

Supplementary Material 1 Chemical structures of *N. sativa* seeds main constituents
(source: Liu *et al.*, 2011)

NIGELLA SATIVA SEEDS

- Whole seeds
- Ground seeds



CONDITION OF STORAGES

Condition	Whole seeds	Ground Seeds	Vial	Nitrogen	Light
A	1/3	-	Amber	-	-
B	Full	-	Amber	-	-
C	Full	-	Transparent	-	-
D	1/3	-	Amber	Flush	-
E	-	1/3	Amber	-	-
F	-	Full	Amber	-	-
G	-	1/3	Amber	Flush	-
H	1/3	-	Amber	-	Expose



STORAGE TIME POINTS

- 1 day
- 14 days
- 28 days



GC/MS ANALYSIS (HEAD SPACE)



MULTIVARIATE DATA ANALYSIS (MVDA)

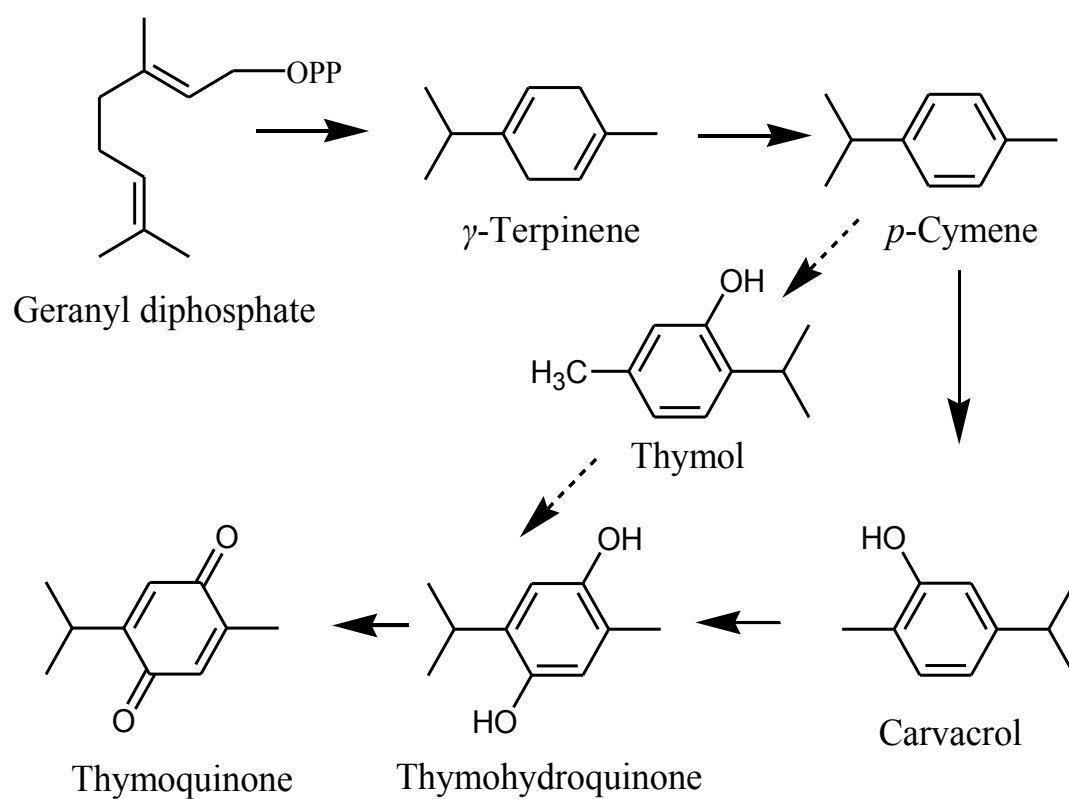
1 Supplementary Material 3 Peak area (10x⁷) of selected constituents

Storage time	Peak area of constituents (10x ⁷)					
	α- Thujene	p-Cymene	Carvone	Thymoquinone	Carvacrol	Longifolene
Condition A						
A0 (1 st day)	6.617±1.074 ^a	26.239±3.638 ^a	8.041±1.363 ^a	10.535±2.100 ^a	6.292±0.980 ^a	2.967±0.441 ^a
A1 (14 th day)	3.233±0.517 ^b	12.542±1.540 ^b	4.235±0.628 ^b	5.062±0.928 ^b	4.426±1.201 ^b	1.561±0.222 ^b
A2 (28 th day)	8.782±0.122 ^c	2.682±0.244 ^c	0.820±0.094 ^c	0.981±0.139 ^c	8.880±0.078 ^c	0.446±0.094 ^c
Condition B						
B0 (1 st day)	6.348±0.820 ^a	26.297±4.633 ^a	11.216±4.811 ^a	12.130±4.198 ^a	11.828±2.453 ^a	3.963±1.678 ^a
B1 (14 th day)	4.821±1.982 ^a	20.999±8.988 ^a	6.544±2.751 ^a	6.934±2.738 ^b	7.851±2.958 ^b	2.660±1.151 ^a
B2 (28 th day)	0.809±0.240 ^b	2.541±0.703 ^b	0.766±0.279 ^b	0.764±0.209 ^c	0.644±0.125 ^c	0.401±0.099 ^b
Condition C						
C0 (1 st day)	5.969±2.128 ^a	23.006±4.940 ^a	7.486±1.333 ^a	9.140±1.407 ^a	6.015±1.738 ^a	2.642±0.471 ^{ab}
C1 (14 th day)	6.752±2.560 ^a	26.297±13.758 ^a	9.697±8.936 ^a	7.380±5.127 ^a	7.257±5.236 ^a	3.812±2.864 ^b
C2 (28 th day)	11.826±7.063 ^b	52.429±13.802 ^b	27.798±15.660 ^b	22.436±14.947 ^a	19.279±9.459 ^b	7.394±2.735 ^{bc}
Condition D						
D0 (1 st day)	6.797±0.899 ^a	25.625±2.935 ^a	8.906±1.104 ^a	7.053±1.289 ^a	14.659±1.237 ^a	3.501±0.399 ^a
D1 (14 th day)	7.885±0.828 ^a	29.919±4.001 ^a	10.787±3.753 ^a	12.958±4.182 ^a	13.291±3.866 ^a	4.285±1.464 ^a

D2 (28 th day)	13.018±1.179 ^b	49.105±4.136 ^b	16.123±1.216 ^b	32.128±11.737 ^b	16.248±1.387 ^a	6.180±0.423 ^b
Condition E						
E0 (1 st day)	938.035±1241.148 ^a	1831.768±1922.327 ^a	4.249±4.046 ^a	42.947±63.688 ^a	10.323±8.767 ^a	24.653±24.701 ^a
E1 (14 th day)	1235.740±201.471 ^a	3922.320±605.098 ^a	2.084±0.555 ^a	24.652±2.479 ^a	8.656±2.758 ^a	18.800±7.039 ^a
E2 (28 th day)	1363.585±843.986 ^a	4304.681±2294.927 ^a	2.975±1.739 ^a	37.720±22.497 ^a	15.199±8.119 ^a	30.582±16.626 ^a
Condition F						
F0 (1 st day)	702.425±943.191 ^{ab}	2408.180±2427.564 ^{ab}	10.214±4.864 ^{ab}	84.896±94.554 ^a	22.714±18.898 ^{ab}	51.315±44.861 ^{ab}
F1 (14 th day)	1359.189±820.535 ^b	4074.124±1111.216 ^b	4.764±1.238 ^b	42.108±16.200 ^a	19.330±5.179 ^b	42.954±12.033 ^b
F2 (28 th day)	77.092±158.586 ^{ac}	480.307±891.473 ^{ac}	1.659±2.481 ^{bc}	8.220±14.150 ^a	1.923±1.668 ^{bc}	3.632±3.482 ^{bc}
Condition G						
G0 (1 st day)	22.786±26.056 ^a	1141.381±850.809 ^a	3.055±0.512 ^a	70.464±43.856 ^a	18.257±4.669 ^a	20.742±4.972 ^a
G1 (14 th day)	2.915±4.695 ^a	110.938±167.432 ^b	0.590±0.168 ^b	23.399±5.982 ^b	2.783±1.662 ^b	4.286±2.267 ^b
G2 (28 th day)	0.561±1.203 ^a	10.916±19.501 ^b	0.015±0.044 ^c	0.428±0.204 ^b	0.038±0.017 ^b	0.159±0.066 ^b
Condition H						
H0 (1 st day)	2.885±0.097 ^a	8.209±0.212 ^a	3.393±1.697 ^a	5.561±2.774 ^a	5.421±1.123 ^a	2.170±0.261 ^a
H1 (14 th day)	0.020±0.005 ^b	0.051±0.008 ^b	0.082±0.009 ^b	0.096±0.010 ^b	0.035±0.004 ^b	0.037±0.003 ^b
H2 (28 th day)	1.828±0.430 ^c	0.247±0.080 ^b	0.391±0.137 ^b	0.460±0.139 ^b	0.294±0.108 ^b	0.274±0.110 ^b

- 2 * Mean values with similar letters within columns for each condition of storages are not significantly different among the storage time points
- 3 (Turkey comparison test, P < 0.05)

1
2



3

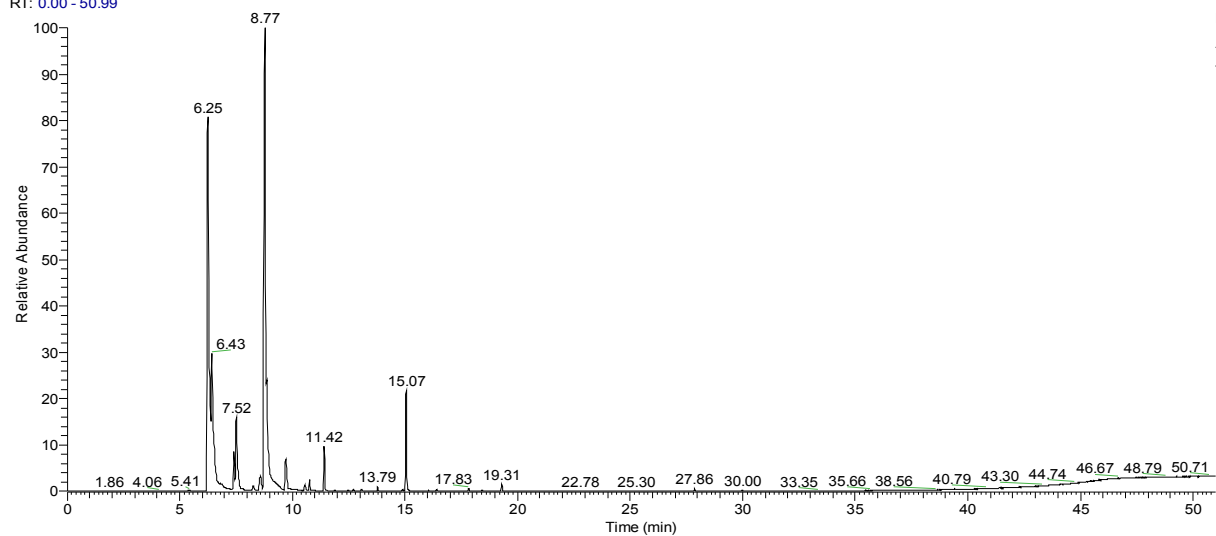
4

5

6 **Supplementary Material 4 Biosynthetic pathway of main of main constituents in *N.***
7 ***sativa* (source : Botnick et al., 2012)**

Incubation temperature 80 degree

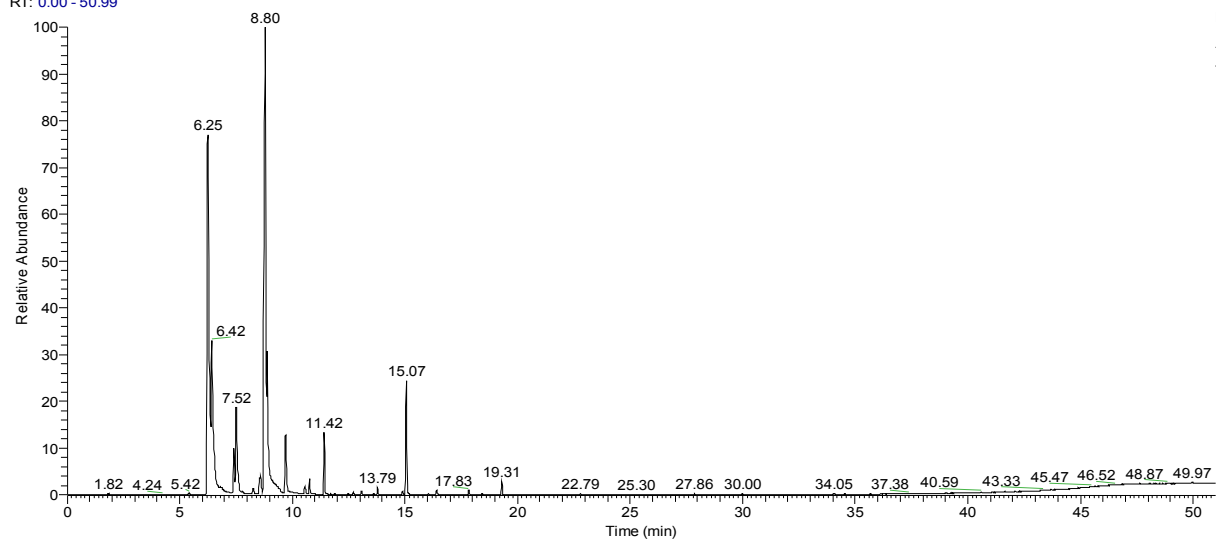
RT: 0.00 - 50.99



NL:
1.49E9
TIC MS
test2

Incubation temperature 100 degree

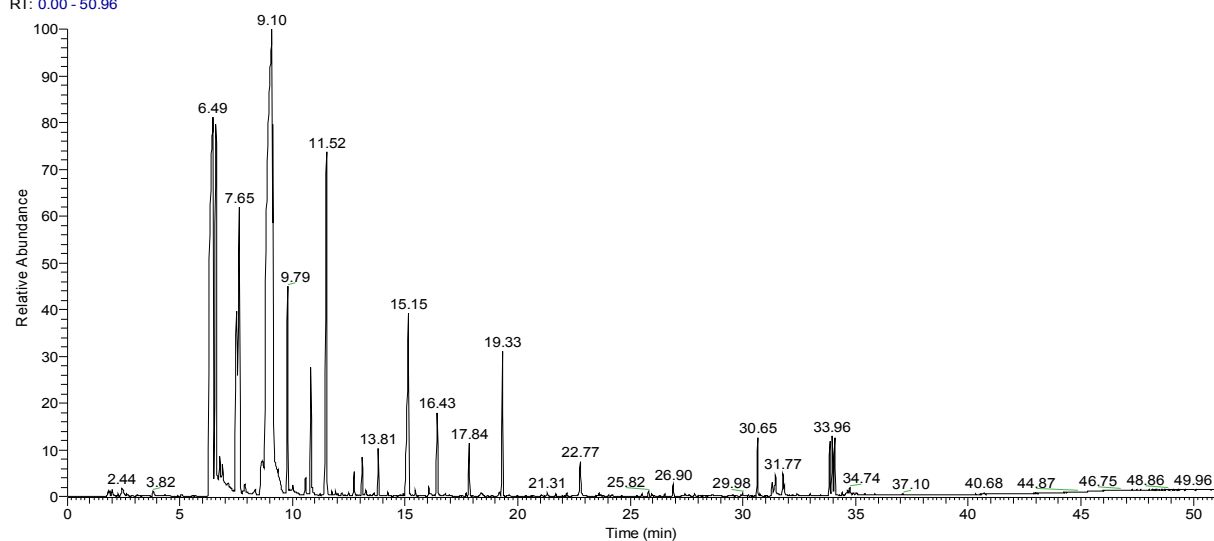
RT: 0.00 - 50.99



NL:
1.81E9
TIC MS
test1

Incubation temperature 160 degree
RT: 0.00 - 50.96

NL:
3.29E9
TIC MS
test3



Supplementary Material 5 Result of peak area from three different incubation temperature

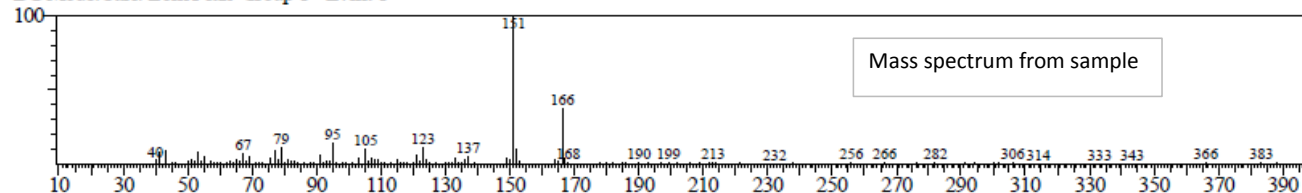
Mass spectrum of thymohydroquinone detected in Flavour and Fragrance Natural and Synthetic Compounds (FFNSC) version 1.3 library

<<Target>>

Line#:26 R.Time:39.961(Scan#:44354) Retention Index:1642 MassPeaks:229

RawMode:Averaged 39.960-39.962(44353-44355) BasePeak:151.05(22404)

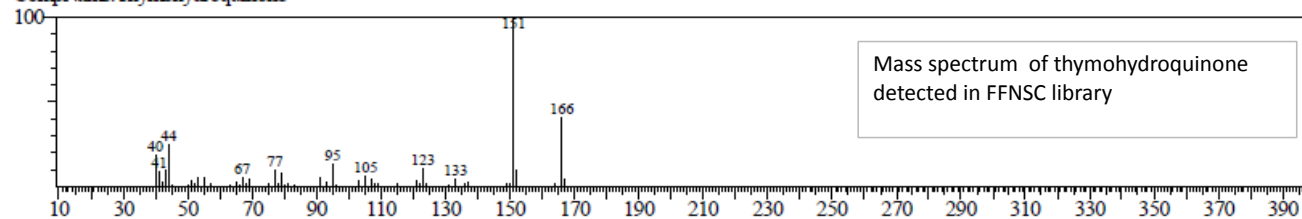
BGMode:Calc. from Peak Group 1 - Event 1



Hit#1 Entry:1823 Library:FFNSC1.3.lib

SI:90 Formula:C10H14O2 CAS:2217-60-9 MolWeight:166 RetIndex:1554

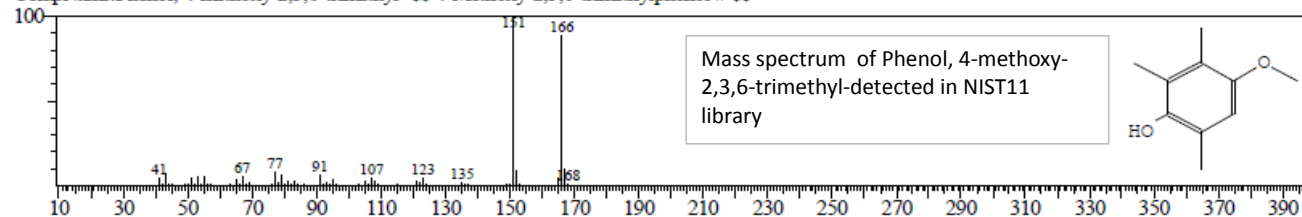
CompName:Thymohydroquinone



Hit#2 Entry:23517 Library:NIST11.lib

SI:86 Formula:C10H14O2 CAS:53651-61-9 MolWeight:166 RetIndex:1430

CompName:Phenol, 4-methoxy-2,3,6-trimethyl- \$\$ 4-Methoxy-2,3,6-trimethylphenol # \$\$



Supplementary Material 6 The molecular weights and mass spectra of phenol,4-methoxy-2,3,6-trimethyl and thymohydroquinone