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Chemical Composition of Essential Oils from Aerial Parts of *Sisymbrium Irio* from Jordan

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Abstract: The volatile compounds obtained from *Sisymbrium irio* growing in Jordan has been analyzed by GC-MS. The major constituents are dioctyladipate (25.44%), *N*-(*n*-proyl) acetamide (14.77%), isopropyl isothiocyanate (11.55%), isobutyl isothiocyanate (6.75%), 3,7,11,15-tetramethyl-2-hexadecen-1-ol (6.52%), *cis*-8,11,14-eicosatrienoic acid (6.30%), heptacosane (3.89%), palmitic acid (3.45%), *n*-butyl isothiocyanate (2.85 %) and dimethoxyacetophenone (2.54 %).

Keywords: *Sisymbrium irio,* Cruciferae, Isopropyl isothiocyanate, Dioctyladipate.

Introduction

The cruciferae family is a large plant family that includes important food crops, herbs, ornamentals and weeds[1]. Forty six genera of this family are distributed in Jordan, including the genus *Sisymbrium*. There are seven species belonging to this genus in Jordan[2]. One of the most important species of this genus is *Sisymbrium irio*, which is grown in many parts of the world. The plant is a rich source of flavoinoids[3,4] and glucosinolates[5, 6]. It has a sharp flavor and can be used in salads. The plant is used in folk medicine as a febrifuge, a stimulating poultice, treating asthma and for infections of the throat and chest[7]. In this paper we report on the isolation and analysis of the volatile compounds from the aerial parts of *Sisymbrium irio* collected from the north of Jordan.

Experimental

Aerial parts of *Sisymbrium irio* ("al-hwarineh or al-shalwa" in Arabic) were collected at the onset of flowering, from Irbid area (north of Jordan). Identification of the plant species was done by professor D. Al-Esawi (Department of Biological Sciences, Faculty of Science, University of Jordan).

Isolation of the volatile components

The fresh aerial parts of *Sisymbrium irio* (30.0 g) were hydrodistilled using a Clevenger-type apparatus to recover the essential oils for 4 h. The oils distillate was separate from trace of water by extraction three times with 3 mL of Ether and dried overnight over 3.0 g of anhydrous sodium sulfate.

GC-MS analysis

Gas chromatography - mass spectrometry (GC-MS) analyses were performed using Agillent 6890 series II-5973 mass spectrometer interfaced with a HP chemstation. The chromatographic conditions were as follow: column oven programe, 40 ºC (10 min, isothermal) to 240 ºC (10 min, isothermal) at 2 ºC/min; the injector and detector temperatures were 270 and 280 ºC, respectively. Helium was the carrier gas (flow rate 0.70 mL/min). A HP-5 MS capillary column (30×0.25 mm *i.d.*, 0.25 µm film thicknesses) was utilized. The actual temperatures in MS source reached approximately 180 ºC. The ionization voltage was 70 eV. The volatile compounds were identified by comparing their MS patterns and retention times with those of known compounds published in the literature[8].

Results and Discussion

Sisymbrium irio is a plant grown in north and middle Jordan. The oil was analyzed by GC-MS; to give the gas chromatogram shown in Figure 1. The chromatogram showed that the volatile oil contains the compounds listed in Table 1.

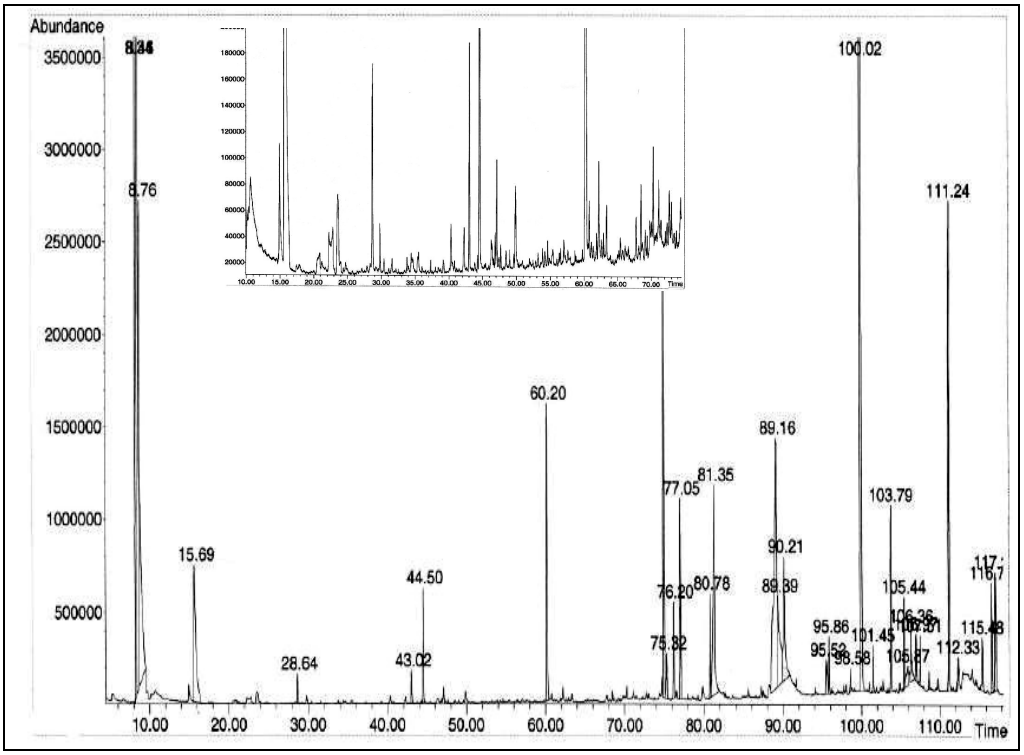


Figure 1. Gas chromatogram of volatile components of *Sisymbrium irio.*

Table 1. Composition and percentage of the essential oil from *Sisymbrium irio*.

No.	Compound	M^+	Retention time, min	Peak area %
1	Isopropyl isothiocyanate	101	8.34	11.55
2	*N*-(*n*-propyl)acetamide	101	8.50	14.77
3	Isobutyl isothiocyanate	115	8.76	6.75
4	2*E*-Hexenal	98	9.65	Trace
5	3-Hexen-1-ol	100	10.11	Trace
6	Dimethyl sulphone	94	14.92	0.10
7	*n*- Butyl isothiocyanate	115	15.69	2.85
8	Tetra acetyl-*d*-xylonic nitrile	343	20.87	Trace
9	3*E*-Hexenoic acid	114	22.80	0.05
10	*β*-Terpinyl acetate	136	23.56	0.12
11	Nonanal	142	29.79	0.07
12	4-(2,5–Dihydro-3-methoxy phenyl)butylamine	181	30.37	Trace
13	trans-*z*-*α*-Bisabolene epoxide	220	30.39	0.05
14	*p*-Anisaldehyde	136	40.35	0.08
15	Indole	117	43.06	0.22
16	*p*-Vinylguaiacol	150	44.47	0.78
17	Nicotine	162	46.40	0.06
18	1,5,8-Trimethyl-1,2-dihydronaphthalene	172	46.84	Trace
19	1,1,6-Trimethyl-1,2-dihydronaphthalene	172	46.85	Trace
20	1,1,6-Trimethyl-1,2,3,4-tetrahydronaphthalene	174	47.13	0.11
21	*o*-Benzyl-*L*-serine	195	47.69	0.06
22	3-Methyl indole	131	48.98	0.05
23	Isovanillin	152	49.88	0.13
24	3′,5′-Dimethoxyacetophenone	180	60.20	2.54
25	1,2,3b,6,7,8,-Hexahdro-6,6-dimethyl cyclopenta[1,3]cyclopropa[1,2]cyclohepten-3(3*H*)-one	190	60.75	Trace
26	8-Isopropyl-1,2,3,7-tetramethylbicyclo[5,1,0] octa-5-en-2-one	218	60.80	0.11
27	Deoxysericealacone	276	61.76	Trace
28	1,2–Dipalmitate glycerol	568	61.84	0.07
29	5-Isopropenyl-2-methylcyclopent-1-enecarboxaaldehyde	150	62.16	0.16
30	Tetrahydrospirilloxanthin	600	62.60	Trace
31	4-(2,4,4-trimethyl-cyclohexa-1,5-dienyl)but-3-*en*-2-one	190	63.31	0.05
32	Methoxyeugenol	194	67.71	Trace
33	13-Heptadecyn-1-ol	252	68.49	0.06
34	2-(2-Methylpropylidene)-1*H*-indene-1,3(2*H*)-dione	200	70.23	0.08
35	2,3,6-Trimethyl-1,4-naphthalenenedione	200	70.25	Trace
36	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	296	74.96	6.52
37	1-Eicosanol	298	75.35	0.39

Contd…

38	Oleic acid	282	76.56	0.67
39	Palmitic acid	256	81.34	3.45
40	*cis*-8,11,14-Eicosatrienoic acid	306	89.16	6.30
41	12-Methyl–*E,E*– 2,13-octadecadien-1-ol	280	89.39	2.04
42	Stearic acid	284	90.21	2.07
43	Docasane	310	95.86	0.36
44	Eicosanoic acid	312	98.57	0.15
45	Dioctyl adipate	370	100.00	25.44
46	Octacosane	394	103.78	1.25
47	1-Hexacosene	364	105.87	0.40
48	Docasanoic	340	106.38	0.60
49	Nonacosane	408	107.51	0.33
50	Heptacosane	380	111.26	3.89
51	Squalene	410	116.71	0.99
52	Octadecanal	268	117.23	1.10
53	Dotriacontane	450	118.70	0.06

**Trace : < 0.01*

The oil contained 53 components, representing 97.48% of the total oil. The main constituents of the oil were dioctyladipate (25.44%), *N*-(*n*-proyl) acetamide (14.77%), isopropyl isothiocyanat (11.55%), isobutyl isothiocyanate (6.75%), 3,7,11,15-tetramethyl-2-hexadecen-1-ol (6.52%), cis-8,11,14-eicosatrienoic acid (6.30%), heptacosane (3.89%), palmitic acid (3.45%), *n*-butyl isothiocyanate (2.85%) and dimethoxyacetophenone (2.54%). A classification of the constituents of the *sisymbrium irio* L. oil is given in Table 2. The oil included seven acids and two esters (38.80%), 11 nitrogen and sulfur containing compounds (36.41%), fifteen terpenoids (8.19%), six aliphatic hydrocarbons (6.29%), five aromatic compounds (3.53%), four fatty alcohols (2.49%) and three of other compounds (1.17%).

Table 2. Classification of the constituents of the *Sisymbrium irio*.

No.	Component	Peak area, %
1	Acids	13.29
2	Esters	25.51
3	Aliphatic hydrocarbons	6.29
4	Aromatic compounds	3.53
5	Terpenoids	8.19
6	Fatty alcohols	2.49
7	Nitrogen containing compounds	15.16
8	Sulfur containing compounds	0.10
9	(Nitrogen + sulfur) containing compounds	21.15
10	Others	1.17

Conclusion

Many crucifers such as *Sisymbrium irio* contain glucosinolates which are precursors of many volatile compounds, in particular nitriles and isothiocyanates. Isothiocyanates, which are strongly odorous and pungent compounds, are formed by the action of the enzyme thioglucoside glucohydrolase (myrosinase) on the glucosinolate when the plant tissue is disrupted[9,10]. In our case, intact plant material was subjected to an isolation procedure so that myrosinase action was restrained; hydrodistillation gave predominantly Isothiocyanates degradation products as observed in the chemical composition of the oil.

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