dSynthetic and computational studies on the tricarboxylate core of 6,7-dideoxysqualestatin H5 involving a carbonyl ylide cycloaddition–rearrangement

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Supplementary Information

Contents:

a. Experimental details for compounds 11-19, 20 (via 19), 21 (via 24), 22-24 and 29

2-Methoxy-6-(trimethylsilyloxy)hept-1-en-3-one 11

TMSCl (9.0 cm^3, 71.2 mmol) was added to a stirred solution of pyridine (7.7 cm^3, 94.8 mmol) in THF (10 cm^3) at 0 °C. After 30 min, a solution of crude alcohol **10** (7.50 g, 47.4 mmol) in THF (10 cm^3) was added and the mixture was allowed to stir at 0 °C for 30 min. Water (5 cm^3) was then added and the mixture extracted with Et_2O (3 × 10 cm^3). The combined organic layers were washed with brine (5 cm^3), water (5 cm^3), dried ($MgSO_4$) and evaporated under reduced pressure to give a yellow oil, *silyl ether* **11** (10.0 g, 92%) which was used directly in the next step; R_f 0.68 (50% Et_2O in light petroleum); ν_{max}/cm^{-1} 2958m, 1709m, 1613s, 1375m, 1251s, 1054s, 841s and 743m; δ_H(400 MHz) 5.18 (1 H, d, *J* 3, H of $=CH_2$), 4.45 (1 H, d, *J* 3, H of $=CH_2$), 3.85–3.75 (1 H, m, CH), 3.62 (3 H, s, OMe), 2.75–2.65 (2 H, m, CH_2), 1.80–1.60 (2 H, m, CH_2), 1.13 (3 H, d, *J* 6, Me) and 0.08 (9 H, s, $SiMe_3$); δ_C(100 MHz) 197.5 (C(3), quat.), 158.4 (C(2), quat), 90.5 ($=CH_2$), 67.5 (CH), 55.2 (OMe), 34.1 (CH_2), 32.9 (CH_2), 23.8 (Me) and 0.1 ($SiMe_3$).

Methyl 5-(trimethylsilyloxy)-2-oxohexanoate 12 and 2-Hydroxy-2-(methoxycarbonyl)-5-methyltetrahydrofuran 13

A mixture of O_3/O_2 was bubbled through a solution of crude silyl ether **11** (5.22 g, 22.7 mmol) in CH_2Cl_2 (50 cm^3) at –78 °C. After 1.5 h, the stream of O_3/O_2 was stopped and argon was bubbled through for 10 min. Ph_3P (6.55 g, 25.0 mmol) was added and the solution allowed to warm to 25 ºC. The reaction mixture was then evaporated under reduced pressure and purified by column chromatography (gradient elution: 10% Et_2O in light petroleum to 20% Et_2O in light petroleum). First to elute was a colourless oil, *α-ketoester* **12** (1.77 g, 33%); R_f 0.34 (20% Et_2O in light petroleum); ν_{max}/cm^{-1} 2957s, 1732s, 1377m, 1251s, 1060s, 842s and 749w; δ_H(400 MHz) 3.90–3.70 (1 H, m, CH), 3.87 (3 H, s, OMe), 3.00–2.80 (2 H, m, CH_2), 1.90–1.70 (2 H, m, CH_2), 1.16 (3 H, d, *J* 6, Me) and 0.10 (9 H, s, $SiMe_3$); δ_C(100 MHz) 194.2 (C(2), quat.), 161.4 (C(1), quat.), 67.1 (CH), 52.8 (OMe), 35.5 (CH_2), 32.7 (CH_2), 23.6 (Me) and 0.1 ($SiMe_3$). Second to elute was *lactol* **13** (1.08 g, 30%, 1:1 mixture of diastereomers, by ^1H NMR analysis of the C-4 methyl signals); R_f 0.42 (50% Et_2O in light petroleum); ν_{max}/cm^{-1} 3460w, 2973w, 1747s, 1441w, 1278m, 1209m, 1150m, 1072s and 882w; δ_H(400 MHz) 4.45–4.37 (1 H, m, CH), 4.32–4.23 (1 H, m, CH), 4.05 (1 H, s, OH), 4.03 (1 H, s, OH), 3.80 (6 H, s, 2 × OMe), 2.51–2.36 (2 H, m, 2 × H of CH_2), 2.22–1.99 (4 H, m, 4 × H of CH_2), 1.84–1.76 (1 H, m, H of CH_2), 1.69–1.60 (1 H, m, H of CH_2), 1.33 (3 H, d, *J* 6, Me) and 1.24 (3 H, d, *J* 6, Me); δ_C(100 MHz) 171.7 (C(2)*C*O, quat.), 171.5 (C(2)*C*O, quat.), 102.2 (C(2), quat.), 101.9 (C(2), quat.), 78.7 (CH), 76.8 (CH), 53.0 (2 × OMe), 35.9 (CH_2), 35.3 (CH_2), 32.8 (CH_2), 32.2 (CH_2), 21.8 (Me) and 20.5 (Me); *m/z* (CI, NH_3) 178 (M + NH_4^+, 55%) and 160 (100) (Found M + NH_4^+: 178.1078. $C_7H_{16}NO_4$ requires *M*, 178.1079).

Methyl 2-diazo-3-hydroxy-3-methoxycarbonyl-6-(trimethylsilyloxy)heptanoate 14

A solution of LDA (7.0 mmol) [prepared from the addition of *n*-BuLi (1.9 mol dm^{-3} in hexanes; 3.7 cm^3, 7.0 mmol) to a solution of diisopropylamine (1.0 cm^3, 7.0 mmol) in THF (10 cm^3) at –78 °C] was slowly added to a stirred solution of α-ketoester **12** (0.96 g, 4.1 mmol) and methyl diazoacetate[1] (92% w/w in CH_2Cl_2; 0.76 g, 7.0 mmol) in THF (10 cm^3) at –78 °C. After 62 h at –78 °C, saturated aq. NH_4Cl (10 cm^3) was added, the mixture allowed to warm to 25 ºC, diluted with Et_2O (10 cm^3) and the layers were separated. The aqueous layer was extracted with Et_2O (3 × 10 cm^3) and the combined organic layers were washed with brine (10 cm^3), water (10 cm^3), dried ($MgSO_4$) and evaporated under reduced pressure. The residue was purified by column

chromatography (40% Et_2O in light petroleum). First to elute was a colourless oil, recovered α-ketoester **12** (161 mg, 17%). Second to elute was a yellow oil, *α-diazoester* **14** [0.61 g, 44% (53% based on recovered **12**); 1:1 mixture of diastereomers by ^1H NMR analysis of the hydroxyl signals]; R_f 0.44 (50% Et_2O in light petroleum); ν_{max}/cm^{-1} 3489w, 2957m, 2099s, 1751s, 1704s, 1439m, 1321s, 1251s, 841s and 750w; δ_H(400 MHz) 4.35 (1 H, s, OH), 4.30 (1 H, s, OH), 3.90–3.70 (2 H, m, 2 × CH), 3.78 (6 H, s, 2 × OMe), 3.75 (6 H, s, 2 × OMe), 2.10–1.15 (8 H, m, 2 × 2 × CH_2), 1.13 (6 H, d, *J* 6, 2 × Me), 0.09 (9 H, s, $SiMe_3$) and 0.08 (9 H, s, $SiMe_3$); δ_C(100 MHz) 173.4 (C, quat.), 173.3 (C, quat.), 166.1 (C, quat.), 166.0 (C, quat.), 73.7 (C, quat.), 73.7 (C, quat.), 68.2 (CH), 67.7 (CH), 53.4 (OMe), 53.4 (OMe), 52.0 (2 × OMe), 32.7 (CH_2), 32.6 (CH_2), 32.5 (CH_2), 32.1 (CH_2), 23.8 (Me), 23.5 (Me) and 0.1 (2 × Me_3Si); *m/z* (ES) 355 (M + Na^+, 50%), 350 (100) and 333 (30) (Found M + NH_4^+: 350.1750. $C_{13}H_{28}N_3O_6Si$ requires *M,* 350.1747).

Methyl 2-diazo-3-methoxycarbonyl-3-(trimethylsilyloxy)-6-oxoheptanoate 17 and Methyl 2-diazo-6-hydroxy-3-methoxycarbonyl-3-(trimethylsilyloxy)heptanoate 16

From **14**: TMS-imidazole (0.8 cm^3, 5.4 mmol) was added to a stirred solution of α-diazoester **14** (0.59 g, 1.7 mmol) in THF (10 cm^3). After 28 h at 25 ºC, the reaction mixture was diluted with Et_2O (5 cm^3), water (5 cm^3) was added and the layers were separated. The aqueous solution was extracted with Et_2O (3 × 5 cm^3) and the combined organic layers were washed with brine (5 cm^3), water (5 cm^3), dried ($MgSO_4$) and evaporated under reduced pressure. The residue contained bis(silyl ether) **15** and silyl ether **16** (1:0.4) as suggested by ^1H NMR analysis of the C-6 methyl signals. PCC (430 mg, 2.0 mmol) was added to a stirred solution of crude mixture containing **15** and **16** obtained above in CH_2Cl_2 (10 cm^3). After 3 h at 25 ºC, a slurry of silica gel in Et_2O (10 cm^3) was added, the mixture was filtered, evaporated under reduced pressure and purified by column chromatography (20% Et_2O in light petroleum). First to elute was a yellow oil, *ketone* **17** (339 mg, 58%); R_f 0.30 (50% Et_2O in light petroleum); ν_{max}/cm^{-1} 2956w, 2099s, 1748m, 1712s, 1438m, 1317m, 1252s, 1137m, 845s and 757w; δ_H(400 MHz) 3.74 (3 H, s, OMe), 3.73 (3 H, s, OMe), 2.57 (1 H, ddd, *J* 17.5, 9, and 6.5, H of CH_2), 2.41 (1 H, ddd, *J* 17.5, 8 and 6.5, H of CH_2), 2.24–2.16 (2 H, m, CH_2), 2.15 (3 H, s, Me) and 0.11 (9 H, s, $SiMe_3$); δ_C(100 MHz) 207.1 (C(6), quat.), 171.3 (C, quat.), 164.9 (C, quat.), 75.6 (C, quat.), 52.8 (OMe), 51.9 (OMe), 37.7 (Me), 32.1 (CH_2), 30.1 (CH_2) and 1.1 ($SiMe_3$); *m/z* (CI, NH_3) 331 (M + H^+, 40%), 259 (30), 241 (40), 215 (30), 199 (30) and 90 (100) (Found M + H^+: 331.1323. $C_{13}H_{23}N_2O_6Si$ requires *M*, 331.1325). Second to elute was silyl ether **16** (41 mg, 7%); R_f 0.24 (60% Et_2O in light petroleum); ν_{max}/cm^{-1} 3416w, 2958w, 2099s, 1748s, 1707s, 1438m, 1317s, 1252s, 1142s, 849s and 756w; δ_H(400 MHz) 3.75 (3 H, s, OMe), 3.74 (3 H, s, OMe), 3.73 (6 H, s, 2 × OMe), 3.90–3.70 (2 H, m, 2 × CH), 2.20–2.00 (2 H, m, 2 × H of CH_2), 2.00–1.80 (2 H, m, 2 × H of CH_2), 1.70 (2H, br, 2 × OH), 1.60–1.50 (2 H, m, 2 × CH-*H*), 1.50–1.30 (2 H, m, 2 × H of CH_2), 1.18 (6 H, d, *J* 6, 2 × Me) and 0.12 (18 H, s, 2 × $SiMe_3$); δ_C(100 MHz) 171.7 (C, quat.), 171.6 (C, quat.), 165.1 (2 × C, quat.), 76.2 (C, quat.), 76.2 (C, quat.), 67.6 (CH), 67.6 (CH), 52.7 (2 × OMe), 51.9 (2 × OMe), 34.5 (CH_2), 34.4 (CH_2), 33.0 (CH_2), 33.0 (CH_2), 23.6 (2 × Me), 1.22 ($SiMe_3$) and 1.21 ($SiMe_3$); *m/z* (ES) 687 (2 × M + Na^+, 70%), 355 (80), 350 (100), 305 (40), 243 (30) and 215 (40) (Found M + NH_4^+: 350.1746. $C_{13}H_{28}N_3O_6Si$ requires *M*, 350.1747).

From **16**: PCC (144 mg, 0.67 mmol) was added to a stirred solution of silyl ether **16** (147 mg, 0.44 mmol) and NaOAc (1 mg, 0.12 mmol) in CH_2Cl_2 (5 cm^3). After 3 h at 25 ºC, a slurry of silica gel in Et_2O (5 cm^3) was added, the mixture was filtered, evaporated under reduced pressure and purified by column chromatography (20% Et_2O in light petroleum) to give a yellow oil, *ketone* **17** (90 mg, 62%); data as above.

4-(Triethylsilyloxy)-1-(pyrrolidin-1-yl)pentan-1-one 19

TESOTf (1.7 cm^3, 7.5 mmol) was added to a solution of 2,6-lutidine (1.7 cm^3, 15 mmol) in CH_2Cl_2 (30 cm^3) at 0 ºC and the resulting mixture was stirred at 0 ºC for 5 min and then at 25 ºC for 30 min. The mixture was re-cooled to 0 ºC and a solution of alcohol **18**[2] (0.85 g, 5.0 mmol) in CH_2Cl_2 (10 cm^3) was slowly added. After 1 h at 0 ºC, saturated aq. NH_4Cl (20 cm^3) was added and the reaction mixture was extracted with CH_2Cl_2 (3 × 20 cm^3). The combined organic layers were washed with water (20 cm^3), brine (20 cm^3), dried ($MgSO_4$) and evaporated under reduced pressure. Purification of the residue by column chromatography (50% Et_2O in light petroleum) gave a colourless oil, *silyl ether* **19** (1.30 g, 92%); R_f 0.36 (60% Et_2O in light petroleum); ν_{max}/cm^{-1} 2954s, 2912s, 1635s, 1438s, 1136m, 1088m, 1004m and 732s; δ_H(200 MHz) 4.00–3.75 (1 H, m, CH), 3.45–3.35 (4 H, m, 2 × CH_2), 2.50–2.10 (2 H, m, CH_2), 2.00–1.50 (6 H, m, 3 × CH_2), 1.13 (3 H, d, *J* 6, Me), 0.93 (9 H, t, *J* 8, Si(CH_2*Me*)$_3$) and 0.56 (6 H, q, *J* 8.0, Si(C*H*$_2$Me)$_3$); δ_C(50 MHz) 171.3 (C, quat.), 67.5 (CH), 46.3 (CH_2), 45.3 (CH_2), 34.1 (CH_2), 30.5 (CH_2), 25.9 (CH_2), 24.2 (CH_2), 23.6 (Me), 6.6 (Si(CH_2*Me*)$_3$) and 4.7 (Si(C*H*$_2$Me)$_3$); *m/z* (CI, NH_3) 286 (M + H^+, 100%) and 256 (5) (Found M + H^+: 286.2204. $C_{15}H_{32}NO_2Si$ requires *M*, 286.2202).

6-(Triethylsilyloxy)-2-methoxyhept-1-en-3-one 20

From **19**: *t*-BuLi (1.7 mol dm^{-3} in pentane; 0.41 cm^3, 0.69 mmol) was added to a stirred solution of methyl vinyl ether (100 mg, 1.7 mmol) in THF (1 cm^3) at –78 °C. The yellow solution obtained was warmed to 0 °C and stirred at this temperature for 10 min. The mixture was then re-cooled to –78 °C and a solution of silyl ether **19** (40 mg, 0.14 mmol) in THF (2 cm^3) was added. After 7 h at –78 °C, saturated aq. NH_4Cl (1 cm^3) was added. The mixture was allowed to warm to 25 ºC, diluted with Et_2O (1 cm^3) and the layers separated. The aqueous layer was extracted with Et_2O (3 × 1 cm^3), the combined organic layers were washed with water (2 cm^3), brine (2 cm^3), dried ($MgSO_4$) and evaporated under reduced pressure to give a colourless oil, *silyl ether* **20** (35 mg, 92%); data as main text.

Triethylsilyl 4-(triethylsilyloxy)pentanoate 22

TESCl (1.2 cm^3, 7.1 mmol) was added to a solution of sodium 4-hydroxypentanoate[3] (333 mg, 2.37 mmol) and imidazole (0.62 g, 9.2 mmol) in DMF (5 cm^3) and the mixture was then heated at 100 ºC for 24 h. The reaction mixture was then diluted with EtOAc (10 cm^3), washed with water (5 cm^3), brine (5 cm^3), dried ($MgSO_4$) and evaporated under reduced pressure. Purification of the residue by column chromatography (20% Et_2O in light petroleum) gave bis(*silyl ether)* **22** (343 mg, 42%); R_f 0.50 (30% Et_2O in light petroleum); ν_{max}/cm^{-1} 2956s, 2878s, 1712s, 1458m, 1415m, 1239m, 1137m, 1091m, 1004m, 823m and 741s; δ_H(400 MHz) 4.00–3.80 (1 H, m, CH), 2.50–2.40 (2 H, m, CH_2), 1.90–1.70 (2 H, m, CH_2), 1.15 (3 H, t, *J* 6, Me), 0.97 (9 H, t, *J* 8, Si(CH_2*Me*)$_3$), 0.95 (9 H, t, *J* 8, Si(CH_2*Me*)$_3$), 0.59 (6 H, q, *J* 8, Si(C*H*$_2$Me)$_3$) and 0.59 (6 H, q, *J* 8, Si(C*H*$_2$Me)$_3$); δ_C(100 MHz) 178.9 (C, quat.), 67.4 (CH), 34.0 (CH_2), 30.2 (CH_2), 23.6 (Me), 6.8 (Si(CH_2*Me*)$_3$), 6.5 (Si(CH_2*Me*)$_3$), 5.7 (Si(*C*H_2Me)$_3$) and 4.8 (Si(*C*H_2Me)$_3$); *m/z* (CI, NH_3) 347 (M + H^+, 2%), 231 (10), 132 (55) and 118 (100) (Found M + H^+: 347.2428. $C_{17}H_{39}O_3Si_2$ requires *M*, 347.2438).

4-(Triethylsilyloxy)pentanoic acid 23

K_2CO_3 (120 mg, 0.99 mmol) was added to a solution of bis(silyl ether) **22** (194 mg, 0.56 mmol) in MeOH:THF:H_2O (3 cm^3: 0.7 cm^3: 0.7 cm^3) at 25 ºC. After 30 min, the solution was concentrated under reduced pressure, the residue was neutralised with 1 M $KHSO_4$, and then diluted with Et_2O (5 cm^3). The layers were separated and the aqueous layer extracted with Et_2O

(3×5 cm^3). The combined organic layers were washed with water (3 cm^3), brine (3 cm^3), dried ($MgSO_4$) and evaporated under reduced pressure. Purification of the residue by column chromatography (40% Et_2O in light petroleum) gave a colourless oil, *acid* **23** (93 mg, 71%); R_f 0.58 (50% Et_2O in light petroleum); ν_{max}/cm^{-1} 2957s, 2858s, 1712s, 1457m, 1415m, 1378m, 1137s, 1190s, 1107s and 742s; δ_H(400 MHz) 3.92–3.86 (1 H, m, CH), 2.47–2.42 (2 H, m, CH_2), 1.80–1.70 (2 H, m, CH_2), 1.17 (3 H, t, *J* 6, Me), 0.96 (9 H, t, *J* 8, Si(CH_2*Me*)$_3$) and 0.60 (6 H, q, *J* 8, Si(C*H*$_2$Me)$_3$); δ_C(100 MHz) 179.4 (C, quat.), 67.4 (CH), 34.0 (CH_2), 30.3 (CH_2), 23.6 (Me), 6.8 (Si(CH_2*Me*)$_3$) and 4.8 (Si(*C*H_2Me)$_3$).

6-Triethylsilyloxy-2-(triphenyl-λ^5-phosphoranylidene)-3-oxoheptanenitrile 24

A solution of (triphenylphosphoranylidene)acetonitrile (220 mg, 0.94 mmol) in CH_2Cl_2 (2 cm^3) was added to a solution of acid **23** (100 mg, 0.43 mmol), DMAP (5 mg, 0.04 mmol) and EDCI (132 mg, 0.68 mmol) in CH_2Cl_2 (5 cm^3) at 0 ºC. The reaction mixture was stirred at 0 ºC for 30 min and then allowed to warm to 25 ºC. After 1.5 h, water (5 cm^3) was added, the layers separated and the organic layer dried ($MgSO_4$) and evaporated under reduced pressure. Purification of the residue by column chromatography (20% EtOAc in light petroleum) gave *phosphoranylidene* **24** (111 mg, 50%); R_f 0.35 (40% EtOAc in light petroleum); ν_{max}/cm^{-1} 3436m, 2956m, 2875m, 2174s, 1584s, 1438s, 1178w, 1108s, 1000m, 719s and 691s; δ_H(400 MHz) 7.70–7.40 (15 H, m, 3 × Ph), 3.90–3.80 (1 H, m, CH), 2.85–2.65 (2 H, m, CH_2), 1.80–1.75 (2 H, m, CH_2), 1.17 (3 H, d, *J* 6, Me), 0.96 (9 H, t, *J* 8, Si(CH_2*Me*)$_3$) and 0.60 (6 H, q, *J* 8, Si(C*H*$_2$Me)$_3$); δ_C(100 MHz) 197.0 (C(3), quat., d, *J* 3.5), 133.5 (6 × ArCH, d, *J* 10) 133.0 (3 × ArCH, d, *J* 3), 129.0 (6 × ArCH, d, *J* 13), 123.3 (3 × ArC, quat., d, *J* 93.5), 68.0 (CH), 35.9 (C(4)H_2, d, *J* 7), 34.9 (C(3)H_2), 23.8 (Me), 6.9 (Si(CH_2*Me*)$_3$) and 4.9 (Si(*C*H_2Me)$_3$); *m/z* (ES) 516 (M + H$^+$, 25%), 263 (100), 187 (90) and 132 (50) (Found M + H$^+$: 516.2479. $C_{31}H_{39}NO_2PSi$ requires *M*, 516.2487).

Methyl-5-(triethylsilyloxy)-2-oxohexanoate 21

From **24**: A mixture of O_3/O_2 was bubbled through a solution of the phosphonoranylidene **24** (100 mg, 0.19 mmol) and pyridine (0.5 cm^3) in CH_2Cl_2 (2 cm^3) and MeOH (2 cm^3) at –78 °C. After 30 min, the stream of O_3/O_2 was stopped and argon was bubbled through for 10 min. and the reaction mixture allowed to warm to 25 ºC and then evaporated under reduced pressure. Purification of the residue by column chromatography (5% Et_2O in light petroleum) gave a colourless oil, *α-ketoester* **21** (18 mg, 34%); data as main text.

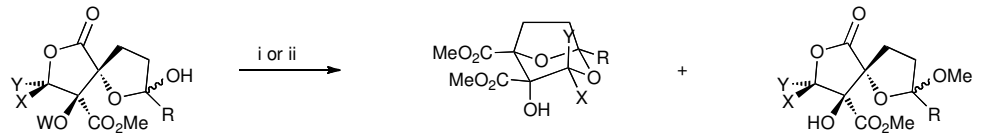
Trimethyl (1*R,2*S**,5*R**,7*R**) 5-methyl-2-trimethylsilyloxy-6,8-dioxabicyclo[3.2.1]octane-1,2,7-tricarboxylate 29**

$Rh_2(OAc)_4$ (cat.) was added to a stirred solution of diazoester **17** (298 mg, 0.9 mmol) in toluene (1 cm^3) and freshly distilled methyl glyoxylate[4] (119 mg, 1.35 mmol) at 110 °C. After 30 min, the reaction mixture was cooled, diluted with Et_2O (3 cm^3), filtered through Celite® and evaporated under reduced pressure. ^{1}H NMR analysis indicated 3 cycloadduct isomers in a ratio 8:1:1, based on the bridge methine singlets (δ_H 5.48, 4.92 and 4.59). Purification of the residue by column chromatography (gradient elution: 10% Et_2O in light petroleum to 20% Et_2O in light petroleum) gave the *cycloadduct* **29** as a colourless oil [two fractions: 167 mg (ratio, 10:0:1) and 23 mg (ratio 1.4:1:0), 54% combined yield]. Data for major fraction: R_f 0.37 (50% Et_2O in light petroleum); ν_{max}/cm^{-1} 2955m, 1753s, 1438m, 1291s, 1204s, 1098s, 844s and 755w; δ_H(500 MHz) (data for major isomer) 5.48 (1 H, s, CH), 3.79 (3 H, s, OMe), 3.69 (3 H, s, OMe), 3.66 (3 H, s, OMe), 2.38 (1 H, ddd, *J* 14, 12 and 6, H*endo* of C(3)H_2), 1.85 (1 H, ddd, *J* 13, 13 and 5, H of

$C(4)H_2$), 1.75 (1 H, ddd, *J* 14, 5 and 1.5, H of CH_2), 1.69 (1 H, ddd, *J* 13, 6 and 1.5, H of CH_2), 1.64 (3 H, s, Me) and 0.11 (9 H, s, $SiMe_3$) [discernible data for minor isomer: 4.59 (1 H, s, CH), 3.79 (3 H, s, OMe), 3.70 (3 H, s, OMe), 3.69 (3 H, s, OMe), 2.70 (1 H, ddd, *J* 14.5, 12 and 6.5, H of CH_2), 1.57 (3 H, s, Me) and 0.10 (9 H, s, $SiMe_3$)]; ^{1}H NMR NOE experiment: irradiation at δ 5.48 saw enhancements at 3.79 (1%), at 3.66 (1.2%) and at 2.38 (6%); δ_C(100 MHz) (data for major isomer) 173.0 (C, quat.), 169.4 (C, quat.), 166.5 (C, quat.), 110.2 (C(5), quat.), 90.2 (C(1), quat.), 77.3 (CH), 77.2 (C(2), quat.), 52.6 (OMe), 52.4 (OMe), 52.4 (OMe), 30.7 ($C(4)H_2$), 29.7 ($C(3)H_2$), 23.7 (Me) and 1.9 ($SiMe_3$) [discernible data for minor isomer: 79.3 (CH)]; *m/z* (CI, NH_3) 408 (M + NH_4^+, 98%), 391 (100) 90 (35) (Found M + H^+: 391.1418. $C_{16}H_{27}O_9Si$ requires *M,* 391.1424).

b. Discussion of structural assignment of spirolactones 34

The two minor less polar compounds isolated from the acid-catalysed rearrangement of cycloadduct alcohol **31** in MeOH are tentatively assigned as a mixture of diastereomeric spirolactones **34**. In the acid-catalysed rearrangement of spirolactones **S1**-**S3** in MeOH to give 2,8-dioxabicyclo[3.2.1]octanes **S4-S6** by Martin and co-workers in their total synthesis of 6,7-dideoxysqualestatin H5 (**2**), structurally closely related spirolactones **S7**-**S9** were observed (Scheme ES1).[5]



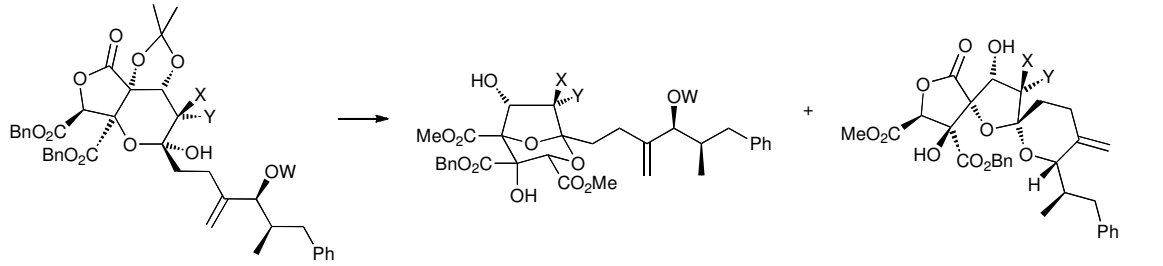
S1 X = $CH_2OTBDMS$, Y = H, W = TMS, R = Me
S2 X = $CH_2OTBDMS$, Y = H, W = TMS, R = full side-chain of **2**
S3 X = H, Y = CO_2Me, W = H, R = H

S4 X = CH_2OH, Y = H, R = Me
S5 X = CH_2OH, Y = H, R = full side-chain of **2**
S6 X = H, Y = CO_2Me, R = H

S7 X = CH_2OH, Y = H, R = Me
S8 X = CH_2OH, Y = H, R = full side-chain of **2**
S9 X = H, Y = CO_2Me, R = H

Scheme ES1[1] *Reagents and conditions:* i, 0.1 M H_2SO_4, MeOH (from **S1**, **S4** : **S7** 1 : 2; 79%; from **S2**, **S5** : **S8** 1 : 2.6; 90%)
ii, HCl, MeOH (from **S3, S6** : **S9** 0 : 1; quant.)

Also, while Nicolaou and co-workers found that lactone **S10** underwent acid-catalysed rearrangement to give the 2,8-dioxabicyclo[3.2.1]octane **S12** in their relay synthesis of zaragozic acid A (**1**), the differentially protected and C7 epimer (zaragozic acid numbering) **S11** gave a product tentatively assigned as spiroketal **S15** (Scheme ES2).[6]



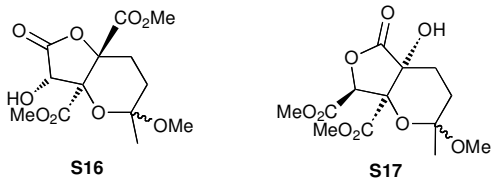
S10 X = OH, Y = H, W = DTBMS
S11 X = H, Y = OH, W = TBDPS

S12 X = OH, Y = H, W = DTBMS (from **S10**, 45%)
S13 X = H, Y = OH, W = H or TBDPS (from **S11**, 0%)

S14 X = OH, Y = H (from **S10**, -%)
S15 X = H, Y = OH (from **S11** yield not given, only product noted)

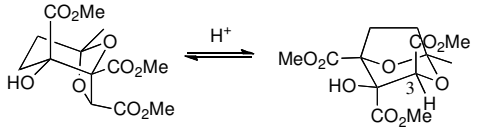
Scheme ES2[2] *Reagents and conditions:* 2% HCl, MeOH

Despite the above precedents, two other lactones **S16** and **S17** are, in principle, possible structures for the minor by-product of the rearrangement reaction. Strain due to *trans*-fusion makes **S16** a less likely candidate. For the minor by-product, the observed ^3J of 8.0 Hz compares well to that found for **S9** by Martin[5] (^3J of 8.1 Hz); however, lactone **S17** is less easily ruled out, as the *cis*-fusion would likely force the 6-membered ring into a twist-boat conformation from which a $^3J_{ax\text{-}eq}$ of 8 Hz would not be unreasonable.



S16 **S17**

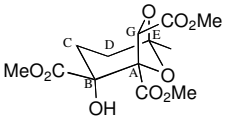
c. Structures arising from opposite facial selectivity in cycloaddition



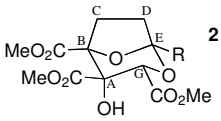
S18 **S19**

In 2,8-dioxabicyclo[3.2.1]octane **S19**, NOE enhancements between the H-3 and the 5-membered ring protons would not be expected.

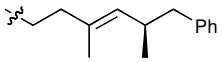
d. Comparison of ^{1}H and ^{13}C NMR data of bicyclic alcohols 31 and 33 with 6,7-dideoxysqualestatin H5 (2)



31



2 Me = H, R =



33 R = Me

Table ES1. Comparison of ^{1}H NMR data.

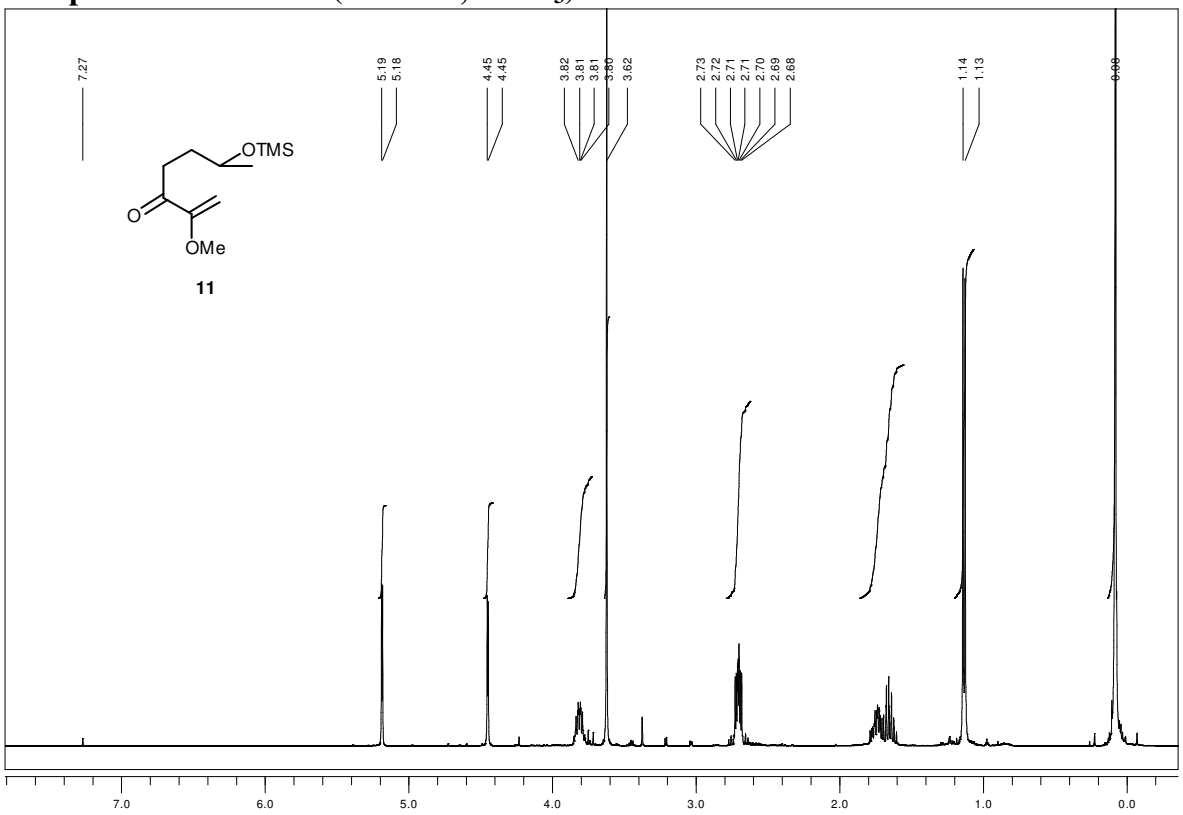
Position no.	**31**	**2**[7]	**33**
G	5.47s	4.87s	4.92s
C	2.32ddd	3.18m	3.15ddd
	1.87-1.74m	2.08-1.98m	2.18-2.05m
D	1.99ddd	2.08-1.98m	2.25ddd
	1.87-1.74m		2.18-2.05m

Table ES2. Comparison of ^{13}C NMR data.

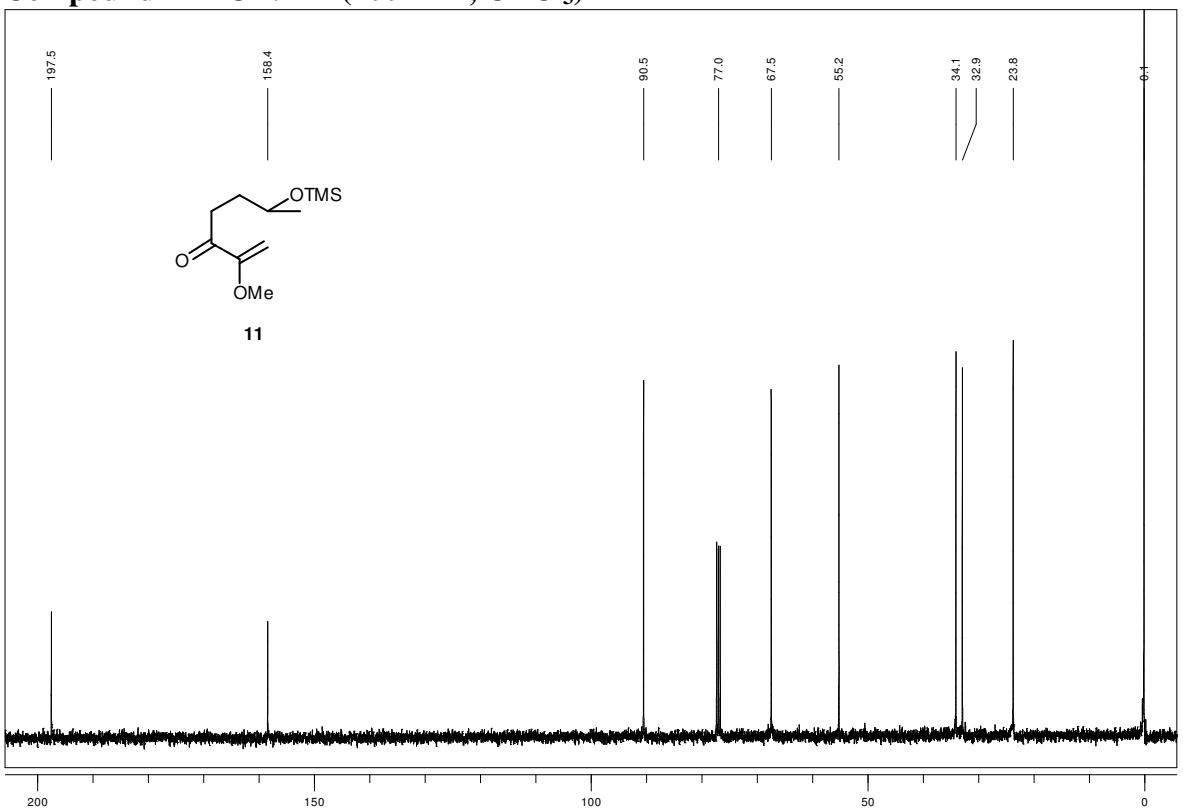
C atom	**31**	**2**[3]	**33**
E	111.0	109.8	107.6
A	89.4	76.0	74.9
G	77.6	75.7	74.9
B	73.7	89.3	88.3
D	30.8	32.0	32.8
C	29.6	30.3	29.4

e. ^{1}H and ^{13}C NMR Spectra

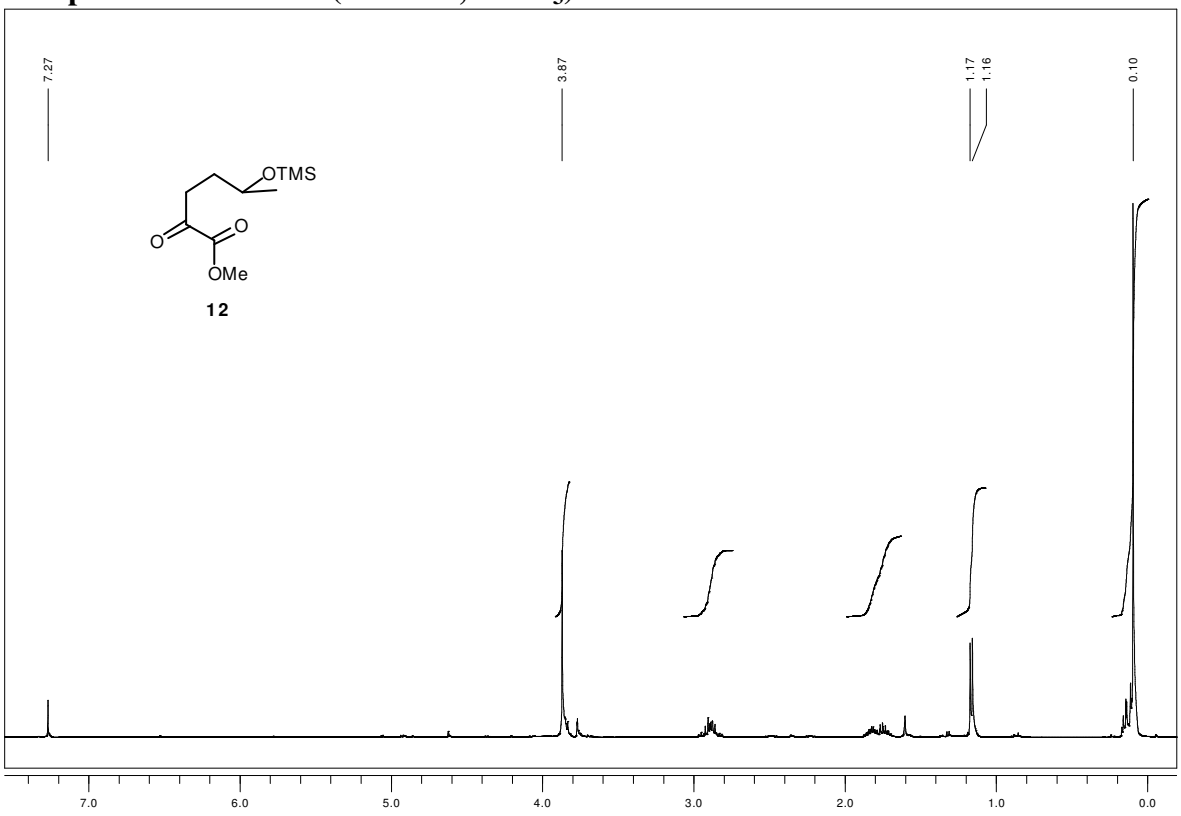
Compound 11 ^{1}H NMR (400MHz, $CDCl_3$)



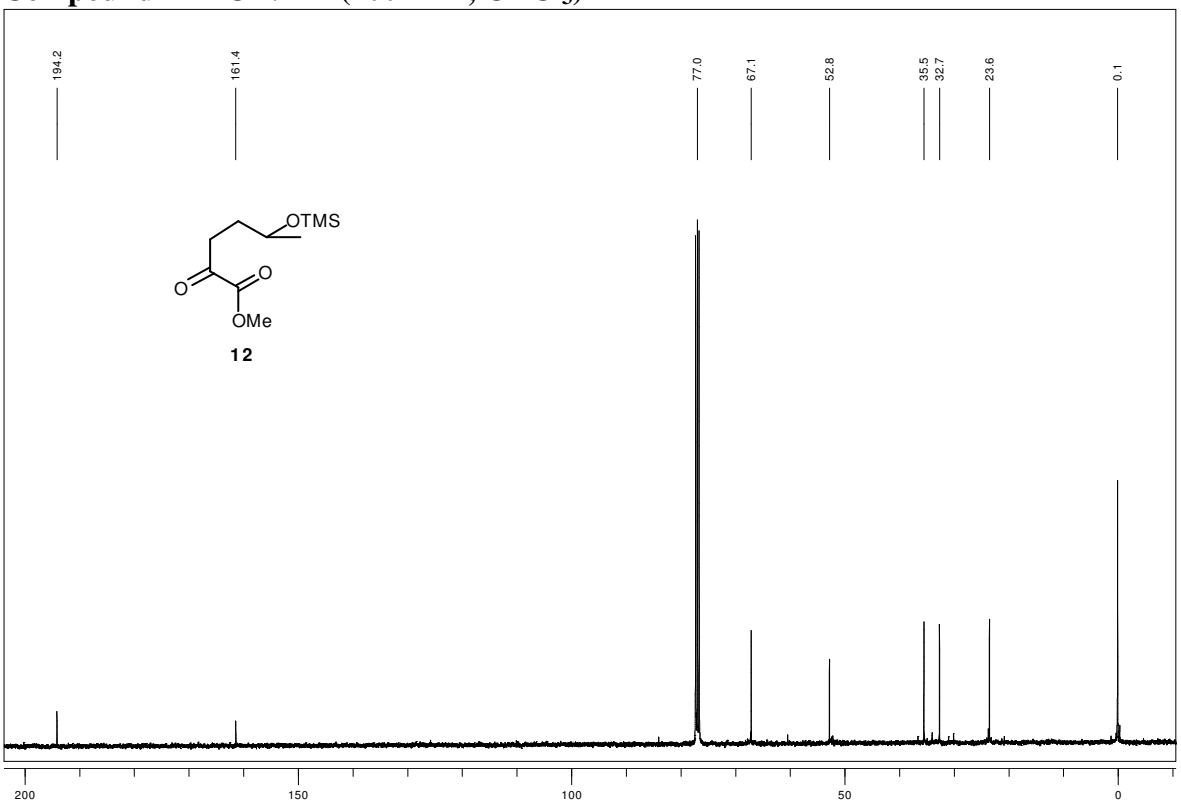
Compound 11 ^{13}C NMR (100MHz, $CDCl_3$)



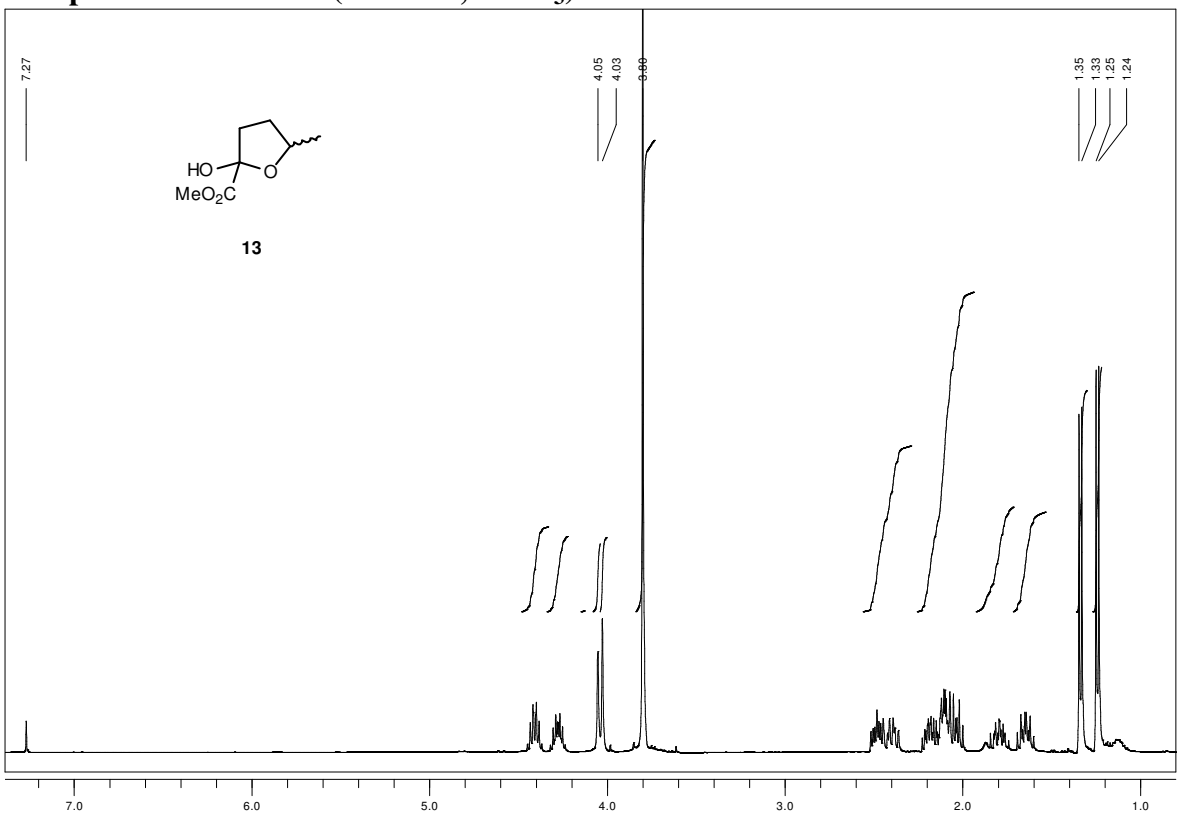
Compound 12 ^{1}H NMR (400MHz, $CDCl_3$)



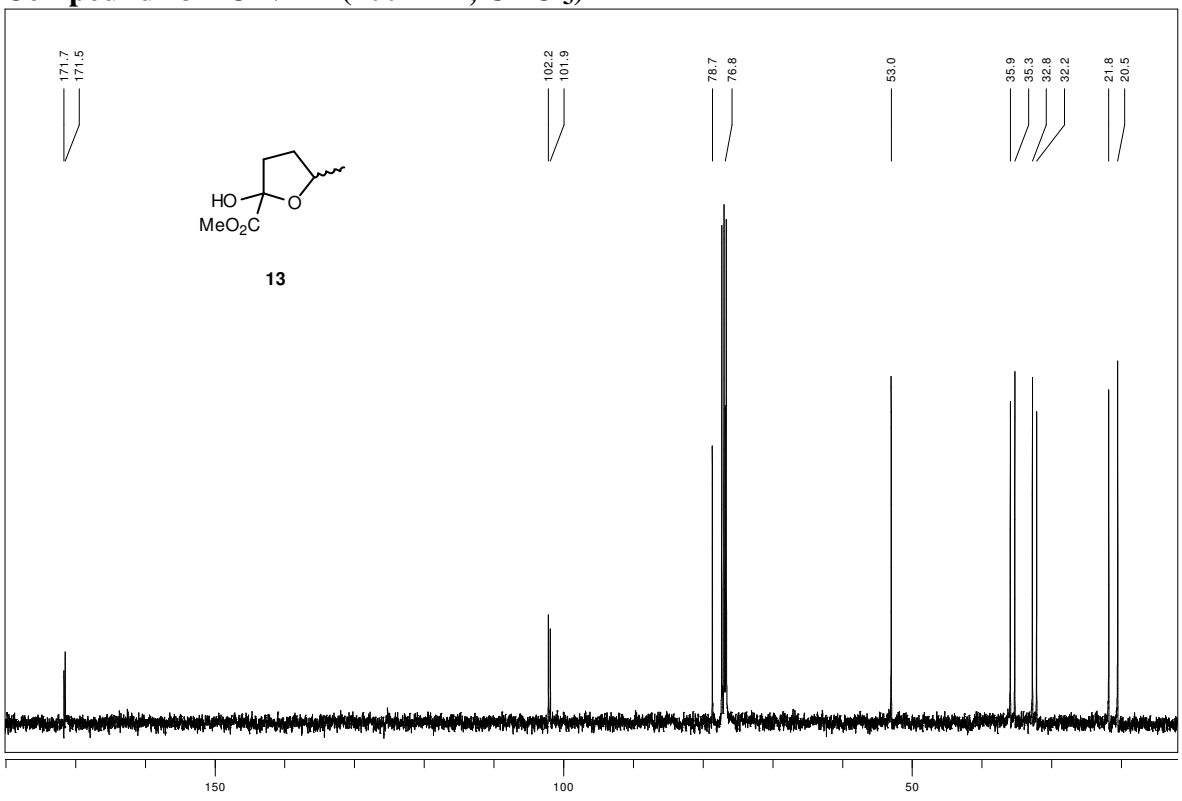
Compound 12 ^{13}C NMR (100MHz, $CDCl_3$)



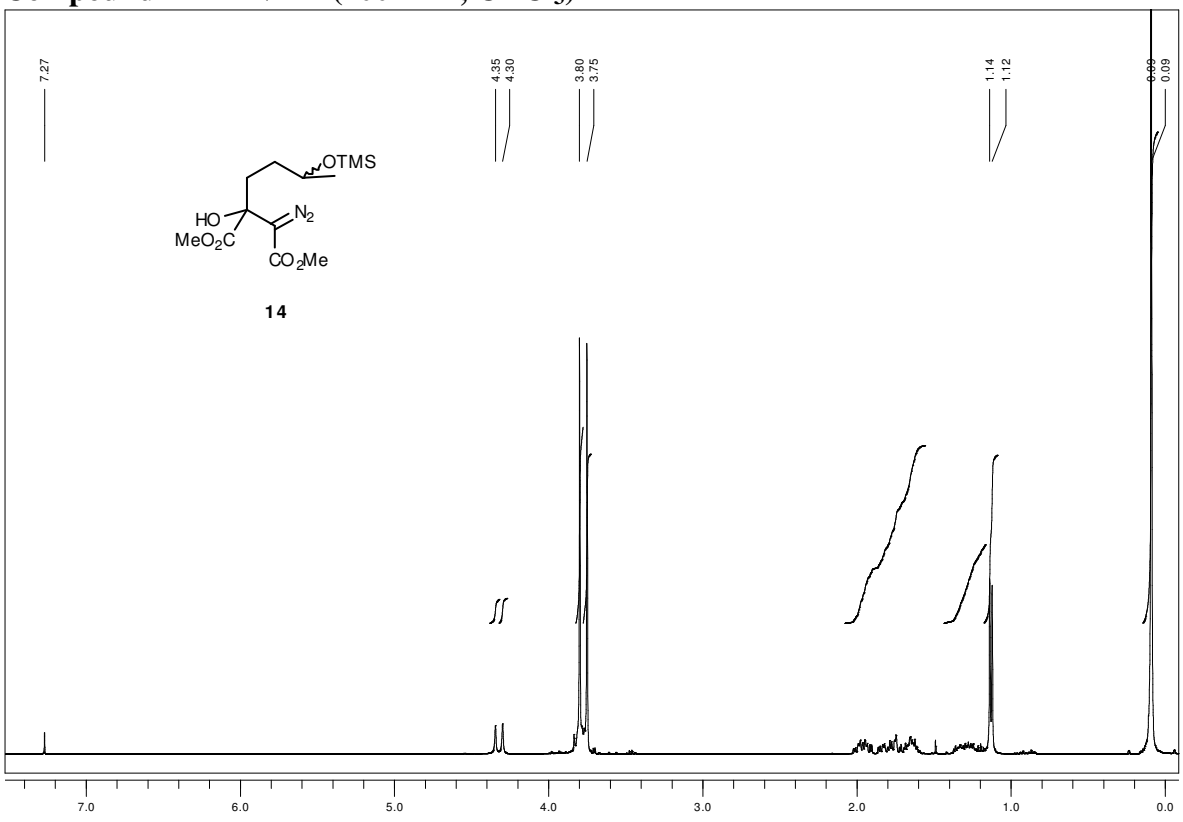
Compound 13 ^{1}H NMR (400MHz, $CDCl_3$)



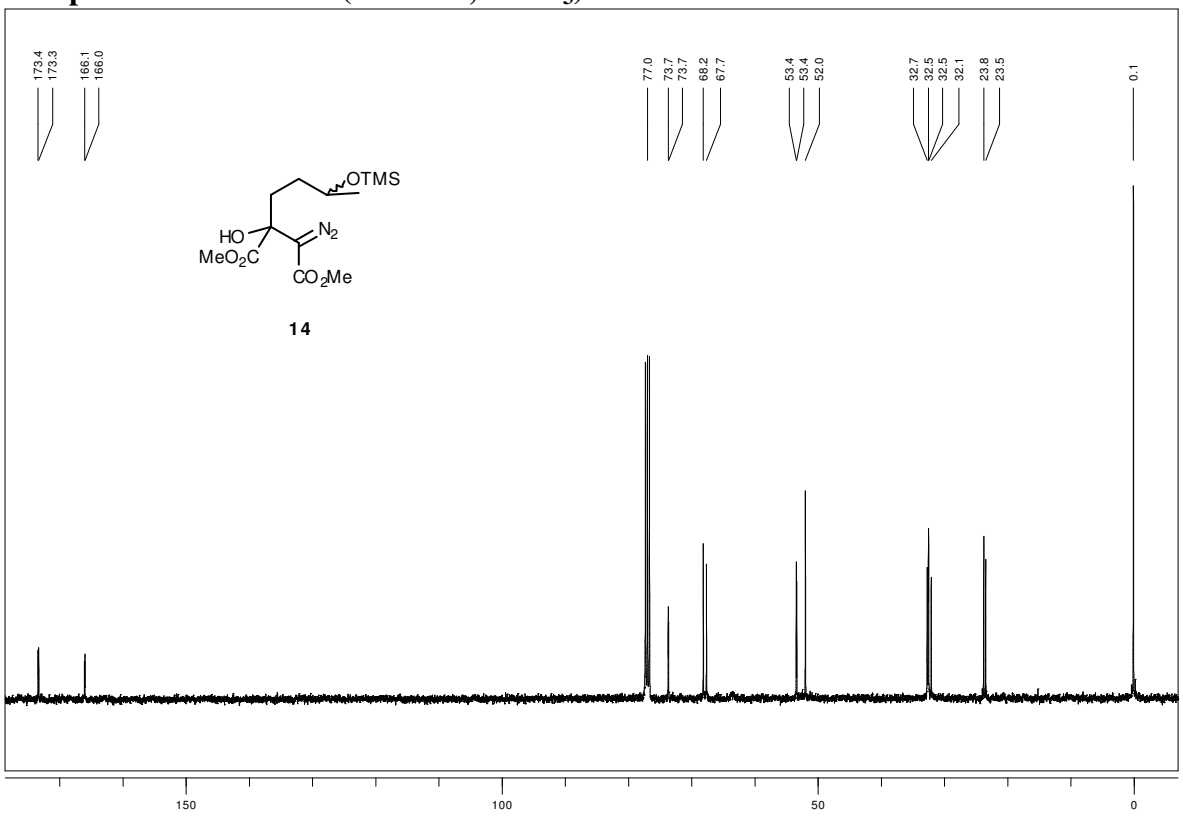
Compound 13 ^{13}C NMR (100MHz, $CDCl_3$)



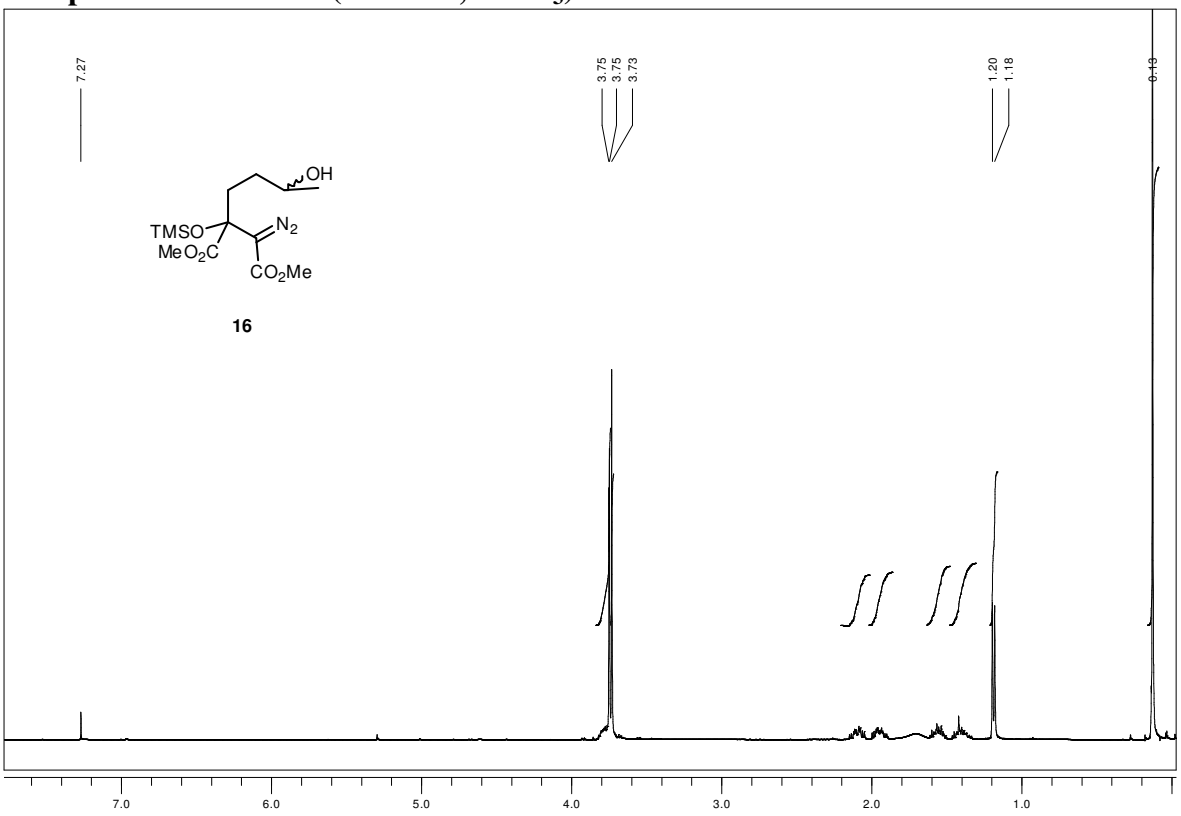
Compound 14 ^{1}H NMR (400MHz, $CDCl_3$)



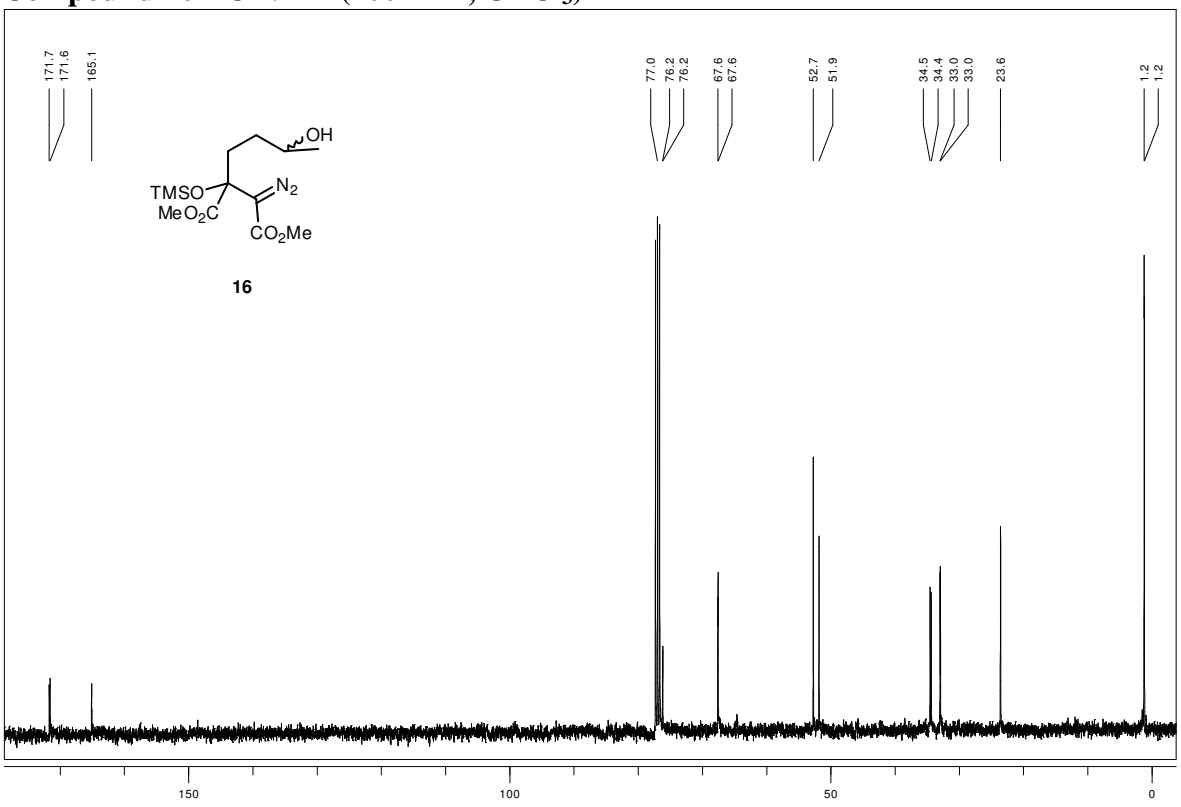
Compound 14 ^{13}C NMR (100MHz, $CDCl_3$)



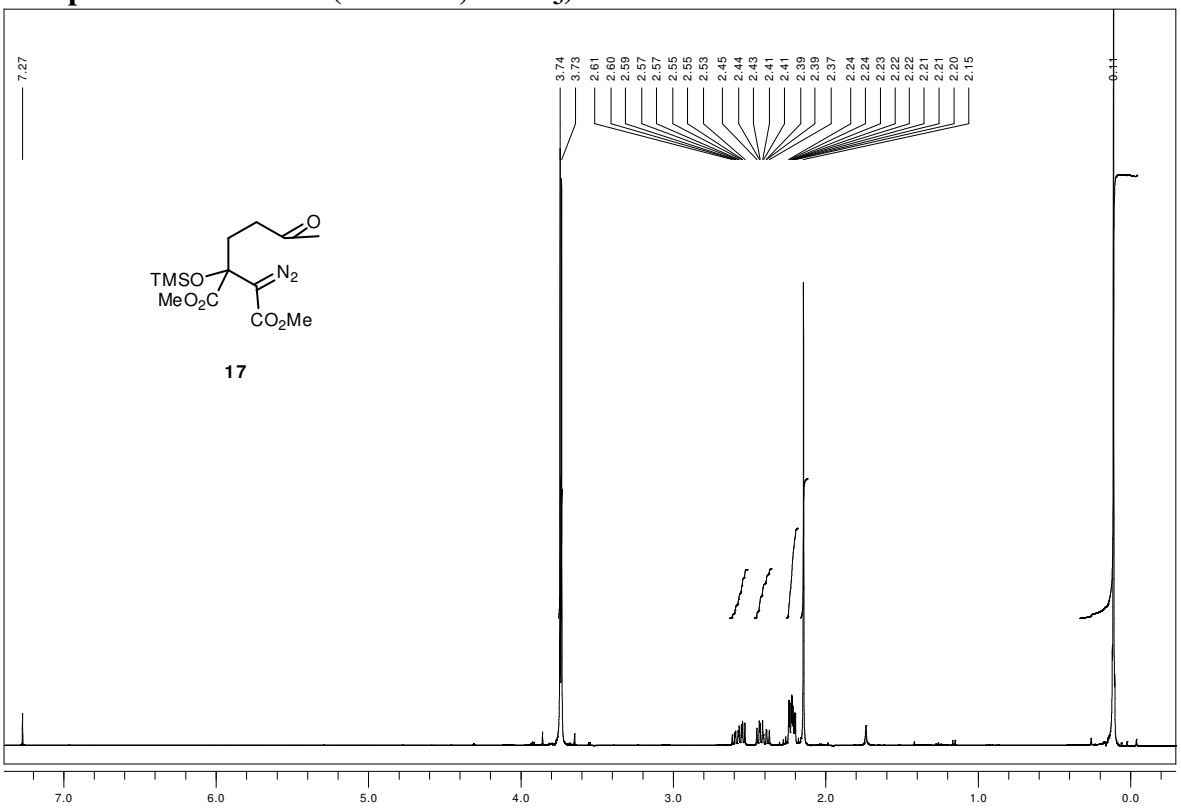
Compound 16 ^{1}H NMR (400MHz, $CDCl_3$)



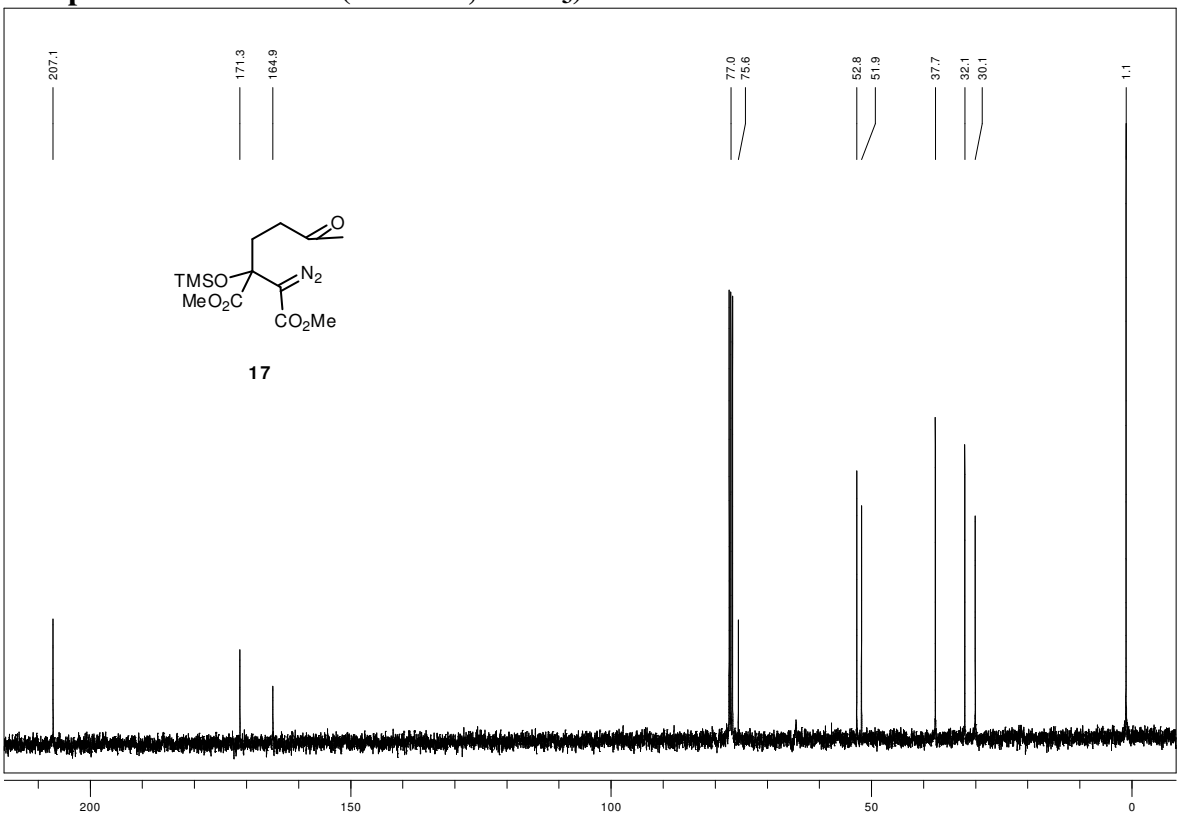
Compound 16 ^{13}C NMR (100MHz, $CDCl_3$)



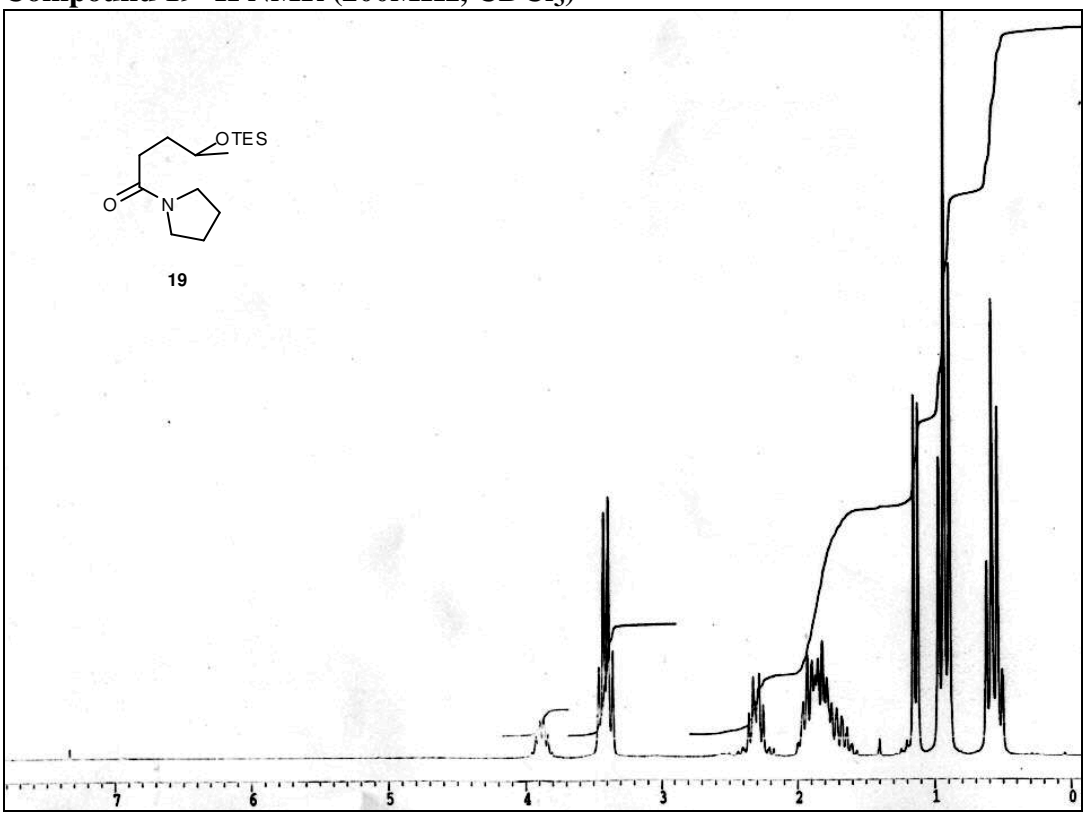
Compound 17 ^{1}H NMR (400MHz, $CDCl_3$)



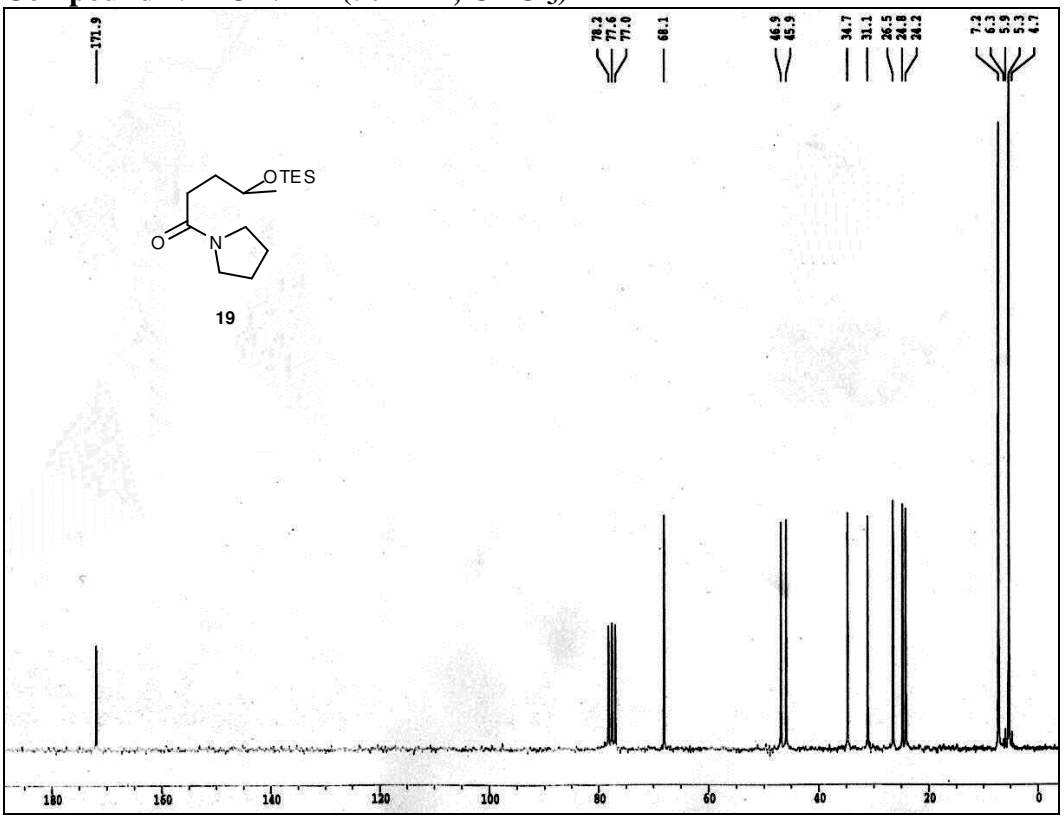
Compound 17 ^{13}C NMR (100MHz, $CDCl_3$)



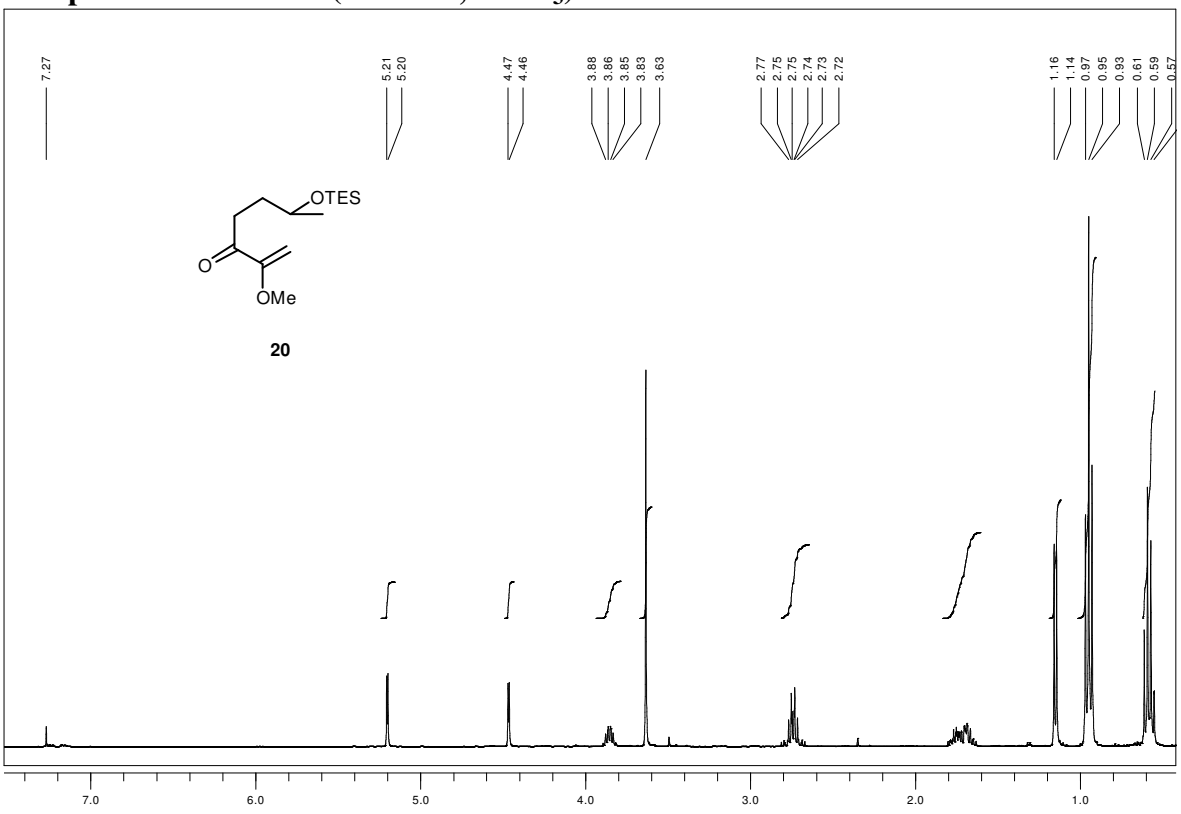
Compound 19 ^{1}H NMR (200MHz, $CDCl_3$)



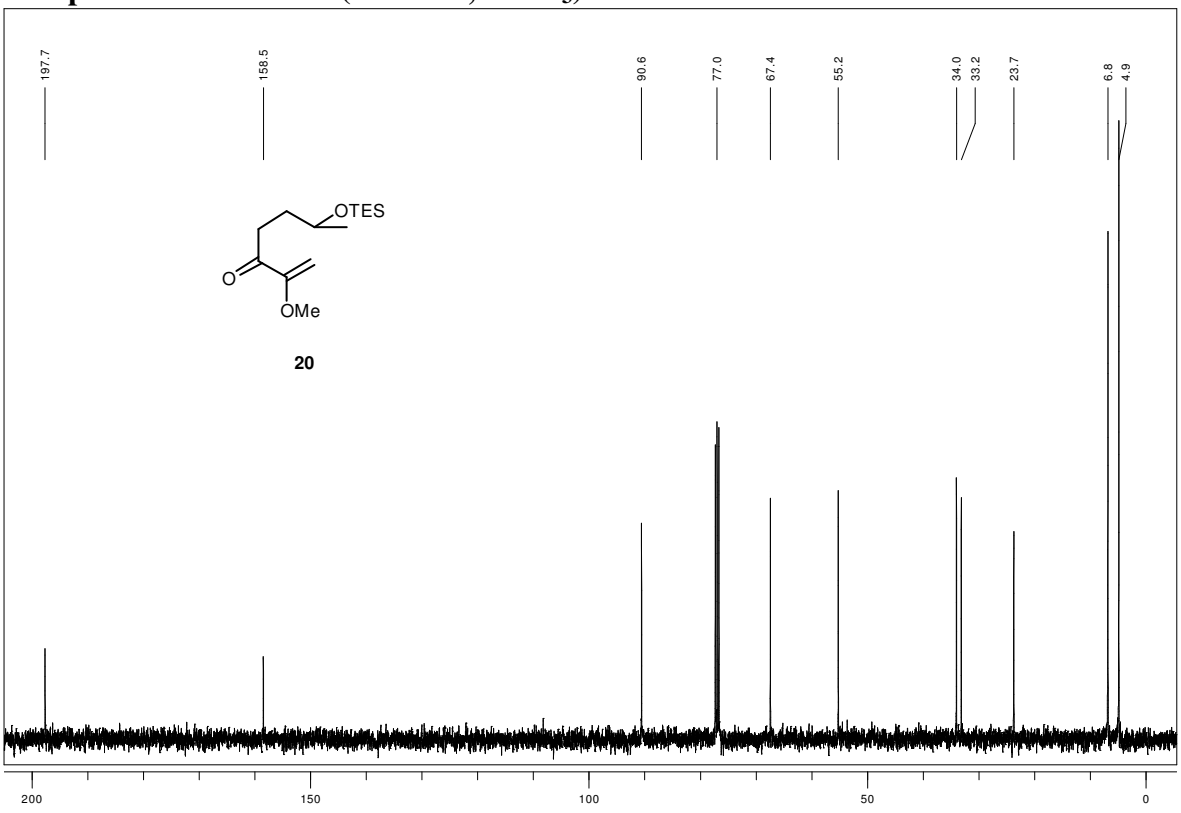
Compound 19 ^{13}C NMR (50MHz, $CDCl_3$)



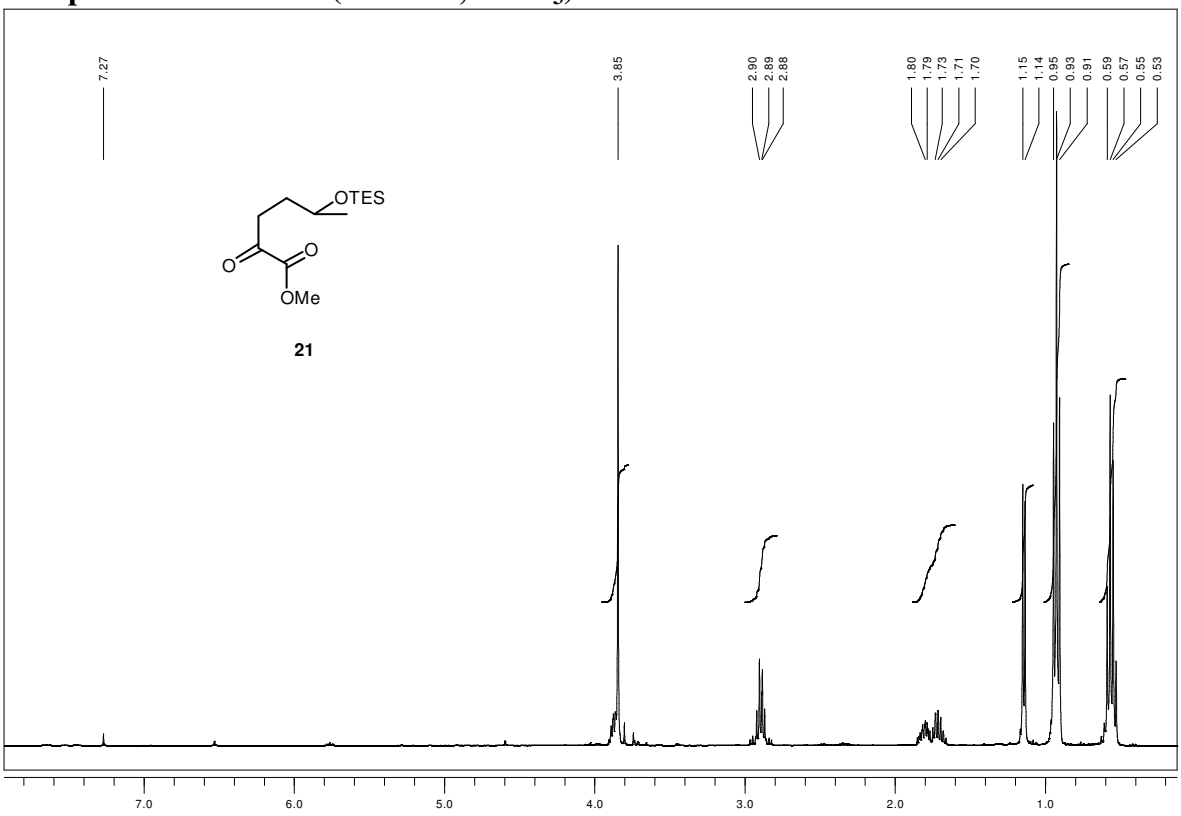
Compound 20 ^{1}H NMR (400MHz, $CDCl_3$)



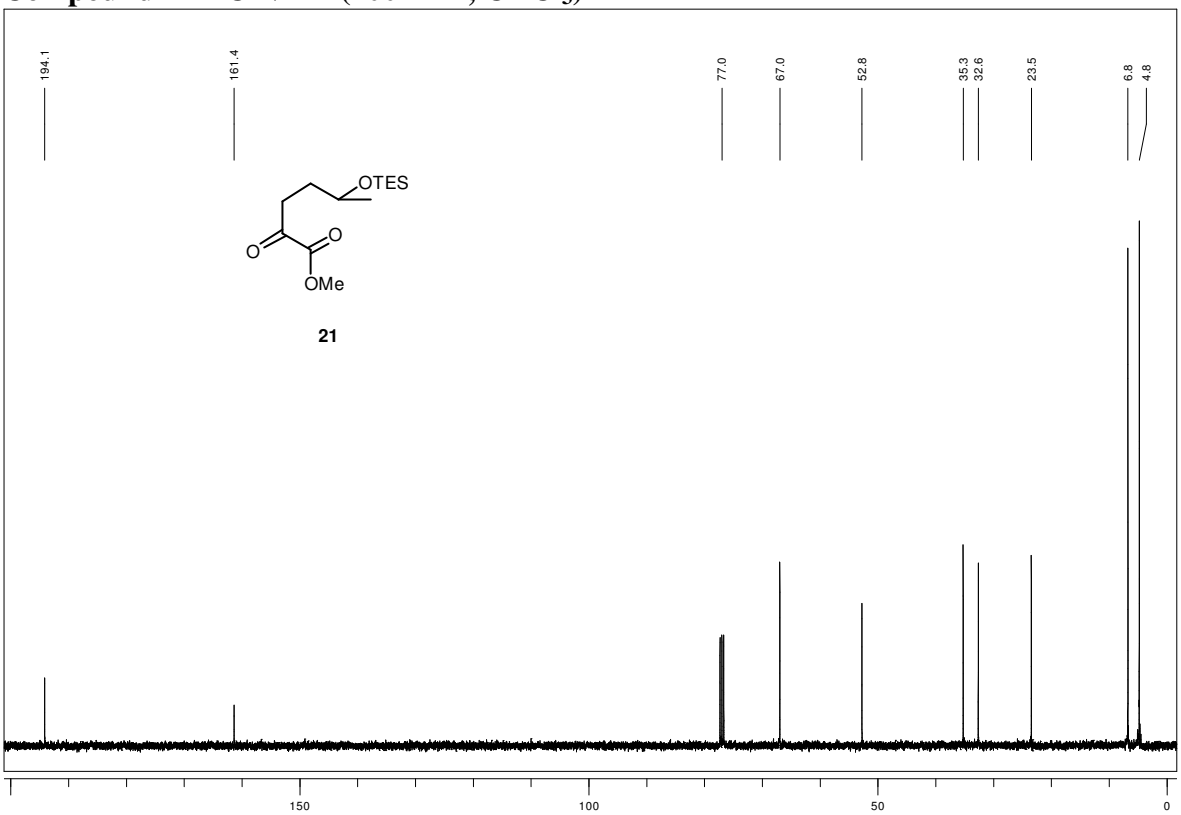
Compound 20 ^{13}C NMR (100MHz, $CDCl_3$)



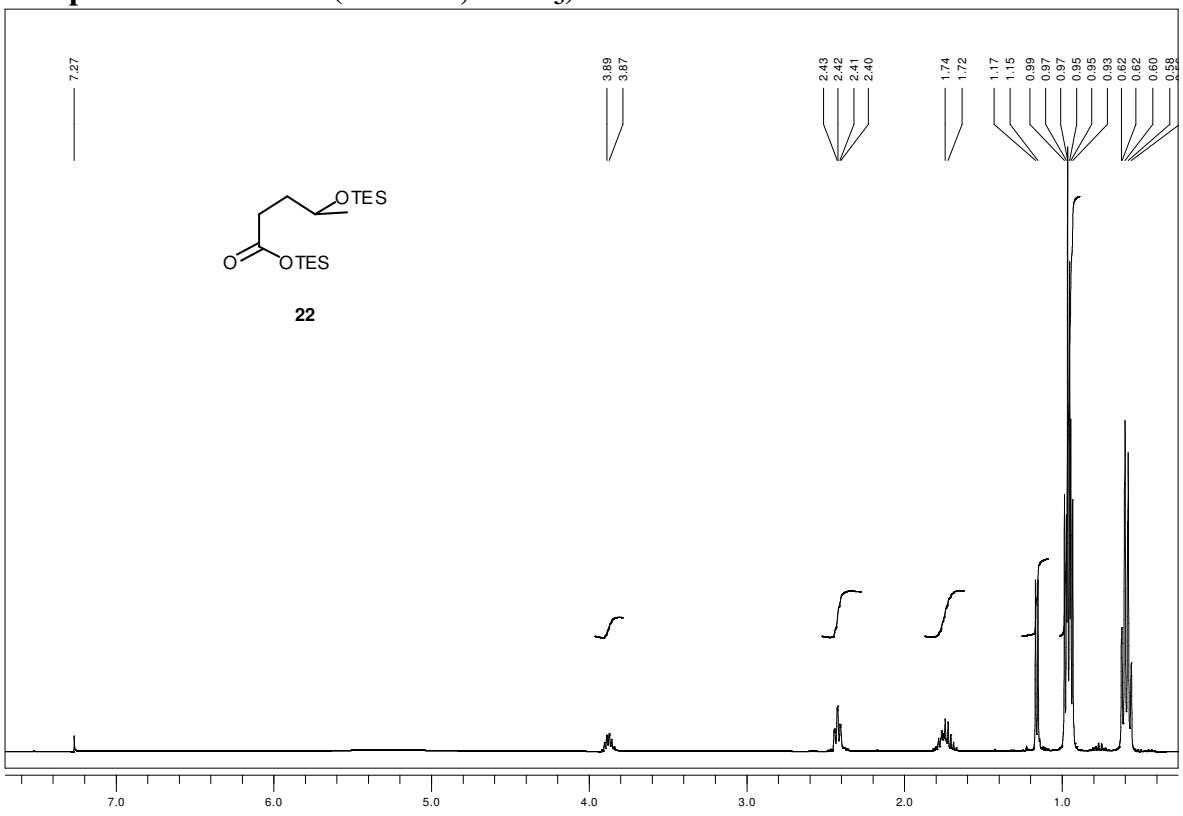
Compound 21 ^{1}H NMR (400MHz, $CDCl_3$)



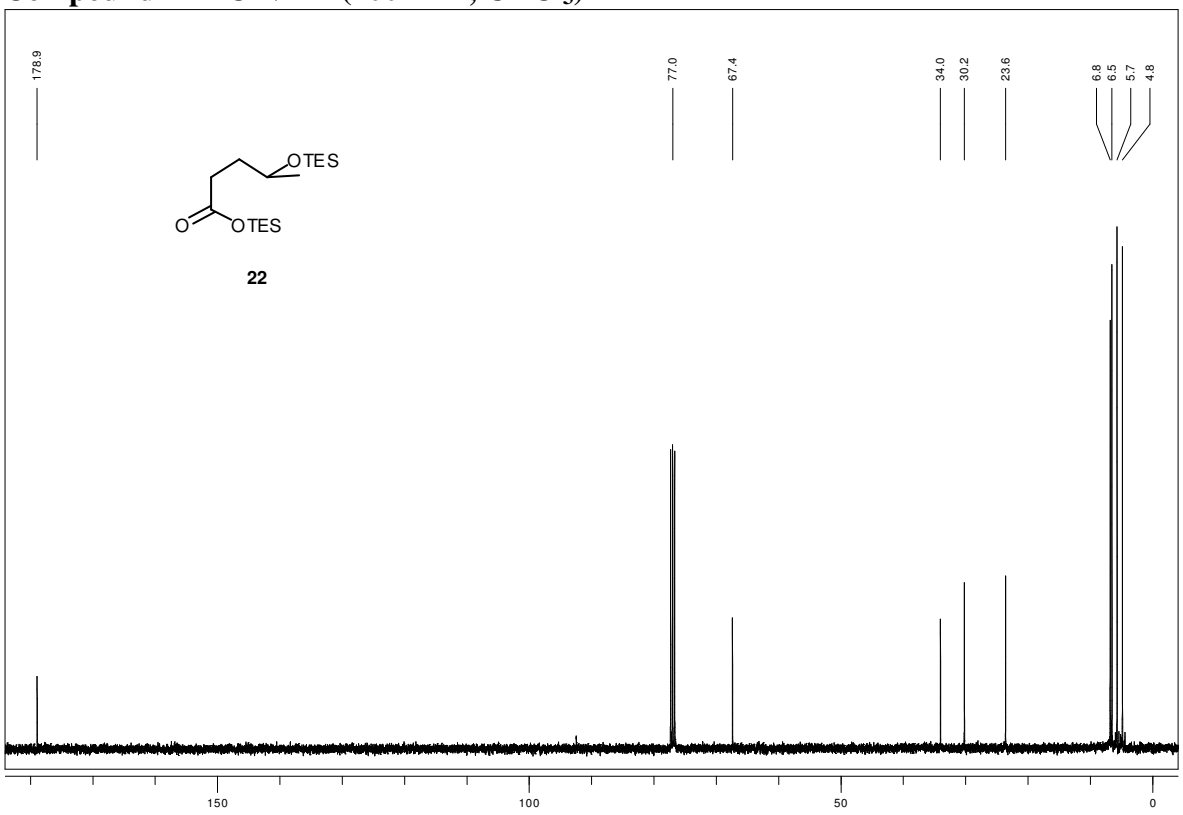
Compound 21 ^{13}C NMR (100MHz, $CDCl_3$)



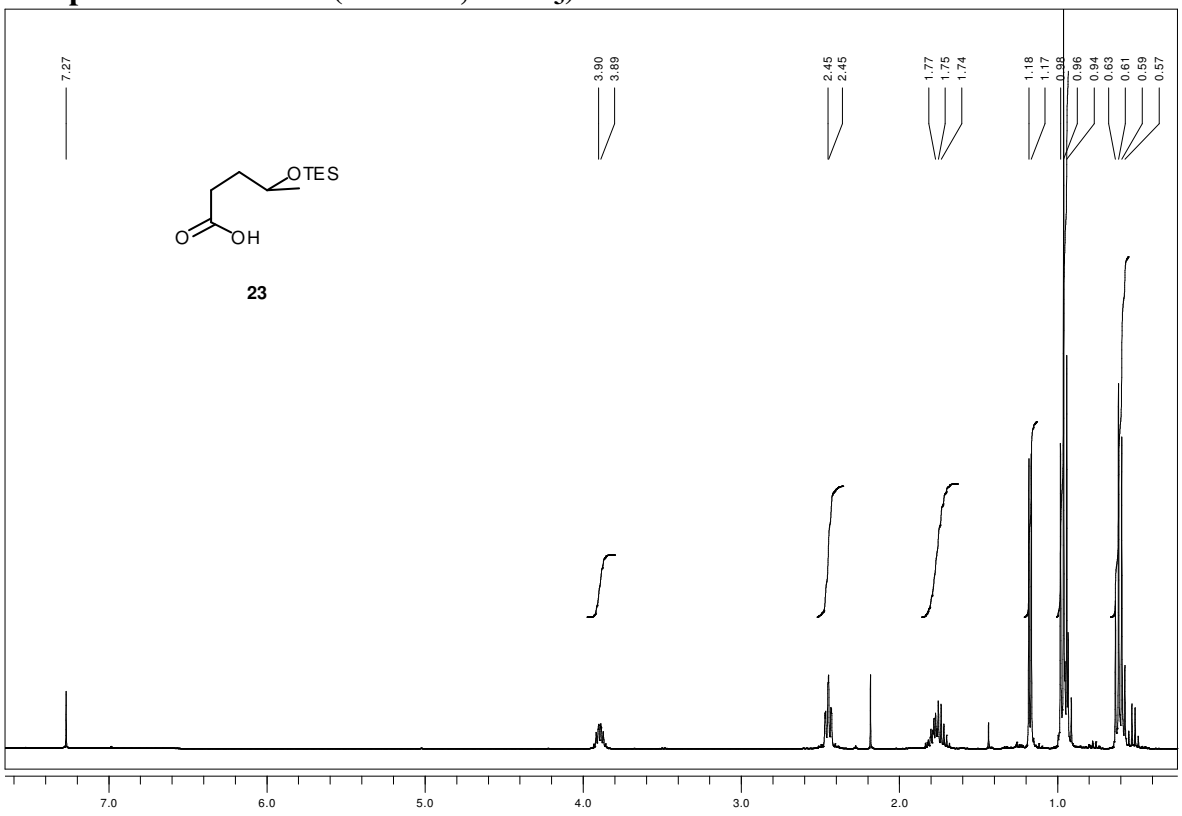
Compound 22 ^{1}H NMR (400MHz, $CDCl_3$)



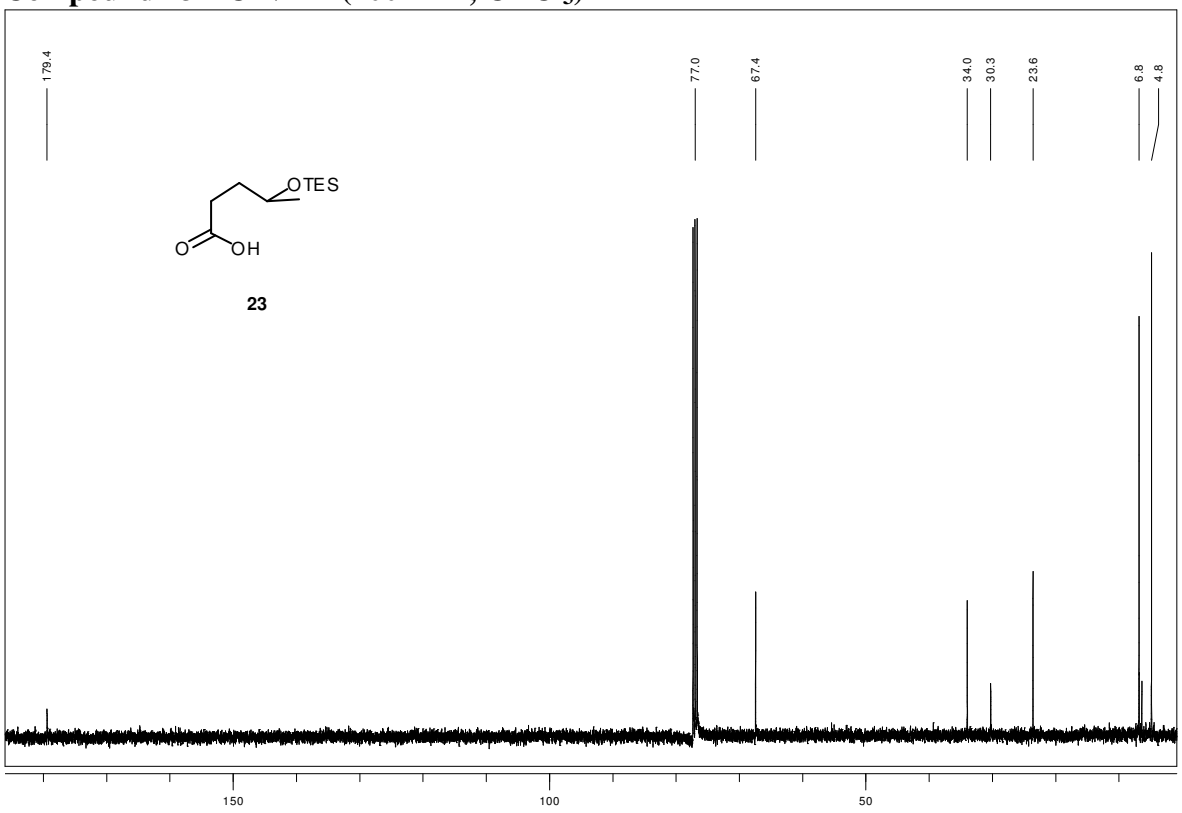
Compound 22 ^{13}C NMR (100MHz, $CDCl_3$)



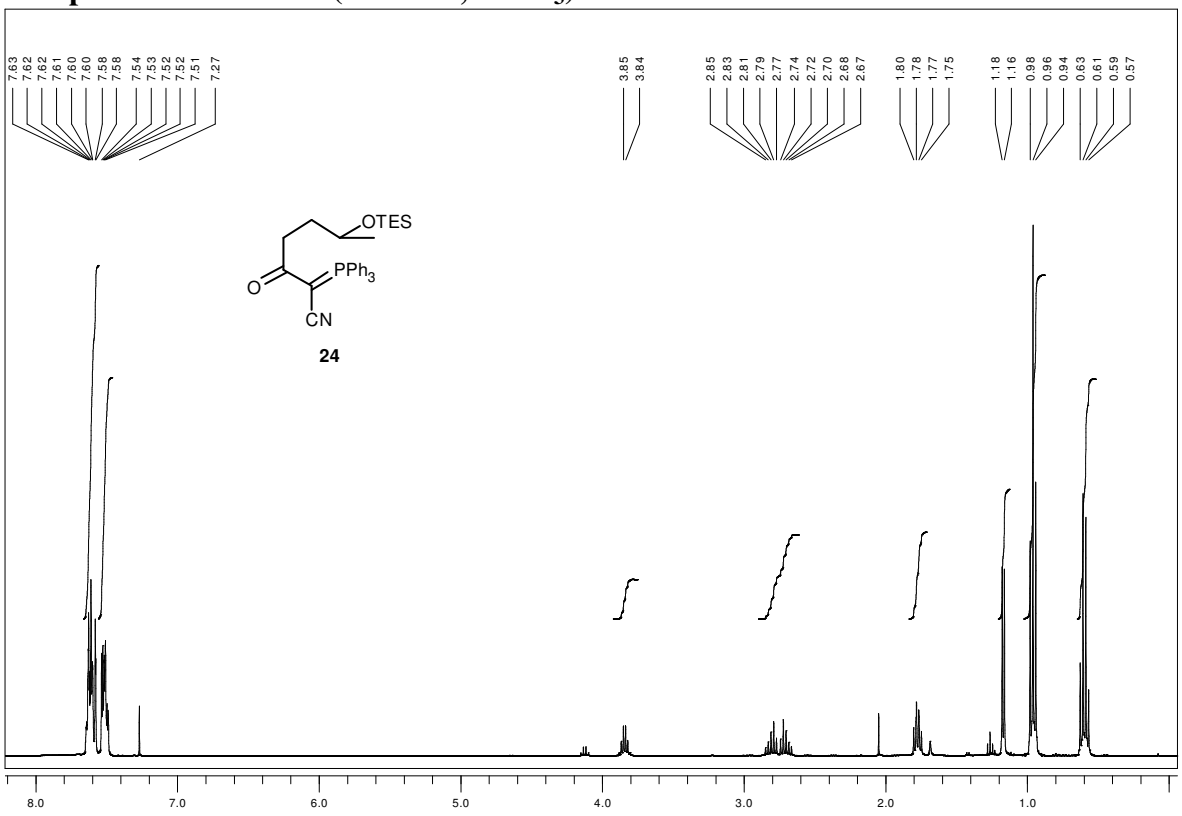
Compound 23 ^{1}H NMR (400MHz, $CDCl_3$)



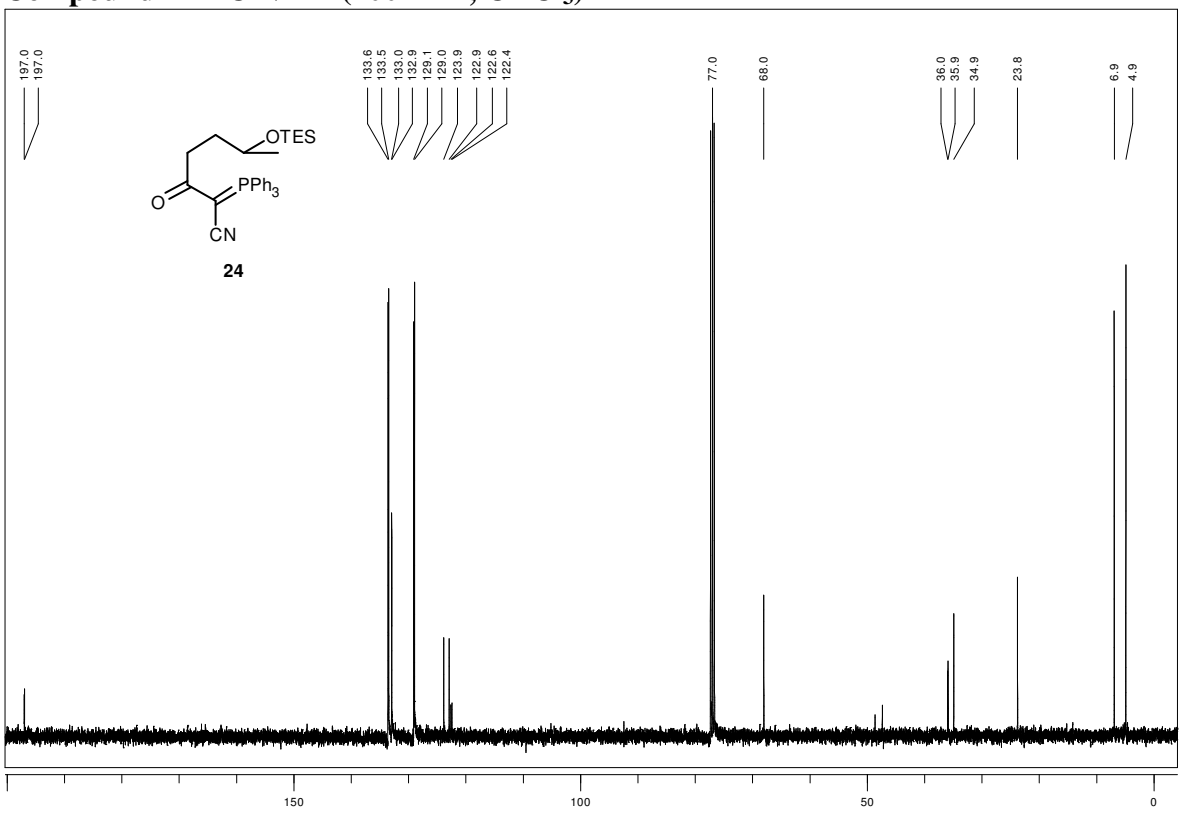
Compound 23 ^{13}C NMR (100MHz, $CDCl_3$)



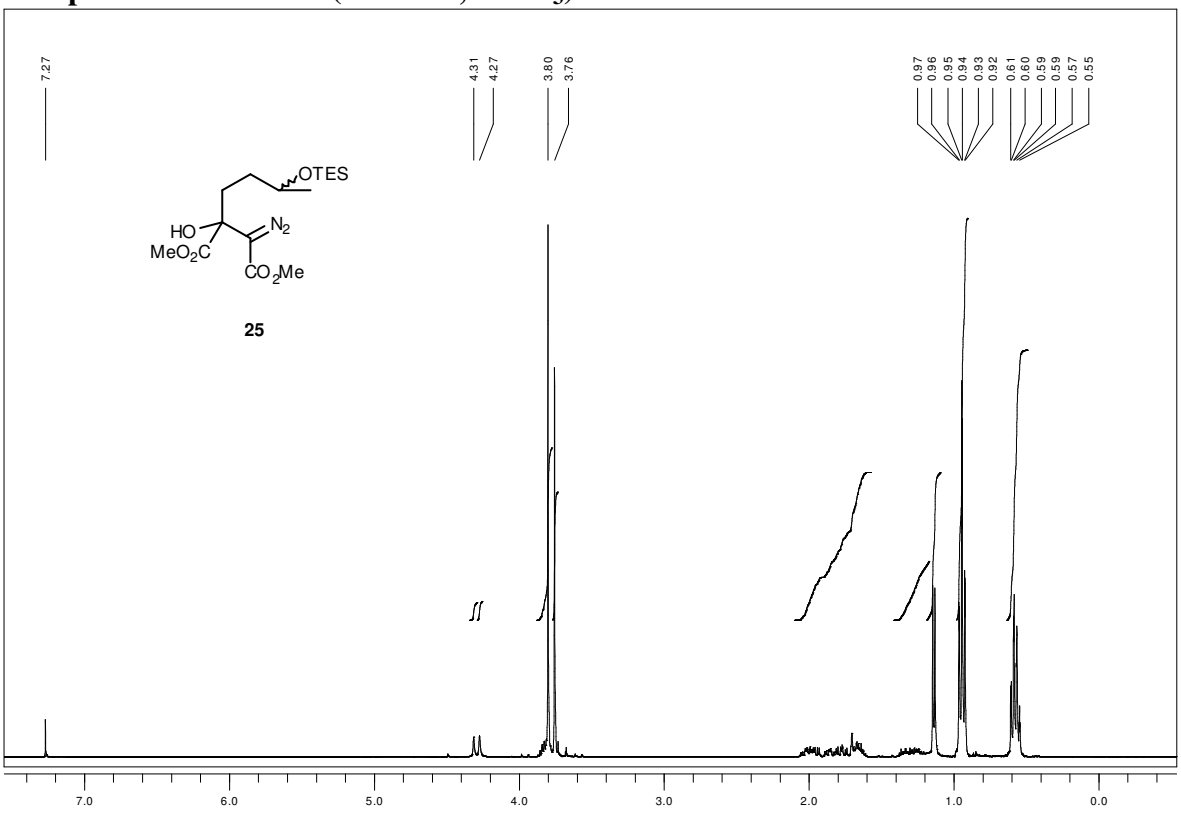
Compound 24 ^{1}H NMR (400MHz, $CDCl_3$)



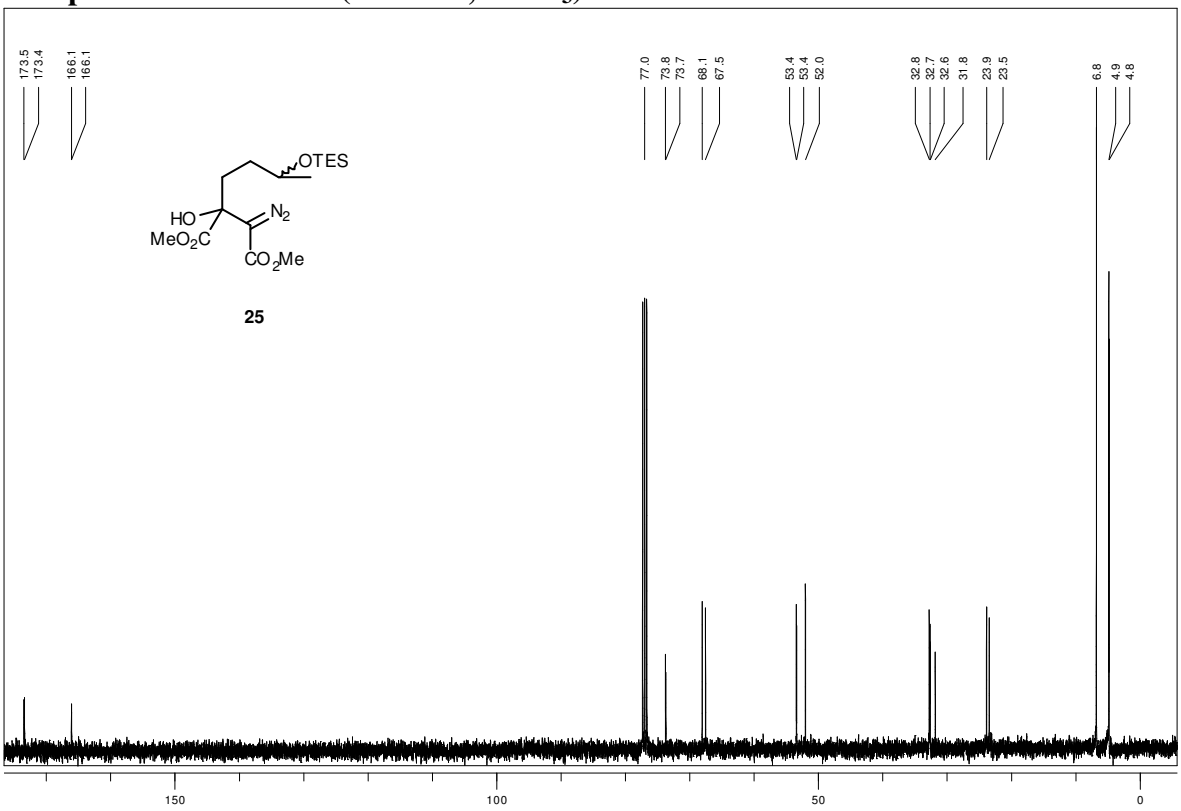
Compound 24 ^{13}C NMR (100MHz, $CDCl_3$)



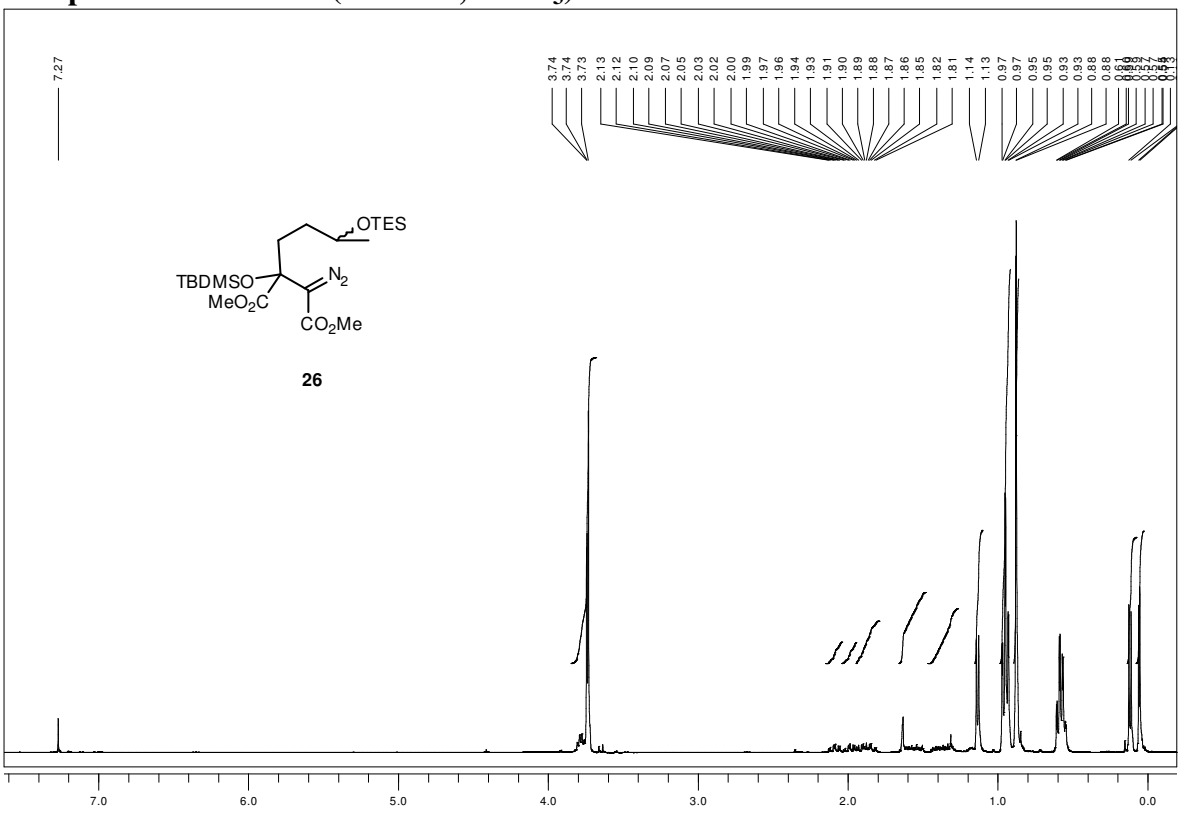
Compound 25 ^{1}H NMR (400MHz, $CDCl_3$)



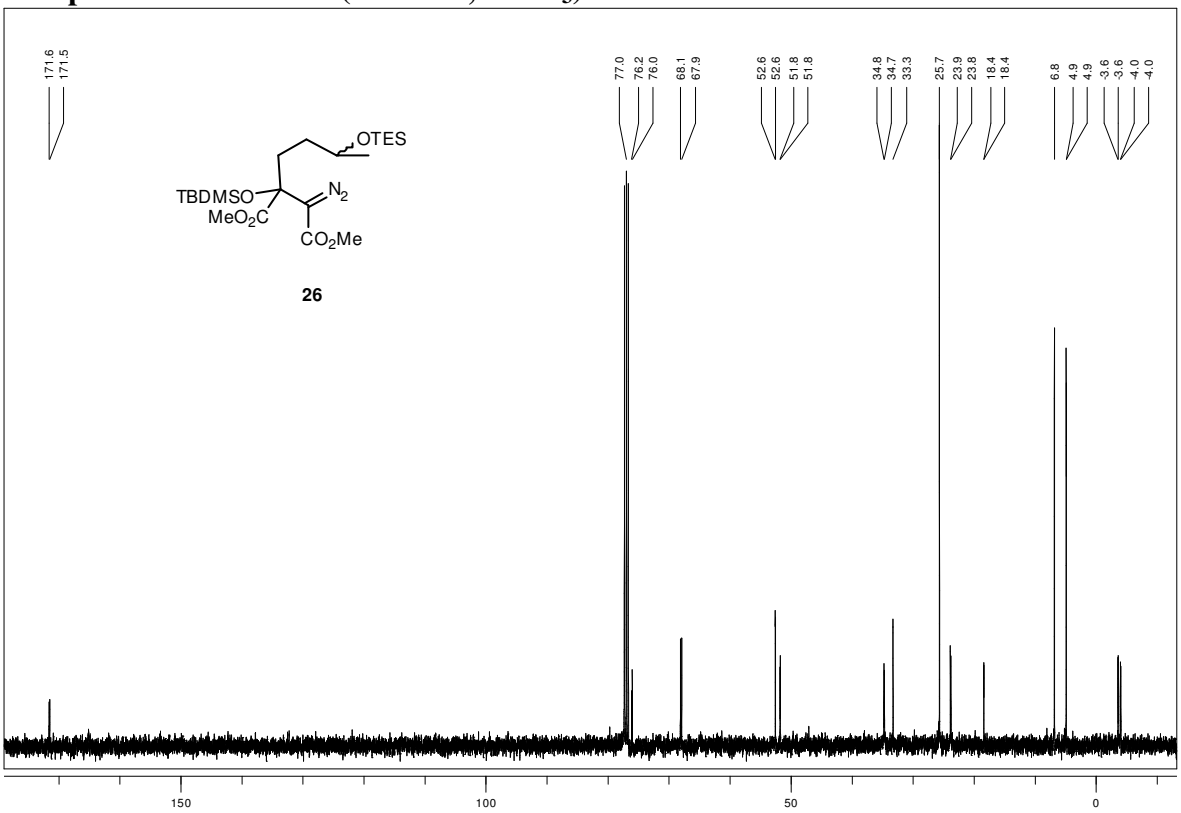
Compound 25 ^{13}C NMR (100MHz, $CDCl_3$)



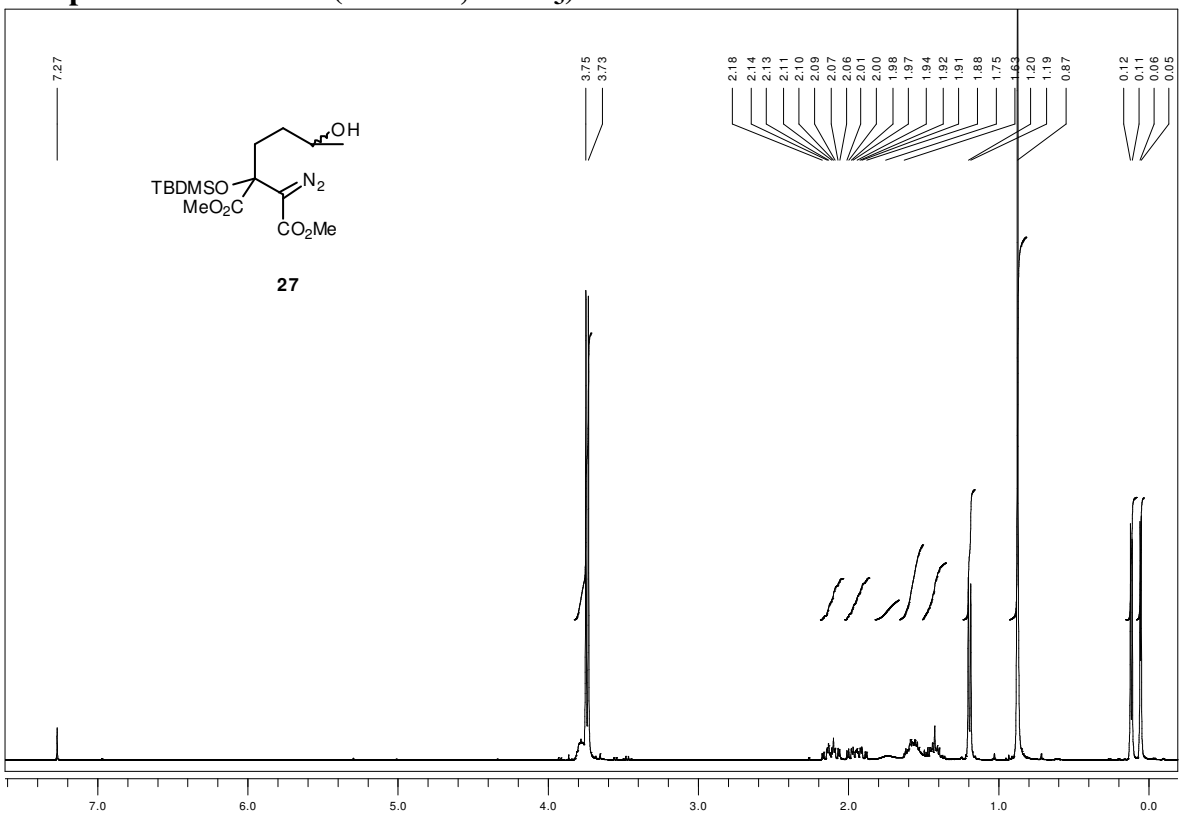
Compound 26 ^{1}H NMR (400MHz, $CDCl_3$)



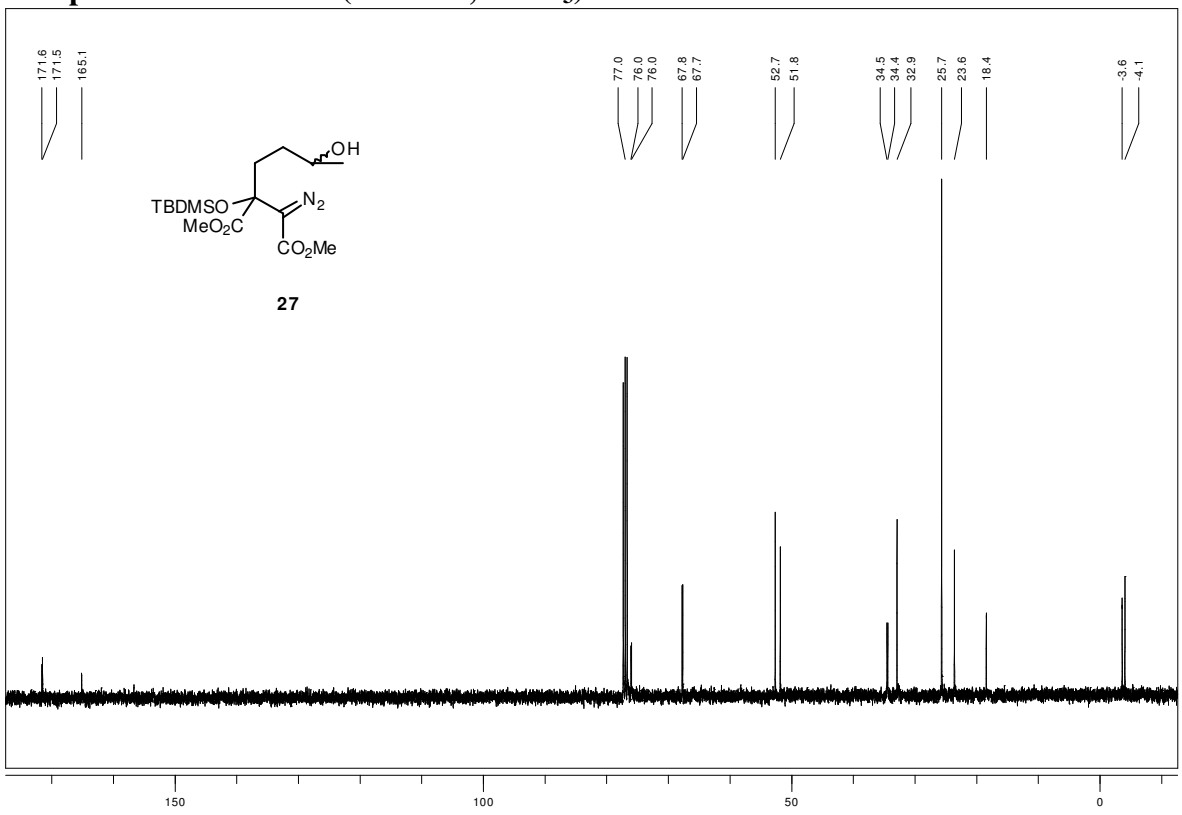
Compound 26 ^{13}C NMR (100MHz, $CDCl_3$)



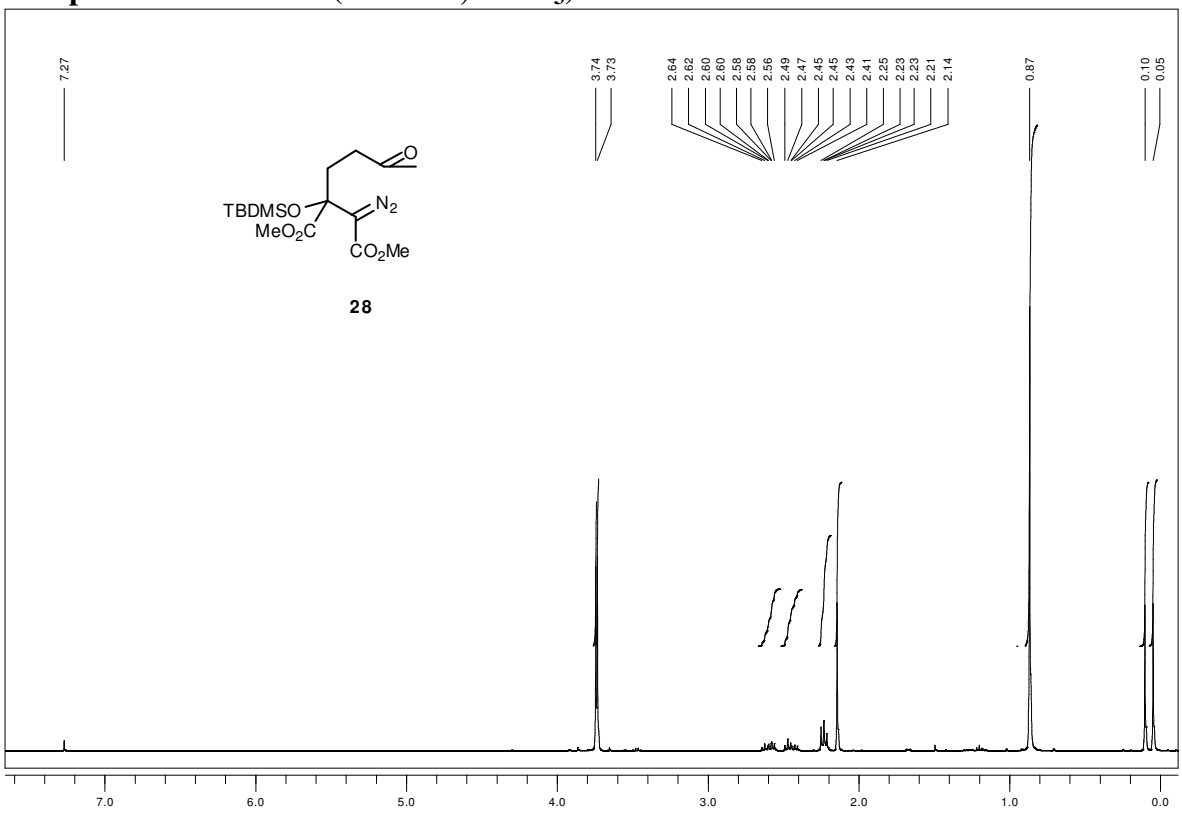
Compound 27 ^{1}H NMR (400MHz, $CDCl_3$)



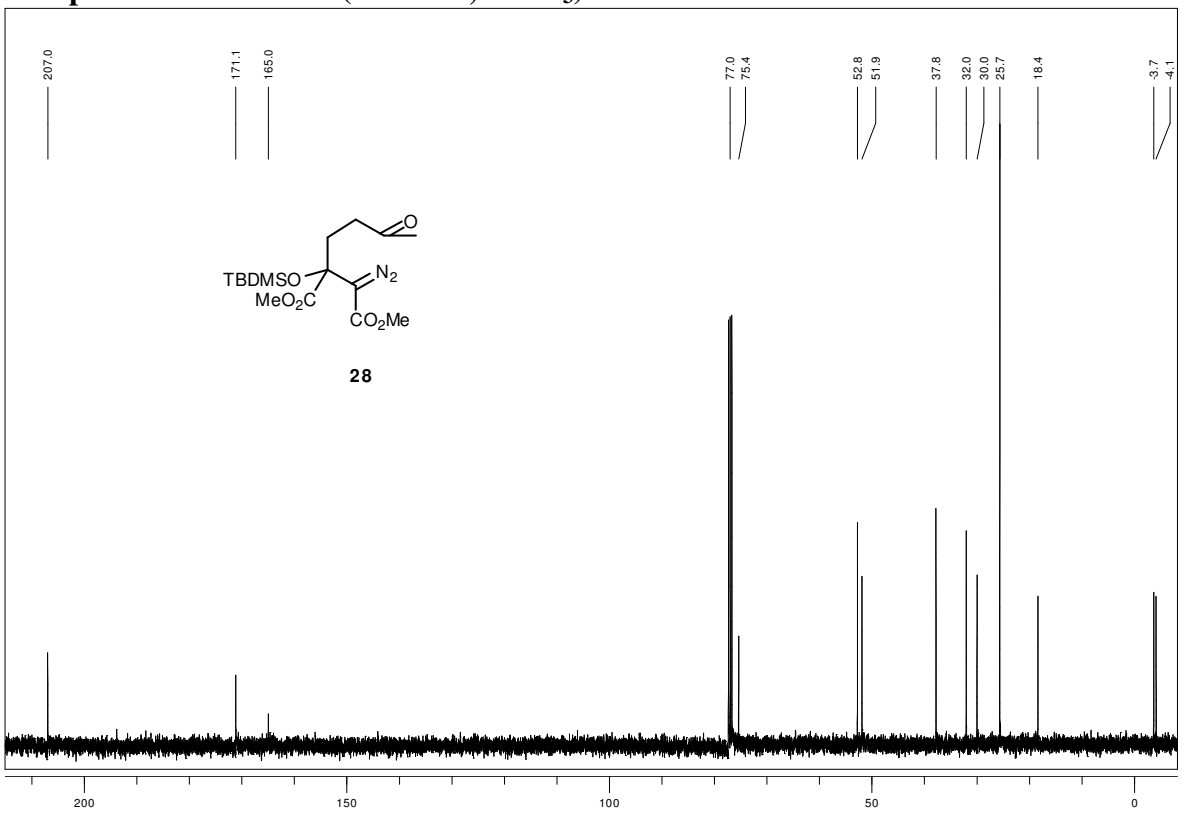
Compound 27 ^{13}C NMR (100MHz, $CDCl_3$)



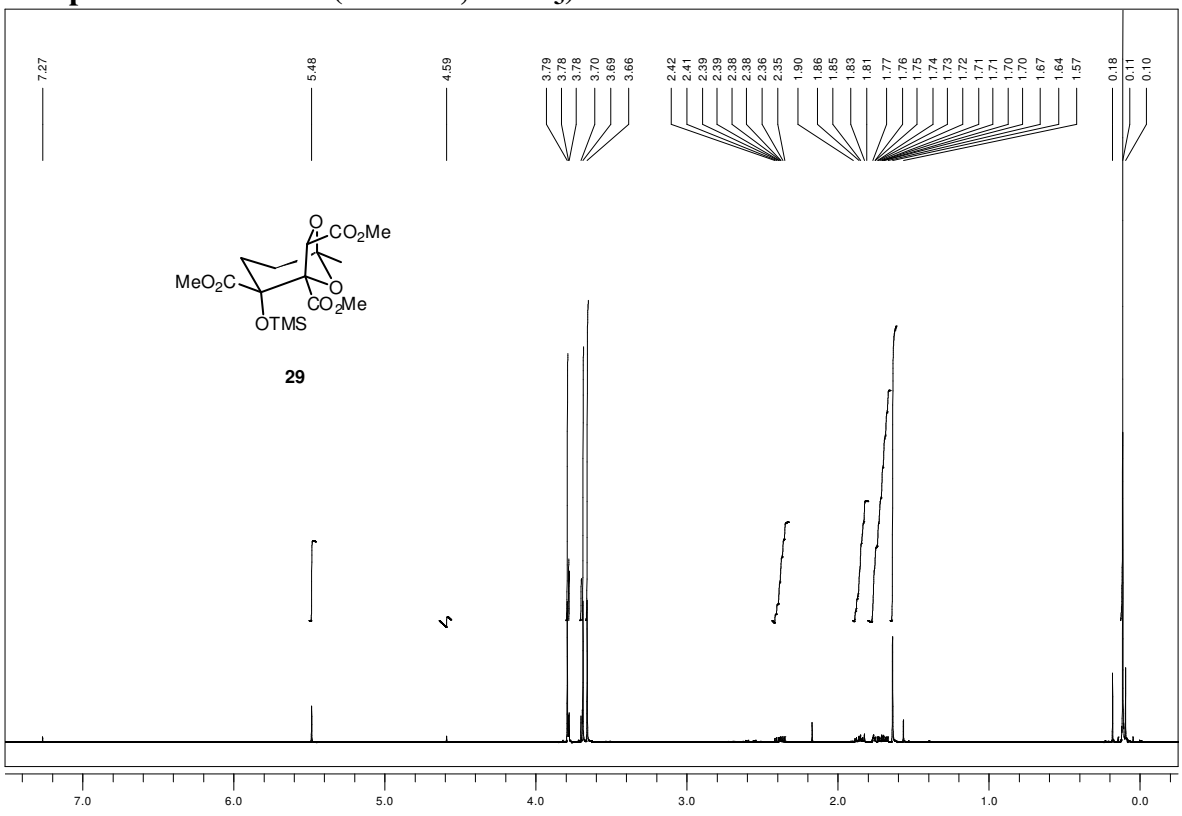
Compound 28 ^{1}H NMR (400MHz, $CDCl_3$)



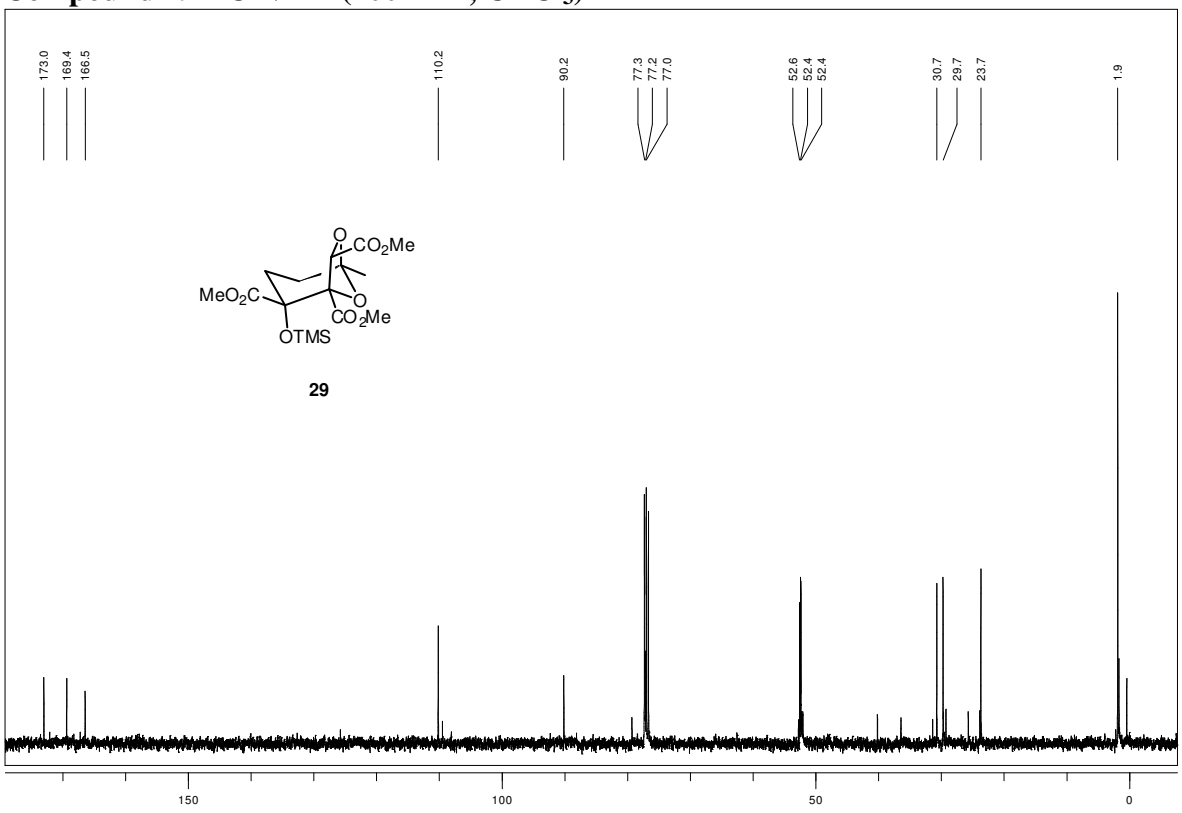
Compound 28 ^{13}C NMR (100MHz, $CDCl_3$)



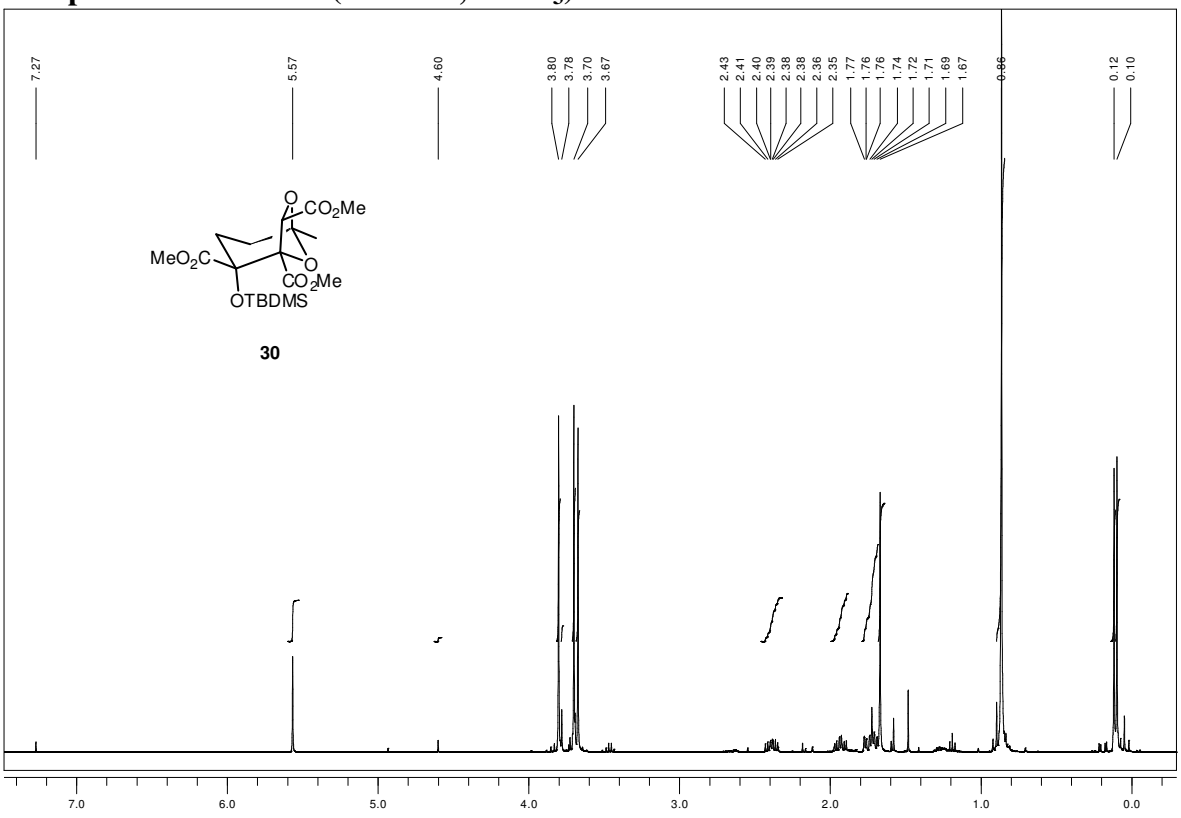
Compound 29 ^{1}H NMR (500MHz, $CDCl_3$)



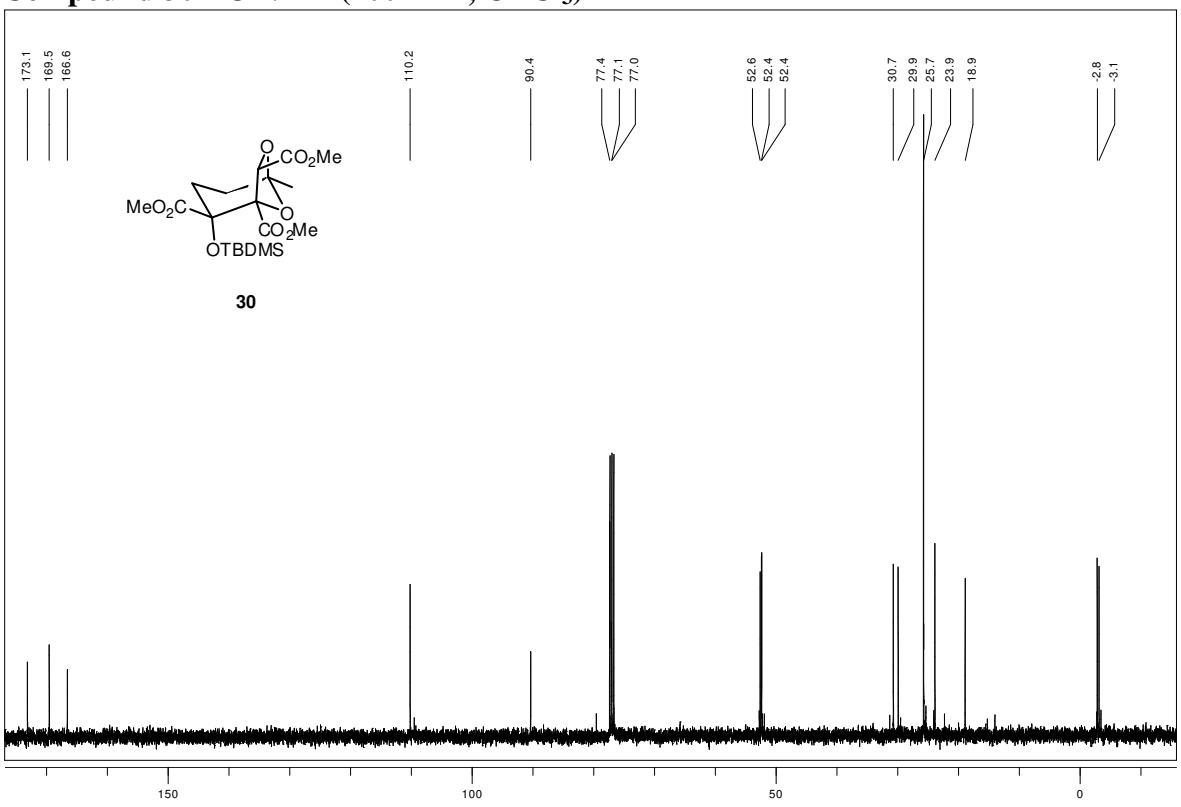
Compound 29 ^{13}C NMR (100MHz, $CDCl_3$)



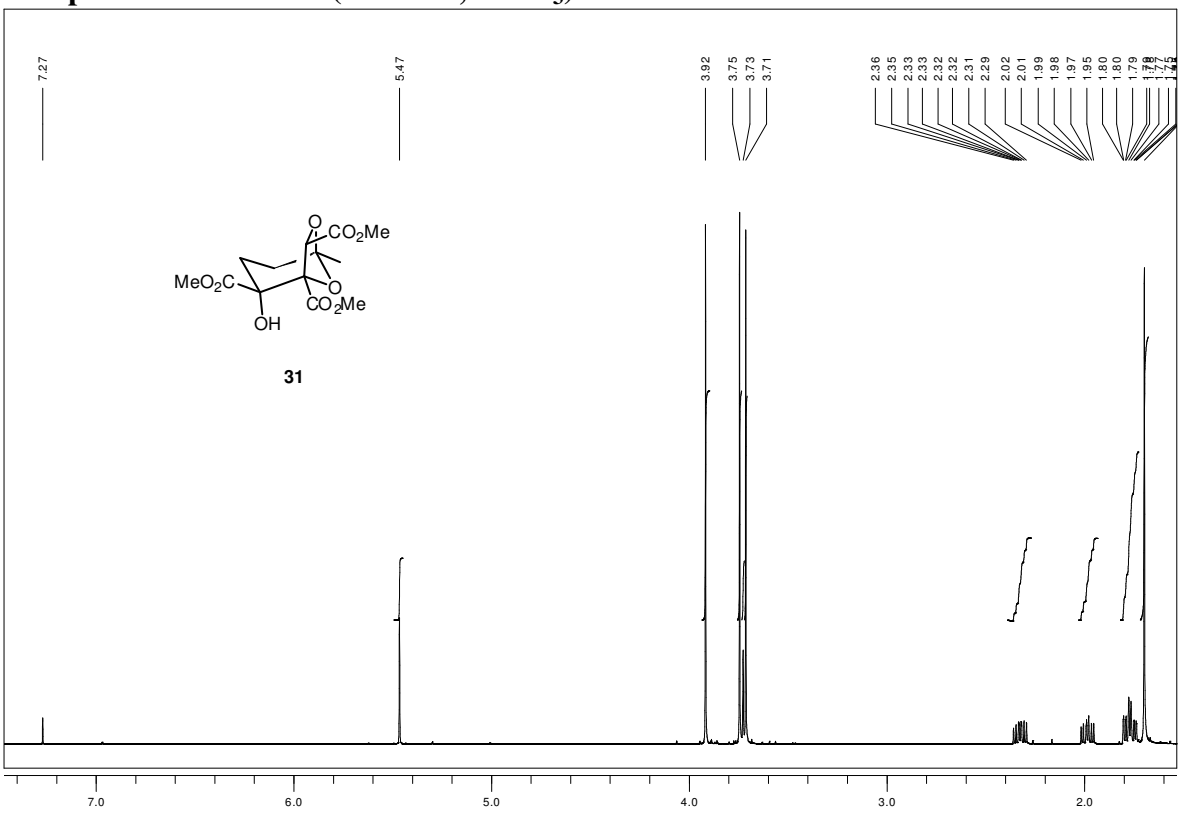
Compound 30 ^{1}H NMR (400MHz, $CDCl_3$)



Compound 30 ^{13}C NMR (100MHz, $CDCl_3$)

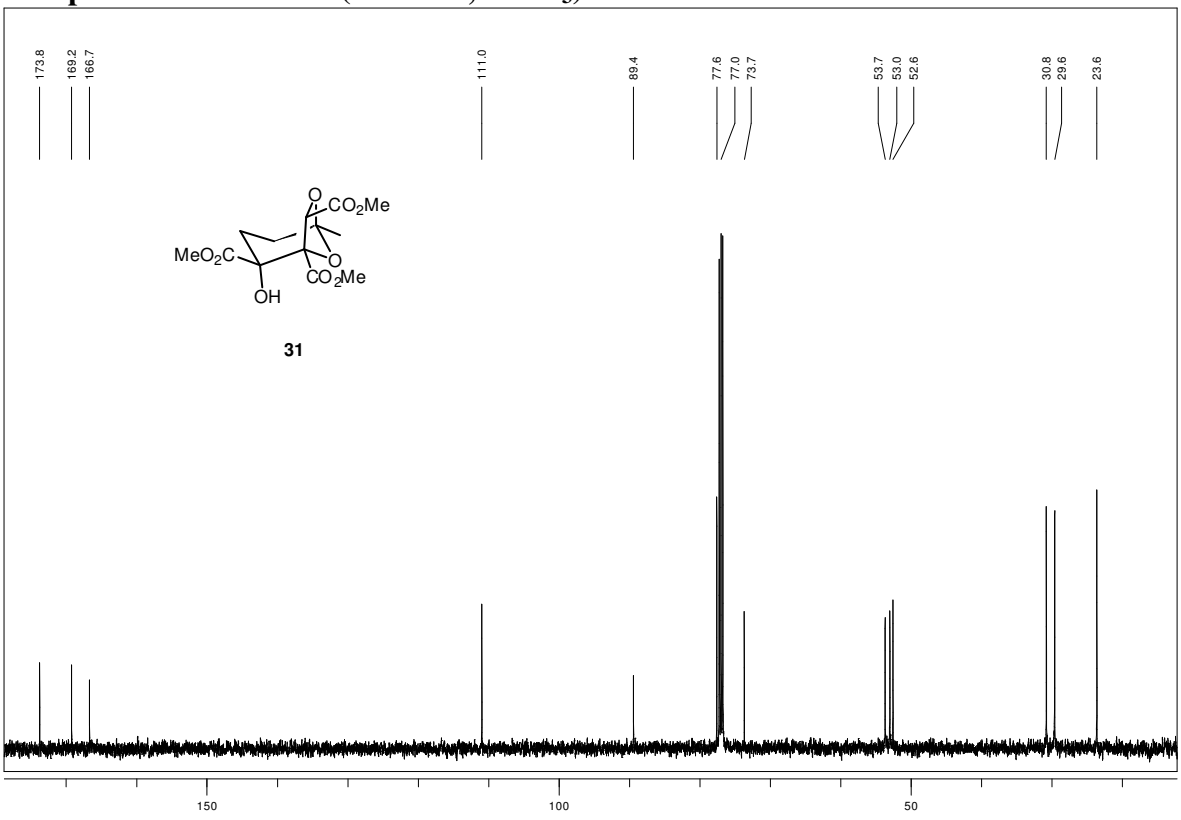


Compound 31 ^{1}H NMR (500MHz, $CDCl_3$)



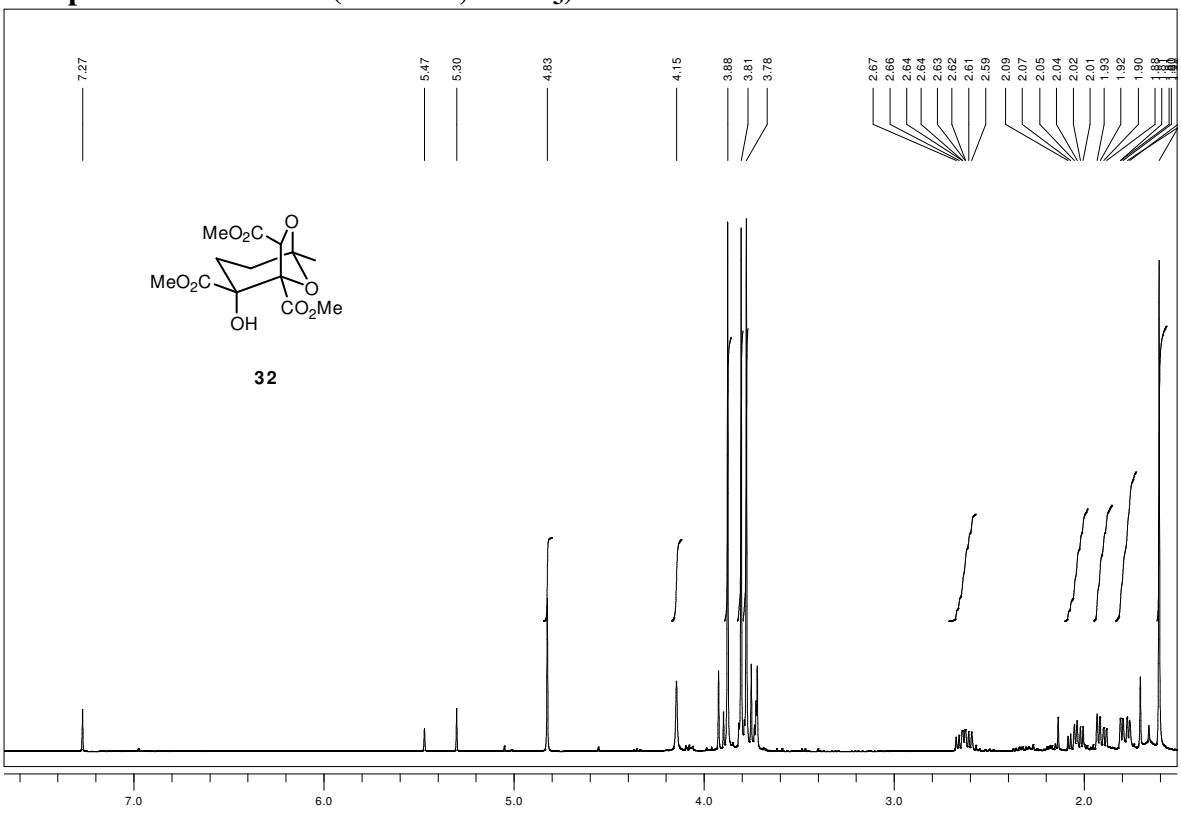
31

Compound 31 ^{13}C NMR (125MHz, $CDCl_3$)

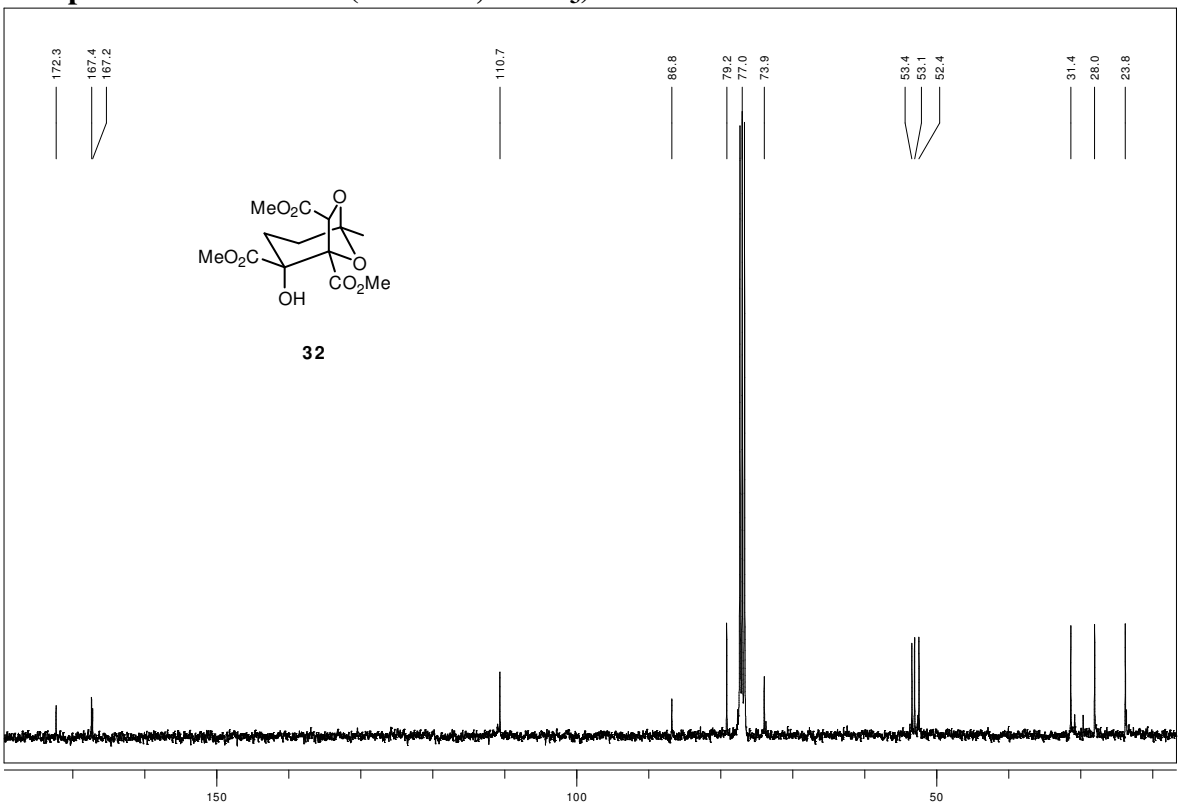


31

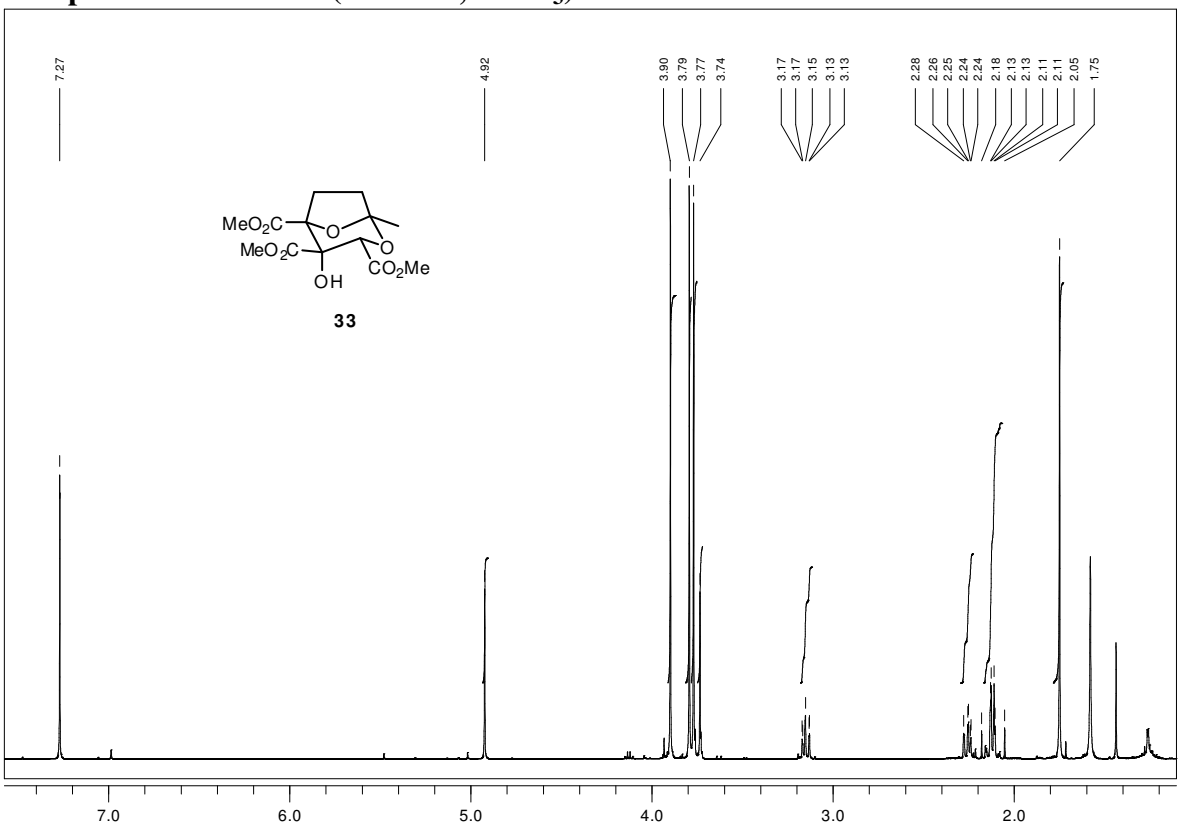
Compound 32 ^{1}H NMR (400MHz, $CDCl_3$)



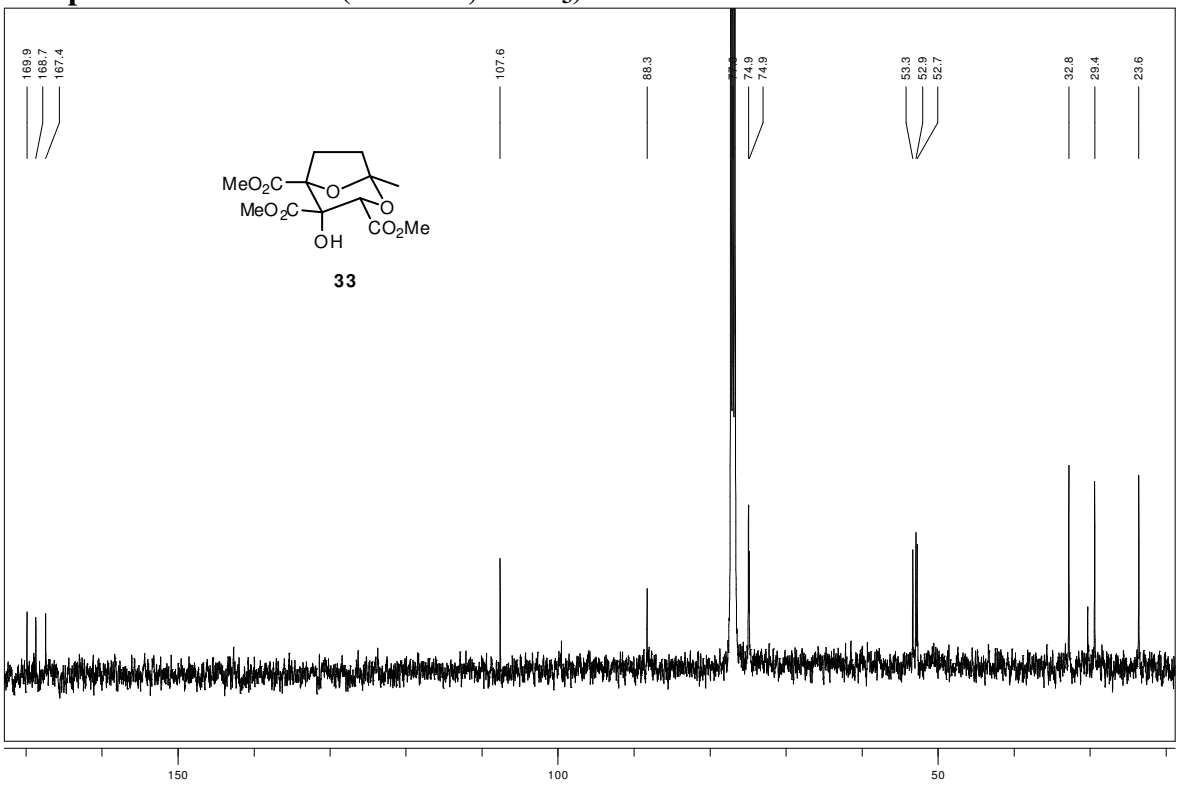
Compound 32 ^{13}C NMR (100MHz, $CDCl_3$)



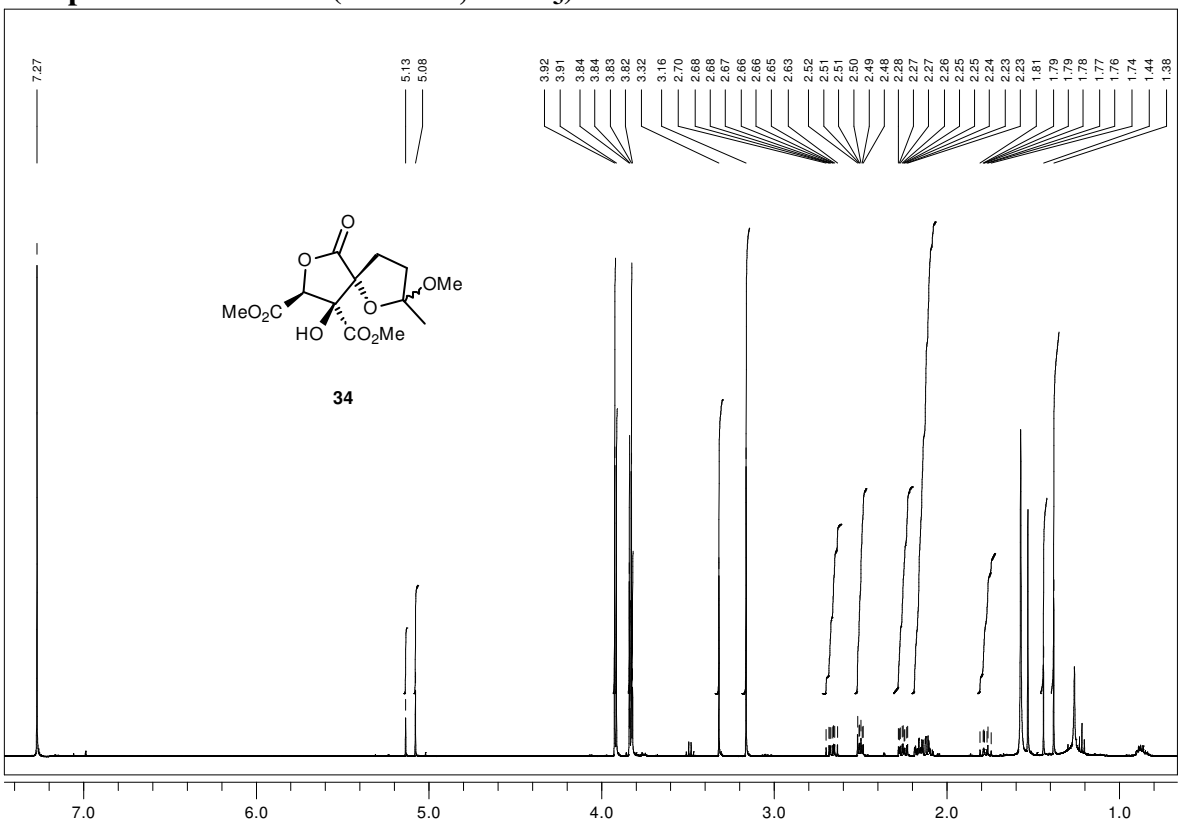
Compound 33 ^{1}H NMR (500MHz, $CDCl_3$)



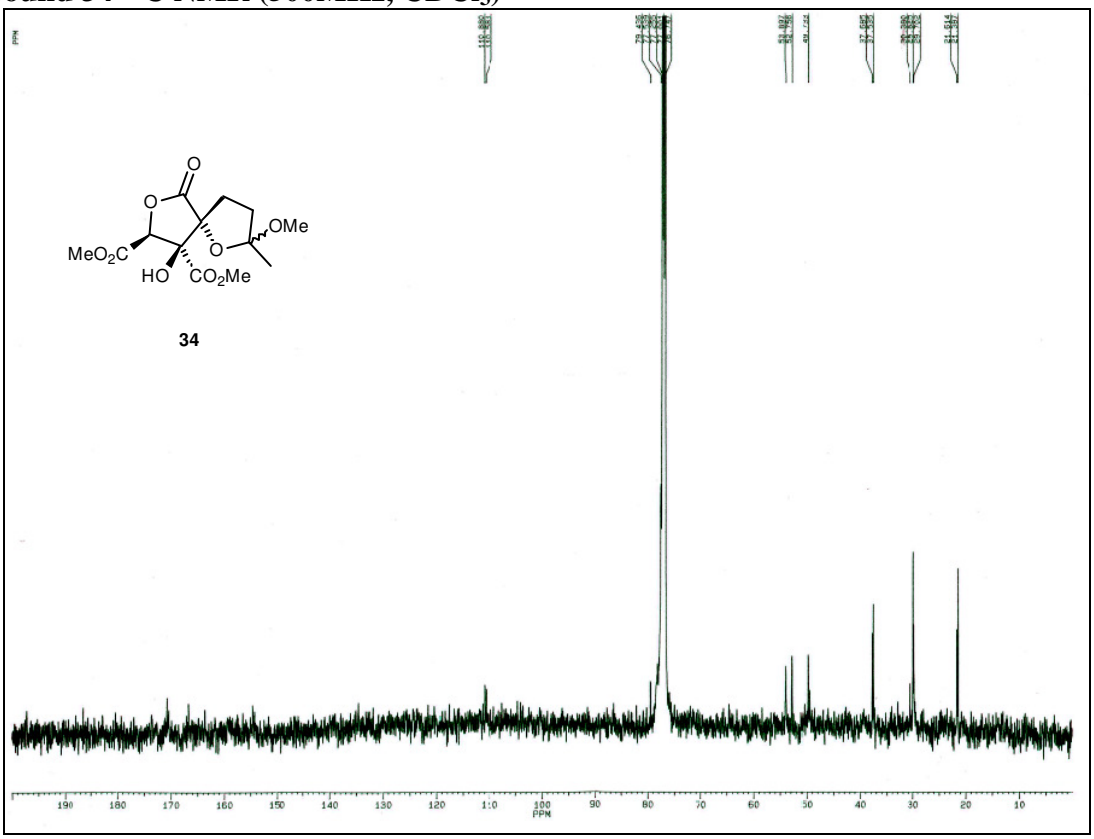
Compound 33 ^{13}C NMR (125MHz, $CDCl_3$)



Compound 34 ^{1}H NMR (500MHz, $CDCl_3$)



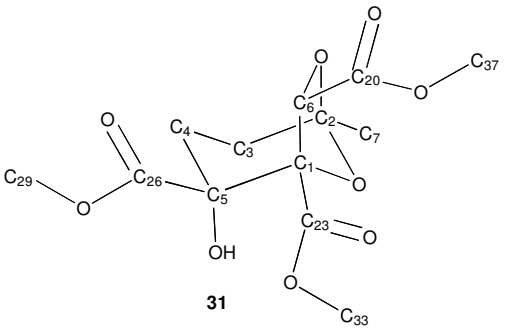
Compound 34 ^{13}C NMR (500MHz, $CDCl_3$)



f. Cartesian coordinates and energies of the DFT structures.

Molecular mechanics calculations were carried out using the MM2* force field[8] and the OPLSAA force field[9] as implemented in MacroModel[10] The DFT methods, used Jaguar,[11] and the DFT methods B3LYP,[12] MPW1PW91,[13] BHandHLYP,[14] M05[15] and M06.[16] The solvent was modelled using a continuum model using Jaguar's Poisson-Boltzmann continuum solvation model and default parameters for dichloromethane.[17]

Structure 31:



31

B3LYP/6-31G**
Energy: -1183.25868266196

C1	-0.4170225062	-3.8537005651	0.0480483349
C2	-2.4658834835	-2.9183516391	-0.1129280290
C3	-2.0998960053	-1.8470832316	-1.1469002541
C4	-0.8422888685	-2.2792368947	-1.9192801097
C5	0.2479514306	-2.8517474952	-0.9728495134
C6	-1.3774806116	-4.9208516713	-0.5658477399
C7	-3.7210224734	-2.6522845799	0.6889012650
O8	-2.5693365713	-4.1875659152	-0.7907212875
O9	-1.3562979806	-3.0704442907	0.7855843526
O10	0.8307482211	-1.8252643611	-0.1915338778
H11	-2.9336075560	-1.6972198106	-1.8400668039
H12	-1.9371867216	-0.8993559933	-0.6212453523
H13	-1.1115706246	-3.0337691016	-2.6615644451
H14	-0.4011706496	-1.4305585295	-2.4506134989
H15	-0.9875833019	-5.3257543616	-1.5008431958
H16	-4.5846704268	-2.6143927905	0.0202499007
H17	-3.8614849286	-3.4570367978	1.4116389460
H18	-3.6417346278	-1.6978499627	1.2163244664
H19	0.1898869104	-1.6257412904	0.5086625121
C20	-1.5834107553	-6.0961229826	0.4004987472
O21	-2.6557059894	-5.9463679010	1.1873008714
O22	-0.8191841280	-7.0376860210	0.4514613613
C23	0.6018554645	-4.4380117902	1.0332807674
O24	1.5645833661	-5.0816303685	0.3586556093
O25	0.5205628110	-4.3662407906	2.2349409596
C26	1.3946822725	-3.4440217352	-1.8077643232
O27	0.9451291162	-4.4398578710	-2.6089322077
O28	2.5330520640	-3.0498143781	-1.8024782066
C29	1.9562579676	-5.0697235766	-3.4155261678
H30	2.7153173968	-5.5296181874	-2.7787926039
H31	1.4365406023	-5.8275760358	-4.0009789149
H32	2.4362930169	-4.3374606602	-4.0684204022
C33	2.5358728650	-5.7739595915	1.1660470953
H34	3.0412934107	-5.0741940381	1.8342015267
H35	2.0410507551	-6.5526703028	1.7497061461
H36	3.2422112086	-6.2102602643	0.4613933273
C37	-2.8309036941	-6.9715935830	2.1839740693

H38	-3.7560751067	-6.7205253451	2.7013462305
H39	-2.9042108536	-7.9545583430	1.7138140600
H40	-1.9876379447	-6.9670797445	2.8782968832

B3LYP/6-31G** with CH_2Cl_2 model (single point)
Energy: -1183.28373536867

B3LYP/6-31G** with CH_2Cl_2 model (optimisation)
Energy: -1183.28425456457

C1	-0.4107769225	-3.8653149136	0.0496531350
C2	-2.4575681211	-2.9101358895	-0.0999317605
C3	-2.0934162687	-1.8560336806	-1.1497504940
C4	-0.8474940089	-2.3046883018	-1.9310451182
C5	0.2461162826	-2.8763094610	-0.9894570106
C6	-1.3878911294	-4.9360221702	-0.5319805021
C7	-3.7026814232	-2.6178596630	0.7078267006
O8	-2.5735879741	-4.1938247216	-0.7599841351
O9	-1.3382389092	-3.0705112272	0.7907259725
O10	0.8425116166	-1.8467782617	-0.2168493540
H11	-2.9325795968	-1.7060470850	-1.8360749576
H12	-1.9225924322	-0.9029910528	-0.6367633794
H13	-1.1263292565	-3.0644341463	-2.6646240534
H14	-0.4090319925	-1.4654414101	-2.4793754233
H15	-1.0168671326	-5.3697188025	-1.4630530433
H16	-4.5693105139	-2.5703730162	0.0423500404
H17	-3.8574292511	-3.4091948519	1.4437580256
H18	-3.6055438460	-1.6560641362	1.2198252746
H19	0.1800620084	-1.5663673541	0.4356749849
C20	-1.5993717091	-6.0874830945	0.4649949996
O21	-2.7345787064	-5.9940989040	1.1545293810
O22	-0.7797320832	-6.9764259897	0.6012706895
C23	0.6221100492	-4.4418296798	1.0274117975
O24	1.6112771973	-5.0404042297	0.3624810508
O25	0.5216784581	-4.3904027001	2.2321480622
C26	1.3862818727	-3.4655050769	-1.8361625440
O27	0.9609263181	-4.4720474644	-2.6153613941
O28	2.5155643417	-3.0294146148	-1.8525703565
C29	1.9640430639	-5.0608858973	-3.4781071047
H30	2.7587198476	-5.5111050517	-2.8798345727
H31	1.4420998084	-5.8208328835	-4.0576172211
H32	2.3905145464	-4.3007684333	-4.1354945962
C33	2.6065144040	-5.7214899086	1.1656667216
H34	3.0694525908	-5.0240790962	1.8668274790
H35	2.1360355502	-6.5417279069	1.7115014043
H36	3.3429757997	-6.1016342913	0.4583729632
C37	-2.9612319721	-7.0304840696	2.1412176068
H38	-3.9322910809	-6.8060956226	2.5808823566
H39	-2.9722677137	-8.0123090004	1.6637529122
H40	-2.1786543728	-7.0014586941	2.9016258886

LMP2/6-31G**
Energy: -1179.86700253829 (single point)
Energy: -1179.86810999377 (minimised)

C1	-0.4377311152	-3.8950317727	0.0181057418
C2	-2.4728605574	-2.9356638773	-0.1398087418
C3	-2.0760577239	-1.8368380828	-1.1266105025
C4	-0.8197223490	-2.2626715160	-1.8931621786
C5	0.2397107084	-2.8695416371	-0.9477817302
C6	-1.3917785603	-4.9352672744	-0.6262985277
C7	-3.7320216746	-2.6709374678	0.6509160424
O8	-2.5834355581	-4.1868286477	-0.8607584566
O9	-1.3871985374	-3.1331385851	0.7823755826
O10	0.8089360655	-1.8693805594	-0.1073964544
H11	-2.8966980098	-1.6523415956	-1.8210633911
H12	-1.9028638198	-0.9166893081	-0.5648579859

H13	-1.0877513071	-2.9947465778	-2.6523007666
H14	-0.3596270863	-1.4091493595	-2.3928849209
H15	-1.0047523609	-5.3354077061	-1.5594596364
H16	-4.5785436919	-2.5856177632	-0.0274712157
H17	-3.8954260504	-3.4939697047	1.3398164496
H18	-3.6278356793	-1.7403043001	1.2066453879
H19	0.1399621336	-1.6990787966	0.5726203193
C20	-1.6131878055	-6.0932889409	0.3490573949
O21	-2.6452080358	-5.8830443471	1.1874059509
O22	-0.8714827029	-7.0650885841	0.3873734026
C23	0.5649808430	-4.4951032759	1.0047710808
O24	1.5646602902	-5.0898658451	0.3233210389
O25	0.4519006182	-4.4718371529	2.2155623362
C26	1.3969395520	-3.4314996299	-1.7840907307
O27	0.9526306836	-4.4292424781	-2.5995814862
O28	2.5418143286	-3.0272296936	-1.7845310357
C29	1.9854186735	-5.0389505205	-3.4036923895
H30	2.7462334643	-5.4786725841	-2.7640821125
H31	1.4803909664	-5.8052279380	-3.9820741516
H32	2.4438405348	-4.3013997110	-4.0570927913
C33	2.5375874152	-5.7612390340	1.1584396959
H34	3.0003504529	-5.0519575230	1.8387887435
H35	2.0524838055	-6.5549826635	1.7199767484
H36	3.2688509987	-6.1666082217	0.4680142301
C37	-2.7436741282	-6.8583105173	2.2512818645
H38	-3.5922474357	-6.5389513112	2.8467469722
H39	-2.9081039184	-7.8521621085	1.8435354943
H40	-1.8321743588	-6.8503541590	2.8436178818

BHandHLYP/6-31G**
Energy: -1172.53004179673

C1	-0.4143368076	-3.8478103584	0.0415515520
C2	-2.4344504625	-2.9243999594	-0.0942387534
C3	-2.0772798143	-1.8521437200	-1.1114615961
C4	-0.8469105445	-2.2962684476	-1.8968767212
C5	0.2377402935	-2.8603813301	-0.9646158329
C6	-1.3679297743	-4.8963231262	-0.5683938909
C7	-3.6722790268	-2.6694191917	0.7133690915
O8	-2.5392149114	-4.1654255722	-0.7731035800
O9	-1.3350848827	-3.0842643070	0.7789879142
O10	0.8197337386	-1.8538550494	-0.1981072064
H11	-2.9218636324	-1.6836455227	-1.7897647773
H12	-1.8924958686	-0.9116613562	-0.5753491609
H13	-1.1341972652	-3.0618795982	-2.6255112664
H14	-0.4035167652	-1.4575277980	-2.4461862416
H15	-0.9790177119	-5.3041149510	-1.5057128290
H16	-4.5416931046	-2.6114872947	0.0509643270
H17	-3.8078979524	-3.4955851390	1.4165748273
H18	-3.5807872298	-1.7277851175	1.2647365114
H19	0.1951038933	-1.6418952765	0.5059143472
C20	-1.5614032251	-6.0450906419	0.4047694013
O21	-2.6813288515	-5.9716884056	1.0913716607
O22	-0.7373821022	-6.9096104062	0.5401132284
C23	0.6057251382	-4.4317913845	1.0001085752
O24	1.5869613464	-5.0015486299	0.3269970373
O25	0.5071833582	-4.4066930523	2.1893042589
C26	1.3528726888	-3.4688807908	-1.8001961785
O27	0.9025631118	-4.4905584548	-2.5294031450
O28	2.4731646285	-3.0648173013	-1.8498155342
C29	1.8901322329	-5.1553388090	-3.2954442134
H30	2.6547413543	-5.5801672275	-2.6370563317
H31	1.3728391698	-5.9477607260	-3.8390355622
H32	2.3716499989	-4.4607399414	-3.9901800490
C33	2.5425336648	-5.6948279943	1.1122424951
H34	2.9571576724	-5.0346559193	1.8789037797

H35	2.0650024396	-6.5562840409	1.5893382691
H36	3.3224872161	-6.0192071669	0.4219925085
C37	-2.8435530048	-6.9765820022	2.0786038273
H38	-3.8125619405	-6.7892672978	2.5435650238
H39	-2.8211124857	-7.9707829384	1.6221327275
H40	-2.0410873846	-6.9092755758	2.8196831982

M05/6-31G**
Energy: -1182.63804390874

C1	-0.4166502569	-3.8208185302	0.0641296255
C2	-2.4753504451	-2.9547239059	-0.1496097286
C3	-2.1166681163	-1.9009103698	-1.1929959550
C4	-0.8285240715	-2.2951169478	-1.9188503897
C5	0.2632614223	-2.8222274438	-0.9537217580
C6	-1.3301151922	-4.9204852571	-0.5687519919
C7	-3.7438423106	-2.7002306933	0.6234719745
O8	-2.5400326821	-4.2373970459	-0.7871922127
O9	-1.3807446955	-3.0558123382	0.7595476938
O10	0.8285638102	-1.7825403328	-0.1990613069
H11	-2.9329831640	-1.7954798588	-1.9125563291
H12	-2.0086203652	-0.9372063642	-0.6850099250
H13	-1.0563925164	-3.0628187015	-2.6597079844
H14	-0.4105783925	-1.4378483068	-2.4523906747
H15	-0.9200226692	-5.3008790005	-1.5054019635
H16	-4.5975731942	-2.6937587242	-0.0564860944
H17	-3.8804730575	-3.4902356029	1.3613990679
H18	-3.6934480182	-1.7350819227	1.1310327425
H19	0.1743979420	-1.5450423637	0.4673468056
C20	-1.4975532672	-6.1086210128	0.3929567206
O21	-2.4807261436	-5.8843207978	1.2682764236
O22	-0.7834832364	-7.0876355790	0.3850008857
C23	0.5457363086	-4.4322975262	1.0860300936
O24	1.4909962567	-5.0943950579	0.4092590512
O25	0.4104766772	-4.4124340737	2.2833890653
C26	1.4420821221	-3.3824660571	-1.7710616372
O27	1.0080379322	-4.3458241312	-2.6116226563
O28	2.5767542454	-2.9860823170	-1.7256841828
C29	2.0023830069	-4.9313851812	-3.4559746068
H30	2.7685649605	-5.4227101754	-2.8538181835
H31	1.4738839042	-5.6580787758	-4.0717565597
H32	2.4702669642	-4.1671021151	-4.0791621380
C33	2.3053545462	-6.0006640085	1.1623391298
H34	2.7675532322	-5.4890769366	2.0068401443
H35	1.6822079543	-6.8254466451	1.5127938657
H36	3.0600016713	-6.3600640887	0.4655628756
C37	-2.6163188633	-6.8326432039	2.3323043057
H38	-3.4817627229	-6.5064629003	2.9071469299
H39	-2.7739877778	-7.8367932873	1.9351508638
H40	-1.7189580848	-6.8194238354	2.9540089579

M06/6-31G**
Energy: -1182.63489771666

C1	-0.4398112947	-3.8436311937	0.0313227628
C2	-2.4625272485	-2.9109399328	-0.1375766356
C3	-2.0787320873	-1.8292392510	-1.1379607969
C4	-0.8154442257	-2.2452516114	-1.8922616623
C5	0.2491589416	-2.8517826029	-0.9528272102
C6	-1.3856174594	-4.8903976565	-0.6138026209
C7	-3.7185568491	-2.6492323202	0.6430052853
O8	-2.5687175468	-4.1620613353	-0.8228119117
O9	-1.3766210156	-3.0768214995	0.7644956359
O10	0.8566373286	-1.8625425863	-0.1621114133
H11	-2.9051636789	-1.6608916114	-1.8390365180
H12	-1.9269238220	-0.8934402856	-0.5819859759
H13	-1.0782314047	-2.9764287248	-2.6643163087
H14	-0.3538982841	-1.3864802466	-2.3932287472

H15	-0.9802743524	-5.2763684051	-1.5546145820
H16	-4.5721448630	-2.5947879288	-0.0394264245
H17	-3.8760182245	-3.4670350272	1.3512609361
H18	-3.6404531671	-1.7032800069	1.1886560151
H19	0.2129162203	-1.6203263715	0.5171324164
C20	-1.5548561640	-6.0690255240	0.3346306476
O21	-2.5658999367	-5.9218684574	1.1859013599
O22	-0.7849784185	-7.0014157308	0.3347995305
C23	0.5264842751	-4.4666771015	1.0293521705
O24	1.5543570576	-5.0149943476	0.3843151399
O25	0.3436746373	-4.5155380879	2.2168397642
C26	1.3769330124	-3.4524926850	-1.7901857184
O27	0.9133577189	-4.4329800499	-2.5903178479
O28	2.5159873752	-3.0775418178	-1.7888009155
C29	1.9144056677	-5.0822018154	-3.3723177993
H30	2.6604577357	-5.5461934902	-2.7188413563
H31	1.3951586809	-5.8414604502	-3.9582665674
H32	2.4161762035	-4.3640608766	-4.0276983654
C33	2.4417829938	-5.7803054752	1.2034214813
H34	2.8227227750	-5.1692669936	2.0261128887
H35	1.9051751036	-6.6453094412	1.6048596143
H36	3.2544320865	-6.0953010255	0.5487176657
C37	-2.6204723821	-6.9130440814	2.2167464800
H38	-3.5048671504	-6.6807192092	2.8106996158
H39	-2.6966332789	-7.9150196031	1.7848306882
H40	-1.7174936466	-6.8542586436	2.8335090990

MPW1PW91/6-31G**
Energy: -1182.98084241531

C1	-0.4283755712	-3.8641502173	0.0319307811
C2	-2.4640672519	-2.9461621987	-0.1267934212
C3	-2.1008177303	-1.8756087273	-1.1520551744
C4	-0.8502620318	-2.3057299939	-1.9191004944
C5	0.2319389232	-2.8509951275	-0.9641451014
C6	-1.3781093344	-4.9257434293	-0.5842998983
C7	-3.7172916732	-2.6836842575	0.6668588314
O8	-2.5635367953	-4.2022522981	-0.8067619599
O9	-1.3658778237	-3.0999099250	0.7711056946
O10	0.7704948370	-1.8244504189	-0.1713896015
H11	-2.9348652021	-1.7259212349	-1.8424556261
H12	-1.9377600554	-0.9297510543	-0.6257703759
H13	-1.1127895412	-3.0737557507	-2.6492443555
H14	-0.4161166139	-1.4622718173	-2.4619298548
H15	-0.9839144382	-5.3381486289	-1.5138108034
H16	-4.5758562638	-2.6425445400	-0.0052338838
H17	-3.8594886287	-3.4911947735	1.3837762042
H18	-3.6390084654	-1.7329896396	1.1974869906
H19	0.1182333873	-1.6566122129	0.5216791199
C20	-1.5802046442	-6.0754622929	0.4035326406
O21	-2.6083543956	-5.8722040609	1.2223802407
O22	-0.8427516919	-7.0328288241	0.4532906590
C23	0.5855013963	-4.4737406453	0.9940662061
O24	1.5197030700	-5.1188210345	0.2966003084
O25	0.5159810564	-4.4287501418	2.1934404538
C26	1.4018249286	-3.4108409829	-1.7744124824
O27	0.9984551312	-4.4037028429	-2.5868826888
O28	2.5261808868	-2.9902404143	-1.7389731894
C29	2.0440537322	-4.9933586497	-3.3607276856
H30	2.8005889785	-5.4277448097	-2.7056701982
H31	1.5696369499	-5.7667409561	-3.9613909718
H32	2.5174532903	-4.2455539521	-3.9984917816
C33	2.4548037226	-5.8743510395	1.0701744246
H34	2.9523494602	-5.2339192190	1.7986014779
H35	1.9334171172	-6.6829929637	1.5835576391
H36	3.1721459961	-6.2736671214	0.3569986604
C37	-2.7502368245	-6.8408814369	2.2639342943

H38	-3.6450062416	-6.5544680930	2.8124030112
H39	-2.8586778185	-7.8424161088	1.8457006390
H40	-1.8767103729	-6.8168355179	2.9171528128

B3LYP/6-31++G**
Energy: -1183.30088421802

C1	-0.4133263496	-3.8369624218	0.0752116735
C2	-2.4488775388	-2.8576638114	-0.0733879965
C3	-2.0722222884	-1.8162506120	-1.1333704514
C4	-0.8281876315	-2.2805883974	-1.9098296722
C5	0.2652167339	-2.8685287693	-0.9741701101
C6	-1.3995600744	-4.8871567198	-0.5404617488
C7	-3.6837755441	-2.5415552051	0.7414740925
O8	-2.5934998266	-4.1416338691	-0.7160589313
O9	-1.3286067170	-3.0233480672	0.8069753281
O10	0.8984041394	-1.8444010912	-0.2255405064
H11	-2.9088659860	-1.6715266940	-1.8245418174
H12	-1.8951423631	-0.8588841948	-0.6295128687
H13	-1.1200964239	-3.0377418097	-2.6414802334
H14	-0.3766227450	-1.4461251878	-2.4552171840
H15	-1.0335112454	-5.2558561219	-1.4991494374
H16	-4.5562183702	-2.4937430163	0.0842100369
H17	-3.8372519832	-3.3255648711	1.4852159395
H18	-3.5690320360	-1.5785111589	1.2468122728
H19	0.2738233802	-1.5635902494	0.4609289671
C20	-1.5971848062	-6.1158352867	0.3572188971
O21	-2.6767844966	-6.0381898310	1.1405703479
O22	-0.8257917392	-7.0557977940	0.3362016042
C23	0.6011779841	-4.4118673382	1.0776364762
O24	1.6317579026	-4.9688297168	0.4326145250
O25	0.4680455676	-4.3765833574	2.2786157142
C26	1.3737779369	-3.4959904422	-1.8403703251
O27	0.9000632930	-4.5424817709	-2.5552507208
O28	2.5009211333	-3.0753236374	-1.9333780397
C29	1.8600911917	-5.2079435538	-3.4003252422
H30	2.6785786339	-5.6059232404	-2.7964953381
H31	1.3106094882	-6.0151109587	-3.8834696668
H32	2.2611265885	-4.5120758683	-4.1406537275
C33	2.6498507034	-5.5722976326	1.2594569348
H34	3.0568965988	-4.8317387741	1.9506053674
H35	2.2240042006	-6.4091907228	1.8168615542
H36	3.4156766495	-5.9163497572	0.5661124365
C37	-2.8891941222	-7.1566450543	2.0278730154
H38	-3.8169686496	-6.9335973161	2.5532672931
H39	-2.9795906251	-8.0822702117	1.4550700753
H40	-2.0566676113	-7.2408930236	2.7298188665

B3LYP/6-311+G**
Energy: -1183.55842245852

C1	-0.4110270165	-3.8468037134	0.0677929615
C2	-2.4489395012	-2.8881119492	-0.0939419782
C3	-2.0737103932	-1.8278238865	-1.1328521648
C4	-0.8253484609	-2.2787371659	-1.9059397600
C5	0.2628760449	-2.8673558823	-0.9682142832
C6	-1.3801348960	-4.9033551457	-0.5489312527
C7	-3.6967592738	-2.6046096005	0.7090756556
O8	-2.5678026177	-4.1607713356	-0.7609819637
O9	-1.3385773528	-3.0472590790	0.7986435295
O10	0.8808213991	-1.8463859720	-0.2062688607
H11	-2.9056968280	-1.6761571564	-1.8249415210
H12	-1.9008931914	-0.8803552578	-0.6134801243
H13	-1.1090596025	-3.0286545321	-2.6446812057
H14	-0.3734635953	-1.4381567469	-2.4375217231
H15	-0.9953139367	-5.2912364369	-1.4900889332
H16	-4.5612495455	-2.5648718595	0.0439683777

H17	-3.8400039907	-3.4025424820	1.4367055856
H18	-3.6051174200	-1.6487910979	1.2288870927
H19	0.2556846701	-1.6098483735	0.4910978854
C20	-1.5870717611	-6.1011575616	0.3855217535
O21	-2.6886566790	-6.0025829152	1.1335268051
O22	-0.8086753107	-7.0231653796	0.4288135949
C23	0.6057308172	-4.4164626291	1.0656575971
O24	1.6091330412	-5.0052979457	0.4080650129
O25	0.4957437617	-4.3583534345	2.2590212528
C26	1.3792229686	-3.4876385493	-1.8247835316
O27	0.8952127534	-4.4992029266	-2.5825674191
O28	2.5103441596	-3.0977581229	-1.8754732869
C29	1.8585695696	-5.1563692293	-3.4266151745
H30	2.6424547680	-5.6112157345	-2.8200229524
H31	1.3013441134	-5.9188163765	-3.9660726832
H32	2.3078807222	-4.4427473139	-4.1181115996
C33	2.6241644847	-5.6228455487	1.2241877187
H34	3.0552160238	-4.8889754713	1.9049812780
H35	2.1893004697	-6.4459698368	1.7915235399
H36	3.3733283425	-5.9876505036	0.5264562071
C37	-2.8978334701	-7.0781638451	2.0708361859
H38	-3.8484866761	-6.8613791651	2.5517405210
H39	-2.9360717843	-8.0346659917	1.5486798843
H40	-2.0901472304	-7.0973299179	2.8034436315

BHandHLYP/6-311+G**
Energy: -1172.83013262383

C1	-0.4206692355	-3.8417054134	0.0578079645
C2	-2.4323688328	-2.9004083896	-0.0862576796
C3	-2.0632284911	-1.8479541300	-1.1160995990
C4	-0.8357727646	-2.3085418728	-1.8927180248
C5	0.2452054541	-2.8694238071	-0.9563645796
C6	-1.3812807315	-4.8816237772	-0.5636270727
C7	-3.6640580388	-2.6139693261	0.7154619685
O8	-2.5541430294	-4.1502942947	-0.7430921335
O9	-1.3333544959	-3.0655986629	0.7842249616
O10	0.8382446583	-1.8579872044	-0.2050258416
H11	-2.9042183916	-1.6871095707	-1.7994056473
H12	-1.8776351478	-0.9012127016	-0.5927949452
H13	-1.1273935979	-3.0816217958	-2.6103230394
H14	-0.3892603155	-1.4797933346	-2.4530630338
H15	-0.9996641196	-5.2648170025	-1.5123199168
H16	-4.5310881914	-2.5540116438	0.0506882284
H17	-3.8149720796	-3.4237776664	1.4340516839
H18	-3.5568284780	-1.6642067087	1.2488369701
H19	0.2211712355	-1.6049134461	0.4879463981
C20	-1.5638787635	-6.0619982728	0.3718677531
O21	-2.6583044162	-5.9953142961	1.0916897817
O22	-0.7550106444	-6.9410391842	0.4447495266
C23	0.5873558386	-4.4365925323	1.0244962476
O24	1.5947115311	-4.9599847585	0.3619597522
O25	0.4580903907	-4.4471857084	2.2060388292
C26	1.3537229827	-3.4879017376	-1.7956665071
O27	0.8990297314	-4.5165380468	-2.5046684070
O28	2.4651579670	-3.0778344385	-1.8648292839
C29	1.8628542279	-5.1870937952	-3.2959686089
H30	2.6540619448	-5.5952075722	-2.6603310626
H31	1.3307292318	-5.9918425748	-3.8038581117
H32	2.3085506303	-4.5013168265	-4.0217903784
C33	2.5711486884	-5.6351079196	1.1375797411
H34	2.9695289310	-4.9697568410	1.9075659503
H35	2.1222617308	-6.5156407359	1.6059485792
H36	3.3570121378	-5.9276704018	0.4415933734
C37	-2.8312062640	-7.0345557885	2.0413101245
H38	-3.7857500099	-6.8376592964	2.5291696789

H39	-2.8470024967	-8.0080573348	1.5435647038
H40	-2.0159531896	-7.0171203818	2.7699721036

M05/6-311+G**
Energy: -1182.88155167771

C1	-0.4199649434	-3.8304342994	0.0675441826
C2	-2.4416472658	-2.8818732371	-0.0879838302
C3	-2.0725128916	-1.8408378965	-1.1378309303
C4	-0.8302715068	-2.2879553711	-1.9013284779
C5	0.2550621930	-2.8595178626	-0.9653116089
C6	-1.3899748137	-4.8809484490	-0.5459892247
C7	-3.6750952840	-2.5757809084	0.7150285632
O8	-2.5713169843	-4.1528123697	-0.7258532069
O9	-1.3352949508	-3.0382352258	0.7891734847
O10	0.8662311631	-1.8412972842	-0.2186701598
H11	-2.9064519034	-1.7030024301	-1.8301786896
H12	-1.9097403209	-0.8835657917	-0.6330240953
H13	-1.1104875439	-3.0467414765	-2.6331725967
H14	-0.3862674063	-1.4523986198	-2.4474120481
H15	-1.0153529477	-5.2539736275	-1.4982865165
H16	-4.5415143472	-2.5208552577	0.0539486176
H17	-3.8345999273	-3.3660241592	1.4479994515
H18	-3.5649939033	-1.6201594723	1.2308478567
H19	0.2445933322	-1.5702460884	0.4624989243
C20	-1.5630962212	-6.0966509141	0.3625697749
O21	-2.6432322597	-6.0250150094	1.1282264760
O22	-0.7711719994	-7.0048677182	0.3706731441
C23	0.5820663719	-4.4223689732	1.0630326649
O24	1.6074202059	-4.9567418661	0.4108556847
O25	0.4316695780	-4.4285494729	2.2509077965
C26	1.3688442451	-3.4785633694	-1.8192806930
O27	0.9000752644	-4.5126655759	-2.5378670078
O28	2.4891227351	-3.0680666081	-1.8898734010
C29	1.8515350808	-5.1975000539	-3.3509022366
H30	2.6390094591	-5.6259521146	-2.7286265640
H31	1.2973888371	-5.9854916024	-3.8563198947
H32	2.2986196281	-4.5157763075	-4.0755381634
C33	2.5912516652	-5.6324994065	1.1967742998
H34	2.9658455663	-4.9755166027	1.9814901997
H35	2.1530378621	-6.5280445516	1.6396190844
H36	3.3880366267	-5.8963259878	0.5055335064
C37	-2.8346731990	-7.0966835736	2.0537873431
H38	-3.7772716273	-6.8871468083	2.5539886782
H39	-2.8819579615	-8.0510946497	1.5283182195
H40	-2.0157056644	-7.1199098099	2.7737638238

M06/6-311+G**
Energy: -1182.91870251479

C1	-0.4392938609	-3.8396007492	0.0488408160
C2	-2.4551252647	-2.8906638963	-0.1030492298
C3	-2.0738442551	-1.8344640951	-1.1273594698
C4	-0.8267252712	-2.2686773106	-1.8879497498
C5	0.2420461044	-2.8516504137	-0.9470802542
C6	-1.4013475380	-4.8769366079	-0.5923900407
C7	-3.6933647638	-2.5894594737	0.6838907327
O8	-2.5877387437	-4.1504466859	-0.7624868566
O9	-1.3616980948	-3.0665786359	0.7870214855
O10	0.8360206190	-1.8453188150	-0.1691648840
H11	-2.9074862016	-1.6807035182	-1.8205800825
H12	-1.9136507425	-0.8868739409	-0.5971564471
H13	-1.0986744060	-3.0165306261	-2.6383224490
H14	-0.3709967629	-1.4240168180	-2.4151450529
H15	-1.0152860951	-5.2419732338	-1.5477069534
H16	-4.5500726204	-2.5231609823	0.0084682930

H17	-3.8651571417	-3.3900209819	1.4057759782
H18	-3.5842562645	-1.6382174106	1.2115607029
H19	0.2039438131	-1.5968331160	0.5156159233
C20	-1.5534799151	-6.0784869693	0.3267731231
O21	-2.5821861314	-5.9721114791	1.1536528388
O22	-0.7686167624	-6.9906998278	0.3140842297
C23	0.5462253157	-4.4703085119	1.0254113295
O24	1.5855184536	-4.9603332175	0.3601092129
O25	0.3709668981	-4.5563610203	2.2048396752
C26	1.3703194360	-3.4525228089	-1.7839561019
O27	0.9188845075	-4.4823445386	-2.5194383428
O28	2.4892973972	-3.0414077056	-1.8258509034
C29	1.9164826368	-5.1788974982	-3.2592172652
H30	2.6681936109	-5.5896830968	-2.5792863348
H31	1.4013147748	-5.9827886640	-3.7824862768
H32	2.4088607904	-4.5125587213	-3.9710305847
C33	2.5203584353	-5.7122821823	1.1324515249
H34	2.9059028833	-5.1100141941	1.9571447218
H35	2.0331991894	-6.6076660151	1.5264342265
H36	3.3247191070	-5.9818040669	0.4504863382
C37	-2.6741325985	-6.9956913993	2.1438925736
H38	-3.5661026175	-6.7711786627	2.7257957480
H39	-2.7600058872	-7.9787945286	1.6758403271
H40	-1.7866953380	-6.9763807072	2.7816114060

MPW1PW91/6-311+G**
Energy: -1183.30088421802

C1	-0.4198716729	-3.8409805709	0.0700607180
C2	-2.4341920382	-2.8716907822	-0.0815275309
C3	-2.0535947721	-1.8331504840	-1.1295632950
C4	-0.8243311424	-2.3072191406	-1.9010888563
C5	0.2592221030	-2.8772513147	-0.9616342734
C6	-1.3953702507	-4.8791870773	-0.5510436792
C7	-3.6654893479	-2.5536592795	0.7213752465
O8	-2.5789151176	-4.1408741536	-0.7240083005
O9	-1.3288015964	-3.0394386113	0.7984943315
O10	0.8710225365	-1.8576866586	-0.2131662331
H11	-2.8885449408	-1.6779065835	-1.8160530098
H12	-1.8667953016	-0.8825291218	-0.6217997416
H13	-1.1192025142	-3.0757556652	-2.6165724950
H14	-0.3738458305	-1.4851818626	-2.4611275022
H15	-1.0220698298	-5.2466652147	-1.5055684626
H16	-4.5303564793	-2.4964431955	0.0597323442
H17	-3.8270086768	-3.3402311866	1.4567526114
H18	-3.5470765848	-1.5967157053	1.2312931366
H19	0.2434428891	-1.6008571560	0.4707110762
C20	-1.5822172934	-6.0938337615	0.3529003619
O21	-2.6539087587	-6.0095558434	1.1275614454
O22	-0.8089070011	-7.0175701025	0.3492448230
C23	0.5836710112	-4.4292709658	1.0618145050
O24	1.6117456820	-4.9596765397	0.4129628234
O25	0.4404820702	-4.4252109801	2.2503237210
C26	1.3681119162	-3.5011712189	-1.8132019075
O27	0.8952611700	-4.5262906538	-2.5394940529
O28	2.4896570050	-3.0942300930	-1.8845094847
C29	1.8523959130	-5.1774086055	-3.3762253551
H30	2.6613844569	-5.5905799815	-2.7739042559
H31	1.3097815010	-5.9726982616	-3.8809821418
H32	2.2669516510	-4.4748603215	-4.0994158400
C33	2.6120303365	-5.5799132857	1.2256371105
H34	2.9981089547	-4.8682337020	1.9542341076
H35	2.1882209889	-6.4424540755	1.7391094937
H36	3.3958245321	-5.8877302878	0.5394757283
C37	-2.8435924203	-7.0997438450	2.0330779298
H38	-3.7687267052	-6.8832526752	2.5604270777

H39	-2.9235655898	-8.0389220072	1.4859456919
H40	-2.0088362595	-7.1576852294	2.7312086043

B3LYP/cc-pVTZ
Energy: -1183.67154512295

C1	-0.3970264370	-3.8863304735	0.0839865122
C2	-2.4240301446	-2.9327992901	-0.0824163999
C3	-2.0502917775	-1.8488137772	-1.0869853412
C4	-0.8090493520	-2.2849920791	-1.8668576819
C5	0.2667435715	-2.8971097236	-0.9468929765
C6	-1.3607609955	-4.9469913333	-0.5015666834
C7	-3.6851586980	-2.6726376419	0.6985397440
O8	-2.5171847021	-4.1849637966	-0.7873284283
O9	-1.3291646865	-3.1057197810	0.8225075065
O10	0.9028206930	-1.9005594456	-0.1696397592
H11	-2.8817962094	-1.6822127335	-1.7724578110
H12	-1.8786228435	-0.9171692253	-0.5448800347
H13	-1.0990784999	-3.0179832226	-2.6159570707
H14	-0.3546263705	-1.4392095119	-2.3832579413
H15	-0.9751702247	-5.3992964487	-1.4110217759
H16	-4.5348122035	-2.6435374473	0.0174454973
H17	-3.8346605044	-3.4694681677	1.4220147150
H18	-3.6171766249	-1.7180889134	1.2194185507
H19	0.2868668138	-1.6488692043	0.5294162226
C20	-1.6319815202	-6.0708441119	0.5084419071
O21	-2.8655712354	-6.0244318930	1.0146006497
O22	-0.8114943151	-6.9070303634	0.7962764506
C23	0.6705546557	-4.4248458778	1.0344676755
O24	1.6158207037	-5.0345552913	0.3137808291
O25	0.6779055270	-4.3004764535	2.2258824745
C26	1.3676346046	-3.5117987984	-1.8212704911
O27	0.8716018499	-4.5036577784	-2.5915081358
O28	2.5048265821	-3.1374013538	-1.8727987028
C29	1.8358008421	-5.1690429564	-3.4179705457
H30	2.5913409126	-5.6494554473	-2.7996014929
H31	1.2785166841	-5.9088240654	-3.9836754355
H32	2.3213074916	-4.4588996359	-4.0843324997
C33	2.7733863921	-5.4736675789	1.0328759271
H34	3.2592115563	-4.6223606619	1.5049206083
H35	2.4908155954	-6.2007813952	1.7907018353
H36	3.4267028267	-5.9223434010	0.2925268031
C37	-3.1750023447	-7.0470925267	1.9745292520
H38	-4.2166662403	-6.8927076735	2.2369511368
H39	-3.0288169818	-8.0334403682	1.5383563511
H40	-2.5366223826	-6.9452575953	2.8497841542

BHandHLYP /cc-pVTZ
Energy: -1172.93422749677

C1	-0.4181783480	-3.8685715607	0.0716668389
C2	-2.4154750170	-2.9204491513	-0.0685383752
C3	-2.0445957787	-1.8542674098	-1.0766249355
C4	-0.8298030479	-2.3140891570	-1.8613519855
C5	0.2402629375	-2.8956421818	-0.9387372319
C6	-1.3816150886	-4.9050932888	-0.5203301289
C7	-3.6526876634	-2.6408420133	0.7192567905
O8	-2.5318242408	-4.1547398989	-0.7474248877
O9	-1.3254752650	-3.0965857203	0.8061482001
O10	0.8478830552	-1.9048106064	-0.1758532113
H11	-2.8866030597	-1.6759026680	-1.7506002963
H12	-1.8470537631	-0.9211662071	-0.5388913671
H13	-1.1329753304	-3.0741379887	-2.5843252870
H14	-0.3751138381	-1.4864241018	-2.4123927283
H15	-1.0047804001	-5.3378543549	-1.4470948380
H16	-4.5069265429	-2.5753629930	0.0420184530

H17	-3.8180454412	-3.4535273090	1.4275840932
H18	-3.5510606985	-1.6971548139	1.2593999007
H19	0.2342059773	-1.6570079173	0.5209116299
C20	-1.6092164800	-6.0336926433	0.4661000058
O21	-2.8028000915	-6.0179617815	1.0100571090
O22	-0.7678897931	-6.8461244618	0.7116739990
C23	0.6369114731	-4.4306454676	0.9972254269
O24	1.5928950125	-4.9731003202	0.2769032700
O25	0.6141016822	-4.3754302129	2.1825714513
C26	1.3326314958	-3.5143045117	-1.7914649864
O27	0.8698613919	-4.5356363571	-2.5032566562
O28	2.4467667597	-3.1142184434	-1.8705085704
C29	1.8426764902	-5.2073916249	-3.2724230334
H30	2.6064519156	-5.6361983311	-2.6196463223
H31	1.3191337302	-5.9944049341	-3.8114511038
H32	2.3262503060	-4.5188542172	-3.9677917774
C33	2.6831127809	-5.4990238067	0.9958093228
H34	3.1458829848	-4.7183952623	1.6021229568
H35	2.3470775923	-6.3089900236	1.6455533888
H36	3.3885975289	-5.8682289709	0.2546001376
C37	-3.0476928366	-7.0419302981	1.9526981302
H38	-4.0774136804	-6.9117742003	2.2792514093
H39	-2.9118051612	-8.0234016535	1.4938986018
H40	-2.3611750233	-6.9510532370	2.7966190590

M05/cc-pVTZ
Energy: -1182.96229519934

C1	-0.4211018944	-3.8575691936	0.0736630351
C2	-2.4261875983	-2.9098156848	-0.0893750415
C3	-2.0503881128	-1.8485895659	-1.1105309327
C4	-0.8121711335	-2.2937734945	-1.8759568490
C5	0.2558375296	-2.8844825709	-0.9440363593
C6	-1.3852841113	-4.9052361342	-0.5225411543
C7	-3.6709527047	-2.6182174057	0.6967243524
O8	-2.5444556763	-4.1607856039	-0.7570681298
O9	-1.3366116154	-3.0768603148	0.8010415867
O10	0.8719470332	-1.8878667763	-0.1753492844
H11	-2.8800773523	-1.6941896998	-1.7990529751
H12	-1.8800772406	-0.9075071616	-0.5866243986
H13	-1.1000523749	-3.0403114275	-2.6118362930
H14	-0.3599334012	-1.4588565971	-2.4092066424
H15	-1.0056243776	-5.3243044413	-1.4497528223
H16	-4.5231431245	-2.5610284911	0.0226900531
H17	-3.8403834725	-3.4142777175	1.4161389767
H18	-3.5717269085	-1.6710678522	1.2228952451
H19	0.2466370075	-1.6355627324	0.5080709582
C20	-1.5981743218	-6.0690039107	0.4427119044
O21	-2.7731878381	-6.0216884259	1.0576044156
O22	-0.7701897520	-6.9250066395	0.6104425334
C23	0.6192085397	-4.4302155756	1.0305670493
O24	1.6127453649	-4.9365186615	0.3108520124
O25	0.5459823832	-4.4291306749	2.2227387407
C26	1.3656711571	-3.5113244118	-1.7924087749
O27	0.8804212403	-4.5117865574	-2.5477441716
O28	2.5005059762	-3.1404040735	-1.8293646839
C29	1.8417976287	-5.2146078257	-3.3223885194
H30	2.5483313012	-5.7249490053	-2.6696249209
H31	1.2854839889	-5.9358690543	-3.9117617735
H32	2.3899783310	-4.5320764763	-3.9678835201
C33	2.7084677758	-5.4911714500	1.0138348518
H34	3.1002544315	-4.7751047933	1.7313808885
H35	2.3988906574	-6.3922026308	1.5383557197
H36	3.4583580780	-5.7215914940	0.2650960464
C37	-3.0200739386	-7.0616437420	1.9979862400
H38	-4.0287961805	-6.9000352002	2.3627435120

H39	-2.9380519129	-8.0360546305	1.5211099504
H40	-2.3042088493	-7.0073587676	2.8151715797

M06/cc-pVTZ
Energy: -1182.98524105097

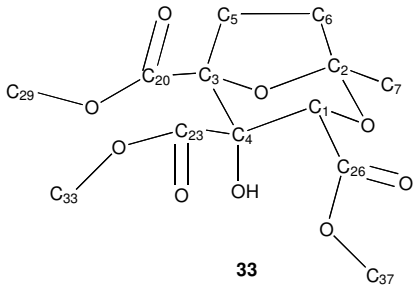
C1	-0.4103681750	-3.8793909033	0.0450372701
C2	-2.4205725805	-2.9328673422	-0.1002516272
C3	-2.0435372367	-1.8522991731	-1.0942156199
C4	-0.8077689088	-2.2789982023	-1.8665934711
C5	0.2573608850	-2.8857618540	-0.9475379811
C6	-1.3726273622	-4.9185230359	-0.5557811779
C7	-3.6708723005	-2.6566959923	0.6688450238
O8	-2.5322113939	-4.1709737698	-0.7941654679
O9	-1.3344837285	-3.1162281711	0.7911015167
O10	0.8733877167	-1.9086407674	-0.1546140655
H11	-2.8780864555	-1.6827612579	-1.7766603056
H12	-1.8769962163	-0.9232756999	-0.5430414819
H13	-1.0909250429	-3.0134655707	-2.6204835594
H14	-0.3465793655	-1.4346992038	-2.3825550426
H15	-0.9888050943	-5.3517072671	-1.4801681498
H16	-4.5119179934	-2.5982150398	-0.0208534021
H17	-3.8465262442	-3.4601421962	1.3801004589
H18	-3.5822324858	-1.7106072463	1.2006830760
H19	0.2457133195	-1.6681931347	0.5353609524
C20	-1.5768133778	-6.0484818247	0.4401683556
O21	-2.7280770404	-5.9624875569	1.0903227074
O22	-0.7525999522	-6.9037903141	0.6170771954
C23	0.6057831529	-4.4727130920	1.0098110539
O24	1.6159678944	-4.9952239623	0.3250087380
O25	0.5023871977	-4.4830564097	2.1966757258
C26	1.3589354819	-3.4677525560	-1.8273275782
O27	0.8810357080	-4.4643152016	-2.5916882764
O28	2.4789082534	-3.0723148465	-1.8881644963
C29	1.8524386234	-5.1312033892	-3.3707113990
H30	2.5898440580	-5.5963918095	-2.7286926161
H31	1.3254359955	-5.8854867834	-3.9456707427
H32	2.3583839686	-4.4353739229	-4.0278720993
C33	2.6328109350	-5.5920600471	1.1067972099
H34	3.0131267690	-4.8763453724	1.8324300018
H35	2.2355755540	-6.4597241466	1.6263714572
H36	3.4153611273	-5.8868271918	0.4149547470
C37	-2.9243714554	-6.9611672083	2.0835380294
H38	-3.9063996793	-6.7777552725	2.5050377703
H39	-2.8776223099	-7.9545969061	1.6420610531
H40	-2.1558317250	-6.8839565964	2.8504358755

MPW1PW91/cc-pVTZ
Energy: -1183.28497130169

C1	-0.4065985668	-3.8825086284	0.0756333890
C2	-2.4137442955	-2.9256546439	-0.0819596233
C3	-2.0382226672	-1.8520807545	-1.0868089582
C4	-0.8128854109	-2.3051811857	-1.8659951862
C5	0.2576468078	-2.9057072521	-0.9459876406
C6	-1.3729977024	-4.9284590646	-0.5070778714
C7	-3.6632682443	-2.6513701016	0.7012786054
O8	-2.5223673554	-4.1690849496	-0.7760655033
O9	-1.3233652011	-3.0989059940	0.8111951465
O10	0.8844492690	-1.9151667999	-0.1737329716
H11	-2.8717690264	-1.6776140594	-1.7672068324
H12	-1.8522292443	-0.9219398405	-0.5471155799
H13	-1.1130844873	-3.0504134442	-2.5997870054
H14	-0.3563309146	-1.4719800524	-2.4002734142
H15	-0.9921846450	-5.3778297360	-1.4207901024
H16	-4.5124432466	-2.6000071876	0.0218492938

H17	-3.8264561783	-3.4542231343	1.4152636855
H18	-3.5757488628	-1.7046496044	1.2316944475
H19	0.2649415053	-1.6766517191	0.5227314808
C20	-1.6247247519	-6.0516588987	0.4952828011
O21	-2.8455967539	-6.0212377680	1.0119249380
O22	-0.7929887125	-6.8764594847	0.7682228322
C23	0.6525749753	-4.4213718456	1.0255128725
O24	1.6059250118	-5.0135256713	0.3163030820
O25	0.6454716432	-4.3065139440	2.2145261341
C26	1.3500404352	-3.5222206439	-1.8168517490
O27	0.8572272527	-4.5122646545	-2.5768676025
O28	2.4821113163	-3.1443210484	-1.8767024333
C29	1.8179930348	-5.1572988337	-3.4052165272
H30	2.5867187808	-5.6264361554	-2.7941564653
H31	1.2711444612	-5.9055803760	-3.9697578812
H32	2.2896912886	-4.4388808699	-4.0730025047
C33	2.7274463786	-5.4717987467	1.0589712625
H34	3.2102318383	-4.6334190229	1.5568314605
H35	2.4130057165	-6.2027159247	1.8002088381
H36	3.3998163492	-5.9211509535	0.3365311829
C37	-3.1209163144	-7.0480139310	1.9617215752
H38	-4.1596438032	-6.9153683786	2.2459170900
H39	-2.9665336428	-8.0291432228	1.5166126742
H40	-2.4687881354	-6.9452703375	2.8268945424

Structure 33



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B3LYP/6-31G**
Energy: -1183.25866512146

C1	0.7001653188	-0.9584324427	-1.0015189185
C2	-1.1758479801	-1.3368264656	0.4464344279
C3	0.8032998195	-2.0645058678	1.2684602935
C4	1.4851695619	-2.0170151465	-0.1557627715
C5	0.6286123652	-0.6846663020	1.9490615619
C6	-0.7262959479	-0.1936004666	1.3863708381
C7	-2.6640290622	-1.5896810907	0.3471250392
O8	-0.5414253658	-2.4961390827	1.0044260477
O9	-0.7037878878	-1.1549532119	-0.8864415594
O10	1.3605403306	-3.2907759881	-0.7402363768
H11	0.9882710410	0.0490100264	-0.6814841731
H12	0.5874081118	-0.8215197058	3.0314629094
H13	1.4645312764	-0.0212764382	1.7321824100
H14	-0.6602062330	0.7533889387	0.8449008359
H15	-1.4630495240	-0.0678019709	2.1832783726
H16	-2.8501750171	-2.4271483594	-0.3286404173
H17	-3.0692767978	-1.8261429784	1.3334630190
H18	-3.1670635991	-0.7034957654	-0.0473162860
H19	0.4381603964	-3.5552948808	-0.5907567165
C20	1.5435105631	-3.0668373844	2.1462105302
O21	0.9655260266	-4.2711227868	2.1817056479
O22	2.5671240569	-2.7699827791	2.7257369717
C23	2.9911125718	-1.7075028565	-0.1018973355
O24	3.2171650942	-0.4140344662	0.2145979765

O25	3.8566721909	-2.5198089359	-0.3031977610
C26	1.1370965319	-1.0889371955	-2.4592317974
O27	0.2144187770	-1.6448875079	-3.2492292261
O28	2.2372007430	-0.7320076707	-2.8251071083
C29	1.6802853388	-5.2695410560	2.9366004871
H30	2.6714103049	-5.4280737310	2.5062942293
H31	1.0778182092	-6.1742268001	2.8644022256
H32	1.7871837586	-4.9577467103	3.9780198759
C33	4.6075974397	-0.0425111123	0.2689138342
H34	5.1304435085	-0.6421343766	1.0168865785
H35	5.0721657649	-0.1939759334	-0.7075308142
H36	4.6185714512	1.0124930285	0.5412063706
C37	0.6278385056	-1.8488499672	-4.6136399541
H38	1.4903143779	-2.5181376293	-4.6510097278
H39	-0.2302411405	-2.2967926128	-5.1136863766
H40	0.8943633640	-0.8980239200	-5.0807772956

B3LYP/6-31G** with CH_2Cl_2 model (single point)
Energy: -1183.28421220437

B3LYP/6-31G** with CH_2Cl_2 model (optimisation)
Energy: -1183.28502064885

C1	0.6922317317	-1.0186524320	-1.0244777589
C2	-1.1803070303	-1.4041292530	0.4279214939
C3	0.8144237285	-2.0853938045	1.2618823600
C4	1.4943565671	-2.0477821957	-0.1636049813
C5	0.6122954963	-0.6974757138	1.9226573010
C6	-0.7458472525	-0.2363860427	1.3408892171
C7	-2.6641299642	-1.6806249304	0.3401566876
O8	-0.5204462500	-2.5450536845	1.0058675215
O9	-0.7060269743	-1.2536331940	-0.9145781238
O10	1.3828522690	-3.3369709958	-0.7249171379
H11	0.9477905532	0.0007473745	-0.7092685001
H12	0.5578016396	-0.8172555167	3.0069971480
H13	1.4381985089	-0.0216398985	1.7054347123
H14	-0.6887846775	0.7005313236	0.7812762016
H15	-1.4877548005	-0.1035255284	2.1314282852
H16	-2.8504247051	-2.5284844687	-0.3236777246
H17	-3.0574052673	-1.9068991051	1.3338840427
H18	-3.1811551905	-0.8023052623	-0.0548171540
H19	0.4587763869	-3.6088204194	-0.5907235779
C20	1.5752425293	-3.0581641854	2.1572391634
O21	0.9221036225	-4.1903962479	2.4093702429
O22	2.6810820959	-2.7836554454	2.5826670207
C23	2.9961454539	-1.7184818161	-0.1244528262
O24	3.2184230443	-0.4343350058	0.1940221810
O25	3.8668201480	-2.5283424141	-0.3433474475
C26	1.1424111748	-1.1340537976	-2.4809910157
O27	0.1594881803	-1.3933429683	-3.3385063066
O28	2.3088805033	-0.9783878205	-2.7896815931
C29	1.6161647730	-5.1502681101	3.2464404923
H30	2.5524892825	-5.4539742780	2.7743974595
H31	0.9376101574	-5.9977045185	3.3363381487
H32	1.8235182756	-4.7170237392	4.2274027126
C33	4.6087165970	-0.0380311208	0.2589376629
H34	5.1340561418	-0.6276170517	1.0130446546
H35	5.0837979795	-0.1790256429	-0.7141671024
H36	4.5994032023	1.0166240539	0.5326477012
C37	0.5471794773	-1.4975544055	-4.7316635648
H38	1.2688554254	-2.3059753948	-4.8631240771
H39	-0.3735544669	-1.7122585154	-5.2726261594
H40	0.9848492442	-0.5575003198	-5.0742569489

LMP2/6-31G**
Energy: -1179.86566809228 (single point)
Energy: -1179.86659914526 (minimised)

C1	0.6858476699	-0.9958182176	-1.0065761616
C2	-1.1924492304	-1.3371008250	0.4376629611
C3	0.7803578015	-2.0403710357	1.2782078135
C4	1.4346878009	-2.0419364695	-0.1448334444
C5	0.6092684018	-0.6472607773	1.9130735881
C6	-0.7315297799	-0.1643194856	1.3224201702
C7	-2.6778246177	-1.5833576753	0.3426873803
O8	-0.5762658963	-2.4831583146	1.0530669613
O9	-0.7214418320	-1.2221939394	-0.9125798089
O10	1.2584738316	-3.3309139369	-0.7021894463
H11	0.9443650528	0.0140450406	-0.6855108622
H12	0.5467219250	-0.7602180783	2.9934699695
H13	1.4490099419	0.0031303956	1.6917927648
H14	-0.6532257931	0.7546856163	0.7449080742
H15	-1.4685507264	-0.0045812183	2.1072654106
H16	-2.8586006092	-2.4392259774	-0.3014319281
H17	-3.0797587824	-1.7815181137	1.3331321662
H18	-3.1667853835	-0.7101688380	-0.0818952448
H19	0.3257095378	-3.5418622035	-0.5419541596
C20	1.5486424770	-3.0110089833	2.1643977191
O21	1.0141253806	-4.2417422261	2.2183529298
O22	2.5826204108	-2.6691084992	2.7213995372
C23	2.9412640008	-1.7779495504	-0.0974603216
O24	3.1843008350	-0.4701841195	0.1735320110
O25	3.8057302005	-2.6164463630	-0.2487980301
C26	1.1560453539	-1.1278553999	-2.4523531754
O27	0.2131840164	-1.5599975839	-3.3041987095
O28	2.3070211828	-0.8603198489	-2.7629962876
C29	1.8416684272	-5.1989401534	2.9232474597
H30	2.8153512980	-5.2697197181	2.4458265461
H31	1.3053148043	-6.1387854839	2.8513760032
H32	1.9664516855	-4.9023726620	3.9613383224
C33	4.5903146740	-0.1439494652	0.2482946932
H34	5.0684223803	-0.7273431347	1.0298309435
H35	5.0674354492	-0.3450247031	-0.7063178956
H36	4.6238723800	0.9148379253	0.4802659565
C37	0.6937695512	-1.7100794107	-4.6604329867
H38	1.4903936320	-2.4479519364	-4.6964982818
H39	-0.1682514332	-2.0430519713	-5.2275251183
H40	1.0632919781	-0.7610342289	-5.0395946761

BHandHLYP/6-31G**
Energy: -1172.52879856130

C1	0.6897035180	-0.9723587279	-0.9815328933
C2	-1.1588699614	-1.3481706858	0.4360222295
C3	0.7923235569	-2.0510642448	1.2566187042
C4	1.4600546709	-2.0174605525	-0.1480727743
C5	0.6313492587	-0.6749556463	1.9126067668
C6	-0.7160915825	-0.1981165012	1.3497006606
C7	-2.6349078108	-1.5981828403	0.3438924652
O8	-0.5307190172	-2.4774199577	1.0047848571
O9	-0.6893615164	-1.1864102635	-0.8770064986
O10	1.3167091218	-3.2723248862	-0.7200650442
H11	0.9720089873	0.0406145515	-0.6617264635
H12	0.5980517206	-0.7951833694	2.9995047921
H13	1.4733460639	-0.0202114807	1.6784683563
H14	-0.6578374657	0.7420788349	0.7911556067
H15	-1.4553183213	-0.0652378366	2.1458457937
H16	-2.8196933072	-2.4416370985	-0.3280081467
H17	-3.0367197270	-1.8291519427	1.3349138896
H18	-3.1379564075	-0.7127000218	-0.0569737386
H19	0.4074959586	-3.5482663426	-0.5441629022
C20	1.5386965692	-3.0383209066	2.1189640229

O21	0.9887116075	-4.2320456035	2.1561592161
O22	2.5562266948	-2.7334748300	2.6782137393
C23	2.9511536665	-1.7186730633	-0.0943937783
O24	3.1863505287	-0.4425065689	0.1917317161
O25	3.7996237061	-2.5366086136	-0.2662489681
C26	1.1497771263	-1.1220668720	-2.4129646842
O27	0.2301976576	-1.5817792392	-3.2309168270
O28	2.2768324152	-0.8574860018	-2.7325480596
C29	1.7282345701	-5.2086573379	2.8716844981
H30	2.7148244578	-5.3410524002	2.4174124094
H31	1.1481737035	-6.1305128926	2.8091254477
H32	1.8575009515	-4.9044141051	3.9148894508
C33	4.5595384463	-0.0938405123	0.2369402921
H34	5.0780957054	-0.6919822357	0.9920600494
H35	5.0210601442	-0.2700082768	-0.7392608323
H36	4.5953556385	0.9665847294	0.4924774754
C37	0.6734947677	-1.8028107650	-4.5590244867
H38	1.4899816117	-2.5313842247	-4.5696806084
H39	-0.1903319477	-2.1847271287	-5.1052852589
H40	1.0304876030	-0.8701045141	-5.0067255877

M05/6-31G**
Energy: -1182.63696376147

C1	0.7375915431	-1.0781535596	-1.0320328944
C2	-1.1631175332	-1.4646294726	0.3752888840
C3	0.8195248577	-2.0677138914	1.2550556704
C4	1.5213710875	-2.1010077721	-0.1603721442
C5	0.5806761443	-0.6584089698	1.8391068865
C6	-0.7938652309	-0.2735542849	1.2697272437
C7	-2.6327491389	-1.7801508577	0.2487267416
O8	-0.4984646131	-2.5603882910	1.0028810740
O9	-0.6558312258	-1.3206484292	-0.9422999109
O10	1.4039738884	-3.3877217164	-0.6883160795
H11	0.9771052928	-0.0605511168	-0.6983596421
H12	0.5539617892	-0.7222511959	2.9275531797
H13	1.3813262155	0.0294177214	1.5735357582
H14	-0.7963505358	0.6593147889	0.7027976042
H15	-1.5364915861	-0.1766136606	2.0639567547
H16	-2.7756449094	-2.6425263968	-0.4032397975
H17	-3.0539495298	-2.0020190906	1.2303231889
H18	-3.1621397021	-0.9281590797	-0.1813032645
H19	0.4913971771	-3.6553691279	-0.5195431131
C20	1.5652590059	-2.9678594039	2.2340742652
O21	0.9397892976	-4.1325260407	2.4050172023
O22	2.5930823373	-2.6308532273	2.7776901932
C23	3.0284956620	-1.8138917421	-0.0983345658
O24	3.2400588281	-0.5019168000	0.1203164272
O25	3.8901641961	-2.6436837283	-0.2097320189
C26	1.1850995053	-1.1287856027	-2.4916477903
O27	0.1432056511	-1.2658148427	-3.3146254048
O28	2.3389058966	-1.0012482687	-2.8331023154
C29	1.5631716586	-5.0667007847	3.2929113703
H30	2.5353413939	-5.3672918044	2.8994562568
H31	0.8860492443	-5.9185170706	3.3390057407
H32	1.6927698893	-4.6242791931	4.2822244188
C33	4.6128613206	-0.1020194245	0.1545381649
H34	5.1526200516	-0.6720942436	0.9118172866
H35	5.0668474377	-0.2672165049	-0.8241262683
H36	4.6040984787	0.9590387996	0.3992125302
C37	0.4199852204	-1.2652158553	-4.7173778781
H38	1.0641359120	-2.1058182845	-4.9800750218
H39	-0.5503769639	-1.3602461222	-5.2039540410
H40	0.9041973931	-0.3322356129	-5.0122335481

M06/6-31G**
Energy: -1182.63314535950

C1	0.6771214584	-0.9575191975	-0.9977310544
C2	-1.1747087960	-1.3669823137	0.4432422806
C3	0.7974643396	-2.0683729099	1.2381911671
C4	1.4580960547	-2.0145589540	-0.1765289942
C5	0.6153916121	-0.7019547451	1.9199097146
C6	-0.7418282743	-0.2314260066	1.3773895992
C7	-2.6511470107	-1.6268357486	0.3555374249
O8	-0.5345003227	-2.5131032378	0.9951169907
O9	-0.7128673783	-1.1742319672	-0.8818727660
O10	1.3178525657	-3.2719638073	-0.7696439104
H11	0.9579109359	0.0555763163	-0.6687514375
H12	0.5840424958	-0.8460204224	3.0043954297
H13	1.4482777127	-0.0299403521	1.7033804403
H14	-0.7054238573	0.7234374806	0.8417118489
H15	-1.4786293471	-0.1294331886	2.1810826595
H16	-2.8400207950	-2.4594886247	-0.3278279450
H17	-3.0431250919	-1.8768603400	1.3458436246
H18	-3.1644751708	-0.7379412384	-0.0232645982
H19	0.3948330372	-3.5291648089	-0.6305347340
C20	1.5813268853	-3.0325945982	2.1021638643
O21	0.9941470323	-4.2128086841	2.2630197059
O22	2.6481370817	-2.7163776939	2.5745192245
C23	2.9595812365	-1.7341764792	-0.1298525839
O24	3.2104583093	-0.4733419611	0.2552685819
O25	3.8026739030	-2.5484491608	-0.3816103510
C26	1.1304684493	-1.0848028170	-2.4389917664
O27	0.1988632375	-1.5687734929	-3.2529675825
O28	2.2537375274	-0.7885935772	-2.7691635320
C29	1.7447361332	-5.1561929531	3.0328995094
H30	2.7022869165	-5.3630159421	2.5466729317
H31	1.1321635723	-6.0570935336	3.0788336420
H32	1.9332748325	-4.7669476994	4.0379763186
C33	4.6007002735	-0.1648343610	0.3615916920
H34	5.0740691741	-0.8220939670	1.0977093093
H35	5.0898435864	-0.2978947891	-0.6079090621
H36	4.6545120950	0.8766490212	0.6808247334
C37	0.6244639951	-1.7639676526	-4.6026045403
H38	1.4546211528	-2.4754137958	-4.6390084141
H39	-0.2430741015	-2.1570241612	-5.1342047727
H40	0.9497236424	-0.8175147082	-5.0449412877

MPW1PW91/6-31G**
Energy: -1182.98179041348

C1	0.6921779584	-0.9695156552	-0.9901826773
C2	-1.1667500005	-1.3512053766	0.4402849659
C3	0.7989961933	-2.0598962756	1.2598133919
C4	1.4705706116	-2.0267228133	-0.1575426986
C5	0.6305227406	-0.6790827457	1.9192995446
C6	-0.7219449429	-0.2022260184	1.3626370181
C7	-2.6485484648	-1.6058745252	0.3463452073
O8	-0.5351257994	-2.4954229782	1.0068526897
O9	-0.6997393378	-1.1806710494	-0.8853081554
O10	1.3294896921	-3.2909682546	-0.7339234270
H11	0.9732037929	0.0364460930	-0.6585737368
H12	0.5997367582	-0.8004305879	3.0027675812
H13	1.4648859026	-0.0202206737	1.6855667547
H14	-0.6659127573	0.7391268621	0.8125187163
H15	-1.4551632137	-0.0749270639	2.1608291497
H16	-2.8330368249	-2.4477372674	-0.3219025876
H17	-3.0498895722	-1.8354926300	1.3340430102
H18	-3.1521147178	-0.7246151959	-0.0535909407
H19	0.4099673812	-3.5446070597	-0.5714367084
C20	1.5456996298	-3.0448955874	2.1400552324

O21	0.9835390024	-4.2471477017	2.1832186605
O22	2.5637068312	-2.7350013152	2.7141469250
C23	2.9706865109	-1.7296434474	-0.1092454363
O24	3.2055784083	-0.4477358076	0.2075949259
O25	3.8248754781	-2.5473664704	-0.3139696913
C26	1.1400649697	-1.0855211293	-2.4378347786
O27	0.2236231079	-1.6141335579	-3.2399410531
O28	2.2445640646	-0.7389862740	-2.7865460663
C29	1.7126176780	-5.2210316304	2.9363899707
H30	2.7027679356	-5.3668112607	2.5027790982
H31	1.1270516962	-6.1357577886	2.8761384382
H32	1.8210812440	-4.9001222890	3.9734272124
C33	4.5901748625	-0.0965209435	0.2613892149
H34	5.1056214390	-0.7036506121	1.0064575841
H35	5.0520874639	-0.2511285811	-0.7142884306
H36	4.6168861082	0.9561160325	0.5358569998
C37	0.6528413387	-1.7995012035	-4.5909652853
H38	1.5081439372	-2.4757814467	-4.6259022827
H39	-0.1993708419	-2.2299134383	-5.1126255631
H40	0.9367232155	-0.8458326478	-5.0384579402

B3LYP/6-31++G**
Energy: -1183.30103901240

C1	0.6990529242	-0.9739642379	-1.0075661193
C2	-1.1760903001	-1.3571208168	0.4476129079
C3	0.8146122414	-2.0773746650	1.2626518244
C4	1.4939837942	-2.0351442869	-0.1677839792
C5	0.6347330589	-0.6925088363	1.9361606917
C6	-0.7252042159	-0.2096411626	1.3789945109
C7	-2.6635089022	-1.6147353090	0.3536398517
O8	-0.5299176739	-2.5119632122	1.0046037206
O9	-0.7033802377	-1.1799726285	-0.8885296365
O10	1.3728873885	-3.3098870999	-0.7531180413
H11	0.9793423994	0.0308855795	-0.6732200845
H12	0.5973062991	-0.8259160286	3.0193182502
H13	1.4662192489	-0.0250564515	1.7148294370
H14	-0.6652391959	0.7365119961	0.8347822721
H15	-1.4581112104	-0.0855013666	2.1798264784
H16	-2.8526376728	-2.4536863409	-0.3200038072
H17	-3.0632602676	-1.8500252353	1.3428952538
H18	-3.1693613139	-0.7287462921	-0.0387738837
H19	0.4575653188	-3.5995272690	-0.6086324179
C20	1.5530180289	-3.0692284105	2.1575863091
O21	0.9500772153	-4.2565317893	2.2541549112
O22	2.5943949277	-2.7732011766	2.7092405653
C23	3.0027768304	-1.7193517197	-0.1237964428
O24	3.2277271649	-0.4386220153	0.2330429931
O25	3.8682172773	-2.5219706848	-0.3695717506
C26	1.1235848846	-1.0662501319	-2.4730397248
O27	0.2098528531	-1.6235119852	-3.2698321800
O28	2.2111113107	-0.6669513043	-2.8399749833
C29	1.6440680173	-5.2481085850	3.0427878420
H30	2.6251705830	-5.4503158022	2.6080388615
H31	1.0121312646	-6.1344457992	3.0068449552
H32	1.7646339053	-4.8978370019	4.0703528239
C33	4.6157868235	-0.0482150860	0.2922964201
H34	5.1471970555	-0.6639651803	1.0209166994
H35	5.0748034680	-0.1610629054	-0.6920301504
H36	4.6089552248	0.9975483346	0.5981277468
C37	0.6019600274	-1.7825443832	-4.6497509315
H38	1.4809118013	-2.4274169547	-4.7169218007
H39	-0.2555721219	-2.2424817093	-5.1393497186
H40	0.8286164242	-0.8110269828	-5.0947015756

B3LYP/6-311+G**
Energy: -1183.55758137712

C1	0.7013257623	-0.9708827804	-1.0063749851
C2	-1.1750137742	-1.3424495067	0.4401695844
C3	0.8049257287	-2.0653369453	1.2646300900
C4	1.4864533142	-2.0277599747	-0.1601277436
C5	0.6310576456	-0.6807519634	1.9320829009
C6	-0.7235519499	-0.1945783790	1.3698308545
C7	-2.6613902438	-1.5930347527	0.3434606538
O8	-0.5386440524	-2.4977989351	1.0034074963
O9	-0.7013176546	-1.1703164987	-0.8922032303
O10	1.3600657592	-3.3034700585	-0.7393195039
H11	0.9840787399	0.0345816861	-0.6821802204
H12	0.5910190015	-0.8091892671	3.0136052161
H13	1.4640977333	-0.0199720458	1.7076830875
H14	-0.6573398169	0.7458968338	0.8209448335
H15	-1.4570213797	-0.0643924789	2.1662063757
H16	-2.8481726868	-2.4276971091	-0.3328992382
H17	-3.0627483171	-1.8301657874	1.3294968294
H18	-3.1618663264	-0.7060763423	-0.0485374407
H19	0.4491832940	-3.5832075003	-0.5730596269
C20	1.5454011121	-3.0587746476	2.1528089153
O21	0.9708024254	-4.2605367578	2.1946309248
O22	2.5594428079	-2.7562465518	2.7329546253
C23	2.9935384119	-1.7188652039	-0.1094778362
O24	3.2175652066	-0.4315993064	0.2224626284
O25	3.8528120470	-2.5232808703	-0.3262434747
C26	1.1387093149	-1.0903213743	-2.4641816015
O27	0.2163447148	-1.6335164049	-3.2577911752
O28	2.2319181582	-0.7285910187	-2.8248389665
C29	1.6807264056	-5.2598143323	2.9555288797
H30	2.6668515041	-5.4268393301	2.5213464032
H31	1.0711371648	-6.1574320681	2.8891617948
H32	1.7905946237	-4.9408340190	3.9926193970
C33	4.6051127525	-0.0459447572	0.2748807200
H34	5.1339845313	-0.6461959146	1.0156191635
H35	5.0644321891	-0.1824547666	-0.7043241493
H36	4.6041068233	1.0046045798	0.5564321755
C37	0.6181909344	-1.8169213255	-4.6300549095
H38	1.4736842783	-2.4912806884	-4.6827574571
H39	-0.2465679791	-2.2496473695	-5.1271886409
H40	0.8856787157	-0.8601932129	-5.0803524821

BHandHLYP/6-311+G**
Energy: -1172.82880880774

C1	0.6925933603	-1.0053215755	-0.9908273166
C2	-1.1554213747	-1.3699713068	0.4276012019
C3	0.7989673619	-2.0607457047	1.2515548505
C4	1.4682144890	-2.0465046521	-0.1557499706
C5	0.6350371199	-0.6746408047	1.8858872690
C6	-0.7135278893	-0.2088950758	1.3225079712
C7	-2.6289524064	-1.6203458038	0.3387186108
O8	-0.5213864231	-2.4897796695	1.0067391049
O9	-0.6824260044	-1.2248350993	-0.8857617776
O10	1.3276183313	-3.3046475441	-0.7183049025
H11	0.9669309152	0.0047631061	-0.6587035031
H12	0.6026564828	-0.7811407480	2.9733426200
H13	1.4730636315	-0.0206267372	1.6426599897
H14	-0.6581587478	0.7228417422	0.7516472893
H15	-1.4498578337	-0.0697427280	2.1185508290
H16	-2.8171110827	-2.4702435704	-0.3232315343
H17	-3.0288915139	-1.8382232994	1.3328582133
H18	-3.1294761061	-0.7378779725	-0.0708075772
H19	0.4313145445	-3.6053058074	-0.5326100587
C20	1.5459108706	-3.0256733613	2.1394107532

O21	0.9861784536	-4.2076607778	2.2239391312
O22	2.5636508289	-2.7094110444	2.6807824404
C23	2.9605977483	-1.7426181895	-0.1071337203
O24	3.1880015052	-0.4738596740	0.1987043561
O25	3.8062231208	-2.5503771270	-0.3015800041
C26	1.1490111196	-1.1202143255	-2.4265064396
O27	0.2185189998	-1.5217931964	-3.2561801671
O28	2.2747798928	-0.8633313135	-2.7374990830
C29	1.7068374753	-5.1735177920	2.9730730814
H30	2.6920575737	-5.3350967471	2.5273392961
H31	1.1116850006	-6.0855028954	2.9331594840
H32	1.8317908573	-4.8396999244	4.0068987388
C33	4.5548705260	-0.1007040375	0.2455006205
H34	5.0826792883	-0.6934903905	0.9975165409
H35	5.0176872527	-0.2593322143	-0.7324062057
H36	4.5697873715	0.9571844702	0.5090543769
C37	0.6334459985	-1.6867024094	-4.6017695806
H38	1.4348678466	-2.4281308336	-4.6618699564
H39	-0.2477426289	-2.0272665047	-5.1452621980
H40	0.9951358172	-0.7387254175	-5.0100364538

M05/6-311+G**
Energy: -1182.88099642716

C1	0.6982172763	-1.0030753401	-1.0062739975
C2	-1.1621162819	-1.3748703106	0.4361183680
C3	0.8059037857	-2.0730382824	1.2538600443
C4	1.4834260353	-2.0525916002	-0.1671238215
C5	0.6235860451	-0.6930679471	1.9085788628
C6	-0.7244898750	-0.2249846717	1.3516566093
C7	-2.6397768948	-1.6320205696	0.3394485372
O8	-0.5212466957	-2.5096166623	1.0045337813
O9	-0.6867120586	-1.2101127007	-0.8873936022
O10	1.3516544125	-3.3195935198	-0.7328640071
H11	0.9763351662	0.0011492349	-0.6699470132
H12	0.5841196377	-0.8171416123	2.9910754646
H13	1.4523430813	-0.0257435540	1.6868512510
H14	-0.6704338930	0.7154134841	0.8010863000
H15	-1.4586854547	-0.0991022895	2.1479130135
H16	-2.8273892809	-2.4748712744	-0.3261796969
H17	-3.0439294698	-1.8574541248	1.3268683884
H18	-3.1429324196	-0.7513240827	-0.0626669470
H19	0.4449074534	-3.6044556313	-0.5784409246
C20	1.5606395935	-3.0386986638	2.1544006270
O21	0.9585810040	-4.2108195696	2.2894929558
O22	2.6056702420	-2.7335385389	2.6680246890
C23	2.9879478731	-1.7481256429	-0.1234290969
O24	3.2129547705	-0.4757291423	0.2243959164
O25	3.8396780663	-2.5504555322	-0.3615472663
C26	1.1403977514	-1.0816640608	-2.4595222545
O27	0.2127551452	-1.5617865603	-3.2738838746
O28	2.2418691018	-0.7323842683	-2.7978464435
C29	1.6544640059	-5.1895373446	3.0659126453
H30	2.6203552374	-5.4106154346	2.6107357655
H31	1.0171147829	-6.0704893986	3.0629854633
H32	1.8091287713	-4.8293794922	4.0837954945
C33	4.5844615931	-0.0806501191	0.2794696516
H34	5.1239407707	-0.6917126124	1.0039386332
H35	5.0427171748	-0.1890543867	-0.7042411736
H36	4.5792265878	0.9633521742	0.5855261193
C37	0.5915092229	-1.6946319933	-4.6450494473
H38	1.4339168983	-2.3808929019	-4.7386158254
H39	-0.2849005922	-2.0906421434	-5.1528380261
H40	0.8708229071	-0.7251589380	-5.0598460636

M06/6-311+G**
Energy: -1182.91643541680

C1	0.6848743348	-0.9948743914	-1.0001380954
C2	-1.1664581419	-1.3665133400	0.4381256946
C3	0.7965351190	-2.0711791703	1.2507560478
C4	1.4646230039	-2.0394500777	-0.1633799876
C5	0.6213172157	-0.6963788347	1.9123623339
C6	-0.7207714408	-0.2174346561	1.3467437926
C7	-2.6419744577	-1.6092436427	0.3527394695
O8	-0.5346501775	-2.5052498362	1.0093428673
O9	-0.6996463452	-1.2093123134	-0.8882645525
O10	1.3305328346	-3.3037163486	-0.7395221882
H11	0.9622557833	0.0167774450	-0.6709185116
H12	0.5731344478	-0.8307746509	2.9959869274
H13	1.4610020712	-0.0344866793	1.7022125885
H14	-0.6598333717	0.7213230036	0.7894238330
H15	-1.4615793763	-0.0829502719	2.1391402439
H16	-2.8414422932	-2.4505726386	-0.3142893878
H17	-3.0383870127	-1.8326911393	1.3458071569
H18	-3.1396860693	-0.7206883709	-0.0437951487
H19	0.4220045496	-3.5925578978	-0.5819148995
C20	1.5655208517	-3.0350047885	2.1289038341
O21	0.9741637341	-4.2100681212	2.2698413649
O22	2.6177794353	-2.7241134330	2.6202175361
C23	2.9638122675	-1.7398950572	-0.1191394179
O24	3.1908636351	-0.4699092116	0.2365279390
O25	3.8127784953	-2.5412596612	-0.3602865935
C26	1.1481714179	-1.1066429651	-2.4384629797
O27	0.2161627994	-1.5454153095	-3.2681053600
O28	2.2736504484	-0.8215885613	-2.7507167809
C29	1.7051585694	-5.1725554320	3.0300393176
H30	2.6715976217	-5.3687212446	2.5609870128
H31	1.0934824006	-6.0726851303	3.0377290371
H32	1.8692710806	-4.8126647571	4.0483689741
C33	4.5671902044	-0.1011682668	0.2778558000
H34	5.1045262294	-0.7226265081	0.9982792104
H35	5.0163874871	-0.2226078864	-0.7111321522
H36	4.5921516718	0.9443311012	0.5811696408
C37	0.6365115209	-1.7040850725	-4.6220697238
H38	1.4585865135	-2.4203690336	-4.6831481037
H39	-0.2332333088	-2.0727798584	-5.1628662205
H40	0.9669964953	-0.7486151292	-5.0363809329

MPW1PW91/6-311+G**
Energy: -1183.28502943178

C1	0.6929121383	-0.9924943187	-0.9954954580
C2	-1.1644615430	-1.3662749330	0.4370307733
C3	0.8038991216	-2.0700372581	1.2564277211
C4	1.4777987290	-2.0464143363	-0.1626769991
C5	0.6337974003	-0.6845039417	1.9041752364
C6	-0.7166609229	-0.2115649536	1.3456489606
C7	-2.6446844241	-1.6166390162	0.3487357582
O8	-0.5278904030	-2.5050960707	1.0071333230
O9	-0.6952692402	-1.2087862892	-0.8893576806
O10	1.3423194861	-3.3124491579	-0.7344361577
H11	0.9679974026	0.0100761109	-0.6533493027
H12	0.6009703273	-0.7995809402	2.9871992893
H13	1.4661421041	-0.0269147380	1.6675217294
H14	-0.6583122275	0.7230281159	0.7866673230
H15	-1.4483660121	-0.0770733865	2.1421706301
H16	-2.8368365857	-2.4606551517	-0.3131798142
H17	-3.0422790772	-1.8368103052	1.3392625036
H18	-3.1440721121	-0.7348332862	-0.0535238363
H19	0.4347060609	-3.5919561835	-0.5661129053
C20	1.5506346380	-3.0427421810	2.1512359539

O21	0.9739525924	-4.2311783853	2.2361298754
O22	2.5735468651	-2.7309408471	2.7036444929
C23	2.9787199085	-1.7401876482	-0.1191046349
O24	3.2065674971	-0.4665004355	0.2187316090
O25	3.8309568220	-2.5444432161	-0.3497139786
C26	1.1382139817	-1.0809309745	-2.4455914100
O27	0.2222719892	-1.5847229501	-3.2568357934
O28	2.2361476033	-0.7237932365	-2.7861258786
C29	1.6858906175	-5.2025130114	3.0088812268
H30	2.6704118944	-5.3768242021	2.5755886093
H31	1.0821051024	-6.1048971835	2.9679674265
H32	1.7993719822	-4.8614709794	4.0379164324
C33	4.5851129652	-0.0906453411	0.2660878917
H34	5.1152379918	-0.6959608795	1.0009999614
H35	5.0405147461	-0.2234720960	-0.7149013679
H36	4.5940048652	0.9578683930	0.5529300574
C37	0.6303127582	-1.7304647117	-4.6192619306
H38	1.4859877270	-2.4020345378	-4.6859368060
H39	-0.2286526516	-2.1498593875	-5.1362423830
H40	0.8991638808	-0.7627191489	-5.0426682971

B3LYP/cc-pVTZ
Energy: -1183.67307230442

C1	0.7156786555	-0.9821280284	-1.0003074259
C2	-1.1450658731	-1.3712105255	0.4432205534
C3	0.8300939270	-2.1105986474	1.2476145648
C4	1.5139361886	-2.0240256945	-0.1607295451
C5	0.6478517881	-0.7571615975	1.9629139132
C6	-0.6856206319	-0.2431426702	1.3868479770
C7	-2.6298165859	-1.6045852669	0.3570334287
O8	-0.5095795738	-2.5335502838	0.9759294387
O9	-0.6807829609	-1.1800093164	-0.8840589900
O10	1.4267133736	-3.2956615673	-0.7562128606
H11	0.9954264006	0.0238570987	-0.6831803627
H12	0.5776899455	-0.9276798503	3.0348074526
H13	1.4839162862	-0.0902330426	1.7894630252
H14	-0.5874228999	0.6958513478	0.8456265707
H15	-1.4273156137	-0.0949382041	2.1687667869
H16	-2.8357698959	-2.4214354211	-0.3312728758
H17	-3.0216165270	-1.8539038991	1.3411275094
H18	-3.1220459380	-0.7052670538	-0.0108844213
H19	0.5172501394	-3.5944982281	-0.6273415993
C20	1.5612895003	-3.1283016102	2.1115414671
O21	0.8690316425	-4.2506605896	2.2990668462
O22	2.6471772101	-2.9032667600	2.5852008127
C23	3.0060185274	-1.6603150480	-0.1071090328
O24	3.1762862105	-0.3584985048	0.1965819109
O25	3.8997352302	-2.4286304780	-0.3084822186
C26	1.1417797847	-1.1031064756	-2.4592371037
O27	0.1860797719	-1.5797076356	-3.2538384840
O28	2.2457698404	-0.7882009963	-2.8286058038
C29	1.5149018543	-5.2353898914	3.1230487863
H30	2.4597597911	-5.5375905125	2.6764548379
H31	0.8231324611	-6.0697436229	3.1714408998
H32	1.7028391285	-4.8315420515	4.1165505166
C33	4.5426764281	0.0798393827	0.2451949239
H34	5.0851973179	-0.4654978078	1.0148671207
H35	5.0199682765	-0.0833270606	-0.7186665401
H36	4.5019207285	1.1393865545	0.4786580216
C37	0.5568935704	-1.7283169034	-4.6338068828
H38	1.3807786353	-2.4330335302	-4.7278346905
H39	-0.3309039065	-2.1028356861	-5.1329400458
H40	0.8592106417	-0.7695913513	-5.0517810679

BHandHLYP /cc-pVTZ
Energy: -1172.93376874458

C1	0.7006583805	-1.0410441199	-0.9869166794
C2	-1.1353953460	-1.3996257572	0.4210838553
C3	0.8103172932	-2.0911800282	1.2478244287
C4	1.4844573665	-2.0567361965	-0.1448490780
C5	0.6445458155	-0.7170146722	1.8931090686
C6	-0.6867752144	-0.2397032215	1.3096353077
C7	-2.6083648522	-1.6308113776	0.3469133353
O8	-0.5073950090	-2.5169458480	0.9972728327
O9	-0.6697372937	-1.2643019870	-0.8894015729
O10	1.3759708562	-3.3190026298	-0.7030461815
H11	0.9648394835	-0.0260692931	-0.6680899812
H12	0.5961315749	-0.8328385461	2.9764426828
H13	1.4850574949	-0.0633260291	1.6709012136
H14	-0.6067925108	0.6825649249	0.7310722435
H15	-1.4300514930	-0.0735957919	2.0905888538
H16	-2.8156450689	-2.4781329337	-0.3083284054
H17	-2.9988901901	-1.8377896865	1.3446127569
H18	-3.0977281679	-0.7433934794	-0.0599997529
H19	0.4811710186	-3.6265542522	-0.5295871854
C20	1.5426094968	-3.0630410383	2.1353885047
O21	0.9332377571	-4.2160651272	2.2693210731
O22	2.5752823591	-2.7763790394	2.6603695991
C23	2.9626331553	-1.7046207812	-0.0928673838
O24	3.1456225633	-0.4112831028	0.1301194341
O25	3.8399366974	-2.4899290192	-0.2191683506
C26	1.1633274709	-1.1649811967	-2.4162225768
O27	0.2026727929	-1.4197628920	-3.2682896616
O28	2.3105741172	-1.0187656939	-2.7155624350
C29	1.6075565404	-5.1532667453	3.0855749542
H30	2.5899488395	-5.3796748453	2.6675648051
H31	0.9807234781	-6.0420786455	3.1042210488
H32	1.7392717357	-4.7539283933	4.0934764449
C33	4.4956757507	-0.0000215804	0.1516961891
H34	5.0364807544	-0.5106036516	0.9506743077
H35	4.9715801266	-0.2304727935	-0.8032928395
H36	4.4853447486	1.0751495313	0.3225858152
C37	0.6135664574	-1.5330485422	-4.6149366784
H38	1.3302530838	-2.3488796644	-4.7262124385
H39	-0.2882207202	-1.7324196003	-5.1899784186
H40	1.0860718350	-0.6074272433	-4.9507493900

M05/cc-pVTZ
Energy: -1182.96284236741

C1	0.7092438436	-1.0084385208	-1.0007460469
C2	-1.1324583188	-1.4040541711	0.4344470304
C3	0.8267931154	-2.1175829019	1.2324091080
C4	1.5051884326	-2.0463317270	-0.1714359449
C5	0.6402662683	-0.7679665420	1.9369803594
C6	-0.6894897835	-0.2710357719	1.3653692669
C7	-2.6112403878	-1.6434115013	0.3494816573
O8	-0.4977322778	-2.5462187557	0.9771113294
O9	-0.6708630965	-1.2188826770	-0.8834469826
O10	1.4048410509	-3.3071097796	-0.7594660790
H11	0.9819739186	-0.0037883252	-0.6723445295
H12	0.5720738393	-0.9343491841	3.0088855059
H13	1.4717323095	-0.0969562280	1.7632052270
H14	-0.6019189799	0.6664992138	0.8215686212
H15	-1.4312748830	-0.1271777546	2.1462482067
H16	-2.8164836202	-2.4604979912	-0.3369817741
H17	-3.0008717319	-1.8933197039	1.3328820067
H18	-3.1071505490	-0.7471961665	-0.0176942951
H19	0.4977391069	-3.5952523333	-0.6233821705
C20	1.5733723434	-3.1072305003	2.1085038707

O21	0.8710378154	-4.2025970814	2.3650290793
O22	2.6734444374	-2.8787030427	2.5341710741
C23	2.9965813374	-1.6972246333	-0.1239251053
O24	3.1761335419	-0.4088264029	0.1995507732
O25	3.8774252837	-2.4679503415	-0.3476629210
C26	1.1466514147	-1.0946384160	-2.4529257208
O27	0.1889336778	-1.5186045441	-3.2654282417
O28	2.2569997362	-0.7925522028	-2.7995803824
C29	1.5120291192	-5.1540127692	3.2093915587
H30	2.4462290938	-5.4868424210	2.7635274847
H31	0.8155584386	-5.9795251202	3.3059189618
H32	1.7223853010	-4.7158954638	4.1832837232
C33	4.5300271346	0.0258159050	0.2358702278
H34	5.0976879288	-0.5636280157	0.9522346733
H35	4.9802583260	-0.0749818416	-0.7493534423
H36	4.5018738808	1.0688529675	0.5344993037
C37	0.5529727641	-1.6189057307	-4.6380929130
H38	1.3670635791	-2.3292832001	-4.7632494348
H39	-0.3364489849	-1.9608386877	-5.1562782489
H40	0.8697250875	-0.6508688338	-5.0214898593

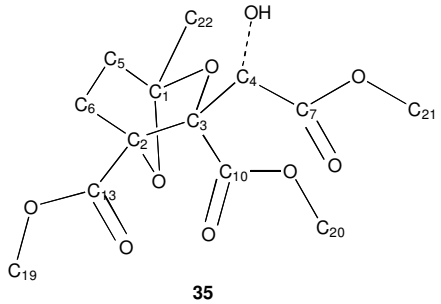
M06/cc-pVTZ
Energy: -1182.98442487055

C1	0.6941782169	-0.9972975269	-1.0016639925
C2	-1.1307780186	-1.3794198616	0.4430998138
C3	0.8269335651	-2.1021847825	1.2262197099
C4	1.4891507927	-2.0243621751	-0.1734316516
C5	0.6544465713	-0.7589687938	1.9358531642
C6	-0.6672528037	-0.2474042984	1.3602260280
C7	-2.6067425971	-1.6005676434	0.3810622219
O8	-0.5032622361	-2.5262932326	0.9845506839
O9	-0.6847842835	-1.2106219751	-0.8807097132
O10	1.3874234811	-3.2845371228	-0.7642312403
H11	0.9721784734	0.0165505810	-0.6913612498
H12	0.5813078756	-0.9366853292	3.0081112224
H13	1.4975961337	-0.0961724140	1.7711105056
H14	-0.5696258689	0.6856503030	0.8057614552
H15	-1.4114678864	-0.0857928125	2.1390063265
H16	-2.8298794054	-2.4231596882	-0.2955935245
H17	-2.9832112343	-1.8358038846	1.3752786894
H18	-3.0954550793	-0.6990047703	0.0128314699
H19	0.4777474381	-3.5752996358	-0.6269162428
C20	1.5836362214	-3.0980059592	2.0727064007
O21	0.9086144365	-4.2148766884	2.2921852055
O22	2.6765627714	-2.8557477462	2.5055356074
C23	2.9726723646	-1.6750282811	-0.1224375637
O24	3.1474196807	-0.3938374236	0.2269521841
O25	3.8556238112	-2.4392049422	-0.3490894162
C26	1.1373596805	-1.1343842947	-2.4409417879
O27	0.1784440734	-1.5467882157	-3.2521713369
O28	2.2620412727	-0.8855757156	-2.7782366826
C29	1.5809660470	-5.1640584398	3.1105236028
H30	2.5298025636	-5.4505092753	2.6599282265
H31	0.9176716636	-6.0195927113	3.1858221557
H32	1.7754017525	-4.7450684857	4.0976699992
C33	4.5053268436	0.0111044201	0.3152027784
H34	5.0258513785	-0.5759810222	1.0714077393
H35	5.0022281405	-0.1257055013	-0.6446449547
H36	4.4940367937	1.0617491790	0.5900839931
C37	0.5755782599	-1.7000518639	-4.6079218269
H38	1.3755347728	-2.4345279922	-4.6892315785
H39	-0.3059835762	-2.0347753812	-5.1451564010
H40	0.9315291036	-0.7533409024	-5.0135917767

MPW1PW91/cc-pVTZ
Energy: -1183.37622928976

C1	0.7034564869	-1.0096019639	-1.0067747891
C2	-1.1296527000	-1.4074954383	0.4242789490
C3	0.8336900159	-2.1309345565	1.2164743234
C4	1.5059003696	-2.0471771472	-0.1854567036
C5	0.6583425943	-0.7795928501	1.9214732790
C6	-0.6689669231	-0.2734639366	1.3478487317
C7	-2.6102433929	-1.6340900554	0.3545006251
O8	-0.4961432942	-2.5563843683	0.9601788100
O9	-0.6792580870	-1.2297658516	-0.8990711686
O10	1.4090412430	-3.3069683214	-0.7809472265
H11	0.9716220637	-0.0044201808	-0.6723641967
H12	0.5914972856	-0.9432089788	2.9948436748
H13	1.4965321163	-0.1170026535	1.7394709243
H14	-0.5737781211	0.6593762225	0.7953628767
H15	-1.4089541869	-0.1165068835	2.1293991788
H16	-2.8278727910	-2.4527403960	-0.3273990492
H17	-2.9916092429	-1.8753834402	1.3441068551
H18	-3.0998933575	-0.7335148652	-0.0121838273
H19	0.4999339770	-3.5929033967	-0.6415265466
C20	1.5721363268	-3.1312419701	2.0814993986
O21	0.8567577383	-4.2111451057	2.3581330309
O22	2.6817570579	-2.9210681703	2.4928110778
C23	2.9889902422	-1.6779817745	-0.1408374731
O24	3.1531920049	-0.3910611730	0.1945751962
O25	3.8822615353	-2.4317495094	-0.3754522388
C26	1.1399638227	-1.1002217004	-2.4566583798
O27	0.1834909008	-1.5144184915	-3.2727858964
O28	2.2532571496	-0.8080990430	-2.8036173373
C29	1.5055304806	-5.1492653543	3.2135801016
H30	2.4296304045	-5.4997169395	2.7588608166
H31	0.8019581253	-5.9650604868	3.3404522682
H32	1.7362927807	-4.6885724253	4.1729234043
C33	4.5095064676	0.0435140195	0.2383947209
H34	5.0624199977	-0.5203201780	0.9871364238
H35	4.9774968653	-0.0944130003	-0.7339055638
H36	4.4752517459	1.0967115445	0.4992319484
C37	0.5713392483	-1.6116805666	-4.6409002196
H38	1.3858675397	-2.3245739546	-4.7527468367
H39	-0.3118804305	-1.9492158015	-5.1731764165
H40	0.8976792072	-0.6422948742	-5.0144694815

Structure 35



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B3LYP/6-31G**
Energy: -1183.24842802730

C1	1.2701456804	0.9012192990	0.2800777556
C2	-0.6007437726	1.2465072939	-0.6790280076
C3	0.2538955665	2.5292468143	-1.0095192891
C4	0.5835007615	2.8226394093	-2.5113378730
C5	1.3155327047	-0.1787324534	-0.8254646908
C6	-0.0793897630	0.0202591699	-1.4831667358
C7	-0.6518157647	3.0839766777	-3.3920451040

O8	−1.3524347339	1.9480604407	−3.6186018642
O9	−0.9381549035	4.1569744851	−3.8626104462
C10	−0.2824753687	3.8209903775	−0.3428914217
O11	−0.5935173019	3.6452153478	0.9460027882
O12	−0.3687568087	4.8917753639	−0.9102415523
C13	−2.1055028369	1.4484622194	−0.6394692055
O14	−2.7282094675	0.3645963889	−0.1572506711
O15	−2.6753844651	2.4571443458	−1.0002317556
O16	1.4871484098	2.1839715745	−0.3502738074
O17	−0.1076297326	0.9303776405	0.6344219079
O18	1.4950385112	3.8750965835	−2.6424627225
C19	−4.1595203215	0.4720742346	−0.0403754971
C20	−1.0945147739	4.8140793833	1.6204328728
C21	−2.5669917221	2.1222260616	−4.3733050054
C22	2.1661398743	0.7643781097	1.4816997148
H23	1.0823194746	1.9305146341	−2.8983643942
H24	2.1501777096	−0.0017692132	−1.5074693928
H25	1.4227748091	−1.1777244509	−0.3944738582
H26	−0.7424625987	−0.8197675710	−1.2697011664
H27	−0.0610220316	0.1756477969	−2.5595812604
H28	0.9887998304	4.6824531505	−2.4486312048
H29	−4.6119607957	0.6433610750	−1.0198303838
H30	−4.4898466920	−0.4786201814	0.3761491782
H31	−4.4254594754	1.2975420660	0.6235242695
H32	−0.3548118000	5.6173210168	1.5944998632
H33	−2.0146846177	5.1606364184	1.1444789601
H34	−1.2847233602	4.4977695204	2.6456530474
H35	−2.9551825086	1.1178084603	−4.5428851937
H36	−3.2777525677	2.7180911608	−3.7967567028
H37	−2.3589715582	2.6213092366	−5.3216169377
H38	1.9770817813	1.5888934424	2.1718201061
H39	1.9762124201	−0.1849725080	1.9884670944
H40	3.2130955066	0.7964375089	1.1697943788

g. CP3 calculations

The calculations were carried out using the data in Table 3 and the program available on: http://www-jmg.ch.cam.ac.uk/tools/nmr/[18]
The CP3 values are 0.58 for the assignment as given in Table 3, and −1.19 for the assignment swapping **31** and **33**. This corresponds to a probability of more than 99.9% that the assignment as given is correct.

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