

## GC- MS study of *Nigella sativa* (seeds) fatty oil

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### RESUMEN

#### Estudio por GC-MS del aceite de la semilla de *Nigella sativa*.

El estudio por GC-MS del aceite de la semilla de *Nigella sativa* reveló la presencia de 26 compuestos los cuales fueron identificados como: hept-6-enoato de metilo, 1-fenilhepta-2,4-diona, pentadecano, hexadec-1-eno, 1-fenildecan-2-ona, octadec-1-eno, octadecano, pentadecanoato de metilo, bis(3-clorofenil) cetona, ftalato de dietilo, octadec-7-enoato de etilo, octadecanoato de metilo, tricos-9-eno, ácido octadeca-9,12-dienoico, ácido hexadecanoico, hexadecanoato de metilo, octadec-15-enoato de metilo, henicusan-10-ona, ácido 2-metil octadecanoico, docos-1-eno, octadecanoato de etilo, octadecanoato de metilo, pentacos-5-eno, 12-metiltricosano, ftalato de dibutilo y 2-metiltetracosano.

**PALABRAS-CLAVE:** Aceite – Cromatografía de gases-Espectrometría de masas – *Nigella sativa* - Semilla.

### SUMMARY

#### GC-MS study of *Nigella sativa* (seeds) fatty oil.

The GC-MS study of *N. sativa* (seeds) fatty oil revealed the presence of 26 compounds which were identified as methyl hept-6-enoate, 1-phenylhepta-2,4-dione, pentadecane, hexadec-1-ene, 1-phenyldecan-2-one, octadec-1-ene, octadecane, methyl pentadecanoate, bis(3-chlorophenyl) ketone, diethyl phthalate, ethyl octadec-7-enoate, methyl octadecanoate, tricos-9-ene, octadeca-9,12-dienoic acid, hexadecanoic acid, methyl hexadecanoate, methyl octadec-15-enoate, henicusan-10-one, 2-methyl octadecanoic acid, docos-1-ene, ethyl octadecanoate, methyl octadecanoate, pentacos-5-ene, 12-methyltricosane, dibutyl phthalate and 2-methyltetracosane.

**KEY WORDS:** Gas chromatography-Mass spectrometry – *Nigella sativa* – Oil - Seed.

### 1. INTRODUCTION

*Nigella sativa* locally known as "Kalaunji" is an spicy plant. Its seeds are believed to have carminative, stimulatory and diaphoretic properties<sup>1-3</sup>. From the oil of its seeds (Nigellidine), sterols like cholesterol, campesterol, stigmasterol,  $\beta$ -sitosterol and  $\alpha$ -spinosterol have been identified<sup>4,5</sup>. Isolation of new saponins, nigelline, nigellimine and nigellicine have also been reported<sup>6-9</sup>. The present communication reports the identification of main constituents of the fatty oil fraction of *N. sativa* seeds by GC- MS study.

### 2. EXPERIMENTAL

The seeds were purchased from the local market, powdered and extracted in a soxhlet extractor with hexane. Removal of the solvent under reduced pressure left an oily mass. The extract was fractionated on a silica gel column. The column was eluted with different solvents in their increasing order of polarity. The benzene fraction have shown broad single spot. All the fractions of similar TLC pattern were mixed together and the solvent was removed to yield an oily mass which was rechromatographed on an alumina grade III column, which afforded two oily fractions using solvent system hexane: benzene (1:3,v/v) and (1:9,v/v), and designated as I and II respectively. Their TLC examination using benzene: ether: acetic acid (9:1:1,v/v) showed single long spot.

The oil was analysed at the Regional Sophisticated Instrumentation Centre, IIT, Powai, Mumbai by GC-MS. The operating parameters are as follows: 5.5x4 mm id glass column, packed with carbowax 20M (10% on chromosorb W, AW and DMCS treated); helium gas was used as a carrier gas at the rate of 40 ml/min, temp. 70°C to 200°C at 4°C/min, detector and injection port heaters maintained at 300°C and 200°C respectively. Significant operating parameters of the MS were: ionisation voltage 70 eV, ionisation current 100  $\mu$ A; source temperature 225°C, accelerating voltage 1.33 KV; resolution 1000; scan speed 3 sec/ decade. Data are processed on a Kratos DS-50 data processing system.

### 3. RESULTS

The GC-MS analysis revealed in all the presence of 26 compounds which were identified by comparing their retention time, kovat indexes and by interpretation of their mass spectra<sup>10</sup>. The results and mass fragmentation data are being given in Table I.

The compounds were identified as methyl hept-6-enoate, 1-phenylhepta-2,4-dione, pentadecane, hexadec-1-ene, 1-phenyldecan-2-one, octadec-1-ene, octadecane, methyl pentadecanoate, bis(3-chlorophenyl) ketone, diethyl phthalate, ethyl octadec-7-enoate, methyl octadecanoate, tricos-9-ene, octadeca-9,12-dienoic acid, hexadecanoic acid,

methyl hexadecanoate, methyl octadec-15-enoate, henicosan-10-one, 2-methyl octadecanoic acid, docos-1-ene, ethyl octadecanoate, methyl octadecanoate, pentacos-5-ene, 12-methyltricosane, dibutyl phthalate and 2-methyltetracosane.

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Table I  
GC-MS data of the oil fraction

Peak No	RT (min)	% in the oil	m/z mol. ion peak	m/z base peak	m/z Other fragments	Compounds identified
1.	12.64	2.7	142	74	111,101,73,60,55,41,29	Methyl hept-6-enoate
2.	12.73	10.2	204	161	119,91,77	1-Phenylhepta-2,4-dione
3.	13.4	2.3	212	57	85,71,43,29	Pentadecane
4.	13.9	2.4	224	57	83,69,41,29	Hexadec-1-ene
5.	14.3	2.3	232	91	175,147,105	1-Phenyldecan-2-one
6.	15.4	2.6	252	85	57,43	Octadec-1-ene
7.	18.3	2.33	254	57	169,85,71,43,29	Octadecane
8.	18.5	7.24	270	74	157,55,43,29	Methyl pentadecanoate
9.	18.8	0.34	250	139	215,113,111,75	Bis(3-Chlorophenyl) ketone
10.	19.9	0.8	222	149	76	Diethyl phthalate
11.	20.2	13.7	310	55	265,264,97,88,83,41	Ethyl octadec-7-enoate
12.	20.3	4.8	298	74	157,101,55,43	Methyl octadecanoate
13.	20.6	4.4	322	57	141,101,71,43	Tricos-9-ene
14.	21.2	1.50	280	55	109,81,67	Octadeca-9,12-dienoic acid
15.	22.2	4.3	256	73	129,43,29	Hexadecanoic acid
16.	22.7	3.2	270	74	129,115,98,56,43	Methyl hexadecanoate
17.	25.9	2.8	296	55	97	Methyl octadec-15-enoate
18.	29.5	2.6	310	183	211,183,113,98,43	Henicosan-10-one
19.	29.7	2.3	298	55	141,112,97,69,41	2-Methyloctadecanoic acid
20.	30.6	11.3	308	55	141,128,98,70,41	Docos-1-ene
21.	30.8	1.17	312	73	284,185,129,98,70,55	Ethyl octadecanoate
22.	31.1	2.5	298	74	157,101,73,55	Methyl octadecanoate
23.	31.8	2.7	350	57	125,112,98,70,55	Pentacos-5-ene
24.	31.9	11.8	338	183	211,155,127,98,55	12-Methyltricosane
25.	32.5	2.4	278	149	167	Dibutyl phthalate
26.	38.5	1.3	352	43	211,155,126,98,70,42	2-Methyltetracosane

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