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SUPPLEMENTARY MATERIAL TO

HPTLC-based metabolomics for the investigation of metabolic changes during plant development: The case study of *Artemisia annua*

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Table S-I. Fractionation by dry-column flash (DF) chromatography

Number of fraction	Hexane:ethyl acetate volume ratio	Volume, mL
DF1-DF9	95:5	400
DF10-DF18	90:10	400
DF19-DF22	85:15	200
DF23-DF26	80:20	200
DF27-DF30	75:25	200
DF31-DF34	70:30	200

IDENTIFICATION OF THE COMPOUNDS – SPECTRAL DATA

Compounds on HPTLC plate (Fig. 1) Triacylglycerol retention factors, R_f = 0.92 – 0.96.

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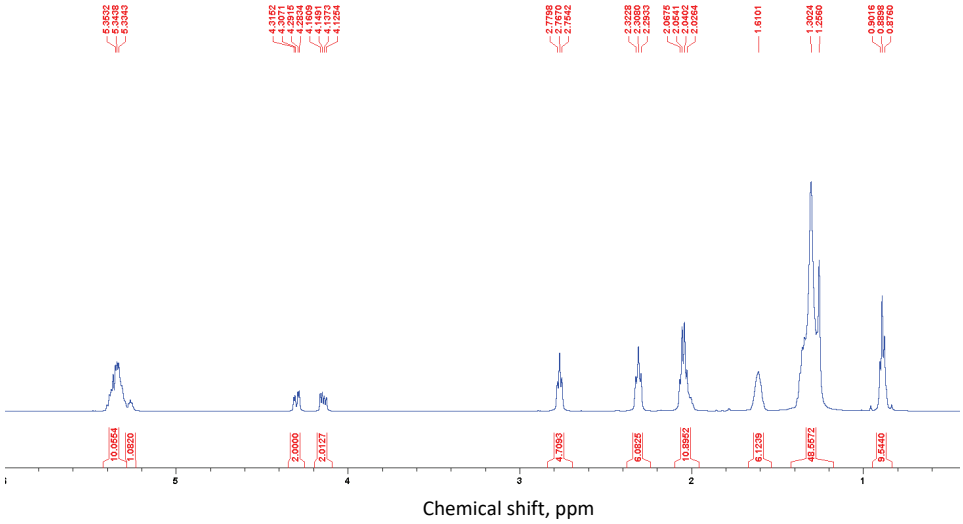

Fig. S-1. ^{1}H NMR spectrum of triacylglycerol.

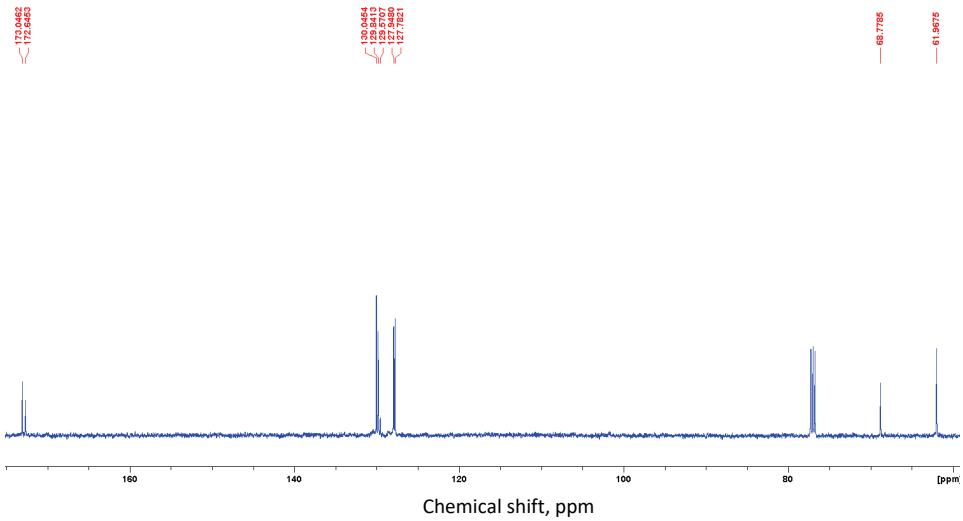

Fig. S-2. ^{13}C NMR spectrum of triacylglycerol.

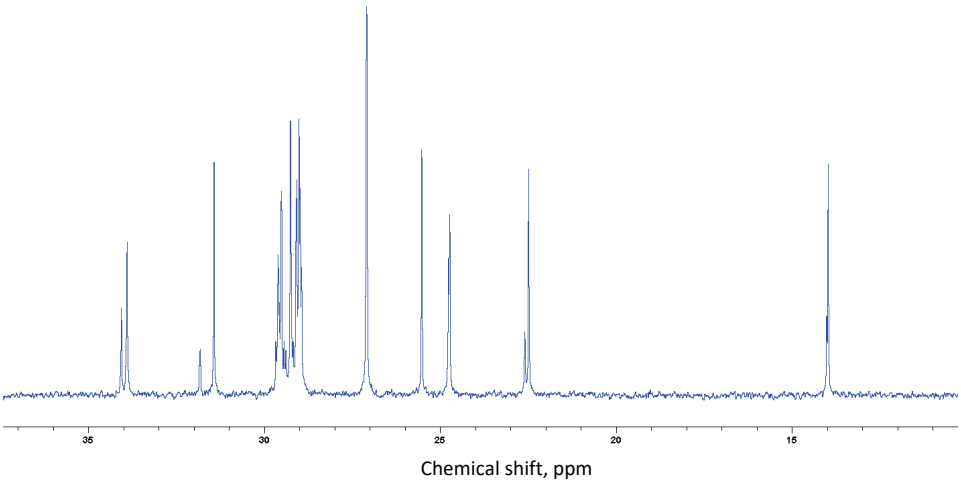

Fig. S-3. ^{13}C NMR spectrum of triacylglycerol.

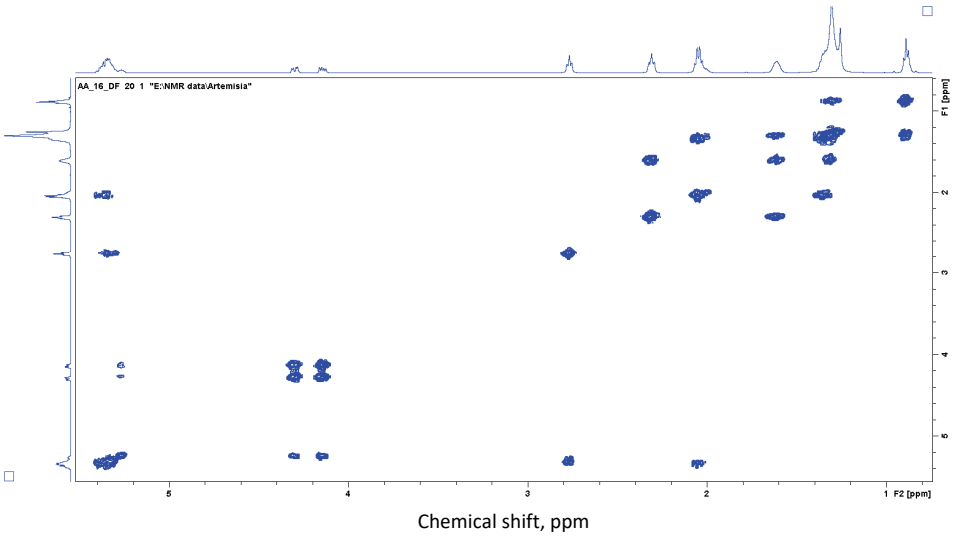

Fig. S-4. COSY spectrum of triacylglycerol.

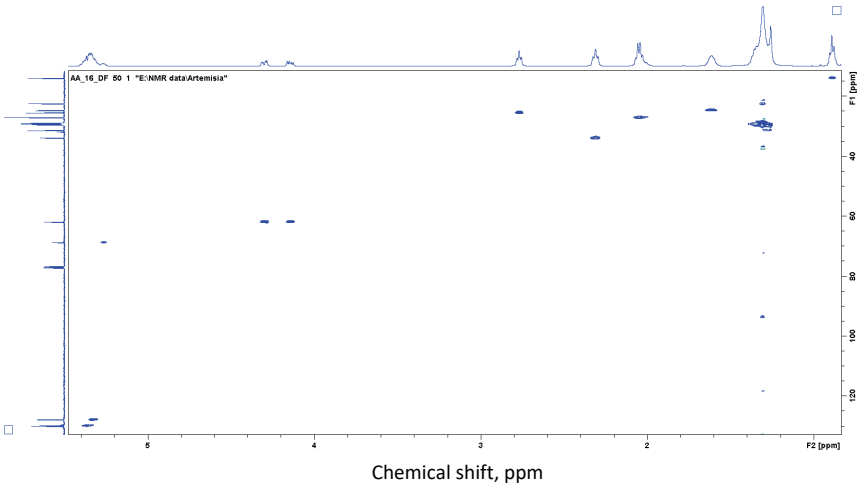

Fig. S-5. HSQC spectrum of triacylglycerol.

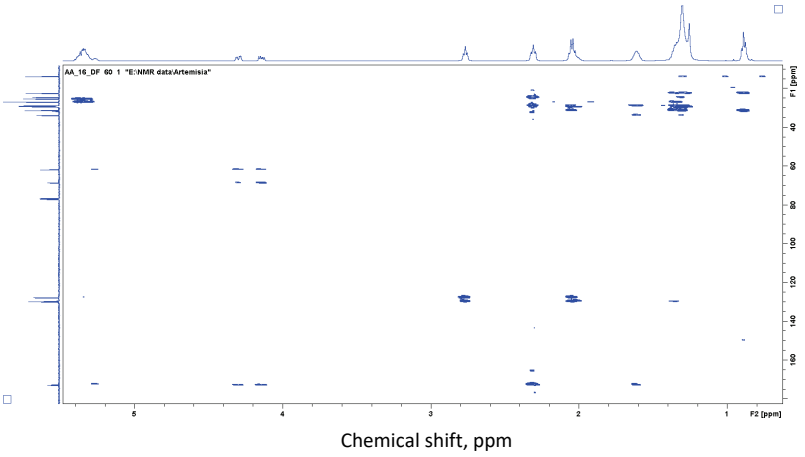

Fig. S-6. HMBC spectrum of triacylglycerol.

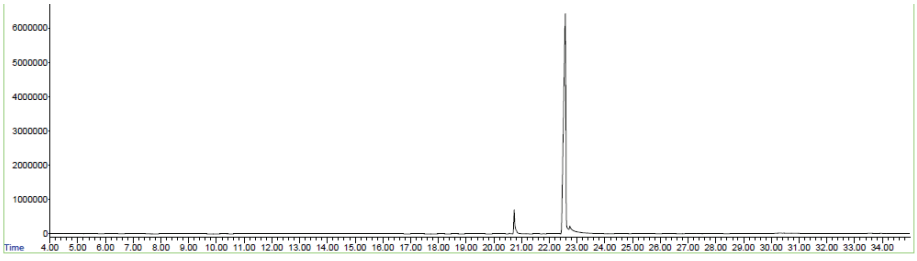

Fig S-7. GC-FID chromatogram of fraction DF16 containing Methyl palmitoleate (Retention time - *RT* = 20.560 min, Retenrion index - *RI* 1935), Methyl Palmitate (*RT* = 20.73 min, *RI* = 1950) and 9,12-Octadecadienoic acid (Z,Z)-, methyl ester (*RT* = 22.53 min, *RI* = 2116).

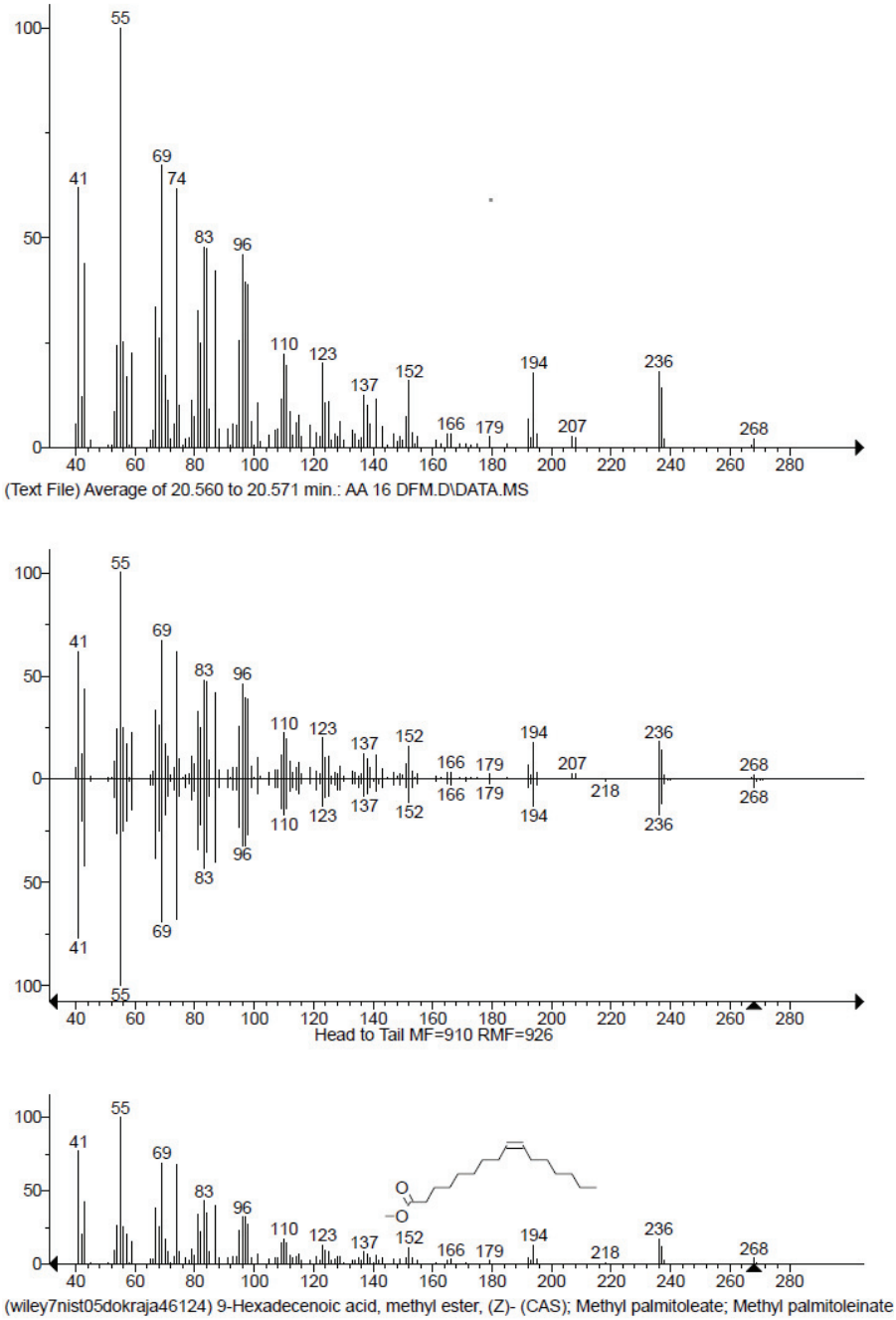

Fig. S-8. MS spectrum of methyl palmitoleate (top) and its comparison with the spectrum from the database (middle and bottom).

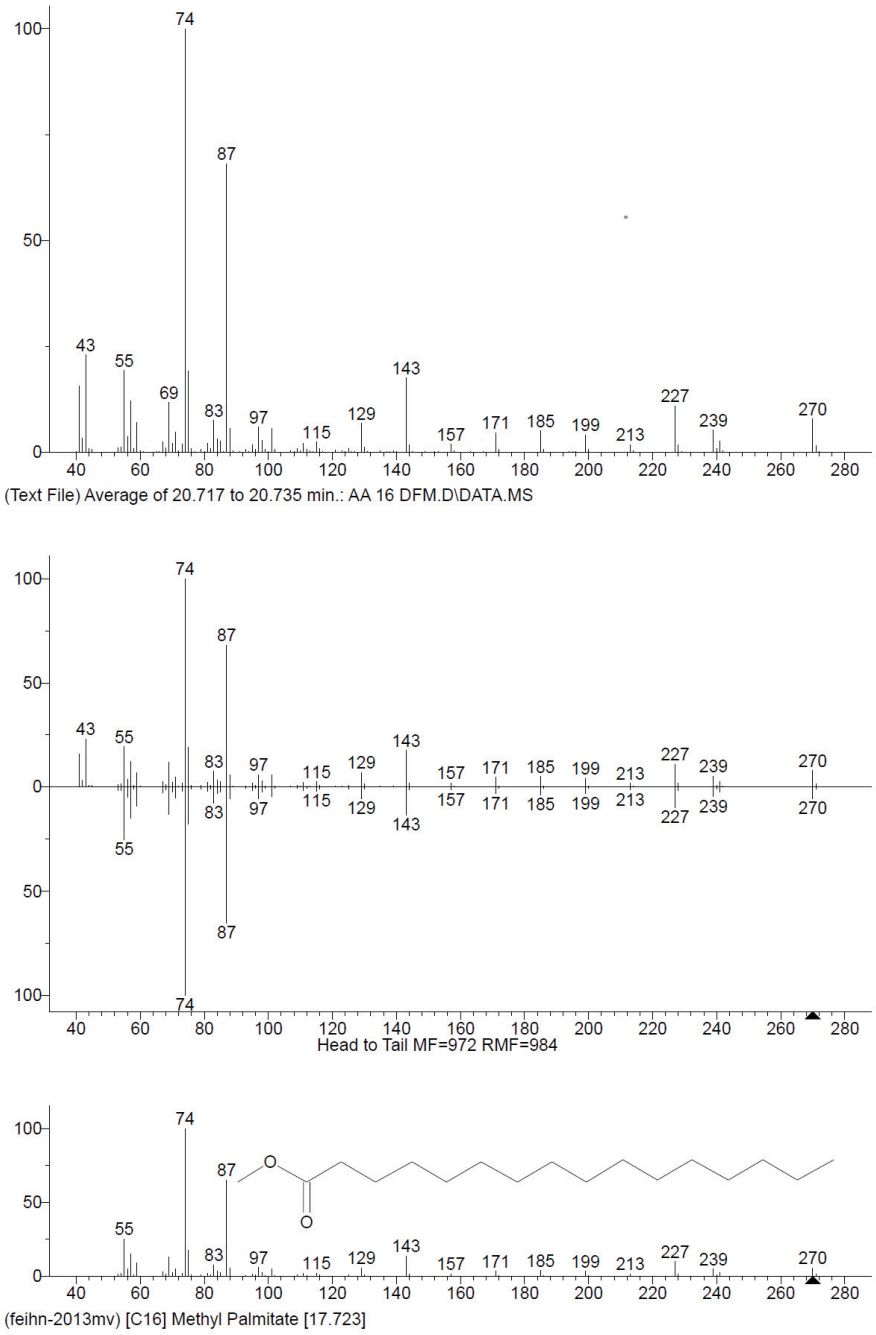

Fig. S-9. MS spectrum of methyl palmitate (top) and its comparison with the spectrum from the database (middle and bottom).

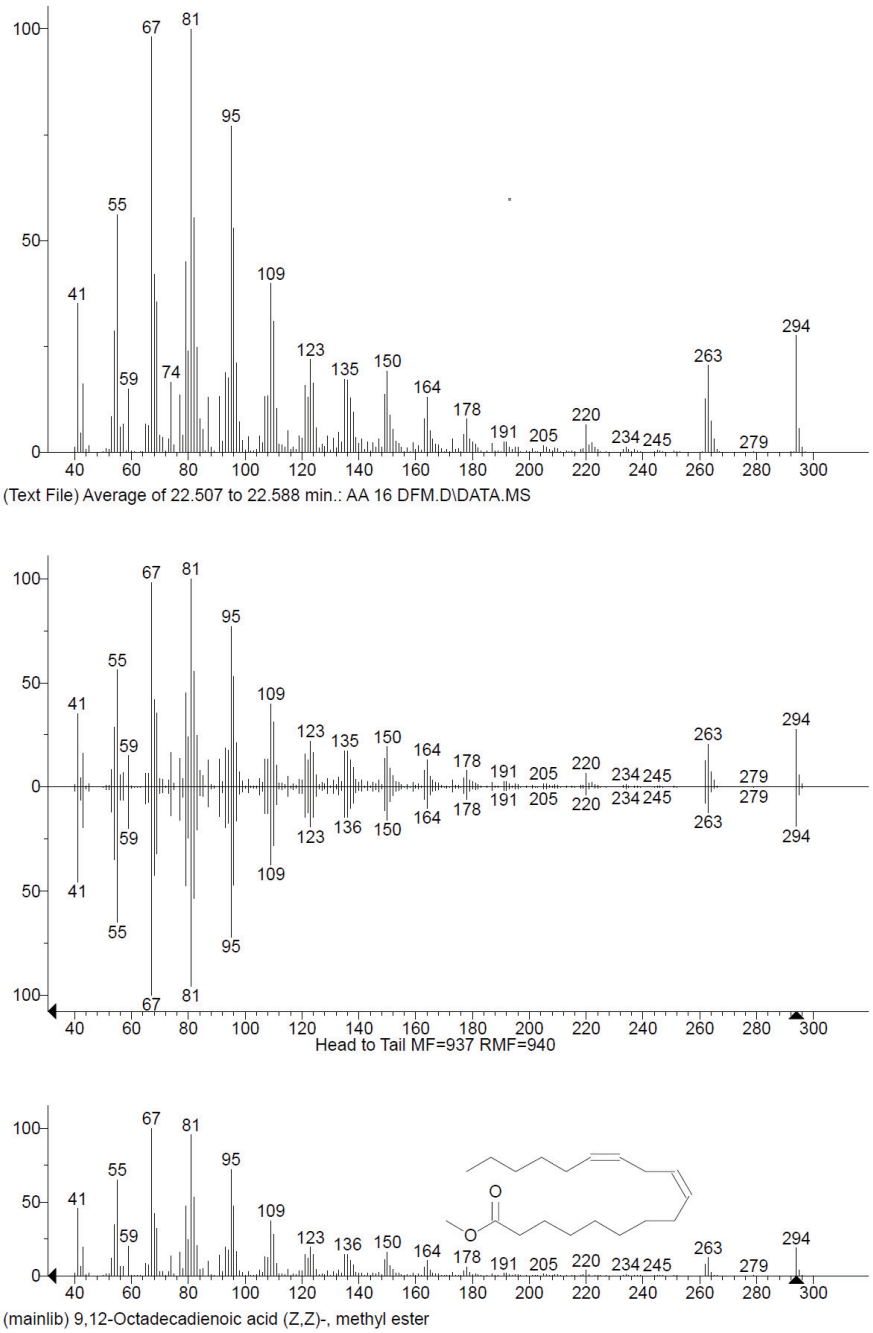

Fig. S-10. MS spectrum 9,12-Octadecadienoic acid (Z,Z)-, methyl ester (top) and its comparison with the spectrum from the database (middle and bottom).

Compounds on HPTLC plate (Fig. 1): *α*-pinene (*RI* = 932), *α*-copaene (*RI* = 1373), E-cariophylene (*RI* = 1416); *β*-selinene (*RI* = 1484), R_f = 0.84 - 0.88

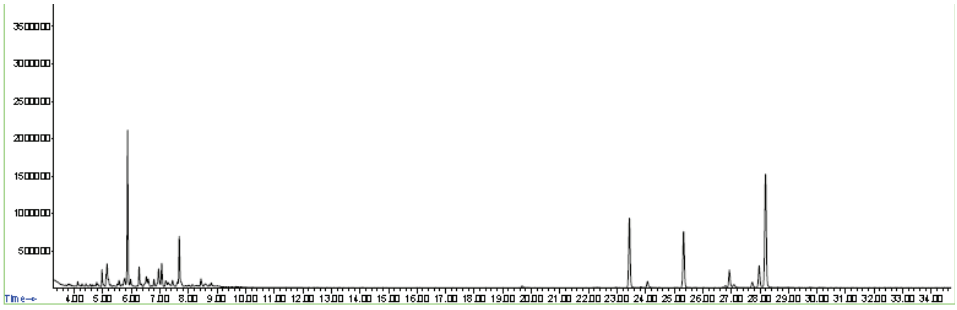

Fig S-11. GC-MS chromatogram of fraction DF1 containing *α*-pinene, *α*-copaene, E-caryophyllene, and *β*-selinene.

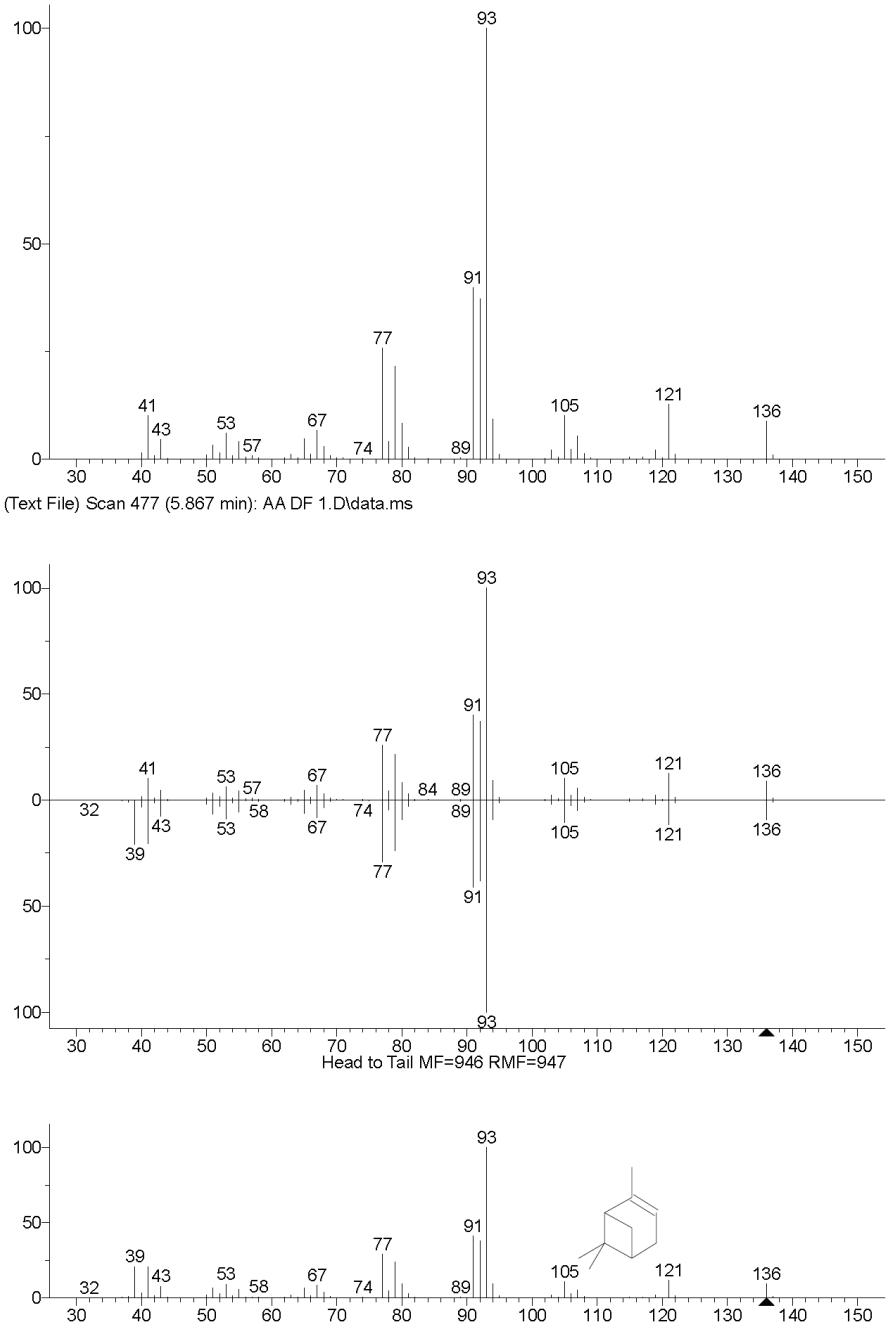

Fig. S-12. MS spectrum of α-pinene (top) and its comparison with the spectrum from the database (middle and bottom).

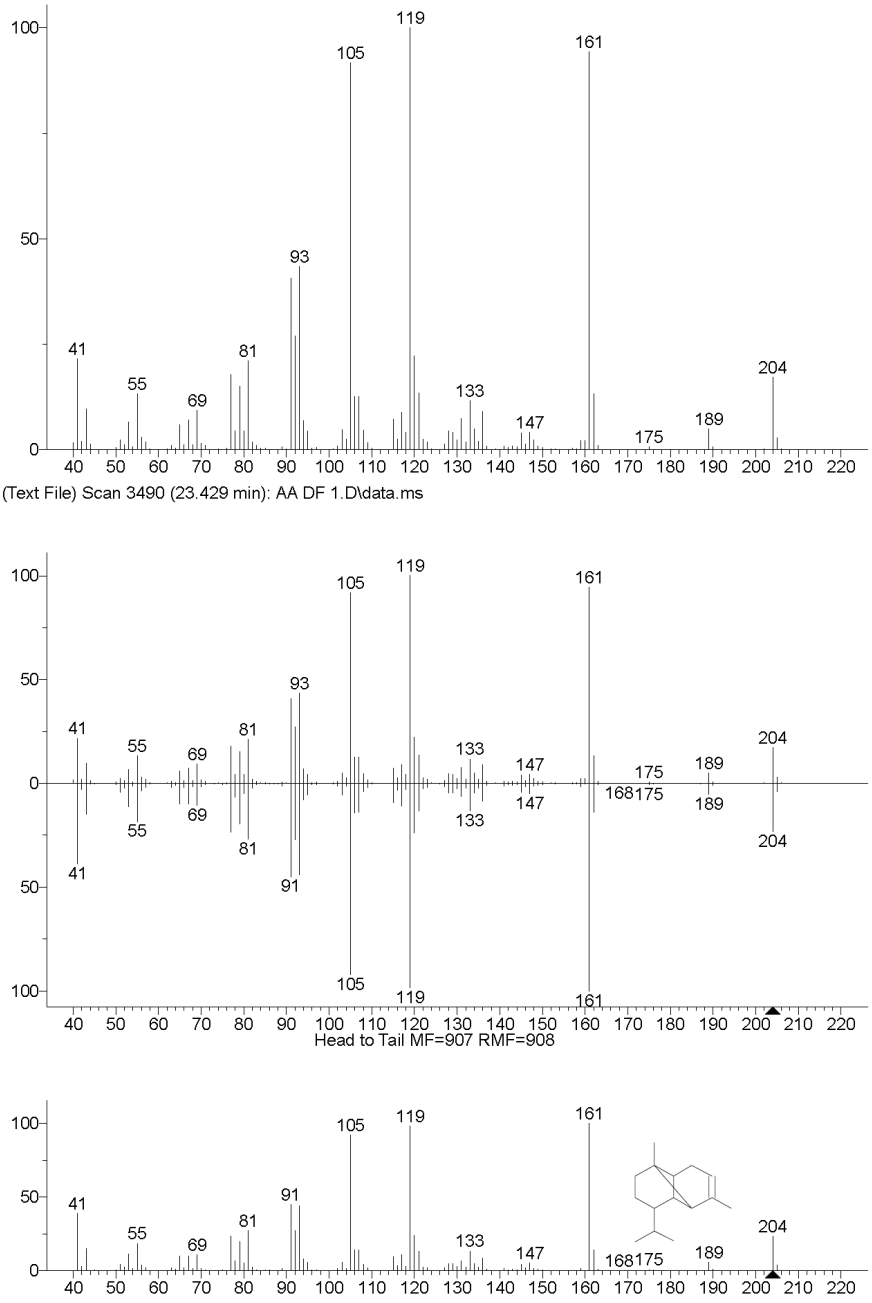

Fig. S-13. MS spectrum of α-copaene (top) and its comparison with the spectrum from the database (middle and bottom).

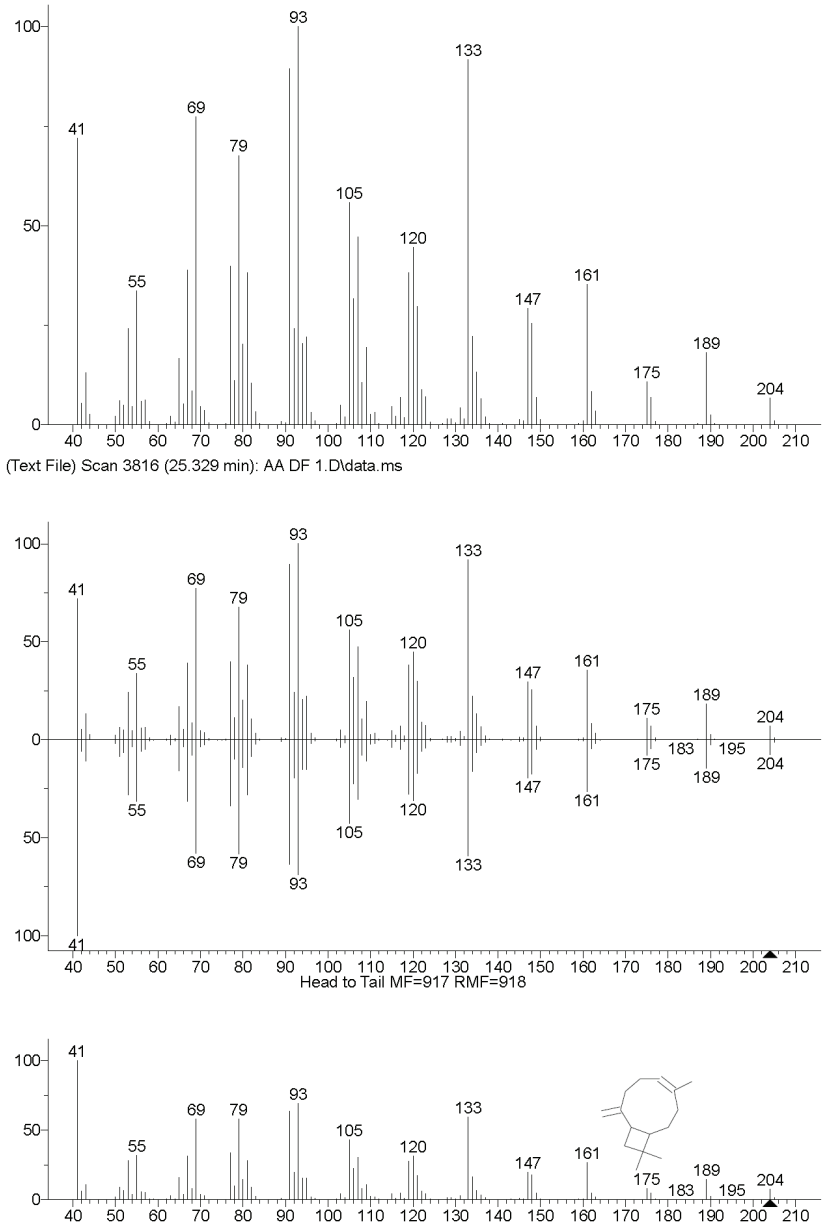

Fig. S-14. MS spectrum of E- β-caryophyllene (top) and its comparison with the spectrum from the database (middle and bottom).

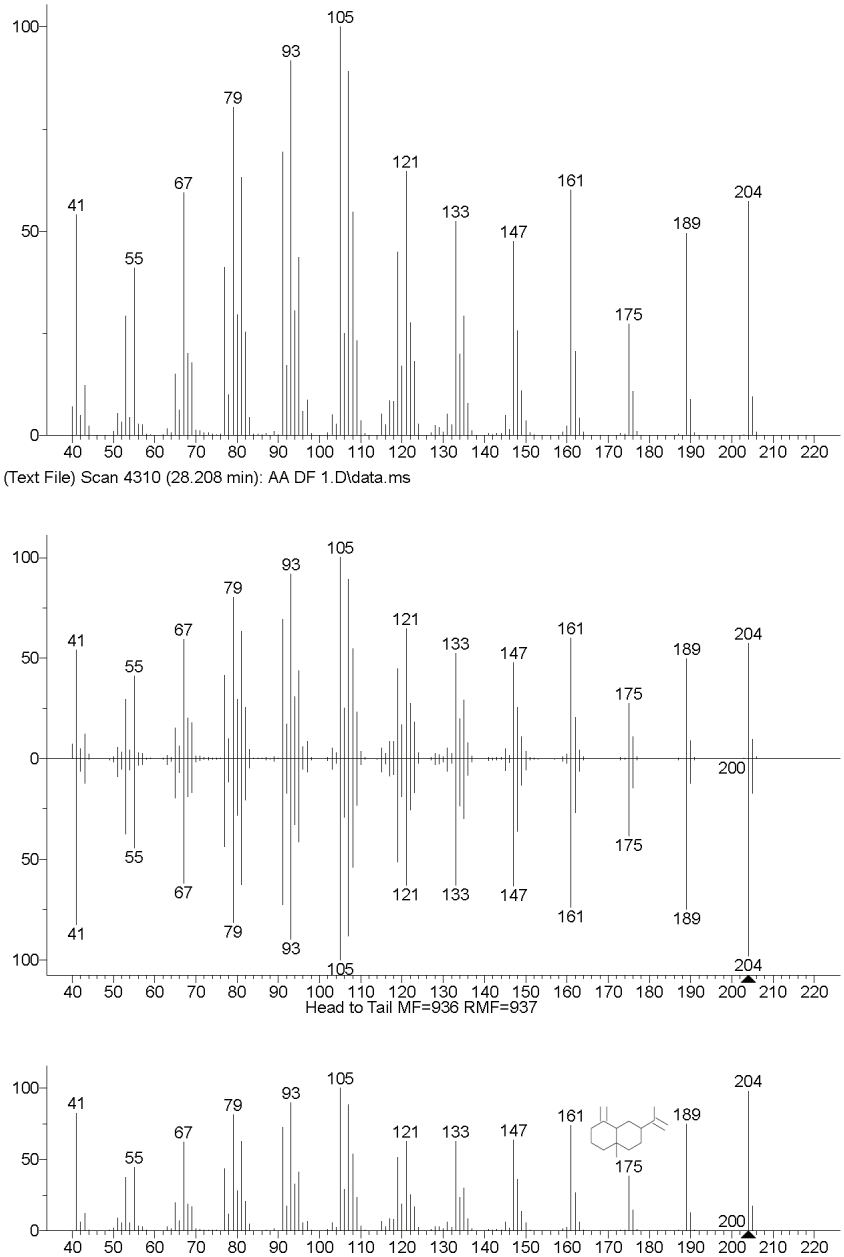

Fig. S-15. MS spectrum of *β*-selinene (top) and its comparison with the spectrum from the database (middle and bottom).

Compound on HPTLC plate (Fig 1.) Artemisia ketone R_f = 0.74 - 0.82.

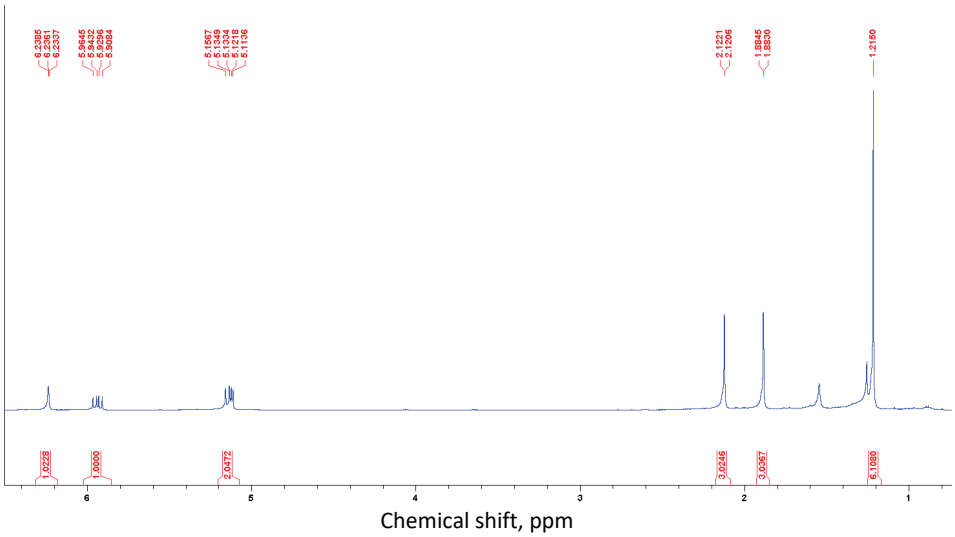

Fig. S-16. ^{1}H NMR spectrum of artemisia ketone.

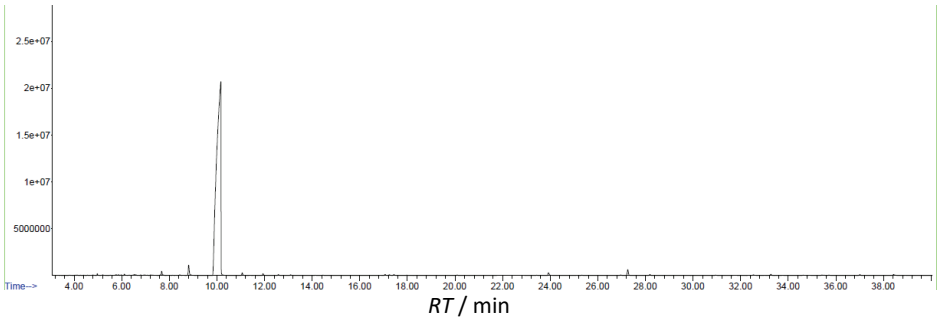

Fig. S-17. GC-MS chromatogram of fraction DF3 containing artemisia ketone (*RI* = 1057.5).

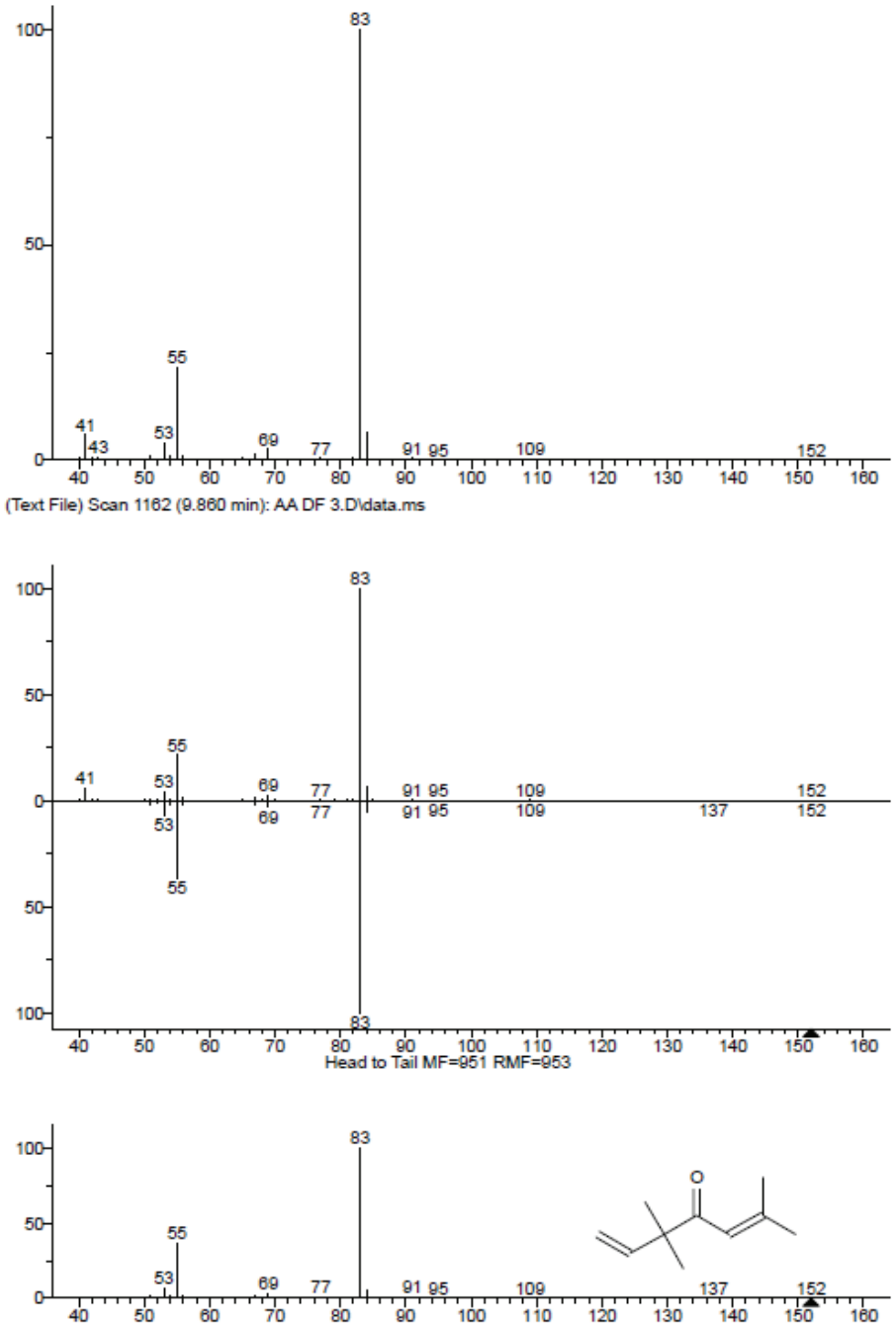

Fig. S-18. MS spectrum of artemisia ketone (top) and its comparison with the spectrum from the database (middle and bottom).

Compound on HPTLC plate (Fig 1.) 1,8-cineole $R_f = 0.68$

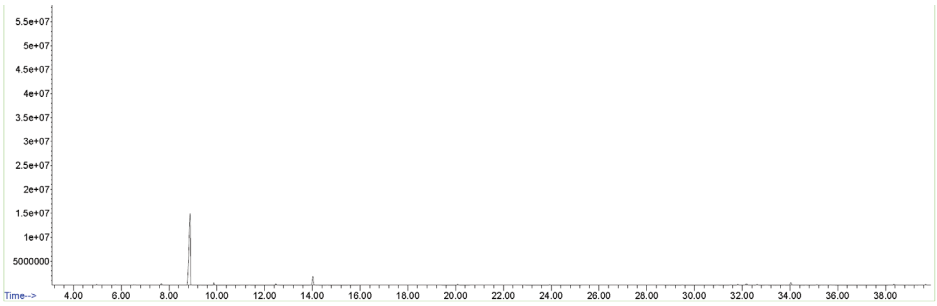

Fig. S-19. GC-MS chromatogram of fraction AA DF5 containing 1,8-cineole (*RI* = 1028).

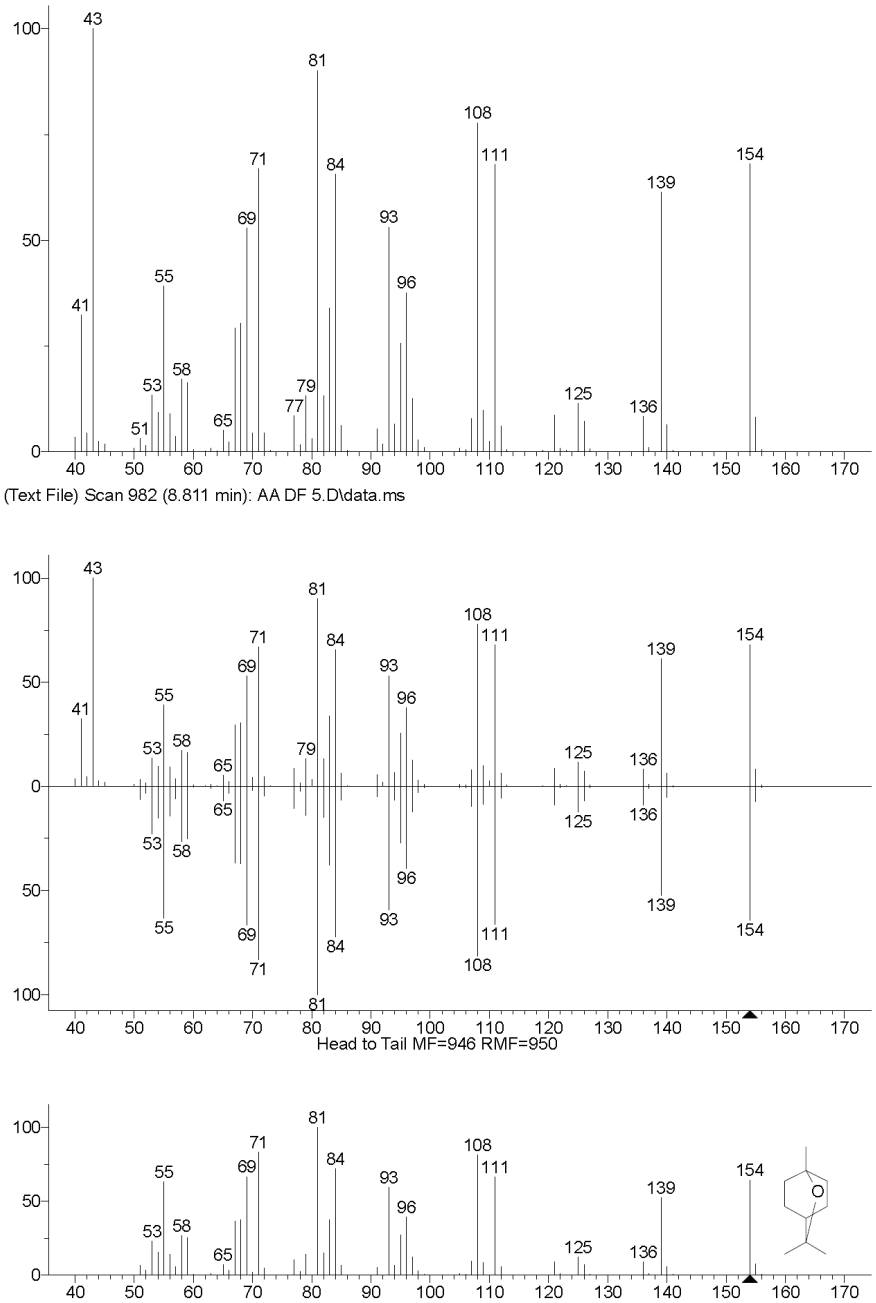

Fig. S-20. MS spectrum of 1,8-cineole (top) and its comparison with the spectrum from the database (middle and bottom).

Compound on HPTLC plate (Fig 1.) Caryophyllene oxide *Rf* = 0.66.

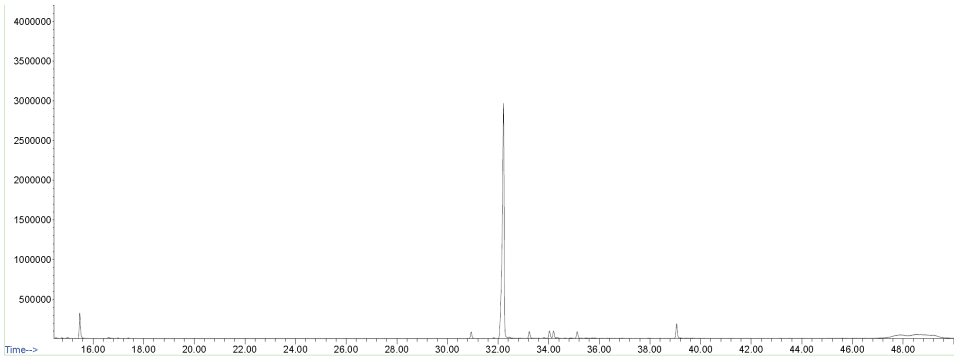

Fig. S-21. GC-MS chromatogram of fraction DF7 containing caryophyllene oxide (*RI* 1581).