Supplemental material

Bioactive compounds from *Curcuma aeruginosa* and the effect of comosone II on the migration and invasion of breast cancer cells

Germacrone (1):

Obtained as colourless prism. IR ν_{max} (KBr) cm^{-1}: 1672.94; ^{1}H-NMR ($CDCl_3$, 500 MHz), δ 1.43 (3H, s, H_3-14), 1.62 (3H, s, H_3-15), 1.72 (3H, s, H_3-12), 1.77 (3H, s, H_3-13), 2.06-2.18 (3H, m, H_1-2, H_2-3), 2.32-2.40 (1H, m, H_1-2), 2.85 (1H, dd, *J* = 11.0, H_1-6), 2.93-2.98 (2H, m, H_1-9, H_1-6), 3.41 (1H, d, *J* = 10.5 Hz, H_1-9), 4.70 (1H, d, *J* =11.5 Hz, H_1-5), 4.98 (1H, d, *J* = 11.5 Hz, H_1-l); ^{13}C-NMR ($CDCl_3$, 500 MHz),), δ 208.0 (C-8), 137.3 (C-11), 135.0 (C-10), 132.7 (C-1), 129.5 (C-7), 126.7 (C-4), 125.4 (C-5), 55.9 (C-9), 38.1 (C-3), 29.3(C-6), 24.1(C-2), 22.4 (C-13), 19.9 (C-12), 16.7 (C-15), 15.6 (C-14). EI-MS, m/z (%): 218.2 $[M]^+$ (10), 175.1 (20), 135.1 (80), 107.1 (100), 67.1 (46).

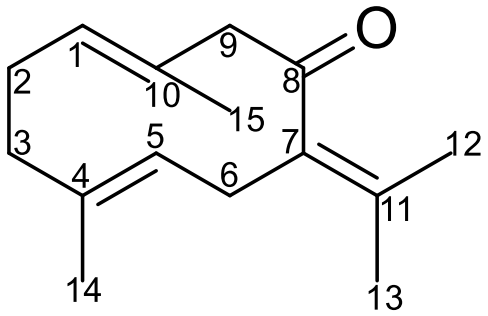
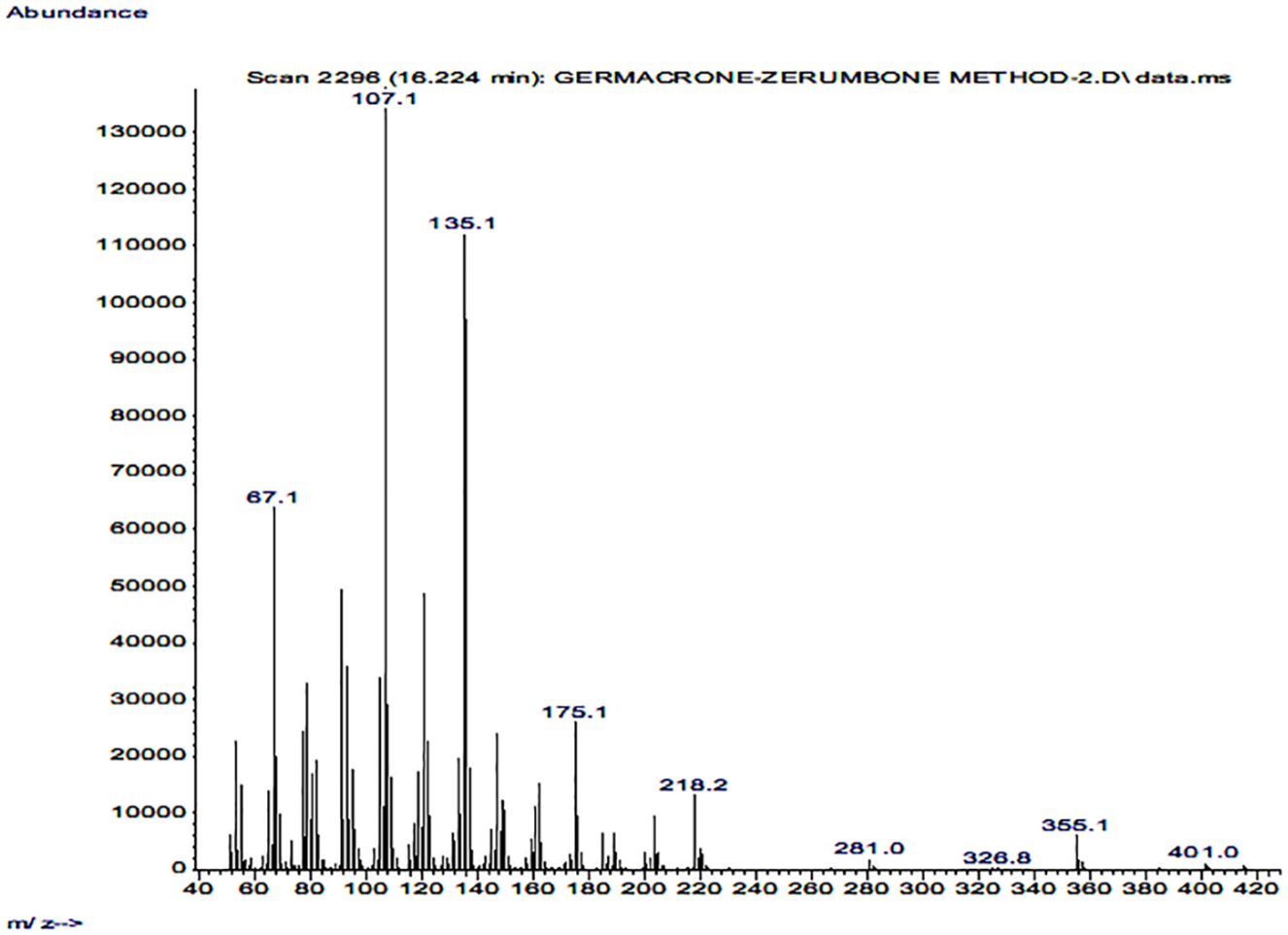


Figure 1S. Chemical structure of germacrone (**1**)



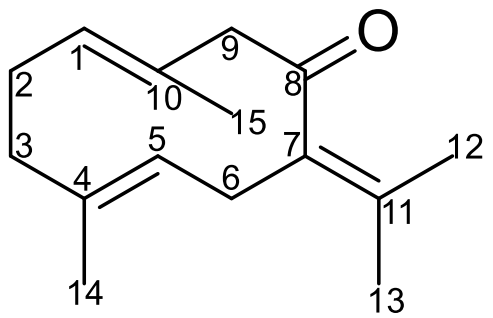
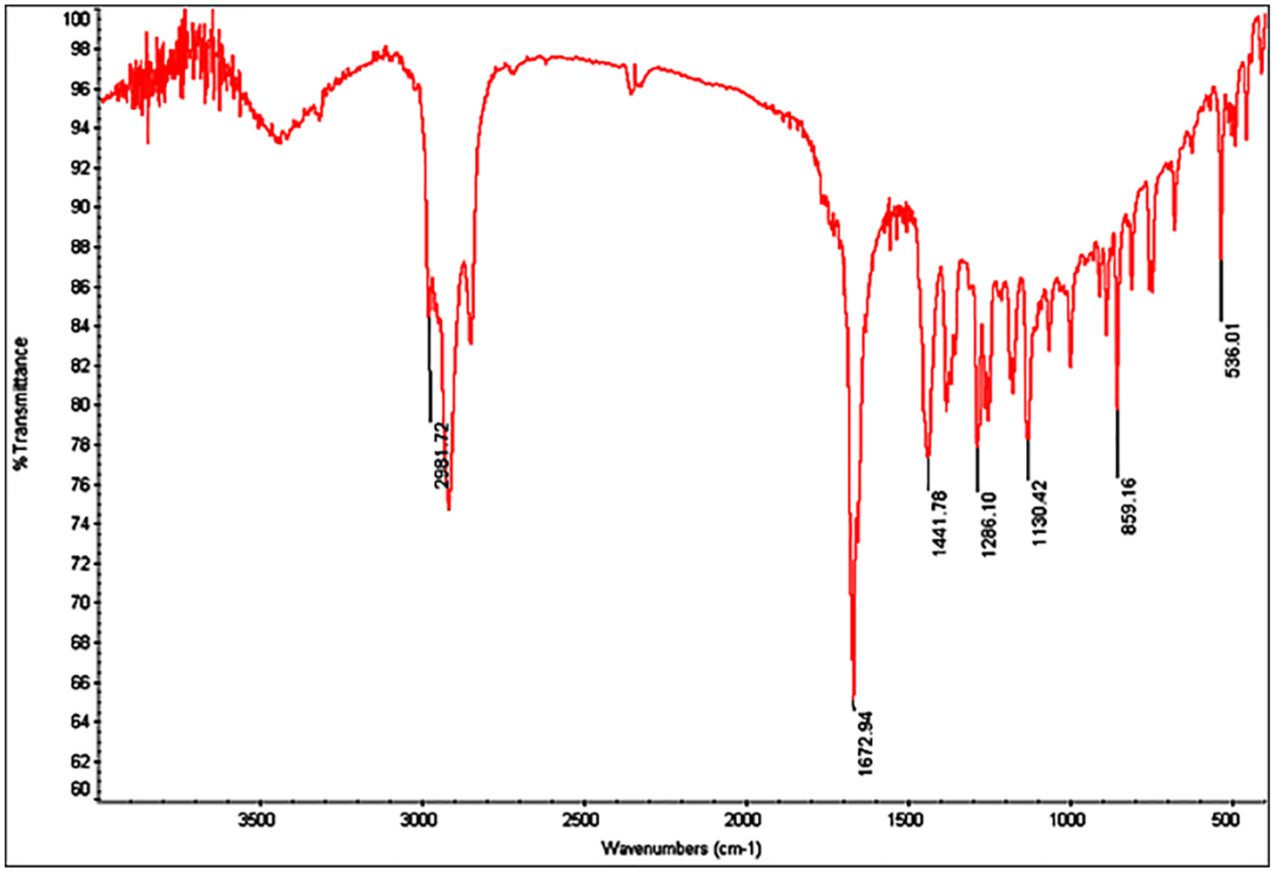


Figure 2S. EI-MS chromatogram of germacrone (**1**)



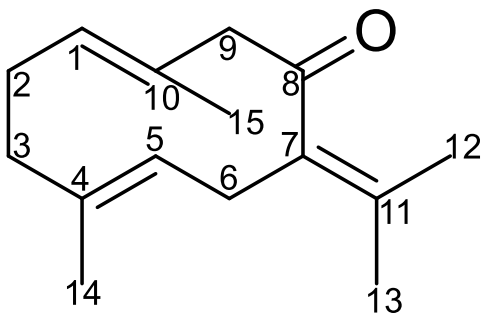
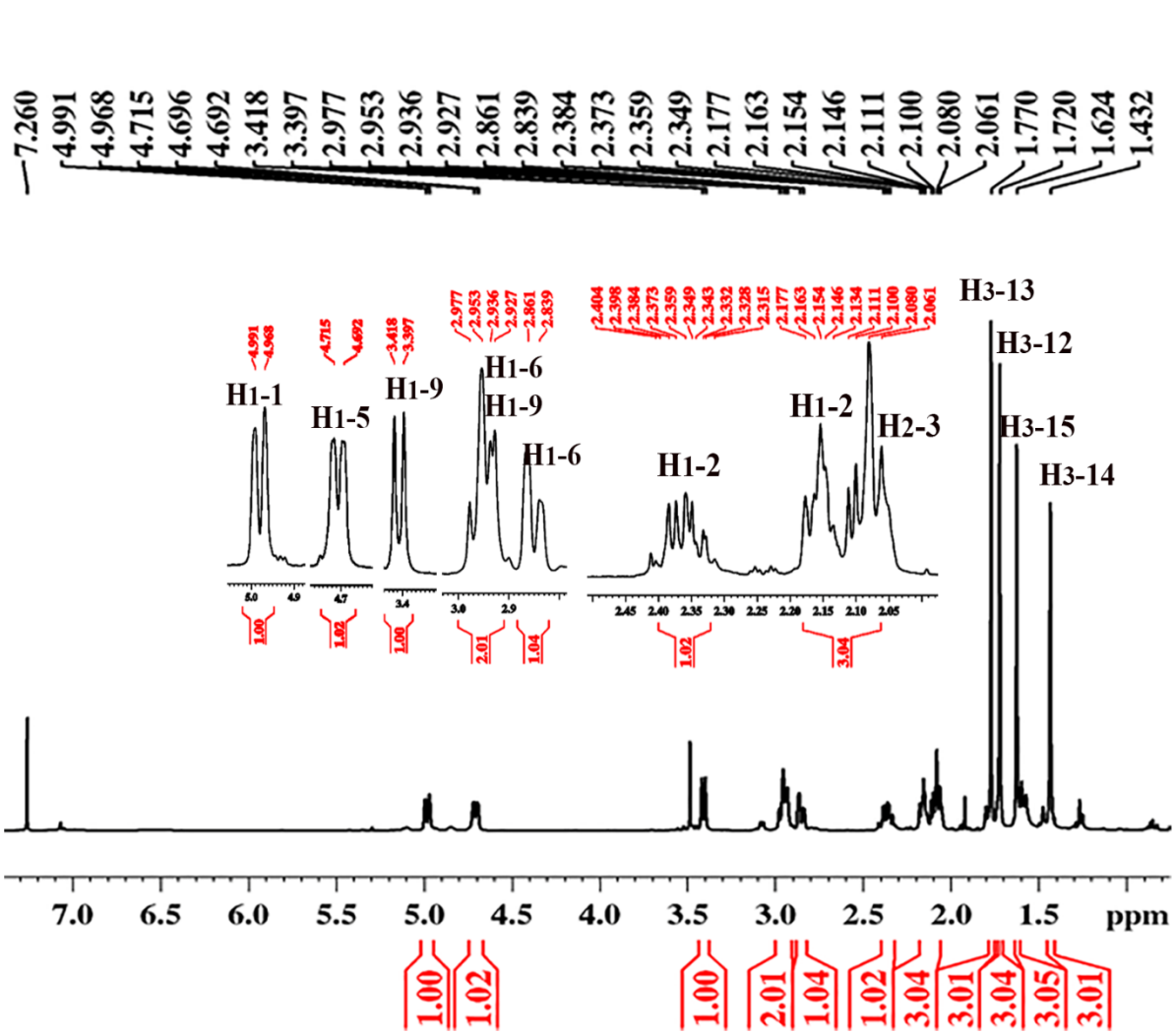


Figure 3S**.** FT-IR spectrum of germacrone (**1**)



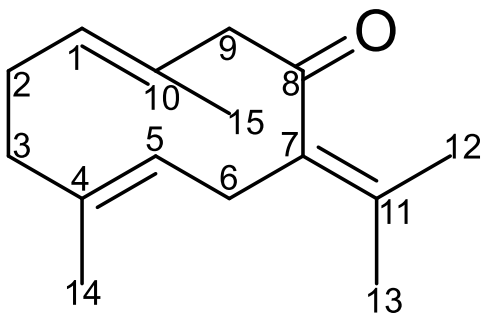
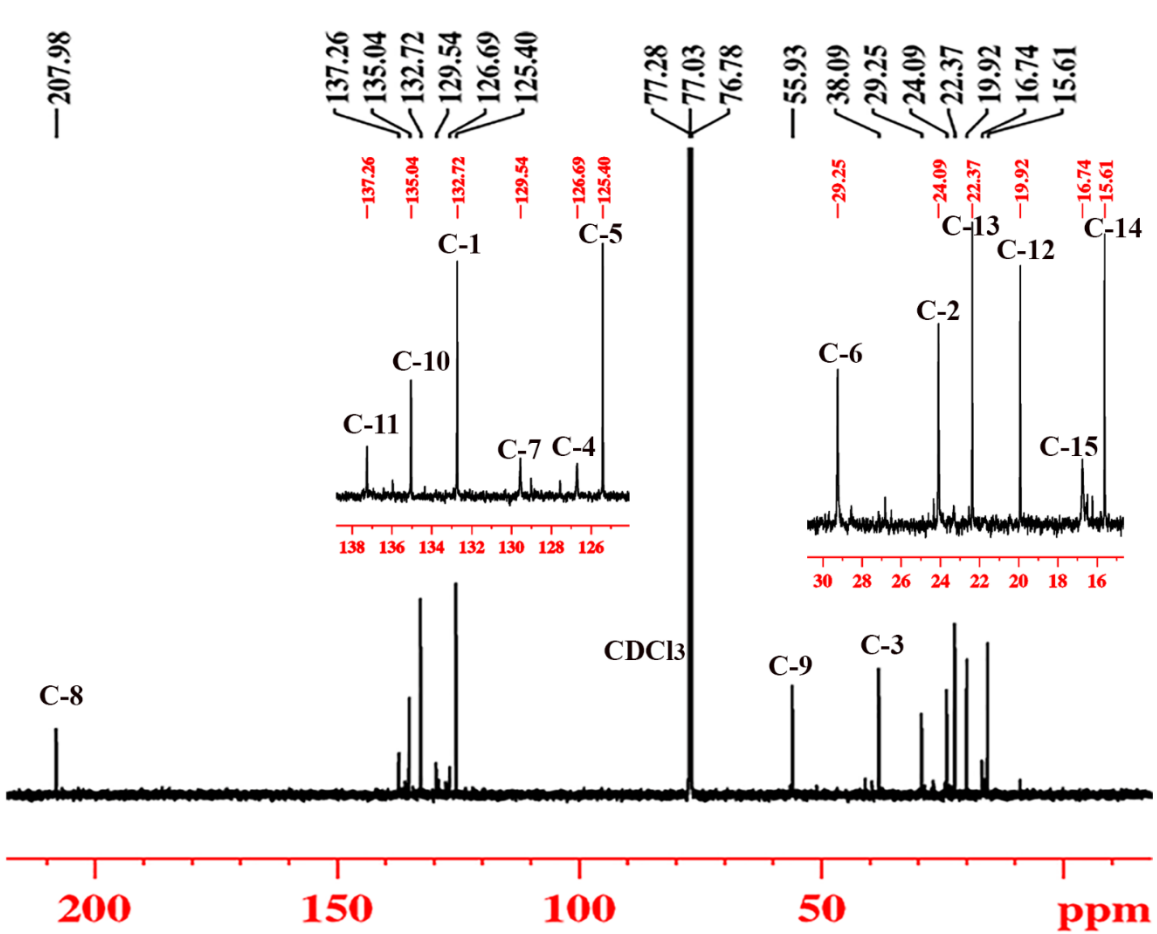


Figure 4S. ^{1}H-NMR spectrum (500 MHz, $CDCl_3$) of germacrone (**1**).



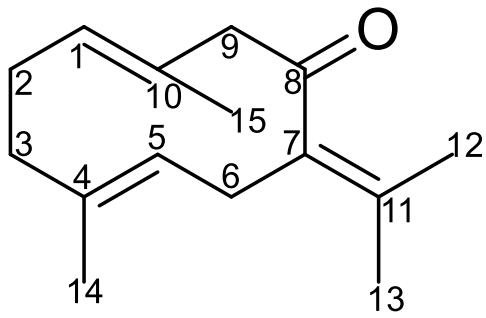


Figure 5S. ^{13}C-NMR spectrum (125 MHz, $CDCl_3$) of germacrone (**1**).

Furanodienone (2):

Obtained as colourless prism. IR ν_{max} (KBr) cm^{-1}: 1644.66, 1610.08; ^{1}H-NMR ($CDCl_3$, 500 MHz), δ 1.29 (3H, s, H_3-15), 1.85-2.47 (4H, m, , H_2-2, H_2-3), 1.98 (3H, s, H_3-14), 2.11 (3H, s, H_3-13), 3.68 (2H, br. d, J = 3.5 Hz H_2-9), 5.16 (1H, dd, J=4.5, 11.5 Hz, H_1-1), 5.79 (1H, s, H_1-5), 7.06 (1H, s, H_1-12); ^{13}C-NMR ($CDCl_3$, 500 MHz),), δ 189.8 (C-6), 156.5 (C-8), 145.8 (C-5), 138.1 (C-12), 135.4 (C-10), 132.5 (C-4), 130.5 (C-1), 123.7 (C-11), 122.2 (C-7), 41.7 (C-3), 40.7 (C-9), 26.5 (C-2), 19.0 (C-14), 15.8 (C-15), 9.6 (C-13). EI-MS, m/z (%): 230.1 $[M]^+$ (50), 215.1 (8), 122.1 (100), 94.1 (36), 65.1 (13).

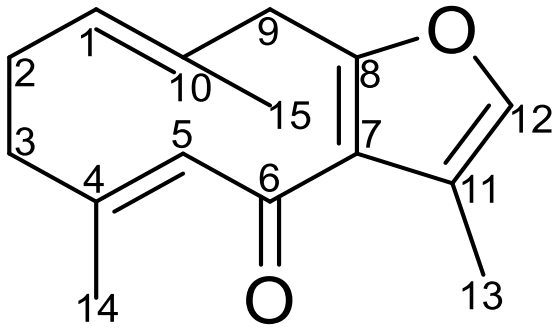
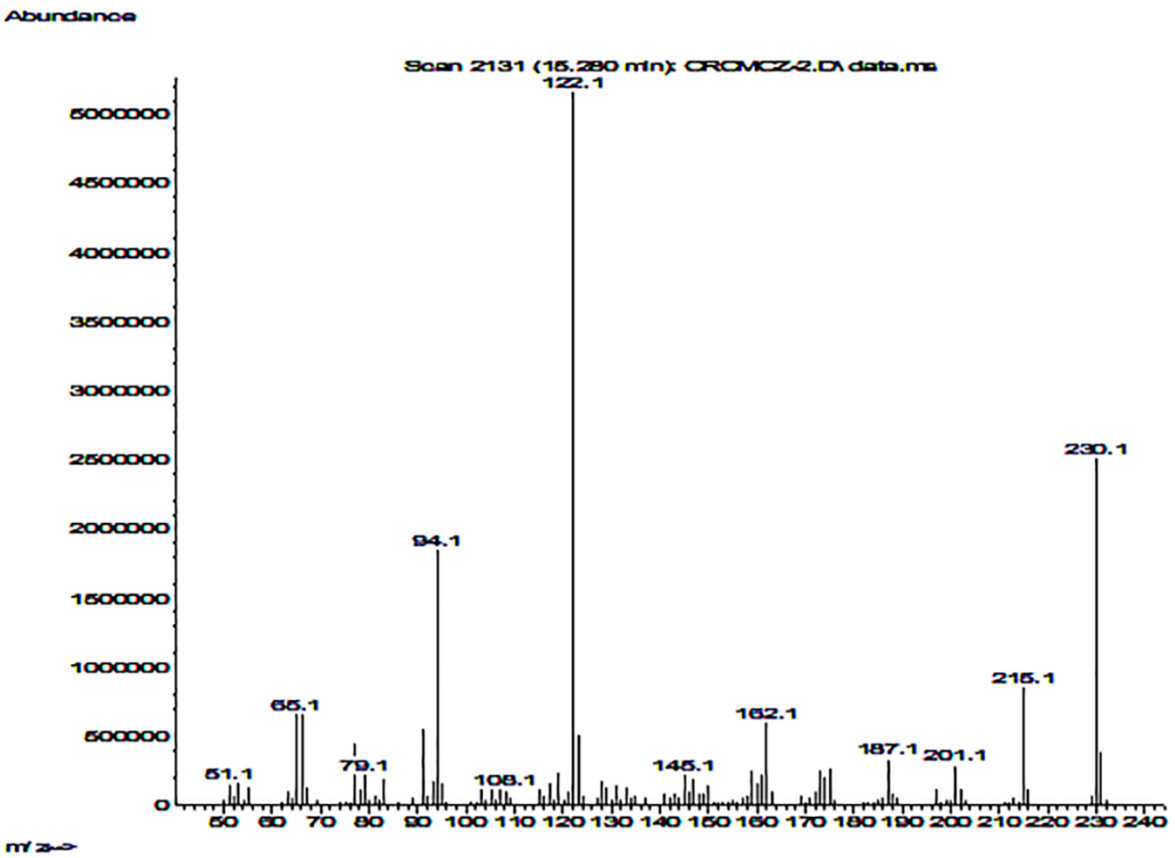


Figure 6S. Chemical structure of furanodienone (**2**)



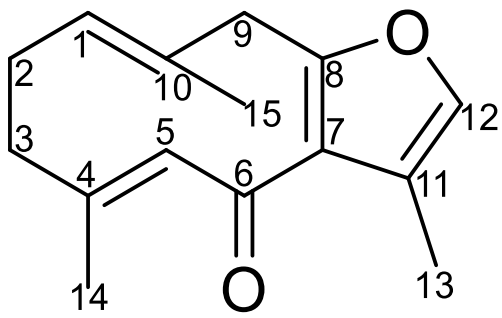
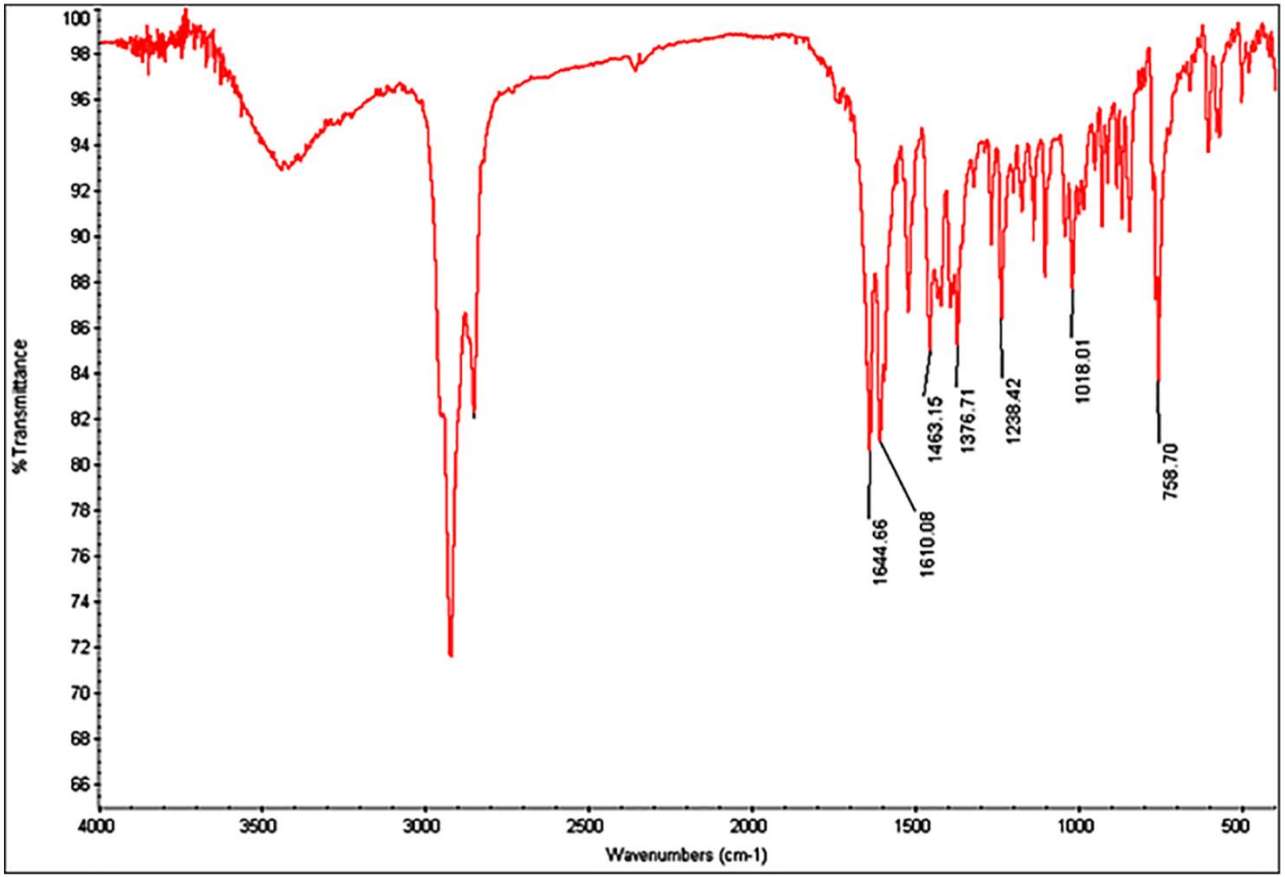


Figure 7S**.** EI-MS chromatogram of furanodienone (**2**)



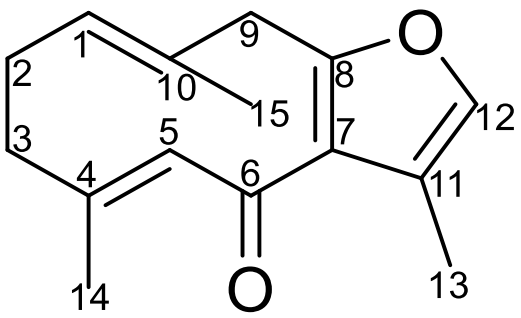
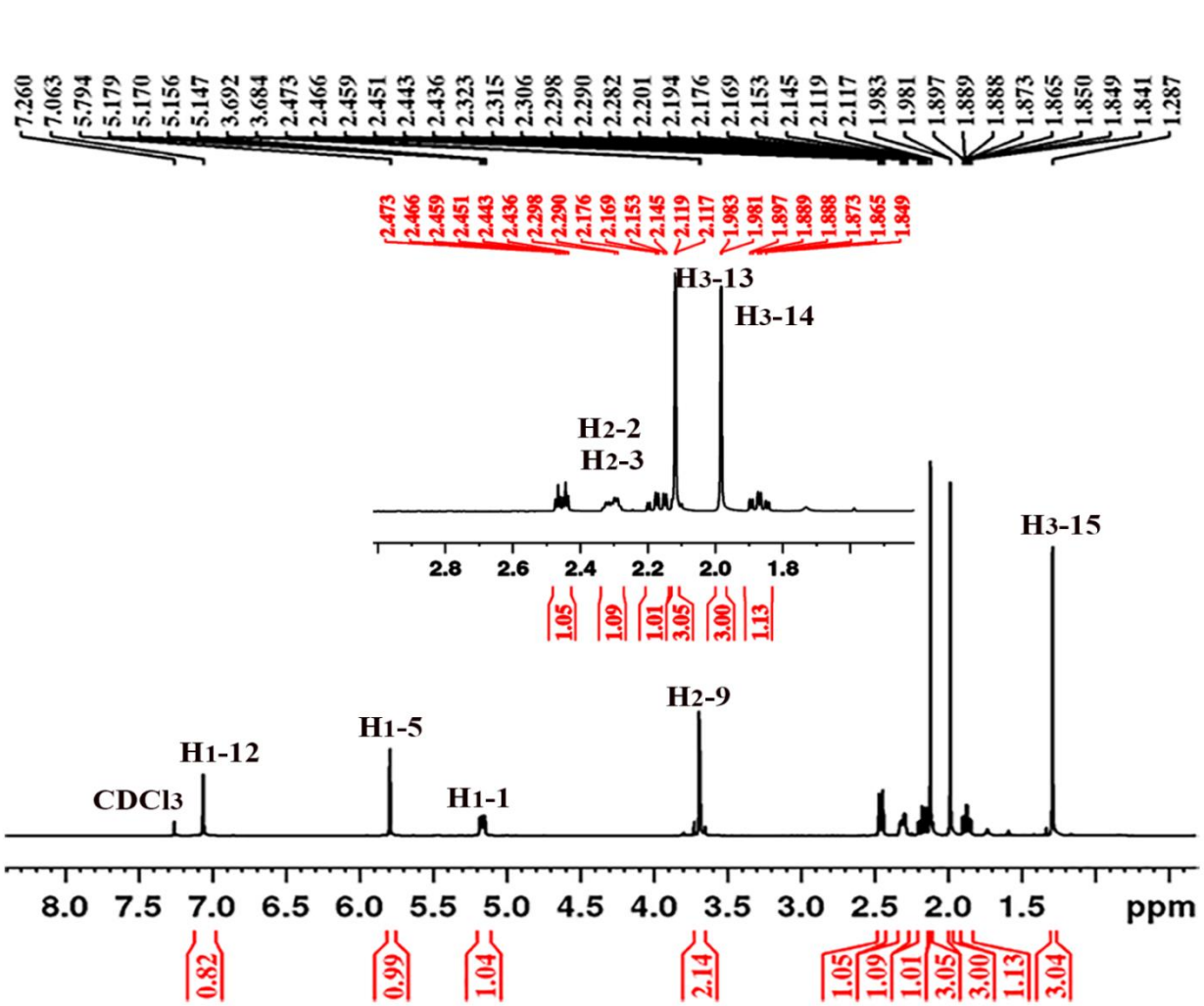


Figure 8S**.** FT-IR spectrum of furanodienone (**2**)



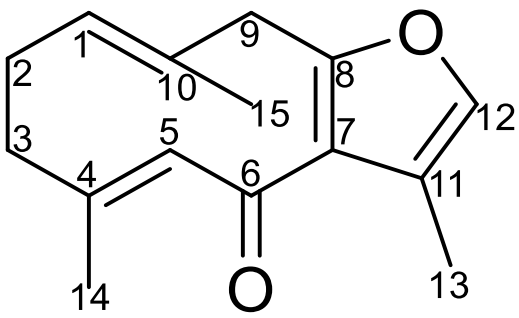
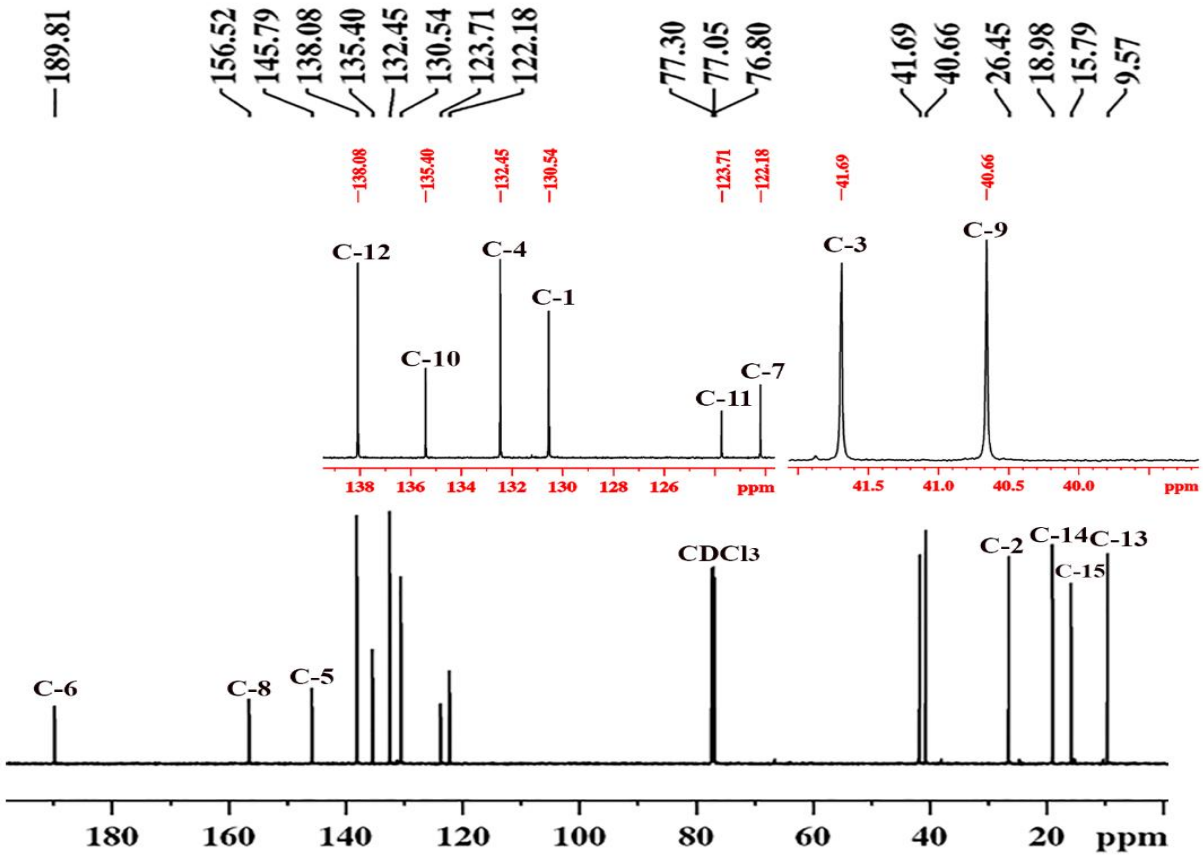


Figure 9S. ^{1}H-NMR spectrum (500 MHz, $CDCl_3$) of furanodienone (**2**)



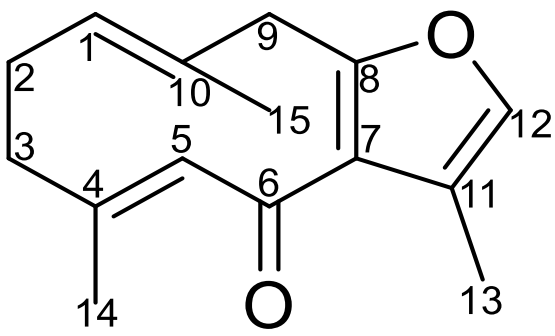


Figure 10S. ^{13}C-NMR spectrum (125 MHz, $CDCl_3$) of furanodienone (**2**)

Curzerenone (3):

Obtained as colourless crystals. ^{1}H-NMR ($CDCl_3$, 500 MHz), δ 1.18 (3H, s, H_3-15), 1.83 (3H, s, H_3-14), 2.17 (3H, s, H_3-13), 2.78 (1H, d, J = 17.5 Hz, H_1-9), 2.90 (1H, d, J = 17.5 Hz, H_1-9), 3.01 (1H, s, H_1-5), 4.75 (2H, s, H_1-3), 4.94-5.0 (3H, m, H_2-2, H_1-3), 5.80 (1H, dd, J = 11.0, 17.5 Hz, H_1-1), 7.08 (1H, s, H_1-12); ^{13}C-NMR ($CDCl_3$, 500 MHz),), δ 194.9 (C-6), 165.5 (C-8), 145.5 (C-1), 141.1 (C-4), 139.5 (C-12), 120.1 (C-7), 119.2 (C-11), 115.6 (C-3), 113.0 (C-2), 64.1 (C-5), 42.8 (C-10), 33.6 (C-9), 24.9 (C-14), 24.8 (C-15), 9.0 (C-13). EI-MS, m/z (%): 230.1 $[M]^+$ (36), 122.0 (100), 94.0 (32), 65.1 (13).

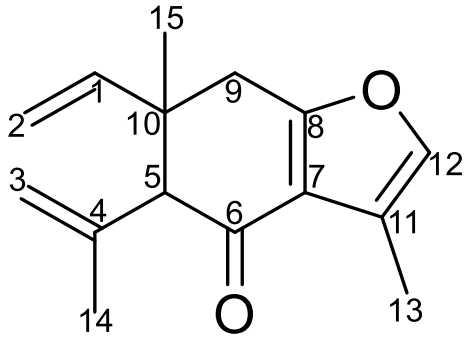
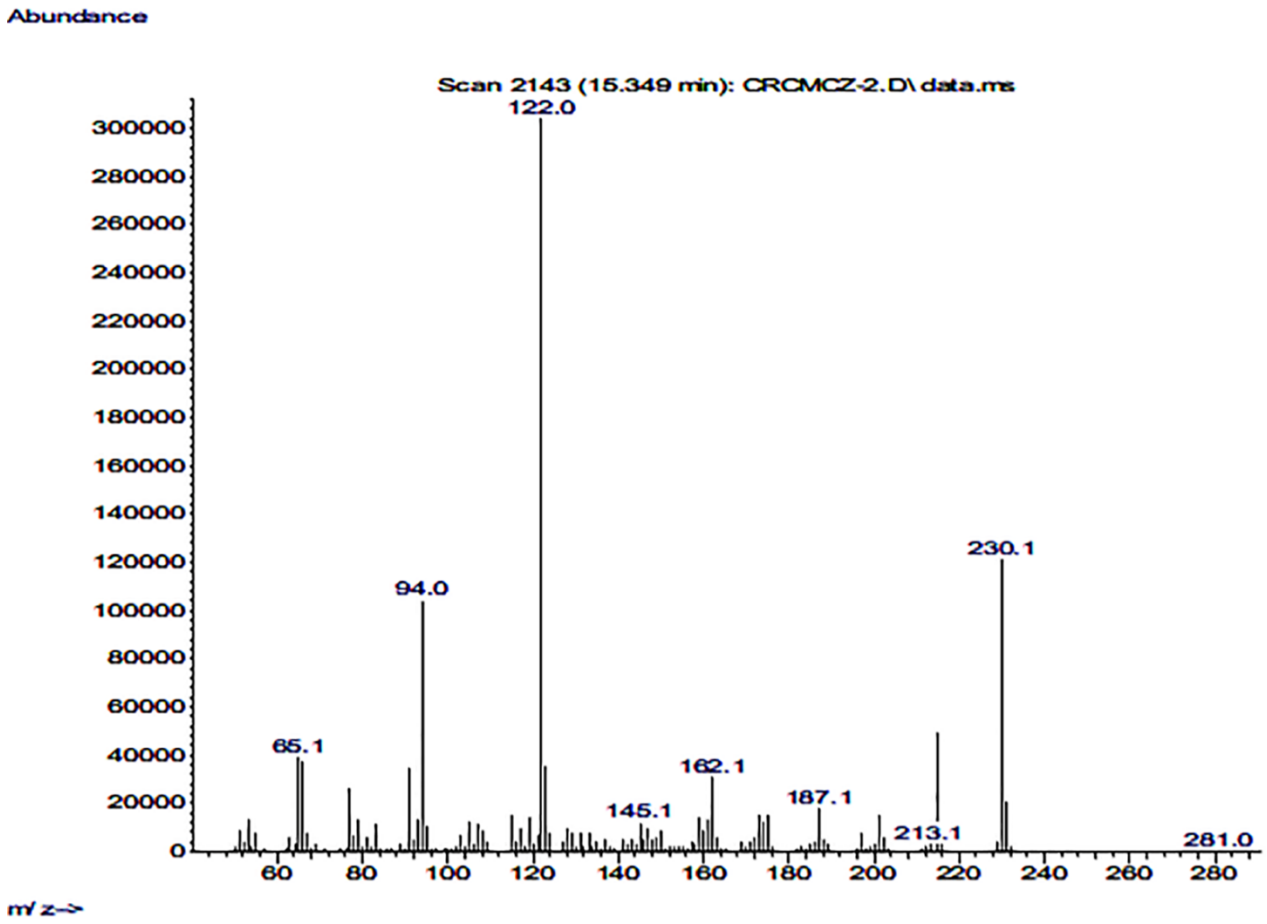


Figure 11S**.** Chemical structure of curzerenone (**3**)



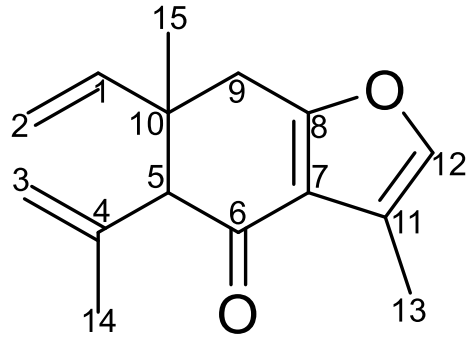
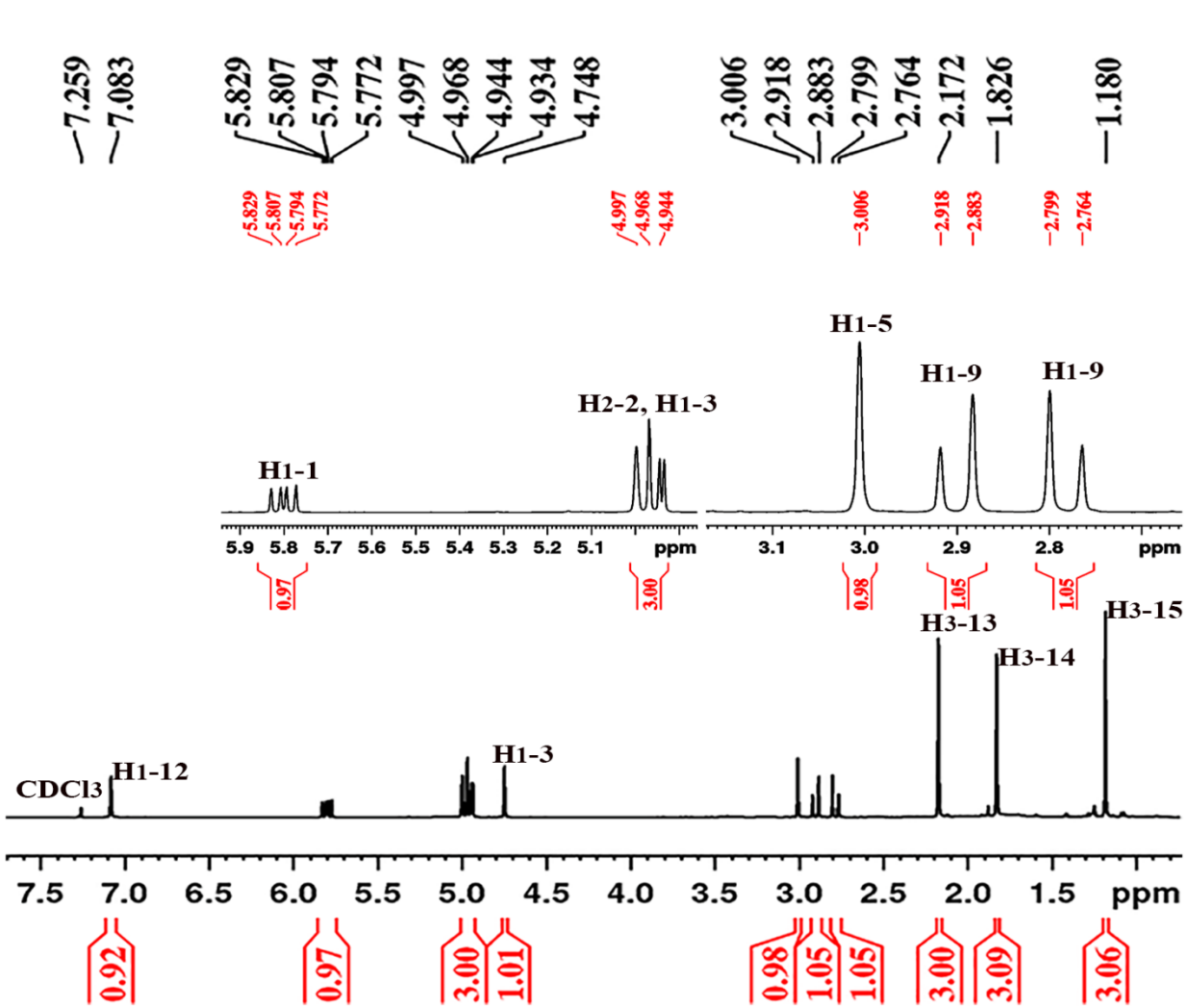


Figure 12S**.** EI-MS chromatogram of curzerenone (**3**)



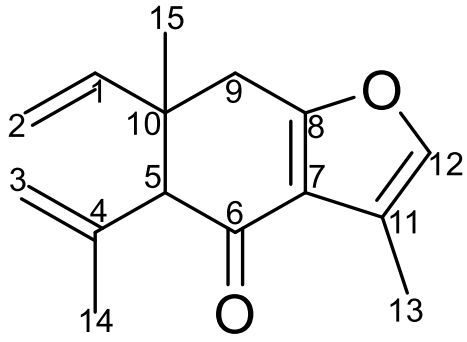


Figure 13S. ^{1}H-NMR spectrum (500 MHz, $CDCl_3$) of curzerenone (**3**)

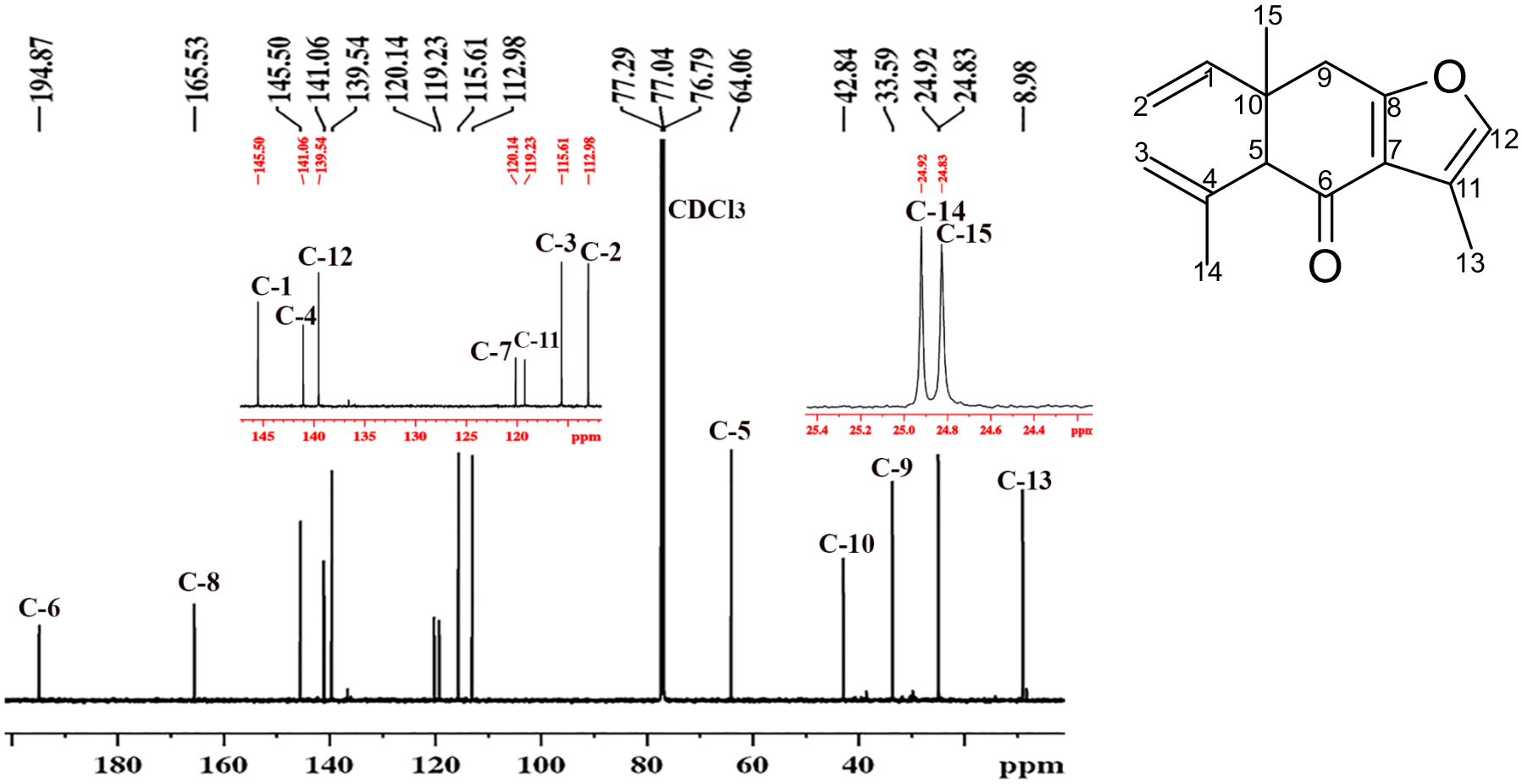


Figure 14S. ^{13}C-NMR spectrum (125 MHz, $CDCl_3$) of curzerenone (**3**)

Curcumenol (4)

Obtained as colourless solid. IR ν_{max} (KBr) cm^{-1}: 3369.03; ^{1}H-NMR ($CDCl_3$, 500 MHz), δ 1.02 (3H, d, J=6.0 Hz, H_3-14), 1.59 (3H, s, H_3-12), 1.66 (3H, s, H_3-13), 1.82 (3H, s, H_3-15), 1.88-1.94 (6H, m, H_2-2, H_2-3, H_1-4), 2.07 (1H, d, J =14.7Hz, H-1), 2.11-2.17 (1H, m, H_1-6), 2.64 (1H, bd, s, H_1-6), 5.76 (1H, bd. s, H_1-9); ^{13}C-NMR ($CDCl_3$, 500 MHz),), δ 139.2 (C-7), 137.3 (C-10), 125.6 (C-9), 122.3 (C-11), 101.5(C-8), 85.7 (C-5), 51.2 (C-1), 40.4 (C-4), 37.2 (C-6), 31.2 (C-3), 27.6 (C-2), 22.3 (C-12), 21.0 (C-15), 18.9 (C-13), 11.9 (C-14). EI-MS, m/z (%): 234.2 $[M]^+$ (41), 189.1 (67), 147.1 (56), 133.1 (67), 105.1 (100).

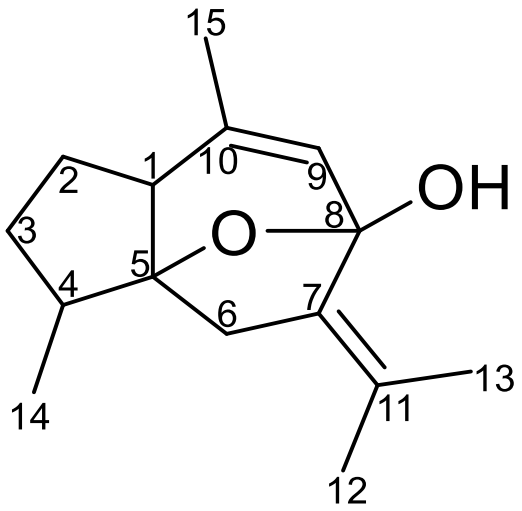
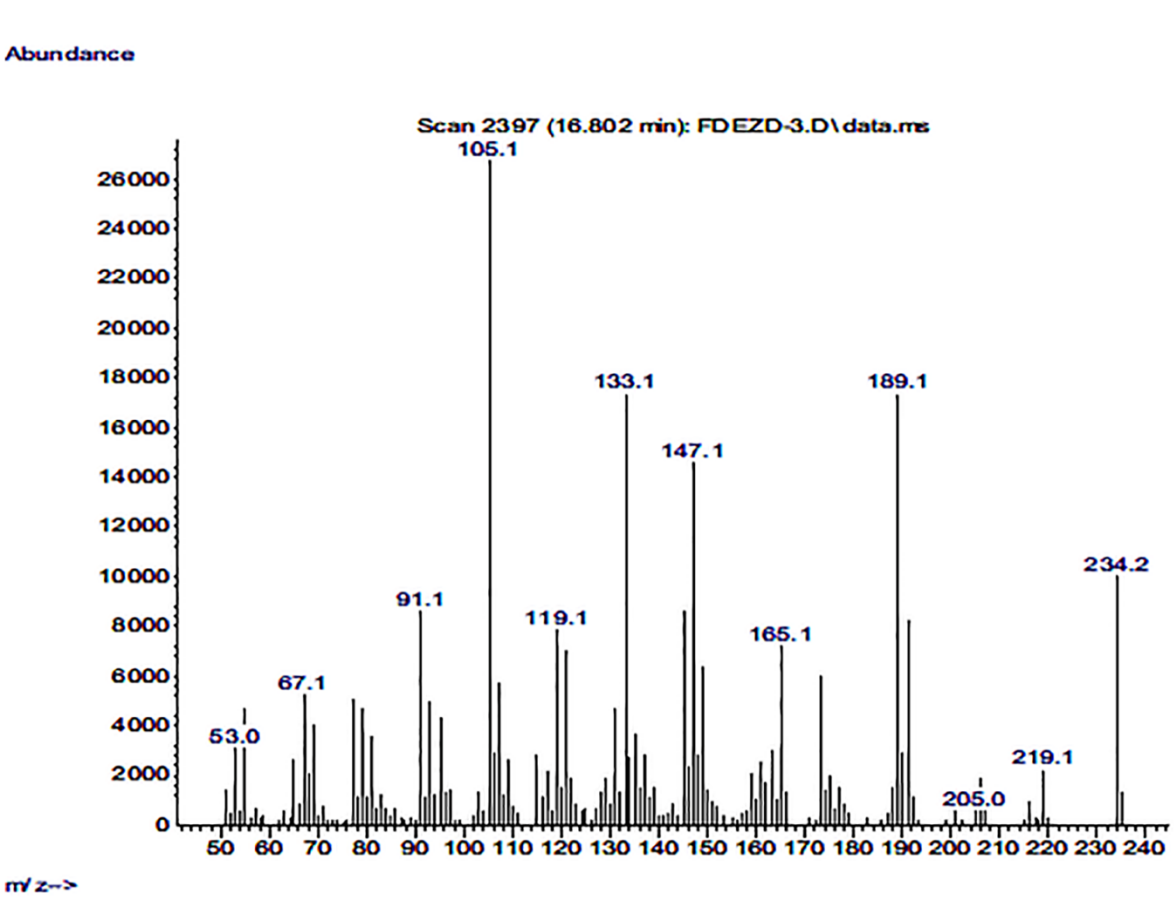


Figure 15S**.** Chemical structure of curcumenol (**4**)



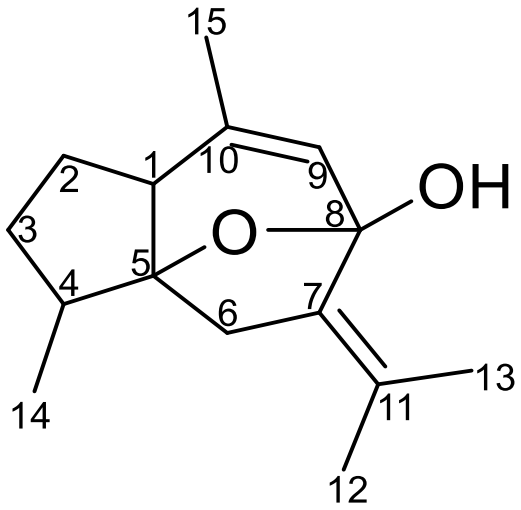
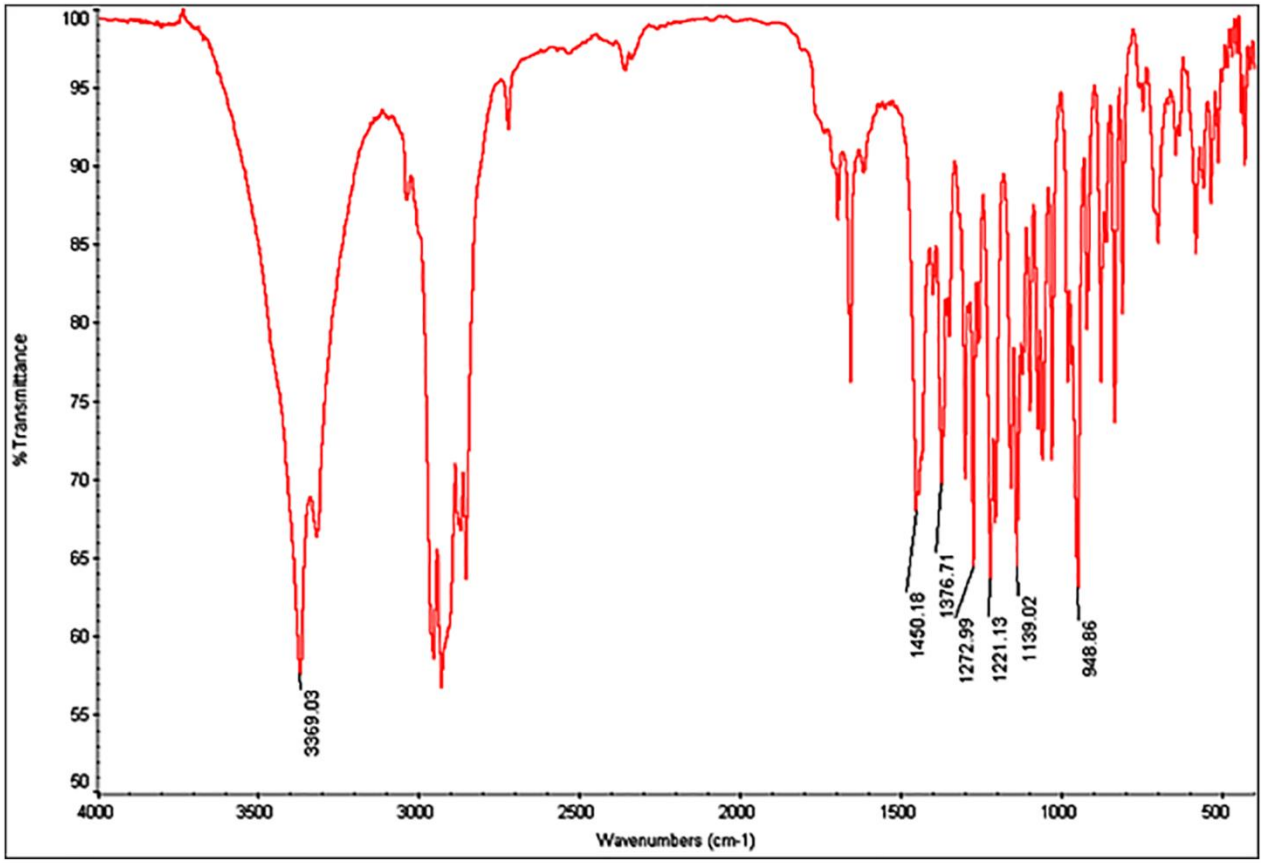


Figure 16S**.** EI-MS chromatogram of curcumenol (**4**)



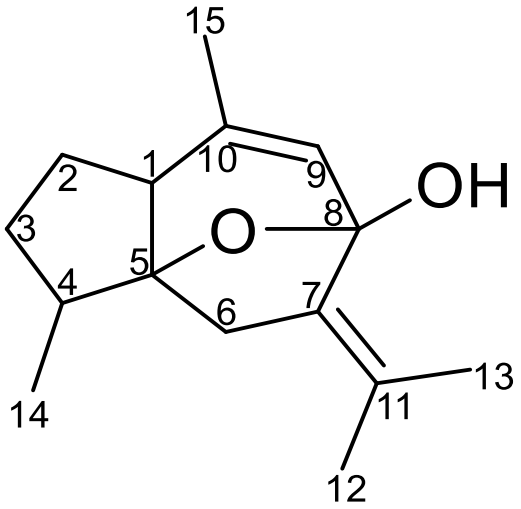
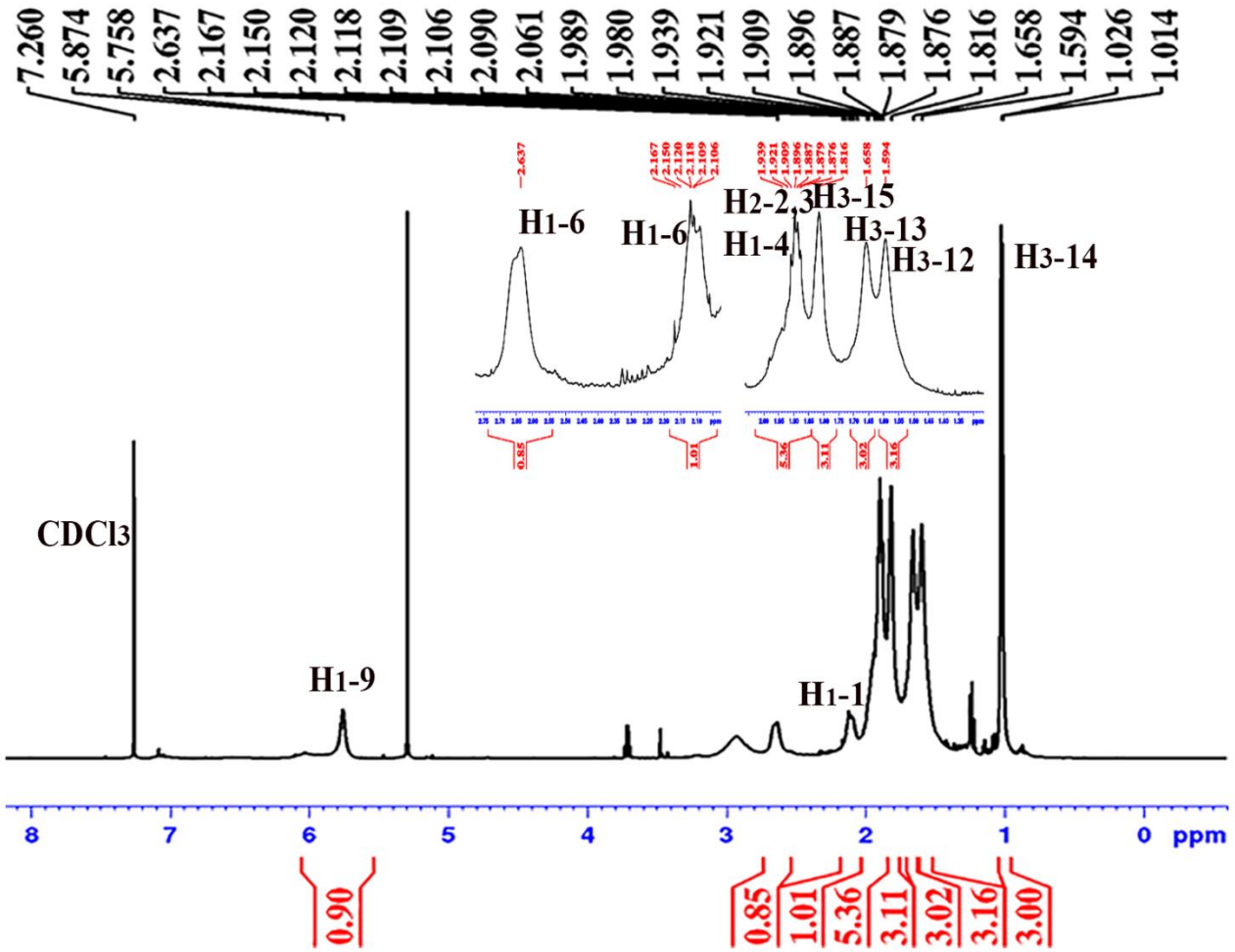


Figure 17S**.** FT-IR spectrum of curcumenol (**4**)



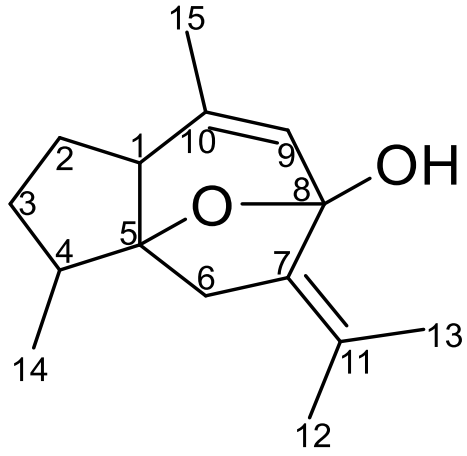
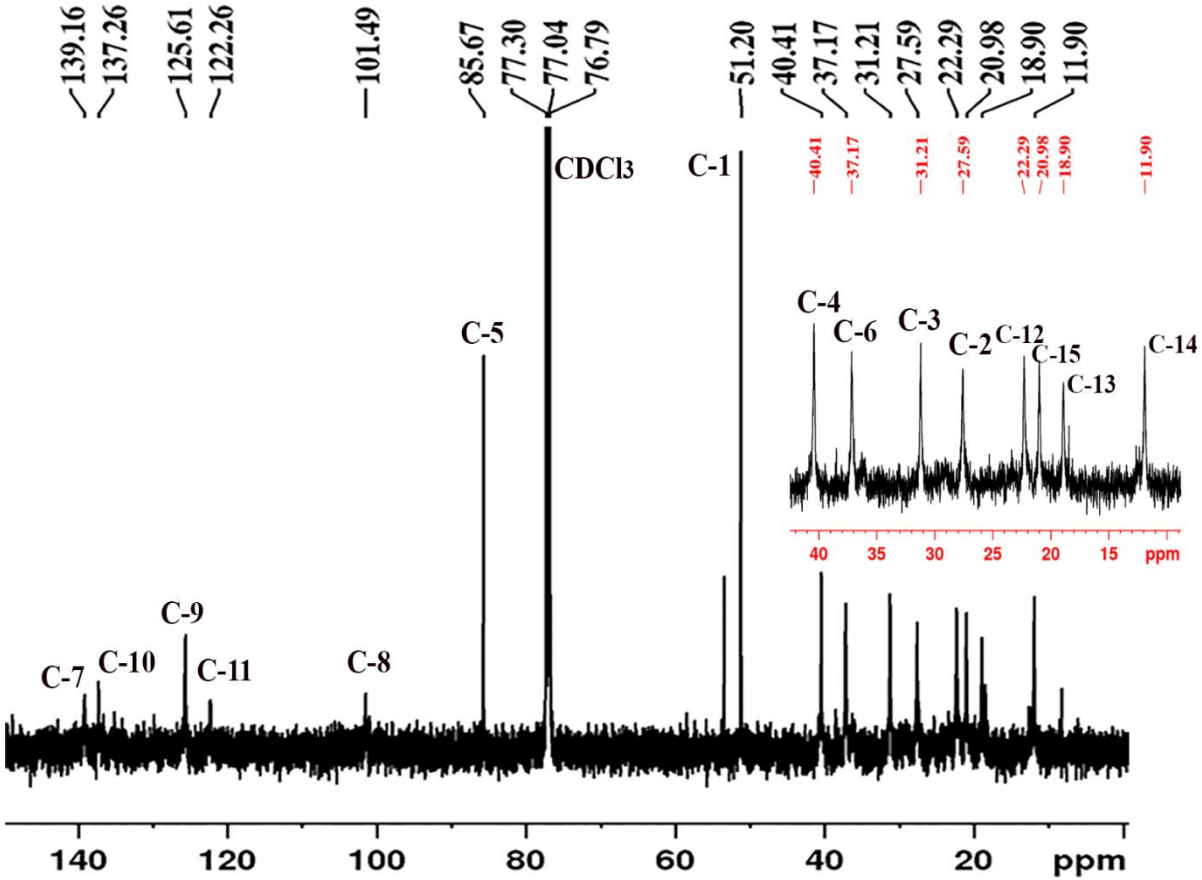


Figure 18S. ^{1}H-NMR spectrum (500 MHz, $CDCl_3$) of curcumenol (**4**)



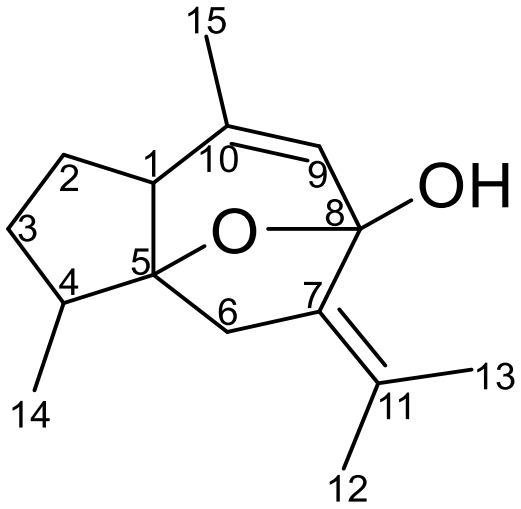


Figure 19S. ^{13}C-NMR spectrum (125 MHz, $CDCl_3$) of curcumenol (**4**)

Zederone (5)

Obtained as colourless crystals. IR ν_{max} (KBr) cm^{-1}: 1661.94; ^{1}H-NMR ($CDCl_3$, 500 MHz), δ 1.24-1.32 (1H, m, H_1-3), 1.33 (3H, s, H_3-14), 1.60 (3H, s, H_3-15), 2.11 (3H, s, H_3-13), 2.21-2.31 (1H, m, H_1-2, H_1-3), 2.50-2.53 (1H, m, H_1-2), 3.66-3.78 (2H, m, H_2-9), 3.81 (1H, s, H_1-5), 5.46-5.49 (1H, m, H_1-1); 7.08 (1H, s, H_1-12), ^{13}C-NMR ($CDCl_3$, 500 MHz),), δ 192.2 (C-6), 157.1 (C-8), 138.1 (C-12), 131.2 (C-1), 131.1 (C-10), 123.3 (C-7), 122.2 (C-11), 66.6 (C-5), 64.0 (C-4), 41.9 (C-9), 38.0 (C-3), 24.7 (C-2), 15.7 (C-15), 15.2 (C-14), 10.3 (C-13). EI-MS, m/z (%): 246.1 $[M]^+$ (36), 175.1 (100), 122.0 (71), 91.0 (36), 65.1 (21).

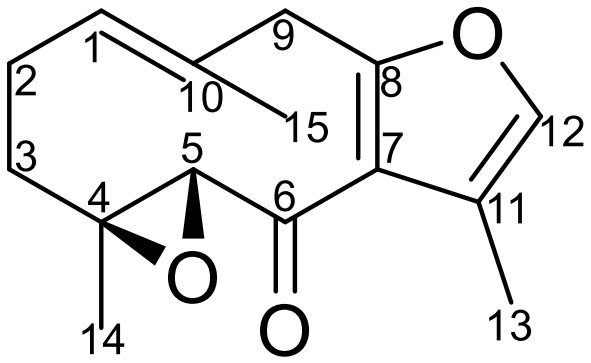


Figure 20S**.** Chemical structure of zederone (**5**)

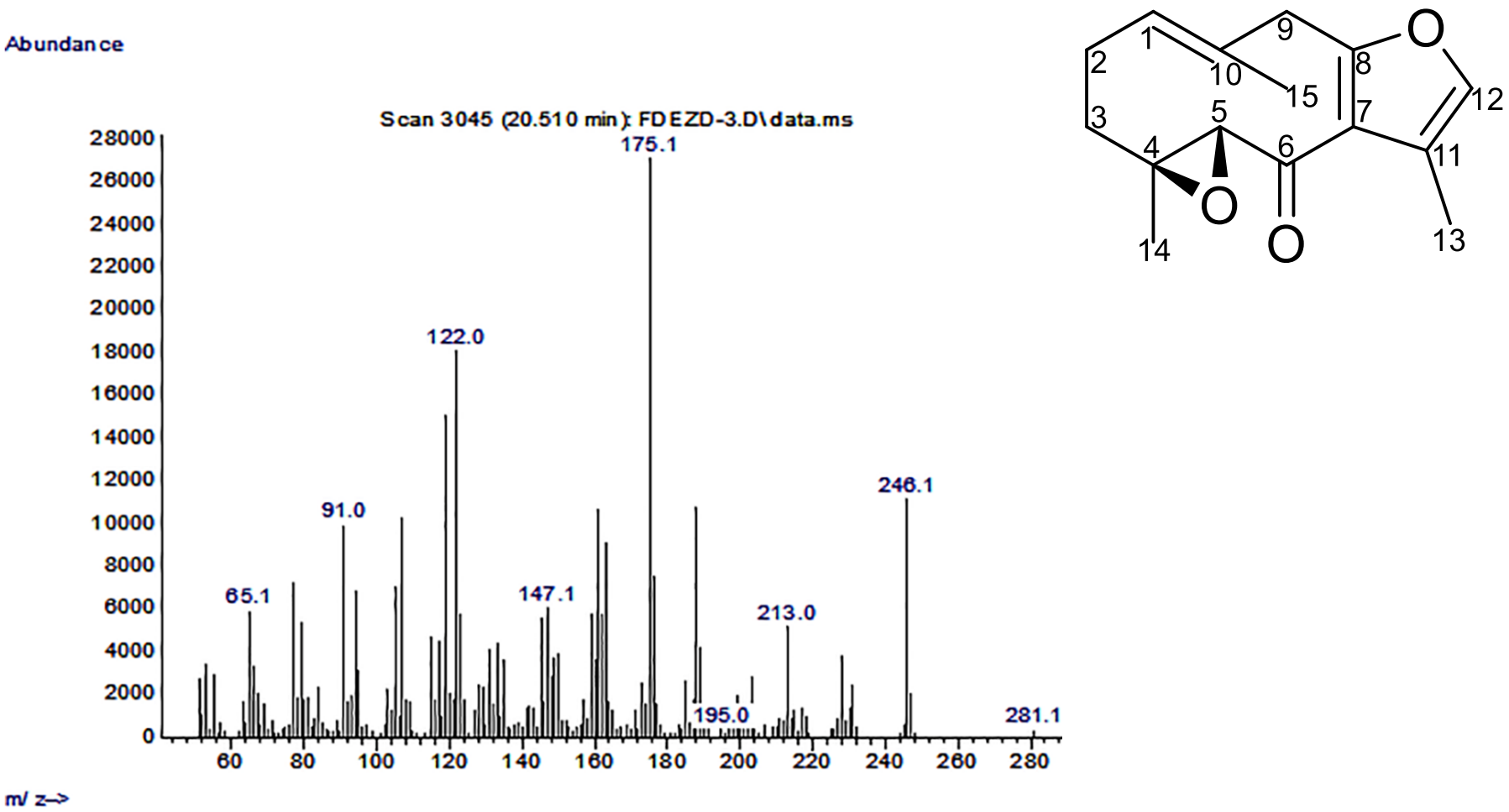
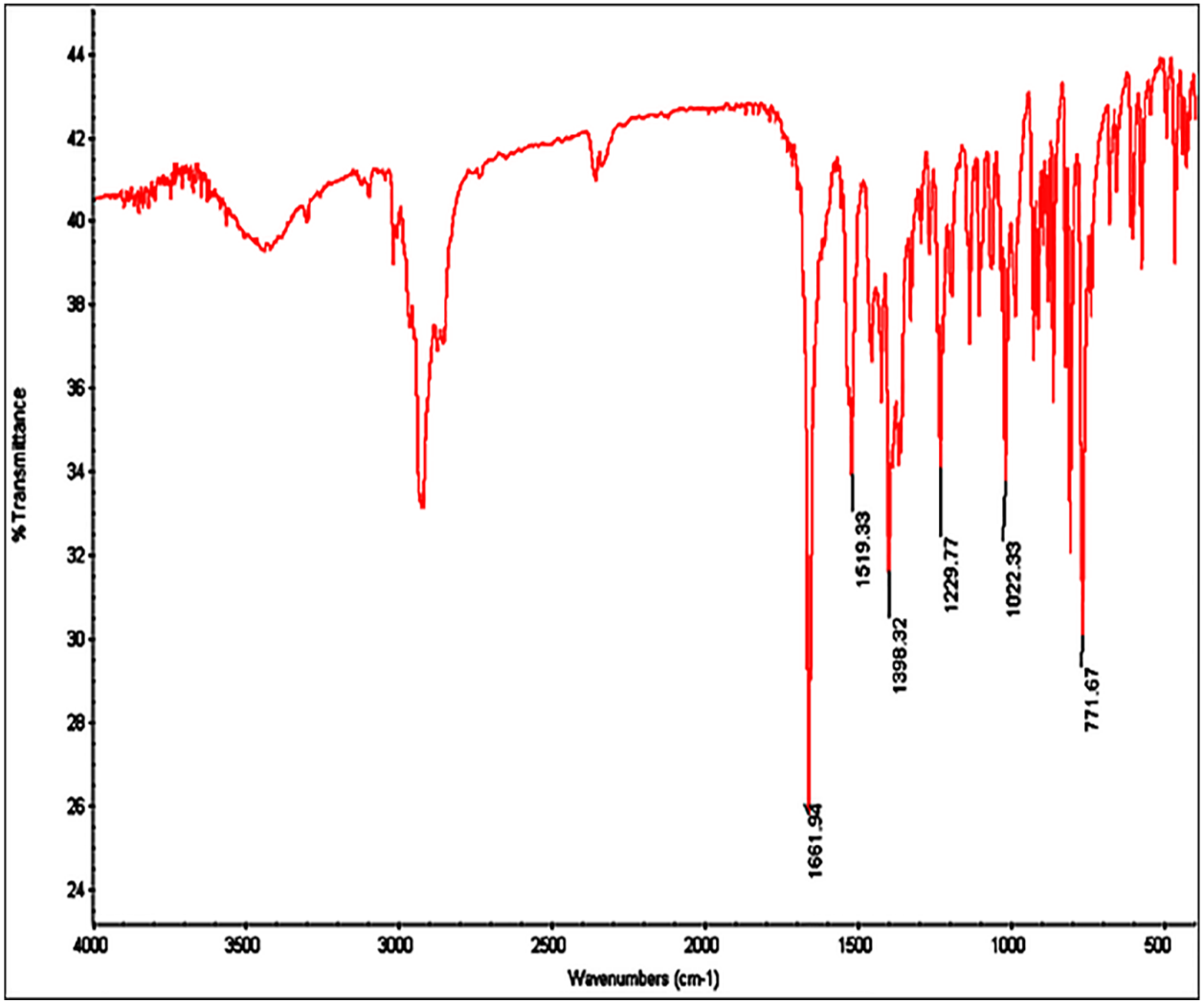


Figure 21S**.** EI-MS chromatogram of zederone (**5**)



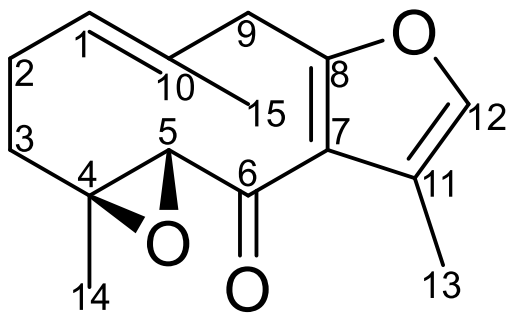
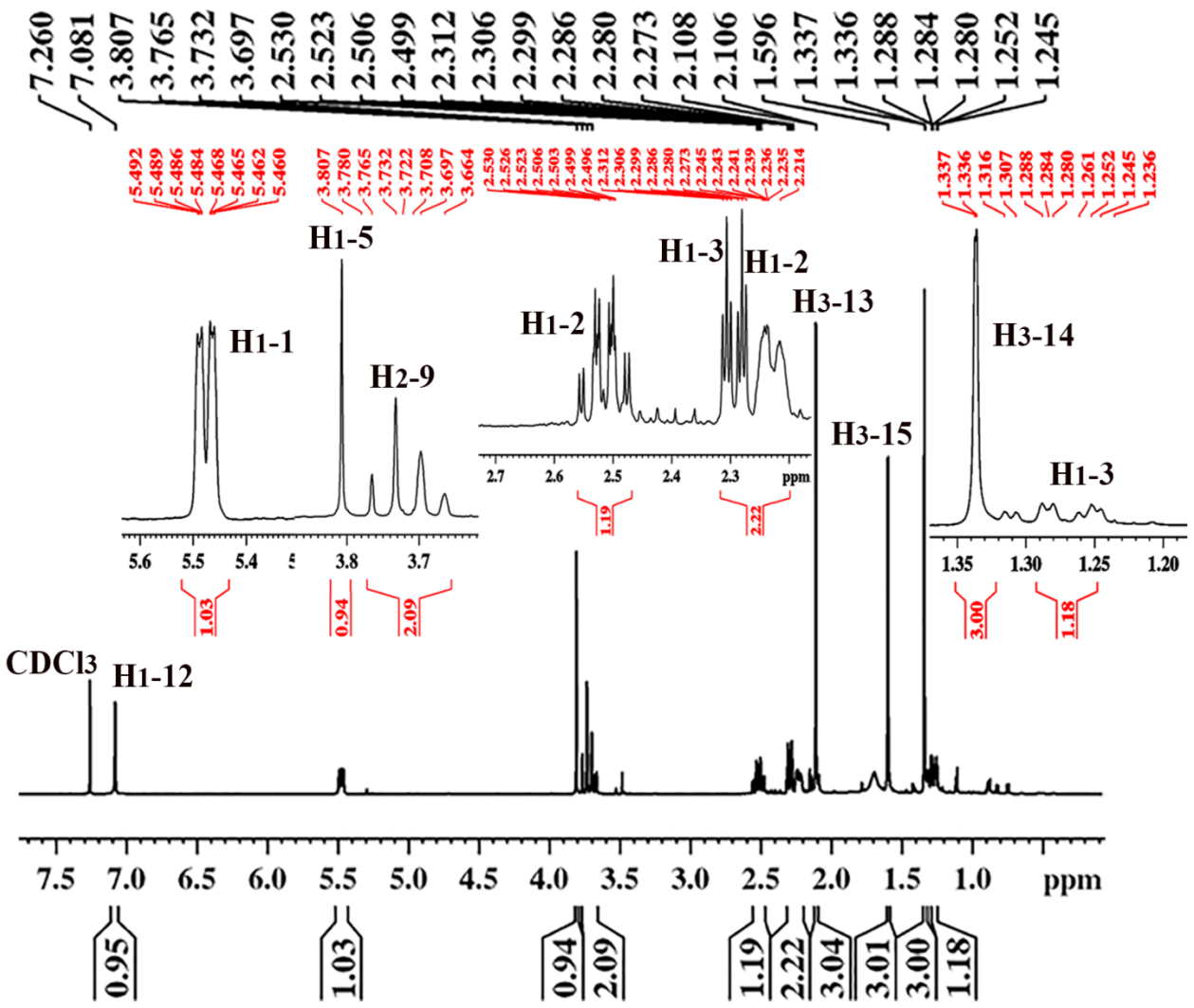


Figure 22S**.** FT-IR spectrum of zederone (**5**)



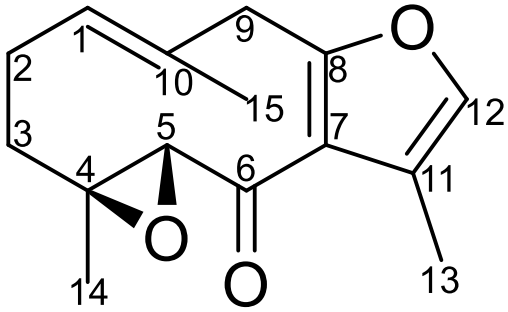
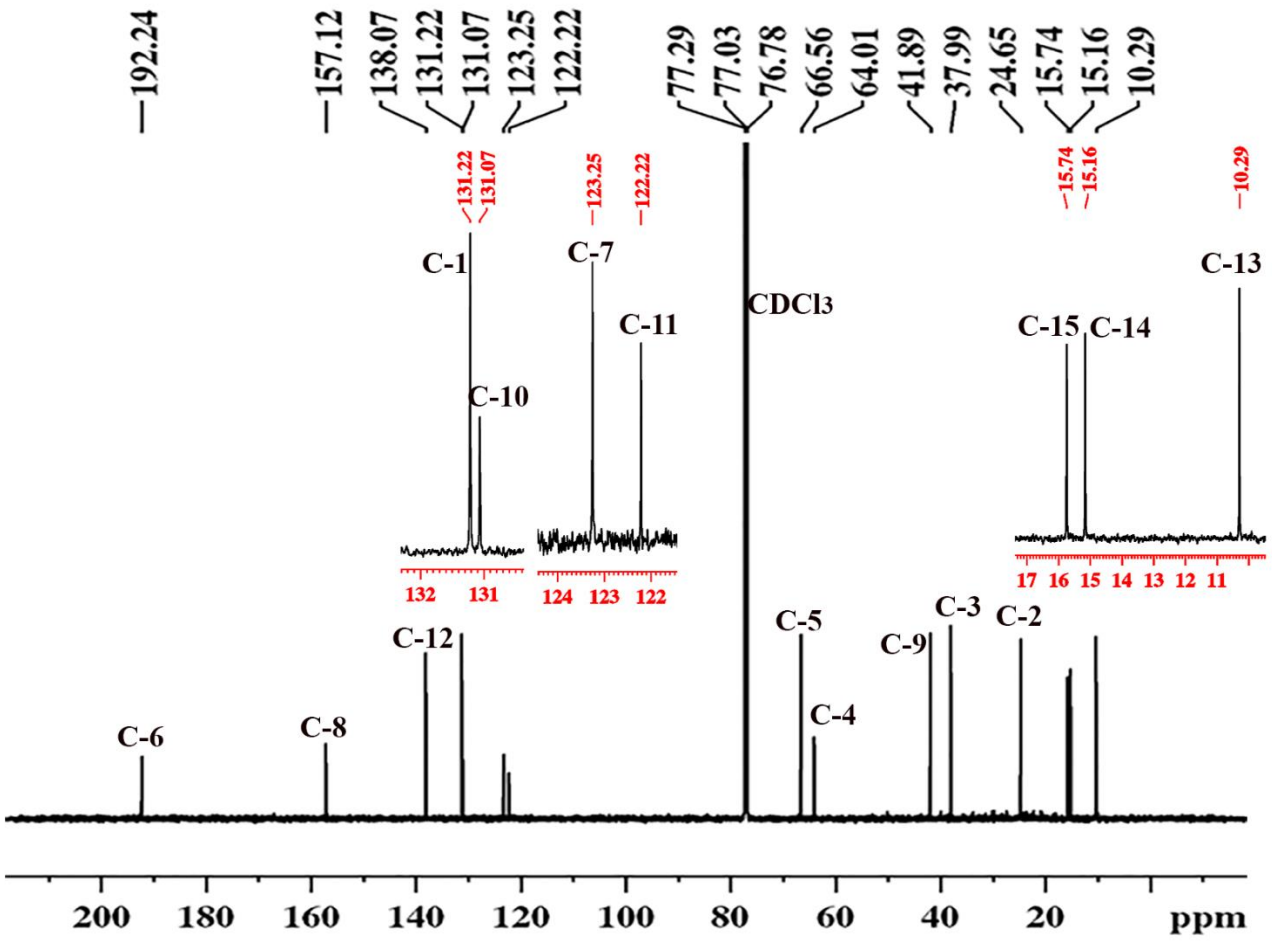


Figure 23S. ^{1}H-NMR spectrum (500 MHz, $CDCl_3$) of zederone (**5**)



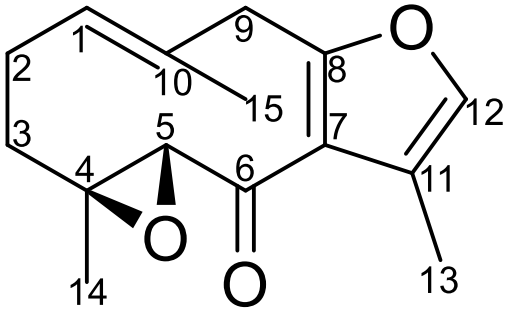


Figure 24S. ^{13}C-NMR spectrum (125 MHz, $CDCl_3$) of zederone (**5**)

Comosone II (6)

Obtained as colorless solid; IR ν_{max} (KBr) cm^{-1}: 1657.62; ^{1}H-NMR ($CDCl_3$, 500 MHz): δ 1.57 (3H, s, H_3-15), 1.75-1.82 (3H, m, H_1-2, H_2-3), 1.86 (3H, s, H_3-13), 1.92 (3H, s, H_3-14), 2.05 (3H, s, H_3-12), 2.18-2.21 (1H, m, H_1-2), 2.73 (1H, br. s, H_1-1), 3.75 (1H, br. s, H_1-6), 4.91 (1H, br. s, H_1-5), 5.89 (1H, s, H_1-9); ^{13}C NMR ($CDCl_3$, 125 MHz) δ: 191.8 (C-8), 158.4 (C-10), 141.7 (C-11), 135.0 (C-4), 133.5 (C-7), 130.8 (C-9), 122.0 (C-5), 39.8 (C-6), 38.3 (C-1), 26.0 (C-3), 25.3 (C-2), 23.4 (C-15), 23.0 (C-12), 21.8 (C-13), 20.8 (C-14); EI-MS, m/z (%): 216.1 $[M]^+$ (100), 201.1 (61), 159.1 (90), 105.1 (56), 77.1 (36). EI-MS, m/z (%): 216.1 $[M]^+$ (100), 201.1 (62), 150.1 (90), 105.1 (56), 77.1 (36).

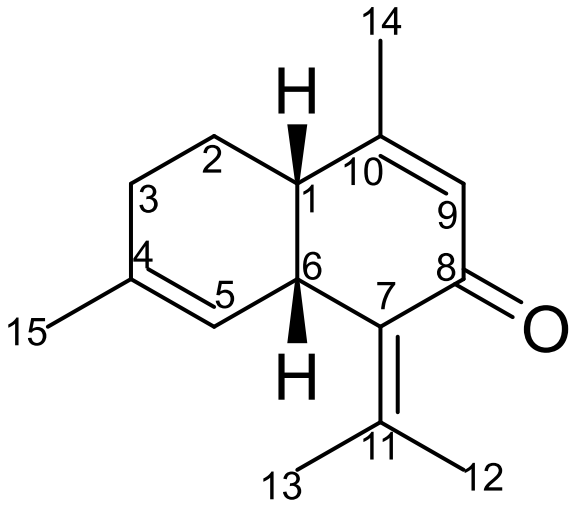
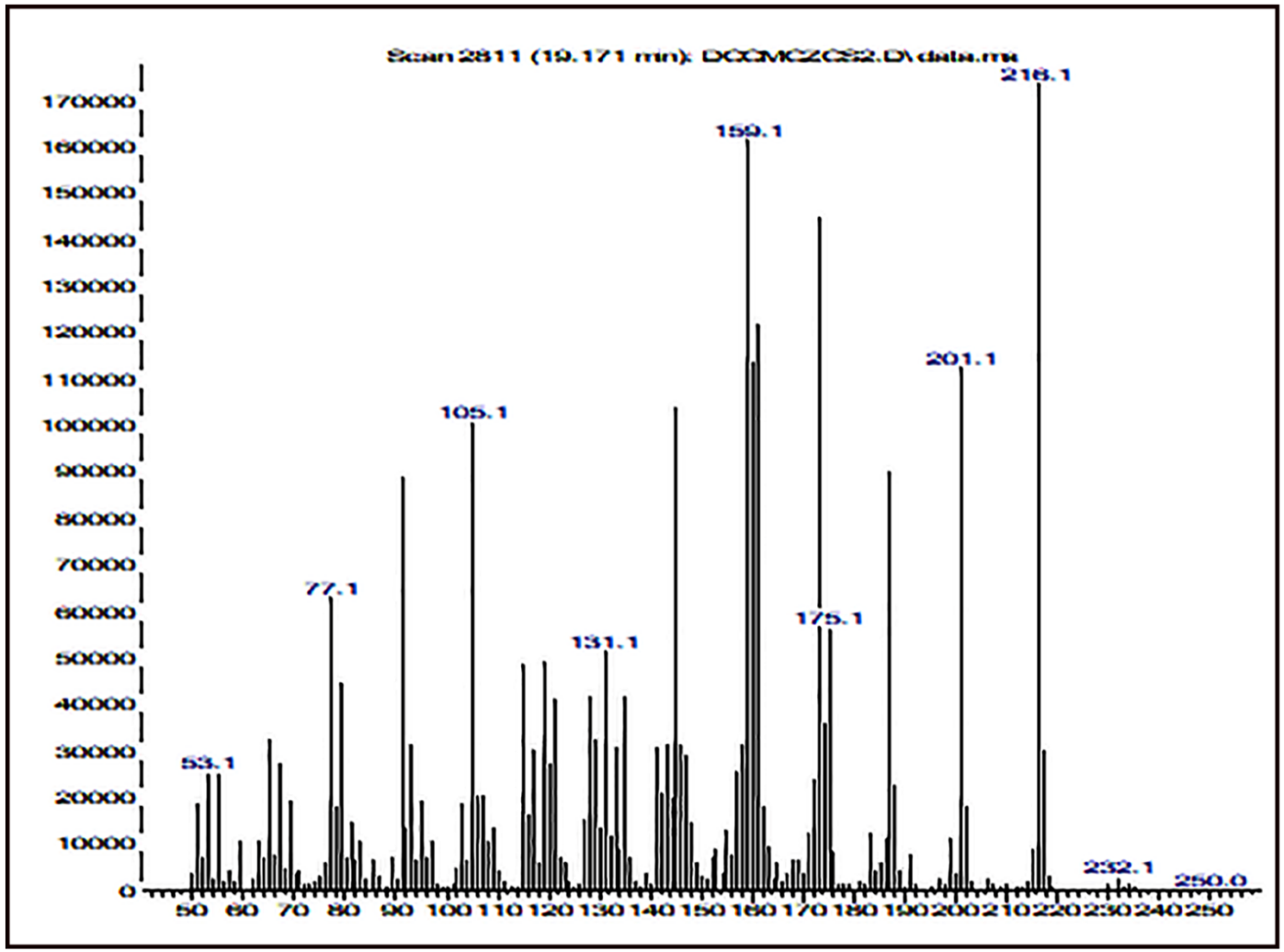


Figure 25S**.** Chemical structure of comosone II (**6**)



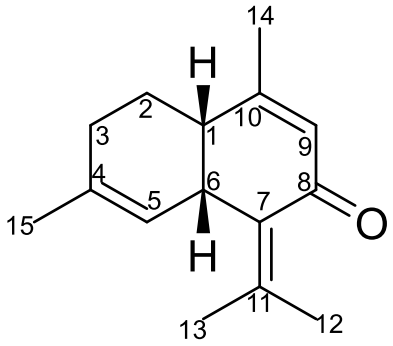
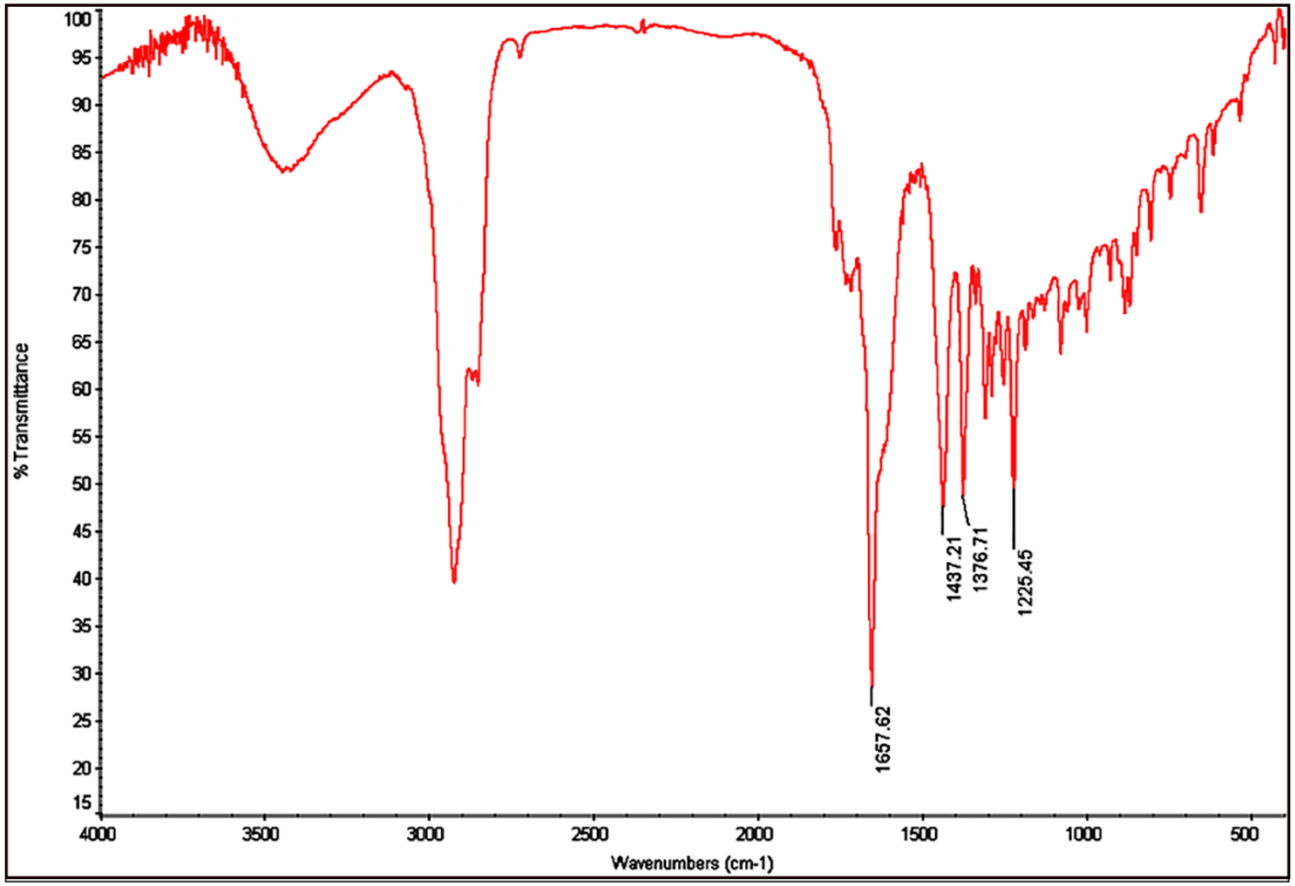


Figure 26S**.** EI-MS chromatogram of comosone II (**6**).



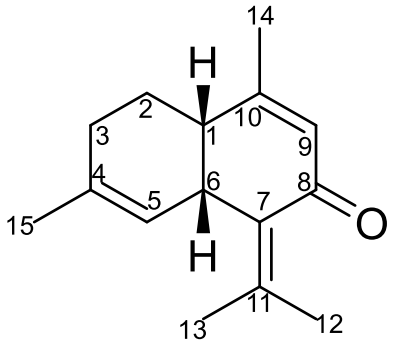
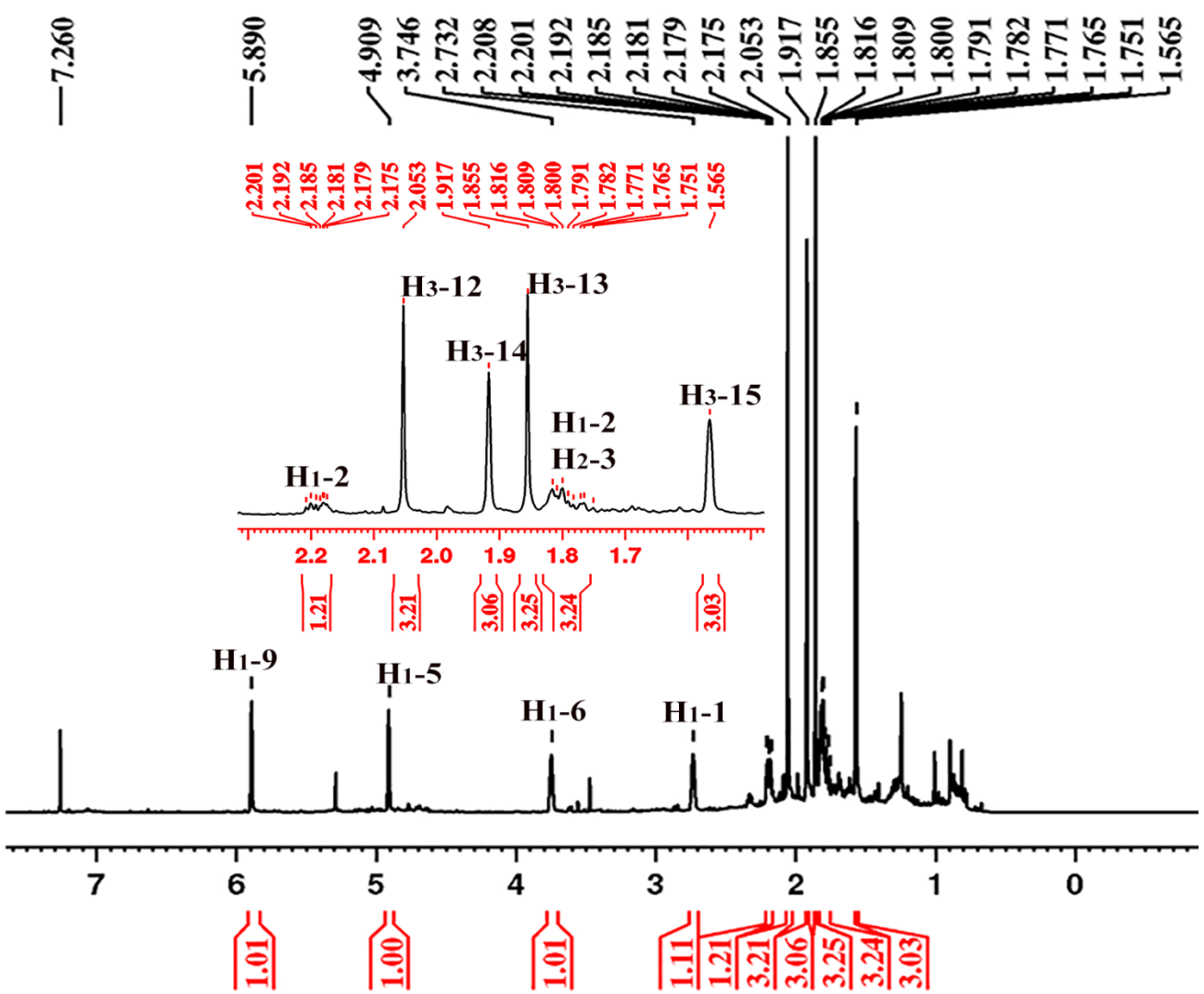


Figure 27S. FT-IR spectrum of comosone II (**6**).



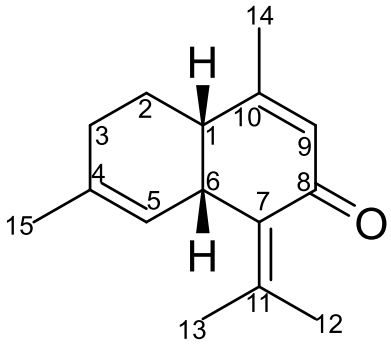
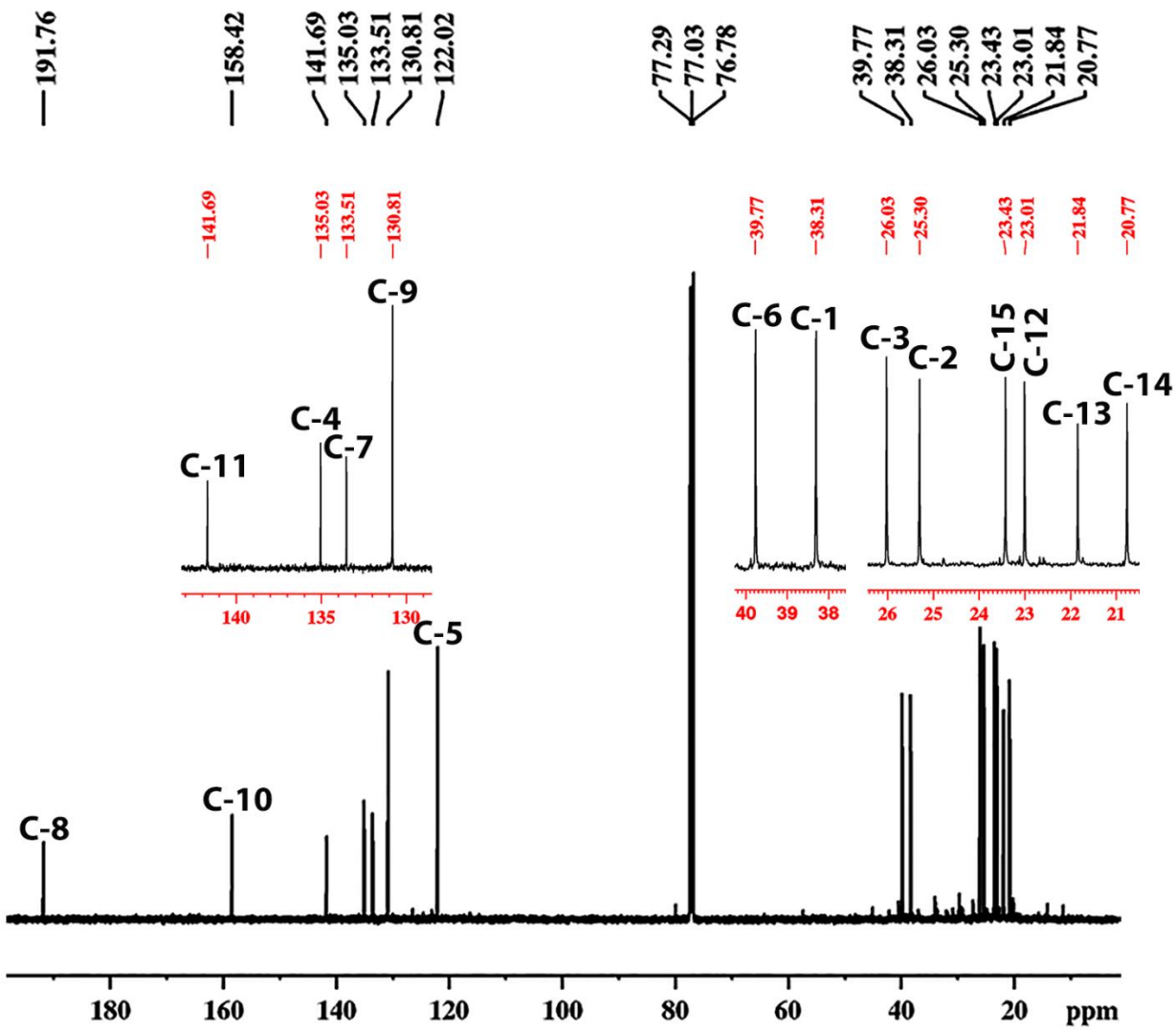


Figure 28S. ^{1}H-NMR spectrum (500 MHz, $CDCl_3$) of comosone II (**6**).



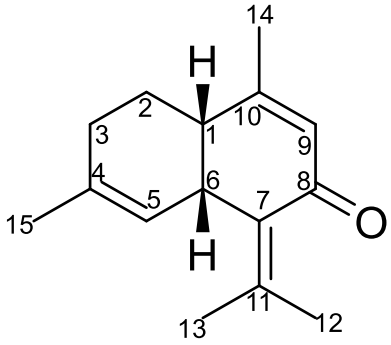


Figure 29S. ^{13}C-NMR spectrum (500 MHz, $CDCl_3$) of comosone II (**6**).

(1*E*,4*E*,8*R*)-8-hydroxygermacra-1(10),4,7(11)-trieno-12,8-lactone (7)

Obtained as colorless solid; ^{1}H-NMR ($CDCl_3$, 500 MHz): δ 1.62 (6H, s, H_3-14 & H_3-15), 1.86 (3H, s, H_3-13), 1.89-1.94 (1H, m, H_1-6), 2.08-2.11 (1H, m, H_1-2), 2.23-2.29 (2H, m, H_1-2 & H_1-6), 2.41 (1H, d, *J* = 14.0 Hz, H_1-9), 3.03-3.09 (2H, m, H_1-3 & H_1-9), 3.19 (1H, d, *J* = 14.0 Hz, H_1-3), 4.27 (1H, d, *J* = 10.5 Hz, H_1-5), 4.80 (1H, d, J = 11.5 Hz, H_1-1). ^{13}C NMR ($CDCl_3$, 125 MHz) δ: 171.2 (C-12), 161.8 (C-7), 134.3 (C-4), 132.8 (C-10), 132.0 (C-1), 127.7 (C-11), 123.4 (C-5), 109.2 (C-8), 51.6 (C-9), 38.4 (C-6), 25.7 (C-2), 25.3 (C-3), 17.4 (C-15), 16.9 (C-14), 8.8 (C-13).

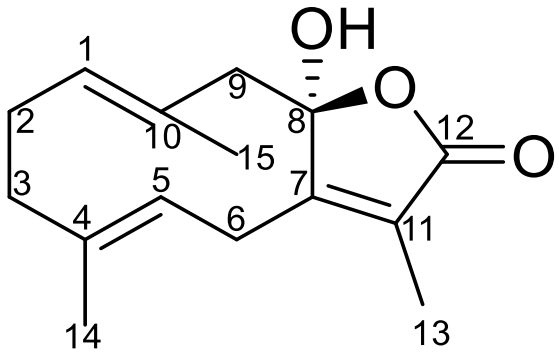
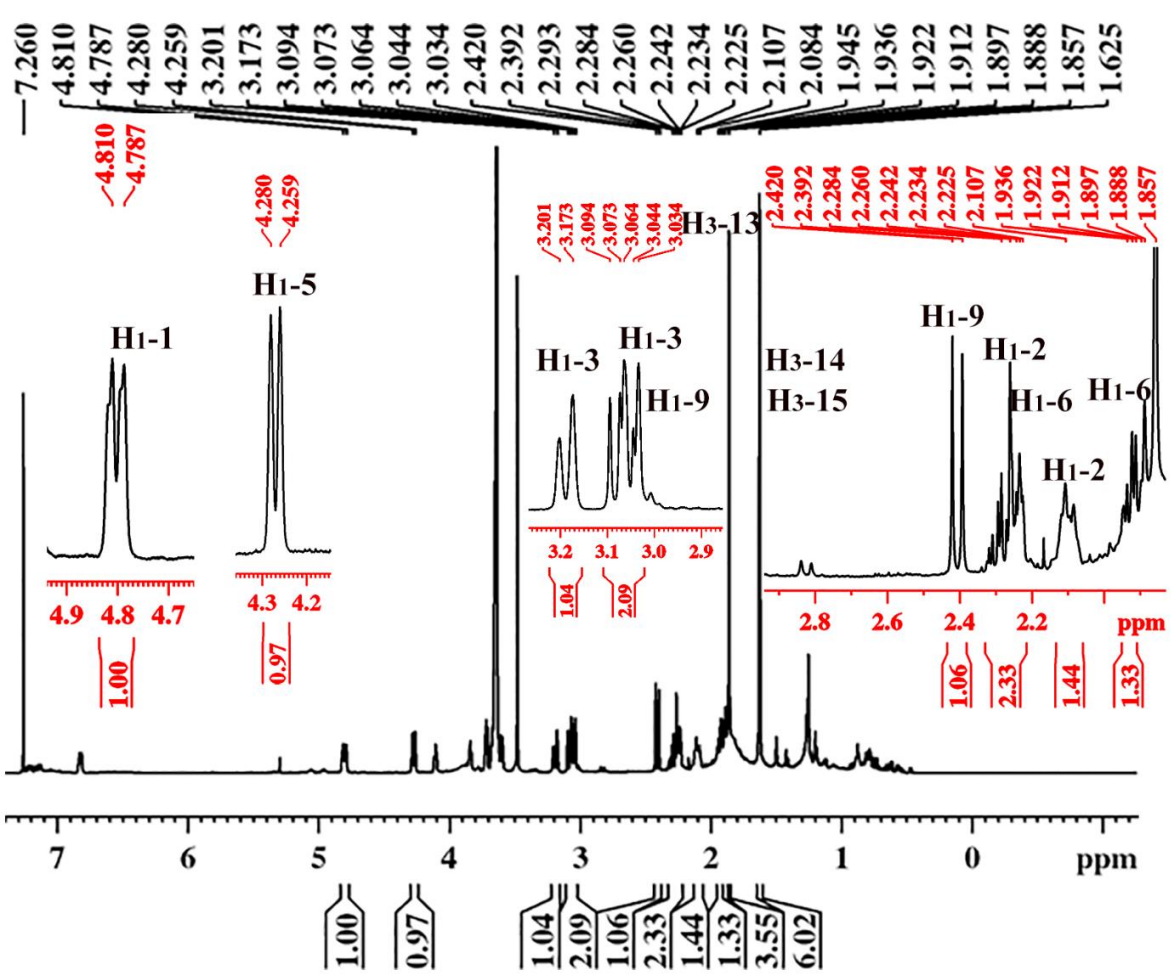


Figure 30S**.** Chemical structure of (1*E*,4*E*,8*R*)-8-hydroxygermacra-1(10),4,7(11)-trieno-12,8-lactone (**7**)



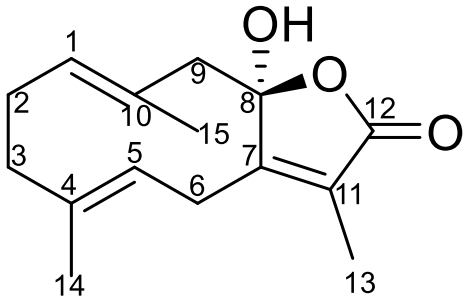
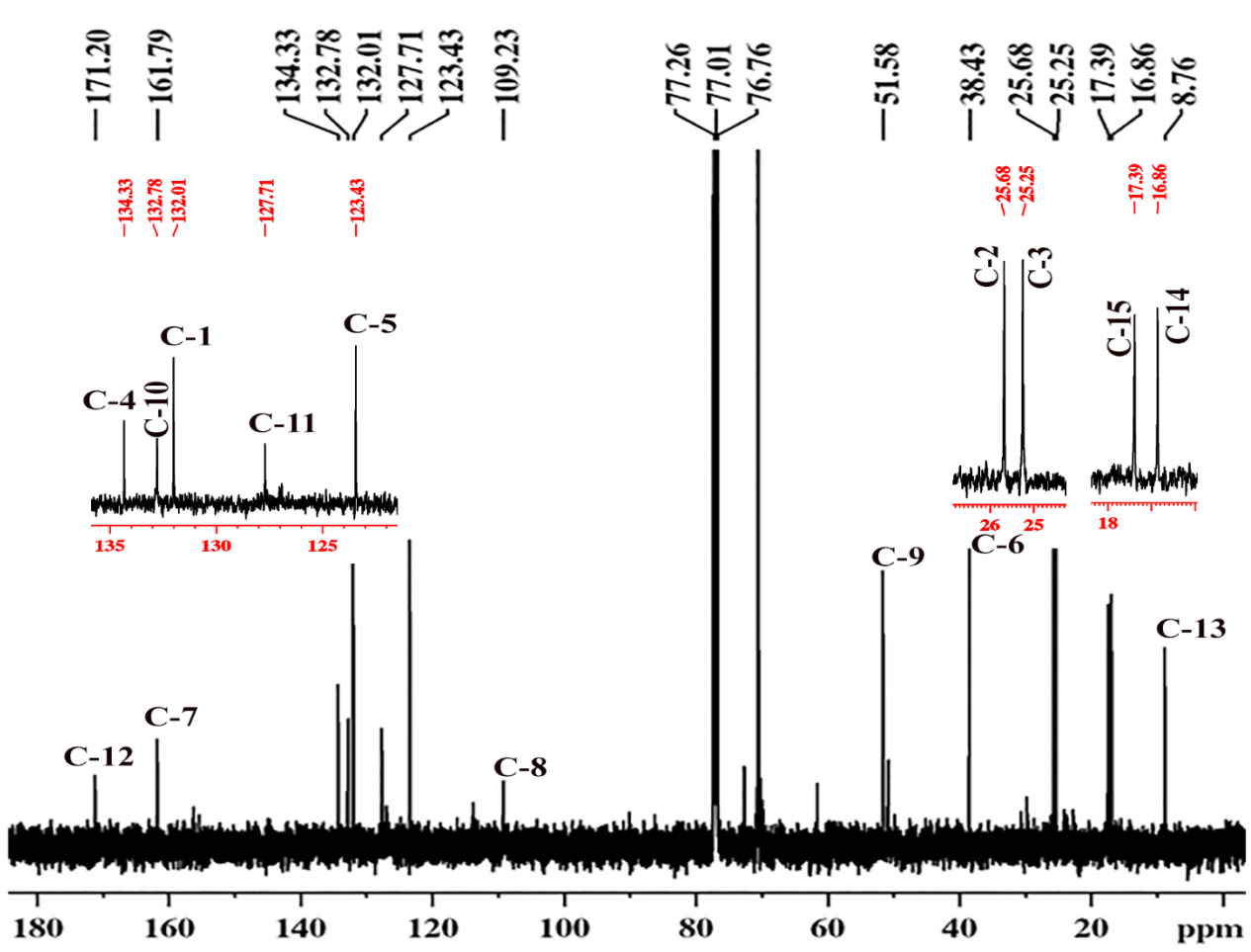


Figure 31S. ^{1}H-NMR spectrum (500 MHz, $CDCl_3$) of (1*E*,4*E*,8*R*)-8-hydroxygermacra-1(10),4,7(11)-trieno-12,8-lactone (**7**)



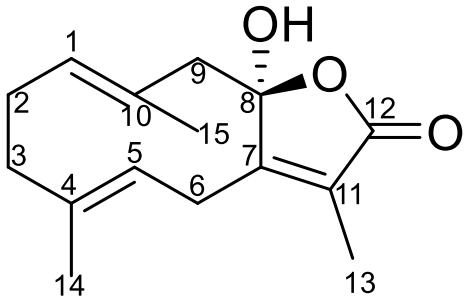


Figure 32S. ^{13}C-NMR spectrum (500 MHz, $CDCl_3$) of (1*E*,4*E*,8*R*)-8-hydroxygermacra-1(10),4,7(11)-trieno-12,8-lactone (**7**)

13-hydroxygermacrone (8)

Obtained as colorless solid; ^{1}H-NMR ($CDCl_3$, 500 MHz): δ 1.42 (3H, s, H_3-14), 1.62 (3H, s, H_3-15), 1.81 (3H, s, H_3-12), 2.04-2.18 (4H, m, H_2-2, H_2-3), 2.91-2.98 (3H, m, H_2-6, H_1-9), 3.43 (1H, d, *J* = 10.5 Hz, H_1-9), 4.18 (1H, d, *J* = 12.0 Hz, H_1-13), 4.29 (1H, d, *J* = 12.5 Hz, H_1-13), 4.66 (1H, d, *J* = 14.0 Hz, H_1-5), 4.98 (1H, d, *J* = 10.5 Hz, H_1-1); ^{13}C NMR ($CDCl_3$, 125 MHz) δ: 207.1 (C-8), 139.8 (C-11), 135.7 (C-4), 133.1 (C-1), 131.3 (C-7), 126.4 (C-10), 125.0 (C-5), 62.8 (C-13), 55.5 (C-9), 38.1(C-3), 28.6 (C-6), 24.1 (C-2), 17.8 (C-12), 16.6 (C-15), 15.6 (C-14).

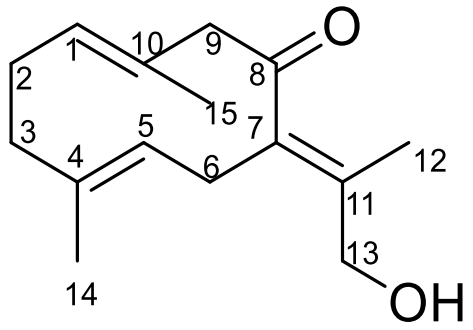


Figure 33S**.** Chemical structure of 13-hydroxygermacrone (**8**)

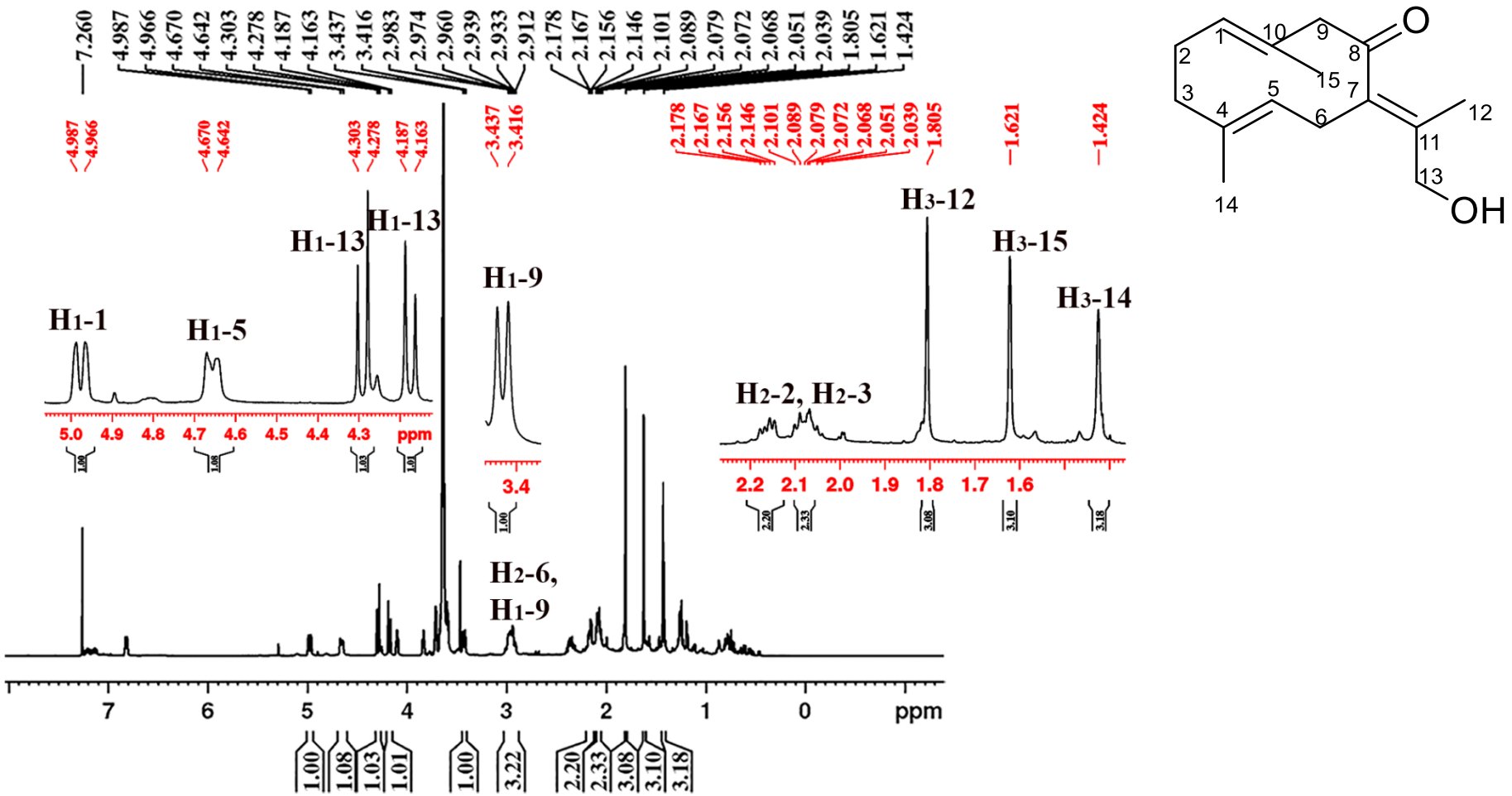
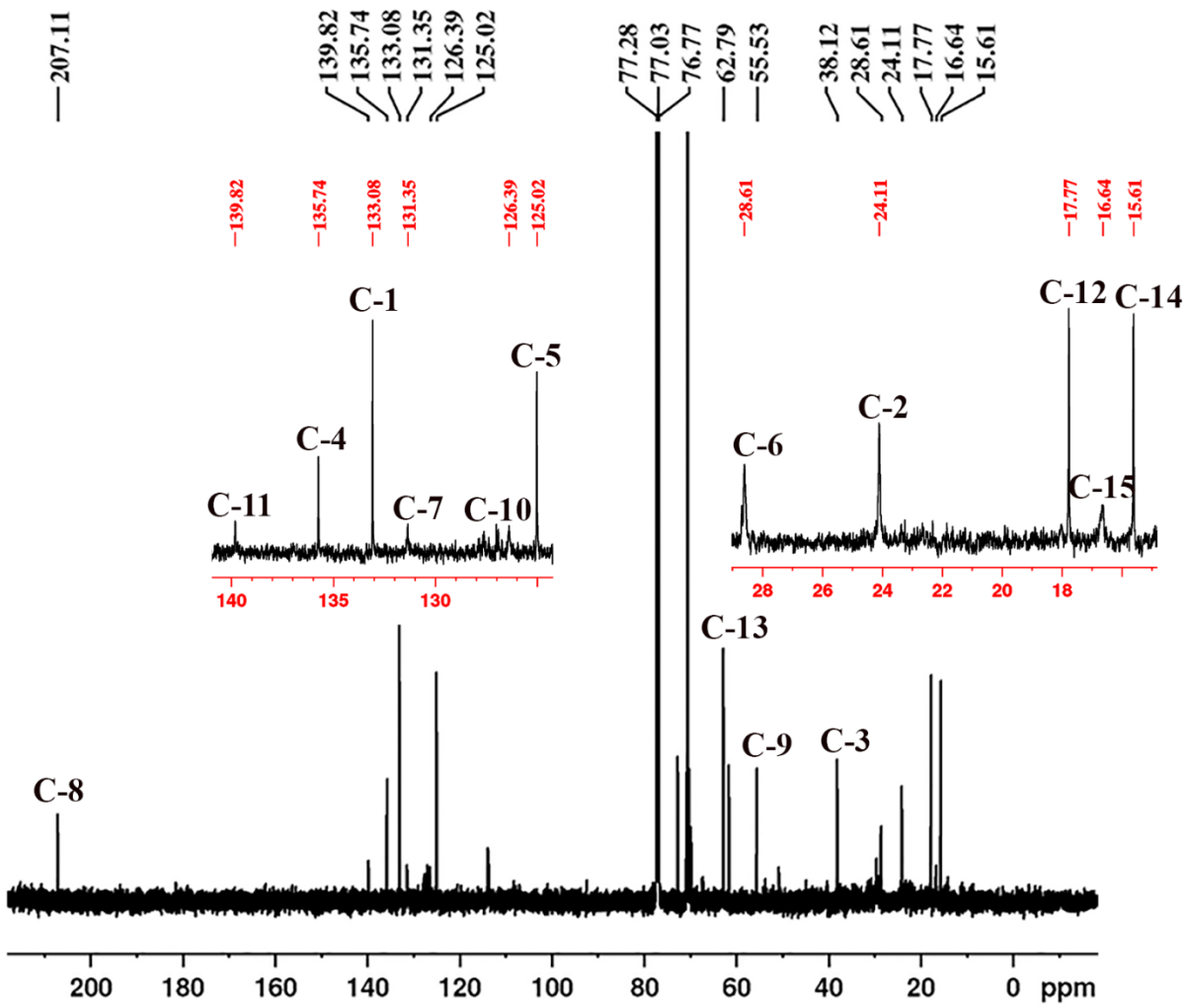


Figure 34S. ^{1}H-NMR spectrum (500 MHz, $CDCl_3$) of 13-hydroxygermacrone (**8**)



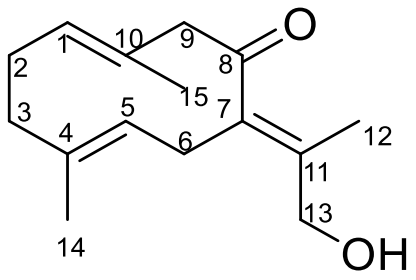


Figure 35S. ^{13}C-NMR spectrum (125 MHz, $CDCl_3$) of 13-hydroxygermacrone (**8**)

Furanodienone 1,10-epoxide (9):

Obtained as colorless solid; IR ν_{max} (KBr) cm^{-1}: 1657.00, 1622.42; ^{1}H-NMR ($CDCl_3$, 500 MHz): δ 1.02 (3H, s, H_3-15), 1.30-1.42 (1H, m, H_α-2), 2.01 (3H, s, H_3-14), 2.18 (3H, s, H_3-13), 2.19-2.23 (2H, m, H_β-2), 2.31-2.42 (2H, m, H_2-3), 2.72 (1H, d, *J* = 17.0 Hz, H_β-9), 2.96 (1H, dd, *J* = 2.5, 11.0 Hz, H_β-1), 3.59 (1H, d, *J* = 17.0 Hz, H_α-9), 6.28 (1H, s, H_β-5), 7.06 (1H, s, H_α-12); ^{13}C NMR ($CDCl_3$, 125 MHz) δ: 189.0 (C-6), 155.7 (C-8), 149.8 (C-4), 138.2 (C-12), 129.1 (C-5), 124.0 (C-7), 122.5 (C-11), 69.9 (C-1), 58.9 (C-10), 40.2 (C-9), 35.6 (C-3), 24.4 (C-2), 19.7 (C-14), 16.6 (C-15), 9.9 (C-13). HRESIMS m/z 247.1327 $[M + H]^+$ (calcd for $C_{15}H_{18}O_3H^+$ 247.1328). EI-MS, m/z (%): 246.1 $[M]^+$ (13), 217.1 (100), 163.1 (82), 122.0 (77), 94.1 (32), 55.1 (26).

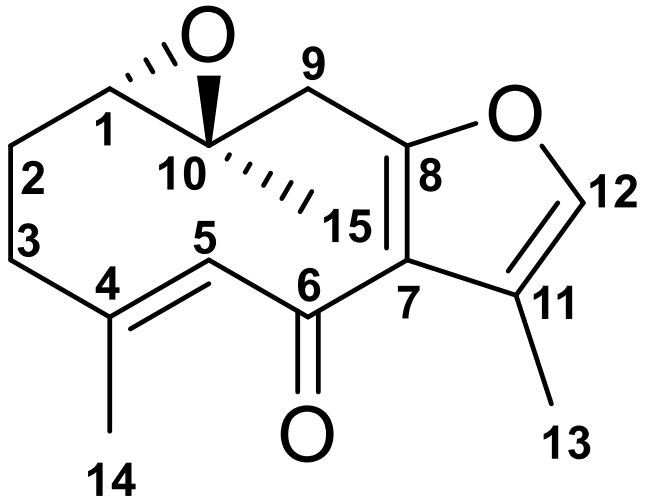
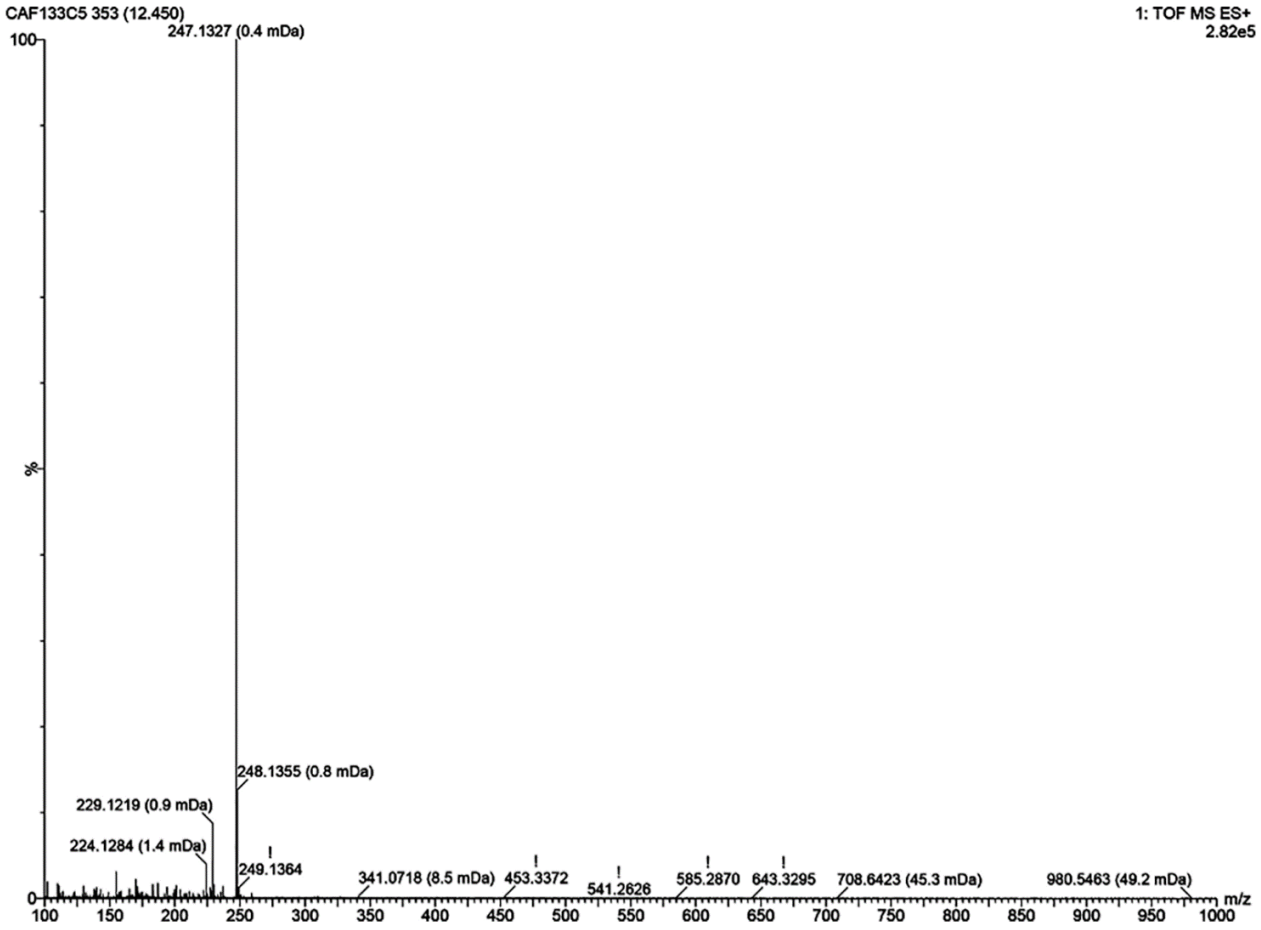


Figure 36S**.** Chemical structure of furanodienone 1,10-epoxide (**9**)



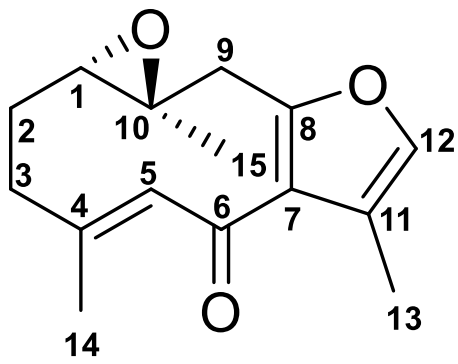
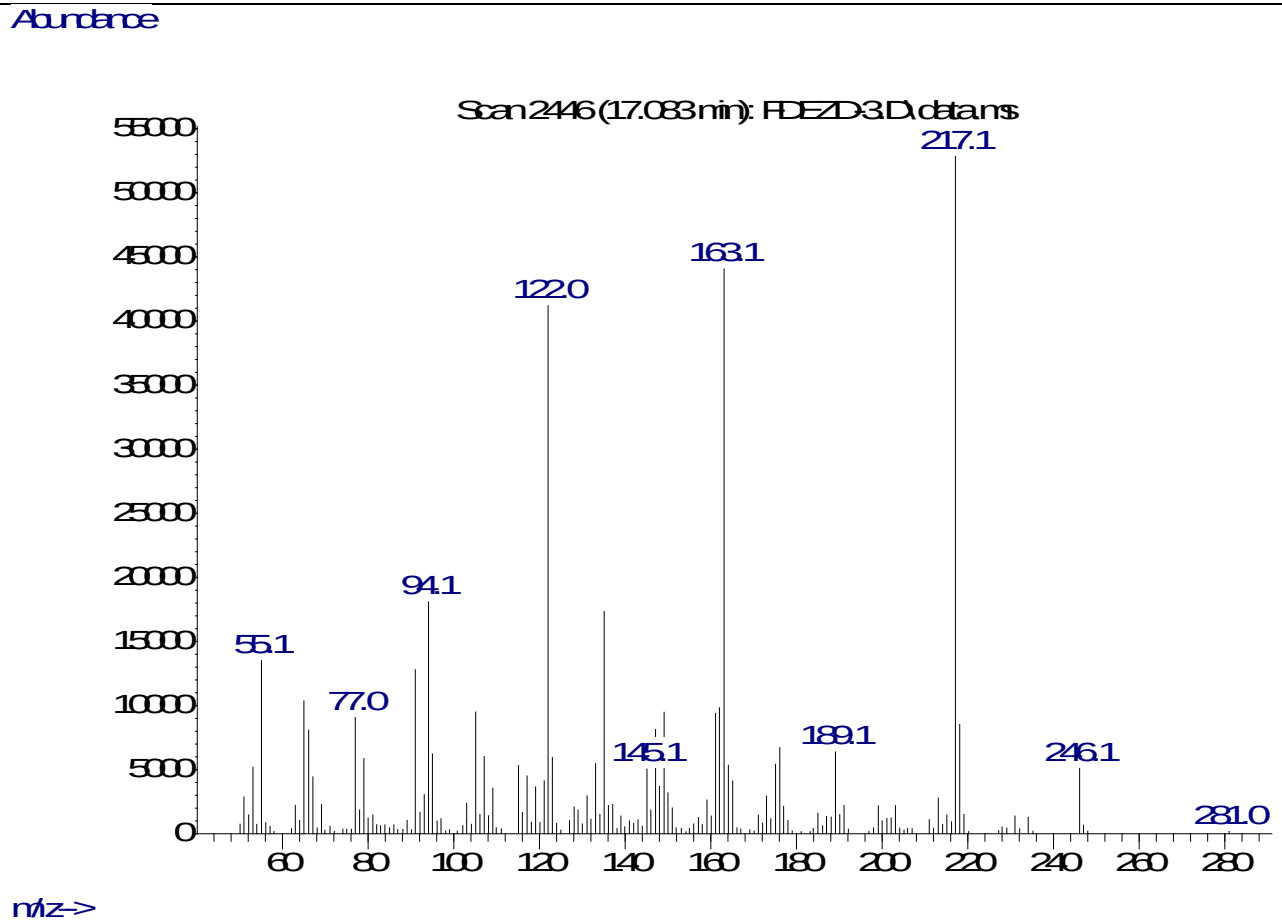


Figure 37S**.** HR-EIMS spectrum of furanodienone 1,10-epoxide (**9**)



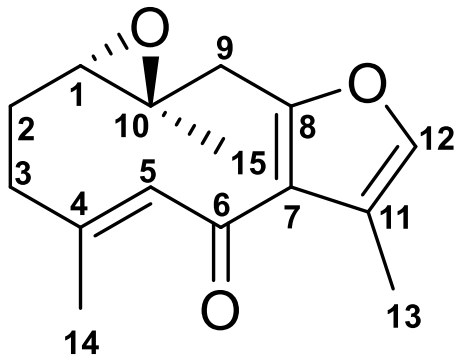
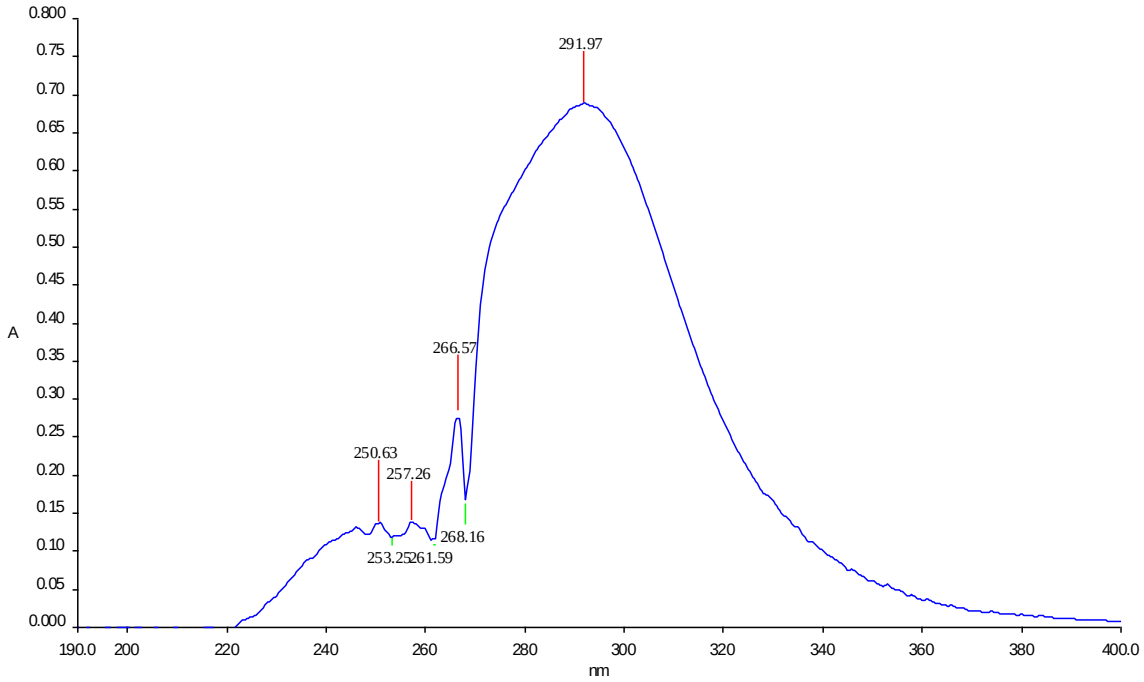


Figure 38S**.** EI-MS spectrum of furanodienone 1,10-epoxide (**9**)



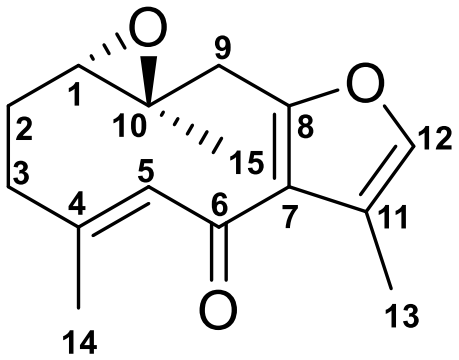
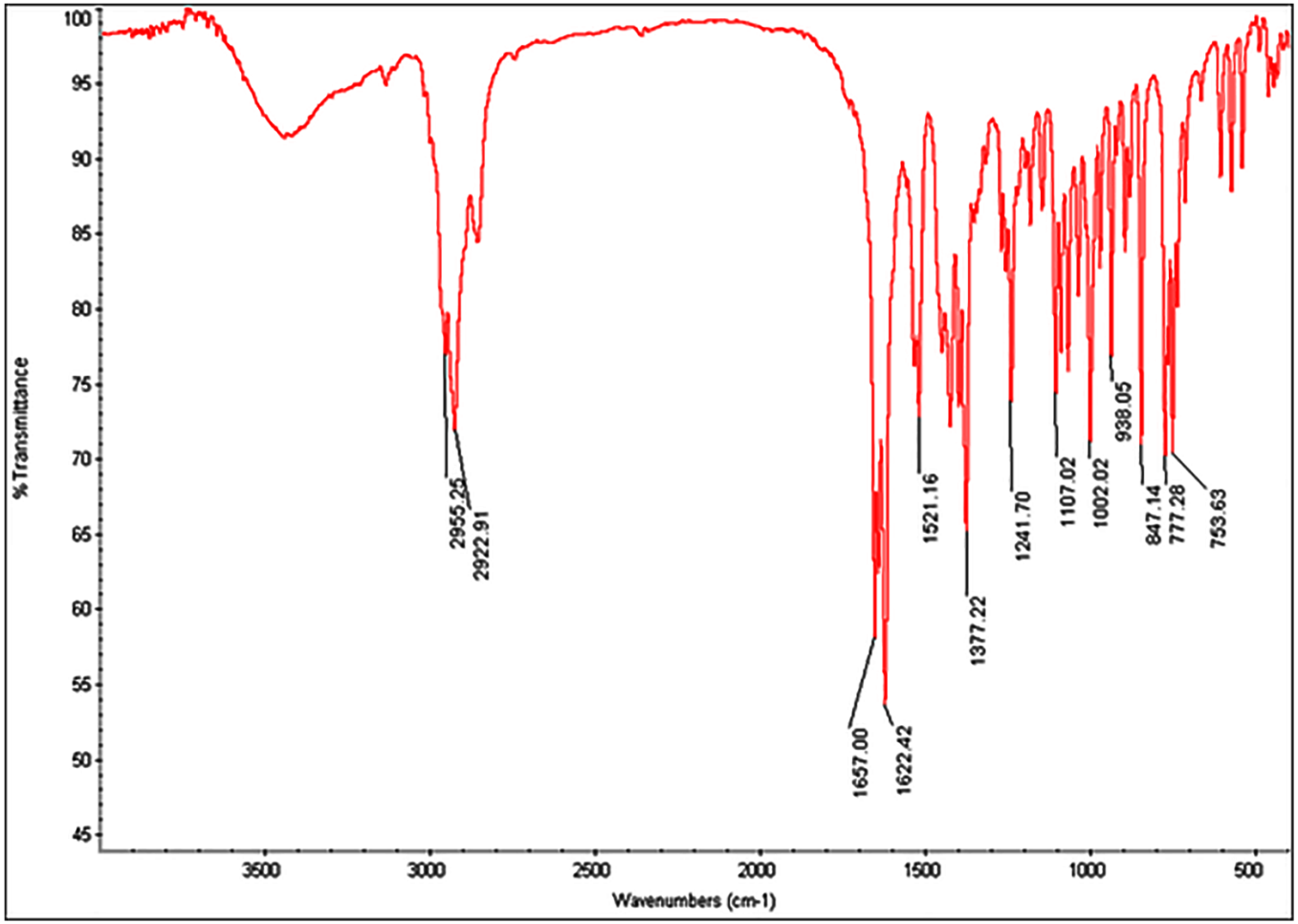


Figure 39S**.** UV spectrum of furanodienone 1,10-epoxide (**9**)



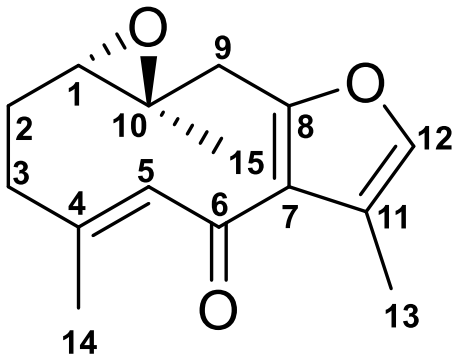
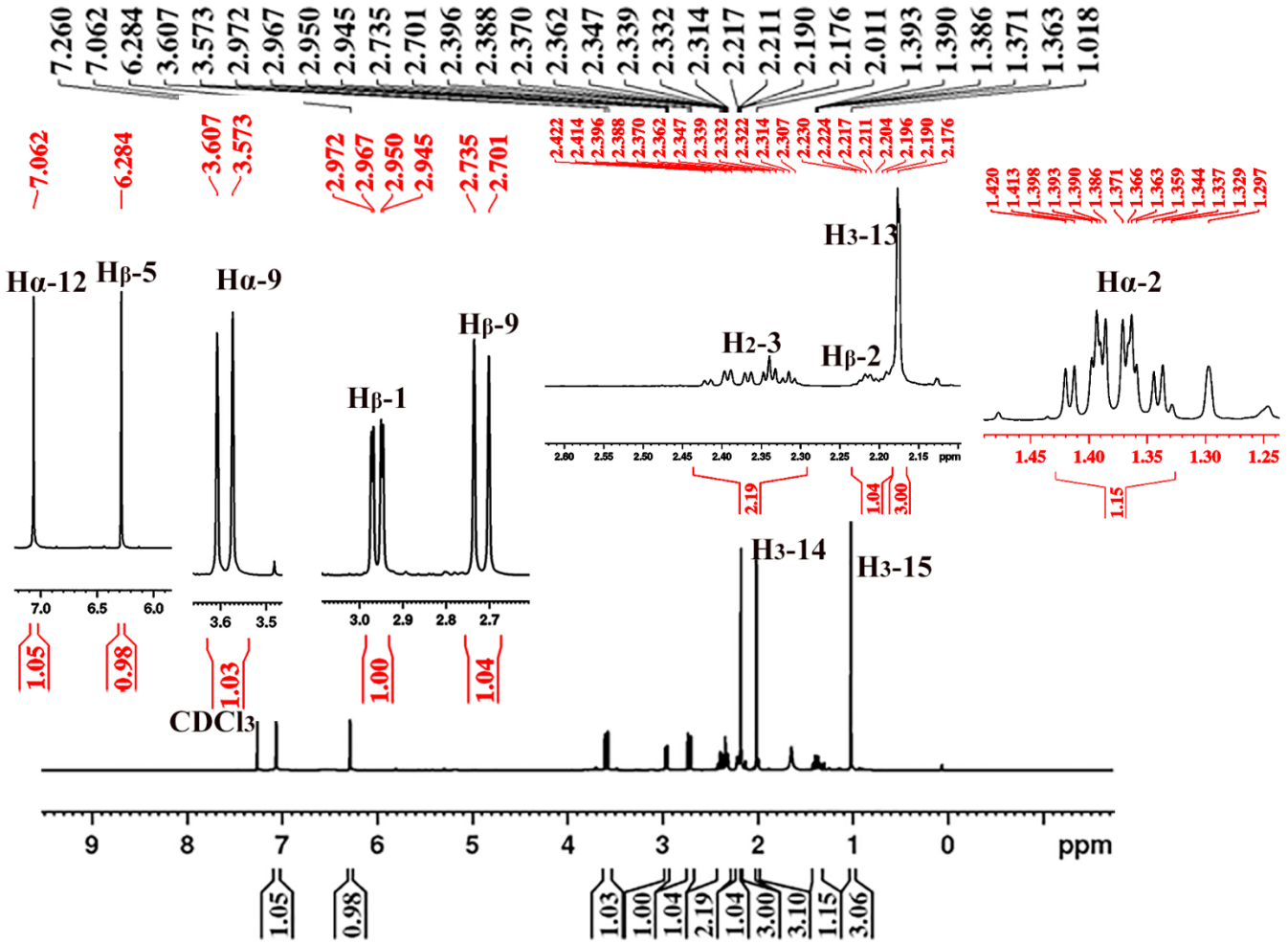


Figure 40S**.** FT-IR spectrum of furanodienone 1,10-epoxide (**9**)



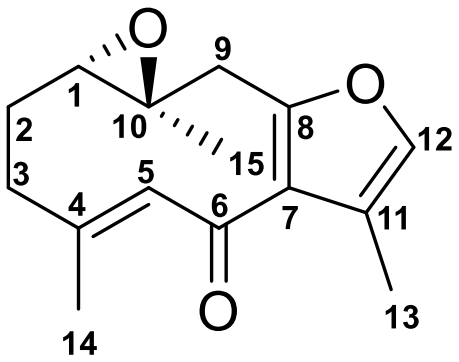
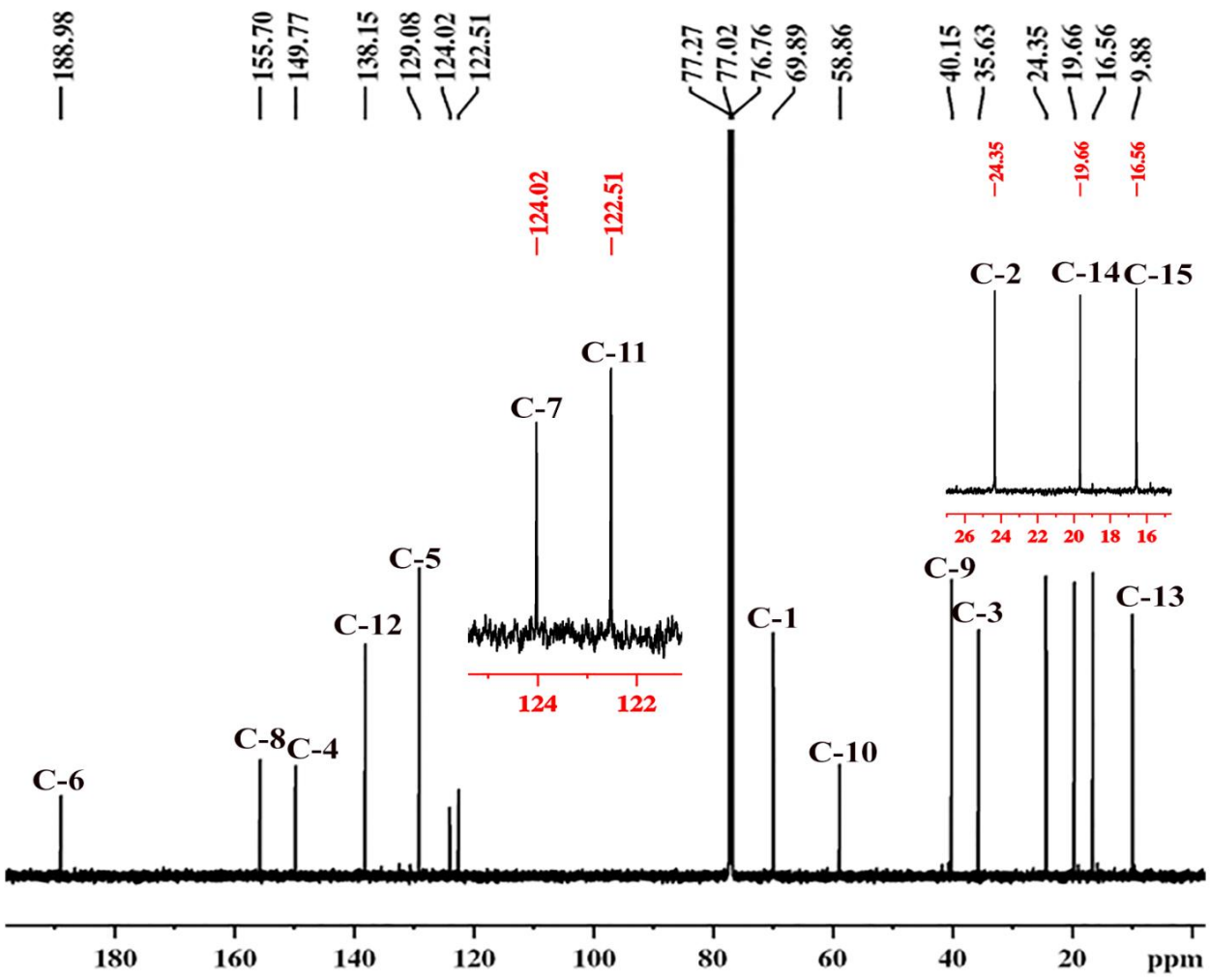


Figure 41S. ^{1}H-NMR spectrum (500 MHz, $CDCl_3$) of furanodienone 1,10-epoxide (**9**)



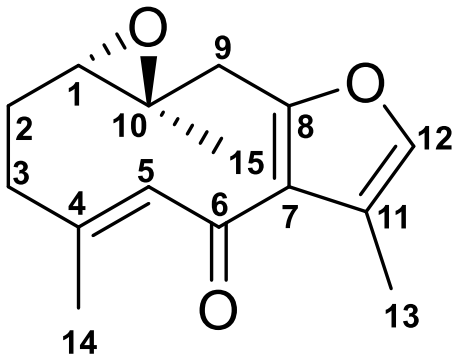


Figure 42S.^{1}H-NMR spectrum (500 MHz, $CDCl_3$) of furanodienone 1,10-epoxide (**9**)

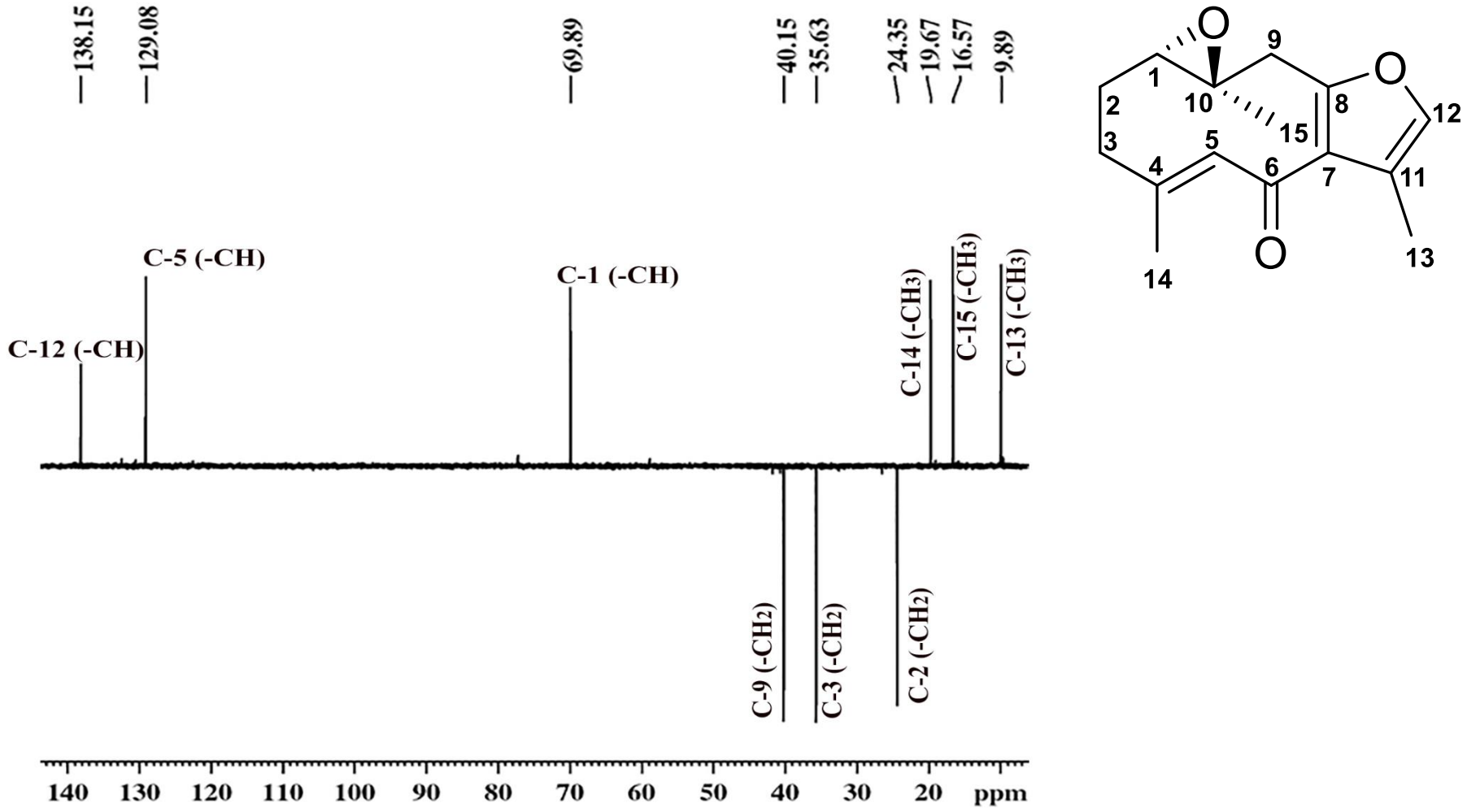
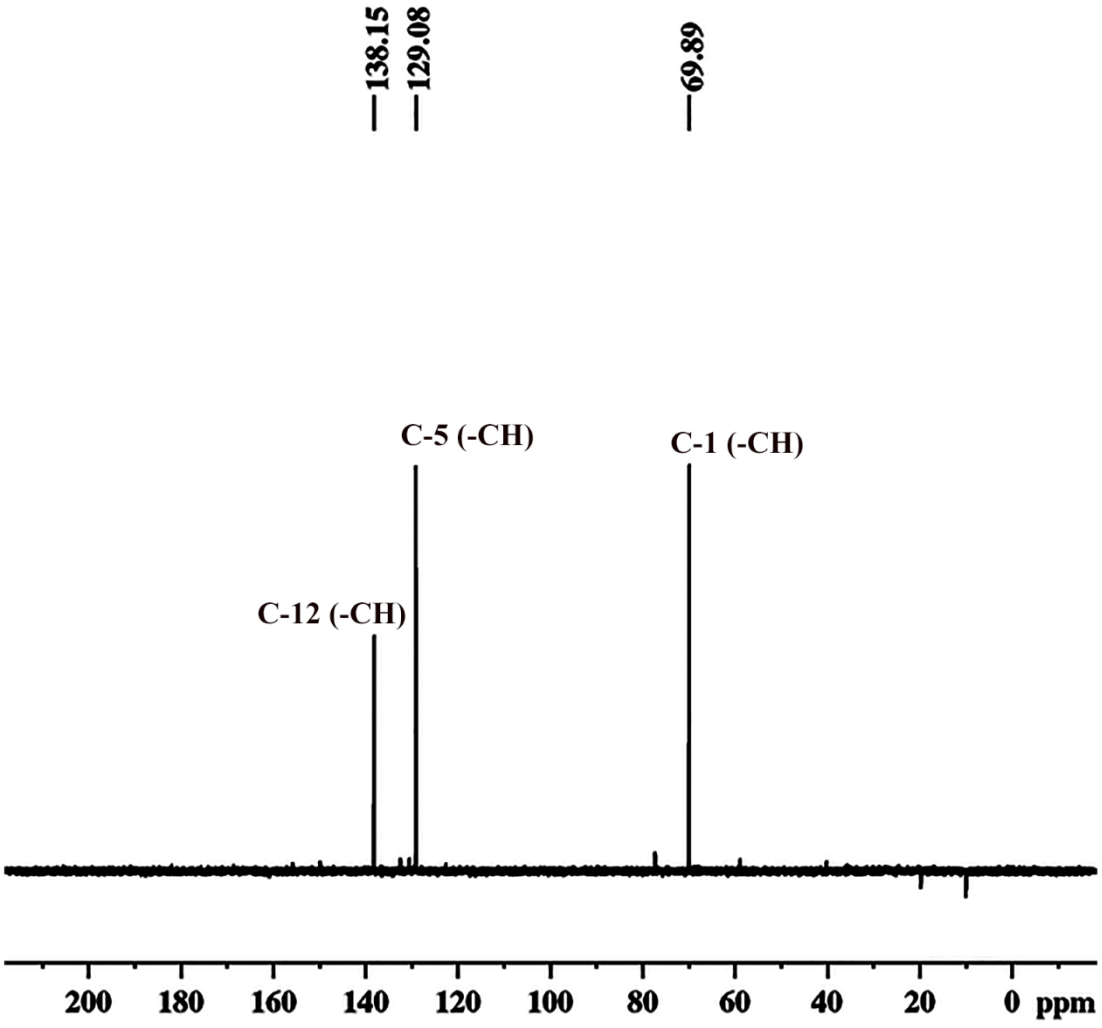


Figure 43S**.** DEPT 135 spectrum of furanodienone 1,10-epoxide (**9**) in $CDCl_3$



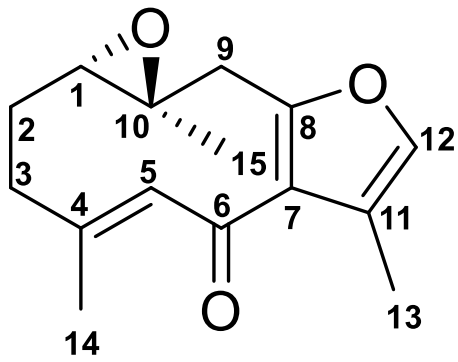


Figure 44S**.** DEPT 90 spectrum of furanodienone 1,10-epoxide (**9**) in $CDCl_3$

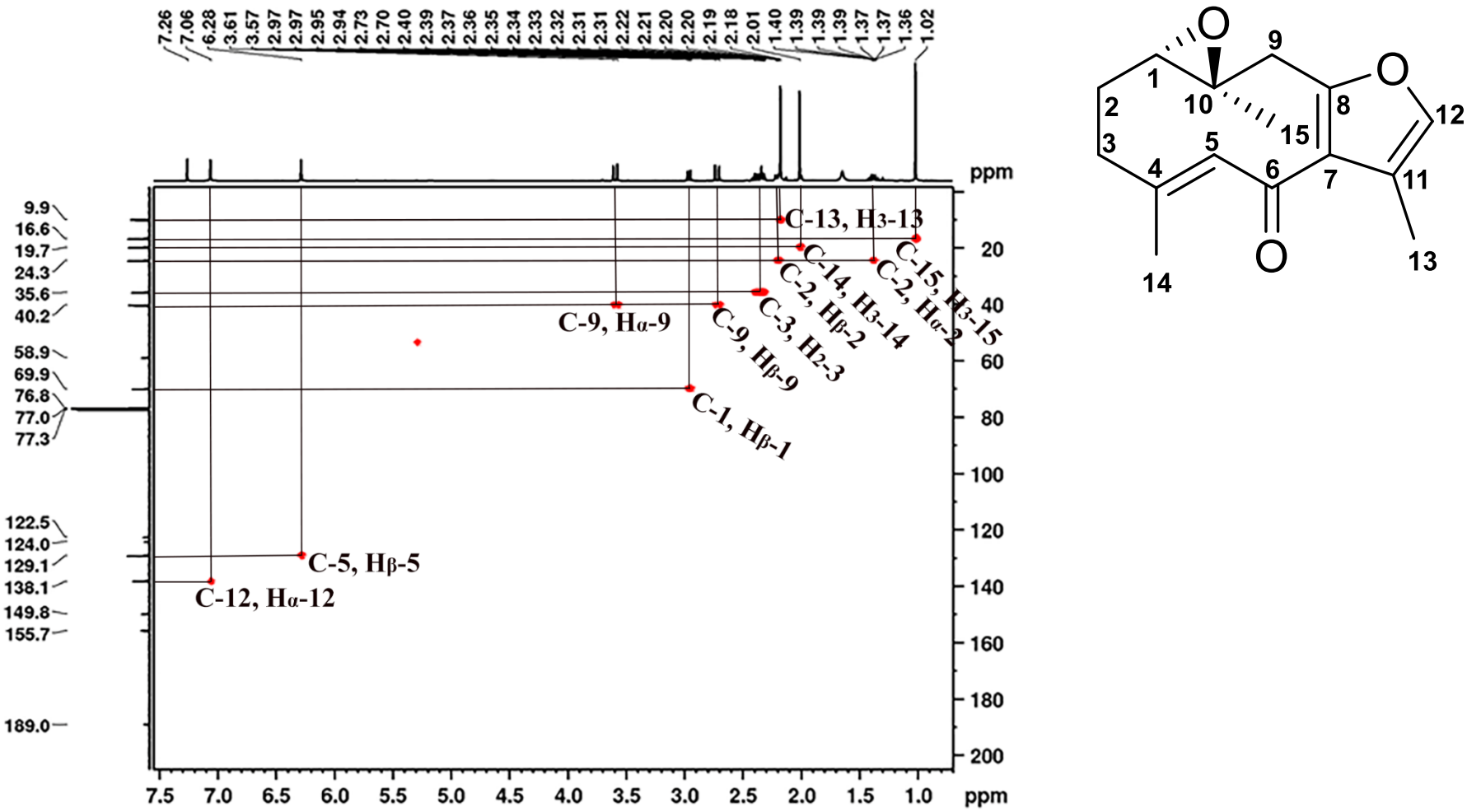
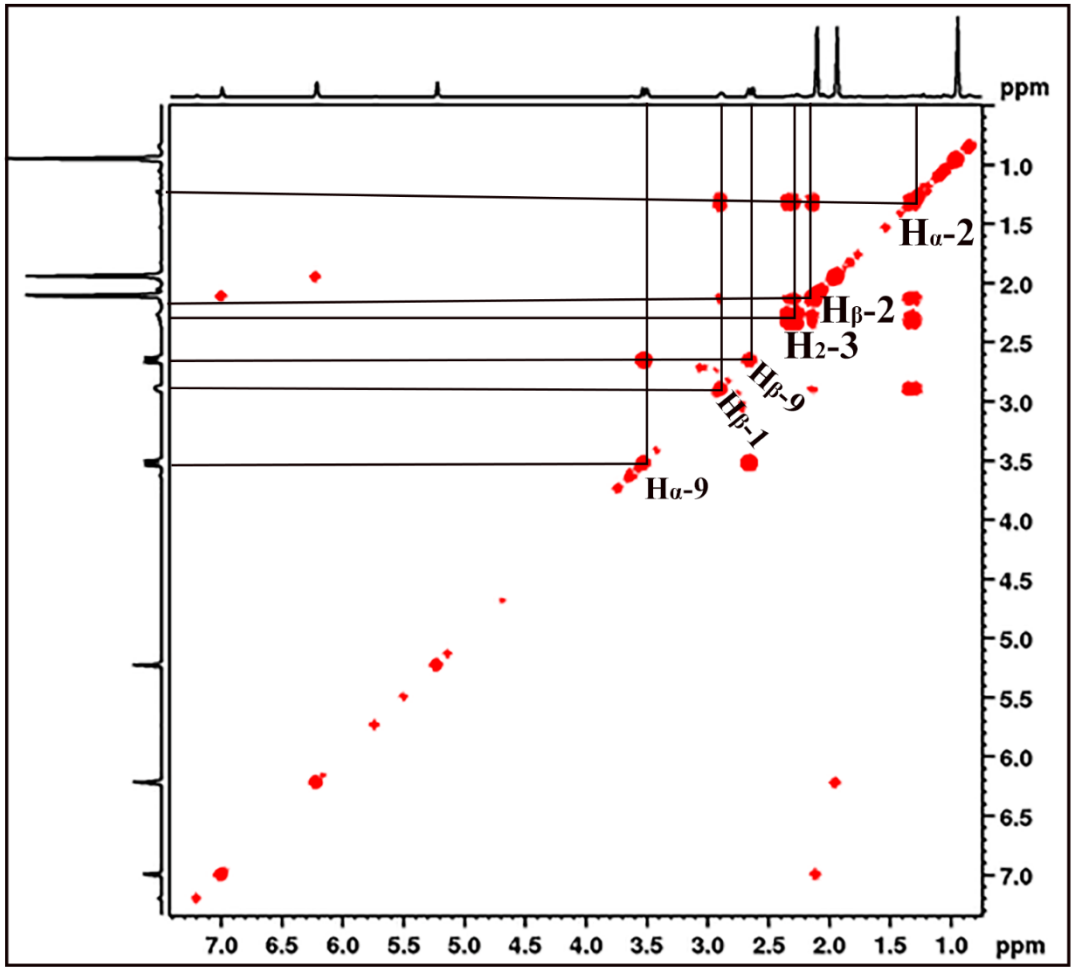
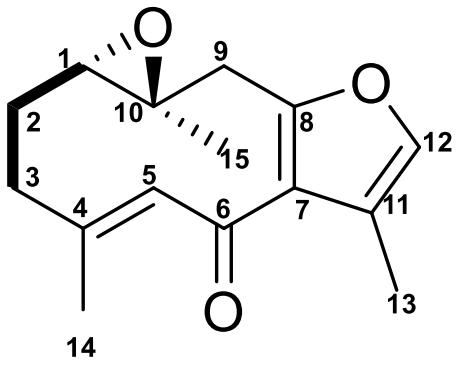


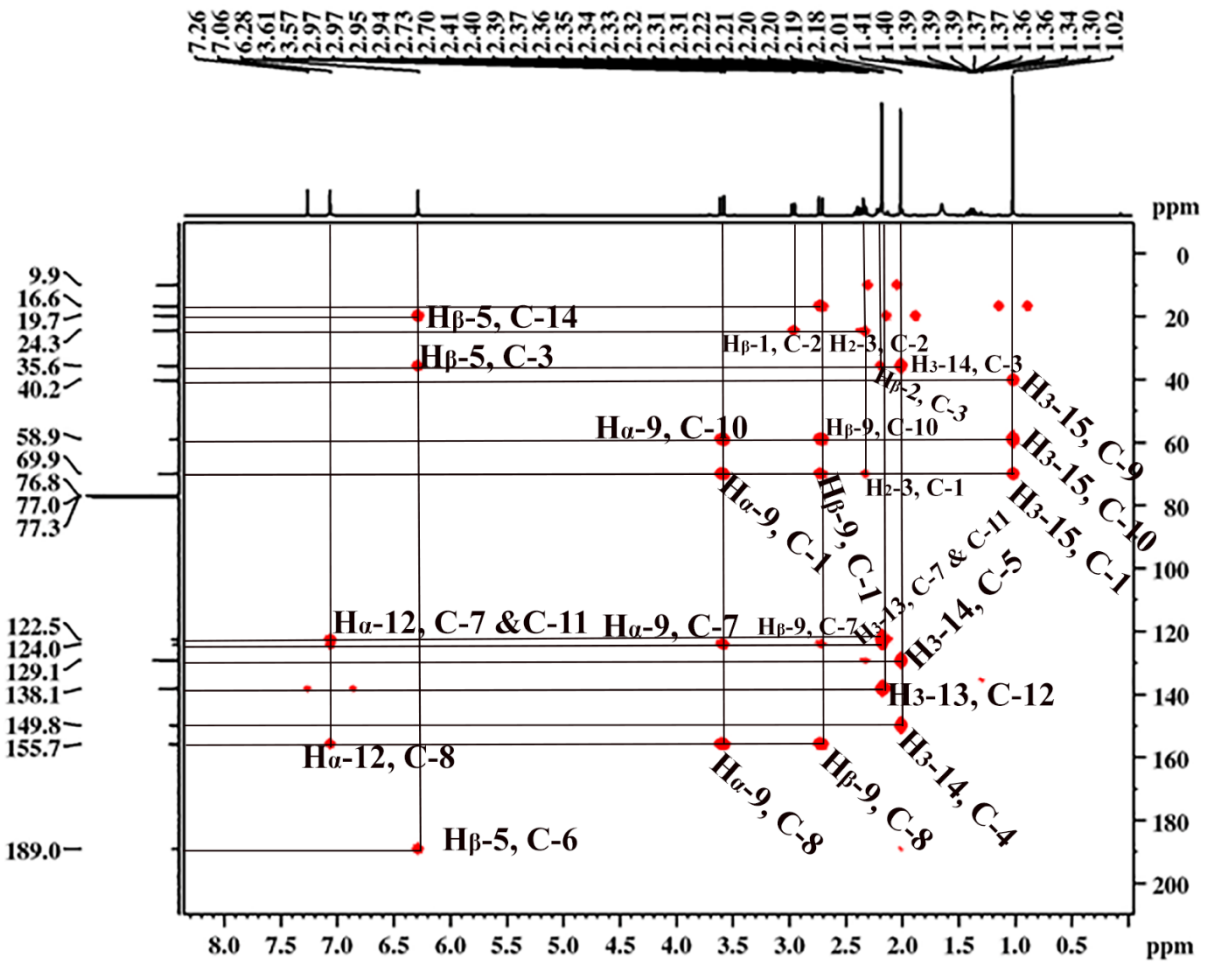
Figure 45S. ^{1}H-^{13}C HSQC spectrum of furanodienone 1,10-epoxide (**9**) in $CDCl_3$

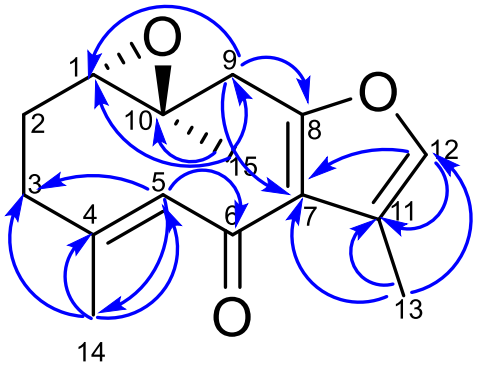




^{1}H-^{1}H COSY: ▬

Figure 46S. ^{1}H-^{1}H-COSY spectrum of furanodienone 1,10-epoxide (**9**) in $CDCl_3$



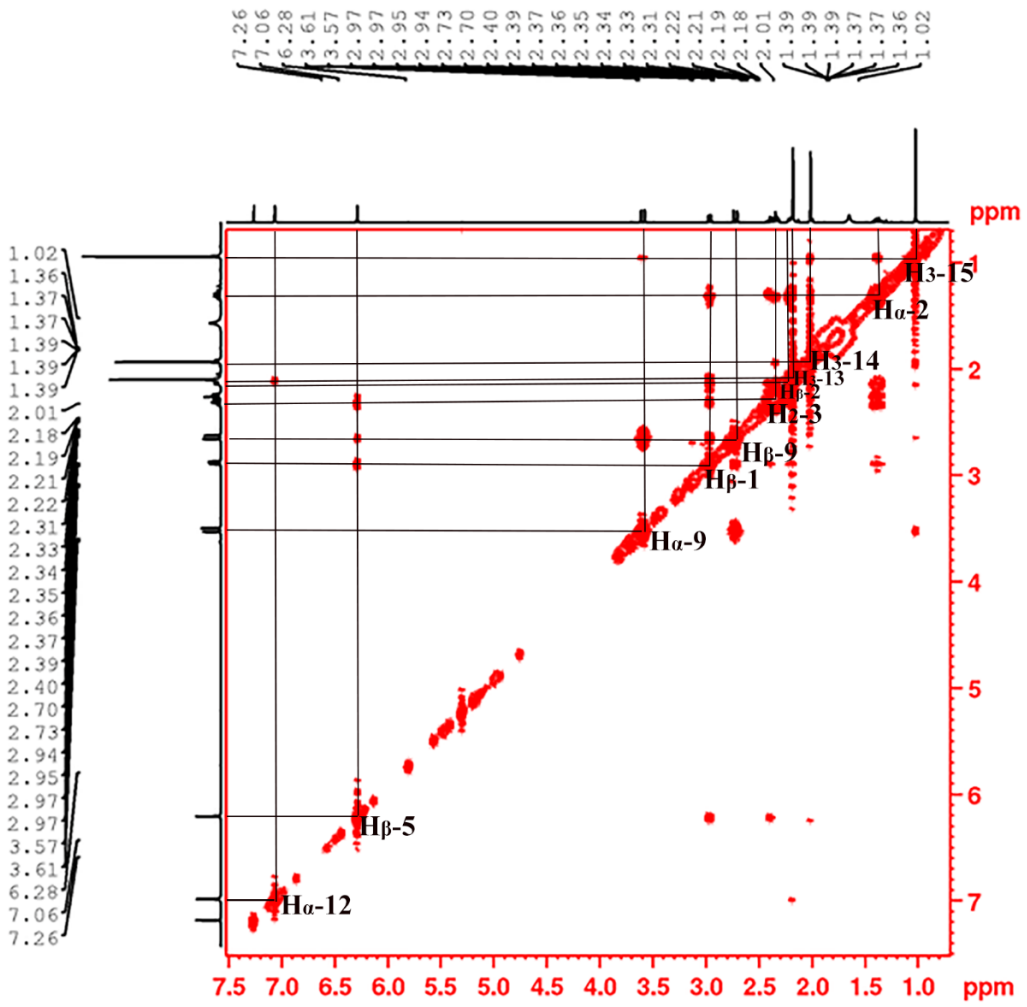


^{1}H-^{13}C HMBC:

HMBC (H ⟶ C)

Position	2*J*	3*J*
1	2	
2	3	
3	2	1
5	6	3, 14
9	8, 10	1, 7
12	11	7, 8
13	11	7, 12
14	4	3, 5
15	10	1, 9

Figure 47S. ^{1}H-^{13}C HMBC spectrum of furanodienone 1,10-epoxide (**9**) in $CDCl_3$



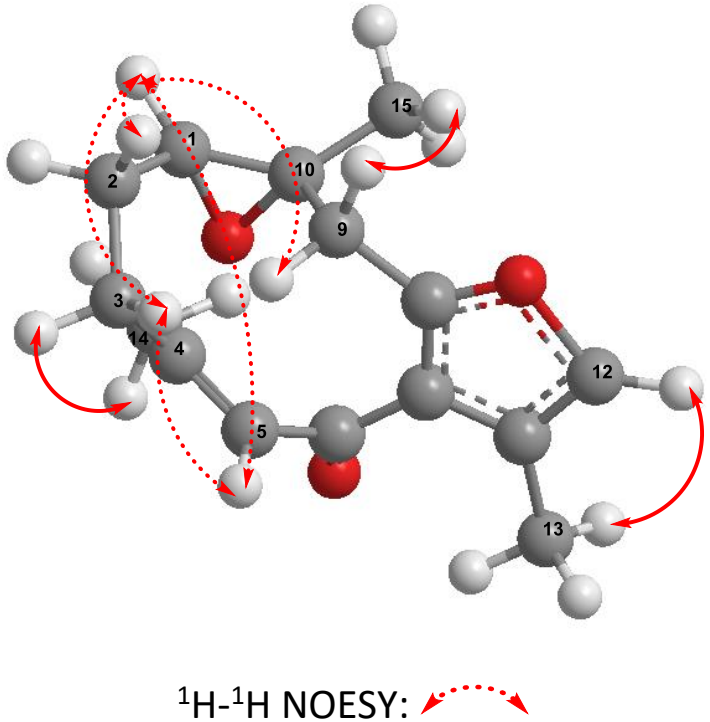


Figure 48S. ^{1}H-^{13}C NOESY spectrum of furanodienone 1,10-epoxide (**9**) in $CDCl_3$

Curcolone (10)

Obtained as colorless solid; ^{1}H-NMR ($CDCl_3$, 500 MHz): δ 1.11 (3H, s, H_3-15), 1.70-1.78 (2H, m, H_2-2), 2.03 (3H, s, H_3-14), 2.22 (3H, d, *J* = 1.5 Hz, H_3-13), 2.29-2.31 (2H, m, H_2-3), 2.75 (1H, d, *J* = 17.0 Hz, H_β-9), 3.09 (1H, d, *J* = 17.0 Hz, H_α-9), 3.80 (1H, dd, *J* = 4.5, 11.5 Hz, H_β-1), 7.06 (1H, s, H_1-12); ^{13}C NMR ($CDCl_3$, 125 MHz) δ: 187.7 (C-6), 164.5 (C-8), 145.6 (C-4), 139.2 (C-12), 134.4 (C-5), 120.0 (C-7), 119.6 (C-11), 76.6 (C-1), 43.3 (C-10), 37.0 (C-9), 33.6 (C-3), 26.9 (C-2), 22.3 (C-14), 19.7 (C-15), 9.2 (C-13).

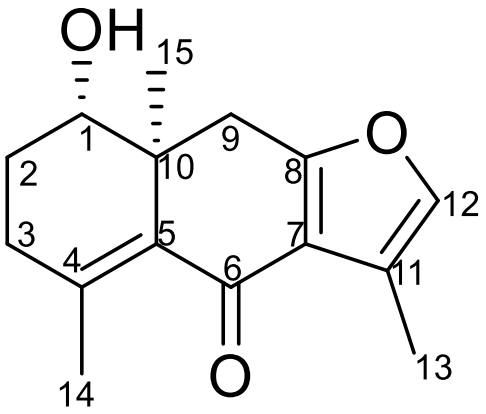


Figure 49S**.** Chemical structure of curcolone (**10**)

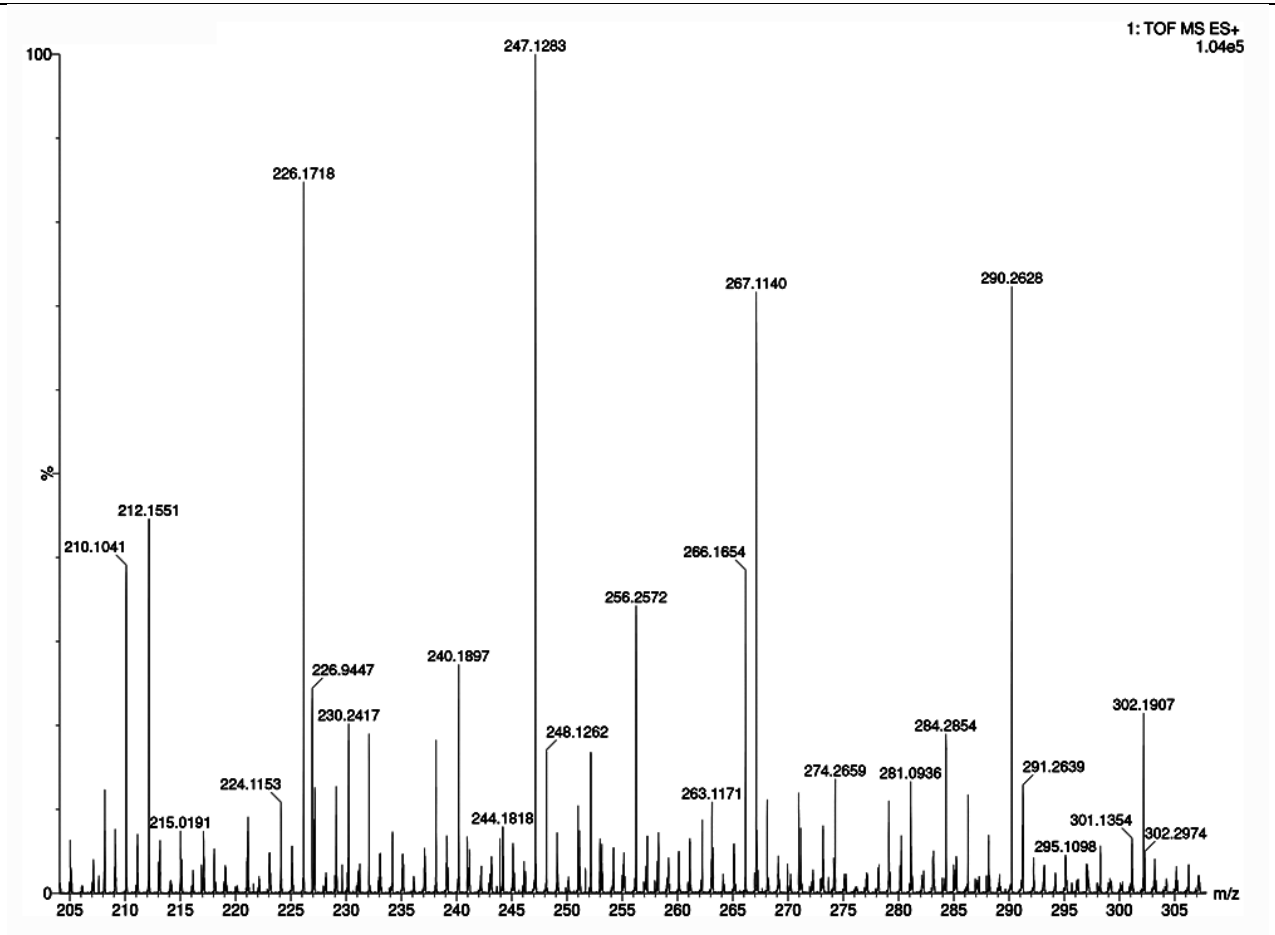
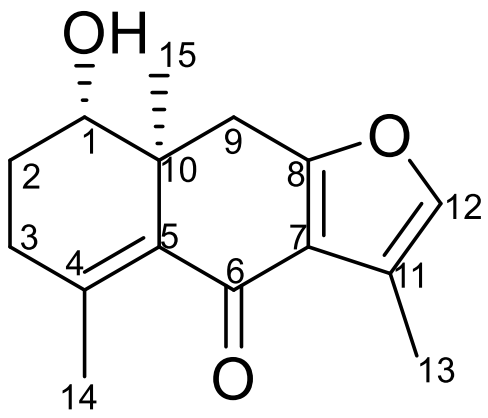


Figure 50S**.** HR-EIMS spectrum of curcolone (**10**)



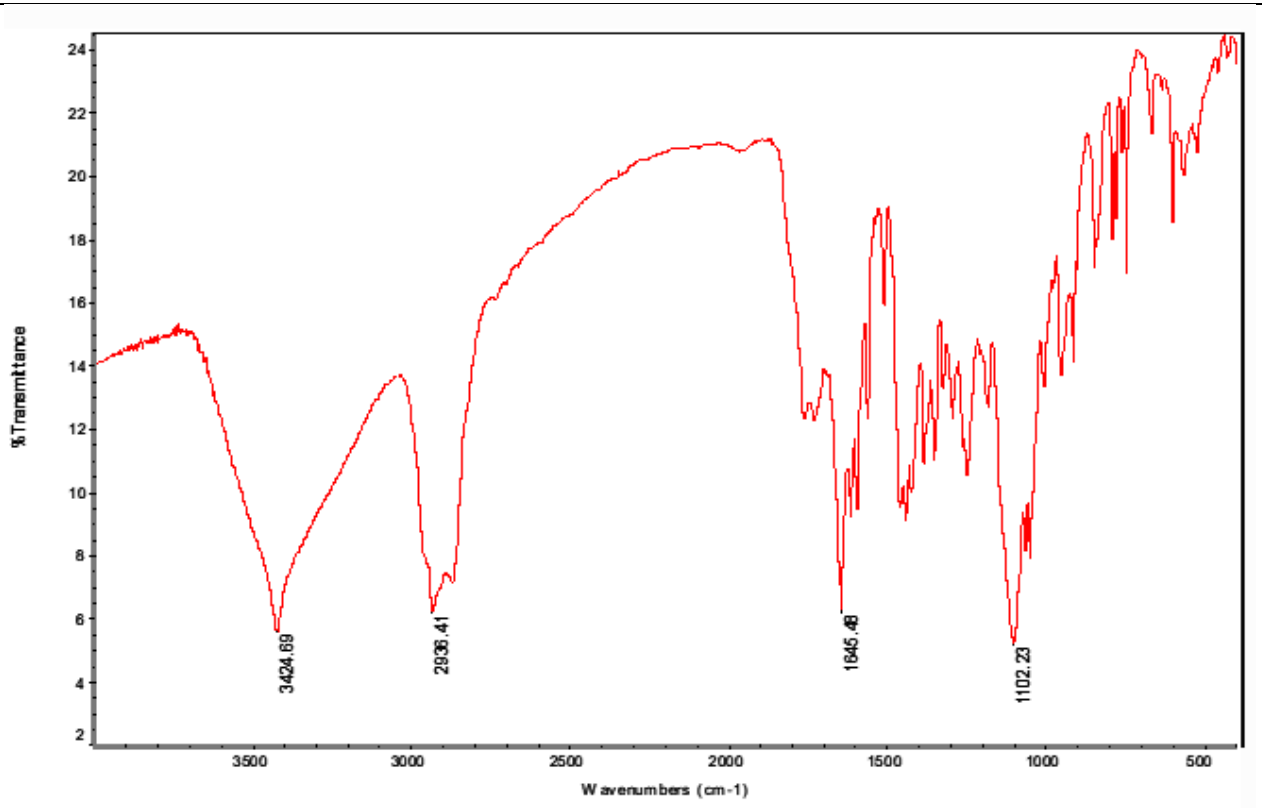
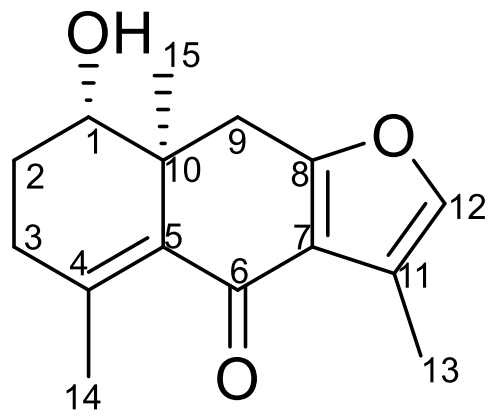


Figure 51S**.** FT-IR spectrum of curcolone (**10**)



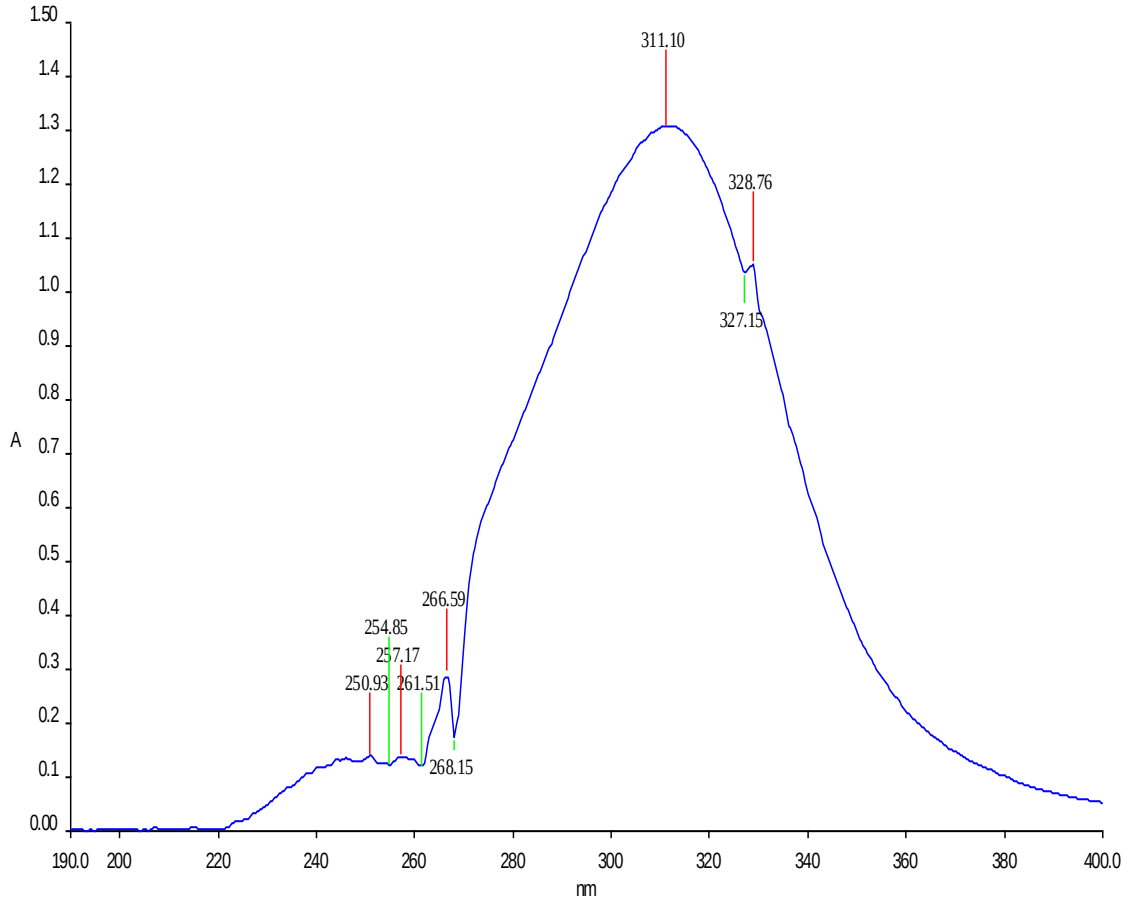
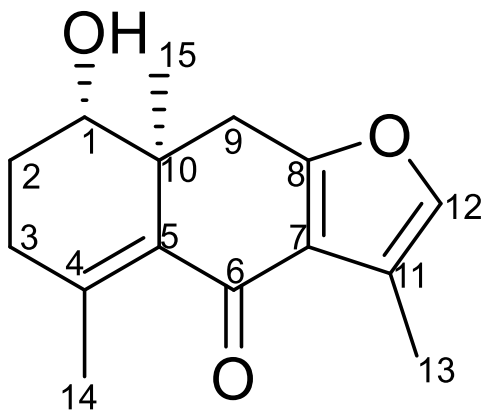


Figure 52S**.** UV spectrum of curcolone (**10**)



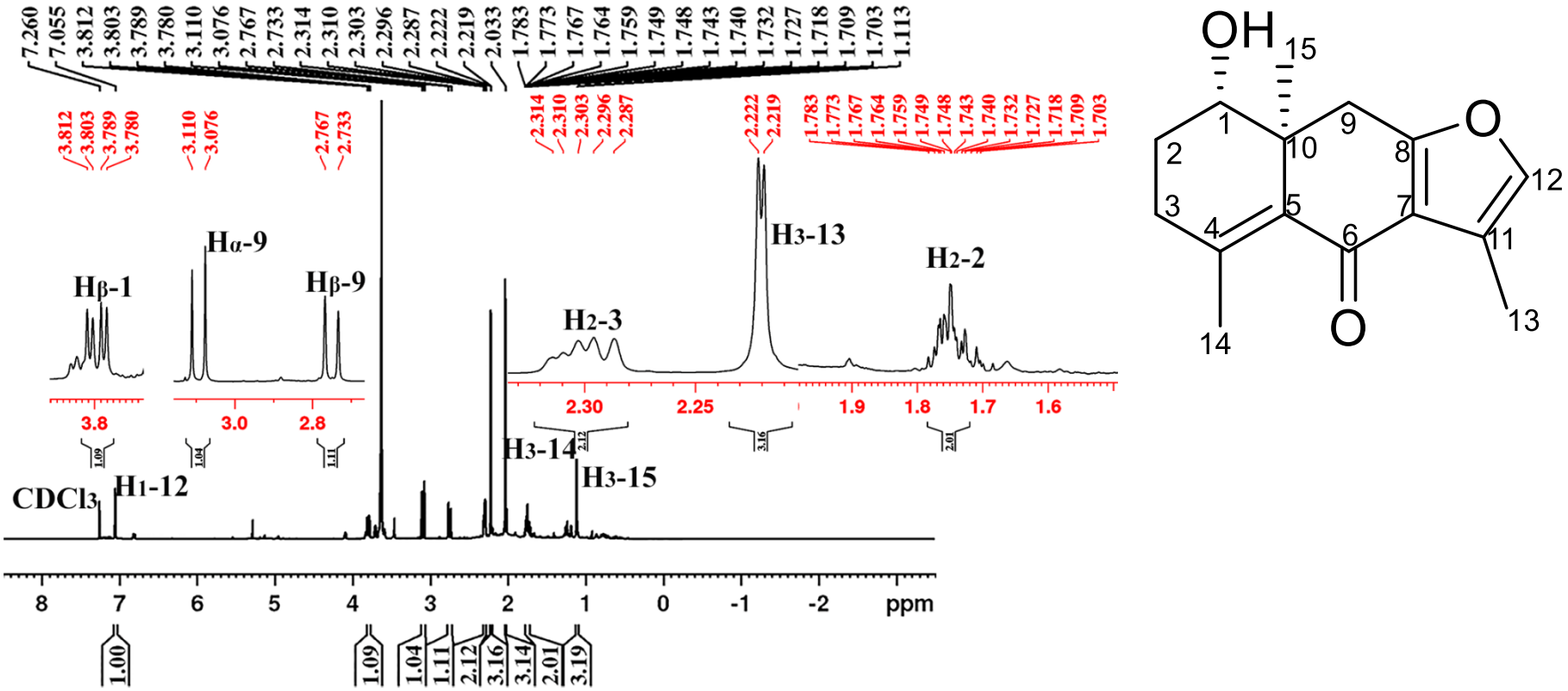
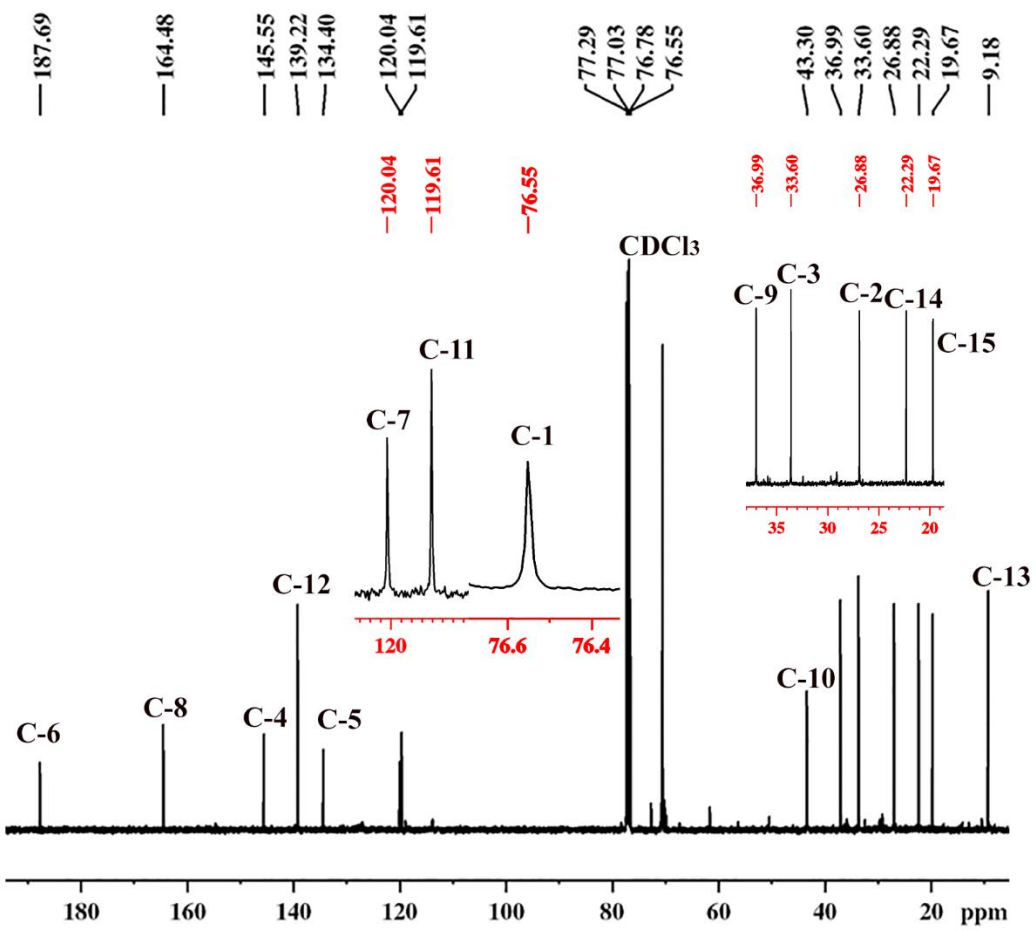


Figure 53S. ^{1}H-NMR spectrum (500 MHz, $CDCl_3$) of curcolone (**10**)



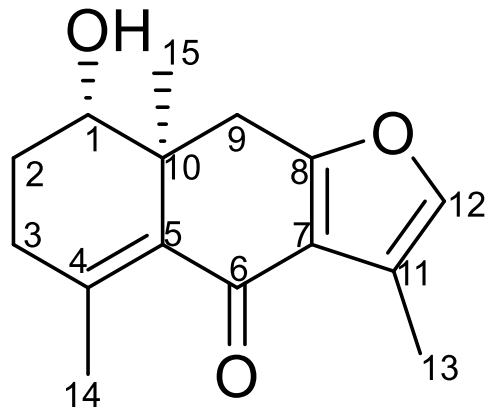
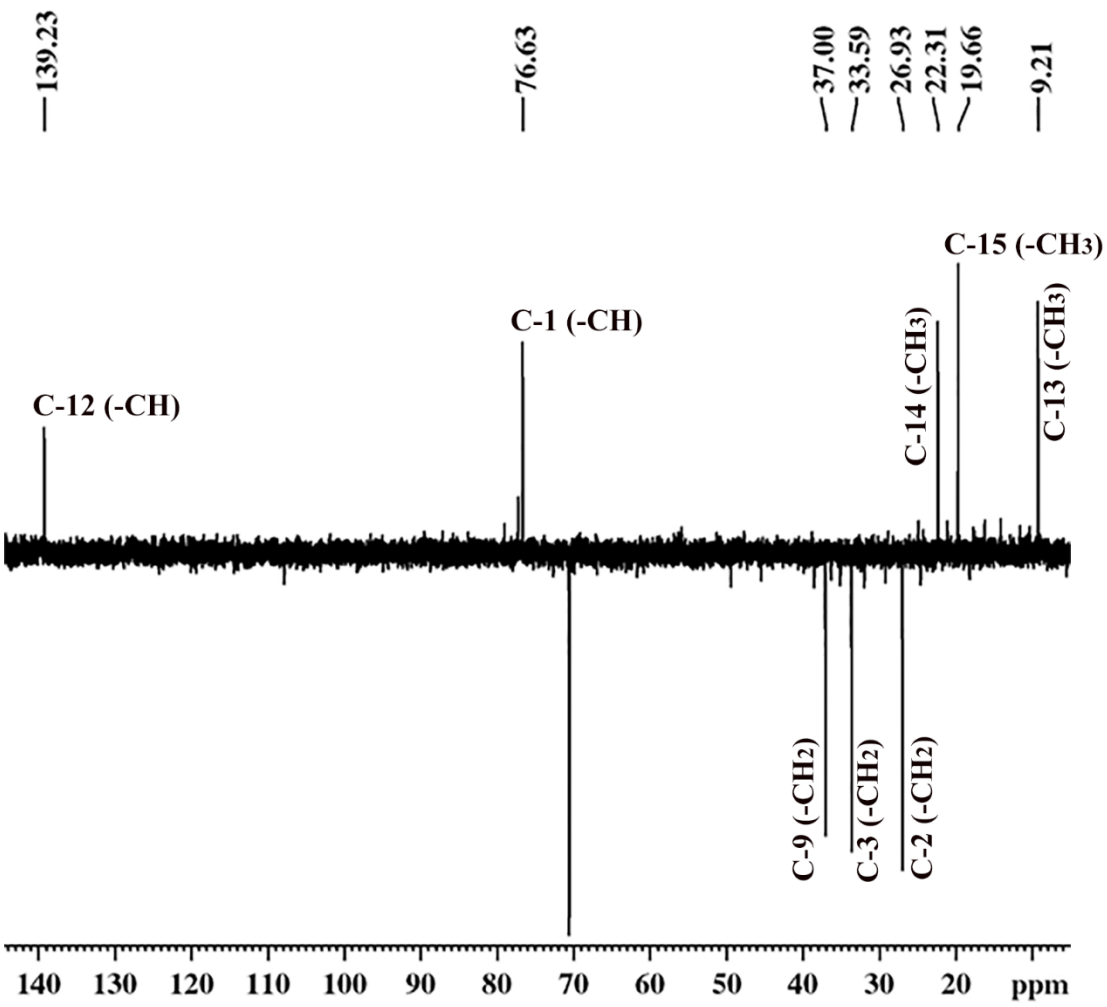


Figure 54S. ^{13}C-NMR spectrum (125 MHz, $CDCl_3$) of curcolone (**10**)



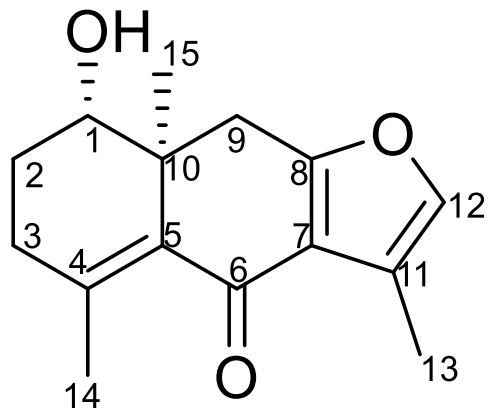
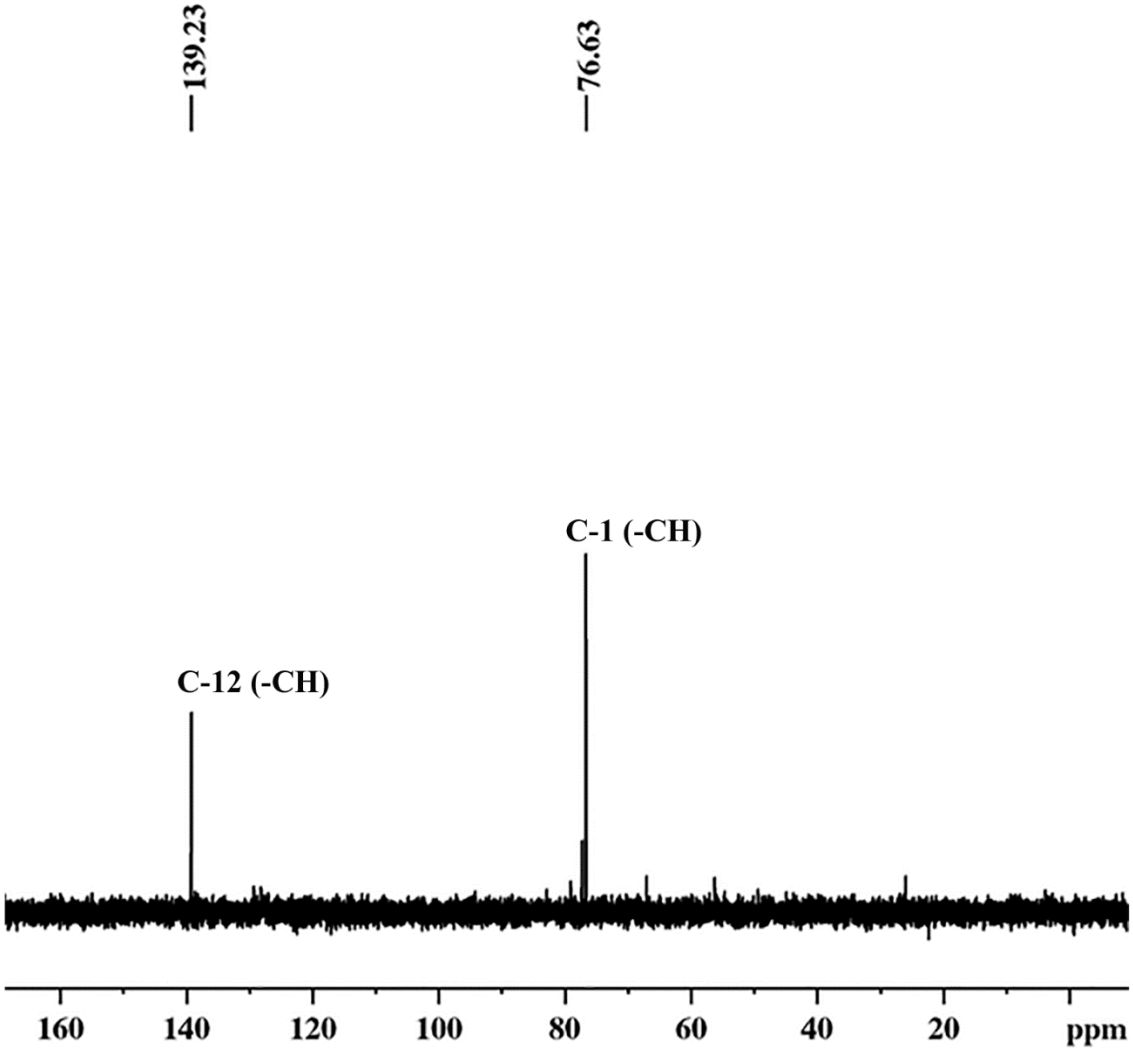


Figure 55S**.** DEPT 135 spectrum of curcolone (**10**) in $CDCl_3$



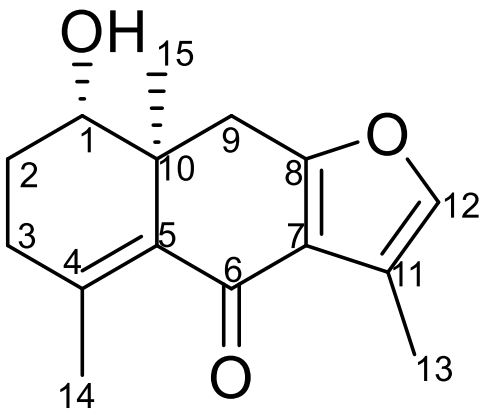
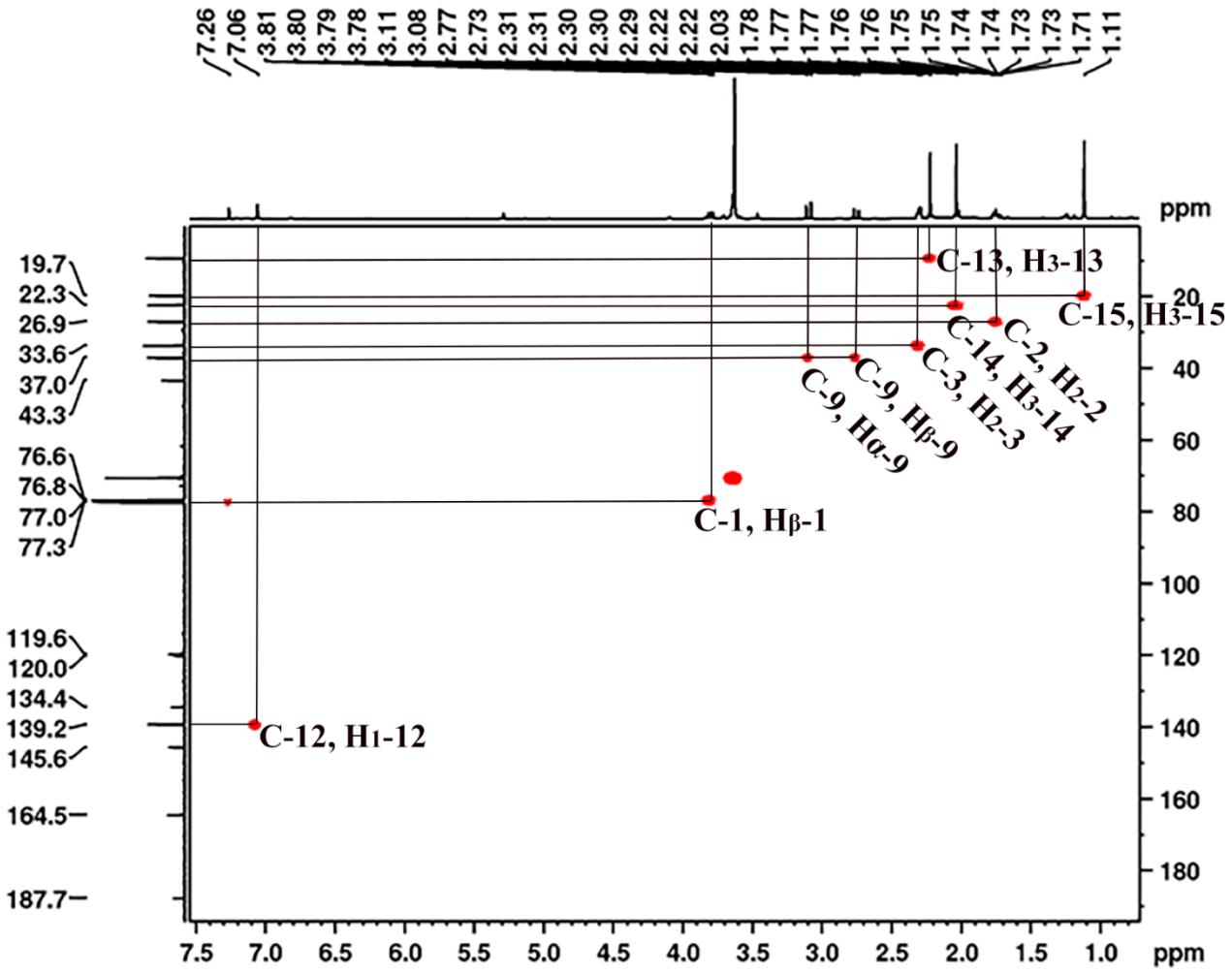


Figure 56S**.** DEPT 90 spectrum of curcolone (**10**) in $CDCl_3$



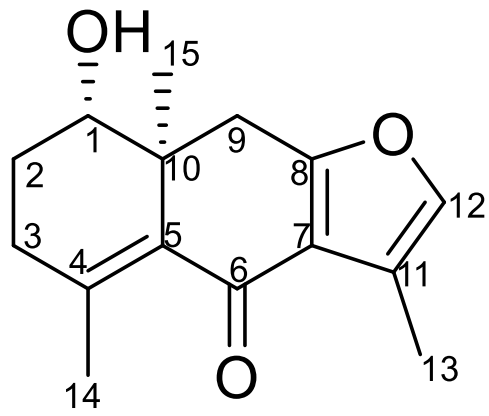


Figure 57S. ^{1}H-^{13}C HSQC spectrum of curcolone (**10**) in $CDCl_3$

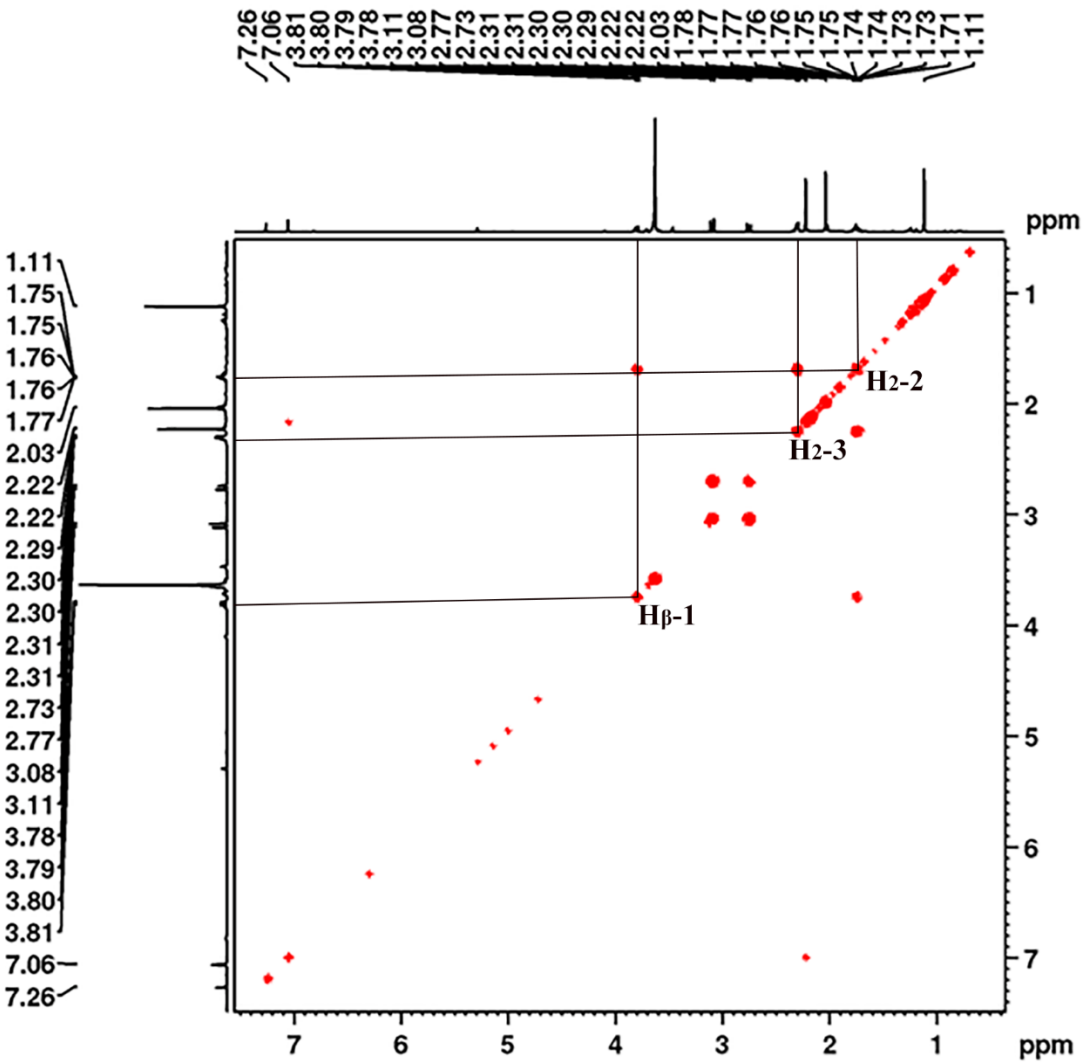
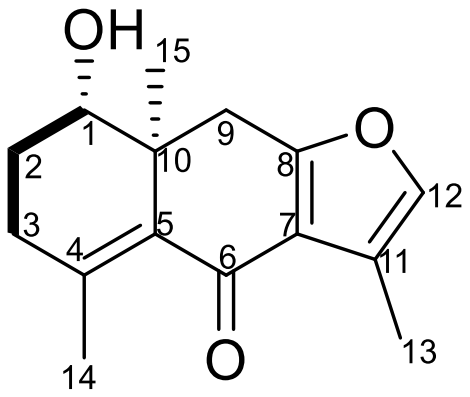
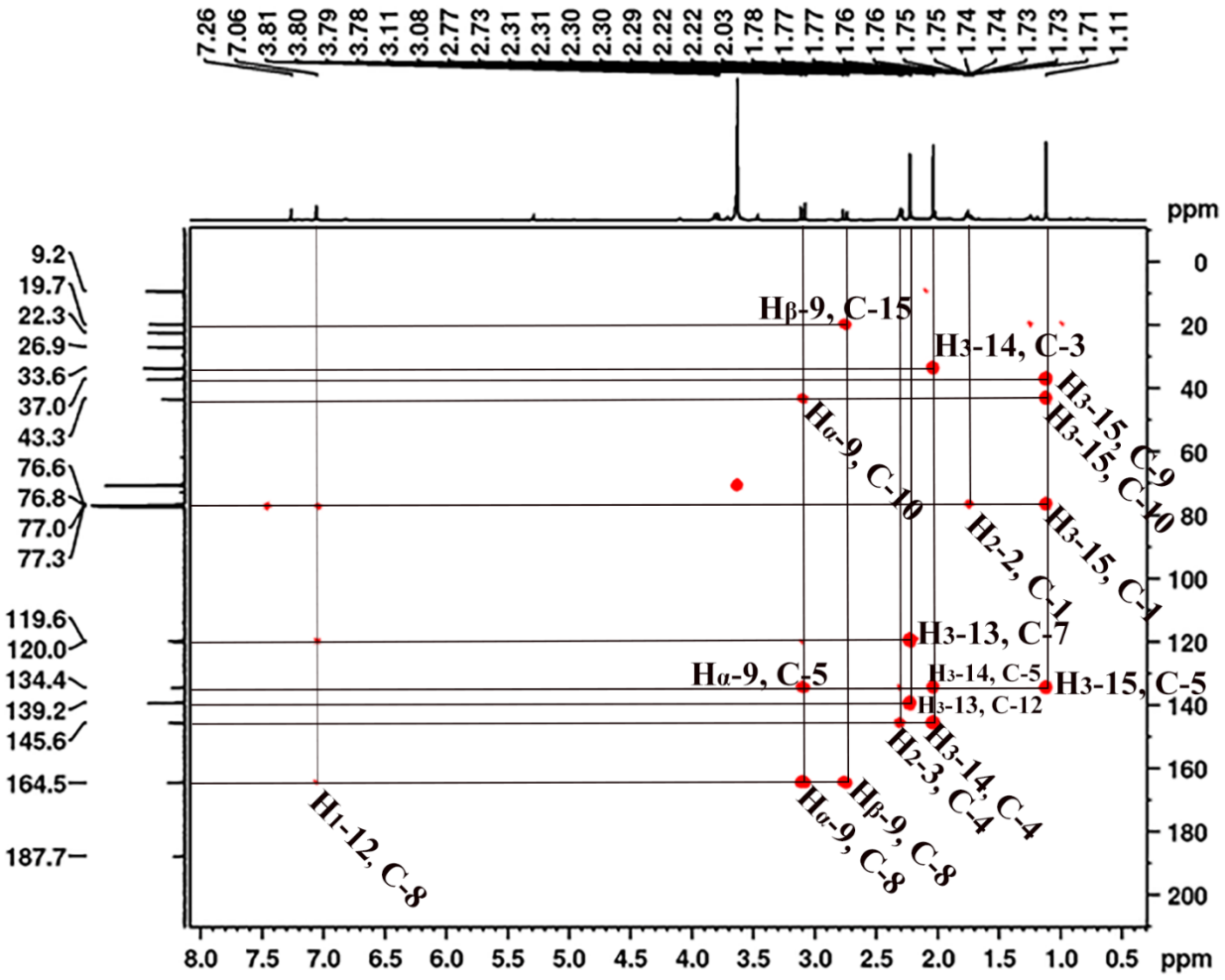
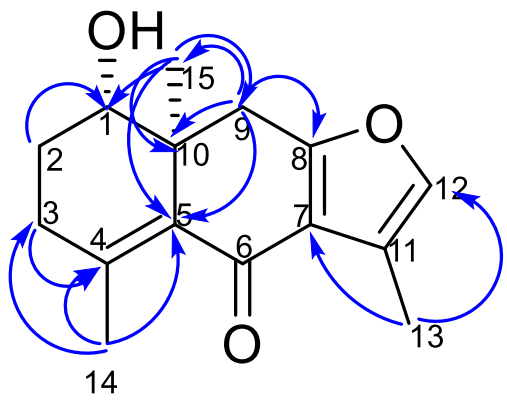


Figure 58S. ^{1}H-^{1}H-COSY spectrum of curcolone (**10**) in $CDCl_3$



^{1}H-^{1}H COSY: ▬

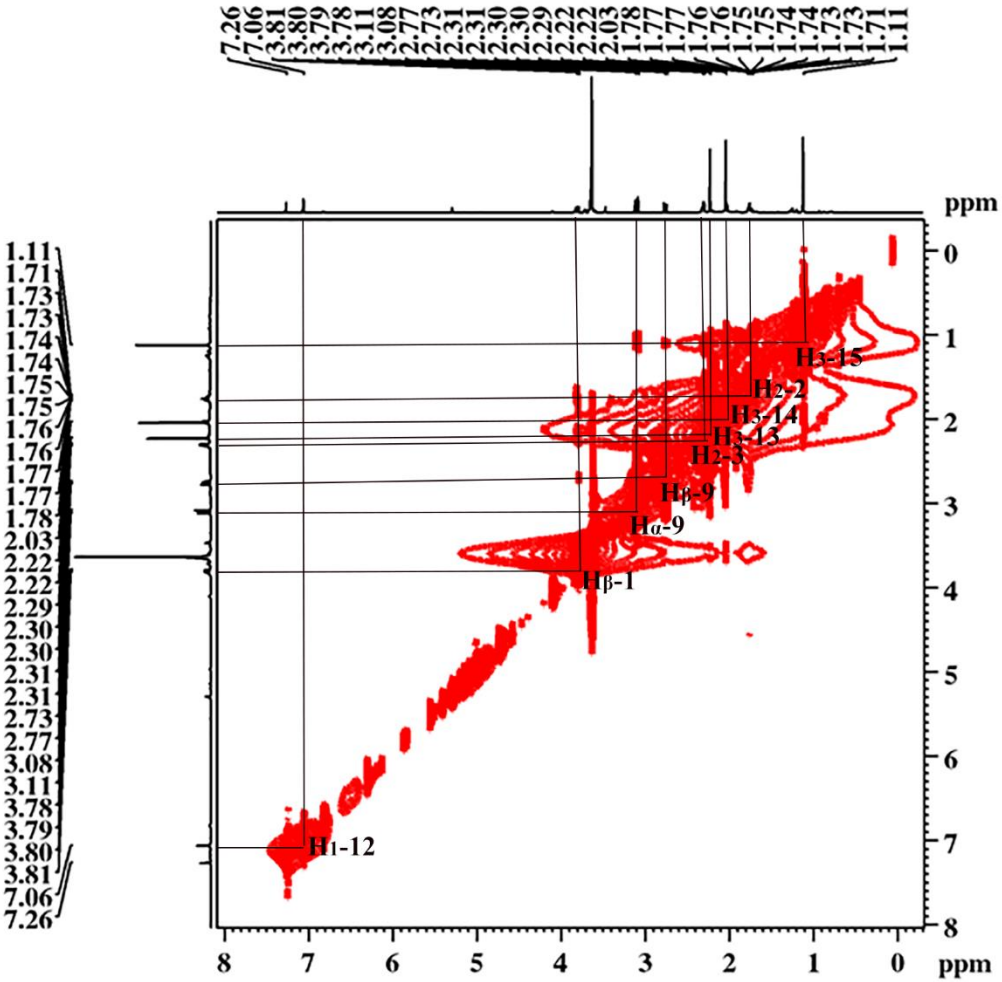


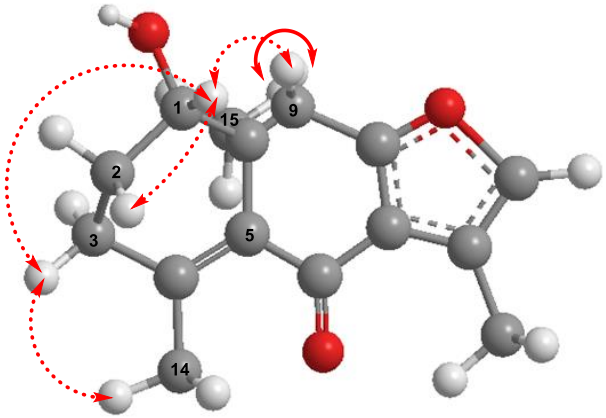


^{1}H-^{13}C HMBC:

HMBC (H ⟶ C)		
Position	2*J*	3*J*
2	1	
3	4	
9	8, 10	5, 15
12		8
13		7, 12
14	4	3, 5
15	10	1, 5, 9,

Figure 59S. ^{1}H-^{13}C HMBC spectrum of curcolone (**10**) in $CDCl_3$





^{1}H-^{1}H NOESY:

Figure 60S. ^{1}H-^{13}C NOESY spectrum of curcolone (**10**) in $CDCl_3$

Curcuzederone (**11**)

Obtained as colourless solid. IR ν_{max} (KBr) cm^{-1}: 3446.82, 1735.41, 1683.55; ^{1}H-NMR ($CDCl_3$, 500 MHz), δ 1.16 (3H, s, H_3-15), 1.33 (3H, s, H_3-14), 1.46-1.58 (1H, m, H_β-2 & H_α-3), 2.18 (3H, s, H_3-13), 2.23 (1H, br. d, *J* =12.0 Hz, H_α -2), 2.41 (1H, br. d, *J* = 13.0 Hz, H_β-3), 2.83 (1H, d, *J* =16.5 Hz, H_β-9), 2.94 (1H, br. d, *J* = 10.0 Hz, H_α-1), 3.69 (1H, d, *J* =17.0 Hz, H_α-9), 3.79 (1H, s, H_β-5), 7.10 (1H, s H_1-12); ^{13}C-NMR ($CDCl_3$, 500 MHz), δ 189.9 (C-6), 156.2 (C-8), 138.5 (C-12), 123.5 (C-11), 122.7 (C-7), 69.1 (C-1), 63.7 (C-4), 63.3 (C-5), 58.0 (C-10), 39.6 (C-9), 36.1(C-3), 23.8 (C-2), 16.8 (C-15), 15.3 (C-14), 10.6 (C-13).

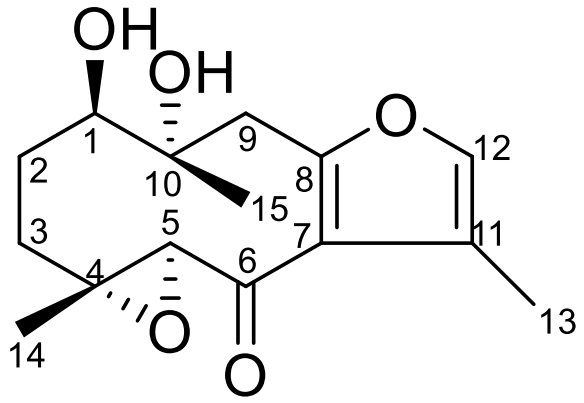
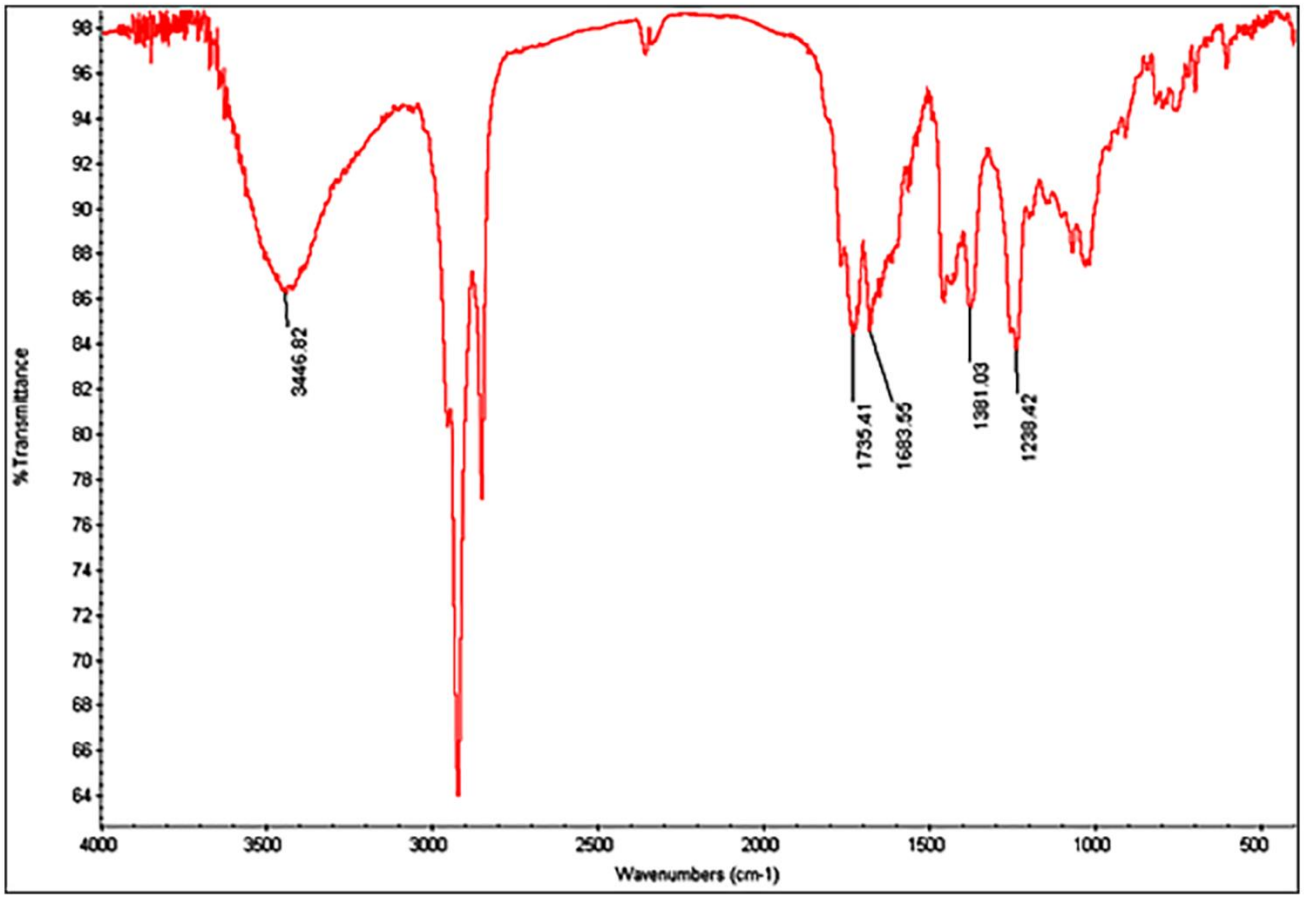


Figure 61S**.** Chemical structure of curcuzederone (**11**)



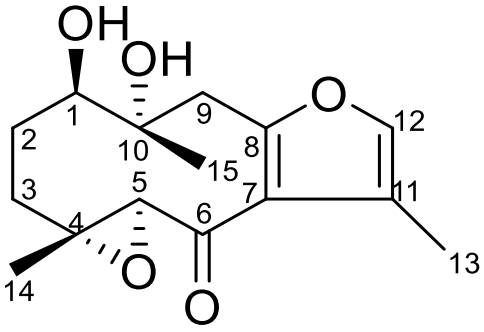
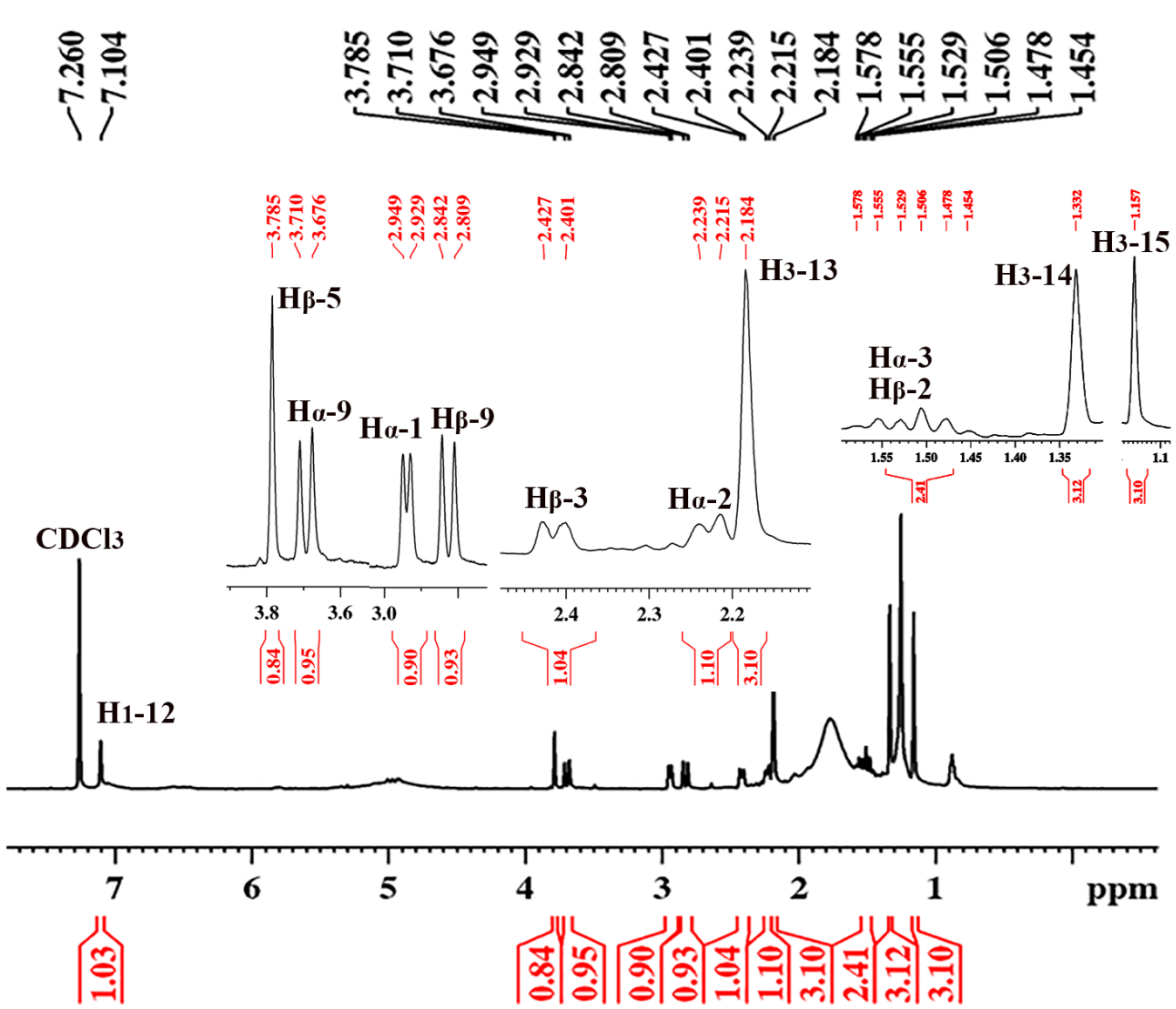


Figure 62S**.** FT-IR spectrum of curcuzederone (**11**)



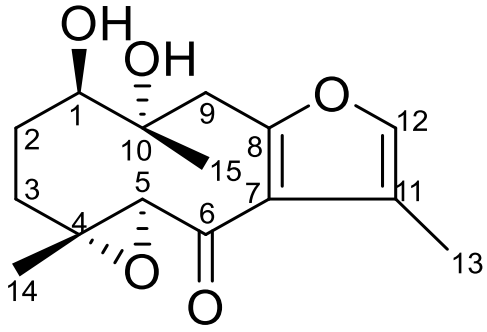


Figure 63S. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of curcuzederone (**11**)

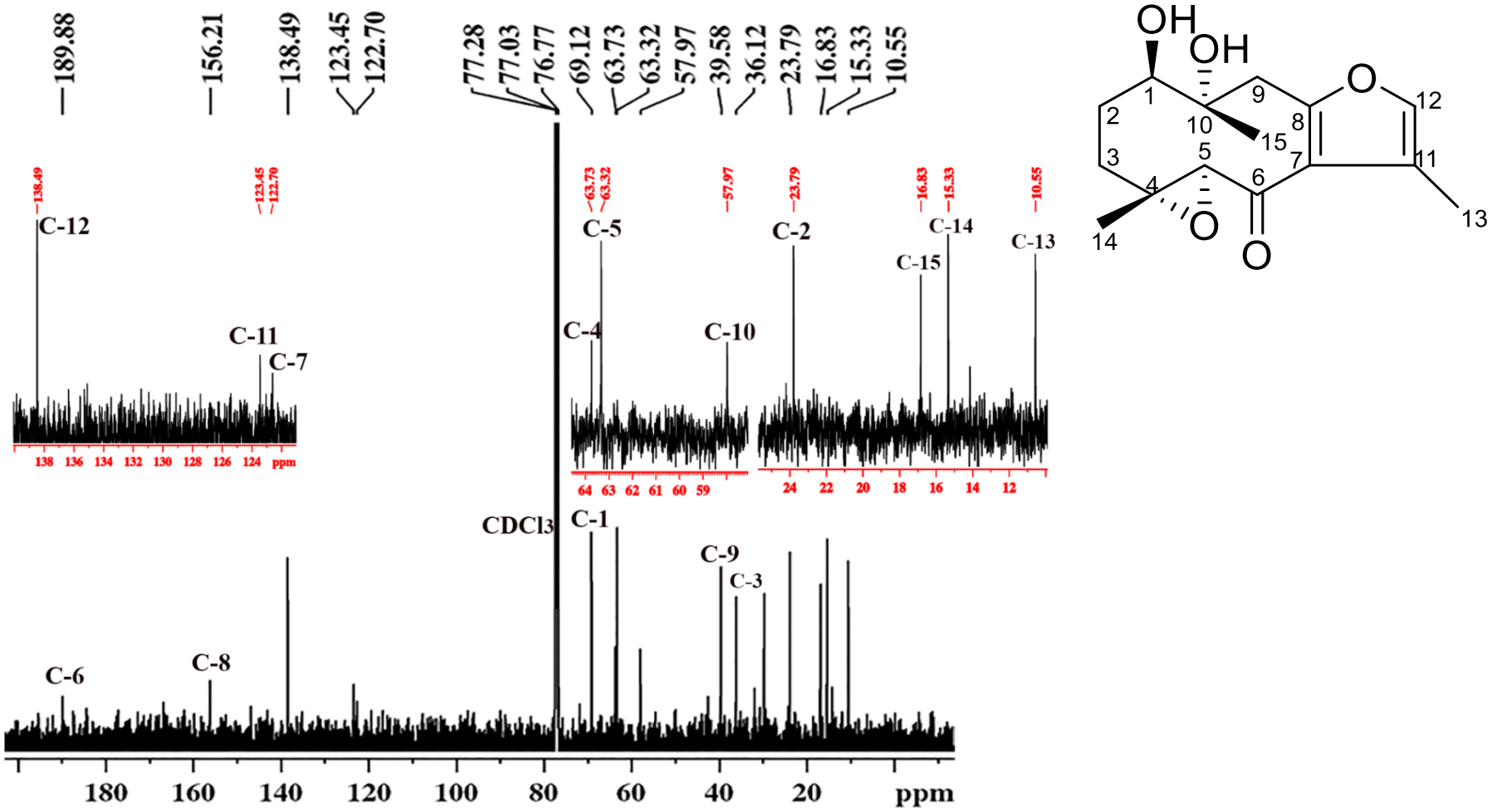


Figure 64S. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of curcuzederone (**11**)

Demethoxycurcumin (12):

Obtained as yellow colored granules; ^{1}H-NMR ($CDCl_3$, 500 MHz): δ 3.95 (3H, s, -OCH3 at C-3′), 5.79 (1H, s, H_1-4), 6.48 (1H, dd, *J* = 2.0, 16.0 Hz, H_1-2 & H_1-6), 6.86 (2H, d, *J* = 8.5 Hz, H_1-3″ & H_1-5″), 6.93 (1H, d, *J* = 8.0 Hz, H_1-5′), 7.05 (1H, d, *J* = 1.5 Hz, H_1-2′), 7.12 (1H, dd, *J* = 1.5, 8.0 Hz, H_1-6′), 7.46 (2H, d, *J* = 8.5 Hz, H1-2″ & H1-6″), 7.60 (1H, dd, *J* = 8.5, 16.0 Hz, H_1-1 & H_1-7); ^{13}C NMR ($CDCl_3$, 125 MHz) δ: 183.4 (C-3/5), 183.3 (C-3/5), 157.7 (C-4″), 147.9 (C-3′) 146.8 (C-4′), 140.6 (C-1), 140.2 (C-7), 130.0 (C-2 & 6), 127.8 (C-1′), 127.7 (C-1″), 123.0 (C-6′), 121.7 (C-6″) , 116.0 (C-3″ & C-5″), 114.8 (C-5′), 109.6 (C-2″), 101.3 (C-2′), 56.0 (OCH3 at C-3′).

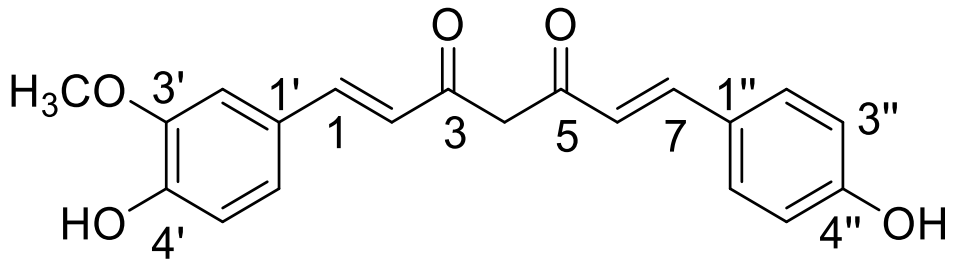
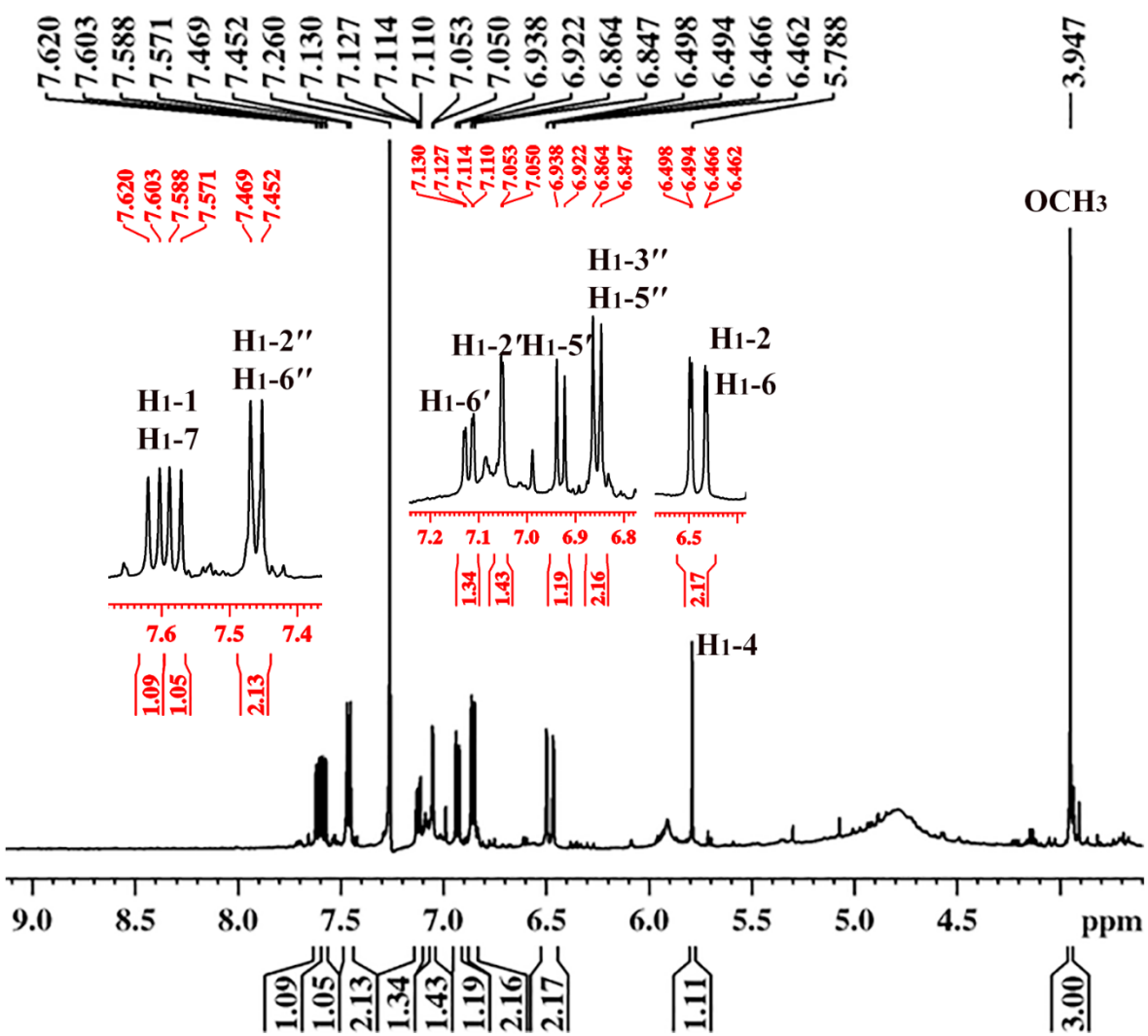


Figure 65S**.** Chemical structure of demethoxycurcumin (**12**)



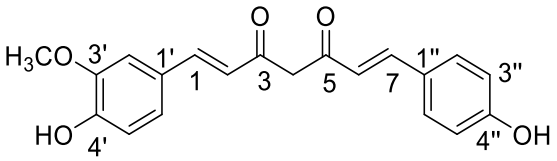
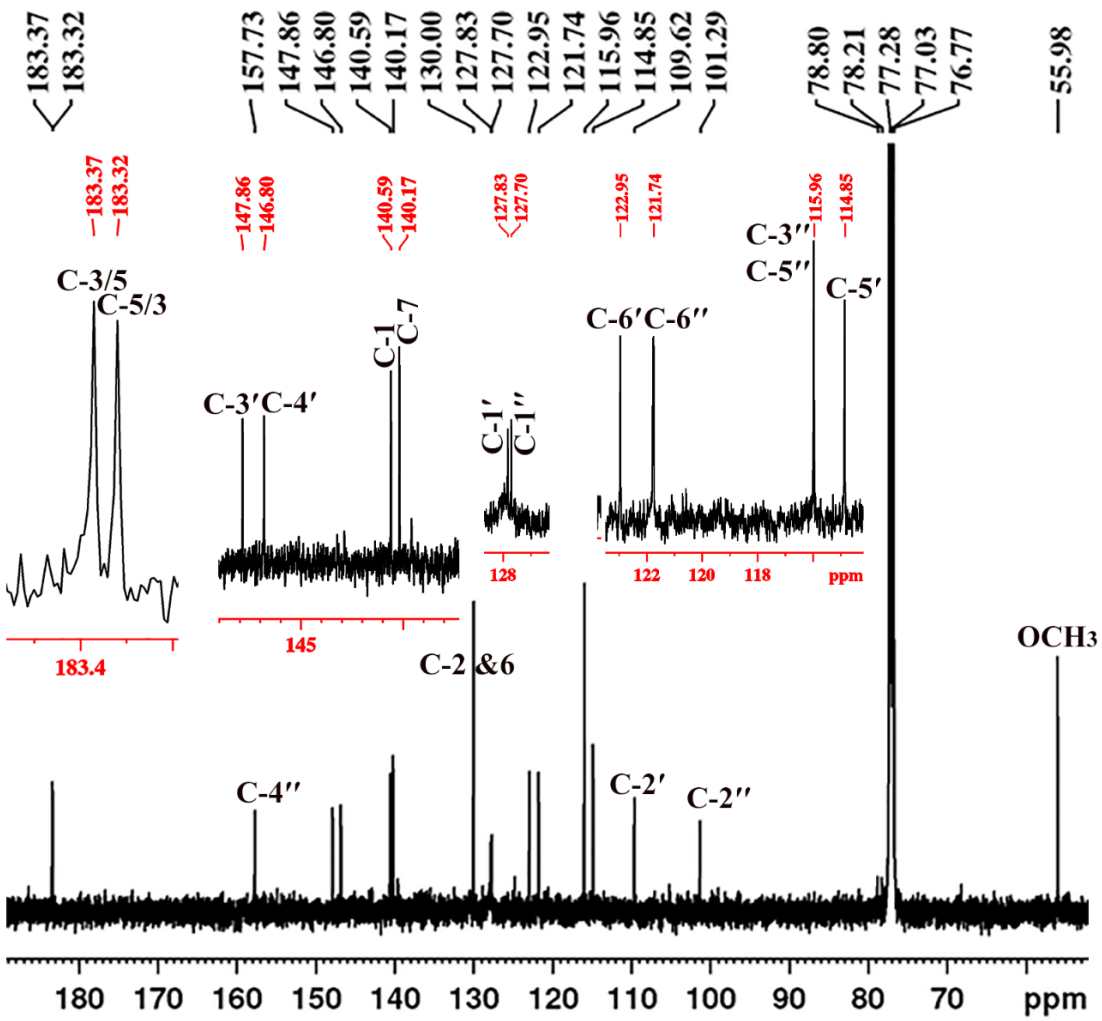


Figure 66S. ^{1}H-NMR spectrum (500 MHz, $CDCl_3$) of demethoxycurcumin (**12**)



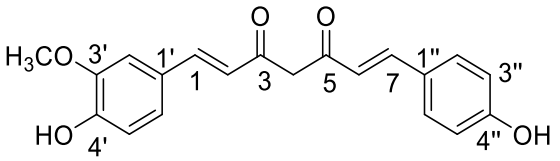


Figure 67S. ^{1}H-NMR spectrum (500 MHz, $CDCl_3$) of demethoxycurcumin (**12**)