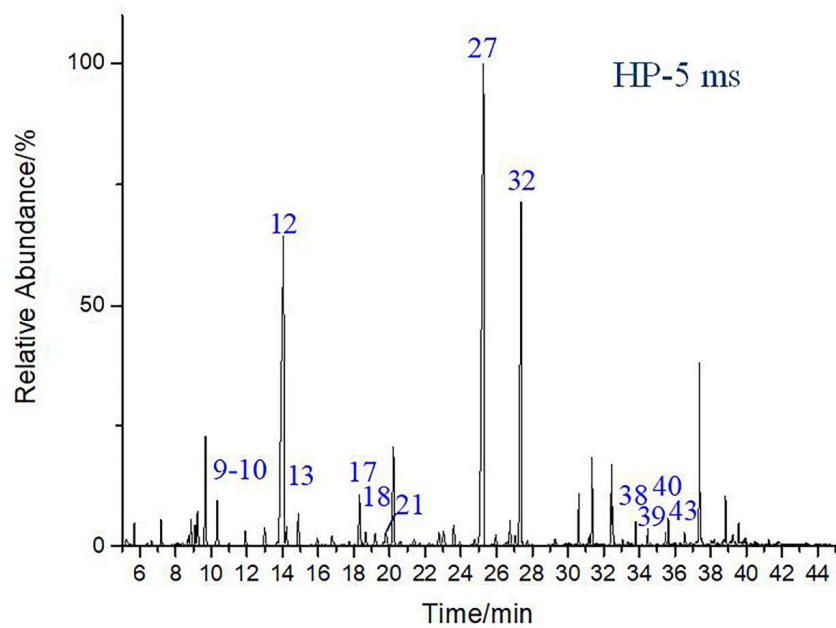
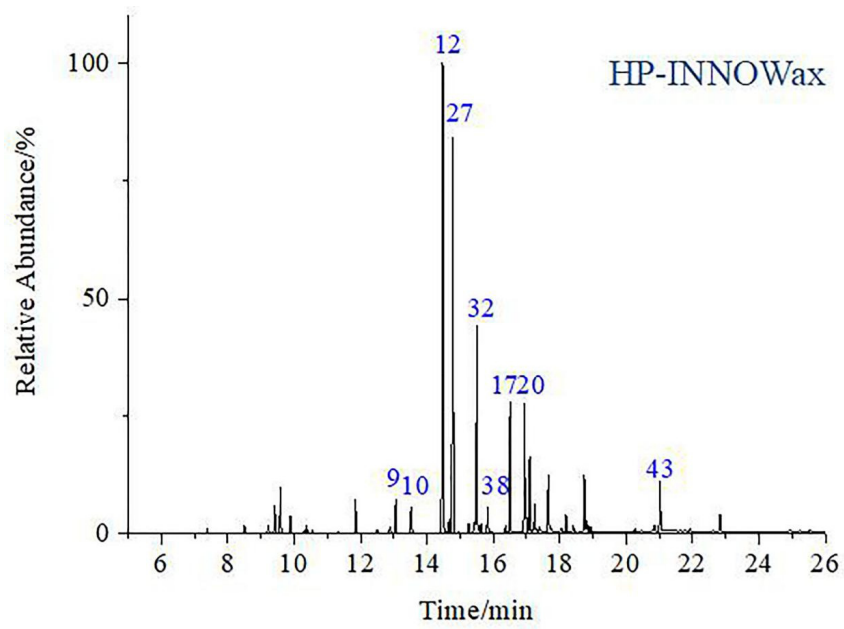
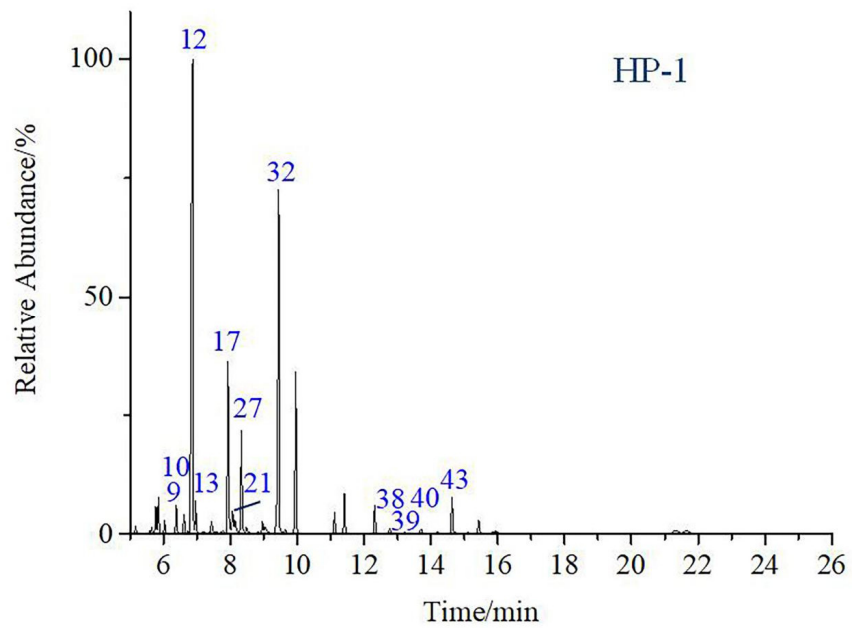


Supplementary Material for:  
**Study on lavender essential oil chemical compositions by  
GC-MS, and improved pGC ~~and autodeck~~**

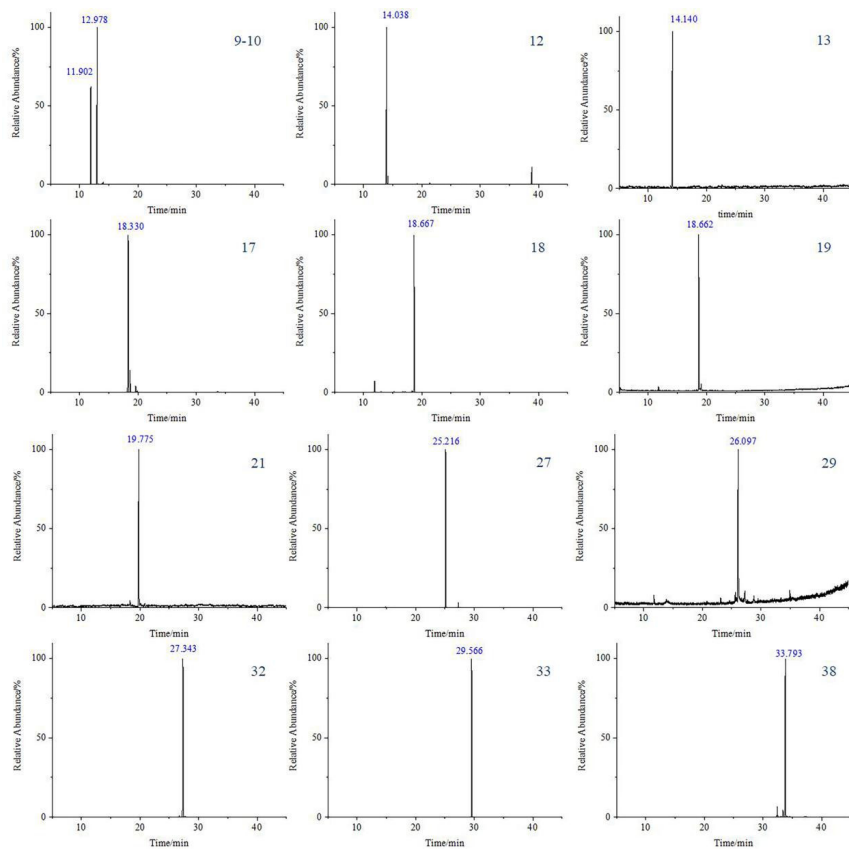
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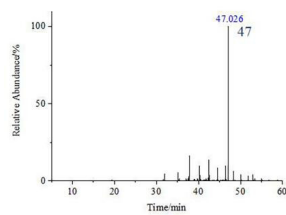
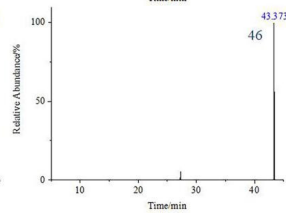
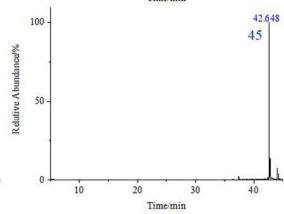
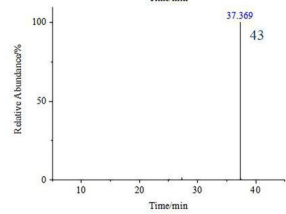
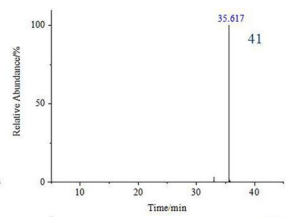
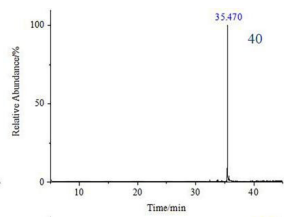
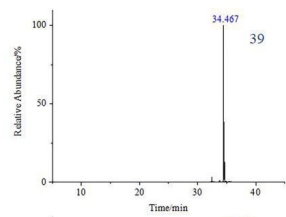
**Figure S1. GC-MS equipped with HP-5 ms, HP-1 and HP-INNOWax capillary columns TiC spectra for Lavender essential oil.**



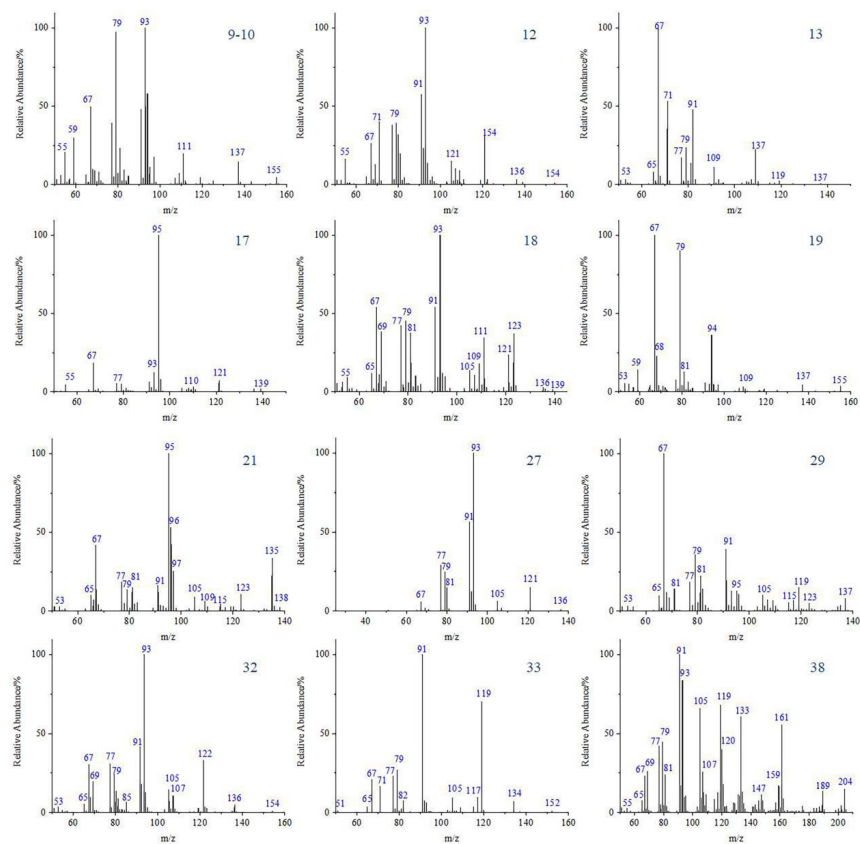


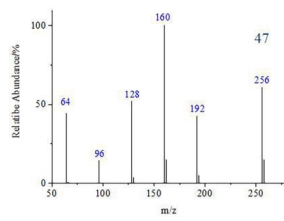
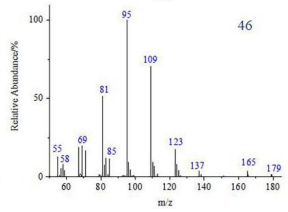
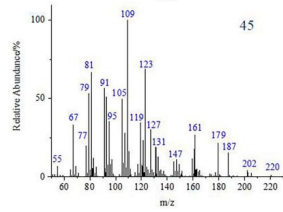
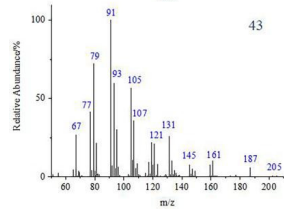
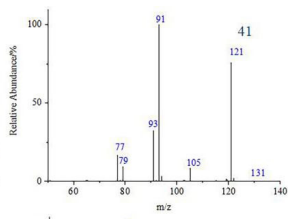
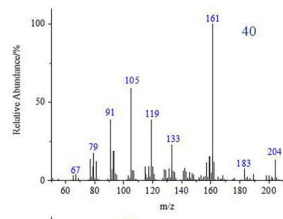
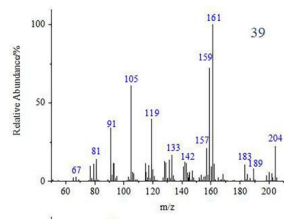
**Figure S2. GC-EI-QTOF-MS Tic spectra for compounds 9, 10, 12, 13, 17, 18, 19, 21, 27, 29, 32, 33, 38, 39, 40, 41, 43, 45, 46, 47.**





**Figure S3. GC-EI-QTOF-MS spectra for compounds 9, 10, 12, 13, 17, 18, 19, 21, 27, 29, 32, 33, 38, 39, 40, 41, 43, 45, 46, 47.**





## Spectral data

*Cis-Linalool oxide and trans-Linalool oxide (9-10)*. C<sub>10</sub>H<sub>18</sub>O<sub>2</sub>; RI (HP-5 ms) 1069; EI-MS 70 eV, m/z (rel. int.): 155(4, M<sup>+</sup>), 137(14, [M-H<sub>2</sub>O]<sup>+</sup>), 125(3), 119(5), 111(20), 109(7), 106(4), 97(17), 95(11), 94(58), 93(100), 91(48), 81(24), 79(97), 77(39), 67(50), 59(30), 55(21), 53(5). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 600 MHz) δ 24.18, 24.33 (8C), 26.02, 26.83 (1C), 26.49 (4C), 27.25, 27.44 (7C), 37.48, 37.93 (3C), 71.12, 71.22 (6C), 82.79, 83.05 (2C), 85.54 (5C), 111.32, 111.58 (10C), 143.71, 144.32 (9C).

*Linalool (12)*. C<sub>10</sub>H<sub>18</sub>O; RI (HP-5 ms) 1102; EI-MS 70 eV, m/z (rel. int.): 154(1, M<sup>+</sup>), 139(2, [M-CH<sub>3</sub>]<sup>+</sup>), 136(3), 121(32), 107(10), 105(15), 96(5), 94(14), 93(100), 92(23), 91(57), 83(5), 82(3), 81(20), 80(32), 79(39), 78(3), 77(38), 72(3), 71(40), 69(13), 67(26), 65(5), 55(16). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 600 MHz) δ 17.67 (8C), 22.78 (10C), 25.67 (9C), 27.85 (5C), 42.04 (4C), 73.44 (3C), 111.64 (1C), 124.29 (6C), 131.91 (7C), 145.02 (2C).

*Hotrienol (13)*. C<sub>10</sub>H<sub>16</sub>O; RI (HP-5 ms) 1105; EI-MS 70 eV, m/z (rel. int.): 137(1, [M-CH<sub>3</sub>]<sup>+</sup>), 119(2), 109(22), 106(2), 105(2), 93(3), 91(11), 83(3), 82(48), 81(14), 80(3), 79(24), 77(17), 71(53), 67(100), 65(8), 53(3). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 600 MHz) δ 18.66 (10C), 27.54 (9C), 45.77 (4C), 72.81 (3C), 112.00 (1C), 115.62 (8C), 124.85 (5C), 137.06 (6C), 139.62 (7C), 144.75 (2C).

*(-)-Borneol (17)*. C<sub>10</sub>H<sub>18</sub>O; RI (HP-5 ms) 1161; EI-MS 70 eV, m/z (rel. int.): 139(2, [M-CH<sub>3</sub>]<sup>+</sup>), 136(2), 121(7), 110(3), 96(8), 95(100), 93(12), 91(5), 81(2), 79(5), 77(6), 67(18), 55(5). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 600 MHz) δ 13.31 (10C), 18.67 (8C), 20.18 (9C), 25.90 (6C), 28.27 (5C), 39.03 (3C), 45.09 (4C), 48.02 (7C), 49.96 (1C), 77.39 (2C).

*Lavandulol (18)*. C<sub>10</sub>H<sub>18</sub>O; RI (HP-5 ms) 1166; EI-MS 70 eV, m/z (rel. int.): 139(1, [M-CH<sub>3</sub>]<sup>+</sup>), 136(2), 135(3), 123(37), 121(24), 111(34), 109(18), 107(10), 105(14), 95(9), 94(12), 93(100), 91(54), 83(11), 81(37), 79(45), 77(42), 71(7), 69(38), 68(11), 67(55), 65(12), 55(10), 53(7), 51(6). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 400 MHz) δ 17.83 (10C), 19.50 (9C), 25.74 (6C), 28.38 (3C), 49.96 (2C), 63.63 (1C), 113.14 (8C), 122.00 (4C), 132.79 (5C), 145.40 (7C).

*2,2,6-trimethyl-6-vinyltetrahydro-2H-pyran-3-ol (19)*. C<sub>10</sub>H<sub>18</sub>O<sub>2</sub>; RI (HP-5 ms) 1166; EI-MS 70 eV, m/z (rel. int.): 155(5, [M-CH<sub>3</sub>]<sup>+</sup>), 137(5), 109(4), 107(3), 97(4), 95(5), 94(36), 93(5), 91(6), 83(6), 81(13), 79(90), 77(7), 68(23), 67(100), 59(15), 55(5), 53(5). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 600 MHz) δ 24.23 (4C), 26.44 (11C), 27.17 (3C), 27.52 (10C), 30.94 (9C), 71.25 (5C), 73.58 (6C), 75.24 (2C), 110.52 (8C), 146.79 (7C).

*Cryptone (21)*. C<sub>9</sub>H<sub>14</sub>O; RI (HP-5 ms) 1182; EI-MS 70 eV, m/z (rel. int.): 138(2, M<sup>+</sup>), 136(4), 135(34), 123(12, [M-CH<sub>3</sub>]<sup>+</sup>), 121(24), 120(3), 119(3), 117(3), 115(5), 110(3), 109(6), 105(9), 97(26), 96(53), 95(100), 91(16), 83(6), 82(5), 81(16), 79(13), 77(19), 67(41), 66(7), 65(10), 53(3), 51(3). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 600 MHz) δ 19.47 (9C), 19.63 (8C), 25.25 (5C), 31.51 (7C), 37.42 (6C), 42.52 (4C), 129.69 (2C), 154.32 (3C), 200.10 (1C).

*Linalyl acetate (27)*. C<sub>12</sub>H<sub>20</sub>O<sub>2</sub>; RI (HP-5 ms) 1263; EI-MS 70 eV, m/z (rel. int.): 136(1), 121(15),

107(2), 105(6), 94(4), 93(100), 92(12), 91(56), 80(15), 79(25), 77(29), 69(2), 67(6), 65(1). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 400 MHz) δ 17.54 (12C), 22.16 (10C), 22.29 (11C), 23.54 (5C), 25.65 (8C), 39.65 (4C), 82.83 (3C), 113.04 (1C), 123.74 (6C), 131.76 (7C), 141.77 (2C), 169.94 (9C).

*3,7-dimethylocta-1,7-diene-3,6-diol (29)*. C<sub>10</sub>H<sub>18</sub>O; RI (HP-5 ms) 1276; EI-MS 70 eV, m/z (rel. int.): 137(8, [M-H<sub>2</sub>O+H]<sup>+</sup>), 135(4), 134(3), 123(5), 119(15), 117(7), 115(6), 109(7), 107(8), 105(10), 96(11), 95(13), 93(13), 91(40), 82(14), 81(22), 79(37), 77(18), 71(14), 69(9), 68(12), 67(100), 65(10), 55(3), 53(3), 51(3). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 600 MHz) δ 17.76, 17.89 (10C), 28.16, 28.28 (9C), 29.16, 29.36 (5C), 37.72, 38.23 (4C), 72.93 (3C), 75.76, 76.22 (6C), 110.94, 110.98 (8C), 111.88, 112.00 (1C), 144.94 (2C), 147.49 (7C).

*Lavandulol acetate (32)*. C<sub>12</sub>H<sub>20</sub>O<sub>2</sub>; RI (HP-5 ms) 1295; EI-MS 70 eV, m/z (rel. int.): 154(1, [M-COCH<sub>3</sub>+H]<sup>+</sup>), 136(5), 123(3), 122(33), 107(11), 105(15), 94(13), 93(100), 92(17), 91(42), 85(7), 81(9), 80(14), 79(24), 77(31), 69(19), 68(9), 67(30), 65(6), 55(1), 53(4), 51(3). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 400 MHz) δ 17.80 (9C), 19.90 (8C), 20.97 (12C), 25.75 (7C), 28.54 (4C), 46.02 (3C), 65.83 (10C), 112.36 (1C), 121.54 (5C), 132.93 (6C), 144.84 (2C), 171.11 (11C).

*(E)-7-hydroxy-3,7-dimethylocta-1,5-dien-3-ylacetate (33)*. C<sub>12</sub>H<sub>20</sub>O<sub>3</sub>; RI (HP-5 ms) 1344; EI-MS 70 eV, m/z (rel. int.): 152(1), 134(7), 120(1), 119(70), 117(10), 115(4), 109(3), 105(9), 103(2), 93(6), 92(8), 91(100), 82(8), 81(2), 79(27), 77(23), 71(16), 67(21), 65(4), 51(1). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 600 MHz) δ 22.15 (12C), 23.65 (9C), 29.88 (10C), 42.05 (4C), 70.73 (7C), 82.35 (3C), 113.50 (1C), 120.96 (5C), 141.49 (6C), 142.13 (2C), 169.89 (11C).

*(E)-β-Fanescene (38)*. C<sub>15</sub>H<sub>24</sub>; RI (HP-5 ms) 1459; EI-MS 70 eV, m/z (rel. int.): 204(15, M<sup>+</sup>), 189(14, [M-CH<sub>3</sub>]<sup>+</sup>), 175(4), 161(55), 159(17), 147(11), 133(61), 121(18), 120(40), 119(68), 117(14), 115(9), 109(12), 107(26), 105(66), 93(84), 91(100), 81(24), 79(45), 77(42), 69(26), 67(23), 65(7), 55(3), 51(3). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 400 MHz) δ 16.02 (14C), 17.68 (15C), 25.69 (12C), 26.61 (5C), 31.41 (4C), 39.70 (8C), 113.03 (1C), 115.70 (13C), 124.01 (6C), 124.34 (10C), 131.30 (11C), 135.38 (7C), 138.99 (2C), 146.12 (3C).

*D-Germacrene (39)*. C<sub>15</sub>H<sub>24</sub>; RI (HP-5 ms) 1480; EI-MS 70 eV, m/z (rel. int.): 204(22, M<sup>+</sup>), 202(5), 200(6), 198(4), 189(8, [M-CH<sub>3</sub>]<sup>+</sup>), 183(11), 161(100), 159(72), 157(21), 143(11), 142(12), 141(9), 133(17), 131(13), 129(12), 128(13), 119(39), 117(10), 115(12), 105(61), 93(11), 91(34), 81(14), 79(11), 77(10), 67(3), 65(3). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 600 MHz) δ 15.91 (14C), 19.33 (13C), 20.76 (12C), 26.51 (8C), 29.24 (2C), 32.75 (11C), 34.50 (3C), 40.71 (9C), 52.91 (7C), 109.02 (15C), 129.65 (1C), 133.55 (6C), 133.99 (10C), 135.49 (5C), 148.88 (4C).

*γ-Cadinene (40)*. C<sub>15</sub>H<sub>24</sub>; RI (HP-5 ms) 1514; EI-MS 70 eV, m/z (rel. int.): 204(13, M<sup>+</sup>), 183(8), 162(12), 161(100), 159(15), 157(11), 133(22), 119(39), 105(59), 93(19), 91(39), 81(12), 79(17), 77(13), 67(4), 65(3). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 600 MHz) δ 15.12 (15C), 21.55 (12C), 23.90 (13C), 25.72 (8C), 26.21 (2C), 26.53 (9C), 30.49 (11C), 36.31 (3C), 44.19 (7C), 45.12 (1C), 46.90 (6C), 103.15 (14C), 122.43 (5C), 134.76 (4C), 153.39 (10C).



*11-hydroxy- $\alpha$ -santal-9-ene* (41). C<sub>15</sub>H<sub>24</sub>O; RI (HP-5 ms) 1519; EI-MS 70 eV, m/z (rel. int.): 131(22), 122(2), 121(76), 119(1), 105(8), 94(3), 93(100), 91(33), 79(9), 77(17), 65(1). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 600 MHz)  $\delta$  10.69 (15C), 17.38 (14C), 19.50 (2C), 19.62 (4C), 26.95 (3C), 29.92 (12C), 29.94 (13C), 30.99 (5C), 31.23 (1C), 37.01 (8C), 38.42 (6C), 46.27 (7C), 70.75 (11C), 124.18 (9C), 139.43 (10C).

*$\beta$ -Caryophyllene oxide* (43). C<sub>15</sub>H<sub>24</sub>O; RI (HP-5 ms) 1585; EI-MS 70 eV, m/z (rel. int.): 205(1, [M-CH<sub>3</sub>]<sup>+</sup>), 187(6), 161(10), 159(8), 145(8), 133(10), 131(26), 121(21), 119(21), 107(36), 105(57), 95(30), 93(60), 91(100), 81(21), 79(72), 77(42), 67(27), 55(3). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 600 MHz)  $\delta$  16.99 (12C), 21.62 (15C), 27.21 (2C), 29.80 (7C), 29.89 (6C), 30.19 (14C), 34.02 (11C), 39.16 (3C), 39.76 (10C), 48.73 (9C), 50.76 (1C), 59.82 (4C), 63.75 (5C), 112.74 (13C), 151.83 (8C).

*(3S,6R,9R)-2-(hydroxymethyl)-5,5,9-trimethyltricyclo[7.2.0.0(3,6)]undecan-2-ol* (45). C<sub>15</sub>H<sub>26</sub>O<sub>2</sub>; RI (HP-5 ms) 1811; EI-MS 70 eV, m/z (rel. int.): 220(1, [M-H<sub>2</sub>O]<sup>+</sup>), 205(2), 202(5), 187(15), 179(21), 161(27), 159(11), 149(7), 147(11), 145(10), 133(13), 131(19), 127(30), 123(69), 121(23), 119(34), 109(100), 107(28), 105(49), 95(35), 93(51), 91(57), 81(67), 79(53), 77(20), 67(33), 55(7). <sup>13</sup>C NMR (CD<sub>3</sub>COCD<sub>3</sub>, 600 MHz)  $\delta$  20.69 (12C), 21.40 (2C), 27.64 (3C), 28.52 (13C), 30.95 (6C), 33.81 (14C), 34.59 (7C), 34.72 (11C), 35.68 (9C), 38.60 (10C), 39.14 (4C), 43.49 (1C), 43.62 (5C), 69.42, 70.65 (8C), 73.31 (15C).

*(6R,10R)-6,10,14-Trimethyl-2-pentadecanone* (46). C<sub>18</sub>H<sub>36</sub>O; RI (HP-5 ms) 1846; EI-MS 70 eV, m/z (rel. int.): 179(1), 165(4), 137(4), 125(4), 124(8), 123(18), 111(7), 110(9), 109(71), 97(4), 96(10), 95(100), 85(11), 83(11), 81(51), 71(16), 69(20), 67(19), 59(4), 58(8), 57(6), 55(13). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 600 MHz)  $\delta$  19.58 (16C), 19.74 (17C), 21.44 (4C), 22.62 (15C), 22.72 (18C), 24.42 (8C), 24.79 (12C), 27.98 (14C), 29.85 (1C), 32.67 (6C), 32.78 (10C), 36.49 (5C), 37.23 (9C), 37.28 (7C), 37.40 (11C), 39.36 (13C), 44.15 (3C), 209.38 (2C).

*S<sub>8</sub>* (47). S<sub>8</sub>; RI (HP-5 ms) 2031; EI-MS 70 eV, m/z (rel. int.): 257(15, [M+H]<sup>+</sup>), 256(60, M<sup>+</sup>), 193(5), 192(43), 161(15), 160(100), 129(3), 128(52), 96(14), 64(45).

Figure S4.  $^{13}\text{C}$  spectra for linalool oxide (9-10).

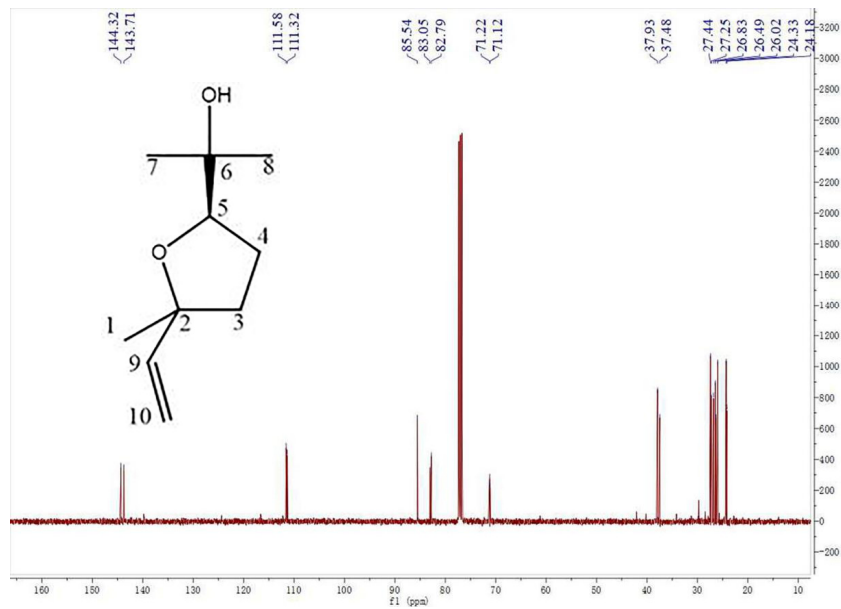


Figure S5.  $^{13}\text{C}$  spectra for Linalool (12).

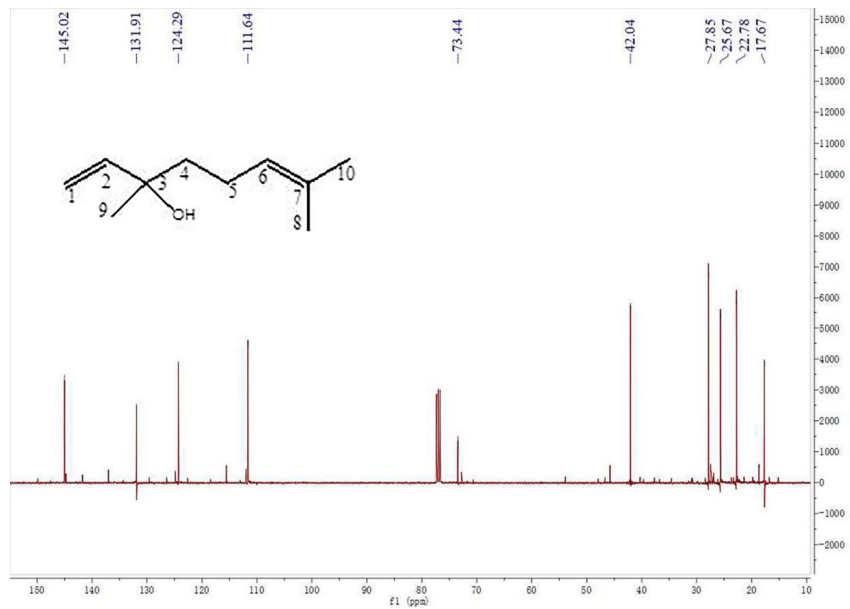


Figure S6.  $^{13}\text{C}$  spectra for Hotrienol (13).

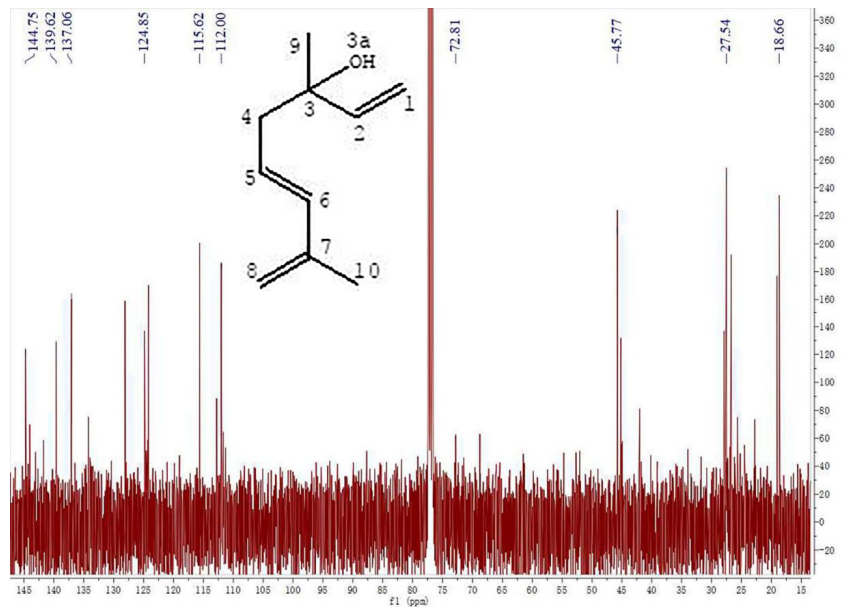


Figure S7.  $^{13}\text{C}$  spectra for (-)-borneol (17).

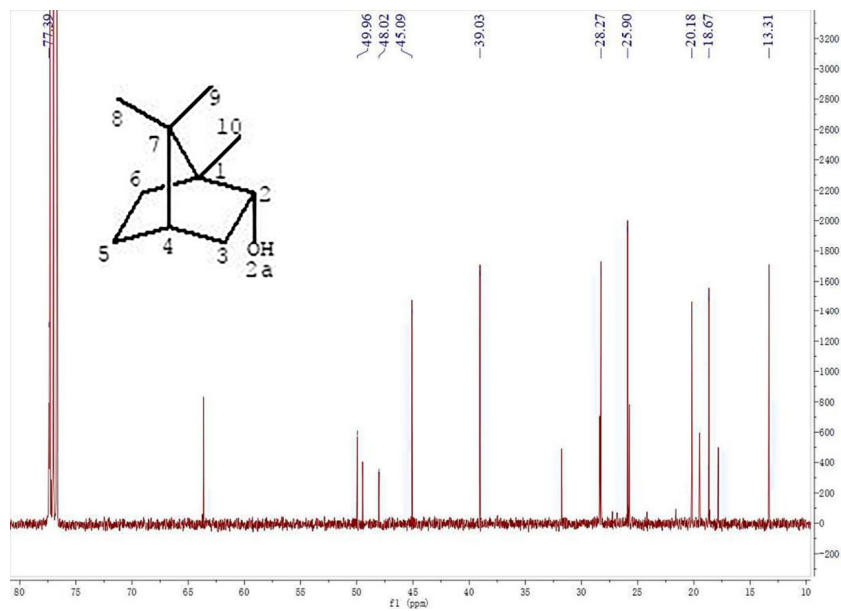


Figure S8.  $^{13}\text{C}$  spectra for lavandulol (18).

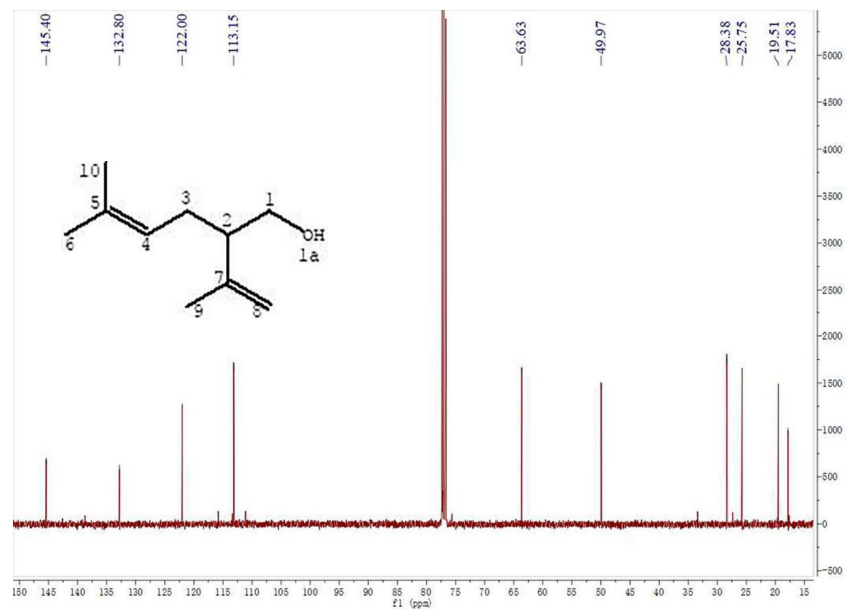


Figure S9.  $^{13}\text{C}$  spectra for 2,2,6-trimethyl-6-vinyltetrahydro-2H-pyran-3-ol (19).

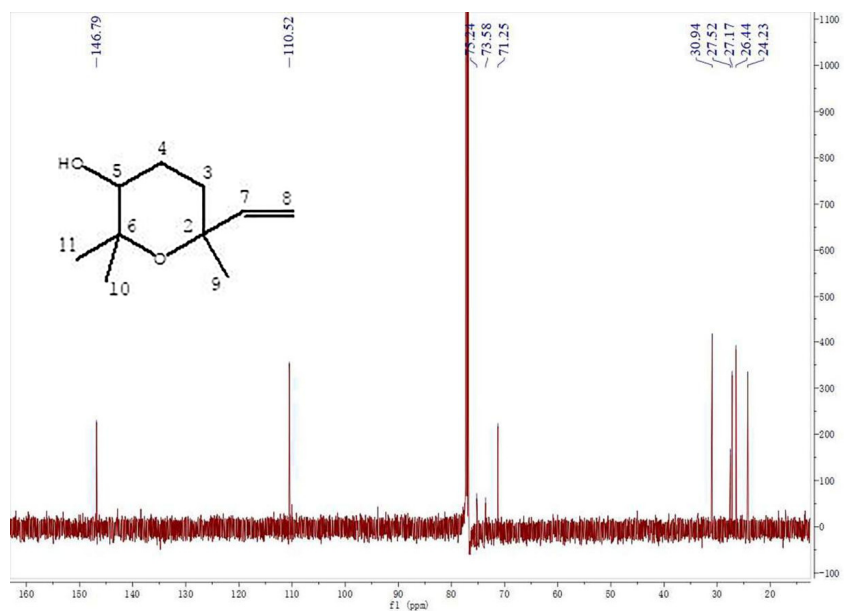


Figure S10.  $^{13}\text{C}$  and  $^1\text{H}$  NMR spectra for cryptone (21).

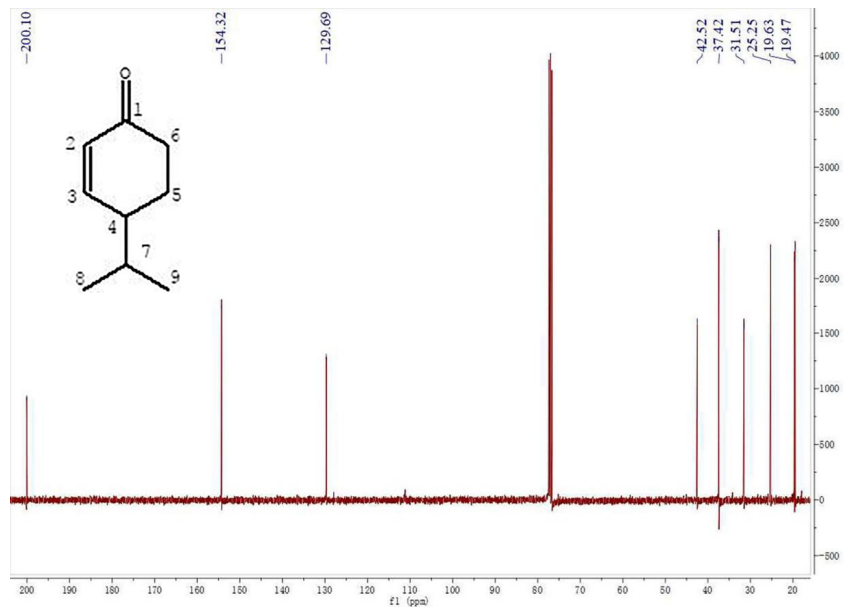




Figure S11.  $^{13}\text{C}$  spectra for linalyl acetate (27).

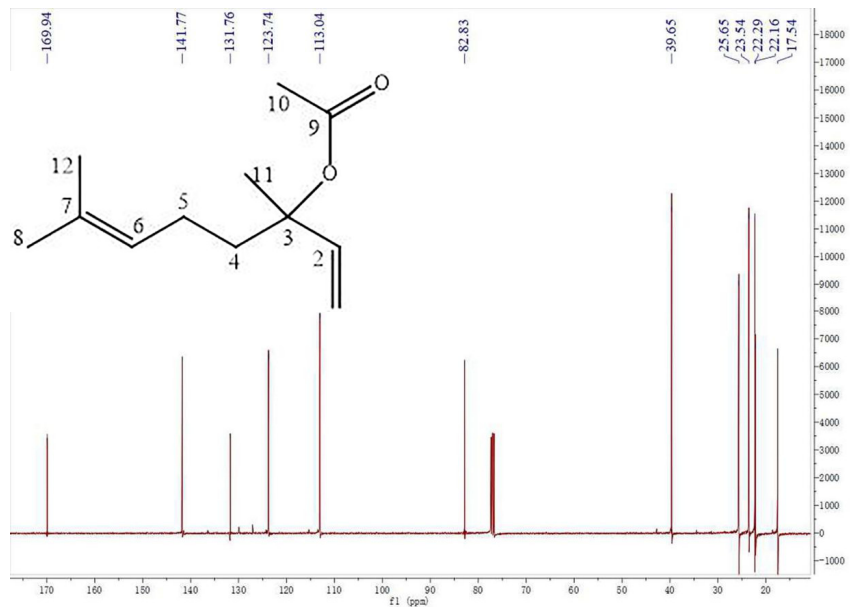


Figure S12.  $^{13}\text{C}$  spectra for 3,7-dimethylocta-1,7-diene-3,6-diol (29).

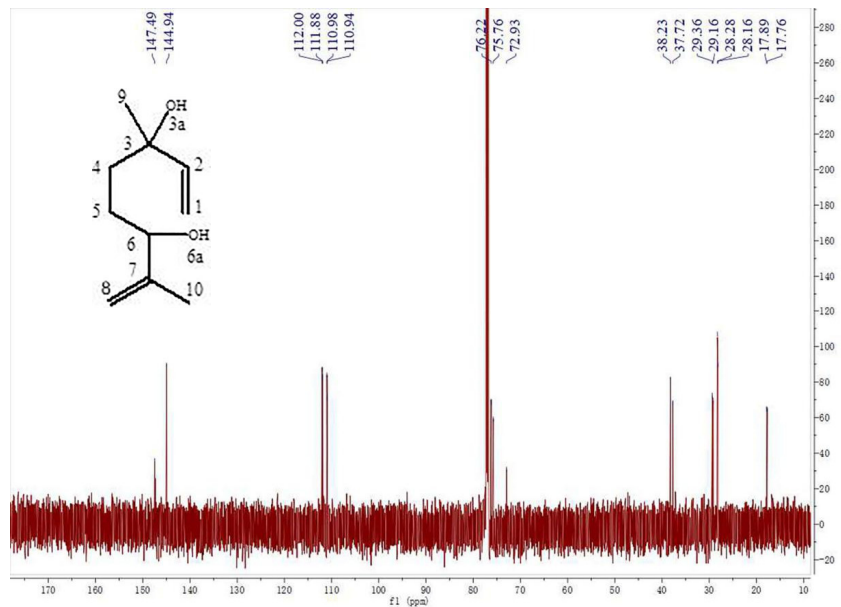


Figure S13.  $^{13}\text{C}$  spectra for Lavandulol acetate (32).

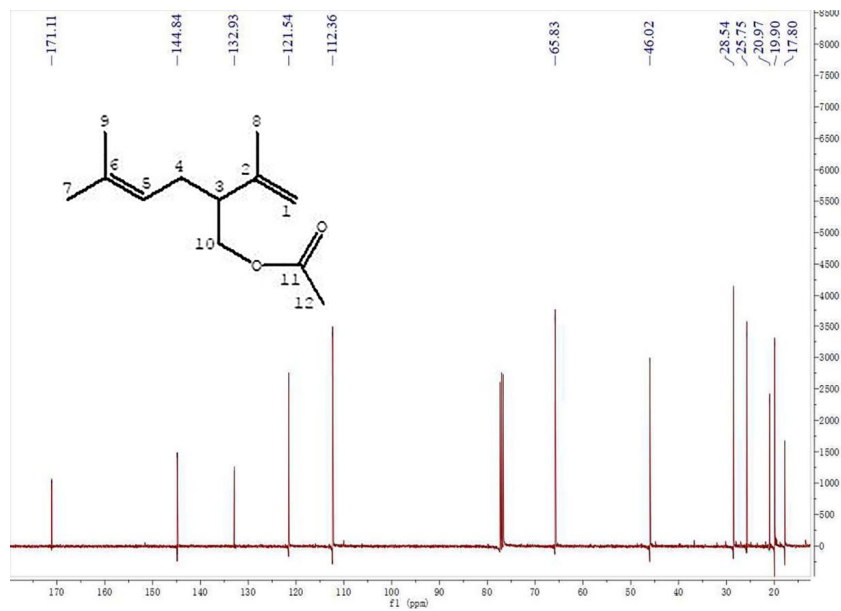


Figure S14.  $^{13}\text{C}$  spectra for (E)-7-hydroxy-3,7-dimethylocta-1,5-dien-3-ylacetate (33).

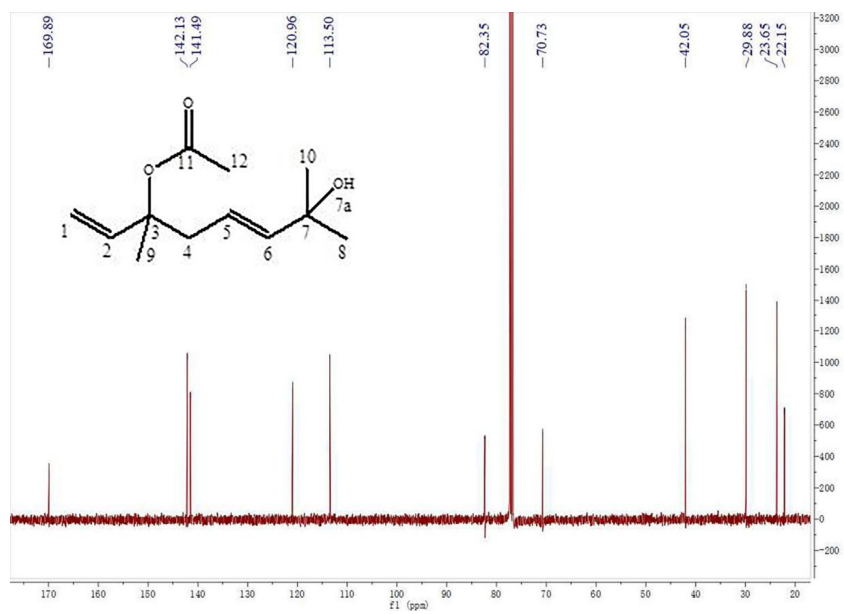


Figure S15.  $^{13}\text{C}$  spectra for (E)- $\beta$ -farnesene (38).

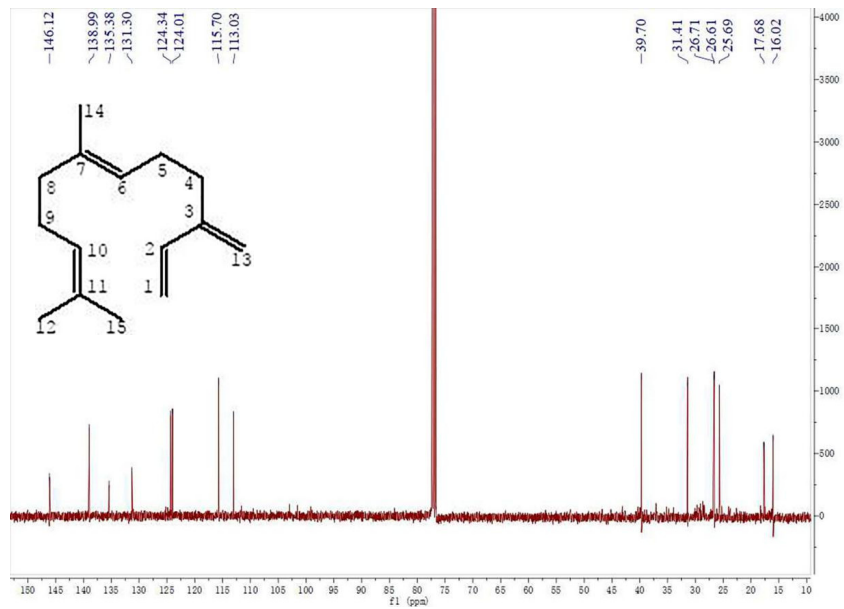


Figure S16.  $^{13}\text{C}$  spectra for germacrene D (39).

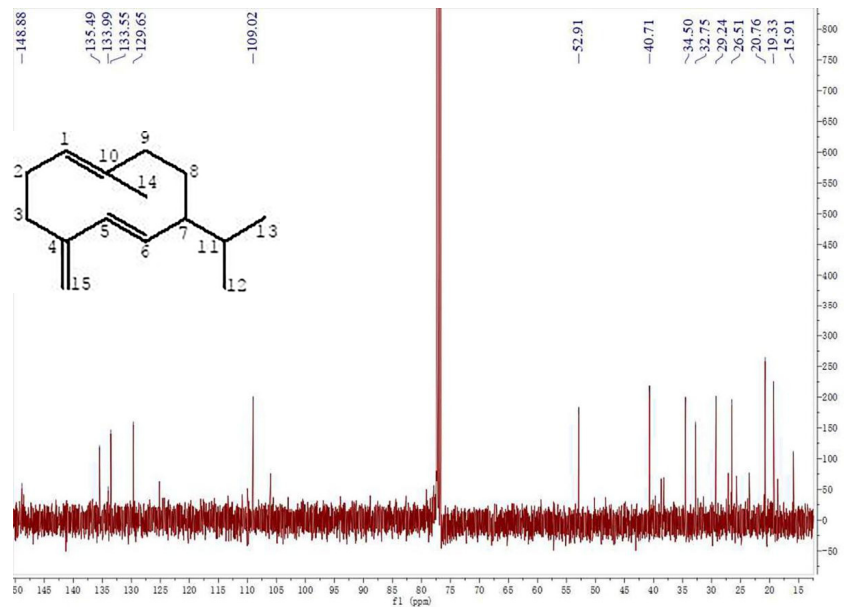


Figure S17.  $^{13}\text{C}$  spectra for  $\gamma$ -cadinene (40).

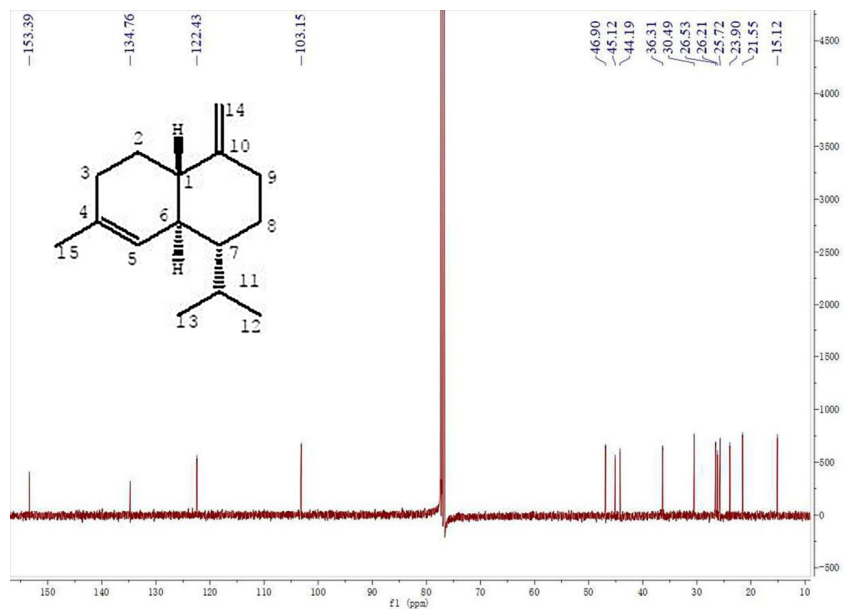


Figure S18.  $^{13}\text{C}$  spectra for 11-hydroxy- $\alpha$ -santal-9-ene (41).

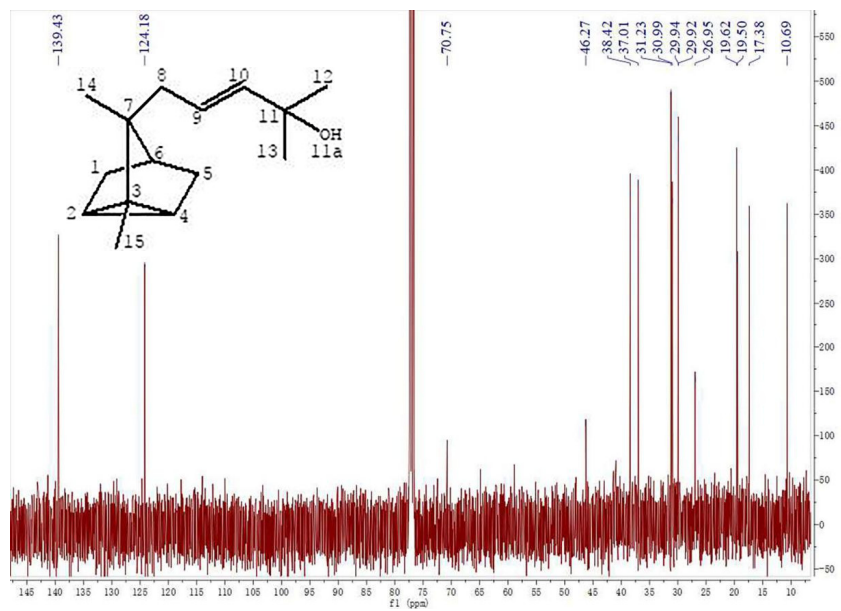




Figure S19.  $^{13}\text{C}$  spectra for  $\beta$ -caryophyllene oxide (43).

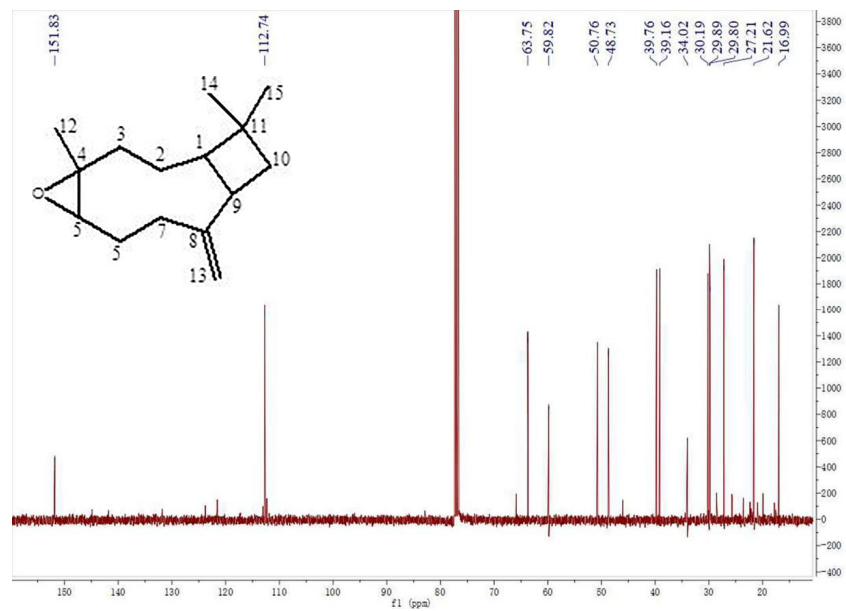


Figure S20.  $^{13}\text{C}$  spectra for (3S,6R,9R)-2-(hydroxymethyl)-5,5,9-trimethyltricyclo[7.2.0.0(3,6)]undecan-2-ol (45).

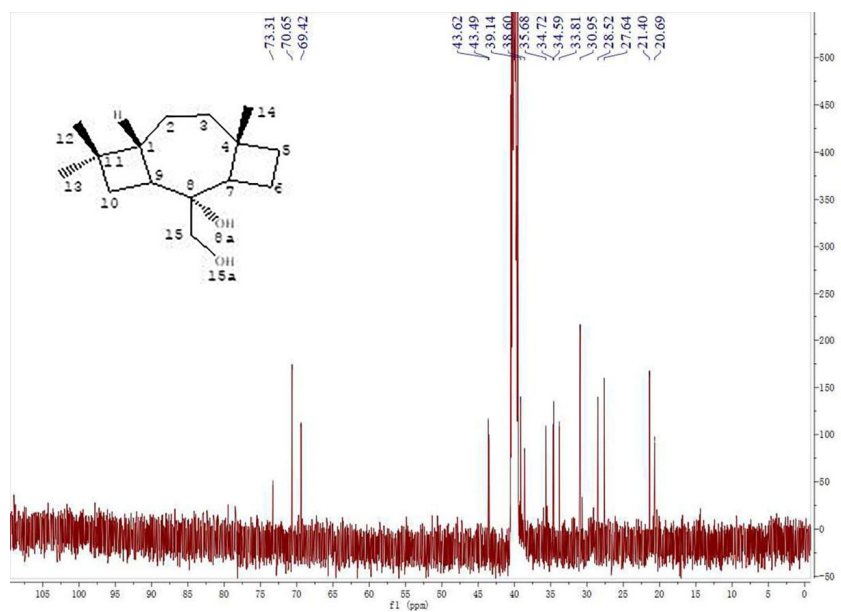


Figure S21.  $^{13}\text{C}$  spectra for (6R,10R)-6,10,14-Trimethyl-2-pentadecanone (46).

