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**General Synthetic Procedures**

Unless stated otherwise, all reactions were performed in flame-dried glassware under an atmosphere of nitrogen or argon. Dry tetrahydrofuran (THF), dichloromethane, diethyl ether, toluene, dimethylformamide (DMF), and hexane were obtained by passing these previously degassed solvents through activated alumina columns. When mentioned, further solvent degassing was performed by bubbling a stream of argon through the solvent in an ultrasound bath for a period of approximately ten minutes. Anhydrous DMSO was purchased from Aldrich stored over molecular sieves and used as received. Compound **20** was prepared according to the procedure of Ting, Xu, Zeng, and Maimone (*JACS*, **2016**, *138*, 14868). All other reagents were used as received, unless stated otherwise. Reactions were monitored by thin layer chromatography (TLC) on Silicycle Siliaplate$^{TM}$ glass backed TLC plates (250 μm thickness, 60 Å porosity, F-254 indicator) and visualized by UV irradiation or development with an anisaldehyde or phosphomolybdic/cerium sulfate stain. Volatile solvents were removed under reduced pressure with a rotary evaporator. All flash column chromatography was performed using Silicycle SiliaFlash® F60, 230-400 mesh silica gel (40-63 μm). $^{1}$H NMR and $^{13}$C NMR spectra were recorded with Bruker AV, AVQ, and DRX spectrometers operating at 300, 400, 500, 600, or 900 MHz for $^{1}$H (75, 100, 125, 150, 225 MHz for $^{13}$C) in $CDCl_3$, benzene-$d_6$, $CD_2Cl_2$, $CD_3OD$, or acetone-$d_6$. Chemical shifts are reported relative to the residual solvent signal ($^{1}$H NMR: δ = 7.26 ($CDCl_3$); $^{13}$C NMR: δ = 77.16 ($CDCl_3$)). NMR data are reported as follows: chemical shift (multiplicity, coupling constants where applicable, number of hydrogens). Splitting is reported with the following symbols: s = singlet, bs = broad singlet, d = doublet, t = triplet, app t = apparent triplet, dd = doublet of doublets, ddd = doublet of doublet of doublets, dt = doublet of triplets, hept = heptet, m = multiplet. IR spectra were taken on a Nicolet 380 spectrometer as thin films and are reported in frequency of absorption ($cm^{-1}$). Only selected resonances are reported. High-resolution mass spectra (HRMS) were obtained by the mass spectral facility at the University of California, Berkeley using a Finnigan LTQFT mass spectrometer (Thermo electron corporation).

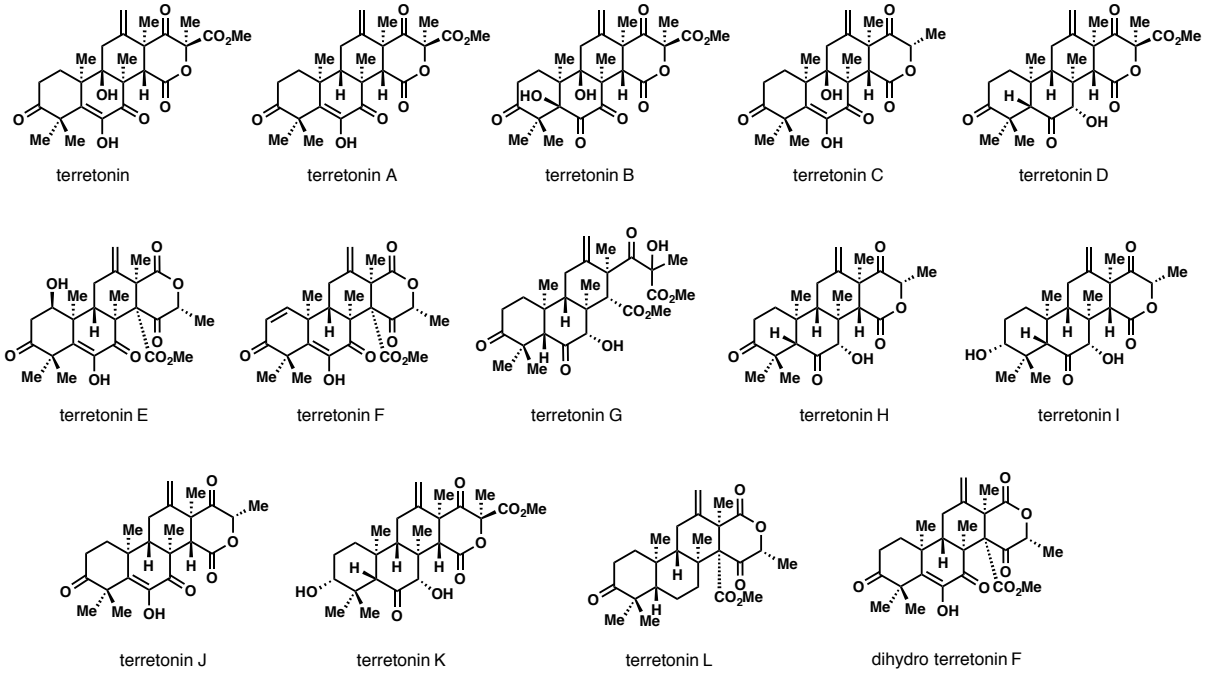
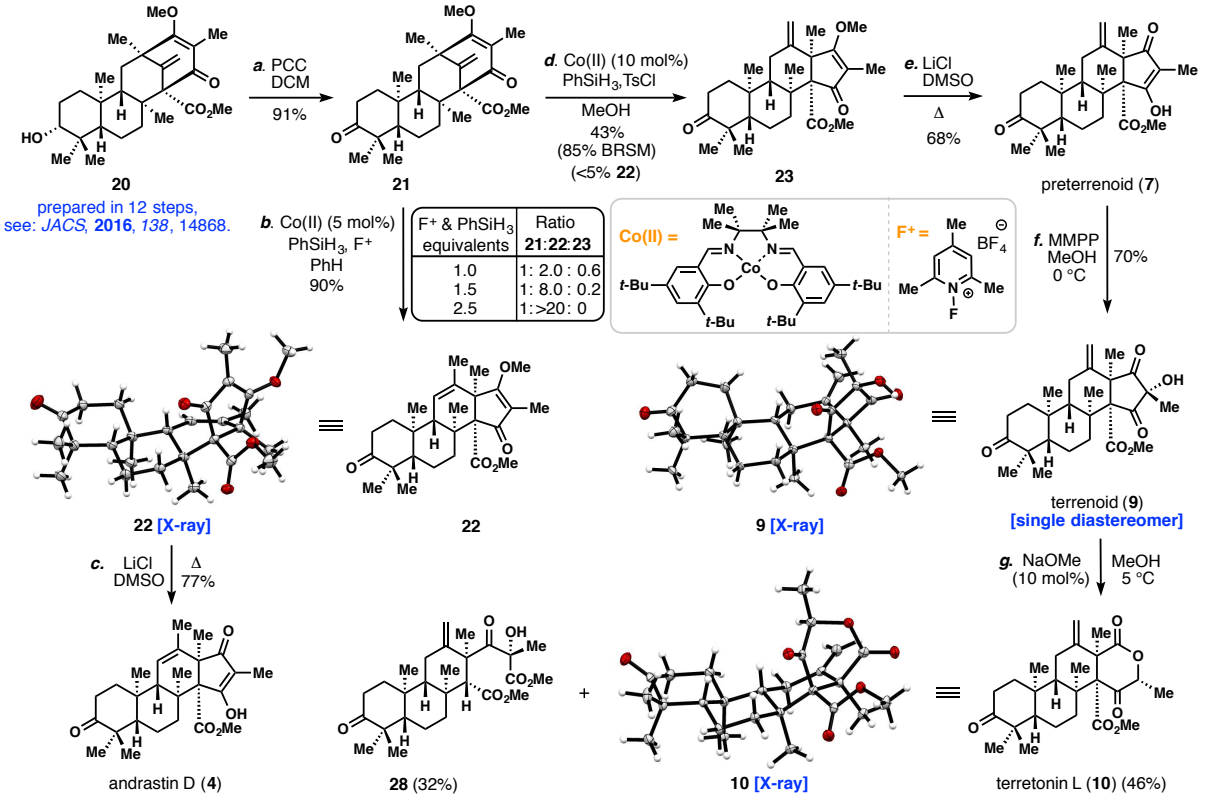
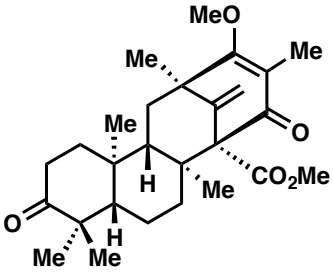


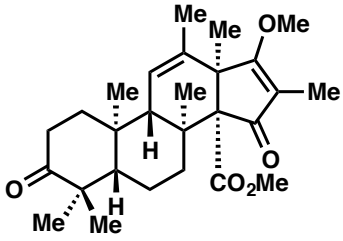

**Figure SI-1**. List of terretonin meroterpenes




**Scheme 1.** Total syntheses of andrastin D (**4**), preterrenoid (**7**), terrenoid (**9**), and terretonin L (**10**).

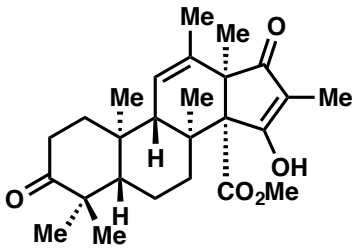



**Ketone 21**. To a solution of alcohol **20** (60.0 mg, 0.14 mmol, 1.0 equiv) in DCM (4.0 mL) was added pyridinium chlorochromate (116 mg, 0.54 mmol, 3.8 equiv) at room temperature. The reaction mixture was stirred for 2 hours at room temperature, filtered through a short pad of celite, and concentrated *in vacuo*. The crude product was purified by silica gel column chromatography (EtOAc/hexane = 1:5) affording ketone **21** (54.4 mg, 91% yield) as a white solid: (mp = 210-212 °C); $^{1}$H NMR (600 MHz, $CDCl_3$) δ 5.05 (s, 1H), 4.47 (s, 1H), 3.89 (s, 3H), 3.64 (s, 3H), 2.47-2.38 (m, 2H), 2.32 (dt, *J* = 13.6, 3.4 Hz, 1H), 1.91 (s, 3H), 1.83 (ddd, *J* = 12.7, 7.6, 4.9 Hz, 1H), 1.73-1.66 (m, 1H), 1.60-1.50 (m, 3H), 1.45 (t, *J* = 13.0 Hz, 1H), 1.40 (s, 3H), 1.36 (dd, *J* = 11.0, 4.2 Hz, 1H), 1.25-1.19 (m, 1H), 1.17 (s, 3H), 1.12 (dd, *J* = 12.6, 3.5 Hz, 1H), 1.05 (s, 3H), 1.02 (s, 3H), 0.95 (s, 3H); $^{13}$C NMR (150 MHz, $CDCl_3$) δ 217.30, 197.14, 175.20, 170.61, 149.14, 120.93, 108.01, 73.24, 61.93, 54.39, 51.55, 50.88, 47.34, 45.17, 42.75, 39.45, 37.19, 33.95, 33.87, 31.98, 27.01, 21.20, 21.03, 19.95, 17.23, 15.79, 10.43; IR (neat) 2978, 2953, 2865, 1733, 1705, 1659, 1623, 1459, 1434, 1387, 1326, 1304, 1217, 1191, 1159, 1106, 905, 751 cm$^{-1}$; HRMS (EI) calcd. for [$C_{27}H_{38}O_5$]: m/z 442.2719, found 442.2719.

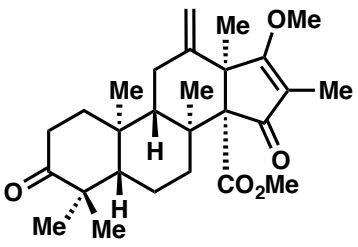



**Ketone 22**. A 15 mL flame-dried reaction tube was charged with ketone **21** (50 mg, 0.11 mmol, 1.0 equiv), Co(II) complex (3.5 mg, 5 mol %) and *N*-fluoro-2,4,6-trimethylpyridinium tetrafluoroborate (64.1 mg, 0.28 mmol, 2.5 equiv). The reaction vessel was evacuated and backfilled with nitrogen and this process was repeated twice. Degassed benzene (3.0 mL) was added, followed by a solution of phenylsilane (10% in degassed benzene, 0.35 mL, 2.5 equiv.) under nitrogen. The resulting mixture was stirred at room temperature for two hours at which point the reaction mixture was concentrated *in vacuo* and the crude material purified by silica gel column chromatography (EtOAc/hexanes = 1:5) affording **22** (45.1 mg, 90%) as a colorless solid: (mp = 174-176 °C); $^{1}$H NMR (600 MHz, $CDCl_3$) δ 5.32 (s, 1H), 4.12 (s, 3H), 3.59 (s, 3H), 3.06 (td, *J* = 13.1, 4.4 Hz, 1H), 2.51 (ddd, *J* = 15.8, 10.8, 7.2 Hz, 1H), 2.37 (ddd, *J* = 15.8, 7.0, 3.9 Hz, 1H), 1.98-1.87 (m, 5H), 1.90 (s, 3H), 1.86-1.83 (m, 1H), 1.65-1.56 (m, 1H), 1.55-1.50 (m, 1H), 1.48 (dd, *J* = 12.3, 2.6 Hz, 1H); 1.38-1.32 (m, 1H), 1.31 (s, 3H), 1.25 (s, 3H), 1.08 (s, 3H), 1.02 (s, 3H), 0.98 (s, 3H); $^{13}$C NMR (150 MHz, $CDCl_3$) δ 217.50, 204.52, 184.40, 170.57, 138.28, 124.97, 110.60, 69.79, 59.49, 53.49, 52.84, 51.86, 51.74,

47.57, 42.89, 38.57, 36.60, 33.96, 31.71, 26.33, 21.24, 21.02, 19.01, 17.50, 16.78, 16.58, 8.75; IR (neat) 2953, 2920, 2851, 1736, 1702, 1627, 1453, 1382, 1310, 1263, 1204, 1151, 1135, 1031, 979 $cm^{-1}$; HRMS (EI) calcd. for [$C_{27}H_{38}O_5$]: m/z 442.2719, found 442.2726.

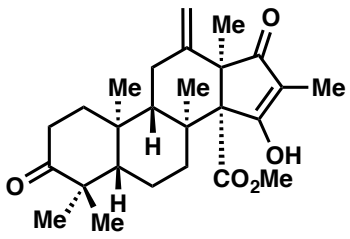



**Andrastin D** (**4**). [Note: Solvents used were degassed with argon for 10 minutes prior to use]. A 10 mL flame-dried reaction tube was charged with ketone **22** (11.7 mg, 0.026 mmol, 1 equiv) and dry lithium chloride (44.8 mg, 1.06 mmol, 40 equiv). The reaction vessel was evacuated and backfilled with nitrogen and this process was repeated twice. DMSO (1.0 mL) was added and the mixture heated to 120 °C for 2 hours. The reaction mixture was then cooled to room temperature, diluted with saturated aq. $NH_4Cl$ solution (5 mL), and extracted with diethyl ether (3 x 2 mL). The combined organic layers extracts were washed with $H_2O$ (3 x 1 mL), brine (1 mL), dried over $MgSO_4$, and concentrated *in vacuo*. The crude residue was purified by column chromatography (EtOAc/hexanes = 2:3) to afford andrastin D (**4**) (8.6 mg, 77% yield) as a colorless solid: $^1$H NMR (600 MHz, $CD_3OD$) δ 5.43 (s, 1H), 3.57 (s, 3H), 2.80 (td, *J* = 13.2, 4.2 Hz, 1H), δ 2.64 (ddd, *J* = 16.0, 11.5, 7.0 Hz, 1H), 2.35 (ddd, *J* = 16.0, 6.5, 3.6 Hz, 1H), 2.14 (dt, *J* = 13.4, 3.4 Hz, 1H), 2.07 (ddd, *J* = 13.3, 7.1, 3.6 Hz, 1H), 1.81 (s, 4H), 1.71 (qd, *J* = 13.3, 3.8 Hz, 1H), 1.60-1.50 (m, 1H), 1.57 (s, 3H), 1.46 (dd, *J* = 12.3, 2.5 Hz, 1H), 1.38-1.26 (m, 1H), 1.34 (s, 3H), 1.20 (s, 3H), 1.09 (s, 3H), 1.07 (s, 3H), 1.06 (s, 3H); $^{13}$C NMR (150 MHz, $CD_3OD$) δ 219.71, 201.29*, 188.16*, 172.05, 137.04, 125.65, 114.50, 68.99, 58.08, 55.64, 54.02, 52.01, 48.57, 43.16, 39.92, 37.74, 34.88, 33.64, 26.57, 21.56, 20.18, 19.87, 18.03, 16.73, 16.21, 6.32; IR (neat) 2951, 2934, 2875, 1737, 1701, 1617, 1454, 1383, 1323, 1210, 1137, 1112, 1029, 1002, 736 $cm^{-1}$; HRMS (EI) calcd. for [$C_{26}H_{36}O_5$]: m/z 428.2563, found 428.2565. [Note: Carbons with an asterisk were identified in the HMBC spectrum]



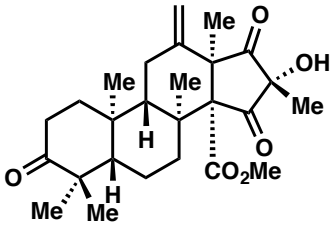

**Ketone 23**. A 10 mL flame-dried reaction tube was charged with ketone **21** (10.2 mg, 0.023 mmol, 1.0 equiv), Co(II) complex (1.4 mg, 10 mol%) and additional Schiff base ligand (6.3 mg, 0.5 equiv). The reaction vessel was evacuated and backfilled with nitrogen (a total of three times) and degassed MeOH (1.0 mL) was

added followed by a solution of phenylsilane (0.14 mL, 5% (v/v) solution in degassed benzene, 2.5 equiv.). A solution of TsCl (6.6 mg, 0.035 mmol, 1.5 equiv) in degassed benzene (0.1 mL) was then added dropwise over 20 min at rt under argon. After 3 hours of stirring, the solvent was evaporated and the residue purified by preparative thin layer chromatograhy (EtOAc/hexanes = 2:3) to afford recovered **21** (5.0 mg) and ketone **23** (4.4 mg, 43% yield) as colorless solid: (mp = 193-195 °C); $^{1}$H NMR (600 MHz, $CDCl_3$) δ 5.09-5.04 (m, 2H), δ 4.07 (s, 3H), 3.61 (s, 3H), 2.80 (td, *J* = 13.0, 4.4 Hz, 1H), 2.49 (ddd, *J* = 16.0, 11.0, 7.3 Hz, 1H), 2.33 (ddd, *J* = 15.9, 6.9, 3.7 Hz, 1H), 2.30-2.19 (m, 2H), 1.97 (s, 3H), 1.77-1.70 (m, 2H), 1.57-1.38 (m, 4H), 1.36 (s, 3H), 1.34-1.27 (m, 1H), 1.33 (s, 3H), 1.07 (s, 3H), 1.04 (s, 3H), 1.02 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 217.43, 204.37, 182.30, 170.64, 148.19, 113.13, 112.72, 70.20, 59.85, 54.13, 53.13, 51.52, 48.92, 47.57, 43.30, 38.25, 37.86, 33.86, 33.26, 29.79, 26.44, 21.41, 19.23, 19.18, 19.12, 15.03, 8.71; IR (neat) 2950, 2849, 1735, 1702, 1627, 1457, 1382, 1308, 1258, 1200, 1155, 1114, 1038, 983, 768, 736 cm$^{-1}$; HRMS (EI) calcd. for [$C_{27}H_{38}O_5$]: m/z 442.2719, found 442.2722.

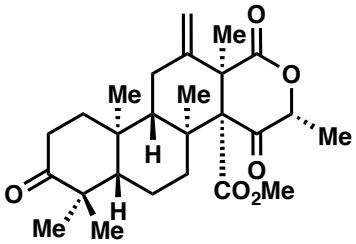



**Preterrenoid (7)**. [Note: Solvents used were degassed with argon for 10 minutes prior to use]. A 10 mL flame-dried reaction tube was charged with ketone **23** (11.1 mg, 0.025 mmol, 1 equiv) and dry lithium chloride (42.4 mg, 1.0 mmol, 40 equiv). The reaction vessel was evacuated and backfilled with nitrogen and this process repeated twice. DMSO (1.0 mL) was added and the reaction mixture heated to 120 °C and kept at this temperature for 1.5 h. The reaction mixture was then cooled to room temperature, diluted with sat. $NH_4Cl$ solution, and extracted with diethyl ether (3 x 2 mL). The combined organic layers extracts were washed with $H_2O$ (3 x 1 mL), washed with brine (1 mL), dried over $MgSO_4$, and concentrated *in vacuo*. The crude residue was purified by preparative thin layer chromatograhy (EtOAc/hexanes = 2:1) to afford preterrenoid (**7**) (7.3 mg, 68% yield) as a foam: $^{1}$H NMR (600 MHz, $CDCl_3$) δ 9.66 (s, 1H), 5.20 (s, 1H), 5.14 (d, *J* = 2.9 Hz, 1H), 3.80 (s, 3H), 2.52-2.33 (m, 3H), 2.26 (dd, *J* = 16.6, 11.9 Hz, 1H), 1.88-1.70 (m, 2H), 1.75 (s, 3H), 1.54-1.46 (m, 2H), 1.45-1.33 (m, 3H), 1.32 (s, 3H), 1.24-1.18 (m, 1H), 1.07 (s, 3H), 1.04 (s, 3H), 1.02 (s, 3H), 0.97 (s, 3H); $^{13}$C NMR (151 MHz, $CDCl_3$) δ 216.97, 205.28, 177.36, 175.33, 143.56, 113.84, 113.09, 68.09, 57.77, 55.15, 52.02, 47.22, 44.73, 44.65, 39.26, 38.04, 37.97, 33.87, 28.84, 27.16, 23.66, 21.63, 19.97, 19.53, 15.91, 6.15; IR (neat) 3214, 2951, 2936, 2873, 1738, 1704,

1632, 1458, 1390, 1345, 1316, 1223, 1202, 1144, 1112, 1034, 1003, 920, 735 $cm^{-1}$; HRMS (EI) calcd. for $[C_{26}H_{36}O_5]$: m/z 428.2563, found 428.2565.




Terrenoid (**9**). [Note: Solvents used were degassed with argon for 10 minutes prior to use.] To a solution of preterrenoid (**7**) (17.6 mg, 0.041 mmol) in a mixture of methanol (1.2 mL) and dichloromethane (0.4 mL) was added a solution of magnesium monoperoxphthalate (80% purity, 50.7 mg, 0.082 mmol, 2 equiv) in MeOH (0.36 mL) dropwise at 0 °C. The solution was stirred at the same temperature for 2 h, and after evaporation of most of the solvent at 0 °C, the residue was diluted with a mixture of saturated aqueous $Na_2S_2O_3$ (0.5 mL) and saturated aqueous $NaHCO_3$ (1.0 mL), and extracted with ethyl acetate (3 x 2 mL). The combined organic layers extracts were washed with brine (1 mL), dried over $MgSO_4$, and concentrated *in vacuo*. The crude residue was purified by preparative thin layer chromatograhy (diethyl ether/hexanes = 2:1) to afford terrenoid (**9**) (12.7 mg, 70% yield) as a colorless solid: (mp = 194-196 °C); $^1$H NMR (900 MHz, $CDCl_3$) δ 5.07 (dd, *J* = 2.6, 1.1 Hz, 1H), 4.91 (d, *J* = 2.7 Hz, 1H), 3.65 (s, 3H), 2.94 (td, *J* = 12.7, 5.2 Hz, 1H), 2.65-2.60 (m, 2H), 2.50 (ddd, *J* = 15.8, 9.8, 7.5 Hz, 1H), 2.45 (ddd, *J* = 15.8, 7.6, 4.5 Hz, 1H), 2.38 (dd, *J* = 16.4, 3.9 Hz, 1H), 2.15 (dt, *J* = 13.6, 3.3 Hz, 1H), 1.95 (ddd, *J* = 13.1, 7.5, 4.5 Hz, 1H), 1.61-1.51 (m, 3H), 1.53 (s, 3H), 1.44-1.40 (m, 1H), 1.39 (s, 3H), 1.38 (s, 3H), 1.30 (dd, *J* = 13.8, 3.9 Hz, 1H), 1.13 (s, 3H), 1.06 (s, 3H), 1.02 (s, 3H); $^{13}$C NMR (225 MHz, $CDCl_3$) δ 217.13, 211.27, 210.14, 168.77, 143.76, 116.55, 75.37, 73.77, 57.60, 53.59, 52.58, 50.46, 47.38, 40.60, 39.24, 37.15, 33.92, 32.94, 28.24, 26.93, 25.84, 23.78, 21.40, 19.08, 18.05, 15.74; IR (neat) 3457, 2953, 2874, 1754, 1729, 1704, 1459, 1389, 1077, 920 $cm^{-1}$; HRMS (ESI) calcd. for $[C_{26}H_{36}O_6Na]^+$ $(M+Na)^+$: m/z 467.2404, found 467.2412.




**Terretonin L (10)**. To a solution of terrenoid (**9**) (3.5 mg, 0.0079 mmol) in dry methanol (0.4 mL) was added a solution of NaOMe (0.043 mg, 0.00080 mmol, 0.1 equiv) in MeOH (0.02 mL) dropwise at 0 °C. The solution was then stirred at 5 °C for 24 h. The reaction mixture was quenched with saturated aq. $NH_4Cl$ solution (1.0 mL) and extracted with diethyl ether (3 x 2 mL). The

combined organic layers extracts were washed with brine (1 mL), dried over $MgSO_4$, and concentrated *in vacuo*. The crude residue was purified by preparative thin layer chromatography (diethyl ether/DCM = 1:20) to afford terretonin L (**10**) (1.6 mg, 46% yield) and diester **24** (1.2 mg, 32% yield). **Terretonin L (10)**: $^1$H NMR (500 MHz, $CDCl_3$) δ 5.04 (d, *J* = 2.3 Hz, 1H), 5.01 (q, *J* = 6.5 Hz, 1H), 4.98 (d, *J* = 2.3 Hz, 1H), 3.64 (s, 3H), 2.69-2.60 (m, 1H), 2.55-2.40 (m, 3H), 2.21 (td, *J* = 12.7, 4.1 Hz, 1H), 2.09 (dt, *J* = 13.7, 3.4 Hz, 1H), 2.02-1.94 (m, 1H), 1.68 (s, 3H), 1.65-1.51 (m, 2H), 1.47 (s, 3H), 1.44-1.38 (m, 1H), 1.41 (d, *J* = 6.4 Hz, 3H), 1.35 (dd, *J* = 12.1, 2.9 Hz, 1H), 1.20 (dd, *J* = 13.6, 3.3 Hz, 1H), 1.09 (s, 3H), 1.05 (s, 3H), 1.00 (s, 3H); $^{13}$C NMR (225 MHz, $CDCl_3$) δ 216.89, 203.11, 172.07, 167.61, 145.37, 113.05, 77.36, 69.06, 54.42, 54.03, 52.48, 51.64, 47.36, 43.63, 39.24, 37.55, 33.86, 33.69, 28.75, 26.88, 25.47, 21.29, 19.81, 19.22, 15.86, 15.44; IR (neat) 2953, 2924, 2872, 1753, 1723, 1704, 1454, 1391, 1229, 1211, 1177, 1156, 1118, 1064, 1034, 918 $cm^{-1}$; HRMS (EI) calcd. for $[C_{26}H_{36}O_6]$: m/z 444.2512, found 444.2505. **Diester 28**: $^1$H NMR (600 MHz, $CDCl_3$) δ 4.77 (s, 1H), 4.24 (d, *J* = 2.3 Hz, 1H), 3.82 (s, 3H), 3.56 (s, 3H), 3.42 (s, 1H), 2.57-2.41 (m, 4H), 1.98 (ddd, *J* = 12.5, 7.5, 4.4 Hz, 1H), 1.95-1.90 (m, 1H), 1.70 (s, 3H), 1.63-1.46 (m, 5H), 1.33-1.18 (m, 2H), 1.32 (s, 3H), 1.29 (s, 3H), 1.09 (s, 3H), 1.05 (s, 3H), 0.98 (s, 3H); $^{13}$C NMR (150 MHz, $CDCl_3$) δ 217.30, 207.31, 174.47, 171.75, 148.46, 111.43, 82.45, 57.48, 55.12, 54.87, 54.20, 53.62, 50.85, 47.43, 40.30, 38.98, 37.21, 36.72, 34.01, 27.89, 26.98, 26.82, 24.81, 21.29, 19.12, 15.53, 15.52; IR (neat) 3472, 2951, 2931, 2852, 1738, 1711, 1451, 1383, 1264, 1193, 1171, 1131, 1007 $cm^{-1}$; HRMS (ESI) calcd. for $[C_{27}H_{40}O_7Na]^{\cdot}$ $(M+Na)^{\cdot}$: m/z 499.2666, found 499.2677.

**X-Ray Crystallography Data**

Table 1. Crystal data and structure refinement for ketone **22**

| | | |
|---|---|---|
| X-ray ID | ketone **22** | |
| Sample/notebook ID | XG-II-75-1 | |
| Empirical formula | C27 H38 O5 | |
| Formula weight | 442.57 | |
| Temperature | 100(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Orthorhombic | |
| Space group | P n a 21 | |
| Unit cell dimensions | a = 14.7846(7) Å | $\alpha$= 90°. |
| | b = 12.5507(5) Å | $\beta$= 90°. |
| | c = 13.1718(6) Å | $\gamma$ = 90°. |
| Volume | 2444.12(19) $Å^3$ | |
| Z | 4 | |
| Density (calculated) | 1.203 $Mg/m^3$ | |
| Absorption coefficient | 0.081 $mm^{-1}$ | |
| F(000) | 960 | |
| Crystal size | 0.070 x 0.050 x 0.050 $mm^3$ | |
| Theta range for data collection | 2.129 to 25.369°. | |
| Index ranges | -17<=h<=17, -15<=k<=15, -15<=l<=15 | |
| Reflections collected | 57579 | |
| Independent reflections | 4465 [R(int) = 0.0382] | |
| Completeness to theta = 25.000° | 100.0 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.928 and 0.898 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 4465 / 1 / 298 | |
| Goodness-of-fit on $F^2$ | 1.057 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0356, wR2 = 0.0863 | |
| R indices (all data) | R1 = 0.0405, wR2 = 0.0894 | |
| Absolute structure parameter | 0.0(2) | |
| Extinction coefficient | n/a | |
| Largest diff. peak and hole | 0.201 and -0.182 $e.Å^{-3}$ | |

Table 2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for ketone **22**. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| C(1) | 6326(2) | 5325(2) | 4640(2) | 19(1) |
| C(2) | 7014(2) | 5093(2) | 5511(2) | 20(1) |
| C(3) | 7016(2) | 5948(2) | 6242(2) | 23(1) |
| C(4) | 6387(2) | 6663(2) | 5950(2) | 21(1) |
| C(5) | 5779(2) | 6301(2) | 5080(2) | 19(1) |
| C(6) | 4891(2) | 5945(2) | 5599(2) | 19(1) |
| C(7) | 4713(2) | 4927(2) | 5777(2) | 20(1) |
| C(8) | 5283(2) | 4016(2) | 5400(2) | 18(1) |
| C(9) | 4806(2) | 2907(2) | 5462(2) | 20(1) |
| C(10) | 4646(2) | 2669(2) | 6596(2) | 22(1) |
| C(11) | 4325(2) | 1524(2) | 6781(2) | 23(1) |
| C(12) | 4944(2) | 702(2) | 6334(2) | 24(1) |
| C(13) | 5297(2) | 876(2) | 5252(2) | 23(1) |
| C(14) | 5505(2) | 2082(2) | 5069(2) | 21(1) |
| C(15) | 5780(2) | 2340(2) | 3976(2) | 24(1) |
| C(16) | 6276(2) | 3403(2) | 3927(2) | 22(1) |
| C(17) | 5715(2) | 4338(2) | 4363(2) | 18(1) |
| C(18) | 6912(2) | 5680(2) | 3729(2) | 21(1) |
| C(19) | 8151(2) | 6725(3) | 3219(2) | 36(1) |
| C(20) | 7668(2) | 5904(2) | 7113(2) | 33(1) |
| C(21) | 6717(2) | 8128(2) | 7071(2) | 28(1) |
| C(22) | 5604(2) | 7202(2) | 4314(2) | 23(1) |
| C(23) | 4246(2) | 6804(2) | 5947(2) | 25(1) |
| C(24) | 3886(2) | 2908(2) | 4908(2) | 25(1) |
| C(25) | 6177(2) | 232(2) | 5126(2) | 31(1) |
| C(26) | 4583(2) | 406(2) | 4526(2) | 28(1) |
| C(27) | 4999(2) | 4652(2) | 3560(2) | 22(1) |
| O(1) | 6818(1) | 5419(1) | 2859(1) | 26(1) |
| O(2) | 7576(1) | 6344(2) | 4031(1) | 27(1) |
| O(3) | 7509(1) | 4310(1) | 5542(2) | 26(1) |
| O(4) | 6170(1) | 7627(1) | 6309(1) | 26(1) |

| | | | | |
|---|---|---|---|---|
| O(5) | 5133(2) | -96(2) | 6810(2) | 40(1) |

Table 3. Bond lengths [Å] and angles [°] for ketone **22**

| | | | |
|---|---|---|---|
| C(1)-C(18) | 1.545(3) | C(14)-H(14) | 1.0000 |
| C(1)-C(2) | 1.561(3) | C(15)-C(16) | 1.524(4) |
| C(1)-C(17) | 1.575(3) | C(15)-H(15A) | 0.9900 |
| C(1)-C(5) | 1.578(3) | C(15)-H(15B) | 0.9900 |
| C(2)-O(3) | 1.226(3) | C(16)-C(17) | 1.547(3) |
| C(2)-C(3) | 1.443(4) | C(16)-H(16A) | 0.9900 |
| C(3)-C(4) | 1.348(4) | C(16)-H(16B) | 0.9900 |
| C(3)-C(20) | 1.499(4) | C(17)-C(27) | 1.548(3) |
| C(4)-O(4) | 1.339(3) | C(18)-O(1) | 1.201(3) |
| C(4)-C(5) | 1.526(3) | C(18)-O(2) | 1.347(3) |
| C(5)-C(22) | 1.537(3) | C(19)-O(2) | 1.448(3) |
| C(5)-C(6) | 1.546(3) | C(19)-H(19A) | 0.9800 |
| C(6)-C(7) | 1.325(4) | C(19)-H(19B) | 0.9800 |
| C(6)-C(23) | 1.511(3) | C(19)-H(19C) | 0.9800 |
| C(7)-C(8) | 1.505(3) | C(20)-H(20A) | 0.9800 |
| C(7)-H(7) | 0.9500 | C(20)-H(20B) | 0.9800 |
| C(8)-C(17) | 1.562(3) | C(20)-H(20C) | 0.9800 |
| C(8)-C(9) | 1.563(3) | C(21)-O(4) | 1.434(3) |
| C(8)-H(8) | 1.0000 | C(21)-H(21A) | 0.9800 |
| C(9)-C(10) | 1.542(3) | C(21)-H(21B) | 0.9800 |
| C(9)-C(24) | 1.544(3) | C(21)-H(21C) | 0.9800 |
| C(9)-C(14) | 1.552(3) | C(22)-H(22A) | 0.9800 |
| C(10)-C(11) | 1.533(3) | C(22)-H(22B) | 0.9800 |
| C(10)-H(10A) | 0.9900 | C(22)-H(22C) | 0.9800 |
| C(10)-H(10B) | 0.9900 | C(23)-H(23A) | 0.9800 |
| C(11)-C(12) | 1.500(4) | C(23)-H(23B) | 0.9800 |
| C(11)-H(11A) | 0.9900 | C(23)-H(23C) | 0.9800 |
| C(11)-H(11B) | 0.9900 | C(24)-H(24A) | 0.9800 |
| C(12)-O(5) | 1.215(3) | C(24)-H(24B) | 0.9800 |
| C(12)-C(13) | 1.533(4) | C(24)-H(24C) | 0.9800 |
| C(13)-C(25) | 1.541(4) | C(25)-H(25A) | 0.9800 |
| C(13)-C(26) | 1.541(4) | C(25)-H(25B) | 0.9800 |
| C(13)-C(14) | 1.564(3) | C(25)-H(25C) | 0.9800 |
| C(14)-C(15) | 1.531(4) | C(26)-H(26A) | 0.9800 |

| | | | |
|---|---|---|---|
| C(26)-H(26B) | 0.9800 | C(27)-H(27B) | 0.9800 |
| C(26)-H(26C) | 0.9800 | C(27)-H(27C) | 0.9800 |
| C(27)-H(27A) | 0.9800 | | |

| | | | |
|---|---|---|---|
| C(18)-C(1)-C(2) | 104.96(18) | C(9)-C(8)-H(8) | 105.2 |
| C(18)-C(1)-C(17) | 111.6(2) | C(10)-C(9)-C(24) | 108.8(2) |
| C(2)-C(1)-C(17) | 113.39(19) | C(10)-C(9)-C(14) | 107.3(2) |
| C(18)-C(1)-C(5) | 110.43(19) | C(24)-C(9)-C(14) | 115.5(2) |
| C(2)-C(1)-C(5) | 102.04(19) | C(10)-C(9)-C(8) | 106.97(19) |
| C(17)-C(1)-C(5) | 113.68(18) | C(24)-C(9)-C(8) | 111.9(2) |
| O(3)-C(2)-C(3) | 125.0(2) | C(14)-C(9)-C(8) | 106.02(18) |
| O(3)-C(2)-C(1) | 124.3(2) | C(11)-C(10)-C(9) | 112.5(2) |
| C(3)-C(2)-C(1) | 110.7(2) | C(11)-C(10)-H(10A) | 109.1 |
| C(4)-C(3)-C(2) | 107.6(2) | C(9)-C(10)-H(10A) | 109.1 |
| C(4)-C(3)-C(20) | 133.3(2) | C(11)-C(10)-H(10B) | 109.1 |
| C(2)-C(3)-C(20) | 119.0(2) | C(9)-C(10)-H(10B) | 109.1 |
| O(4)-C(4)-C(3) | 131.8(2) | H(10A)-C(10)-H(10B) | 107.8 |
| O(4)-C(4)-C(5) | 113.1(2) | C(12)-C(11)-C(10) | 113.2(2) |
| C(3)-C(4)-C(5) | 115.0(2) | C(12)-C(11)-H(11A) | 108.9 |
| C(4)-C(5)-C(22) | 111.9(2) | C(10)-C(11)-H(11A) | 108.9 |
| C(4)-C(5)-C(6) | 104.75(19) | C(12)-C(11)-H(11B) | 108.9 |
| C(22)-C(5)-C(6) | 111.11(19) | C(10)-C(11)-H(11B) | 108.9 |
| C(4)-C(5)-C(1) | 101.84(19) | H(11A)-C(11)-H(11B) | 107.8 |
| C(22)-C(5)-C(1) | 114.6(2) | O(5)-C(12)-C(11) | 120.4(3) |
| C(6)-C(5)-C(1) | 111.91(19) | O(5)-C(12)-C(13) | 121.3(2) |
| C(7)-C(6)-C(23) | 120.6(2) | C(11)-C(12)-C(13) | 118.3(2) |
| C(7)-C(6)-C(5) | 121.7(2) | C(12)-C(13)-C(25) | 108.2(2) |
| C(23)-C(6)-C(5) | 117.6(2) | C(12)-C(13)-C(26) | 106.8(2) |
| C(6)-C(7)-C(8) | 124.3(2) | C(25)-C(13)-C(26) | 108.1(2) |
| C(6)-C(7)-H(7) | 117.9 | C(12)-C(13)-C(14) | 110.4(2) |
| C(8)-C(7)-H(7) | 117.9 | C(25)-C(13)-C(14) | 108.9(2) |
| C(7)-C(8)-C(17) | 108.7(2) | C(26)-C(13)-C(14) | 114.2(2) |
| C(7)-C(8)-C(9) | 114.00(19) | C(15)-C(14)-C(9) | 110.4(2) |
| C(17)-C(8)-C(9) | 117.43(19) | C(15)-C(14)-C(13) | 113.7(2) |
| C(7)-C(8)-H(8) | 105.2 | C(9)-C(14)-C(13) | 117.6(2) |
| C(17)-C(8)-H(8) | 105.2 | C(15)-C(14)-H(14) | 104.5 |

| | | | |
|---|---|---|---|
| C(9)-C(14)-H(14) | 104.5 | O(4)-C(21)-H(21B) | 109.5 |
| C(13)-C(14)-H(14) | 104.5 | H(21A)-C(21)-H(21B) | 109.5 |
| C(16)-C(15)-C(14) | 110.6(2) | O(4)-C(21)-H(21C) | 109.5 |
| C(16)-C(15)-H(15A) | 109.5 | H(21A)-C(21)-H(21C) | 109.5 |
| C(14)-C(15)-H(15A) | 109.5 | H(21B)-C(21)-H(21C) | 109.5 |
| C(16)-C(15)-H(15B) | 109.5 | C(5)-C(22)-H(22A) | 109.5 |
| C(14)-C(15)-H(15B) | 109.5 | C(5)-C(22)-H(22B) | 109.5 |
| H(15A)-C(15)-H(15B) | 108.1 | H(22A)-C(22)-H(22B) | 109.5 |
| C(15)-C(16)-C(17) | 112.97(19) | C(5)-C(22)-H(22C) | 109.5 |
| C(15)-C(16)-H(16A) | 109.0 | H(22A)-C(22)-H(22C) | 109.5 |
| C(17)-C(16)-H(16A) | 109.0 | H(22B)-C(22)-H(22C) | 109.5 |
| C(15)-C(16)-H(16B) | 109.0 | C(6)-C(23)-H(23A) | 109.5 |
| C(17)-C(16)-H(16B) | 109.0 | C(6)-C(23)-H(23B) | 109.5 |
| H(16A)-C(16)-H(16B) | 107.8 | H(23A)-C(23)-H(23B) | 109.5 |
| C(16)-C(17)-C(27) | 107.84(19) | C(6)-C(23)-H(23C) | 109.5 |
| C(16)-C(17)-C(8) | 110.32(19) | H(23A)-C(23)-H(23C) | 109.5 |
| C(27)-C(17)-C(8) | 112.59(19) | H(23B)-C(23)-H(23C) | 109.5 |
| C(16)-C(17)-C(1) | 112.01(18) | C(9)-C(24)-H(24A) | 109.5 |
| C(27)-C(17)-C(1) | 110.5(2) | C(9)-C(24)-H(24B) | 109.5 |
| C(8)-C(17)-C(1) | 103.62(18) | H(24A)-C(24)-H(24B) | 109.5 |
| O(1)-C(18)-O(2) | 122.3(2) | C(9)-C(24)-H(24C) | 109.5 |
| O(1)-C(18)-C(1) | 126.7(2) | H(24A)-C(24)-H(24C) | 109.5 |
| O(2)-C(18)-C(1) | 111.0(2) | H(24B)-C(24)-H(24C) | 109.5 |
| O(2)-C(19)-H(19A) | 109.5 | C(13)-C(25)-H(25A) | 109.5 |
| O(2)-C(19)-H(19B) | 109.5 | C(13)-C(25)-H(25B) | 109.5 |
| H(19A)-C(19)-H(19B) | 109.5 | H(25A)-C(25)-H(25B) | 109.5 |
| O(2)-C(19)-H(19C) | 109.5 | C(13)-C(25)-H(25C) | 109.5 |
| H(19A)-C(19)-H(19C) | 109.5 | H(25A)-C(25)-H(25C) | 109.5 |
| H(19B)-C(19)-H(19C) | 109.5 | H(25B)-C(25)-H(25C) | 109.5 |
| C(3)-C(20)-H(20A) | 109.5 | C(13)-C(26)-H(26A) | 109.5 |
| C(3)-C(20)-H(20B) | 109.5 | C(13)-C(26)-H(26B) | 109.5 |
| H(20A)-C(20)-H(20B) | 109.5 | H(26A)-C(26)-H(26B) | 109.5 |
| C(3)-C(20)-H(20C) | 109.5 | C(13)-C(26)-H(26C) | 109.5 |
| H(20A)-C(20)-H(20C) | 109.5 | H(26A)-C(26)-H(26C) | 109.5 |
| H(20B)-C(20)-H(20C) | 109.5 | H(26B)-C(26)-H(26C) | 109.5 |
| O(4)-C(21)-H(21A) | 109.5 | C(17)-C(27)-H(27A) | 109.5 |

| | |
|---|---|
| C(17)-C(27)-H(27B) | 109.5 |
| H(27A)-C(27)-H(27B) | 109.5 |
| C(17)-C(27)-H(27C) | 109.5 |
| H(27A)-C(27)-H(27C) | 109.5 |
| H(27B)-C(27)-H(27C) | 109.5 |
| C(18)-O(2)-C(19) | 114.5(2) |
| C(4)-O(4)-C(21) | 120.51(19) |

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for ketone **22**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| C(1) | 18(1) | 20(1) | 17(1) | 1(1) | 2(1) | 0(1) |
| C(2) | 15(1) | 24(1) | 20(1) | 3(1) | 2(1) | -1(1) |
| C(3) | 21(1) | 25(1) | 22(1) | 1(1) | -2(1) | 1(1) |
| C(4) | 23(1) | 20(1) | 19(1) | 2(1) | 2(1) | -4(1) |
| C(5) | 20(1) | 19(1) | 18(1) | 1(1) | 0(1) | 2(1) |
| C(6) | 18(1) | 24(1) | 16(1) | -1(1) | -2(1) | 4(1) |
| C(7) | 18(1) | 27(1) | 15(1) | -3(1) | 0(1) | -1(1) |
| C(8) | 19(1) | 21(1) | 15(1) | -2(1) | 1(1) | 0(1) |
| C(9) | 21(1) | 22(1) | 17(1) | -2(1) | 1(1) | -1(1) |
| C(10) | 24(1) | 21(1) | 20(1) | -3(1) | 1(1) | -2(1) |
| C(11) | 26(1) | 23(1) | 19(1) | 0(1) | 1(1) | -5(1) |
| C(12) | 28(1) | 23(1) | 21(1) | 0(1) | -4(1) | -4(1) |
| C(13) | 28(1) | 20(1) | 22(1) | -2(1) | 2(1) | -2(1) |
| C(14) | 24(1) | 21(1) | 19(1) | -2(1) | 0(1) | -1(1) |
| C(15) | 28(1) | 23(1) | 21(1) | -2(1) | 8(1) | 1(1) |
| C(16) | 24(1) | 23(1) | 20(1) | -2(1) | 4(1) | 1(1) |
| C(17) | 19(1) | 21(1) | 15(1) | -1(1) | 2(1) | 0(1) |
| C(18) | 19(1) | 22(1) | 22(1) | 3(1) | 0(1) | 3(1) |
| C(19) | 30(2) | 46(2) | 31(2) | 8(1) | 6(1) | -13(1) |
| C(20) | 33(2) | 39(2) | 28(2) | -3(1) | -11(1) | 5(1) |
| C(21) | 31(2) | 31(2) | 23(1) | -7(1) | -2(1) | -2(1) |
| C(22) | 25(1) | 23(1) | 22(1) | 2(1) | -1(1) | 3(1) |
| C(23) | 24(1) | 27(1) | 25(1) | -1(1) | 2(1) | 5(1) |
| C(24) | 24(1) | 28(1) | 22(1) | -4(1) | -2(1) | -4(1) |
| C(25) | 33(2) | 24(1) | 35(2) | -1(1) | 4(1) | 3(1) |
| C(26) | 38(2) | 25(1) | 23(1) | -7(1) | 1(1) | -6(1) |
| C(27) | 22(1) | 25(1) | 19(1) | -1(1) | 0(1) | 1(1) |
| O(1) | 27(1) | 32(1) | 18(1) | 0(1) | 2(1) | -3(1) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O(2) | 24(1) | 35(1) | 23(1) | 1(1) | 3(1) | -8(1) |
| O(3) | 23(1) | 26(1) | 29(1) | -1(1) | -3(1) | 6(1) |
| O(4) | 28(1) | 22(1) | 27(1) | -7(1) | -6(1) | 0(1) |
| O(5) | 56(1) | 34(1) | 31(1) | 10(1) | 10(1) | 11(1) |

Table 5. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters ($Å^2$x $10^3$) for ketone **22**.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(7) | 4191 | 4762 | 6167 | 24 |
| H(8) | 5801 | 3970 | 5887 | 22 |
| H(10A) | 5215 | 2790 | 6974 | 26 |
| H(10B) | 4187 | 3171 | 6864 | 26 |
| H(11A) | 4275 | 1402 | 7521 | 27 |
| H(11B) | 3714 | 1436 | 6483 | 27 |
| H(14) | 6062 | 2223 | 5478 | 26 |
| H(15A) | 6177 | 1769 | 3712 | 29 |
| H(15B) | 5233 | 2372 | 3543 | 29 |
| H(16A) | 6430 | 3561 | 3211 | 27 |
| H(16B) | 6849 | 3345 | 4312 | 27 |
| H(19A) | 8462 | 6120 | 2903 | 54 |
| H(19B) | 8600 | 7222 | 3496 | 54 |
| H(19C) | 7782 | 7091 | 2709 | 54 |
| H(20A) | 8192 | 6355 | 6963 | 50 |
| H(20B) | 7868 | 5167 | 7215 | 50 |
| H(20C) | 7370 | 6161 | 7730 | 50 |
| H(21A) | 6669 | 7727 | 7707 | 43 |
| H(21B) | 6506 | 8859 | 7180 | 43 |
| H(21C) | 7349 | 8139 | 6847 | 43 |
| H(22A) | 5301 | 7795 | 4657 | 35 |
| H(22B) | 5219 | 6936 | 3764 | 35 |
| H(22C) | 6181 | 7447 | 4033 | 35 |
| H(23A) | 3960 | 7135 | 5355 | 38 |
| H(23B) | 4580 | 7345 | 6330 | 38 |
| H(23C) | 3780 | 6489 | 6382 | 38 |
| H(24A) | 3985 | 2847 | 4175 | 37 |
| H(24B) | 3565 | 3573 | 5055 | 37 |
| H(24C) | 3522 | 2303 | 5143 | 37 |
| H(25A) | 6640 | 515 | 5585 | 46 |

| | | | | |
|---|---|---|---|---|
| H(25B) | 6389 | 289 | 4423 | 46 |
| H(25C) | 6062 | -518 | 5289 | 46 |
| H(26A) | 4773 | 523 | 3822 | 43 |
| H(26B) | 4000 | 757 | 4643 | 43 |
| H(26C) | 4521 | -360 | 4652 | 43 |
| H(27A) | 5286 | 5077 | 3025 | 33 |
| H(27B) | 4520 | 5072 | 3884 | 33 |
| H(27C) | 4737 | 4006 | 3262 | 33 |

Table 6. Crystal data and structure refinement for terretonin L (**10**)

| | | |
|---|---|---|
| Identification code | terretonin L | |
| Empirical formula | C26 H36 O6 | |
| Formula weight | 444.55 | |
| Temperature | 100(2) K | |
| Wavelength | 1.54178 ≈ | |
| Crystal system | Monoclinic | |
| Space group | P 21/n | |
| Unit cell dimensions | a = 9.7395(8) ≈ | α= 90∞. |
| | b = 23.1865(18) ≈ | β= 99.380(3)∞. |
| | c = 9.9111(8) ≈ | γ = 90∞. |
| Volume | 2208.2(3) ≈$^3$ | |
| Z | 4 | |
| Density (calculated) | 1.337 Mg/m$^3$ | |
| Absorption coefficient | 0.758 mm$^{-1}$ | |
| F(000) | 960 | |

| | |
|---|---|
| Crystal size | 0.100 x 0.100 x 0.080 $mm^3$ |
| Theta range for data collection | 3.813 to 68.341∞. |
| Index ranges | -11<=h<=11, -27<=k<=23, -11<=l<=11 |
| Reflections collected | 38470 |
| Independent reflections | 4040 [R(int) = 0.0283] |
| Completeness to theta = 67.000∞ | 99.9 % |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 0.753 and 0.706 |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 4040 / 0 / 296 |
| Goodness-of-fit on $F^2$ | 1.029 |
| Final R indices [I>2sigma(I)] | R1 = 0.0345, wR2 = 0.0877 |
| R indices (all data) | R1 = 0.0358, wR2 = 0.0888 |
| Extinction coefficient | n/a |
| Largest diff. peak and hole | 0.322 and -0.185 $e.\approx^{-3}$ |

Table 7. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($\approx^2$x $10^3$) for terretonin L (**10**). U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| C(1) | 5082(1) | 2509(1) | 7678(1) | 17(1) |
| C(2) | 4269(1) | 2848(1) | 6467(1) | 14(1) |
| C(3) | 4452(1) | 2523(1) | 5152(1) | 16(1) |
| C(4) | 3353(1) | 3354(1) | 3939(1) | 17(1) |
| C(5) | 3150(1) | 3565(1) | 2478(1) | 22(1) |
| C(6) | 4387(1) | 3717(1) | 4903(1) | 15(1) |
| C(7) | 4803(1) | 3494(1) | 6394(1) | 13(1) |
| C(8) | 6408(1) | 3470(1) | 6585(1) | 15(1) |
| C(9) | 8229(1) | 2959(1) | 5798(1) | 21(1) |
| C(10) | 4247(1) | 3920(1) | 7454(1) | 13(1) |
| C(11) | 4803(1) | 3744(1) | 8949(1) | 17(1) |
| C(12) | 2624(1) | 3895(1) | 7112(1) | 13(1) |
| C(13) | 2111(1) | 3284(1) | 7367(1) | 16(1) |
| C(14) | 2711(1) | 2817(1) | 6582(1) | 15(1) |
| C(15) | 1948(1) | 2366(1) | 6095(1) | 20(1) |
| C(16) | 4769(1) | 4543(1) | 7279(1) | 16(1) |
| C(17) | 3960(1) | 4998(1) | 7945(1) | 16(1) |
| C(18) | 2408(1) | 4960(1) | 7364(1) | 14(1) |

| | | | | |
|---|---|---|---|---|
| C(19) | 1803(1) | 4376(1) | 7767(1) | 14(1) |
| C(20) | 1850(1) | 4290(1) | 9317(1) | 17(1) |
| C(21) | 267(1) | 4339(1) | 7073(1) | 18(1) |
| C(22) | -600(1) | 4869(1) | 7335(1) | 20(1) |
| C(23) | 43(1) | 5428(1) | 6994(1) | 19(1) |
| C(24) | 1582(1) | 5520(1) | 7579(1) | 17(1) |
| C(25) | 1657(1) | 5703(1) | 9086(1) | 20(1) |
| C(26) | 2142(2) | 6018(1) | 6811(2) | 26(1) |
| O(1) | 4953(1) | 2050(1) | 5124(1) | 21(1) |
| O(2) | 3948(1) | 2778(1) | 3943(1) | 18(1) |
| O(3) | 6770(1) | 3110(1) | 5640(1) | 18(1) |
| O(4) | 4922(1) | 4136(1) | 4492(1) | 20(1) |
| O(5) | 7229(1) | 3714(1) | 7418(1) | 22(1) |
| O(6) | -644(1) | 5792(1) | 6302(1) | 29(1) |

Table 8. Bond lengths [≈] and angles [∞] for terretonin L (**10**)

| | |
|---|---|
| C(1)-C(2) | 1.5422(16) |
| C(1)-H(1A) | 0.9800 |
| C(1)-H(1B) | 0.9800 |
| C(1)-H(1C) | 0.9800 |
| C(2)-C(3) | 1.5412(17) |
| C(2)-C(14) | 1.5417(16) |
| C(2)-C(7) | 1.5900(16) |
| C(3)-O(1) | 1.2018(16) |
| C(3)-O(2) | 1.3537(15) |
| C(4)-O(2) | 1.4566(14) |
| C(4)-C(5) | 1.5104(17) |
| C(4)-C(6) | 1.5233(17) |
| C(4)-H(4) | 1.0000 |
| C(5)-H(5A) | 0.9800 |
| C(5)-H(5B) | 0.9800 |
| C(5)-H(5C) | 0.9800 |
| C(6)-O(4) | 1.2048(15) |
| C(6)-C(7) | 1.5563(16) |
| C(7)-C(8) | 1.5440(16) |
| C(7)-C(10) | 1.5991(16) |
| C(8)-O(5) | 1.1946(15) |

| | |
|---|---|
| C(8)-O(3) | 1.3443(15) |
| C(9)-O(3) | 1.4471(14) |
| C(9)-H(9A) | 0.9800 |
| C(9)-H(9B) | 0.9800 |
| C(9)-H(9C) | 0.9800 |
| C(10)-C(11) | 1.5474(16) |
| C(10)-C(16) | 1.5506(16) |
| C(10)-C(12) | 1.5625(15) |
| C(11)-H(11A) | 0.9800 |
| C(11)-H(11B) | 0.9800 |
| C(11)-H(11C) | 0.9800 |
| C(12)-C(13) | 1.5368(16) |
| C(12)-C(19) | 1.5716(16) |
| C(12)-H(12) | 1.0000 |
| C(13)-C(14) | 1.5067(17) |
| C(13)-H(13A) | 0.9900 |
| C(13)-H(13B) | 0.9900 |
| C(14)-C(15) | 1.3273(18) |
| C(15)-H(15A) | 0.9500 |
| C(15)-H(15B) | 0.9500 |
| C(16)-C(17) | 1.5298(16) |
| C(16)-H(16A) | 0.9900 |
| C(16)-H(16B) | 0.9900 |

| | |
|---|---|
| C(17)-C(18) | 1.5300(16) |
| C(17)-H(17A) | 0.9900 |
| C(17)-H(17B) | 0.9900 |
| C(18)-C(19) | 1.5540(16) |
| C(18)-C(24) | 1.5615(16) |
| C(18)-H(18) | 1.0000 |
| C(19)-C(20) | 1.5430(16) |
| C(19)-C(21) | 1.5441(16) |
| C(20)-H(20A) | 0.9800 |
| C(20)-H(20B) | 0.9800 |
| C(20)-H(20C) | 0.9800 |
| C(21)-C(22) | 1.5358(17) |
| C(21)-H(21A) | 0.9900 |
| C(21)-H(21B) | 0.9900 |
| C(22)-C(23) | 1.5030(19) |
| C(22)-H(22A) | 0.9900 |
| C(22)-H(22B) | 0.9900 |
| C(23)-O(6) | 1.2168(16) |
| C(23)-C(24) | 1.5316(18) |
| C(24)-C(26) | 1.5306(17) |
| C(24)-C(25) | 1.5423(17) |
| C(25)-H(25A) | 0.9800 |
| C(25)-H(25B) | 0.9800 |

| | |
|---|---|
| C(25)-H(25C) | 0.9800 |
| C(26)-H(26A) | 0.9800 |
| C(26)-H(26B) | 0.9800 |
| C(26)-H(26C) | 0.9800 |

| | |
|---|---|
| C(2)-C(1)-H(1A) | 109.5 |
| C(2)-C(1)-H(1B) | 109.5 |
| H(1A)-C(1)-H(1B) | 109.5 |
| C(2)-C(1)-H(1C) | 109.5 |
| H(1A)-C(1)-H(1C) | 109.5 |
| H(1B)-C(1)-H(1C) | 109.5 |
| C(3)-C(2)-C(14) | 106.89(9) |
| C(3)-C(2)-C(1) | 107.07(10) |
| C(14)-C(2)-C(1) | 107.79(9) |
| C(3)-C(2)-C(7) | 109.81(9) |
| C(14)-C(2)-C(7) | 112.33(9) |
| C(1)-C(2)-C(7) | 112.65(9) |
| O(1)-C(3)-O(2) | 117.90(11) |
| O(1)-C(3)-C(2) | 124.67(11) |
| O(2)-C(3)-C(2) | 117.35(10) |
| O(2)-C(4)-C(5) | 106.88(10) |
| O(2)-C(4)-C(6) | 106.40(9) |
| C(5)-C(4)-C(6) | 113.08(10) |

| | |
|---|---|
| O(2)-C(4)-H(4) | 110.1 |
| C(5)-C(4)-H(4) | 110.1 |
| C(6)-C(4)-H(4) | 110.1 |
| C(4)-C(5)-H(5A) | 109.5 |
| C(4)-C(5)-H(5B) | 109.5 |
| H(5A)-C(5)-H(5B) | 109.5 |
| C(4)-C(5)-H(5C) | 109.5 |
| H(5A)-C(5)-H(5C) | 109.5 |
| H(5B)-C(5)-H(5C) | 109.5 |
| O(4)-C(6)-C(4) | 120.77(11) |
| O(4)-C(6)-C(7) | 121.96(11) |
| C(4)-C(6)-C(7) | 117.10(10) |
| C(8)-C(7)-C(6) | 103.27(9) |
| C(8)-C(7)-C(2) | 107.05(9) |
| C(6)-C(7)-C(2) | 108.62(9) |
| C(8)-C(7)-C(10) | 112.69(9) |
| C(6)-C(7)-C(10) | 110.79(9) |
| C(2)-C(7)-C(10) | 113.81(9) |
| O(5)-C(8)-O(3) | 123.64(11) |
| O(5)-C(8)-C(7) | 128.17(11) |
| O(3)-C(8)-C(7) | 108.19(10) |
| O(3)-C(9)-H(9A) | 109.5 |
| O(3)-C(9)-H(9B) | 109.5 |

| | |
|---|---|
| H(9A)-C(9)-H(9B) | 109.5 |
| O(3)-C(9)-H(9C) | 109.5 |
| H(9A)-C(9)-H(9C) | 109.5 |
| H(9B)-C(9)-H(9C) | 109.5 |
| C(11)-C(10)-C(16) | 106.43(9) |
| C(11)-C(10)-C(12) | 112.43(9) |
| C(16)-C(10)-C(12) | 110.37(9) |
| C(11)-C(10)-C(7) | 111.28(9) |
| C(16)-C(10)-C(7) | 110.47(9) |
| C(12)-C(10)-C(7) | 105.92(9) |
| C(10)-C(11)-H(11A) | 109.5 |
| C(10)-C(11)-H(11B) | 109.5 |
| H(11A)-C(11)-H(11B) | 109.5 |
| C(10)-C(11)-H(11C) | 109.5 |
| H(11A)-C(11)-H(11C) | 109.5 |
| H(11B)-C(11)-H(11C) | 109.5 |
| C(13)-C(12)-C(10) | 110.03(9) |
| C(13)-C(12)-C(19) | 112.60(9) |
| C(10)-C(12)-C(19) | 116.73(9) |
| C(13)-C(12)-H(12) | 105.5 |
| C(10)-C(12)-H(12) | 105.5 |
| C(19)-C(12)-H(12) | 105.5 |
| C(14)-C(13)-C(12) | 114.42(10) |

| | |
|---|---|
| C(14)-C(13)-H(13A) | 108.7 |
| C(12)-C(13)-H(13A) | 108.7 |
| C(14)-C(13)-H(13B) | 108.7 |
| C(12)-C(13)-H(13B) | 108.7 |
| H(13A)-C(13)-H(13B) | 107.6 |
| C(15)-C(14)-C(13) | 120.85(11) |
| C(15)-C(14)-C(2) | 120.60(11) |
| C(13)-C(14)-C(2) | 118.33(10) |
| C(14)-C(15)-H(15A) | 120.0 |
| C(14)-C(15)-H(15B) | 120.0 |
| H(15A)-C(15)-H(15B) | 120.0 |
| C(17)-C(16)-C(10) | 113.13(10) |
| C(17)-C(16)-H(16A) | 109.0 |
| C(10)-C(16)-H(16A) | 109.0 |
| C(17)-C(16)-H(16B) | 109.0 |
| C(10)-C(16)-H(16B) | 109.0 |
| H(16A)-C(16)-H(16B) | 107.8 |
| C(16)-C(17)-C(18) | 110.19(10) |
| C(16)-C(17)-H(17A) | 109.6 |
| C(18)-C(17)-H(17A) | 109.6 |
| C(16)-C(17)-H(17B) | 109.6 |
| C(18)-C(17)-H(17B) | 109.6 |
| H(17A)-C(17)-H(17B) | 108.1 |

| | |
|---|---|
| C(17)-C(18)-C(19) | 110.26(9) |
| C(17)-C(18)-C(24) | 113.58(10) |
| C(19)-C(18)-C(24) | 117.73(9) |
| C(17)-C(18)-H(18) | 104.6 |
| C(19)-C(18)-H(18) | 104.6 |
| C(24)-C(18)-H(18) | 104.6 |
| C(20)-C(19)-C(21) | 107.78(10) |
| C(20)-C(19)-C(18) | 114.68(10) |
| C(21)-C(19)-C(18) | 108.33(9) |
| C(20)-C(19)-C(12) | 112.61(9) |
| C(21)-C(19)-C(12) | 107.36(9) |
| C(18)-C(19)-C(12) | 105.80(9) |
| C(19)-C(20)-H(20A) | 109.5 |
| C(19)-C(20)-H(20B) | 109.5 |
| H(20A)-C(20)-H(20B) | 109.5 |
| C(19)-C(20)-H(20C) | 109.5 |
| H(20A)-C(20)-H(20C) | 109.5 |
| H(20B)-C(20)-H(20C) | 109.5 |
| C(22)-C(21)-C(19) | 113.56(10) |
| C(22)-C(21)-H(21A) | 108.9 |
| C(19)-C(21)-H(21A) | 108.9 |
| C(22)-C(21)-H(21B) | 108.9 |
| C(19)-C(21)-H(21B) | 108.9 |

| | |
|---|---|
| H(21A)-C(21)-H(21B) | 107.7 |
| C(23)-C(22)-C(21) | 113.09(10) |
| C(23)-C(22)-H(22A) | 109.0 |
| C(21)-C(22)-H(22A) | 109.0 |
| C(23)-C(22)-H(22B) | 109.0 |
| C(21)-C(22)-H(22B) | 109.0 |
| H(22A)-C(22)-H(22B) | 107.8 |
| O(6)-C(23)-C(22) | 121.00(12) |
| O(6)-C(23)-C(24) | 122.05(12) |
| C(22)-C(23)-C(24) | 116.93(10) |
| C(26)-C(24)-C(23) | 108.83(11) |
| C(26)-C(24)-C(25) | 108.14(11) |
| C(23)-C(24)-C(25) | 107.11(10) |
| C(26)-C(24)-C(18) | 109.02(10) |
| C(23)-C(24)-C(18) | 109.02(10) |
| C(25)-C(24)-C(18) | 114.59(10) |
| C(24)-C(25)-H(25A) | 109.5 |
| C(24)-C(25)-H(25B) | 109.5 |
| H(25A)-C(25)-H(25B) | 109.5 |
| C(24)-C(25)-H(25C) | 109.5 |
| H(25A)-C(25)-H(25C) | 109.5 |
| H(25B)-C(25)-H(25C) | 109.5 |
| C(24)-C(26)-H(26A) | 109.5 |

| | |
|---|---|
| C(24)-C(26)-H(26B) | 109.5 |
| H(26A)-C(26)-H(26B) | 109.5 |
| C(24)-C(26)-H(26C) | 109.5 |
| H(26A)-C(26)-H(26C) | 109.5 |
| H(26B)-C(26)-H(26C) | 109.5 |
| C(3)-O(2)-C(4) | 119.34(9) |
| C(8)-O(3)-C(9) | 116.06(10) |

Symmetry transformations used to generate equivalent atoms:

Table 9. Anisotropic displacement parameters ($\approx^2$x $10^3$) for terretonin L (**10**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12} ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| C(1) | 16(1) | 16(1) | 19(1) | 3(1) | 2(1) | 1(1) |
| C(2) | 14(1) | 12(1) | 16(1) | 1(1) | 2(1) | 0(1) |
| C(3) | 14(1) | 16(1) | 19(1) | 0(1) | 3(1) | -2(1) |
| C(4) | 18(1) | 16(1) | 16(1) | 1(1) | 2(1) | 2(1) |
| C(5) | 25(1) | 24(1) | 16(1) | 2(1) | 2(1) | 2(1) |
| C(6) | 13(1) | 15(1) | 17(1) | -1(1) | 5(1) | 3(1) |
| C(7) | 12(1) | 12(1) | 15(1) | 1(1) | 2(1) | -1(1) |
| C(8) | 15(1) | 13(1) | 19(1) | 3(1) | 4(1) | 1(1) |
| C(9) | 14(1) | 22(1) | 28(1) | 1(1) | 7(1) | 4(1) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(10) | 12(1) | 13(1) | 15(1) | 0(1) | 2(1) | 0(1) |
| C(11) | 16(1) | 18(1) | 15(1) | -1(1) | 0(1) | 2(1) |
| C(12) | 12(1) | 14(1) | 13(1) | 0(1) | 2(1) | -1(1) |
| C(13) | 13(1) | 16(1) | 20(1) | 0(1) | 5(1) | -2(1) |
| C(14) | 14(1) | 15(1) | 16(1) | 4(1) | 1(1) | 0(1) |
| C(15) | 16(1) | 18(1) | 25(1) | -1(1) | 3(1) | -1(1) |
| C(16) | 13(1) | 14(1) | 22(1) | -2(1) | 5(1) | -2(1) |
| C(17) | 16(1) | 13(1) | 19(1) | -1(1) | 4(1) | -1(1) |
| C(18) | 15(1) | 14(1) | 13(1) | 1(1) | 4(1) | 1(1) |
| C(19) | 13(1) | 15(1) | 14(1) | 0(1) | 3(1) | 0(1) |
| C(20) | 19(1) | 17(1) | 16(1) | 1(1) | 6(1) | 0(1) |
| C(21) | 14(1) | 20(1) | 20(1) | -2(1) | 2(1) | 1(1) |
| C(22) | 14(1) | 25(1) | 23(1) | -2(1) | 3(1) | 3(1) |
| C(23) | 22(1) | 24(1) | 14(1) | -1(1) | 5(1) | 9(1) |
| C(24) | 20(1) | 15(1) | 19(1) | 1(1) | 7(1) | 3(1) |
| C(25) | 20(1) | 19(1) | 22(1) | -5(1) | 6(1) | 1(1) |
| C(26) | 30(1) | 17(1) | 34(1) | 7(1) | 16(1) | 6(1) |
| O(1) | 23(1) | 15(1) | 26(1) | -2(1) | 5(1) | 3(1) |
| O(2) | 23(1) | 16(1) | 16(1) | -2(1) | 2(1) | 2(1) |
| O(3) | 13(1) | 19(1) | 22(1) | -2(1) | 5(1) | 1(1) |
| O(4) | 23(1) | 18(1) | 19(1) | 3(1) | 7(1) | -1(1) |
| O(5) | 13(1) | 24(1) | 28(1) | -6(1) | 2(1) | -2(1) |
| O(6) | 30(1) | 31(1) | 25(1) | 7(1) | 3(1) | 13(1) |

Table 10. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters (≈$^2$x $10^3$) for terretonin L (**10**).

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(1A) | 4790 | 2636 | 8531 | 25 |
| H(1B) | 6081 | 2579 | 7726 | 25 |
| H(1C) | 4892 | 2096 | 7548 | 25 |
| H(4) | 2439 | 3340 | 4273 | 20 |
| H(5A) | 4041 | 3554 | 2141 | 33 |
| H(5B) | 2798 | 3962 | 2438 | 33 |
| H(5C) | 2478 | 3317 | 1907 | 33 |
| H(9A) | 8762 | 3291 | 5555 | 31 |
| H(9B) | 8351 | 2634 | 5197 | 31 |
| H(9C) | 8564 | 2850 | 6750 | 31 |
| H(11A) | 5764 | 3606 | 9018 | 26 |
| H(11B) | 4220 | 3435 | 9227 | 26 |
| H(11C) | 4777 | 4078 | 9550 | 26 |
| H(12) | 2393 | 3956 | 6102 | 16 |
| H(13A) | 2346 | 3198 | 8356 | 20 |
| H(13B) | 1084 | 3276 | 7121 | 20 |
| H(15A) | 1011 | 2335 | 6240 | 24 |

| | | | | |
|---|---|---|---|---|
| H(15B) | 2339 | 2075 | 5601 | 24 |
| H(16A) | 5766 | 4567 | 7686 | 19 |
| H(16B) | 4690 | 4629 | 6291 | 19 |
| H(17A) | 4312 | 5387 | 7770 | 19 |
| H(17B) | 4101 | 4936 | 8946 | 19 |
| H(18) | 2371 | 4934 | 6352 | 17 |
| H(20A) | 1110 | 4517 | 9622 | 26 |
| H(20B) | 2755 | 4416 | 9808 | 26 |
| H(20C) | 1716 | 3880 | 9507 | 26 |
| H(21A) | 232 | 4294 | 6075 | 21 |
| H(21B) | -158 | 3991 | 7411 | 21 |
| H(22A) | -1538 | 4834 | 6780 | 24 |
| H(22B) | -711 | 4874 | 8310 | 24 |
| H(25A) | 2633 | 5746 | 9511 | 30 |
| H(25B) | 1213 | 5407 | 9576 | 30 |
| H(25C) | 1171 | 6071 | 9129 | 30 |
| H(26A) | 2198 | 5896 | 5875 | 38 |
| H(26B) | 3071 | 6126 | 7280 | 38 |
| H(26C) | 1516 | 6350 | 6786 | 38 |

## Computational Section

## Table of Contents



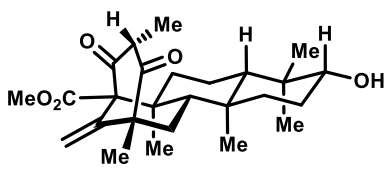
## Computational General Information

DFT optimizations were performed using Gaussian '09[1] (on the Omega and Grace Clusters at Yale University)[2] at both the mPW1PW91/6-31+G(d,p)//B3LYP/6-31G* and B3LYP/6-31+G(d,p)//B3LYP/6-31G* levels of theory[3] using gas-phase geometries at 298K. Natural bond order (NBO)[4] analysis was conducted using the mPW1PW91 functional with the 6-31+G(d,p) basis set.

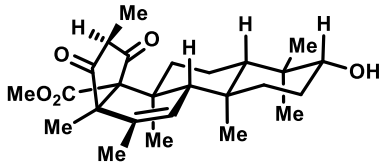
Optimized structures are displayed visually and listed with energies and geometric coordinates. Ground state structures display no imaginary frequencies while transition state structures display one imaginary frequency that corresponds to the transition state movement.

The following abbreviations are used:
PA – protoaustinoid A
AN – andrastin E
TE – preterretonin A
PAC – protoaustinoid A carbocation
ATC – andrastin E/preterretonin A carbocation
TS – transition state
DK – diketone isomer
EN – enol north isomer
ES – enol south isomer

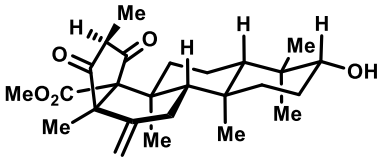
# Summary of Minimized Structures and Energies (Neutral Structures)



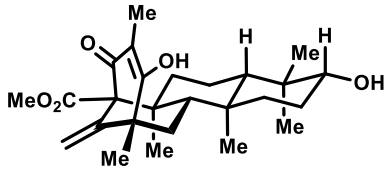
**PA-DK**
B3LYP: 0.0 kcal/mol
mPW1PW91: 0.0 kcal/mol



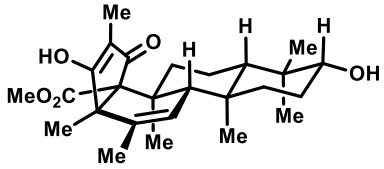
**AN-DK**
B3LYP: -2.8 kcal/mol
mPW1PW91: -2.8 kcal/mol



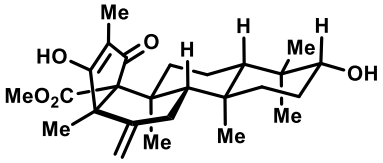
**TE-DK**
B3LYP: +5.0 kcal/mol
mPW1PW91: +5.2 kcal/mol



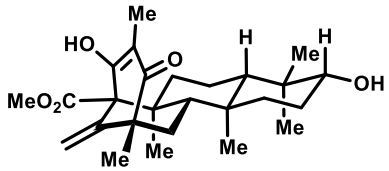
**PA-EN**
B3LYP: +3.5 kcal/mol
mPW1PW91: +3.1 kcal/mol



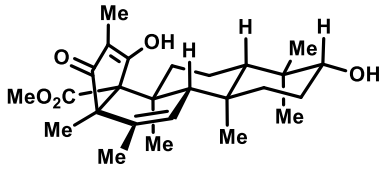
**AN-EN**
B3LYP: -0.6 kcal/mol
mPW1PW91: -0.6 kcal/mol



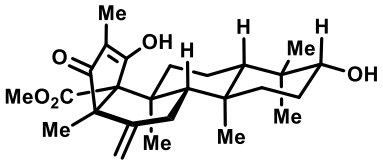
**TE-EN**
B3LYP: +4.9 kcal/mol
mPW1PW91: +4.5 kcal/mol



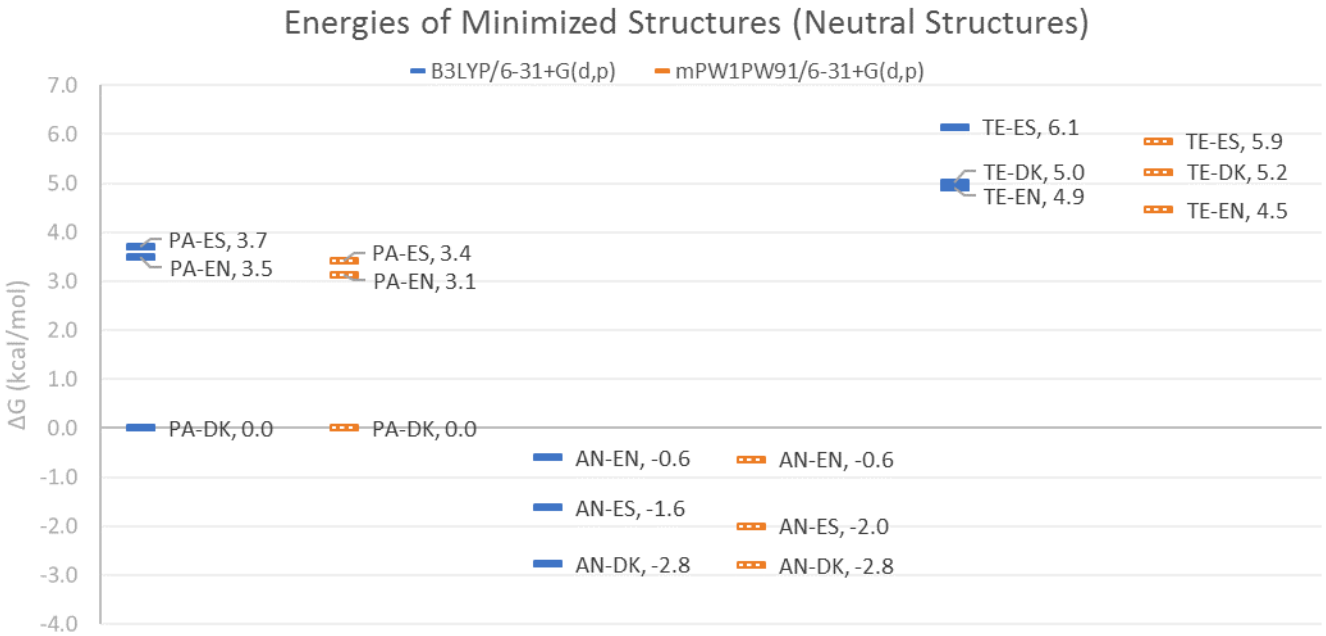
**PA-ES**
B3LYP: +3.7 kcal/mol
mPW1PW91: +3.4 kcal/mol



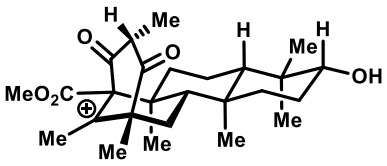
**AN-ES**
B3LYP: -1.6 kcal/mol
mPW1PW91: -2.0 kcal/mol



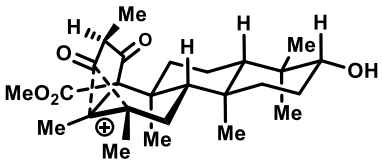
**TE-ES**
B3LYP: +6.1 kcal/mol
mPW1PW91: +5.9 kcal/mol



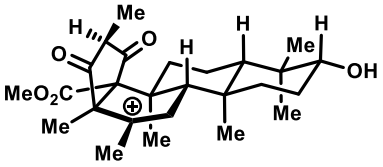
# Summary of Minimized Structures and Energies (Charged Structures)



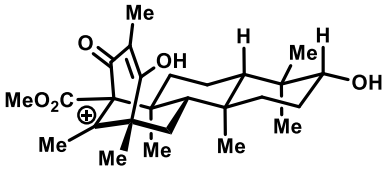
**PAC-DK**
B3LYP: 0.0 kcal/mol
mPW1PW91: 0.0 kcal/mol



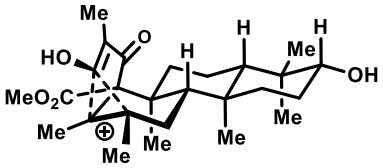
**TS-DK**
B3LYP: +5.7 kcal/mol
mPW1PW91:+6.8 kcal/mol



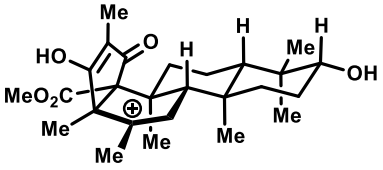
**ATC-DK**
B3LYP: -1.2 kcal/mol
mPW1PW91: -1.5 kcal/mol



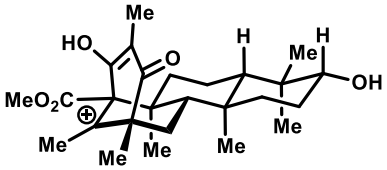
**PAC-EN**
B3LYP: -3.1 kcal/mol
mPW1PW91: -3.2 kcal/mol



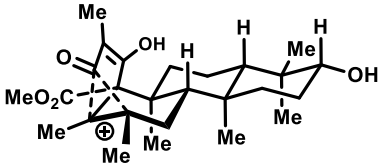
**TS-EN**
B3LYP: +8.9 kcal/mol
mPW1PW91: +5.9 kcal/mol



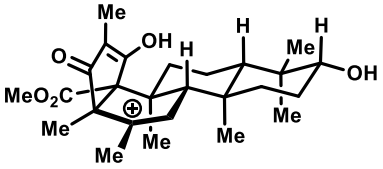
**ATC-EN**
B3LYP: -1.4 kcal/mol
mPW1PW91: -2.8 kcal/mol



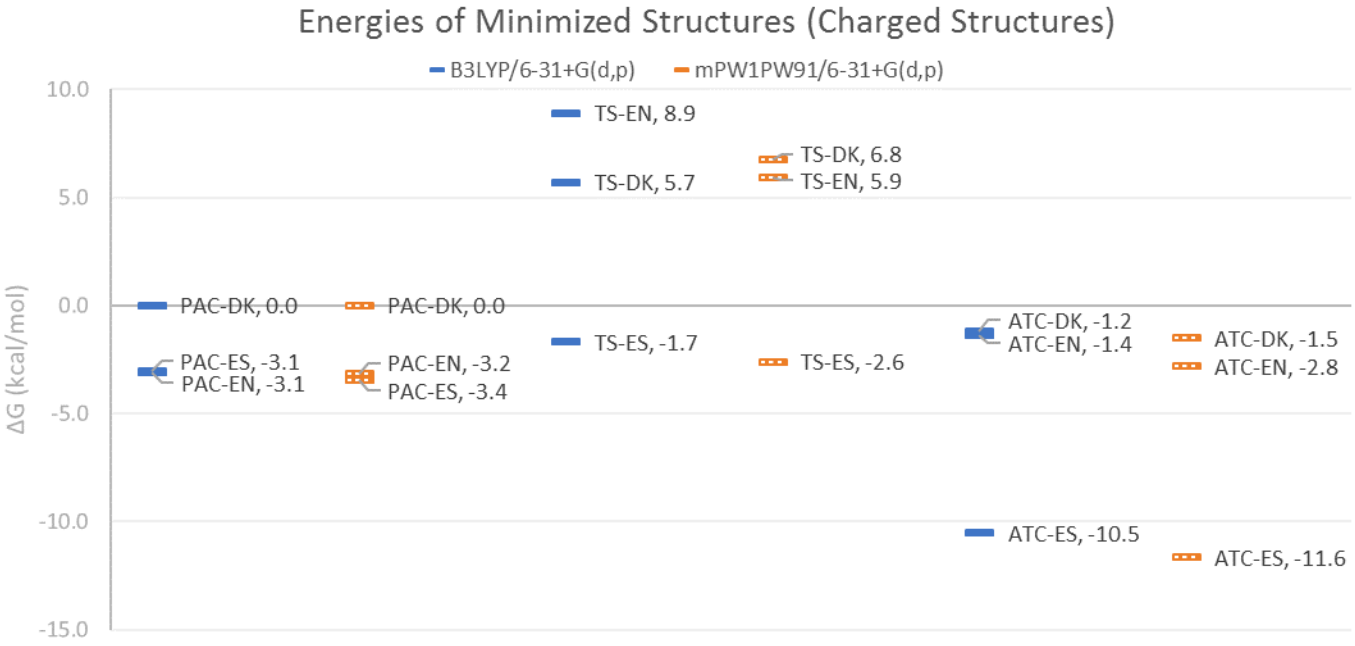
**PAC-ES**
B3LYP: -3.1 kcal/mol
mPW1PW91: -3.4 kcal/mol



**TS-ES**
B3LYP: -1.7 kcal/mol
mPW1PW91: -2.6 kcal/mol

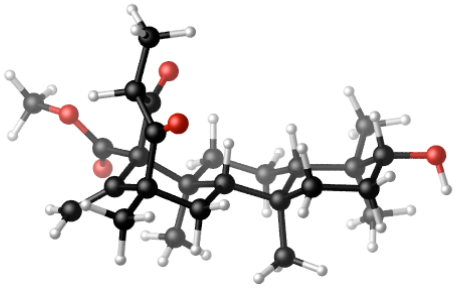


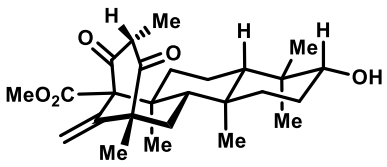
**ATC-ES**
B3LYP: -10.5 kcal/mol
mPW1PW91: -11.6 kcal/mol



# Minimized Structures and Energies

## PA-DK






**B3LYP/6-31+G(d,p)//B3LYP/6-31G***

Zero-point correction= 0.602720 (Hartree/Particle)
Thermal correction to Energy= 0.633568
Thermal correction to Enthalpy= 0.634512
Thermal correction to Gibbs Free Energy= 0.545705
Sum of electronic and zero-point Energies= -1389.238802
Sum of electronic and thermal Energies= -1389.207954
Sum of electronic and thermal Enthalpies= -1389.207010
Sum of electronic and thermal Free Energies= -1389.295816

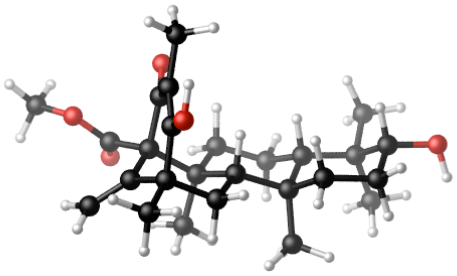
**MPW1PW91/6-31+G(d,p)//B3LYP/G-31G***

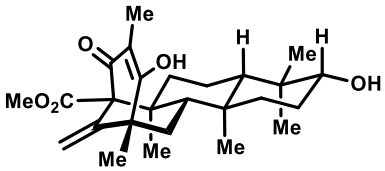
Zero-point correction= 0.605391 (Hartree/Particle)
Thermal correction to Energy= 0.635691
Thermal correction to Enthalpy= 0.636635
Thermal correction to Gibbs Free Energy= 0.550332
Sum of electronic and zero-point Energies= -1388.929778
Sum of electronic and thermal Energies= -1388.899478
Sum of electronic and thermal Enthalpies= -1388.898534
Sum of electronic and thermal Free Energies= -1388.984837

| | | | |
|---|---|---|---|
| C | -4.44701300 | 0.51914900 | 0.88007700 |
| C | -3.93121600 | -0.87107300 | 0.40106500 |
| C | -2.38094500 | -0.75653500 | 0.18283400 |
| C | -1.86555400 | 0.41660700 | -0.72608800 |
| C | -2.48732200 | 1.73851300 | -0.19245300 |
| C | -4.01023000 | 1.67498200 | -0.01955600 |
| O | -5.86108200 | 0.54072700 | 1.09256200 |
| C | -0.29954800 | 0.49142300 | -0.50022700 |
| C | -1.69198800 | -2.07871800 | -0.19311300 |
| C | -0.17490400 | -2.00653000 | 0.03564600 |
| C | 0.50758800 | -0.84174100 | -0.72630700 |
| C | 1.98670500 | -0.55514500 | -0.15432400 |
| C | 2.61456800 | 0.55252400 | -1.00992300 |
| C | 1.87940000 | 1.87812700 | -0.85416900 |
| C | 0.37330600 | 1.68052800 | -1.21834100 |
| C | 3.65426100 | 0.36665900 | -1.82746300 |
| C | 1.91949700 | 2.31750400 | 0.62943700 |
| C | 1.94906600 | -0.06806200 | 1.33416600 |
| C | 2.52539400 | 1.32218800 | 1.61549200 |
| O | 1.46968100 | 3.38742500 | 0.98628700 |

| | | | |
|---|---|---|---|
| O | 1.52043100 | -0.76226900 | 2.23185900 |
| C | -2.24234200 | 0.27734000 | -2.22343200 |
| C | 0.62180100 | -1.23185500 | -2.22047700 |
| C | -4.21603500 | -1.87087500 | 1.54700200 |
| C | -4.71661700 | -1.35877100 | -0.83581500 |
| C | 2.40859300 | 1.74713000 | 3.07314400 |
| C | 2.89062200 | -1.80471200 | -0.13100200 |
| O | 2.72509300 | -2.85082300 | -0.71597000 |
| O | 3.96970000 | -1.57222400 | 0.65122800 |
| C | 4.89762000 | -2.66445200 | 0.77740000 |
| C | 2.45479800 | 3.02493400 | -1.70147600 |
| H | -4.02781600 | 0.69069900 | 1.88064500 |
| H | -2.00005400 | -0.50292200 | 1.18690600 |
| H | -2.03593300 | 1.97867200 | 0.78115700 |
| H | -2.24238800 | 2.57330600 | -0.85943600 |
| H | -4.37350800 | 2.61221700 | 0.41856300 |
| H | -4.50598300 | 1.58558800 | -0.99700600 |
| H | -6.28480300 | 0.53047300 | 0.21968800 |
| H | -0.22551700 | 0.69689800 | 0.57884100 |
| H | -2.08107900 | -2.89508300 | 0.42381200 |
| H | -1.91836600 | -2.35578000 | -1.22981200 |
| H | 0.29180100 | -2.94942600 | -0.26511200 |
| H | 0.00134400 | -1.89700400 | 1.10849800 |
| H | -0.13358700 | 2.61539000 | -0.96476100 |
| H | 0.31368800 | 1.56800300 | -2.30560900 |
| H | 4.14338000 | -0.59676900 | -1.93354200 |
| H | 4.05128000 | 1.16801100 | -2.44085800 |
| H | 3.58425300 | 1.23260000 | 1.31438800 |
| H | -2.22499200 | -0.75390800 | -2.58033700 |
| H | -3.24520700 | 0.66450800 | -2.41989900 |
| H | -1.56146300 | 0.85262400 | -2.85763400 |
| H | 0.93407000 | -0.40448500 | -2.86082000 |
| H | 1.34395100 | -2.04084700 | -2.33850500 |
| H | -0.33707600 | -1.59495100 | -2.59323300 |
| H | -4.06576300 | -2.91036100 | 1.23762600 |
| H | -5.25539800 | -1.76417900 | 1.87180300 |
| H | -3.57014500 | -1.68023300 | 2.41326400 |
| H | -4.71635700 | -0.64725500 | -1.66584200 |
| H | -4.30542600 | -2.30045500 | -1.21408700 |
| H | -5.75971800 | -1.55555400 | -0.56193300 |
| H | 2.86292500 | 2.73056500 | 3.21738900 |
| H | 2.90223000 | 1.02050600 | 3.72304100 |
| H | 1.35966700 | 1.81260900 | 3.37469900 |
| H | 5.67601500 | -2.30724100 | 1.45164100 |
| H | 4.39739100 | -3.54167600 | 1.19450100 |
| H | 5.32020900 | -2.92223700 | -0.19727800 |
| H | 3.51017600 | 3.20826900 | -1.47146500 |
| H | 2.36975800 | 2.79914200 | -2.76947500 |
| H | 1.90081800 | 3.94274800 | -1.49011900 |

## PA-EN






**B3LYP/6-31+G(d,p)//B3LYP/6-31G***

Zero-point correction= 0.603688 (Hartree/Particle)
Thermal correction to Energy= 0.634381
Thermal correction to Enthalpy= 0.635325
Thermal correction to Gibbs Free Energy= 0.547373
Sum of electronic and zero-point Energies= -1389.233931
Sum of electronic and thermal Energies= -1389.203238
Sum of electronic and thermal Enthalpies= -1389.202293
Sum of electronic and thermal Free Energies= -1389.290246

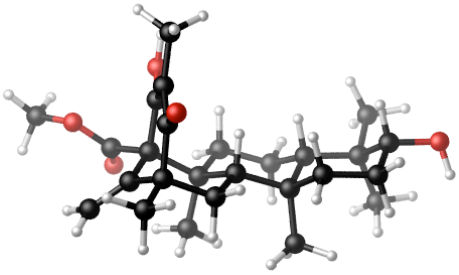
**MPW1PW91/6-31+G(d,p)//B3LYP/G-31G***

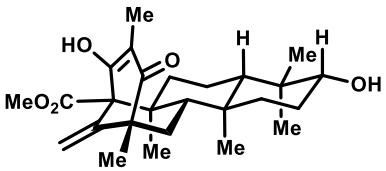
Zero-point correction= 0.606481 (Hartree/Particle)
Thermal correction to Energy= 0.636588
Thermal correction to Enthalpy= 0.637533
Thermal correction to Gibbs Free Energy= 0.551987
Sum of electronic and zero-point Energies= -1388.925361
Sum of electronic and thermal Energies= -1388.895253
Sum of electronic and thermal Enthalpies= -1388.894309
Sum of electronic and thermal Free Energies= -1388.979855

| | | | |
|---|---|---|---|
| C | -4.47652400 | 0.54658000 | 0.81202700 |
| C | -3.94801000 | -0.85835600 | 0.39470200 |
| C | -2.39392300 | -0.74423900 | 0.20485300 |
| C | -1.86317500 | 0.39195900 | -0.74165300 |
| C | -2.49996400 | 1.73061400 | -0.27152300 |
| C | -4.02596300 | 1.66812600 | -0.12410900 |
| O | -5.89425300 | 0.57384500 | 0.99872100 |
| C | -0.30195000 | 0.47600600 | -0.48731900 |
| C | -1.68701300 | -2.07621400 | -0.09417900 |
| C | -0.17316000 | -1.98079800 | 0.14861200 |
| C | 0.51246600 | -0.85860200 | -0.67106100 |
| C | 2.00421500 | -0.56399300 | -0.12208700 |
| C | 2.61708900 | 0.52635500 | -0.99643000 |
| C | 1.89202400 | 1.85904700 | -0.83362300 |
| C | 0.38098400 | 1.65834000 | -1.20122900 |
| C | 3.62898900 | 0.33592700 | -1.84562800 |
| C | 1.98763900 | 2.23871500 | 0.63527900 |
| C | 1.96805000 | -0.08797500 | 1.36461600 |
| C | 2.04209900 | 1.34482100 | 1.65632900 |
| O | 1.95222400 | 3.57540500 | 0.84960500 |
| O | 1.86889300 | -0.92349700 | 2.25871500 |

| | | | |
|---|---|---|---|
| C | -2.21574100 | 0.19497500 | -2.23895000 |
| C | 0.61847800 | -1.30652200 | -2.14927600 |
| C | -4.25327600 | -1.81782700 | 1.56938800 |
| C | -4.70706700 | -1.39179500 | -0.83970400 |
| C | 2.08661900 | 1.77488600 | 3.10412100 |
| C | 2.89815200 | -1.82480800 | -0.09432100 |
| O | 2.64035600 | -2.92282600 | -0.53667900 |
| O | 4.07700700 | -1.54462100 | 0.50039100 |
| C | 4.97138500 | -2.65707300 | 0.65535800 |
| C | 2.46438400 | 2.97953100 | -1.71855900 |
| H | -4.07570300 | 0.75692100 | 1.81280700 |
| H | -2.03783600 | -0.44374600 | 1.20527000 |
| H | -2.06794600 | 2.00900900 | 0.70118300 |
| H | -2.24652200 | 2.54013400 | -0.96621900 |
| H | -4.40201900 | 2.62045600 | 0.26881000 |
| H | -4.50166200 | 1.53743300 | -1.10671700 |
| H | -6.30262900 | 0.50783600 | 0.12097800 |
| H | -0.24891500 | 0.69761300 | 0.58628300 |
| H | -2.07836400 | -2.86390300 | 0.55775600 |
| H | -1.89689900 | -2.40708600 | -1.11871100 |
| H | 0.30231600 | -2.93659600 | -0.08464600 |
| H | -0.00964000 | -1.80686300 | 1.21677000 |
| H | -0.13693900 | 2.59490600 | -0.97140000 |
| H | 0.33963100 | 1.53680700 | -2.28894700 |
| H | 4.11748000 | -0.62680000 | -1.95209800 |
| H | 4.01630600 | 1.13293400 | -2.46981700 |
| H | -2.20162800 | -0.84981400 | -2.55407600 |
| H | -3.21117100 | 0.58305300 | -2.46997400 |
| H | -1.51671000 | 0.73743200 | -2.88255800 |
| H | 0.90934400 | -0.49770200 | -2.82321300 |
| H | 1.35456700 | -2.10585000 | -2.24389600 |
| H | -0.33498100 | -1.70324200 | -2.50023600 |
| H | -4.09497000 | -2.86692800 | 1.29922200 |
| H | -5.29876800 | -1.70195800 | 1.87083500 |
| H | -3.62386200 | -1.59612900 | 2.44042600 |
| H | -4.69760400 | -0.70636100 | -1.69124400 |
| H | -4.28065000 | -2.34078700 | -1.18054900 |
| H | -5.75339000 | -1.59026200 | -0.57906700 |
| H | 2.98486600 | 2.36421300 | 3.33598000 |
| H | 2.09992900 | 0.88368100 | 3.73480100 |
| H | 1.20727900 | 2.36815900 | 3.39601700 |
| H | 5.85480100 | -2.25240400 | 1.15002600 |
| H | 4.50838100 | -3.43361500 | 1.26957300 |
| H | 5.23479300 | -3.08098100 | -0.31755200 |
| H | 3.51140000 | 3.19089800 | -1.48010600 |
| H | 2.39962000 | 2.69152000 | -2.77217000 |
| H | 1.89623600 | 3.90217800 | -1.58076600 |
| H | 1.96718400 | 3.74332500 | 1.80738700 |

## PA-ES






**B3LYP/6-31+G(d,p)//B3LYP/6-31G***

Zero-point correction= 0.603453 (Hartree/Particle)
Thermal correction to Energy= 0.634236
Thermal correction to Enthalpy= 0.635180
Thermal correction to Gibbs Free Energy= 0.546935
Sum of electronic and zero-point Energies= -1389.233408
Sum of electronic and thermal Energies= -1389.202625
Sum of electronic and thermal Enthalpies= -1389.201681
Sum of electronic and thermal Free Energies= -1389.289926

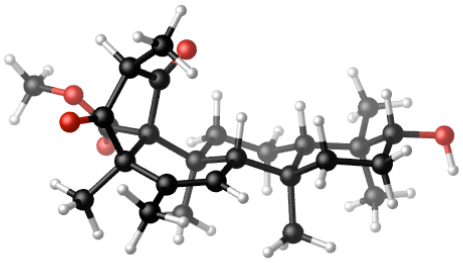
**MPW1PW91/6-31+G(d,p)//B3LYP/G-31G***

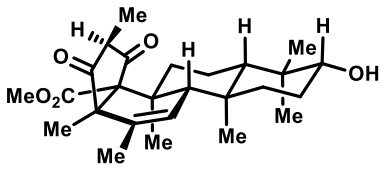
Zero-point correction= 0.606266 (Hartree/Particle)
Thermal correction to Energy= 0.636446
Thermal correction to Enthalpy= 0.637390
Thermal correction to Gibbs Free Energy= 0.551656
Sum of electronic and zero-point Energies= -1388.924790
Sum of electronic and thermal Energies= -1388.894610
Sum of electronic and thermal Enthalpies= -1388.893666
Sum of electronic and thermal Free Energies= -1388.979400

| | | | |
|---|---|---|---|
| C | -4.49451800 | 0.50659100 | 0.81669300 |
| C | -3.94907700 | -0.88256300 | 0.36779100 |
| C | -2.39615200 | -0.74649700 | 0.18825900 |
| C | -1.87321400 | 0.41790000 | -0.72801200 |
| C | -2.52573100 | 1.73792600 | -0.22751500 |
| C | -4.05159400 | 1.65591300 | -0.08833900 |
| O | -5.91323200 | 0.51160800 | 0.99713400 |
| C | -0.31389100 | 0.51416800 | -0.46372700 |
| C | -1.67295800 | -2.06413700 | -0.13625700 |
| C | -0.16128000 | -1.95306600 | 0.11404200 |
| C | 0.51165100 | -0.80689900 | -0.68176800 |
| C | 2.00817500 | -0.51313600 | -0.13244000 |
| C | 2.60310700 | 0.60933900 | -0.99252300 |
| C | 1.87461000 | 1.92645900 | -0.79150900 |
| C | 0.36072800 | 1.72398400 | -1.14156300 |
| C | 3.60079500 | 0.43244100 | -1.86148700 |
| C | 1.96063600 | 2.33591900 | 0.70066400 |
| C | 2.01074300 | -0.02788300 | 1.31509000 |
| C | 2.04064100 | 1.26991500 | 1.70729700 |
| O | 1.90600800 | 3.51825700 | 1.02301900 |

| | | | |
|---|---|---|---|
| O | 1.97314300 | -1.04797700 | 2.20960300 |
| C | -2.21941500 | 0.25387200 | -2.23073600 |
| C | 0.61586000 | -1.21395100 | -2.17219700 |
| C | -4.25051500 | -1.87286500 | 1.51759500 |
| C | -4.69710400 | -1.39458400 | -0.88224100 |
| C | 2.06894500 | 1.66471300 | 3.16520900 |
| C | 2.92407900 | -1.76513800 | -0.16577300 |
| O | 2.67461800 | -2.84415400 | -0.65585800 |
| O | 4.10398500 | -1.49702900 | 0.43102200 |
| C | 5.02964600 | -2.59378500 | 0.49190400 |
| C | 2.42298100 | 3.07750400 | -1.64473600 |
| H | -4.10059900 | 0.69635500 | 1.82441400 |
| H | -2.04914400 | -0.46455600 | 1.19758000 |
| H | -2.10014800 | 1.99821400 | 0.75270300 |
| H | -2.27715600 | 2.56593000 | -0.90124000 |
| H | -4.43809500 | 2.59408100 | 0.32749300 |
| H | -4.52275100 | 1.54551100 | -1.07570700 |
| H | -6.31703200 | 0.48830100 | 0.11511800 |
| H | -0.26761000 | 0.70441500 | 0.61532700 |
| H | -2.05680800 | -2.87086800 | 0.49681100 |
| H | -1.87369200 | -2.37570900 | -1.16822300 |
| H | 0.32938600 | -2.89951900 | -0.12799400 |
| H | -0.01348000 | -1.79022400 | 1.18709200 |
| H | -0.15514300 | 2.64915200 | -0.86713200 |
| H | 0.30032000 | 1.64249300 | -2.23257800 |
| H | 4.09161700 | -0.52518400 | -1.99981600 |
| H | 3.96929300 | 1.24458800 | -2.47751000 |
| H | -2.19746600 | -0.78283100 | -2.57136500 |
| H | -3.21667600 | 0.64060900 | -2.45577700 |
| H | -1.52240700 | 0.81700400 | -2.85825800 |
| H | 0.86992200 | -0.37639600 | -2.82473700 |
| H | 1.37458800 | -1.98608900 | -2.30152900 |
| H | -0.32941800 | -1.63078200 | -2.52131600 |
| H | -4.07917600 | -2.91381800 | 1.22441600 |
| H | -5.29904100 | -1.77557300 | 1.81476900 |
| H | -3.62975700 | -1.66397900 | 2.39824300 |
| H | -4.68710100 | -0.69127000 | -1.71891400 |
| H | -4.26309000 | -2.33369600 | -1.24086900 |
| H | -5.74351400 | -1.60405400 | -0.63130800 |
| H | 2.10686800 | 2.75406800 | 3.23048700 |
| H | 2.94937700 | 1.26518200 | 3.68819900 |
| H | 1.17197100 | 1.33470500 | 3.70967700 |
| H | 5.90983500 | -2.20229600 | 1.00243600 |
| H | 4.59710400 | -3.42744000 | 1.05129700 |
| H | 5.28886800 | -2.93635900 | -0.51342700 |
| H | 3.48015800 | 3.26589000 | -1.43190100 |
| H | 2.31575300 | 2.85487500 | -2.71149000 |
| H | 1.87523500 | 3.99416300 | -1.41744400 |
| H | 1.98994400 | -0.68336100 | 3.11079900 |

**AN-DK**






**B3LYP/6-31+G(d,p)//B3LYP/6-31G***

Zero-point correction= 0.602333 (Hartree/Particle)
Thermal correction to Energy= 0.633519
Thermal correction to Enthalpy= 0.634463
Thermal correction to Gibbs Free Energy= 0.545164
Sum of electronic and zero-point Energies= -1389.243068
Sum of electronic and thermal Energies= -1389.211883
Sum of electronic and thermal Enthalpies= -1389.210939
Sum of electronic and thermal Free Energies= -1389.300237

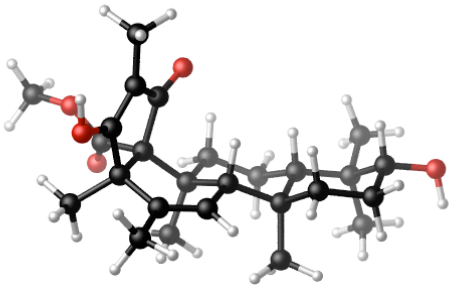
**MPW1PW91/6-31+G(d,p)//B3LYP/G-31G***

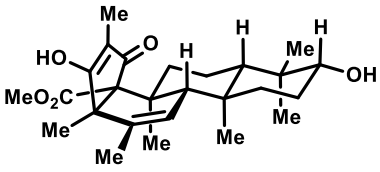
Zero-point correction= 0.605059 (Hartree/Particle)
Thermal correction to Energy= 0.635691
Thermal correction to Enthalpy= 0.636635
Thermal correction to Gibbs Free Energy= 0.549772
Sum of electronic and zero-point Energies= -1388.934002
Sum of electronic and thermal Energies= -1388.903370
Sum of electronic and thermal Enthalpies= -1388.902425
Sum of electronic and thermal Free Energies= -1388.989288

| | | | |
|---|---|---|---|
| C | 4.64648100 | -0.53071000 | 0.95440100 |
| C | 4.14313500 | 0.75864400 | 0.23650100 |
| C | 2.57982600 | 0.66524600 | 0.13416200 |
| C | 1.98389500 | -0.63814500 | -0.50826100 |
| C | 2.58309300 | -1.84887400 | 0.26113300 |
| C | 4.11515600 | -1.82425800 | 0.33551100 |
| O | 6.07005700 | -0.57256500 | 1.08338800 |
| C | 0.43457100 | -0.59558700 | -0.21080300 |
| C | 1.89952000 | 1.92349300 | -0.43317300 |
| C | 0.38954500 | 1.94306400 | -0.14012200 |
| C | -0.34407100 | 0.68349400 | -0.67439100 |
| C | -1.79667700 | 0.52341400 | -0.06208900 |
| C | -2.59051700 | -0.73171000 | -0.63290500 |
| C | -1.63265400 | -1.91217400 | -0.88637200 |
| C | -0.31166600 | -1.82985300 | -0.65619900 |
| C | -3.49865800 | -0.47950500 | -1.85388200 |
| C | -3.46242700 | -1.20458600 | 0.56313700 |
| C | -1.80305500 | 0.26644100 | 1.49370900 |
| C | -2.86876900 | -0.74746600 | 1.88153300 |
| O | -4.46122100 | -1.88370300 | 0.45280000 |
| O | -1.07443800 | 0.80756700 | 2.29674300 |

| | | | |
|---|---|---|---|
| C | 2.27772500 | -0.82511100 | -2.01824300 |
| C | -0.44929900 | 0.79921700 | -2.21740800 |
| C | 4.53123600 | 1.95151100 | 1.14197300 |
| C | 4.86048300 | 0.95803000 | -1.11575900 |
| C | -2.33946100 | -1.89300000 | 2.76312800 |
| C | -2.66356700 | 1.78458300 | -0.24486400 |
| O | -2.44641300 | 2.73911500 | -0.95416400 |
| O | -3.77775200 | 1.69698200 | 0.52716800 |
| C | -4.68971600 | 2.80912300 | 0.44551800 |
| C | -2.24353300 | -3.19303400 | -1.41198200 |
| H | 4.29014400 | -0.47979800 | 1.99208300 |
| H | 2.25666000 | 0.61075700 | 1.18748700 |
| H | 2.18530000 | -1.85169300 | 1.28627700 |
| H | 2.26597100 | -2.79465900 | -0.19470700 |
| H | 4.47372400 | -2.66866400 | 0.93626600 |
| H | 4.55130500 | -1.95782500 | -0.66514600 |
| H | 6.43568700 | -0.74045000 | 0.20039600 |
| H | 0.40700200 | -0.57203300 | 0.88754400 |
| H | 2.33508100 | 2.82048400 | 0.01889600 |
| H | 2.08773300 | 2.01353900 | -1.51009900 |
| H | -0.05820900 | 2.83681600 | -0.58381500 |
| H | 0.25048300 | 2.01500300 | 0.94126700 |
| H | 0.27233100 | -2.73006300 | -0.83519900 |
| H | -2.92132000 | -0.32301700 | -2.76690900 |
| H | -4.15700800 | -1.33944900 | -1.99382200 |
| H | -4.14336600 | 0.38991800 | -1.69839700 |
| H | -3.64861300 | -0.21238000 | 2.43705400 |
| H | 2.30239200 | 0.11443000 | -2.57311400 |
| H | 3.23894100 | -1.31824100 | -2.18435200 |
| H | 1.51457800 | -1.45902100 | -2.48230500 |
| H | -0.67053800 | -0.15697100 | -2.69535800 |
| H | -1.22100200 | 1.51977700 | -2.49080000 |
| H | 0.48733300 | 1.16558300 | -2.63969500 |
| H | 4.40193500 | 2.91421200 | 0.63676600 |
| H | 5.58309100 | 1.86164500 | 1.42961700 |
| H | 3.93015900 | 1.96906300 | 2.05979000 |
| H | 4.78951800 | 0.09442000 | -1.78242800 |
| H | 4.44770200 | 1.81901500 | -1.65166400 |
| H | 5.92344400 | 1.16806400 | -0.94887400 |
| H | -3.15946300 | -2.56898700 | 3.02144100 |
| H | -1.90852600 | -1.48093200 | 3.67988500 |
| H | -1.56686900 | -2.46716200 | 2.24254700 |
| H | -5.50546500 | 2.56542800 | 1.12591000 |
| H | -4.19001500 | 3.73088500 | 0.75206300 |
| H | -5.06037600 | 2.92287200 | -0.57607800 |
| H | -2.57658600 | -3.07749900 | -2.45136000 |
| H | -1.50821300 | -4.00321100 | -1.39009800 |
| H | -3.12038500 | -3.50253000 | -0.83407700 |

## AN-EN






**B3LYP/6-31+G(d,p)//B3LYP/6-31G***

Zero-point correction= 0.602439 (Hartree/Particle)
Thermal correction to Energy= 0.633785
Thermal correction to Enthalpy= 0.634729
Thermal correction to Gibbs Free Energy= 0.544990
Sum of electronic and zero-point Energies= -1389.239263
Sum of electronic and thermal Energies= -1389.207917
Sum of electronic and thermal Enthalpies= -1389.206973
Sum of electronic and thermal Free Energies= -1389.296712

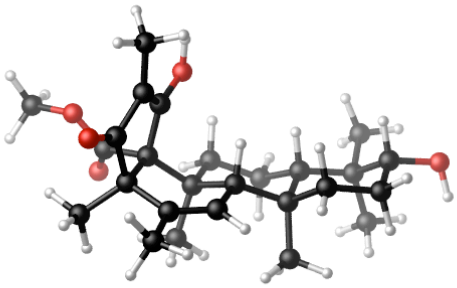
**MPW1PW91/6-31+G(d,p)//B3LYP/G-31G***

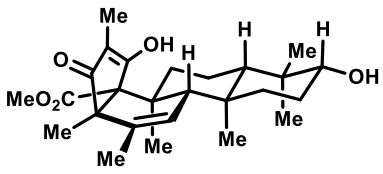
Zero-point correction= 0.605409 (Hartree/Particle)
Thermal correction to Energy= 0.636079
Thermal correction to Enthalpy= 0.637024
Thermal correction to Gibbs Free Energy= 0.550174
Sum of electronic and zero-point Energies= -1388.930500
Sum of electronic and thermal Energies= -1388.899830
Sum of electronic and thermal Enthalpies= -1388.898885
Sum of electronic and thermal Free Energies= -1388.985735

| | | | |
|---|---|---|---|
| C | -4.61173000 | 0.45515000 | 1.08696400 |
| C | -4.12848200 | -0.76877300 | 0.25064500 |
| C | -2.57171900 | -0.65482200 | 0.08998700 |
| C | -2.01012700 | 0.70188500 | -0.46323600 |
| C | -2.58802800 | 1.84274900 | 0.42069400 |
| C | -4.11594400 | 1.79842500 | 0.54906900 |
| O | -6.02996700 | 0.47207400 | 1.27494100 |
| C | -0.45064700 | 0.66127800 | -0.22972500 |
| C | -1.91130400 | -1.84928400 | -0.62014200 |
| C | -0.39439400 | -1.88575300 | -0.37648100 |
| C | 0.32832400 | -0.57779300 | -0.79989800 |
| C | 1.77301500 | -0.47768500 | -0.15715800 |
| C | 2.54767100 | 0.87167100 | -0.53708200 |
| C | 1.57602400 | 2.03193500 | -0.85752600 |
| C | 0.25653400 | 1.92255500 | -0.65596800 |
| C | 3.60906800 | 0.71486500 | -1.64968700 |
| C | 3.19048200 | 1.23485800 | 0.79399900 |
| C | 1.77351700 | -0.43647900 | 1.42156200 |
| C | 2.70431600 | 0.58680800 | 1.87419000 |
| O | 4.13738600 | 2.19567300 | 0.78053900 |

| | | | |
|---|---|---|---|
| O | 1.13942800 | -1.18307900 | 2.15385500 |
| C | -2.36699500 | 0.99919500 | -1.94327700 |
| C | 0.42209700 | -0.55609600 | -2.34878600 |
| C | -4.47202000 | -2.03375400 | 1.07222800 |
| C | -4.90199900 | -0.86402500 | -1.08263800 |
| C | 3.05417700 | 0.77811900 | 3.31909300 |
| C | 2.64613700 | -1.70715000 | -0.50772500 |
| O | 2.43429000 | -2.53332700 | -1.36777200 |
| O | 3.73223500 | -1.78923500 | 0.29997900 |
| C | 4.58350600 | -2.92588800 | 0.07304200 |
| C | 2.16687700 | 3.32980700 | -1.36429100 |
| H | -4.21351400 | 0.32877100 | 2.10268500 |
| H | -2.20060400 | -0.69185200 | 1.12810700 |
| H | -2.15232000 | 1.76687200 | 1.42735500 |
| H | -2.28995100 | 2.82390300 | 0.03081500 |
| H | -4.45892000 | 2.59066600 | 1.22536800 |
| H | -4.59019200 | 2.00183700 | -0.42196000 |
| H | -6.43102800 | 0.69404100 | 0.41973000 |
| H | -0.36525900 | 0.58134800 | 0.86420900 |
| H | -2.32920600 | -2.78874500 | -0.24349900 |
| H | -2.13488900 | -1.83435400 | -1.69405800 |
| H | 0.04380400 | -2.72738500 | -0.92107600 |
| H | -0.22126900 | -2.06670300 | 0.68676100 |
| H | -0.35026900 | 2.80357100 | -0.85313400 |
| H | 3.13928400 | 0.44005800 | -2.59777600 |
| H | 4.15601600 | 1.64915200 | -1.79322800 |
| H | 4.34298800 | -0.05125200 | -1.38886300 |
| H | -2.43035700 | 0.10110100 | -2.56095400 |
| H | -3.32795700 | 1.51339300 | -2.03037900 |
| H | -1.61725600 | 1.65408000 | -2.39916700 |
| H | 0.71597900 | 0.41887400 | -2.74341600 |
| H | 1.13355400 | -1.30653200 | -2.69212300 |
| H | -0.54452300 | -0.80475600 | -2.79022200 |
| H | -4.35707600 | -2.95146700 | 0.48638500 |
| H | -5.51204500 | -1.97766300 | 1.40796800 |
| H | -3.83352100 | -2.11907600 | 1.96029800 |
| H | -4.86696300 | 0.05430500 | -1.67472100 |
| H | -4.50559200 | -1.67049700 | -1.70797900 |
| H | -5.95488100 | -1.10059600 | -0.88903200 |
| H | 3.95319200 | 0.21474400 | 3.60348100 |
| H | 2.23297800 | 0.40535400 | 3.93851700 |
| H | 3.22019200 | 1.83271500 | 3.57823600 |
| H | 5.37930600 | -2.84368700 | 0.81380700 |
| H | 4.02347200 | -3.85414600 | 0.20922400 |
| H | 4.99493500 | -2.90329800 | -0.93959500 |
| H | 2.56862000 | 3.22367000 | -2.38030600 |
| H | 1.39599600 | 4.10617300 | -1.39769400 |
| H | 2.98726400 | 3.68877200 | -0.73405300 |
| H | 4.44289500 | 2.35098700 | 1.69081300 |

**AN-ES**






**B3LYP/6-31+G(d,p)//B3LYP/6-31G***

Zero-point correction= 0.602349 (Hartree/Particle)
Thermal correction to Energy= 0.633706
Thermal correction to Enthalpy= 0.634650
Thermal correction to Gibbs Free Energy= 0.545025
Sum of electronic and zero-point Energies= -1389.241087
Sum of electronic and thermal Energies= -1389.209731
Sum of electronic and thermal Enthalpies= -1389.208786
Sum of electronic and thermal Free Energies= -1389.298411

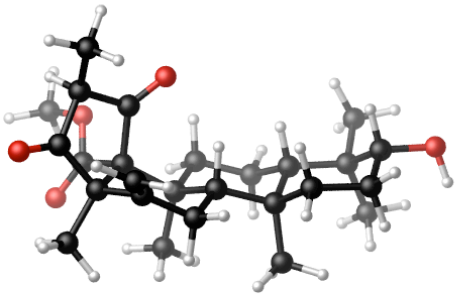
**MPW1PW91/6-31+G(d,p)//B3LYP/G-31G***

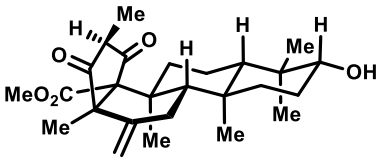
Zero-point correction= 0.605280 (Hartree/Particle)
Thermal correction to Energy= 0.635984
Thermal correction to Enthalpy= 0.636928
Thermal correction to Gibbs Free Energy= 0.550040
Sum of electronic and zero-point Energies= -1388.932704
Sum of electronic and thermal Energies= -1388.902001
Sum of electronic and thermal Enthalpies= -1388.901056
Sum of electronic and thermal Free Energies= -1388.987945

| | | | |
|---|---|---|---|
| C | -4.61432700 | 0.43102600 | 1.06142500 |
| C | -4.11995100 | -0.77997900 | 0.21272500 |
| C | -2.56179000 | -0.66043900 | 0.07119800 |
| C | -1.99598500 | 0.70444600 | -0.45725700 |
| C | -2.58738900 | 1.83204200 | 0.43477200 |
| C | -4.11652100 | 1.78243100 | 0.54674300 |
| O | -6.03365000 | 0.44024800 | 1.23739600 |
| C | -0.43775000 | 0.66636100 | -0.20854800 |
| C | -1.89138700 | -1.84556000 | -0.64527500 |
| C | -0.37755200 | -1.88140100 | -0.38031500 |
| C | 0.34590400 | -0.56665200 | -0.78030900 |
| C | 1.79861200 | -0.45708600 | -0.14001400 |
| C | 2.56448900 | 0.88113100 | -0.57178800 |
| C | 1.58683300 | 2.03708300 | -0.84696000 |
| C | 0.27025500 | 1.93389500 | -0.61553700 |
| C | 3.60108100 | 0.72410100 | -1.69846700 |
| C | 3.26497000 | 1.32573700 | 0.74451600 |
| C | 1.82892900 | -0.31990900 | 1.38589100 |
| C | 2.62031500 | 0.66148000 | 1.86989000 |
| O | 4.18935200 | 2.12330500 | 0.80315300 |

| | | | |
|---|---|---|---|
| O | 1.16888800 | -1.23688200 | 2.12838800 |
| C | -2.33596500 | 1.02140500 | -1.93709800 |
| C | 0.44948400 | -0.53589800 | -2.32858600 |
| C | -4.47127000 | -2.05709900 | 1.01172800 |
| C | -4.87763000 | -0.85664400 | -1.13071100 |
| C | 2.95380400 | 0.96211400 | 3.30011900 |
| C | 2.67297300 | -1.69570900 | -0.48200000 |
| O | 2.47660900 | -2.50461200 | -1.36174200 |
| O | 3.74358200 | -1.78185000 | 0.34024900 |
| C | 4.63325600 | -2.88222900 | 0.08120600 |
| C | 2.18768900 | 3.34108700 | -1.32081400 |
| H | -4.22455100 | 0.29148800 | 2.07895300 |
| H | -2.20350500 | -0.70974400 | 1.11404500 |
| H | -2.16245200 | 1.74511300 | 1.44537200 |
| H | -2.28751100 | 2.81839800 | 0.06102800 |
| H | -4.46795500 | 2.56479800 | 1.23007800 |
| H | -4.58138900 | 1.99785400 | -0.42605300 |
| H | -6.42867400 | 0.68581500 | 0.38581400 |
| H | -0.36261000 | 0.57724500 | 0.88762000 |
| H | -2.31345500 | -2.79060100 | -0.28769200 |
| H | -2.09837400 | -1.81627200 | -1.72152600 |
| H | 0.07290000 | -2.71641100 | -0.92502200 |
| H | -0.23307900 | -2.08328900 | 0.68328100 |
| H | 3.12829600 | 0.51385800 | -2.66142400 |
| H | 4.18479600 | 1.64308200 | -1.78237000 |
| H | 4.30970800 | -0.07771500 | -1.47563100 |
| H | -2.38519800 | 0.13300300 | -2.56988200 |
| H | -3.29889100 | 1.53098800 | -2.02900900 |
| H | -1.58382700 | 1.68807800 | -2.37082000 |
| H | 0.72331300 | 0.44757400 | -2.71385800 |
| H | 1.17910800 | -1.26794000 | -2.67251800 |
| H | -0.50902200 | -0.80312700 | -2.77619500 |
| H | -4.34712400 | -2.96653500 | 0.41499100 |
| H | -5.51545000 | -2.00748000 | 1.33504600 |
| H | -3.84444800 | -2.15320800 | 1.90730500 |
| H | -4.83235000 | 0.06881400 | -1.71031800 |
| H | -4.47636500 | -1.65649600 | -1.76147800 |
| H | -5.93335600 | -1.09210800 | -0.95232400 |
| H | 3.85306800 | 1.58487900 | 3.32630200 |
| H | 3.16045100 | 0.05485700 | 3.88619700 |
| H | 2.15344400 | 1.51528000 | 3.80918800 |
| H | 5.42109500 | -2.79925100 | 0.83004900 |
| H | 4.10249700 | -3.83251200 | 0.17883900 |
| H | 5.05023000 | -2.80916700 | -0.92654100 |
| H | 2.55339100 | 3.26373200 | -2.35295400 |
| H | 1.43758800 | 4.13788100 | -1.29556800 |
| H | 1.34887000 | -1.06367900 | 3.06875400 |
| H | 3.03976800 | 3.64140100 | -0.70186300 |
| H | -0.33366000 | 2.82532300 | -0.76857000 |

## TE-DK






**B3LYP/6-31+G(d,p)//B3LYP/6-31G***

Zero-point correction= 0.602371 (Hartree/Particle)
Thermal correction to Energy= 0.633530
Thermal correction to Enthalpy= 0.634475
Thermal correction to Gibbs Free Energy= 0.544866
Sum of electronic and zero-point Energies= -1389.230311
Sum of electronic and thermal Energies= -1389.199152
Sum of electronic and thermal Enthalpies= -1389.198208
Sum of electronic and thermal Free Energies= -1389.287817

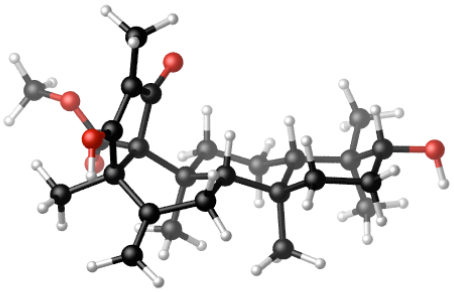
**MPW1PW91/6-31+G(d,p)//B3LYP/G-31G***

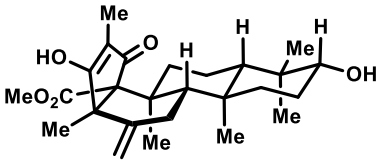
Zero-point correction= 0.605029 (Hartree/Particle)
Thermal correction to Energy= 0.635660
Thermal correction to Enthalpy= 0.636604
Thermal correction to Gibbs Free Energy= 0.549367
Sum of electronic and zero-point Energies= -1388.920835
Sum of electronic and thermal Energies= -1388.890204
Sum of electronic and thermal Enthalpies= -1388.889260
Sum of electronic and thermal Free Energies= -1388.976497

| | | | |
|---|---|---|---|
| C | 4.57453700 | -0.60103300 | 1.01172000 |
| C | 4.06210600 | 0.72592300 | 0.37422300 |
| C | 2.51357900 | 0.58358900 | 0.16302200 |
| C | 2.00612700 | -0.68214300 | -0.61999500 |
| C | 2.62311000 | -1.93426100 | 0.06618800 |
| C | 4.14449500 | -1.85148400 | 0.24441200 |
| O | 5.98723300 | -0.59734100 | 1.23406400 |
| C | 0.44275100 | -0.73081800 | -0.39504400 |
| C | 1.82675000 | 1.86009100 | -0.35297400 |
| C | 0.30702400 | 1.80688600 | -0.13607000 |
| C | -0.36137400 | 0.55977800 | -0.77918300 |
| C | -1.83337600 | 0.37488800 | -0.18823300 |
| C | -2.61608200 | -0.92328300 | -0.69168000 |
| C | -1.68077400 | -2.14025000 | -0.50352600 |
| C | -0.25211100 | -1.97977300 | -0.98016900 |
| C | -3.21382400 | -0.95938000 | -2.11126300 |
| C | -3.73746600 | -1.05269900 | 0.36498600 |
| C | -1.91276200 | 0.13070100 | 1.36247200 |
| C | -3.29873100 | -0.41677900 | 1.68133400 |
| O | -4.80650500 | -1.59396800 | 0.18305900 |

| | | | |
|---|---|---|---|
| O | -1.03554400 | 0.28088800 | 2.18290100 |
| C | 2.39584700 | -0.71665600 | -2.11880900 |
| C | -0.42519800 | 0.80743500 | -2.30914100 |
| C | 4.34346300 | 1.84950300 | 1.39950100 |
| C | 4.85363500 | 1.06654800 | -0.90728300 |
| C | -3.37807900 | -1.32989300 | 2.90787000 |
| C | -2.64819200 | 1.66125500 | -0.45066300 |
| O | -3.17983800 | 1.98454500 | -1.49102400 |
| O | -2.68497900 | 2.44827900 | 0.64960000 |
| C | -3.37522500 | 3.70386200 | 0.50047100 |
| C | -2.10917200 | -3.30838200 | -0.00894800 |
| H | 4.14879400 | -0.65849200 | 2.02254300 |
| H | 2.12603400 | 0.43542300 | 1.18433400 |
| H | 2.16345100 | -2.06077200 | 1.05699400 |
| H | 2.38464700 | -2.84007400 | -0.50397200 |
| H | 4.50372700 | -2.73297000 | 0.78891600 |
| H | 4.64917100 | -1.87319800 | -0.73250100 |
| H | 6.41620000 | -0.68312100 | 0.36797100 |
| H | 0.34914300 | -0.81749100 | 0.69155300 |
| H | 2.20747200 | 2.73631200 | 0.18165400 |
| H | 2.06567200 | 2.03020700 | -1.40968100 |
| H | -0.14898800 | 2.71678300 | -0.54987200 |
| H | 0.11525200 | 1.81397600 | 0.93852000 |
| H | 0.29669100 | -2.88486800 | -0.70741800 |
| H | -0.24877700 | -1.94271000 | -2.07707000 |
| H | -2.44954200 | -1.13124800 | -2.87157700 |
| H | -3.92349400 | -1.79024500 | -2.14497300 |
| H | -3.73963900 | -0.03596900 | -2.35353700 |
| H | -3.95155500 | 0.45426000 | 1.84413300 |
| H | 2.37988000 | 0.26465500 | -2.59678000 |
| H | 3.40093900 | -1.12119100 | -2.26308500 |
| H | 1.72065400 | -1.36582200 | -2.68528300 |
| H | -0.59949000 | -0.09793900 | -2.89177900 |
| H | -1.22053000 | 1.51111000 | -2.56038000 |
| H | 0.51245300 | 1.23984900 | -2.66205000 |
| H | 4.20841700 | 2.84724300 | 0.96931300 |
| H | 5.37801900 | 1.77192600 | 1.74697500 |
| H | 3.68590900 | 1.76656500 | 2.27384200 |
| H | 4.86910100 | 0.25626300 | -1.64095100 |
| H | 4.43388700 | 1.94805700 | -1.40312100 |
| H | 5.89189500 | 1.30972500 | -0.65285400 |
| H | -4.40268600 | -1.68951000 | 3.03737700 |
| H | -3.07116800 | -0.78388700 | 3.80392000 |
| H | -2.71621900 | -2.19288800 | 2.79070300 |
| H | -3.30549200 | 4.18837400 | 1.47411700 |
| H | -2.89411100 | 4.31168300 | -0.26954600 |
| H | -4.41862500 | 3.53502100 | 0.22310000 |
| H | -3.13391800 | -3.48031200 | 0.30269500 |
| H | -1.43247400 | -4.15569700 | 0.06965100 |

## TE-EN






**B3LYP/6-31+G(d,p)//B3LYP/6-31G***

Zero-point correction= 0.603332 (Hartree/Particle)
Thermal correction to Energy= 0.634352
Thermal correction to Enthalpy= 0.635296
Thermal correction to Gibbs Free Energy= 0.545950
Sum of electronic and zero-point Energies= -1389.230618
Sum of electronic and thermal Energies= -1389.199597
Sum of electronic and thermal Enthalpies= -1389.198653
Sum of electronic and thermal Free Energies= -1389.287999

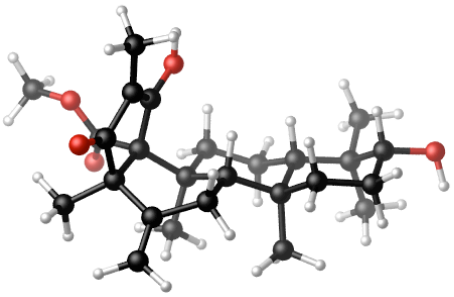
**MPW1PW91/6-31+G(d,p)//B3LYP/G-31G***

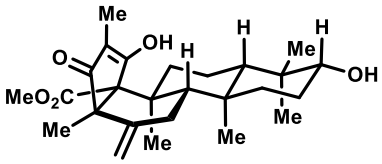
Zero-point correction= 0.606160 (Hartree/Particle)
Thermal correction to Energy= 0.636553
Thermal correction to Enthalpy= 0.637497
Thermal correction to Gibbs Free Energy= 0.551009
Sum of electronic and zero-point Energies= -1388.922589
Sum of electronic and thermal Energies= -1388.892197
Sum of electronic and thermal Enthalpies= -1388.891253
Sum of electronic and thermal Free Energies= -1388.977741

| | | | |
|---|---|---|---|
| C | 4.57247500 | -0.40604500 | 1.05675200 |
| C | 4.06899100 | 0.81005600 | 0.22039200 |
| C | 2.51182900 | 0.67806500 | 0.07431600 |
| C | 1.96042600 | -0.68776300 | -0.46821600 |
| C | 2.56201400 | -1.82117900 | 0.40896500 |
| C | 4.09008000 | -1.75724900 | 0.52546500 |
| O | 5.99161900 | -0.40500400 | 1.23572100 |
| C | 0.40500000 | -0.66709200 | -0.20668400 |
| C | 1.82988500 | 1.85864900 | -0.63883200 |
| C | 0.31226200 | 1.86728200 | -0.39673100 |
| C | -0.39322600 | 0.54211100 | -0.79969800 |
| C | -1.83914600 | 0.46079800 | -0.13393500 |
| C | -2.60909400 | -0.88986100 | -0.50508100 |
| C | -1.67719200 | -1.94759400 | -1.10778100 |
| C | -0.28183500 | -2.03291300 | -0.51742800 |
| C | -3.88351000 | -0.67682300 | -1.35192300 |
| C | -2.98946500 | -1.44582500 | 0.86643300 |
| C | -1.80300800 | 0.41334200 | 1.44433100 |
| C | -2.56623000 | -0.73097700 | 1.92753200 |
| O | -3.67837800 | -2.60019100 | 0.95133500 |
| O | -1.21868100 | 1.21722200 | 2.15572900 |

| | | | |
|---|---|---|---|
| C | 2.31693100 | -0.96952200 | -1.95224500 |
| C | -0.49621000 | 0.50645300 | -2.34793600 |
| C | 4.40372200 | 2.08202800 | 1.03463700 |
| C | 4.83239300 | 0.90938200 | -1.11836900 |
| C | -2.75763200 | -1.02022600 | 3.38268800 |
| C | -2.70325800 | 1.69536500 | -0.47850000 |
| O | -2.58387000 | 2.43483200 | -1.43098000 |
| O | -3.67179400 | 1.88061300 | 0.44913900 |
| C | -4.51517900 | 3.02817200 | 0.24743300 |
| C | -2.09040500 | -2.84974600 | -2.01120100 |
| H | 4.17911300 | -0.28199200 | 2.07463000 |
| H | 2.15097300 | 0.71767100 | 1.11564300 |
| H | 2.13546300 | -1.75062500 | 1.42017100 |
| H | 2.26933900 | -2.80418000 | 0.01909300 |
| H | 4.44813900 | -2.54317300 | 1.20121700 |
| H | 4.56014100 | -1.95719300 | -0.44833300 |
| H | 6.39065300 | -0.62481700 | 0.37900800 |
| H | 0.34358800 | -0.52937000 | 0.87877000 |
| H | 2.22991600 | 2.80657000 | -0.26397500 |
| H | 2.05411000 | 1.84610200 | -1.71261200 |
| H | -0.14130200 | 2.69336200 | -0.95397900 |
| H | 0.13467300 | 2.06145900 | 0.66368100 |
| H | -0.33733800 | -2.61014900 | 0.41491800 |
| H | 0.32540600 | -2.63563600 | -1.19831400 |
| H | -3.63150300 | -0.30681900 | -2.34960800 |
| H | -4.44902800 | -1.60600600 | -1.46669400 |
| H | -4.55048300 | 0.03693100 | -0.86524500 |
| H | 2.40015000 | -0.06235700 | -2.55366700 |
| H | 3.26992700 | -1.49790200 | -2.04152700 |
| H | 1.56586700 | -1.60304700 | -2.43385700 |
| H | -0.77138600 | -0.47245000 | -2.74513100 |
| H | -1.22795000 | 1.23800300 | -2.68984300 |
| H | 0.46320300 | 0.77560500 | -2.79305200 |
| H | 4.27032900 | 2.99597700 | 0.44676500 |
| H | 5.44771400 | 2.04116600 | 1.35995300 |
| H | 3.77339700 | 2.16180200 | 1.92899600 |
| H | 4.80553100 | -0.01174600 | -1.70645600 |
| H | 4.42289800 | 1.70867700 | -1.74448400 |
| H | 5.88336500 | 1.15947800 | -0.93191700 |
| H | -2.99685200 | -2.07420800 | 3.55145200 |
| H | -3.57274700 | -0.41632600 | 3.80146000 |
| H | -1.85109000 | -0.75909700 | 3.93822000 |
| H | -5.21223600 | 3.02495100 | 1.08546300 |
| H | -3.91718600 | 3.94256900 | 0.24612200 |
| H | -5.05082100 | 2.95017200 | -0.70246300 |
| H | -3.07370000 | -2.83561600 | -2.46892800 |
| H | -1.41534800 | -3.62479300 | -2.36613700 |
| H | -3.59981300 | -3.06609400 | 0.09680200 |

## TE-ES






**B3LYP/6-31+G(d,p)//B3LYP/6-31G***

Zero-point correction= 0.602968 (Hartree/Particle)
Thermal correction to Energy= 0.634071
Thermal correction to Enthalpy= 0.635015
Thermal correction to Gibbs Free Energy= 0.545535
Sum of electronic and zero-point Energies= -1389.228592
Sum of electronic and thermal Energies= -1389.197490
Sum of electronic and thermal Enthalpies= -1389.196546
Sum of electronic and thermal Free Energies= -1389.286026

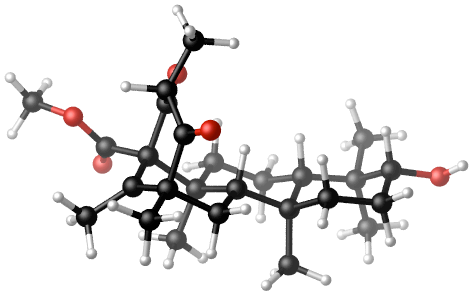
**MPW1PW91/6-31+G(d,p)//B3LYP/G-31G***

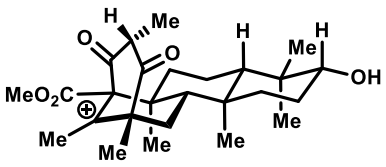
Zero-point correction= 0.605800 (Hartree/Particle)
Thermal correction to Energy= 0.636287
Thermal correction to Enthalpy= 0.637231
Thermal correction to Gibbs Free Energy= 0.550541
Sum of electronic and zero-point Energies= -1388.920240
Sum of electronic and thermal Energies= -1388.889753
Sum of electronic and thermal Enthalpies= -1388.888809
Sum of electronic and thermal Free Energies= -1388.975498

| | | | |
|---|---|---|---|
| C | 4.60149600 | -0.36178400 | 1.06106700 |
| C | 4.08635600 | 0.81555900 | 0.17752200 |
| C | 2.52727000 | 0.67674800 | 0.06112600 |
| C | 1.96901800 | -0.71085900 | -0.41651900 |
| C | 2.58264600 | -1.80283300 | 0.50381400 |
| C | 4.11230500 | -1.73509500 | 0.59744900 |
| O | 6.02254000 | -0.35106900 | 1.22212800 |
| C | 0.41732200 | -0.67858800 | -0.14013000 |
| C | 1.83282100 | 1.83031100 | -0.68390300 |
| C | 0.31652400 | 1.84310400 | -0.42534000 |
| C | -0.38336900 | 0.50165300 | -0.78232400 |
| C | -1.84472100 | 0.41328900 | -0.13747000 |
| C | -2.62492800 | -0.92461900 | -0.56253400 |
| C | -1.64684900 | -2.00275100 | -1.03926800 |
| C | -0.28726400 | -2.05220300 | -0.36547600 |
| C | -3.79295200 | -0.71675300 | -1.53857900 |
| C | -3.19807400 | -1.46222000 | 0.78658600 |
| C | -1.85719100 | 0.28139300 | 1.38667100 |
| C | -2.58328200 | -0.74133500 | 1.89092300 |
| O | -4.02979900 | -2.35088900 | 0.86555000 |

| | | | |
|---|---|---|---|
| O | -1.22318200 | 1.22435800 | 2.11618600 |
| C | 2.30430800 | -1.06156200 | -1.89009300 |
| C | -0.47765800 | 0.42234100 | -2.32984700 |
| C | 4.43502600 | 2.12266600 | 0.92713400 |
| C | 4.82808500 | 0.85196000 | -1.17659800 |
| C | -2.85586600 | -1.05417500 | 3.33228800 |
| C | -2.69860200 | 1.65856200 | -0.49053500 |
| O | -2.57329700 | 2.37370100 | -1.45998400 |
| O | -3.66779400 | 1.86760900 | 0.43049200 |
| C | -4.53351000 | 2.98700900 | 0.17090500 |
| C | -1.98585100 | -2.93997200 | -1.93196500 |
| H | 4.22085900 | -0.19185100 | 2.07742800 |
| H | 2.18444500 | 0.75643900 | 1.10709700 |
| H | 2.16998900 | -1.68517800 | 1.51677400 |
| H | 2.28335500 | -2.80195700 | 0.16497900 |
| H | 4.47885100 | -2.49013000 | 1.30324700 |
| H | 4.56997000 | -1.97892200 | -0.37199100 |
| H | 6.41125500 | -0.62310900 | 0.37572000 |
| H | 0.37133900 | -0.48271500 | 0.93824400 |
| H | 2.23502700 | 2.79196700 | -0.34810300 |
| H | 2.04263500 | 1.78036400 | -1.75886300 |
| H | -0.14582700 | 2.65122400 | -1.00077900 |
| H | 0.16245500 | 2.07782100 | 0.63075500 |
| H | -0.40474300 | -2.54136400 | 0.61113700 |
| H | 0.34414300 | -2.72545000 | -0.95206300 |
| H | -3.44324800 | -0.44430400 | -2.53797200 |
| H | -4.37428400 | -1.63939700 | -1.59802700 |
| H | -4.47493400 | 0.05798200 | -1.17854000 |
| H | 2.37286200 | -0.18479100 | -2.53669400 |
| H | 3.25803900 | -1.59013200 | -1.97068700 |
| H | 1.54645400 | -1.72056100 | -2.32402600 |
| H | -0.72623200 | -0.57409900 | -2.69567600 |
| H | -1.22647700 | 1.12529000 | -2.69388500 |
| H | 0.47545600 | 0.70610400 | -2.77865900 |
| H | 4.29093000 | 3.00941500 | 0.30141200 |
| H | 5.48438700 | 2.09584100 | 1.23597100 |
| H | 3.82065600 | 2.24191100 | 1.82856400 |
| H | 4.78336000 | -0.09271900 | -1.72424100 |
| H | 4.41419700 | 1.62754400 | -1.82921200 |
| H | 5.88400500 | 1.10075800 | -1.01837100 |
| H | -3.64803200 | -1.80698300 | 3.38300200 |
| H | -3.19722000 | -0.17357100 | 3.89539600 |
| H | -1.97635200 | -1.46202700 | 3.84827600 |
| H | -5.24002200 | 3.00470100 | 1.00096000 |
| H | -3.95657200 | 3.91434200 | 0.13254500 |
| H | -5.05777700 | 2.85380600 | -0.77883400 |
| H | -2.95750900 | -2.98648000 | -2.40874600 |
| H | -1.27934000 | -3.71821500 | -2.21059100 |
| H | -1.38221500 | 1.04968400 | 3.06002300 |

**PAC-DK**






**B3LYP/6-31+G(d,p)//B3LYP/6-31G***

| | |
|---|---|
| Zero-point correction= | 0.611808 (Hartree/Particle) |
| Thermal correction to Energy= | 0.643649 |
| Thermal correction to Enthalpy= | 0.644593 |
| Thermal correction to Gibbs Free Energy= | 0.553703 |
| Sum of electronic and zero-point Energies= | -1389.564292 |
| Sum of electronic and thermal Energies= | -1389.532451 |
| Sum of electronic and thermal Enthalpies= | -1389.531506 |
| Sum of electronic and thermal Free Energies= | -1389.622397 |

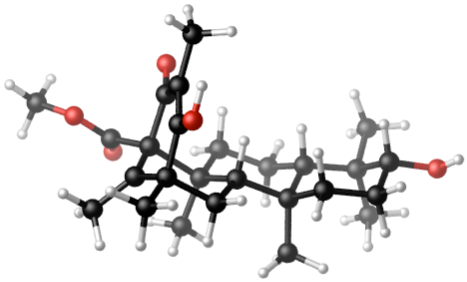
**MPW1PW91/6-31+G(d,p)//B3LYP/G-31G***

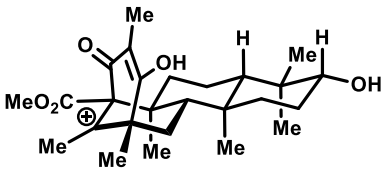
| | |
|---|---|
| Zero-point correction= | 0.614545 (Hartree/Particle) |
| Thermal correction to Energy= | 0.645793 |
| Thermal correction to Enthalpy= | 0.646737 |
| Thermal correction to Gibbs Free Energy= | 0.558566 |
| Sum of electronic and zero-point Energies= | -1389.254526 |
| Sum of electronic and thermal Energies= | -1389.223278 |
| Sum of electronic and thermal Enthalpies= | -1389.222334 |
| Sum of electronic and thermal Free Energies= | -1389.310504 |

| | | | |
|---|---|---|---|
| C | -4.47440500 | 0.50986600 | 0.80993200 |
| C | -3.94800000 | -0.88551400 | 0.37506900 |
| C | -2.39293900 | -0.75910300 | 0.18490400 |
| C | -1.88287400 | 0.39379200 | -0.75086500 |
| C | -2.51456600 | 1.72815700 | -0.26461200 |
| C | -4.03979400 | 1.64538800 | -0.12061800 |
| O | -5.89300100 | 0.43010300 | 0.89148700 |
| C | -0.30895500 | 0.48265000 | -0.49066000 |
| C | -1.68849800 | -2.08288300 | -0.14306000 |
| C | -0.16487600 | -1.99933800 | 0.10452700 |
| C | 0.46330900 | -0.85039300 | -0.70385200 |
| C | 2.04410300 | -0.52354300 | -0.07270100 |
| C | 2.53835200 | 0.52214900 | -0.95589600 |
| C | 1.91274800 | 1.84645100 | -0.83597300 |
| C | 0.36236800 | 1.64491000 | -1.21784300 |
| C | 3.57321600 | 0.25805400 | -1.98163700 |
| C | 1.86570100 | 2.33964900 | 0.66789500 |
| C | 1.92201700 | -0.04905900 | 1.42333900 |
| C | 2.33719600 | 1.38184100 | 1.74352200 |
| O | 1.46802200 | 3.45321700 | 0.89376000 |
| O | 1.60898700 | -0.83878500 | 2.27769800 |

| | | | |
|---|---|---|---|
| C | -2.22152900 | 0.20796500 | -2.25074300 |
| C | 0.64124100 | -1.28005500 | -2.17063000 |
| C | -4.23429600 | -1.86019500 | 1.54342700 |
| C | -4.70934900 | -1.40912300 | -0.86133300 |
| C | 1.97822900 | 1.82298200 | 3.16050800 |
| C | 2.95804800 | -1.77493500 | -0.04492800 |
| O | 2.72583100 | -2.85793200 | -0.52006400 |
| O | 4.09244400 | -1.44521600 | 0.59402900 |
| C | 5.05275200 | -2.52018500 | 0.78576100 |
| C | 2.50037400 | 2.96775700 | -1.70825700 |
| H | -4.05351300 | 0.71163200 | 1.81188200 |
| H | -2.03404900 | -0.47281200 | 1.18835500 |
| H | -2.08259700 | 1.99794400 | 0.71070400 |
| H | -2.26588700 | 2.54390700 | -0.95430500 |
| H | -4.40870000 | 2.60000700 | 0.27828300 |
| H | -4.52716100 | 1.51763700 | -1.09326500 |
| H | -6.22228900 | 1.24808900 | 1.29476500 |
| H | -0.25954800 | 0.69740800 | 0.58652000 |
| H | -2.06045000 | -2.88197200 | 0.50408500 |
| H | -1.90093400 | -2.40496400 | -1.16790500 |
| H | 0.31421500 | -2.94314000 | -0.16426400 |
| H | -0.00696300 | -1.84992100 | 1.17396100 |
| H | -0.09357100 | 2.60510100 | -0.96602800 |
| H | 0.32035300 | 1.53442700 | -2.30403200 |
| H | 3.73038100 | -0.80329700 | -2.17724400 |
| H | 3.36977900 | 0.79000900 | -2.91533700 |
| H | 4.52363800 | 0.67367100 | -1.60251800 |
| H | 3.43868900 | 1.35206900 | 1.62301700 |
| H | -2.18172300 | -0.83063000 | -2.58318100 |
| H | -3.22905100 | 0.56612200 | -2.46586700 |
| H | -1.55034700 | 0.78624900 | -2.89357000 |
| H | 0.93225800 | -0.46576800 | -2.84141000 |
| H | 1.38232400 | -2.07753100 | -2.24329000 |
| H | -0.29768100 | -1.68588500 | -2.54757600 |
| H | -4.06329500 | -2.90421000 | 1.26219200 |
| H | -5.28170400 | -1.76654600 | 1.84116100 |
| H | -3.61171600 | -1.63693200 | 2.41937300 |
| H | -4.69500200 | -0.72174800 | -1.70939200 |
| H | -4.29789700 | -2.36714100 | -1.19761400 |
| H | -5.75731000 | -1.57185200 | -0.59893100 |
| H | 2.36913100 | 2.82484100 | 3.34918700 |
| H | 2.39758200 | 1.12515300 | 3.88763200 |
| H | 0.89371300 | 1.84924200 | 3.29731800 |
| H | 5.88751600 | -2.06478400 | 1.31574900 |
| H | 4.59915400 | -3.31530200 | 1.37986800 |
| H | 5.36900400 | -2.91554600 | -0.18134400 |
| H | 3.56931800 | 3.11424000 | -1.52116700 |
| H | 2.35848200 | 2.76515700 | -2.77380400 |
| H | 1.99013800 | 3.90227600 | -1.46893400 |

**PAC-EN**






**B3LYP/6-31+G(d,p)//B3LYP/6-31G***

Zero-point correction= 0.612772 (Hartree/Particle)
Thermal correction to Energy= 0.644767
Thermal correction to Enthalpy= 0.645711
Thermal correction to Gibbs Free Energy= 0.554594
Sum of electronic and zero-point Energies= -1389.569135
Sum of electronic and thermal Energies= -1389.537140
Sum of electronic and thermal Enthalpies= -1389.536196
Sum of electronic and thermal Free Energies= -1389.627313

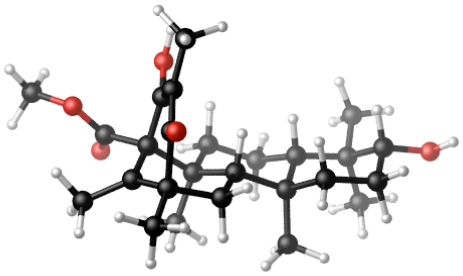
**MPW1PW91/6-31+G(d,p)//B3LYP/G-31G***

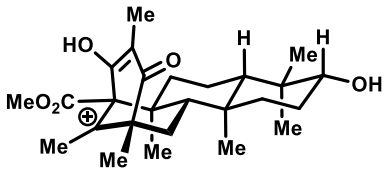
Zero-point correction= 0.615652 (Hartree/Particle)
Thermal correction to Energy= 0.646985
Thermal correction to Enthalpy= 0.647929
Thermal correction to Gibbs Free Energy= 0.559703
Sum of electronic and zero-point Energies= -1389.259588
Sum of electronic and thermal Energies= -1389.228255
Sum of electronic and thermal Enthalpies= -1389.227310
Sum of electronic and thermal Free Energies= -1389.315536

| | | | |
|---|---|---|---|
| C | -4.51230900 | 0.53893600 | 0.73757400 |
| C | -3.96619400 | -0.87523600 | 0.39887400 |
| C | -2.40917600 | -0.74185300 | 0.23043800 |
| C | -1.89390900 | 0.34981400 | -0.77453400 |
| C | -2.54255400 | 1.70597000 | -0.38042700 |
| C | -4.06955300 | 1.61897800 | -0.25355600 |
| O | -5.93169100 | 0.45186400 | 0.79782800 |
| C | -0.32324400 | 0.46507400 | -0.50146400 |
| C | -1.68001600 | -2.07639600 | 0.01768900 |
| C | -0.15808400 | -1.94990500 | 0.26833000 |
| C | 0.44509300 | -0.87072000 | -0.64128000 |
| C | 2.08933000 | -0.52081500 | -0.03262900 |
| C | 2.52174400 | 0.49489500 | -0.94230700 |
| C | 1.88816700 | 1.83670500 | -0.80792300 |
| C | 0.35981400 | 1.60394900 | -1.25510200 |
| C | 3.47880800 | 0.22390700 | -2.03900900 |
| C | 1.88520300 | 2.25354400 | 0.66297600 |
| C | 1.97716800 | -0.03205400 | 1.45574700 |
| C | 1.92663400 | 1.39819000 | 1.71536600 |
| O | 1.78309200 | 3.58506900 | 0.79959200 |
| O | 1.96943600 | -0.88666300 | 2.32242100 |

| | | | |
|---|---|---|---|
| C | -2.21344000 | 0.07024100 | -2.26368900 |
| C | 0.62037600 | -1.40252100 | -2.07067700 |
| C | -4.26564000 | -1.78000600 | 1.61906700 |
| C | -4.69913800 | -1.47956000 | -0.81742300 |
| C | 1.88208500 | 1.86995200 | 3.14996600 |
| C | 2.98850500 | -1.78253700 | -0.00973400 |
| O | 2.68112900 | -2.90236000 | -0.33628800 |
| O | 4.20207400 | -1.42101200 | 0.42992900 |
| C | 5.15320800 | -2.50072900 | 0.62193600 |
| C | 2.49876100 | 2.93883700 | -1.69559300 |
| H | -4.11222800 | 0.80572500 | 1.73302900 |
| H | -2.07500600 | -0.37786400 | 1.21684900 |
| H | -2.12709100 | 2.03939500 | 0.58256900 |
| H | -2.29160500 | 2.47981200 | -1.11620200 |
| H | -4.45303000 | 2.59315800 | 0.07940700 |
| H | -4.53965800 | 1.42741000 | -1.22430100 |
| H | -6.27529900 | 1.29211800 | 1.13834200 |
| H | -0.28948100 | 0.72362200 | 0.56196400 |
| H | -2.04543900 | -2.82674700 | 0.72411900 |
| H | -1.87630900 | -2.48289000 | -0.98010300 |
| H | 0.33628800 | -2.90673200 | 0.09295200 |
| H | -0.00718000 | -1.69649700 | 1.32043500 |
| H | -0.13186900 | 2.56320600 | -1.07588100 |
| H | 0.36656600 | 1.44451200 | -2.33701700 |
| H | 3.65546100 | -0.83815100 | -2.20758400 |
| H | 3.18063000 | 0.70962300 | -2.97270700 |
| H | -2.18952400 | -0.98889700 | -2.52613600 |
| H | -3.20993700 | 0.43204000 | -2.52101800 |
| H | -1.51878700 | 0.59169700 | -2.93027200 |
| H | 0.87745800 | -0.63167500 | -2.80287800 |
| H | 1.37847100 | -2.18615100 | -2.09660900 |
| H | -0.31253800 | -1.86054200 | -2.40062700 |
| H | -4.08127000 | -2.83736600 | 1.40418600 |
| H | -5.31871400 | -1.67829000 | 1.89332200 |
| H | -3.65979400 | -1.49905100 | 2.49020300 |
| H | -4.67751700 | -0.84182400 | -1.70323500 |
| H | -4.26944500 | -2.44990400 | -1.08926100 |
| H | -5.74962800 | -1.64063100 | -0.56414300 |
| H | 2.70261100 | 2.56291800 | 3.37794100 |
| H | 1.98211900 | 1.01238200 | 3.81771100 |
| H | 0.93323900 | 2.36638100 | 3.39345900 |
| H | 6.06500200 | -2.01822100 | 0.97015500 |
| H | 4.76993100 | -3.19667000 | 1.37033000 |
| H | 5.32121900 | -3.02688700 | -0.31983100 |
| H | 3.55529800 | 3.10791800 | -1.46558700 |
| H | 2.40648100 | 2.68819900 | -2.75520800 |
| H | 1.97005800 | 3.87780900 | -1.53056200 |
| H | 1.74907700 | 3.82587200 | 1.74263300 |
| H | 4.43927300 | 0.68604700 | -1.75398200 |

**PAC-ES**






**B3LYP/6-31+G(d,p)//B3LYP/6-31G***

Zero-point correction= 0.612968 (Hartree/Particle)
Thermal correction to Energy= 0.644915
Thermal correction to Enthalpy= 0.645859
Thermal correction to Gibbs Free Energy= 0.554362
Sum of electronic and zero-point Energies= -1389.568666
Sum of electronic and thermal Energies= -1389.536719
Sum of electronic and thermal Enthalpies= -1389.535775
Sum of electronic and thermal Free Energies= -1389.627272

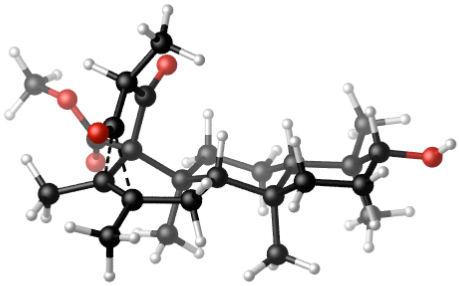
**MPW1PW91/6-31+G(d,p)//B3LYP/G-31G***

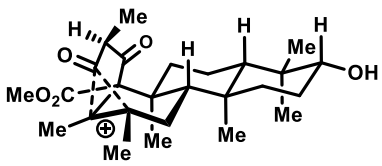
Zero-point correction= 0.615882 (Hartree/Particle)
Thermal correction to Energy= 0.647131
Thermal correction to Enthalpy= 0.648075
Thermal correction to Gibbs Free Energy= 0.559921
Sum of electronic and zero-point Energies= -1389.260029
Sum of electronic and thermal Energies= -1389.228779
Sum of electronic and thermal Enthalpies= -1389.227835
Sum of electronic and thermal Free Energies= -1389.315989

| | | | |
|---|---|---|---|
| C | -4.52448300 | 0.50792700 | 0.87162400 |
| C | -4.01650900 | -0.84637600 | 0.30593100 |
| C | -2.45859100 | -0.73084700 | 0.15110600 |
| C | -1.91264200 | 0.49680800 | -0.66210300 |
| C | -2.52850400 | 1.78818300 | -0.05438400 |
| C | -4.05655300 | 1.72298900 | 0.06613700 |
| O | -5.94582700 | 0.44770600 | 0.92947600 |
| C | -0.34686600 | 0.53070000 | -0.37334000 |
| C | -1.76417000 | -2.02775700 | -0.29334200 |
| C | -0.24781200 | -1.98297100 | -0.03033300 |
| C | 0.43384700 | -0.77532900 | -0.71355000 |
| C | 1.95213800 | -0.54183600 | -0.10721900 |
| C | 2.55459000 | 0.54244000 | -0.94945200 |
| C | 1.91979800 | 1.82471600 | -0.87351700 |
| C | 0.34019400 | 1.77586200 | -0.94429300 |
| C | 3.77196600 | 0.29276900 | -1.75645900 |
| C | 2.23128700 | 2.27131400 | 0.71717800 |
| C | 1.92810600 | -0.04361800 | 1.34036700 |
| C | 2.09271400 | 1.25085400 | 1.72841700 |
| O | 2.46830600 | 3.43920400 | 0.87688800 |
| O | 1.75886400 | -1.04716900 | 2.20628200 |

| | | | |
|---|---|---|---|
| C | -2.25096500 | 0.45727100 | -2.17423000 |
| C | 0.59110200 | -1.03911200 | -2.22883600 |
| C | -4.34118100 | -1.92837000 | 1.36425500 |
| C | -4.76816400 | -1.22617000 | -0.98804100 |
| C | 2.10688100 | 1.67242300 | 3.18003300 |
| C | 2.83859000 | -1.82618800 | -0.13754900 |
| O | 2.58377700 | -2.84636900 | -0.72848300 |
| O | 3.96766900 | -1.61527600 | 0.55620200 |
| C | 4.88082000 | -2.74129000 | 0.63730100 |
| C | 2.45248400 | 2.93091900 | -1.78664100 |
| H | -4.11406100 | 0.60123500 | 1.89438300 |
| H | -2.11066300 | -0.54776300 | 1.18259300 |
| H | -2.10421100 | 1.95139000 | 0.94821600 |
| H | -2.25516800 | 2.66397600 | -0.65588100 |
| H | -4.41257000 | 2.63938400 | 0.55663600 |
| H | -4.53521200 | 1.70504400 | -0.91909000 |
| H | -0.31124000 | 0.62031500 | 0.71853600 |
| H | -2.16003100 | -2.88057900 | 0.26539100 |
| H | -1.96828500 | -2.24545700 | -1.34738000 |
| H | 0.21919900 | -2.91013800 | -0.36934900 |
| H | -0.09621200 | -1.92783100 | 1.05227500 |
| H | -0.03068900 | 2.68467800 | -0.46456200 |
| H | 0.12834800 | 1.88320200 | -2.01311300 |
| H | 3.73620900 | -0.70324000 | -2.21251100 |
| H | 3.93918500 | 1.04723200 | -2.52313600 |
| H | -2.29263500 | -0.55337700 | -2.58353700 |
| H | -3.22503700 | 0.90953000 | -2.36702800 |
| H | -1.53052100 | 1.02287200 | -2.77307000 |
| H | 0.92606300 | -0.15651800 | -2.78872300 |
| H | 1.29881500 | -1.85106300 | -2.40404100 |
| H | -0.35964600 | -1.34398700 | -2.66437100 |
| H | -4.18041600 | -2.94131300 | 0.98196100 |
| H | -5.39231000 | -1.84751200 | 1.65237400 |
| H | -3.73211700 | -1.80518000 | 2.26927800 |
| H | -4.74621800 | -0.44596200 | -1.75146700 |
| H | -4.35296000 | -2.14001600 | -1.42731000 |
| H | -5.81866600 | -1.41649600 | -0.75571800 |
| H | 2.43119800 | 2.71192400 | 3.25857700 |
| H | 2.80736700 | 1.06850000 | 3.77234300 |
| H | 1.11286100 | 1.60230100 | 3.63992500 |
| H | 5.72000900 | -2.38535700 | 1.23277700 |
| H | 4.38525100 | -3.58381100 | 1.12296400 |
| H | 5.20598000 | -3.03478000 | -0.36279700 |
| H | 3.51591200 | 3.12743100 | -1.63108300 |
| H | 2.28751600 | 2.66716200 | -2.83649100 |
| H | 1.91868900 | 3.86037700 | -1.58022600 |
| H | 4.64140300 | 0.27701500 | -1.07981700 |
| H | 1.79034100 | -0.72403100 | 3.12513600 |
| H | -6.26625400 | 1.24420900 | 1.38006100 |

## TS-DK






**B3LYP/6-31+G(d,p)//B3LYP/6-31G***

| | |
|---|---|
| Zero-point correction= | 0.611276 (Hartree/Particle) |
| Thermal correction to Energy= | 0.642934 |
| Thermal correction to Enthalpy= | 0.643878 |
| Thermal correction to Gibbs Free Energy= | 0.552689 |
| Sum of electronic and zero-point Energies= | -1389.554706 |
| Sum of electronic and thermal Energies= | -1389.523048 |
| Sum of electronic and thermal Enthalpies= | -1389.522104 |
| Sum of electronic and thermal Free Energies= | -1389.613292 |

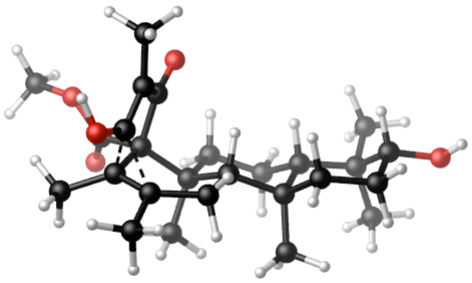
**MPW1PW91/6-31+G(d,p)//B3LYP/G-31G***

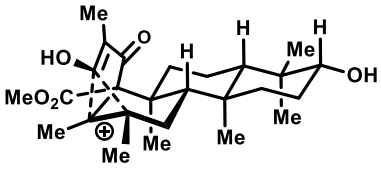
| | |
|---|---|
| Zero-point correction= | 0.614129 (Hartree/Particle) |
| Thermal correction to Energy= | 0.645125 |
| Thermal correction to Enthalpy= | 0.646070 |
| Thermal correction to Gibbs Free Energy= | 0.558321 |
| Sum of electronic and zero-point Energies= | -1389.243901 |
| Sum of electronic and thermal Energies= | -1389.212905 |
| Sum of electronic and thermal Enthalpies= | -1389.211961 |
| Sum of electronic and thermal Free Energies= | -1389.299709 |

| | | | |
|---|---|---|---|
| C | -4.50133200 | 0.51917000 | 0.93012500 |
| C | -4.03004100 | -0.80039700 | 0.25972800 |
| C | -2.47132800 | -0.71098700 | 0.09936600 |
| C | -1.90177400 | 0.56364400 | -0.62134300 |
| C | -2.48492000 | 1.81945600 | 0.08448800 |
| C | -4.01301100 | 1.78074500 | 0.21147000 |
| O | -5.92354400 | 0.48931100 | 0.99744500 |
| C | -0.34396900 | 0.54221200 | -0.34286600 |
| C | -1.81101000 | -1.98499700 | -0.45432600 |
| C | -0.29184900 | -1.99941000 | -0.20720500 |
| C | 0.42262900 | -0.74786400 | -0.77586900 |
| C | 1.90628400 | -0.57361500 | -0.14212200 |
| C | 2.59629300 | 0.55204100 | -0.89058500 |
| C | 1.88548700 | 1.74492200 | -1.04848800 |
| C | 0.37595300 | 1.81670900 | -0.82993500 |
| C | 3.96663200 | 0.34084700 | -1.46067900 |
| C | 2.69666800 | 2.09734300 | 0.80228500 |
| C | 1.79899100 | -0.21130600 | 1.38336000 |
| C | 2.45617100 | 1.09024900 | 1.86947800 |
| O | 3.15257100 | 3.17658500 | 0.78626000 |
| O | 1.29330600 | -0.95405800 | 2.18448200 |
| C | -2.24778500 | 0.64351100 | -2.13040900 |

| | | | |
|---|---|---|---|
| C | 0.56956800 | -0.90484900 | -2.30896700 |
| C | -4.37258800 | -1.95110800 | 1.23676200 |
| C | -4.80108900 | -1.06411300 | -1.05138000 |
| C | 1.77505500 | 1.70971000 | 3.10618200 |
| C | 2.75870100 | -1.87237300 | -0.19495200 |
| O | 2.62167000 | -2.77505500 | -0.98173900 |
| O | 3.71663000 | -1.83376500 | 0.75090100 |
| C | 4.56805900 | -3.00859200 | 0.84132200 |
| C | 2.41766700 | 2.89156700 | -1.87858600 |
| H | -4.08052700 | 0.52591800 | 1.95261000 |
| H | -2.10920800 | -0.61826600 | 1.13768400 |
| H | -2.05434600 | 1.89502400 | 1.09535200 |
| H | -2.19083300 | 2.73206300 | -0.45004200 |
| H | -4.34690700 | 2.66615500 | 0.76982500 |
| H | -4.49775400 | 1.84354100 | -0.76907000 |
| H | -6.21919500 | 1.24636800 | 1.52611800 |
| H | -0.30298200 | 0.55334200 | 0.75426300 |
| H | -2.22467700 | -2.86854000 | 0.03979500 |
| H | -2.03299100 | -2.11221800 | -1.51979500 |
| H | 0.14813800 | -2.89644500 | -0.65220200 |
| H | -0.12650600 | -2.06467600 | 0.87097700 |
| H | 0.14250800 | 2.67079500 | -0.18242400 |
| H | -0.00685100 | 2.11860500 | -1.81384900 |
| H | 3.88840500 | -0.43301600 | -2.23825300 |
| H | 4.38929500 | 1.23317100 | -1.91918100 |
| H | 4.66136700 | -0.05047700 | -0.71099800 |
| H | 3.47760300 | 0.77157100 | 2.14593600 |
| H | -2.30902900 | -0.33335100 | -2.61207200 |
| H | -3.21316300 | 1.12819400 | -2.28342400 |
| H | -1.51935900 | 1.23615300 | -2.69400000 |
| H | 0.88088800 | 0.01440000 | -2.81774700 |
| H | 1.28961500 | -1.69183400 | -2.53976600 |
| H | -0.38088900 | -1.20283300 | -2.75110500 |
| H | -4.24416800 | -2.93492500 | 0.77466400 |
| H | -5.41763500 | -1.86523800 | 1.54487700 |
| H | -3.74911000 | -1.91570200 | 2.13944500 |
| H | -4.75959400 | -0.23376600 | -1.75938200 |
| H | -4.41563800 | -1.95700500 | -1.55567800 |
| H | -5.85543900 | -1.23868700 | -0.82419300 |
| H | 2.37348300 | 2.53402900 | 3.49967700 |
| H | 1.67964300 | 0.93036900 | 3.86482600 |
| H | 0.77508600 | 2.07794700 | 2.86143800 |
| H | 5.25561100 | -2.80042600 | 1.65940300 |
| H | 3.95882600 | -3.88774000 | 1.05694900 |
| H | 5.10586500 | -3.15383100 | -0.09750700 |
| H | 3.48124700 | 3.08644700 | -1.73824900 |
| H | 2.24887800 | 2.66435900 | -2.93872500 |
| H | 1.87450600 | 3.81129900 | -1.64609400 |

## TS-EN






**B3LYP/6-31+G(d,p)//B3LYP/6-31G***

Zero-point correction= 0.611885 (Hartree/Particle)
Thermal correction to Energy= 0.643360
Thermal correction to Enthalpy= 0.644304
Thermal correction to Gibbs Free Energy= 0.554862
Sum of electronic and zero-point Energies= -1389.551267
Sum of electronic and thermal Energies= -1389.519792
Sum of electronic and thermal Enthalpies= -1389.518848
Sum of electronic and thermal Free Energies= -1389.608291

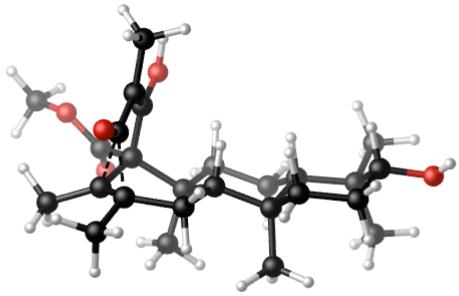
**MPW1PW91/6-31+G(d,p)//B3LYP/G-31G***

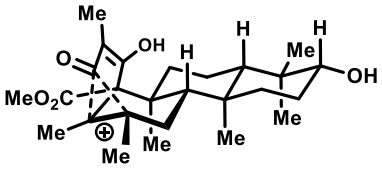
Zero-point correction= 0.614821 (Hartree/Particle)
Thermal correction to Energy= 0.645627
Thermal correction to Enthalpy= 0.646572
Thermal correction to Gibbs Free Energy= 0.559758
Sum of electronic and zero-point Energies= -1389.246028
Sum of electronic and thermal Energies= -1389.215222
Sum of electronic and thermal Enthalpies= -1389.214277
Sum of electronic and thermal Free Energies= -1389.301091

| | | | |
|---|---|---|---|
| C | 4.55544300 | -0.51043400 | 1.02459900 |
| C | 4.09819400 | 0.75818400 | 0.25369700 |
| C | 2.53962300 | 0.67099600 | 0.09211200 |
| C | 1.95939500 | -0.65111800 | -0.52724300 |
| C | 2.52709500 | -1.85169200 | 0.28013000 |
| C | 4.05552100 | -1.81886000 | 0.40565500 |
| O | 5.97807000 | -0.49004500 | 1.09359700 |
| C | 0.40014800 | -0.58931900 | -0.25979600 |
| C | 1.89398000 | 1.90299400 | -0.56535100 |
| C | 0.37579400 | 1.94867100 | -0.33049000 |
| C | -0.35792700 | 0.66614300 | -0.80414900 |
| C | -1.81184400 | 0.58090700 | -0.15187300 |
| C | -2.59399600 | -0.62459800 | -0.73460500 |
| C | -1.83454000 | -1.83635800 | -0.84805400 |
| C | -0.32694500 | -1.88988600 | -0.64340700 |
| C | -3.88608800 | -0.40496300 | -1.48459300 |
| C | -2.79624700 | -1.69976500 | 0.65209100 |
| C | -1.73336600 | 0.30355100 | 1.37627400 |
| C | -2.38851600 | -0.98451400 | 1.73341500 |
| O | -3.69495300 | -2.70289200 | 0.64245600 |
| O | -1.28352000 | 1.05875900 | 2.20883800 |

| | | | |
|---|---|---|---|
| C | 2.31241800 | -0.85561900 | -2.02347300 |
| C | -0.49969100 | 0.69025900 | -2.34410900 |
| C | 4.44609600 | 1.97589200 | 1.14446000 |
| C | 4.87810200 | 0.91734600 | -1.06893600 |
| C | -2.69526100 | -1.30316500 | 3.15690300 |
| C | -2.65091900 | 1.87788600 | -0.32571700 |
| O | -2.49661500 | 2.70586100 | -1.18893000 |
| O | -3.61402600 | 1.93817900 | 0.61156800 |
| C | -4.44412100 | 3.12946100 | 0.58969400 |
| C | -2.34411500 | -3.01721300 | -1.65313400 |
| H | 4.13283600 | -0.43372700 | 2.04336200 |
| H | 2.17149500 | 0.66446900 | 1.13233700 |
| H | 2.09399000 | -1.84013600 | 1.29222400 |
| H | 2.22476800 | -2.80206400 | -0.17904200 |
| H | 4.38063900 | -2.66143000 | 1.03147600 |
| H | 4.53978100 | -1.96190800 | -0.56666100 |
| H | 6.26374700 | -1.20712800 | 1.68027400 |
| H | 0.35285200 | -0.51179500 | 0.83369900 |
| H | 2.31528000 | 2.81948300 | -0.14265200 |
| H | 2.12097100 | 1.94075500 | -1.63686800 |
| H | -0.05207000 | 2.81623000 | -0.84036800 |
| H | 0.20138000 | 2.09224900 | 0.74078100 |
| H | -0.09722900 | -2.69686800 | 0.05996200 |
| H | 0.04015700 | -2.25414200 | -1.61107800 |
| H | -3.64360800 | 0.11130400 | -2.42213300 |
| H | -4.39477500 | -1.33571900 | -1.73241700 |
| H | -4.56704200 | 0.23066000 | -0.91647800 |
| H | 2.39034000 | 0.07922800 | -2.58045300 |
| H | 3.27146400 | -1.36483400 | -2.13070100 |
| H | 1.57814600 | -1.48054900 | -2.54312300 |
| H | -0.85742500 | -0.25642300 | -2.76645800 |
| H | -1.18521000 | 1.48423700 | -2.64463900 |
| H | 0.46169000 | 0.89750800 | -2.81343600 |
| H | 4.32833000 | 2.92390700 | 0.61030700 |
| H | 5.48909200 | 1.90453500 | 1.46340600 |
| H | 3.81796400 | 2.01256100 | 2.04384600 |
| H | 4.82541400 | 0.04030300 | -1.71742300 |
| H | 4.50861600 | 1.77815700 | -1.63688700 |
| H | 5.93424200 | 1.09136400 | -0.84969100 |
| H | -2.78939200 | -2.37844300 | 3.33716200 |
| H | -3.62617900 | -0.80849500 | 3.47044900 |
| H | -1.90554000 | -0.89297000 | 3.79352800 |
| H | -5.14547200 | 3.00369200 | 1.41301400 |
| H | -3.82263900 | 4.01392600 | 0.73916700 |
| H | -4.96788100 | 3.20577800 | -0.36526000 |
| H | -2.05347700 | -2.83274600 | -2.69529700 |
| H | -1.85504500 | -3.93812600 | -1.32579700 |
| H | -3.42057600 | -3.16523900 | -1.62192100 |
| H | -4.24065900 | -2.67521200 | 1.44894500 |

## TS-ES






**B3LYP/6-31+G(d,p)//B3LYP/6-31G***

Zero-point correction= 0.612830 (Hartree/Particle)
Thermal correction to Energy= 0.644079
Thermal correction to Enthalpy= 0.645023
Thermal correction to Gibbs Free Energy= 0.556138
Sum of electronic and zero-point Energies= -1389.568488
Sum of electronic and thermal Energies= -1389.537239
Sum of electronic and thermal Enthalpies= -1389.536295
Sum of electronic and thermal Free Energies= -1389.625181

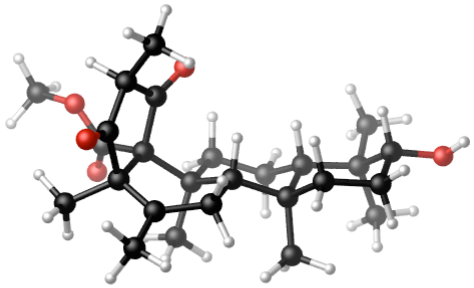
**MPW1PW91/6-31+G(d,p)//B3LYP/G-31G***

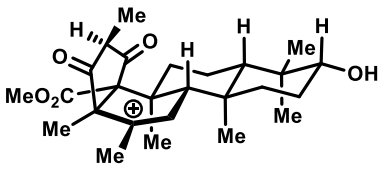
Zero-point correction= 0.615670 (Hartree/Particle)
Thermal correction to Energy= 0.646295
Thermal correction to Enthalpy= 0.647239
Thermal correction to Gibbs Free Energy= 0.560811
Sum of electronic and zero-point Energies= -1389.259820
Sum of electronic and thermal Energies= -1389.229195
Sum of electronic and thermal Enthalpies= -1389.228251
Sum of electronic and thermal Free Energies= -1389.314680

| | | | |
|---|---|---|---|
| C | -4.52153600 | 0.50398100 | 0.90834400 |
| C | -4.02789600 | -0.83180400 | 0.28837500 |
| C | -2.47015100 | -0.72299300 | 0.13128600 |
| C | -1.91666000 | 0.52997300 | -0.63725800 |
| C | -2.52125200 | 1.80282400 | 0.01896200 |
| C | -4.04903700 | 1.74481100 | 0.14544100 |
| O | -5.94307500 | 0.45312400 | 0.97368500 |
| C | -0.35386400 | 0.54301500 | -0.35370400 |
| C | -1.78608100 | -2.00712900 | -0.36543900 |
| C | -0.26942600 | -1.98299300 | -0.10726200 |
| C | 0.42577300 | -0.75252200 | -0.73811100 |
| C | 1.92826700 | -0.54607700 | -0.13132100 |
| C | 2.57280500 | 0.56498600 | -0.93217400 |
| C | 1.89991900 | 1.80992700 | -0.92356600 |
| C | 0.34297000 | 1.80492300 | -0.88531400 |
| C | 3.87556600 | 0.34675800 | -1.61349000 |
| C | 2.36290700 | 2.22112500 | 0.74864800 |
| C | 1.90867200 | -0.07617600 | 1.32529700 |
| C | 2.14170600 | 1.20514800 | 1.73547800 |
| O | 2.70463300 | 3.35967500 | 0.86410800 |
| O | 1.66849100 | -1.07061500 | 2.17843000 |

| | | | |
|---|---|---|---|
| C | -2.26338400 | 0.54715100 | -2.14848800 |
| C | 0.57568400 | -0.95990100 | -2.26438800 |
| C | -4.35783200 | -1.95164500 | 1.30462000 |
| C | -4.78847800 | -1.15390600 | -1.01588500 |
| C | 2.15922400 | 1.60801300 | 3.19358300 |
| C | 2.80122800 | -1.84038600 | -0.18703900 |
| O | 2.57476600 | -2.80812600 | -0.87034800 |
| O | 3.88047400 | -1.70948000 | 0.60022100 |
| C | 4.76949200 | -2.85677100 | 0.65018300 |
| C | 2.42521400 | 2.93925300 | -1.80552900 |
| H | -4.10393500 | 0.55534100 | 1.93125400 |
| H | -2.11631500 | -0.58185200 | 1.16752300 |
| H | -2.09164400 | 1.92723200 | 1.02499800 |
| H | -2.24350100 | 2.69779100 | -0.55169600 |
| H | -4.39600500 | 2.64507100 | 0.67121300 |
| H | -4.53309000 | 1.76622600 | -0.83720800 |
| H | -6.25396800 | 1.23768000 | 1.45113100 |
| H | -0.31396500 | 0.59638200 | 0.74123100 |
| H | -2.18823500 | -2.87814300 | 0.15974400 |
| H | -1.99488400 | -2.18104600 | -1.42679200 |
| H | 0.18906400 | -2.89831800 | -0.48915800 |
| H | -0.11467800 | -1.97951100 | 0.97635600 |
| H | 0.01001200 | 2.69286400 | -0.34090500 |
| H | 0.06684000 | 1.98034100 | -1.93176200 |
| H | 3.80640200 | -0.56280400 | -2.22636200 |
| H | 4.17347100 | 1.17926100 | -2.24737400 |
| H | 4.66237900 | 0.14505900 | -0.87459200 |
| H | -2.32550300 | -0.44843000 | -2.59079200 |
| H | -3.22996600 | 1.02326400 | -2.32067800 |
| H | -1.53602900 | 1.11818700 | -2.73385900 |
| H | 0.91658500 | -0.06024600 | -2.79138900 |
| H | 1.27454400 | -1.77143300 | -2.47223600 |
| H | -0.37977000 | -1.23867300 | -2.70724500 |
| H | -4.21012800 | -2.94975200 | 0.88041100 |
| H | -5.40609900 | -1.87180000 | 1.60317600 |
| H | -3.74151600 | -1.87194800 | 2.20963400 |
| H | -4.76361600 | -0.34406100 | -1.74767300 |
| H | -4.38147900 | -2.05256900 | -1.49249000 |
| H | -5.83937500 | -1.34542600 | -0.78630900 |
| H | 1.15682000 | 1.58142200 | 3.63947900 |
| H | 2.53565100 | 2.62778300 | 3.29449400 |
| H | 2.82165100 | 0.96034200 | 3.78342500 |
| H | 5.56571600 | -2.57057300 | 1.33546000 |
| H | 4.22712900 | -3.72817800 | 1.02121100 |
| H | 5.16578700 | -3.06860400 | -0.34483000 |
| H | 3.48197000 | 3.15572500 | -1.64009300 |
| H | 2.27435400 | 2.68327500 | -2.85995700 |
| H | 1.86973400 | 3.85579700 | -1.59538900 |
| H | 1.70028700 | -0.75981200 | 3.10179900 |

**ATC-DK**






**B3LYP/6-31+G(d,p)//B3LYP/6-31G***

Zero-point correction= 0.611334 (Hartree/Particle)
Thermal correction to Energy= 0.643132
Thermal correction to Enthalpy= 0.644076
Thermal correction to Gibbs Free Energy= 0.552582
Sum of electronic and zero-point Energies= -1389.565515
Sum of electronic and thermal Energies= -1389.533717
Sum of electronic and thermal Enthalpies= -1389.532773
Sum of electronic and thermal Free Energies= -1389.624268

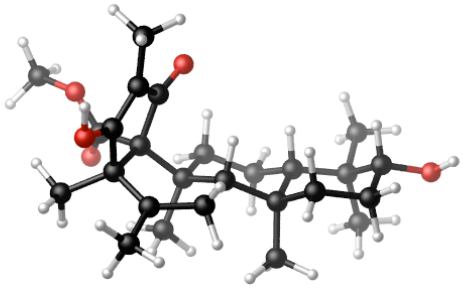
**MPW1PW91/6-31+G(d,p)//B3LYP/G-31G***

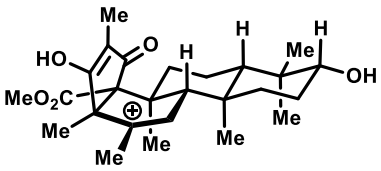
Zero-point correction= 0.614102 (Hartree/Particle)
Thermal correction to Energy= 0.645275
Thermal correction to Enthalpy= 0.646219
Thermal correction to Gibbs Free Energy= 0.558117
Sum of electronic and zero-point Energies= -1389.256930
Sum of electronic and thermal Energies= -1389.225757
Sum of electronic and thermal Enthalpies= -1389.224812
Sum of electronic and thermal Free Energies= -1389.312915

| | | | |
|---|---|---|---|
| C | 4.57414200 | -0.44054400 | 1.03121400 |
| C | 4.09502000 | 0.78906000 | 0.21110100 |
| C | 2.53692000 | 0.67494100 | 0.06047300 |
| C | 1.97776200 | -0.68054500 | -0.50419900 |
| C | 2.56266000 | -1.83791000 | 0.35270700 |
| C | 4.09114000 | -1.78162200 | 0.46894500 |
| O | 5.99623900 | -0.39744000 | 1.09044300 |
| C | 0.42411400 | -0.63403900 | -0.22835500 |
| C | 1.86943300 | 1.86867800 | -0.64524300 |
| C | 0.35368500 | 1.90702300 | -0.39168100 |
| C | -0.37078300 | 0.58952600 | -0.78631800 |
| C | -1.81399400 | 0.50346000 | -0.11256400 |
| C | -2.58213700 | -0.78388500 | -0.60456400 |
| C | -1.71225800 | -1.87126800 | -1.02632400 |
| C | -0.29170700 | -1.94878900 | -0.61956100 |
| C | -3.82822600 | -0.55190000 | -1.49431700 |
| C | -3.22290700 | -1.46309100 | 0.80843200 |
| C | -1.77672900 | 0.38023000 | 1.45145200 |
| C | -2.82278100 | -0.60428600 | 1.97436200 |
| O | -3.91114700 | -2.43563900 | 0.78147300 |
| O | -1.04111300 | 0.98772700 | 2.18872800 |

| | | | |
|---|---|---|---|
| C | 2.32971100 | -0.94012400 | -1.99242100 |
| C | -0.52131100 | 0.53710500 | -2.32429700 |
| C | 4.42922000 | 2.04733700 | 1.04899700 |
| C | 4.86658600 | 0.90214500 | -1.12118700 |
| C | -2.41958200 | -1.39516500 | 3.22880600 |
| C | -2.67303000 | 1.76887000 | -0.40597100 |
| O | -2.56370600 | 2.49632200 | -1.36139100 |
| O | -3.59441000 | 1.94679200 | 0.56143200 |
| C | -4.43648800 | 3.12480900 | 0.43047000 |
| C | -2.29205900 | -3.03007200 | -1.73673800 |
| H | 4.15531500 | -0.32875500 | 2.04802900 |
| H | 2.17139300 | 0.70522900 | 1.10078700 |
| H | 2.13534600 | -1.78382300 | 1.36559200 |
| H | 2.26719200 | -2.81262800 | -0.05991700 |
| H | 4.42967700 | -2.59233900 | 1.12838100 |
| H | 4.57376300 | -1.95872300 | -0.49851000 |
| H | 6.29545100 | -1.07311900 | 1.71808400 |
| H | 0.37244100 | -0.55127900 | 0.86099600 |
| H | 2.28424400 | 2.80724800 | -0.26719200 |
| H | 2.08462200 | 1.86220000 | -1.71976000 |
| H | -0.09478400 | 2.73721600 | -0.94539000 |
| H | 0.19256700 | 2.10242200 | 0.67083400 |
| H | -3.52369800 | -0.12131600 | -2.45265100 |
| H | -4.37356800 | -1.47932700 | -1.66951800 |
| H | -4.51592400 | 0.14364900 | -1.01002500 |
| H | 2.41270400 | -0.02608300 | -2.58271400 |
| H | 3.28584400 | -1.45801400 | -2.08261700 |
| H | 1.59172700 | -1.57728900 | -2.49298400 |
| H | -0.89224900 | -0.42858900 | -2.70237600 |
| H | -1.20444300 | 1.31280500 | -2.66931700 |
| H | 0.44187100 | 0.69934600 | -2.80716600 |
| H | 4.29622400 | 2.97052100 | 0.47630500 |
| H | 5.47451400 | 2.00348800 | 1.36540500 |
| H | 3.80435200 | 2.11258500 | 1.94887600 |
| H | 4.82636000 | -0.00491100 | -1.72766600 |
| H | 4.48076100 | 1.72967600 | -1.72646600 |
| H | 5.92046200 | 1.10348100 | -0.91517100 |
| H | -3.25333300 | -2.00734200 | 3.57930800 |
| H | -2.13740700 | -0.68555300 | 4.00989700 |
| H | -1.56250300 | -2.04665500 | 3.03356800 |
| H | -5.09872800 | 3.09942400 | 1.29425400 |
| H | -3.81641900 | 4.02255800 | 0.43921900 |
| H | -5.00291300 | 3.07733900 | -0.50141500 |
| H | -2.70246500 | -2.72476500 | -2.70915600 |
| H | -1.57441200 | -3.83856800 | -1.88448700 |
| H | -3.15874200 | -3.39289600 | -1.15709100 |
| H | -0.27343600 | -2.66666000 | 0.22437800 |
| H | 0.23182400 | -2.50125800 | -1.40920500 |
| H | -3.70893200 | 0.00893800 | 2.20208700 |

## ATC-EN






**B3LYP/6-31+G(d,p)//B3LYP/6-31G***

Zero-point correction= 0.611647 (Hartree/Particle)
Thermal correction to Energy= 0.643609
Thermal correction to Enthalpy= 0.644553
Thermal correction to Gibbs Free Energy= 0.553165
Sum of electronic and zero-point Energies= -1389.566103
Sum of electronic and thermal Energies= -1389.534141
Sum of electronic and thermal Enthalpies= -1389.533197
Sum of electronic and thermal Free Energies= -1389.624585

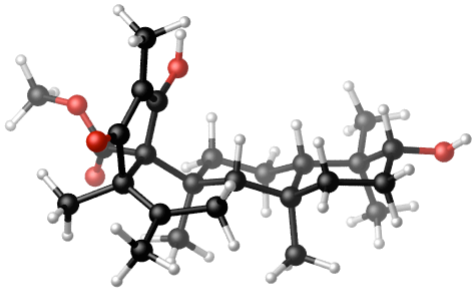
**MPW1PW91/6-31+G(d,p)//B3LYP/G-31G***

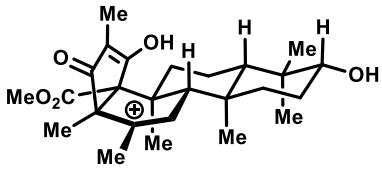
Zero-point correction= 0.614569 (Hartree/Particle)
Thermal correction to Energy= 0.645852
Thermal correction to Enthalpy= 0.646796
Thermal correction to Gibbs Free Energy= 0.558535
Sum of electronic and zero-point Energies= -1389.258929
Sum of electronic and thermal Energies= -1389.227647
Sum of electronic and thermal Enthalpies= -1389.226702
Sum of electronic and thermal Free Energies= -1389.314963

| | | | |
|---|---|---|---|
| C | 4.58190100 | -0.41299500 | 1.08611800 |
| C | 4.11379600 | 0.77932600 | 0.20710800 |
| C | 2.55651400 | 0.66455200 | 0.04967100 |
| C | 1.99667200 | -0.71317500 | -0.45750100 |
| C | 2.57191900 | -1.83379000 | 0.45294400 |
| C | 4.09973300 | -1.77663300 | 0.57961600 |
| O | 6.00383300 | -0.37214500 | 1.15583300 |
| C | 0.44167900 | -0.64644000 | -0.19573300 |
| C | 1.89849600 | 1.82566600 | -0.71665200 |
| C | 0.38047500 | 1.87754900 | -0.48290900 |
| C | -0.35006100 | 0.54748900 | -0.82067200 |
| C | -1.78332500 | 0.50421200 | -0.14329500 |
| C | -2.59924000 | -0.79756500 | -0.54979900 |
| C | -1.69578000 | -1.93367400 | -0.90166800 |
| C | -0.27053900 | -1.97360600 | -0.52764400 |
| C | -3.77308100 | -0.59605500 | -1.53395100 |
| C | -3.11143400 | -1.32802800 | 0.81662000 |
| C | -1.73372900 | 0.41698700 | 1.41875100 |
| C | -2.60242600 | -0.67878800 | 1.88638700 |
| O | -4.00557900 | -2.33071200 | 0.76813900 |
| O | -1.10867900 | 1.15571800 | 2.15253100 |

| | | | |
|---|---|---|---|
| C | 2.35847800 | -1.03749800 | -1.93068200 |
| C | -0.49878700 | 0.41763900 | -2.35259800 |
| C | 4.44689300 | 2.07384900 | 0.98801100 |
| C | 4.89575200 | 0.82709300 | -1.12344100 |
| C | -2.90989200 | -0.88014400 | 3.33471400 |
| C | -2.63754900 | 1.75778500 | -0.48400900 |
| O | -2.50924200 | 2.45689900 | -1.46078500 |
| O | -3.57374200 | 1.96118100 | 0.45832100 |
| C | -4.40979300 | 3.13298900 | 0.27860100 |
| C | -2.24944100 | -3.13073500 | -1.57253300 |
| H | 4.15466800 | -0.25486000 | 2.09312400 |
| H | 2.18222400 | 0.74410800 | 1.08422100 |
| H | 2.13598400 | -1.73566500 | 1.45883600 |
| H | 2.27790700 | -2.82477800 | 0.07918900 |
| H | 4.43046100 | -2.55820800 | 1.27719000 |
| H | 4.58999000 | -1.99748400 | -0.37484400 |
| H | 6.29450200 | -1.01699400 | 1.81888200 |
| H | 0.37834300 | -0.51042000 | 0.88782400 |
| H | 2.31129500 | 2.77936700 | -0.37605000 |
| H | 2.12672600 | 1.77137300 | -1.78737000 |
| H | -0.05942800 | 2.68369500 | -1.07685500 |
| H | 0.20389000 | 2.11907900 | 0.56876800 |
| H | -3.41139800 | -0.21616800 | -2.49254100 |
| H | -4.32668900 | -1.52106600 | -1.69938400 |
| H | -4.47433800 | 0.12799500 | -1.11604100 |
| H | 2.44163000 | -0.15009000 | -2.56026400 |
| H | 3.31674200 | -1.55553900 | -1.99264000 |
| H | 1.62636900 | -1.69879900 | -2.40890100 |
| H | -0.89062000 | -0.56102700 | -2.67630600 |
| H | -1.17435500 | 1.18340900 | -2.73422400 |
| H | 0.46354100 | 0.53744800 | -2.84967900 |
| H | 4.31833800 | 2.96965800 | 0.37256300 |
| H | 5.49048400 | 2.04244700 | 1.31161100 |
| H | 3.81712600 | 2.18117400 | 1.88026000 |
| H | 4.85643900 | -0.10756400 | -1.68638300 |
| H | 4.51692700 | 1.62600100 | -1.77012200 |
| H | 5.94894400 | 1.03476700 | -0.92001800 |
| H | -3.19793400 | -1.91110800 | 3.57186500 |
| H | -3.71922400 | -0.21469500 | 3.66026700 |
| H | -2.02908200 | -0.61990200 | 3.92984900 |
| H | -5.08757900 | 3.13265200 | 1.13078900 |
| H | -3.79066100 | 4.03179600 | 0.27347300 |
| H | -4.96077100 | 3.06270100 | -0.66152800 |
| H | -2.49694300 | -2.86392300 | -2.61238700 |
| H | -1.54724700 | -3.96650800 | -1.58575800 |
| H | -3.19868100 | -3.43004100 | -1.11179800 |
| H | -0.21445300 | -2.67650200 | 0.32527300 |
| H | 0.23077700 | -2.54326300 | -1.32247700 |
| H | -4.29001300 | -2.57664600 | 1.66655500 |

## ATC-ES






**B3LYP/6-31+G(d,p)//B3LYP/6-31G***

Zero-point correction= 0.612463 (Hartree/Particle)
Thermal correction to Energy= 0.644392
Thermal correction to Enthalpy= 0.645337
Thermal correction to Gibbs Free Energy= 0.554276
Sum of electronic and zero-point Energies= -1389.580970
Sum of electronic and thermal Energies= -1389.549041
Sum of electronic and thermal Enthalpies= -1389.548096
Sum of electronic and thermal Free Energies= -1389.639157

**MPW1PW91/6-31+G(d,p)//B3LYP/G-31G***

Zero-point correction= 0.615325 (Hartree/Particle)
Thermal correction to Energy= 0.646594
Thermal correction to Enthalpy= 0.647538
Thermal correction to Gibbs Free Energy= 0.559514
Sum of electronic and zero-point Energies= -1389.273245
Sum of electronic and thermal Energies= -1389.241976
Sum of electronic and thermal Enthalpies= -1389.241032
Sum of electronic and thermal Free Energies= -1389.329056

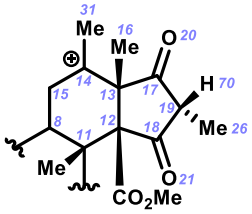
| | | | |
|---|---|---|---|
| C | 4.55712800 | -0.38576500 | 1.07414500 |
| C | 4.08122800 | 0.79875000 | 0.18857100 |
| C | 2.52614200 | 0.66738400 | 0.02243700 |
| C | 1.97897800 | -0.71821200 | -0.47513600 |
| C | 2.56529800 | -1.82919000 | 0.44023100 |
| C | 4.09201400 | -1.75541200 | 0.56969200 |
| O | 5.97729800 | -0.32557400 | 1.15410900 |
| C | 0.42205600 | -0.67173300 | -0.21585800 |
| C | 1.86483700 | 1.81763100 | -0.75815600 |
| C | 0.34561100 | 1.86126800 | -0.52533600 |
| C | -0.37002400 | 0.51882800 | -0.84089800 |
| C | -1.82098100 | 0.45753000 | -0.16322000 |
| C | -2.57629200 | -0.85596100 | -0.59114400 |
| C | -1.71845800 | -1.95466100 | -0.93685500 |
| C | -0.28466800 | -2.00571100 | -0.54598000 |
| C | -3.87265400 | -0.69062900 | -1.39940700 |
| C | -3.09070500 | -1.51148100 | 0.93511400 |
| C | -1.81522000 | 0.35973200 | 1.35780100 |
| C | -2.50162200 | -0.67406300 | 1.92875000 |
| O | -3.83597700 | -2.44997400 | 0.98674700 |
| O | -1.19845800 | 1.31878500 | 2.03939700 |

| | | | |
|---|---|---|---|
| C | 2.34787600 | -1.04668000 | -1.94603200 |
| C | -0.51029200 | 0.38681700 | -2.37672500 |
| C | 4.39863400 | 2.09938000 | 0.96582100 |
| C | 4.86829000 | 0.84937800 | -1.13878100 |
| C | -2.74401500 | -0.88287000 | 3.39987800 |
| C | -2.68609700 | 1.70610600 | -0.53853300 |
| O | -2.62661400 | 2.30837800 | -1.58284300 |
| O | -3.53880000 | 2.01393200 | 0.45123600 |
| C | -4.39034200 | 3.16589000 | 0.21613400 |
| C | -2.30373700 | -3.16971700 | -1.54810000 |
| H | 4.12092500 | -0.22937300 | 2.07833100 |
| H | 2.14560900 | 0.75323700 | 1.05525300 |
| H | 2.12664200 | -1.73337200 | 1.44540800 |
| H | 2.28030900 | -2.82315900 | 0.06979000 |
| H | 4.42937300 | -2.53165400 | 1.27018800 |
| H | 4.58686000 | -1.97369100 | -0.38293300 |
| H | 6.27474400 | -0.99075500 | 1.79376300 |
| H | 0.35668800 | -0.53649500 | 0.87041900 |
| H | 2.27214100 | 2.77803100 | -0.42988500 |
| H | 2.09332300 | 1.75078600 | -1.82734000 |
| H | -0.10264800 | 2.65267300 | -1.13440000 |
| H | 0.18072600 | 2.13520600 | 0.51897200 |
| H | -3.64662700 | -0.31211000 | -2.40090600 |
| H | -4.41123900 | -1.63481100 | -1.48310500 |
| H | -4.53995900 | 0.01907500 | -0.90656800 |
| H | 2.42861700 | -0.16231800 | -2.58003100 |
| H | 3.30955400 | -1.55914400 | -2.00169600 |
| H | 1.62119100 | -1.71390400 | -2.42208200 |
| H | -0.85259000 | -0.60310300 | -2.70840200 |
| H | -1.20878500 | 1.12749700 | -2.76358900 |
| H | 0.45365600 | 0.55337600 | -2.85690100 |
| H | 4.26063600 | 2.99250200 | 0.34839100 |
| H | 5.44177500 | 2.08125300 | 1.29160600 |
| H | 3.76694100 | 2.20164800 | 1.85776000 |
| H | 4.83466100 | -0.08579000 | -1.70094100 |
| H | 4.48843900 | 1.64604900 | -1.78763300 |
| H | 5.91963400 | 1.06196700 | -0.93125100 |
| H | -3.24071000 | -1.84117100 | 3.56759400 |
| H | -3.38881600 | -0.10071700 | 3.82003300 |
| H | -1.80393600 | -0.89745700 | 3.96666300 |
| H | -5.00087800 | 3.25621900 | 1.11315500 |
| H | -3.77686100 | 4.05640300 | 0.06793200 |
| H | -5.01204500 | 2.99865600 | -0.66546000 |
| H | -2.73900800 | -2.94284200 | -2.53037200 |
| H | -1.58072400 | -3.98071700 | -1.65016000 |
| H | -1.33141900 | 1.20440800 | 2.99845100 |
| H | -3.14834300 | -3.49839400 | -0.91779200 |
| H | -0.23218200 | -2.70194300 | 0.31028100 |
| H | 0.22683200 | -2.56008600 | -1.34217800 |

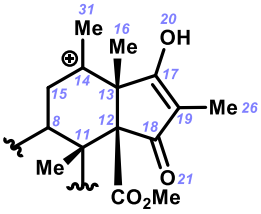
# NBO Analysis

## Comparison of Bond Donor/Acceptor Interactions for ATC-DK, ATC-EN, ATC-ES

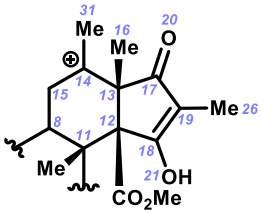
Interactions are taken from the second order perturbation theory analysis of Fock matrix in NBO basis at the mPW1PW91/6-31+G(d,p) level of theory. Hydrogen atoms are not numbered and can be assumed to be substituted on the atom to which they are bound. Interactions for the structures shown are listed from greatest to least energy and separated by interactions involving the $C_{14}$ empty p orbital.




ATC-DK




ATC-EN

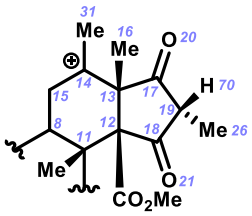



ATC-ES

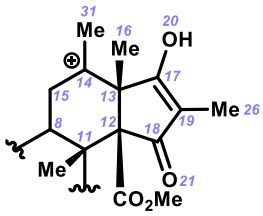
| Interaction | E (kcal/mol) | Interaction | E (kcal/mol) | Interaction | E (kcal/mol) |
|---|---|---|---|---|---|
| $\boldsymbol{n_{O20} \rightarrow \sigma^*_{C13\text{-}C17}}$ | ***37.34*** | $n_{O20} \rightarrow \pi^*_{C17\text{-}C19}$ | 34.34 | $n_{O21} \rightarrow \pi^*_{C18\text{-}C19}$ | 43.48 |
| $n_{O21} \rightarrow \sigma^*_{C12\text{-}C18}$ | 25.99 | $\boldsymbol{n_{O21} \rightarrow \sigma^*_{C12\text{-}C18}}$ | ***26.15*** | $\boldsymbol{n_{O20} \rightarrow \sigma^*_{C13\text{-}C17}}$ | ***42.26*** |
| $n_{O21} \rightarrow \sigma^*_{C18\text{-}C19}$ | 23.68 | $\pi_{C17\text{-}C19} \rightarrow \pi^*_{C18\text{-}O21}$ | 22.74 | $\pi_{C18\text{-}C19} \rightarrow \pi^*_{C17\text{-}C20}$ | 39.46 |
| $n_{O20} \rightarrow \sigma^*_{C17\text{-}C19}$ | 18.66 | $n_{O21} \rightarrow \sigma^*_{C18\text{-}C19}$ | 21.83 | $n_{O20} \rightarrow \sigma^*_{C17\text{-}C19}$ | 15.90 |
| $\sigma_{C19\text{-}H70} \rightarrow \pi^*_{C17\text{-}O20}$ | 7.96 | $\sigma_{C18\text{-}C19} \rightarrow \sigma^*_{C17\text{-}O20}$ | 9.42 | $n_{O21} \rightarrow \sigma^*_{C18\text{-}C19}$ | 7.05 |
| $\sigma_{C19\text{-}H70} \rightarrow \pi^*_{C18\text{-}O21}$ | 7.26 | $n_{O20} \rightarrow \sigma^*_{C17\text{-}C19}$ | 7.67 | $\sigma_{O21\text{-}H67} \rightarrow \sigma^*_{C12\text{-}C18}$ | 6.64 |
| | | $\sigma_{O20\text{-}H70} \rightarrow \sigma^*_{C13\text{-}C17}$ | 6.57 | $\sigma_{C17\text{-}C19} \rightarrow \sigma^*_{C18\text{-}O21}$ | 6.35 |
| | | $\pi_{C18\text{-}O21} \rightarrow \pi^*_{C17\text{-}C19}$ | 5.24 | $\sigma_{C26\text{-}H59} \rightarrow \sigma^*_{C18\text{-}C19}$ | 5.41 |
| $\boldsymbol{\sigma_{C13\text{-}C17} \rightarrow p_{C14}}$ | ***28.09*** | $\boldsymbol{\sigma_{C13\text{-}C17} \rightarrow p_{C14}}$ | ***18.63*** | $\boldsymbol{\sigma_{C13\text{-}C17} \rightarrow p_{C14}}$ | ***42.13*** |
| $\sigma_{C15\text{-}H68} \rightarrow p_{C14}$ | 16.61 | $\sigma_{C15\text{-}H68} \rightarrow p_{C14}$ | 17.18 | $\sigma_{C15\text{-}H69} \rightarrow p_{C14}$ | 13.81 |
| $\sigma_{C31\text{-}H67} \rightarrow p_{C14}$ | 11.33 | $\sigma_{C31\text{-}H65} \rightarrow p_{C14}$ | 13.59 | $\sigma_{C31\text{-}H68} \rightarrow p_{C14}$ | 11.10 |
| $\sigma_{C31\text{-}H65} \rightarrow p_{C14}$ | 9.42 | $\pi_{C17\text{-}C19} \rightarrow p_{C14}$ | 10.51 | $\sigma_{C31\text{-}C65} \rightarrow p_{C14}$ | 8.63 |
| $\sigma_{C15\text{-}H69} \rightarrow p_{C14}$ | 5.73 | $\sigma_{C31\text{-}H67} \rightarrow p_{C14}$ | 7.98 | $\sigma_{C15\text{-}H70} \rightarrow p_{C14}$ | 6.57 |
| | | $\sigma_{C15\text{-}H69} \rightarrow p_{C14}$ | 7.75 | | |

## Comparison of Bond Orders and Bond Lengths for ATC-DK, ATC-EN, ATC-ES

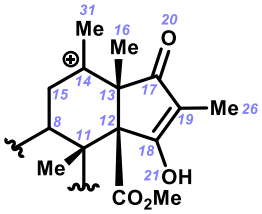
Bond orders are taken from the Wiberg bond index matrix in the NAO basis at the mPW1PW91/6-31+G(d,p) level of theory. Bond lengths are calculated from geometric coordinates.




ATC-DK




ATC-EN




ATC-ES

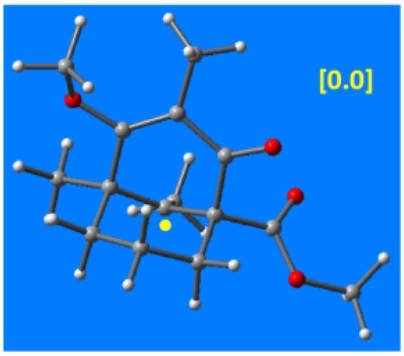
| | Bond Order | | |
|---|---|---|---|
| bond | ATC-DK | ATC-EN | ATC-ES |
| C12-C13 | 0.952 | 0.935 | 0.947 |
| ***C13-C14*** | ***1.160*** | ***1.039*** | ***1.214*** |
| C14-C15 | 1.124 | 1.149 | 1.102 |
| C11-C12 | 0.945 | 0.953 | 0.936 |
| C12-C18 | 0.922 | 0.922 | 0.982 |
| C18-C19 | 0.959 | 1.049 | 1.522 |
| C19-C17 | 0.999 | 1.616 | 1.172 |
| ***C17-C13*** | ***0.715*** | ***0.893*** | ***0.645*** |
| C17-O20 | 1.933 | 1.078 | 1.807 |
| C19-C26 | 0.982 | 1.032 | 1.011 |
| C18-O21 | 1.872 | 1.778 | 1.138 |
| C13-C16 | 0.975 | 0.974 | 0.988 |
| C14-C31 | 1.134 | 1.139 | 1.121 |

| | Bond Length (Å) | | |
|---|---|---|---|
| bond | ATC-DK | ATC-EN | ATC-ES |
| C12-C13 | 1.58 | 1.59 | 1.57 |
| ***C13-C14*** | ***1.45*** | ***1.49*** | ***1.44*** |
| C14-C15 | 1.48 | 1.47 | 1.49 |
| C11-C12 | 1.60 | 1.59 | 1.60 |
| C12-C18 | 1.57 | 1.57 | 1.52 |
| C18-C19 | 1.53 | 1.47 | 1.37 |
| C19-C17 | 1.50 | 1.35 | 1.43 |
| ***C17-C13*** | ***1.69*** | ***1.55*** | ***1.74*** |
| C17-O20 | 1.19 | 1.34 | 1.20 |
| C19-C26 | 1.54 | 1.49 | 1.51 |
| C18-O21 | 1.21 | 1.21 | 1.33 |
| C13-C16 | 1.55 | 1.55 | 1.54 |
| C14-C31 | 1.48 | 1.48 | 1.48 |

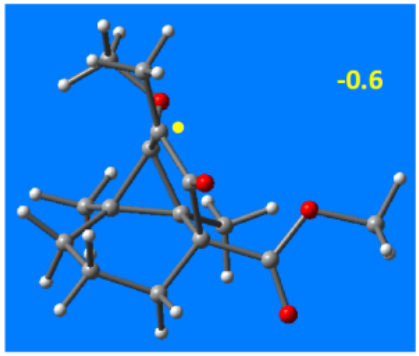
# Truncated Model System Cation and Radical Pathway Minimization and Energies

## Summary of Truncated System Minimized Structures and Energies

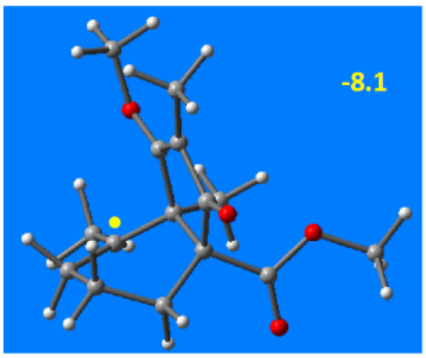
*radical (all minima)* *TSS @ +11.6* *TSS @ +4.9*




Sum of electronic and thermal Free Energies=
-884.629514

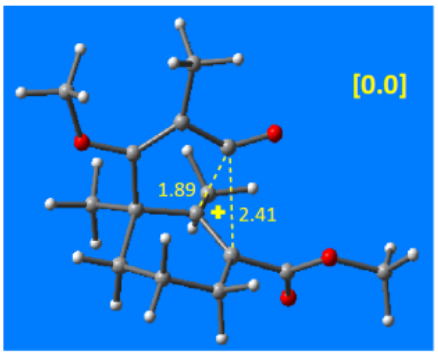



Sum of electronic and thermal Free Energies=
-884.630405

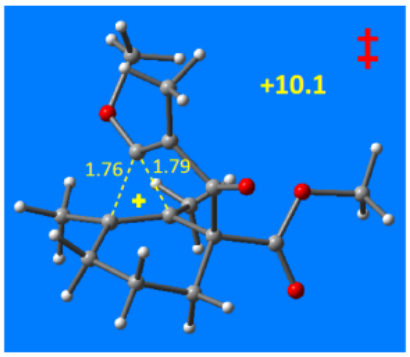



Sum of electronic and thermal Free Energies=
-884.642465

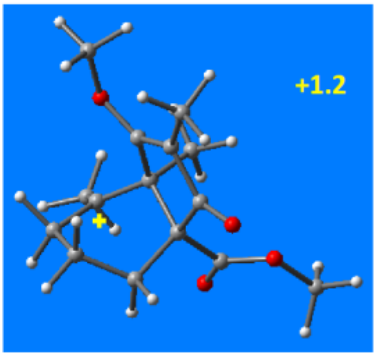
*cation*




Sum of electronic and thermal Free Energies=
-884.403063

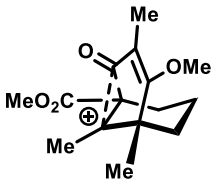



Sum of electronic and thermal Free Energies=
-884.387008




Sum of electronic and thermal Free Energies=
-884.401102

### Truncated Cation Reactant

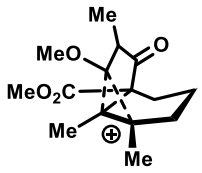



Zero-point correction= 0.340793 (Hartree/Particle)
Thermal correction to Energy= 0.361524
Thermal correction to Enthalpy= 0.362468
Thermal correction to Gibbs Free Energy= 0.291345
Sum of electronic and zero-point Energies= -884.353615
Sum of electronic and thermal Energies= -884.332884
Sum of electronic and thermal Enthalpies= -884.331940

Sum of electronic and thermal Free Energies= -884.403063

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.408838 | -1.434980 | -1.995929 |
| 2 | 6 | 0 | -1.029474 | -1.075215 | -1.657252 |
| 3 | 1 | 0 | 0.947186 | -0.543758 | -2.334638 |
| 4 | 6 | 0 | -1.250497 | -0.593398 | -0.272216 |
| 5 | 6 | 0 | -0.272189 | -0.464563 | 0.716772 |
| 6 | 6 | 0 | 1.121607 | -1.057318 | 0.418804 |
| 7 | 6 | 0 | 1.088498 | -2.035635 | -0.777575 |
| 8 | 1 | 0 | 2.112513 | -2.335067 | -1.009680 |
| 9 | 6 | 0 | 1.709690 | -1.802959 | 1.631124 |
| 10 | 1 | 0 | 2.665010 | -2.246565 | 1.348709 |
| 11 | 1 | 0 | 1.884271 | -1.151102 | 2.487865 |
| 12 | 6 | 0 | 2.012956 | 0.118242 | 0.066448 |
| 13 | 8 | 0 | 3.258727 | -0.246612 | -0.107783 |
| 14 | 6 | 0 | 1.442655 | 1.363639 | -0.023633 |
| 15 | 6 | 0 | 0.056472 | 1.352755 | 0.302273 |
| 16 | 6 | 0 | 2.034914 | 2.728218 | -0.286223 |
| 17 | 1 | 0 | 2.568796 | 3.113085 | 0.585968 |
| 18 | 1 | 0 | 2.711940 | 2.722032 | -1.139172 |
| 19 | 1 | 0 | 1.233813 | 3.432727 | -0.510744 |
| 20 | 8 | 0 | -0.784200 | 2.156138 | 0.491080 |
| 21 | 6 | 0 | -0.693165 | -0.309327 | 2.172308 |
| 22 | 1 | 0 | -0.942901 | -1.286976 | 2.589505 |
| 23 | 1 | 0 | 0.108146 | 0.127749 | 2.767875 |
| 24 | 6 | 0 | -2.694594 | -0.301016 | 0.047259 |
| 25 | 8 | 0 | -3.294687 | -0.996225 | 0.831217 |
| 26 | 8 | 0 | -3.176085 | 0.693939 | -0.669123 |
| 27 | 6 | 0 | -4.562300 | 1.036254 | -0.440292 |
| 28 | 1 | 0 | -4.712144 | 1.284423 | 0.610058 |
| 29 | 1 | 0 | -4.750070 | 1.897733 | -1.074516 |
| 30 | 1 | 0 | -5.198566 | 0.196634 | -0.718961 |
| 31 | 1 | 0 | 0.557479 | -2.939367 | -0.457411 |
| 32 | 1 | 0 | -1.571054 | 0.326945 | 2.268858 |
| 33 | 1 | 0 | 0.422145 | -2.139620 | -2.830138 |
| 34 | 1 | 0 | -1.469573 | -0.347529 | -2.351316 |
| 35 | 1 | 0 | -1.682635 | -1.959409 | -1.752371 |
| 36 | 6 | 0 | 4.330369 | 0.651998 | -0.439347 |
| 37 | 1 | 0 | 4.380807 | 1.473672 | 0.273242 |
| 38 | 1 | 0 | 5.231046 | 0.046952 | -0.370450 |
| 39 | 1 | 0 | 4.210995 | 1.017810 | -1.459039 |
| 40 | 1 | 0 | 1.040078 | -2.608449 | 1.938107 |

## Truncated Cation TS




Imaginary: -245.5974 cm-1
Zero-point correction= 0.339899 (Hartree/Particle)
Thermal correction to Energy= 0.359688
Thermal correction to Enthalpy= 0.360632
Thermal correction to Gibbs Free Energy= 0.293343
Sum of electronic and zero-point Energies= -884.340452
Sum of electronic and thermal Energies= -884.320663
Sum of electronic and thermal Enthalpies= -884.319718
Sum of electronic and thermal Free Energies= -884.387008

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.353801 | 2.481001 | 1.304076 |
| 2 | 6 | 0 | -0.941174 | 2.109766 | 0.596227 |
| 3 | 6 | 0 | -0.868696 | 0.640211 | 0.141866 |
| 4 | 6 | 0 | 0.243228 | 0.422737 | -0.887203 |
| 5 | 6 | 0 | 1.462979 | 1.120356 | -0.614439 |
| 6 | 6 | 0 | 1.563427 | 2.237622 | 0.408872 |
| 7 | 6 | 0 | -0.068373 | -0.164308 | -2.230064 |
| 8 | 6 | 0 | 1.464124 | -0.515293 | 0.022106 |
| 9 | 6 | 0 | -0.479201 | -0.207191 | 1.361532 |
| 10 | 6 | 0 | 0.848442 | -0.848002 | 1.195535 |
| 11 | 8 | 0 | 2.428056 | -1.178274 | -0.605853 |
| 12 | 8 | 0 | -1.180469 | -0.360224 | 2.330713 |
| 13 | 6 | 0 | 1.319968 | -1.813426 | 2.218125 |
| 14 | 6 | 0 | -2.234321 | 0.184577 | -0.395991 |
| 15 | 8 | 0 | -3.062854 | 0.949067 | -0.815352 |
| 16 | 8 | 0 | -2.362366 | -1.140201 | -0.346525 |
| 17 | 6 | 0 | -3.638067 | -1.665950 | -0.769716 |
| 18 | 6 | 0 | 2.535886 | 1.242060 | -1.671723 |
| 19 | 1 | 0 | 2.484590 | 2.117316 | 0.985691 |
| 20 | 1 | 0 | 1.728845 | 3.125027 | -0.215704 |
| 21 | 1 | 0 | -0.613990 | 0.596084 | -2.802203 |
| 22 | 1 | 0 | 0.825501 | -0.421430 | -2.793852 |
| 23 | 1 | 0 | -0.708911 | -1.041309 | -2.144294 |
| 24 | 1 | 0 | 2.407223 | -1.848932 | 2.285713 |
| 25 | 1 | 0 | 0.944654 | -2.822711 | 2.013205 |
| 26 | 1 | 0 | 0.895833 | -1.524669 | 3.182681 |
| 27 | 1 | 0 | -3.564198 | -2.742003 | -0.636568 |
| 28 | 1 | 0 | -4.430472 | -1.252337 | -0.146699 |
| 29 | 1 | 0 | -3.821607 | -1.412294 | -1.813962 |
| 30 | 1 | 0 | 2.247308 | 2.082229 | -2.311874 |
| 31 | 1 | 0 | 3.495373 | 1.482138 | -1.211883 |

| | | | | | |
|---|---|---|---|---|---|
| 32 | 1 | 0 | 2.663259 | 0.364967 | -2.297522 |
| 33 | 6 | 0 | 2.402571 | -2.620152 | -0.604513 |
| 34 | 1 | 0 | 2.983737 | -2.917475 | -1.474881 |
| 35 | 1 | 0 | 2.869572 | -3.012806 | 0.297780 |
| 36 | 1 | 0 | 1.374403 | -2.976972 | -0.694108 |
| 37 | 1 | 0 | 0.336834 | 3.533639 | 1.596606 |
| 38 | 1 | 0 | 0.443596 | 1.918639 | 2.238941 |
| 39 | 1 | 0 | -1.796531 | 2.221018 | 1.264754 |
| 40 | 1 | 0 | -1.131542 | 2.744867 | -0.273819 |

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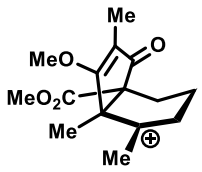
**Truncated Cation Product**




Zero-point correction= 0.340050 (Hartree/Particle)
Thermal correction to Energy= 0.360328
Thermal correction to Enthalpy= 0.361272
Thermal correction to Gibbs Free Energy= 0.291975
Sum of electronic and zero-point Energies= -884.353028
Sum of electronic and thermal Energies= -884.332750
Sum of electronic and thermal Enthalpies= -884.331805
Sum of electronic and thermal Free Energies= -884.401102

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.675714 | 0.889457 | 2.322013 |
| 2 | 6 | 0 | -0.695797 | 0.348058 | 1.933316 |
| 3 | 1 | 0 | 1.445284 | 0.119595 | 2.236902 |
| 4 | 6 | 0 | -0.728644 | -0.154542 | 0.465454 |
| 5 | 6 | 0 | 0.282467 | 0.590606 | -0.517829 |
| 6 | 6 | 0 | 0.528258 | 1.934736 | 0.028615 |
| 7 | 6 | 0 | 0.970222 | 2.082521 | 1.418786 |
| 8 | 1 | 0 | 2.055049 | 2.286825 | 1.328139 |
| 9 | 6 | 0 | 0.275662 | 3.138160 | -0.755159 |
| 10 | 1 | 0 | 0.672379 | 4.043087 | -0.295670 |
| 11 | 1 | 0 | 0.581596 | 3.039676 | -1.798812 |
| 12 | 6 | 0 | 1.517968 | -0.317713 | -0.411529 |
| 13 | 8 | 0 | 2.613275 | 0.292165 | -0.857610 |
| 14 | 6 | 0 | 1.239088 | -1.575014 | -0.000101 |
| 15 | 6 | 0 | -0.152304 | -1.589474 | 0.472054 |
| 16 | 6 | 0 | 2.035639 | -2.841626 | 0.046023 |
| 17 | 1 | 0 | 2.162403 | -3.273993 | -0.950096 |
| 18 | 1 | 0 | 3.022245 | -2.713865 | 0.491599 |
| 19 | 1 | 0 | 1.480247 | -3.566339 | 0.644914 |
| 20 | 8 | 0 | -0.744435 | -2.535198 | 0.935253 |

| | | | | | |
|---|---|---|---|---|---|
| 21 | 6 | 0 | -0.173085 | 0.567285 | -1.985182 |
| 22 | 1 | 0 | -1.026788 | 1.222638 | -2.160837 |
| 23 | 1 | 0 | 0.645448 | 0.864211 | -2.644143 |
| 24 | 6 | 0 | -2.142910 | 0.072981 | -0.069163 |
| 25 | 8 | 0 | -2.593683 | 1.199604 | -0.132322 |
| 26 | 8 | 0 | -2.763209 | -1.021996 | -0.443984 |
| 27 | 6 | 0 | -4.119051 | -0.866884 | -0.910829 |
| 28 | 1 | 0 | -4.136642 | -0.250650 | -1.809871 |
| 29 | 1 | 0 | -4.461982 | -1.875753 | -1.122641 |
| 30 | 1 | 0 | -4.726897 | -0.403483 | -0.134196 |
| 31 | 1 | 0 | 0.561847 | 3.021314 | 1.814384 |
| 32 | 1 | 0 | -0.461001 | -0.449710 | -2.256889 |
| 33 | 1 | 0 | 0.674222 | 1.219311 | 3.362806 |
| 34 | 1 | 0 | -0.996156 | -0.481033 | 2.577997 |
| 35 | 1 | 0 | -1.439272 | 1.142283 | 2.050730 |
| 36 | 6 | 0 | 3.851712 | -0.427655 | -0.964545 |
| 37 | 1 | 0 | 3.729071 | -1.310788 | -1.591268 |
| 38 | 1 | 0 | 4.546095 | 0.265515 | -1.433574 |
| 39 | 1 | 0 | 4.215519 | -0.703495 | 0.025994 |
| 40 | 1 | 0 | -0.827881 | 3.222680 | -0.777704 |

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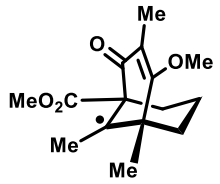
**Truncated Radical Reactant**




Zero-point correction= 0.340679 (Hartree/Particle)
Thermal correction to Energy= 0.360612
Thermal correction to Enthalpy= 0.361556
Thermal correction to Gibbs Free Energy= 0.292312
Sum of electronic and zero-point Energies= -884.581147
Sum of electronic and thermal Energies= -884.561214
Sum of electronic and thermal Enthalpies= -884.560270
Sum of electronic and thermal Free Energies= -884.629514

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.438865 | -0.667988 | 2.256004 |
| 2 | 6 | 0 | 0.973598 | -0.443617 | 1.722564 |
| 3 | 1 | 0 | -0.965063 | 0.290804 | 2.324026 |
| 4 | 6 | 0 | 0.983111 | -0.087147 | 0.211448 |
| 5 | 6 | 0 | 0.246966 | -1.150098 | -0.561943 |
| 6 | 6 | 0 | -1.195907 | -1.257512 | -0.127971 |
| 7 | 6 | 0 | -1.232653 | -1.633325 | 1.382707 |
| 8 | 1 | 0 | -2.275583 | -1.688675 | 1.715020 |

| | | | | | |
|---|---|---|---|---|---|
| 9 | 6 | 0 | -1.979593 | -2.318375 | -0.909067 |
| 10 | 1 | 0 | -2.995263 | -2.404533 | -0.522578 |
| 11 | 1 | 0 | -2.043973 | -2.081333 | -1.973493 |
| 12 | 6 | 0 | -1.857188 | 0.111098 | -0.286817 |
| 13 | 8 | 0 | -3.200128 | -0.007286 | -0.357766 |
| 14 | 6 | 0 | -1.169695 | 1.284845 | -0.311719 |
| 15 | 6 | 0 | 0.256093 | 1.273231 | 0.040322 |
| 16 | 6 | 0 | -1.739718 | 2.641073 | -0.633417 |
| 17 | 1 | 0 | -2.508273 | 2.578794 | -1.404901 |
| 18 | 1 | 0 | -2.156948 | 3.157477 | 0.236407 |
| 19 | 1 | 0 | -0.929980 | 3.270364 | -1.005349 |
| 20 | 8 | 0 | 0.869540 | 2.308225 | 0.252750 |
| 21 | 6 | 0 | 0.735166 | -1.707662 | -1.855010 |
| 22 | 1 | 0 | 1.811943 | -1.886447 | -1.840217 |
| 23 | 1 | 0 | 0.241874 | -2.651365 | -2.093234 |
| 24 | 6 | 0 | 2.393194 | 0.151253 | -0.325784 |
| 25 | 8 | 0 | 2.631372 | 0.489915 | -1.461681 |
| 26 | 8 | 0 | 3.348797 | -0.061757 | 0.587974 |
| 27 | 6 | 0 | 4.682855 | 0.200496 | 0.146985 |
| 28 | 1 | 0 | 4.777975 | 1.240899 | -0.167305 |
| 29 | 1 | 0 | 5.319482 | -0.002333 | 1.006053 |
| 30 | 1 | 0 | 4.945357 | -0.450326 | -0.688797 |
| 31 | 1 | 0 | -0.813191 | -2.642833 | 1.469772 |
| 32 | 1 | 0 | 0.557355 | -1.019660 | -2.695864 |
| 33 | 1 | 0 | -0.381875 | -1.056073 | 3.278222 |
| 34 | 1 | 0 | 1.474629 | 0.351386 | 2.280503 |
| 35 | 1 | 0 | 1.566757 | -1.354415 | 1.848983 |
| 36 | 6 | 0 | -4.063238 | 0.970715 | 0.213168 |
| 37 | 1 | 0 | -4.307375 | 1.761386 | -0.497293 |
| 38 | 1 | 0 | -4.975346 | 0.436545 | 0.481485 |
| 39 | 1 | 0 | -3.614994 | 1.404659 | 1.109609 |
| 40 | 1 | 0 | -1.488904 | -3.289009 | -0.800093 |

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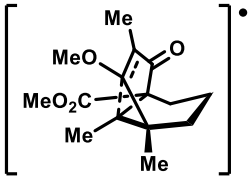
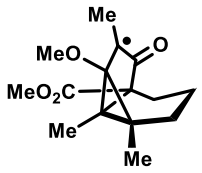
**Truncated Radical TS1**




Imaginary: -357.5498 cm-1
Zero-point correction= 0.338726 (Hartree/Particle)
Thermal correction to Energy= 0.358487
Thermal correction to Enthalpy= 0.359431
Thermal correction to Gibbs Free Energy= 0.291165
Sum of electronic and zero-point Energies= -884.563439
Sum of electronic and thermal Energies= -884.543678
Sum of electronic and thermal Enthalpies= -884.542733
Sum of electronic and thermal Free Energies= -884.611000

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.433652 | 1.736970 | 2.004619 |
| 2 | 6 | 0 | -0.937779 | 1.637193 | 1.349357 |
| 3 | 1 | 0 | 0.613478 | 0.847000 | 2.616161 |
| 4 | 6 | 0 | -0.950980 | 0.479365 | 0.327550 |
| 5 | 6 | 0 | 0.054263 | 0.713836 | -0.775147 |
| 6 | 6 | 0 | 1.432960 | 1.027833 | -0.295670 |
| 7 | 6 | 0 | 1.534967 | 1.904951 | 0.964338 |
| 8 | 1 | 0 | 2.522173 | 1.754707 | 1.415849 |
| 9 | 6 | 0 | 2.355512 | 1.616776 | -1.363091 |
| 10 | 1 | 0 | 3.319810 | 1.885691 | -0.924425 |
| 11 | 1 | 0 | 2.537846 | 0.936433 | -2.194254 |
| 12 | 6 | 0 | 1.522125 | -0.490625 | -0.164938 |
| 13 | 8 | 0 | 2.386562 | -1.151480 | -1.002869 |
| 14 | 6 | 0 | 0.770232 | -1.285887 | 0.711796 |
| 15 | 6 | 0 | -0.518876 | -0.793971 | 1.112700 |
| 16 | 6 | 0 | 1.182593 | -2.670007 | 1.103257 |
| 17 | 1 | 0 | 1.590722 | -3.214240 | 0.247873 |
| 18 | 1 | 0 | 1.947213 | -2.660618 | 1.889031 |
| 19 | 1 | 0 | 0.318993 | -3.207844 | 1.497385 |
| 20 | 8 | 0 | -1.240208 | -1.274517 | 1.980278 |
| 21 | 6 | 0 | -0.329914 | 0.635075 | -2.215958 |
| 22 | 1 | 0 | -0.720015 | -0.353399 | -2.477702 |
| 23 | 1 | 0 | -1.128768 | 1.357341 | -2.430904 |
| 24 | 6 | 0 | -2.366279 | 0.282869 | -0.200457 |
| 25 | 8 | 0 | -3.252205 | 1.101269 | -0.113845 |
| 26 | 8 | 0 | -2.518682 | -0.908158 | -0.792667 |
| 27 | 6 | 0 | -3.831824 | -1.193605 | -1.278423 |
| 28 | 1 | 0 | -4.128836 | -0.464297 | -2.034394 |
| 29 | 1 | 0 | -3.773947 | -2.191484 | -1.708426 |
| 30 | 1 | 0 | -4.550072 | -1.171200 | -0.457538 |
| 31 | 1 | 0 | 1.511187 | 2.941344 | 0.603489 |
| 32 | 1 | 0 | 0.502379 | 0.861663 | -2.880234 |
| 33 | 1 | 0 | 0.457549 | 2.588273 | 2.692393 |
| 34 | 1 | 0 | -1.708028 | 1.438044 | 2.097944 |
| 35 | 1 | 0 | -1.207305 | 2.568515 | 0.842304 |
| 36 | 6 | 0 | 3.756054 | -1.129756 | -0.615977 |
| 37 | 1 | 0 | 4.312953 | -1.592331 | -1.431066 |
| 38 | 1 | 0 | 4.122411 | -0.111727 | -0.459244 |
| 39 | 1 | 0 | 3.905464 | -1.710546 | 0.299776 |
| 40 | 1 | 0 | 1.910821 | 2.535657 | -1.754930 |

## Truncated Radical Intermediate




Zero-point correction= 0.340083 (Hartree/Particle)
Thermal correction to Energy= 0.359938
Thermal correction to Enthalpy= 0.360882
Thermal correction to Gibbs Free Energy= 0.292919
Sum of electronic and zero-point Energies= -884.583242
Sum of electronic and thermal Energies= -884.563387
Sum of electronic and thermal Enthalpies= -884.562442
Sum of electronic and thermal Free Energies= -884.630405

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.400129 | -2.276367 | 1.468160 |
| 2 | 6 | 0 | 0.909308 | -1.991219 | 0.741807 |
| 3 | 1 | 0 | -0.462481 | -1.645907 | 2.360688 |
| 4 | 6 | 0 | 0.912375 | -0.551143 | 0.207409 |
| 5 | 6 | 0 | -0.204707 | -0.319015 | -0.839347 |
| 6 | 6 | 0 | -1.526328 | -0.955082 | -0.481275 |
| 7 | 6 | 0 | -1.615879 | -2.062548 | 0.563974 |
| 8 | 1 | 0 | -2.524144 | -1.928368 | 1.163236 |
| 9 | 6 | 0 | -2.502671 | -1.224627 | -1.614841 |
| 10 | 1 | 0 | -3.474428 | -1.523394 | -1.209652 |
| 11 | 1 | 0 | -2.656065 | -0.365541 | -2.266245 |
| 12 | 6 | 0 | -1.269102 | 0.549739 | -0.160072 |
| 13 | 8 | 0 | -1.934410 | 1.496840 | -0.932907 |
| 14 | 6 | 0 | -0.746601 | 0.968277 | 1.144013 |
| 15 | 6 | 0 | 0.548724 | 0.390370 | 1.374461 |
| 16 | 6 | 0 | -1.358049 | 1.929675 | 2.090510 |
| 17 | 1 | 0 | -1.514534 | 2.905755 | 1.616564 |
| 18 | 1 | 0 | -2.334201 | 1.584719 | 2.450557 |
| 19 | 1 | 0 | -0.693733 | 2.062557 | 2.946766 |
| 20 | 8 | 0 | 1.250799 | 0.551136 | 2.370662 |
| 21 | 6 | 0 | 0.186880 | -0.105952 | -2.280873 |
| 22 | 1 | 0 | 0.651744 | -1.009114 | -2.688658 |
| 23 | 1 | 0 | -0.677014 | 0.140646 | -2.895790 |
| 24 | 6 | 0 | 2.287988 | -0.202277 | -0.338300 |
| 25 | 8 | 0 | 3.139674 | -1.006799 | -0.636709 |
| 26 | 8 | 0 | 2.447656 | 1.122570 | -0.463624 |
| 27 | 6 | 0 | 3.723060 | 1.550450 | -0.945782 |
| 28 | 1 | 0 | 3.910899 | 1.147898 | -1.942935 |
| 29 | 1 | 0 | 3.675540 | 2.637175 | -0.972749 |
| 30 | 1 | 0 | 4.512975 | 1.217493 | -0.270900 |
| 31 | 1 | 0 | -1.771788 | -2.985504 | -0.009101 |
| 32 | 1 | 0 | 0.896152 | 0.718446 | -2.374528 |

| | | | | | |
|---|---|---|---|---|---|
| 33 | 1 | 0 | -0.405456 | -3.308667 | 1.831352 |
| 34 | 1 | 0 | 1.755672 | -2.117815 | 1.420751 |
| 35 | 1 | 0 | 1.059838 | -2.681430 | -0.094675 |
| 36 | 6 | 0 | -3.292378 | 1.720313 | -0.592316 |
| 37 | 1 | 0 | -3.725247 | 2.301329 | -1.408027 |
| 38 | 1 | 0 | -3.842436 | 0.779350 | -0.489122 |
| 39 | 1 | 0 | -3.389935 | 2.291524 | 0.335847 |
| 40 | 1 | 0 | -2.136077 | -2.054691 | -2.227922 |

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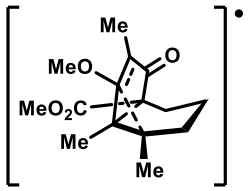
## Truncated Radical TS2




Imaginary: -491.8588 cm-1
Zero-point correction= 0.338711 (Hartree/Particle)
Thermal correction to Energy= 0.358486
Thermal correction to Enthalpy= 0.359431
Thermal correction to Gibbs Free Energy= 0.291484
Sum of electronic and zero-point Energies= -884.574441
Sum of electronic and thermal Energies= -884.554665
Sum of electronic and thermal Enthalpies= -884.553721
Sum of electronic and thermal Free Energies= -884.621668

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.349891 | 2.376223 | 1.437108 |
| 2 | 6 | 0 | -0.933790 | 2.032249 | 0.694663 |
| 3 | 1 | 0 | 0.417576 | 1.759264 | 2.337488 |
| 4 | 6 | 0 | -0.879118 | 0.581956 | 0.207017 |
| 5 | 6 | 0 | 0.262851 | 0.338149 | -0.823525 |
| 6 | 6 | 0 | 1.506172 | 1.113185 | -0.512352 |
| 7 | 6 | 0 | 1.580205 | 2.179017 | 0.552014 |
| 8 | 1 | 0 | 2.481641 | 2.036920 | 1.161349 |
| 9 | 6 | 0 | 2.575784 | 1.253561 | -1.557730 |
| 10 | 1 | 0 | 3.522676 | 1.556909 | -1.100694 |
| 11 | 1 | 0 | 2.742844 | 0.340372 | -2.128028 |
| 12 | 6 | 0 | 1.117052 | -0.726033 | -0.183214 |
| 13 | 8 | 0 | 1.901115 | -1.481539 | -0.995272 |
| 14 | 6 | 0 | 0.694235 | -1.051455 | 1.119497 |
| 15 | 6 | 0 | -0.520987 | -0.336462 | 1.399859 |
| 16 | 6 | 0 | 1.258615 | -2.025548 | 2.094748 |
| 17 | 1 | 0 | 1.241223 | -3.051379 | 1.709987 |
| 18 | 1 | 0 | 2.291432 | -1.792863 | 2.374233 |
| 19 | 1 | 0 | 0.644716 | -1.997433 | 2.997900 |

| | | | | | |
|---|---|---|---|---|---|
| 20 | 8 | 0 | -1.196502 | -0.395088 | 2.422993 |
| 21 | 6 | 0 | -0.141160 | 0.186507 | -2.279240 |
| 22 | 1 | 0 | -0.627699 | 1.100455 | -2.631280 |
| 23 | 1 | 0 | 0.723870 | -0.007431 | -2.912383 |
| 24 | 6 | 0 | -2.232317 | 0.177192 | -0.358479 |
| 25 | 8 | 0 | -3.105925 | 0.947938 | -0.682045 |
| 26 | 8 | 0 | -2.346700 | -1.154065 | -0.467764 |
| 27 | 6 | 0 | -3.600303 | -1.628919 | -0.962723 |
| 28 | 1 | 0 | -3.785700 | -1.247404 | -1.968652 |
| 29 | 1 | 0 | -3.518450 | -2.713930 | -0.972341 |
| 30 | 1 | 0 | -4.410770 | -1.311163 | -0.305106 |
| 31 | 1 | 0 | 1.759707 | 3.113356 | -0.002819 |
| 32 | 1 | 0 | -0.832302 | -0.648270 | -2.405223 |
| 33 | 1 | 0 | 0.318080 | 3.414197 | 1.781610 |
| 34 | 1 | 0 | -1.796881 | 2.146860 | 1.353567 |
| 35 | 1 | 0 | -1.091418 | 2.696479 | -0.162010 |
| 36 | 6 | 0 | 3.155153 | -1.916516 | -0.486131 |
| 37 | 1 | 0 | 3.721802 | -2.279075 | -1.344117 |
| 38 | 1 | 0 | 3.691669 | -1.085048 | -0.017693 |
| 39 | 1 | 0 | 3.038968 | -2.728923 | 0.233847 |
| 40 | 1 | 0 | 2.297414 | 2.041503 | -2.272005 |

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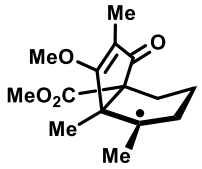
**Truncated Radical Product**




Zero-point correction= 0.339699 (Hartree/Particle)
Thermal correction to Energy= 0.360260
Thermal correction to Enthalpy= 0.361204
Thermal correction to Gibbs Free Energy= 0.289466
Sum of electronic and zero-point Energies= -884.592232
Sum of electronic and thermal Energies= -884.571671
Sum of electronic and thermal Enthalpies= -884.570727
Sum of electronic and thermal Free Energies= -884.642465

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.583631 | 1.376765 | 2.286693 |
| 2 | 6 | 0 | -0.806892 | 1.240286 | 1.686115 |
| 3 | 1 | 0 | 0.974359 | 0.388695 | 2.552523 |
| 4 | 6 | 0 | -0.797929 | 0.290701 | 0.476685 |
| 5 | 6 | 0 | 0.386084 | 0.576727 | -0.531071 |
| 6 | 6 | 0 | 1.188509 | 1.801872 | -0.142414 |
| 7 | 6 | 0 | 1.510797 | 2.079465 | 1.293436 |
| 8 | 1 | 0 | 2.565038 | 1.830163 | 1.505443 |

| | | | | | |
|---|---|---|---|---|---|
| 9 | 6 | 0 | 1.941350 | 2.587549 | -1.165380 |
| 10 | 1 | 0 | 2.368964 | 3.487146 | -0.713877 |
| 11 | 1 | 0 | 2.774742 | 2.011304 | -1.594323 |
| 12 | 6 | 0 | 1.233492 | -0.686535 | -0.379279 |
| 13 | 8 | 0 | 2.352112 | -0.646293 | -1.107977 |
| 14 | 6 | 0 | 0.724282 | -1.646777 | 0.435251 |
| 15 | 6 | 0 | -0.525091 | -1.133058 | 0.986153 |
| 16 | 6 | 0 | 1.180976 | -3.017852 | 0.836405 |
| 17 | 1 | 0 | 1.122961 | -3.734528 | 0.012318 |
| 18 | 1 | 0 | 2.197069 | -3.037351 | 1.234613 |
| 19 | 1 | 0 | 0.505760 | -3.369122 | 1.620326 |
| 20 | 8 | 0 | -1.238119 | -1.704208 | 1.794101 |
| 21 | 6 | 0 | -0.070256 | 0.658135 | -1.999847 |
| 22 | 1 | 0 | -0.710233 | 1.530326 | -2.156162 |
| 23 | 1 | 0 | 0.792875 | 0.739349 | -2.661391 |
| 24 | 6 | 0 | -2.162234 | 0.370982 | -0.197117 |
| 25 | 8 | 0 | -2.860005 | 1.359270 | -0.219069 |
| 26 | 8 | 0 | -2.509679 | -0.781047 | -0.786682 |
| 27 | 6 | 0 | -3.791317 | -0.791724 | -1.417593 |
| 28 | 1 | 0 | -3.827980 | -0.059110 | -2.226152 |
| 29 | 1 | 0 | -3.917021 | -1.800265 | -1.806379 |
| 30 | 1 | 0 | -4.572036 | -0.560891 | -0.691357 |
| 31 | 1 | 0 | 1.446265 | 3.167148 | 1.442672 |
| 32 | 1 | 0 | -0.624800 | -0.238768 | -2.280577 |
| 33 | 1 | 0 | 0.535515 | 1.946189 | 3.219353 |
| 34 | 1 | 0 | -1.516201 | 0.840165 | 2.415908 |
| 35 | 1 | 0 | -1.182373 | 2.215253 | 1.361932 |
| 36 | 6 | 0 | 3.275697 | -1.727054 | -1.073391 |
| 37 | 1 | 0 | 2.798915 | -2.663436 | -1.367722 |
| 38 | 1 | 0 | 4.052226 | -1.471918 | -1.793103 |
| 39 | 1 | 0 | 3.719538 | -1.826519 | -0.080663 |
| 40 | 1 | 0 | 1.315345 | 2.907505 | -2.004247 |

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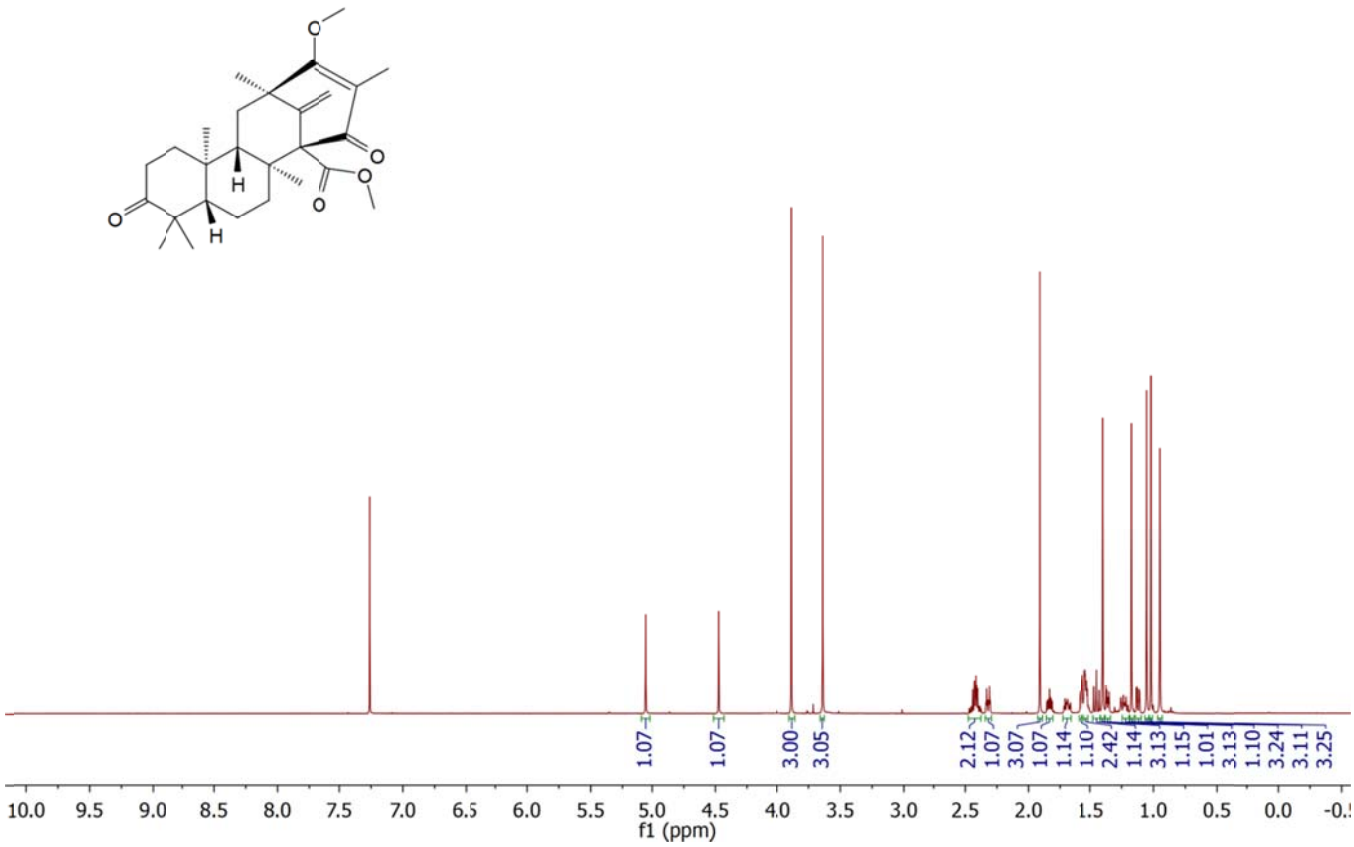
## Computational References

[1] Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

[2] This work was supported by the HPC facilities operated by, and the staff of, the Yale Center for Research Computing. We gratefully acknowledge the National Science Foundation for financial support in the establishment of the Yale University High Performance Computing (HPC) Center (CNS 08-21132).

[3] For systematic evaluation and recommendation of using B3LYP geometries and mPW1PW91 single point energies, see: S. P. T. Matsuda, W. K. Wilson, Q. Xiong, *Org. Biomol. Chem.* **2006**, *4*, 530.

[4] NBO 6.0. E. D. Glendening, J, K. Badenhoop, A. E. Reed, J. E. Carpenter, J. A. Bohmann, C. M. Morales, C. R. Landis, and F. Weinhold, Theoretical Chemistry Institute, University of Wisconsin, Madison (2013).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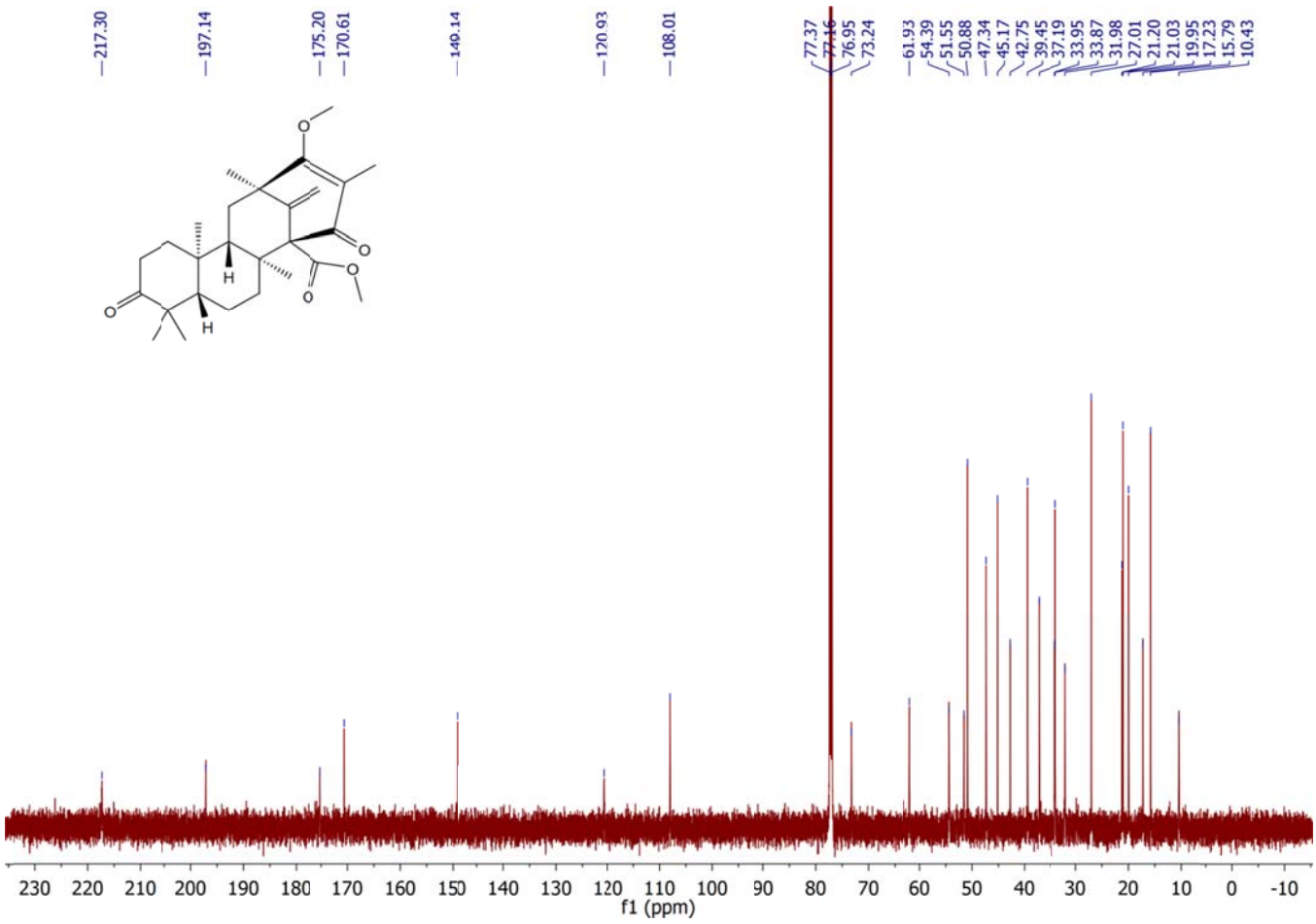
1.07
3.00
3.05
2.12
1.07
3.07
1.07
1.14
1.10
2.42
1.14
3.13
1.15
1.01
3.13
1.10
3.24
3.11
3.25
f1 (ppm)


217.30
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175.20
170.61
140.14
120.93
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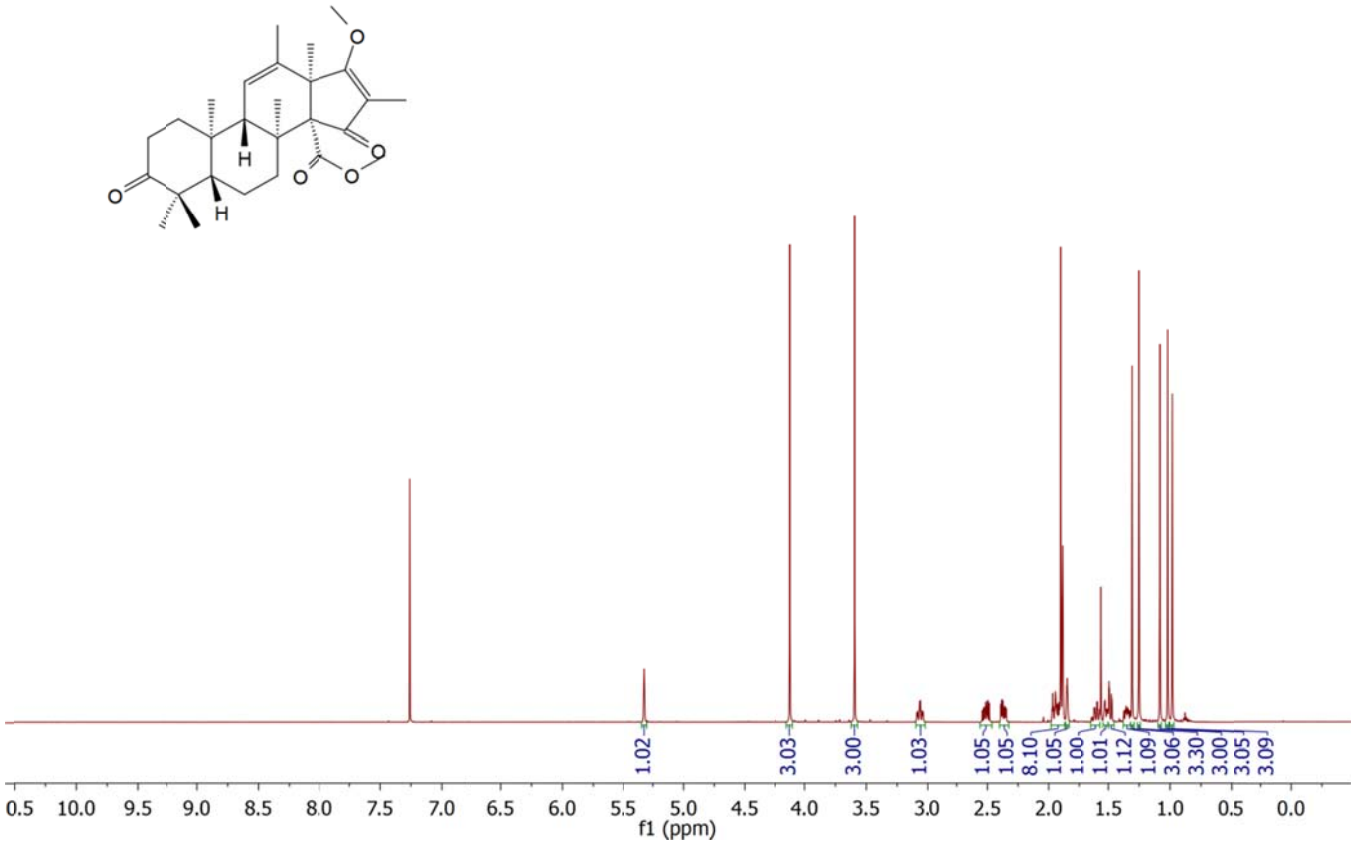
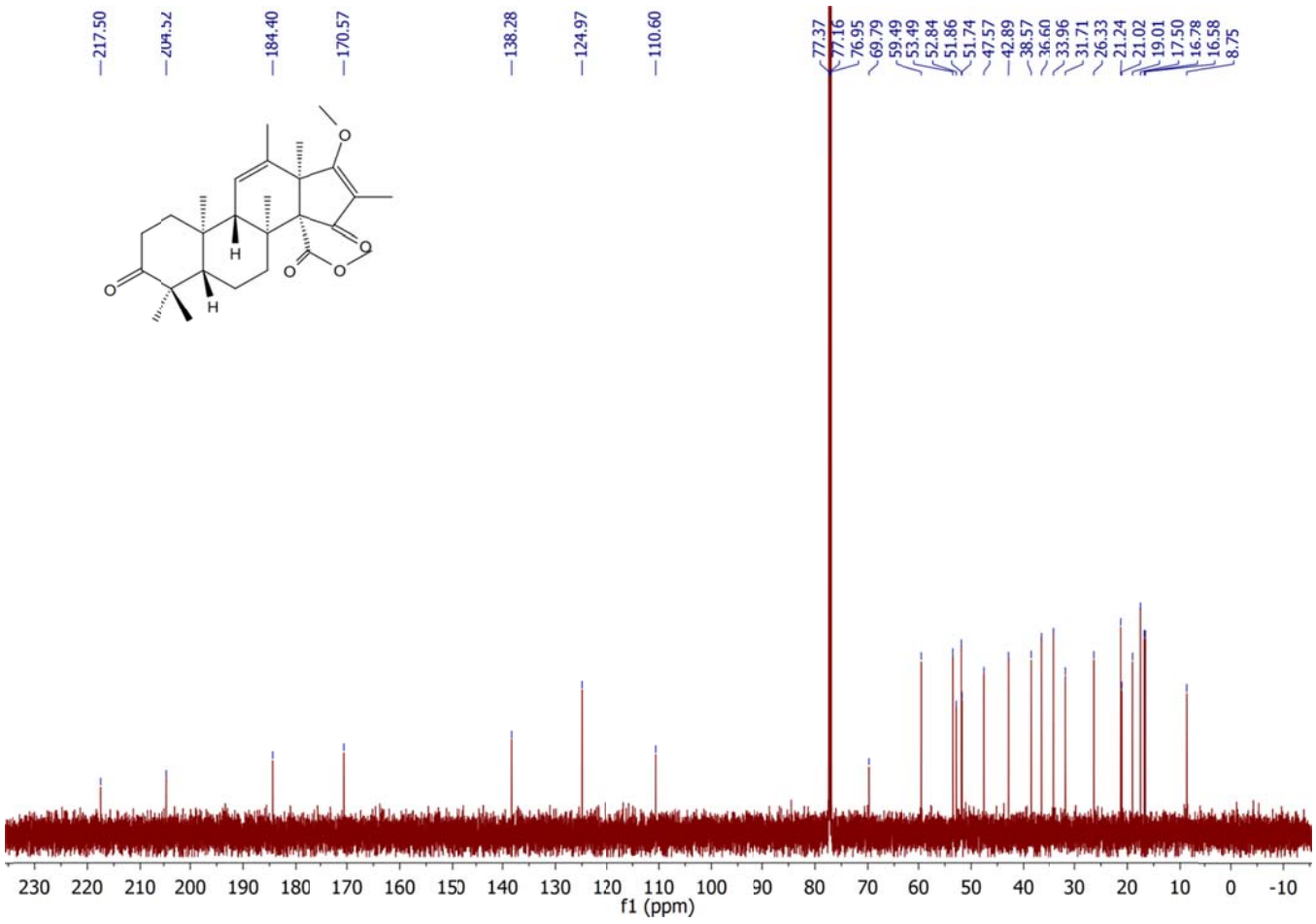
77.37
77.16
76.95
73.24
61.93
54.39
51.55
50.88
47.34
45.17
42.75
39.45
37.19
33.95
33.87
31.98
27.01
21.20
21.03
19.95
17.23
15.79
10.43
f1 (ppm)


1.02
3.03
3.00
1.03
1.05
1.05
8.10
1.05
1.00
1.01
1.12
1.09
3.06
3.30
3.00
3.05
3.09
f1 (ppm)


217.50
184.40
170.57
138.28
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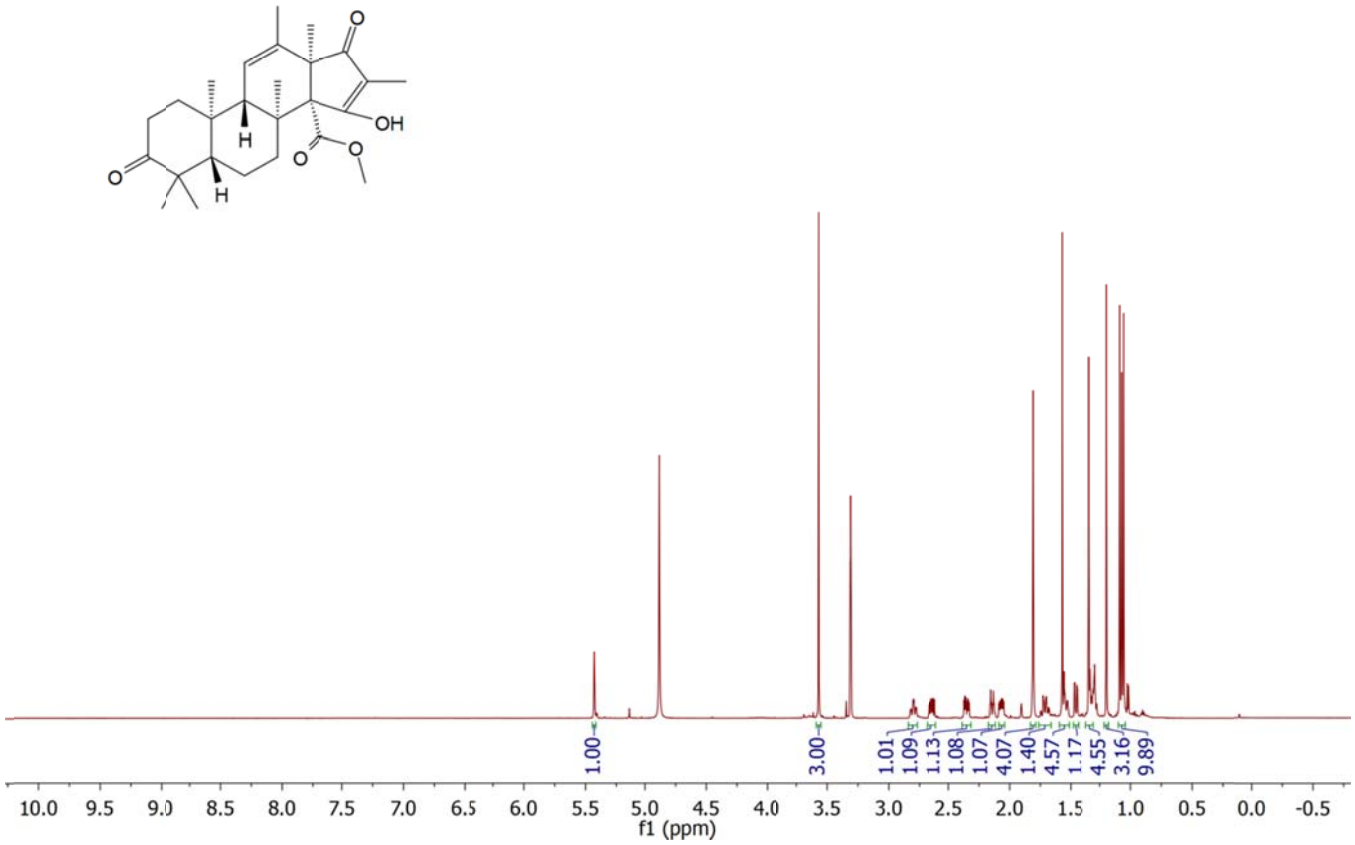
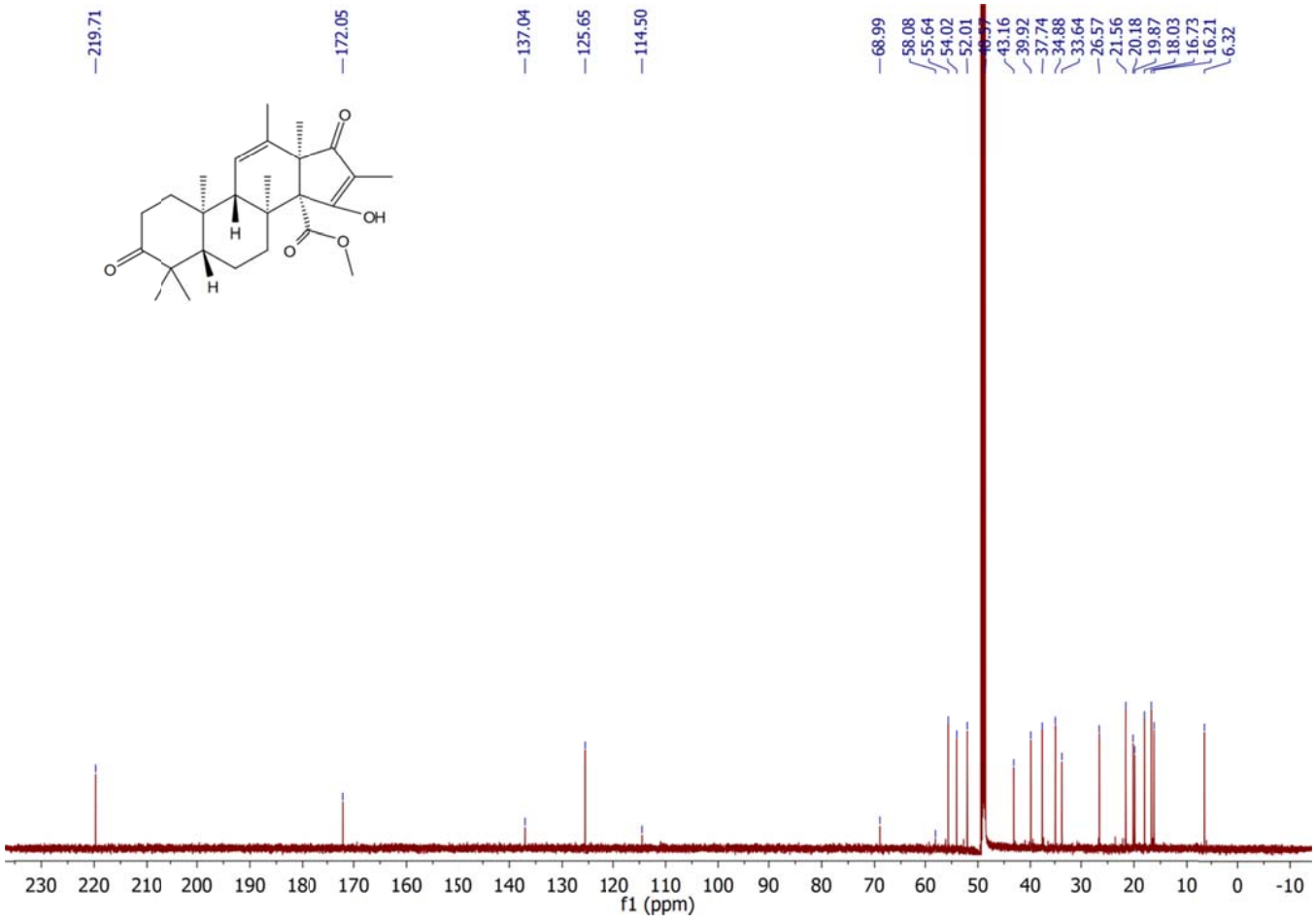
77.16
76.95
69.79
59.49
53.49
52.84
51.86
51.74
47.57
42.89
38.57
36.60
33.96
31.71
26.33
21.24
21.02
19.01
17.50
16.78
16.58
8.75
f1 (ppm)


O
OH
O
O
H
H
1.00
3.00
1.01
1.09
1.13
1.08
1.07
4.07
1.40
4.57
1.17
4.55
3.16
9.89
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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52.01
43.16
39.92
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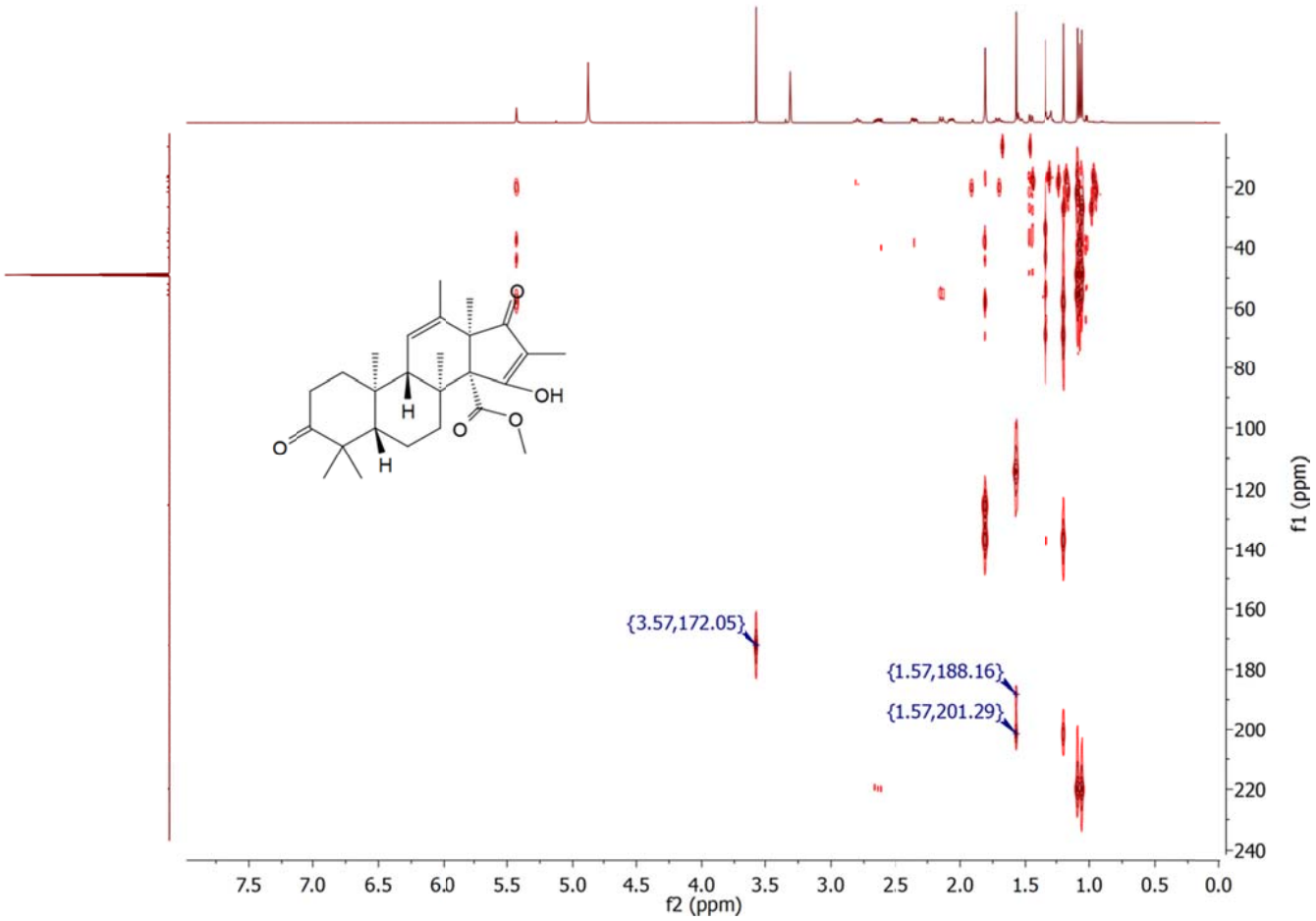
34.88
33.64
26.57
21.56
20.18
19.87
18.03
16.73
16.21
6.32
O
OH
O
O
H
H
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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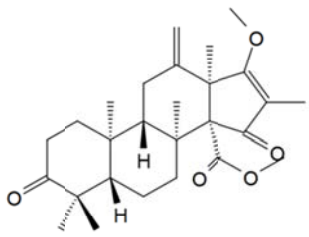
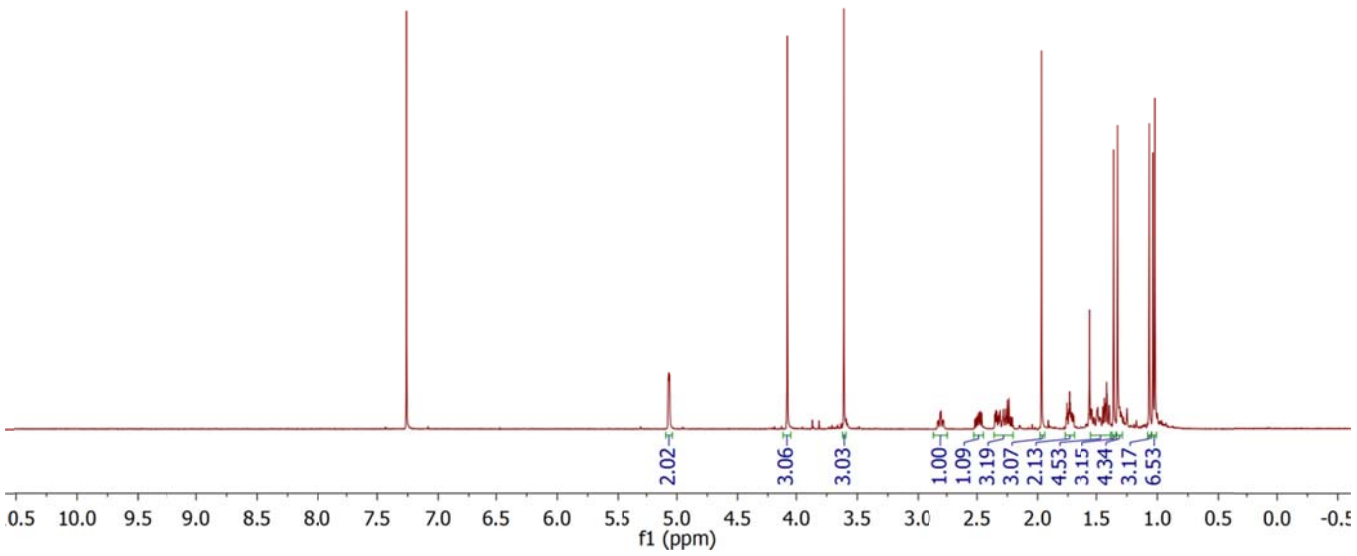
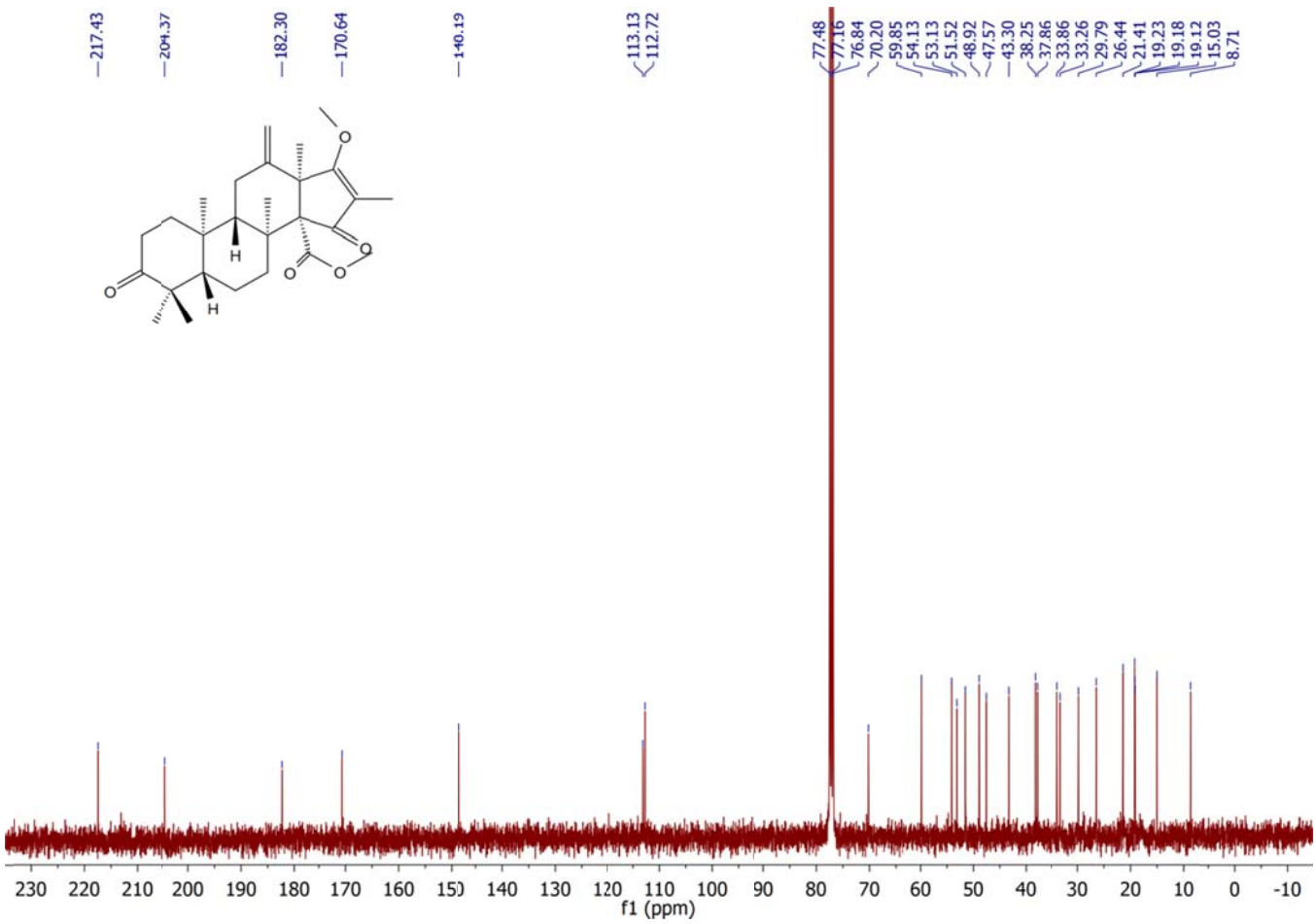
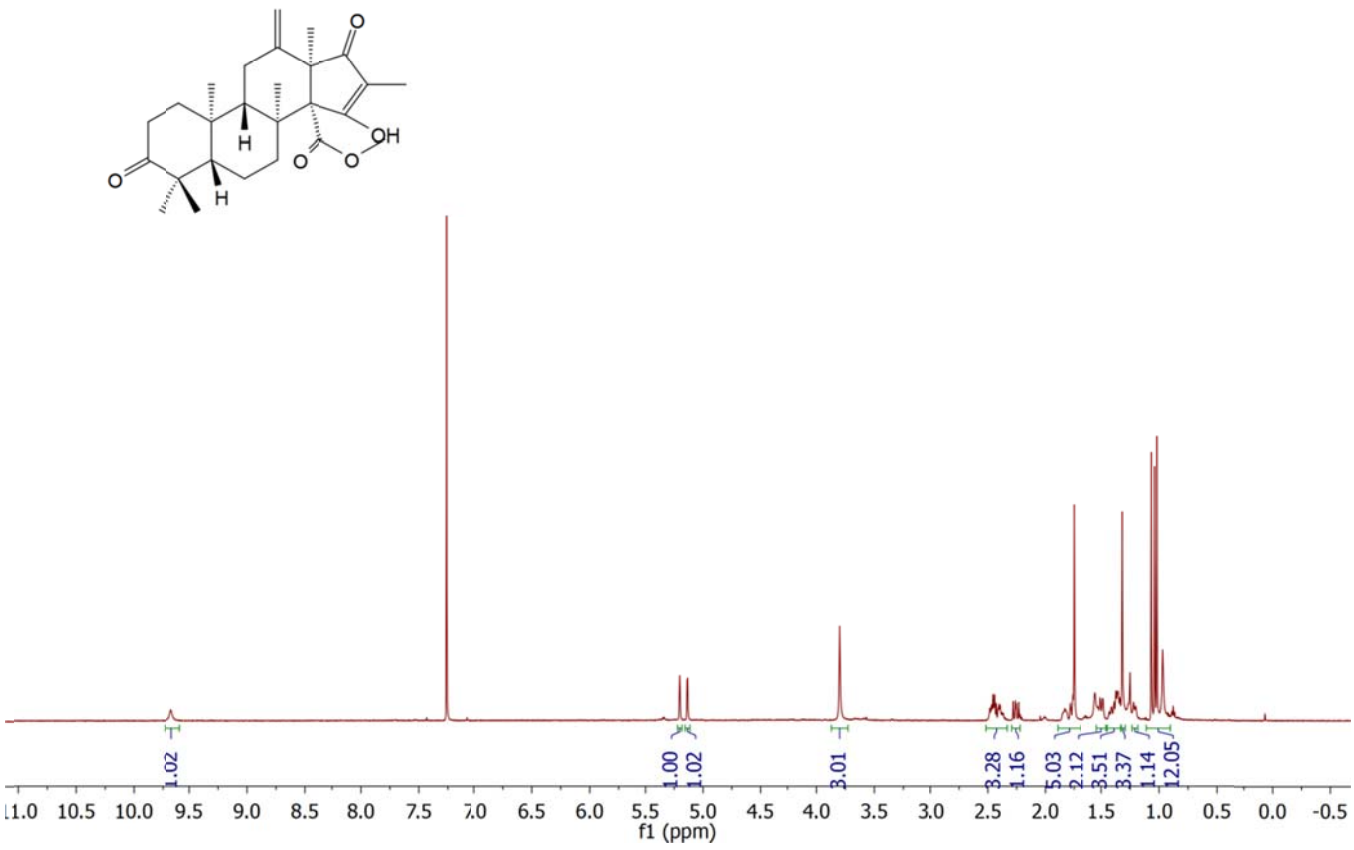
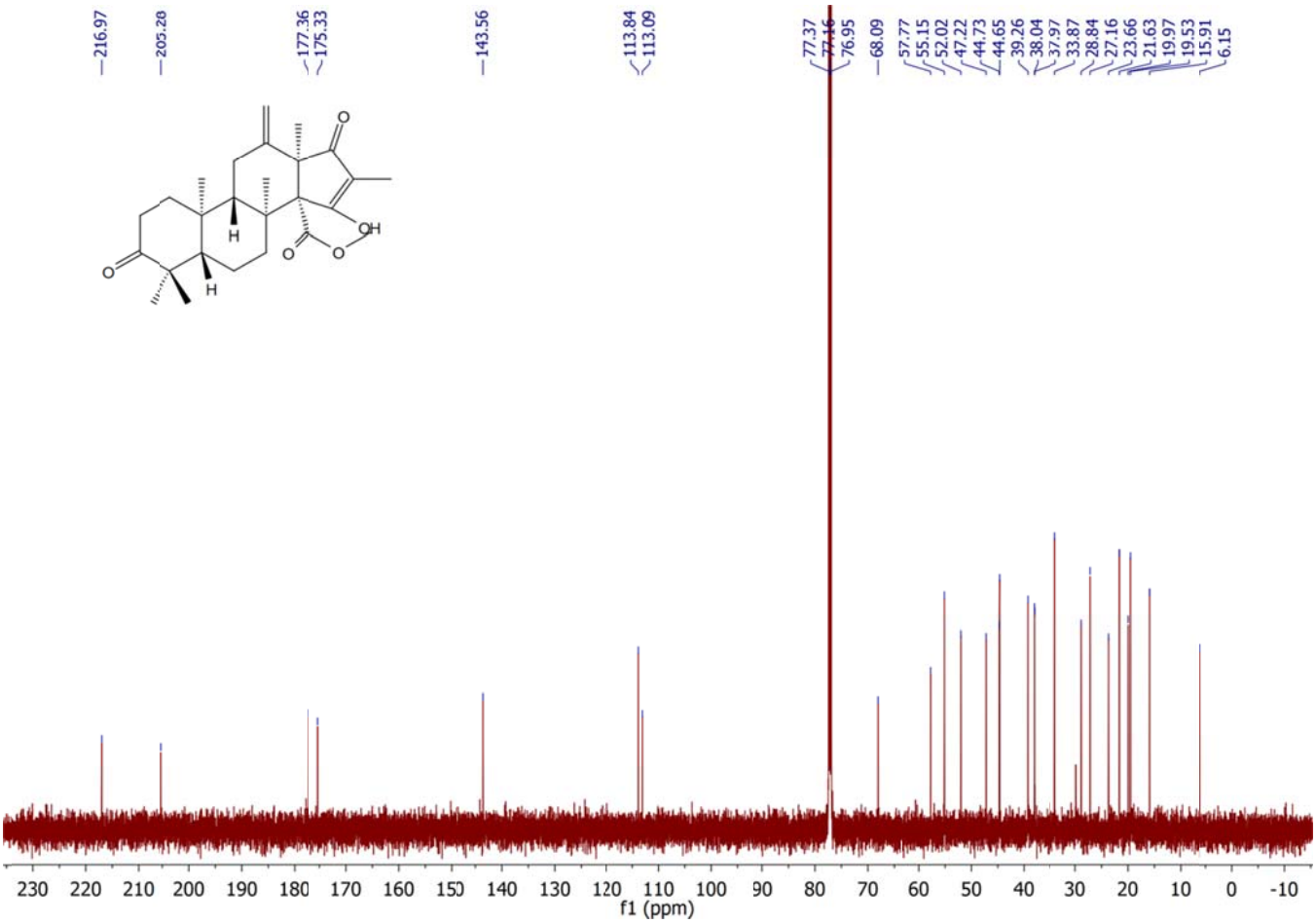
{1.57,188.16}
{1.57,201.29}
f2 (ppm)
f1 (ppm)

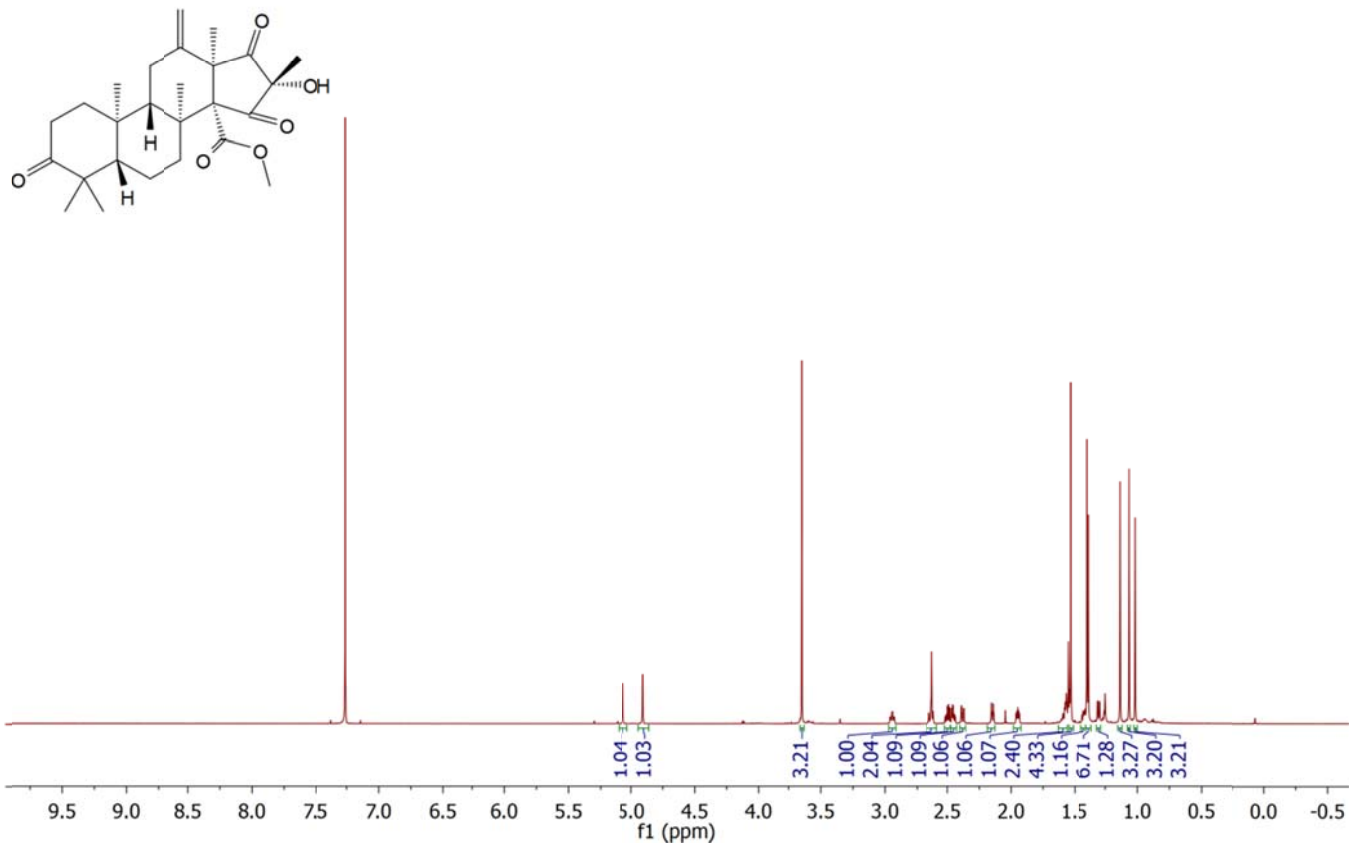


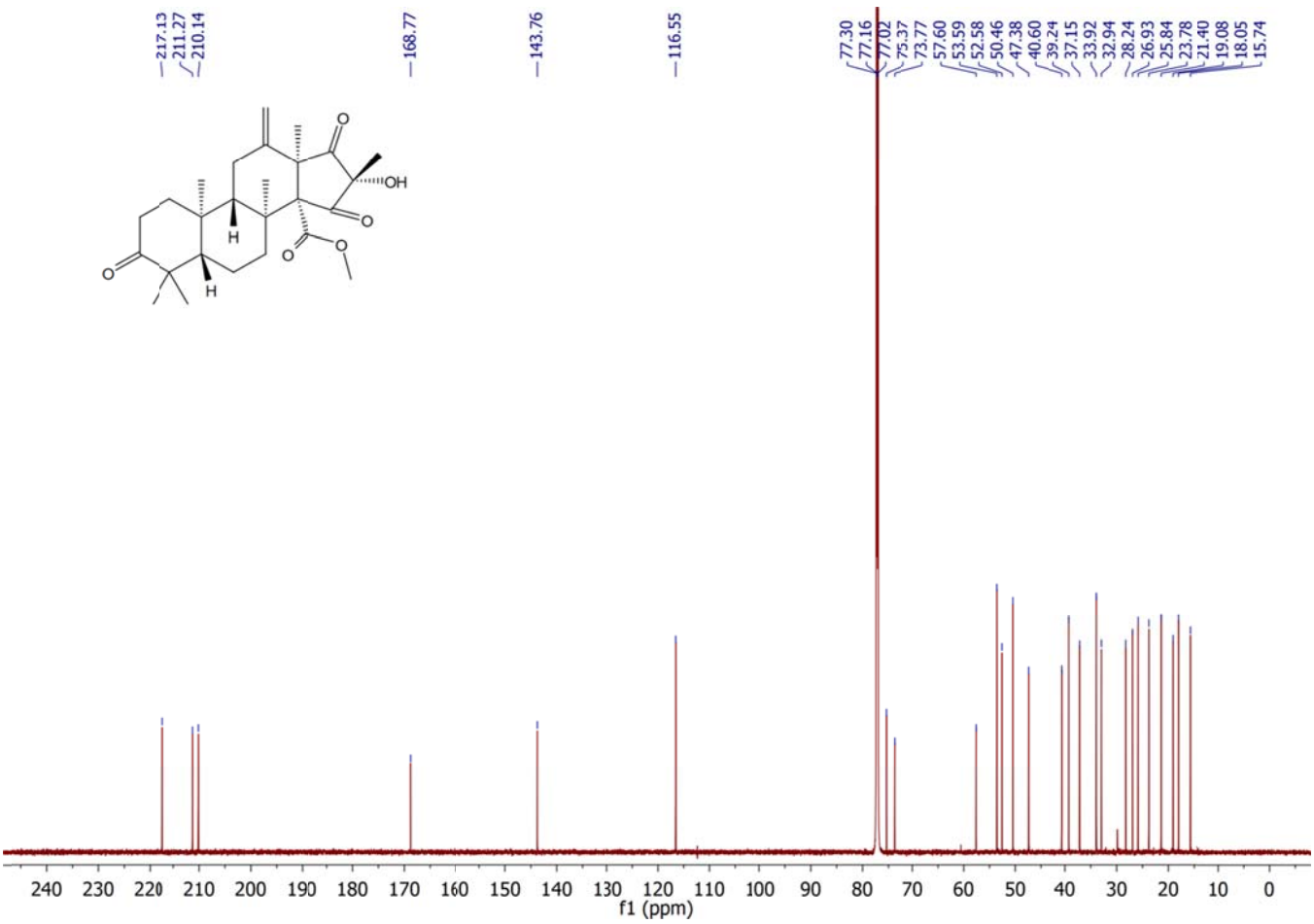

2.02
3.06
3.03
1.00
1.09
3.19
3.07
2.13
4.53
3.15
4.34
3.17
6.53
f1 (ppm)

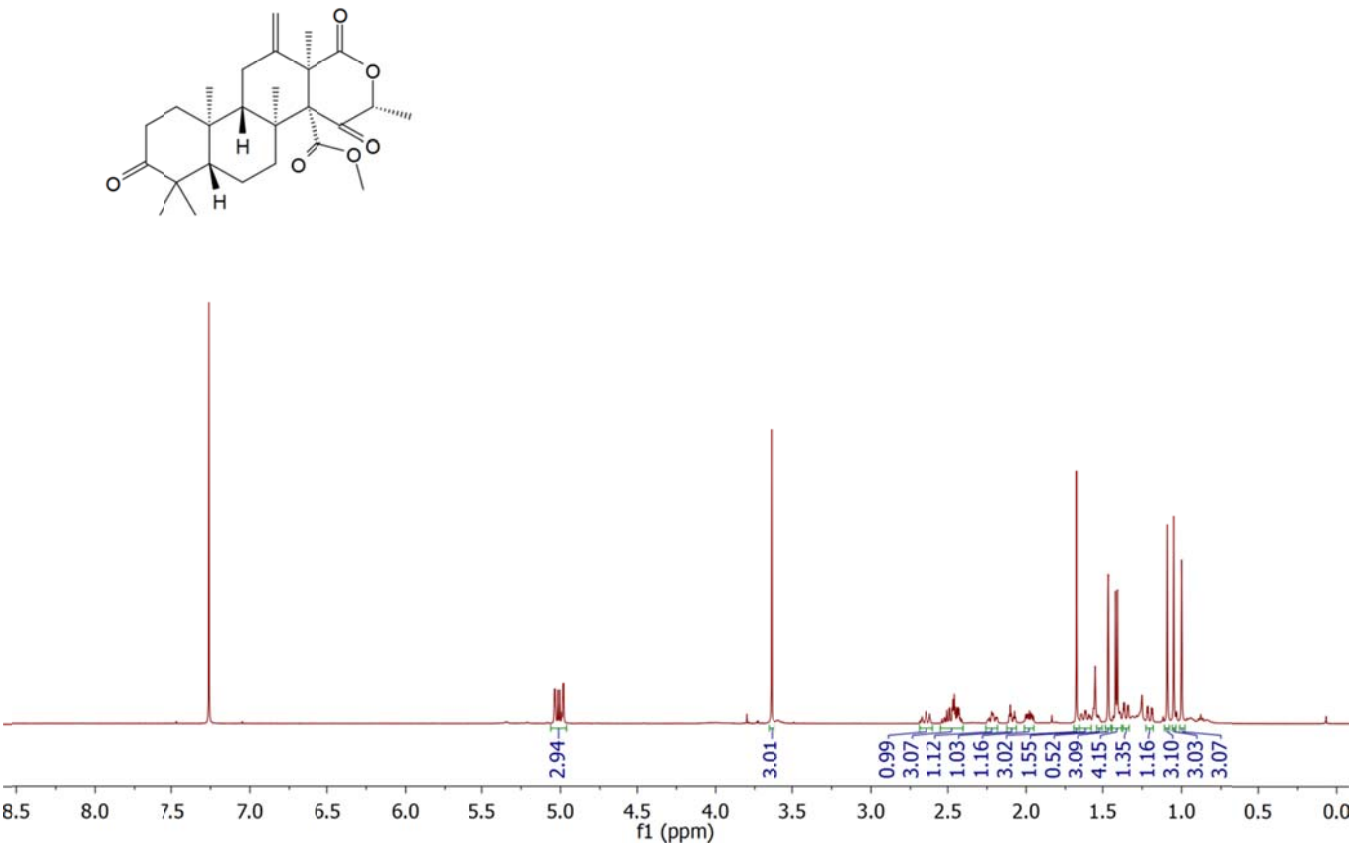

217.43
204.37
182.30
170.64
140.19
113.13
112.72
77.48
77.16
76.84
70.20
59.85
54.13
53.13
51.52
48.92
47.57
43.30
38.25
37.86
33.86
33.26
29.79
26.44
21.41
19.23
19.18
19.12
15.03
8.71
O
H
H
O
O
O
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

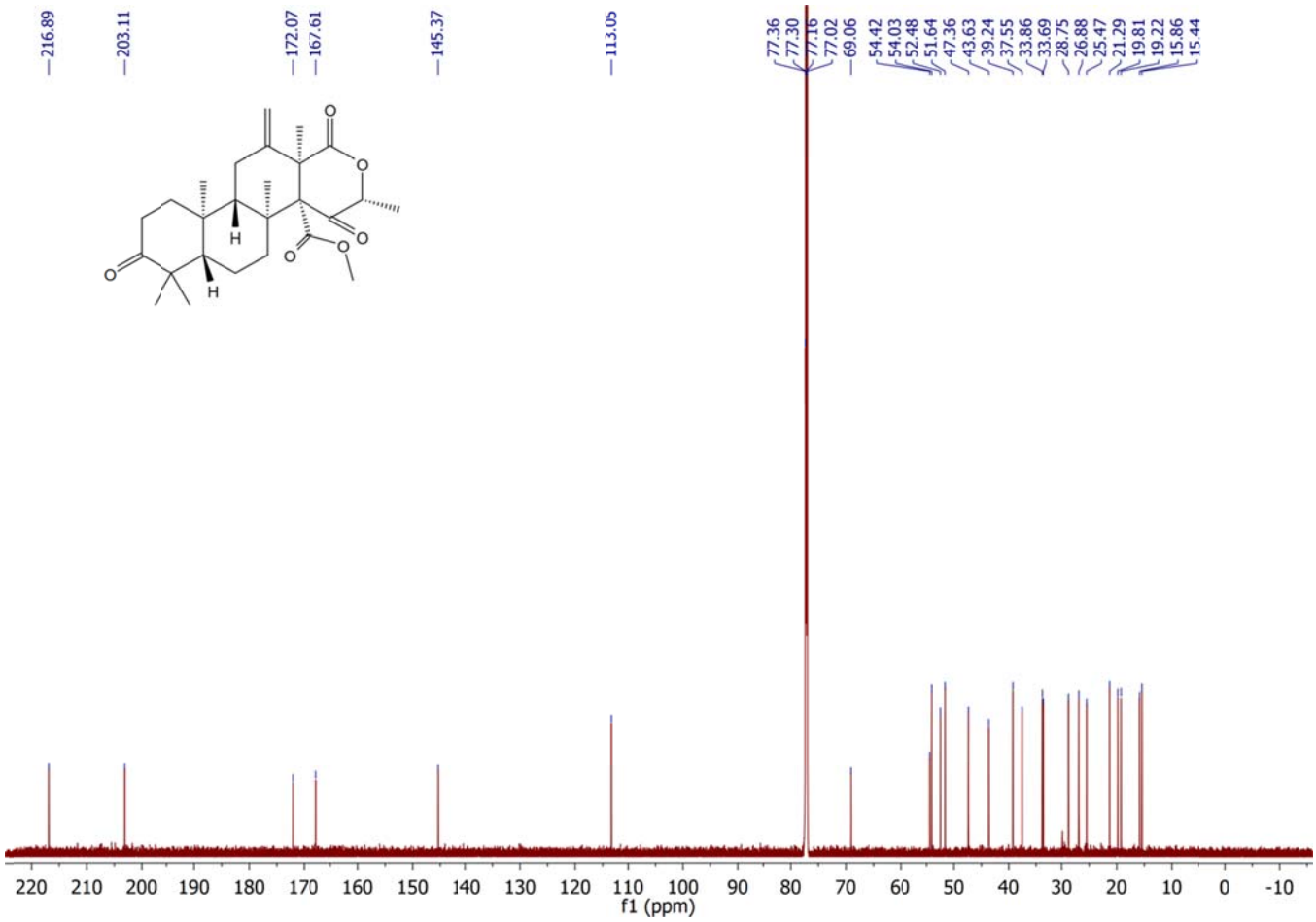

O
H
OH
O
O
H
1.02
1.00
1.02
3.01
3.28
1.16
5.03
2.12
3.51
3.37
1.14
12.05
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

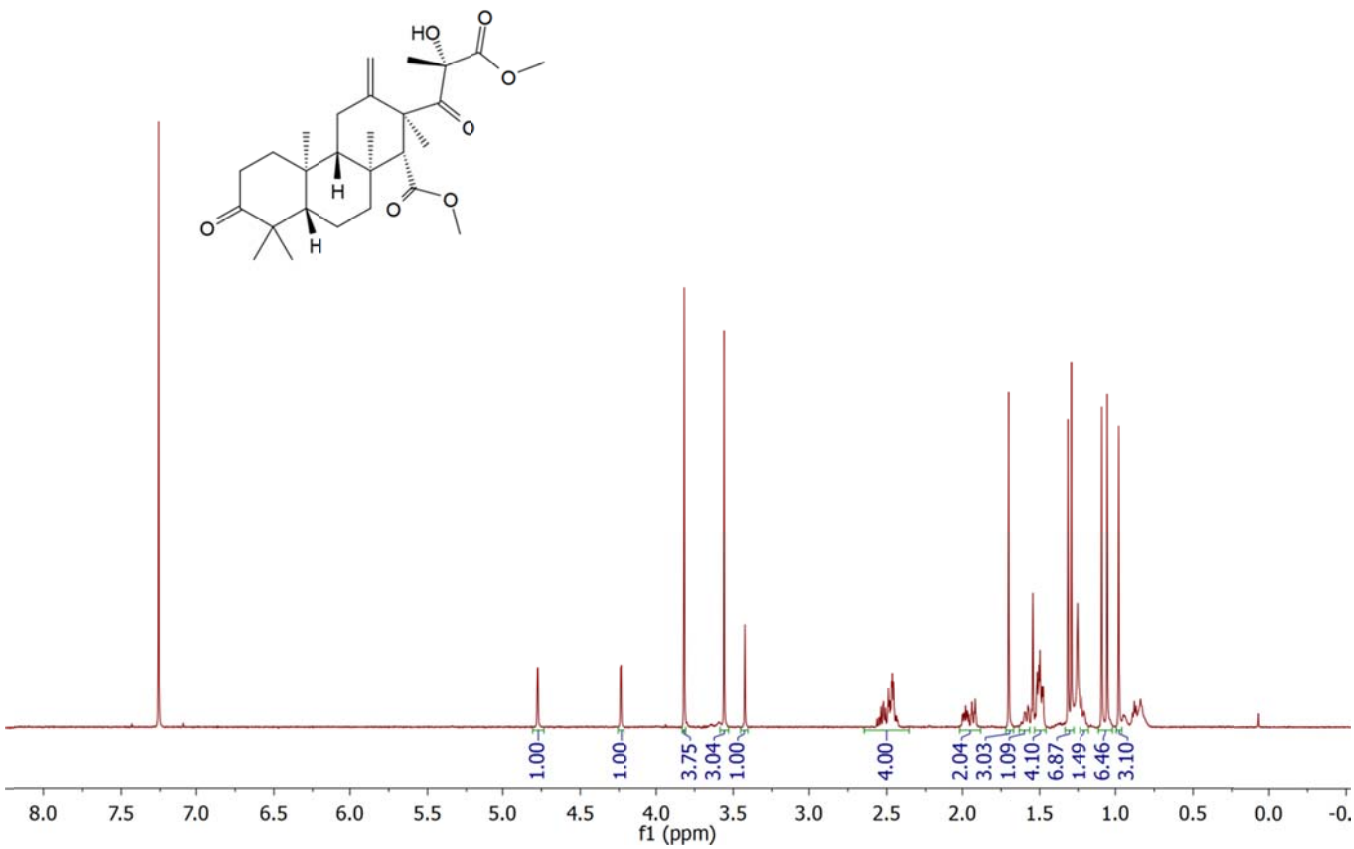

216.97
205.28
177.36
175.33
143.56
113.84
113.09
77.37
77.16
76.95
68.09
57.77
55.15
52.02
47.22
44.73
44.65
39.26
38.04
37.97
33.87
28.84
27.16
23.66
21.63
19.97
19.53
15.91
6.15
OH
H
H
O
O
O
O
f1 (ppm)

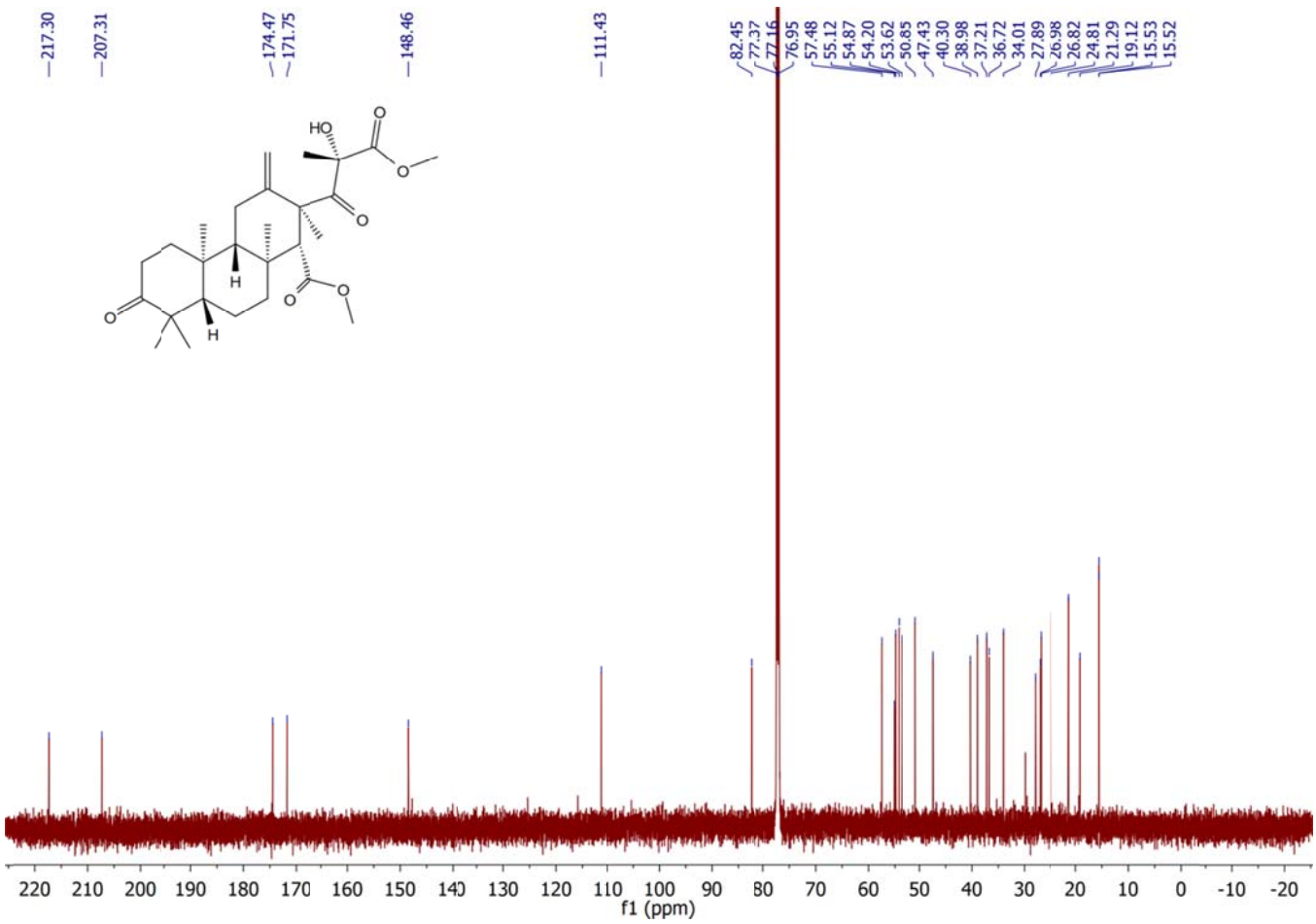

OH
H
H
O
O
O
O
O
1.04
1.03
3.21
1.00
2.04
1.09
1.09
1.06
1.06
1.07
2.40
4.33
1.16
6.71
1.28
3.27
3.20
3.21
f1 (ppm)


217.13
211.27
210.14
168.77
143.76
116.55
77.30
77.16
77.02
75.37
73.77
57.60
53.59
52.58
50.46
47.38
40.60
39.24
37.15
33.92
32.94
28.24
26.93
25.84
23.78
21.40
19.08
18.05
15.74
OH
H
H
O
O
O
O
O
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


H
H
O
O
O
O
O
2.94
3.01
0.99
3.07
1.12
1.03
1.16
3.02
1.55
0.52
3.09
4.15
1.35
1.16
3.10
3.03
3.07
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


216.89
203.11
172.07
167.61
145.37
113.05
77.36
77.30
77.16
77.02
69.06
54.42
54.03
52.48
51.64
47.36
43.63
39.24
37.55
33.86
33.69
28.75
26.88
25.47
21.29
19.81
19.22
15.86
15.44
f1 (ppm)


1.00
1.00
3.75
3.04
1.00
4.00
2.04
3.03
1.09
4.10
6.87
1.49
6.46
3.10
f1 (ppm)


217.30
207.31
174.47
171.75
148.46
111.43
82.45
77.37
77.16
76.95
57.48
55.12
54.87
54.20
53.62
50.85
47.43
40.30
38.98
37.21
36.72
34.01
27.89
26.98
26.82
24.81
21.29
19.12
15.53
15.52
HO
O
O
O
O
O
H
H
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)