Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supplementary Information

for

Free Radical 5-*Exo*-Dig Cyclization as the Key Step in the Synthesis of Bis-Butyrolactone Natural Products: Experimental and Theoretical Studies

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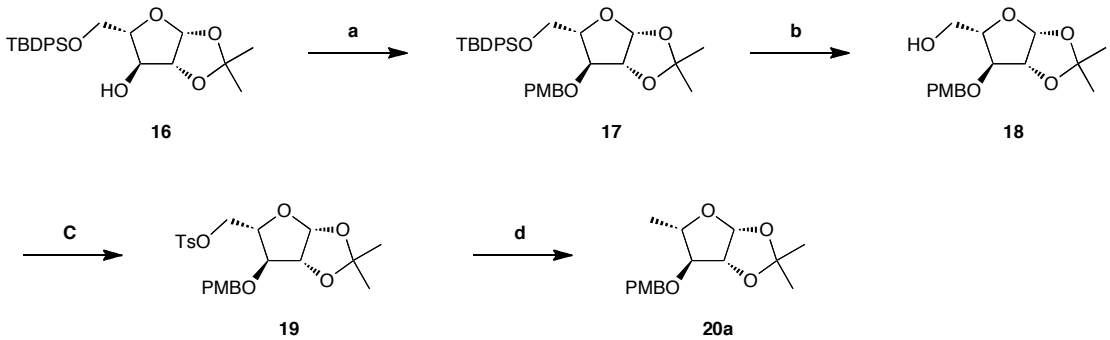
1. Syntheses of Radical Precursors

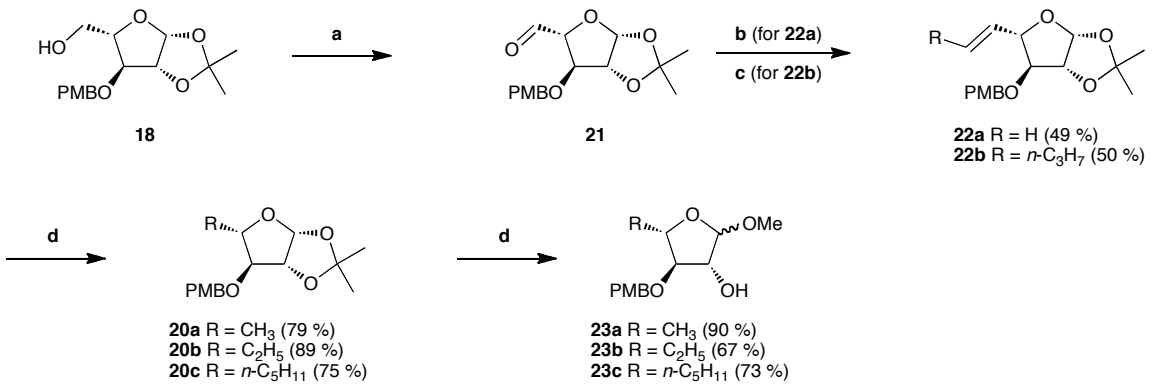
Accordingly, readily available **11** (Scheme 1) was converted into **16** by a known procedure.[1] Alcohol **16** on reaction with PMBBr in the presence of NaH in dry THF at 0 °C to room temperature for 4 h (Scheme 3) furnished **17** in 81% yield. Desilylation of **17** with TBAF at 0 °C to room temperature for 4 h gave alcohol **18** in 89% yield, which on reaction with *p*-TsCl and Et_3N in CH_2Cl_2 at 0 °C to room temperature for 14 h furnished tosylate **19** in 81% yield. Deoxygenation of **19** using $NaBH_4$ in dry DMSO[2] at 160 °C for 15 min under nitrogen atmosphere gave **20a** in 79% yield.



Reagents and conditions: (a) PMBr, NaH, THF, 4h, 81 %; (b) TBAF, THF 14 h, 89 %; (c) TsCl, Et_3N, CH_2Cl_2, 0 °C - RT, 14 h, 81 %; (d) $NaBH_4$, DMSO, 160 °C, 15 min, 79 %.

Scheme 1 Synthesis of intermediates for **12a** and **13a.**

Oxidation of alcohol **18** (Scheme 2) with IBX in dry DMSO gave aldehyde **21** in 80% yield. Wittig olefination of **21** with methyl triphenylphosphonium iodide and *t*-BuOK in THF afforded the olefin **22a** in 49% yield, while a similar reaction of **21** with *n*-butyl triphenylphosphonium bromide and *t*-BuOK in THF afforded **22b** in 50% yield. Further, hydrogenation of olefins **22a** and **22b** with PtO_2 in EtOAc afforded **20b** (89%) and **20c** (75%) respectively. Compounds **20a, 20b** and **20c** on methanolysis with 2-3 drops of conc. HCl in methanol at 0 °C to room temperature gave diastereomeric mixtures of methyl glycosides **23a** (1:1.5), **23b** (1:1.5) and **23c** (4.5:5.5) respectively as α- and β-anomers.



18 **21**

22a R = H (49 %)
22b R = *n*-C_3H_7 (50 %)

20a R = CH_3 (79 %)
20b R = C_2H_5 (89 %)
20c R = *n*-C_5H_{11} (75 %)

23a R = CH_3 (90 %)
23b R = C_2H_5 (67 %)
23c R = *n*-C_5H_{11} (73 %)

Reagents and conditions: (a) IBX, DMSO, 3h, 80 %; (b) $CH_3PPh_3^+I^-$, *t*-BuO^-K^+, THF, 7 h, -4 °C, 49 % (for **22a**); (c) *n*-$C_4H_9PPh_3^+Br^-$, *t*-BuO^-K^+, THF, 7 h, -4 °C, 50 % (for **22b**); (d) PtO_2, EtOAc, 2 h: (e) H^+, MeOH, 6 h.

Scheme 2 Synthesis of intermediates for **12** and **13.**

[1] A. P. Rauter, F. Ramoa-Ribeiro, A. Fernandes and J. A. Figueiredo, *Tetrahedron*, 1995, **51**, 6529.
[2] G. Mehta, N. Mohal and S. Lakshminath, *Tetrahedron Lett.*, 2000, **41**, 3505.

6-(4-Methoxybenzyloxy)-2,2-dimethyl-(3aR,5S,6S,6aR)-perhydrofuro[2,3-d][1,3]dioxol-5-(*tert*-butyldiphenylsilyl)-methylether (17). A stirred suspension of sodium hydride (0.96 g, 40.28 mmol) in dry THF (30 mL) under N_2 atmosphere was treated with a solution of **16** (8.62 g, 20.14 mmol) in THF (25 ml) at 0 °C and stirred for 30 min. PMBBr (4.5 mL, 24.16 mmol) was added to the reaction mixture at 0 °C and stirred at room temperature for 4 h. Reaction mixture was quenched with aq. NH_4Cl solution (20 mL) and extracted with ethyl acetate (2 x 100 mL). Organic layer was washed with water (100 mL), brine (100 mL), dried (Na_2SO_4) and evaporated. Purification of residue by column chromatography (60-120 Silica gel, ethyl acetate:*n*-hexane, 0.5:9.5) afforded **17** (8.94 g, 81%) as a colorless liquid; $[\alpha]_D$ = +12.12 (*c* 1.25, $CHCl_3$); IR (Neat): ν_{max} 3451, 3069, 2934, 2859, 1723, 1612, 1513, 1464, 1249, 1214, 1107, 1030, 820, 704 cm^{-1}; ^1H NMR: (200 MHz, $CDCl_3$): δ 1.06 (s, 9H, $3CH_3$), 1.26 (s, 3H, CH_3), 1.30 (s , 3H, CH_3), 3.70-3.80 (m, 5H, H-6, H-5a, OCH_3), 4.08-4.18 (m, 2H, H-5, H-5b), 4.42-4.54 (m, 2H, OCH_2), 4.60 (d, 1H, *J* = 3.6 Hz, H-6a), 5.82 (d, 1H, *J* = 3.6 Hz, H-3a), 6.82 and 7.22 (2d, 2H each, *J* = 8.6 Hz, Ar-H), 7.30-7.42 (m, 6H, Ar-H), 7.56-7.74 (m, 4H, Ar-H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 159.3, 136.3, 135.8, 135.5 (4C), 129.6 (2C), 129.3 (2C), 127.7 (4C), 127.3, 113.9 (2C), 112.4, 105.7, 85.2 (2C), 82.4, 71.3, 63.4, 55.2, 26.9, 26.8 (3C), 26.1, 19.2; HRMS (ESI): *m/z* calculated for $C_{32}H_{40}NaO_6Si(M^+$+Na) 571.2491, found 571.2507.

6-(4-Methoxybenzyloxy)-2,2-dimethyl-(3aR,5S,6S,6aR)-perhydrofuro[2,3-d][1,3]dioxol-5-yl-methanol (18). A solution of **17** (8.56 g, 15.62 mmol) in dry THF (20 mL) under N_2 atmosphere was treated with tetra *n*-butylammonium fluoride (17.2 mL, 1.0 M, 17.18 mmol) at 0 °C and stirred at room temperature for 4 h. Evaporation of solvent and purification of the residue by chromatography (60-120 Silica gel, ethyl acetate:*n*-hexane, 2:3) afforded **18** (4.30 g, 89%) as a colorless liquid; $[\alpha]_D$ = +16.18 (*c* 0.85, $CHCl_3$); IR (Neat): ν_{max} 3450, 2927, 2855, 1756, 1612, 1513, 1461, 1377, 1301, 1247, 1168, 1074, 1030, 821, 517 cm^{-1}; ^1H NMR (200 MHz, $CDCl_3$): δ 1.35 (s, 3H, CH_3), 1.54 (s, 3H, CH_3), 1.94 (br. s, 1H, OH), 3.64 (d, 2H, *J* = 5.5 Hz, H-5a, H-5b), 3.82 (s, 3H, OCH_3), 3.90 (d, 1H, *J* = 2.4 Hz, H-6), 4.06-4.17 (m, 1H, H-5), 4.50-4.57 (m, 2H, OCH_2), 4.60 (d, 1H, *J* = 5.5 Hz, H-6a), 5.82 (d, 1H, *J* = 5.5 Hz, H-3a), 6.82, 7.22 (2d, 2H each, *J* = 8.6 Hz, Ar-H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 159.3, 129.3 (3C), 113.8 (2C), 112.7, 105.5, 85.5, 85.1, 82.3, 71.4, 62.5, 55.1, 27.0, 26.2; HRMS (ESI): *m/z* calculated for $C_{16}H_{22}NaO_6(M^+$+Na) 333.1314, found 333.1315.

6-(4-Methoxybenzyloxy)-5-(4-methylphenylsulphonyloxy-methyl)-2,2-dimethyl-(3aR,5S,6S,6aR)-perhydrofuro[2,3-d][1,3]dioxole (19). A solution of **18** (2.5 g, 8.06 mmol) in dry CH_2Cl_2 (30 mL) at 0 °C was treated with Et_3N (3.2 mL, 24.19 mmol) and *p*-toluenesulphonyl chloride (2.3 g, 12.09 mmol) at 0 °C and stirred at room temperature for 14 h. After completion of the reaction, dichloromethane (50 mL) was added to the reaction mixture and washed with water (2 x 50 mL), brine (50 mL) and dried (Na_2SO_4). Evaporation of solvent and purification of the residue by column chromatography (60-120 Silica gel, ethyl acetate:*n*-hexane, 1:9) afforded **19** (3.05 g, 81%) as white solid, m.p. 131 °C; $[\alpha]_D$ = +16.18 (*c* 0.85, $CHCl_3$); IR (Neat): ν_{max} 3310, 2987, 1782, 1237, 1019, 765 cm^{-1}; ^1H NMR (200 MHz, $CDCl_3$): δ 1.27 (s, 3H, CH_3), 1.35 (s, 3H, CH_3), 2.45 (s, 3H, CH_3), 3.82 (s, 3H, OCH_3), 3.90 (d, 1H, *J* = 1.8 Hz, H-6), 4.08 (d, 2H, *J* = 6.4 Hz, H-5a, H-5b), 4.18 (dd, 1H, *J* = 6.4, 1.8 Hz, H-5), 4.48 (s, 2H, OCH_2), 4.53 (d, 1H, *J* = 4.1 Hz, H-6a), 5.82 (d, 1H, *J* = 4.1 Hz, H-3a), 6.87 (d, 2H, *J* = 8.2 Hz, Ar-H), 7.22 (d, 2H, *J* = 8.2 Hz, Ar-H), 7.32 (d, 2H, *J* = 7.6 Hz, Ar-H), 7.75 (d, 2H, *J* = 7.6 Hz, Ar-H); ^{13}C NMR ($CDCl_3$, 75 MHz): δ 159.4, 144.9, 132.6, 129.8, 129.5, 128.8, 128.0, 114.0, 112.6, 105.9,

84.4, 81.8 (2C), 71.4, 68.5, 55.2, 26.6, 25.8, 21.6; HRMS (ESI): *m/z* calculated for $C_{23}H_{28}NaO_8S(M^+Na)$ 487.1402, found 487.1388.

6-(4-Methoxybenzyloxy)-2,2,5-trimethyl-(3a*R*,5*S*,6*S*,6a*R*)-perhydrofuro[2,3-*d*][1,3]dioxole (20a). A solution of **19** (8.56 g, 18.44 mmol) in dry DMSO (40 mL) under N_2 atmosphere was treated with $NaBH_4$ (1.39 g, 36.89 mmol) at 0 °C and heated upto 160 °C for 10 min. The reaction mixture was cooled to room temperature, extracted into EtOAc (2 x 100 mL) and washed with water (75 mL) and dried (Na_2SO_4). Evaporation of solvent and purification of the residue by column chromatography (60-120 Silica gel, ethyl acetate:*n*-hexane, 1.7:8.3) afforded **20a** (4.30 g, 79%) as a colorless liquid; $[\alpha]_D$ = -27.25 (*c* 1.6, $CHCl_3$); IR (neat): ν_{max} 2940, 1450, 1080, 700 cm^{-1}; ^1H NMR (75 MHz, $CDCl_3$): δ 1.32 (d, 6H, *J* = 6.7 Hz, $2CH_3$), 1.49 (s, 3H, CH_3), 3.62 (d, 1H, *J* = 3.7 Hz, H-6), 3.78 (s, 3H, Ar-OCH_3), 4.03 (m, 1H, H-5), 4.40-4.56 (m, 3H, H-6a, -OCH_2 Ar), 5.74 (d, 1H, *J* = 4.1 Hz, H-3a), 6.82 (d, 2H, *J* = 8.3 Hz, Ar-H), 7.19 (d, 2H, *J* = 8.3 Hz, Ar-H); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 159.3, 129.3 (3C), 113.8 (2C), 112.8, 105.3, 86.8, 85.6, 80.3, 71.4, 55.2, 27.1, 26.5, 19.9; HRMS (ESI): *m/z* calculated for $C_{16}H_{22}NaO_5(M^+Na)$ 317.1364, found 317.1355.

6-(4-Methoxybenzyloxy)-2,2-dimethyl-(3aR,5R,6R,6aR)-perhydrofuro[2,3-d][1,3]dioxol-5-carbaldehyde (21). A solution of **18** (2.5 g, 8.06 mmol) in dry DMSO (10 mL) was treated with IBX (3.38 g, 12.09 mmol) at 10 °C and stirred at room temperature for 3 h. Reaction mixture was quenched with ice cold water (10 mL) and stirred at room temperature for 15 min, filtered and extracted with ethyl acetate (2 x 75 mL). Organic layer was washed with aq. $NaHCO_3$ solution (50 mL), water (50 mL), brine (50 mL) and dried (Na_2SO_4). Solvent was evaporated to afford **21** (1.98 g, 80%) as a liquid; $[\alpha]_D$ = -2.64 (*c* 0.8, $CHCl_3$); IR (Neat): ν_{max} 3290 cm^{-1}; ^1H NMR (200 MHz, $CDCl_3$): δ 1.35 (s, 3H, CH_3), 1.54 (s, 3H, CH_3), 3.84 (s, 3H, OCH_3), 3.92 (d, 1H, *J* = 2.4 Hz, H-6), 4.22-4.54 (m, 3H, H-5, H-8, H-8a), 4.60 (d, 1H, *J* = 5.4 Hz, H-6a), 5.82 (d, 1H, *J* = 5.4 Hz, H-3a), 6.95 and 7.80 (2d, 2H each, *J* = 8.6 Hz, Ar-H), 9.02 (s, 1H, CHO).

(3aR,5S,6S,6aR)-6-(4-Methoxybenzyloxy)-tetrahydro-2,2-dimethyl-5-vinylfuro[3,2-d][1,3] dioxole (22a). A solution of methyltriphenylphosphonium iodide (18.75 g, 46.42 mmol) in dry THF (50 mL) under N_2 atmosphere was treated with $^tBuO^-K^+$ (5.19 g, 46.42 mmol) at 0 °C and stirred for 6 h. A solution of **21** (7.10 g, 23.21 mmol) in THF (30 mL) was added to the reaction mixture at 0 °C. Reaction mixture was stirred at 0 °C for 1 h, warmed to room temperature and stirred for 30 min. It was quenched with aq. NH_4Cl solution (30 mL) and extracted with ethyl acetate (2 x 100 mL). The organic layers were washed with water (100 mL), brine (100 mL), dried (Na_2SO_4) and evaporated. Purification of residue by column chromatography (60-120 Silica gel, ethyl acetate:*n*-hexane, 0.5:9.5) afforded **22a** (3.48 g, 49%) as a colorless liquid; $[\alpha]_D$ = -47.2 (*c* 0.68, $CHCl_3$); IR (Neat): ν_{max} 2931, 1722, 1614, 1514, 1376, 1247, 1081, 1025, 824, 580 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 1.32 (s, 3H, CH_3), 1.48 (s, 3H, CH_3), 3.79 (s, 4H, H-6, OCH_3), 4.40-4.56 (m, 4H, H-5, H-6a, Ar-OCH_2), 5.11-5.31 (dd, 2H, *J* =10.6 Hz, olefinic), 5.83 (d, 1H, *J* = 3.81 Hz, H-3a), 5.94 (m, 1H, olefinic), 6.82 and 7.20 (2d, 2H each, *J* = 8.6 Hz, Ar-H); ^{13}C NMR ($CDCl_3$, 75 MHz): δ 159.2, 136.6, 129.1 (2C), 116.1, 113.6 (2C), 112.5, 105.3, 96.0, 85.9, 85.1, 84.8, 71.2, 54.7, 27.0, 26.5; HRMS (ESI): *m/z* calculated for $C_{17}H_{22}NaO_5(M^+Na)$ 329.1364, found 329.1366.

(3aR,5S,6S,6aR)-6-(4-Methoxybenzyloxy)-tetrahydro-2,2-dimethyl-5-((E)-pent-1-enyl)furo- [3,2-d][1,3]dioxole (22b). A solution of **21** (7.80 g, 25.32 mmol) in THF (40 mL) was treated with *n*-butyltriphenylphosphonium bromide (30.23 g, 75.97 mmol) in dry THF (30 mL) and $^tBuO^-K^+$ (8.51 g, 75.97 mmol), work up as described for **22a** and after purification of

residue by column chromatography (60-120 Silica gel, ethyl acetate:*n*-hexane, 0.5:9.5) gave **22b** (4.40 g, 50%) as a colorless liquid; $[\alpha]_D$ = -12.0 (*c* 0.73, $CHCl_3$); IR (Neat): ν_{max} 2931, 1722, 1614, 1514, 1376, 1247, 1081, 1025, 824, 580 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 0.90 (t, 3H, *J* = 7.3 Hz, CH_3), 1.25-1.45 (m, 8H, $2CH_3$, CH_2), 1.93-2.15 (m, 2H, allylic-CH_2), 3.75-3.78 (m, 4H, H-4, OCH_3), 4.42-4.56 (m, 3H, H-5, OCH_2), 4.70-4.72 (dd, 1H, *J* = 3.5, 7.9 Hz, H-3), 5.52-5.59 (m, 2H, olefinic), 5.80 (d, 1H, *J* = 3.9 Hz, H-2), 6.81 and 7.20 (2d, 2H each, *J* = 8.6 Hz, Ar-H); ^{13}C NMR ($CDCl_3$, 75 MHz): δ 159.3, 135.5, 133.4, 129.3, 128.2, 127.6, 113.8, 112.6, 105.5, 86.7, 85.2, 80.7, 71.5, 55.2, 29.4, 27.0, 26.4, 22.6, 13.7; HRMS (ESI): *m/z* calculated for $C_{20}H_{28}NaO_5(M^+$+Na) 371.1834, found 371.1841.

(3aR,5S,6S,6aR)-6-(4-Methoxybenzyloxy)-5-ethyl-tetrahydro-2,2-dimethylfuro[3,2-d][1,3] dioxole (20b). A solution of **22a** (2.80 g, 9.15 mmol) in dry EtOAc (20 mL) was treated with catalytic amount of PtO_2 (0.02 g) under H_2 atmosphere and stirred at room temperature for 2 h. It was filtered, solvent was removed and residue purified by column chromatography (60-120 Silica gel, ethyl acetate:*n*-hexane, 0.7:9.3) afforded **20b** (2.50 g, 89%) as a colorless liquid; $[\alpha]_D$ = -82.49 (*c* 1.4, $CHCl_3$); IR (Neat): ν_{max} 2941, 1450, 1100, 720 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 0.93 (t, 3H, *J* = 7.4 Hz, CH_3), 1.31 (s, 3H, CH_3), 1.47 (s, 3H, CH_3), 1.66 (m, 2H, allylic-CH_2), 3.67 (d, 1H, *J* = 3.6 Hz, H-6), 3.77 (m, 4H, H-5,OCH_3), 4.40-4.55 (m, 3H, H-6a, OCH_2), 5.76(d, 1H, *J* = 3.9 Hz, H-3a), 6.82 - 7.20 (2d, 2H each, *J* = 8.4 Hz, Ar-H); ^{13}C NMR ($CDCl_3$, 75 MHz): δ 159.2, 131.7, 129.1 (2C), 113.6 (2C), 112.5, 105.0, 96.1, 85.3 (2C), 85.0, 71.1, 54.8, 27.3, 27.0, 26.6, 10.3; HRMS (ESI): *m/z* calculated for $C_{17}H_{24}NaO_5(M^+$+Na) 331.1624, found 331.1627.

(3aR,5S,6S,6aR)-6-(4-Methoxybenzyloxy)-tetrahydro-2,2-dimethyl-5-pentylfuro[3,2-d][1,3] dioxole (20c). A solution of **22b** (2.20 g, 6.32 mmol) in dry EtOAc (15 mL) was treated with catalytic amount of PtO_2 (0.02 g), worked up as described for **20b** and purified the residue by column chromatography (60-120 Silica gel, ethyl acetate:*n*-hexane, 0.5:9.5) gave **20c** (1.66 g, 75%) as a colorless liquid; $[\alpha]_D$ = -120.1 (*c* 0.3, $CHCl_3$); IR (Neat): ν_{max} 2941, 1450, 1100, 720 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 0.88 (t, 3H, *J* = 6.4 Hz, CH_3), 1.28-1.69 (m, 14H, $2CH_3$, $4CH_2$), 3.66 (d, 1H, *J* = 3.4 Hz, H-6), 3.78 (s, 3H, OCH_3), 3.85 (m, 1H, H-5), 4.40-4.56 (m, 3H, H-6a, OCH_2), 5.75 (d, 1H, *J* = 4.1 Hz, H-3a), 6.81 and 7.21 (2d, 2H each, *J* = 8.3 Hz, Ar-H); ^{13}C NMR ($CDCl_3$, 75 MHz): δ 159.2, 135.4, 131.8, 129.3, 128.2, 127.5, 113.7, 112.5, 105.1, 87.7, 87.2, 85.3 (2C), 84.5, 78.4, 71.2, 55.0, 33.9, 31.4, 27.0, 26.3, 25.5, 22.4, 13.8; HRMS (ESI): *m/z* calculated for $C_{20}H_{31}O_5(M^+$+H) 351.2093, found 351.2097.

Hydrolysis of 20a

To a solution of **20a** (1.50 g, 5.10 mmol) in dry methanol (20 mL) under N_2 atmosphere 3 drops of conc. HCl was added at 0 °C and stirred for 4-5 hours. The reaction mixture was cooled to 0 °C and neutralized with solid $NaHCO_3$ (0.3 g) at 0 °C. It was filtered, solvent evaporated and the residue purified by column chromatography (60-120 Silica gel; ethyl acetate:*n*-hexane, 1.8:8.2) to afford anomeric mixture of **23a** (1.23 g, 90%) in 1.5:1 ratio as a liquid; IR (neat): ν_{max} 3590, 3500, 2237, 1724, 1256,867,793 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 1.27 (t, 6H, *J* = 6.1 Hz, $2CH_3$), 3.33 (s, 3H, anomeric-OCH_3), 3.36 (m, 2H, *J* = 3.2, 6.9 Hz, 2H-4), 3.41 (s, 3H, anomeric-OCH_3), 3.57 (t, 2H, *J* = 6.1 Hz, 2H-5), 3.78 (s, 6H, 2Ar-OCH_3), 4.13-3.90 (m, 2H, 2H-3), 4.73-4.49 (m, 6H, 2H-2 and $2OCH_2$), 6.82 (q, 4H, *J* = 3.6, 8.2, 12.2 Hz, Ar-H), 7.22 (d, 4H, *J* = 8.19 Hz, Ar-H); HRMS (ESI): *m/z* calculated for $C_{14}H_{20}NaO_5(M^+$+Na) 291.1208, found 291.1210.

Hydrolysis of 20b

To a solution of **20b** (1.95 g, 6.33 mmol) in dry methanol (20 mL) under N_2 atmosphere 3 drops of conc. HCl was added at 0 °C worked up as described for **20a** and purified the residue by column chromatography (60-120 Silica gel, ethyl acetate:*n*-hexane, 1.8:8.2) to give **23b** (1.20 g, 67%) in 1.5:1 ratio as a colorless liquid; IR (neat): ν_{max} 3500, 3590, 1765, 879 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 0.92 (m, 6H, $2CH_3$), 1.60 (m, 4H, $2CH_2$), 2.38 (bs, 2H, 2OH), 3.32 (s, 3H, anomeric-OCH_3), 3.40-3.44 (m, 4H, anomeric-OCH_3, H-4), 3.62 (t, 1H, *J* = 6.1 Hz, H-4), 3.70-3.85 (m, 8H, 2H-5, 2Ar-OCH_3), 4.06–4.17 (m, 2H, 2H-3), 4.45–4.74 (m, 6H, $2OCH_2$, 2H-2), 6.82 (d, 4H, *J* = 8.3 Hz, Ar-H), 7.21 (d, 4H, *J* = 7.6 Hz, Ar-H); HRMS (ESI): *m/z* calculated for $C_{15}H_{22}NaO_5$(M^++Na) 305.1364, found 305.1356.

Hydrolysis of 20c

A solution of **20c** (1.2 g, 3.42 mmol) was treated with catalytic amount of conc. HCl in methanol (15 mL) worked up as described for **20a** and purified the residue by column chromatography (60-120 Silica gel, ethyl acetate:*n*-hexane, 1.8:8.2) to give **23c** (0.81 g, 73%) in 5.5:4.5 ratio as a liquid; IR (neat): ν_{max} 3500, 3590, 2867, 1734, 1198, 867 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 0.89 (t, 6H, *J* = 5.4 Hz, $2CH_3$), 1.28-1.57 (m, 16H, $8CH_2$), 2.41 (d, 2H, 2OH), 3.32 (s, 3H, anomeric-OCH_3), 3.40 (s, 3H, anomeric-OCH_3), 3.65 (t, 2H, *J* = 5.4 Hz, 2H-4), 3.78 (s, 6H, 2Ar-OCH_3), 3.86 (q, 2H, 2H-5), 4.06-4.18 (m, 2H, 2H-3), 4.47-4.58 (m, 4H, $2OCH_2$), 4.66-4.74 (m, 2H, H-2), 6.81 (m, 4H, Ar-H), 7.23 (d, 4H, *J* = 8.4 Hz, Ar-H); HRMS (ESI): *m/z* calculated for $C_{18}H_{28}NaO_5$(M^++Na) 347.1834, found 347.1846.

(2S,3S,4R,5R)-3-(4-Methoxybenzyloxy)-2-ethyl-tetrahydro-5-methoxy-4-(prop-2-ynyloxy)furan (24b) and (2S,3S,4R,5S)-3-(4-methoxybenzyloxy)-2-ethyl-tetrahydro-5-methoxy-4-(prop-2-ynyloxy)furan (25b). Reaction of **23b** (1.10 g, 3.90 mmol) with sodium hydride (0.23 g, 9.75 mmol) and propargyl bromide (0.58 mL, 3.90 mmol) in dry THF (12 mL) as described for **23a** and purified. First eluted on purification by column chromatography (60-120 Silica gel; ethyl acetate:*n*-hexane, 1.2:8.8) was **24b** (0.54 g, 43%) as liquid; $[\alpha]_D$ = -252.8 (*c* 0.54, chloroform); IR (neat): ν_{max} 3442, 2921, 1728, 1612, 1247, 1110, 1050, 1036, 894, 772 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 0.93 (t, 3H, *J* = 7.5 Hz, CH_3), 1.48-1.70 (m, 2H, CH_2), 2.41 (t, 1H, *J* = 2.2 Hz, acetylinic), 3.33 (s, 3H, OCH_3), 3.50 (m, 1H, H-3), 3.77- 3.85 (m, 4H, Ar-OCH_3, H-2), 4.03–4.19 (m, 3H, OCH_2, H-4), 4.62-4.42 (dd, 2H, *J* = 11.7 Hz, Ar-OCH_2) 4.78 (s, 1H, H-5), 6.80 (d, 2H, *J* = 8.7 Hz, Ar-H), 7.20 (d, 2H, *J* = 8.7 Hz, Ar-H); ^{13}C NMR ($CDCl_3$, 75 MHz): δ 159.2, 129.9, 129.4 (2C), 113.7 (2C), 106.3, 96.1, 88.0, 86.0, 81.8, 74.9, 71.6, 57.0, 55.0, 54.3, 26.1, 9.9; HRMS (ESI): *m/z* calculated for $C_{18}H_{24}NaO_5$(M^++Na) 343.1521, found 343.1524.

Second eluted on purification by column chromatography (60-120 Silica gel; ethyl acetate:*n*-hexane, 1.2:8.8) was **25b** (0.36 g, 29%) as liquid; $[\alpha]_D$ = +119.4 (*c* 0.70, chloroform); IR (neat): ν_{max} 3431, 2924, 1713, 1631, 1460, 776 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): ^1H NMR (300 MHz, $CDCl_3$): δ 0.93 (t, 3H, *J* = 7.2 Hz, CH_3), 1.60 (m, 2H, CH_2), 2.41 (t, 1H, *J* = 2.2 Hz, acetylinic), 3.37 (s, 3H, OCH_3), 3.70-3.78 (m, 4H, Ar-OCH_3, H-3), 3.89 (t, 1H, *J* = 6.8 Hz, H-2), 4.14–4.31 (m, 3H, OCH_2, H-4), 4.46-4.65 (dd, 2H, *J* = 11.3 Hz, Ar-OCH_2), 4.85 (d, 1H, *J* = 4.1 Hz, H-5), 6.82 (d, 2H, *J* = 8.6 Hz, Ar-H), 7.20 (d, 2H, *J* = 8.3 Hz, Ar-H); ^{13}C NMR ($CDCl_3$, 75 MHz): δ 159.3, 130.3, 129.5 (2C), 113.8 (2C), 101.2, 96.2, 84.5, 84.0, 82.5, 75.2, 71.8, 57.3, 55.1, 54.7, 29.2, 10.2; HRMS (ESI): *m/z* calculated for $C_{18}H_{24}NaO_5$(M^++Na) 343.1521, found 343.1522.

(2S,3S,4R,5R)-3-(4-Methoxybenzyloxy)-tetrahydro-5-meth-oxy-2-pentyl-4-(prop-2-ynyloxy)furan (24c) and (2S,3S,4R,5S)-3-(4-methoxybenzyloxy)-tetrahydro-5-meth-oxy-2-pentyl-4-(prop-2-ynyloxy)furan (25c). Reaction of **23c** (0.76 g, 2.34 mmol) with sodium hydride (0.14 g, 5.86 mmol) and propargyl bromide (0.34 mL, 2.34 mmol) in dry THF (10 mL) as described for **24a** and purified. First eluted on purification by column chromatography (60-120 Silica gel, ethyl acetate:*n*-hexane, 0.7:9.3) was **24c** (0.30 g, 35%) as a liquid; $[\alpha]_D$ = -240.7 (*c* 0.93, $CDCl_3$); IR (neat): ν_{max} 3279, 2929, 1712, 1525, 1050, 929, 780 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 0.88 (t, 3H, *J* = 6.7 Hz, CH_3), 1.27-1.63 (m, 8H, $4CH_2$), 2.42 (t, 1H, *J* = 2.4 Hz, acetylinic), 3.33 (s, 3H, OCH_3), 3.49 (dd, 1H, *J* = 2.8 Hz, H-3), 3.78 (s, 3H, Ar-OCH_3), 3.84 (m, 1H, H-2), 4.02-4.20 (m, 3H, H-4, OCH_2), 4.42-4.63 (dd, 2H, *J* = 11.5 Hz, Ar-OCH_2), 4.77 (s, 1H, H-5), 6.81 (d, 2H, *J* = 8.6 Hz, Ar-H), 7.23 (d, 2H, *J* = 8.6 Hz, Ar-H); ^{13}C NMR ($CDCl_3$, 75 MHz): δ 159.3, 129.9, 129.6 (2C), 113.8 (2C), 106.3, 87.9, 86.5, 80.9, 79.2, 75.0, 71.8, 57.1, 55.2, 54.5, 33.3, 31.8, 25.4, 22.5, 14.0; HRMS (ESI): *m/z* calculated for $C_{21}H_{30}NaO_5$(M^++Na) 385.1990, found 385.1988.

Second eluted on purification by column chromatography (60-120 Silica gel, ethyl acetate:*n*-hexane, 0.7:9.3) was **25c** (0.26 g, 30%) as a liquid; $[\alpha]_D$ = +95.0 (*c* 0.84, $CDCl_3$); IR (neat): ν_{max} 3272, 2942, 1743, 1576, 1057, 996, 732 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 0.88 (t, 3H, *J* = 6.6 Hz, CH_3), 1.27-1.59 (m, 8H, 4 CH_2), 2.42 (t, 1H, *J* = 2.4 Hz, acetylinic), 3.37 (s, 3H, OCH_3), 3.47 (dd, 1H, *J* = 2.8 Hz, H-3), 3.78 (s, 4H, H-3, Ar-OCH_3), 3.86 (m, 1H, H-2), 4.02-4.20 (m, 3H, H-4, OCH_2), 4.42-4.63 (dd, 2H, *J* = 11.5 Hz, Ar-OCH_2), 4.84 (d, 1H, *J* = 4.3 Hz, H-5), 6.82 (d, 2H, *J* = 8.6 Hz, Ar-H), 7.20 (d, 2H, *J* = 8.6 Hz, Ar-H); ^{13}C NMR ($CDCl_3$, 75 MHz): δ 159.2, 130.2, 129.5 (2C), 113.8 (2C), 101.2, 85.0, 83.9, 81.3, 79.3, 75.1, 71.8, 57.4, 55.2, 54.7, 36.2, 31.6, 25.3, 22.5, 14.0; HRMS (ESI): *m/z* calculated for $C_{21}H_{30}NaO_5$(M^++Na) 385.1990, found 385.2003.

(2S,3S,4R,5R)-2-Ethyl-tetrahydro-5-methoxy-4-(prop-2-ynyloxy)furan-3-ol (26b). A solution of **24b** (0.39 g, 1.21 mmol) in aq. CH_2Cl_2 (1:19, H_2O:CH_2Cl_2, 10 mL) was treated with DDQ (0.55 g, 2.43 mmol) at 0 °C as described for **24a.** Work up and purification by column chromatography (60-120 Silica gel; ethyl acetate:*n*-hexane, 1:4) afforded **26b** (0.20 g, 82%) as a colorless liquid; $[\alpha]_D$ = -176.5 (*c* 0.67, $CDCl_3$); IR (neat): ν_{max} 3447, 2925, 2854, 1741, 1219, 771 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 0.99 (t, 3H, *J* = 7.5 Hz, CH_3), 1.58-1.69 (m, 2H, CH_2), 2.43 (t, 1H, *J* = 2.2 Hz, acetylinic), 3.36 (s, 3H, OCH_3), 3.77 (m, 2H, H-3, H-2), 3.89 (s, 1H, H-4), 4.38-4.16 (dd, 2H, *J* = 2.2, 15.8 Hz, OCH_2), 4.85 (s, 1H, H-5); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 106.2, 96.3, 88.7, 86.0, 78.9, 75.1, 57.3, 54.6, 26.4, 10.2; HRMS (ESI): *m/z* calculated for $C_{10}H_{16}NaO_4$(M^++Na) 223.0946, found 223.0945.

(2S,3S,4R,5S)-2-Ethyl-tetrahydro-5-methoxy-4-(prop-2-ynyloxy)furan-3-ol (27b). A solution of **25b** (0.38 g, 1.18 mmol) in aq. CH_2Cl_2 (1:19, H_2O:CH_2Cl_2, 10 mL) was treated with DDQ (0.53 g, 2.37 mmol) at 0 °C as described **25a.** Work up and purification by column chromatography (60-120 Silica gel; ethyl acetate:*n*-hexane, 1:4) gave **27b** (0.19 g, 80%) as a colorless liquid; $[\alpha]_D$ = +138.2 (*c* 0.48, $CDCl_3$); IR (neat): ν_{max} 3437, 2926, 2856, 1737, 1219, 1051, 769 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 0.99 (t, 3H, *J* = 7.5 Hz, CH_3), 1.57-1.71 (m, 2H, CH_2), 2.21 (bs, 1H, OH), 2.45 (t, 1H, *J* = 2.2 Hz, acetylinic), 3.37 (s, 3H, OCH_3), 3.69 (q, 1H, *J* = 6.4, 13.2 Hz, H-2), 3.98 (m, 1H, H-3), 4.10 (t, 1H, *J* = 7.1 Hz, H-4), 4.16-4.38 (ddd, 2H, *J* = 2.2 Hz, OCH_2), 4.82 (d, 1H, *J* = 4.1 Hz, H-5);^{13}C NMR ($CDCl_3$, 75 MHz): δ 100.7, 96.2, 84.5, 82.7, 79.8, 75.2, 57.5, 54.5, 28.6, 9.9; HRMS (ESI): *m/z* calculated for $C_{10}H_{16}NaO_4$(M^++Na) 223.0946, found 223.0947.

(2S,3S,4R,5R)-Tetrahydro-5-methoxy-2-pentyl-4-(prop-2-ynyloxy)furan-3-ol (26c). A solution of **24c** (0.26 g, 0.71 mmol) in aq. CH_2Cl_2 (1:19, H_2O:CH_2Cl_2, 10 mL) was treated with DDQ (0.32 g, 1.43 mmol) as described for **26a.** Work up and purification of residue obtained by column chromatography (60-120 Silica gel, ethyl acetate:*n*-hexane, 0.7:9.3) gave **26c** (0.11 g, 65%) as a liquid; $[\alpha]_D$ = -164.8 (*c* 1.30, $CDCl_3$); IR (neat): ν_{max}3380, 2856, 2115, 1211, 764 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$): δ 0.90 (t, 3H, *J* = 6.6 Hz, CH_3), 1.25-1.60 (m, 8H, $4CH_2$), 2.24 (d, 1H, *J* = 8.1 Hz, OH), 2.41 (t, 1H, *J* = 2.2 Hz, acetylinic), 3.36 (s, 3H, OCH_3), 3.74 (bs, 1H, H-3), 3.83 (q, 1H, *J* = 5.6, 12.2 Hz, H-2), 3.88 (d, 1H, *J* = 2.2 Hz, H-4), 4.22 (dd, 2H, *J* = 2.0, 15.7 Hz, OCH_2), 4.84 (s, 1H, H-5); ^{13}C NMR ($CDCl_3$, 75 MHz): δ 106.2, 96.2, 88.6, 84.8, 79.3, 75.1, 57.4, 54.7, 33.5, 31.8, 25.6, 22.6, 14.1; HRMS (ESI): *m/z* calculated for $C_{13}H_{22}NaO_4(M^+$+Na) 265.1415, found 265.1427.

(2S,3S,4R,5S)-Tetrahydro-5-methoxy-2-pentyl-4-(prop-2-ynyloxy)furan-3-ol (27c). A solution of **25c** (0.25 g, 0.70 mmol) in aq. CH_2Cl_2 (1:19, H_2O:CH_2Cl_2, 10 mL) was treated with DDQ (0.32 g, 1.41 mmol) as described for **26c.** Work up and purification by column chromatography (60-120 Silica gel; ethyl acetate:*n*-hexane, 1:4) afforded **27c** (0.12 g, 72%) as a liquid; $[\alpha]_D$ = +149.7 (*c* 0.7, $CDCl_3$); IR (neat): ν_{max} ethyl acetate:*n*-hexane 3378, 2860, 2215, 1223, 698 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 0.90 (t, 3H, *J* = 6.4 Hz, CH_3), 1.25-1.67 (m, 8H, $4CH_2$), 2.45 (t, 1H, *J* = 2.2 Hz, acetylinic), 2.59 (bs, 1H, OH), 3.37 (s, 3H, OCH_3), 3.72 (q, 1H, *J* = 6.7, 13.2 Hz, H-3), 3.94-4.10 (m, 2H, H-2, H-4), 4.17-4.37 (ddd, 2H, *J* = 2.2, 15.8 Hz, OCH_2), 4.81 (d, 1H, *J* = 4.1 Hz, H-5); ^{13}C NMR ($CDCl_3$, 75 MHz): δ 100.7, 96.1, 84.5, 81.7, 78.4, 75.3, 57.7, 54.7, 35.8, 31.7, 25.2, 22.6, 14.0; HRMS (ESI): *m/z* calculated for $C_{13}H_{22}NaO_4(M^+$+Na) 265.1415, found 265.1420.

O-(2S,3S,4R,5R)-2-Ethyl-tetrahydro-5-methoxy-4-(prop-2-ynyloxy)furan-3-yl-S-methyl carbonodithioate (14b). A solution of **26b** (0.19 g, 0.95 mmol) with NaH (0.05 g, 2.37 mmol), carbon disulphide (0.08 mL, 1.42 mmol) and methyl iodide (0.09 mL, 1.42 mmol) was added at 0 °C and stirred at room temperature for 30 min.. Methyl iodide (0.07 mL, 1.12 mmol) was added at 0 °C work up as described for **14a** and purification of the residue by column chromatography (60-120 Silica gel; ethyl acetate:*n*-hexane, 1:9) gave **14b** (0.19 g, 70%) as liquid; $[\alpha]_D$ = -370.5 (*c* 0.28, $CDCl_3$); IR (neat): ν_{max} 3448, 2921, 2851, 1724, 1460, 1250, 1071, 771 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 0.98 (t, 3H, *J* = 7.5 Hz, CH_3), 1.75 (m, 2H, CH_2), 2.46 (t, 1H, *J* = 2.2 Hz, acetylinic), 2.57 (s, 3H, SCH_3), 3.40 (s, 3H, OCH_3), 4.11-4.15 (m, 2H, H-4, H-2), 4.32 (d, 2H, *J* = 2.3 Hz, OCH_2), 4.98 (s, 1H, H-5), 5.67 (d, 1H, *J* = 4.6 Hz, H-3); ^{13}C NMR ($CDCl_3$, 100 Hz): δ 214.9, 106.7, 87.4, 86.2, 82.9, 78.8, 75.2, 57.7, 54.5, 26.2, 19.0, 9.7; HRMS (ESI): *m/z* calculated for $C_{12}H_{18}NaO_4S_2(M^+$+Na) 313.0544, found 313.0547.

O-(2S,3S,4R,5S)-2-Ethyl-tetrahydro-5-methoxy-4-(prop-2-nyloxy)furan-3-yl-S-methyl carbonodithioate (15b). A solution of **27b** (0.16 g, 0.82 mmol) with sodium hydride (0.05 g, 2.06 mmol), carbon disulphide (0.07 mL, 1.23 mmol) and methyl iodide (0.07 mL, 1.23 mmol) was added at 0 °C work up as described for **27a** and purification of the residue by column chromatography (60-120 Silica gel; ethyl acetate:*n*-hexane, 1:9) gave **15b** (0.21 g, 88%) as a liquid; $[\alpha]_D$ = +206.3 (*c* 1.25, $CDCl_3$); IR (neat): ν_{max} 3285, 2924, 2858, 2120, 1712, 1446, 1210, 1064, 669 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 0.99 (t, 3H, *J* = 7.3 Hz, CH_3), 1.67-2.0 (m, 2H, CH_2), 2.48 (t, 1H, *J* = 2.2 Hz, acetylinic), 2.58 (s, 3H, SCH_3), 3.46 (s, 3H, OCH_3), 3.87-3.93 (m, 1H, H-2), 4.29-4.27 (dd, 2H, *J* = 2.4 Hz, OCH_2), 4.48 (dd, 1H, *J* = 4.5 Hz, H-4), 5.01 (d, 1H, *J* = 4.5 Hz, H-5), 6.12 (dd, 1H, *J* = 4.5 Hz, H-3); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 215.1, 101.8, 88.0, 83.1, 81.9, 78.8, 75.5, 57.8, 55.2, 28.5, 19.3, 10.1; HRMS (ESI): *m/z* calculated for $C_{12}H_{18}NaO_4S_2(M^+$+Na) 313.0544, found 313.0549.

O-(2S,3S,4R,5R)-Tetrahydro-5-methoxy-2-pentyl-4-(prop-2-ynyloxy)furan-3-yl-S-methyl carbonodithioate (14c). A solution of **26c** (0.09 g, 0.37 mmol) with sodium hydride (0.02 g, 0.74 mmol), carbon disulphide (0.03 mL, 0.55 mmol) and methyl iodide (0.03 mL, 0.55 mmol) was added at 0 °C work up as described for **14a** and purification of the residue by column chromatography (60-120 Silica gel; ethyl acetate:*n*-hexane, 1:9) gave **14c** (0.09 g, 73%) as light yellow liquid; $[\alpha]_D$ = -327.0 (*c* 0.4, $CDCl_3$); IR (neat): ν_{max} 3440, 2922, 2115, 1724, 1469, 1255, 1072, 778 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 0.89 (t, 3H, *J* = 6.6 Hz, CH_3), 1.25-1.72 (m, 8H, 4 CH_2), 2.39 (t, 1H, *J* = 2.2 Hz, acetylinic), 2.57 (s, 3H, SCH_3), 3.36 (s, 3H, OCH_3), 4.08-4.14 (m, 2H, H-4, H-2), 4.28 (d, 2H, *J* = 2.2 Hz, OCH_2), 4.91 (s, 1H, H-5), 5.59 (d, 1H, *J* = 4.7 Hz, H-3); ^{13}C NMR ($CDCl_3$, 75 MHz): δ 214.8, 106.8, 87.9, 86.2, 81.8, 78.9, 75.3, 57.7, 54.5, 33.3, 31.6, 25.3, 22.6, 19.1, 14.1; HRMS (ESI): *m/z* calculated for $C_{15}H_{24}NaO_4S_2$(M^++Na) 355.1013, found 355.1008.

O-(2S,3S,4R,5S)-Tetrahydro-5-methoxy-2-pentyl-4-(prop-2-ynyloxy)furan-3-yl-S-methyl carbonodithioate (15c). A solution of **27c** (0.10 g, 0.41 mmol) with sodium hydride (0.02 g, 1.03 mmol), carbon disulphide (0.03 mL, 0.62 mmol) and methyl iodide (0.03 mL, 0.62 mmol) was added at 0 °C work up as described for **14c** and purification of the residue by column chromatography (60-120 Silica gel; ethyl acetate:*n*-hexane, 1:9) gave **15c** (0.11 g, 81%) as light yellow liquid; $[\alpha]_D$ = +158.9 (*c* 0.58, $CDCl_3$); IR (neat): ν_{max} 3356, 2861, 2167, 1718, 1532, 1209, 1132, 761 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$): δ 0.88 (t, 3H, *J* = 6.6 Hz, CH_3), 1.25-1.92 (m, 8H, 4CH_2), 2.35 (s, 1H, H-acetylinic), 2.58 (s, 3H, SCH_3), 3.45 (s, 3H, OCH_3), 3.95 (m, 1H, H-2), 4.27 (m, 2H, OCH_2), 4.46 (t, 1H, *J* = 4.9 Hz, H-4), 4.99 (d, 1H, *J* = 4.5 Hz, H-5), 6.0 (t, 1H, *J* = 4.7 Hz, H-3); ^{13}C NMR ($CDCl_3$, 150 MHz): δ 215.1, 101.7, 101.1, 88.4, 82.0, 81.8, 78.6, 75.6, 57.8, 55.2, 35.5, 31.4, 25.4, 22.6, 19.4, 14.1; HRMS (ESI): *m/z* calculated for $C_{15}H_{24}NaO_4S_2$(M^++Na) 355.1013, found 355.1023.

2. NMR Spectra

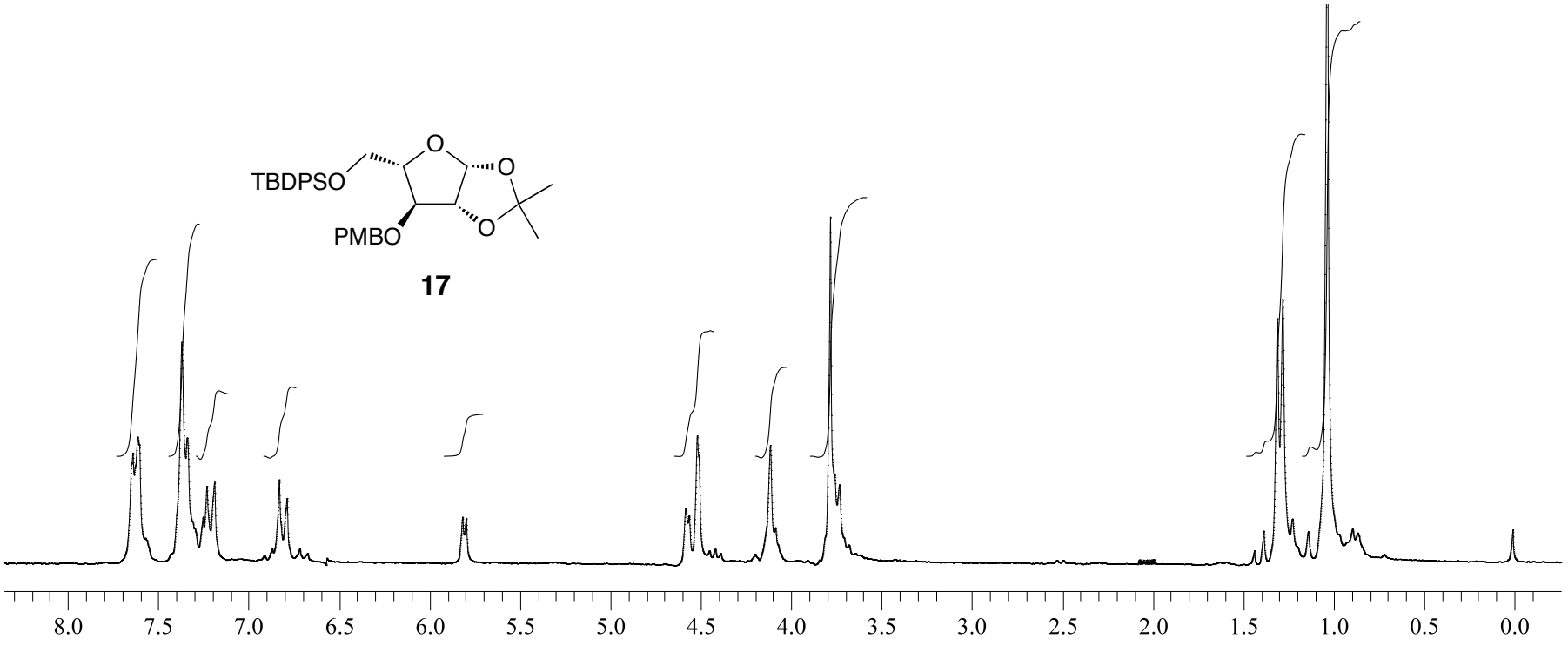


Figure S1 ^{1}H NMR Spectrum of **17** ($CDCl_3$, 303 K, 200 MHz).

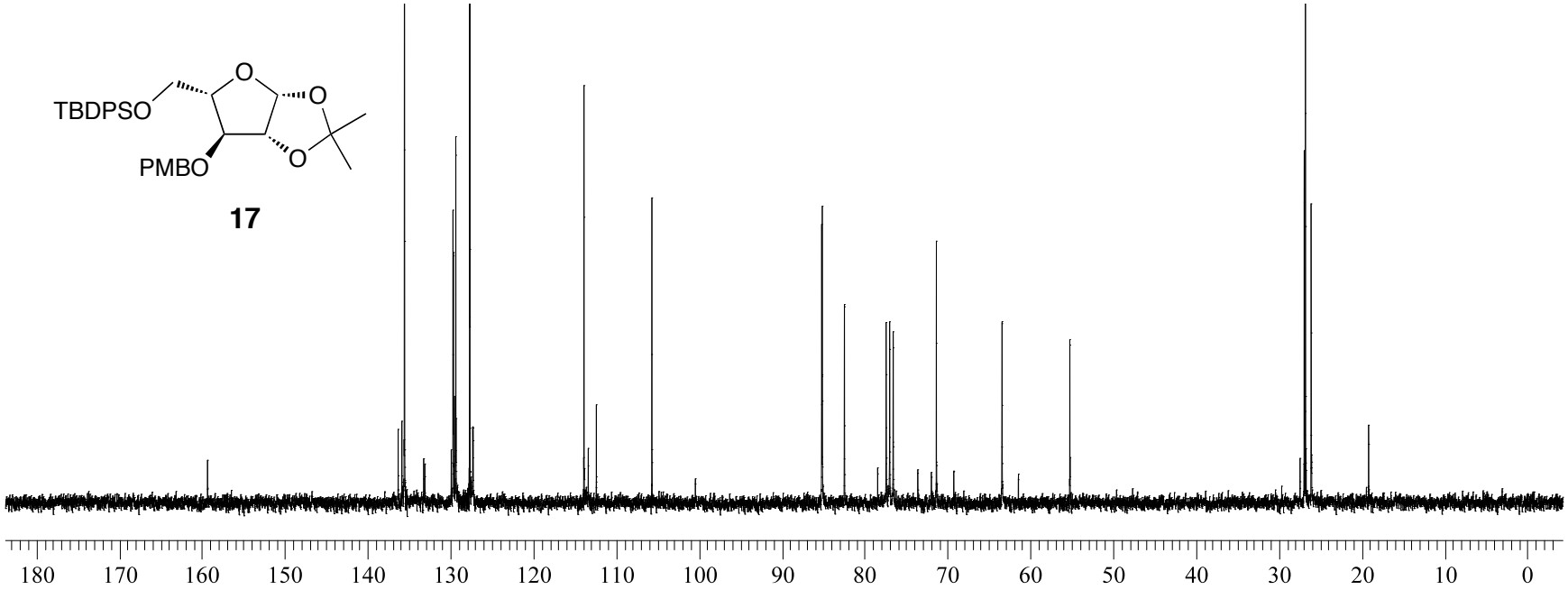


Figure S2 ^{13}C NMR Spectrum of **17** ($CDCl_3$, 303 K, 75 MHz).

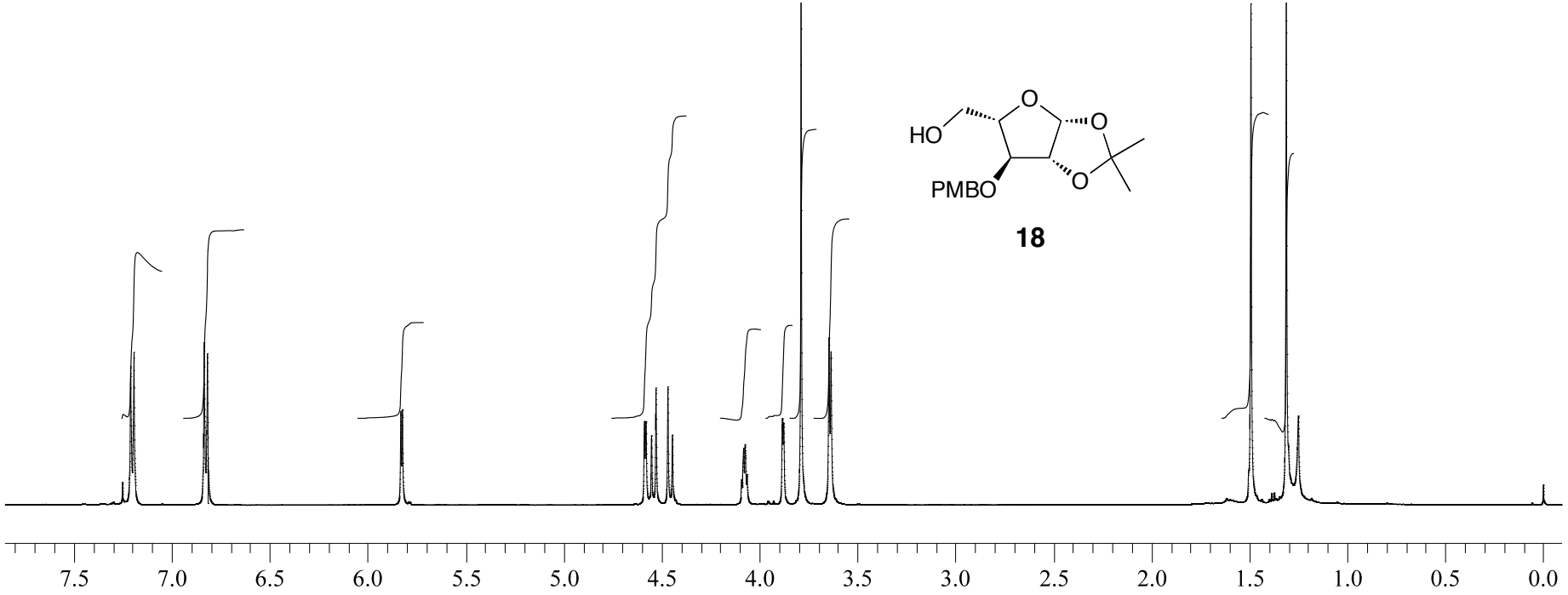


Figure S3 ^{1}H NMR Spectrum of **18** ($CDCl_3$, 303 K, 500 MHz).

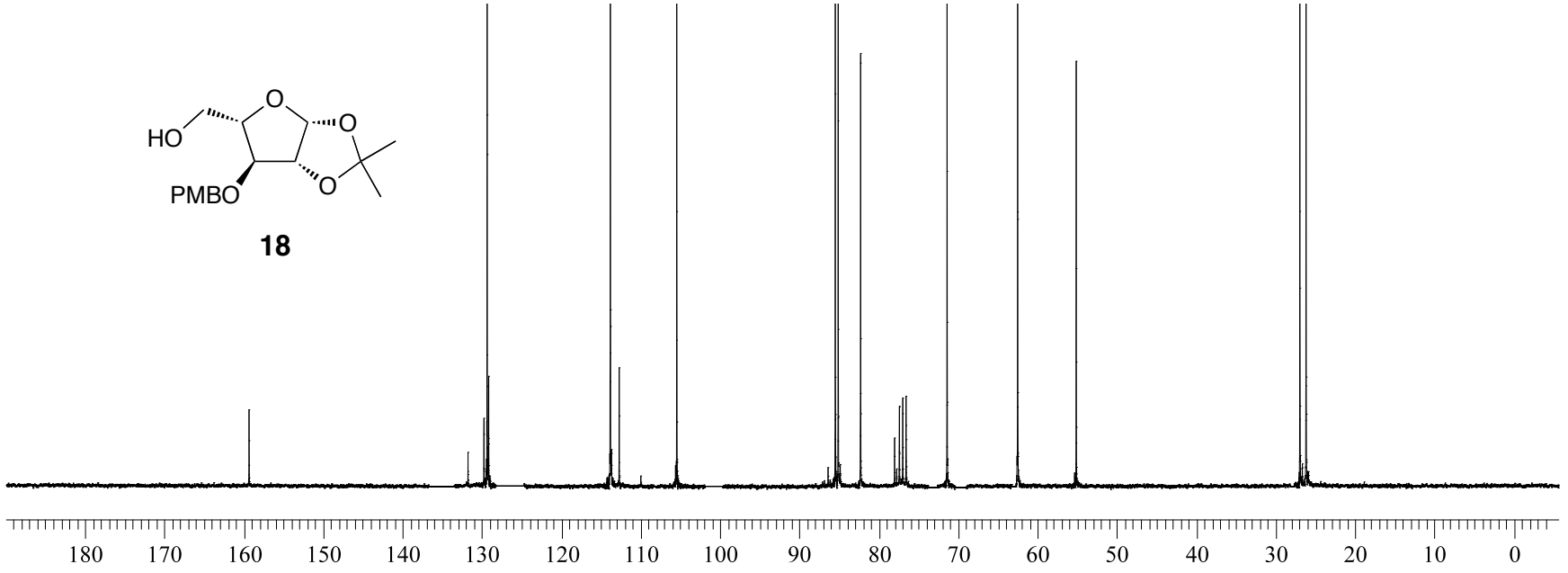


Figure S4 ^{13}C NMR Spectrum of **18** ($CDCl_3$, 303 K, 75 MHz).

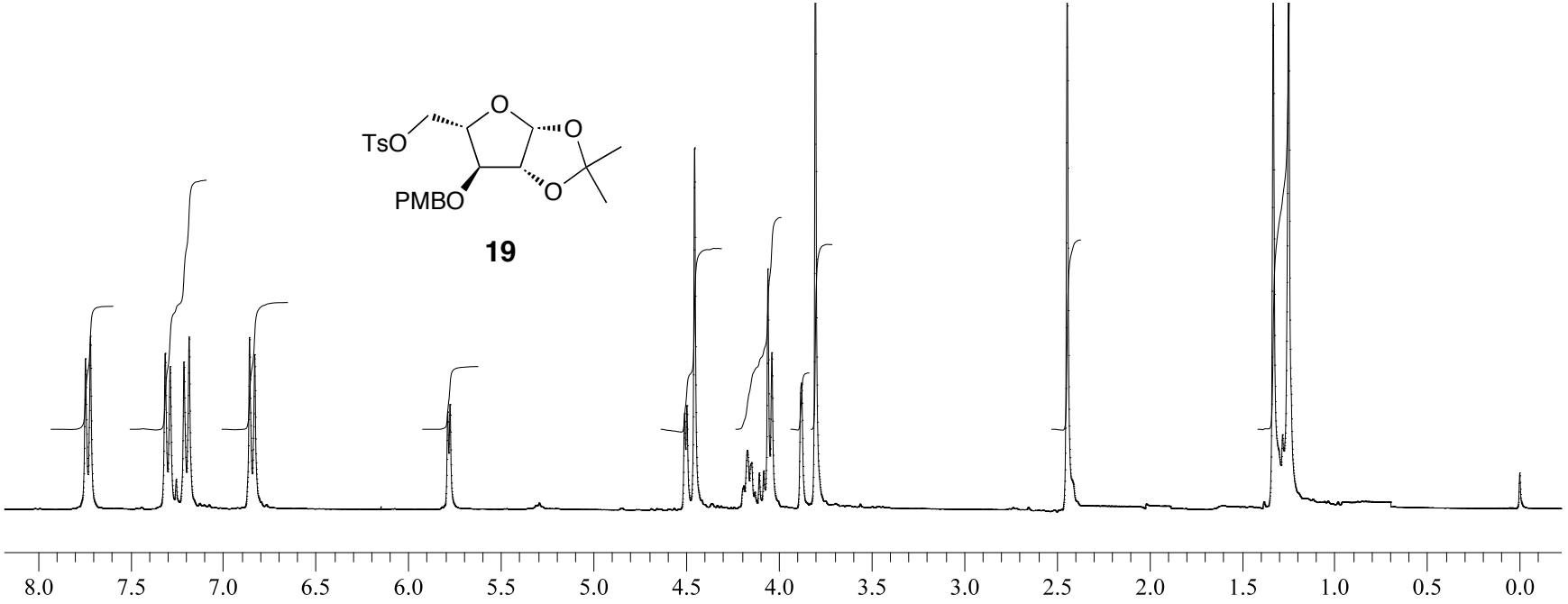


Figure S5 ^{1}H NMR Spectrum of **19** ($CDCl_3$, 303 K, 300 MHz).

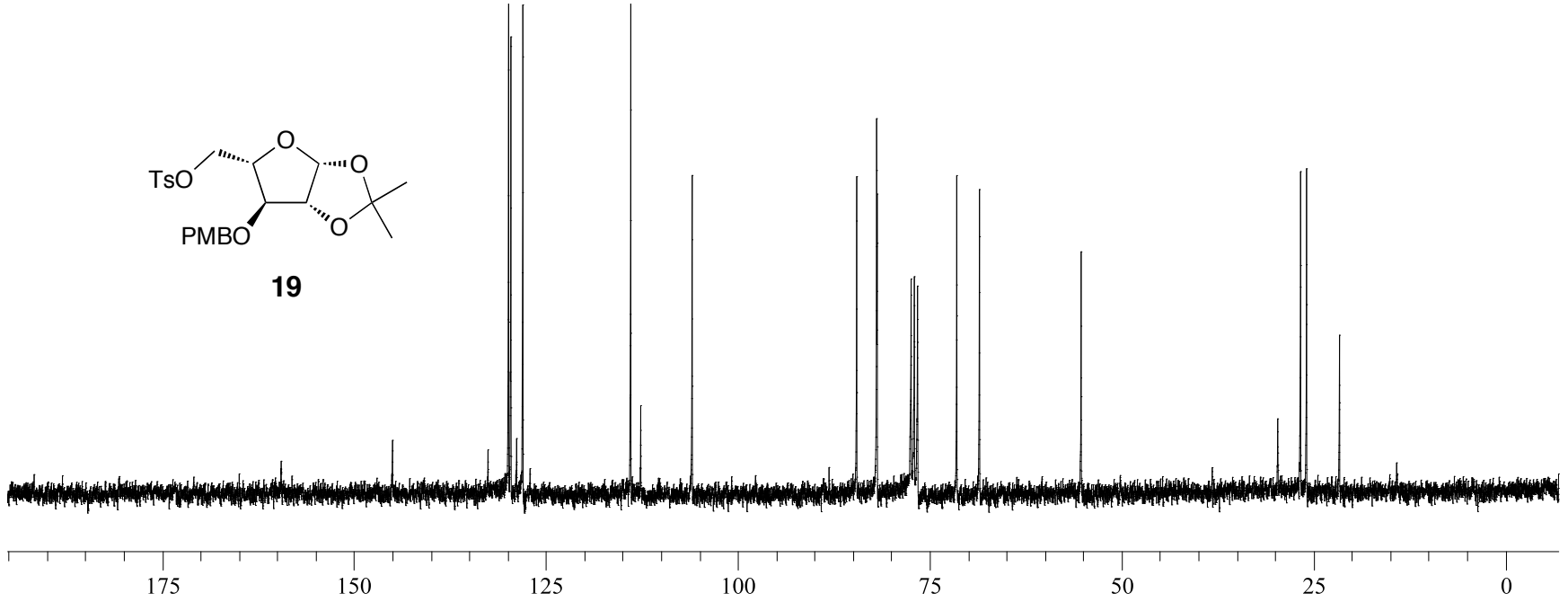


Figure S6 ^{13}C NMR Spectrum of **19** ($CDCl_3$, 303 K, 75 MHz).

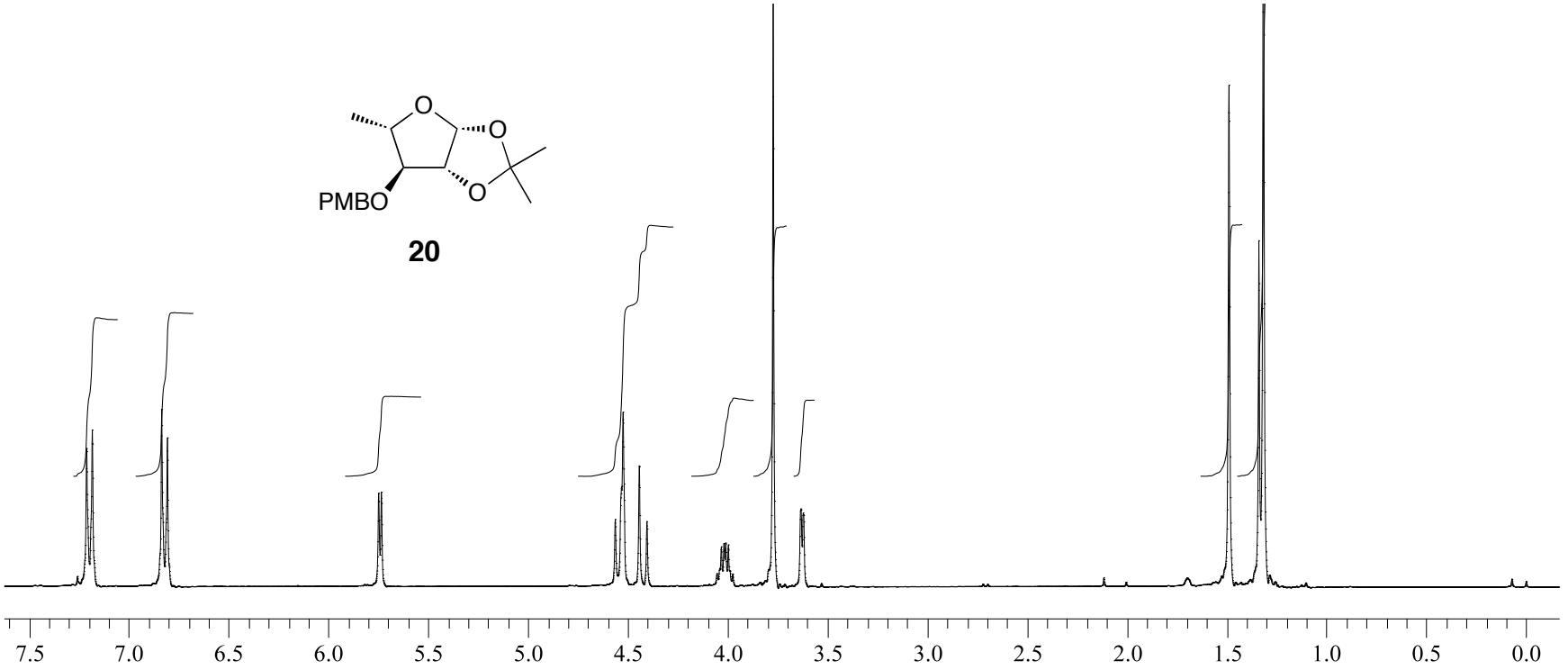


Figure S7 ^{1}H NMR Spectrum of **20a** ($CDCl_3$, 303 K, 300 MHz).

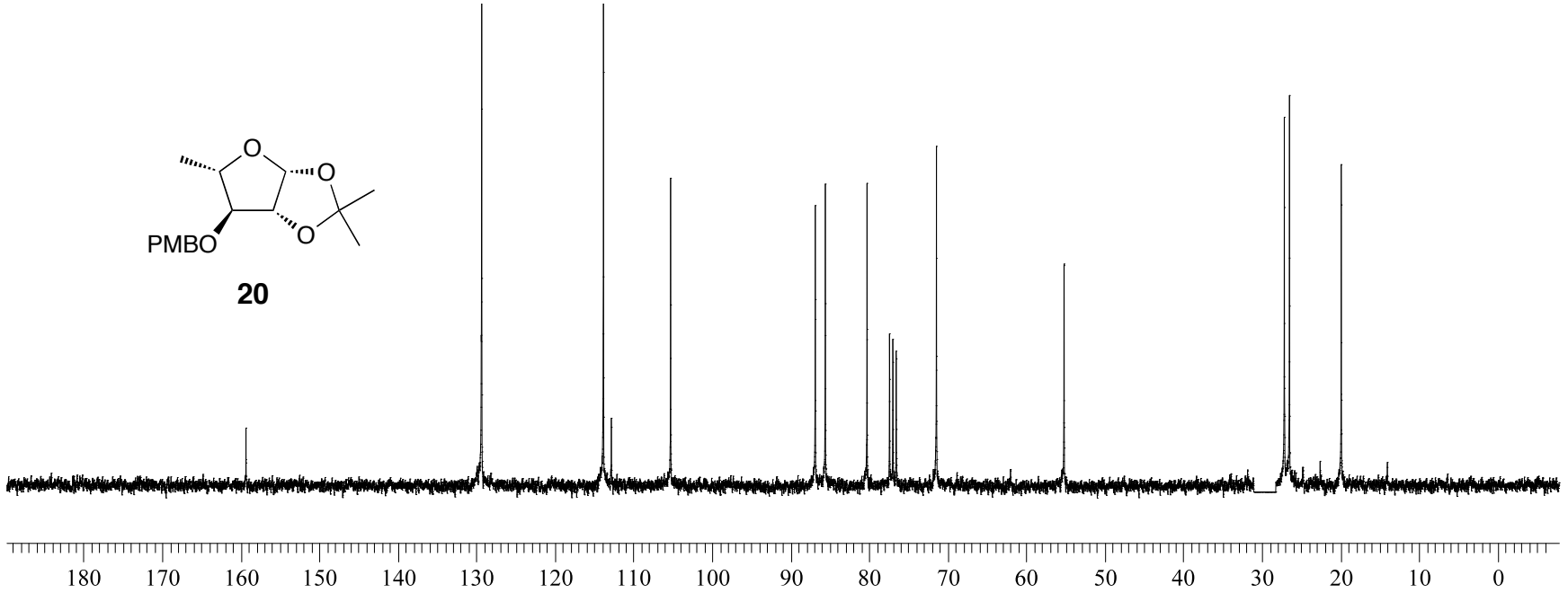


Figure S8 ^{13}C NMR Spectrum of **20a** ($CDCl_3$, 303 K, 75 MHz).

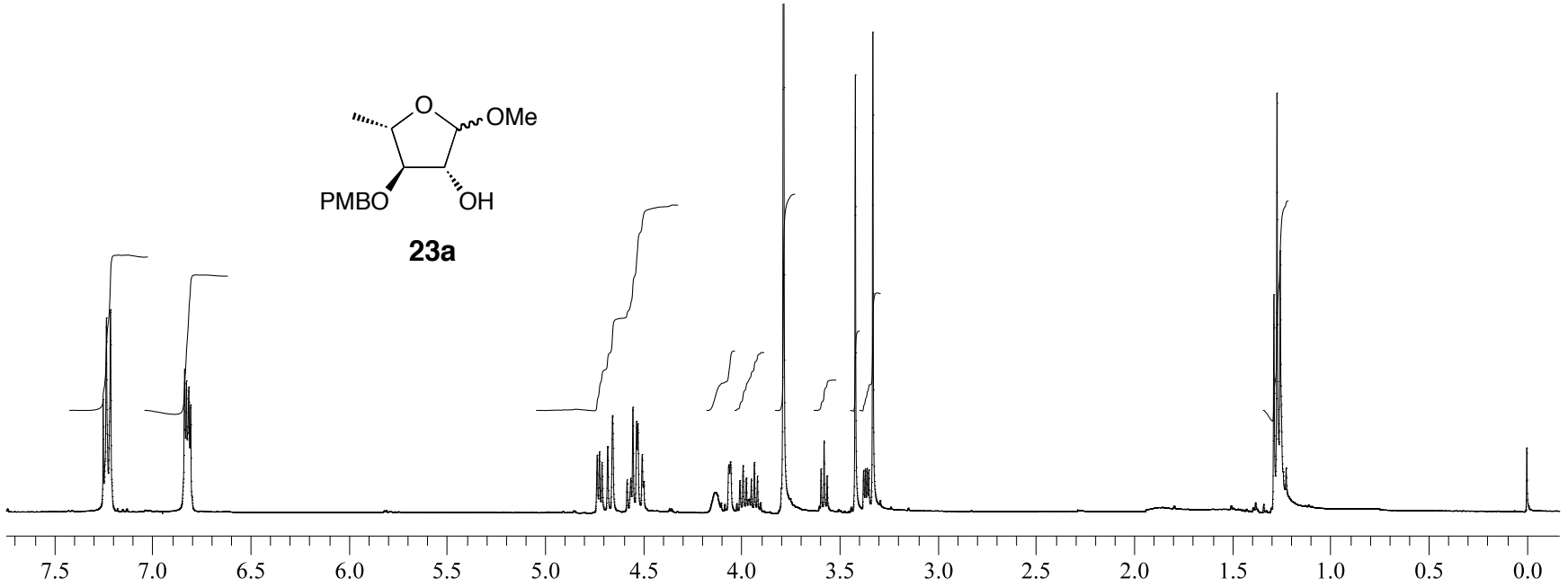


Figure S9 ^{1}H NMR Spectrum of **23a** ($CDCl_3$, 303 K, 400 MHz).

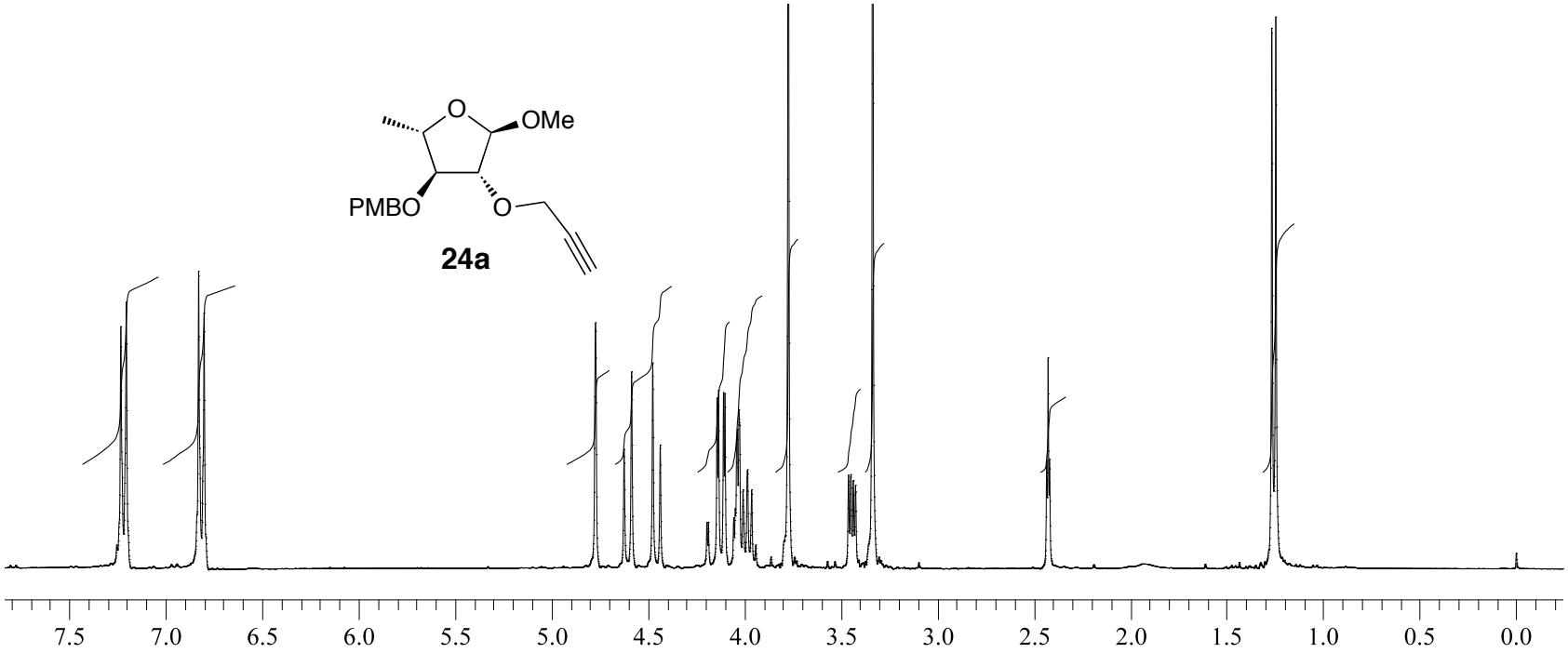


Figure S10 ^{1}H NMR Spectrum of **24a** ($CDCl_3$, 303 K, 300 MHz).

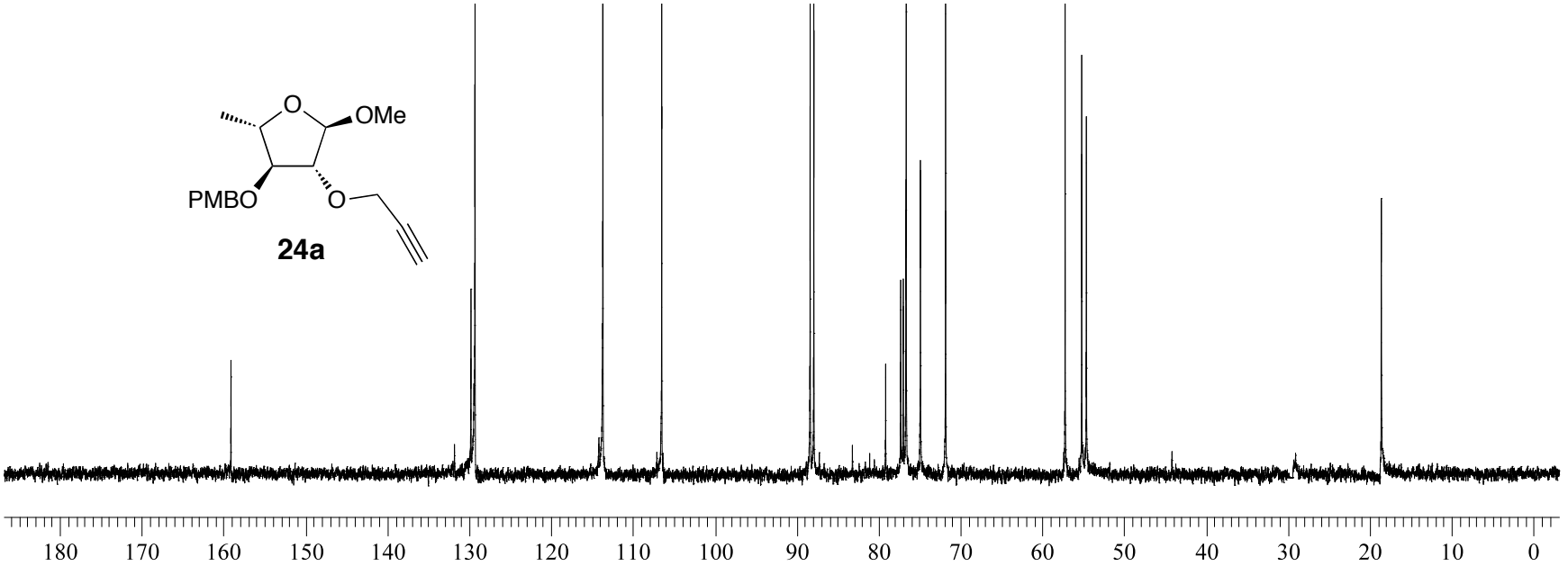


Figure S11 ^{13}C NMR Spectrum of **24a** ($CDCl_3$, 303 K, 100 MHz).

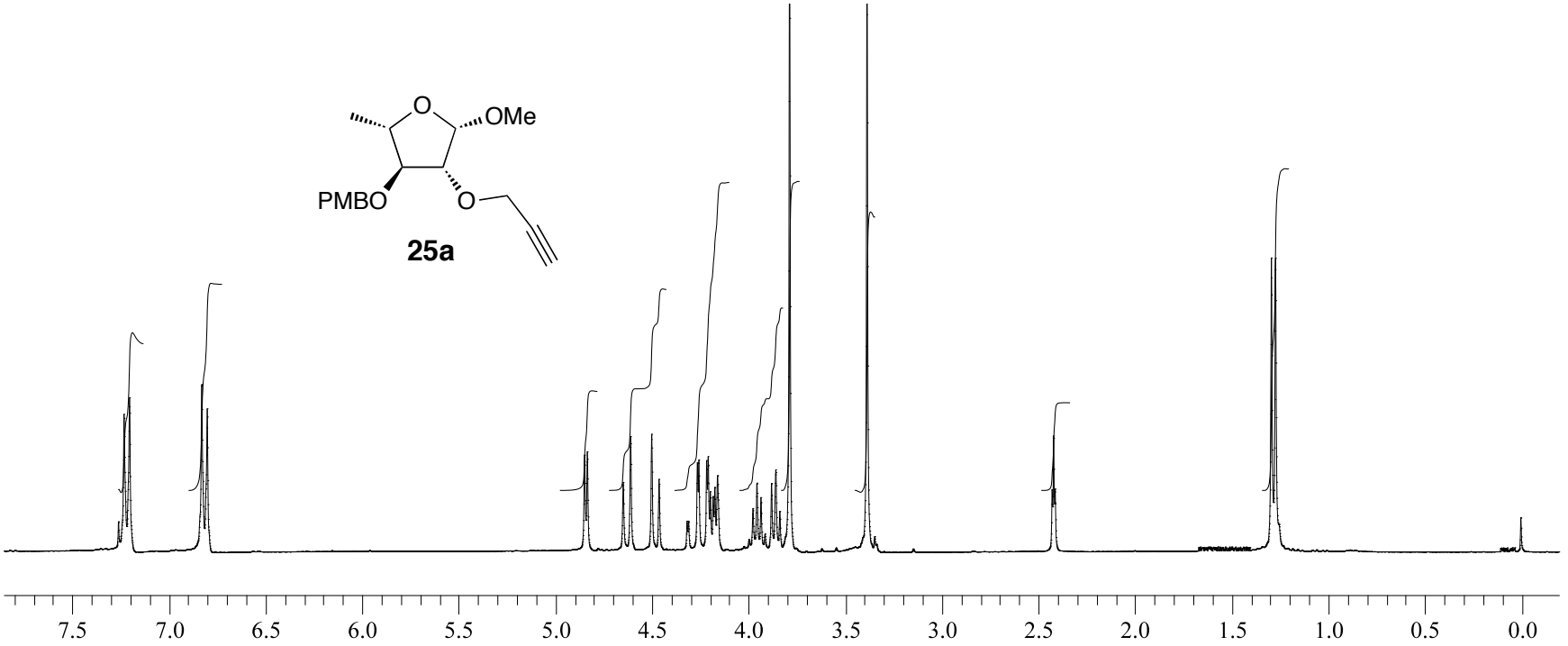


Figure S12 ^{1}H NMR Spectrum of **25a** ($CDCl_3$, 303 K, 300 MHz).

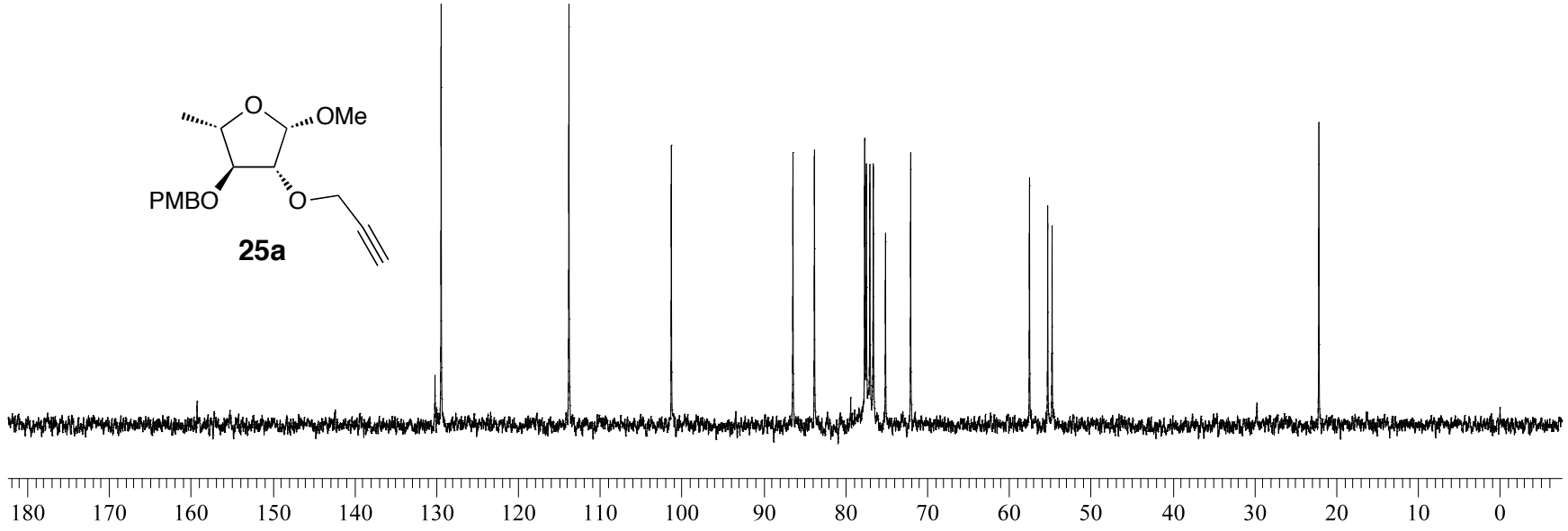


Figure S13 ^{13}C NMR Spectrum of **25a** ($CDCl_3$, 303 K, 75 MHz).

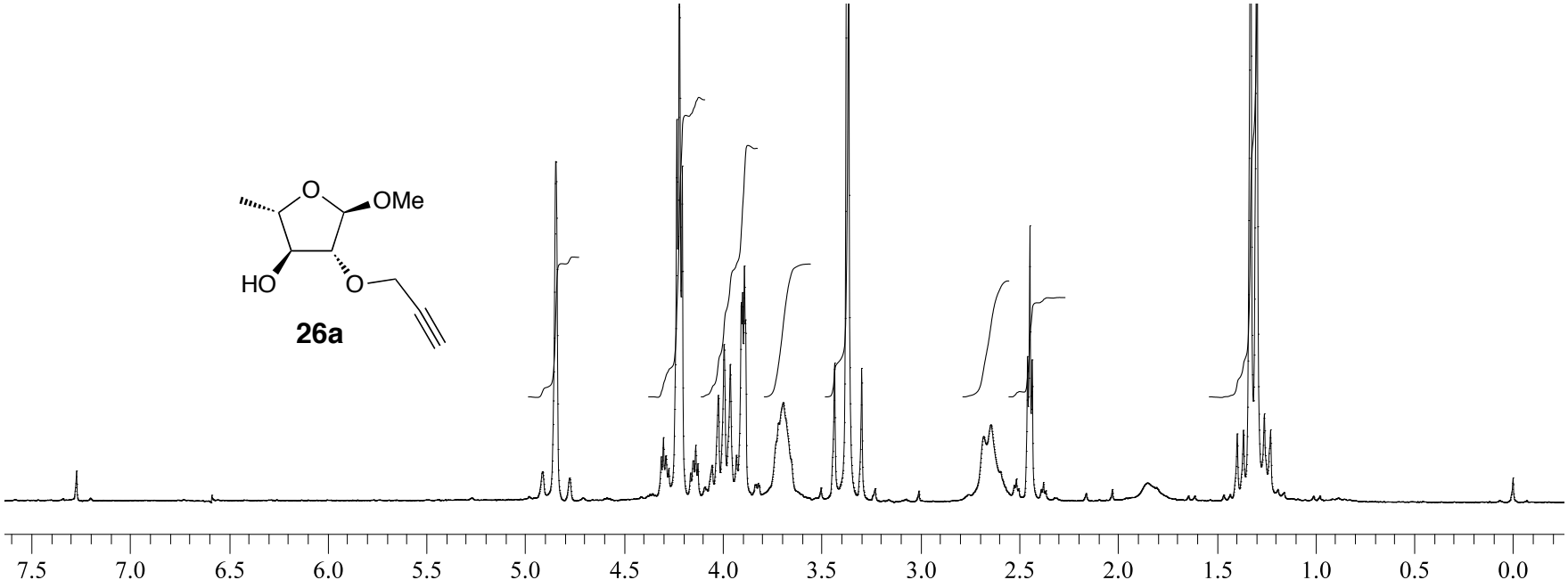


Figure S14 ^{1}H NMR Spectrum of **26a** ($CDCl_3$, 303 K, 200 MHz).

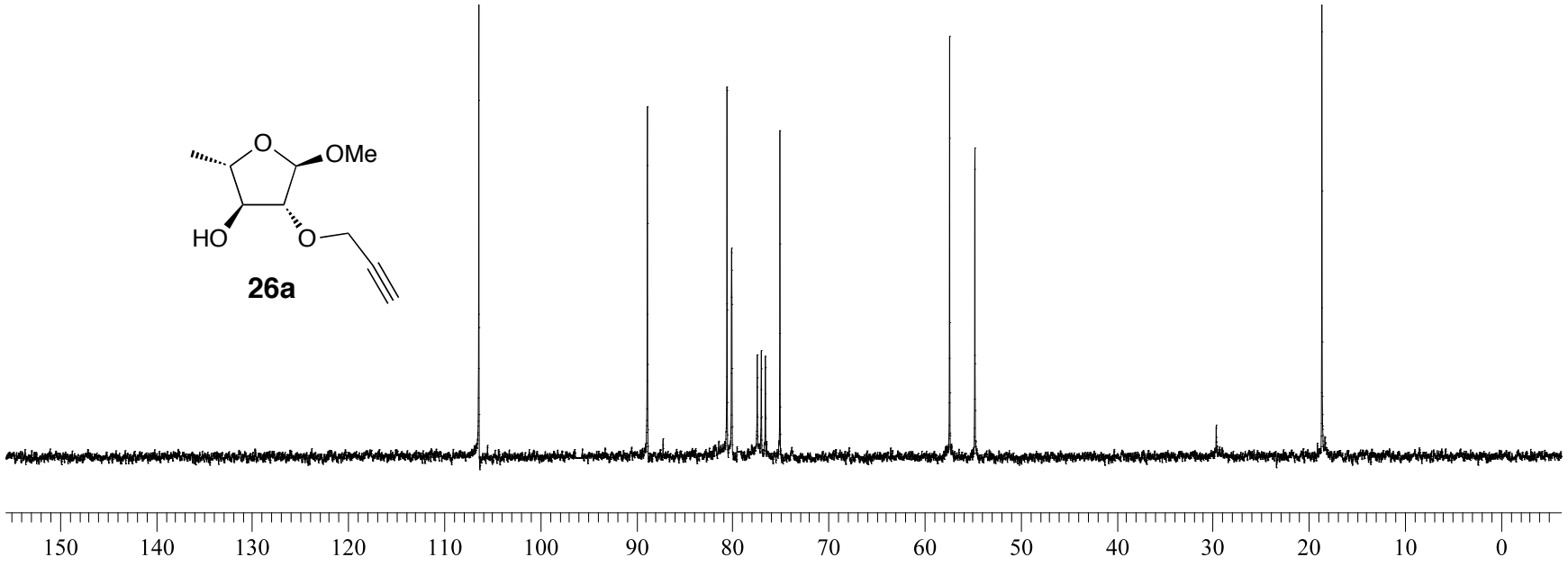


Figure S15 ^{13}C NMR Spectrum of **26a** ($CDCl_3$, 303 K, 75 MHz).

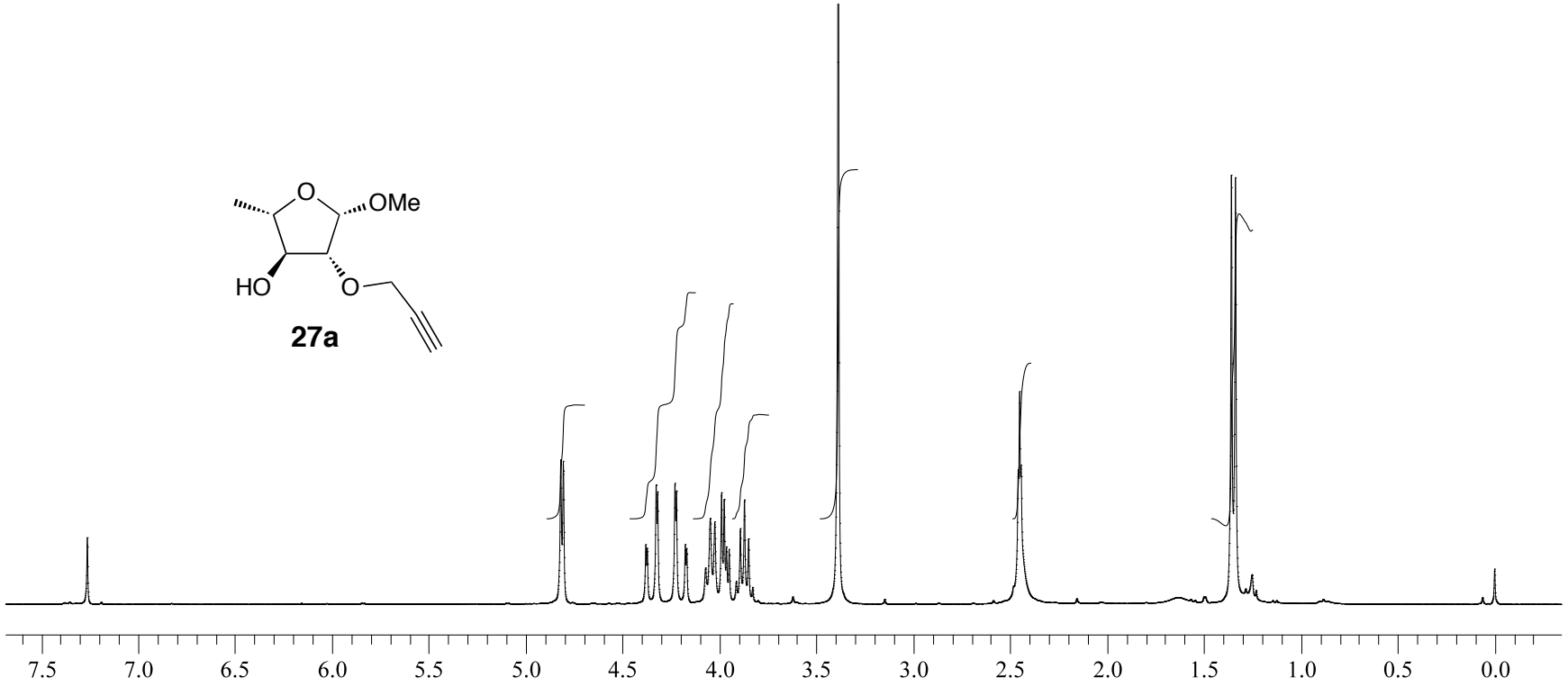


Figure S16 ^{1}H NMR Spectrum of **27a** ($CDCl_3$, 303 K, 300 MHz).

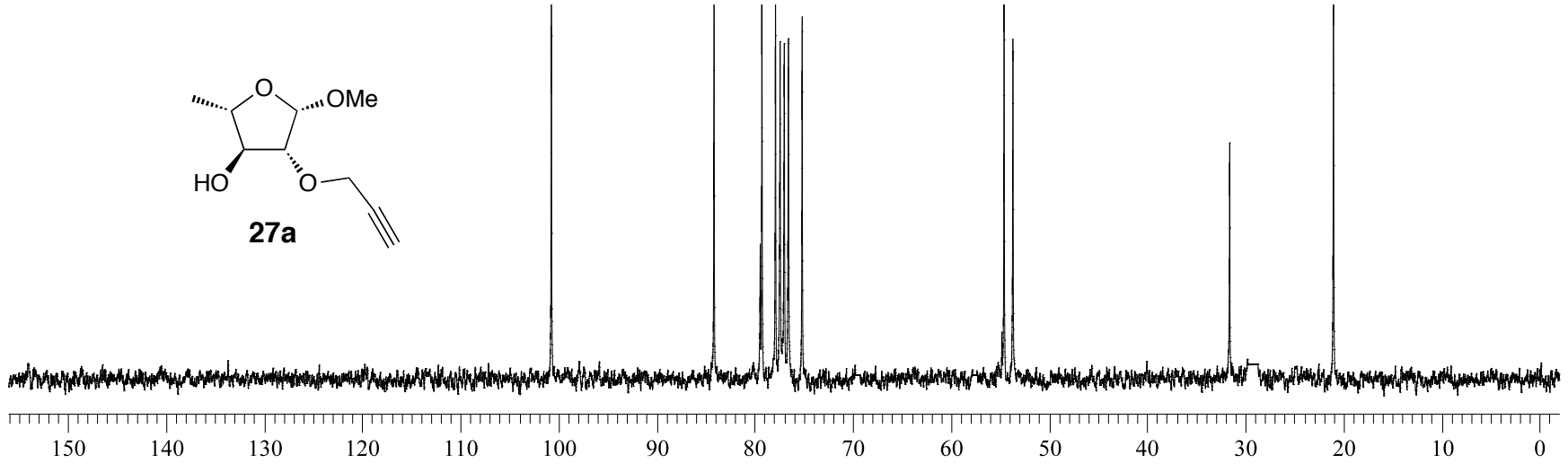


Figure S17 ^{13}C NMR Spectrum of **27a** ($CDCl_3$, 303 K, 75 MHz).

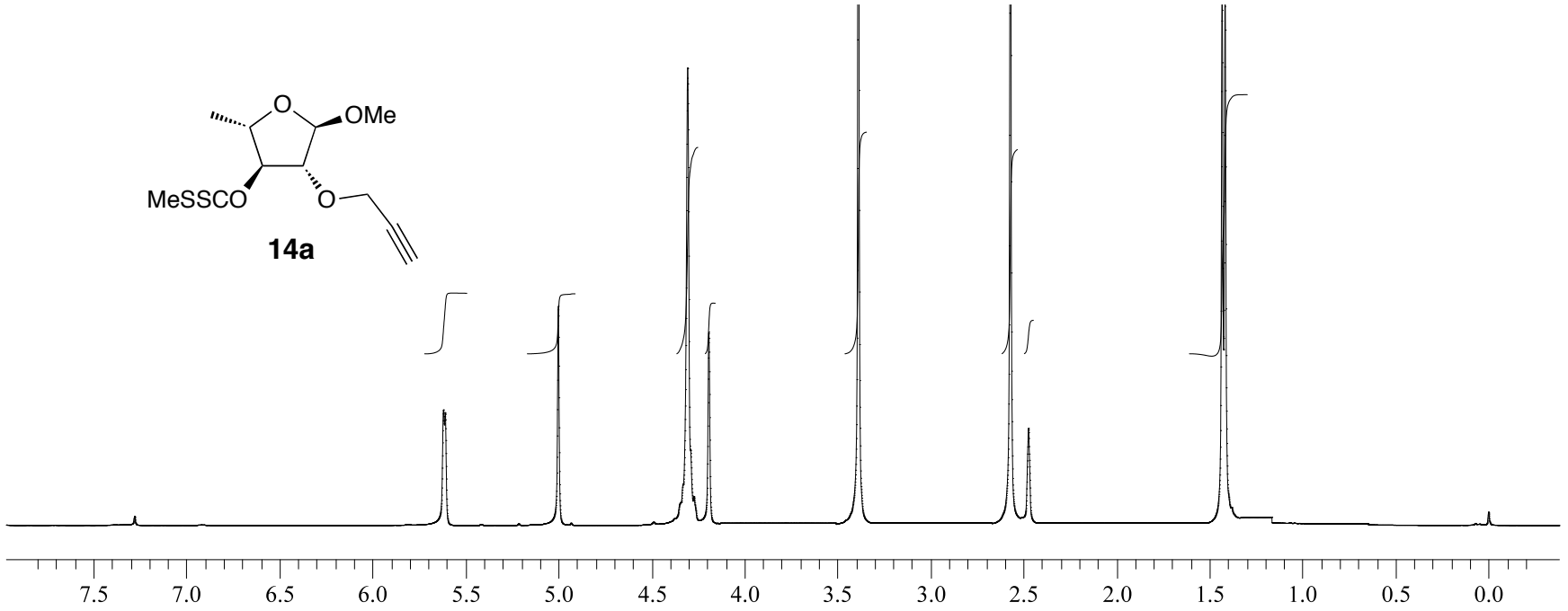


Figure S18 ^{1}H NMR Spectrum of **14a** ($CDCl_3$, 303 K, 400 MHz).

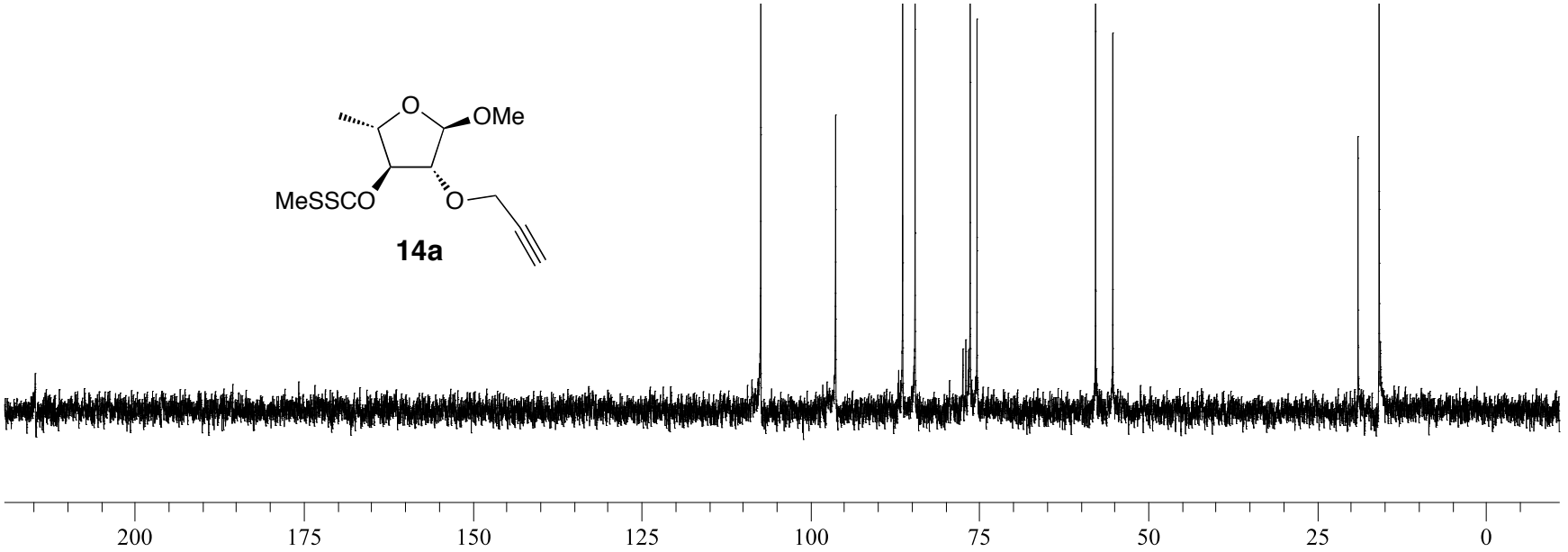


Figure S19 ^{13}C NMR Spectrum of **14a** ($CDCl_3$, 303 K, 75 MHz).

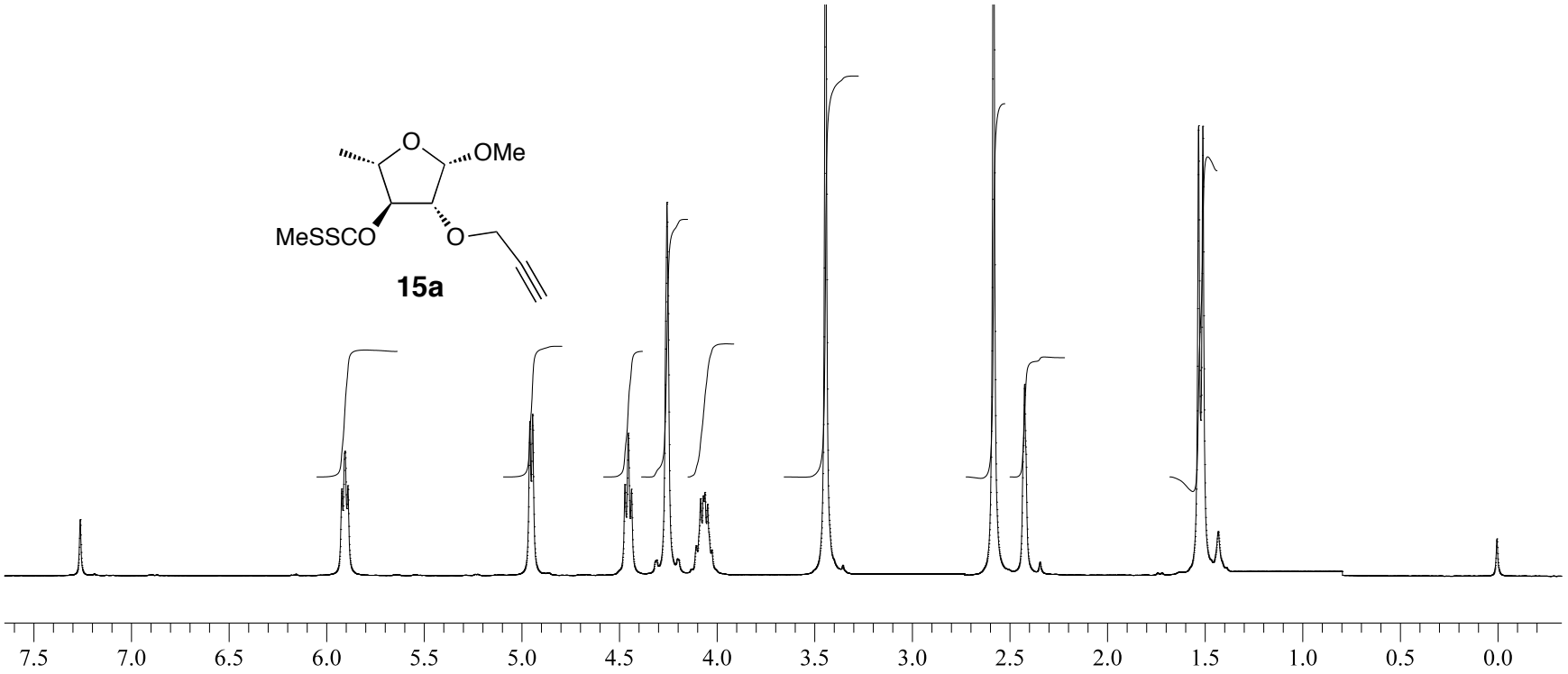


Figure S20 ^{1}H NMR Spectrum of **15a** ($CDCl_3$, 303 K, 300 MHz).

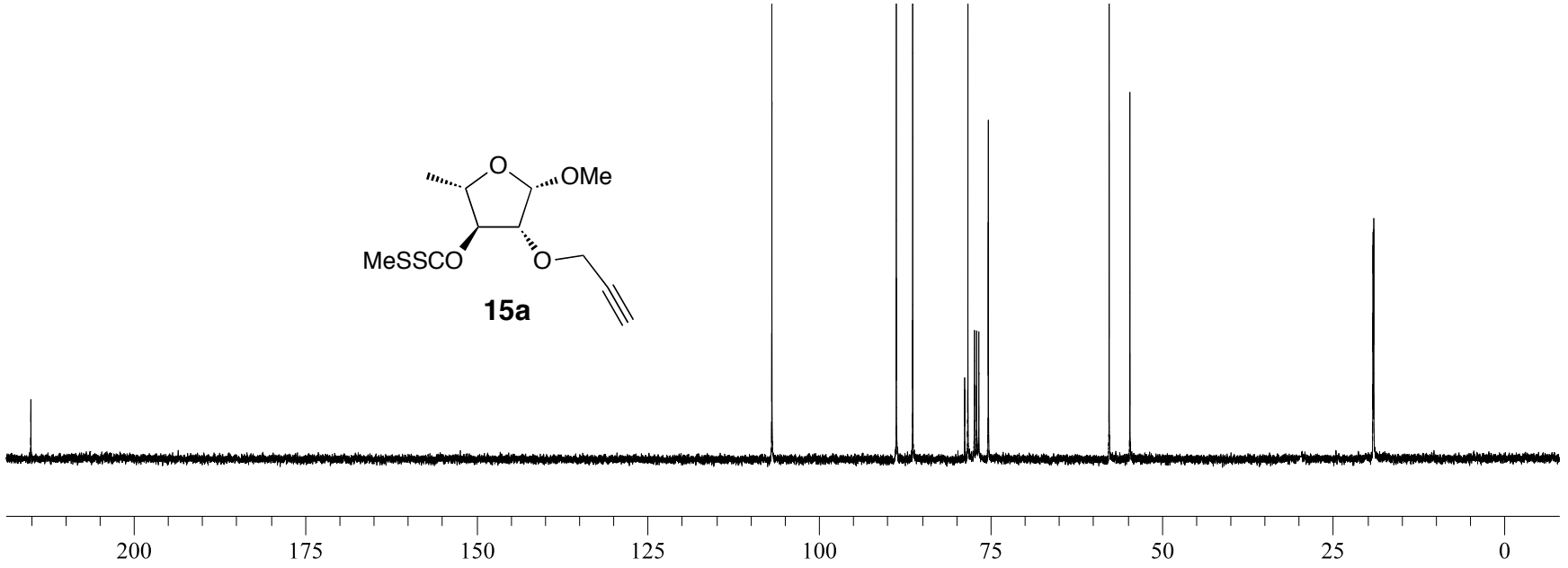


Figure S21 ^{13}C NMR Spectrum of **15a** ($CDCl_3$, 303 K, 100 MHz).

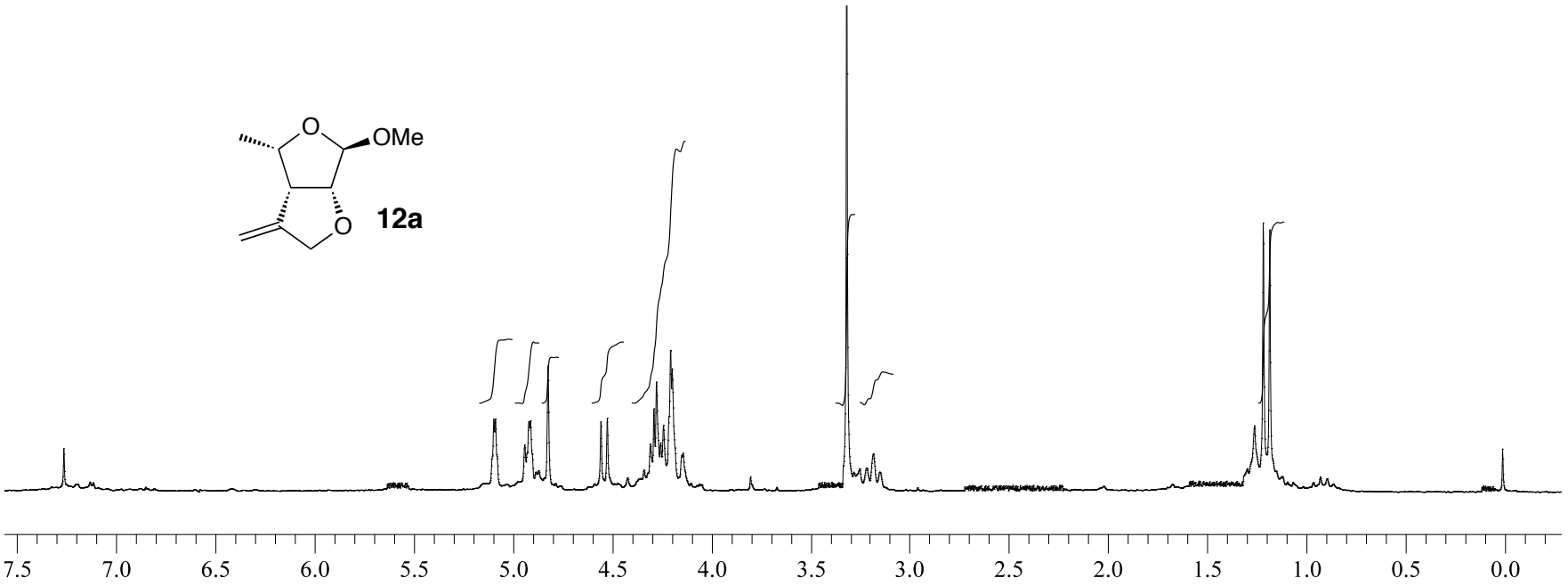


Figure S22 ^{1}H NMR Spectrum of **12a** ($CDCl_3$, 303 K, 200 MHz).

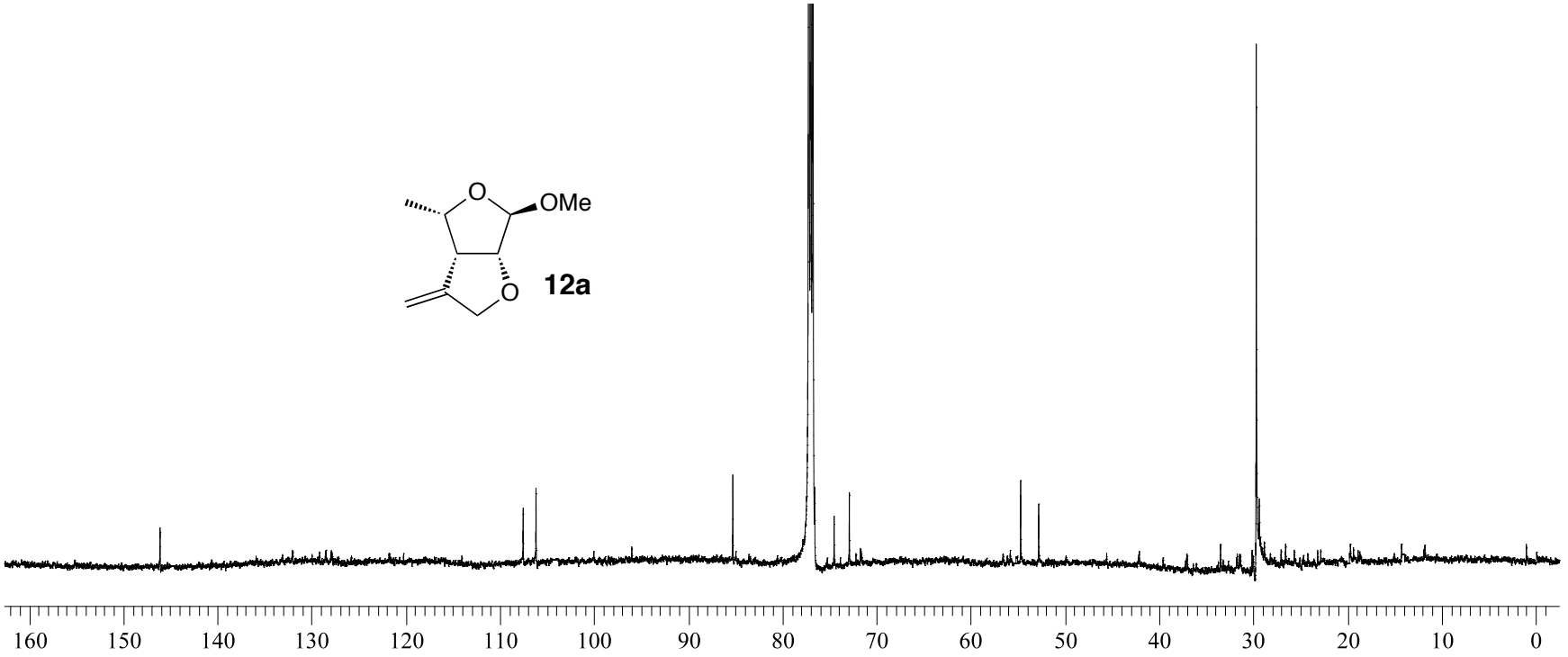


Figure S23 ^{13}C NMR Spectrum of **12a** ($CDCl_3$, 303 K, 75 MHz).

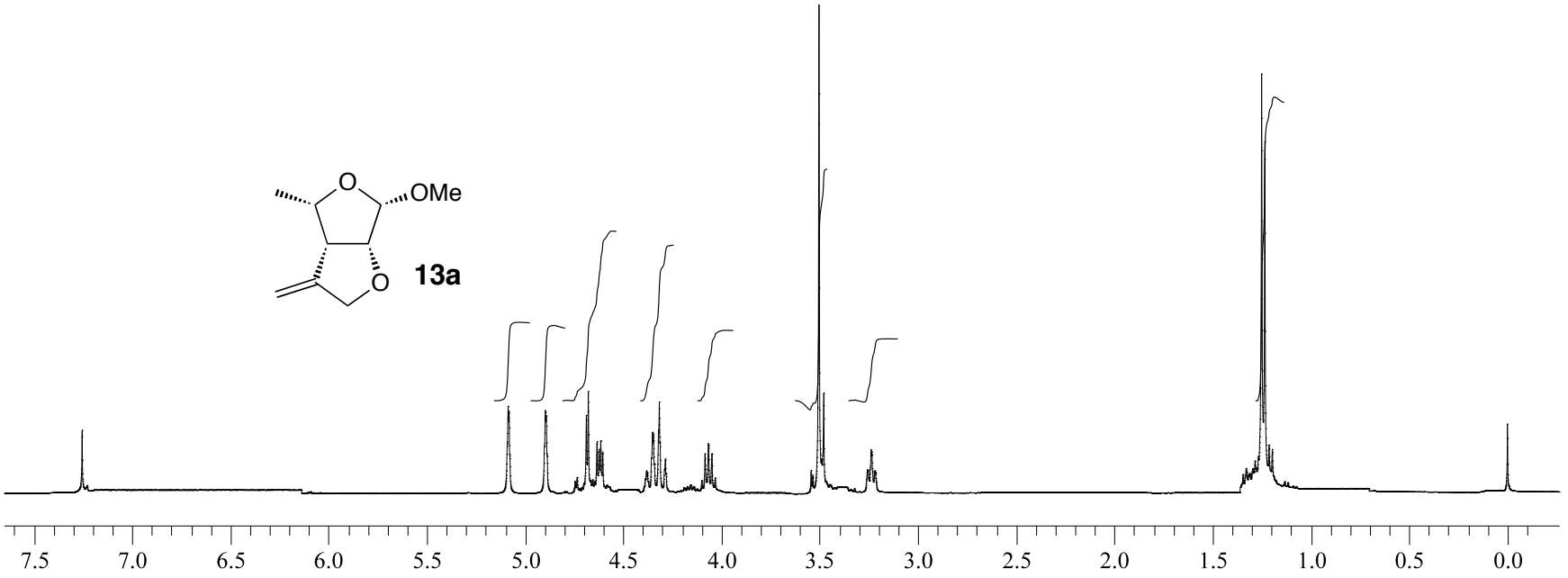


Figure S24 ^{1}H NMR Spectrum of **13a** ($CDCl_3$, 303 K, 400 MHz).

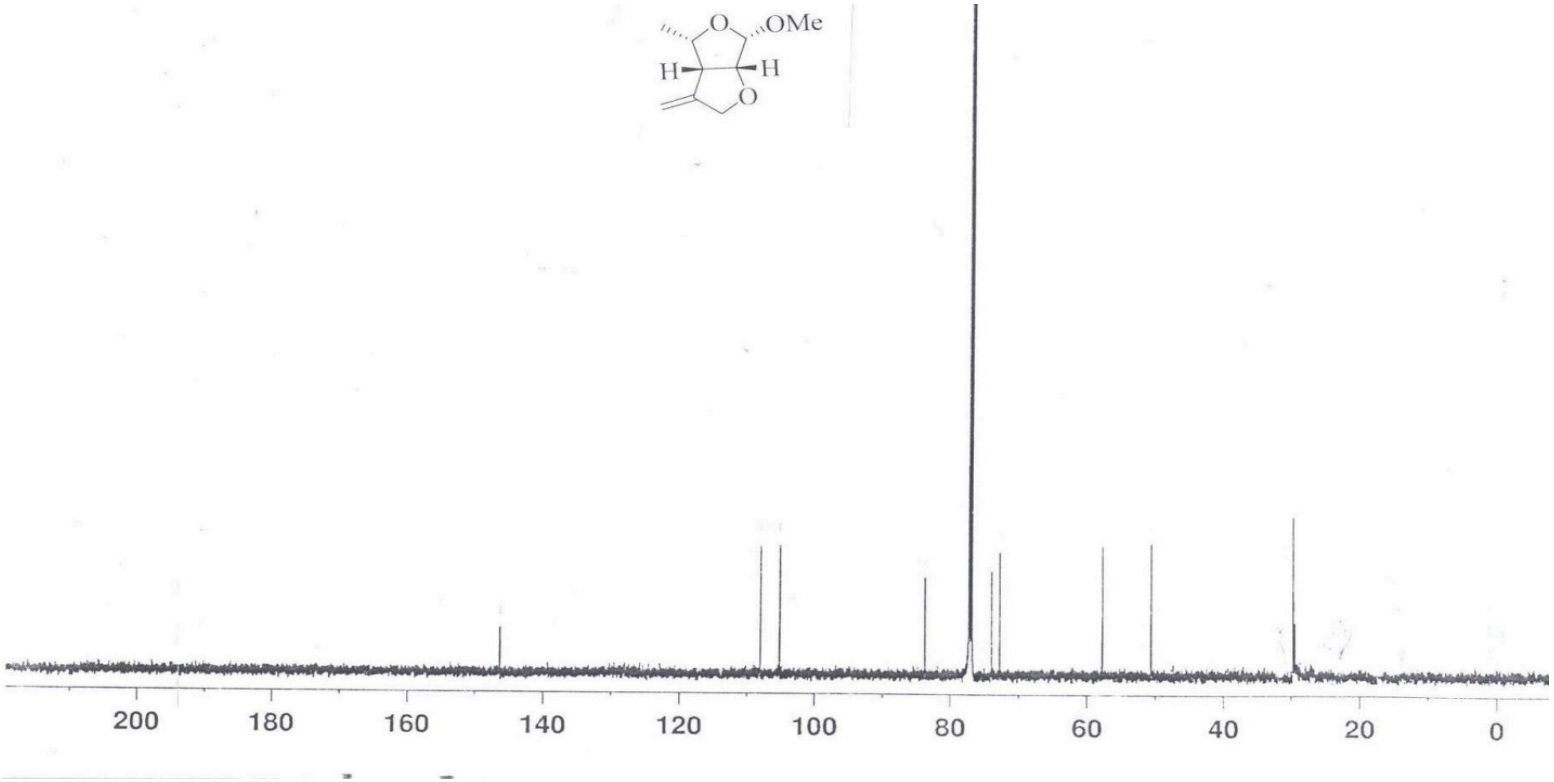


Figure S25 ^{13}C NMR Spectrum of **13a** ($CDCl_3$, 303 K, 75 MHz).

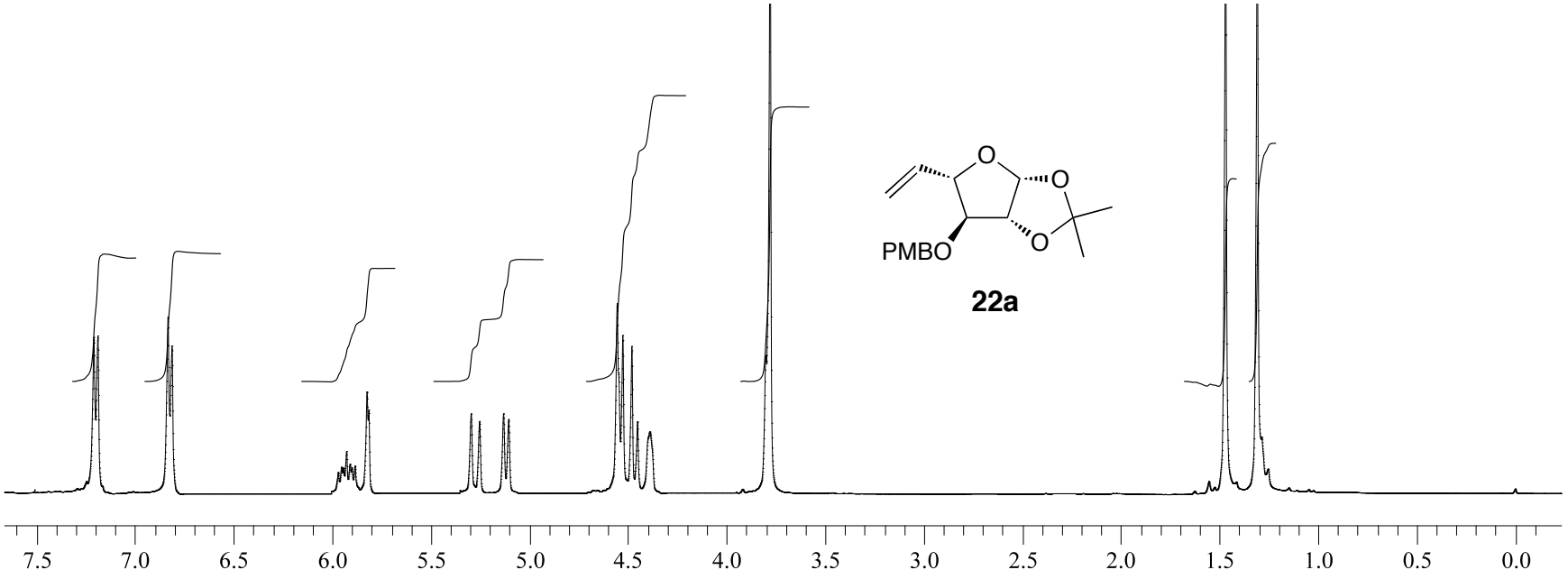


Figure S26 ^{1}H NMR Spectrum of **22a** ($CDCl_3$, 303 K, 400 MHz).

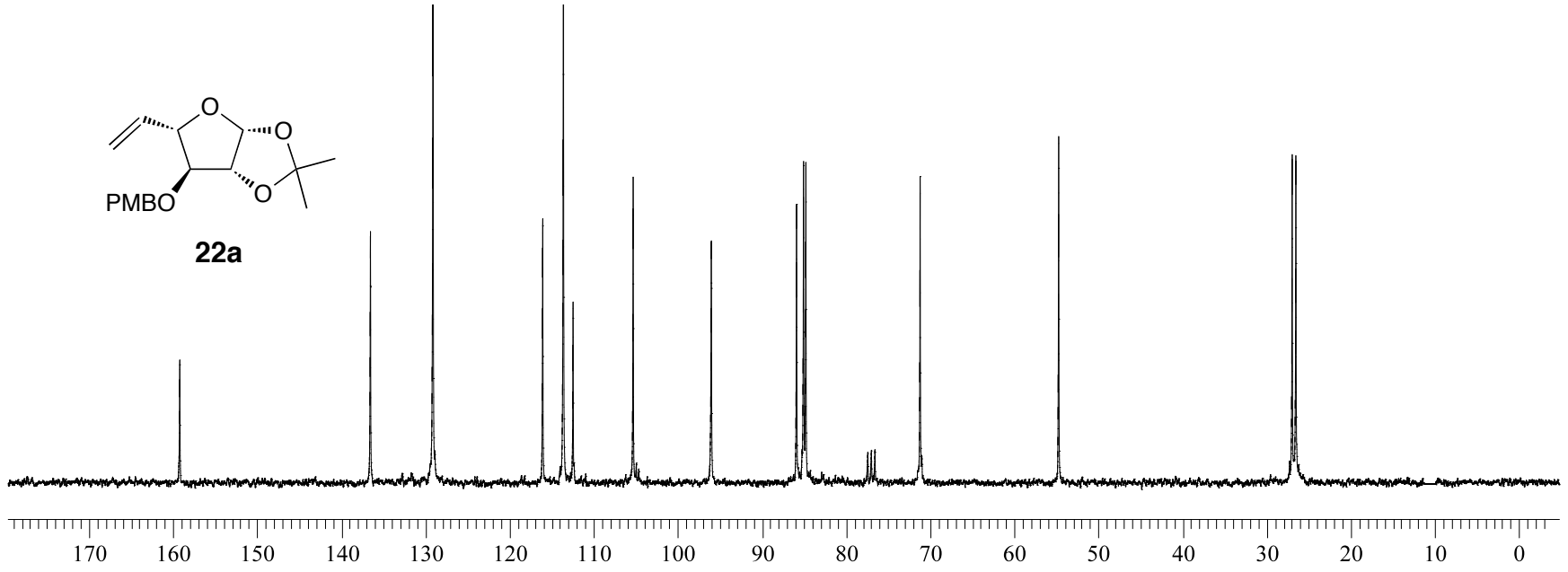


Figure S27 ^{13}C NMR Spectrum of **22a** ($CDCl_3$, 303 K, 75 MHz).

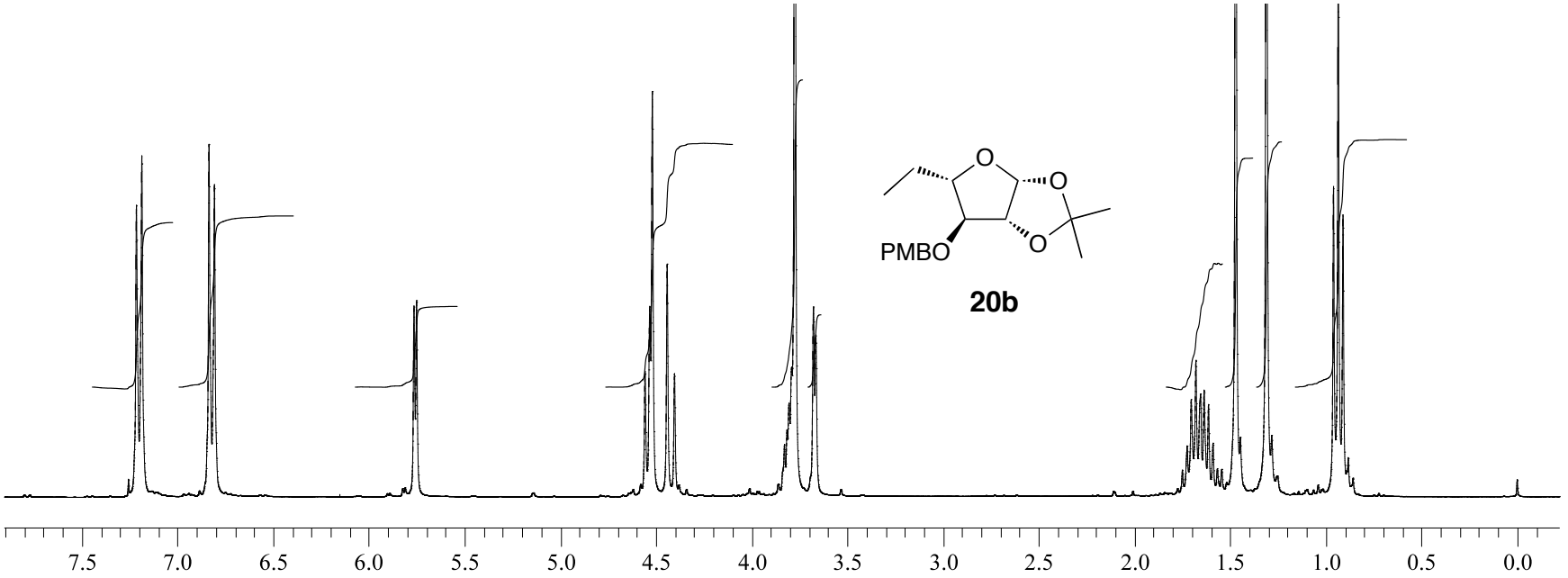


Figure S28 ^{1}H NMR Spectrum of **20b** ($CDCl_3$, 303 K, 300 MHz).

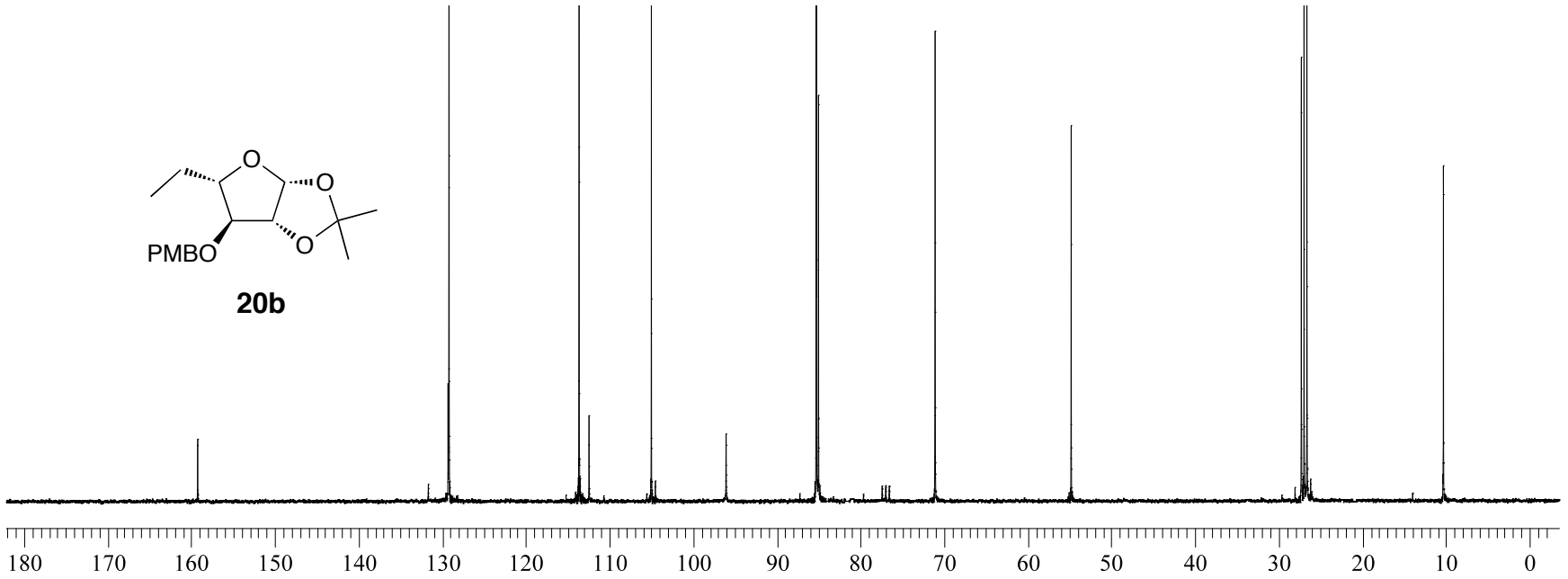


Figure S29 ^{13}C NMR Spectrum of **20b** ($CDCl_3$, 303 K, 75 MHz).

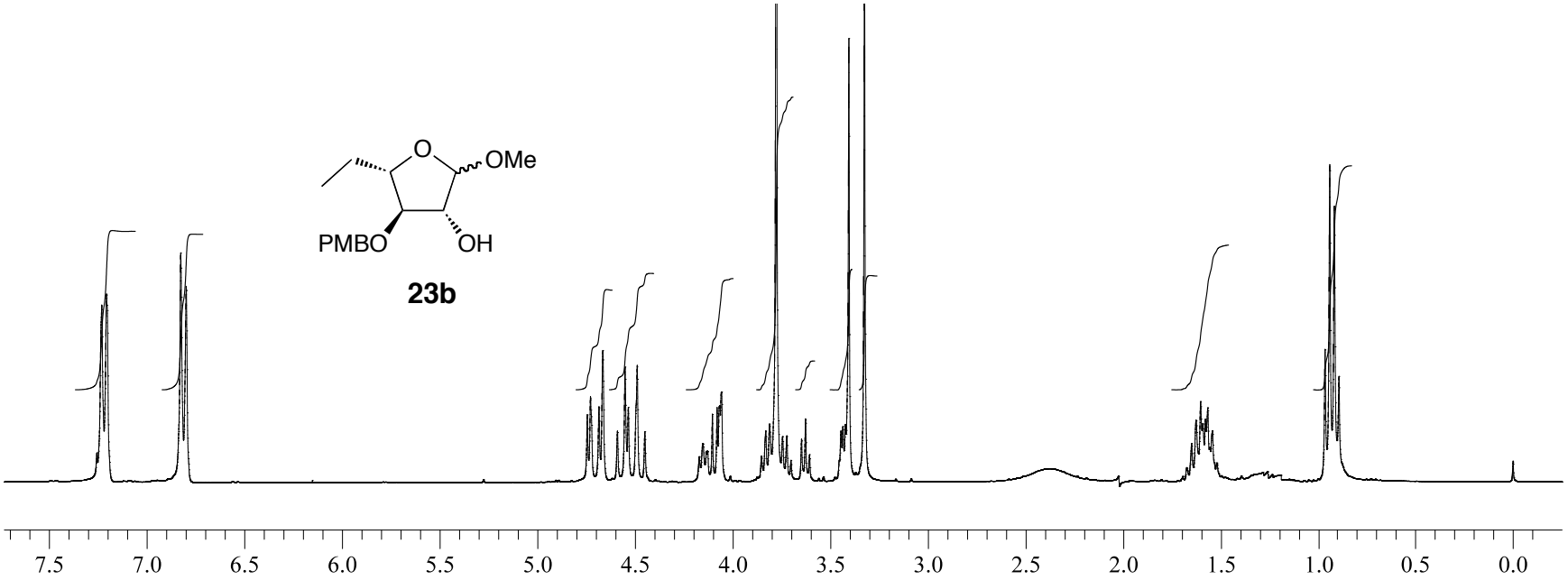


Figure S30 ^{1}H NMR Spectrum of **23b** ($CDCl_3$, 303 K, 300 MHz).

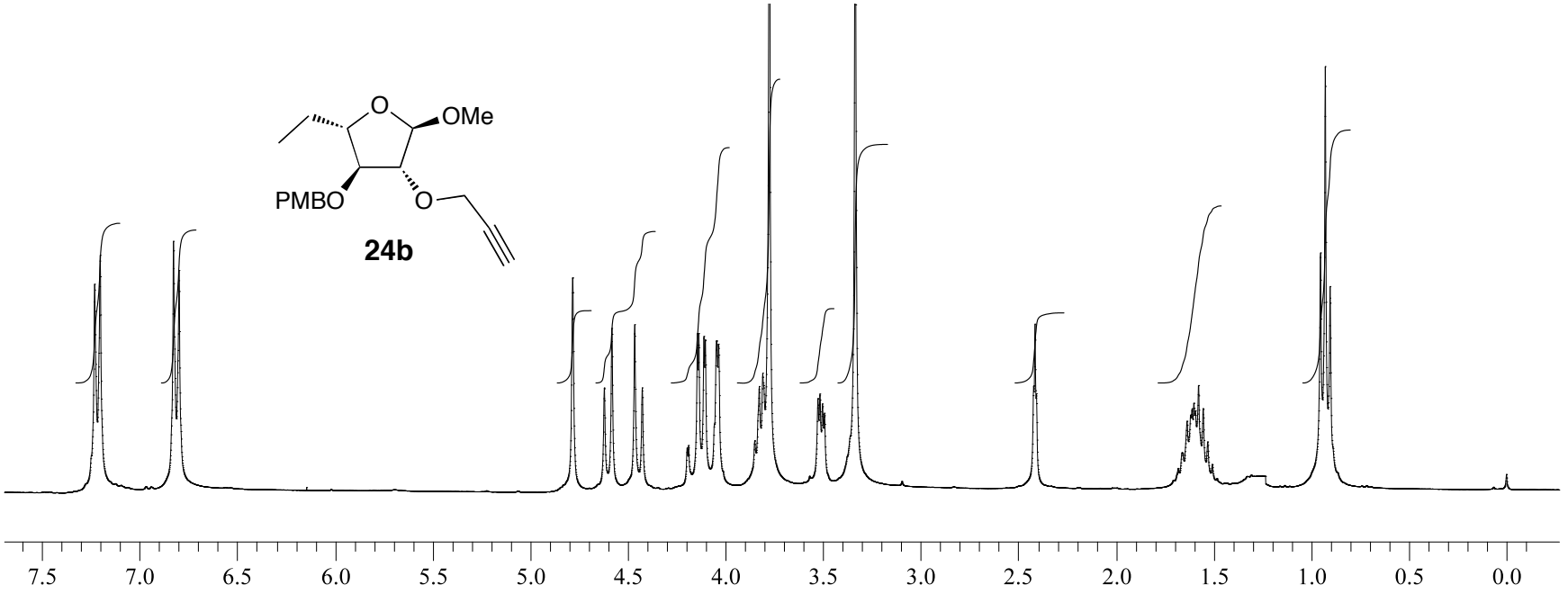


Figure S31 ^{1}H NMR Spectrum of **24b** ($CDCl_3$, 303 K, 300 MHz).

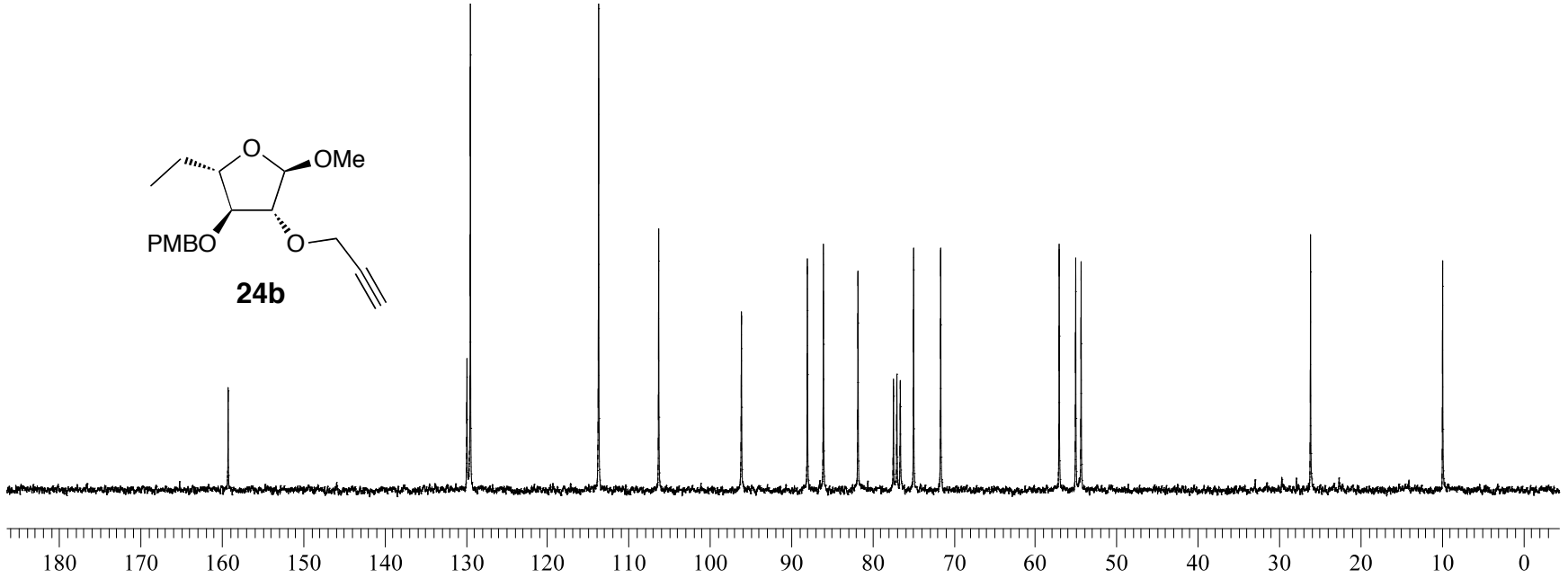


Figure S32 ^{13}C NMR Spectrum of **24b** ($CDCl_3$, 303 K, 75 MHz).

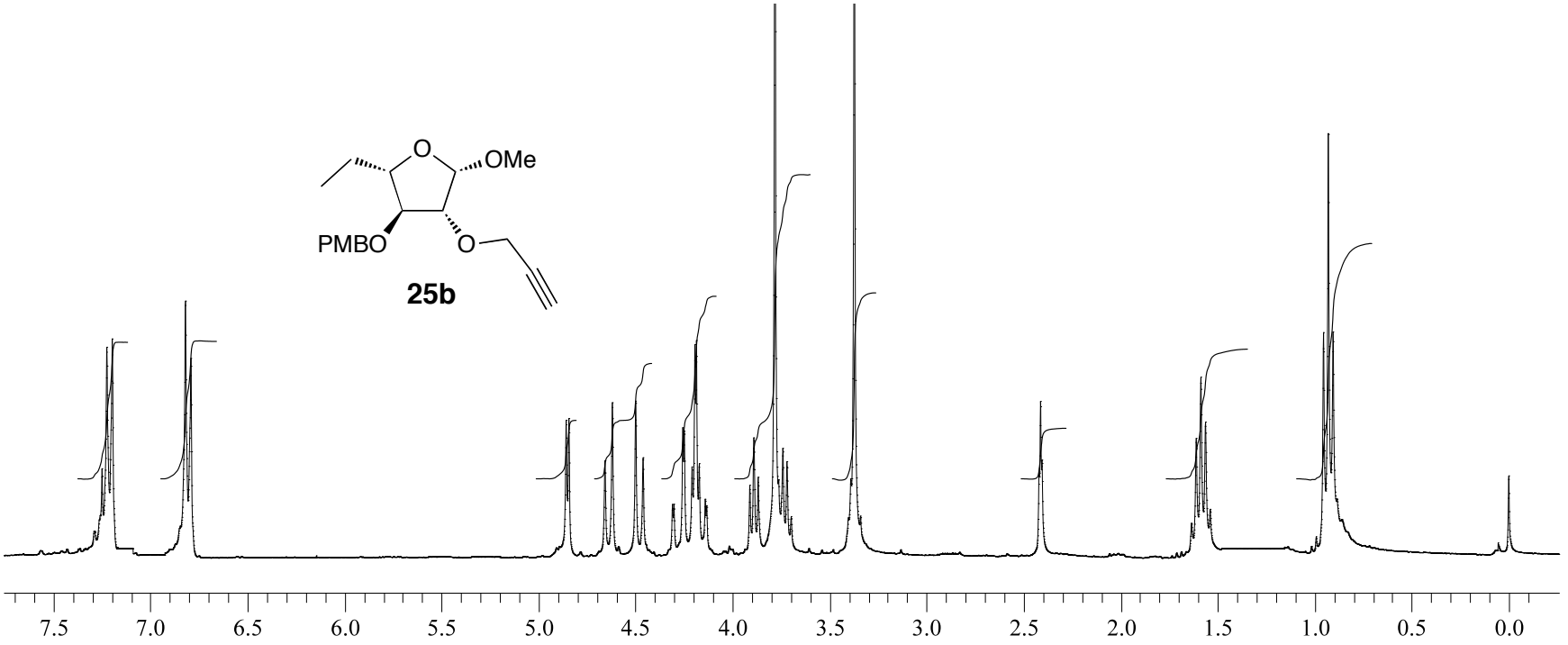


Figure S33 ^{1}H NMR Spectrum of **25b** ($CDCl_3$, 303 K, 300 MHz).

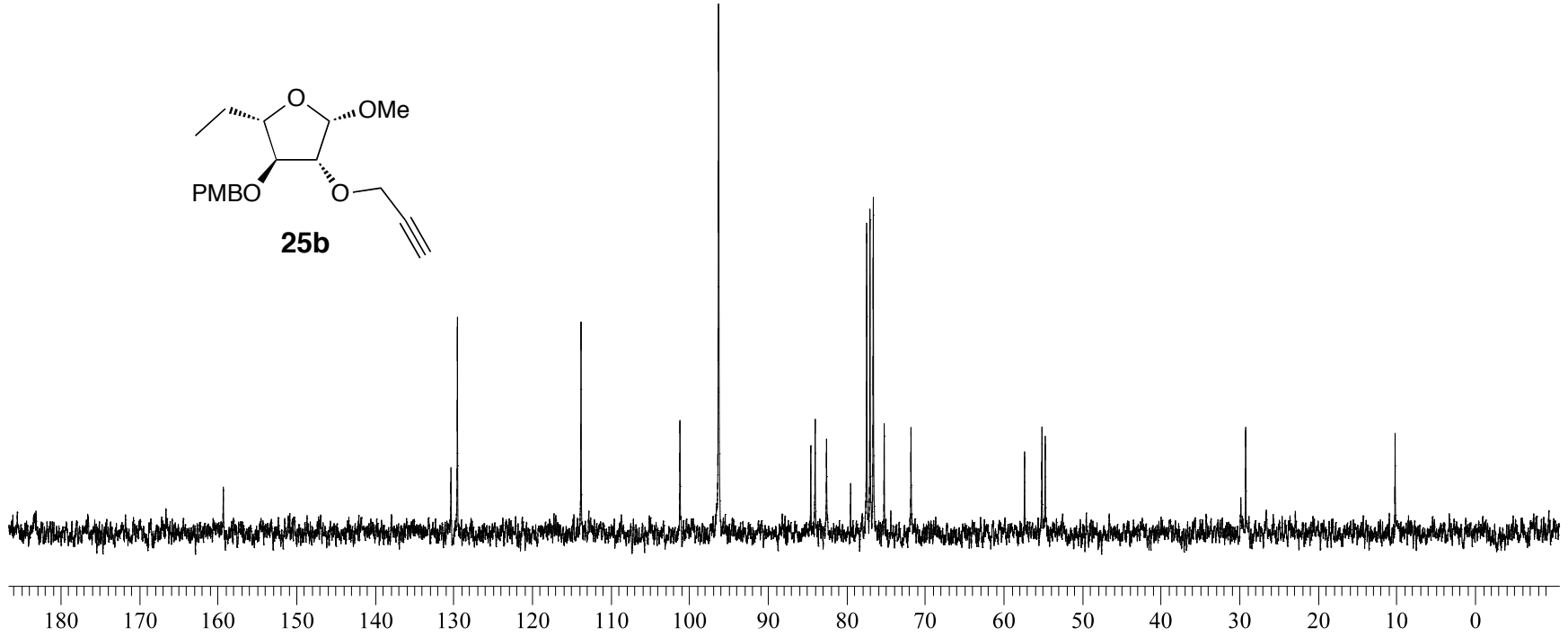


Figure S34 ^{13}C NMR Spectrum of **25b** ($CDCl_3$, 303 K, 75 MHz).

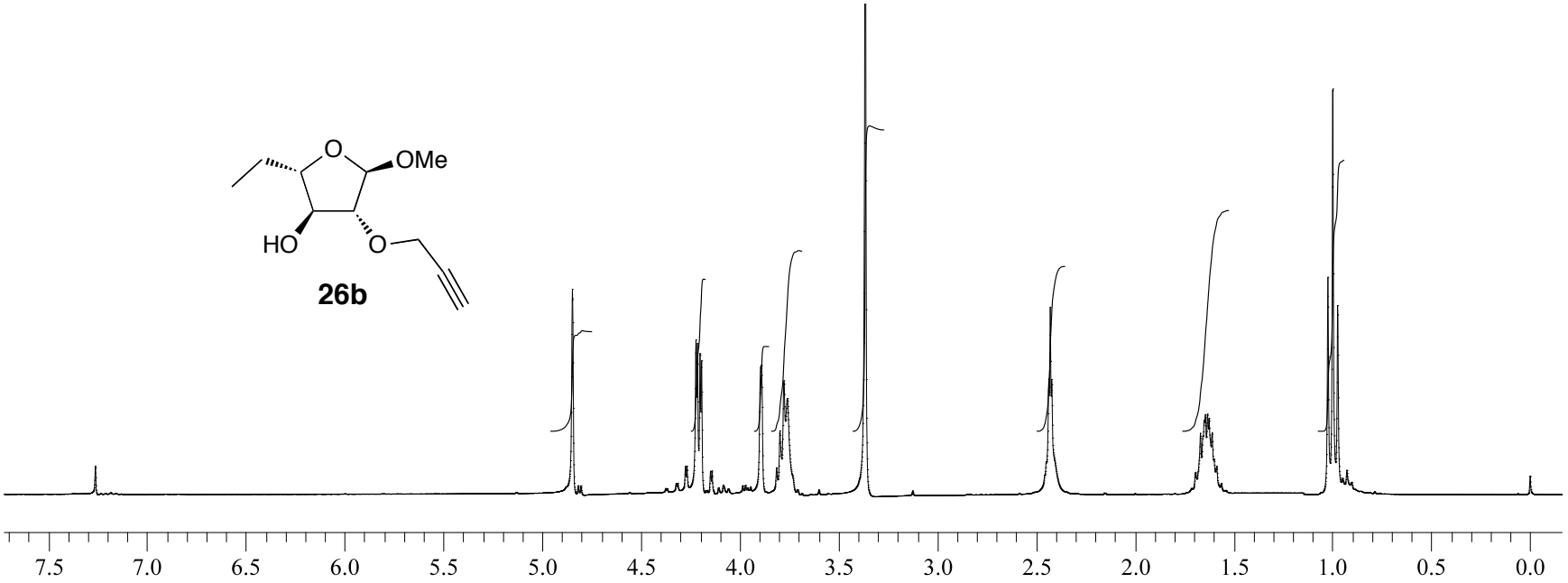


Figure S35 ^{1}H NMR Spectrum of **26b** ($CDCl_3$, 303 K, 300 MHz).

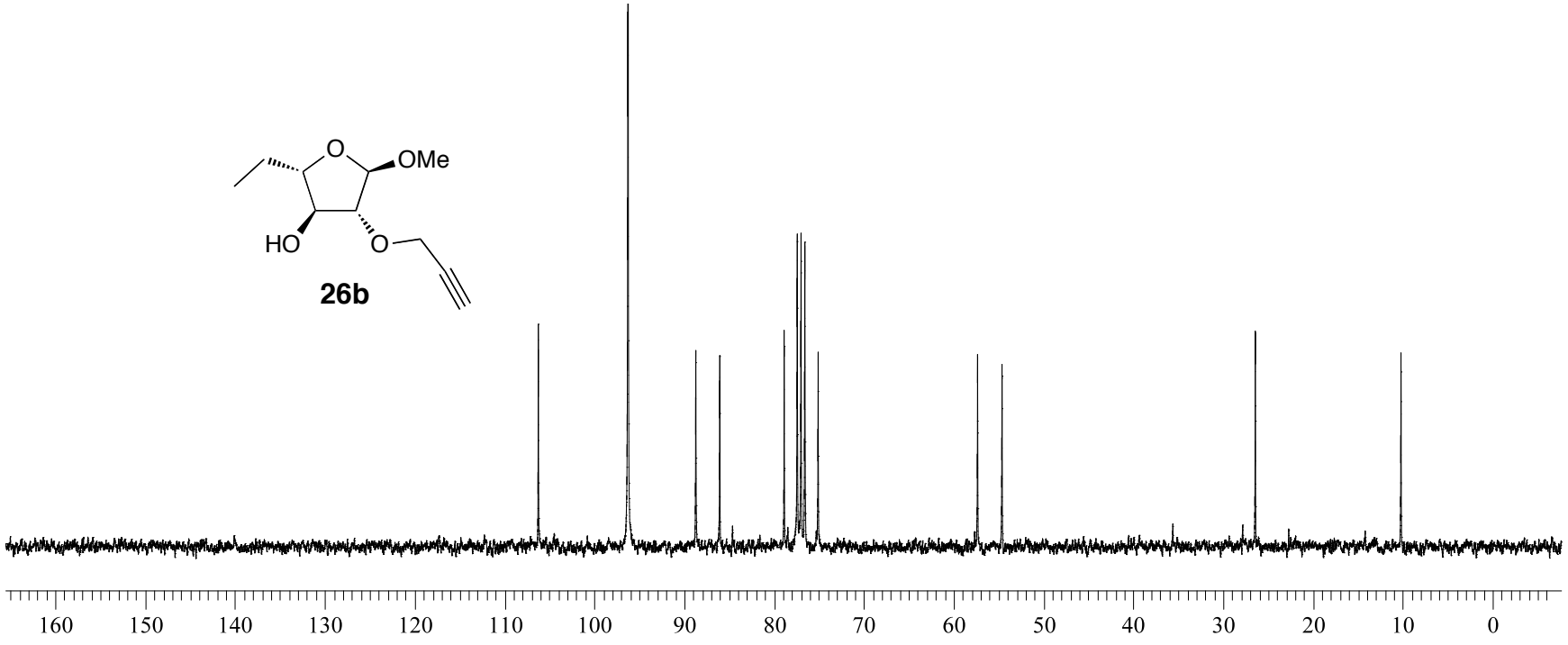


Figure S36 ^{13}C NMR Spectrum of **26b** ($CDCl_3$, 303 K, 75 MHz).

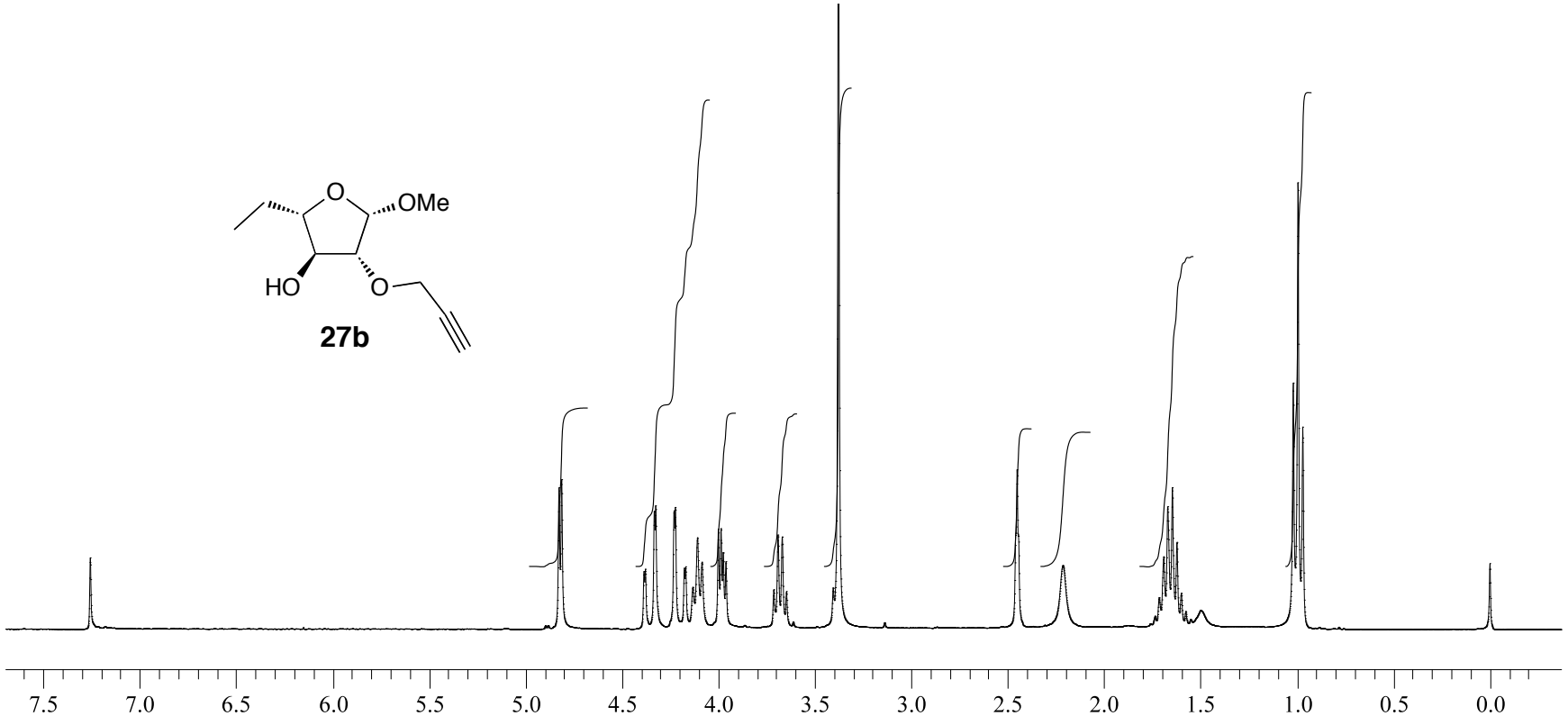


Figure S37 ^{1}H NMR Spectrum of **27b** ($CDCl_3$, 303 K, 300 MHz).

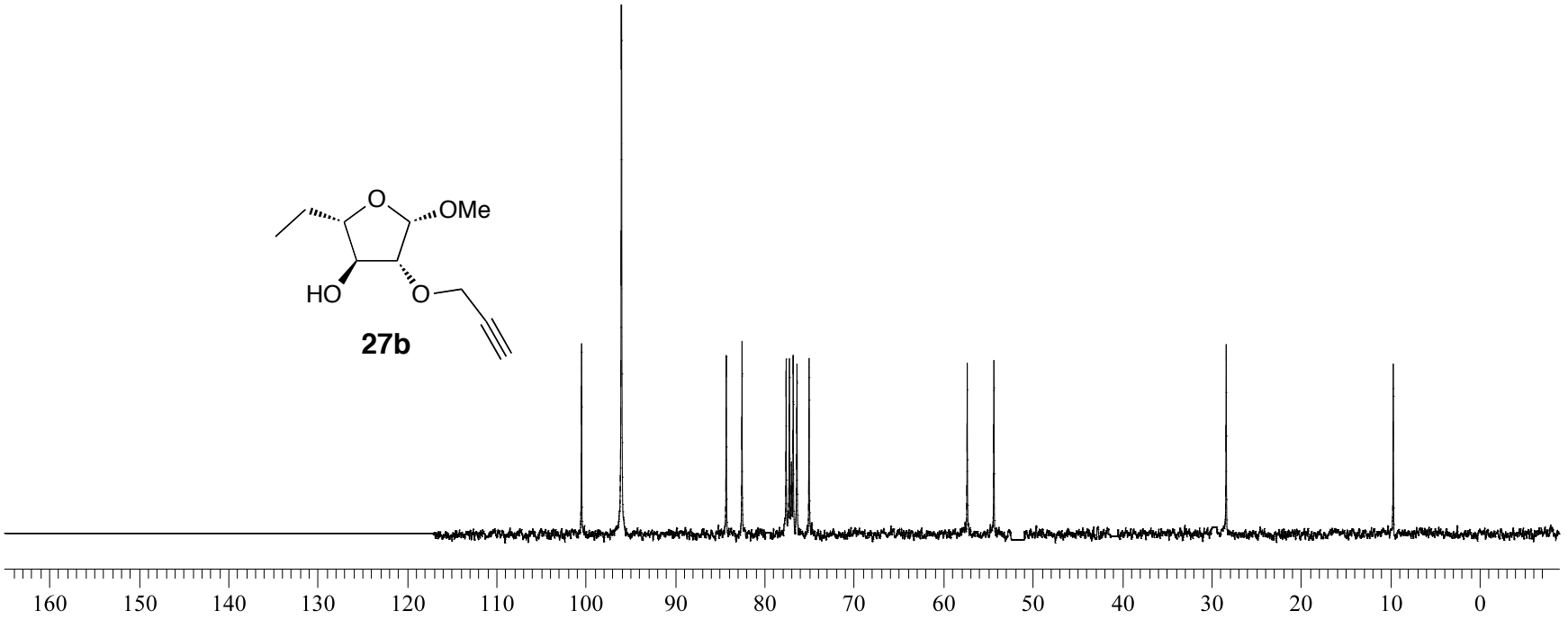


Figure S38 ^{13}C NMR Spectrum of **27b** ($CDCl_3$, 303 K, 75 MHz).

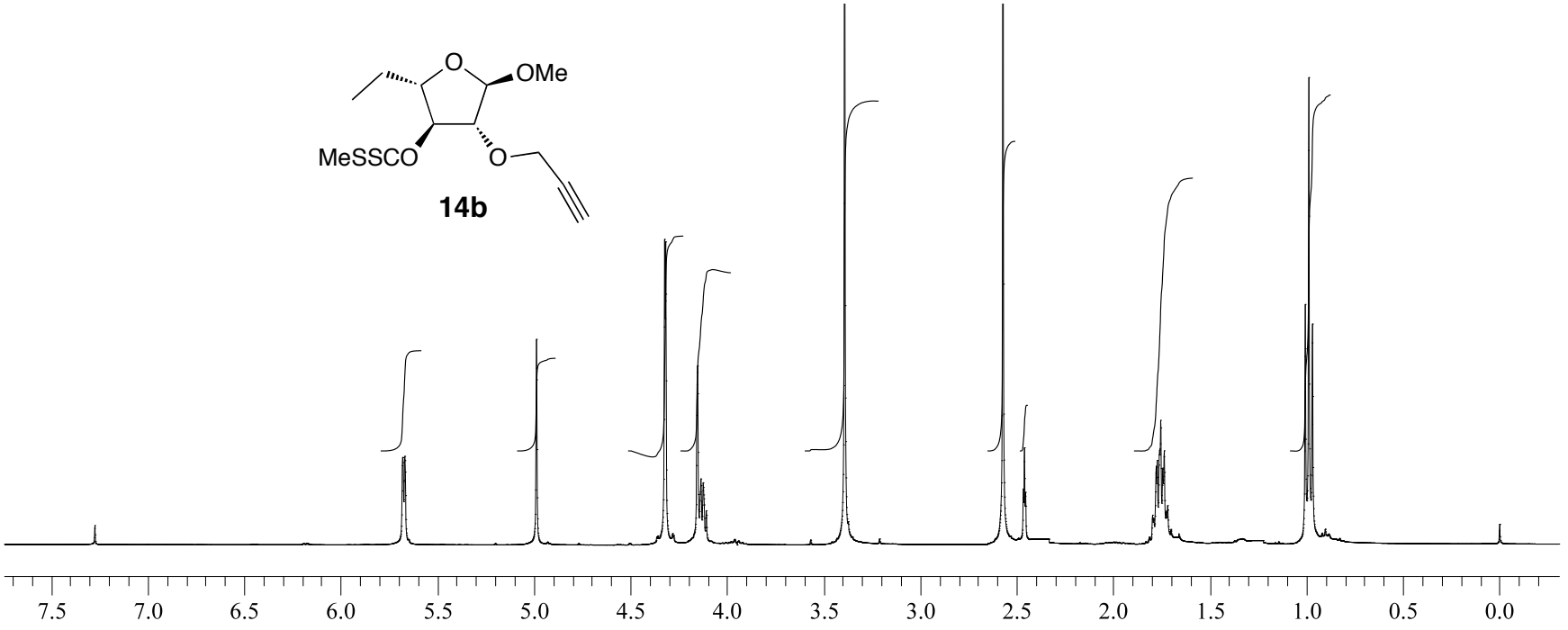


Figure S39 ^{1}H NMR Spectrum of **14b** ($CDCl_3$, 303 K, 400 MHz).

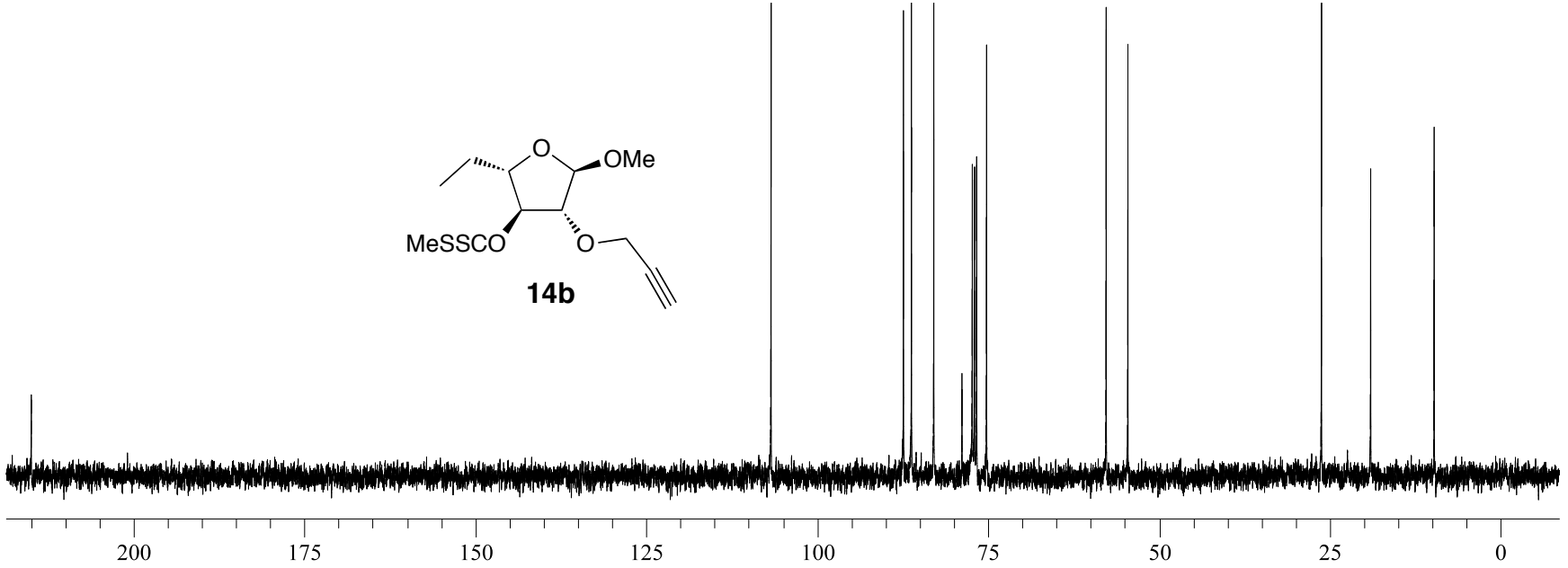


Figure S40 ^{13}C NMR Spectrum of **14b** ($CDCl_3$, 303 K, 100 MHz).

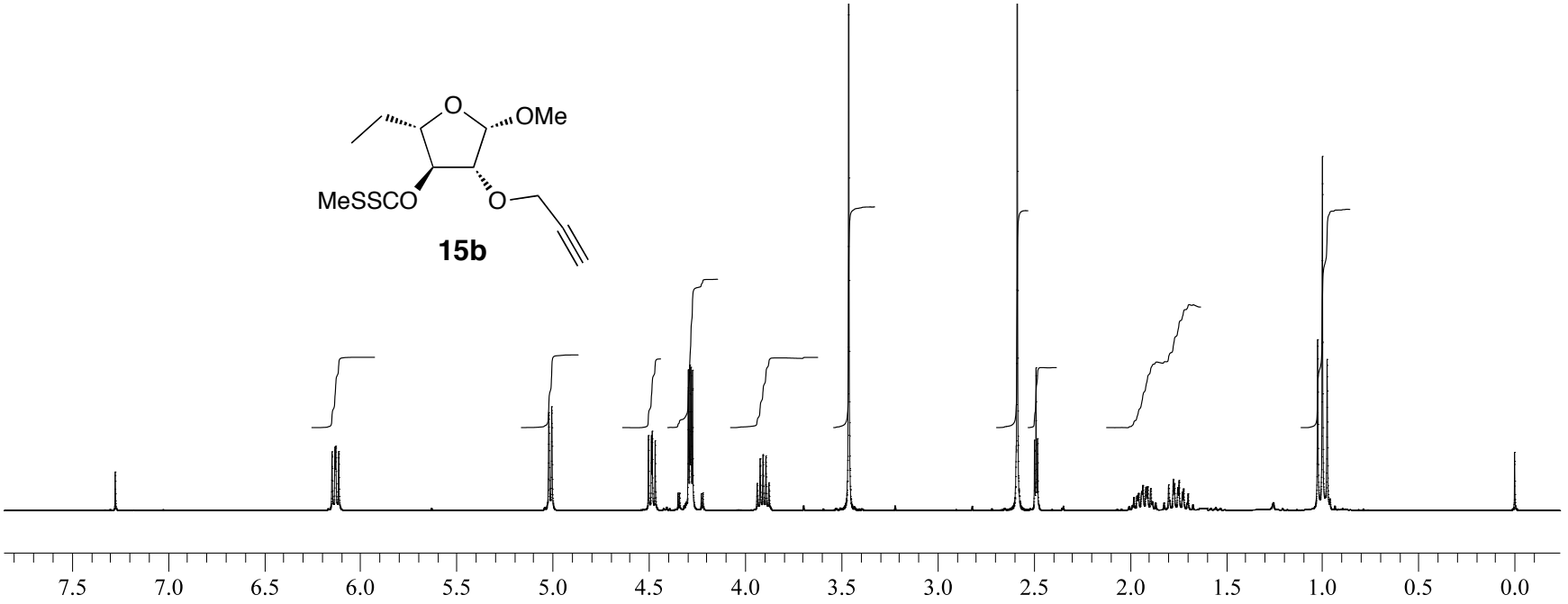


Figure S41 ^{1}H NMR Spectrum of **15b** ($CDCl_3$, 303 K, 300 MHz).

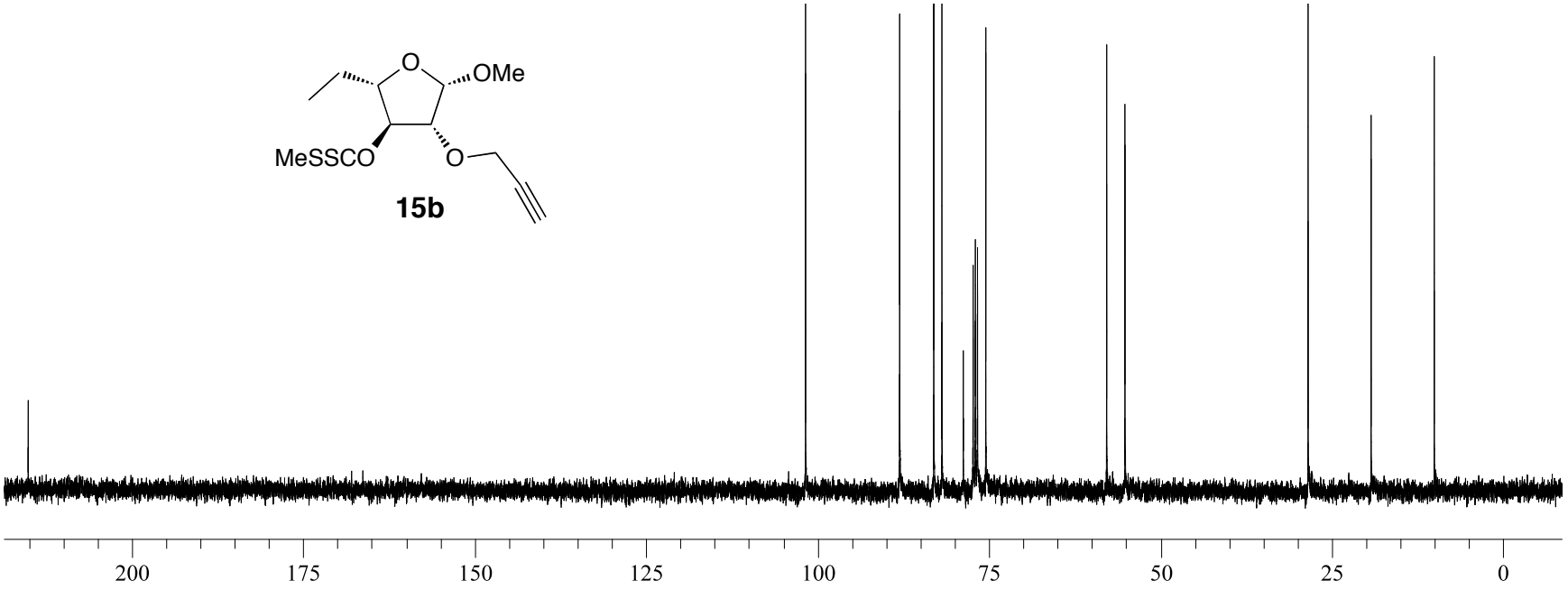


Figure S42 ^{13}C NMR Spectrum of **15b** ($CDCl_3$, 303 K, 100 MHz).

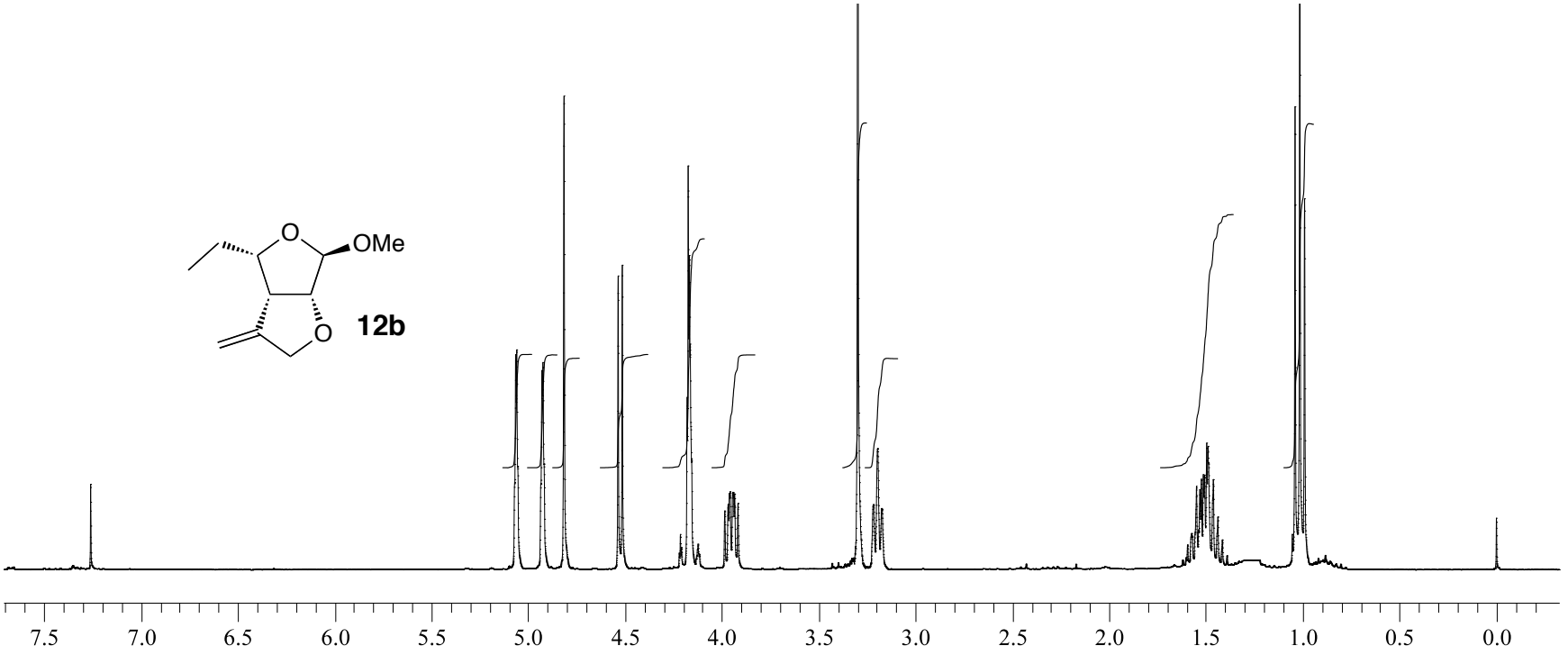


Figure S43 ^{1}H NMR Spectrum of **12b** ($CDCl_3$, 303 K, 300 MHz).

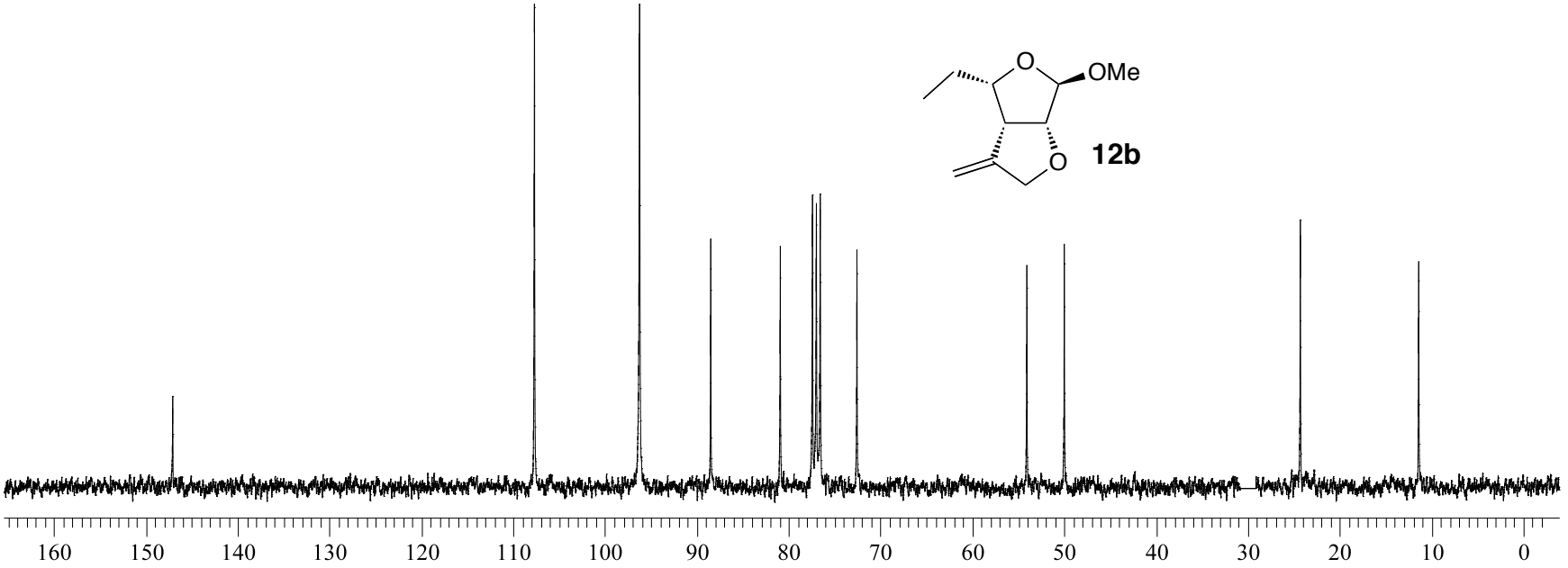


Figure S44 ^{13}C NMR Spectrum of **12b** ($CDCl_3$, 303 K, 75 MHz).

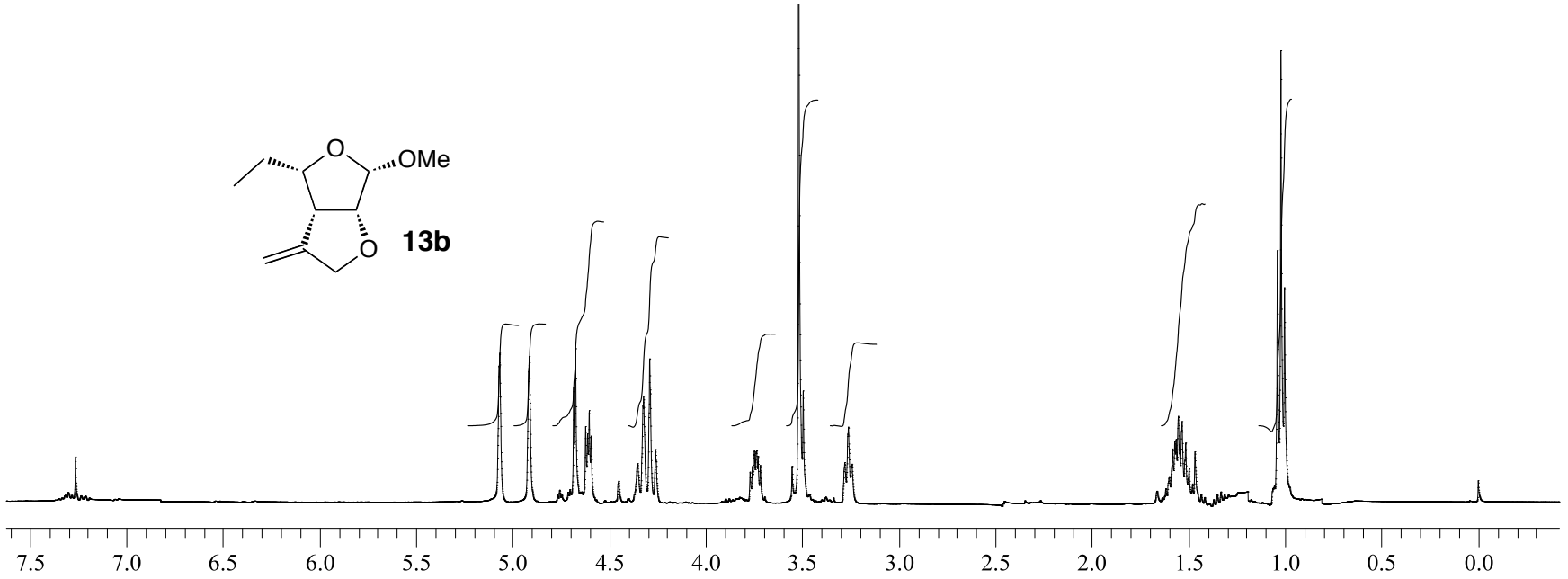


Figure S45 ^{1}H NMR Spectrum of **13b** ($CDCl_3$, 303 K, 400 MHz).

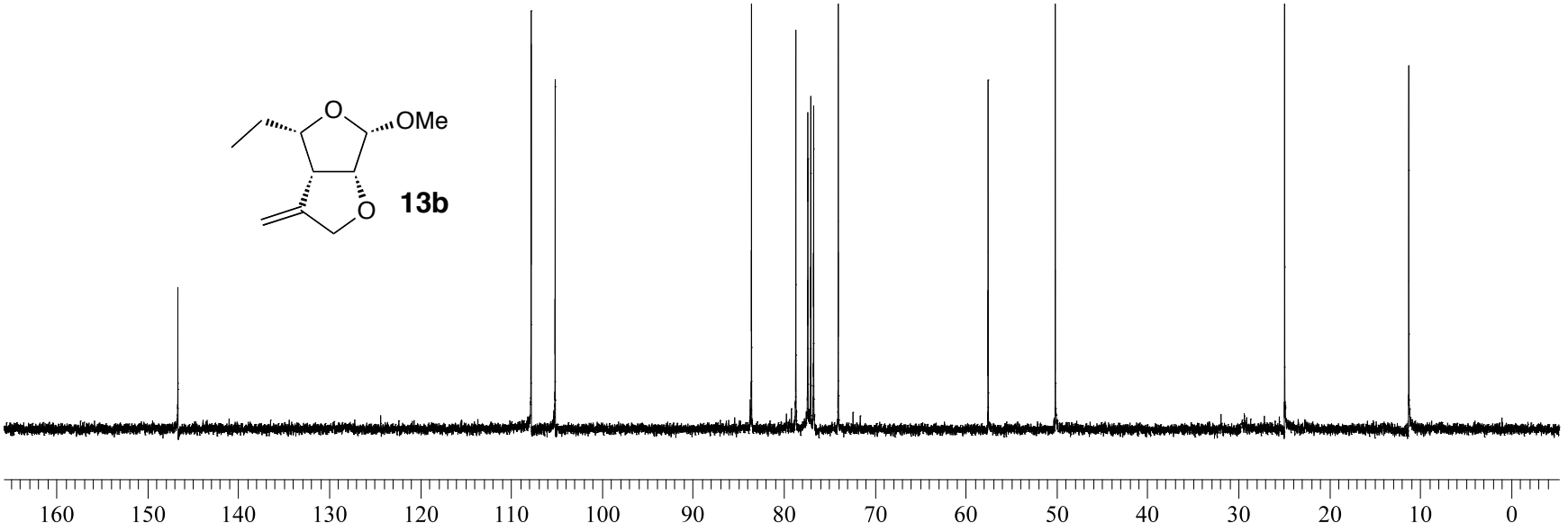


Figure S46 ^{13}C NMR Spectrum of **13b** ($CDCl_3$, 303 K, 100 MHz).

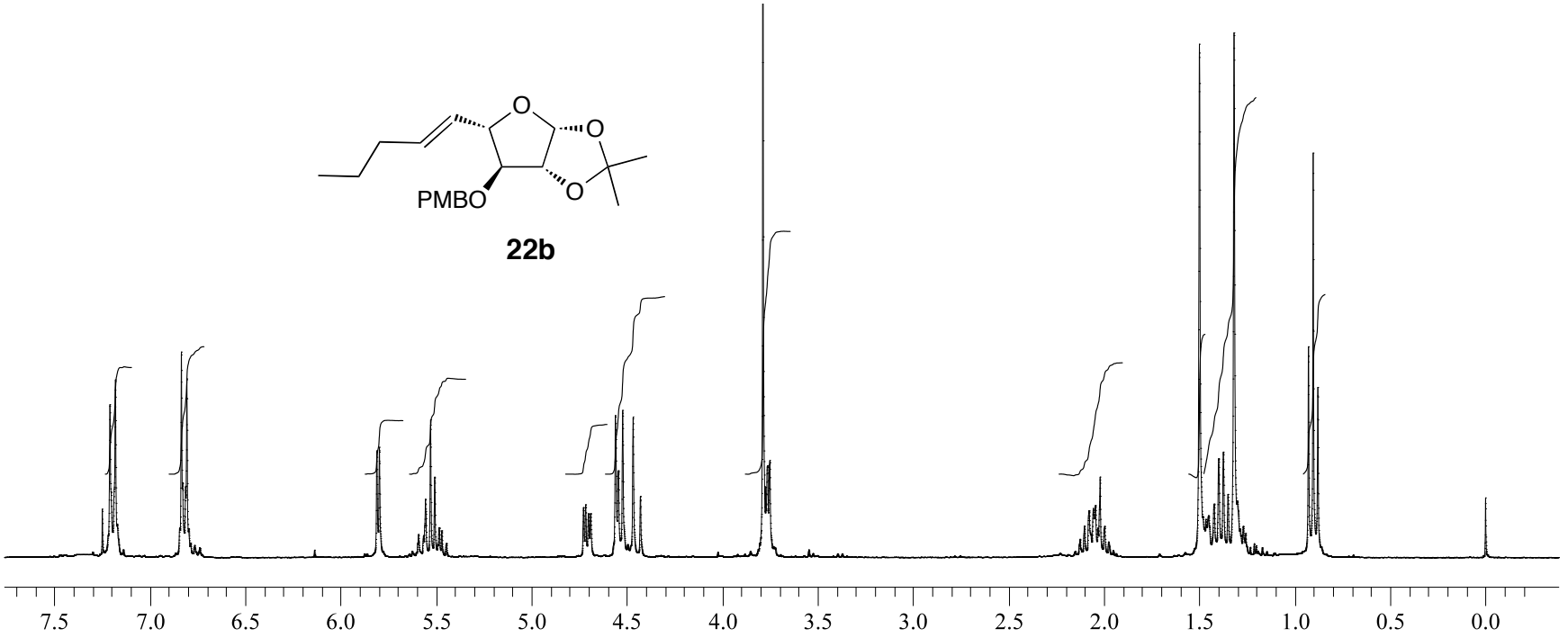


Figure S47 ^{1}H NMR Spectrum of **22b** ($CDCl_3$, 303 K, 300 MHz).

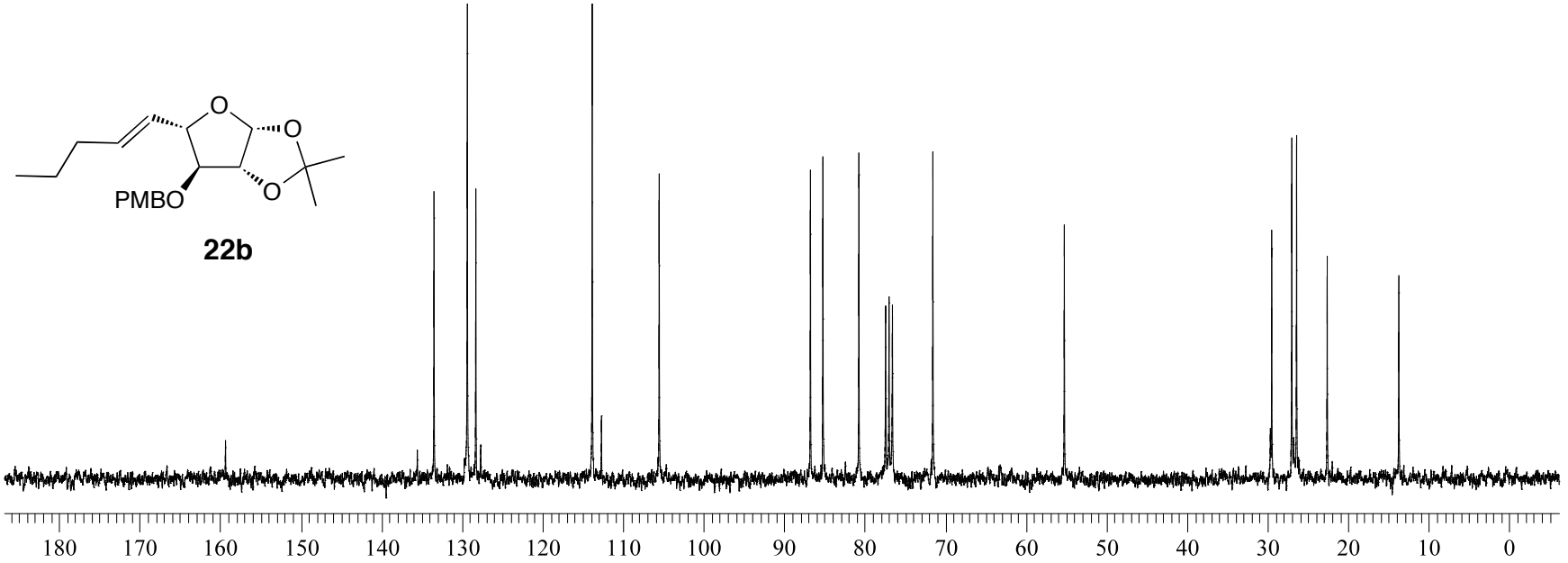


Figure S48 ^{13}C NMR Spectrum of **22b** ($CDCl_3$, 303 K, 75 MHz).

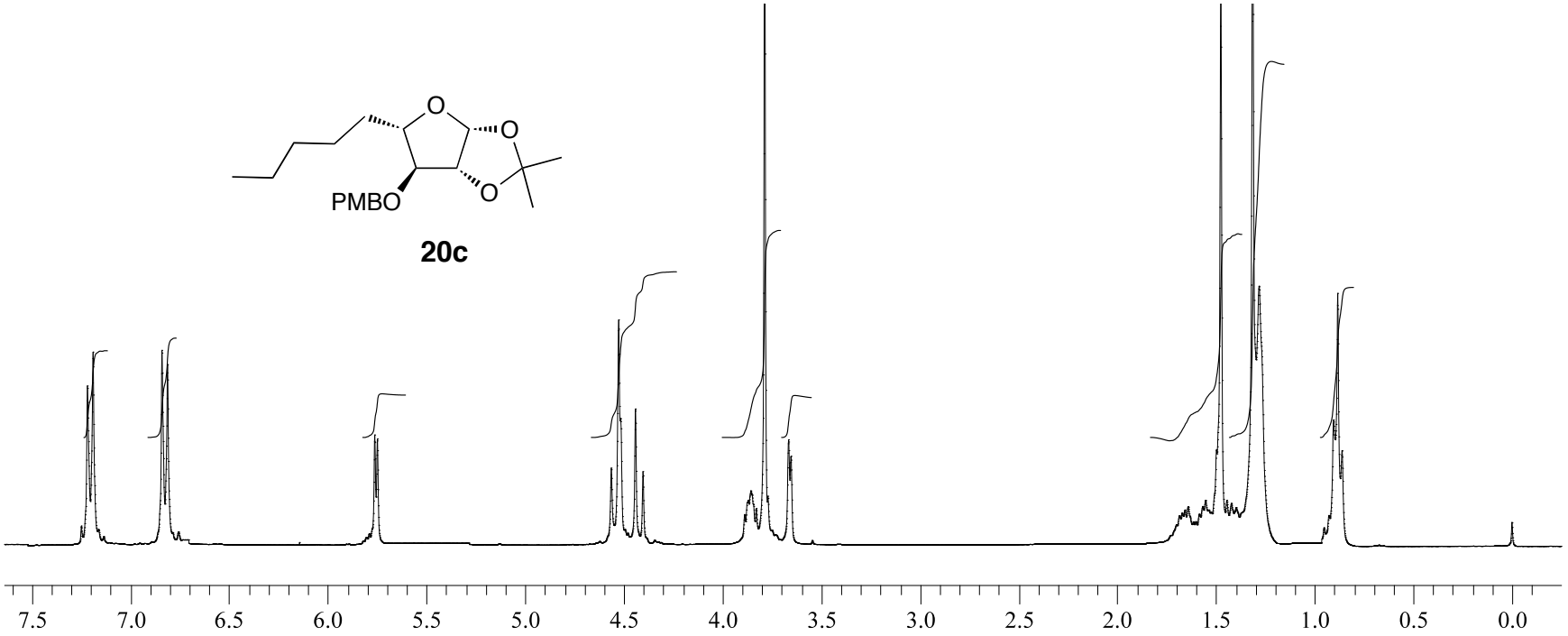


Figure S49 ^{1}H NMR Spectrum of **20c** ($CDCl_3$, 303 K, 300 MHz).

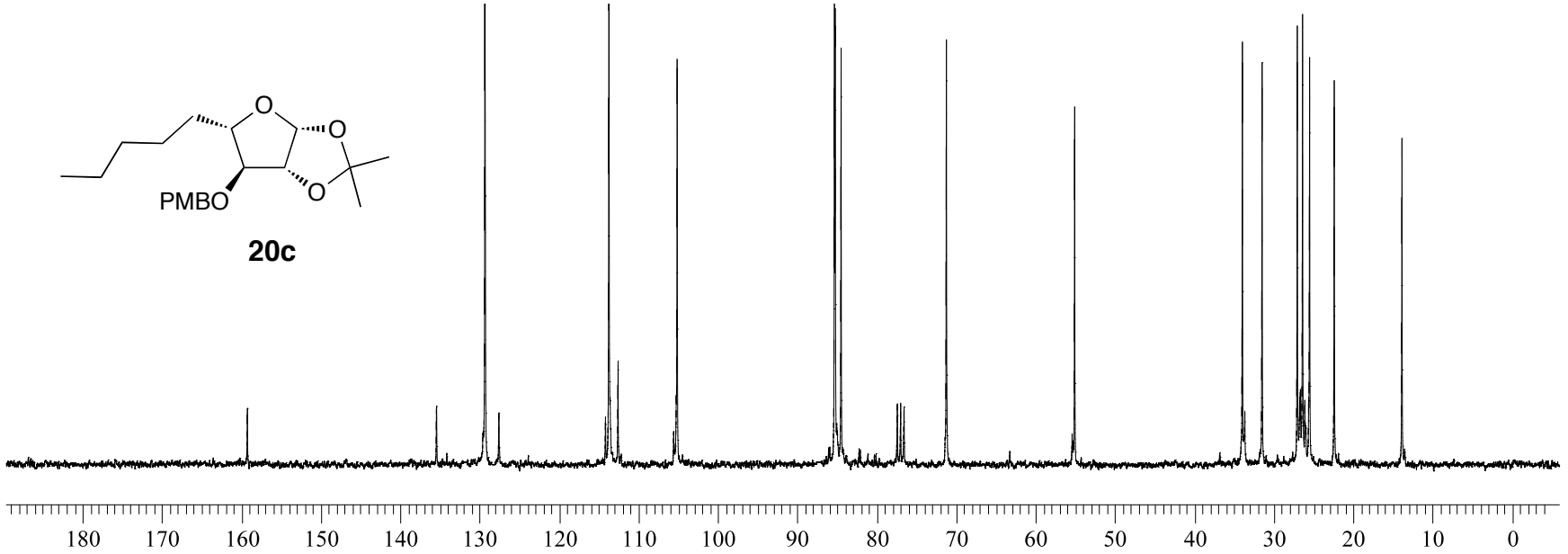


Figure S50 ^{13}C NMR Spectrum of **20c** ($CDCl_3$, 303 K, 75 MHz).

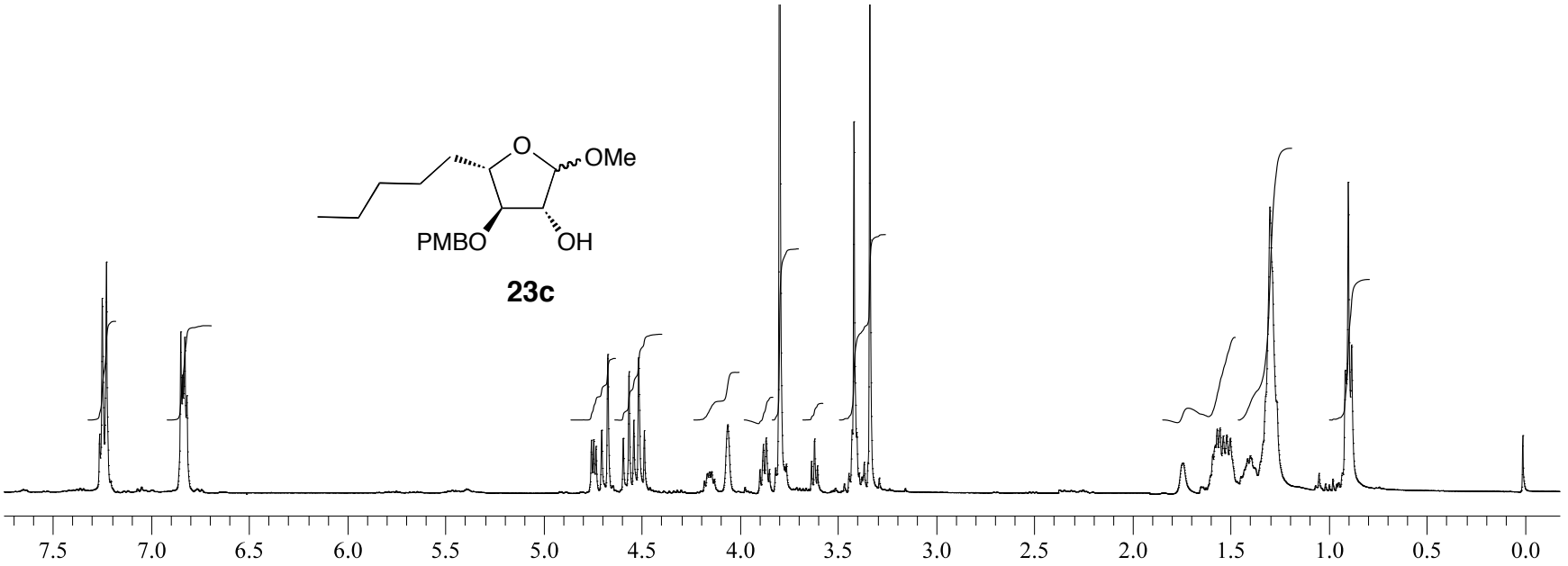


Figure S51 ^{1}H NMR Spectrum of **23c** ($CDCl_3$, 303 K, 400 MHz).

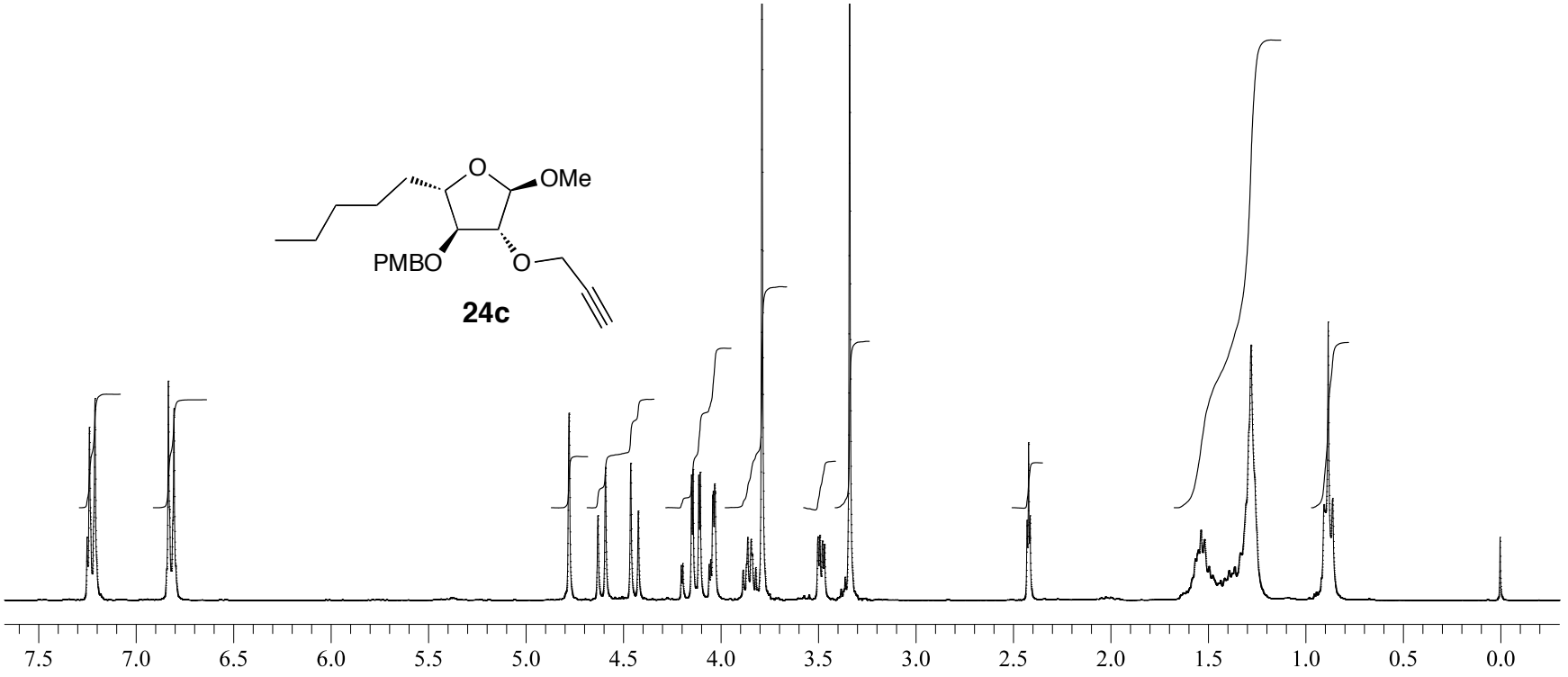


Figure S52 ^{1}H NMR Spectrum of **24c** ($CDCl_3$, 303 K, 300 MHz).

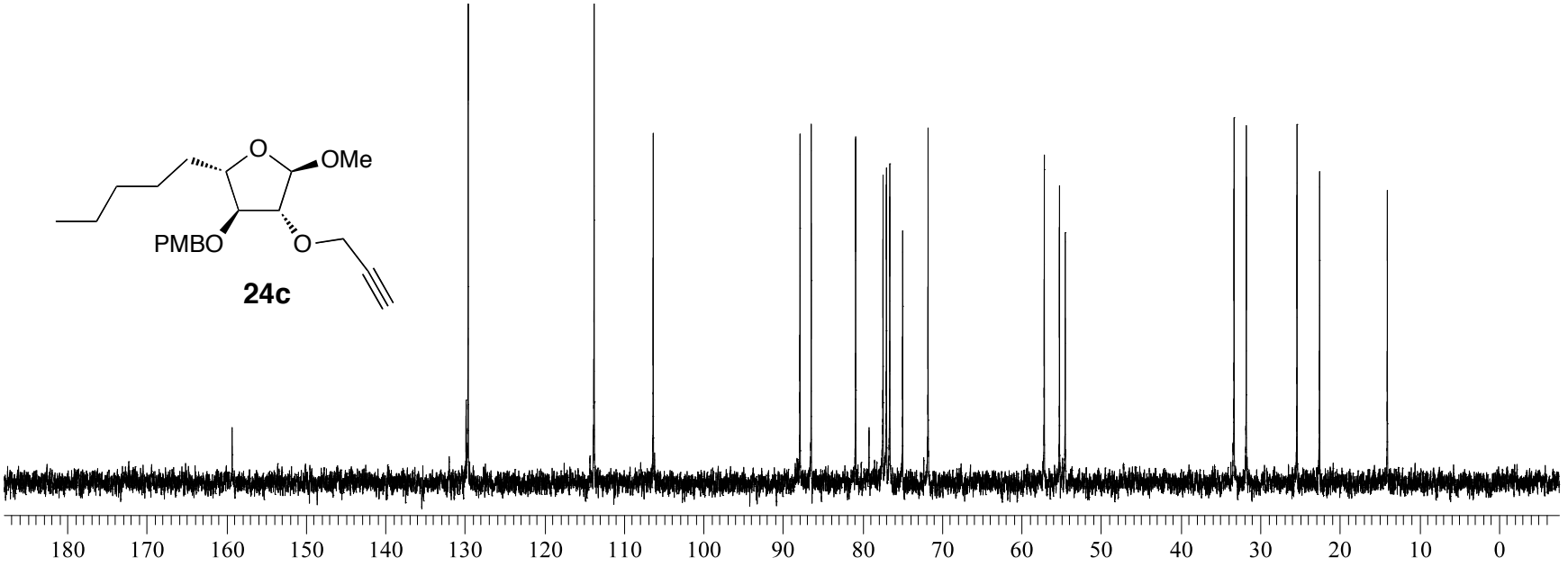


Figure S53 ^{13}C NMR Spectrum of **24c** ($CDCl_3$, 303 K, 75 MHz).

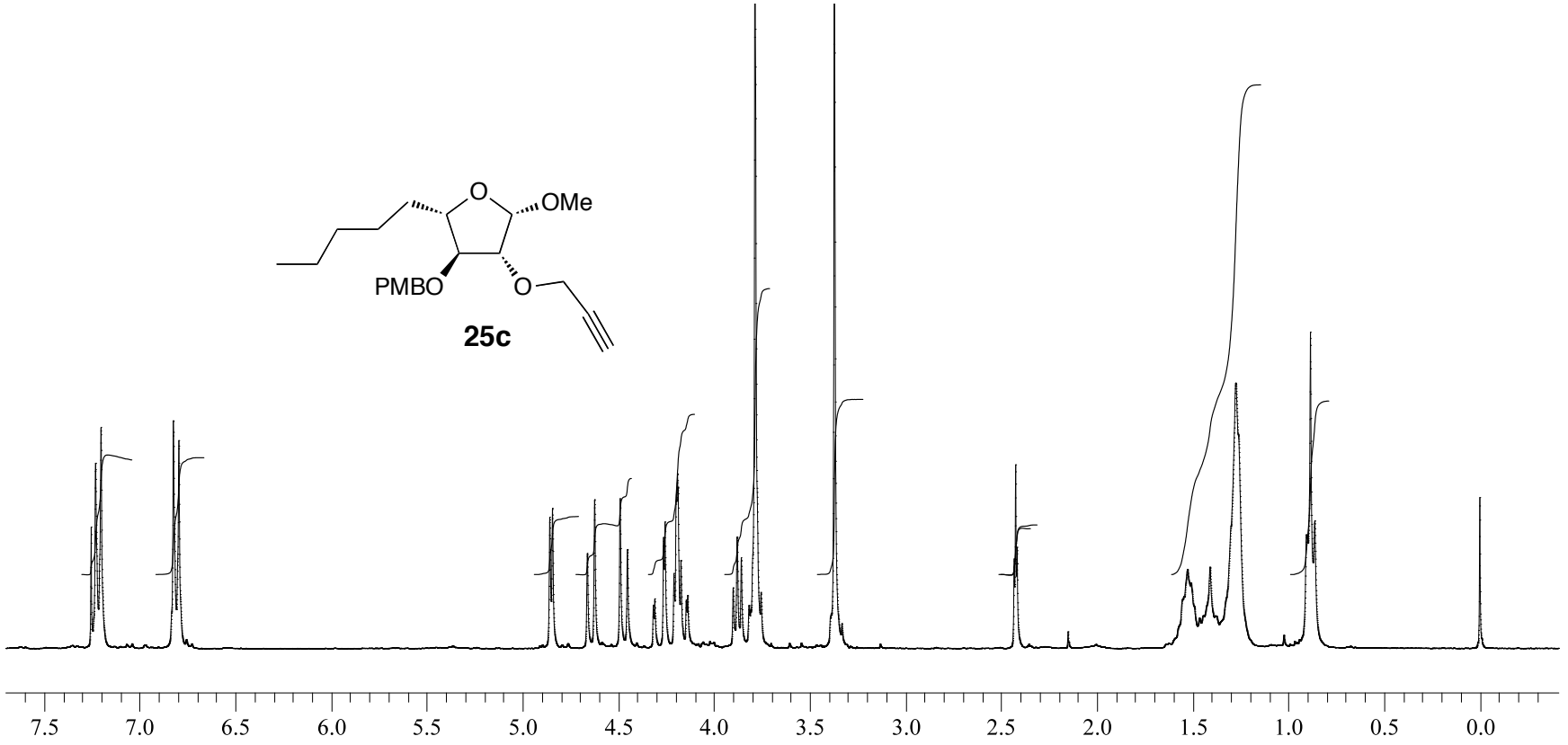


Figure S54 ^{1}H NMR Spectrum of **25c** ($CDCl_3$, 303 K, 300 MHz).

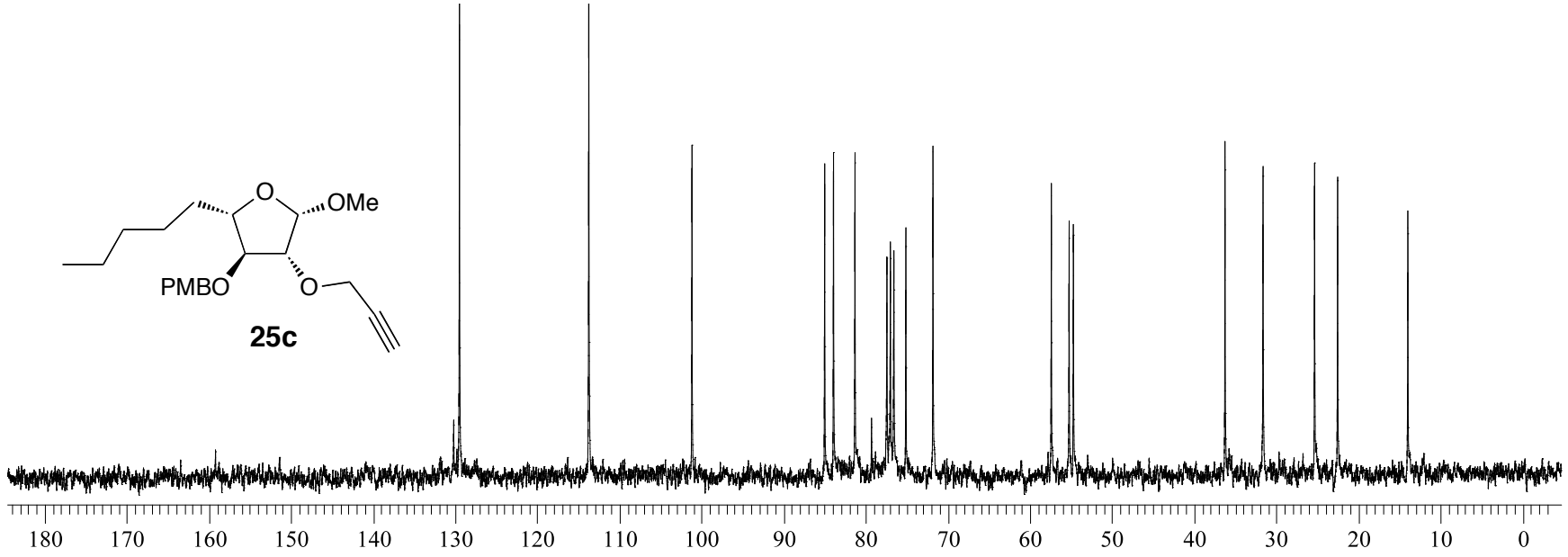


Figure S55 ^{13}C NMR Spectrum of **25c** ($CDCl_3$, 303 K, 75 MHz).

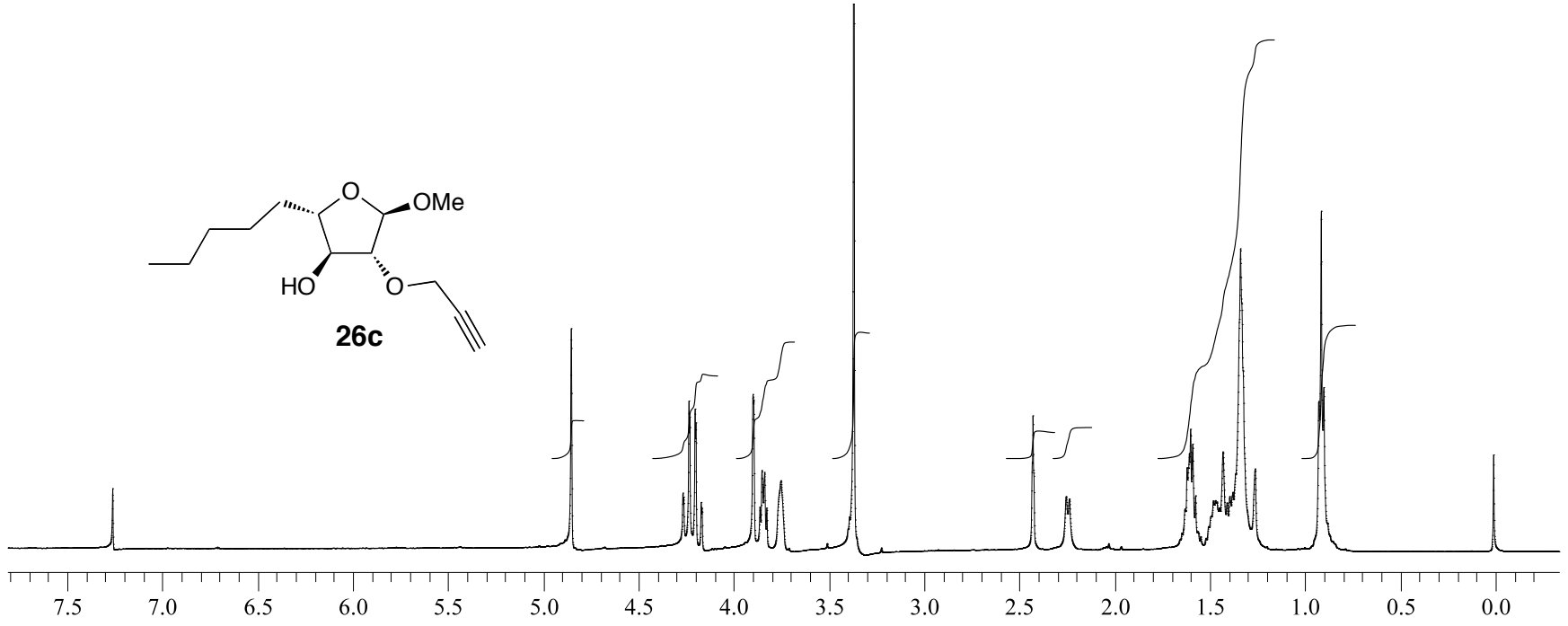


Figure S56 ^{1}H NMR Spectrum of **26c** ($CDCl_3$, 303 K, 500 MHz).

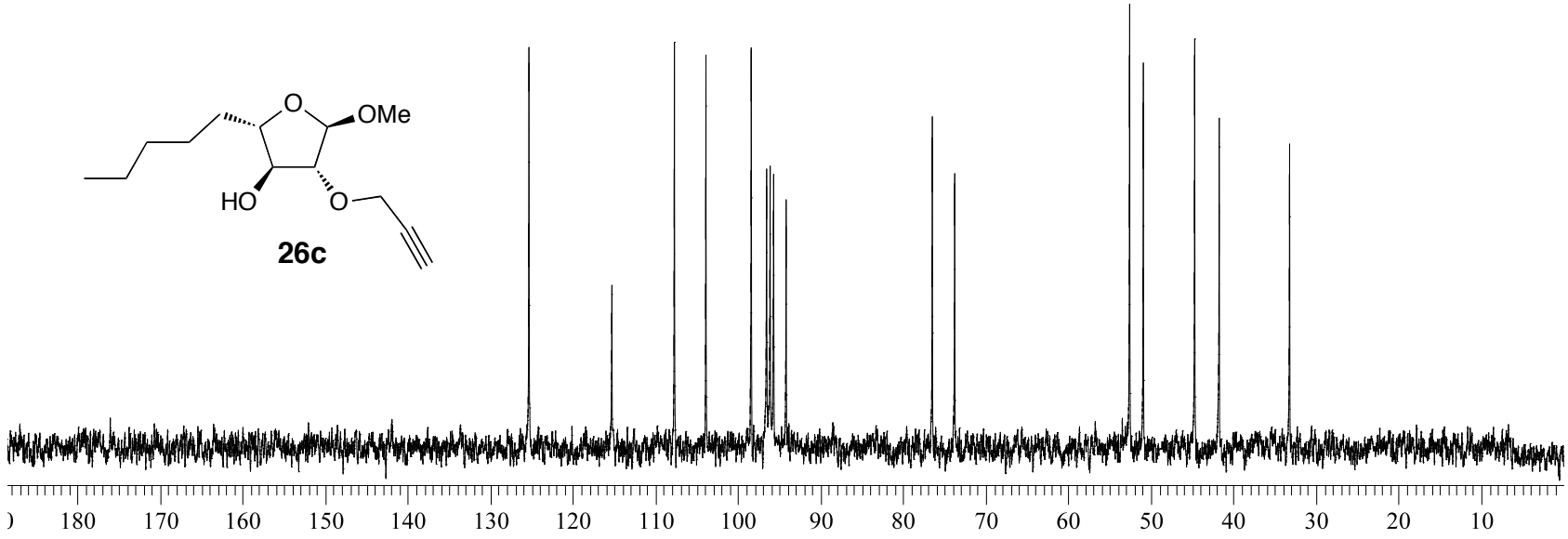


Figure S57 ^{13}C NMR Spectrum of **26c** ($CDCl_3$, 303 K, 75 MHz).

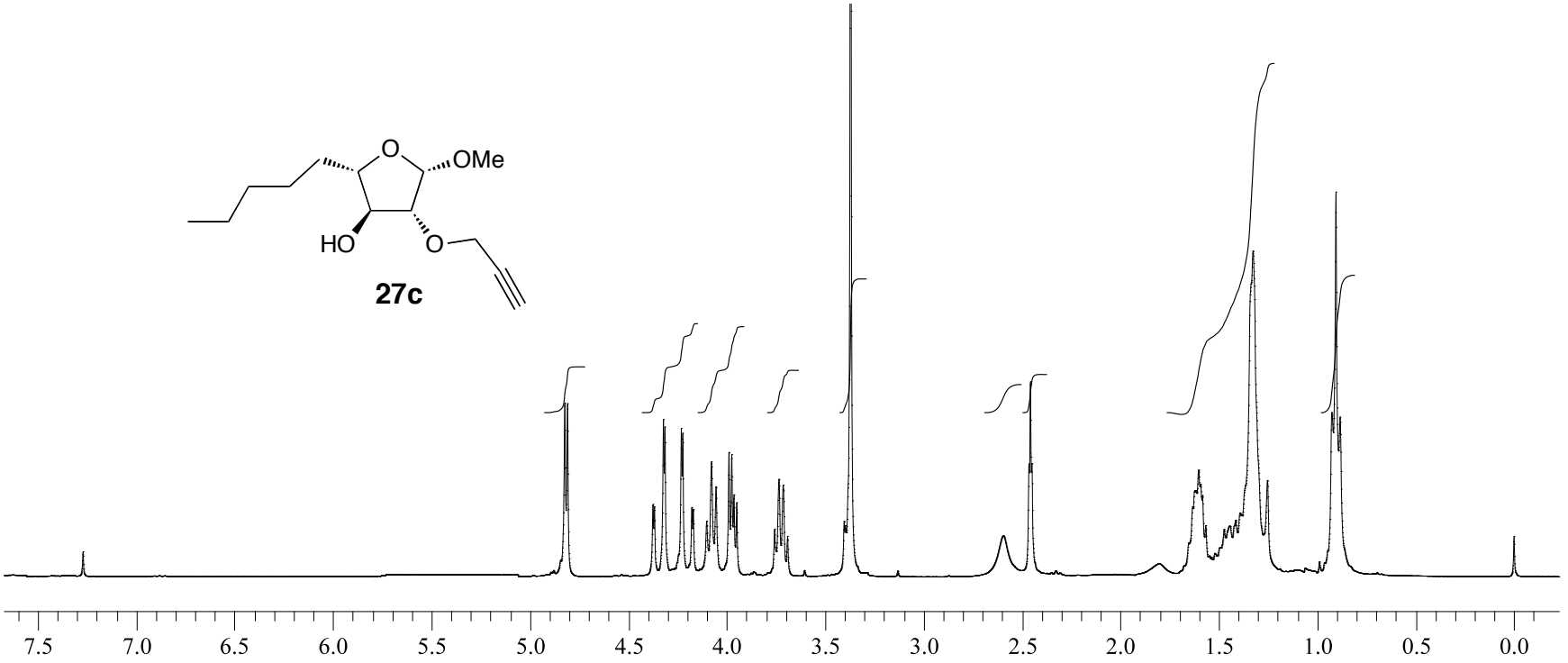


Figure S58 ^{1}H NMR Spectrum of **27c** ($CDCl_3$, 303 K, 300 MHz).

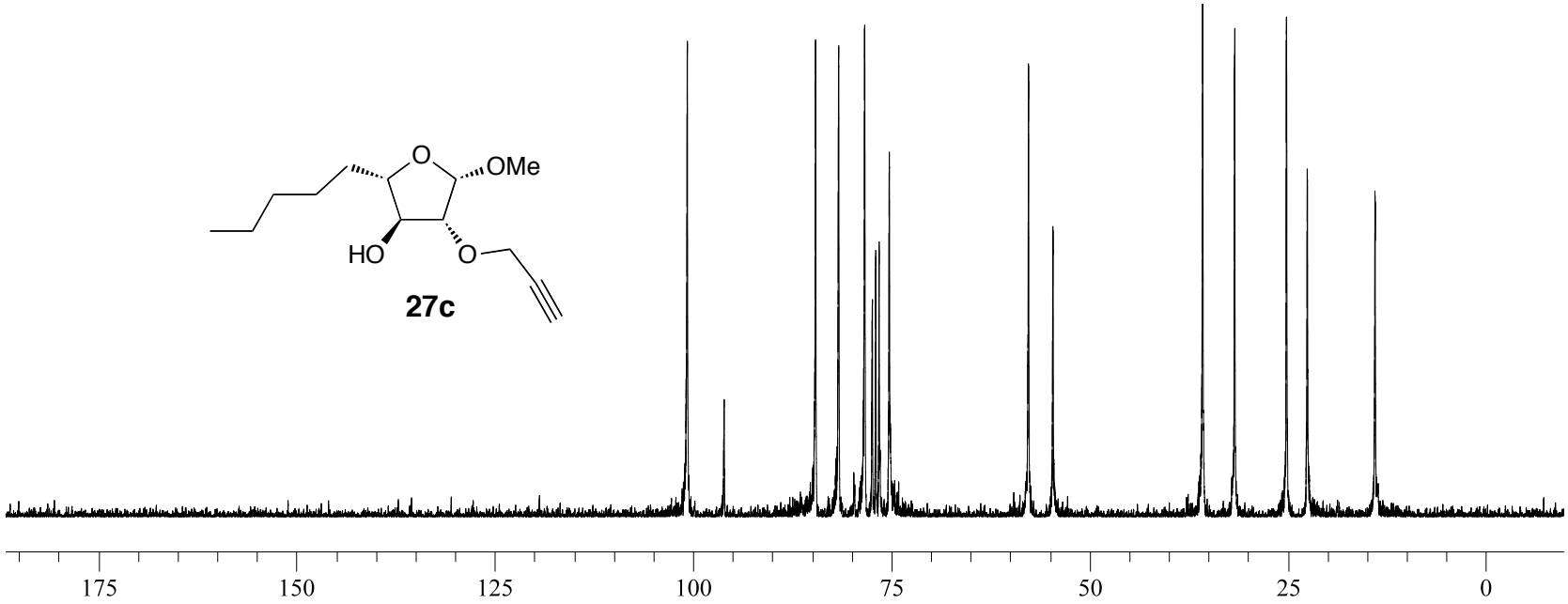


Figure S59 ^{13}C NMR Spectrum of **27c** ($CDCl_3$, 303 K, 75 MHz).

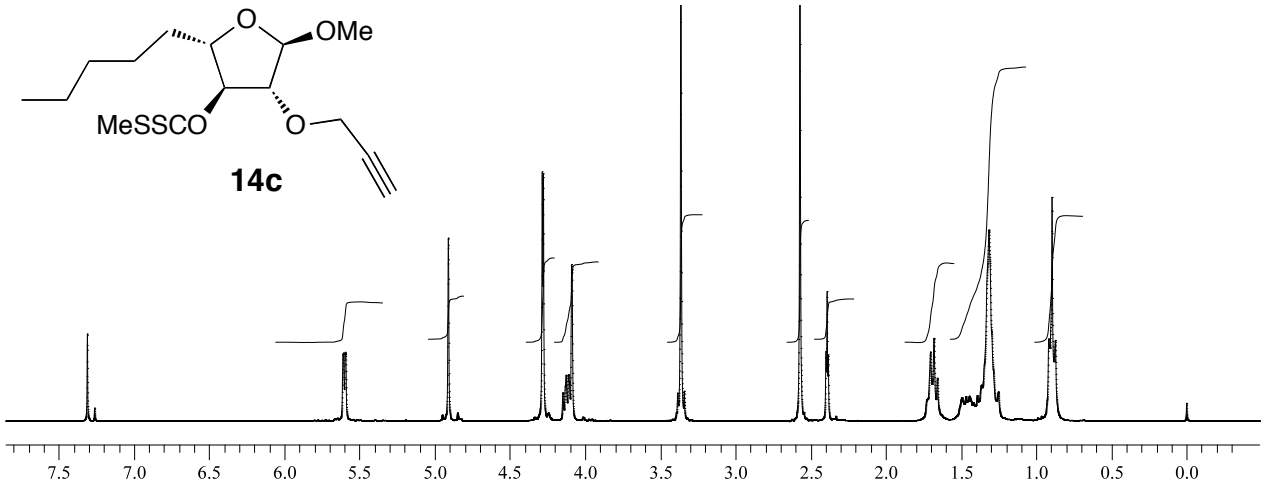


Figure S60 ^{1}H NMR Spectrum of **14c** ($CDCl_3$, 303 K, 300 MHz).

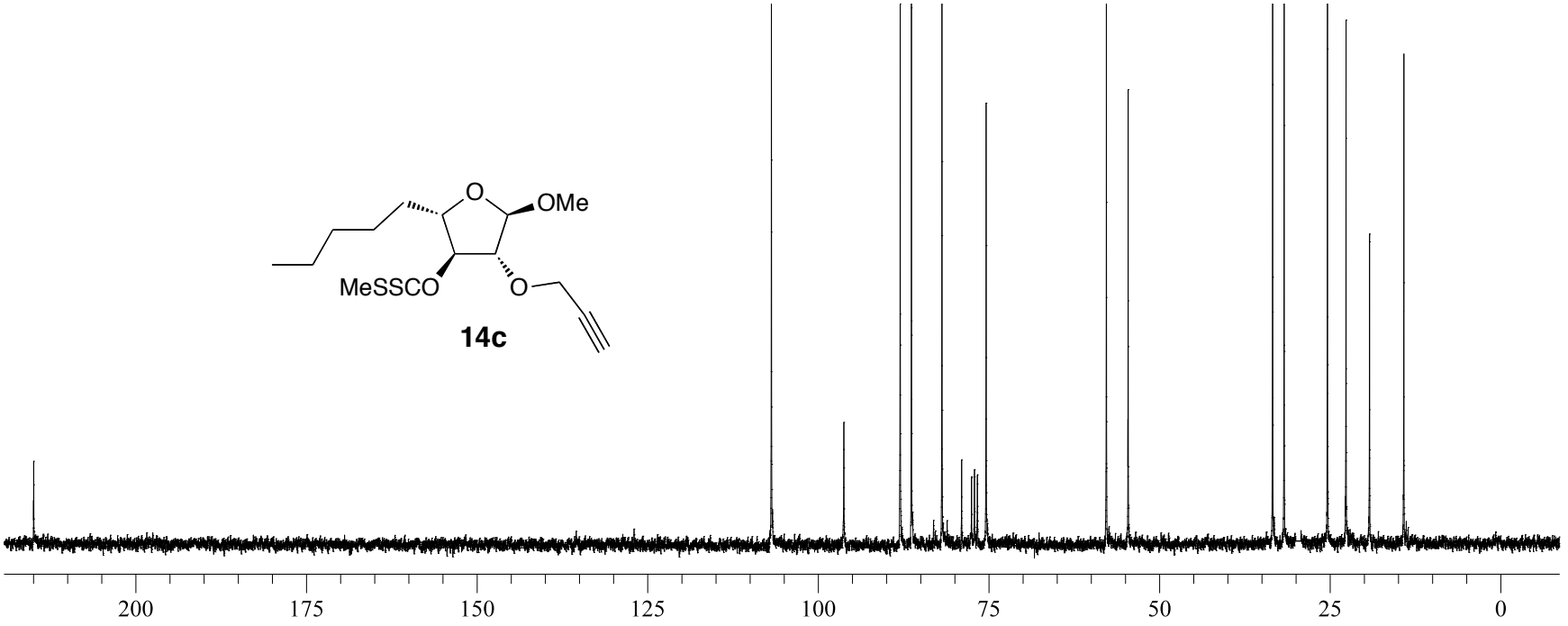


Figure S61 ^{13}C NMR Spectrum of **14c** ($CDCl_3$, 303 K, 75 MHz).

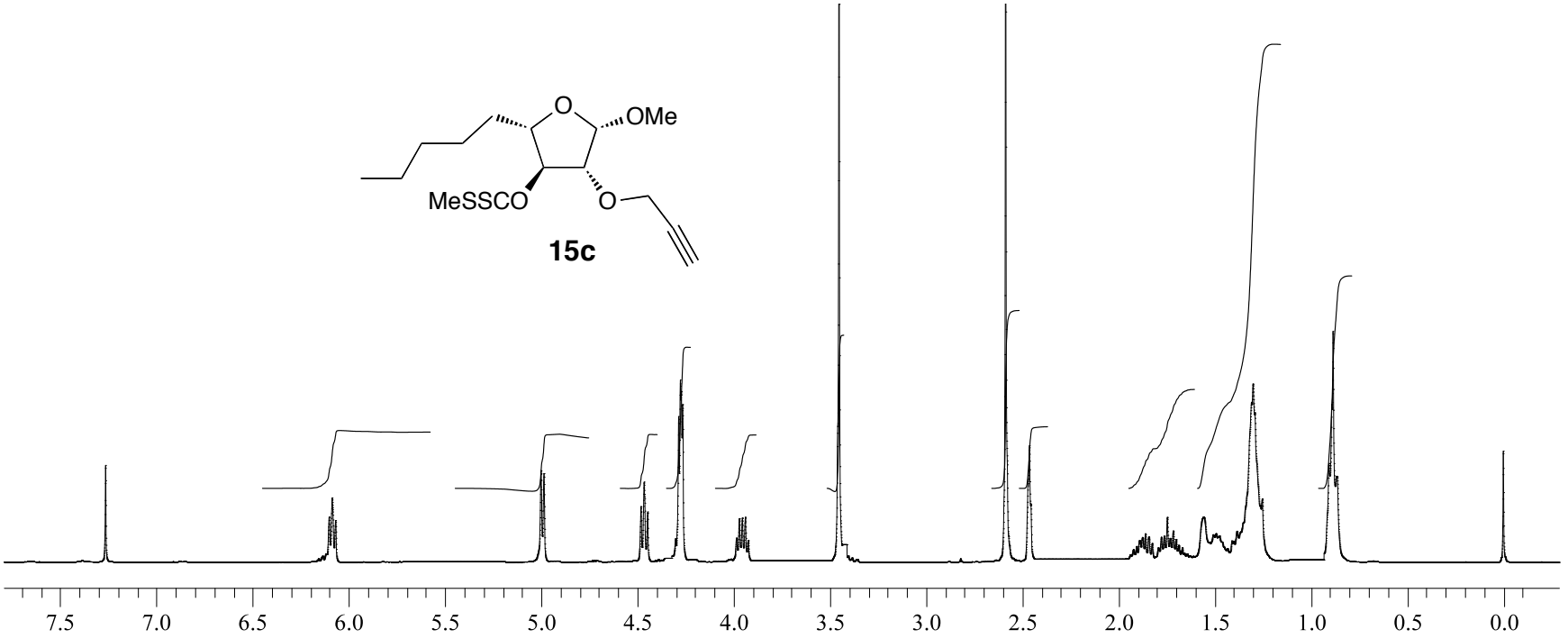


Figure S62 ^{1}H NMR Spectrum of **15c** ($CDCl_3$, 303 K, 300 MHz).

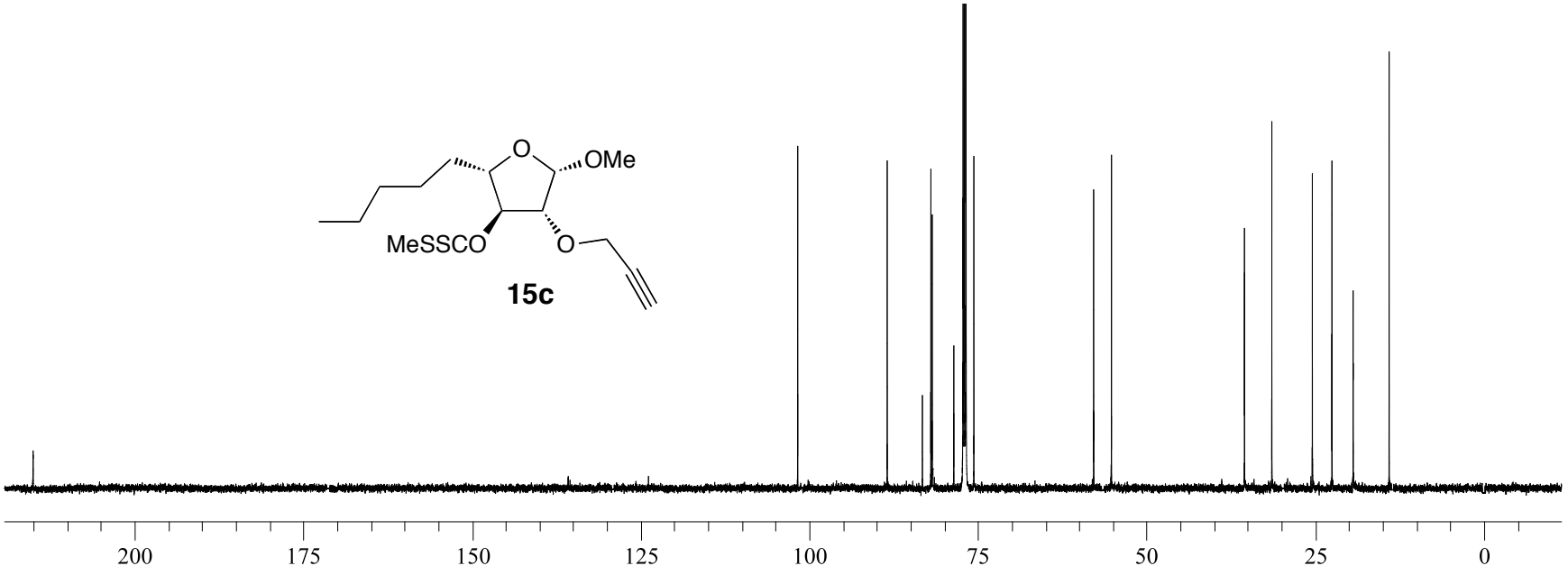


Figure S63 ^{13}C NMR Spectrum of **15c** ($CDCl_3$, 303 K, 75 MHz).

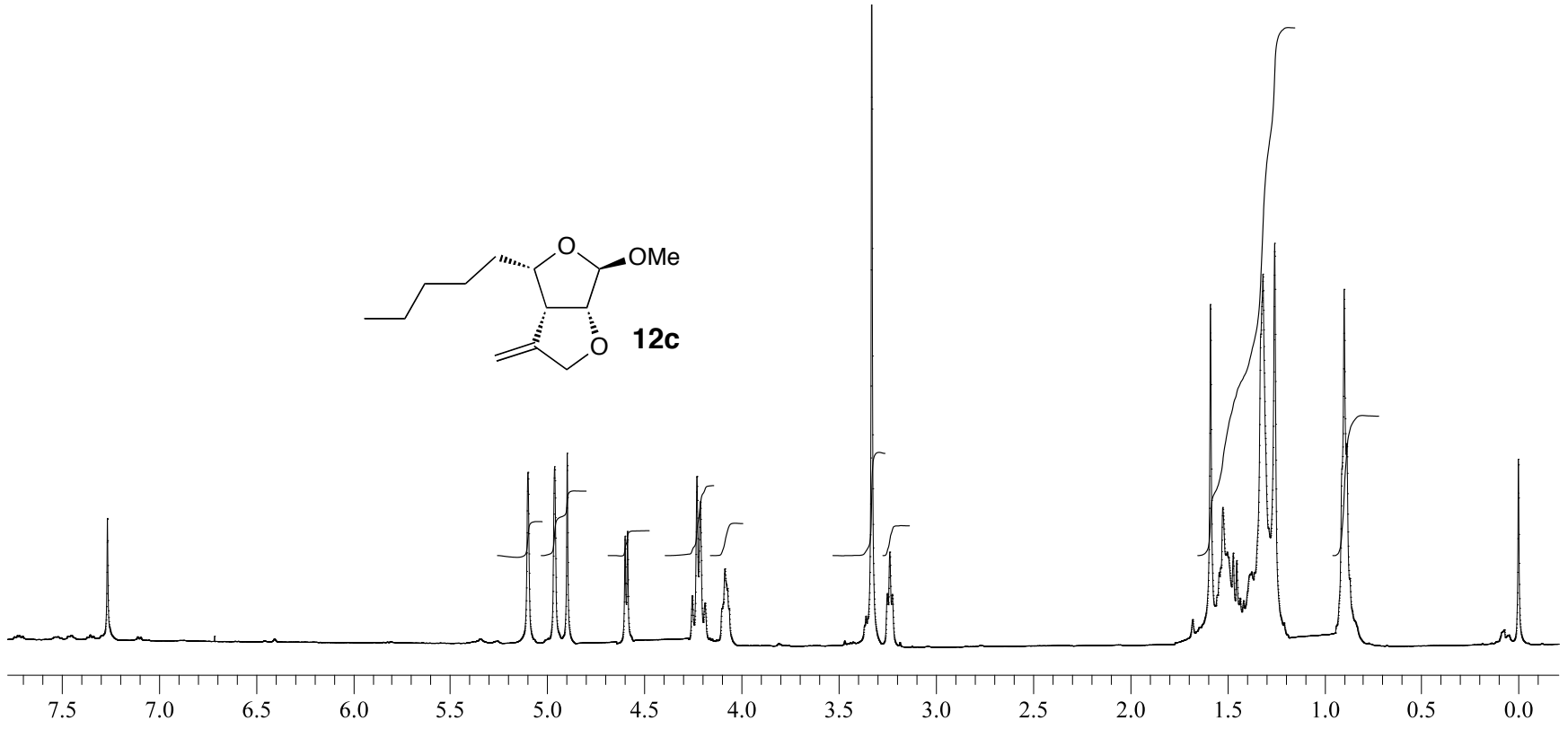


Figure S64 ^{1}H NMR Spectrum of **12c** ($CDCl_3$, 303 K, 500 MHz).

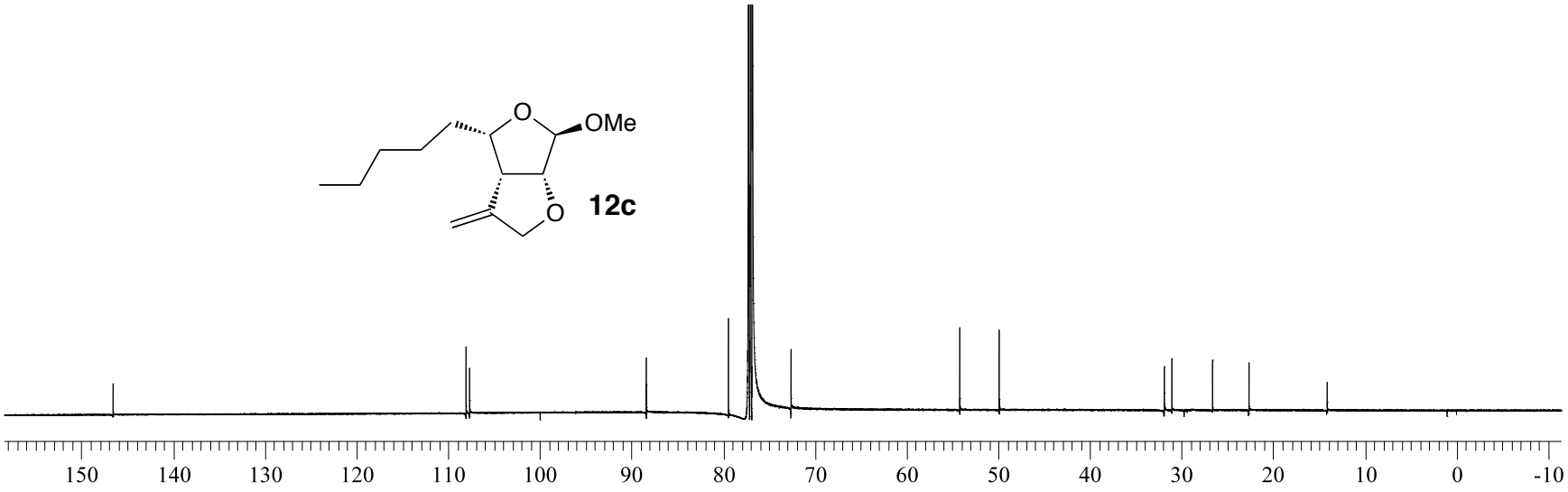
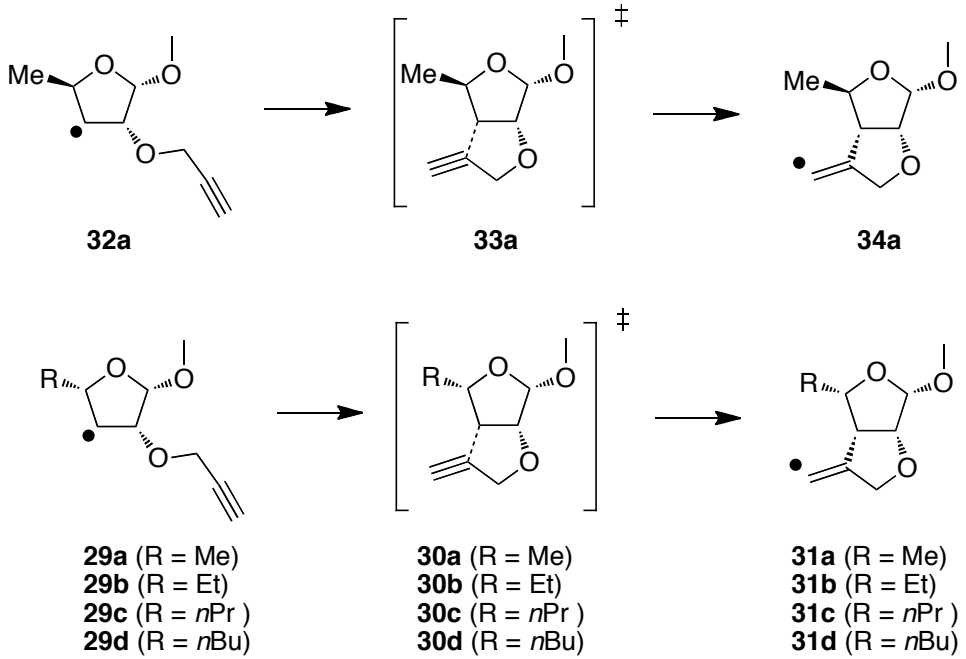


Figure S65 ^{13}C NMR Spectrum of **12c** ($CDCl_3$, 303 K, 75 MHz).

3. Theoretical Studies to the 5-*Exo*-Dig Cyclzation

In order to study the intramolecular 5-exo-dig-cyclization reaction in propargyloxy-substituted radicals **29** and **32** for each stage along the reaction pathway the conformational space has been searched extensively with the MM3* force field[3] and the systematic search routine implemented in *MACROMODEL 9.7*.[4] in order to identify all possible low energy conformations. The structures of reactants, products, and transition states have been optimized at the UB3LYP/6-31G(d) level of theory. Energy differences between stationary points have been calculated using Boltzmann-averaged values with weighting factors w ≥ 1% of the energetically most favourable conformers. The nature of all stationary points has been verified through calculation of analytical second derivatives and thermal corrections to enthalpies at 298.15 have been calculated at this same level. Single point energies have subsequently been calculated at the UB3LYP/6-311+G(d,p) level of theory. Combination of this total energies with thermal corrections calculated at UB3LYP/6-31G(d) level yield the enthalpies "H_{298}" tabled below. Single point calculations have also been performed at the (RO)MP2(FC)/G3MP2large level and combined with thermochemical corrections to 298.15 K obtained at UB3LYP/6-31G(d) level using a scaling factor of 0.9806. These results are termed as "H_{298}(ROMP2)" in the text. The G3MP2large basis set is a large triple-zeta basis set used in the G3(MP2) compound energy scheme.[5] All calculations have been performed with *Gaussian 03*.[6]

[3] N. L. Allinger, Y. H. Yuh, J. H. Lii, *J. Am. Chem. Soc.* **1989**, *111*, 8551. J. H. Lii, N. L. Allinger, *J. Am. Chem. Soc.* **1989**, 111, 8566. J. H. Lii, N. L. Allinger, *J. Am. Chem. Soc.* **1989**, 111, 8576.
[4] Schrödinger, LLC., *MacroModel 9.7*, **2009**.
[5] L. A. Curtiss, P. C. Redfern, K. Raghavachari, V. Rassolov, J. A. Pople, *J. Chem. Phys.* 1999, **110**, 4703.
[6] Gaussian 03, Revision E.01, **2006**, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, **2004**.



Scheme 3 Studied Systems in the 5-*Exo*-Dig cyclizations.

Table S1: Total energies and enthalpies (in Hartree, by 0.9806 scaled enthalpies in parentheses) for all systems described in scheme 1

System	E(UB3LYP/6-31G(d))	H(UB3LYP/6-31G(d))	E(UB3LYP/6-311+G(d,p))	E(ROMP2(FC)/G3MP2large)
32a gags_5	-576.2831005	-576.063423 (-576.067220)	-576.454725	-575.1452307
Gats_1b	-576.2821099	-576.062308 (-576.066108)	-576.453513	-575.1437222
33a	-576.2726830	-576.053686 (-576.057495)	-576.442695	-575.1356677

gats_1				
34a ga_5	-576.320173	-576.097499 (-576.101395)	-576.485813	-575.1807414
ga_8	-576.319733	-576.097110 (-576.101005)	-576.485311	-575.1804539
29a (R=Me) xags_5sp	-576.282835	-576.063064 (-576.066864)	-576.453719	-575.1446680
xats_1bsp	-576.281731	-576.061886 (-576.065687)	-576.452350	-575.1432474
30a (R=Me) xats_1	-576.2711661	-576.052036 (-576.055849)	-576.440061	-575.1340226
31a (R=Me) xylalpha_5	-576.3166655	-576.093877 (-576.097776)	-576.481384	-575.1775110
xylalpha_8	-576.3161315	-576.093355 (-576.097255)	-576.480830	-575.1771844
29b (R=Et) ShaC2 alpha_001	-615.5968431	-615.347119 (-615.351454)	-615.7779406	-614.3629413
ShaC2 alpha_024	-615.5964869	-615.346680 (-615.351017)	-615.7777136	-614.3626044
ShaC2 alpha_060	-615.5957930	-615.345921 (-615.350260)	-615.7766876	-614.3616171
ShaC2 alpha_09	-615.5948569	-615.345336 (-615.349667)	-615.7762117	-614.3603232
ShaC2 alpha_066	-615.5955401	-615.345588 (-615.349928)	-615.7764714	-614.3615387
ShaC2 alpha_010	-615.5938687	-615.344053 (-615.348390)	-615.7761907	-614.3591678
ShaC2 alpha_014	-615.5944866	-615.344905 (-615.349238)	-615.7759469	-614.3599948
ShaC2 alpha_090	-615.5938639	-615.344044 (-615.348382)	-615.7760844	-614.3590353
ShaC2	-615.5946950	-615.344928	-615.7759745	-614.3599826

alpha_051		(-615.349265)		
ShaC2 alpha_013	-615.5949856	-615.345210 (-615.349547)	-615.7759440	-614.3608783
ShaC2 alpha_028	-615.5949862	-615.345207 (-615.349544)	-615.7759423	-614.3608737
ShaC2 alpha_057	-615.5943736	-615.344521 (-615.348860)	-615.7757663	-614.3596725
ShaC2 alpha_05	-615.5947314	-615.345157 (-615.349489)	-615.7754552	-614.3615387
ShaC2 alpha_02	-615.5939013	-615.344301 (-615.348632)	-615.7752422	-614.3598498
ShaC2 alpha_06	-615.5943293	-615.344694 (-615.349028)	-615.7752559	-614.3610328
ShaC2 alpha_019	-615.5938494	-615.344018 (-615.348356)	-615.7754227	-614.3596994
ShaC2 alpha_07	-615.5935059	-615.343962 (-615.348293)	-615.7745471	-614.3590933
30b (R=Et) TSSC2 alpha_001	-615.5851852	-615.3360490 (-615.340399)	-615.7642868	-614.3524689
TSC2 alpha_002	-615.5843188	-615.3351690 (-615.339520)	-615.7633766	-614.3520835
TSC2 alpha_ special	-615.5808382	-615.3315530 (-615.335908)	-615.7597984	-614.3484727
31b (R=Et) cShaC2 alpha_010	-615.6303486	-615.3776260 (-615.382061)	-615.8052405	-614.3955838
cShaC2 alpha_001	-615.6287211	-615.3762120 (-615.380643)	-615.8041176	-614.3940570
cShaC2 alpha_002	-615.6284599	-615.3759110 (-615.380343)	-615.8036578	-614.3941450
cShaC2 alpha_016	-615.6290016	-615.3763130 (-615.380747)	-615.8037036	-614.3939728
cShaC2 alpha_023	-615.6276904	-615.3749840 (-615.379419)	-615.8022465	-614.3922469
cShaC2	-615.6265240	-615.3740940	-615.8015272	-614.3915832

alpha_013		(-615.378523)		
cShaC2 alpha_004	-615.6266049	-615.3741990 (-615.378626)	-615.8009299	-614.3916813
29c (R=Pr) ShaC3 alpha_001	-654.9105332	-654.6308380 (-654.635709)	-655.1022224	-653.5805674
ShaC3 alpha_003	-654.9100962	-654.6302940 (-654.635168)	-655.1019744	-653.5800724
ShaC3 alpha_105	-654.9094548	-654.6297200 (-654.634592)	-655.1009362	-653.5792413
ShaC3 alpha_006	-654.9093123	-654.6295140 (-654.634389)	-655.1009720	-653.5797683
ShaC3 alpha_013	-654.9085568	-654.6290860 (-654.633953)	-655.1004971	-653.5780210
ShaC3 alpha_015	-654.9076224	-654.6278600 (-654.632734)	-655.1004990	-653.5766866
ShaC3 alpha_115	-654.9090776	-654.6291190 (-654.633997)	-655.1006519	-653.5791266
ShaC3 alpha_019	-654.9080846	-654.6285170 (-654.633386)	-655.1001997	-653.5775178
ShaC3 alpha_087	-654.9084147	-654.6287030 (-654.633576)	-655.1002762	-653.5776505
ShaC3 alpha_020	-654.9086677	-654.6289270 (-654.633800)	-655.1002259	-653.5786187
ShaC3 alpha_008	-654.9084996	-654.6286580 (-654.633533)	-655.1002770	-653.5788295
ShaC3 alpha_005	-654.9084358	-654.6289210 (-654.633789)	-655.0998070	-653.5790770
ShaC3 alpha_099	-654.9079826	-654.6281310 (-654.633007)	-655.0999793	-653.5772888
ShaC3 alpha_002	-654.9076229	-654.6279930 (-654.632863)	-655.0995810	-653.5774901
ShaC3 alpha_014	-654.9084179	-654.6286090 (-654.633484)	-655.0997229	-653.5786130
ShaC3 alpha_009	-654.9079146	-654.6282610 (-654.633132)	-655.0994384	-653.5785992
30c (R=Pr)	-654.8988376	-654.6197720	-655.0885455	-653.5700373

TSC3 alpha_001		(-654.624658)		
TSC3 alpha_002	-654.8979443	-654.6187670 (-654.623655)	-655.0876124	-653.5699353
TSC3 alpha_003	-654.8976207	-654.6183860 (-654.623276)	-655.0872952	-653.5691124
TSC3 alpha_004	-654.8966328	-654.6174760 (-654.621944)	-655.0859096	-653.5682786
TSC3 alpha_005	-654.8962776	-654.6170540 (-654.622365)	-655.0859229	-653.5680325
31c (R=Pr) cShaC3 alpha_016	-654.9440436	-654.6613680 (-654.666339)	-655.1295293	-653.6133235
cShaC3 alpha_001	-654.9424015	-654.6600420 (-654.665006)	-655.1283842	-653.6116614
cShaC3 alpha_002	-654.9421111	-654.6595910 (-654.664560)	-655.1279545	-653.6120127
cShaC3 alpha_025	-654.9426700	-654.6598870 (-654.664861)	-655.1281710	-653.6123811
cShaC3 alpha_031	-654.9427088	-654.6600250 (-654.664996)	-655.1280496	-653.6120582
cShaC3 alpha_003	-654.9411079	-654.6585970 (-654.663565)	-655.1270827	-653.6108901
cShaC3 alpha_039	-654.9415569	-654.6588780 (-654.663850)	-655.1266115	-653.6107848
cShaC3 alpha_004	-654.9406389	-654.6582390 (-654.663205)	-655.1261645	-653.6100206
cShaC3 alpha_007	-654.9404354	-654.6579020 (-654.662871)	-655.1261953	-653.6107519
cShaC3 alpha_019	-654.9402675	-654.6578990 (-654.662864)	-655.1258666	-653.6091621
cShaC3 alpha_006	-654.9403604	-654.6579620 (-654.662927)	-655.1253330	-653.6095097
29d (R=Bu) ShaC4 alpha_001	-694.2242624	-693.9146170 (-693.920025)	-694.4265725	-692.7981525
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alpha_003		(-693.919484)		
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ShaC4 alpha_005	-694.2229601	-693.9132440 (-693.918654)	-694.4252084	-692.7975407
ShaC4 alpha_021	-694.2223049	-693.9128080 (-693.918212)	-694.4248763	-692.7955821
ShaC4 alpha_011	-694.2225940	-693.9127530 (-693.918166)	-694.4250335	-692.7970611
ShaC4 alpha_015	-694.2225030	-693.9126460 (-693.918056)	-694.4249878	-692.7968043
ShaC4 alpha_027	-694.2219064	-693.9123360 (-693.917742)	-694.4246409	-692.7951057
ShaC4 alpha_026	-694.2223327	-693.9127310 (-693.918138)	-694.4244960	-692.7963324
ShaC4 alpha_013	-694.2222194	-693.9124440 (-693.917856)	-694.4246046	-692.7965489
ShaC4 alpha_006	-694.2221835	-693.9127010 (-693.918105)	-694.4241691	-692.7967040
ShaC4 alpha_187	-694.2217257	-693.9119620 (-693.917374)	-694.4243576	-692.7948786
ShaC4 alpha_022	-694.2222185	-693.9125500 (-693.917959)	-694.4240987	-692.7964777
ShaC4 alpha_002	-694.2213377	-693.9117660 (-693.917172)	-694.4239091	-692.7950134
ShaC4 alpha_014	-694.2216769	-693.9121650 (-693.917570)	-694.4238327	-692.7961614
ShaC4 alpha_029	-694.2216406	-693.9117830 (-693.917197)	-694.4239372	-692.7966260
30d (R=Bu) TSC4 alpha_001	-694.2125451	-693.9035660 (-693.908987)	-694.4128788	-692.7876813
TSC4 alpha_002	-694.2116537	-693.9025570 (-693.907981)	-694.4119221	-692.7876534
TSC4 alpha_007	-694.2113279	-693.9021330 (-693.907559)	-694.4116137	-692.7867843

TSC4 alpha_003	-694.2112160	-693.9021180 (-693.907542)	-694.4114532	-692.7872186
TSC4 alpha_008	-694.2103953	-693.9011790 (-693.906606)	-694.4106952	-692.7868436
TSC4 alpha_009	-694.2104550	-693.9014390 (-693.906862)	-694.4103212	-692.7858790
TSC4 alpha_006	-694.2100309	-693.9008380 (-693.906264)	-694.4102952	-692.7860398
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31d (R=Bu) cShaC4 alpha_028	-694.2577541	-693.9451760 (-693.950682)	-694.4538738	-692.8309687
cShaC4 alpha_001	-694.2561801	-693.9438120 (-693.949314)	-694.4528163	-692.8292485
cShaC4 alpha_054	-694.2564810	-693.9437950 (-693.949303)	-694.4526198	-692.8303523
cShaC4 alpha_002	-694.2558469	-693.9434180 (-693.948922)	-694.4523145	-692.8297470
cShaC4 alpha_045	-694.2564351	-693.9437200 (-693.949229)	-694.4524669	-692.8304018
cShaC4 alpha_059	-694.2563608	-693.9436150 (-693.949125)	-694.4524773	-692.8300608
cShaC4 alpha_071	-694.2564706	-693.9437830 (-693.949292)	-694.4524128	-692.8298374
cShaC4 alpha_004	-694.2548619	-693.9424280 (-693.947931)	-694.4514507	-692.8285453
cShaC4 alpha_003	-694.2547585	-693.9423770 (-693.947880)	-694.4513463	-692.8284710
cShaC4 alpha_005	-694.2547958	-693.9423220 (-693.947827)	-694.4514030	-692.8285394
cShaC4 alpha_010	-694.2544655	-693.9420000 (-693.947504)	-694.4508961	-692.8287892
cShaC4 alpha_094	-694.2550916	-693.9423850 (-693.947894)	-694.4510422	-692.8289176
cShaC4	-694.2545405	-693.9420200	-694.4508505	-692.8291304

alpha_009		(-693.947526)		
cShaC4 alpha_079	-694.2550503	-693.9422050 (-693.947718)	-694.4511643	-692.8293687
cShaC4 alpha_008	-694.2544787	-693.9421780 (-693.947678)	-694.4505819	-692.8278188
cShaC4 alpha_087	-694.2550514	-693.9423360 (-693.947846)	-694.4508090	-692.8290529

Table S2: Boltzmann-averaged enthalpies $<H_{298}>$ at UB3LYP/6-311+G(d,p)//UB3LYP/6-31G(d) level of theory (in Hartree) for all systems described in scheme 1

System	E(UB3LYP/6-311+G(d,p))	H(UB3LYP/6-311+G(d,p))	w	$<H_{298}>$
32a gags_5	-576.454725	-576.2350475	0.8046149	**-576.2347822**
Gats_1b	-576.453513	-576.2337111	0.1953850	
33a gats_1	-576.442695	-576.223698	1.0000000	**-576.2236980**
34a ga_5	-576.485813	-576.263139	0.6171525	**-576.2629740**
ga_8	-576.485311	-576.262688	0.3827793	
29a (R=Me) xags_5sp	-576.453719	-576.233948	0.8217564	**-576.2336954**
xats_1bsp	-576.452350	-576.232505	0.1782436	
30a (R=Me) xats_1	-576.440061	-576.220931	1.0000000	**-576.2209309**
31a (R=Me) xylalpha_5	-576.481384	-576.2585955	0.6396941	**-576.2584153**
xylalpha_8	-576.480830	-576.2580535	0.3603060	
29b (R=Et)	-615.7779406	-615.5282165	0.2886641	**-615.5271813**

ShaC2 alpha_001				
ShaC2 alpha_024	-615.7777136	-615.5279067	0.2079197	
ShaC2 alpha_060	-615.7766876	-615.5268156	0.0654679	
ShaC2 alpha_009	-615.7762117	-615.5266908	0.0573621	
ShaC2 alpha_066	-615.7764714	-615.5265193	0.0478344	
ShaC2 alpha_010	-615.7761907	-615.5263750	0.0410552	
ShaC2 alpha_014	-615.7759469	-615.5263653	0.0406356	
ShaC2 alpha_090	-615.7760844	-615.5262645	0.0365209	
ShaC2 alpha_051	-615.7759745	-615.5262075	0.0343814	
ShaC2 alpha_013	-615.7759440	-615.5261684	0.0329867	
ShaC2 alpha_028	-615.7759423	-615.5261631	0.0328021	
ShaC2 alpha_057	-615.7757663	-615.5259137	0.0251876	
ShaC2 alpha_005	-615.7754552	-615.5258808	0.0243250	
ShaC2 alpha_002	-615.7752422	-615.5256419	0.0188872	
ShaC2 alpha_006	-615.7752559	-615.5256206	0.0184659	
ShaC2 alpha_019	-615.7754227	-615.5255913	0.0179017	
ShaC2 alpha_007	-615.7745471	-615.5250032	0.0096026	
30b (R=Et)	-615.7642868	-615.5151506	0.7229236	**-615.5148967**

TSC2 alpha_001				
TSC2 alpha_002	-615.7633766	-615.5142268	0.2717547	
TSC2alpha_ special	-615.7597984	-615.5105132	0.0053217	
31b (R=Et) cShaC2 alpha_010	-615.8052405	-615.5525179	0.5279647	**-615.5518718**
cShaC2 alpha_001	-615.8041176	-615.5516085	0.2015176	
cShaC2 alpha_002	-615.8036578	-615.5511089	0.1187175	
cShaC2 alpha_016	-615.8037036	-615.5510150	0.1074791	
cShaC2 alpha_023	-615.8022465	-615.5495401	0.0225383	
cShaC2 alpha_013	-615.8015272	-615.5490972	0.0140995	
cShaC2 alpha_004	-615.8009299	-615.5485240	0.0076834	
29c (R=Pr) ShaC3 alpha_001	-655.1022224	-654.8225272	0.2851318	**-654.8215091**
ShaC3 alpha_003	-655.1019744	-654.8221722	0.1957755	
ShaC3 alpha_105	-655.1009362	-654.8212014	0.0700204	
ShaC3 alpha_006	-655.1009720	-654.8211737	0.0679960	
ShaC3 alpha_013	-655.1004971	-654.8210263	0.0581681	
ShaC3 alpha_015	-655.1004990	-654.8207366	0.0427989	
ShaC3	-655.1006519	-654.8206933	0.0408805	

alpha_115				
ShaC3 alpha_019	-655.1001997	-654.8206321	0.0383148	
ShaC3 alpha_087	-655.1002762	-654.8205645	0.0356675	
ShaC3 alpha_020	-655.1002259	-654.8204852	0.0327943	
ShaC3 alpha_008	-655.1002770	-654.8204354	0.0311094	
ShaC3 alpha_005	-655.0998070	-654.8202922	0.0267316	
ShaC3 alpha_099	-655.0999793	-654.8201277	0.0224575	
ShaC3 alpha_002	-655.0995810	-654.8199511	0.0186265	
ShaC3 alpha_014	-655.0997229	-654.8199140	0.0179088	
ShaC3 alpha_009	-655.0994384	-654.8197848	0.0156185	
30c (R=Pr) TSC3 alpha_001	-655.0885455	-654.8094799	0.6019139	**-654.8088832**
TSC3 alpha_002	-655.0876124	-654.8084351	0.1990505	
TSC3 alpha_003	-655.0872952	-654.8080605	0.1338630	
TSSC3 alpha_004	-655.0859096	-654.8067528	0.0335093	
TSC3 alpha_005	-655.0859229	-654.8066993	0.0316633	
31c (R=Pr) cShaC3 alpha_016	-655.1295293	-654.8468537	0.4333702	**-654.8459759**
cShaC3 alpha_001	-655.1283842	-654.8460247	0.1801144	
cShaC3 alpha_002	-655.1279545	-654.8454344	0.0963898	

cShaC3 alpha_025	-655.1281710	-654.8453880	0.0917675	
cShaC3 alpha_031	-655.1280496	-654.8453658	0.0896350	
cShaC3 alpha_003	-655.1270827	-654.8445718	0.0386603	
cShaC3 alpha_039	-655.1266115	-654.8439326	0.0196452	
cShaC3 alpha_004	-655.1261645	-654.8437646	0.0164430	
cShaC3 alpha_007	-655.1261953	-654.8436619	0.0147484	
cShaC3 alpha_019	-655.1258666	-654.8434981	0.0123994	
cShaC3 alpha_006	-655.1253330	-654.8429346	0.0068267	
29d (R=Bu) ShaC4 alpha_001	-694.4265725	-694.1169271	0.2727817	**-694.1158870**
ShaC4 alpha_003	-694.4264259	-694.1165743	0.1877326	
ShaC4 alpha_007	-694.4253413	-694.1155911	0.0662678	
ShaC4 alpha_009	-694.4253092	-694.1155122	0.0609553	
ShaC4 alpha_005	-694.4252084	-694.1154923	0.0596840	
ShaC4 alpha_021	-694.4248763	-694.1153794	0.0529576	
ShaC4 alpha_011	-694.4250335	-694.1151925	0.0434471	
ShaC4 alpha_015	-694.4249878	-694.1151308	0.0406987	
ShaC4 alpha_027	-694.4246409	-694.1150705	0.0381808	
ShaC4 alpha_026	-694.4244960	-694.1148943	0.0316810	
ShaC4	-694.4246046	-694.1148292	0.0295703	

alpha_013				
ShaC4 alpha_006	-694.4241691	-694.1146866	0.0254252	
ShaC4 alpha_187	-694.4243576	-694.1145939	0.0230476	
ShaC4 alpha_022	-694.4240987	-694.1144302	0.0193789	
ShaC4 alpha_002	-694.4239091	-694.1143374	0.0175649	
ShaC4 alpha_014	-694.4238327	-694.1143208	0.0172587	
ShaC4 alpha_029	-694.4239372	-694.1140796	0.0133680	
30d (R=Bu) TSC4 alpha_001	-694.4128788	-694.1038997	0.4980720	**-694.1030420**
TSC4 alpha_002	-694.4119221	-694.1028254	0.1596438	
TSC4 alpha_007	-694.4116137	-694.1024188	0.1037840	
TSC4 alpha_003	-694.4114532	-694.1023552	0.0970234	
TSC4 alpha_008	-694.4106952	-694.1014789	0.0383539	
TSC4 alpha_009	-694.4103212	-694.1013052	0.0319090	
TSC4 alpha_006	-694.4102952	-694.1011023	0.0257387	
TSC4 alpha_005	-694.4101422	-694.1009981	0.0230493	
TSC4 alpha_010	-694.4101750	-694.1009722	0.0224257	
31d (R=Bu) cShaC4 alpha_028	-694.4538738	-694.1412957	0.3387804	**-694.1401913**
cShaC4 alpha_001	-694.4528163	-694.1404482	0.1380697	

cShaC4 alpha_054	-694.4526198	-694.1399338	0.0800742	
cShaC4 alpha_002	-694.4523145	-694.1398856	0.0760890	
cShaC4 alpha_045	-694.4524669	-694.1397518	0.0660357	
cShaC4 alpha_059	-694.4524773	-694.1397315	0.0646311	
cShaC4 alpha_071	-694.4524128	-694.1397252	0.0642013	
cShaC4 alpha_004	-694.4514507	-694.1390168	0.0303183	
cShaC4 alpha_003	-694.4513463	-694.1389648	0.0286937	
cShaC4 alpha_005	-694.4514030	-694.1389292	0.0276320	
cShaC4 alpha_010	-694.4508961	-694.1384306	0.0162957	
cShaC4 alpha_094	-694.4510422	-694.1383356	0.0147359	
cShaC4 alpha_009	-694.4508505	-694.1383300	0.0146488	
cShaC4 alpha_079	-694.4511643	-694.1383190	0.0144791	
cShaC4 alpha_008	-694.4505819	-694.1382812	0.0139109	
cShaC4 alpha_087	-694.4508090	-694.1380936	0.0114042	

Table S3: Boltzmann-averaged enthalpies $<H_{298}ROMP2>$ at (RO)MP2(FC)/G3MP2large//UB3LYP/6-31G(d) level of theory (in Hartree) for all systems described in scheme 1

System	E((RO)MP2(FC)/ G3MP2large)	H((RO)MP2(FC)/ G3MP2large)	w	$<H_{298}ROMP2>$
32a gags_5	-575.1452307	-574.9293502	0.8489308	**-574.9291005**
Gats_1b	-575.1437222	-574.9277203	0.1510692	

33a gats_1	-575.1356677	-574.9110528	1.0000000	**-574.9204797**
34a ga_5	-575.1807414	-574.9619634	0.5625551	**-574.9618695**
ga_8	-575.1804539	-574.9617259	0.4374450	
29a (R=Me) xags_5sp	-575.1446680	-574.9286970	0.8294711	**-574.9284574**
xats_1bsp	-575.1432474	-574.9272034	0.1705289	
30a (R=Me) xats_1	-575.1340226	-574.9187055	1.0000000	**-574.9187055**
31a (R=Me) xylalpha_5	-575.1775110	-574.9586215	0.5822791	**-574.9584926**
xylalpha_8	-575.1771844	-574.9583079	0.4177209	
29b (R=Et) ShaC2 alpha_001	-614.3629413	-614.1175522	0.3360249	**-614.1165830**
ShaC2 alpha_024	-614.3626044	-614.1171345	0.2158958	
ShaC2 alpha_060	-614.3616171	-614.1160841	0.2112155	
ShaC2 alpha_09	-614.3603232	-614.1151333	0.0259276	
ShaC2 alpha_066	-614.3615387	-614.1159266	0.0600693	
ShaC2 alpha_010	-614.3591678	-614.1136891	0.0056167	
ShaC2 alpha_014	-614.3599948	-614.1147462	0.0512082	
ShaC2 alpha_090	-614.3590353	-614.1135534	0.0048648	
ShaC2	-614.3599826	-614.1145526	0.0140172	

alpha_051				
ShaC2 alpha_013	-614.3608783	-614.1154397	0.0358671	
ShaC2 alpha_028	-614.3608737	-614.1154315	0.0355569	
ShaC2 alpha_057	-614.3596725	-614.1141589	0.0092379	
ShaC2 alpha_05	-614.3615387	-614.1162963	0.0888591	
ShaC2 alpha_02	-614.3598498	-614.1145805	0.0144376	
ShaC2 alpha_06	-614.3610328	-614.1157315	0.0488555	
ShaC2 alpha_019	-614.3596994	-614.1142060	0.0097104	
ShaC2 alpha_07	-614.3590933	-614.1138804	0.0068782	
30b (R=Et) TSC2 alpha_001	-614.3524689	-614.1076827	0.5993373	**-614.1074987**
TSC2 alpha_002	-614.3520835	-614.1072847	0.3931926	
TSC2alpha_ special	-614.3484727	-614.1035425	0.0074701	
31b (R=Et) cShaC2 alpha_010	-614.3955838	-614.1472962	0.5655011	**-614.1466011**
cShaC2 alpha_001	-614.3940570	-614.1459789	0.1401271	
cShaC2 alpha_002	-614.3941450	-614.1460281	0.1476224	
cShaC2 alpha_016	-614.3939728	-614.1457182	0.1063186	
cShaC2 alpha_023	-614.3922469	-614.1439755	0.0167892	
cShaC2	-614.3915832	-614.1435822	0.0110694	

alpha_013				
cShaC2 alpha_004	-614.3916813	-614.1437024	0.0125722	
29c (R=Pr) ShaC3 alpha_001	-653.5805674	-653.3057432	0.3007596	**-653.3047448**
ShaC3 alpha_003	-653.5800724	-653.3051442	0.1594779	
ShaC3 alpha_105	-653.5792413	-653.3043785	0.0708771	
ShaC3 alpha_006	-653.5797683	-653.3048450	0.1161660	
ShaC3 alpha_013	-653.5780210	-653.3034172	0.0256060	
ShaC3 alpha_015	-653.5766866	-653.3017982	0.0046096	
ShaC3 alpha_115	-653.5791266	-653.3040460	0.0410533	
ShaC3 alpha_019	-653.5775178	-653.3028192	0.0135920	
ShaC3 alpha_087	-653.5776505	-653.3028118	0.0134859	
ShaC3 alpha_020	-653.5786187	-653.3037510	0.0364651	
ShaC3 alpha_008	-653.5788295	-653.3038629	0.0410533	
ShaC3 alpha_005	-653.5790770	-653.3044302	0.0748662	
ShaC3 alpha_099	-653.5772888	-653.3023132	0.0079532	
ShaC3 alpha_002	-653.5774901	-653.3027302	0.0123693	
ShaC3 alpha_014	-653.5786130	-653.3036791	0.0337914	
ShaC3 alpha_009	-653.5785992	-653.3038166	0.0390887	
30c (R=Pr)	-653.5700373	-653.2958577	0.4230728	**-653.2954370**

TSC3 alpha_001				
TSC3 alpha_002	-653.5699353	-653.2956460	0.3380965	
TSC3 alpha_003	-653.5691124	-653.2947677	0.1333686	
TSC3 alpha_004	-653.5682786	-653.2935898	0.0383055	
TSC3 alpha_005	-653.5680325	-653.2941199	0.0671566	
31c (R=Pr) cShaC3 alpha_016	-653.6133235	-653.3356189	0.4104482	**-653.3347402**
cShaC3 alpha_001	-653.6116614	-653.3342659	0.0979323	
cShaC3 alpha_002	-653.6120127	-653.3344616	0.1204873	
cShaC3 alpha_025	-653.6123811	-653.3345721	0.1354464	
cShaC3 alpha_031	-653.6120582	-653.3343454	0.1065353	
cShaC3 alpha_003	-653.6108901	-653.3333472	0.0370132	
cShaC3 alpha_039	-653.6107848	-653.3330779	0.0278284	
cShaC3 alpha_004	-653.6100206	-653.3325867	0.0165407	
cShaC3 alpha_007	-653.6107519	-653.3331875	0.0312536	
cShaC3 alpha_019	-653.6091621	-653.3317586	0.0068811	
cShaC3 alpha_006	-653.6095097	-653.3320763	0.0096336	
29d (R=Bu) ShaC4 alpha_001	-692.7981525	-692.4939151	0.2261856	**-692.4929673**
ShaC4	-692.7975998	-692.4931612	0.1017882	

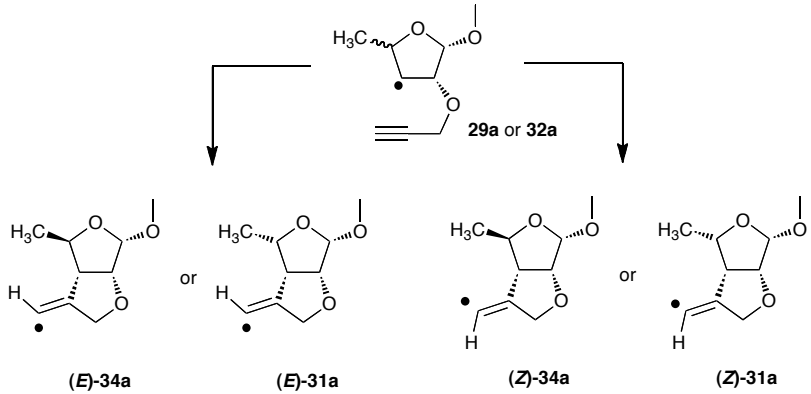
alpha_003				
ShaC4 alpha_007	-692.7974547	-692.4931155	0.0969789	
ShaC4 alpha_009	-692.7974074	-692.4930224	0.0878728	
ShaC4 alpha_005	-692.7975407	-692.4932346	0.1100168	
ShaC4 alpha_021	-692.7955821	-692.4914892	0.0173235	
ShaC4 alpha_011	-692.7970611	-692.4926331	0.0581822	
ShaC4 alpha_015	-692.7968043	-692.4923573	0.0434442	
ShaC4 alpha_027	-692.7951057	-692.4909413	0.0096967	
ShaC4 alpha_026	-692.7963324	-692.4921377	0.0344289	
ShaC4 alpha_013	-692.7965489	-692.4921855	0.0362168	
ShaC4 alpha_006	-692.7967040	-692.4926255	0.0577158	
ShaC4 alpha_187	-692.7948786	-692.4905269	0.0062519	
ShaC4 alpha_022	-692.7964777	-692.4922182	0.0374931	
ShaC4 alpha_002	-692.7950134	-692.4908477	0.0087815	
ShaC4 alpha_014	-692.7961614	-692.4920545	0.0315250	
ShaC4 alpha_029	-692.7966260	-692.4921824	0.0360981	
30d (R=Bu) TSC4 alpha_001	-692.7876813	-692.4841232	0.2695989	**-692.4835254**
TSC4 alpha_002	-692.7876534	-692.4839807	0.2318318	
TSC4 alpha_007	-692.7867843	-692.4830154	0.0834006	

TSC4 alpha_003	-692.7872186	-692.4835446	0.1460772	
TSC4 alpha_008	-692.7868436	-692.4830543	0.0869084	
TSC4 alpha_009	-692.7858790	-692.4822860	0.0385186	
TSC4 alpha_006	-692.7860398	-692.4822729	0.0379879	
TSShaC4 alpha_005	-692.7865460	-692.4828269	0.0683071	
TSC4 alpha_010	-692.7860332	-692.4822574	0.0373694	
31d (R=Bu) cShaC4 alpha_028	-692.8309687	-692.5238966	0.2512805	**-692.5229069**
cShaC4 alpha_001	-692.8292485	-692.5223824	0.0505452	
cShaC4 alpha_054	-692.8303523	-692.5231743	0.1169301	
cShaC4 alpha_002	-692.8297470	-692.5228221	0.0805243	
cShaC4 alpha_045	-692.8304018	-692.5231957	0.1196106	
cShaC4 alpha_059	-692.8300608	-692.5228250	0.0807720	
cShaC4 alpha_071	-692.8298374	-692.5226588	0.0677352	
cShaC4 alpha_004	-692.8285453	-692.5216144	0.0224093	
cShaC4 alpha_003	-692.8284710	-692.5215925	0.0218955	
cShaC4 alpha_005	-692.8285394	-692.5215706	0.0213935	
cShaC4 alpha_010	-692.8287892	-692.5218277	0.0280891	
cShaC4 alpha_094	-692.8289176	-692.5217200	0.0250611	
cShaC4	-692.8291304	-692.5221159	0.0381153	

alpha_009				
cShaC4 alpha_079	-692.8293687	-692.5220364	0.0350375	
cShaC4 alpha_008	-692.8278188	-692.5210181	0.0119165	
cShaC4 alpha_087	-692.8290529	-692.5218475	0.0286844	

Table S4: Boltzmann-averaged reaction and activation enthalpies (in kJ/mol) for the reactions described in scheme 3

Reaction	$<H_{298}>$(UB3LYP/6-311+G(d,p))	$<H_{298}>$((RO)MP2(FC)/G3MP2large)
33a – 32a	+29.10	+22.63
34a – 32a	-74.02	-86.03
30a – 29a	+33.51	+25.60
31a – 29a	-64.90	-78.86
30b – 29b	+32.30	+23.83
31b – 29b	-64.82	-78.81
30c – 29c	+33.15	+24.44
31c – 29c	-64.24	-78.75
30d – 29d	+33.72	+24.79
31d – 29d	-63.81	-78.66



Scheme 4 Possible configuration of the σ-type product radicals **31** and **34.**

Table S5: Reaction enthalpies (in kJ/mol) for the reactions described in scheme 4 (using Boltzmann-averaged enthalpies for **29a** and **32a**)

Reaction	$<H_{298}>$(UB3LYP/6-311+G(d,p))	$<H_{298}>$((RO)MP2(FC)/G3MP2large)
32a to **(*E*)-34a** H(**ga_8**)–$<H_{298}>$(**1**)	-73.27	-85.66
32a to **(*Z*)-34a** H(**ga_5**)–$<H_{298}>$(**1**)	-74.45	-86.28
29a to **(*E*)-31a** H(**xylalpha_8**)–$<H_{298}>$(**4a**)	-63.95	-78.37
29a to **(*Z*)-31a** H(**xylalpha_5**)–$<H_{298}>$(**4a**)	-65.38	-79.20

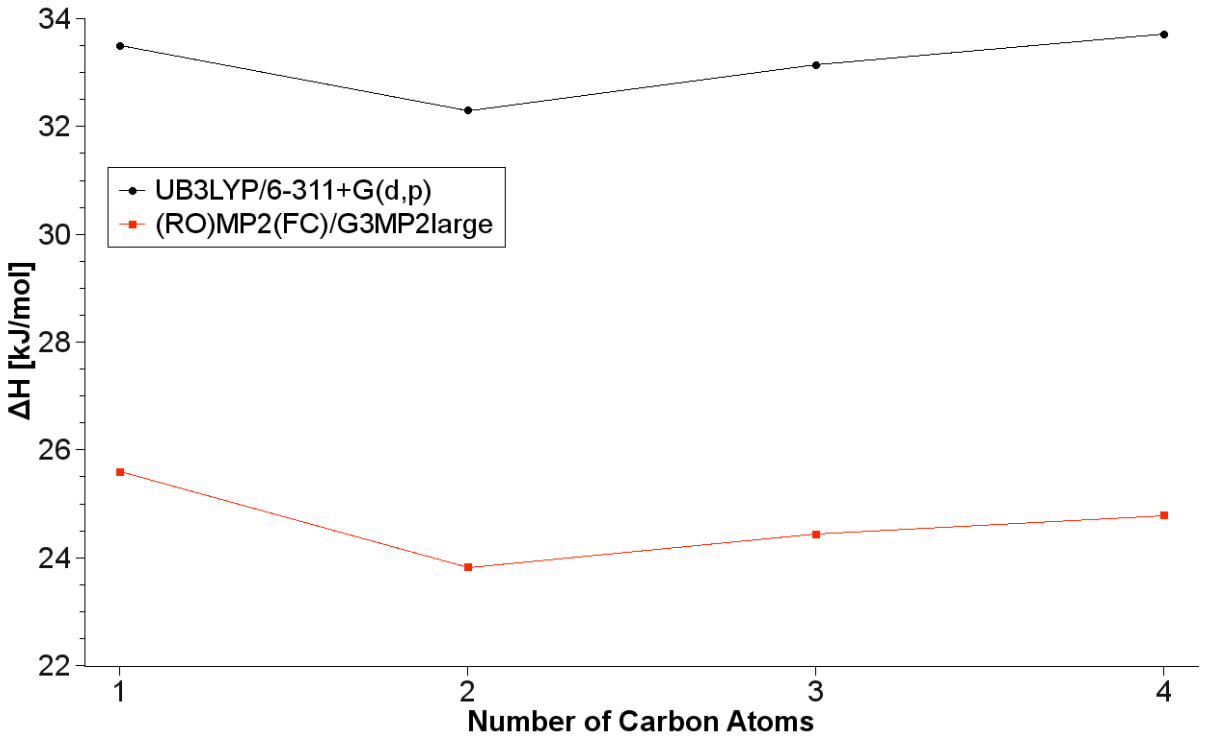


Figure S66 Graphical trend of the activation enthalpies as a function of the length of the alkyl chain.

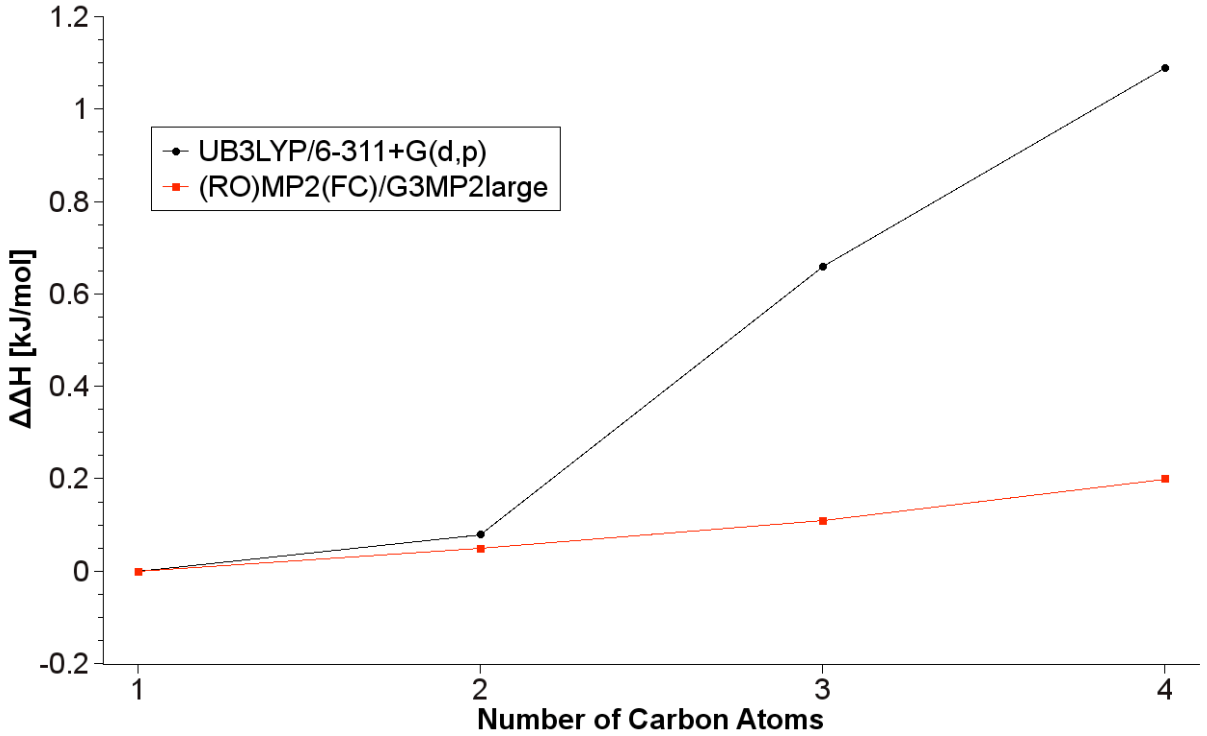


Figure S67 Graphical trend of the reaction enthalpies as a function of the length of the alkyl chain.

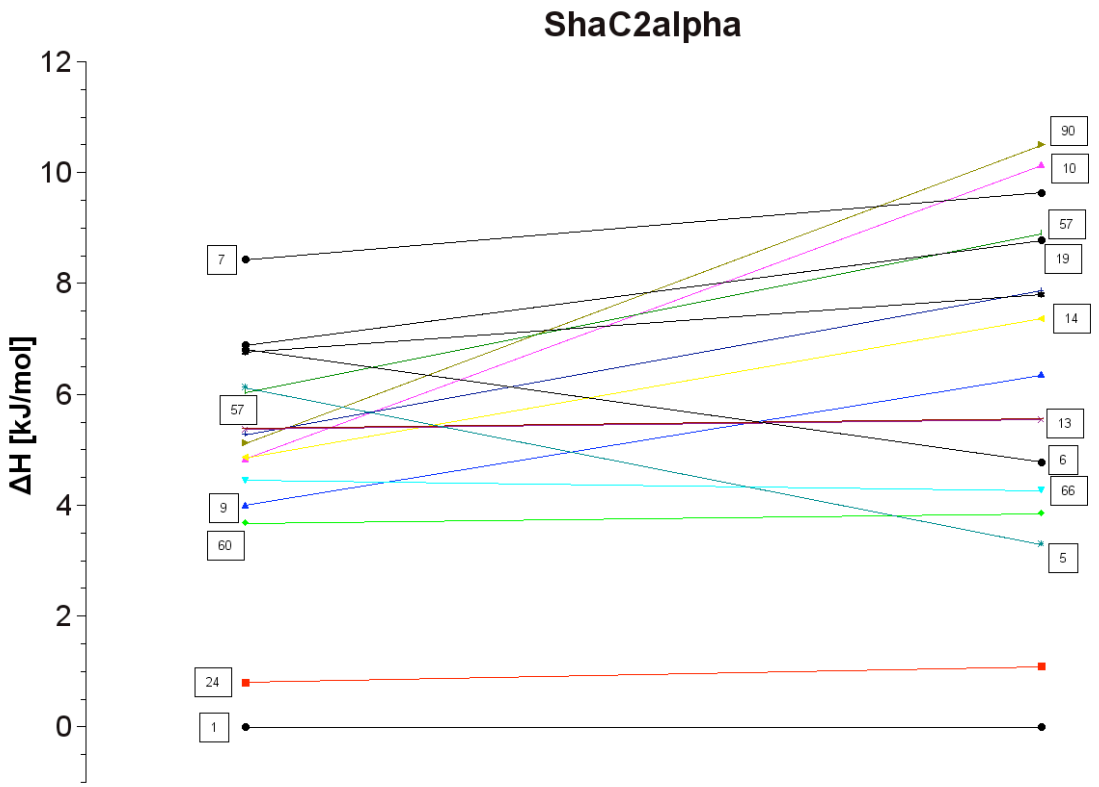


Figure S68 Relative enthalpies of conformers of **29b.**
Left UB3LYP/6-311+G(d,p), Right (RO)MP2(FC)/G3MP2large.

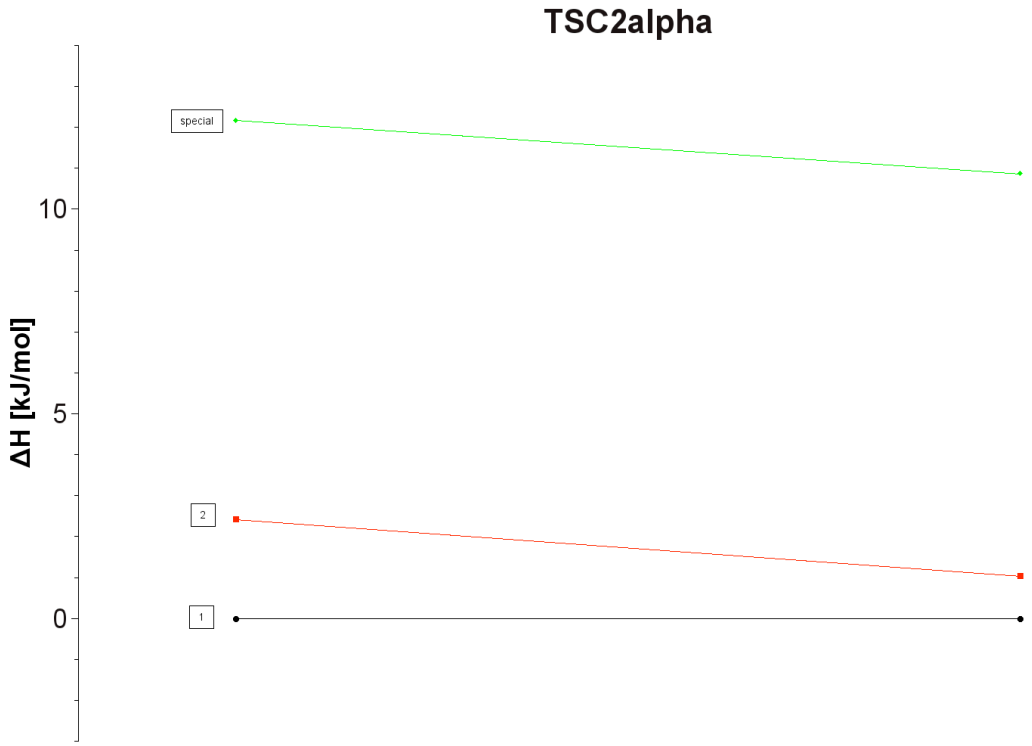


Figure S69 Relative enthalpies of conformers of **30b**.
Left UB3LYP/6-311+G(d,p), Right (RO)MP2(FC)/G3MP2large.

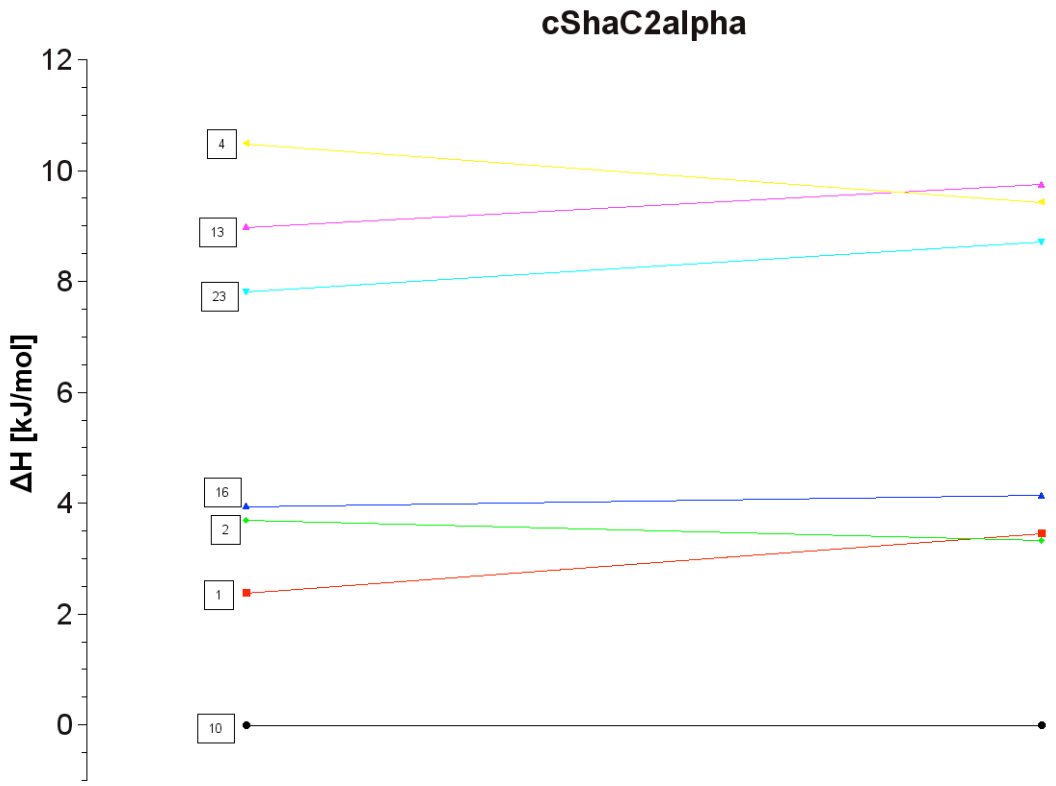


Figure S70 Relative enthalpies of conformers of **31b**.
Left UB3LYP/6-311+G(d,p), Right (RO)MP2(FC)/G3MP2large.

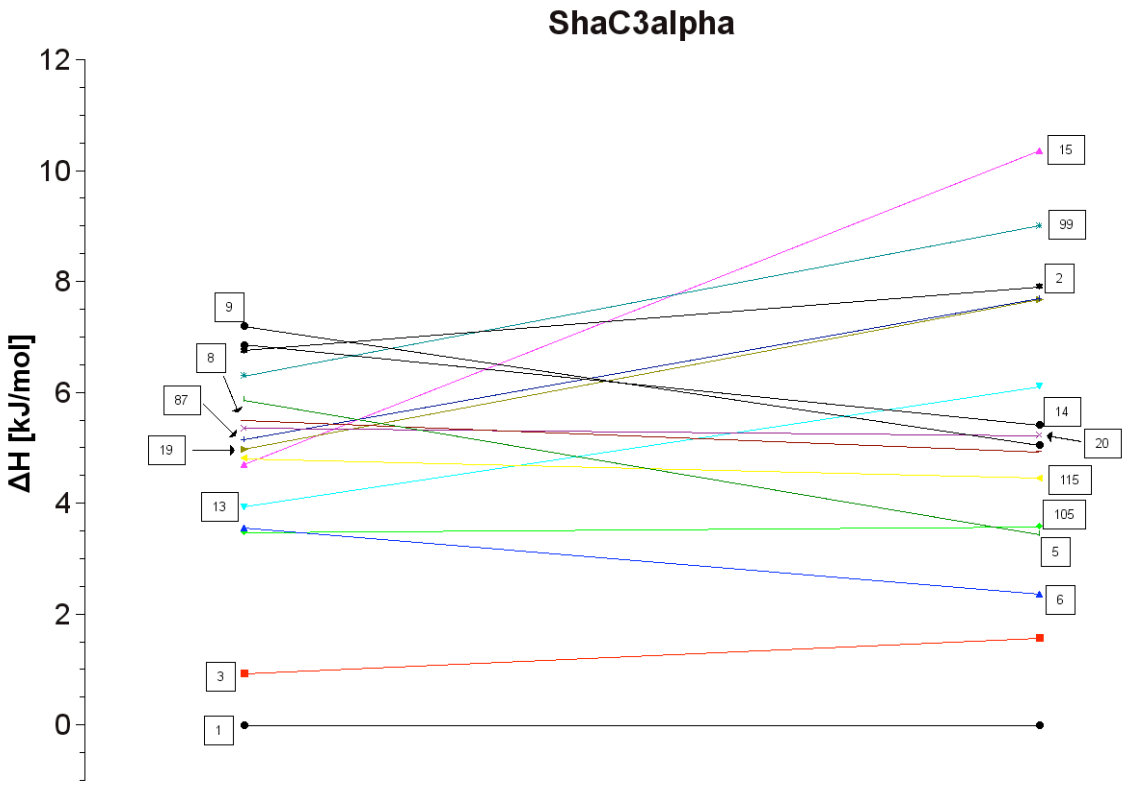


Figure S71 Relative enthalpies of conformers of **29c**.
Left UB3LYP/6-311+G(d,p), Right (RO)MP2(FC)/G3MP2large.

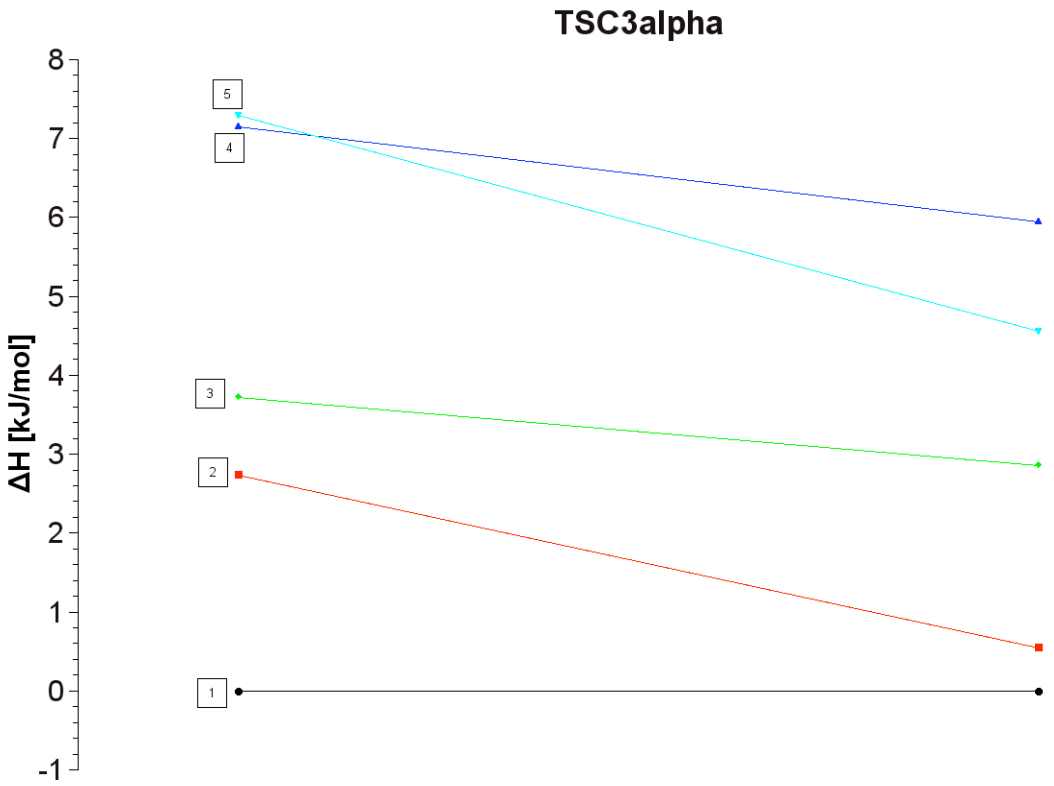


Figure S72 Relative enthalpies of conformers of **30c**.
Left UB3LYP/6-311+G(d,p), Right (RO)MP2(FC)/G3MP2large.

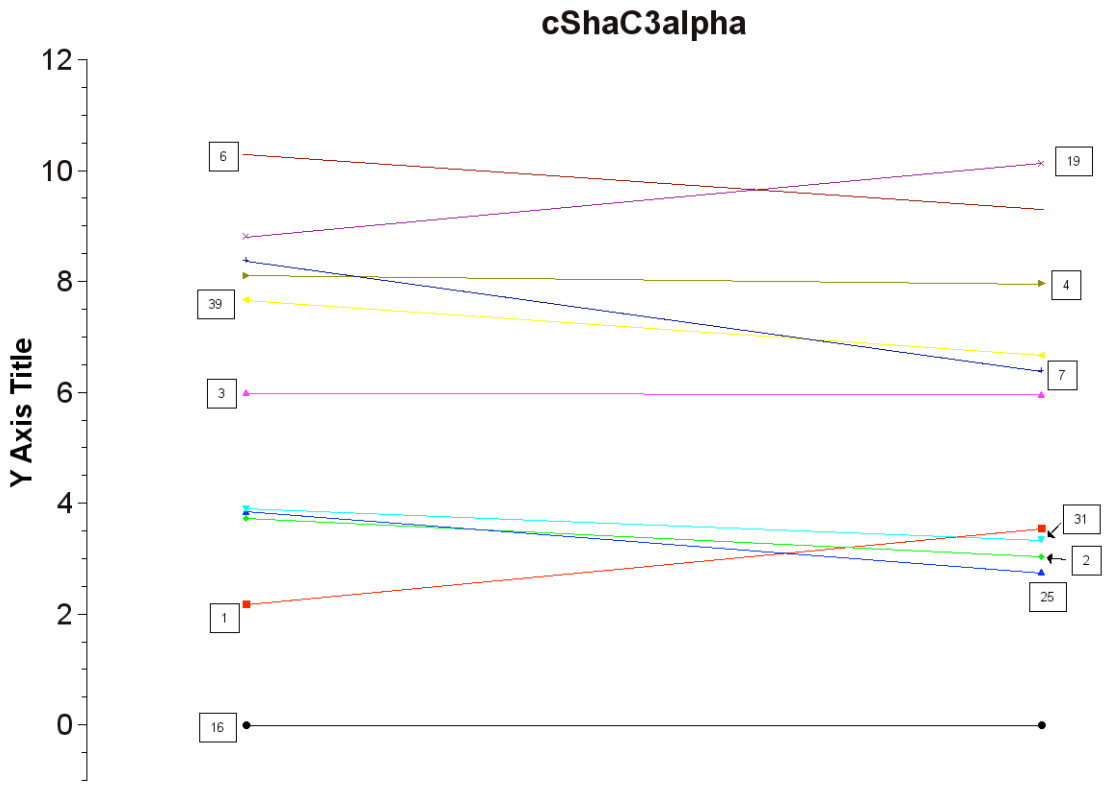


Figure S73 Relative enthalpies of conformers of **31c**.
Left UB3LYP/6-311+G(d,p), Right (RO)MP2(FC)/G3MP2large.

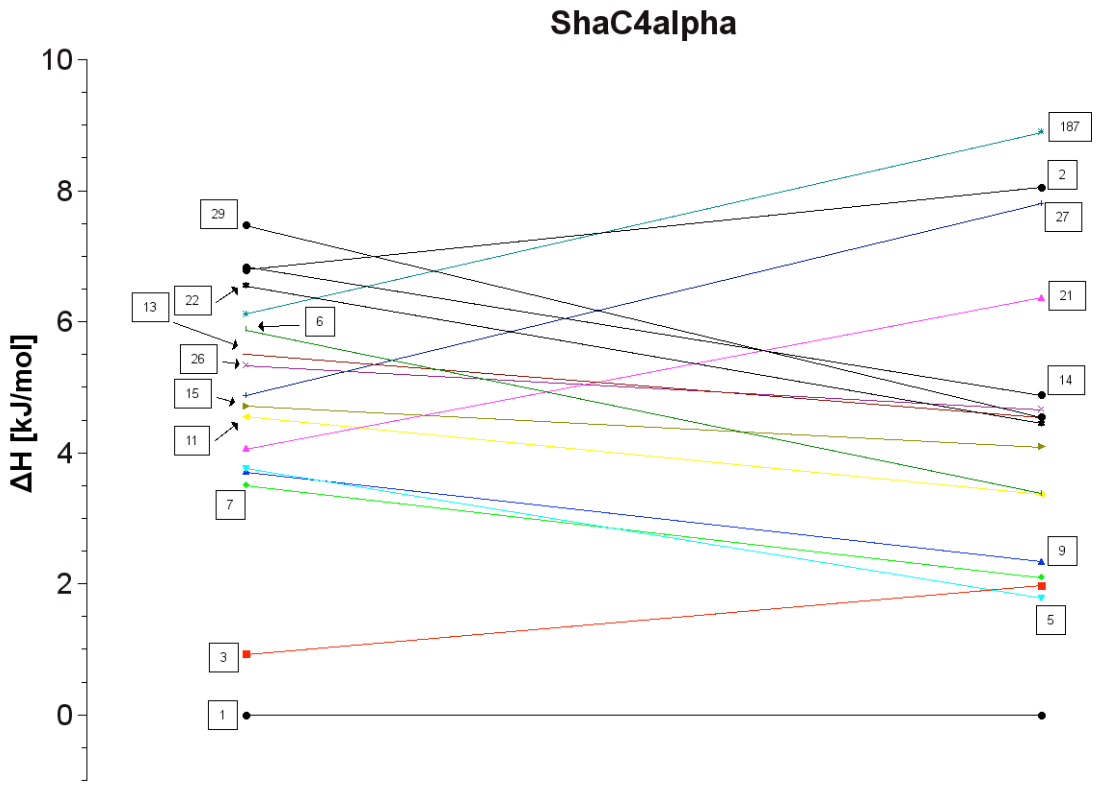


Figure S74 Relative enthalpies of conformers of **29d.**
Left UB3LYP/6-311+G(d,p), Right (RO)MP2(FC)/G3MP2large.

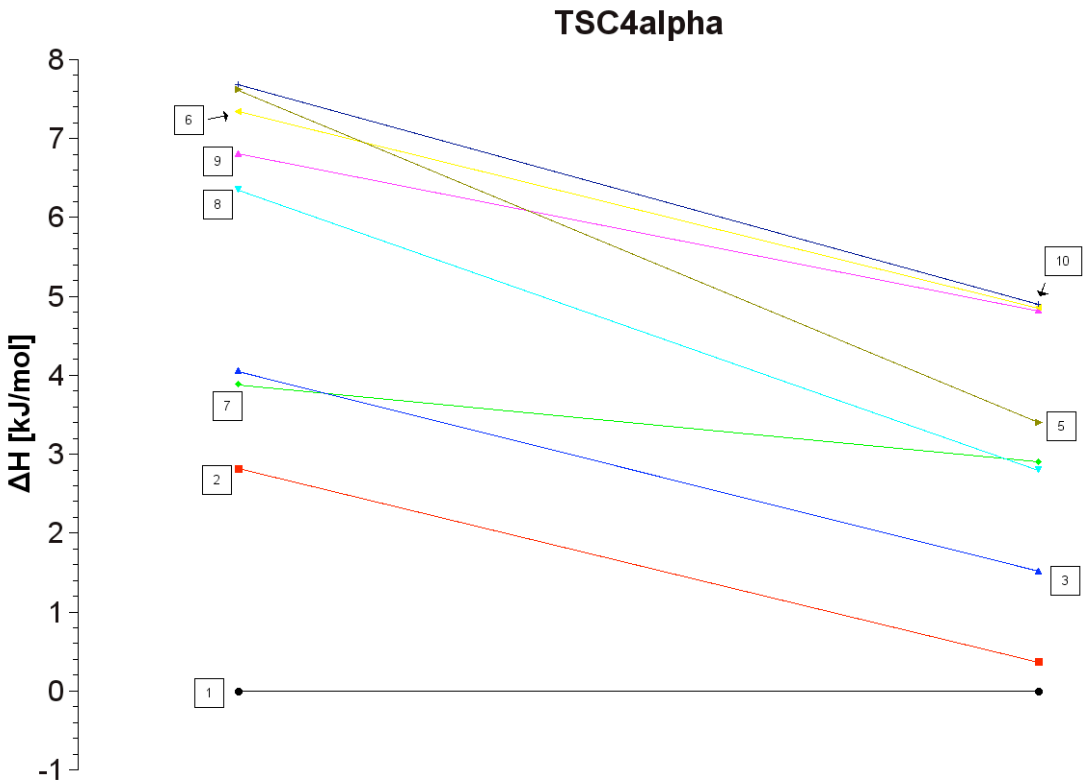


Figure S75 Relative enthalpies of conformers of **30d**.
Left UB3LYP/6-311+G(d,p), Right (RO)MP2(FC)/G3MP2large.

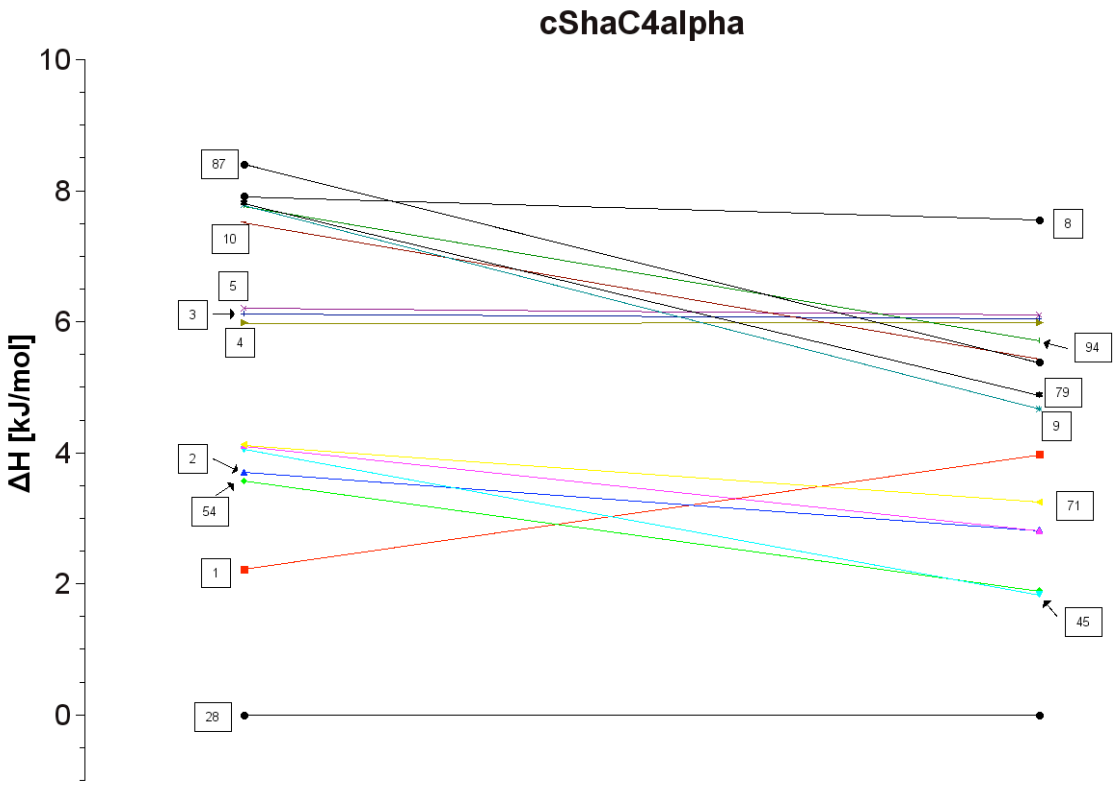


Figure S76 Relative enthalpies of conformers of **31d**.
Left UB3LYP/6-311+G(d,p), Right (RO)MP2(FC)/G3MP2large.

4. Theoretical Appendix

Structures of all stationary points
(optimized at UB3LYP/6-31G(d) level of theory)

32a

gags_5.log

```
1\1\GINC-TERMINUS\SP\UB3LYP\6-311+G(d,p)\C9H13O3(2)\SHARMA\05-Jan-2008
 \0\\#P UBECKE3LYP/6-311+G(D,P)\\gags_5sp ub3lyp/6-311+G(d,p)//ub3lyp/6
 -31G(d) sp of reactant radical\\0,2\C,0,-3.218766,-0.437367,-0.291445\
 C,0,-2.428175,0.387347,0.634833\O,0,-1.26465,-0.256842,1.141432\C,0,-0
 .297516,-0.600901,0.161327\C,0,0.848042,-1.316908,0.786289\C,0,0.43087
 ,0.588911,-0.537872\O,0,1.734986,0.114895,-0.800449\C,0,2.138874,-0.77
 8812,0.266562\O,0,0.405524,1.690959,0.329861\C,0,1.019388,2.849695,-0.
 217972\C,0,-3.866263,-1.109681,-1.058369\H,0,0.744978,-2.049529,1.5765
 64\H,0,-0.782053,-1.211518,-0.622547\H,0,-3.027575,0.625996,1.519998\H
 ,0,-2.160741,1.339455,0.155044\H,0,-4.444995,-1.70466,-1.728164\H,0,0.
 009466,0.864967,-1.514974\H,0,0.917485,3.641402,0.527908\H,0,2.081159,
 2.678509,-0.430114\H,0,0.519968,3.1635,-1.14802\C,0,3.10941,-1.808725,
 -0.308759\H,0,3.979895,-1.306026,-0.74303\H,0,3.457792,-2.484553,0.479
 987\H,0,2.620306,-2.40022,-1.088803\H,0,2.662245,-0.190777,1.041832\\V
 ersion=x86-Linux-G03RevB.03\State=2-A\HF=-576.4547249\S2=0.753898\S2-1
 =0.\S2A=0.750011\RMSD=5.683e-05\Dipole=0.0723486,0.0747932,-0.3397376\
 PG=C01 [X(C9H13O3)]\\@
```

Gats_1b.log

```
1\1\GINC-TICHY\SP\UB3LYP\6-311+G(d,p)\C9H13O3(2)\SHARMA\19-Jan-2008\0\
 \#P UBecke3LYP/6-311+G(d,p) geom=check guess=read scf=tight\\gats_1b u
 b3lyp/6-311+G(d,p)//ub3lyp/6-31G(d) reverse irc opt + freq\\0,2\C,0,-0
 .4978366306,0.7550755282,0.1115819765\C,0,-0.2482728434,-0.1939561183,
 1.2058057265\O,0,1.0515862144,-0.0479752863,1.7829966272\C,0,2.1049602
 245,-0.8168221671,1.2232440933\C,0,2.1441310762,-1.0313406342,-0.25376
 62051\C,0,2.2243797798,-2.2804203965,1.7394372178\O,0,2.9943582457,-2.
 9402255353,0.7583359732\C,0,2.6474637744,-2.4067776804,-0.5468447166\O
 ,0,0.9344208636,-2.8209662872,1.8764041022\C,0,0.9267849793,-4.1398245
 682,2.4056104021\C,0,-0.720870073,1.5298843483,-0.7881276133\H,0,1.940
 5673882,-0.2712751068,-0.996395023\H,0,3.0105841137,-0.2864986893,1.56
 10314649\H,0,-0.4144917593,-1.2216746908,0.8693301695\H,0,-0.950654054
 8,0.001068251,2.0243641556\H,0,-0.9146330994,2.2145532868,-1.582417552
 8\H,0,2.7740259464,-2.3746513078,2.6855336052\H,0,-0.1201080716,-4.441
```

305959,2.4868423664\H,0,1.4609266788,-4.8375205221,1.7499205124\H,0,1.
3879788384,-4.1671738113,3.404515583\C,0,3.8834912512,-2.4845157737,-1
.4416781409\H,0,4.2289170854,-3.5208885388,-1.5165657169\H,0,3.6473474
818,-2.1245119361,-2.4490746052\H,0,4.6938238937,-1.8746281017,-1.0303
577662\H,0,1.8538868294,-3.0380523916,-0.9846643257\\Version=IA32L-G03
RevD.01\State=2-A\HF=-576.4535129\S2=0.754154\S2-1=0.\S2A=0.750013\RMS
D=6.796e-09\Thermal=0.\Dipole=0.0512041,-0.4755132,-0.3956192\PG=C01 [
X(C9H13O3)]\\@

33a

gats_1.log

1\1\GINC-MORITZ\SP\UB3LYP\6-311+G(d,p)\C9H13O3(2)\SHARMA\23-Nov-2007\0
\\#P UBecke3LYP/6-311+G(d,p) geom=check guess=read scf=tight\\gats_1 u
b3lyp/6-311+G(d,p)//ub3lyp/6-31G(d) ts opt -3- finally do sp\\0,2\C,0,
0.0335560541,-0.0744728791,0.0227094839\C,0,-0.0001585053,0.0229139109
,1.5063449407\O,0,1.2763749222,0.031056968,2.1356535307\C,0,2.25754917
77,-0.7689525281,1.497880643\C,0,2.2436016596,-0.6836749275,0.00303431
11\C,0,2.1888219419,-2.3053329773,1.7356494147\O,0,2.7960081574,-2.871
8378369,0.5960211994\C,0,2.4873872681,-2.0532424896,-0.566071443\O,0,0
.8458315296,-2.6880435809,1.8888832276\C,0,0.6803425603,-4.0761585971,
2.1425535461\C,0,-0.4831450505,-0.0099593432,-1.0903792268\H,0,2.59027
11803,0.2056765527,-0.5122861483\H,0,3.2069340225,-0.4069081462,1.9171
669646\H,0,-0.6047467108,-0.8063528373,1.8886398316\H,0,-0.4755217977,
0.9671647017,1.7939133025\H,0,-0.720437496,-0.0261603381,-2.1307664547
\H,0,2.7747880069,-2.6458346601,2.6007324898\H,0,-0.3916087366,-4.2494
545282,2.262143727\H,0,1.0612587445,-4.6825092629,1.3126662795\H,0,1.1
989020116,-4.3736792995,3.0669879628\C,0,3.655232801,-2.1567947884,-1.
5412764022\H,0,3.8257441121,-3.2022542419,-1.8183259848\H,0,3.44123838
21,-1.5880950784,-2.4531498069\H,0,4.5720588222,-1.7643048424,-1.08906
6278\H,0,1.5782102652,-2.4508610232,-1.0437230722\\Version=IA32L-G03Re
vD.01\State=2-A\HF=-576.4426947\S2=0.770531\S2-1=0.\S2A=0.75016\RMSD=3
.030e-09\Thermal=0.\Dipole=0.0312599,-0.2698983,-0.4671053\PG=C01 [X(C
9H13O3)]\\@

34a

ga_5.log

1\1\GINC-MORITZ\SP\UB3LYP\6-311+G(d,p)\C9H13O3(2)\SHARMA\21-Nov-2007\0
\\#P UBecke3LYP/6-311+G(d,p) geom=check guess=read scf=tight\\ga_5sp u
b3lyp/6-311+G(d,p)//UB3LYP/6-31G(d) sp\\0,2\C,0,-0.2410642192,0.071438
8311,-0.0073187871\O,0,-0.0208248045,0.2074150334,1.3797542618\C,0,1.3
856082858,-0.0208250377,1.624028357\C,0,2.1008201489,0.6064952284,0.39
7553676\C,0,0.9768871847,0.7794504462,-0.6602443537\H,0,2.5519447379,1

.5634163825,0.6755077399\H,0,0.7197084926,1.8268006915,-0.8424627844\O
,0,1.4342408779,0.2392405539,-1.8850487697\C,0,2.4374614337,-0.7373286
096,-1.6182788711\H,0,1.9847442769,-1.728408189,-1.4847758822\H,0,3.12
03055197,-0.763191928,-2.4724353094\C,0,3.1112484602,-0.2795267342,-0.
3169929053\C,0,4.3192615741,-0.576590966,0.0932015492\H,0,5.1658256235
,-1.1566980678,-0.2505533368\H,0,-1.2056228434,0.5547853382,-0.2146628
32\O,0,-0.2654991581,-1.2657216126,-0.4322754131\C,0,-1.3726818835,-1.
9988684316,0.0738779234\H,0,-1.2988656883,-3.006812462,-0.3408245598\H
,0,-1.3564943821,-2.0488968883,1.1691357714\H,0,-2.3239028901,-1.54684
00822,-0.2458954106\H,0,1.5710304027,-1.1024406204,1.6428577532\C,0,1.
7490226034,0.5909675167,2.9646164608\H,0,1.1522522078,0.1443836534,3.7
664429791\H,0,2.8084641775,0.4174348361,3.1830731951\H,0,1.5646860653,
1.6710669443,2.9580850741\\Version=IA32L-G03RevD.01\State=2-A\HF=-576.
4858131\S2=0.760219\S2-1=0.\S2A=0.750047\RMSD=7.814e-09\Thermal=0.\Dip
ole=0.03205,-0.2543873,0.2823395\PG=C01 [X(C9H13O3)]\\@

ga_8.log

1\1\GINC-GRETEL\SP\UB3LYP\6-311+G(d,p)\C9H13O3(2)\SHARMA\21-Nov-2007\0
\\#P UBecke3LYP/6-311+G(d,p) geom=check guess=read scf=tight\\ga_8sp u
b3lyp/6-311+G(d,p)//UB3LYP/6-31G(d) sp\\0,2\C,0,-0.2383266548,0.073812
2067,-0.0132785796\O,0,-0.0368211554,0.2053837943,1.3780281633\C,0,1.3
632899617,-0.0343805767,1.6412151348\C,0,2.1005787542,0.5937472604,0.4
286809466\C,0,0.9941166373,0.7739523818,-0.6481961197\H,0,2.5519218451
,1.5481978947,0.7148085074\H,0,0.7470092939,1.8240130902,-0.8304321004
\O,0,1.4641101034,0.2326237881,-1.8651763759\C,0,2.460711923,-0.750503
9905,-1.5841983056\H,0,1.9991422031,-1.7390978915,-1.4625811189\H,0,3.
155648088,-0.7795154672,-2.427942471\C,0,3.1186726838,-0.300064651,-0.
2822522437\C,0,4.3250217573,-0.6054531942,0.1267494986\H,0,-1.19576777
58,0.5658515893,-0.2327360344\O,0,-0.2669840722,-1.2617070034,-0.43974
78607\C,0,-1.3893874882,-1.986724794,0.0442611978\H,0,-1.3150790743,-2
.9947605391,-0.3699967149\H,0,-1.3946972063,-2.0379906176,1.1396242821
\H,0,-2.330721927,-1.5271238404,-0.2933845497\H,0,1.5411419732,-1.1174
760594,1.6575035966\C,0,1.7060874755,0.5690869988,2.9916047337\H,0,1.0
866499559,0.1264945234,3.7782123\H,0,2.7579447527,0.3837989407,3.23670
837\H,0,1.5333685767,1.651036657,2.9850675162\H,0,4.967652809,-0.39923
23043,0.9726404316\\Version=IA32L-G03RevD.01\State=2-A\HF=-576.4853105
\S2=0.760209\S2-1=0.\S2A=0.750047\RMSD=9.523e-09\Thermal=0.\Dipole=-0.
061406,0.0066104,0.6803264\PG=C01 [X(C9H13O3)]\\@

29a

xags_5sp.log

1\1\GINC-HAENSEL\SP\UB3LYP\6-311+G(d,p)\C9H13O3(2)\SHARMA\24-Nov-2007\

0\\#P UBecke3LYP/6-311+G(d,p) scf=tight geom=check guess=read\\xags_5s
p ub3lyp/6-311+G(d,p)//ub3lyp/6-31G(d) sp of reactant radical\\0,2\C,0
,-0.1062421178,-0.417218245,-0.0014144708\C,0,0.0721196195,0.194525997
5,1.3240947307\O,0,1.4173717482,0.1958741565,1.788495309\C,0,2.3203645
317,0.9579070117,1.0027797023\C,0,3.7066711153,0.8247938898,1.52467603
41\C,0,2.1245358001,2.50521742,1.0330983982\O,0,3.4253143361,3.0458917
423,0.9240825476\C,0,4.3861395132,2.1517767689,1.5409237827\O,0,1.4737
008986,2.847180937,2.2298505574\C,0,1.1874988431,4.2355198911,2.334567
7237\C,0,4.7916889256,2.6487480069,2.9355388237\C,0,-0.2542696022,-0.9
131751794,-1.092985047\H,0,4.1407762315,-0.1076227655,1.8620997718\H,0
,2.248859696,0.6264136706,-0.0499556551\H,0,-0.4849898815,-0.378478546
7,2.0731288196\H,0,-0.3354054819,1.2153215911,1.3249220953\H,0,-0.3893
662924,-1.359419572,-2.0522410825\H,0,5.2731671513,2.1714721567,0.8885
408116\H,0,5.5580485723,1.9935565486,3.3662623238\H,0,5.2029175319,3.6
61845093,2.8668073035\H,0,3.923064587,2.6595235537,3.5993867214\H,0,1.
562439528,2.9030105107,0.1761332362\H,0,0.6512042777,4.3755740945,3.27
59958727\H,0,2.1055922033,4.8343841497,2.341774013\H,0,0.5506930388,4.
5743808633,1.5024834077\\Version=IA32L-G03RevD.01\State=2-A\HF=-576.45
37195\S2=0.754102\S2-1=0.\S2A=0.750012\RMSD=8.063e-09\Thermal=0.\Dipol
e=-0.0397944,0.2263842,-0.2305977\PG=C01 [X(C9H13O3)]\\@

xats_1bsp.log

1\1\GINC-Z7\SP\UB3LYP\6-311+G(d,p)\C9H13O3(2)\SHARMA\19-Jan-2008\0\\#P
UBecke3LYP/6-311+G(d,p) geom=check guess=read\\xats_1b ub3lyp/6-311+G
(d,p)//ub3lyp/6-31G(d) sp\\0,2\C,0,-0.6163802311,0.9198398714,0.314379
5034\C,0,-0.2428275531,-0.1210361477,1.2823759467\O,0,1.1111064562,-0.
0062132817,1.7270256289\C,0,2.1027931427,-0.6999798143,0.9887909217\C,
0,1.9855359503,-0.7799448814,-0.4968125677\C,0,2.2955242351,-2.1996393
044,1.3538528103\O,0,2.9689558679,-2.7551005548,0.2445598982\C,0,2.551
4181365,-2.0773839496,-0.9711295273\O,0,1.0346897562,-2.7795082171,1.5
821927602\C,0,1.1038048581,-4.128597375,2.0240393798\C,0,1.5916929451,
-2.9508227974,-1.7887911772\C,0,-0.9432629313,1.7711199088,-0.47803527
43\H,0,1.7066255001,0.0440929948,-1.1404032653\H,0,3.036509464,-0.1849
456636,1.2718467995\H,0,-0.4373778953,-1.1160693577,0.8711006836\H,0,-
0.853222861,-0.0137131572,2.1863958614\H,0,-1.2293754326,2.5228203174,
-1.1782507689\H,0,3.4710332744,-1.9265493185,-1.5589984427\H,0,1.32888
19415,-2.4513948338,-2.7286891718\H,0,2.0681393269,-3.9078372738,-2.02
75898084\H,0,0.6752240593,-3.1424062015,-1.2240287144\H,0,2.9421404131
,-2.3626599273,2.2263905035\H,0,0.0765523173,-4.4572090041,2.197955930
2\H,0,1.5731714957,-4.7725307279,1.2710239022\H,0,1.6709500741,-4.2071
008082,2.9638363053\\Version=IA32L-G03RevD.01\State=2-A\HF=-576.452349

9\S2=0.754118\S2-1=0.\S2A=0.750012\RMSD=4.772e-05\Thermal=0.\Dipole=-0
.0230551,-0.4166828,-0.4198594\PG=C01 [X(C9H13O3)]\\@

30a

xats_1.log

1\1\GINC-TICHY\SP\UB3LYP\6-311+G(d,p)\C9H13O3(2)\SHARMA\23-Nov-2007\0\
\#P UBecke3LYP/6-311+G(d,p) scf=tight geom=check guess=read\\xats_1 ub
3lyp/6-311+G(d,p)//ub3lyp/6-31G(d) sp ts\\0,2\C,0,-0.1308350032,0.0998
763631,0.0294407449\C,0,-0.0381515086,-0.0312131609,1.5083467504\O,0,1
.2905491963,0.0105249713,2.015977467\C,0,2.2386546128,-0.6765762425,1.
2185858508\C,0,2.0507101854,-0.4982933383,-0.2585774684\C,0,2.29456594
1,-2.2236394717,1.360029738\O,0,2.8139136193,-2.6801833368,0.131553086
2\C,0,2.3942647758,-1.7949656658,-0.9440331142\O,0,1.0050596735,-2.716
2468814,1.6304334365\C,0,0.9738240457,-4.1191851584,1.8551130709\C,0,1
.2896385038,-2.4472340963,-1.7784145563\C,0,-0.7524227352,0.3721190479
,-0.9978869978\H,0,2.3045740731,0.4433075677,-0.7333936018\H,0,3.20772
55707,-0.2779091761,1.5515801581\H,0,-0.531621267,-0.9621731443,1.8068
485411\H,0,-0.5572389152,0.8105167857,1.9785029259\H,0,-1.0696354992,0
.5239060472,-2.005805498\H,0,3.2822181365,-1.6646430715,-1.5802347797\
H,0,1.0194085202,-1.8047507315,-2.6241487863\H,0,1.6403656186,-3.40815
9689,-2.1699363597\H,0,0.3984546812,-2.6099105865,-1.1680265534\H,0,2.
9897518897,-2.5674598035,2.138557438\H,0,-0.0623239469,-4.3796950396,2
.0831362393\H,0,1.3062588815,-4.6736530222,0.9698897893\H,0,1.61110654
29,-4.3961412699,2.7087744078\\Version=IA32L-G03RevD.01\State=2-A\HF=-
576.440061\S2=0.772567\S2-1=0.\S2A=0.750181\RMSD=4.275e-09\Thermal=0.\
Dipole=-0.0207913,-0.2306583,-0.4719012\PG=C01 [X(C9H13O3)]\\@

31a

xylalpha_5.log

1\1\GINC-GRETEL\SP\UB3LYP\6-311+G(d,p)\C9H13O3(2)\SHARMA\14-Nov-2007\0
\\#P UBecke3LYP/6-311+G(d,p) geom=check guess=read scf=tight\\xyl-alph
a_5sp ub3lyp/6-311+G(d,p)//UB3LYP/6-31G(d) sp\\0,2\C,0,-0.1920330147,0
.010923817,0.0872436322\O,0,0.0180816601,0.049616111,1.4778925346\C,0,
1.4373086247,-0.0516370777,1.7690256797\C,0,2.1577022324,0.4811500782,
0.4926610012\C,0,1.0101384994,0.7836897318,-0.5068897463\H,0,2.7154407
802,1.3871577047,0.7445226489\H,0,0.7537484914,1.8460474103,-0.5533894
184\O,0,1.4315869139,0.3935379615,-1.7969688625\C,0,2.3840076555,-0.66
08004296,-1.6760247516\H,0,1.883613844,-1.6361730922,-1.7032141444\H,0
,3.0784996515,-0.584189233,-2.5180567556\C,0,3.0626559215,-0.447519884
2,-0.3147708995\C,0,4.2288245342,-0.9194658676,0.0504479414\H,0,5.0096
072306,-1.542175924,-0.3668443812\H,0,1.6043467553,0.6465524655,2.5961
652831\C,0,1.7960919068,-1.458970079,2.2306998303\H,0,2.8488453186,-1.

5113646477,2.5287758712\H,0,1.1757117164,-1.7263833265,3.0926140962\H,
0,1.6274294558,-2.1891059089,1.4351712382\H,0,-1.162670399,0.494310743
9,-0.0909428746\O,0,-0.205022627,-1.2920793856,-0.4418074631\C,0,-1.32
37055489,-2.0606311926,-0.0210607648\H,0,-1.2447459962,-3.0308278914,-
0.5169981366\H,0,-1.3281526724,-2.2025957624,1.0660904096\H,0,-2.26705
00421,-1.5792634407,-0.3205126023\\Version=IA32L-G03RevD.01\State=2-A\
HF=-576.481385\S2=0.760435\S2-1=0.\S2A=0.750049\RMSD=8.707e-09\Thermal
=0.\Dipole=0.0602188,-0.2616626,0.2144047\PG=C01 [X(C9H13O3)]\\@

xylalpha_8.log

1\1\GINC-GRETEL\SP\UB3LYP\6-311+G(d,p)\C9H13O3(2)\SHARMA\14-Nov-2007\0
\\#P UBecke3LYP/6-311+G(d,p) geom=check guess=read scf=tight\\xyl-alph
a_8sp ub3lyp/6-311+G(d,p)//UB3LYP/6-31G(d) sp\\0,2\C,0,-0.013995052,-0
.0015668007,-0.0031751984\O,0,-0.0195052484,0.006660651,1.4048369934\C
,0,1.3423077314,0.0019990662,1.9049952078\C,0,2.1953843843,0.656729180
3,0.7754645605\C,0,1.1953519256,0.8831128539,-0.3921137825\H,0,2.60754
86481,1.6035618303,1.1343176431\H,0,0.8584062107,1.9215214904,-0.46479
40917\O,0,1.8425249256,0.5612980908,-1.6032014439\C,0,2.8609659744,-0.
4053408578,-1.3420049626\H,0,2.4594800653,-1.4209076151,-1.4447473028\
H,0,3.6607355034,-0.2577790078,-2.0732094798\C,0,3.3120690489,-0.14703
74655,0.0939562335\C,0,4.4693094185,-0.488394853,0.6039241446\H,0,1.32
29209662,0.6651522989,2.7765660826\C,0,1.7464863201,-1.3967013327,2.35
82534419\H,0,2.7296711099,-1.3823786629,2.8412491238\H,0,1.0131481239,
-1.7654554818,3.0830208677\H,0,1.7870132078,-2.0898663185,1.5144798047
\H,0,-0.9832014427,0.4114279979,-0.3155203727\O,0,0.1582607922,-1.2824
857193,-0.5553038566\C,0,-0.9471219771,-2.1472938416,-0.3328701239\H,0
,-0.7159914339,-3.0900082069,-0.8341130374\H,0,-1.107368792,-2.3292263
087,0.7364738062\H,0,-1.8684969664,-1.7271242911,-0.763820937\H,0,4.99
79798555,-0.4045837509,1.5441068626\\Version=IA32L-G03RevD.01\State=2-
A\HF=-576.48083\S2=0.760495\S2-1=0.\S2A=0.750049\RMSD=4.924e-09\Therma
l=0.\Dipole=-0.0928672,-0.0703464,0.626723\PG=C01 [X(C9H13O3)]\\@

29b

ShaC2alpha_001_sp.log

1\1\GINC-NODE-31\SP\UB3LYP\6-311+G(d,p)\C10H15O3(2)\ZIP06\31-May-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC2alpha_00
1 sp\\0,2\C,0,-1.642975,-1.16265,0.353795\O,0,-1.258277,-0.005173,1.14
0061\C,0,-0.04796,0.533961,0.647213\H,0,-2.039263,-1.894434,1.077279\H
,0,0.438613,1.013242,1.508648\C,0,2.676047,0.397343,-0.833324\C,0,-0.3
67942,-1.617939,-0.267461\C,0,0.738188,-0.683531,0.070465\O,0,1.540948
,-0.427401,-1.071302\H,0,2.362367,1.388094,-0.475414\H,0,1.378928,-1.0
87078,0.876638\O,0,-0.22897,1.473851,-0.380409\C,0,-0.856061,2.67189,0

.056255\H,0,-0.898295,3.337696,-0.808898\H,0,-1.871812,2.484083,0.4235
15\H,0,-0.275137,3.156509,0.856462\C,0,-2.761379,-0.821096,-0.649608\H
,0,-2.961574,-1.7192,-1.250308\H,0,-2.381469,-0.055043,-1.334578\C,0,-
4.048186,-0.349507,0.032928\H,0,-4.81328,-0.089615,-0.707015\H,0,-3.85
8643,0.532783,0.652656\H,0,-4.462929,-1.130525,0.682672\H,0,3.135122,0
.537691,-1.817866\C,0,3.658956,-0.184031,0.09349\C,0,4.465572,-0.65677
,0.858543\H,0,5.183548,-1.075596,1.526874\H,0,-0.251349,-2.494836,-0.8
9125\\Version=IA32L-G03RevD.01\State=2-A\HF=-615.7779406\S2=0.754115\S
2-1=0.\S2A=0.750012\RMSD=9.385e-09\Thermal=0.\Dipole=-0.0141637,0.1669
014,0.2897763\PG=C01 [X(C10H15O3)]\\@

ShaC2alpha_024_sp.log

1\1\GINC-NODE-31\SP\UB3LYP\6-311+G(d,p)\C10H15O3(2)\ZIP06\01-Jun-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC2alpha_02
4 sp\\0,2\C,0,-1.769439,-0.656236,0.761945\O,0,-1.138762,0.520649,1.32
8442\C,0,0.0725,0.791535,0.653632\H,0,-2.185536,-1.215914,1.615825\H,0
,0.711623,1.310885,1.381787\C,0,2.587176,0.027403,-0.985131\C,0,-0.647
202,-1.387507,0.107555\C,0,0.611919,-0.602818,0.21402\O,0,1.331514,-0.
642053,-1.008205\H,0,2.447852,1.096364,-0.770578\H,0,1.259288,-0.98618
2,1.024862\O,0,-0.089378,1.58772,-0.491934\C,0,-0.519388,2.910572,-0.1
9927\H,0,0.195955,3.424211,0.461931\H,0,-0.571304,3.442125,-1.152313\H
,0,-1.506139,2.914975,0.278008\C,0,-2.934819,-0.261265,-0.166373\H,0,-
2.525569,0.30174,-1.012223\H,0,-3.58274,0.421975,0.39781\C,0,-3.744092
,-1.464802,-0.65813\H,0,-4.146045,-2.047064,0.180852\H,0,-3.133703,-2.
138096,-1.270892\H,0,-4.591769,-1.139826,-1.270921\H,0,2.969077,-0.051
941,-2.00865\C,0,3.561096,-0.550129,-0.046496\C,0,4.360829,-1.017558,0
.728982\H,0,5.07213,-1.434044,1.405855\H,0,-0.711593,-2.364912,-0.3521
79\\Version=IA32L-G03RevD.01\State=2-A\HF=-615.7777136\S2=0.754115\S2-
1=0.\S2A=0.750012\RMSD=8.998e-09\Thermal=0.\Dipole=0.0018882,0.1953579
,0.2546716\PG=C01 [X(C10H15O3)]\\@

ShaC2alpha_060_sp.log

1\1\GINC-NODE-28\SP\UB3LYP\6-311+G(d,p)\C10H15O3(2)\ZIP06\31-May-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC2alpha_06
0 sp\\0,2\C,0,-1.159694,-1.104739,0.74074\O,0,-1.656053,0.243449,0.965
982\C,0,-0.617697,1.175635,0.74814\H,0,-1.583341,-1.717029,1.554645\H,
0,-0.851942,2.053977,1.364199\C,0,2.30776,0.582202,-0.616065\C,0,0.321
814,-0.978983,0.860167\C,0,0.677484,0.43315,1.184614\O,0,1.893886,0.97
3018,0.695242\H,0,2.89022,1.428398,-0.998249\H,0,0.762618,0.565373,2.2
76569\O,0,-0.491563,1.560709,-0.598441\C,0,-1.565585,2.366436,-1.06354
1\H,0,-2.51834,1.824672,-1.029611\H,0,-1.656821,3.285423,-0.465225\H,0
,-1.335043,2.634379,-2.097259\C,0,-1.662849,-1.674037,-0.598369\H,0,-1

.206252,-2.663754,-0.737049\H,0,-1.289748,-1.032923,-1.404725\C,0,-3.1
88748,-1.785488,-0.660993\H,0,-3.656406,-0.808108,-0.505055\H,0,-3.569
544,-2.464841,0.111911\H,0,-3.515282,-2.169802,-1.633629\H,0,1.44556,0
.452082,-1.276887\C,0,3.14585,-0.625179,-0.615588\C,0,3.847353,-1.6086
03,-0.631228\H,0,4.468876,-2.475112,-0.640252\H,0,1.011169,-1.812508,0
.891083\\Version=IA32L-G03RevD.01\State=2-A\HF=-615.7766876\S2=0.75411
\S2-1=0.\S2A=0.750012\RMSD=4.873e-09\Thermal=0.\Dipole=-0.4476122,-0.2
676776,-0.2705621\PG=C01 [X(C10H15O3)]\\@

ShaC2alpha_009_sp.log

1\1\GINC-NODE-25\SP\UB3LYP\6-311+G(d,p)\C10H15O3(2)\ZIP06\31-May-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC2alpha_00
9 sp\\0,2\C,0,1.889987,-1.05143,-0.353468\O,0,1.65371,0.202432,-1.0453
47\C,0,0.30543,0.596267,-0.885918\H,0,2.54946,-1.636145,-1.016254\H,0,
0.061316,1.19074,-1.778293\C,0,-2.706159,0.072803,-0.442137\C,0,0.5352
77,-1.658359,-0.231442\C,0,-0.499927,-0.735299,-0.767131\O,0,-1.63738,
-0.713208,0.073604\H,0,-2.904026,-0.196699,-1.4947\H,0,-0.81534,-1.028
001,-1.790618\O,0,0.072172,1.354725,0.270515\C,0,0.685832,2.636248,0.2
38967\H,0,1.778575,2.558431,0.197166\H,0,0.339872,3.221628,-0.627257\H
,0,0.390745,3.147829,1.157877\C,0,2.620782,-0.834484,0.985288\H,0,2.70
9339,-1.81032,1.482632\H,0,1.987488,-0.206829,1.621724\C,0,4.007368,-0
.208554,0.811409\H,0,4.489354,-0.046497,1.781856\H,0,3.938884,0.756716
,0.2994\H,0,4.663695,-0.855789,0.216092\H,0,-2.439463,1.139394,-0.4188
8\C,0,-3.910161,-0.152491,0.354671\C,0,-4.922482,-0.314202,0.990593\H,
0,-5.808795,-0.467526,1.563352\H,0,0.315198,-2.621514,0.210733\\Versio
n=IA32L-G03RevD.01\State=2-A\HF=-615.7762117\S2=0.754102\S2-1=0.\S2A=0
.750012\RMSD=8.659e-09\Thermal=0.\Dipole=0.2185375,0.1943818,-0.394089
2\PG=C01 [X(C10H15O3)]\\@

ShaC2alpha_066_sp.log

1\1\GINC-NODE-31\SP\UB3LYP\6-311+G(d,p)\C10H15O3(2)\ZIP06\31-May-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC2alpha_06
6 sp\\0,2\C,0,1.161778,1.142508,0.789245\O,0,1.895944,-0.106272,0.9013
19\C,0,1.030479,-1.191853,0.645418\H,0,1.512143,1.774964,1.621846\H,0,
1.443257,-2.054656,1.18505\C,0,-2.003598,-1.026398,-0.587416\C,0,-0.26
6801,0.748509,0.965692\C,0,-0.354478,-0.726269,1.177899\O,0,-1.480562,
-1.430625,0.680271\H,0,-2.465864,-1.927552,-1.006439\H,0,-0.369942,-0.
956122,2.256679\O,0,0.91759,-1.498849,-0.722491\C,0,2.108076,-2.037777
,-1.281906\H,0,2.405751,-2.959919,-0.760391\H,0,1.888611,-2.272436,-2.
326051\H,0,2.934381,-1.319046,-1.232392\C,0,1.503394,1.858854,-0.53059
9\H,0,2.596576,1.941609,-0.583759\H,0,1.18679,1.219762,-1.362253\C,0,0
.864204,3.246234,-0.643274\H,0,-0.230015,3.18498,-0.654593\H,0,1.17700

5,3.744518,-1.567137\H,0,1.156393,3.891126,0.195226\H,0,-1.1996,-0.724
243,-1.265075\C,0,-3.015731,0.03414,-0.480795\C,0,-3.861362,0.894342,-
0.412529\H,0,-4.609586,1.651321,-0.346364\H,0,-1.085431,1.437931,1.122
46\\Version=IA32L-G03RevD.01\State=2-A\HF=-615.7764714\S2=0.754105\S2-
1=0.\S2A=0.750012\RMSD=4.312e-09\Thermal=0.\Dipole=0.3772677,0.391572,
-0.2728041\PG=C01 [X(C10H15O3)]\\@

ShaC2alpha_010_sp.log

1\1\GINC-NODE-31\SP\UB3LYP\6-311+G(d,p)\C10H15O3(2)\ZIP06\01-Jun-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC2alpha_01
0 sp\\0,2\C,0,1.747135,-0.855984,-0.690531\O,0,1.541636,0.549057,-0.46
3102\C,0,0.184783,0.905969,-0.714594\H,0,2.363247,-0.976697,-1.601486\
H,0,0.112886,1.293869,-1.749018\C,0,-2.412114,-0.015036,1.024804\C,0,0
.378624,-1.421228,-0.88282\C,0,-0.6519,-0.392968,-0.581399\O,0,-1.1500
17,-0.622872,0.744\H,0,-2.369507,1.064892,0.841623\H,0,-1.492665,-0.39
5649,-1.289096\O,0,-0.242858,1.879849,0.180017\C,0,0.434106,3.123035,0
.042517\H,0,1.493359,3.0287,0.305363\H,0,0.35222,3.50819,-0.985411\H,0
,-0.052577,3.821082,0.727574\C,0,2.521952,-1.459002,0.496423\H,0,2.632
723,-2.537201,0.317327\H,0,1.904206,-1.341079,1.394139\C,0,3.894956,-0
.812498,0.698007\H,0,3.791996,0.261594,0.879156\H,0,4.531217,-0.946658
,-0.185863\H,0,4.414031,-1.256387,1.55475\H,0,-2.564006,-0.165133,2.09
9208\C,0,-3.527349,-0.611896,0.275211\C,0,-4.440304,-1.094494,-0.35198
\H,0,-5.251036,-1.52579,-0.89427\H,0,0.164489,-2.477393,-0.995151\\Ver
sion=IA32L-G03RevD.01\State=2-A\HF=-615.7761967\S2=0.75402\S2-1=0.\S2A
=0.750012\RMSD=6.115e-09\Thermal=0.\Dipole=-0.0134656,0.112872,-0.5547
194\PG=C01 [X(C10H15O3)]\\@

ShaC2alpha_014_sp.log

1\1\GINC-NODE-31\SP\UB3LYP\6-311+G(d,p)\C10H15O3(2)\ZIP06\01-Jun-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC2alpha_01
4 sp\\0,2\C,0,2.050048,-0.456908,-0.660523\O,0,1.615961,0.880213,-1.01
7498\C,0,0.238814,1.029093,-0.739849\H,0,2.759377,-0.763257,-1.446785\
H,0,-0.126903,1.792504,-1.441716\C,0,-2.650897,0.000004,-0.415219\C,0,
0.796583,-1.263057,-0.693048\C,0,-0.376051,-0.387595,-0.960683\O,0,-1.
467811,-0.739307,-0.132364\H,0,-2.858715,-0.013654,-1.499773\H,0,-0.69
5532,-0.45162,-2.022059\O,0,-0.029638,1.424528,0.579081\C,0,0.430653,2
.736011,0.877614\H,0,1.520044,2.809374,0.781683\H,0,-0.034748,3.48114,
0.213692\H,0,0.138322,2.943515,1.909422\C,0,2.799299,-0.450897,0.68667
2\H,0,2.097326,-0.144618,1.469799\H,0,3.575638,0.322411,0.622533\C,0,3
.433281,-1.802932,1.026427\H,0,4.129304,-2.127569,0.242504\H,0,2.67534
8,-2.585432,1.146852\H,0,3.996233,-1.743587,1.96407\H,0,-2.523059,1.05
0676,-0.116964\C,0,-3.779843,-0.583685,0.305897\C,0,-4.734927,-1.03828

2,0.88599\H,0,-5.568914,-1.451555,1.40635\H,0,0.72641,-2.332327,-0.543
031\\Version=IA32L-G03RevD.01\State=2-A\HF=-615.7759469\S2=0.754103\S2
-1=0.\S2A=0.750012\RMSD=8.169e-09\Thermal=0.\Dipole=0.2011217,0.301639
8,-0.3103267\PG=C01 [X(C10H15O3)]\\@

ShaC2alpha_090_sp.log

1\1\GINC-NODE-21\SP\UB3LYP\6-311+G(d,p)\C10H15O3(2)\ZIP06\01-Jun-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC2alpha_09
0 sp\\0,2\C,0,1.741855,-0.871783,-0.697742\O,0,1.5494,0.541595,-0.5118
66\C,0,0.187586,0.903919,-0.725761\H,0,2.367637,-1.021337,-1.597049\H,
0,0.09427,1.305496,-1.752747\C,0,-2.405038,-0.003565,1.026041\C,0,0.37
0202,-1.427754,-0.889566\C,0,-0.65284,-0.39285,-0.586358\O,0,-1.147283
,-0.61845,0.741295\H,0,-2.356441,1.076257,0.843622\H,0,-1.49674,-0.393
16,-1.290316\O,0,-0.217785,1.868715,0.190141\C,0,0.457659,3.112362,0.0
50311\H,0,1.522934,3.013332,0.285792\H,0,0.351312,3.509661,-0.970773\H
,0,-0.010573,3.8033,0.755193\C,0,2.495142,-1.4531,0.514498\H,0,2.59651
2,-2.536632,0.364125\H,0,1.867261,-1.306181,1.400842\C,0,3.872316,-0.8
16074,0.717451\H,0,3.778543,0.263433,0.869127\H,0,4.518568,-0.979972,-
0.154083\H,0,4.375319,-1.242751,1.592343\H,0,-2.555054,-0.153526,2.100
727\C,0,-3.525762,-0.593427,0.279053\C,0,-4.444044,-1.072774,-0.342817
\H,0,-5.259048,-1.499074,-0.882661\H,0,0.148392,-2.483447,-0.991373\\V
ersion=IA32L-G03RevD.01\State=2-A\HF=-615.7760844\S2=0.754011\S2-1=0.\
S2A=0.750012\RMSD=6.391e-09\Thermal=0.\Dipole=-0.0314102,0.1093237,-0.
5314063\PG=C01 [X(C10H15O3)]\\@

ShaC2alpha_051_sp.log

1\1\GINC-NODE-21\SP\UB3LYP\6-311+G(d,p)\C10H15O3(2)\ZIP06\01-Jun-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC2alpha_05
1 sp\\0,2\C,0,-1.563556,-1.092584,0.550265\O,0,-1.752028,0.289248,0.96
2775\C,0,-0.520408,0.979513,0.894474\H,0,-2.14975,-1.698176,1.261673\H
,0,-0.580708,1.797238,1.624846\C,0,2.23259,0.0595,-0.510625\C,0,-0.098
923,-1.327744,0.705615\C,0,0.549828,-0.092122,1.240569\O,0,1.888197,0.
179765,0.87464\H,0,2.115099,1.027748,-1.010076\H,0,0.599509,-0.140579,
2.34137\O,0,-0.249967,1.498368,-0.383313\C,0,-1.099557,2.577157,-0.750
919\H,0,-2.148145,2.261536,-0.804689\H,0,-1.013838,3.408265,-0.034903\
H,0,-0.769977,2.917782,-1.735133\C,0,-2.121669,-1.338963,-0.863698\H,0
,-1.900374,-2.379798,-1.137997\H,0,-1.573302,-0.698676,-1.563585\C,0,-
3.627615,-1.079322,-0.959879\H,0,-3.863661,-0.052177,-0.664496\H,0,-4.
18952,-1.753646,-0.301584\H,0,-3.988398,-1.233498,-1.982741\H,0,1.5554
03,-0.645415,-1.012609\C,0,3.613487,-0.410763,-0.624811\C,0,4.750978,-
0.793566,-0.753743\H,0,5.757196,-1.131672,-0.854592\H,0,0.36992,-2.304
603,0.678211\\Version=IA32L-G03RevD.01\State=2-A\HF=-615.7759745\S2=0.

754063\S2-1=0.\S2A=0.750012\RMSD=7.154e-09\Thermal=0.\Dipole=-0.650918
3,-0.1636545,-0.311161\PG=C01 [X(C10H15O3)]\\@

ShaC2alpha_013_sp.log

1\1\GINC-NODE-28\SP\UB3LYP\6-311+G(d,p)\C10H15O3(2)\ZIP06\31-May-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC2alpha_01
3 sp\\0,2\C,0,1.712513,-1.143175,-0.800023\O,0,1.346443,0.156806,-1.32
5133\C,0,0.122866,0.619101,-0.787038\H,0,1.933595,-1.76936,-1.682199\H
,0,-0.410387,1.104647,-1.6179\C,0,-2.460783,0.330715,0.949746\C,0,0.49
2003,-1.619144,-0.094828\C,0,-0.617202,-0.641228,-0.234126\O,0,-1.2864
16,-0.472718,1.007023\H,0,-2.215667,1.343349,0.601307\H,0,-1.35304,-0.
969326,-0.991802\O,0,0.292581,1.54533,0.253718\C,0,0.852543,2.776963,-
0.184002\H,0,1.862992,2.636805,-0.585265\H,0,0.225178,3.245128,-0.9584
65\H,0,0.892887,3.432004,0.689368\C,0,3.005257,-1.081321,0.038566\H,0,
3.772,-0.605242,-0.586118\H,0,3.336805,-2.116651,0.201293\C,0,2.882677
,-0.354925,1.379792\H,0,2.182112,-0.868766,2.047275\H,0,2.511389,0.664
322,1.244954\H,0,3.856105,-0.306823,1.880762\H,0,-2.796129,0.415443,1.
988978\C,0,-3.537014,-0.24007,0.125783\C,0,-4.420247,-0.704642,-0.5551
24\H,0,-5.205295,-1.116798,-1.14793\H,0,0.390911,-2.577715,0.3984\\Ver
sion=IA32L-G03RevD.01\State=2-A\HF=-615.775944\S2=0.754137\S2-1=0.\S2A
=0.750012\RMSD=7.706e-09\Thermal=0.\Dipole=-0.0907861,0.0923477,-0.375
2549\PG=C01 [X(C10H15O3)]\\@

ShaC2alpha_028_sp.log

1\1\GINC-NODE-25\SP\UB3LYP\6-311+G(d,p)\C10H15O3(2)\ZIP06\01-Jun-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC2alpha_02
8 sp\\0,2\C,0,1.713252,-1.1425,-0.801199\O,0,1.348087,0.15821,-1.32490
3\C,0,0.123902,0.620032,-0.787904\H,0,1.936752,-1.767003,-1.683893\H,0
,-0.408346,1.106061,-1.619126\C,0,-2.459576,0.329815,0.950549\C,0,0.49
1124,-1.619925,-0.099779\C,0,-0.617011,-0.640461,-0.236572\O,0,-1.2848
39,-0.47327,1.005643\H,0,-2.215239,1.342904,0.602941\H,0,-1.354068,-0.
966619,-0.9938\O,0,0.29229,1.545891,0.253483\C,0,0.853267,2.777499,-0.
182952\H,0,0.227191,3.246194,-0.958134\H,0,0.892518,3.432154,0.690741\
H,0,1.864223,2.637187,-0.582802\C,0,3.003752,-1.082012,0.040935\H,0,3.
772471,-0.605682,-0.58112\H,0,3.334306,-2.11771,0.203312\C,0,2.878089,
-0.357166,1.382672\H,0,3.849956,-0.311692,1.886869\H,0,2.174315,-0.870
464,2.04718\H,0,2.509216,0.66297,1.248055\H,0,-2.79369,0.413258,1.9902
68\C,0,-3.536521,-0.240382,0.127133\C,0,-4.419871,-0.703836,-0.554384\
H,0,-5.205303,-1.115376,-1.147087\H,0,0.388955,-2.579216,0.391813\\Ver
sion=IA32L-G03RevD.01\State=2-A\HF=-615.7759423\S2=0.754138\S2-1=0.\S2
A=0.750012\RMSD=7.732e-09\Thermal=0.\Dipole=-0.0907994,0.0923706,-0.37
48343\PG=C01 [X(C10H15O3)]\\@

ShaC2alpha_057_sp.log

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1\1\GINC-NODE-25\SP\UB3LYP\6-311+G(d,p)\C10H15O3(2)\ZIP06\01-Jun-2010\
 0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC2alpha_05
 7 sp\\0,2\C,0,-1.779482,-0.68633,0.691575\O,0,-1.863139,0.755349,0.848
 102\C,0,-0.580215,1.326942,0.692961\H,0,-2.435981,-1.113607,1.467431\H
 ,0,-0.586719,2.266607,1.261058\C,0,2.098475,-0.05707,-0.449451\C,0,-0.
 344514,-1.00266,0.954035\C,0,0.39628,0.259918,1.259876\O,0,1.756041,0.
 350227,0.880416\H,0,2.0345,0.797904,-1.13164\H,0,0.434069,0.417173,2.3
 50748\O,0,-0.251774,1.58232,-0.649739\C,0,-1.023439,2.624995,-1.232448
 \H,0,-2.090795,2.375409,-1.240798\H,0,-0.882114,3.570763,-0.688056\H,0
 ,-0.667582,2.745831,-2.258096\C,0,-2.320244,-1.118402,-0.684446\H,0,-1
 .679063,-0.68274,-1.458683\H,0,-3.315768,-0.670648,-0.798521\C,0,-2.40
 6461,-2.638932,-0.844257\H,0,-1.417215,-3.107618,-0.785438\H,0,-2.8400
 01,-2.904495,-1.814317\H,0,-3.036485,-3.088302,-0.066295\H,0,1.386284,
 -0.811906,-0.811733\C,0,3.45257,-0.610933,-0.449862\C,0,4.568678,-1.06
 9132,-0.486993\H,0,5.555972,-1.471341,-0.507799\H,0,0.041983,-1.996576
 ,1.145967\\Version=IA32L-G03RevD.01\State=2-A\HF=-615.7757663\S2=0.754
 067\S2-1=0.\S2A=0.750012\RMSD=6.829e-09\Thermal=0.\Dipole=-0.6750784,-
 0.2027118,-0.3084708\PG=C01 [X(C10H15O3)]\\@
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ShaC2alpha_005_sp.log

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1\1\GINC-NODE-28\SP\UB3LYP\6-311+G(d,p)\C10H15O3(2)\ZIP06\01-Jun-2010\
 0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC2alpha_00
 5 sp\\0,2\C,0,-1.881236,-0.870276,0.474457\O,0,-1.216068,0.255919,1.10
 3376\C,0,0.101418,0.373954,0.592688\H,0,-2.465865,-1.35483,1.274642\H,
 0,0.686834,0.879745,1.37016\C,0,2.845141,-1.206879,-0.340433\C,0,-0.76
 1092,-1.731958,0.00022\C,0,0.544932,-1.093412,0.316648\O,0,1.482701,-1
 .276803,-0.731438\H,0,3.411392,-1.545876,-1.214718\H,0,0.971288,-1.498
 242,1.256516\O,0,0.167798,1.084802,-0.610475\C,0,-0.036467,2.479915,-0
 .453728\H,0,-1.030841,2.701216,-0.045867\H,0,0.726229,2.918636,0.20764
 2\H,0,0.055586,2.924966,-1.447344\C,0,-2.858386,-0.415205,-0.62644\H,0
 ,-3.282989,-1.314724,-1.093869\H,0,-2.282396,0.107167,-1.397509\C,0,-3
 .980425,0.476929,-0.089072\H,0,-3.567464,1.364584,0.400444\H,0,-4.5939
 15,-0.056077,0.648381\H,0,-4.641879,0.807784,-0.897452\H,0,3.044131,-1
 .919556,0.478071\C,0,3.319325,0.125101,0.064248\C,0,3.74715,1.197737,0
 .418176\H,0,4.120481,2.152024,0.713944\H,0,-0.868198,-2.693591,-0.4853
 35\\Version=IA32L-G03RevD.01\State=2-A\HF=-615.7754552\S2=0.754139\S2-
 1=0.\S2A=0.750012\RMSD=4.087e-09\Thermal=0.\Dipole=0.1590917,-0.081320
 5,0.3283587\PG=C01 [X(C10H15O3)]\\@
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ShaC2alpha_002_sp.log

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1\1\GINC-NODE-28\SP\UB3LYP\6-311+G(d,p)\C10H15O3(2)\ZIP06\01-Jun-2010\
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0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC2alpha_00
2 sp\\0,2\C,0,-1.398863,-1.199949,0.386208\O,0,-1.305619,0.034683,1.14
5457\C,0,-0.252097,0.828102,0.628616\H,0,-1.60325,-1.989058,1.129599\H
,0,0.081858,1.472424,1.452958\C,0,2.852562,-0.377406,-1.05537\C,0,-0.0
48304,-1.349104,-0.230477\C,0,0.813424,-0.196355,0.171283\O,0,1.652615
,0.349316,-0.837923\H,0,3.315879,0.089497,-1.931257\H,0,1.431604,-0.44
7109,1.052648\O,0,-0.635029,1.605251,-0.470424\C,0,-1.501319,2.676537,
-0.128871\H,0,-2.453326,2.314563,0.279155\H,0,-1.032567,3.347114,0.607
89\H,0,-1.688635,3.234381,-1.049335\C,0,-2.5683,-1.168207,-0.615348\H,
0,-2.54775,-2.107008,-1.186633\H,0,-2.386452,-0.355253,-1.326466\C,0,-
3.929171,-1.00002,0.065877\H,0,-3.956896,-0.078115,0.65541\H,0,-4.1402
99,-1.836257,0.744361\H,0,-4.736713,-0.957761,-0.673431\H,0,2.640031,-
1.425634,-1.320333\C,0,3.788967,-0.343685,0.079252\C,0,4.556471,-0.318
966,1.011519\H,0,5.239228,-0.291087,1.830498\H,0,0.261333,-2.190388,-0
.838086\\Version=IA32L-G03RevD.01\State=2-A\HF=-615.7752422\S2=0.75412
2\S2-1=0.\S2A=0.750012\RMSD=6.694e-09\Thermal=0.\Dipole=0.1105296,-0.4
508317,0.0930066\PG=C01 [X(C10H15O3)]\\@

ShaC2alpha_006_sp.log

1\1\GINC-NODE-21\SP\UB3LYP\6-311+G(d,p)\C10H15O3(2)\ZIP06\01-Jun-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC2alpha_00
6 sp\\0,2\C,0,-1.938534,-0.255868,0.761806\O,0,-1.015085,0.74933,1.251
094\C,0,0.248119,0.573713,0.633046\H,0,-2.535832,-0.568555,1.634747\H,
0,0.987982,1.003093,1.319534\C,0,2.540125,-1.590319,-0.372078\C,0,-1.0
52724,-1.352536,0.274745\C,0,0.37508,-0.965884,0.440868\O,0,1.163507,-
1.395696,-0.657295\H,0,2.950295,-2.078309,-1.262903\H,0,0.79639,-1.388
904,1.374776\O,0,0.337767,1.180119,-0.62446\C,0,0.372875,2.59755,-0.56
3193\H,0,0.464284,2.9545,-1.591778\H,0,-0.541236,3.00533,-0.114104\H,0
,1.241101,2.947084,0.016386\C,0,-2.899901,0.338815,-0.28582\H,0,-2.311
05,0.65616,-1.15283\H,0,-3.343223,1.240666,0.155733\C,0,-4.004008,-0.6
34925,-0.707876\H,0,-4.590003,-0.97574,0.155268\H,0,-3.592703,-1.52143
5,-1.204472\H,0,-4.696712,-0.157367,-1.409231\H,0,2.659765,-2.290685,0
.472057\C,0,3.304975,-0.367218,-0.086704\C,0,3.963924,0.612707,0.16683
4\H,0,4.542314,1.48445,0.37428\H,0,-1.380474,-2.316517,-0.091949\\Vers
ion=IA32L-G03RevD.01\State=2-A\HF=-615.7752559\S2=0.754136\S2-1=0.\S2A
=0.750012\RMSD=8.011e-09\Thermal=0.\Dipole=0.1210993,-0.0953652,0.3153
022\PG=C01 [X(C10H15O3)]\\@

ShaC2alpha_019_sp.log

1\1\GINC-NODE-28\SP\UB3LYP\6-311+G(d,p)\C10H15O3(2)\ZIP06\01-Jun-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC2alpha_01
9 sp\\0,2\C,0,1.891606,-0.729617,-0.934997\O,0,1.692837,0.64128,-0.552

733\C,0,0.326218,1.013733,-0.705052\H,0,2.409402,-0.750386,-1.912833\H
,0,0.207346,1.505022,-1.689932\C,0,-2.261586,-0.036575,0.970686\C,0,0.
516191,-1.298199,-1.059794\C,0,-0.508494,-0.296603,-0.665678\O,0,-1.00
6226,-0.630865,0.63656\H,0,-2.209688,1.053996,0.872801\H,0,-1.353791,-
0.241244,-1.366652\O,0,-0.058593,1.88908,0.303727\C,0,0.604596,3.14672
2,0.255636\H,0,0.159438,3.764406,1.039007\H,0,1.678487,3.035725,0.4407
52\H,0,0.456943,3.636454,-0.719064\C,0,2.812641,-1.42222,0.08965\H,0,3
.783586,-0.911135,0.059322\H,0,2.988127,-2.448336,-0.261923\C,0,2.2636
46,-1.424939,1.518018\H,0,1.304813,-1.950213,1.57817\H,0,2.097476,-0.4
01124,1.865357\H,0,2.968484,-1.91212,2.200978\H,0,-2.409705,-0.268907,
2.030824\C,0,-3.38541,-0.563428,0.182513\C,0,-4.306172,-0.988332,-0.47
4284\H,0,-5.123719,-1.369557,-1.043209\H,0,0.29923,-2.34179,-1.254216\
\Version=IA32L-G03RevD.01\State=2-A\HF=-615.7754227\S2=0.754069\S2-1=0
.\S2A=0.750012\RMSD=9.053e-09\Thermal=0.\Dipole=-0.0562715,0.1810392,-
0.5824992\PG=C01 [X(C10H15O3)]\\@

30b

TSC2alpha_001_sp.log

1\1\GINC-NODE-25\SP\UB3LYP\6-311+G(d,p)\C10H15O3(2)\ZIP06\04-Jun-2010\
0\\#P UBecke3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) TSC2alpha
_001 sp\\0,2\C,0,1.753735,-1.387292,-0.621587\C,0,2.415938,-0.055214,-
0.619961\O,0,2.28036,0.662885,0.601152\C,0,1.005348,0.542238,1.206389\
C,0,0.416173,-0.834816,1.139891\C,0,-0.138227,1.420519,0.62584\O,0,-1.
324506,0.722562,0.933704\C,0,-1.071628,-0.710711,0.949593\O,0,0.0598,1
.592763,-0.755557\C,0,-0.884197,2.46691,-1.358167\C,0,-1.667442,-1.390
77,-0.292217\C,0,1.621503,-2.529686,-1.061875\H,0,1.171748,0.858538,2.
246235\H,0,2.016667,0.531618,-1.453722\H,0,3.493422,-0.187074,-0.76356
7\H,0,1.301585,-3.526232,-1.272026\H,0,-1.602466,-1.09143,1.83659\H,0,
-1.399653,-2.455273,-0.255753\H,0,-1.179067,-0.973995,-1.178909\H,0,-0
.222586,2.403883,1.109145\H,0,-0.854514,3.462864,-0.890446\H,0,-0.6042
85,2.557604,-2.410261\H,0,-1.903594,2.070545,-1.283025\C,0,-3.187606,-
1.232725,-0.380353\H,0,-3.46928,-0.175006,-0.398325\H,0,-3.580192,-1.7
06171,-1.287219\H,0,-3.686925,-1.695458,0.480462\H,0,0.81233,-1.630802
,1.761105\\Version=IA32L-G03RevD.01\State=2-A\HF=-615.7642868\S2=0.772
673\S2-1=0.\S2A=0.750182\RMSD=5.722e-09\Thermal=0.\Dipole=-0.4219929,-
0.2669273,-0.1178852\PG=C01 [X(C10H15O3)]\\@

TSC2alpha_002_sp.log

1\1\GINC-NODE-28\SP\UB3LYP\6-311+G(d,p)\C10H15O3(2)\ZIP06\04-Jun-2010\
0\\#P UBecke3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) TSC2alpha
_002 sp\\0,2\C,0,-0.471115,1.987059,0.55012\C,0,1.001523,2.155723,0.41
1498\O,0,1.538317,1.652543,-0.805877\C,0,0.924329,0.4625,-1.261546\C,0

,-0.568993,0.440721,-1.116421\C,0,1.340151,-0.86201,-0.566513\O,0,0.25
048,-1.731986,-0.770937\C,0,-0.991489,-0.979756,-0.842798\O,0,1.598151
,-0.615985,0.793576\C,0,2.053721,-1.763202,1.497389\C,0,-1.851509,-1.2
38756,0.403101\C,0,-1.533116,2.307497,1.087735\H,0,1.225687,0.391101,-
2.317003\H,0,1.485608,1.674969,1.267728\H,0,1.243966,3.223609,0.420437
\H,0,-2.547506,2.392318,1.408756\H,0,-1.531069,-1.383772,-1.715025\H,0
,-1.370677,-0.767988,1.266478\H,0,-1.852116,-2.322439,0.57569\H,0,2.21
5,-1.343313,-1.02561\H,0,2.987173,-2.149927,1.060392\H,0,2.244208,-1.4
47895,2.525838\H,0,1.301971,-2.56081,1.490545\C,0,-3.290254,-0.739205,
0.244443\H,0,-3.790828,-1.22798,-0.600946\H,0,-3.878679,-0.950929,1.14
4023\H,0,-3.322438,0.342008,0.071133\H,0,-1.185362,1.071037,-1.748586\
\Version=IA32L-G03RevD.01\State=2-A\HF=-615.7633766\S2=0.773445\S2-1=0
.\S2A=0.750191\RMSD=6.525e-09\Thermal=0.\Dipole=-0.4231821,-0.2856628,
0.1695321\PG=C01 [X(C10H15O3)]\\@

31b

cShaC2alpha_010_sp.log

1\1\GINC-NODE-28\SP\UB3LYP\6-311+G(d,p)\C10H15O3(2)\ZIP06\05-Jun-2010\
0\\#P UBecke3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) cShaC2alp
ha_010 sp\\0,2\C,0,-0.874344,-0.826588,0.867118\O,0,-1.226053,0.57101,
1.057335\C,0,-0.151611,1.398124,0.680678\H,0,-1.272673,-1.337655,1.751
873\H,0,-0.285347,2.343746,1.224238\C,0,2.285999,-0.053375,-0.774577\C
,0,1.474884,-1.280669,-0.332602\C,0,0.683189,-0.869942,0.909067\C,0,1.
110077,0.607987,1.101883\O,0,2.276876,0.835618,0.340436\H,0,3.329059,-
0.290878,-1.005184\H,0,1.81818,0.418593,-1.646699\H,0,1.004292,-1.4904
7,1.750197\H,0,1.343979,0.853001,2.142006\C,0,1.517353,-2.470041,-0.87
9955\H,0,2.017646,-2.954987,-1.708247\O,0,-0.093131,1.64871,-0.70162\C
,0,-1.157983,2.459741,-1.177241\H,0,-0.975051,2.62933,-2.240866\H,0,-2
.129528,1.968257,-1.046633\H,0,-1.177496,3.429217,-0.656652\C,0,-1.553
805,-1.40201,-0.375353\H,0,-1.220443,-2.440616,-0.498762\H,0,-1.201959
,-0.855415,-1.256979\C,0,-3.081787,-1.347999,-0.285113\H,0,-3.542821,-
1.745748,-1.196019\H,0,-3.451161,-1.940957,0.561252\H,0,-3.430055,-0.3
19494,-0.146166\\Version=IA32L-G03RevD.01\State=2-A\HF=-615.8052404\S2
=0.760436\S2-1=0.\S2A=0.750049\RMSD=7.942e-09\Thermal=0.\Dipole=-0.221
5869,-0.1289065,-0.2107877\PG=C01 [X(C10H15O3)]\\@

cShaC2alpha_001_sp.log

1\1\GINC-NODE-31\SP\UB3LYP\6-311+G(d,p)\C10H15O3(2)\ZIP06\05-Jun-2010\
0\\#P UBecke3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) Z-Butene
sp\\0,2\C,0,-0.921827,0.799554,0.639631\O,0,0.274009,1.11596,-0.077712
\C,0,1.33365,0.419171,0.576019\H,0,-0.901437,1.322841,1.614159\H,0,1.6
39061,1.009079,1.463791\C,0,0.118569,-2.065107,-0.882963\C,0,-1.194216

,-1.647312,-0.217845\C,0,-0.804036,-0.720924,0.931579\C,0,0.736327,-0.
946946,1.029792\O,0,1.068756,-2.026717,0.17412\H,0,0.104168,-3.078334,
-1.292323\H,0,0.389796,-1.354417,-1.677781\H,0,-1.342867,-0.98637,1.84
4562\H,0,1.095419,-1.211739,2.027622\C,0,-2.39865,-2.060514,-0.523631\
H,0,-2.857822,-2.714121,-1.254262\O,0,2.403639,0.236078,-0.277367\C,0,
3.065624,1.443345,-0.634976\H,0,3.932113,1.155856,-1.234741\H,0,2.4128
78,2.099129,-1.222289\H,0,3.408852,1.987065,0.258401\C,0,-2.131759,1.2
82206,-0.147663\H,0,-3.035899,0.936559,0.370788\H,0,-2.129352,0.79378,
-1.127715\C,0,-2.164647,2.805194,-0.312828\H,0,-1.269701,3.158195,-0.8
34282\H,0,-3.042066,3.116245,-0.890432\H,0,-2.208591,3.311673,0.659477
\\Version=IA32L-G03RevD.01\State=2-A\HF=-615.8041176\S2=0.760083\S2-1=
0.\S2A=0.750047\RMSD=3.771e-09\Thermal=0.\Dipole=-0.3055859,0.5006982,
0.2441362\PG=C01 [X(C10H15O3)]\\@

cShaC2alpha_002_sp.log

1\1\GINC-NODE-21\SP\UB3LYP\6-311+G(d,p)\C10H15O3(2)\ZIP06\05-Jun-2010\
0\\#P UBecke3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) cShaC2alp
ha_002 sp\\0,2\C,0,0.801017,-1.05552,0.394179\O,0,-0.463058,-1.234884,
-0.248291\C,0,-1.431093,-0.553721,0.546959\H,0,0.825737,-1.669519,1.31
4284\H,0,-1.739989,-1.228893,1.369909\C,0,-0.248076,2.043331,-0.67651\
C,0,1.101555,1.457177,-0.252206\C,0,0.794882,0.431071,0.838178\C,0,-0.
712666,0.704432,1.128747\O,0,-1.062516,1.914025,0.481926\H,0,-0.203947
,3.101529,-0.946214\H,0,-0.669648,1.469964,-1.515073\H,0,1.436643,0.58
7967,1.708412\H,0,-0.955707,0.830198,2.186848\C,0,2.282077,1.821899,-0
.68633\H,0,2.688,2.525442,-1.402009\O,0,-2.525262,-0.188627,-0.214736\
C,0,-3.288116,-1.2919,-0.688255\H,0,-3.623977,-1.927723,0.145045\H,0,-
4.160915,-0.871574,-1.193046\H,0,-2.713597,-1.902876,-1.39372\C,0,1.90
5818,-1.535266,-0.537181\H,0,1.894071,-0.923643,-1.445486\H,0,1.656176
,-2.560454,-0.837354\C,0,3.295398,-1.500521,0.10743\H,0,4.047123,-1.91
3289,-0.573818\H,0,3.596726,-0.475278,0.349686\H,0,3.325218,-2.091852,
1.031271\\Version=IA32L-G03RevD.01\State=2-A\HF=-615.8036578\S2=0.7600
99\S2-1=0.\S2A=0.750047\RMSD=5.111e-09\Thermal=0.\Dipole=0.3003078,-0.
5245311,0.1428029\PG=C01 [X(C10H15O3)]\\@

cShaC2alpha_016_sp.log

1\1\GINC-NODE-25\SP\UB3LYP\6-311+G(d,p)\C10H15O3(2)\ZIP06\05-Jun-2010\
0\\#P UBecke3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) cShaC2alp
ha_016 sp\\0,2\C,0,-0.860019,-0.86844,-0.867728\O,0,0.441785,-1.502541
,-0.99454\C,0,1.461346,-0.607627,-0.629167\H,0,-1.404382,-1.165811,-1.
772266\H,0,2.374151,-0.95364,-1.133821\C,0,0.5571,2.130905,0.69744\C,0
,-0.812241,1.567506,0.284777\C,0,-0.580551,0.666789,-0.931038\C,0,0.95
6624,0.767555,-1.12154\O,0,1.419435,1.896764,-0.413704\H,0,0.535545,3.

209097,0.883241\H,0,0.928819,1.613502,1.58918\H,0,-1.113479,1.095424,-
1.784166\H,0,1.249369,0.892139,-2.168141\C,0,-1.958354,1.89427,0.82905
6\H,0,-2.306836,2.524593,1.637236\O,0,1.677638,-0.547137,0.758954\C,0,
2.214646,-1.745834,1.300709\H,0,3.177609,-1.994248,0.829228\H,0,2.3744
69,-1.566709,2.366455\H,0,1.527741,-2.590149,1.169253\C,0,-1.608518,-1
.423627,0.34648\H,0,-1.400009,-2.500288,0.373736\H,0,-1.193273,-0.9928
06,1.263941\C,0,-3.122978,-1.199838,0.281103\H,0,-3.372422,-0.132688,0
.272675\H,0,-3.551006,-1.655651,-0.62091\H,0,-3.619479,-1.649411,1.148
127\\Version=IA32L-G03RevD.01\State=2-A\HF=-615.8037036\S2=0.760414\S2
-1=0.\S2A=0.750049\RMSD=4.687e-09\Thermal=0.\Dipole=-0.201302,-0.19973
2,0.2203137\PG=C01 [X(C10H15O3)]\\@

cShaC2alpha_023_sp.log

1\1\GINC-NODE-31\SP\UB3LYP\6-311+G(d,p)\C10H15O3(2)\ZIP06\05-Jun-2010\
0\\#P UBecke3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) cShaC2alp
ha_023 sp\\0,2\C,0,1.371864,0.051884,0.77165\O,0,0.804868,-1.256551,1.
032034\C,0,-0.553874,-1.270731,0.72462\H,0,2.111467,0.199107,1.567114\
H,0,-1.015523,-2.074746,1.314624\C,0,-1.503732,1.420849,-0.768731\C,0,
-0.202677,1.975531,-0.180987\C,0,0.185477,1.048479,0.966187\C,0,-1.067
833,0.143649,1.116605\O,0,-2.095326,0.661514,0.284351\H,0,-2.213308,2.
198819,-1.064779\H,0,-1.286421,0.779318,-1.633008\H,0,0.360433,1.64178
1,1.866788\H,0,-1.45916,0.124141,2.13827\C,0,0.411692,3.072163,-0.5497
05\H,0,0.285253,3.853179,-1.288278\O,0,-0.736703,-1.538941,-0.654644\C
,0,-1.951657,-2.207703,-0.96297\H,0,-2.036946,-3.150216,-0.400097\H,0,
-2.827165,-1.582464,-0.751963\H,0,-1.919612,-2.437958,-2.030919\C,0,2.
090949,0.088745,-0.578018\H,0,2.504352,1.096245,-0.714481\H,0,1.361148
,-0.066518,-1.380041\C,0,3.202089,-0.960177,-0.675003\H,0,3.698141,-0.
913926,-1.650833\H,0,3.967682,-0.804777,0.096035\H,0,2.79315,-1.96631,
-0.544245\\Version=IA32L-G03RevD.01\State=2-A\HF=-615.8022465\S2=0.760
349\S2-1=0.\S2A=0.750048\RMSD=3.969e-09\Thermal=0.\Dipole=-0.3323747,0
.2604119,-0.130533\PG=C01 [X(C10H15O3)]\\@

cShaC2alpha_013_sp.log

1\1\GINC-NODE-28\SP\UB3LYP\6-311+G(d,p)\C10H15O3(2)\ZIP06\05-Jun-2010\
0\\#P UBecke3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) cShaC2alp
ha_013 sp\\0,2\C,0,1.271896,-0.527092,0.599674\O,0,0.335765,-1.269764,
-0.188407\C,0,-0.952277,-1.080568,0.34603\H,0,1.446785,-1.068712,1.547
783\H,0,-1.171721,-1.863251,1.099694\C,0,-0.921195,1.824852,-0.719547\
C,0,0.490536,1.865433,-0.128403\C,0,0.534301,0.785789,0.953335\C,0,-0.
95109,0.338176,1.030896\O,0,-1.728402,1.294422,0.329344\H,0,-1.314922,
2.808781,-0.98693\H,0,-0.951307,1.165643,-1.5983\H,0,0.91065,1.20147,1
.891939\H,0,-1.351536,0.285071,2.046811\C,0,1.445397,2.706289,-0.43864

2\H,0,1.595925,3.529489,-1.125194\O,0,-1.838281,-1.195255,-0.725732\C,
0,-3.188289,-1.395277,-0.338161\H,0,-3.599764,-0.515418,0.171286\H,0,-
3.750523,-1.570889,-1.258227\H,0,-3.290156,-2.276043,0.315197\C,0,2.59
0542,-0.427085,-0.15407\H,0,3.261708,0.225784,0.419626\H,0,2.406913,0.
073893,-1.110203\C,0,3.247777,-1.791888,-0.385065\H,0,2.591496,-2.4445
67,-0.968519\H,0,4.192973,-1.682455,-0.928032\H,0,3.465235,-2.295789,0
.565149\\Version=IA32L-G03RevD.01\State=2-A\HF=-615.8015272\S2=0.76021
5\S2-1=0.\S2A=0.750048\RMSD=4.370e-09\Thermal=0.\Dipole=-0.037398,0.15
5141,0.5649994\PG=C01 [X(C10H15O3)]\\@

cShaC2alpha_004_sp.log

1\1\GINC-NODE-25\SP\UB3LYP\6-311+G(d,p)\C10H15O3(2)\ZIP06\05-Jun-2010\
0\\#P UBecke3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) cShaC2alp
ha_004 sp\\0,2\C,0,-0.089255,1.089526,0.797079\O,0,1.16309,0.46653,1.1
47206\C,0,1.183666,-0.882269,0.693878\H,0,-0.251519,1.865973,1.553466\
H,0,1.683646,-1.453477,1.490791\C,0,-2.038694,-1.215077,-0.962188\C,0,
-2.330277,-0.117337,0.078512\C,0,-1.108772,-0.071883,0.981749\C,0,-0.2
96964,-1.303302,0.52976\O,0,-0.656737,-1.513778,-0.831154\H,0,-2.65555
3,-2.104137,-0.749823\H,0,-2.221793,-0.901409,-1.99392\H,0,-1.385359,-
0.128405,2.038301\H,0,-0.520848,-2.201806,1.123468\C,0,-3.422672,0.597
942,0.182684\H,0,-4.368477,0.704346,-0.332439\O,0,1.868348,-1.056842,-
0.509789\C,0,3.268684,-0.850667,-0.395271\H,0,3.503302,0.181304,-0.107
747\H,0,3.712874,-1.534339,0.345255\H,0,3.696418,-1.061847,-1.378053\C
,0,-0.042354,1.73861,-0.590006\H,0,-1.034591,2.153705,-0.806312\H,0,0.
155509,0.963971,-1.339146\C,0,1.014992,2.842539,-0.680346\H,0,1.037634
,3.282021,-1.683705\H,0,0.809731,3.650747,0.033379\H,0,2.011292,2.4475
81,-0.458721\\Version=IA32L-G03RevD.01\State=2-A\HF=-615.8009299\S2=0.
760521\S2-1=0.\S2A=0.75005\RMSD=3.968e-09\Thermal=0.\Dipole=-0.3767318
,-0.1281707,0.1953832\PG=C01 [X(C10H15O3)]\\@

29c

ShaC3alpha_001_sp.log

1\1\GINC-NODE-21\SP\UB3LYP\6-311+G(d,p)\C11H17O3(2)\ZIP06\05-Jun-2010\
0\\#P UBecke3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC3alph
a_001 sp\\0,2\C,0,-1.21707,-1.168608,0.50684\O,0,-0.786012,-0.012021,1
.270903\C,0,0.392103,0.528578,0.707311\H,0,-1.565621,-1.903132,1.25160
1\H,0,0.929701,1.006191,1.538825\C,0,3.021211,0.401124,-0.930874\C,0,0
.017979,-1.620075,-0.193342\C,0,1.142543,-0.687198,0.0817\O,0,1.877218
,-0.427468,-1.104195\H,0,2.72474,1.389908,-0.553502\H,0,1.829233,-1.09
3365,0.847776\O,0,0.14954,1.47054,-0.305718\C,0,-0.449834,2.667896,0.1
70099\H,0,0.177363,3.149803,0.936267\H,0,-0.541757,3.336113,-0.689332\
H,0,-1.442644,2.480115,0.595681\C,0,-2.394998,-0.827147,-0.425156\H,0,

-2.063656,-0.049602,-1.12368\H,0,-2.624433,-1.720294,-1.024543\C,0,-3.
650376,-0.373539,0.329853\H,0,-3.39283,0.482502,0.965495\H,0,-3.972766
,-1.174725,1.010745\H,0,3.421935,0.544867,-1.940082\C,0,4.058346,-0.17
7651,-0.063455\C,0,4.909119,-0.647401,0.654141\H,0,5.666131,-1.064068,
1.279351\C,0,-4.805045,-0.000636,-0.604991\H,0,-5.101138,-0.850963,-1.
231892\H,0,-5.68803,0.319714,-0.040105\H,0,-4.522262,0.82008,-1.275574
\H,0,0.096204,-2.493596,-0.827714\\Version=IA32L-G03RevD.01\State=2-A\
HF=-655.1022224\S2=0.754118\S2-1=0.\S2A=0.750012\RMSD=4.550e-09\Therma
l=0.\Dipole=-0.0089692,0.1741132,0.3221462\PG=C01 [X(C11H17O3)]\\@

ShaC3alpha_003_sp.log

1\1\GINC-NODE-28\SP\UB3LYP\6-311+G(d,p)\C11H17O3(2)\ZIP06\05-Jun-2010\
0\\#P UBecke3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC3alph
a_003 sp\\0,2\C,0,-1.33912,-0.39134,1.060345\O,0,-0.581456,0.78012,1.4
57318\C,0,0.580882,0.896505,0.662476\H,0,-1.718362,-0.83511,1.995373\H
,0,1.317413,1.424339,1.284877\C,0,2.862788,-0.202235,-1.129513\C,0,-0.
329746,-1.264716,0.396712\C,0,0.981285,-0.56781,0.308296\O,0,1.566593,
-0.767713,-0.969051\H,0,2.824794,0.888345,-0.997912\H,0,1.682819,-0.92
5497,1.084871\O,0,0.374194,1.603831,-0.53318\C,0,0.063896,2.975453,-0.
325944\H,0,0.868492,3.486389,0.225747\H,0,-0.035429,3.427977,-1.315314
\H,0,-0.873936,3.094476,0.228691\C,0,-2.548504,0.005336,0.190969\H,0,-
2.175586,0.455513,-0.736481\H,0,-3.099377,0.786155,0.733265\C,0,-3.485
753,-1.167656,-0.120757\H,0,-3.810063,-1.637198,0.819402\H,0,-2.937134
,-1.939615,-0.676996\H,0,3.127885,-0.394647,-2.174728\C,0,3.885562,-0.
780074,-0.244581\C,0,4.726737,-1.249257,0.484605\H,0,5.473314,-1.66734
2,1.121297\C,0,-4.717135,-0.742262,-0.927586\H,0,-5.369999,-1.596685,-
1.139103\H,0,-5.308774,0.003948,-0.383326\H,0,-4.426221,-0.298218,-1.8
87198\H,0,-0.499848,-2.274401,0.046704\\Version=IA32L-G03RevD.01\State
=2-A\HF=-655.1019744\S2=0.754116\S2-1=0.\S2A=0.750012\RMSD=6.891e-09\T
hermal=0.\Dipole=0.0354329,0.185287,0.2316266\PG=C01 [X(C11H17O3)]\\@

ShaC3alpha_105_sp.log

1\1\GINC-NODE-25\SP\UB3LYP\6-311+G(d,p)\C11H17O3(2)\ZIP06\05-Jun-2010\
0\\#P UBecke3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC3alph
a_105 sp\\0,2\C,0,-0.918324,-0.490364,1.170083\O,0,-1.060085,0.95685,1
.147877\C,0,0.116884,1.543423,0.632964\H,0,-1.344591,-0.815036,2.13418
2\H,0,0.180782,2.549472,1.068637\C,0,2.586647,-0.007265,-0.869731\C,0,
0.554653,-0.718846,1.114857\C,0,1.263469,0.593488,1.083474\O,0,2.47975
9,0.70802,0.363473\H,0,3.278799,0.58028,-1.483822\H,0,1.544503,0.90148
5,2.104882\O,0,0.122508,1.633561,-0.770253\C,0,-0.801783,2.583006,-1.2
83246\H,0,-0.595531,3.58837,-0.886188\H,0,-0.674026,2.594291,-2.368184
\H,0,-1.835467,2.310423,-1.038932\C,0,-1.72576,-1.155051,0.040604\H,0,

-1.526782,-2.236188,0.072233\H,0,-1.343288,-0.787887,-0.919424\C,0,-3.
234511,-0.901857,0.146764\H,0,-3.412824,0.180196,0.163345\H,0,-3.59922
6,-1.287565,1.109843\H,0,1.625916,-0.033897,-1.392556\C,0,3.120699,-1.
365757,-0.698494\C,0,3.572961,-2.479306,-0.576213\H,0,3.974518,-3.4608
12,-0.46397\C,0,-4.026936,-1.544535,-0.995759\H,0,-3.887309,-2.632599,
-1.01517\H,0,-5.100633,-1.348509,-0.895912\H,0,-3.706112,-1.153897,-1.
969337\H,0,1.035816,-1.677191,1.259776\\Version=IA32L-G03RevD.01\State
=2-A\HF=-655.1009362\S2=0.754113\S2-1=0.\S2A=0.750012\RMSD=4.735e-09\T
hermal=0.\Dipole=-0.5586971,-0.1739005,-0.1353949\PG=C01 [X(C11H17O3)]
\\@

ShaC3alpha_006_sp.log

1\1\GINC-NODE-31\SP\UB3LYP\6-311+G(d,p)\C11H17O3(2)\ZIP06\05-Jun-2010\
0\\#P UBecke3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC3alph
a_006 sp\\0,2\C,0,1.377895,-0.941959,-0.163847\O,0,0.913599,0.113406,-
1.046892\C,0,-0.360493,0.564137,-0.632663\H,0,1.858544,-1.685114,-0.81
8707\H,0,-0.857134,0.934091,-1.540871\C,0,-3.117579,0.268226,0.746347\
C,0,0.129783,-1.470964,0.454632\C,0,-1.047447,-0.682649,0.003489\O,0,-
1.926205,-0.430958,1.088644\H,0,-2.876428,1.263134,0.346236\H,0,-1.604
832,-1.205889,-0.795884\O,0,-0.310333,1.584235,0.331258\C,0,0.217141,2
.805667,-0.168087\H,0,-0.372425,3.173905,-1.022145\H,0,0.157405,3.5303
61,0.647314\H,0,1.261341,2.694557,-0.483182\C,0,2.416611,-0.416717,0.8
47394\H,0,2.680937,-1.243566,1.52287\H,0,1.926135,0.350153,1.456759\C,
0,3.690267,0.154129,0.202736\H,0,4.265359,0.674215,0.980261\H,0,3.4034
15,0.91657,-0.532053\H,0,-3.640665,0.41774,1.697027\C,0,-3.991616,-0.4
51566,-0.192342\C,0,-4.708995,-1.035102,-0.969702\H,0,-5.348746,-1.552
85,-1.648111\C,0,4.589809,-0.893331,-0.464555\H,0,5.499115,-0.430864,-
0.865297\H,0,4.897806,-1.665808,0.251469\H,0,4.087402,-1.395769,-1.299
309\H,0,0.07402,-2.307554,1.139134\\Version=IA32L-G03RevD.01\State=2-A
\HF=-655.100972\S2=0.754116\S2-1=0.\S2A=0.750012\RMSD=5.385e-09\Therma
l=0.\Dipole=0.0476064,0.1819903,-0.3144683\PG=C01 [X(C11H17O3)]\\@

ShaC3alpha_013_sp.log

1\1\GINC-NODE-28\SP\UB3LYP\6-311+G(d,p)\C11H17O3(2)\ZIP06\05-Jun-2010\
0\\#P UBecke3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC3alph
a_013 sp\\0,2\C,0,1.454637,-1.07742,-0.68535\O,0,1.141436,0.162073,-1.
373816\C,0,-0.176059,0.567575,-1.062274\H,0,2.033957,-1.677716,-1.4061
61\H,0,-0.523494,1.14653,-1.93023\C,0,-3.112938,0.075308,-0.253715\C,0
,0.121469,-1.676589,-0.397281\C,0,-0.966544,-0.756541,-0.822556\O,0,-1
.995984,-0.710823,0.146954\H,0,-3.43781,-0.213337,-1.269042\H,0,-1.403
328,-1.065861,-1.7953\O,0,-0.265944,1.349255,0.099152\C,0,0.348381,2.6
24259,-0.029081\H,0,-0.096726,3.19915,-0.856111\H,0,0.171722,3.153051,

0.910281\H,0,1.427145,2.535385,-0.202842\C,0,2.331448,-0.834571,0.5577
11\H,0,2.474061,-1.799493,1.06566\H,0,1.775907,-0.189174,1.248261\C,0,
3.695453,-0.218872,0.223261\H,0,3.538005,0.71484,-0.330248\H,0,4.23903
8,-0.890395,-0.457167\H,0,-2.836906,1.139226,-0.285334\C,0,-4.214672,-
0.121774,0.685699\C,0,-5.144629,-0.261738,1.441286\H,0,-5.958058,-0.39
4702,2.117839\C,0,4.547719,0.049255,1.46759\H,0,5.516081,0.487896,1.20
0799\H,0,4.043697,0.743858,2.150674\H,0,4.743034,-0.876002,2.023781\H,
0,-0.047978,-2.630653,0.085069\\Version=IA32L-G03RevD.01\State=2-A\HF=
-655.1004971\S2=0.754105\S2-1=0.\S2A=0.750012\RMSD=9.020e-09\Thermal=0
.\Dipole=0.1916634,0.1987121,-0.4432014\PG=C01 [X(C11H17O3)]\\@

ShaC3alpha_015_sp.log

1\1\GINC-NODE-21\SP\UB3LYP\6-311+G(d,p)\C11H17O3(2)\ZIP06\09-Jun-2010\
0\\#P UBecke3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC3alph
a_015 sp\\0,2\C,0,1.356114,-0.470064,-1.078584\O,0,1.026241,0.872047,-
0.678686\C,0,-0.382844,1.082219,-0.725305\H,0,1.880701,-0.424696,-2.05
1048\H,0,-0.629101,1.572362,-1.686706\C,0,-2.62546,-0.341362,1.163533\
C,0,0.043616,-1.170943,-1.200661\C,0,-1.047839,-0.317201,-0.66259\O,0,
-1.348422,-0.751229,0.671357\H,0,-2.727855,0.748803,1.111001\H,0,-1.96
4925,-0.346517,-1.267365\O,0,-0.797178,1.887949,0.329033\C,0,-0.289626
,3.215172,0.271554\H,0,0.799501,3.22849,0.388678\H,0,-0.554317,3.7007,
-0.680238\H,0,-0.753376,3.762907,1.095187\C,0,2.311147,-1.095877,-0.04
4855\H,0,2.51356,-2.13286,-0.34952\H,0,1.785464,-1.138356,0.917046\C,0
,3.630605,-0.327975,0.099791\H,0,3.406513,0.709172,0.374887\H,0,4.1357
9,-0.288064,-0.876266\H,0,-2.623557,-0.625194,2.221548\C,0,-3.751764,-
0.989137,0.475353\C,0,-4.676499,-1.512731,-0.0995\H,0,-5.495543,-1.981
524,-0.596261\C,0,4.568454,-0.952545,1.137586\H,0,4.829186,-1.984413,0
.870669\H,0,5.502162,-0.384838,1.222842\H,0,4.101208,-0.976193,2.12960
7\H,0,-0.065966,-2.227241,-1.415622\\Version=IA32L-G03RevD.01\State=2-
A\HF=-655.100499\S2=0.754014\S2-1=0.\S2A=0.750012\RMSD=5.461e-09\Therm
al=0.\Dipole=-0.0901965,0.1978591,-0.5268918\PG=C01 [X(C11H17O3)]\\@

ShaC3alpha_115_sp.log

1\1\GINC-NODE-21\SP\UB3LYP\6-311+G(d,p)\C11H17O3(2)\ZIP06\05-Jun-2010\
0\\#P UBecke3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC3alph
a_115 sp\\0,2\C,0,-1.088703,-0.468087,-1.149145\O,0,-0.497943,-1.79087
2,-1.028877\C,0,0.809558,-1.682475,-0.508367\H,0,-1.622584,-0.463536,-
2.113826\H,0,1.363776,-2.558713,-0.870397\C,0,2.185936,0.99451,0.79573
\C,0,0.081519,0.45809,-1.168174\C,0,1.343729,-0.331775,-1.063371\O,0,2
.454147,0.226001,-0.379436\H,0,3.083363,0.890889,1.416387\H,0,1.746155
,-0.542107,-2.06868\O,0,0.844769,-1.647235,0.89716\C,0,0.474004,-2.877
438,1.504933\H,0,1.137222,-3.693227,1.179949\H,0,0.577933,-2.740579,2.

583808\H,0,-0.561928,-3.145543,1.266647\C,0,-2.119744,-0.228256,-0.030
54\H,0,-1.600328,-0.266397,0.934327\H,0,-2.826867,-1.068808,-0.049922\
C,0,-2.880902,1.095425,-0.174355\H,0,-3.352994,1.140987,-1.166642\H,0,
-2.171485,1.932609,-0.131487\H,0,1.347514,0.57201,1.357208\C,0,1.95323
1,2.417629,0.511042\C,0,1.775128,3.593094,0.296013\H,0,1.621769,4.6303
66,0.101648\C,0,-3.951179,1.28193,0.906373\H,0,-4.478668,2.234689,0.78
4249\H,0,-4.697553,0.479171,0.867945\H,0,-3.506226,1.272781,1.908715\H
,0,0.037658,1.506368,-1.431538\\Version=IA32L-G03RevD.01\State=2-A\HF=
-655.1006519\S2=0.754101\S2-1=0.\S2A=0.750012\RMSD=5.026e-09\Thermal=0
.\Dipole=-0.5883586,-0.0334203,0.1522088\PG=C01 [X(C11H17O3)]\\@

ShaC3alpha_019_sp.log

1\1\GINC-NODE-31\SP\UB3LYP\6-311+G(d,p)\C11H17O3(2)\ZIP06\09-Jun-2010\
0\\#P UBecke3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC3alph
a_019 sp\\0,2\C,0,1.619296,0.136264,-1.074211\O,0,0.987564,1.442098,-1
.033136\C,0,-0.347231,1.318184,-0.58778\H,0,2.238159,0.130925,-1.98648
1\H,0,-0.891183,2.163062,-1.034518\C,0,-3.027829,-0.164227,-0.241772\C
,0,0.475153,-0.814137,-1.170809\C,0,-0.816543,-0.080915,-1.092713\O,0,
-1.74088,-0.771641,-0.274025\H,0,-3.375984,0.046262,-1.268528\H,0,-1.2
63553,0.059847,-2.099271\O,0,-0.480167,1.348984,0.808305\C,0,-0.13944,
2.605872,1.378395\H,0,0.913759,2.853255,1.202455\H,0,-0.766347,3.41210
1,0.966539\H,0,-0.322416,2.522837,2.452076\C,0,2.549354,-0.063544,0.13
8452\H,0,1.939919,-0.047493,1.049517\H,0,3.221369,0.804635,0.180441\C,
0,3.374316,-1.354311,0.068088\H,0,3.934351,-1.380442,-0.878137\H,0,2.7
00784,-2.221612,0.051353\H,0,-2.982307,0.794768,0.294451\C,0,-3.976063
,-1.056006,0.422179\C,0,-4.786607,-1.765966,0.964698\H,0,-5.490937,-2.
404575,1.447596\C,0,4.351027,-1.496014,1.240514\H,0,4.925397,-2.426643
,1.170159\H,0,5.064557,-0.66339,1.263982\H,0,3.818647,-1.503399,2.1991
94\H,0,0.551063,-1.886863,-1.290229\\Version=IA32L-G03RevD.01\State=2-
A\HF=-655.1001997\S2=0.754104\S2-1=0.\S2A=0.750012\RMSD=8.954e-09\Ther
mal=0.\Dipole=0.1304435,0.3651491,-0.2586586\PG=C01 [X(C11H17O3)]\\@

ShaC3alpha_087_sp.log

1\1\GINC-NODE-21\SP\UB3LYP\6-311+G(d,p)\C11H17O3(2)\ZIP06\05-Jun-2010\
0\\#P UBecke3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC3alph
a_087 sp\\0,2\C,0,-1.196004,-0.52583,1.160729\O,0,-1.208838,0.927368,1
.105357\C,0,0.053688,1.40127,0.68119\H,0,-1.719545,-0.792728,2.094055\
H,0,0.166195,2.408553,1.103783\C,0,2.4771,-0.260831,-0.642543\C,0,0.25
1382,-0.87994,1.224145\C,0,1.071159,0.369443,1.241104\O,0,2.356688,0.3
39292,0.65259\H,0,2.41409,0.511971,-1.416998\H,0,1.28213,0.667815,2.28
1724\O,0,0.182017,1.45254,-0.717325\C,0,-0.621267,2.454911,-1.325857\H
,0,-1.688714,2.27151,-1.155413\H,0,-0.365363,3.453274,-0.940401\H,0,-0

.411476,2.420804,-2.397385\C,0,-1.970223,-1.143083,-0.017965\H,0,-1.86
5621,-2.236329,0.041734\H,0,-1.488018,-0.825713,-0.950366\C,0,-3.45637
2,-0.764825,-0.028502\H,0,-3.544849,0.32831,-0.034493\H,0,-3.922763,-1
.105337,0.907299\H,0,1.647899,-0.959652,-0.817751\C,0,3.753975,-0.9704
86,-0.731347\C,0,4.801924,-1.560161,-0.8374\H,0,5.730524,-2.077763,-0.
919544\C,0,-4.212259,-1.356968,-1.221978\H,0,-4.161865,-2.452951,-1.22
1908\H,0,-5.270536,-1.07265,-1.203883\H,0,-3.789682,-1.007736,-2.17212
\H,0,0.630041,-1.865971,1.467247\\Version=IA32L-G03RevD.01\State=2-A\H
F=-655.1002762\S2=0.754067\S2-1=0.\S2A=0.750012\RMSD=7.648e-09\Thermal
=0.\Dipole=-0.7289396,-0.1496427,-0.1456503\PG=C01 [X(C11H17O3)]\\@

ShaC3alpha_020_sp.log

1\1\GINC-NODE-25\SP\UB3LYP\6-311+G(d,p)\C11H17O3(2)\ZIP06\05-Jun-2010\
0\\#P UBecke3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC3alph
a_020 sp\\0,2\C,0,1.257371,-1.04723,-1.178892\O,0,0.787906,0.25782,-1.
6005\C,0,-0.355674,0.665895,-0.875472\H,0,1.359473,-1.639311,-2.105403
\H,0,-1.010133,1.171862,-1.600615\C,0,-2.6806,0.242308,1.166605\C,0,0.
16364,-1.57885,-0.321509\C,0,-0.982641,-0.635211,-0.281204\O,0,-1.4927
25,-0.532613,1.039752\H,0,-2.499841,1.276813,0.843915\H,0,-1.798723,-0
.961738,-0.952682\O,0,-0.059627,1.550742,0.172975\C,0,0.408568,2.81455
1,-0.280264\H,0,-0.329357,3.297856,-0.939372\H,0,0.554902,3.432715,0.6
08512\H,0,1.356911,2.719449,-0.821794\C,0,2.658366,-0.980349,-0.538897
\H,0,3.029513,-2.013142,-0.460698\H,0,3.318789,-0.469525,-1.252959\C,0
,2.73621,-0.299773,0.831719\H,0,2.095612,-0.839331,1.541622\H,0,2.3162
21,0.708858,0.760618\H,0,-2.887569,0.267449,2.241862\C,0,-3.839132,-0.
313342,0.451041\C,0,-4.790677,-0.762856,-0.142294\H,0,-5.635144,-1.162
738,-0.656627\C,0,4.168413,-0.235851,1.371628\H,0,4.201125,0.250303,2.
353398\H,0,4.600139,-1.238605,1.483155\H,0,4.823743,0.331051,0.698249\
H,0,0.156847,-2.555308,0.146235\\Version=IA32L-G03RevD.01\State=2-A\HF
=-655.1002259\S2=0.754141\S2-1=0.\S2A=0.750012\RMSD=9.633e-09\Thermal=
0.\Dipole=-0.1719044,0.1244401,-0.3328681\PG=C01 [X(C11H17O3)]\\@

ShaC3alpha_008_sp.log

1\1\GINC-NODE-28\SP\UB3LYP\6-311+G(d,p)\C11H17O3(2)\ZIP06\05-Jun-2010\
0\\#P UBecke3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC3alph
a_008 sp\\0,2\C,0,1.507478,-0.262741,-0.707034\O,0,0.717847,0.797101,-
1.307008\C,0,-0.543142,0.879067,-0.676214\H,0,2.031365,-0.748796,-1.54
3707\H,0,-1.233042,1.271508,-1.43699\C,0,-2.930456,-0.244134,0.959951\
C,0,0.492349,-1.160255,-0.085907\C,0,-0.868904,-0.574844,-0.215599\O,0
,-1.583064,-0.700305,1.004772\H,0,-2.965079,0.825449,0.70951\H,0,-1.44
5905,-1.066586,-1.020742\O,0,-0.553175,1.717388,0.450833\C,0,-0.333359
,3.085003,0.131774\H,0,-1.096569,3.457298,-0.569437\H,0,-0.405777,3.64

1979,1.068819\H,0,0.657209,3.238565,-0.311719\C,0,2.551895,0.325012,0.
26524\H,0,3.119403,1.087348,-0.286355\H,0,2.00796,0.839922,1.064705\C,
0,3.520356,-0.704669,0.869571\H,0,2.951243,-1.462446,1.425049\H,0,4.13
8132,-0.189394,1.616542\H,0,-3.299302,-0.35007,1.985857\C,0,-3.792523,
-1.004221,0.042258\C,0,-4.500873,-1.622817,-0.716049\H,0,-5.131044,-2.
173567,-1.377186\C,0,4.441764,-1.392083,-0.146567\H,0,5.017425,-0.6542
92,-0.719366\H,0,5.156375,-2.052702,0.35731\H,0,3.88331,-2.004059,-0.8
64469\H,0,0.693912,-2.113534,0.384866\\Version=IA32L-G03RevD.01\State=
2-A\HF=-655.100277\S2=0.754114\S2-1=0.\S2A=0.750012\RMSD=4.092e-09\The
rmal=0.\Dipole=0.0003425,0.1620581,-0.2339331\PG=C01 [X(C11H17O3)]\\@

ShaC3alpha_005_sp.log

1\1\GINC-NODE-31\SP\UB3LYP\6-311+G(d,p)\C11H17O3(2)\ZIP06\05-Jun-2010\
0\\#P UBecke3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC3alph
a_005 sp\\0,2\C,0,-1.380402,-1.073357,0.627429\O,0,-0.751518,0.071246,
1.260829\C,0,0.510661,0.312271,0.660965\H,0,-1.857255,-1.640314,1.4448
43\H,0,1.116734,0.824677,1.41795\C,0,3.283652,-1.033462,-0.546257\C,0,
-0.242366,-1.821155,0.021315\C,0,1.035285,-1.102846,0.276889\O,0,1.902
306,-1.164793,-0.843926\H,0,3.801669,-1.277803,-1.480006\H,0,1.55827,-
1.519202,1.16113\O,0,0.432492,1.080885,-0.505128\C,0,0.12822,2.445154,
-0.262528\H,0,0.891478,2.912614,0.378278\H,0,0.125262,2.944368,-1.2344
3\H,0,-0.854261,2.563766,0.211636\C,0,-2.476503,-0.646629,-0.366681\H,
0,-2.86411,-1.552442,-0.855867\H,0,-2.010915,-0.0343,-1.147531\C,0,-3.
6281,0.11586,0.299391\H,0,-3.218517,0.985924,0.826742\H,0,-4.087503,-0
.521281,1.069163\H,0,3.58561,-1.783684,0.204272\C,0,3.70665,0.297058,-
0.084211\C,0,4.09027,1.371257,0.312978\H,0,4.42458,2.326941,0.648282\C
,0,-4.699181,0.566746,-0.698599\H,0,-5.506556,1.113456,-0.197863\H,0,-
4.273798,1.227512,-1.463982\H,0,-5.148402,-0.290021,-1.216232\H,0,-0.3
17643,-2.764292,-0.504742\\Version=IA32L-G03RevD.01\State=2-A\HF=-655.
099807\S2=0.754142\S2-1=0.\S2A=0.750012\RMSD=4.630e-09\Thermal=0.\Dipo
le=0.1801006,-0.0817171,0.3453776\PG=C01 [X(C11H17O3)]\\@

ShaC3alpha_099_sp.log

1\1\GINC-NODE-28\SP\UB3LYP\6-311+G(d,p)\C11H17O3(2)\ZIP06\09-Jun-2010\
0\\#P UBecke3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC3alph
a_099 sp\\0,2\C,0,1.445622,0.237062,-1.081593\O,0,1.105276,1.63587,-0.
87915\C,0,-0.242727,1.743684,-0.470308\H,0,2.052482,0.204614,-2.001459
\H,0,-0.584456,2.740118,-0.780311\C,0,-2.238101,-0.586902,0.517034\C,0
,0.128184,-0.437697,-1.273658\C,0,-0.966221,0.578478,-1.198439\O,0,-2.
224927,0.174242,-0.696376\H,0,-2.360532,0.08296,1.375589\H,0,-1.208935
,0.94367,-2.210347\O,0,-0.410832,1.590194,0.916952\C,0,0.131762,2.6635
75,1.675406\H,0,-0.086048,2.450902,2.724529\H,0,1.215777,2.744649,1.53

4166\H,0,-0.33699,3.619325,1.396772\C,0,2.309613,-0.286727,0.080798\H,
0,1.718001,-0.237982,1.002741\H,0,3.152207,0.40782,0.200457\C,0,2.8367
46,-1.709222,-0.143213\H,0,3.38089,-1.752087,-1.097914\H,0,1.99143,-2.
403974,-0.239977\H,0,-1.280127,-1.108372,0.650113\C,0,-3.330696,-1.559
033,0.466193\C,0,-4.225487,-2.369213,0.45734\H,0,-5.019592,-3.080535,0
.437627\C,0,3.75598,-2.183883,0.987333\H,0,3.23195,-2.180935,1.950725\
H,0,4.116624,-3.202711,0.806533\H,0,4.632019,-1.531317,1.085045\H,0,0.
001115,-1.43932,-1.667061\\Version=IA32L-G03RevD.01\State=2-A\HF=-655.
0999793\S2=0.75406\S2-1=0.\S2A=0.750012\RMSD=5.349e-09\Thermal=0.\Dipo
le=0.7477637,-0.0746665,0.1794407\PG=C01 [X(C11H17O3)]\\@

ShaC3alpha_002_sp.log

1\1\GINC-NODE-21\SP\UB3LYP\6-311+G(d,p)\C11H17O3(2)\ZIP06\09-Jun-2010\
0\\#P UBecke3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC3alph
a_002 sp\\0,2\C,0,-1.033793,-1.034928,0.583225\O,0,-0.838038,0.231158,
1.267494\C,0,0.226212,0.938721,0.657047\H,0,-1.235982,-1.772357,1.3783
29\H,0,0.636231,1.604558,1.428268\C,0,3.152153,-0.531336,-1.139101\C,0
,0.272592,-1.28785,-0.092178\C,0,1.211994,-0.163393,0.201604\O,0,2.022
342,0.286845,-0.875732\H,0,3.596833,-0.120447,-2.051926\H,0,1.863646,-
0.402608,1.061863\O,0,-0.173721,1.679902,-0.460769\C,0,-0.962968,2.813
094,-0.132919\H,0,-1.911622,2.52539,0.337503\H,0,-0.422567,3.490533,0.
546214\H,0,-1.165711,3.336187,-1.070384\C,0,-2.251555,-0.994916,-0.358
154\H,0,-2.306836,-1.96082,-0.881898\H,0,-2.072119,-0.227441,-1.120014
\C,0,-3.572196,-0.727722,0.373883\H,0,-3.485595,0.21379,0.929604\H,0,-
3.73552,-1.513605,1.125754\H,0,2.849172,-1.566801,-1.363103\C,0,4.1526
89,-0.540929,-0.060006\C,0,4.971589,-0.552508,0.82774\H,0,5.700342,-0.
556889,1.606578\C,0,-4.774913,-0.666891,-0.572757\H,0,-5.704569,-0.474
432,-0.024962\H,0,-4.65452,0.131156,-1.315695\H,0,-4.899849,-1.60976,-
1.119775\H,0,0.513188,-2.187737,-0.644597\\Version=IA32L-G03RevD.01\St
ate=2-A\HF=-655.099581\S2=0.754116\S2-1=0.\S2A=0.750012\RMSD=6.910e-09
\Thermal=0.\Dipole=0.0771339,-0.449308,0.1432723\PG=C01 [X(C11H17O3)]\
\@

ShaC3alpha_014_sp.log

1\1\GINC-NODE-28\SP\UB3LYP\6-311+G(d,p)\C11H17O3(2)\ZIP06\09-Jun-2010\
0\\#P UBecke3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC3alph
a_014 sp\\0,2\C,0,-1.295266,-1.2046,0.290494\O,0,-0.962463,0.003486,1.
024926\C,0,0.257567,0.542999,0.554318\H,0,-1.672327,-1.915395,1.045505
\H,0,0.700647,1.070581,1.410857\C,0,3.050581,0.386912,-0.784791\C,0,0.
007493,-1.645271,-0.283532\C,0,1.085323,-0.684939,0.06824\O,0,1.941397
,-0.466634,-1.0417\H,0,2.704589,1.388792,-0.493814\H,0,1.688757,-1.045
9,0.922227\O,0,0.102473,1.429923,-0.522358\C,0,-0.535625,2.647913,-0.1

62976\H,0,0.022385,3.170277,0.629732\H,0,-0.549885,3.271321,-1.060135\
H,0,-1.562035,2.47843,0.181723\C,0,-2.406755,-0.984479,-0.756599\H,0,-
2.116457,-0.1371,-1.388962\H,0,-2.417077,-1.872736,-1.403852\C,0,-3.81
8911,-0.786565,-0.179869\H,0,-4.050923,-1.631924,0.484882\H,0,-4.53672
4,-0.851655,-1.008804\H,0,3.560299,0.486352,-1.74917\C,0,3.989786,-0.1
31826,0.221204\C,0,4.758948,-0.551712,1.052771\H,0,5.445052,-0.924862,
1.779125\C,0,-4.04514,0.529984,0.572512\H,0,-3.857647,1.390348,-0.0821
56\H,0,-5.080602,0.601995,0.925894\H,0,-3.379726,0.621101,1.435452\H,0
,0.162423,-2.544319,-0.866086\\Version=IA32L-G03RevD.01\State=2-A\HF=-
655.0997229\S2=0.754129\S2-1=0.\S2A=0.750012\RMSD=5.191e-09\Thermal=0.
\Dipole=-0.0146283,0.153665,0.3056256\PG=C01 [X(C11H17O3)]\\@

ShaC3alpha_009_sp.log

1\1\GINC-NODE-31\SP\UB3LYP\6-311+G(d,p)\C11H17O3(2)\ZIP06\09-Jun-2010\
0\\#P UBecke3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC3alph
a_009 sp\\0,2\C,0,-1.448608,-0.279556,1.066202\O,0,-0.482806,0.728305,
1.461761\C,0,0.705607,0.565782,0.707206\H,0,-1.950412,-0.597555,1.9951
43\H,0,1.513114,0.99854,1.310403\C,0,2.888516,-1.57405,-0.558031\C,0,-
0.611637,-1.369928,0.486543\C,0,0.822749,-0.971629,0.494623\O,0,1.4871
11,-1.390241,-0.686815\H,0,3.200633,-2.055172,-1.491331\H,0,1.348703,-
1.394827,1.373656\O,0,0.651955,1.178004,-0.549881\C,0,0.674035,2.59561
2,-0.485286\H,0,-0.196545,2.988913,0.054059\H,0,1.590337,2.955144,0.00
7669\H,0,0.658637,2.957496,-1.516085\C,0,-2.513287,0.3153,0.12434\H,0,
-2.016044,0.641499,-0.796114\H,0,-2.916143,1.21335,0.612693\C,0,-3.656
333,-0.654769,-0.198519\H,0,-4.113887,-1.007997,0.737257\H,0,-3.253453
,-1.54554,-0.699386\H,0,3.107299,-2.276447,0.264232\C,0,3.67051,-0.345
424,-0.354241\C,0,4.345194,0.639517,-0.171424\H,0,4.935759,1.515592,-0
.02575\C,0,-4.734992,-0.022877,-1.084792\H,0,-4.314558,0.309684,-2.041
485\H,0,-5.53952,-0.73447,-1.302651\H,0,-5.184718,0.851793,-0.599154\H
,0,-0.969803,-2.336414,0.156595\\Version=IA32L-G03RevD.01\State=2-A\HF
=-655.0994384\S2=0.754137\S2-1=0.\S2A=0.750012\RMSD=8.817e-09\Thermal=
0.\Dipole=0.1444695,-0.1188942,0.2960639\PG=C01 [X(C11H17O3)]\\@

30c

TSC3alpha_001_sp.log

1\1\GINC-NODE-28\SP\UB3LYP\6-311+G(d,p)\C11H17O3(2)\ZIP06\05-Aug-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) TSC3alpha_001
\\0,2\C,0,-1.428088,1.870225,-0.622292\C,0,-2.47857,0.845457,-0.864413
\O,0,-2.783144,0.040106,0.268629\C,0,-1.656481,-0.313258,1.051193\C,0,
-0.657812,0.789712,1.231968\C,0,-0.771043,-1.479119,0.529442\O,0,0.505
277,-1.240759,1.080026\C,0,0.722111,0.189453,1.242469\O,0,-0.776017,-1
.47661,-0.876401\C,0,-0.072852,-2.571327,-1.446798\C,0,1.714032,0.7218

96,0.198395\C,0,-0.860114,2.924686,-0.908751\H,0,-0.880714,1.629939,1.
880655\H,0,-2.087118,-0.627999,2.012786\H,0,-2.163916,0.217616,-1.7046
28\H,0,-3.416484,1.345129,-1.128524\H,0,-0.202333,3.763934,-0.959729\H
,0,1.178398,0.304519,2.238572\H,0,1.795366,1.810123,0.331277\H,0,1.288
209,0.558773,-0.79788\H,0,-1.087335,-2.466072,0.895012\H,0,-0.189372,-
2.4921,-2.530168\H,0,0.992578,-2.542508,-1.189696\H,0,-0.49413,-3.5303
24,-1.108504\C,0,3.102198,0.079979,0.306621\H,0,3.00048,-1.008125,0.21
3586\H,0,3.510512,0.264302,1.311097\C,0,4.082937,0.603735,-0.747193\H,
0,5.066573,0.130562,-0.647553\H,0,3.718092,0.403695,-1.762171\H,0,4.22
4355,1.688014,-0.656009\\Version=IA32L-G03RevD.01\State=2-A\HF=-655.08
85455\S2=0.77271\S2-1=0.\S2A=0.750182\RMSD=5.013e-09\Thermal=0.\Dipole
=0.5084292,0.0912817,-0.003938\PG=C01 [X(C11H17O3)]\\@

TSC3alpha_002_sp.log

1\1\GINC-NODE-28\SP\UB3LYP\6-311+G(d,p)\C11H17O3(2)\ZIP06\05-Aug-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) TSC3alpha_002
\\0,2\C,0,0.118602,2.065127,0.504313\C,0,1.594977,1.946384,0.655412\O,
0,2.256221,1.400433,-0.479554\C,0,1.541509,0.360762,-1.119681\C,0,0.06
4497,0.602379,-1.234636\C,0,1.594733,-1.044926,-0.463258\O,0,0.428576,
-1.694618,-0.913785\C,0,-0.637262,-0.727527,-1.125436\O,0,1.642234,-0.
907544,0.935559\C,0,1.762009,-2.146996,1.620194\C,0,-1.716754,-0.87480
3,-0.043586\C,0,-0.949871,2.575234,0.848067\H,0,-0.310588,1.349287,-1.
926171\H,0,2.01194,0.280741,-2.110597\H,0,1.804469,1.34347,1.545006\H,
0,2.024343,2.944128,0.793842\H,0,-1.973627,2.850169,0.973371\H,0,-1.08
7561,-0.994329,-2.094995\H,0,-1.308589,-0.522692,0.910159\H,0,-1.92484
7,-1.947985,0.063146\H,0,2.443338,-1.655701,-0.801648\H,0,0.894671,-2.
791223,1.435586\H,0,2.674134,-2.681268,1.313015\H,0,1.8256,-1.914466,2
.685701\C,0,-3.01602,-0.133751,-0.379967\H,0,-3.40729,-0.503022,-1.339
104\H,0,-2.803185,0.93311,-0.52619\C,0,-4.087696,-0.297219,0.702956\H,
0,-5.011191,0.228909,0.435057\H,0,-4.33836,-1.354167,0.855058\H,0,-3.7
41854,0.100888,1.664742\\Version=IA32L-G03RevD.01\State=2-A\HF=-655.08
76124\S2=0.773533\S2-1=0.\S2A=0.750192\RMSD=5.920e-09\Thermal=0.\Dipol
e=-0.499299,-0.200664,0.0583517\PG=C01 [X(C11H17O3)]\\@

TSC3alpha_003_sp.log

1\1\GINC-NODE-28\SP\UB3LYP\6-311+G(d,p)\C11H17O3(2)\ZIP06\05-Aug-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) TSC3alpha_003
\\0,2\C,0,1.614557,-1.808692,-0.609933\C,0,2.648196,-0.742474,-0.52548
9\O,0,2.670149,-0.050109,0.717661\C,0,1.386246,0.218022,1.253363\C,0,0
.402457,-0.902683,1.094066\C,0,0.612056,1.427538,0.658168\O,0,-0.74942
2,1.128145,0.871629\C,0,-0.957349,-0.312369,0.832217\O,0,0.941496,1.57
0324,-0.701542\C,0,0.358996,2.714996,-1.308727\C,0,-1.64502,-0.731532,

-0.477185\C,0,1.170264,-2.849071,-1.096804\H,0,0.489443,-1.79697,1.701
62\H,0,1.578906,0.436139,2.313676\H,0,2.491066,-0.039694,-1.350431\H,0
,3.641333,-1.192186,-0.627021\H,0,0.575027,-3.696204,-1.357064\H,0,-1.
629332,-0.533349,1.674345\H,0,-1.73536,-1.827056,-0.478751\H,0,-0.9758
13,-0.470532,-1.303194\H,0,0.807633,2.373082,1.18291\H,0,0.664563,3.63
5949,-0.789082\H,0,0.7245,2.746966,-2.337746\H,0,-0.735777,2.655993,-1
.310496\C,0,-3.026872,-0.093624,-0.69201\H,0,-3.342133,-0.298904,-1.72
3731\H,0,-2.93113,0.996016,-0.608881\C,0,-4.115632,-0.590027,0.267153\
H,0,-5.083756,-0.13359,0.031297\H,0,-4.236901,-1.678816,0.200932\H,0,-
3.887455,-0.344236,1.310717\\Version=IA32L-G03RevD.01\State=2-A\HF=-65
5.0872952\S2=0.772771\S2-1=0.\S2A=0.750183\RMSD=5.517e-09\Thermal=0.\D
ipole=-0.5088436,-0.0826017,-0.1642609\PG=C01 [X(C11H17O3)]\\@

TSC3alpha_004_sp.log

1\1\GINC-NODE-31\SP\UB3LYP\6-311+G(d,p)\C11H17O3(2)\ZIP06\05-Aug-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) TSC3alpha_004
\\0,2\C,0,0.440017,2.09664,0.528038\C,0,1.89192,1.858336,0.302211\O,0,
2.195486,1.209933,-0.927083\C,0,1.261888,0.216024,-1.303853\C,0,-0.171
843,0.588363,-1.062348\C,0,1.367661,-1.161223,-0.595782\O,0,0.077271,-
1.71777,-0.695872\C,0,-0.929023,-0.666638,-0.71177\O,0,1.784771,-0.972
013,0.733518\C,0,1.980767,-2.187802,1.442279\C,0,-1.720551,-0.671881,0
.605587\C,0,-0.463247,2.702919,1.10773\H,0,-0.646028,1.344849,-1.67868
6\H,0,1.4584,0.053955,-2.373878\H,0,2.280956,1.277785,1.145033\H,0,2.4
13408,2.82046,0.263438\H,0,-1.398694,3.060606,1.476869\H,0,-1.610785,-
0.931525,-1.533812\H,0,-1.051714,-0.334157,1.403617\H,0,-1.986453,-1.7
15835,0.819944\H,0,2.049711,-1.861554,-1.098087\H,0,2.735947,-2.816549
,0.946137\H,0,2.338593,-1.918501,2.438732\H,0,1.047454,-2.756226,1.528
296\C,0,-2.99591,0.187249,0.584098\H,0,-2.74384,1.211053,0.27804\H,0,-
3.372361,0.264097,1.612717\C,0,-4.117546,-0.356372,-0.311081\H,0,-3.82
6089,-0.390146,-1.367248\H,0,-4.399904,-1.374139,-0.014742\H,0,-5.0136
2,0.270939,-0.241525\\Version=IA32L-G03RevD.01\State=2-A\HF=-655.08590
96\S2=0.773433\S2-1=0.\S2A=0.750191\RMSD=5.792e-09\Thermal=0.\Dipole=-
0.502621,-0.1429633,0.2130613\PG=C01 [X(C11H17O3)]\\@

TSC3alpha_005_sp.log

1\1\GINC-NODE-28\SP\UB3LYP\6-311+G(d,p)\C11H17O3(2)\ZIP06\05-Aug-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) TSC3alpha_005
\\0,2\C,0,1.923117,-1.467162,-0.702248\C,0,2.694013,-0.19482,-0.693074
\O,0,2.649989,0.50856,0.543289\C,0,1.391655,0.466421,1.191484\C,0,0.70
959,-0.86612,1.131725\C,0,0.289915,1.42465,0.659849\O,0,-0.929044,0.80
468,1.007389\C,0,-0.775354,-0.642879,1.023525\O,0,0.448013,1.59605,-0.
725768\C,0,-0.434041,2.56031,-1.28366\C,0,-1.477068,-1.322203,-0.16453

1\C,0,1.683531,-2.580739,-1.170443\H,0,1.082702,-1.700482,1.715936\H,0
,1.614768,0.758753,2.227907\H,0,2.324867,0.439916,-1.505356\H,0,3.7527
63,-0.413079,-0.867856\H,0,1.27945,-3.542129,-1.39846\H,0,-1.272686,-0
.979024,1.947912\H,0,-1.147423,-2.369783,-0.170376\H,0,-1.099691,-0.87
4042,-1.090782\H,0,0.289678,2.406636,1.153093\H,0,-0.179712,2.645207,-
2.342781\H,0,-1.481351,2.253703,-1.181682\H,0,-0.301179,3.541224,-0.80
2286\C,0,-3.014307,-1.293461,-0.121896\H,0,-3.351537,-1.690645,0.84714
9\H,0,-3.386429,-1.997571,-0.878689\C,0,-3.658283,0.077052,-0.363217\H
,0,-3.359684,0.802471,0.398149\H,0,-3.360815,0.479682,-1.339749\H,0,-4
.751977,-0.001457,-0.356486\\Version=IA32L-G03RevD.01\State=2-A\HF=-65
5.0859229\S2=0.772766\S2-1=0.\S2A=0.750183\RMSD=4.954e-09\Thermal=0.\D
ipole=-0.4247958,-0.2375968,-0.0729211\PG=C01 [X(C11H17O3)]\\@

31c

cShaC3alpha_016_sp.log

1\1\GINC-NODE-31\SP\UB3LYP\6-311+G(d,p)\C11H17O3(2)\ZIP06\05-Jun-2010\
0\\#P UBecke3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) cShaC3alp
ha_016 sp\\0,2\C,0,-0.600485,-0.380082,1.13485\O,0,-0.431685,1.061759,
1.220213\C,0,0.775235,1.447092,0.608018\H,0,-0.987337,-0.674002,2.1178
69\H,0,1.056017,2.409169,1.058719\C,0,2.316983,-0.832722,-1.007007\C,0
,1.228057,-1.677717,-0.328933\C,0,0.838171,-0.95403,0.959862\C,0,1.755
869,0.295179,0.931298\O,0,2.787306,0.066266,-0.004637\H,0,3.168795,-1.
428722,-1.348821\H,0,1.897134,-0.278573,-1.854818\H,0,1.073709,-1.6010
93,1.809326\H,0,2.227703,0.500046,1.896699\C,0,0.778935,-2.835041,-0.7
47163\H,0,0.941942,-3.506115,-1.580577\O,0,0.677843,1.586531,-0.787743
\C,0,-0.120625,2.688733,-1.194171\H,0,-1.162887,2.572778,-0.873434\H,0
,0.273218,3.632089,-0.78645\H,0,-0.076481,2.725434,-2.285155\C,0,-1.63
311,-0.753195,0.072116\H,0,-1.684564,-1.848989,0.010864\H,0,-1.280219,
-0.404492,-0.90557\C,0,-3.025964,-0.183381,0.36833\H,0,-2.95222,0.9054
33,0.478126\H,0,-3.37565,-0.564792,1.338918\C,0,-4.05218,-0.530191,-0.
714846\H,0,-3.748473,-0.131633,-1.690781\H,0,-4.165269,-1.616019,-0.82
373\H,0,-5.038439,-0.114836,-0.47797\\Version=IA32L-G03RevD.01\State=2
-A\HF=-655.1295293\S2=0.760442\S2-1=0.\S2A=0.750049\RMSD=4.465e-09\The
rmal=0.\Dipole=-0.2907076,-0.0397571,-0.1352071\PG=C01 [X(C11H17O3)]\\
@

cShaC3alpha_001_sp.log

1\1\GINC-NODE-25\SP\UB3LYP\6-311+G(d,p)\C11H17O3(2)\ZIP06\05-Jun-2010\
0\\#P UBecke3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) cShaC3alp
ha_001 sp\\0,2\C,0,0.782354,-0.035932,0.812784\O,0,0.07679,-1.01984,0.
05139\C,0,-1.25156,-1.063412,0.569523\H,0,0.973499,-0.43846,1.825305\H
,0,-1.251172,-1.711655,1.468736\C,0,-1.619978,1.614944,-0.982414\C,0,-

0.361069,2.061791,-0.23594\C,0,-0.231399,1.128472,0.966494\C,0,-1.6106
64,0.401226,0.968977\O,0,-2.446037,1.059399,0.033339\H,0,-2.166616,2.4
33777,-1.456935\H,0,-1.369501,0.856852,-1.739207\H,0,-0.037372,1.69737
,1.879334\H,0,-2.133611,0.420659,1.928513\C,0,0.405637,3.082666,-0.527
303\H,0,0.459344,3.850659,-1.288346\O,0,-2.133522,-1.547992,-0.376972\
C,0,-1.93308,-2.918575,-0.700425\H,0,-2.740213,-3.197622,-1.381535\H,0
,-0.966227,-3.077174,-1.191549\H,0,-1.985265,-3.549893,0.199699\C,0,2.
11747,0.26349,0.147217\H,0,2.585562,1.104191,0.678327\H,0,1.930373,0.6
08346,-0.876054\C,0,3.068171,-0.941211,0.133792\H,0,2.57584,-1.77665,-
0.37799\H,0,3.247457,-1.274567,1.166249\C,0,4.407039,-0.631557,-0.5426
2\H,0,5.068082,-1.50572,-0.53684\H,0,4.262866,-0.330384,-1.587429\H,0,
4.93157,0.186316,-0.032854\\Version=IA32L-G03RevD.01\State=2-A\HF=-655
.1283842\S2=0.760104\S2-1=0.\S2A=0.750047\RMSD=2.162e-09\Thermal=0.\Di
pole=0.5006382,-0.2532645,0.2942003\PG=C01 [X(C11H17O3)]\\@

cShaC3alpha_002_sp.log

1\1\GINC-NODE-25\SP\UB3LYP\6-311+G(d,p)\C11H17O3(2)\ZIP06\05-Jun-2010\
0\\#P UBecke3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) cShaC3alp
ha_002 sp\\0,2\C,0,0.612052,-0.744791,0.538105\O,0,-0.533511,-1.227233
,-0.167871\C,0,-1.678868,-0.749662,0.534936\H,0,0.705525,-1.300564,1.4
90124\H,0,-1.87564,-1.436163,1.382731\C,0,-0.998141,1.986223,-0.780676
\C,0,0.407532,1.743545,-0.224338\C,0,0.247253,0.720389,0.898889\C,0,-1
.301524,0.665267,1.07328\O,0,-1.8569,1.730383,0.323206\H,0,-1.168991,3
.012519,-1.115357\H,0,-1.208999,1.29278,-1.608111\H,0,0.771526,1.04885
9,1.79943\H,0,-1.647649,0.789576,2.102481\C,0,1.508596,2.349859,-0.591
967\H,0,1.804891,3.09763,-1.316552\O,0,-2.777887,-0.685088,-0.300137\C
,0,-3.242501,-1.957677,-0.734242\H,0,-3.475537,-2.607523,0.123049\H,0,
-4.155726,-1.776213,-1.305481\H,0,-2.503619,-2.458221,-1.370285\C,0,1.
85818,-1.002986,-0.297557\H,0,1.779797,-0.445744,-1.237933\H,0,1.86239
9,-2.069856,-0.557359\C,0,3.164354,-0.639492,0.421035\H,0,3.208856,-1.
160215,1.388511\H,0,3.170543,0.435588,0.644029\C,0,4.406254,-0.990945,
-0.40441\H,0,5.326511,-0.720074,0.125298\H,0,4.448614,-2.065532,-0.620
693\H,0,4.404755,-0.459721,-1.363801\\Version=IA32L-G03RevD.01\State=2
-A\HF=-655.1279545\S2=0.760092\S2-1=0.\S2A=0.750047\RMSD=4.196e-09\The
rmal=0.\Dipole=0.4152867,-0.4260132,0.2228441\PG=C01 [X(C11H17O3)]\\@

cShaC3alpha_025_sp.log

1\1\GINC-NODE-28\SP\UB3LYP\6-311+G(d,p)\C11H17O3(2)\ZIP06\05-Jun-2010\
0\\#P UBecke3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC3alph
a_025 sp\\0,2\C,0,-0.852753,-0.389357,0.744474\O,0,-0.643791,1.027815,
0.99493\C,0,0.690603,1.378963,0.719271\H,0,-1.478117,-0.729393,1.57637
3\H,0,0.899333,2.282399,1.309102\C,0,2.451994,-0.875122,-0.691969\C,0,

1.211803,-1.709149,-0.33727\C,0,0.557608,-1.042689,0.87324\C,0,1.51423
4,0.144423,1.157168\O,0,2.722069,-0.08211,0.462048\H,0,3.336544,-1.486
925,-0.893275\H,0,2.245583,-0.235509,-1.558407\H,0,0.550236,-1.754618,
1.703068\H,0,1.761375,0.24857,2.21766\C,0,0.837661,-2.820404,-0.921318
\H,0,1.170279,-3.448903,-1.737372\O,0,0.93598,1.633736,-0.641494\C,0,0
.317371,2.820544,-1.117534\H,0,0.653024,3.697118,-0.542876\H,0,0.62203
8,2.939143,-2.15994\H,0,-0.775947,2.757809,-1.060538\C,0,-1.596832,-0.
612311,-0.572818\H,0,-1.69581,-1.694794,-0.73309\H,0,-0.973744,-0.2333
47,-1.390044\C,0,-2.98403,0.049901,-0.625345\H,0,-3.349458,-0.00233,-1
.659448\H,0,-2.879953,1.115532,-0.386605\C,0,-4.02868,-0.585079,0.3009
49\H,0,-5.005157,-0.102608,0.178671\H,0,-4.155925,-1.652902,0.082143\H
,0,-3.752233,-0.493091,1.357619\\Version=IA32L-G03RevD.01\State=2-A\HF
=-655.128171\S2=0.760425\S2-1=0.\S2A=0.750049\RMSD=8.376e-09\Thermal=0
.\Dipole=-0.2598389,0.0083851,-0.2398598\PG=C01 [X(C11H17O3)]\\@

cShaC3alpha_031_sp.log

1\1\GINC-NODE-21\SP\UB3LYP\6-311+G(d,p)\C11H17O3(2)\ZIP06\05-Jun-2010\
0\\#P UBecke3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) cShaC3alp
ha_031 sp\\0,2\C,0,-0.587995,-0.453246,-1.132289\O,0,0.450348,-1.47097
3,-1.138077\C,0,1.621449,-0.979173,-0.537549\H,0,-1.040632,-0.51233,-2
.129359\H,0,2.450699,-1.579982,-0.936317\C,0,1.410438,1.838682,0.91520
6\C,0,0.026885,1.776161,0.249721\C,0,0.168354,0.906801,-1.002083\C,0,1
.667877,0.508468,-0.954099\O,0,2.333357,1.387187,-0.073117\H,0,1.69867
8,2.854368,1.203202\H,0,1.439416,1.187307,1.796266\H,0,-0.048374,1.525
28,-1.877368\H,0,2.160628,0.582992,-1.927896\C,0,-1.034432,2.433318,0.
64791\H,0,-1.300576,3.105138,1.453979\O,0,1.605016,-1.061297,0.866319\
C,0,1.624578,-2.395127,1.355209\H,0,1.64999,-2.331407,2.445517\H,0,0.7
34039,-2.951462,1.040113\H,0,2.520465,-2.930134,1.005126\C,0,-1.66156,
-0.791006,-0.095227\H,0,-1.289581,-0.561216,0.909903\H,0,-1.810571,-1.
87791,-0.141391\C,0,-3.003087,-0.089126,-0.344398\H,0,-3.360426,-0.342
591,-1.353227\H,0,-2.858409,0.99948,-0.329732\C,0,-4.069476,-0.471427,
0.686717\H,0,-4.254749,-1.55283,0.685156\H,0,-3.756897,-0.19052,1.6997
61\H,0,-5.021657,0.030547,0.480563\\Version=IA32L-G03RevD.01\State=2-A
\HF=-655.1280496\S2=0.760424\S2-1=0.\S2A=0.750049\RMSD=6.722e-09\Therm
al=0.\Dipole=-0.3048346,-0.1099615,0.1467864\PG=C01 [X(C11H17O3)]\\@

cShaC3alpha_003_sp.log

1\1\GINC-NODE-21\SP\UB3LYP\6-311+G(d,p)\C11H17O3(2)\ZIP06\05-Jun-2010\
0\\#P UBecke3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) cShaC3alp
ha_003 sp\\0,2\C,0,-0.939538,-0.192013,0.499521\O,0,-0.312773,0.894676
,-0.187511\C,0,0.861585,1.224085,0.552156\H,0,-1.38263,0.188303,1.4371
32\H,0,0.567684,1.88583,1.391532\C,0,2.043138,-1.362672,-0.724698\C,0,

0.774911,-2.03627,-0.195548\C,0,0.237141,-1.120084,0.902012\C,0,1.4191
49,-0.123555,1.106978\O,0,2.53203,-0.621781,0.386525\H,0,2.820397,-2.0
65822,-1.034392\H,0,1.801563,-0.693402,-1.563643\H,0,-0.007628,-1.6942
6,1.799273\H,0,1.740916,-0.007147,2.145013\C,0,0.293447,-3.198627,-0.5
59148\H,0,0.53955,-3.978954,-1.267983\O,0,1.792493,1.849625,-0.254708\
C,0,1.39117,3.139083,-0.701251\H,0,2.238151,3.553786,-1.252494\H,0,0.5
16914,3.080851,-1.359569\H,0,1.156196,3.797435,0.148965\C,0,-2.038976,
-0.779709,-0.374463\H,0,-2.455515,-1.654779,0.144109\H,0,-1.581798,-1.
1532,-1.296754\C,0,-3.166815,0.207009,-0.724414\H,0,-3.825869,-0.27930
9,-1.455593\H,0,-2.731266,1.076691,-1.230643\C,0,-4.008103,0.672598,0.
469858\H,0,-3.415544,1.249818,1.188685\H,0,-4.832809,1.314573,0.139878
\H,0,-4.444966,-0.179641,1.006022\\Version=IA32L-G03RevD.01\State=2-A\
HF=-655.1270827\S2=0.76011\S2-1=0.\S2A=0.750047\RMSD=4.759e-09\Thermal
=0.\Dipole=-0.5938261,0.1427752,0.1474615\PG=C01 [X(C11H17O3)]\\@

cShaC3alpha_039_sp.log

1\1\GINC-NODE-31\SP\UB3LYP\6-311+G(d,p)\C11H17O3(2)\ZIP06\05-Jun-2010\
0\\#P UBecke3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) cShaC3alp
ha_039 sp\\0,2\C,0,-0.650313,-0.731339,0.885824\O,0,-0.85121,0.698038,
1.066352\C,0,0.303519,1.410801,0.692572\H,0,-1.068353,-1.188279,1.7912
01\H,0,0.272146,2.360272,1.244647\C,0,2.568848,-0.263057,-0.788533\C,0
,1.62838,-1.401182,-0.364159\C,0,0.897262,-0.932441,0.89435\C,0,1.4760
58,0.489128,1.10298\O,0,2.658704,0.603639,0.340677\H,0,3.579156,-0.610
138,-1.025952\H,0,2.154261,0.271132,-1.651363\H,0,1.165913,-1.597419,1
.719937\H,0,1.73579,0.696993,2.145019\C,0,1.538351,-2.576928,-0.934737
\H,0,1.976879,-3.096582,-1.776833\O,0,0.383325,1.665377,-0.68714\C,0,-
0.555265,2.628701,-1.144871\H,0,-0.420372,3.58801,-0.622593\H,0,-0.364
217,2.773449,-2.210801\H,0,-1.587315,2.288371,-1.000772\C,0,-1.40955,-
1.277456,-0.325054\H,0,-1.051726,-2.301127,-0.497009\H,0,-1.12545,-0.6
99754,-1.21286\C,0,-2.940021,-1.31887,-0.167231\H,0,-3.185986,-1.85776
,0.75994\H,0,-3.34598,-1.931134,-0.983941\C,0,-3.650267,0.039928,-0.16
89\H,0,-3.452424,0.582389,-1.102193\H,0,-4.735976,-0.090304,-0.086712\
H,0,-3.314915,0.671733,0.65772\\Version=IA32L-G03RevD.01\State=2-A\HF=
-655.1266115\S2=0.760408\S2-1=0.\S2A=0.750049\RMSD=2.455e-09\Thermal=0
.\Dipole=-0.2136439,-0.1023424,-0.1767713\PG=C01 [X(C11H17O3)]\\@

cShaC3alpha_004_sp.log

1\1\GINC-NODE-25\SP\UB3LYP\6-311+G(d,p)\C11H17O3(2)\ZIP06\05-Jun-2010\
0\\#P UBecke3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) cShaC3alp
ha_004 sp\\0,2\C,0,-0.858579,-0.376632,0.743527\O,0,-0.461548,0.809077
,0.047102\C,0,0.767741,1.238723,0.631078\H,0,-1.202868,-0.097165,1.756
972\H,0,0.532543,1.821154,1.544233\C,0,2.018392,-1.126715,-0.96835\C,0

,0.921559,-1.966296,-0.309319\C,0,0.461823,-1.174383,0.913489\C,0,1.54
5177,-0.059334,1.011331\O,0,2.584799,-0.388316,0.10726\H,0,2.8117,-1.7
20539,-1.429386\H,0,1.58588,-0.4503,-1.720292\H,0,0.417635,-1.817292,1
.796369\H,0,2.004458,0.043853,1.997707\C,0,0.514341,-3.155502,-0.67643
9\H,0,0.729111,-3.86667,-1.463798\O,0,1.493518,2.005702,-0.259453\C,0,
0.894521,3.259885,-0.562062\H,0,-0.047459,3.133326,-1.107862\H,0,0.702
764,3.838877,0.354144\H,0,1.608867,3.801991,-1.185831\C,0,-2.002869,-1
.072538,0.014667\H,0,-2.067652,-2.094099,0.41233\H,0,-1.73287,-1.17188
,-1.043068\C,0,-3.377644,-0.396399,0.155496\H,0,-3.600927,-0.256754,1.
223386\H,0,-4.137276,-1.094989,-0.22036\C,0,-3.525298,0.941478,-0.5791
57\H,0,-2.816462,1.685317,-0.205368\H,0,-3.336447,0.820376,-1.652911\H
,0,-4.540131,1.339372,-0.461105\\Version=IA32L-G03RevD.01\State=2-A\HF
=-655.1261645\S2=0.760103\S2-1=0.\S2A=0.750047\RMSD=5.430e-09\Thermal=
0.\Dipole=-0.5397474,0.0352534,0.2775804\PG=C01 [X(C11H17O3)]\\@

cShaC3alpha_007_sp.log

1\1\GINC-NODE-21\SP\UB3LYP\6-311+G(d,p)\C11H17O3(2)\ZIP06\05-Jun-2010\
0\\#P UBecke3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) cShaC3alp
ha_007 sp\\0,2\C,0,0.766715,-0.711953,0.163405\O,0,-0.459763,-1.168132
,-0.414943\C,0,-1.492756,-0.854497,0.516412\H,0,1.026022,-1.376206,1.0
06807\H,0,-1.527379,-1.658165,1.279059\C,0,-1.159342,2.066291,-0.48914
5\C,0,0.330324,1.835053,-0.220952\C,0,0.408496,0.671755,0.767048\C,0,-
1.08407,0.496132,1.183867\O,0,-1.800642,1.615983,0.697254\H,0,-1.42178
5,3.116288,-0.641367\H,0,-1.489493,1.478243,-1.358076\H,0,1.063065,0.9
20938,1.60599\H,0,-1.252974,0.457597,2.262976\C,0,1.326362,2.544485,-0
.689632\H,0,1.462009,3.391832,-1.349611\O,0,-2.713524,-0.741407,-0.121
775\C,0,-3.192987,-1.967473,-0.660861\H,0,-4.191089,-1.763676,-1.05517
9\H,0,-2.545616,-2.330851,-1.466995\H,0,-3.263209,-2.74187,0.118235\C,
0,1.862102,-0.788277,-0.893018\H,0,1.5784,-0.138254,-1.727672\H,0,1.87
1552,-1.816682,-1.278056\C,0,3.26855,-0.408137,-0.400082\H,0,3.26194,0
.629282,-0.040377\H,0,3.940013,-0.417304,-1.268505\C,0,3.846006,-1.331
178,0.68071\H,0,3.270882,-1.289002,1.613112\H,0,3.855266,-2.376126,0.3
46066\H,0,4.877434,-1.050799,0.92279\\Version=IA32L-G03RevD.01\State=2
-A\HF=-655.1261953\S2=0.760106\S2-1=0.\S2A=0.750047\RMSD=5.195e-09\The
rmal=0.\Dipole=0.4873361,-0.4222792,0.0605199\PG=C01 [X(C11H17O3)]\\@

cShaC3alpha_019_sp.log

1\1\GINC-NODE-31\SP\UB3LYP\6-311+G(d,p)\C11H17O3(2)\ZIP06\05-Jun-2010\
0\\#P UBecke3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) cShaC3alp
ha_019 sp\\0,2\C,0,0.90643,-0.193566,0.783567\O,0,0.204218,-1.13156,-0
.038974\C,0,-1.138978,-1.17771,0.378497\H,0,1.093729,-0.656595,1.77003
5\H,0,-1.270801,-1.956462,1.156346\C,0,-1.554158,1.636735,-0.842866\C,

0,-0.241685,1.974878,-0.131004\C,0,-0.097079,0.962947,1.005476\C,0,-1.
471858,0.240084,0.978813\O,0,-2.344381,1.000191,0.158692\H,0,-2.100076
,2.513718,-1.199939\H,0,-1.371924,0.950714,-1.681976\H,0,0.104815,1.47
5706,1.949738\H,0,-1.951273,0.150616,1.957259\C,0,0.558377,2.976569,-0
.39847\H,0,0.613579,3.788712,-1.111974\O,0,-1.885858,-1.508609,-0.7525
48\C,0,-3.205043,-1.94371,-0.463916\H,0,-3.6363,-2.271505,-1.412607\H,
0,-3.20145,-2.792476,0.238047\H,0,-3.818766,-1.133666,-0.05146\C,0,2.2
44273,0.135138,0.137125\H,0,2.717309,0.939785,0.717519\H,0,2.05862,0.5
39959,-0.864246\C,0,3.187027,-1.072946,0.052377\H,0,2.68934,-1.872954,
-0.508089\H,0,3.364088,-1.467657,1.063461\C,0,4.52785,-0.731904,-0.604
736\H,0,4.385629,-0.370553,-1.630531\H,0,5.057097,0.052257,-0.048764\H
,0,5.183624,-1.608873,-0.649353\\Version=IA32L-G03RevD.01\State=2-A\HF
=-655.1258666\S2=0.760207\S2-1=0.\S2A=0.750047\RMSD=4.151e-09\Thermal=
0.\Dipole=-0.1199572,0.1340666,0.5554025\PG=C01 [X(C11H17O3)]\\@

cShaC3alpha_006_sp.log

1\1\GINC-NODE-28\SP\UB3LYP\6-311+G(d,p)\C11H17O3(2)\ZIP06\05-Jun-2010\
0\\#P UBecke3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) cShaC3alp
ha_006 sp\\0,2\C,0,0.052202,0.553096,1.148039\O,0,0.848464,-0.632425,1
.347281\C,0,0.357951,-1.697301,0.540617\H,0,0.121061,1.112441,2.088028
\H,0,0.431747,-2.599581,1.166744\C,0,-2.391847,-0.127369,-1.250898\C,0
,-2.34971,0.699181,0.048757\C,0,-1.380966,-0.027668,0.967029\C,0,-1.11
3708,-1.346895,0.213773\O,0,-1.30855,-1.040847,-1.16246\H,0,-3.353333,
-0.662578,-1.321839\H,0,-2.257798,0.471644,-2.156223\H,0,-1.81438,-0.2
00672,1.956083\H,0,-1.791209,-2.157215,0.520801\C,0,-3.037172,1.78182,
0.315301\H,0,-3.755356,2.422779,-0.179251\O,0,1.080676,-1.883538,-0.63
8789\C,0,2.400219,-2.360151,-0.419817\H,0,2.393417,-3.318232,0.123424\
H,0,2.844543,-2.512263,-1.406168\H,0,3.001504,-1.638049,0.145507\C,0,0
.583433,1.422966,0.004947\H,0,-0.092554,2.280089,-0.114073\H,0,0.54749
1,0.851134,-0.929952\C,0,2.01037,1.925078,0.257372\H,0,2.672362,1.0629
86,0.401205\H,0,2.035313,2.491736,1.199847\C,0,2.539971,2.803456,-0.88
0433\H,0,1.912042,3.691868,-1.022957\H,0,3.561034,3.146837,-0.677729\H
,0,2.554931,2.254276,-1.829813\\Version=IA32L-G03RevD.01\State=2-A\HF=
-655.125333\S2=0.76052\S2-1=0.\S2A=0.75005\RMSD=8.473e-09\Thermal=0.\D
ipole=-0.4040231,0.0063476,0.1683208\PG=C01 [X(C11H17O3)]\\@

29d

ShaC4alpha_001_sp.log

1\1\GINC-NODE-25\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\04-Oct-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC4alpha_00
1\\0,2\C,0,0.758353,-1.219851,-0.481604\O,0,0.366778,-0.049194,-1.2454
53\C,0,-0.804055,0.519286,-0.694112\H,0,1.095306,-1.960665,-1.225462\H

,0,-1.318399,1.014317,-1.53014\C,0,-3.459612,0.448469,0.908342\C,0,-0.
495995,-1.641075,0.202823\C,0,-1.59313,-0.679516,-0.083618\O,0,-2.3370
77,-0.406386,1.093398\H,0,-3.136324,1.431807,0.53874\H,0,-2.279213,-1.
065453,-0.860631\O,0,-0.550453,1.450094,0.326455\C,0,0.085186,2.633985
,-0.135509\H,0,1.078145,2.422998,-0.549757\H,0,-0.519825,3.135678,-0.9
06819\H,0,0.183369,3.295309,0.728557\C,0,1.935063,-0.913037,0.464169\H
,0,1.616808,-0.128145,1.160375\H,0,2.132355,-1.813516,1.063811\C,0,3.2
09882,-0.493256,-0.27723\H,0,2.982887,0.368806,-0.918088\H,0,3.520842,
-1.303777,-0.953967\H,0,-3.870192,0.597582,1.912806\C,0,-4.498115,-0.1
03655,0.025292\C,0,-5.349536,-0.551541,-0.705395\H,0,-6.107379,-0.9488
99,-1.342063\C,0,4.370575,-0.145685,0.663189\H,0,4.587509,-1.008738,1.
308974\H,0,4.059685,0.665608,1.336559\C,0,5.644929,0.267815,-0.08034\H
,0,5.468416,1.149325,-0.708931\H,0,6.45397,0.512615,0.61741\H,0,6.0014
5,-0.537432,-0.734535\H,0,-0.604669,-2.515165,0.831919\\Version=IA32L-
G03RevD.01\State=2-A\HF=-694.4265725\S2=0.75412\S2-1=0.\S2A=0.750012\R
MSD=8.861e-09\Thermal=0.\Dipole=0.0162613,0.1732463,-0.291285\PG=C01 [
X(C12H19O3)]\\@

ShaC4alpha_003_sp.log

1\1\GINC-NODE-28\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\04-Oct-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC4alpha_00
3\\0,2\C,0,-0.888056,0.024944,1.228299\O,0,0.023902,1.134753,1.427959\
C,0,1.141595,1.003552,0.5738\H,0,-1.261909,-0.241737,2.230228\H,0,1.97
2843,1.505119,1.089585\C,0,3.143652,-0.589388,-1.187625\C,0,-0.029116,
-1.046166,0.648253\C,0,1.342963,-0.532445,0.393056\O,0,1.804083,-0.959
106,-0.879914\H,0,3.24756,0.504752,-1.195729\H,0,2.054739,-0.876617,1.
166217\O,0,0.950013,1.581187,-0.692029\C,0,0.827648,2.996648,-0.648422
\H,0,1.722259,3.459541,-0.203242\H,0,0.726061,3.335255,-1.682135\H,0,-
0.052306,3.305652,-0.072486\C,0,-2.090848,0.449424,0.362211\H,0,-2.518
406,1.353774,0.816529\H,0,-1.719269,0.728555,-0.630612\C,0,-3.169433,-
0.634184,0.246827\H,0,-3.492988,-0.941616,1.253076\H,0,-2.743265,-1.53
0726,-0.225507\H,0,3.305038,-0.939051,-2.213039\C,0,4.151698,-1.183889
,-0.29691\C,0,4.98143,-1.665424,0.437335\H,0,5.716869,-2.097169,1.0778
56\C,0,-4.394925,-0.180939,-0.557951\H,0,-4.071527,0.133951,-1.559942\
H,0,-4.829611,0.710684,-0.084236\C,0,-5.467764,-1.267206,-0.684414\H,0
,-6.329104,-0.912598,-1.2619\H,0,-5.07276,-2.157793,-1.18851\H,0,-5.83
3918,-1.580379,0.301183\H,0,-0.337341,-2.063839,0.447795\\Version=IA32
L-G03RevD.01\State=2-A\HF=-694.4264259\S2=0.754115\S2-1=0.\S2A=0.75001
2\RMSD=6.987e-09\Thermal=0.\Dipole=0.067038,0.2295924,0.1838818\PG=C01
[X(C12H19O3)]\\@

ShaC4alpha_007_sp.log

1\1\GINC-NODE-21\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\04-Oct-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC4alpha_00
7\\0,2\C,0,0.849894,-0.968588,-0.792745\O,0,0.308272,0.240149,-1.38644
4\C,0,-0.855772,0.640625,-0.691719\H,0,1.190788,-1.587243,-1.639184\H,
0,-1.47212,1.178414,-1.426087\C,0,-3.350322,0.170705,1.089488\C,0,-0.3
12527,-1.5742,-0.084425\C,0,-1.498571,-0.681657,-0.171092\O,0,-2.15840
4,-0.606941,1.083141\H,0,-3.128399,1.214452,0.826084\H,0,-2.217551,-1.
033325,-0.934337\O,0,-0.594273,1.471997,0.409629\C,0,-0.090154,2.74911
3,0.043877\H,0,-0.790323,3.277671,-0.62174\H,0,0.023359,3.31888,0.9691
37\H,0,0.881005,2.67008,-0.458708\C,0,2.064178,-0.669612,0.107807\H,0,
1.734182,-0.006135,0.916323\H,0,2.373622,-1.615169,0.573242\C,0,3.2351
83,-0.04107,-0.65943\H,0,2.863927,0.840102,-1.196953\H,0,3.584827,-0.7
45803,-1.42958\H,0,-3.687396,0.16274,2.131658\C,0,-4.415759,-0.35142,0
.220423\C,0,-5.291579,-0.774111,-0.496309\H,0,-6.06958,-1.149704,-1.12
1772\C,0,4.423272,0.371168,0.224716\H,0,4.077378,1.088623,0.98246\H,0,
5.148517,0.912965,-0.39742\C,0,5.137001,-0.796152,0.917348\H,0,4.47885
,-1.317764,1.621294\H,0,5.49031,-1.532862,0.184683\H,0,6.0084,-0.44556
3,1.48217\H,0,-0.303613,-2.520801,0.440477\\Version=IA32L-G03RevD.01\S
tate=2-A\HF=-694.4253413\S2=0.754118\S2-1=0.\S2A=0.750012\RMSD=5.433e-
09\Thermal=0.\Dipole=-0.0087611,0.2362597,-0.2837316\PG=C01 [X(C12H19O
3)]\\@

ShaC4alpha_009_sp.log

1\1\GINC-NODE-25\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\04-Oct-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC4alpha_00
9\\0,2\C,0,0.96802,-0.919098,-0.025392\O,0,0.538757,0.120217,-0.94429\
C,0,-0.759398,0.562624,-0.601663\H,0,1.486298,-1.666515,-0.645853\H,0,
-1.21266,0.914752,-1.5392\C,0,-3.581848,0.251822,0.636848\C,0,-0.30423
6,-1.451505,0.53825\C,0,-1.464969,-0.683058,0.015847\O,0,-2.401419,-0.
427247,1.050324\H,0,-3.332545,1.244584,0.236288\H,0,-1.974086,-1.22368
9,-0.80398\O,0,-0.768971,1.596096,0.349104\C,0,-0.229262,2.816391,-0.1
39877\H,0,0.830132,2.711891,-0.402037\H,0,-0.779804,3.167807,-1.026446
\H,0,-0.335744,3.550684,0.662057\C,0,1.951477,-0.37051,1.028264\H,0,1.
423626,0.398095,1.603245\H,0,2.190522,-1.185807,1.726676\C,0,3.248648,
0.207623,0.439712\H,0,3.773082,0.758961,1.232934\H,0,2.990873,0.946395
,-0.330556\H,0,-4.155886,0.40676,1.556751\C,0,-4.396458,-0.491553,-0.3
36325\C,0,-5.064649,-1.095001,-1.141813\H,0,-5.661216,-1.630118,-1.845
626\C,0,4.209468,-0.834157,-0.15138\H,0,3.716946,-1.379875,-0.967502\H
,0,4.448098,-1.583488,0.617315\C,0,5.507145,-0.21277,-0.678996\H,0,6.1
76951,-0.974638,-1.09396\H,0,5.301657,0.517744,-1.470954\H,0,6.049393,
0.309249,0.119156\H,0,-0.38621,-2.280157,1.229738\\Version=IA32L-G03Re

vD.01\State=2-A\HF=-694.4253092\S2=0.754117\S2-1=0.\S2A=0.750012\RMSD=
6.169e-09\Thermal=0.\Dipole=0.0517889,0.1453363,-0.321515\PG=C01 [X(C1
2H19O3)]\\@

ShaC4alpha_005_sp.log

1\1\GINC-NODE-28\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\04-Oct-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC4alpha_00
5\\0,2\C,0,0.780069,-1.377422,-0.474442\O,0,0.371892,-0.309383,-1.3683
28\C,0,-0.740557,0.376151,-0.828946\H,0,1.03959,-2.227673,-1.126859\H,
0,-1.297926,0.766872,-1.692183\C,0,-3.274939,0.635905,0.94539\C,0,-0.4
3453,-1.647868,0.344502\C,0,-1.519365,-0.69178,-0.000992\O,0,-2.165881
,-0.226162,1.173287\H,0,-2.953318,1.543006,0.414476\H,0,-2.272488,-1.1
54202,-0.666032\O,0,-0.388711,1.432539,0.027016\C,0,0.251099,2.510123,
-0.642704\H,0,-0.386847,2.915855,-1.443317\H,0,0.424402,3.286932,0.105
697\H,0,1.208592,2.201308,-1.078239\C,0,2.031113,-0.991336,0.33808\H,0
,1.782957,-0.109027,0.937374\H,0,2.24355,-1.809652,1.041905\C,0,3.2603
62,-0.738663,-0.544821\H,0,3.02659,0.058034,-1.263224\H,0,3.456283,-1.
640963,-1.14255\H,0,-3.604376,0.943122,1.943808\C,0,-4.391865,0.002726
,0.227955\C,0,-5.308119,-0.512734,-0.367191\H,0,-6.122519,-0.968301,-0
.883679\C,0,4.535016,-0.373521,0.233863\H,0,5.379418,-0.356001,-0.4684
14\H,0,4.759123,-1.170587,0.957547\C,0,4.468656,0.973828,0.963222\H,0,
5.42016,1.201246,1.457474\H,0,4.254962,1.790259,0.261754\H,0,3.68784,0
.985282,1.731648\H,0,-0.526031,-2.423921,1.093518\\Version=IA32L-G03Re
vD.01\State=2-A\HF=-694.4252084\S2=0.754118\S2-1=0.\S2A=0.750012\RMSD=
3.038e-09\Thermal=0.\Dipole=0.0205476,0.109417,-0.332943\PG=C01 [X(C12
H19O3)]\\@

ShaC4alpha_021_sp.log

1\1\GINC-NODE-21\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\04-Oct-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC4alpha_02
1\\0,2\C,0,0.950976,-1.222572,-0.714114\O,0,0.64712,-0.031143,-1.48587
1\C,0,-0.638745,0.448226,-1.148124\H,0,1.471876,-1.90098,-1.409744\H,0
,-1.008709,0.967424,-2.044038\C,0,-3.546259,0.136133,-0.158072\C,0,-0.
385928,-1.744761,-0.31514\C,0,-1.461662,-0.820638,-0.762142\O,0,-2.436
832,-0.656963,0.249776\H,0,-3.930987,-0.218154,-1.130771\H,0,-1.958967
,-1.19029,-1.683328\O,0,-0.644131,1.324662,-0.052959\C,0,-0.001815,2.5
64394,-0.317815\H,0,-0.115484,3.174662,0.580989\H,0,1.063915,2.427527,
-0.535898\H,0,-0.472669,3.082568,-1.167741\C,0,1.896669,-0.916443,0.46
2772\H,0,1.399809,-0.195075,1.122037\H,0,2.026979,-1.84259,1.041227\C,
0,3.264528,-0.387499,0.015682\H,0,3.118123,0.508024,-0.602132\H,0,3.74
7983,-1.132215,-0.634895\H,0,-3.237939,1.183825,-0.286736\C,0,-4.60501
3,0.053462,0.845651\C,0,-5.499637,0.008197,1.653695\H,0,-6.281564,-0.0

4037,2.377088\C,0,4.197572,-0.057703,1.187954\H,0,4.33657,-0.955844,1.
806509\H,0,3.713406,0.685383,1.837231\C,0,5.564031,0.469608,0.73817\H,
0,6.206423,0.700834,1.595535\H,0,6.088824,-0.267277,0.117636\H,0,5.458
299,1.385409,0.143616\H,0,-0.563437,-2.64774,0.254746\\Version=IA32L-G
03RevD.01\State=2-A\HF=-694.4248763\S2=0.754106\S2-1=0.\S2A=0.750012\R
MSD=9.117e-09\Thermal=0.\Dipole=0.1673283,0.1558873,-0.4360412\PG=C01
[X(C12H19O3)]\\@

ShaC4alpha_011_sp.log

1\1\GINC-NODE-21\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\04-Oct-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC4alpha_01
1\\0,2\C,0,0.8934,-0.331502,-1.331119\O,0,0.085967,0.83983,-1.615807\C
,0,-0.987912,0.920009,-0.701807\H,0,1.178895,-0.745622,-2.31198\H,0,-1
.790672,1.455301,-1.228671\C,0,-3.06702,-0.253581,1.275691\C,0,-0.0324
88,-1.235112,-0.590446\C,0,-1.335084,-0.558173,-0.350142\O,0,-1.787634
,-0.798769,0.973193\H,0,-3.053342,0.840123,1.16738\H,0,-2.10729,-0.904
309,-1.062289\O,0,-0.663822,1.596914,0.485539\C,0,-0.393571,2.978151,0
.286339\H,0,-0.189286,3.403614,1.271621\H,0,0.475047,3.12663,-0.365476
\H,0,-1.260313,3.493349,-0.156408\C,0,2.181469,0.059309,-0.579862\H,0,
2.664988,0.859904,-1.157086\H,0,1.89546,0.482715,0.388641\C,0,3.156704
,-1.112669,-0.405533\H,0,3.340693,-1.574482,-1.386866\H,0,2.692293,-1.
889986,0.218142\H,0,-3.224749,-0.473407,2.337059\C,0,-4.166797,-0.8230
53,0.482352\C,0,-5.070813,-1.283517,-0.173508\H,0,-5.872226,-1.695502,
-0.744096\C,0,4.508421,-0.717743,0.213062\H,0,4.981022,0.051178,-0.414
706\H,0,5.175308,-1.589822,0.179332\C,0,4.41978,-0.214416,1.658587\H,0
,5.416322,-0.00058,2.061658\H,0,3.829305,0.705184,1.735926\H,0,3.95125
5,-0.963786,2.308861\H,0,0.184656,-2.250525,-0.286118\\Version=IA32L-G
03RevD.01\State=2-A\HF=-694.4250335\S2=0.754117\S2-1=0.\S2A=0.750012\R
MSD=5.852e-09\Thermal=0.\Dipole=-0.0388108,0.196776,-0.2210115\PG=C01
[X(C12H19O3)]\\@

ShaC4alpha_015_sp.log

1\1\GINC-NODE-21\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\04-Oct-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC4alpha_01
5\\0,2\C,0,-0.915737,-0.414809,1.098447\O,0,-0.165729,0.766353,1.48181
4\C,0,0.98281,0.894772,0.669118\H,0,-1.277541,-0.85963,2.039788\H,0,1.
722295,1.433095,1.2789\C,0,3.248947,-0.180865,-1.156472\C,0,0.094982,-
1.27858,0.424206\C,0,1.395553,-0.565538,0.312653\O,0,1.962696,-0.76192
9,-0.973493\H,0,3.199607,0.909458,-1.026637\H,0,2.113878,-0.912221,1.0
78785\O,0,0.749381,1.596313,-0.525057\C,0,0.427218,2.964981,-0.316782\
H,0,1.235327,3.486823,0.219343\H,0,0.305773,3.413135,-1.305688\H,0,-0.
502236,3.07545,0.253559\C,0,-2.141334,-0.033007,0.244309\H,0,-2.678,0.

753667,0.789393\H,0,-1.784816,0.40604,-0.695119\C,0,-3.071267,-1.22020
9,-0.039288\H,0,-3.413961,-1.653519,0.912908\H,0,-2.501489,-2.009085,-
0.548701\H,0,3.49923,-0.372463,-2.20549\C,0,4.293184,-0.743929,-0.2872
23\C,0,5.152033,-1.200794,0.429069\H,0,5.914138,-1.608138,1.054223\C,0
,-4.295526,-0.869917,-0.902469\H,0,-4.817854,-1.80133,-1.159002\H,0,-3
.952235,-0.441488,-1.854686\C,0,-5.289582,0.090243,-0.23868\H,0,-5.653
926,-0.314892,0.71396\H,0,-4.839183,1.067535,-0.032415\H,0,-6.16057,0.
259619,-0.882009\H,0,-0.066908,-2.292049,0.081449\\Version=IA32L-G03Re
vD.01\State=2-A\HF=-694.4249878\S2=0.754114\S2-1=0.\S2A=0.750012\RMSD=
4.457e-09\Thermal=0.\Dipole=0.0220643,0.1866096,0.2033004\PG=C01 [X(C1
2H19O3)]\\@

ShaC4alpha_027_sp.log

1\1\GINC-NODE-21\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\04-Oct-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC4alpha_02
7\\0,2\C,0,1.107139,0.714681,-1.14406\O,0,0.268492,1.872503,-0.894367\
C,0,-0.997068,1.458205,-0.423912\H,0,1.668368,0.943415,-2.064664\H,0,-
1.70119,2.247319,-0.725172\C,0,-3.358872,-0.510082,-0.185218\C,0,0.134
024,-0.396567,-1.34434\C,0,-1.254995,0.079696,-1.107127\O,0,-1.992464,
-0.868955,-0.359749\H,0,-3.804434,-0.222416,-1.153937\H,0,-1.785385,0.
274017,-2.062906\O,0,-1.049685,1.276706,0.966188\C,0,-0.89665,2.485575
,1.698256\H,0,0.085448,2.93946,1.522248\H,0,-1.677081,3.214453,1.42937
2\H,0,-0.997093,2.22699,2.754783\C,0,2.120049,0.511793,-0.000038\H,0,2
.635677,1.469929,0.151805\H,0,1.564224,0.292452,0.918895\C,0,3.146851,
-0.591494,-0.282364\H,0,3.661502,-0.382388,-1.232749\H,0,2.630687,-1.5
52523,-0.41773\H,0,-3.441094,0.356694,0.486408\C,0,-4.096387,-1.640487
,0.374764\C,0,-4.737045,-2.552556,0.836344\H,0,-5.289356,-3.367895,1.2
45323\C,0,4.190658,-0.73885,0.832913\H,0,3.676444,-0.942939,1.782416\H
,0,4.712176,0.219126,0.968711\C,0,5.214279,-1.844751,0.557068\H,0,5.94
4032,-1.925839,1.370651\H,0,4.724491,-2.820512,0.450561\H,0,5.768634,-
1.650433,-0.369507\H,0,0.3813,-1.411916,-1.624794\\Version=IA32L-G03Re
vD.01\State=2-A\HF=-694.4246409\S2=0.754103\S2-1=0.\S2A=0.750012\RMSD=
6.164e-09\Thermal=0.\Dipole=0.055353,0.4259283,-0.1731368\PG=C01 [X(C1
2H19O3)]\\@

ShaC4alpha_026_sp.log

1\1\GINC-NODE-25\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\04-Oct-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC4alpha_02
6\\0,2\C,0,-0.71166,-1.670566,0.829858\O,0,-0.232964,-0.648337,1.73995
2\C,0,0.777475,0.148004,1.153151\H,0,-0.651832,-2.619254,1.39188\H,0,1
.510104,0.345337,1.949652\C,0,2.818094,0.88622,-1.09148\C,0,0.259903,-
1.652661,-0.296953\C,0,1.359202,-0.690533,-0.028495\O,0,1.683852,0.033

552,-1.205552\H,0,2.650419,1.647063,-0.316669\H,0,2.267733,-1.207636,0
.333316\O,0,0.300473,1.370888,0.65476\C,0,-0.145131,2.253263,1.676715\
H,0,-0.996629,1.833743,2.224962\H,0,0.663299,2.473459,2.391211\H,0,-0.
448497,3.179023,1.182311\C,0,-2.194132,-1.466055,0.460497\H,0,-2.53976
4,-2.390505,-0.025452\H,0,-2.754136,-1.385911,1.402289\C,0,-2.497391,-
0.263443,-0.438655\H,0,-1.983814,-0.389139,-1.401982\H,0,-2.07089,0.64
1944,0.007842\H,0,2.876829,1.407904,-2.05276\C,0,4.079729,0.175219,-0.
835142\C,0,5.116756,-0.405886,-0.61976\H,0,6.035294,-0.916497,-0.43788
6\C,0,-3.999682,-0.069198,-0.680685\H,0,-4.509946,0.05627,0.285325\H,0
,-4.419795,-0.981938,-1.127882\C,0,-4.312826,1.129708,-1.581804\H,0,-3
.939359,2.062639,-1.142074\H,0,-3.841606,1.018828,-2.566095\H,0,-5.391
738,1.242852,-1.739072\H,0,0.231411,-2.311444,-1.155675\\Version=IA32L
-G03RevD.01\State=2-A\HF=-694.424496\S2=0.75414\S2-1=0.\S2A=0.750012\R
MSD=8.575e-09\Thermal=0.\Dipole=0.1987179,-0.0421251,0.3429542\PG=C01
[X(C12H19O3)]\\@

ShaC4alpha_013_sp.log

1\1\GINC-NODE-25\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\04-Oct-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC4alpha_01
3\\0,2\C,0,-1.091878,0.096329,0.781088\O,0,-0.135521,1.048931,1.315283
\C,0,1.099405,0.926009,0.640665\H,0,-1.644542,-0.285919,1.652608\H,0,1
.866982,1.244153,1.360531\C,0,3.25222,-0.593219,-0.993907\C,0,-0.24103
8,-0.954807,0.154098\C,0,1.19491,-0.57564,0.233587\O,0,1.853065,-0.853
828,-0.992532\H,0,3.443981,0.471709,-0.801075\H,0,1.711286,-1.116074,1
.048808\O,0,1.184577,1.70993,-0.521909\C,0,1.173497,3.106404,-0.257044
\H,0,2.011754,3.393736,0.396843\H,0,1.281703,3.609894,-1.220527\H,0,0.
234926,3.416635,0.216448\C,0,-2.081428,0.800332,-0.171415\H,0,-2.51619
7,1.647912,0.376316\H,0,-1.501393,1.215198,-1.002879\C,0,-3.204023,-0.
097859,-0.714758\H,0,-2.766886,-0.951788,-1.251957\H,0,-3.761389,0.473
503,-1.470104\H,0,3.577898,-0.802254,-2.018591\C,0,4.020011,-1.420876,
-0.051222\C,0,4.652941,-2.095174,0.726052\H,0,5.215343,-2.695087,1.405
284\C,0,-4.196862,-0.610977,0.339604\H,0,-4.61043,0.245098,0.891629\H,
0,-3.67433,-1.227725,1.083444\C,0,-5.341087,-1.427324,-0.270447\H,0,-4
.959487,-2.306337,-0.804479\H,0,-6.035863,-1.781228,0.499668\H,0,-5.91
5337,-0.829148,-0.988729\H,0,-0.594999,-1.881727,-0.277783\\Version=IA
32L-G03RevD.01\State=2-A\HF=-694.4246046\S2=0.754115\S2-1=0.\S2A=0.750
012\RMSD=8.263e-09\Thermal=0.\Dipole=0.0275983,0.1736818,0.2597467\PG=
C01 [X(C12H19O3)]\\@

ShaC4alpha_006_sp.log

1\1\GINC-NODE-28\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\04-Oct-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC4alpha_00

6\\0,2\C,0,-0.868674,-1.248481,0.616679\O,0,-0.33395,-0.058503,1.25351
5\C,0,0.906814,0.28199,0.657712\H,0,-1.301613,-1.852542,1.431886\H,0,1
.467677,0.841766,1.416036\C,0,3.783659,-0.83637,-0.531522\C,0,0.326849
,-1.902734,0.012971\C,0,1.543079,-1.087176,0.276375\O,0,2.419744,-1.08
0219,-0.838376\H,0,4.327127,-1.044027,-1.459677\H,0,2.091058,-1.461928
,1.164178\O,0,0.772212,1.040897,-0.509644\C,0,0.352444,2.374927,-0.270
96\H,0,1.066427,2.904397,0.378423\H,0,0.318679,2.872478,-1.243126\H,0,
-0.641748,2.41088,0.192136\C,0,-1.992988,-0.90743,-0.379423\H,0,-1.574
349,-0.261267,-1.159393\H,0,-2.307748,-1.840793,-0.8689\C,0,-3.20058,-
0.23697,0.285991\H,0,-2.860673,0.660874,0.818255\H,0,-3.614013,-0.9093
38,1.053302\H,0,4.138934,-1.555203,0.226378\C,0,4.094235,0.526878,-0.0
75601\C,0,4.38662,1.631082,0.31687\H,0,4.639783,2.612912,0.647683\C,0,
-4.307334,0.139449,-0.707097\H,0,-4.638831,-0.761938,-1.24252\H,0,-3.8
92959,0.810768,-1.472564\C,0,-5.51328,0.808168,-0.039037\H,0,-5.970449
,0.146153,0.706752\H,0,-5.219329,1.731159,0.475727\H,0,-6.28541,1.0668
68,-0.772727\H,0,0.328331,-2.848625,-0.513538\\Version=IA32L-G03RevD.0
1\State=2-A\HF=-694.4241691\S2=0.754143\S2-1=0.\S2A=0.750012\RMSD=9.80
1e-09\Thermal=0.\Dipole=0.1808011,-0.0715312,0.316025\PG=C01 [X(C12H19
O3)]\\@

ShaC4alpha_187_sp.log

1\1\GINC-NODE-28\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\04-Oct-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC4alpha_18
7\\0,2\C,0,-0.865666,-0.905421,-1.128467\O,0,-0.097127,-2.102313,-0.82
7331\C,0,1.191968,-1.740361,-0.37759\H,0,-1.406774,-1.122428,-2.06413\
H,0,1.85362,-2.584266,-0.613924\C,0,2.272911,1.164434,0.509204\C,0,0.1
66959,0.153697,-1.328019\C,0,1.528302,-0.441513,-1.159748\O,0,2.562905
,0.378374,-0.652439\H,0,2.556784,0.613631,1.412987\H,0,1.922062,-0.759
002,-2.139768\O,0,1.237594,-1.467966,1.000859\C,0,1.038201,-2.61751,1.
813468\H,0,0.04691,-3.055899,1.649755\H,0,1.804045,-3.381215,1.610813\
H,0,1.126398,-2.289419,2.851706\C,0,-1.905376,-0.634002,-0.025369\H,0,
-2.474807,-1.561804,0.121105\H,0,-1.372091,-0.431677,0.911007\C,0,-2.8
62503,0.51748,-0.356938\H,0,-3.353319,0.322638,-1.322669\H,0,-2.29172,
1.448254,-0.485829\H,0,1.193698,1.359705,0.577322\C,0,3.003773,2.42968
4,0.430328\C,0,3.597317,3.480232,0.396565\H,0,4.126954,4.404774,0.3558
37\C,0,-3.935987,0.733753,0.717867\H,0,-3.446377,0.923819,1.683284\H,0
,-4.510756,-0.194274,0.845778\C,0,-4.890833,1.886756,0.392193\H,0,-5.6
4405,2.016135,1.177629\H,0,-4.348395,2.834975,0.291882\H,0,-5.421156,1
.708259,-0.551422\H,0,-0.022392,1.119667,-1.781045\\Version=IA32L-G03R
evD.01\State=2-A\HF=-694.4243576\S2=0.754059\S2-1=0.\S2A=0.750012\RMSD
=9.697e-09\Thermal=0.\Dipole=-0.7560986,-0.1737819,0.1830812\PG=C01 [X

(C12H19O3)]\\@

ShaC4alpha_022_sp.log

```
1\1\GINC-NODE-28\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\04-Oct-2010\
 0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC4alpha_02
 2\\0,2\C,0,-0.86314,-1.280434,0.224278\O,0,-0.610295,-0.028135,0.91586
 9\C,0,0.612153,0.534331,0.479414\H,0,-1.25174,-1.969653,0.993317\H,0,0
 .991898,1.119061,1.329149\C,0,3.47122,0.427042,-0.705707\C,0,0.481592,
 -1.697209,-0.264491\C,0,1.506153,-0.683738,0.09733\O,0,2.414357,-0.487
 247,-0.974344\H,0,3.068044,1.428316,-0.498333\H,0,2.073134,-0.98234,0.
 999149\O,0,0.481346,1.360969,-0.647177\C,0,-0.219407,2.569075,-0.38349
 2\H,0,0.274333,3.149695,0.411328\H,0,-0.206067,3.148034,-1.309968\H,0,
 -1.256708,2.376177,-0.087033\C,0,-1.928859,-1.150117,-0.883752\H,0,-1.
 634827,-0.326292,-1.544747\H,0,-1.87905,-2.069089,-1.484597\C,0,-3.373
 644,-0.972827,-0.386717\H,0,-3.611014,-1.78664,0.316092\H,0,-4.049761,
 -1.111342,-1.242702\H,0,4.034898,0.490837,-1.642691\C,0,4.367025,0.010
 808,0.384008\C,0,5.10113,-0.324432,1.282967\H,0,5.756098,-0.622162,2.0
 70343\C,0,-3.692136,0.37477,0.276271\H,0,-3.456784,1.183356,-0.430916\
 H,0,-3.035066,0.525693,1.139456\C,0,-5.158393,0.485952,0.707196\H,0,-5
 .835809,0.367741,-0.148073\H,0,-5.416171,-0.288674,1.44038\H,0,-5.3684
 11,1.45903,1.166041\H,0,0.697578,-2.615763,-0.794827\\Version=IA32L-G0
 3RevD.01\State=2-A\HF=-694.4240987\S2=0.754128\S2-1=0.\S2A=0.750012\RM
 SD=6.237e-09\Thermal=0.\Dipole=-0.0039057,0.1951789,0.3016559\PG=C01 [
 X(C12H19O3)]\\@
```

ShaC4alpha_002_sp.log

```
1\1\GINC-NODE-25\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\04-Oct-2010\
 0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC4alpha_00
 2\\0,2\C,0,-0.622665,-1.004257,0.553912\O,0,-0.41071,0.254121,1.247642
 \C,0,0.672517,0.945248,0.65206\H,0,-0.84807,-1.742036,1.34232\H,0,1.08
 6435,1.59973,1.430864\C,0,3.591499,-0.567455,-1.119384\C,0,0.686499,-1
 .278188,-0.107798\C,0,1.642965,-0.172324,0.201102\O,0,2.472228,0.26814
 7,-0.865781\H,0,4.052231,-0.16175,-2.026542\H,0,2.281444,-0.427153,1.0
 66768\O,0,0.297769,1.699079,-0.466081\C,0,-0.473886,2.845014,-0.140802
 \H,0,0.071842,3.509306,0.547006\H,0,-0.657407,3.376062,-1.077766\H,0,-
 1.432402,2.572585,0.318585\C,0,-1.828036,-0.935542,-0.401867\H,0,-1.62
 3047,-0.168241,-1.15731\H,0,-1.895154,-1.89772,-0.930898\C,0,-3.15163,
 -0.645474,0.315522\H,0,-3.054523,0.29197,0.878258\H,0,-3.342213,-1.431
 881,1.06185\H,0,3.274357,-1.597463,-1.348936\C,0,4.580347,-0.595224,-0
 .029884\C,0,5.390144,-0.620638,0.865888\H,0,6.110602,-0.637827,1.65223
 \C,0,-4.348452,-0.55295,-0.639437\H,0,-4.437769,-1.492407,-1.203725\H,
 0,-4.156024,0.231074,-1.385547\C,0,-5.670135,-0.261419,0.078746\H,0,-5
```

.908616,-1.048392,0.804892\H,0,-5.622018,0.688145,0.625884\H,0,-6.5049
35,-0.196834,-0.628591\H,0,0.915967,-2.178692,-0.663931\\Version=IA32L
-G03RevD.01\State=2-A\HF=-694.4239091\S2=0.754118\S2-1=0.\S2A=0.750012
\RMSD=9.039e-09\Thermal=0.\Dipole=0.068391,-0.4520615,0.1110124\PG=C01
[X(C12H19O3)]\\@

ShaC4alpha_014_sp.log

1\1\GINC-NODE-25\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\04-Oct-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC4alpha_01
4\\0,2\C,0,-0.957753,-0.042479,1.234862\O,0,0.092293,0.927086,1.484357
\C,0,1.217346,0.625769,0.677045\H,0,-1.411923,-0.253803,2.217263\H,0,2
.0869,1.049425,1.19435\C,0,3.178095,-1.745265,-0.532223\C,0,-0.230544,
-1.227307,0.693924\C,0,1.22366,-0.928022,0.586302\O,0,1.784176,-1.4852
54,-0.591719\H,0,3.398239,-2.331524,-1.431029\H,0,1.776174,-1.314545,1
.466122\O,0,1.122257,1.139829,-0.620897\C,0,1.244236,2.552655,-0.67515
3\H,0,2.213133,2.881614,-0.268984\H,0,1.186147,2.833046,-1.729563\H,0,
0.439365,3.049374,-0.119242\C,0,-2.047617,0.547214,0.31913\H,0,-2.3533
97,1.508097,0.755311\H,0,-1.598869,0.762204,-0.65723\C,0,-3.271429,-0.
362963,0.161266\H,0,-3.678174,-0.609442,1.154128\H,0,-2.968466,-1.3179
35,-0.291519\H,0,3.411192,-2.379302,0.340148\C,0,4.041463,-0.555338,-0
.499354\C,0,4.783901,0.396374,-0.457461\H,0,5.432767,1.242558,-0.43675
8\C,0,-4.379988,0.26526,-0.694011\H,0,-3.974262,0.51081,-1.685341\H,0,
-4.684624,1.221056,-0.244776\C,0,-5.605684,-0.640021,-0.852202\H,0,-6.
054263,-0.874333,0.121224\H,0,-6.377447,-0.164719,-1.468356\H,0,-5.337
475,-1.590713,-1.329468\H,0,-0.668943,-2.190427,0.467049\\Version=IA32
L-G03RevD.01\State=2-A\HF=-694.4238327\S2=0.754136\S2-1=0.\S2A=0.75001
2\RMSD=9.715e-09\Thermal=0.\Dipole=0.1513182,-0.0737021,0.2813573\PG=C
01 [X(C12H19O3)]\\@

ShaC4alpha_029_sp.log

1\1\GINC-NODE-21\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\04-Oct-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) ShaC4alpha_02
9\\0,2\C,0,-1.078846,-0.706157,0.21543\O,0,-0.511474,0.332608,1.056636
\C,0,0.794554,0.650174,0.619124\H,0,-1.612577,-1.382772,0.900966\H,0,1
.331722,1.001404,1.511606\C,0,3.504169,0.047373,-0.760659\C,0,0.108726
,-1.364182,-0.398497\C,0,1.357671,-0.674455,0.019392\O,0,2.246825,-0.5
38596,-1.077796\H,0,3.366113,1.068533,-0.378156\H,0,1.871065,-1.222041
,0.832023\O,0,0.829326,1.639458,-0.377018\C,0,0.425767,2.920722,0.0862
43\H,0,-0.620667,2.920204,0.413278\H,0,1.057092,3.258413,0.922945\H,0,
0.544961,3.609953,-0.753019\C,0,-2.081829,-0.12787,-0.802531\H,0,-1.53
1596,0.554789,-1.459391\H,0,-2.437708,-0.954408,-1.432432\C,0,-3.26887
3,0.615792,-0.166263\H,0,-3.829226,1.116465,-0.968643\H,0,-2.87141,1.4

11313,0.476082\H,0,4.028916,0.127152,-1.71878\C,0,4.313957,-0.736981,0
.18401\C,0,4.97943,-1.375604,0.964222\H,0,5.572521,-1.941616,1.646462\
C,0,-4.246959,-0.243401,0.65462\H,0,-4.976957,0.428997,1.12509\H,0,-3.
715277,-0.727638,1.484948\C,0,-5.002184,-1.302436,-0.157613\H,0,-5.730
824,-1.831712,0.46712\H,0,-5.549389,-0.843919,-0.991029\H,0,-4.328207,
-2.055978,-0.581486\H,0,0.080521,-2.222739,-1.057022\\Version=IA32L-G0
3RevD.01\State=2-A\HF=-694.4239372\S2=0.754119\S2-1=0.\S2A=0.750012\RM
SD=1.411e-09\Thermal=0.\Dipole=-0.0350329,0.1880681,0.3416168\PG=C01 [
X(C12H19O3)]\\@

30d

TSC4alpha_001_sp.log

1\1\GINC-NODE-21\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\30-Sep-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) TSC4alpha_001
\\0,2\C,0,-1.820137,1.854468,-0.67022\C,0,-2.848185,0.8169,-0.95104\O,
0,-3.190187,0.012484,0.172027\C,0,-2.093197,-0.324438,1.002399\C,0,-1.
115847,0.790638,1.220346\C,0,-1.172673,-1.4812,0.523139\O,0,0.075074,-
1.227142,1.129637\C,0,0.268635,0.206151,1.295178\O,0,-1.115235,-1.4802
46,-0.881604\C,0,-0.374116,-2.566456,-1.41912\C,0,1.30137,0.743998,0.2
93686\C,0,-1.251802,2.91403,-0.935899\H,0,-1.376152,1.631435,1.854171\
H,0,-2.559753,-0.641085,1.946476\H,0,-2.491919,0.189344,-1.774655\H,0,
-3.779928,1.304896,-1.255714\H,0,-0.602071,3.760642,-0.962046\H,0,0.67
821,0.330645,2.310191\H,0,1.358196,1.834781,0.416938\H,0,0.926453,0.56
1667,-0.719524\H,0,-1.493612,-2.471222,0.876071\H,0,-0.443247,-2.48889
6,-2.50667\H,0,0.678348,-2.524342,-1.114822\H,0,-0.798212,-3.530488,-1
.099192\C,0,2.692325,0.126058,0.4772\H,0,2.613167,-0.966229,0.40058\H,
0,3.053361,0.33537,1.495882\C,0,3.720778,0.640191,-0.538214\H,0,3.3615
17,0.429142,-1.555416\H,0,3.791025,1.734975,-0.463024\C,0,5.111613,0.0
25514,-0.349726\H,0,5.823111,0.407976,-1.090601\H,0,5.513139,0.25176,0
.645782\H,0,5.078557,-1.066245,-0.451276\\Version=IA32L-G03RevD.01\Sta
te=2-A\HF=-694.4128788\S2=0.772631\S2-1=0.\S2A=0.750181\RMSD=4.616e-09
\Thermal=0.\Dipole=0.5028045,0.1164461,-0.0064857\PG=C01 [X(C12H19O3)]
\\@

TSC4alpha_002_sp.log

1\1\GINC-NODE-21\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\01-Oct-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) TSC4alpha_002
\\0,2\C,0,0.396831,2.054054,0.480393\C,0,1.873523,2.010627,0.665393\O,
0,2.587019,1.488298,-0.448971\C,0,1.938337,0.411346,-1.09718\C,0,0.454
615,0.580725,-1.249296\C,0,2.042811,-0.985678,-0.428853\O,0,0.921836,-
1.694099,-0.904692\C,0,-0.184297,-0.781198,-1.148848\O,0,2.04656,-0.83
7191,0.969608\C,0,2.214352,-2.064171,1.666491\C,0,-1.281357,-0.976402,

-0.092406\C,0,-0.70309,2.511912,0.79753\H,0,0.061041,1.304811,-1.95468
6\H,0,2.435701,0.347018,-2.076051\H,0,2.092164,1.426877,1.56552\H,0,2.
249478,3.029749,0.803528\H,0,-1.741782,2.736102,0.89815\H,0,-0.596814,
-1.074804,-2.127371\H,0,-0.912402,-0.601608,0.868703\H,0,-1.437988,-2.
058188,0.014485\H,0,2.928725,-1.556364,-0.740555\H,0,2.233064,-1.82262
5,2.731733\H,0,1.389986,-2.756732,1.461018\H,0,3.16354,-2.548403,1.390
271\C,0,-2.607025,-0.301817,-0.463149\H,0,-2.958095,-0.692265,-1.43061
7\H,0,-2.446848,0.775339,-0.608652\C,0,-3.702707,-0.511171,0.590519\H,
0,-3.857272,-1.588838,0.741779\H,0,-3.354642,-0.116664,1.555644\C,0,-5
.034085,0.148235,0.217047\H,0,-4.919638,1.232174,0.090083\H,0,-5.42528
7,-0.253288,-0.72596\H,0,-5.793704,-0.017145,0.989572\\Version=IA32L-G
03RevD.01\State=2-A\HF=-694.4119221\S2=0.773559\S2-1=0.\S2A=0.750193\R
MSD=8.414e-09\Thermal=0.\Dipole=-0.4912665,-0.2459943,0.0769351\PG=C01
[X(C12H19O3)]\\@

TSC4alpha_007_sp.log

1\1\GINC-NODE-21\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\01-Oct-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) TSC4alpha_007
\\0,2\C,0,2.018457,-1.800479,-0.615125\C,0,3.045946,-0.727728,-0.53839
8\O,0,3.071551,-0.033671,0.703723\C,0,1.789678,0.226339,1.248193\C,0,0
.81231,-0.901054,1.097063\C,0,1.003117,1.429812,0.657013\O,0,-0.354689
,1.121725,0.881209\C,0,-0.553458,-0.320045,0.845031\O,0,1.32143,1.5726
39,-0.705324\C,0,0.724738,2.711073,-1.310487\C,0,-1.248385,-0.74546,-0
.458991\C,0,1.577727,-2.844233,-1.097954\H,0,0.909961,-1.794434,1.7043
03\H,0,1.988364,0.447081,2.30686\H,0,2.879241,-0.02698,-1.363183\H,0,4
.041185,-1.171402,-0.645786\H,0,0.986619,-3.695673,-1.353516\H,0,-1.21
7269,-0.544232,1.692735\H,0,-1.328933,-1.841646,-0.460214\H,0,-0.58688
5,-0.479451,-1.289524\H,0,1.196223,2.377485,1.178837\H,0,1.024256,3.63
5438,-0.793377\H,0,1.084422,2.745461,-2.341476\H,0,-0.369402,2.641525,
-1.306301\C,0,-2.636405,-0.118325,-0.664954\H,0,-2.950838,-0.308892,-1
.700917\H,0,-2.553526,0.971824,-0.563974\C,0,-3.72901,-0.637801,0.2805
37\H,0,-3.793164,-1.732302,0.193346\H,0,-3.453999,-0.430386,1.323483\C
,0,-5.102845,-0.021763,-0.004627\H,0,-5.86593,-0.406802,0.681491\H,0,-
5.076432,1.069379,0.104181\H,0,-5.43144,-0.243558,-1.027648\\Version=I
A32L-G03RevD.01\State=2-A\HF=-694.4116137\S2=0.772755\S2-1=0.\S2A=0.75
0183\RMSD=5.617e-09\Thermal=0.\Dipole=-0.5030894,-0.1043286,-0.1344596
\PG=C01 [X(C12H19O3)]\\@

TSC4alpha_003_sp.log

1\1\GINC-NODE-28\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\01-Oct-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) TSC4alpha_003
\\0,2\C,0,1.574445,1.908087,0.675406\C,0,2.564198,0.892313,1.124329\O,

0,3.069026,0.068322,0.080005\C,0,2.096688,-0.319131,-0.875041\C,0,1.12
8565,0.763782,-1.246922\C,0,1.151181,-1.489708,-0.485444\O,0,-0.018546
,-1.28057,-1.24502\C,0,-0.226053,0.14371,-1.462388\O,0,0.922744,-1.463
101,0.90159\C,0,0.149766,-2.558815,1.370649\C,0,-1.374037,0.673831,-0.
589871\C,0,0.96867,2.969819,0.823461\H,0,1.445102,1.589827,-1.874364\H
,0,2.688945,-0.644389,-1.742461\H,0,2.102501,0.278805,1.90514\H,0,3.43
8598,1.400415,1.544088\H,0,0.317421,3.810532,0.730213\H,0,-0.523973,0.
237786,-2.518573\H,0,-1.444504,1.760168,-0.743579\H,0,-1.098917,0.5218
42,0.458262\H,0,1.535785,-2.477793,-0.774307\H,0,0.087407,-2.45926,2.4
56777\H,0,-0.859998,-2.5505,0.943575\H,0,0.632439,-3.516726,1.123771\C
,0,-2.721219,0.016461,-0.915777\H,0,-2.629503,-1.070576,-0.791497\H,0,
-2.94888,0.183578,-1.978921\C,0,-3.897123,0.533686,-0.070539\H,0,-3.97
6549,1.624366,-0.187116\H,0,-4.82884,0.117421,-0.476922\C,0,-3.808081,
0.185813,1.420467\H,0,-3.729423,-0.898996,1.566389\H,0,-2.936674,0.647
614,1.897915\H,0,-4.698731,0.529588,1.959028\\Version=IA32L-G03RevD.01
\State=2-A\HF=-694.4114532\S2=0.77256\S2-1=0.\S2A=0.750181\RMSD=4.204e
-09\Thermal=0.\Dipole=-0.5231529,0.0996646,-0.0834745\PG=C01 [X(C12H19
O3)]\\@

TSC4alpha_008_sp.log

1\1\GINC-NODE-28\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\01-Oct-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) TSC4alpha_008
\\0,2\C,0,0.77461,2.050308,0.597418\C,0,2.195744,1.672525,0.829573\O,0
,2.833974,1.078015,-0.294206\C,0,2.001994,0.208904,-1.038632\C,0,0.598
098,0.705413,-1.227231\C,0,1.773729,-1.21608,-0.466916\O,0,0.546446,-1
.632345,-1.019574\C,0,-0.323293,-0.487405,-1.240564\O,0,1.754285,-1.15
9501,0.937984\C,0,1.621036,-2.433795,1.552134\C,0,-1.48927,-0.499492,-
0.240954\C,0,-0.215913,2.716795,0.904693\H,0,0.403339,1.539088,-1.8933
21\H,0,2.520377,0.099365,-2.002421\H,0,2.237823,0.999637,1.692262\H,0,
2.77609,2.573594,1.053916\H,0,-1.186516,3.154296,0.981489\H,0,-0.74098
8,-0.626453,-2.250687\H,0,-1.101106,-0.26179,0.755765\H,0,-1.869595,-1
.527772,-0.210854\H,0,2.527275,-1.94595,-0.794465\H,0,1.648953,-2.2686
5,2.631687\H,0,0.674044,-2.912895,1.277914\H,0,2.451535,-3.098004,1.26
7772\C,0,-2.614756,0.470588,-0.624274\H,0,-3.012104,0.194573,-1.61301\
H,0,-2.197371,1.480219,-0.73313\C,0,-3.77284,0.522831,0.38671\H,0,-3.3
77655,0.814268,1.370315\H,0,-4.462868,1.322809,0.085655\C,0,-4.559875,
-0.786048,0.521422\H,0,-5.402377,-0.667748,1.212395\H,0,-4.966498,-1.1
03174,-0.447258\H,0,-3.93558,-1.602027,0.902072\\Version=IA32L-G03RevD
.01\State=2-A\HF=-694.4106952\S2=0.773454\S2-1=0.\S2A=0.750191\RMSD=5.
739e-09\Thermal=0.\Dipole=-0.5455038,-0.1048968,0.0320002\PG=C01 [X(C1
2H19O3)]\\@

TSC4alpha_009_sp.log

```
1\1\GINC-NODE-21\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\01-Oct-2010\
 0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) TSC4alpha_009
 \\0,2\C,0,2.274453,-1.469303,-0.741831\C,0,3.050602,-0.200246,-0.75306
 4\O,0,3.042949,0.503102,0.484037\C,0,1.803314,0.464212,1.167523\C,0,1.
 116773,-0.866739,1.127414\C,0,0.689198,1.424756,0.666733\O,0,-0.520844
 ,0.807506,1.04893\C,0,-0.370134,-0.640364,1.061874\O,0,0.808496,1.5954
 69,-0.722803\C,0,-0.087607,2.560788,-1.25596\C,0,-1.107873,-1.318829,-
 0.104643\C,0,2.017215,-2.58115,-1.204744\H,0,1.504584,-1.702137,1.7004
 96\H,0,2.056245,0.756407,2.197112\H,0,2.662601,0.436288,-1.555079\H,0,
 4.103322,-0.423037,-0.956336\H,0,1.603201,-3.540549,-1.423097\H,0,-0.8
 41131,-0.974582,2.000594\H,0,-0.780301,-2.366893,-0.11949\H,0,-0.75608
 2,-0.872397,-1.041659\H,0,0.704892,2.406903,1.159399\H,0,-1.132009,2.2
 53868,-1.127962\H,0,0.057482,3.540689,-0.776044\H,0,0.13953,2.647896,-
 2.321064\C,0,-2.643106,-1.287827,-0.017582\H,0,-2.955084,-1.676035,0.9
 6455\H,0,-3.040211,-1.998111,-0.75741\C,0,-3.302645,0.078702,-0.252597
 \H,0,-2.939935,0.797072,0.490182\H,0,-2.982301,0.463931,-1.231619\C,0,
 -4.832864,0.008618,-0.208987\H,0,-5.283999,0.991597,-0.387361\H,0,-5.2
 23546,-0.679841,-0.969103\H,0,-5.186019,-0.345386,0.767773\\Version=IA
 32L-G03RevD.01\State=2-A\HF=-694.4103212\S2=0.772772\S2-1=0.\S2A=0.750
 184\RMSD=5.225e-09\Thermal=0.\Dipole=-0.396701,-0.2031492,-0.0615055\P
 G=C01 [X(C12H19O3)]\\@
```

TSC4alpha_006_sp.log

```
1\1\GINC-NODE-28\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\01-Oct-2010\
 0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) TSC4alpha_006
 \\0,2\C,0,0.721537,2.096389,0.539759\C,0,2.1813,1.938777,0.29455\O,0,2
 .504295,1.313846,-0.942013\C,0,1.621404,0.272397,-1.312345\C,0,0.17290
 7,0.565064,-1.05113\C,0,1.811025,-1.100476,-0.613276\O,0,0.55128,-1.72
 5647,-0.699929\C,0,-0.510364,-0.730477,-0.696609\O,0,2.234633,-0.89665
 3,0.711861\C,0,2.505948,-2.104531,1.409404\C,0,-1.280874,-0.783551,0.6
 32544\C,0,-0.206032,2.648765,1.134819\H,0,-0.349533,1.297219,-1.657714
 \H,0,1.812834,0.12614,-2.385568\H,0,2.611767,1.375924,1.129198\H,0,2.6
 49385,2.927931,0.254816\H,0,-1.155655,2.950949,1.517207\H,0,-1.188813,
 -1.028299,-1.510007\H,0,-0.620075,-0.408617,1.420489\H,0,-1.48141,-1.8
 41517,0.848843\H,0,2.523142,-1.760283,-1.128555\H,0,3.289468,-2.686662
 ,0.900484\H,0,2.859221,-1.822573,2.403968\H,0,1.606748,-2.724619,1.500
 988\C,0,-2.604054,0.000131,0.633885\H,0,-2.422128,1.034118,0.309205\H,
 0,-2.960757,0.069822,1.671206\C,0,-3.721945,-0.613762,-0.223113\H,0,-3
 .40784,-0.669716,-1.274179\H,0,-3.891964,-1.651275,0.097803\C,0,-5.035
 635,0.17015,-0.135698\H,0,-4.905629,1.202961,-0.482351\H,0,-5.818662,-
```

0.289945,-0.749085\H,0,-5.403069,0.212817,0.89716\\Version=IA32L-G03Re
vD.01\State=2-A\HF=-694.4102952\S2=0.773465\S2-1=0.\S2A=0.750191\RMSD=
5.900e-09\Thermal=0.\Dipole=-0.4948316,-0.2008678,0.1971234\PG=C01 [X(
C12H19O3)]\\@

TSC4alpha_005_sp.log

1\1\GINC-NODE-21\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\01-Oct-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) TSC4alpha_005
\\0,2\C,0,0.419983,2.07686,0.398445\C,0,1.864464,1.932105,0.728663\O,0
,2.643901,1.343139,-0.30555\C,0,1.984656,0.307323,-1.007241\C,0,0.5399
29,0.581587,-1.308605\C,0,1.917157,-1.082693,-0.320942\O,0,0.804722,-1
.717022,-0.907724\C,0,-0.19899,-0.732283,-1.281014\O,0,1.782162,-0.912
748,1.068307\C,0,1.781233,-2.137686,1.78852\C,0,-1.427925,-0.850258,-0
.366864\C,0,-0.667904,2.620955,0.5994\H,0,0.272935,1.326587,-2.050656\
H,0,2.570948,0.191502,-1.930685\H,0,1.952215,1.348852,1.651166\H,0,2.2
97167,2.924326,0.893886\H,0,-1.691218,2.923778,0.594965\H,0,-0.511181,
-1.004696,-2.302266\H,0,-1.153497,-0.498455,0.63258\H,0,-1.66304,-1.92
0607,-0.287533\H,0,2.787838,-1.719439,-0.531056\H,0,1.705469,-1.88143,
2.847776\H,0,0.932811,-2.76973,1.501667\H,0,2.714563,-2.696102,1.61879
6\C,0,-2.653157,-0.100621,-0.906904\H,0,-2.810179,-0.388585,-1.956944\
H,0,-2.452216,0.979416,-0.913207\C,0,-3.952452,-0.374588,-0.130494\H,0
,-4.785037,0.105914,-0.662042\H,0,-4.161157,-1.453772,-0.152442\C,0,-3
.943597,0.110569,1.32375\H,0,-3.173613,-0.393396,1.91791\H,0,-3.750106
,1.189271,1.38096\H,0,-4.909351,-0.078004,1.806573\\Version=IA32L-G03R
evD.01\State=2-A\HF=-694.4101422\S2=0.773587\S2-1=0.\S2A=0.750193\RMSD
=6.120e-09\Thermal=0.\Dipole=-0.5289467,-0.2077496,0.0027803\PG=C01 [X
(C12H19O3)]\\@

TSC4alpha_010_sp.log

1\1\GINC-NODE-28\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\01-Oct-2010\
0\\#P UB3LYP/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) TSC4alpha_010
\\0,2\C,0,-1.547314,2.020952,-0.618064\C,0,-2.784444,1.201286,-0.51631
1\O,0,-2.940722,0.532503,0.729961\C,0,-1.7381,0.002045,1.258121\C,0,-0
.541617,0.88968,1.086773\C,0,-1.239398,-1.345406,0.665256\O,0,0.154827
,-1.339969,0.877853\C,0,0.66178,0.024256,0.822852\O,0,-1.592301,-1.419
381,-0.694037\C,0,-1.273076,-2.666849,-1.294351\C,0,1.411389,0.279875,
-0.494566\C,0,-0.895017,2.938038,-1.11811\H,0,-0.434539,1.785745,1.688
498\H,0,-1.963953,-0.167003,2.320849\H,0,-2.79169,0.479654,-1.339922\H
,0,-3.658953,1.853561,-0.609624\H,0,-0.135472,3.636092,-1.392847\H,0,1
.371543,0.104598,1.659163\H,0,1.708982,1.336226,-0.517507\H,0,0.698527
,0.143767,-1.314161\H,0,-1.630228,-2.226189,1.19355\H,0,-1.62972,-2.62
1542,-2.325954\H,0,-0.192306,-2.85092,-1.288123\H,0,-1.778015,-3.49538

2,-0.774661\C,0,2.631094,-0.633289,-0.706716\H,0,2.974379,-0.513697,-1
.744245\H,0,2.302533,-1.675359,-0.608169\C,0,3.826408,-0.394211,0.2335
81\H,0,3.516321,-0.528016,1.279093\H,0,4.57113,-1.179249,0.045415\C,0,
4.498971,0.974265,0.070871\H,0,4.834708,1.127979,-0.962503\H,0,3.82183
8,1.798549,0.323074\H,0,5.376424,1.062105,0.721846\\Version=IA32L-G03R
evD.01\State=2-A\HF=-694.410175\S2=0.772701\S2-1=0.\S2A=0.750182\RMSD=
4.823e-09\Thermal=0.\Dipole=0.5237634,-0.0470275,-0.1517358\PG=C01 [X(
C12H19O3)]\\@

31d

cShaC4alpha_028_sp.log

1\1\GINC-NODE-31\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\24-Aug-2010\
0\\#P ubecke3lyp/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) cShaC4alp
ha_028\\0,2\C,0,-0.169333,-0.391765,1.166546\O,0,-0.012527,1.0512,1.25
2038\C,0,1.170879,1.451208,0.604414\H,0,-0.52528,-0.692518,2.159078\H,
0,1.45578,2.414208,1.050576\C,0,2.678003,-0.810006,-1.06737\C,0,1.6276
89,-1.671558,-0.350558\C,0,1.269792,-0.950446,0.948956\C,0,2.173318,0.
308288,0.89159\O,0,3.174149,0.091692,-0.080132\H,0,3.523896,-1.392885,
-1.444498\H,0,2.217619,-0.258487,-1.895608\H,0,1.537101,-1.594113,1.79
1518\H,0,2.6766,0.516027,1.84032\C,0,1.18465,-2.837846,-0.749938\H,0,1
.330949,-3.508533,-1.586771\O,0,1.028682,1.595854,-0.787009\C,0,0.2046
6,2.690075,-1.162835\H,0,0.213225,2.731535,-2.254506\H,0,-0.825265,2.5
60439,-0.80921\H,0,0.600279,3.636477,-0.764013\C,0,-1.227228,-0.773534
,0.131938\H,0,-1.26709,-1.869677,0.069619\H,0,-0.905094,-0.418622,-0.8
54046\C,0,-2.617385,-0.220364,0.468677\H,0,-2.554986,0.870112,0.578859
\H,0,-2.93697,-0.607512,1.448446\C,0,-3.677128,-0.572867,-0.582784\H,0
,-3.732307,-1.665471,-0.692038\H,0,-3.357585,-0.186968,-1.561417\C,0,-
5.06675,-0.022545,-0.246251\H,0,-5.800251,-0.287264,-1.016503\H,0,-5.4
29897,-0.419733,0.709782\H,0,-5.050166,1.071183,-0.163077\\Version=IA3
2L-G03RevD.01\State=2-A\HF=-694.4538738\S2=0.76043\S2-1=0.\S2A=0.75004
9\RMSD=5.603e-09\Thermal=0.\Dipole=-0.2923063,-0.0588154,-0.1501568\PG
=C01 [X(C12H19O3)]\\@

cShaC4alpha_001_sp.log

1\1\GINC-NODE-21\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\24-Aug-2010\
0\\#P ubecke3lyp/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) cShaC4alp
ha_001\\0,2\C,0,-0.3395,-0.184403,0.858094\O,0,0.139026,0.925424,0.093
441\C,0,1.451478,1.214077,0.572533\H,0,-0.567928,0.161919,1.883573\H,0
,1.356937,1.829706,1.489684\C,0,2.254516,-1.331203,-1.052313\C,0,1.138
017,-2.018234,-0.262899\C,0,0.88194,-1.136654,0.957394\C,0,2.09805,-0.
161412,0.921363\O,0,3.000987,-0.634643,-0.062428\H,0,2.927518,-2.02596
6,-1.561147\H,0,1.831238,-0.630343,-1.787216\H,0,0.833832,-1.739592,1.

867696\H,0,2.657278,-0.096141,1.858215\C,0,0.571142,-3.166082,-0.53863
7\H,0,0.633948,-3.924457,-1.308561\O,0,2.190072,1.881087,-0.385251\C,0
,1.716826,3.193101,-0.664569\H,0,1.675754,3.80301,0.250775\H,0,2.43100
7,3.63871,-1.360699\H,0,0.721485,3.170882,-1.122723\C,0,-1.615591,-0.7
26284,0.23051\H,0,-1.891264,-1.649178,0.759666\H,0,-1.402436,-1.014386
,-0.805111\C,0,-2.781881,0.269802,0.272643\H,0,-2.485026,1.191354,-0.2
43985\H,0,-2.984362,0.553556,1.316595\C,0,-4.065959,-0.28423,-0.357797
\H,0,-4.351833,-1.212965,0.156655\H,0,-3.863979,-0.565368,-1.401085\C,
0,-5.234555,0.705331,-0.31274\H,0,-6.134586,0.283703,-0.774728\H,0,-5.
48602,0.975542,0.720384\H,0,-4.989142,1.632219,-0.845597\\Version=IA32
L-G03RevD.01\State=2-A\HF=-694.4528163\S2=0.760103\S2-1=0.\S2A=0.75004
7\RMSD=5.444e-09\Thermal=0.\Dipole=-0.538615,0.1150161,0.3056608\PG=C0
1 [X(C12H19O3)]\\@

cShaC4alpha_054_sp.log

1\1\GINC-NODE-25\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\24-Aug-2010\
0\\#P ubecke3lyp/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) cShaC4alp
ha_054\\0,2\C,0,0.235026,0.123066,1.237567\O,0,-0.223904,-1.256067,1.2
30753\C,0,-1.426314,-1.364578,0.507582\H,0,0.604269,0.288835,2.256557\
H,0,-1.929516,-2.267049,0.881534\C,0,-2.31559,1.25746,-1.080322\C,0,-1
.175032,1.850838,-0.240865\C,0,-1.045954,0.982868,1.01037\C,0,-2.18526
,-0.052363,0.818877\O,0,-3.052864,0.424301,-0.188143\H,0,-2.998853,2.0
16707,-1.472533\H,0,-1.909845,0.667327,-1.910865\H,0,-1.220352,1.60746
6,1.89059\H,0,-2.783194,-0.200822,1.722722\C,0,-0.497438,2.937526,-0.5
16575\H,0,-0.460745,3.68392,-1.299564\O,0,-1.240155,-1.465864,-0.88235
8\C,0,-0.656283,-2.694761,-1.290343\H,0,-0.608097,-2.67417,-2.381578\H
,0,0.353852,-2.818522,-0.881699\H,0,-1.27436,-3.548591,-0.973863\C,0,1
.391963,0.327908,0.259196\H,0,1.651833,1.393888,0.260683\H,0,1.045593,
0.091812,-0.754264\C,0,2.617149,-0.525914,0.61407\H,0,2.298022,-1.5704
57,0.715564\H,0,2.995558,-0.224014,1.602883\C,0,3.761058,-0.446433,-0.
410041\H,0,3.385014,-0.759298,-1.394822\H,0,4.530188,-1.179822,-0.1323
3\C,0,4.41308,0.936144,-0.530788\H,0,3.703271,1.692979,-0.882923\H,0,4
.804086,1.273407,0.437622\H,0,5.250232,0.916881,-1.238095\\Version=IA3
2L-G03RevD.01\State=2-A\HF=-694.4526198\S2=0.760405\S2-1=0.\S2A=0.7500
49\RMSD=5.434e-09\Thermal=0.\Dipole=0.3095095,-0.0375845,-0.1304052\PG
=C01 [X(C12H19O3)]\\@

cShaC4alpha_002_sp.log

1\1\GINC-NODE-21\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\24-Aug-2010\
0\\#P ubecke3lyp/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) cShaC4alp
ha_002\\0,2\C,0,0.244719,-0.700356,0.503464\O,0,-0.895195,-1.2286,-0.1
78701\C,0,-2.044262,-0.803702,0.550991\H,0,0.384655,-1.256069,1.449719

\H,0,-2.195509,-1.503832,1.396916\C,0,-1.515095,1.964229,-0.760118\C,0
,-0.086574,1.779614,-0.241145\C,0,-0.174297,0.745694,0.880645\C,0,-1.7
14744,0.622495,1.09206\O,0,-2.333298,1.667998,0.364136\H,0,-1.738027,2
.983595,-1.085203\H,0,-1.717729,1.26552,-1.585113\H,0,0.357335,1.09311
4,1.769671\H,0,-2.040678,0.72443,2.130265\C,0,0.977171,2.435502,-0.632
771\H,0,1.221524,3.199029,-1.360305\O,0,-3.161884,-0.778582,-0.261569\
C,0,-3.57871,-2.065585,-0.701684\H,0,-4.511482,-1.918602,-1.250837\H,0
,-2.832357,-2.524872,-1.359743\H,0,-3.763421,-2.735251,0.152097\C,0,1.
480624,-0.90047,-0.362891\H,0,1.352364,-0.346703,-1.29978\H,0,1.526499
,-1.965774,-0.6248\C,0,2.785447,-0.477482,0.324219\H,0,2.878007,-0.993
262,1.292174\H,0,2.750288,0.598168,0.546324\C,0,4.029242,-0.771815,-0.
524396\H,0,3.933787,-0.259232,-1.491868\H,0,4.067262,-1.846688,-0.7516
69\C,0,5.335044,-0.344855,0.153187\H,0,5.476142,-0.866447,1.10805\H,0,
6.203705,-0.565388,-0.477676\H,0,5.339261,0.73213,0.361499\\Version=IA
32L-G03RevD.01\State=2-A\HF=-694.4523145\S2=0.760089\S2-1=0.\S2A=0.750
047\RMSD=5.188e-09\Thermal=0.\Dipole=0.4425281,-0.4201248,0.1766626\PG
=C01 [X(C12H19O3)]\\@

cShaC4alpha_045_sp.log

1\1\GINC-NODE-25\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\24-Aug-2010\
0\\#P ubecke3lyp/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) cShaC4alp
ha_045\\0,2\C,0,0.135063,-0.404918,-1.307002\O,0,-0.040126,1.035917,-1
.389866\C,0,-1.146003,1.437511,-0.618064\H,0,0.374242,-0.716034,-2.330
991\H,0,-1.48786,2.391742,-1.042577\C,0,-2.429276,-0.805229,1.247843\C
,0,-1.464168,-1.672886,0.426085\C,0,-1.264528,-0.969322,-0.916378\C,0,
-2.165727,0.283938,-0.772927\O,0,-3.04619,0.075323,0.310857\H,0,-3.219
755,-1.386209,1.732626\H,0,-1.877784,-0.235625,2.005075\H,0,-1.621674,
-1.62785,-1.712888\H,0,-2.776619,0.474959,-1.659915\C,0,-0.971097,-2.8
31473,0.787377\H,0,-1.016211,-3.490775,1.644586\O,0,-0.848738,1.604351
,0.746096\C,0,-0.000987,2.712523,1.012269\H,0,0.98567,2.586688,0.55057
2\H,0,-0.448692,3.648173,0.644364\H,0,0.109222,2.772091,2.097553\C,0,1
.309988,-0.768302,-0.39934\H,0,1.358169,-1.863552,-0.322318\H,0,1.1034
38,-0.393519,0.608555\C,0,2.647359,-0.228087,-0.924146\H,0,2.582847,0.
863889,-1.019568\H,0,2.808494,-0.613623,-1.941662\C,0,3.862074,-0.5990
49,-0.057392\H,0,4.775398,-0.30292,-0.59089\H,0,3.912848,-1.692462,0.0
47363\C,0,3.86964,0.046847,1.333478\H,0,3.830979,1.14113,1.258793\H,0,
3.014257,-0.274226,1.93829\H,0,4.779438,-0.215925,1.88551\\Version=IA3
2L-G03RevD.01\State=2-A\HF=-694.4524669\S2=0.760419\S2-1=0.\S2A=0.7500
49\RMSD=4.531e-09\Thermal=0.\Dipole=0.3321532,-0.0551663,0.0888965\PG=
C01 [X(C12H19O3)]\\@

cShaC4alpha_059_sp.log

1\1\GINC-NODE-21\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\24-Aug-2010\
 0\\#P ubecke3lyp/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) cShaC4alp
 ha_059\\0,2\C,0,-0.461404,-0.401737,0.738439\O,0,-0.270513,1.017877,0.
 988931\C,0,1.060886,1.384788,0.719267\H,0,-1.088675,-0.748003,1.566266
 \H,0,1.255795,2.291082,1.309451\C,0,2.853038,-0.851526,-0.681654\C,0,1
 .623817,-1.701608,-0.327287\C,0,0.955749,-1.038346,0.877353\C,0,1.8973
 67,0.160639,1.162187\O,0,3.110131,-0.052855,0.471413\H,0,3.746273,-1.4
 51356,-0.880484\H,0,2.639094,-0.216277,-1.549506\H,0,0.951751,-1.74733
 1,1.709698\H,0,2.139849,0.26956,2.223265\C,0,1.267919,-2.821233,-0.906
 712\H,0,1.612561,-3.449203,-1.718168\O,0,1.309809,1.641664,-0.640414\C
 ,0,0.678349,2.820071,-1.120545\H,0,-0.414345,2.743089,-1.069466\H,0,0.
 999469,3.701247,-0.544618\H,0,0.987129,2.942026,-2.161348\C,0,-1.19288
 6,-0.634913,-0.584557\H,0,-1.276121,-1.718483,-0.745652\H,0,-0.56735,-
 0.248718,-1.396428\C,0,-2.587426,0.01044,-0.650125\H,0,-2.934798,-0.02
 4304,-1.692326\H,0,-2.503792,1.073277,-0.387793\C,0,-3.649087,-0.65307
 4,0.239286\H,0,-3.343214,-0.603503,1.293002\H,0,-3.713454,-1.72202,-0.
 010659\C,0,-5.032284,-0.010164,0.091324\H,0,-5.38922,-0.073062,-0.9442
 16\H,0,-5.774389,-0.502602,0.730164\H,0,-5.006206,1.051076,0.367521\\V
 ersion=IA32L-G03RevD.01\State=2-A\HF=-694.4524773\S2=0.760419\S2-1=0.\
 S2A=0.750049\RMSD=5.524e-09\Thermal=0.\Dipole=-0.2517048,-0.017095,-0.
 2180676\PG=C01 [X(C12H19O3)]\\@

cShaC4alpha_071_sp.log

1\1\GINC-NODE-21\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\24-Aug-2010\
 0\\#P ubecke3lyp/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) cShaC4alp
 ha_071\\0,2\C,0,-0.149888,-0.487893,-1.164742\O,0,0.916618,-1.475822,-
 1.129797\C,0,2.053479,-0.946068,-0.496495\H,0,-0.566994,-0.564105,-2.1
 76009\H,0,2.91187,-1.526323,-0.862649\C,0,1.727294,1.875952,0.924752\C
 ,0,0.362077,1.761496,0.22819\C,0,0.562599,0.89381,-1.016682\C,0,2.0705
 55,0.538334,-0.925456\O,0,2.687691,1.443007,-0.035942\H,0,1.975971,2.9
 03721,1.206805\H,0,1.755947,1.236141,1.814191\H,0,0.353285,1.504353,-1
 .899362\H,0,2.586661,0.61756,-1.886708\C,0,-0.730167,2.381904,0.600899
 \H,0,-1.036657,3.046208,1.398849\O,0,1.993539,-1.01641,0.90689\C,0,2.0
 35855,-2.344825,1.409001\H,0,1.17293,-2.929976,1.070171\H,0,2.958172,-
 2.856075,1.093809\H,0,2.0231,-2.270915,2.498882\C,0,-1.246308,-0.85261
 1,-0.161384\H,0,-0.909597,-0.612489,0.853639\H,0,-1.36446,-1.943077,-0
 .210631\C,0,-2.597186,-0.186137,-0.452178\H,0,-2.921042,-0.451905,-1.4
 7023\H,0,-2.482436,0.906943,-0.438175\C,0,-3.689656,-0.587263,0.547155
 \H,0,-3.367128,-0.312733,1.561345\H,0,-3.797415,-1.681464,0.547624\C,0
 ,-5.045916,0.060057,0.249773\H,0,-5.410994,-0.223297,-0.745216\H,0,-5.
 803712,-0.243822,0.981065\H,0,-4.976713,1.154514,0.276391\\Version=IA3

2L-G03RevD.01\State=2-A\HF=-694.4524128\S2=0.760441\S2-1=0.\S2A=0.7500
49\RMSD=7.388e-09\Thermal=0.\Dipole=-0.3011833,-0.135088,0.1641013\PG=
C01 [X(C12H19O3)]\\@

cShaC4alpha_004_sp.log

1\1\GINC-NODE-25\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\24-Aug-2010\
0\\#P ubecke3lyp/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) cShaC4alp
ha_004\\0,2\C,0,0.406718,-0.076887,0.807504\O,0,-0.340939,-1.033914,0.
051802\C,0,-1.667579,-1.022699,0.575529\H,0,0.585735,-0.48387,1.820415
\H,0,-1.688584,-1.664487,1.479197\C,0,-1.926038,1.664674,-0.98857\C,0,
-0.652238,2.064507,-0.240834\C,0,-0.559358,1.127625,0.962061\C,0,-1.96
7213,0.457041,0.966886\O,0,-2.774537,1.143823,0.02696\H,0,-2.439995,2.
502818,-1.465913\H,0,-1.703614,0.89587,-1.743399\H,0,-0.341077,1.68876
1,1.874206\H,0,-2.489914,0.502702,1.925703\C,0,0.152503,3.055966,-0.53
1184\H,0,0.235558,3.821352,-1.292246\O,0,-2.571643,-1.478929,-0.364079
\C,0,-2.425165,-2.85814,-0.679712\H,0,-2.497058,-3.48151,0.224599\H,0,
-3.245576,-3.110354,-1.355385\H,0,-1.467389,-3.056598,-1.174092\C,0,1.
750047,0.168134,0.135267\H,0,2.242977,0.997655,0.658321\H,0,1.570147,0
.509057,-0.890881\C,0,2.647136,-1.078367,0.127079\H,0,2.089124,-1.9031
81,-0.331708\H,0,2.85575,-1.384428,1.163601\C,0,3.977064,-0.891716,-0.
621396\H,0,3.767838,-0.595301,-1.659186\H,0,4.482789,-1.864872,-0.6805
21\C,0,4.930213,0.12568,0.017215\H,0,4.504809,1.135584,0.026804\H,0,5.
1609,-0.147143,1.054961\H,0,5.877992,0.175207,-0.53101\\Version=IA32L-
G03RevD.01\State=2-A\HF=-694.4514507\S2=0.760098\S2-1=0.\S2A=0.750047\
RMSD=2.272e-09\Thermal=0.\Dipole=0.5059767,-0.2787511,0.2690203\PG=C01
[X(C12H19O3)]\\@

cShaC4alpha_003_sp.log

1\1\GINC-NODE-25\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\24-Aug-2010\
0\\#P ubecke3lyp/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) cShaC4alp
ha_003\\0,2\C,0,-0.349834,0.019451,-1.011986\O,0,0.216409,-1.001427,-0
.185533\C,0,1.59743,-1.090333,-0.530485\H,0,-0.423717,-0.361421,-2.048
066\H,0,1.689257,-1.732766,-1.429073\C,0,1.887332,1.553082,1.092654\C,
0,0.734877,2.050922,0.216979\C,0,0.717215,1.144959,-1.0133\C,0,2.05770
8,0.363107,-0.86527\O,0,2.803729,0.979615,0.168656\H,0,2.403934,2.3482
37,1.636182\H,0,1.529452,0.79681,1.806863\H,0,0.658902,1.738143,-1.929
526\H,0,2.68885,0.369345,-1.757565\C,0,-0.030659,3.089311,0.442077\H,0
,-0.14785,3.844654,1.208648\O,0,2.332934,-1.61363,0.515771\C,0,2.03710
7,-2.97559,0.800101\H,0,2.178177,-3.606275,-0.090878\H,0,2.73845,-3.28
9655,1.576462\H,0,1.009687,-3.095066,1.162275\C,0,-1.747774,0.359985,-
0.516248\H,0,-2.118563,1.215376,-1.098816\H,0,-1.673234,0.698095,0.521
932\C,0,-2.72686,-0.816834,-0.638037\H,0,-2.346323,-1.659362,-0.046507

\H,0,-2.744111,-1.158086,-1.683321\C,0,-4.164055,-0.488094,-0.201918\H
,0,-4.806944,-1.34303,-0.451303\H,0,-4.539814,0.357347,-0.796427\C,0,-
4.31856,-0.170798,1.290528\H,0,-5.370997,-0.009616,1.551004\H,0,-3.944
979,-0.996555,1.908968\H,0,-3.768311,0.73235,1.577417\\Version=IA32L-G
03RevD.01\State=2-A\HF=-694.4513463\S2=0.760118\S2-1=0.\S2A=0.750047\R
MSD=4.367e-09\Thermal=0.\Dipole=-0.4874405,-0.2253603,-0.3581211\PG=C0
1 [X(C12H19O3)]\\@

cShaC4alpha_005_sp.log

1\1\GINC-NODE-25\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\24-Aug-2010\
0\\#P ubecke3lyp/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) cShaC4alp
ha_005\\0,2\C,0,-0.49701,-0.403453,0.497982\O,0,-0.079266,0.776743,-0.
193958\C,0,1.009681,1.319384,0.55065\H,0,-1.001043,-0.105856,1.434676\
H,0,0.593596,1.908407,1.392665\C,0,2.643844,-1.01141,-0.730336\C,0,1.5
25318,-1.905879,-0.190534\C,0,0.830347,-1.098295,0.903955\C,0,1.809828
,0.098952,1.101689\O,0,2.99119,-0.185578,0.374019\H,0,3.536985,-1.5599
22,-1.040191\H,0,2.279408,-0.404321,-1.57238\H,0,0.695151,-1.702989,1.
804313\H,0,2.111171,0.273967,2.137681\C,0,1.268002,-3.140477,-0.543571
\H,0,1.65283,-3.866761,-1.248105\O,0,1.806221,2.114733,-0.249893\C,0,1
.167842,3.307295,-0.689988\H,0,0.326082,3.088611,-1.356884\H,0,0.80373
1,3.899862,0.163175\H,0,1.923376,3.882558,-1.229836\C,0,-1.470224,-1.1
86997,-0.372654\H,0,-1.714857,-2.124143,0.147057\H,0,-0.951994,-1.4699
88,-1.294741\C,0,-2.76169,-0.427155,-0.720294\H,0,-3.308747,-1.011126,
-1.473727\H,0,-2.496238,0.523476,-1.199956\C,0,-3.699347,-0.158844,0.4
6565\H,0,-3.1905,0.46417,1.213455\H,0,-3.932974,-1.109559,0.966751\C,0
,-5.002209,0.530118,0.046026\H,0,-5.654788,0.713495,0.907297\H,0,-4.80
136,1.49657,-0.432434\H,0,-5.561279,-0.083075,-0.671615\\Version=IA32L
-G03RevD.01\State=2-A\HF=-694.451403\S2=0.760107\S2-1=0.\S2A=0.750047\
RMSD=4.740e-09\Thermal=0.\Dipole=-0.6080756,0.0218389,0.1822584\PG=C01
[X(C12H19O3)]\\@

cShaC4alpha_010_sp.log

1\1\GINC-NODE-21\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\25-Aug-2010\
0\\#P ubecke3lyp/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) cShaC4alp
ha_010\\0,2\C,0,0.360526,-0.475276,0.622293\O,0,-0.645365,-1.199016,-0
.091323\C,0,-1.886315,-0.920042,0.553008\H,0,0.522617,-0.96136,1.60271
1\H,0,-1.980387,-1.592501,1.429303\C,0,-1.680393,1.828481,-0.885342\C,
0,-0.281194,1.892777,-0.267688\C,0,-0.290008,0.906983,0.899425\C,0,-1.
806551,0.564015,1.027072\O,0,-2.521798,1.466087,0.201926\H,0,-2.031176
,2.783132,-1.285375\H,0,-1.715367,1.06544,-1.676801\H,0,0.125251,1.367
473,1.798943\H,0,-2.21295,0.668415,2.036234\C,0,0.695494,2.688697,-0.6
24949\H,0,0.872433,3.448752,-1.375264\O,0,-2.944984,-1.105698,-0.31561

1\C,0,-3.136432,-2.46054,-0.704537\H,0,-4.043797,-2.483365,-1.312332\H
,0,-2.289687,-2.831608,-1.293029\H,0,-3.273584,-3.109407,0.173928\C,0,
1.66209,-0.528476,-0.166117\H,0,1.513981,-0.030685,-1.131448\H,0,1.863
391,-1.585333,-0.377882\C,0,2.848116,0.106167,0.573872\H,0,2.967683,-0
.373026,1.557741\H,0,2.623282,1.16344,0.76681\C,0,4.17999,0.022801,-0.
191003\H,0,4.925832,0.625265,0.344514\H,0,4.058471,0.495548,-1.175798\
C,0,4.72663,-1.398717,-0.369283\H,0,4.055509,-2.025223,-0.967346\H,0,5
.698392,-1.384346,-0.876051\H,0,4.865559,-1.892816,0.600697\\Version=I
A32L-G03RevD.01\State=2-A\HF=-694.4508961\S2=0.760075\S2-1=0.\S2A=0.75
0047\RMSD=5.211e-09\Thermal=0.\Dipole=0.5093126,-0.3167427,0.234858\PG
=C01 [X(C12H19O3)]\\@

cShaC4alpha_094_sp.log

1\1\GINC-NODE-21\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\24-Aug-2010\
0\\#P ubecke3lyp/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) cShaC4alp
ha_094\\0,2\C,0,-0.268058,0.227935,1.202474\O,0,0.559996,1.423214,1.19
5149\C,0,1.7783,1.175496,0.540624\H,0,-0.660991,0.167593,2.224699\H,0,
2.497845,1.906361,0.935264\C,0,2.040059,-1.578077,-1.015744\C,0,0.6868
53,-1.782755,-0.315854\C,0,0.718123,-0.961042,0.975188\C,0,2.11476,-0.
289529,0.898461\O,0,2.898568,-0.999912,-0.034865\H,0,2.49433,-2.517262
,-1.346267\H,0,1.926329,-0.905041,-1.872985\H,0,0.656476,-1.649338,1.8
22687\H,0,2.647808,-0.302499,1.853649\C,0,-0.260126,-2.590653,-0.72487
9\H,0,-0.433771,-3.258161,-1.559267\O,0,1.693467,1.297441,-0.85773\C,0
,1.46993,2.630343,-1.295887\H,0,1.45515,2.605718,-2.387959\H,0,0.51550
8,3.022058,-0.924566\H,0,2.28088,3.295597,-0.962251\C,0,-1.448154,0.39
0991,0.24186\H,0,-1.10118,0.273189,-0.79145\H,0,-1.790996,1.426875,0.3
50185\C,0,-2.60493,-0.575435,0.533029\H,0,-2.969394,-0.403569,1.557551
\H,0,-2.228362,-1.606907,0.505401\C,0,-3.782787,-0.462319,-0.448917\H,
0,-4.498491,-1.265477,-0.227588\H,0,-3.418688,-0.652591,-1.468458\C,0,
-4.518629,0.882561,-0.411365\H,0,-3.867962,1.713624,-0.705634\H,0,-5.3
76517,0.880715,-1.093668\H,0,-4.896268,1.09807,0.596281\\Version=IA32L
-G03RevD.01\State=2-A\HF=-694.4510422\S2=0.760464\S2-1=0.\S2A=0.75005\
RMSD=6.592e-09\Thermal=0.\Dipole=-0.3287617,0.0420947,-0.1450094\PG=C0
1 [X(C12H19O3)]\\@

cShaC4alpha_009_sp.log

1\1\GINC-NODE-25\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\25-Aug-2010\
0\\#P ubecke3lyp/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) cShaC4alp
ha_009\\0,2\C,0,0.24445,-0.703238,0.695555\O,0,-0.815663,-1.229332,-0.
106559\C,0,-2.03583,-0.775796,0.475824\H,0,0.262094,-1.240995,1.662104
\H,0,-2.297074,-1.459402,1.308289\C,0,-1.325464,1.965409,-0.80525\C,0,
0.034291,1.766094,-0.129617\C,0,-0.193611,0.755522,0.993525\C,0,-1.749

388,0.654317,1.031109\O,0,-2.26785,1.696395,0.224967\H,0,-1.49407,2.98
3607,-1.164893\H,0,-1.447501,1.258939,-1.639549\H,0,0.237711,1.115327,
1.930712\H,0,-2.188433,0.775623,2.024611\C,0,1.146165,2.396604,-0.4150
34\H,0,1.481126,3.141415,-1.125709\O,0,-3.049457,-0.748877,-0.463304\C
,0,-3.433265,-2.037461,-0.928041\H,0,-2.6205,-2.522629,-1.480398\H,0,-
3.734828,-2.686401,-0.09167\H,0,-4.288217,-1.886203,-1.590924\C,0,1.57
0301,-0.938631,-0.015276\H,0,1.556809,-0.398437,-0.967137\H,0,1.626361
,-2.009407,-0.253377\C,0,2.789103,-0.530868,0.825015\H,0,2.714045,-0.9
98256,1.817865\H,0,2.771276,0.555511,0.989953\C,0,4.139292,-0.920813,0
.200044\H,0,4.170026,-2.010698,0.057806\H,0,4.935569,-0.685433,0.91890
2\C,0,4.446297,-0.223482,-1.13028\H,0,3.729537,-0.501316,-1.910858\H,0
,4.409666,0.867392,-1.020273\H,0,5.44612,-0.490068,-1.491733\\Version=
IA32L-G03RevD.01\State=2-A\HF=-694.4508505\S2=0.760092\S2-1=0.\S2A=0.7
50047\RMSD=4.614e-09\Thermal=0.\Dipole=0.4253622,-0.4236001,0.2598309\
PG=C01 [X(C12H19O3)]\\@

cShaC4alpha_079_sp.log

1\1\GINC-NODE-25\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\25-Aug-2010\
0\\#P ubecke3lyp/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) cShaC4alp
ha_079\\0,2\C,0,-0.582985,-0.117755,0.737328\O,0,-0.0712,1.221497,0.98
284\C,0,1.309863,1.270408,0.717488\H,0,-1.264243,-0.312194,1.572348\H,
0,1.706818,2.110542,1.30418\C,0,2.560944,-1.313741,-0.668524\C,0,1.156
63,-1.844962,-0.344516\C,0,0.651232,-1.061742,0.867033\C,0,1.838881,-0
.111734,1.168342\O,0,2.978729,-0.598743,0.492672\H,0,3.288173,-2.11075
5,-0.851197\H,0,2.524078,-0.647115,-1.538124\H,0,0.483625,-1.762062,1.
689973\H,0,2.085365,-0.060392,2.232846\C,0,0.547844,-2.83383,-0.950734
\H,0,0.739932,-3.513106,-1.771217\O,0,1.615342,1.454858,-0.642633\C,0,
1.272159,2.742998,-1.133285\H,0,1.602016,2.78246,-2.174052\H,0,0.19090
9,2.919474,-1.085251\H,0,1.786391,3.531455,-0.56308\C,0,-1.362735,-0.1
75772,-0.576911\H,0,-1.679561,-1.212999,-0.744252\H,0,-0.677575,0.0694
1,-1.395531\C,0,-2.573783,0.773222,-0.622696\H,0,-2.95644,0.790976,-1.
653031\H,0,-2.226505,1.790519,-0.403566\C,0,-3.738305,0.429531,0.32395
9\H,0,-4.481939,1.234784,0.254612\H,0,-3.391301,0.438514,1.366209\C,0,
-4.426883,-0.907755,0.025243\H,0,-3.750264,-1.759358,0.160737\H,0,-5.2
86064,-1.064552,0.687549\H,0,-4.79355,-0.939705,-1.008545\\Version=IA3
2L-G03RevD.01\State=2-A\HF=-694.4511643\S2=0.760432\S2-1=0.\S2A=0.7500
49\RMSD=5.347e-09\Thermal=0.\Dipole=-0.260932,0.0738277,-0.2201476\PG=
C01 [X(C12H19O3)]\\@

cShaC4alpha_008_sp.log

1\1\GINC-NODE-21\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\25-Aug-2010\
0\\#P ubecke3lyp/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) cShaC4alp

ha_008\\0,2\C,0,-0.359407,-0.585942,0.786797\O,0,-0.242894,0.657132,0.
087552\C,0,0.88636,1.333872,0.63958\H,0,-0.717838,-0.385575,1.813961\H
,0,0.563969,1.8427,1.569986\C,0,2.54262,-0.712536,-1.033965\C,0,1.6739
66,-1.76575,-0.34208\C,0,1.103859,-1.090302,0.904055\C,0,1.933146,0.22
6811,0.973359\O,0,2.981584,0.127632,0.026398\H,0,3.425131,-1.124878,-1
.529633\H,0,1.948863,-0.141958,-1.76342\H,0,1.227309,-1.729593,1.78191
5\H,0,2.399608,0.420176,1.942735\C,0,1.513844,-3.013926,-0.704336\H,0,
1.843831,-3.663235,-1.505153\O,0,1.4008,2.247328,-0.259251\C,0,0.54118
1,3.351579,-0.514407\H,0,0.269057,3.866068,0.41979\H,0,1.100944,4.0392
1,-1.152398\H,0,-0.374381,3.036674,-1.028024\C,0,-1.3587,-1.504324,0.0
91959\H,0,-1.200493,-2.515401,0.490264\H,0,-1.105268,-1.553142,-0.9732
97\C,0,-2.838528,-1.125605,0.276004\H,0,-3.055334,-1.026825,1.350782\H
,0,-3.45014,-1.969154,-0.075041\C,0,-3.294259,0.146854,-0.452592\H,0,-
3.06518,0.046903,-1.523041\H,0,-2.709004,1.00275,-0.099584\C,0,-4.7902
61,0.424451,-0.272105\H,0,-5.399486,-0.405071,-0.652886\H,0,-5.044945,
0.560049,0.786724\H,0,-5.095487,1.332477,-0.804897\\Version=IA32L-G03R
evD.01\State=2-A\HF=-694.4505819\S2=0.760102\S2-1=0.\S2A=0.750047\RMSD
=6.759e-09\Thermal=0.\Dipole=-0.4903026,-0.0571028,0.2817934\PG=C01 [X
(C12H19O3)]\\@

cShaC4alpha_087_sp.log

1\1\GINC-NODE-21\SP\UB3LYP\6-311+G(d,p)\C12H19O3(2)\ZIP06\24-Aug-2010\
0\\#P ubecke3lyp/6-311+G(d,p) scf=tight\\UB3LYP/6-311+G(d,p) cShaC4alp
ha_087\\0,2\C,0,-0.141176,-0.429695,-1.309781\O,0,0.857887,-1.475967,-
1.160107\C,0,1.949772,-1.009612,-0.409126\H,0,-0.433979,-0.473249,-2.3
65858\H,0,2.810022,-1.633161,-0.68977\C,0,1.636955,1.817285,1.001123\C
,0,0.338626,1.767023,0.178996\C,0,0.620008,0.909561,-1.057359\C,0,2.08
99,0.47296,-0.820717\O,0,2.662861,1.339211,0.13359\H,0,1.905659,2.8325
94,1.309018\H,0,1.552009,1.177697,1.886905\H,0,0.534193,1.54543,-1.942
937\H,0,2.702509,0.527454,-1.725407\C,0,-0.756745,2.428686,0.46053\H,0
,-1.106216,3.094856,1.239028\O,0,1.740512,-1.081922,0.979661\C,0,1.669
979,-2.41265,1.472393\H,0,2.599327,-2.962022,1.25799\H,0,1.538703,-2.3
42016,2.55463\H,0,0.826378,-2.959408,1.034987\C,0,-1.370172,-0.747272,
-0.454797\H,0,-1.140415,-0.548462,0.597108\H,0,-1.541911,-1.828028,-0.
548795\C,0,-2.635744,0.000557,-0.897966\H,0,-2.789574,-0.174676,-1.973
079\H,0,-2.487026,1.083141,-0.778404\C,0,-3.909011,-0.420449,-0.145268
\H,0,-4.061213,-1.502312,-0.270824\H,0,-4.771652,0.064723,-0.621542\C,
0,-3.90826,-0.076139,1.349037\H,0,-3.111917,-0.601017,1.888347\H,0,-3.
759491,0.999458,1.504608\H,0,-4.860281,-0.353109,1.816451\\Version=IA3
2L-G03RevD.01\State=2-A\HF=-694.450809\S2=0.76046\S2-1=0.\S2A=0.750049
\RMSD=6.742e-09\Thermal=0.\Dipole=-0.337911,-0.110155,0.0961607\PG=C01

[X(C12H19O3)]\\@