

Essential Oil Constituents of *Nigella sativa* from Iran

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ABSTRACT

The essential oil of *Nigella sativa* L. collected from Kurdistan Mountain, Iran, was obtained by hydrodistillation. The oil was analyzed by chromatography/mass spectrophotometry (GC/MS). *P*-cymene (40.7%) and thymoquinone (20.32%) were the major components of the essential oil from *Nigella sativa* L.

Keywords: *Nigella sativa*, Hydrodistillation, *P*-Cymene, Thymoquinone

İran'daki *Nigella sativa*'ların Esansiyel Yağlarının Bileşenleri

ÖZ

Nigella sativa L.'nin esansiyel yağları İran'da bulunan Kürd Dağları'ndan hidrodistilasyon yöntemi ile toplanmıştır. Yağ GC/MS yöntemi kullanılarak analiz edilmiştir. *P*-cymene (%40.7) ve timokinon (%20.32) *N. sativa*'dan elde edilen esansiyel yağın ana bileşenleri olarak belirlenmiştir.

Anahtar Kelimeler: *Nigella sativa*, Hidrodistilasyon, *P*-Cymene, Timokinon

INTRODUCTION

Aromatic plants are potential natural sources of novel antibiotics and particular interest has focused on their essential oils as main sources of potent antimicrobial and antifungal compounds classified as terpenoids, flavonoids and phenolics. As an aromatic plant, *Nigella sativa* is widely grown in north, west and east of the Iran and the seeds of black cumin have been used to promote health and antioxidant properties (Hedrick 1972). *Nigella sativa* seeds yield esters of fatty acids, free sterols and steryl esters (Menounos *et al.* 1986). The seeds also contain lipase, phytosterols and sitosterol (Duke 1992). Among the different groups of plant products, essential oils are especially considered as one of the most promising groups of natural products for the formulation of safer antifungal agents (Ali 2003, Celiktas *et al.* 2007). The present work was undertaken to determine the chemical composition of essential oils from *Nigella sativa* wild in Kurdistan Mountain, Iran.

MATERIALS AND METHODS

Plant material and extraction of essential oils

Seeds of *Nigella sativa* were collected during 2013-2014. Voucher specimens was identified by Dr. Esmaili and deposited, under the numbers *Nigella sativa* (no. 421), in the private herbarium of Dr F. Esmaili. Essential oils were isolated by hydrodistillation for 3 h using a Clevenger-type apparatus, according to the procedure described in the European Pharmacopoeia (2013). The obtained EOs were dried over Na₂SO₄ and stored in a sealed dark vials, at 4°C.

Essential oil analysis

Composition of the essential oils was determined by gas chromatography (GC) and mass spectrophotometry (GC/MS). The GC analysis was done on an Agilent Technologies 7890 GC equipped with a single injector and a flame ionization detector (FID). The analysis was carried out on fused silica capillary HP-5 column (30 m×0.32 mm i.d.; film thickness 0.25 µm). The injector and detector temperatures were kept at 250°C and 280°C, respectively. Nitrogen was used as carrier gas at a flow rate of 1 ml/min; oven temperature program was 60–210°C at the rate of 4°C/min and then programmed to 240°C at the rate of 20°C/min and finally held isothermally for 8.5 min; split ratio was 1:50. GC–MS analysis was carried out by use of Agilent gas chromatograph equipped with fused silica capillary HP-5MS column (30 m×0.25 mm i.d.; film thickness 0.25 µm) coupled with 5975-C mass spectrometer. Helium was used as carrier gas with ionization voltage of 70 eV. Ion source and interface temperatures were 230°C and 280°C, respectively. Mass range was from 45 to 550 amu. Oven temperature program was the same given above for the GC. The constituents of the EOs were identified by calculation of

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their retention indices under temperature-programmed conditions for *n*-alkanes (C₈–C₂₅) and the oil on a HP-5 column under the same chromatographic conditions. Identification of individual compounds was made by comparison of their mass spectra with those of the internal reference mass spectra library or with authentic compounds and confirmed by comparison of their retention indices with authentic compounds or with those of reported in the literature (Adams 2001). For quantification purpose, relative area percentages obtained by FID were used without the use of correction factors.

RESULTS AND DISCUSSION

Chemical composition of the essential oils

The essential oil obtained in yields of 0.84 % (*N. sativa*) (v/w) dried mass. This is comparable to the yield of the EOs obtained from the aerial part and seeds of other species considered economically important, such as *N. sativa* (Burits and Bucar 2000). Results obtained by the GC–MS chemical analysis of *N. sativa* essential oil are presented in Table 1. In total, 18 compounds were identified. Eighteen compounds were identified in *N. sativa* oil, which accounted for 98.39% of the total oil; the major constituent was *p*-cymene (32.05%), followed by thymoquinone (20.32%). Our results on chemical profiling of the *N. sativa* EO are in agreement with some other studies (Burits and Bucar 2000). In addition, chemical profile of our *N. sativa* EO sample is in opposition with report of Iran, Algeria and India (Hajhashemi *et al.* 2004, Singhet *et al.* 2005, Benkaci-Ali *et al.* 2007). The chemical compositions revealed that this seeds had compositions relatively similar to those of other *N. sativa* essential oils analyzed by Fatima *et al.* (2002) and Shareef (2011). The different qualitative and quantitative chemical compositions of these EOs with respect to previous investigations could be related first and foremost to the different environmental conditions, genetics (degree of hybridization), geographical origin and harvest period. Iran is one of the richest countries of the world in terms of having a substantial number of different medicinal plants species grown in various ecological conditions.

Table 1. Chemical composition of *Nigella sativa* volatile oil constituents.

Compound	%	RI	Compound	%	RI
α -Thujene	6	916	γ -Terpinene	5.12	1068
α -Pinene	1.11	920	Terpinolene	0.23	1080
Camphene	11	928	Camphor	1	1120
Sabinene	1	956	Borneol	0.43	1168
β -Pinene	7	960	Carvone	0.32	1240
β -Myrcene	0.21	968	Thymoquinone	20.32	1252
α -Phellandrene	0.45	1000	Thymol	10.12	1290
Limonene	0.13	1020	Carvacrol	1	1301
<i>p</i> -Cymene	32.05	1022	Longicyclene	0.9	1387
Total	98.39				

^a The retention Kovats indices were determined on HP5 capillary column.

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