

Survey of the impacts of soil and climatic variations on the production of essential oils in *Heracleum persicum*

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Abstract. *Hasani R, Mehregan I, Larijani K, Nejdassattari T, Scalone R. 2017. Survey of the impacts of soil and climatic variations on the production of essential oils in Heracleum persicum Biodiversitas 18: 365-377.* Essential oils have been extracted from different parts of the *Heracleum persicum* plants (Apiaceae) since many years. However, the effect of the climate and the soil composition on their quality and quantity of the essential oils have never been investigated in this species. For this aim, ten populations of Persian hogweed were selected regarding their different localities in Iran and their essential oils were extracted from dry fruits by hydrodistillation clevenger type, GC-FID and GC-MS analyses. During the sampling of the *Heracleum* populations, certain climatic and edaphic parameters were also recorded. Within these ten populations, 18 to 43 different oil compounds were identified expanding the diversity of chemical compounds found in Iranian populations. Certain rare molecules as per example the isopropyl-2-methyl butyrate, the isopropyl-3-methyl butyrate, the γ -terpinene or the *p*-cymene should be considered to categorize the different populations between them within the species. Certain environmental factors (e.g., EC, Cl, P) are related with the production of certain essential oils within the studied populations and are providing crucial information for the production of these oils by this aromatic herb. To conclude, the study of the environment of the populations can help to improve the utility of this aromatic plant, although certain preliminary results have still to be confirmed by controlled-environment experiments.

Keywords: Apiaceae, chemotaxonomy, ecological factors, Persian hogweed

INTRODUCTION

Since ancient time, essential oils of plants have been utilized as natural active products for medicinal and agronomic purposes (Djilani and Dicko 2012). Certain plant species are containing a large variety of essential oils extracted from their different organs: leaves, stems, flowers, buds, roots, seeds, fruits. Although certain species have been grown and used to extract these essential oils during centuries, the factors determining the quality and the quantity of the essential oils present in the plants are still not completely understood. Indeed, certain environmental and climatic factors (altitude, latitude, soil type, water availability, etc.) influencing the growing conditions of the plant during the season as well as the precise harvest time are impacting significantly the chemical composition of these natural products. However, these quantitative and qualitative variations of the chemical compounds present in the plant are limited within a definite plant species. Genetic factors are fixing the possibility to find (or not) certain essential oils within the different organs of a specific plant species. Thus, different chemical compositions of essential oils can be found between different species but also, at a lower level, within the same species present in different habitats (Djilani and Dicko 2012; Sadgrove and Jones 2015). Although the use of this chemotaxonomy can help botanists to select species or varieties presenting economic

values due to their contents of specific essential oils, this selective process will still be limited by the unknown impact of the environment on the plant growth and its essential oils production (Sadgrove and Jones 2015).

One of the species representing high economic values for its essential oils content is the genus *Heracleum* L. (hogweed in English) composed by more than 100 species and considered as one of the most widespread genera of the Apiaceae family (Umbelliferae). Aromatic species of *Heracleum* are known to be rich sources of essential oils in the Persian culture since centuries (Kuljanabagavad et al. 2010). In Iran, eight species of this genus can be found growing often along rivers or humid mountains (Saeidnia et al. 2005; Torbati et al. 2013; Radjabian et al. 2014). One of the eight Iranian hogweed species, *Heracleum persicum* Desf. ex Fischer (Persian hogweed) also named *Golpar* has been cultivated and used for its culinary and medicinal properties. This plant is a perennial and polycarpic herb present in Iran, Iraq and Turkey, tall between 150 and 200cm with a stem with sparse hairs large more than 1cm. The leaves are pinnate usually with 5 leaflets. Each flower is constituted by white petals with hairy ovary, while fruits are schizocarp, cuneate-obovate with 13-15×6-7mm and clavate vittae (Davis 1965; Mozaffarian 1986; Reching 1987; Asgarpanah et al. 2012).

The fruits of *H. persicum* are the organs of the plant widely used as carminative, antiseptic, anthelmintic,

diuretic, digestive, tonic, aphrodisiac and analgesic agents in traditional and contemporain Iranian medicines (Sefidkon et al. 2004; Torbati et al. 2013; Radjabian et al. 2014). However, other parts of the *Heracleum* plant possess various chemical compounds and different amounts of essential oils (Scheffer et al. 1984; Mojab et al. 2002; Sefidkon et al. 2002; Mojab and Nickavar 2003; Sefidkon et al. 2004; Kuljanabagavad et al. 2010; Mazandarani, et al. 2012; Radjabian, et al. 2013; Torbati, et al. 2013; Kharkwal, et al. 2014; Radjabian et al. 2014; Torbati et al. 2014). Anti-inflammatory, analgesic (Hajhashemi et al. 2009), antioxidant (Firuzi et al. 2010; Mazandarani, et al. 2012; Torbati, et al. 2014) anticonvulsant (Sayyah, et al. 2005), antitumor (Firuzi, et al. 2010), cytotoxic (Saeidnia et al. 2005; Moshafi et al. 2009; Sharififar et al. 2009), immunomodulatory effects, antimicrobial and antifungal activities (Habibi, et al. 2010; Kuljanabagavad et al. 2010; Najafabadi et al. 2011; Akcin et al. 2013; Torbati et al. 2013; Kharkwal et al. 2014; Torbati et al. 2014), antidermatophytic (Sefidkon et al. 2004), contraceptive (Hemati et al. 2010) and adjunctive treatment for hypertriglyceridemia patients (Dadjo et al. 2014) have been reported as effects provided by the essential oils of this *Heracleum* species. Monoterpenes, oxygenated monoterpenes, sesquiterpenes, and aliphatic esters are the most important chemical compounds composing the essential oils extracted from the different parts of this *Heracleum* species (Sefidkon et al. 2004, Radjabian et al. 2013, Radjabian et al. 2014). In addition, coumarins, furanocoumarins, anthraquinones, stilbenes, furanocoumarin dimers, flavonoids and other types of secondary metabolites have also been identified in *Heracleum* essential oils (Kuljanabagavad et al. 2010).

According to previous studies, a large variability can be observed in the type, in the number and in the proportions of the chemical compounds present in the essential oils extracted from *Heracleum* materials (Radjabian et al. 2013, Radjabian et al. 2014). Although the co-occurrence of the chemical compounds of octyl acetate and hexyl butyrate is specific to the *H. persicum* species and its Iranian populations, the amount and the proportions of other chemical compounds of the essential oils can be highly variable depending to the population locations. Environmental factors including edaphic and climatic

characteristics, as per example the temperatures or the precipitations, could affect the quantity and the quality of the production of these active products in the *Golpar* plants. In order to evaluate whether certain climatic and edaphic conditions have an impact on the production of the chemical compounds present in the *H. persicum* plants, we extracted the essential oils from ripen fruits of ten different *Heracleum persicum* populations growing in various places in Iran and analyzed their contents. Soil samples and climatic information of these various Iranian places were collected and the soil proprieties tested at the light of the variations of the essential oils extracted.

MATERIALS AND METHODS

Essential oils data

Plant material. Ten populations of *Heracleum persicum* Desf. ex Fischer were selected from different regions of Iran, however selected populatios did not show the same size (with at least 50 individuals in each population). The fruits were collected randomly from ten individuals (about 400 to 800 fruits per individual) between July and August 2014 (Table 1 and Figure 1).

Isolation of essential oils. Hydrodistillation clevenger-type apparatus was used during three hours to extract the essential oils from the air dried fruits. The pale yellow obtained essential oils were mixed with hexane, then dried by anhydrous Na₂SO₄ and, at the last step, stored in sealed dark vials at 4-5°C until gas chromatography analysis. Essential oils percentage were calculated as w/w.

Gas Chromatography (GC) analysis. Shimadzu 15A gas chromatography with a split/splitless injector (250°C) and a flame ionization detector (FID) (250°C) were carried out for GC analyses. DB-5 capillary (30m × 0.25mm, film thickness 0.32µm) with N₂ (1mL/min) as carrier gas was the type of column used. The program for oven temperature was adjusted at 60°C for 3min, then rising to 250°C with a 6°C/min rate and, finally, stay constant at 250°C for 5min. For the qualification part, the relative contents of the essential-oil components were calculated by the peak areas in the GC-FID profiles without using internal standards or correction factors and expressed as percentage.

Table 1. Geographical location of the ten Iranian populations of *Heracleum persicum* investigated here

Pop. code	Collection Site	Province	Latitude (N)	Longitude (E)	Altitude (m asl.)	Collection date (2014)
P1	SRN Sareyn, Vila Darreh	Ardabil	38° 10' 45.4''	048° 03' 50.2''	1757 m	8 Aug.
P2	HMD Hamedan, Darreh Morad Beik	Hamedan	34° 44' 53.8''	048° 30' 25.1''	2027 m	16 Aug.
P3	RMS Ramsar, Javaher Deh	Mazandaran	36° 51' 20.0''	050° 28' 28.0''	1800 m	11 Aug.
P4	KND Karaj to Chalus road, after Kandovan tunnel, Dona	Mazandaran	36° 10' 46.3''	051° 19' 08.0''	2511 m	24 Jul.
P5	TNG Firuzkuh, Tangeh Vashi	Tehran	35° 52' 33.0''	052° 43' 37.0''	2000 m	4 Sep.
P6	PLR Polur	Mazandaran	35° 50' 48.6''	052° 03' 03.2''	2224 m	9 Jul.
P7	ZSK Mashhad, Zoshk	Razavi Khorasan	36° 19' 28.3''	059° 10' 59.2''	1770 m	31 Jul
P8	AKM Chenaran, Akhلامad	Razavi Khorasan	36° 35' 41.0''	058° 56' 33.2''	1500 m	1 Aug
P9	YZD Taft, Shahkuh, Dehbala	Yazd	31° 36' 17.9''	054° 07' 06.5''	2470 m	17 Jul.
P10	LZR Bardsir, Lalehzar	Kerman	29° 30' 49.8''	056° 41' 06.5''	2879 m	15 Jul.



Figure 1. Geographic distribution of the collected plant and soil materials examined in this study (more details in Table 1)

Gas Chromatography-Mass Spectrometry (GC-MS) analysis. Hewlett-Packard (HP-6890/5973) GC-MS system coupled with a HP-5MS column (30m × 0.25mm, film thickness 0.32µm) was used for GC/MS analyses. The temperature of the column adjusted as described above (cf. GC analysis). Helium (1ml/min) with 70eV ionization energy in MS, 40-300amu mass range and 1s scan time was performed as a carrier gas. GC peak areas without correction factors was used to calculate the percentage of essential oil components. Individual compounds were identified by comparison of their mass spectra, retention times and indexes with corresponding data in the literature (Adams 2007) and websites (El-Sayed 2016, <http://www.pherobase.com>; NIST 2016, <http://webbook.nist.gov/chemistry/>). Retention times for n-alkanes were determined by injection with the same chromatographic conditions to identify retention times.

Soil data

In all localities, soil samples were collected from the base of the plants (20cm depth). Bouyoucos hydrometer method was performed to determine the soil texture as a physical analysis (Gee and Bauder 1979). For chemical analysis different factors were analyzed; the acidity rate (pH) of the soil samples, the electrical conductivity (EC) with a portable CPD-65N multi-meter (ISTEK, South Korea) by saturation extract examined by pH meter, the amount of organic carbon (OC) by the modified Walkley and Black method (Najafabadi et al. 2011), Ca²⁺, K⁺ and Na⁺ by atomic absorption spectroscopy (AAS) (Richards

1954), Cl⁻ by ion chromatography (Khym 1974), CaCO₃ as the total amount of carbonates included in 100gr of dry soil corresponding to the calcimeter Bernard method, phosphor by the Olsen method (Buurman et al. 1996), and the availability of nitrogen by the Kjeldahl method corresponding to the estimation of the changes of the various nitrogen types into NH₄⁺ (Bremner and Mulvaney 1982).

Climatic data

Climatic information such as precipitations and minimal, average and maximal temperatures were collected for the ten studied populations from the internet website: www.en.climate-data.org. Then, 19 climatic variables were obtained for each location including: annual mean temperature (CLIM1), annual mean diurnal range (CLIM2), isothermality (CLIM3), temperature seasonality (CLIM4), maximal temperature of warmest month (CLIM5), minimal temperature of coldest month (CLIM6), annual temperature range (CLIM7), mean temperature of wettest quarter (CLIM8), mean temperature of driest quarter (CLIM9), mean temperature of warmest quarter (CLIM10), mean temperature of coldest quarter (CLIM11), annual precipitations (CLIM12), precipitations of wettest month (CLIM13), precipitations of driest month (CLIM14), precipitations seasonality (CLIM15), precipitations of wettest quarter (CLIM16), precipitations of driest quarter (CLIM17), precipitations of warmest quarter (CLIM18) and precipitations of coldest quarter (CLIM19) (O'Donnell and Ignizio 2012).

Table 2. Compositions of the essential oils and oil yields obtained after extraction of the fruits of the ten investigated populations of *H. persicum*

No.	Compound name	CAS#	KI	SRN	HMD	RMS	KND	TNG	PLR	ZSK	AKM	YZD	LZR
1	Octane	111-65-9	800	-	0.38	-	-	-	1.79	-	-	-	-
2	Isopropyl butyrate	638-11-9	844	-	0.57	-	-	0.19	-	-	-	-	-
3	Hexanol	111-27-3	870	-	-	0.86	-	-	-	-	-	-	-
4	Isopropyl-2-methyl butyrate	66576-71-4	885	2.55	1.05	4.43	2.45	3.51	0.49	3.50	2.81	4.89	1.15
5	Isopropyl 3-methyl butyrate	32665-23-9	904	2.93	1.69	2.92	2.84	3.34	2.15	4.22	3.05	4.35	1.38
6	Isobutyl isobutyrate	97-85-8	911	-	0.43	0.74	0.86	0.92	0.36	0.36	-	0.54	-
7	α -Pinene	90-56-8	939	0.38	-	0.42	0.38	-	-	-	-	-	-
8	Butyl isobutyrate	97-87-0	955	0.37	-	2.15	1.21	0.81	0.38	0.61	-	1.09	1.07
9	Isobutyl butyrate	539-90-2	961	-	-	-	-	0.66	0.37	-	-	-	-
10	Isopropyl 3-methyl-2-butenolate	25859-51-2	965	1.22	0.74	1.38	0.90	1.15	1.09	1.52	-	1.95	-
11	Butyl butyrate	109-21-7	994	1.22	1.61	1.67	0.52	1.01	0.75	-	0.78	0.46	-
12	<i>n</i> -Octanal	124-13-0	998	0.56	1.72	0.81	1.13	1.62	1.05	0.45	0.45	0.87	-
13	Isobutyl 2-methylbutanoate	2445-67-2	1004	-	-	1.23	0.75	2.41	0.43	0.79	-	0.79	-
14	Isobutyl isovalerate	589-59-3	1006	-	-	0.48	0.50	-	0.55	-	-	-	-
15	Hexyl acetate	142-92-4	1009	4.70	1.68	2.57	-	1.05	0.66	1.09	4.60	3.13	1.31
16	Isopentyl isobutyrate	2050_3_1	1013	-	-	0.31	0.31	0.30	-	-	-	-	-
17	<i>p</i> -Cymene	99-87-6	1026	3.12	-	1.61	0.94	1.54	0.83	1.97	2.39	2.81	-
18	Limonene	138-86-3	1031	0.61	-	-	-	-	-	-	-	-	-
19	Butyl 2-methylbutanoate	15706-73-7	1042	-	-	2.49	1.01	1.37	0.44	0.67	0.38	1.19	-
20	Butyl 3-methylbutanoate	109-19-3	1047	-	-	1.82	0.98	1.14	1.20	0.58	-	0.69	0.77
21	Pentyl isobutyrate	2445-72-9	1057	-	-	0.62	-	0.85	0.55	-	-	-	-
22	γ -Terpinene	99-85-4	1059	3.89	0.83	2.24	1.82	2.01	1.21	3.19	2.94	4.67	-
23	Linalool	78_70_6	1096	-	1.61	-	-	-	0.73	-	-	-	3.39
24	Hexyl propanoate	2445-76-3	1101	0.64	-	0.53	-	0.33	-	1.13	0.55	0.55	-
25	2-Methyl butyl isovalerate	2445-77-4	1104	-	-	0.44	0.23	0.93	-	-	-	-	-
26	Hexyl isobutyrate	2349_7_7	1151	5.33	2.16	7.12	5.17	1.24	7.54	6.06	4.75	3.59	6.29
27	Hexyl butyrate	2639-63-6	1192	17.94	21.77	19.56	14.53	19.95	17.47	16.54	20.78	22.98	26.41
28	Octenol acetate	26806-12-2	1198	2.64	4.89	2.48	2.56	2.59	2.07	2.89	3.67	4.41	7.93
29	<i>n</i> -Decanal	112-31-2	1201	-	-	-	0.98	-	1.96	1.09	0.77	2.24	-
30	<i>n</i>-Octyl acetate	112-14-1	1211	18.28	16.09	16.43	13.79	17.10	10.11	17.71	24.54	20.83	16.93
31	Hexyl 2-methyl butyrate	10032-15-2	1236	5.68	3.03	8.46	5.46	1.70	6.43	8.58	6.44	4.83	9.53
32	Hexyl isovalerate	10032-13-0	1244	1.63	0.81	-	-	-	1.27	-	-	0.82	-
33	Hexyl pentanoate	1117-59-5	1275	-	-	-	-	0.94	-	-	2.14	-	-
34	<i>E</i> -Anethole	4180-23-8	1284	0.80	-	-	1.21	1.88	2.14	1.21	-	0.76	-
35	Octyl propionate	142-60-9	1302	0.26	1.16	-	0.55	0.17	0.33	0.36	-	-	-

Table 2. Compositions of the essential oils and oil yields obtained after extraction of the fruits of the ten investigated populations of *H. persicum* (continued)

No.	Compound name	CAS#	KI	SRN	HMD	RMS	KND	TNG	PLR	ZSK	AKM	YZD	LZR
36	Octyl isobutyrate	109-15-9	1317	3.11	4.91	3.88	9.04	0.54	9.77	5.44	3.03	2.06	5.73
37	Hexyl hexanoate	6378-65-0	1383	5.64	7.45	3.35	4.25	8.84	2.34	4.40	4.77	3.51	5.94
38	<i>n</i> -Octyl butyrate	110-39-4	1434	3.73	7.50	2.63	5.59	6.32	5.75	3.92	3.50	2.19	1.32
39	Dodecanal	112-54-9	1435	0.90	-	-	0.57	1.15	-	0.42	0.54	0.72	-
40	<i>N</i> -Octyl 2-methyl butyrate	29811-50-5	1436	6.08	9.95	4.92	9.19	1.15	9.15	6.81	4.71	2.45	7.65
41	E,E- α -farnesene	502-61-4	1508	0.53	-	-	-	-	-	-	-	-	-
42	Octyl hexanoate	4887-30-3	1570	-	1.72	-	-	2.81	-	1.58	-	-	0.97
43	Octyl octanoate	2306-88-9	1771	0.55	0.69	-	-	-	-	0.98	-	-	1.01
Aldehyde				1.46	1.72	0.81	2.68	2.77	3.01	1.96	1.76	3.83	-
Aliphatic esters				84.50	89.90	92.61	82.69	83.32	81.65	89.74	90.50	87.30	95.39
Monoterpene hydrocarbons				8.00	0.83	4.27	3.14	1.54	2.04	5.16	5.33	7.48	-
Oxygenated monoterpenes				0.80	1.61	-	1.21	1.88	2.87	1.21	-	0.76	3.39
Hydrocarbon				-	-	-	-	-	1.79	-	-	-	-
Sesquiterpene				0.53	-								
Alcohol				-	-	0.86	-						
oil yield %				6.29	6.01	3.40	8.32	4.59	2.22	3.26	4.07	2.55	2.24
The number of different chemical compounds identified				33	30	32	40	43	37	31	24	29	18
Total identified %				95.29	94.06	98.55	89.72	89.51	91.36	98.07	97.59	99.37	98.78
The percentage of unknown components in each population				4.71	5.94	1.45	10.28	10.49	8.64	1.93	2.41	0.63	1.22

Note: The code of the *Golpar* populations are referring to their names listed in Table 1, as following, Sareyn (SRN), Hamedan (HMD), Ramsar (RMS), Kandovan (KND), Tangeh Vashi (TNG), Polur (PLR), Mashhad, Zoshk (ZSK), Mashhad, Akhlamad (AKM), Yazd (YZD) & Kerman, Lalehzar (LZR)

Table 3. Edaphic information obtained for the ten investigated populations of *H. persicum*.

Pop. Code	EC (ms/cm)	pH	Ca (meq/lit)	Na (meq/lit)	Cl (meq/lit)	CaCo3 (%)	Sand (%)	Silt (%)	Clay (%)	Texture	OC (%)	N (%)	P (ppm)	K (ppm)
SRN	1.615	7.56	3.8	9.9	11.6	15.3	48.3	26.1	25.6	Loam	0.38	0.046	7.42	218.3
HMD	1.614	7.19	2.8	7.3	12.8	7.3	45.9	32.3	21.8	Loam	0.31	0.039	8.34	231.7
RMS	1.587	7.12	9.6	1.2	8.0	8.1	42.8	35.1	22.1	Loam	1.22	0.160	8.07	231.5
KND	1.390	7.43	3.5	6.3	7.2	10.2	50.2	32.8	17.0	Loam	1.31	0.220	7.19	221.0
TNG	1.283	7.80	1.9	6.1	5.9	17.3	49.8	26.2	24.0	Loam	0.37	0.050	4.35	192.1
PLR	1.616	7.83	2.8	10.2	9.4	13.1	44.1	28.2	27.7	Clay loam	0.23	0.035	4.01	186.2
ZSK	1.909	7.59	4.6	10.9	13.1	11.8	57.3	27.9	14.8	Sandy loam	0.16	0.180	6.07	201.9
AKM	1.536	7.52	2.6	8.3	10.7	14.1	55.2	23.1	21.7	Sandy clay loam	0.25	0.032	5.33	182.5
YZD	2.270	7.84	3.8	10.1	17.4	15.9	56.1	24.3	16.6	Sandy loam	0.18	0.024	3.85	174.2
LZR	2.760	7.77	5.1	14.7	18.9	14.6	53.2	30.1	16.7	Loam	0.13	0.019	4.51	191.7

Note: The code of the *Golpar* populations are referring to their names listed in Table 1

Table 4. Climatic information obtained for the ten investigated populations of *H. persicum*

Pop. Code	CLIM1	CLIM2	CLIM3	CLIM4	CLIM5	CLIM6	CLIM7	CLIM8	CLIM9	CLIM10	CLIM11	CLIM12	CLIM13	CLIM14	CLIM15	CLIM16	CLIM17	CLIM18	CLIM19
SRN	8.19	12.12	33.20	8.37	28.6	-7.9	36.5	5.57	17.87	18.07	-2.07	312	49	11	41.96	125	39	42	94
HMD	9.14	15.12	39.16	8.58	31.0	-7.6	38.6	6.57	19.67	19.93	-1.07	364	71	0	83.99	182	2	9	137
RMS	10.55	13.21	36.09	8.65	30.0	-6.6	36.6	4.00	20.60	20.93	-0.07	326	59	6	60.70	146	25	26	97
KND	10.19	13.84	34.09	9.70	31.1	-9.5	40.6	3.53	21.13	21.77	-2.03	206	37	1	73.28	101	7	11	76
TNG	10.09	14.44	34.55	9.85	31.8	-10	41.8	9.67	21.10	22.00	-2.30	149	28	1	75.24	75	5	8	5.4
PLR	10.79	14.33	34.44	9.85	32.4	-9.2	41.6	4.47	21.87	22.67	-1.60	159	28	1	74.75	78	4	7	60
ZSK	9.21	14.73	37.28	8.77	30.0	-9.5	39.5	8.03	19.40	19.87	-1.60	279	58	2	78.97	149	6	14	82
AKM	10.29	14.56	36.49	8.93	31.3	-8.6	39.9	9.10	20.70	21.10	-0.70	268	57	1	79.37	145	5	13	74
YZD	15.01	16.12	38.84	9.38	36.7	-4.8	41.5	5.70	26.57	26.57	3.37	85	17	0	87.39	46	1	1	40
LZR	10.33	16.44	42.49	8.22	30.3	-8.4	38.7	2.33	15.17	20.43	0.17	241	46	2	86.65	134	10	12	116

Note: The code of the *Golpar* populations are referring to their names listed in Table 1. CLIM1: annual mean temperature, CLIM2: annual mean diurnal range, CLIM3: isothermality, CLIM4: temperature seasonality, CLIM5: maximal temperature of warmest month, CLIM6: minimal temperature of coldest month, CLIM7: annual temperature range, CLIM8: mean temperature of wettest quarter, CLIM9: mean temperature of driest quarter, CLIM10: mean temperature of warmest quarter, CLIM11: mean temperature of coldest quarter, CLIM12: annual precipitations, CLIM13: precipitations of wettest month, CLIM14: precipitations of driest month, CLIM15: precipitations seasonality, CLIM16: precipitations of wettest quarter, CLIM17: precipitations of driest quarter, CLIM18: precipitations of warmest quarter, CLIM19: precipitations of coldest quarter

Table 5. Correlation coefficients among the different chemical compounds of the essential oils extracted from the ten investigated populations of *H. persicum*

	4	5	8	10	11	12	15	17	19	22	26	27	28	30	31	34	36	37	38	40
4	1																			
5	0.839**	1																		
8	0.529	0.161	1																	
10	0.605	0.697*	0.345	1																
11	0.040	-0.223	0.031	0.106	1															
12	-0.050	-0.033	-0.130	0.287	0.571	1														
15	0.324	0.218	-0.225	-0.052	0.308	-0.347	1													
17	0.683*	0.779**	-0.018	0.476	0.021	-0.245	0.711*	1												
19	0.724*	0.441	0.812**	0.505	0.284	0.212	-0.119	0.197	1											
22	0.742*	0.867**	0.006	0.626	-0.018	-0.133	0.603	0.954**	0.227	1										
26	-0.173	-0.153	0.321	-0.049	-0.246	-0.647*	-0.040	-0.020	-0.063	-0.103	1									
27	-0.057	-0.332	-0.013	-0.362	-0.085	-0.254	0.245	-0.235	-0.194	-0.244	-0.217	1								
28	-0.284	-0.466	-0.042	-0.521	-0.358	-0.391	0.007	-0.448	-0.436	-0.419	-0.090	0.861**	1							
30	0.523	0.428	-0.179	-0.160	-0.069	-0.353	-0.753*	0.585	-0.038	0.552	-0.326	0.386	0.243	1						
31	-0.031	-0.100	0.358	-0.193	-0.435	-0.857**	0.031	-0.049	0.016	-0.113	0.867**	0.092	0.268	-0.004	1					
34	-0.081	0.282	-0.104	0.426	-0.224	0.355	-0.491	0.083	0.072	0.082	-0.024	-0.563	-0.587	-0.542	-0.333	1				
36	-0.631	-0.429	-0.015	-0.172	-0.262	-0.061	-0.590	-0.531	-0.232	-0.487	0.606	-0.415	-0.079	-0.730*	0.363	0.259	1			
37	-0.117	-0.213	-0.213	-0.285	0.211	0.391	-0.035	-0.224	-0.243	-0.265	-0.789**	0.295	0.275	0.186	-0.581	-0.078	-0.523	1		
38	-0.399	-0.195	-0.461	0.026	0.412	0.856**	-0.414	-0.346	-0.150	-0.287	-0.481	-0.459	-0.426	-0.449	-0.719*	0.444	0.213	0.397	1	
40	-0.774**	-0.636*	-0.253	-0.334	-0.033	-0.005	-0.398	-0.625	-0.501	-0.569	0.400	-0.234	0.140	-0.578	0.269	-0.085	0.848**	-0.217	0.319	1

Note: The numbers are referring to the number of essential oils components presented in Table 2. Pearson's correlation coefficient is indicated with levels of significance (* for $P \leq 0.05$ and ** for $P \leq 0.01$ are indicated in bold). Negative and positive correlation between factors are shown by minus and plus signs

Table 6. Correlation coefficients between the different chemical compounds of the essential oils present in the *Golpar* population and the edaphic information

	Altitude	EC	pH	Ca	Na	Cl	CaCo3	Sand	Silt	Clay	OC	N	P	K
Isopropyl-2-methyl butyrate	-0.275	-0.060	-0.062	0.384	-0.427	-0.079	0.172	0.333	-0.185	-0.340	0.250	0.301	-0.007	-0.091
Isopropyl 3-methyl butyrate	-0.343	-0.136	0.209	0.010	-0.154	-0.081	0.315	0.531	-0.462	-0.324	-0.015	0.304	-0.194	-0.307
Butyl isobutyrate	0.312	0.160	-0.196	0.797**	-0.440	-0.109	-0.181	-0.200	0.544	-0.293	0.657*	0.495	0.107	0.231
Isopropyl 3-methyl-2-butenate	-0.091	-0.129	0.079	0.201	-0.267	-0.102	0.026	-0.050	-0.014	-0.047	0.127	0.283	0.010	0.048
Butyl butyrate	-0.481	-0.596	-0.654*	0.201	-0.741*	-0.492	-0.425	-0.768**	0.333	0.647*	0.357	-0.081	0.609	0.613
n-Octanal	-0.083	-0.644*	-0.217	-0.365	-0.540	-0.547	-0.254	-0.476	0.215	0.365	0.221	0.022	0.201	0.299
Hexyl acetate	-0.539	0.017	-0.113	0.077	-0.015	0.204	0.264	0.157	-0.515	0.230	-0.220	-0.420	0.118	-0.104
p-Cymene	-0.523	-0.163	0.173	0.010	-0.085	-0.046	0.466	0.354	-0.633*	0.063	-0.081	-0.016	-0.089	-0.263
Butyl 2-methylbutanoate	-0.125	-0.279	-0.261	0.602	-0.762*	-0.462	-0.179	-0.240	0.332	-0.060	0.063*	0.483	0.090	0.155
γ -Terpinene	-0.426	-0.111	0.136	-0.003	-0.089	0.043	0.351	0.415	-0.568	-0.105	-0.070	0.060	-0.058	-0.234
Hexyl isobutyrate	0.063	0.260	-0.042	0.564	0.145	0.090	-0.218	-0.172	0.274	0.005	0.199	0.299	0.026	0.040
Hexyl butyrate	0.375	0.709*	0.201	0.076	0.378	0.701*	0.247	0.199	-0.150	-0.171	-0.489	-0.701*	-0.336	-0.337
Octenol acetate	0.580	0.824**	0.147	0.027	0.589	0.809**	0.085	0.337	0.027	-0.455	-0.413	-0.451	-0.198	-0.193
n-Octyl acetate	-0.394	0.161	-0.007	-0.050	0.065	0.314	0.333	-0.641*	-0.592	-0.293	-0.292	-0.268	-0.079	-0.319
Hexyl 2-methyl butyrate	0.112	0.553	-0.062	0.648*	0.294	0.384	-0.176	-0.164	0.228	-0.361	0.048	0.270	0.011	-0.018
E-Anethole	0.750	-0.366	0.575	-0.450	0.065	-0.447	0.383	-0.080	-0.229	0.304	-0.071	0.117	-0.448	-0.305
Octyl isobutyrate	0.377	0.014	-0.051	0.007	0.178	-0.076	-0.444	-0.275	0.461	-0.021	0.254	0.366	0.084	0.171
Hexyl hexanoate	-0.054	-0.151	-0.024	-0.403	-0.001	-0.084	0.196	0.041	-0.073	0.077	-0.220	-0.283	0.105	0.161
n-Octyl butyrate	-0.202	-0.715*	-0.203	-0.559	-0.316	-0.589	-0.295	-0.419	0.168	0.421	0.094	0.082	0.258	0.330
N-Octyl 2-methyl butyrate	0.240	0.045	-0.336	-0.022	0.210	0.084	-0.634*	-0.322	0.537	-0.007	0.130	0.221	0.413	0.450
Oil yield	-0.122	-0.588	-0.467	-0.249	-0.363	-0.469	-0.302	-0.183	0.267	0.041	0.543	0.416	0.644*	0.622
The number of components	-0.153	-0.770**	0.013	-0.244	-0.521	-0.808**	-0.001	-0.401	0.124	0.387	0.427	0.387	0.092	0.222

Note: Pearson's correlation coefficient is indicated with levels of significance (* for $P \leq 0.05$ and ** for $P \leq 0.01$ are indicated in bold). Negative and positive correlation between factors are shown by minus and plus signs.

Table 7. Correlation coefficients between the different chemical compounds of the essential oils present in the *Golpar* population and the climatic information

	CLIM1	CLIM2	CLIM3	CLIM4	CLIM5	CLIM6	CLIM7	CLIM8	CLIM9	CLIM10	CLIM11	CLIM12	CLIM13	CLIM14	CLIM15	CLIM16	CLIM17	CLIM18	CLIM19
Isopropyl-2-methyl butyrate	0.456	-0.100	-0.121	0.082	0.316	0.457	-0.018	0.300	0.520	0.380	0.441	-0.224	-0.199	0.135	-0.115	-0.282	0.134	0.070	-0.457
Isopropyl 3-methyl butyrate	0.397	-0.090	-0.288	0.299	0.387	0.205	0.266	0.492	0.615	0.401	0.262	-0.383	-0.326	0.005	-0.048	-0.407	-0.054	-0.059	-0.605
Butyl isobutyrate	0.333	-0.068	0.048	0.022	0.052	0.315	-0.199	-0.509	0.115	0.254	0.315	-0.135	-0.198	0.174	-0.132	-0.208	0.249	0.094	-0.094
Isopropyl 3-methyl-2-butenate	0.381	-0.208	-0.322	0.309	0.382	0.390	0.110	0.073	0.622	0.398	0.252	-0.318	-0.384	0.156	-0.222	-0.461	0.112	0.022	-0.406
Butyl butyrate	-0.250	-0.553	-0.359	-0.091	-0.209	0.251	-0.437	0.110	0.082	-0.234	-0.179	0.471	0.360	0.354	-0.485	0.285	0.393	0.391	0.185
n-Octanal	0.000	-0.116	-0.338	0.549	0.248	-0.087	0.347	0.305	0.424	0.202	-0.247	-1.000	-0.112	-0.330	0.072	-0.156	-0.316	-0.320	-0.261
Hexyl acetate	0.030	-0.286	-0.070	-0.462	-0.048	0.491	-0.453	0.267	0.039	-0.141	0.287	0.255	0.210	0.523	-0.411	0.151	0.500	0.523	0.089
p-Cymene	0.207	-0.407	-0.441	0.021	0.155	0.316	-0.084	0.404	0.399	0.135	0.201	-0.175	-0.222	0.464	-0.467	-0.309	0.405	0.389	-0.433
Butyl 2-methylbutanoate	0.367	-0.205	-0.244	0.322	0.203	0.256	0.020	-0.009	0.462	0.382	0.214	-0.191	-0.198	0.025	-0.126	-0.267	0.076	-0.031	-0.403
γ -Terpinene	0.347	-0.275	-0.345	0.073	0.320	0.437	0.003	0.380	0.556	0.279	0.335	-0.229	-0.250	0.308	-0.313	-0.340	0.247	0.235	-0.410
Hexyl isobutyrate	-0.077	-0.219	-0.047	-0.212	-0.303	-0.019	-0.324	-0.600	-0.253	-0.169	-0.006	0.145	0.089	0.340	-0.269	0.110	0.344	0.322	0.307
Hexyl buyrate	0.352	0.689*	0.828**	-0.441	0.270	0.462	-0.073	-0.123	-0.171	0.192	0.617	-0.052	0.012	-0.202	0.471	0.066	-0.173	-0.248	0.205
Octenol acetate	0.156	0.744*	0.920**	-0.543	0.076	0.246	-0.114	-0.328	-0.417	-0.001	0.455	0.070	0.142	-0.253	0.545	0.236	-0.220	-0.249	0.458
n-Octyl acetate	0.196	0.162	0.243	-0.352	0.140	0.348	-0.126	0.511	0.104	0.053	0.406	0.077	0.181	0.042	0.103	0.145	0.025	0.082	-0.075
Hexyl 2-methyl butyrate	-0.059	0.066	0.336	-0.504	-0.337	-0.053	-0.420	-0.509	-0.424	-0.230	0.186	0.252	0.267	0.251	-0.041	0.308	0.260	0.261	0.433
E-Anethole	0.036	-0.173	-0.588	0.788**	0.207	-0.503	0.640*	0.189	0.318	0.258	-0.402	-0.607	-0.648*	-0.142	-0.082	-0.655*	-0.200	-0.234	-0.698*
Octyl isobutyrate	-0.157	-0.021	-0.082	0.196	-0.146	-0.347	0.118	-0.592	-0.150	-0.074	-0.285	0.023	0.004	-0.184	0.088	0.060	-0.169	-0.148	0.328
Hexyl hexanoate	-0.405	0.094	0.128	-0.140	-0.244	-0.308	-0.022	0.451	-0.368	-0.347	-0.342	0.193	0.202	-0.052	-0.052	0.069	0.224	-0.047	0.006
n-Octyl butyrate	-0.382	-0.223	-0.430	0.467	-0.073	-0.479	0.308	0.360	0.115	-0.143	-0.619	0.097	0.098	-0.288	0.013	0.078	-0.302	-0.211	-0.088
N-Octyl 2-methyl butyrate	-0.429	-0.034	0.104	-0.202	-0.375	-0.259	-0.208	-0.516	-0.408	-0.403	-0.339	0.441	0.415	-0.062	0.042	0.473	-0.048	0.034	0.716*
Oil yield	-0.458	-0.514	-0.477	0.077	-0.347	-0.264	-0.173	0.034	-0.102	-0.369	-0.517	0.315	0.221	0.199	-0.379	0.204	0.230	0.304	0.160
The number of components	-0.114	-0.513	-0.798**	0.738*	0.045	-0.375	0.355	0.226	0.380	0.116	-0.513	-0.286	-0.375	0.020	-0.336	-0.428	0.010	-0.014	-0.565

Note: Pearson's correlation coefficient is indicated with levels of significance (* for $P \leq 0.05$ and ** for $P \leq 0.01$ are indicated in bold). Negative and positive correlation between factors are shown by minus and plus signs.

Statistical analyses

For statistical analysis, the normality of frequency distributions was analyzed by Kolmogorov–Smirnov test. One-way ANOVA test was done to compare the means for normal distribution. In order to find any relationship between different factors, bivariate analysis with Pearson and Spearman correlation coefficient were performed.

Average-linkage method with standard Euclidean coefficient was performed for hierarchical cluster analysis (HCA) using essential oils components from the different populations. Principal component analysis (PCA) was carried out based on the relative contents of oil components from different populations as dependent variables (Radjabian et al. 2014). The statistical SPSS v. 21 software (IBM Inc, Chicago, IL) was used to conduct the different statistical tests in this study.

RESULTS AND DISCUSSION

Characterization of essential oils

The composition of the essential oils, their relative percentages and the oil yields of the ten studied populations of *H. persicum* are listed in Table 2. Essential oils with yellow color and strong odor exhibited a considerable variation between populations both in their oil yields and in their chemical compositions. The yield of the essential oil extracted from the *Heracleum* fruits is varying from the lowest value of 2.22% of the extraction for the population of Polur (PLR) to the maximal value of 8.32% for the populations of Dona (KND), both localities closed to Tehran. A significant variation in the number of chemical oils components was observed through all the localities, with an average of 32 different chemical compounds found in the extracted essential oils (Table 2). The minimal number of oil compounds was found in the population of Bardsir-Lalehzar (LZR) with a total of 18 different components, while the maximal number was found in the population of Firuzkuh Tangeh Vashi (TNG) with a total of 43 different compounds identified, representing two times more than the number identified in the previous population (Table 2).

Based on the GC/MS results, 43 different chemical compounds were identified within the ten populations of *H. persicum* studied here accounting for 89.51–99.37% of the total extracted oils (Table 2). The essential oils were complex mixtures of alcohol (0–0.86%), aldehyde (0–3.83%), aliphatic esters (with the highest amount comprised between 81.65 and 95.39%), monoterpene hydrocarbons (0–8%), oxygenated monoterpenes (0–3.39%), hydrocarbon (0–1.79%) and sesquiterpene (0–0.53%). Aliphatic esters were the main category of the chemical components present in the *Golpar* essential oils and some of these components were present in all populations: isopropyl-2-methyl butyrate (from 0.49% in PLR to 4.89% in YZD), isopropyl-3-methyl butyrate (from 1.38% in LZR to 4.35% in YAD), hexyl isobutyrate (from 1.24% in TNG to 7.54% in PLR), hexyl butyrate (from 14.53% in KND to 22.98% in YZD), octenol acetate (from 2.07% in AKM to 7.93% in LZR), octyl acetate (from

10.11% in PLR to 24.54% in AKM), hexyl-2-methyl butyrate (from 1.7% in TNG to 9.53% in LZR), octyl isobutyrate (from 0.54% in TNG to 9.04% in KND), hexyl hexanoate (from 2.34% in PLR to 8.84% in TNG), octyl butyrate (from 1.32% in LZR to 7.5% in HMD) and *n*-octyl-2-methyl butyrate (from 1.15% in TNG to 9.95% in HMD).

Hexyl butyrate with contents included between 14.53% in the population of Dona (KND) to 26.41% in the population Lalehzar (LZR) as well as octyl acetate representing 10.11% in the population of Polur (PLR) to 24.54% in the population of Akhlamad (AKM) of the chemical compounds were recognized as the two main oil compounds specific of the *Golpar* species showing equally high amounts in different populations of *H. persicum*. Hexyl 2-methyl butyrate (from 1.7% in TNG to 9.53% in LZR) and *N*-Octyl 2-methyl butyrate (from 1.15% in TNG to 9.95% in HMD) are the second highest oils amounts identified in our sampling.

The alcohol molecule as hexanol was recorded to be present only in the population of Ramsar (RMS) (0.86%), while the sesquiterpene *E*, *E*-alpha-farnesene was found only in the locality of Sareyn (SRN) (0.53%). Three aldehydes consisting of *n*-octanal (from 0.45% in AKM and ZSK to 1.72% in HMD), *n*-decanal (from 0% in SRN, HMD, RMS, TNG and LZR to 2.24% in YZD) and dodecanal (from 0% in HMD, RMS, PLR and LZR to 1.15% in TNG) were also identified within our populations. Four monoterpene hydrocarbons were recorded to be present in our study: α -pinene (0–0.42%), *p*-cymene (0–2.81%), γ -terpinene (0–4.67%) and limonene (0–0.61%). Two oxygenated monoterpenes were also found: linalool (0–3.39%) and *E*-anethole (0–2.14%).

Climatic and edaphic properties

The results of soil analysis for the ten locations are presented in Table 3. Among these data, the electrical conductivity (EC) (from 1.283 ms/cm in TNG to 2.76 ms/cm in LZR), Na⁺ (from 1.2% in RMS to 14.7% in LZR), Cl⁻ (from 5.9% in TNG to 18.9% in LZR), Ca²⁺ (from 1.9% in TNG to 9.6% in RMS) and CaCO₃ (from 7.3% in HMD to 17.3% in TNG) showed considerable variabilities between the ten *Golpar* locations (from 2-fold for EC to more than 10-fold for Na⁺).

The information about the 19 climatic factors applied to the ten populations are shown in Table 4. Annual mean diurnal range (CLIM2) showed a range from 12.12°C (SRN) to 16.44°C (LZR). A range of 33.20°C (SRN) to 42.49°C was achieved for the isothermality (CLIM3). Precipitations of wettest month (CLIM13) showed a large range from 17mm (YZD) to 5 times more with 71mm (HMD), while the wettest month (CLIM16) received between 1mm (YZD) to 39mm (SRN) of precipitations.

Statistical analyses

Correlations among different components of essential oils are represented in Table 5. Positive correlations were found between pairs of isopropyl-3-methyl butyrate and isopropyl-2-methyl butyrate, *p*-cymene and isopropyl-3-methyl butyrate, butyl 2-methyl butanoate and butyl

isobutyrate, terpinene and isopropyl 3-methyl butyrate, terpinene and *p*-cymene, octanol acetate and hexyl butyrate, hexyl 2-methyl butyrate and hexyl acetate, *n*-octyl butyrate and octanal, *n*-octyl-2-methyl butyrate and octyl isobutyrate, and negative correlations are between hexyl 2-methyl butyrate and *n*-octanal, hexyl hexanoate and hexyl isobutyrate, *n*-octyl 2-methyl butyrate and isopropyl 2-methyl butyrate.

Interactions between edaphic and climatic factors and the essence oils characteristics of the ten *Golpar* populations are presented in Tables 6 and 7. The number of chemical components present in the essential oils of each population was negatively correlated with the electrical conductivity (EC) and the chloride content (Cl⁻) of the soil. Oil yields are positively correlated with phosphor content of the soil. Hexyl butyrate and octenol acetate are positively correlated with the electrical conductivity (EC) and the chloride content (Cl⁻) of the soil content too as well as with the annual mean diurnal range (CLIM2) and strongly with the isothermality (CLIM3) applied to the plants. Except these two compounds specific to *H. persicum*, *E*-anethol and *N*-octyl-2-methyl-butyrate are the only two chemical compounds correlated with one climatic variable, the quantity of precipitations received during the coldest quarter of the season (CLIM19).

The dendrogram obtained by hierarchical cluster analysis (HCA) of the relative contents of the essential oils (Figure 2) indicated that the ten populations of *H. persicum* were divided into two main clusters at an average distance value (ADV) of 25: cluster A1 including PLR and KND and cluster A2 including the rest of the populations. The cluster A2 in itself is sub-divided into two smaller sub-clusters at ADV 24: cluster B1 including LZR and cluster B2. The cluster B2 is also sub-divided into two sub-clusters at ADV 20: cluster C1 including HMD and TNG and cluster C2 (including YZD, AKM, SRN, ZSK and RMS).

The graph obtained from principal component analysis (PCA) of the relative contents of the essential oils (Figure 3) indicated that ten populations of *H. persicum* were placed into five groups; SRN, ZSK, AKM, YZD and RMS in the first group, KND and PLR in the second one and HMD, TNG and LZR each located in one of the three separate groups.

Discussion

Expanded variability of chemical compounds/oil yields

Significant variations within the essential oil components present among Iranian populations of Persian hogweed have been recorded in our study. Although similar variations and differences have already been recorded before within a larger sampling of 17 Iranian populations in Radjabian et al. (2013), certain different results should be enlightened here. First, the number of chemical components of essential oils identified in our study varied from 18 to 43 with a average per population of 32 different molecules identified. A similar average number per population (31.1) has been identified by Radjabian and his colleagues (2013) and similar numbers and ranges have been recorded in previous studies: 33 (Radjabian et al. 2014), 21-35 (Radjabian et al. 2013), 32

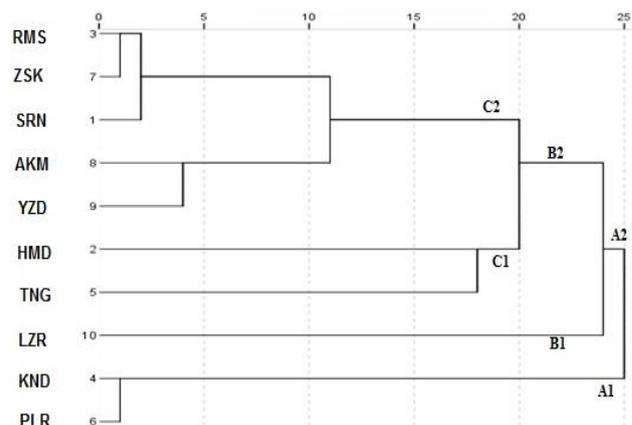


Figure 2. Dendrogram obtained by hierarchical cluster analysis of the distribution of the essential oil compounds of the ten *H. persicum* populations, using average linkage between groups (rescales distance cluster combine)

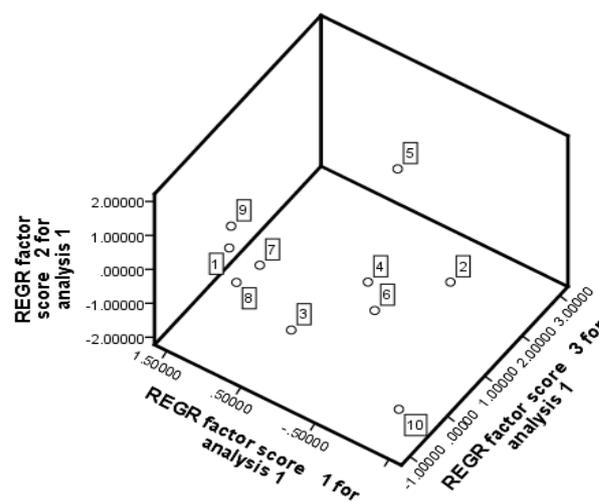


Figure 3. Principal component analysis of the distribution of the essential oil compounds of ten populations of *H. persicum*. The numbers are referring to the sample numbers P of the populations listed in Table 1.

Table 8. Component matrix of the principal component analysis (PCA) with the essential oils information obtained for the ten different populations of *H. persicum*.

	Components		
	1	2	3
Isopropyl-2-methyl butyrate	0.945	0.030	0.149
Isopropyl-3-methyl butyrate	0.876	0.042	0.103
γ -terpinene	0.870	-0.202	0.001
<i>p</i> -cymene	0.846	-0.295	0.010
Isopropyl 3-methyl-2-butanoate	0.644	0.440	0.188
Butyl 2-methyl butanoate	0.600	0.517	0.386
Isobutyl isobutyrate	0.301	0.882	0.016
<i>n</i> -octanal	0.013	0.792	-0.572
<i>n</i> -octyl butyrate	-0.297	0.679	-0.577
Butyl 3-methyl butanoate	0.122	0.590	0.615
Hexyl isobutyrate	-0.235	-0.172	0.888
Hexyl 2-methyl butyrate	-0.184	-0.459	0.823
Butyl isobutyrate	0.317	0.300	0.645

(Saeidnia et al. 2005; Firuzi et al. 2010; Ebadollahi, et al. 2014), 23 (Hajhashemi et al. 2009). However, our results are expanding the existing diversity of chemical molecules present and identified in hogweed populations with lower (18) and higher numbers (43) never obtained before. Indeed, three populations possessed more than 35 different chemical compounds in their essential oils (Kandovan, Tangeh Vashi and Polur) which has never been reported so far. It should be noticed that these three locations are geographically close to each other and located in the neighborhood of Tehran. Second, the oil yields obtained from the fruits extraction represented variable rates from 2.22% for the Polur population to 8.32% for the Dona population. Similarly to the number of chemical compounds identified, the range of the oils yields present in Iranian populations of *H. persicum* was also expanded by our results compared to the existing literature. Indeed, several rates obtained here were largely higher than the ones published in previous studies: 3.8% (Radjabian et al. 2013), 1.6-4.9% (Radjabian et al. 2013), 4 (Hajhashemi et al. 2009), 1.6 (Ebadollahi et al. 2014), 1.8 (Firuzi et al. 2010). The populations located in Polur, Lalehzar and Yazd presented the lowest oil yields of our study, with respectively 2.22%, 2.24% and 2.55%. These hogweed populations are located near the regions of Damavand and Aliabad, where the lower amounts of oil yields have been recorded in Radjabian et al. (2013) with 1.6% and 2.2%. Moreover, the population of Kandovan presenting the highest amount of oil yield of our study is also located near to Gajere, where was detected one of the highest amount of the previous study of Radjabian et al. (2013). These two similarities are indicating that the oil yield is fixed geographically and that the plants grown in certain regions will produce more oils than the ones grown in another region. In average, our GC and GC-MS methods have identified the same number of different chemical compounds than previous studies, but these active molecules are constituting higher percentages of oil yields in our extractions than in the ones done by Radjabian et al. using similar methods on Iranian *Golpar* fruits (average of 4.3% of oil yields compared to 2.8% in Radjabian et al. 2013). Then, these global higher results in the chemical identification and in the oil yields are probably due to a different sampling than the similar work of Radjabian et al. her colleagues. Indeed, even if our sampling of Iranian hogweed populations is smaller ($10 < 17$), the diversities of Iranian regions investigated are similar (7) than the sampling of Radjabian et al. (2013). Moreover, two populations present in locations shared by both samplings (Polur & Tangeh Vashi) are presenting similar (2.22% compared to 2.1% for Polur) or equivalent (4.59% compared to 3.0 % for Tangeh Vashi) oil yields results, confirming the accuracy of our method and the pertinence of our results.

Dominant essential oils influenced by the environment

Similarly to previous results, the molecules of hexyl butyrate and octyl acetate are the two main chemical components presenting the largest quantities within the essential oils extracted (14.53%-26.41%, 10.11%-24.54%

respectively). Based on the literature, the co-occurrence of these two main compounds within fruits oils is a taxonomic trait specific to *H. persicum* samples (Radjabian et al. 2013; Radjabian et al. 2014). Additionally, the variations in the proportions between these two molecules allowed Radjabian and his colleagues to group Iranian populations of *H. persicum* into three groups: one group of populations containing equal amounts of these two molecules, one group of populations containing more octyl acetate than hexyl butyrate and a third group of populations containing the inverse (octyl acetate < hexyl butyrate; Radjabian et al. 2013). This categorization motivated by chemotaxonomic reasons is dividing our smaller sampling in three groups too: populations of Sareyn, Kandovan and Zoshk belonging to the first category (octyl acetate = hexyl butyrate), the single population of Akhlamad belonging to the second category (octyl acetate > hexyl butyrate) and the rest of our investigated populations belonging to the last category. However, no clear relationship between these two components have been detected (Table 5), justifying the creation of this categorization, at the light of edaphic and climatic information (Table 6 and 7) and genetic tools should be used to verify the pertinence of this categorization. It should be mentioned that the two populations sharing the same locations than the ones of Radjabian et al. (2013) (Polur & Tangeh Vashi) have different octyl acetate/hexyl butyrate ratios and are classified in different chemotaxonomic categories than in the previous study. On the other hand, the concentrations of the hexyl butyrate molecule in fruits oils are explained by the variations of the electrical conductivity and of the chloride and nitrogen content of the soil where the *Golpar* plants grew. The annual mean diurnal range and the isothermality applied to the populations are also affecting strongly the variations of the concentration of this molecule. To summarize our findings about the different impacts of the edaphic and climatic factors, the concentration of this important chemical compound in the fruit oils is increased if the plants are growing in a soil rich in salts with a low level of nitrogen and under constant high temperatures. These new information can be crucial in the production of essential oils using *Heracleum persicum* plants. These findings about the optimal conditions for the hexyl butyrate production should be, however, confirmed by growth chamber experiments under controlled-environments.

Variations of the secondary chemical compounds

Hexyl isobutyrate, octenol acetate, hexyl-2-methyl butyrate, octyl isobutyrate, hexyl hexanoate, n-octyl butyrate and n-octyl-2-methyl butyrate are the molecules with the secondary higher amounts identified in our study (~5%). Their identifications and their quantifications are in accordance with previous reports (Saeidnia et al. 2005, Hajhashemi et al. 2009, Radjabian et al. 2013, Ebadollahi et al. 2014, Radjabian et al. 2014). Three of these secondary compounds were determinant in the principal component analysis (Figure 3) and were presenting high variability: n-octyl butyrate was representing 68% of the variability on the second axis, while hexyl isobutyrate and

hexyl-2-methyl butyrate were representing 89% and 82% of the variability represented on the third axis. Moreover, rare chemical compounds (<5%) as isopropyl-2-methyl butyrate, isopropyl-3-methyl butyrate, γ -terpinene and *p*-cymene were composing the majority of the variability represented on the first axis (94.5%, 88%, 87%, and 85% respectively). These four last chemical compounds were affected highly the grouping of the different populations of *H. persicum* tested in this study. Moreover, the amount of these components are positively correlated to each other. To conclude, although hexyl butyrate and octyl acetate are the chemical components with the highest amounts in all populations and can be used to separate *Heracleum persicum* from the other species of *Heracleum*, these “rare” chemical compounds are more useful on the species level to separate the different populations of *H. persicum*. However, additional factors such as genetic background and environmental variables, in particular the date of collection can affect these essential oils components within *H. persicum*. Moreover, environmental stresses can have important effects on the genes expression, the enzyme production and the synthetisation of the chemical compounds constituting the essential oils present in the plant metabolism (Lantemona et al. 2013). If a genetic background can explain the fact that certain populations, as per example the populations of Sareyn, Hamedan and Kandovan, are producing three times more oils than other Iranian populations (oil yield rates higher than 6%), certain environmental factor can participate to this higher production. Inversely to the main chemical compounds of *H. persicum* (hexyl butyrate), the number of components identified in the essential oils is increased if the plants are growing in soils presenting low electrical conductivity and low chloride content. These two edaphic factors are blocking the production of hexyl butyrate in the plant and favouring the production of other chemical compounds. In addition, this production of diverse chemical compounds necessitates a large range of extrem and instable temperatures applied to the plants. These new findings are providing crucial information in order to increase the production of chemical compounds present in *Heracleum persicum*. In the perspective of producing *Golpar* to extract its essential oils, our results are providing important information about which populations the botanists should select and the soil and thermic conditions required by the plants, as well as which nutrient should be provide to the plants. Indeed, the increase of phosphore (P) in the soil is increasing the oil yields produced by the fruits of the plant.

To conclude, certain new results are providing important information for the production of essential oils in *Golpar*, while other results confirmed previous conclusions. Indeed, certain rare chemical compounds such as γ -terpinene or *p*-cymene seem to be more pertinent in chemotaxonomy than the two main molecules (hexyl butyrate & octyl acetate) in order to differentiate populations within the *H. persicum* species. New findings enlightened the impacts of certain environmental parameters on the production of the essential oils by the *Golpar* plant (EC, Cl, P, variable temperatures). Although these preliminary results have to be confirmed by

controlled-environment experiments, they are providing new ways to explore in order to improve the use of *Heracleum persicum* as aromatic plant.

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