Composition of essential oils from roots and aerial parts of *Carpesium divaricatum*, a traditional herbal medicine and wild edible plant from South-East Asia, grown in Poland

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Supplementary material:

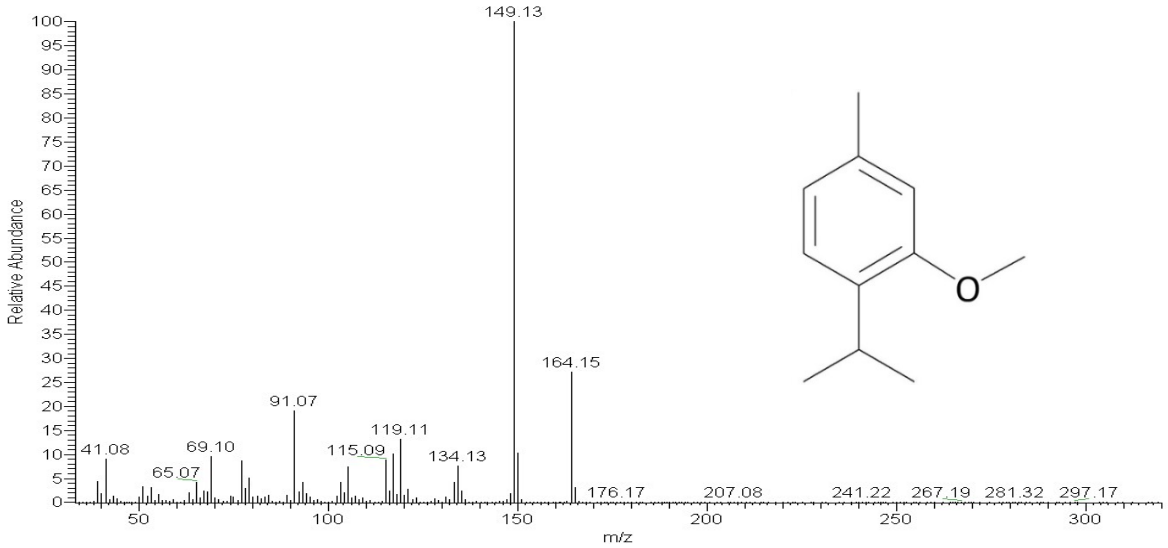
Figure S1. Mass spectra and retention indices (RI) together with chemical structures of thymol derivatives detected in *C. divaricatum* essential oils (the numbering of the compounds corresponds to that in Table 1) – pp. 2-9.

Figure S2. Mass spectra and experimental retention indices (RI) of unidentified compounds from *C. divaricatum* essential oils (the numbering of the compounds corresponds to that Table 1) - pp. 10-15.

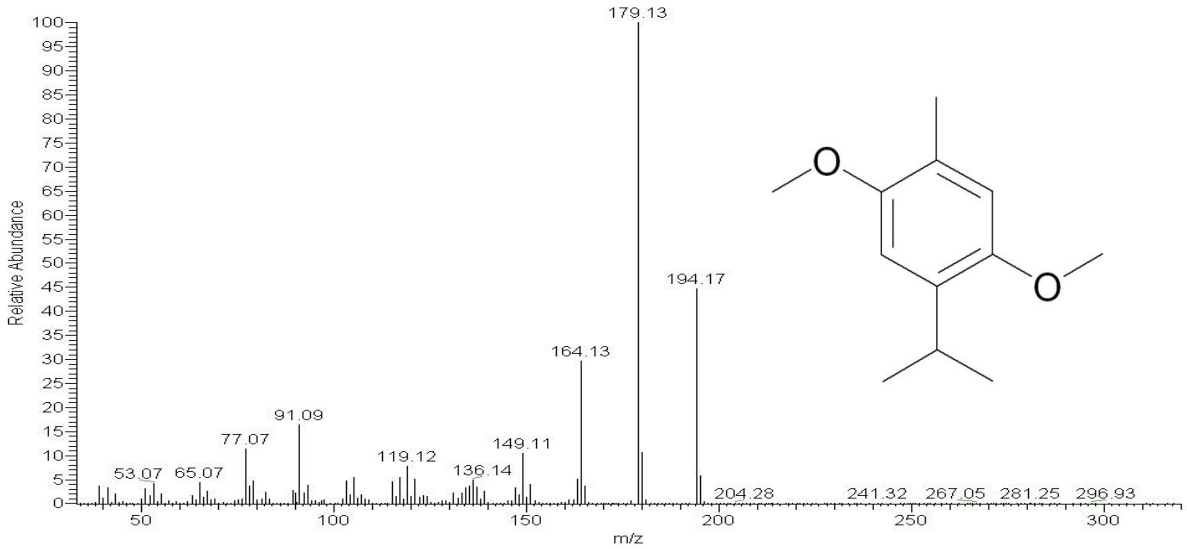
Figure S3. Results of NMR analyses of crude fractions (obtained by flash chromatography) from *C. divaricatum* essential oils – pp. 16-21.

Figure S1. Mass spectra and retention indices (RI), together with chemical structures, of thymol derivatives detected in *C. divaricatum* essential oils (the numbering of the compounds corresponds to that in Table 1).

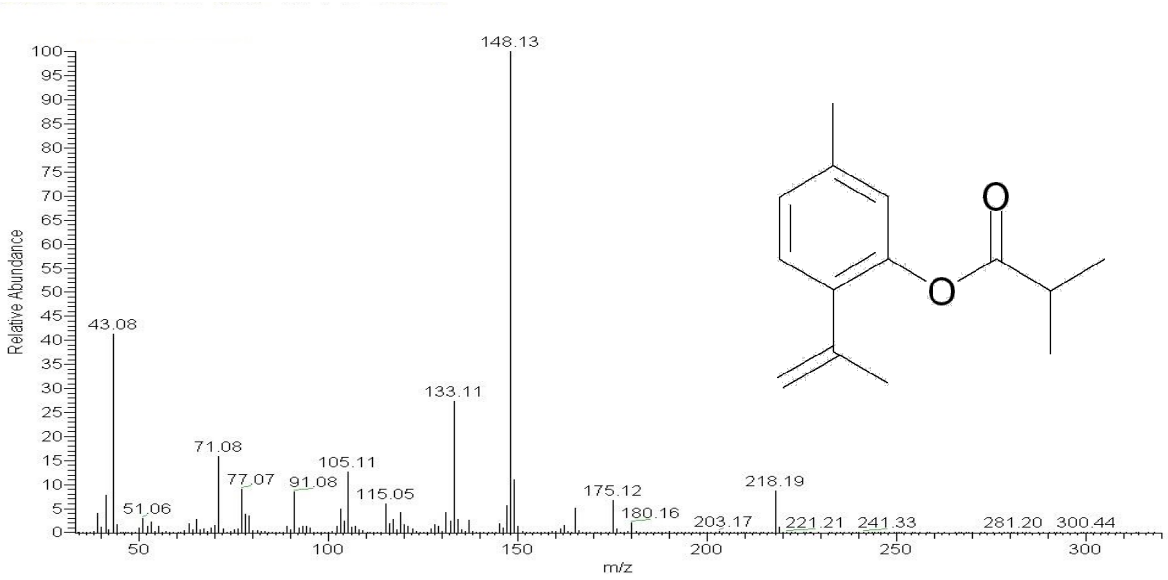
50. Thymol methyl ether (RI $_{exp..}$ 1211/RI $_{lit.}$ 1215)



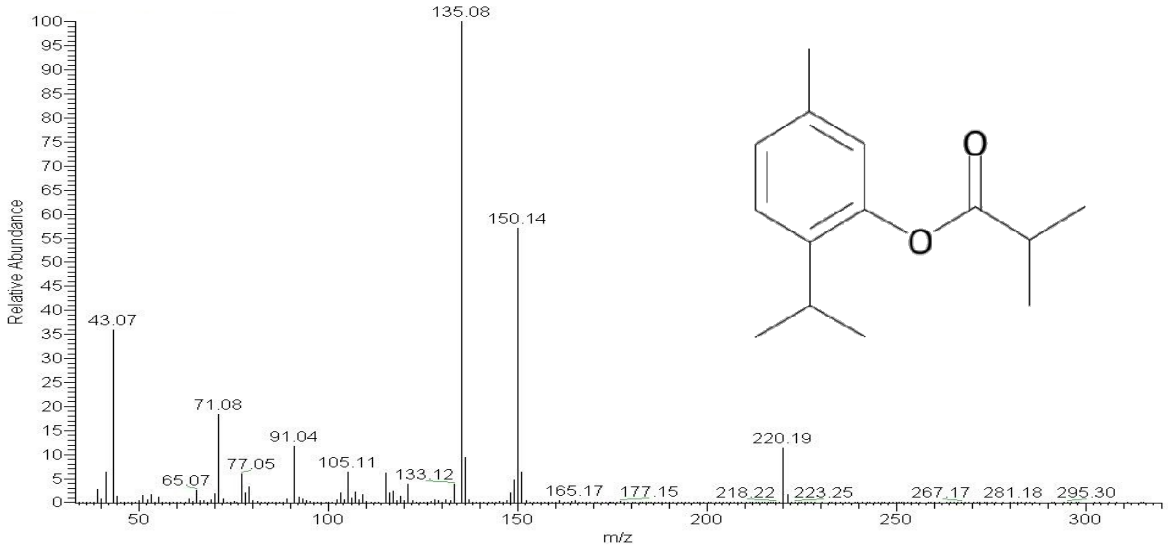
73. 6-Methoxythymol methyl ether (RI $_{exp.}$ 1394/RI $_{lit.}$ 1399)



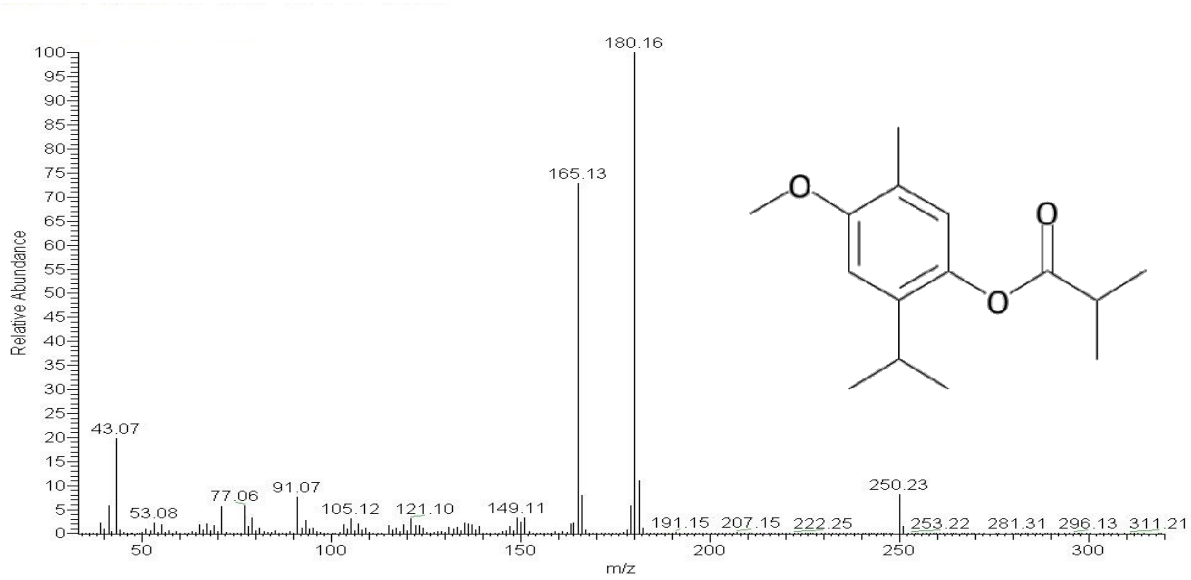
84. 8,9-Didehydrothymyl isobutryate (RI $_{exp.}$ 1461/RI $_{lit.}$ 1458)



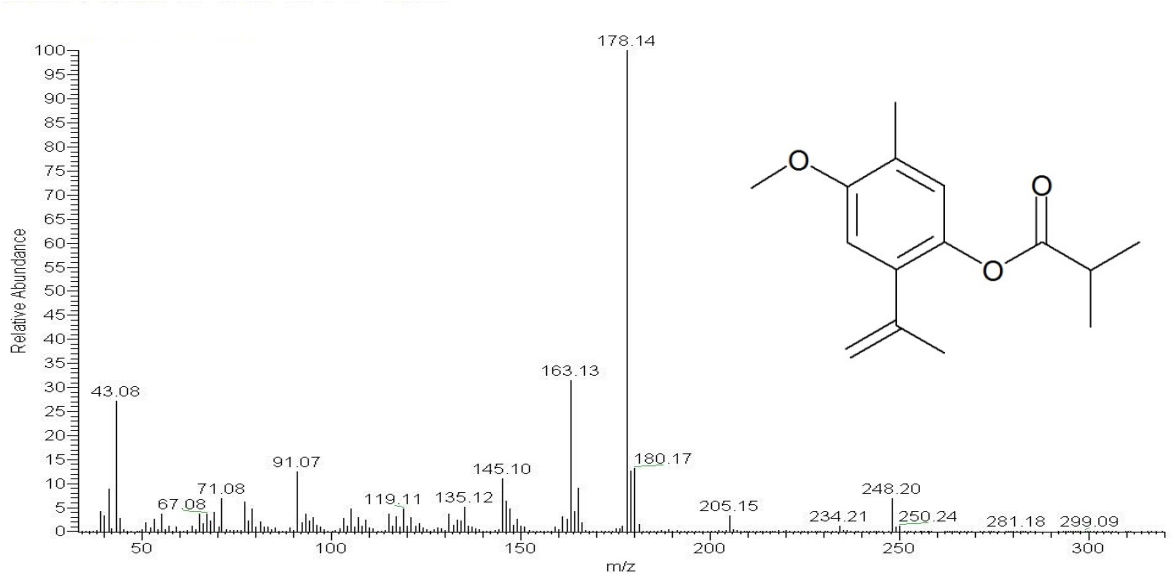
85. Thymyl isobutyrate (RI $_{exp.}$ 1467/RI $_{lit.}$ 1462)



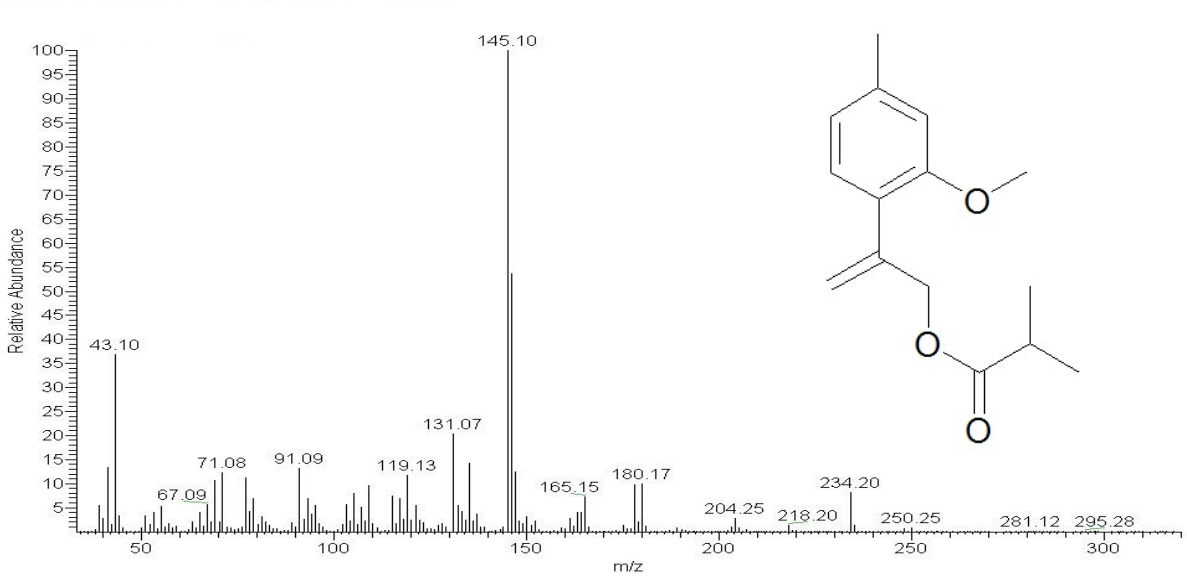
130. 6-Methoxythymyl isobutyrate (RI $_{exp.}$ 1657/RI $_{lit.}$ 1658)



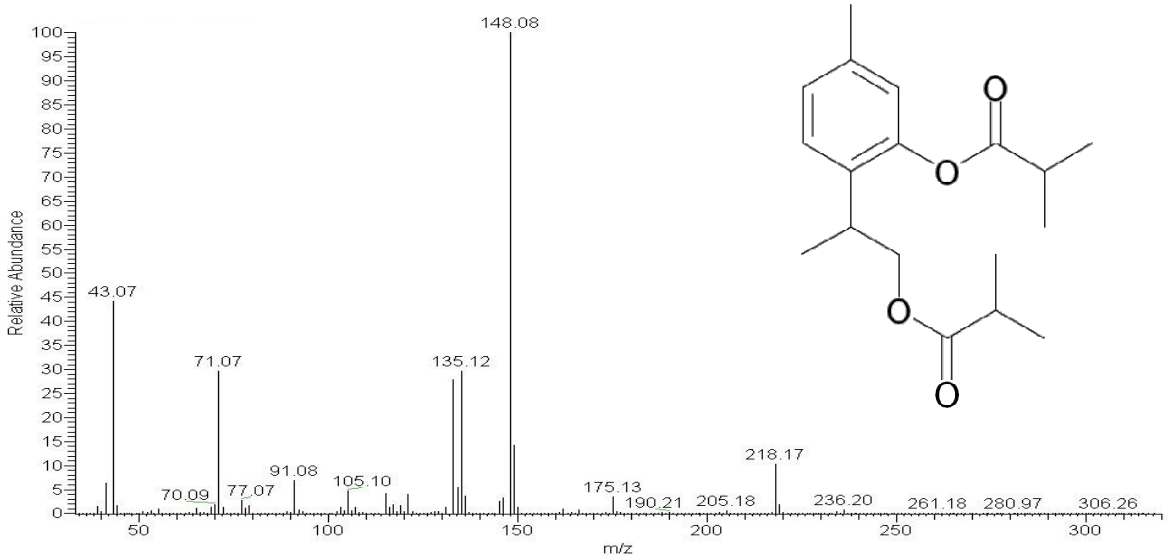
131. 6-Methoxy-8,9-didehydrotymyl isobutyrate (RI $_{exp.}$ 1665/RI $_{lit.}$ 1676)



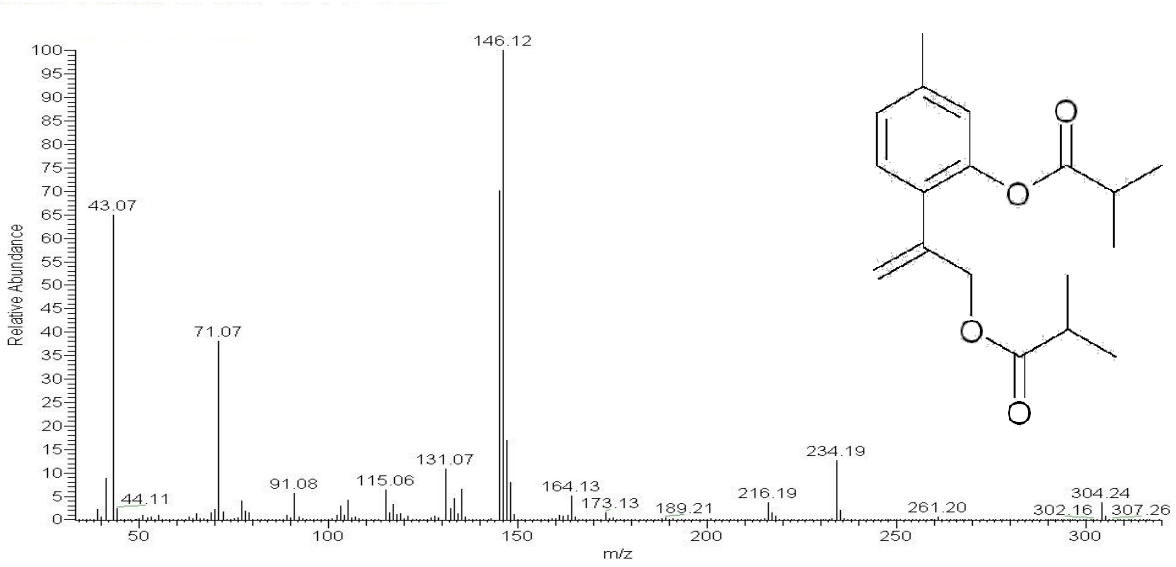
132. 10-Isobutyryloxy-8,9-didehydrothymol methyl ether (RI $_{exp.}$ 1666/RI $_{lit.}$ 1684)



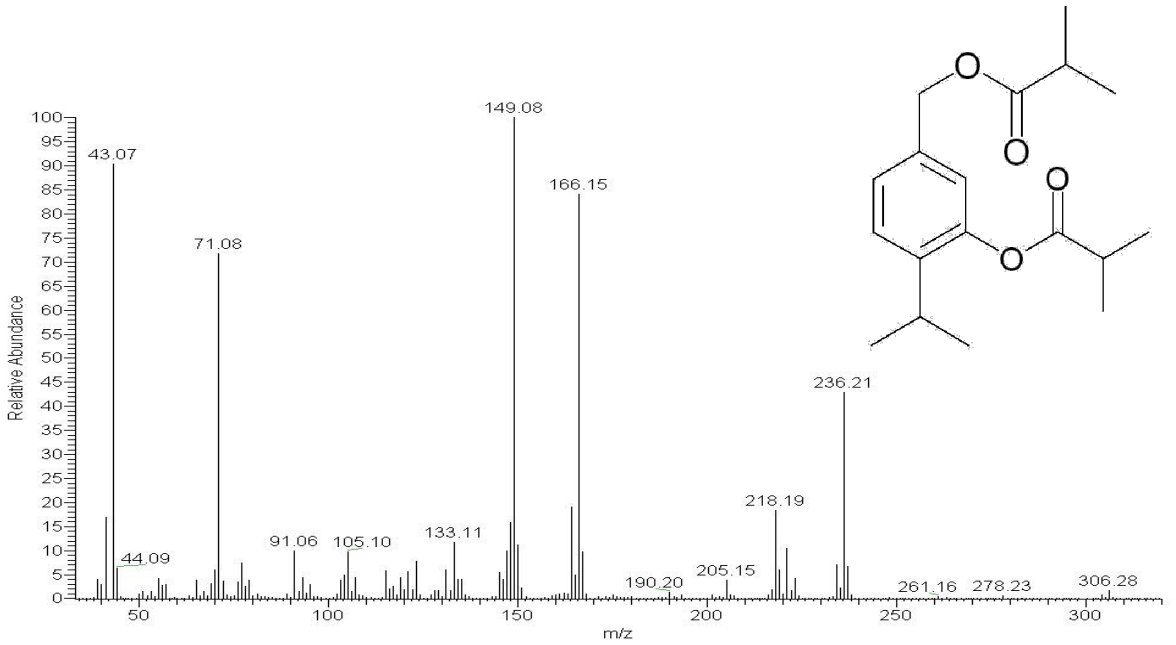
142. 9-Isobutyryloxytymyl isobutyrate (RI $_{exp.}$ 1879/RI $_{lit.}$ 1891)



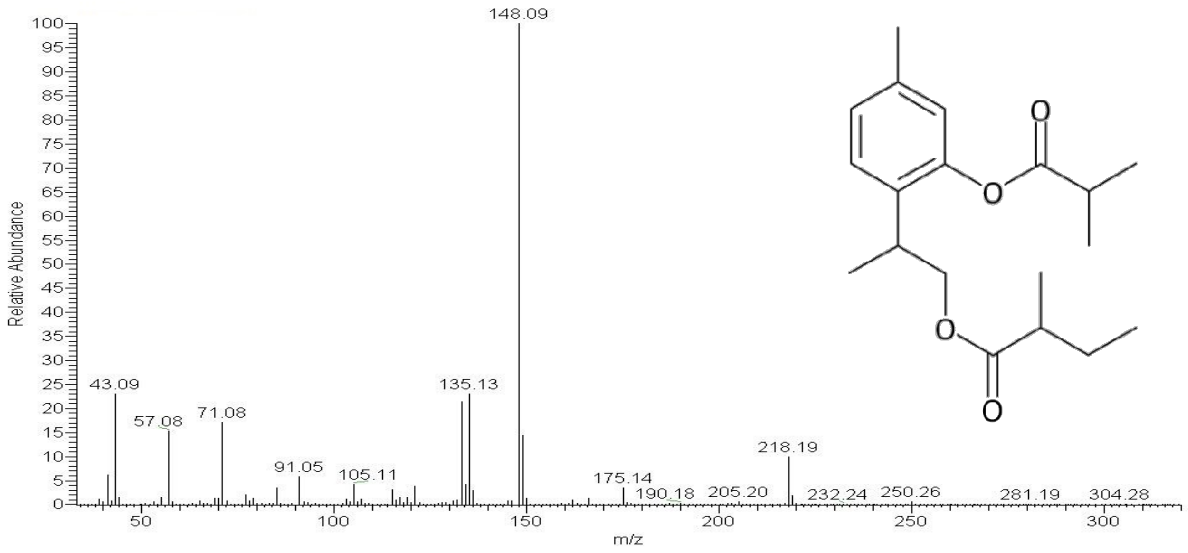
143. 10-Isobutyryloxy-8,9-didehydrothymyl isobutyrate (RI $_{exp.}$ 1882/RI $_{lit.}$ 1891)



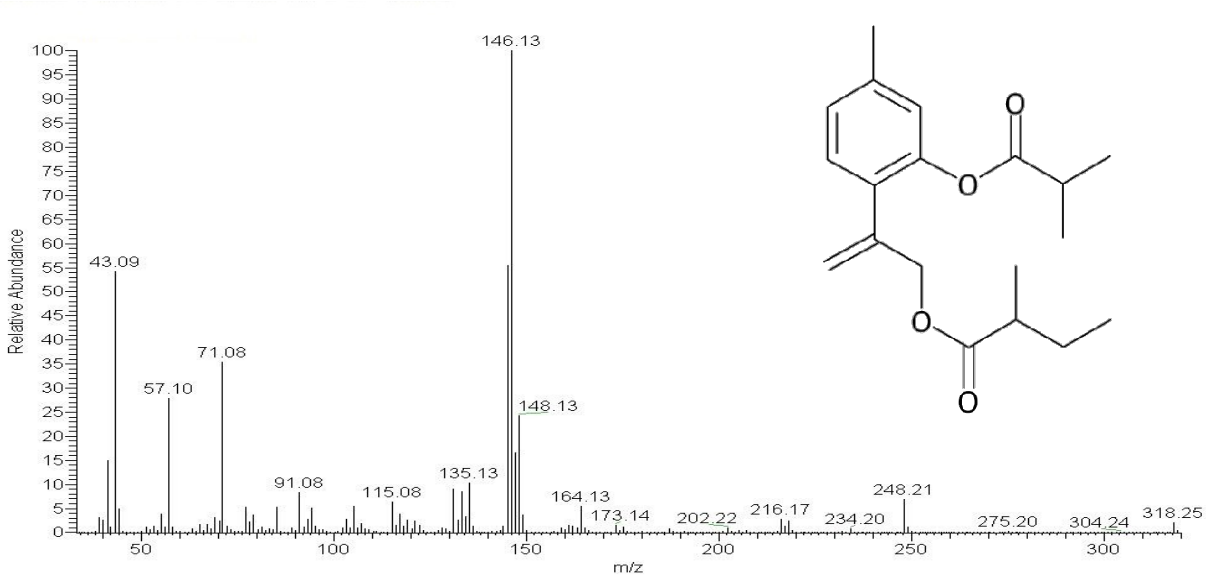
146. 7-Isobutyryloxythymyl isobutyrate (RI $_{exp.}$ 1914/RI $_{lit.}$ 1924)



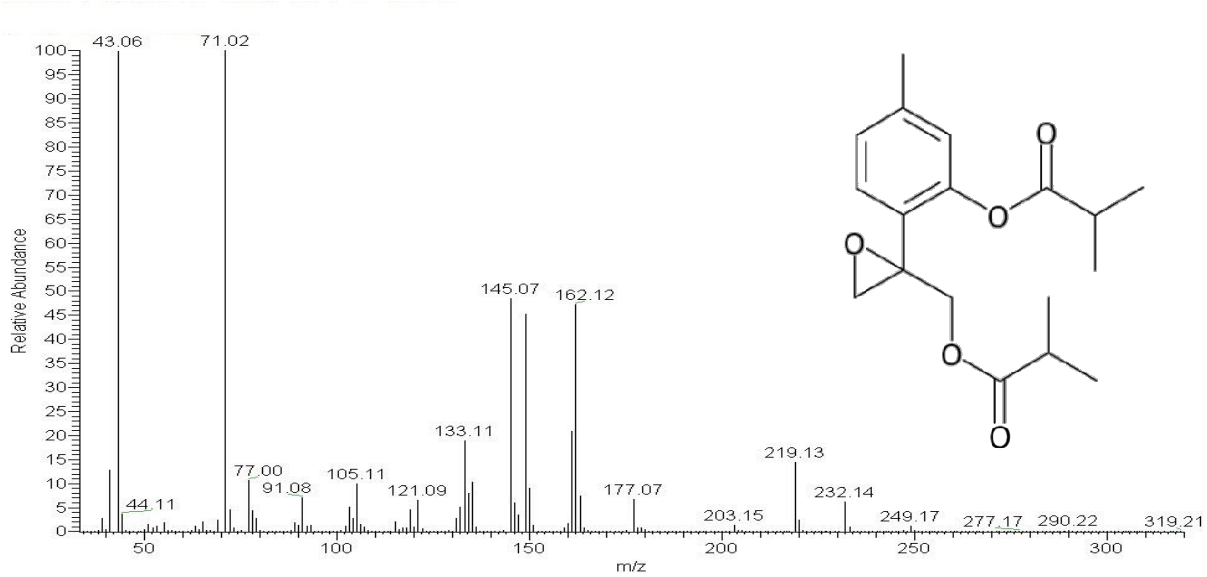
147. 9-(2-Methylbutyryloxy)thymyl isobutyrate (RI $_{exp..}$ 1964/RI $_{lit.}$1970)



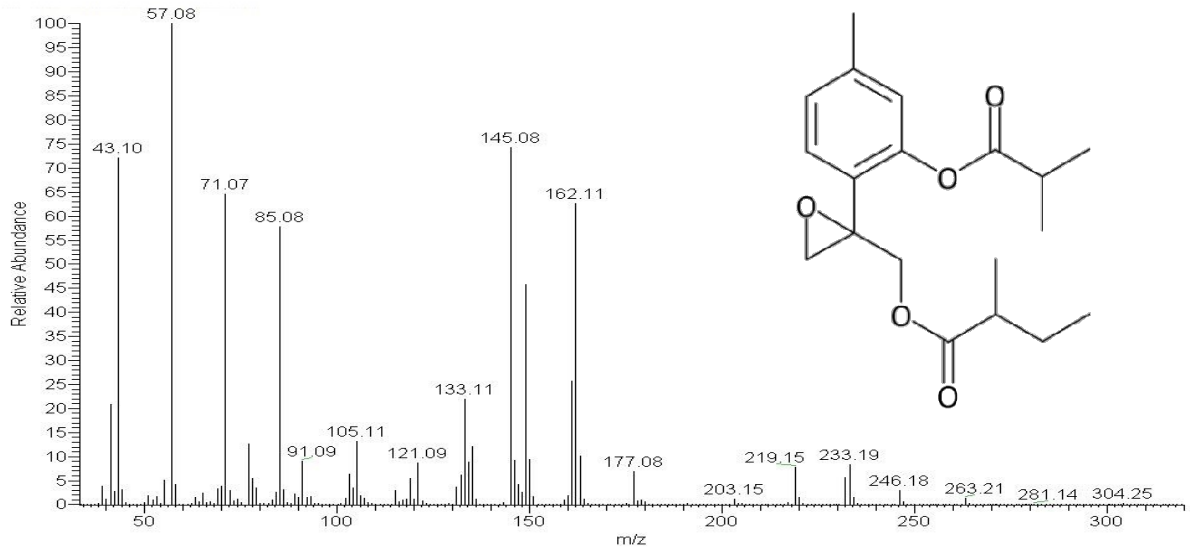
148. 10-(2-Methylbutyryloxy)-8,9-didehydrotymyl isobutyrate (RI $_{exp..}$ 1967/RI $_{lit.}$ 1970)



149. 10-Isobutyryloxy-8,9-epoxythymyl isobutyrate (RI $_{exp..}$ 2002/RI $_{lit.}$ 2036 [HP-5 column])



151. 10-(2-Methylbutyryloxy)-8,9-epoxythymyl isobutyrate (RI $_{exp.}$ 2077/RI $_{lit.}$ 2056 [BP-1 column])



152. 10-Isovaleroxy-8,9-epoxythymyl isobutyrate (RI $_{exp.}$ 2097/RI $_{lit.}$ 2122 [HP-5 column])

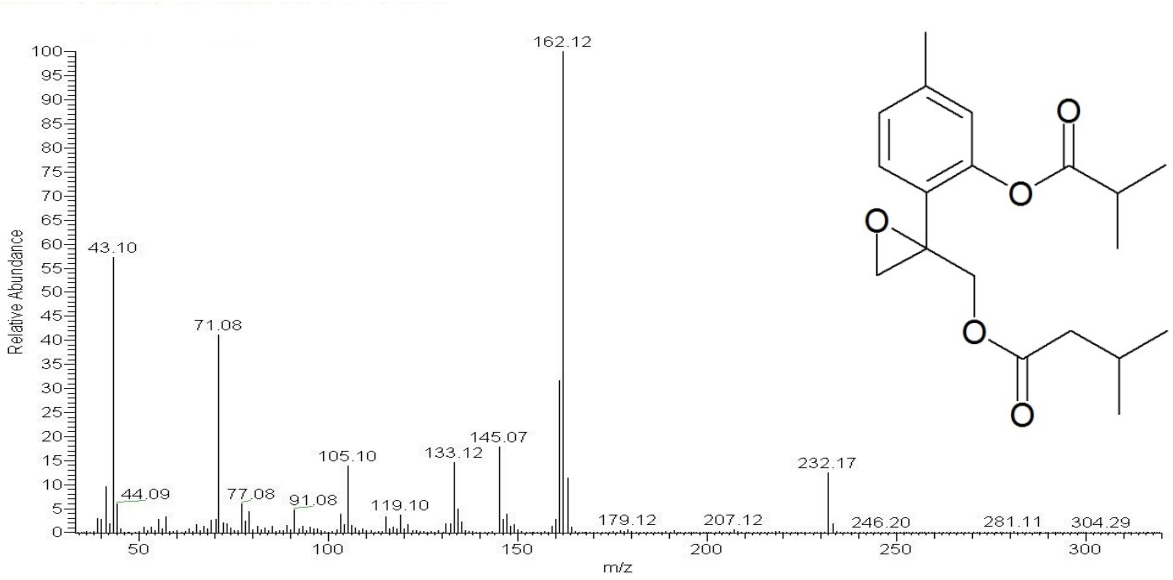
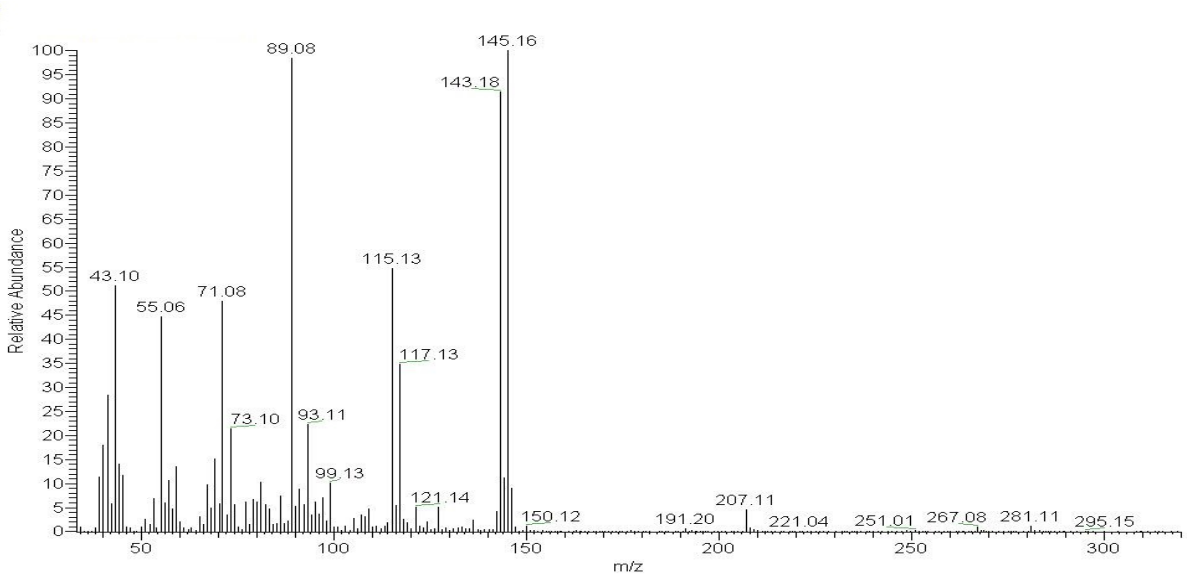
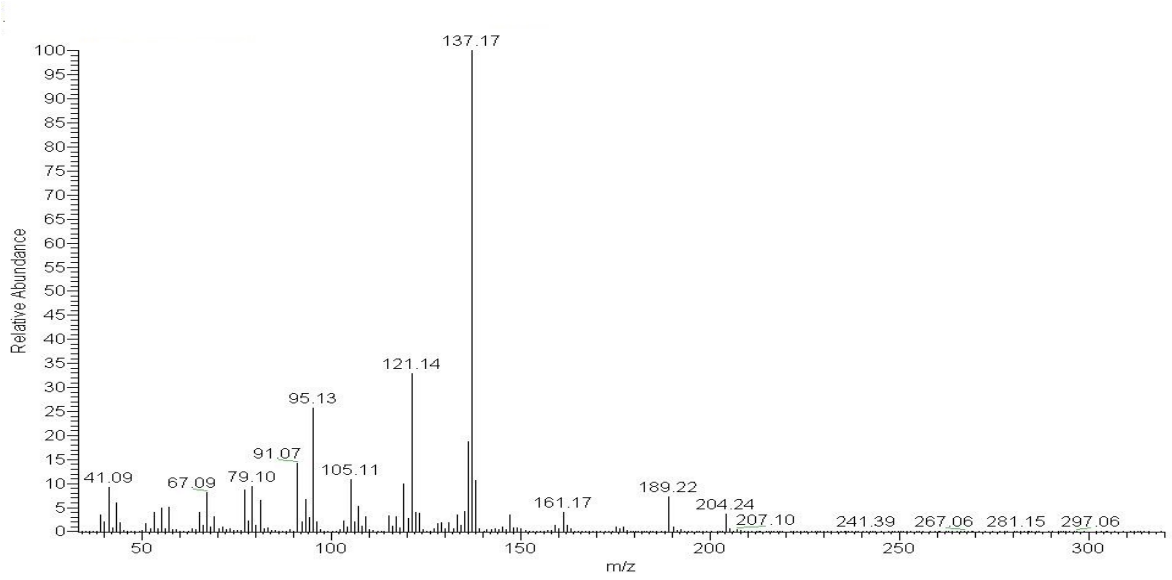


Figure S2. Mass spectra and experimental retention indices (RI) of unidentified compounds from *C. divaricatum* essential oils (the numbering of the compounds corresponds to that in Table 1).

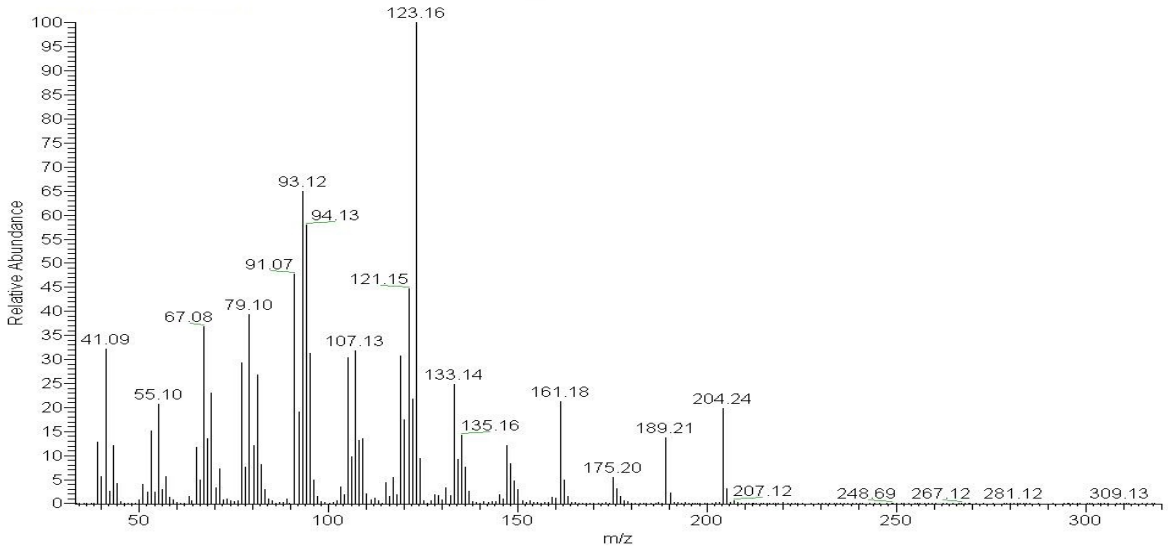
Compound 25: RI $_{exp.}$ 1091



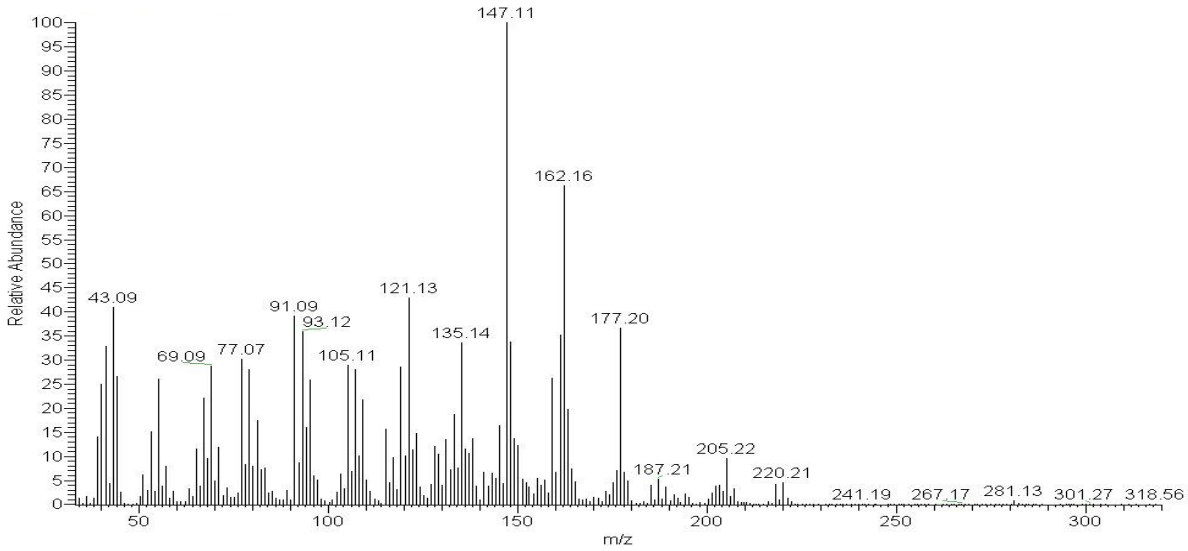
Compound 72: RI $_{exp.}$ 1391



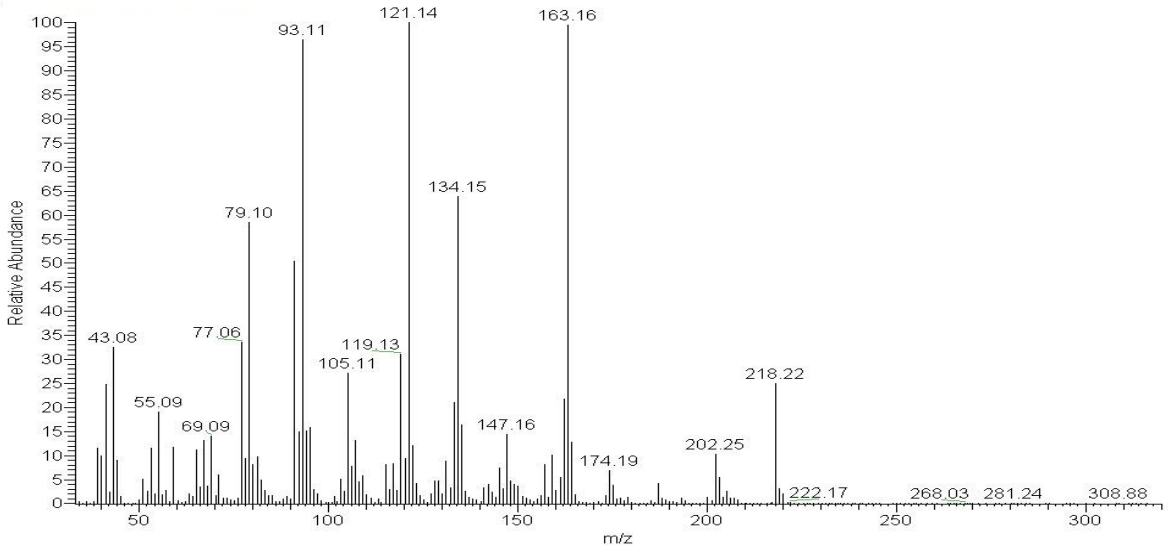
Compound 89: RI $_{exp.}$1484



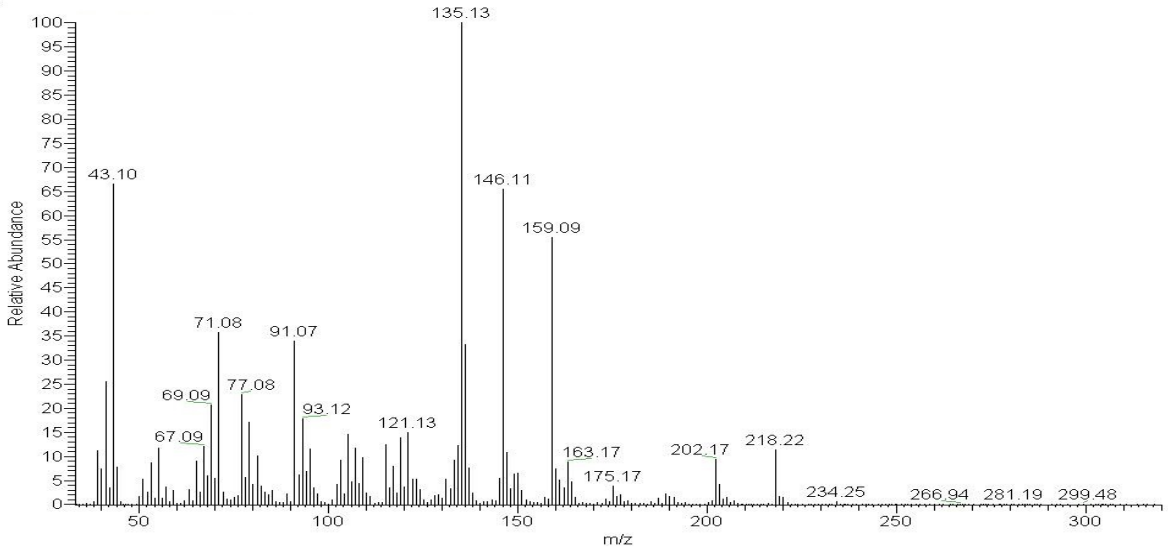
Compound 106: RI $_{exp.}$1531



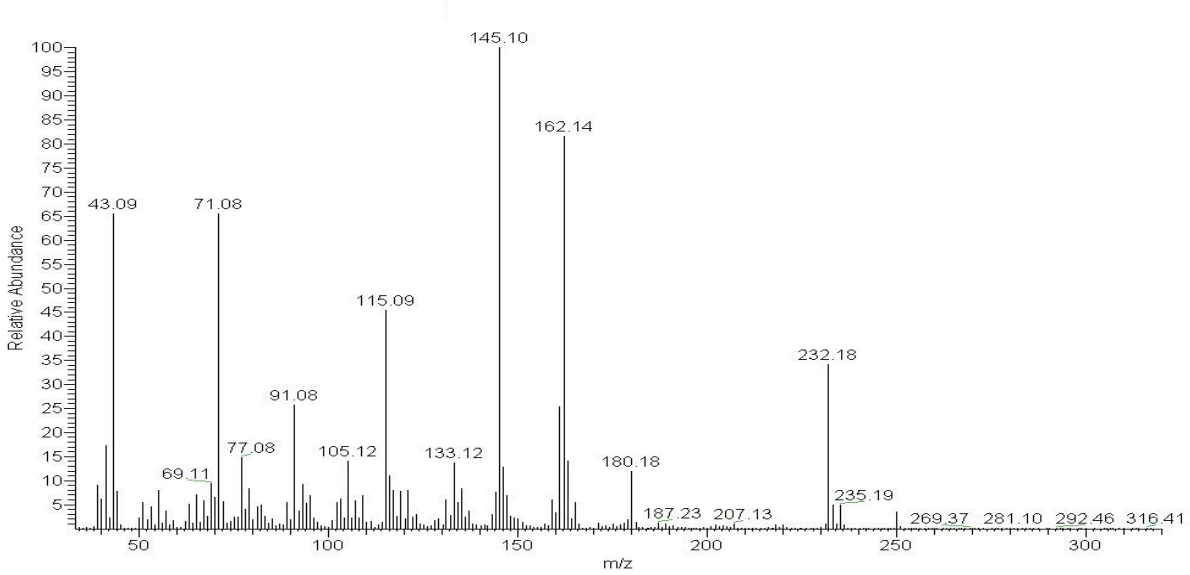
Compound 107: RI $_{exp.}$1534



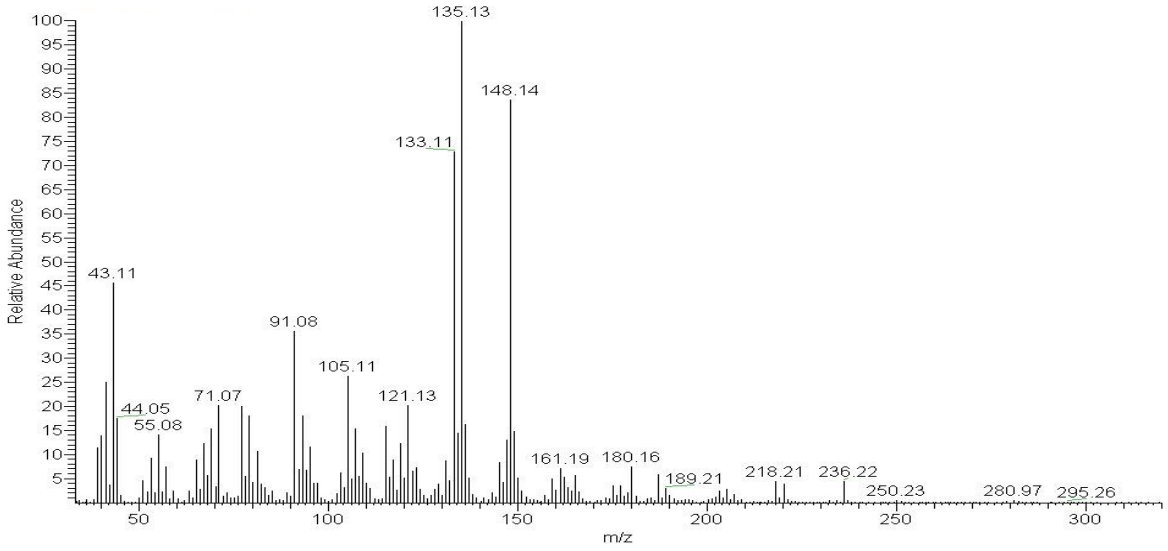
Compound 120: RI $_{exp.}$1602



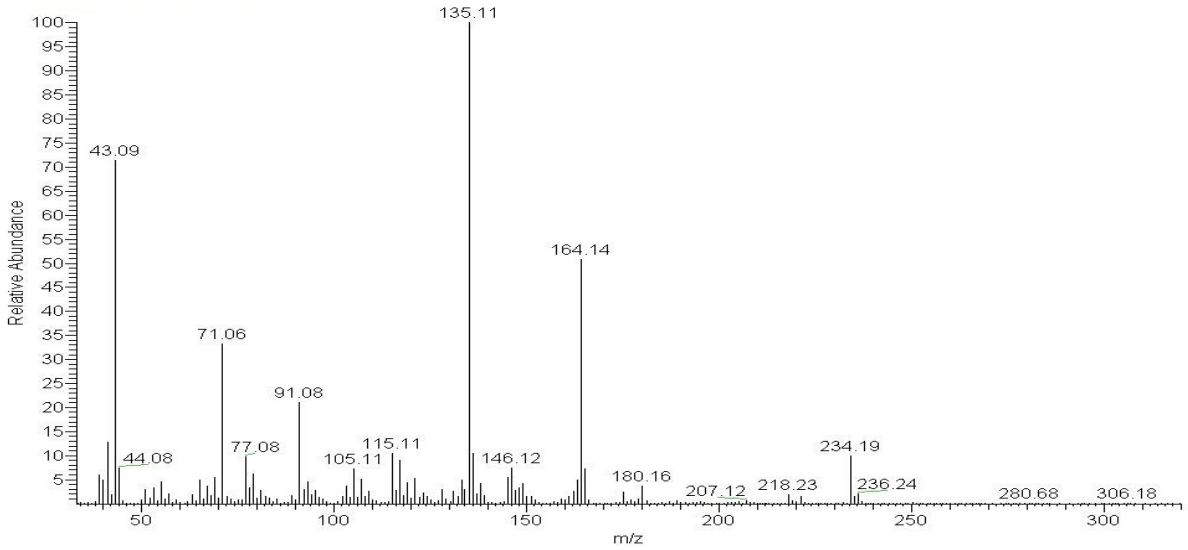
Compound 134: $RI_{exp.}$ 1681



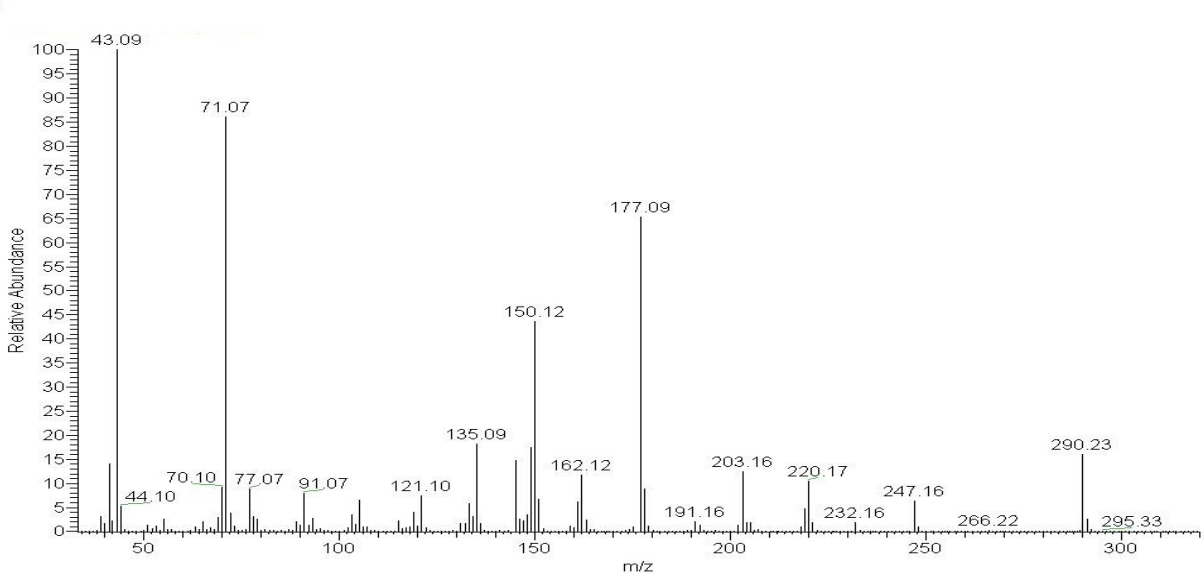
Compound 136: $RI_{exp.}$ 1725



Compound 137. $RI_{exp.}$ 1733



Compound 150: $RI_{exp.}$ 2048



Compound 154: $RI_{exp.}$ 2149

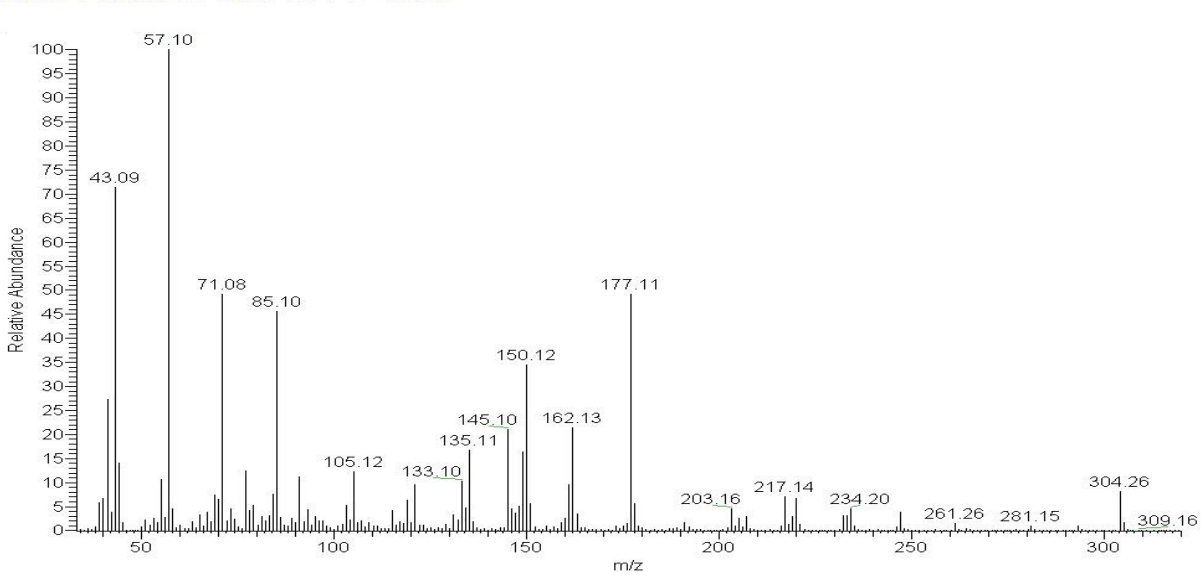
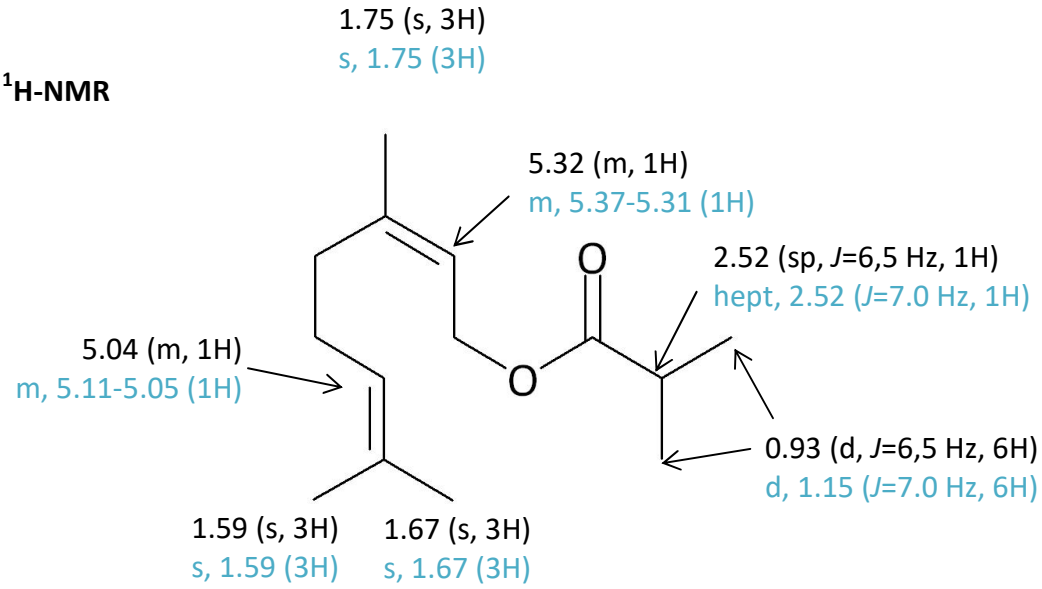


Figure S3. Results of NMR analyses of crude fractions (obtained by flash chromatography) from *C. divaricatum* essential oils (chemical shifts given in the literature are printed in blue).

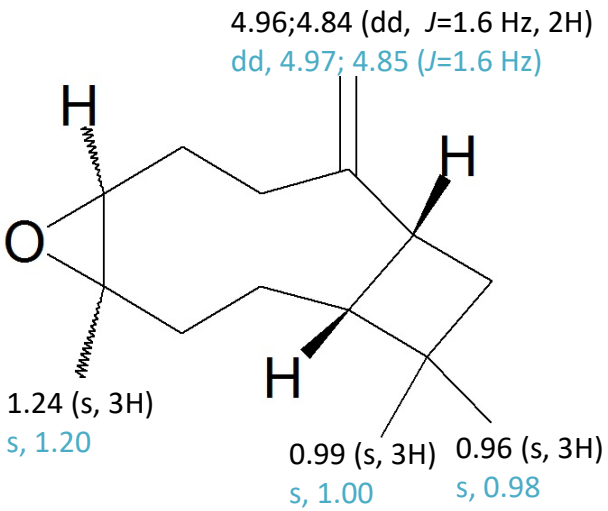
Fraction 1a: neryl isobutyrate (25.5% of the fraction)

- **^{1}H-NMR**



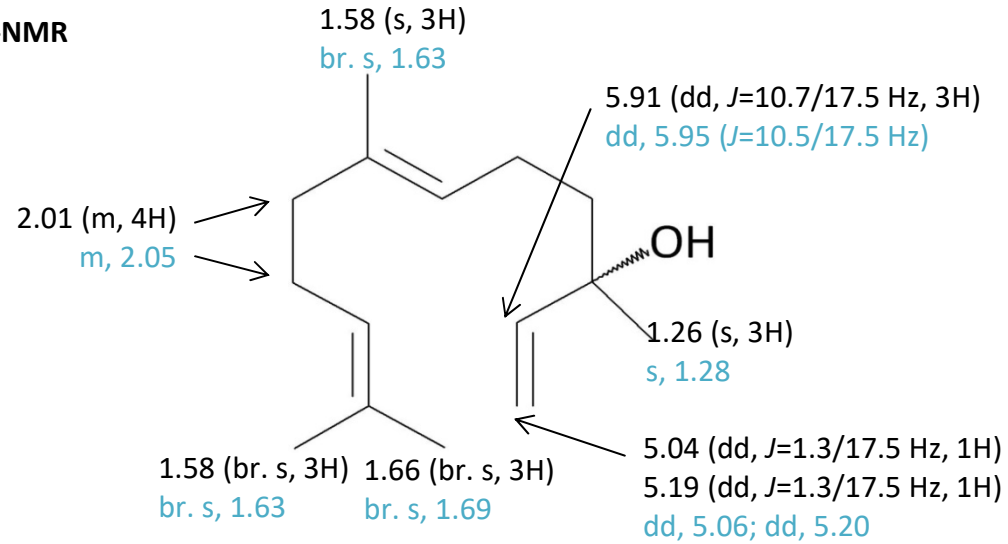
Fraction 13b: (*E*)-β-caryophyllene oxide (51.5% of the fraction)

- **^{1}H-NMR**



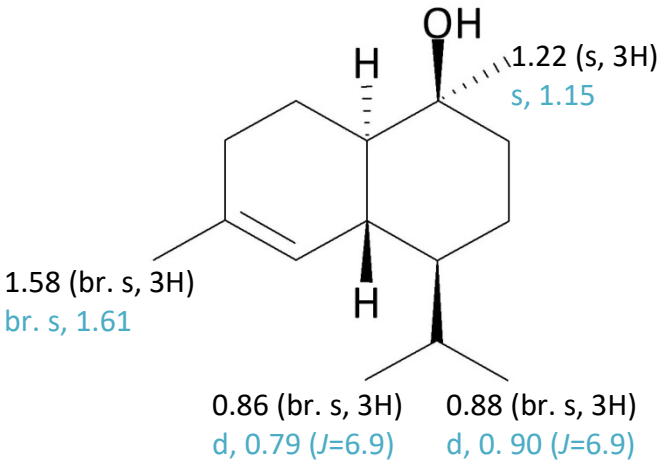
Fraction 13a: (*E*)-nerolidol (24.6% of the fraction)

- **^{1}H-NMR**



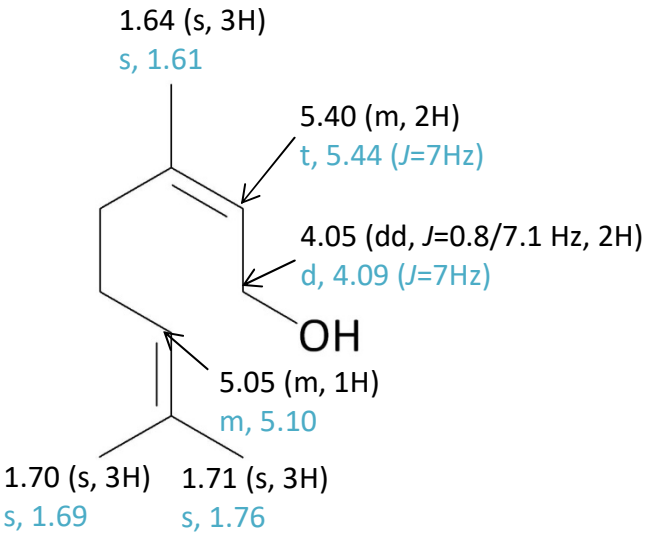
Fraction 18b: τ-cadinol (20,7% of the fraction)

- **^{1}H-NMR**



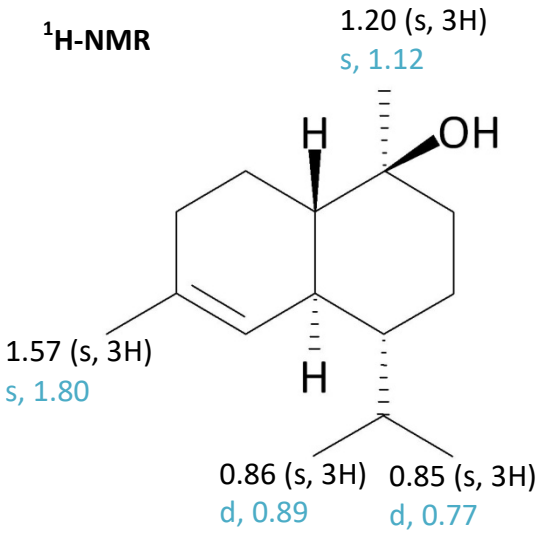
Fraction 17a: nerol (25,2% of the fraction)

- **^{1}H-NMR**



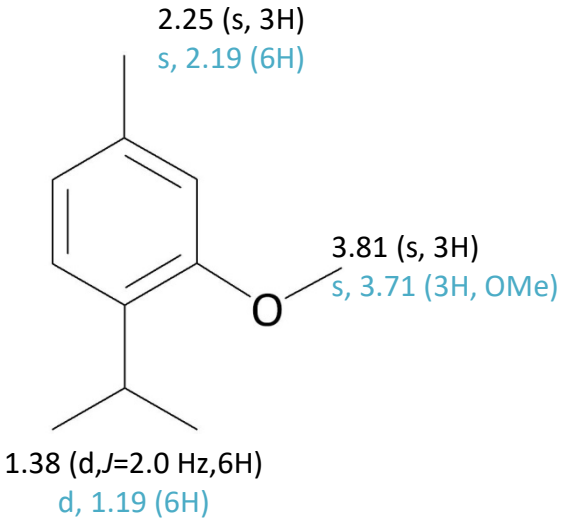
Fraction 18a: α-cadinol (22.8% of the fraction)

- **^{1}H-NMR**



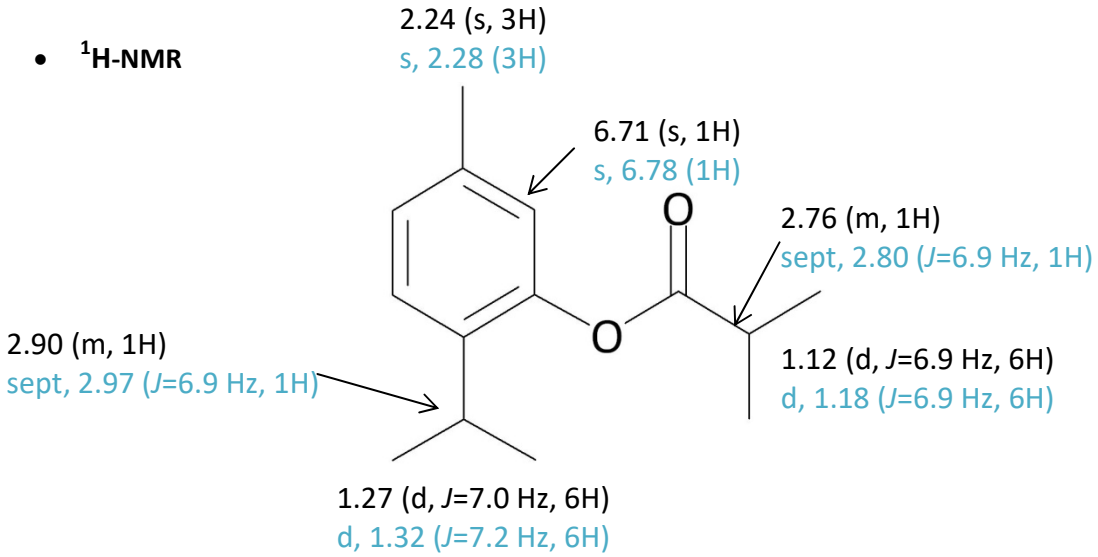
Fraction 3b: thymol methyl ether (33.0% of the fraction)

- **^{1}H-NMR**



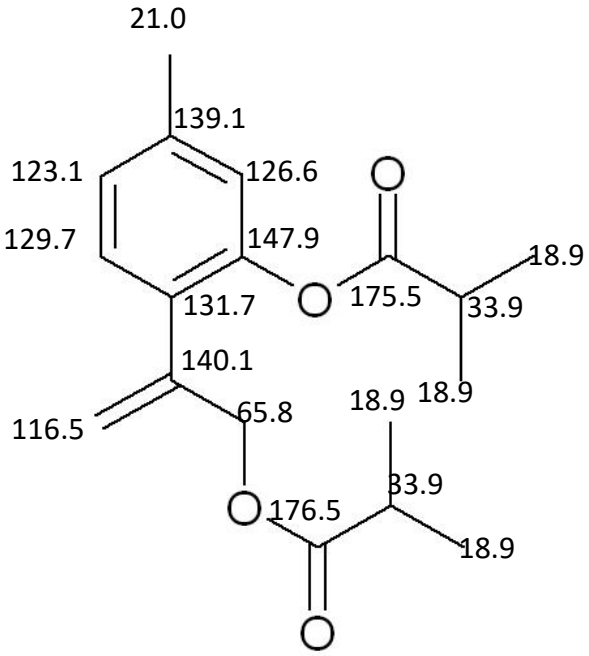
Fraction 7b: thymyl isobutyrate (57.2% of the fraction)

- **^{1}H-NMR**



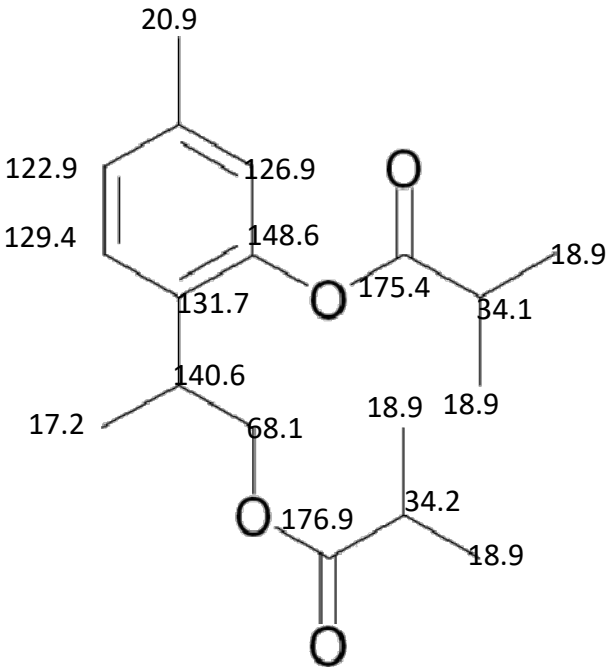
Fraction 14b: 10-isobutyryloxy-8,9-didehydrothymyl isobutyrate (45,5%)

^{13}C-NMR



Fraction 15 b: 9-isobutyryloxythymyl isobutyrate (54.6%)

- **^{13}C-NMR**



Fraction 17 b: 10-isobutyryloxy-8,9-epoxytymyl isobutyrate (54.6%)

^{1}H-NMR: δ 7.35 (d, J=7.8Hz, 1H), 7.03 (d, J=7.8 Hz, 1H), 6.86 (s, 1H), 4.56 (d, J=12.2 Hz, 1H), 4.18 (d, J=12.2 Hz, 1Hz), 3.02 (d, J=5.4Hz, 1H), 2.85 (hept.,1H), 2.78 (d, J=5.4Hz, 1H), 2.50 (hept.1H), 2.33 (s, 3H), 1.32 (d, J=7.0 Hz, 6H), 1.10 (d, J=7.O Hz, 3H), 1.07 (s, J=7.0 Hz, 3H)

^{13}C-NMR: δ 175.4 (C1'), 174.3 (C1"), 147.6 (C3), 138.9 (C1), 127.9 (C5), 125.7 (C6), 125.0 (C4), 121.9 (C2), 63.9 (C10), 55.9 (C8), 49.7 (C9), 33.2 (C2'), 32.8 (C2"), 19.9 (C7), 17.9 (C3',C4',C3",C4")

Literature:

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