Supporting Information

Alkyne and Reversible Nitrile Activation: N,N'-Diamidocarbene Facilitated Synthesis of Cyclopropenes, Cyclopropenones, and Azirines

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General Considerations. All procedures were performed using standard Schlenk techniques under an atmosphere of nitrogen or in a nitrogen-filled glove box unless otherwise noted. *N,N′*-dimesityl-4,6-diketo-5,5-dimethylpyrimidin-2-ylidene (**1**) was synthesized according to literature procedures.[1] Dimethyl acetylenedicarboxylate was distilled prior to use. All commercial liquid substrates were dried over molecular sieves prior to use. All commercial solid substrates were dried under reduced pressure for 24 h prior to use. Benzene, toluene, pentane, and diethyl ether were dried and degassed using a Vacuum Atmospheres Company solvent purification system (model number 103991-0319) and stored over molecular sieves in a nitrogen-filled glove box. Infrared (IR) spectra were recorded on a Perkin Elmer Spectrum BX FTIR spectrophotometer. High resolution mass spectra (HRMS) were obtained with a VG analytical ZAB2-E instrument (CI or ESI). NMR spectra were recorded on Varian Unity+ 300, Varian Mercury 400, Varian MR-400, or Varian Inova 500 spectrometers. Chemical shifts (δ) are given in ppm and are referenced to the residual solvent (^{1}H: $CDCl_3$, 7.24 ppm; C_6D_6, 7.15 ppm; C_7D_8, 7.09 ppm; ^{13}C: $CDCl_3$, 77.0 ppm; C_6D_6, 128.0 ppm). Elemental analyses were performed at Midwest Microlab, LLC (Indianapolis, IN). Melting points were obtained using a Stanford Research Systems automated melting point system and are uncorrected.

Synthesis of 2a. A 100 mL Schlenk flask was charged with **1** (1.0 g, 2.66 mmol, 1 eq), benzene (20 mL), and a stir bar, and then capped with a rubber septum. A needle, attached to a balloon of acetylene, was inserted through the septum into the reaction flask. The septum was then punctured with another needle to relieve pressure, enabling bubbling of acetylene through the reaction mixture. After approximately one minute of bubbling, the needles were removed from the reaction flask, and the mixture was stirred at 23 °C. A white solid was observed to precipitate from the reaction mixture over time. After 8 h, the volatiles were removed under reduced pressure and the residue was repeatedly washed with dry diethyl ether. Removal of the residual solvent under reduced pressure afforded **2a** as a white solid (0.87 g, 2.16 mmol, 81% yield). mp = 166-168 °C (decomp.) ^{1}H NMR ($CDCl_3$, 399.68 MHz): δ 1.72 (s, 6H, C(C*H*$_3$)$_2$), 2.13 (s, 12H, Ar-C*H*$_3$), 2.23 (s, 6H, Ar-C*H*$_3$), 6.84 (s, 4H, Ar-*H*), 7.23 (s, 2H, *H*C=C*H*). ^{13}C NMR ($CDCl_3$, 100.50 MHz): δ 19.76, 21.87, 23.78, 48.57, 57.60, 117.93, 130.27, 132.68, 137.25, 139.00, 172.76. IR (KBr): ν = 3135.9, 2978.0, 29.19.4, 2861.3, 1695.4, 1654.0, 1620.0, 1462.7, 1407.4, 1223.1, 1039.0, 861.4 cm^{-1}. HRMS (CI): $[M+H]^+$ calcd. for $C_{26}H_{31}N_2O_2$: 403.2386; Found: 403.2385. Anal. calcd. for $C_{26}H_{30}N_2O_2$: C,77.58 ; H, 7.51; N, 6.96; Found: C, 77.46; H, 7.56; N, 7.02.

Synthesis of 2b. An 8 mL vial was charged with **1** (0.075 g, 0.199 mmol, 1 eq), benzene (1 mL), and a stir bar. The vial was then charged with 4-tert-butylphenylacetylene (0.032 g, 35.9 μL, 0.199 mmol, 1 eq) and the resultant mixture stirred at 23 °C. After 16 h, the volatiles were removed under reduced pressure and the residue was purified by silica gel column chromatography using 2:1 hexanes/ethyl acetate as the eluent (R_f = 0.28). Removal of the residual solvent under reduced pressure afforded **2b** as a white solid (0.079 g, 0.148 mmol, 74% yield). mp = 144-145 °C. ^{1}H NMR (C_6D_6, 399.68 MHz): δ 1.04 (s, 9H, C(C*H*$_3$)$_3$), 1.94 (s, 6H, Ar-C*H*$_3$), 2.00 (s, 3H, C(C*H*$_3$)), 2.16 (bs, 9H, Ar-C*H*$_3$/C(C*H*$_3$)), 2.18 (s, 6H, Ar-C*H*$_3$), 6.47 (s, 2H, Ar-*H*), 6.65 (s, 1H, *H*C=C), 6.66 (s, 2H, Ar-*H*), 6.96-7.02 (m, 4H, Ar-*H*). ^{13}C NMR (C_6D_6,100.50 MHz): δ 19.22, 19.46, 20.75, 23.14, 24.18, 30.97, 34.65, 48.02, 61.39, 109.21, 123.97, 125.48, 127.33, 128.94, 129.30, 129.63, 133.63, 136.81, 137.37, 137.69, 153.33, 171.81. IR (KBr): ν = 3087.7, 2966.5, 2928.2, 2868.2, 1680.8, 1649.9, 1461.8, 1405.7, 1354.8, 1216.0,

844.7 cm^{-1}. HRMS (CI): $[M+H]^+$ calcd. for $C_{36}H_{43}N_2O_2$: 535.3325; Found: 535.3312. Anal. calcd. for $C_{36}H_{42}N_2O_2$: C, 80.86; H, 7.92; N, 5.24; Found: C, 80.57; H, 7.69; N, 4.90.

Synthesis of 2c. An 8 mL vial was charged with **1** (0.075 g, 0.199 mmol, 1 eq), benzene (1 mL), and a stir bar. To this vial, cyclohexylacetylene (0.022 g, 26 μL, 0.199 mmol, 1 eq), was added and the resultant mixture was stirred at 60 °C. After 16 h, the reaction mixture was cooled to ambient temperature and the volatiles were removed under reduced pressure. Recrystallization of the residue from toluene at -20 °C followed by washing with cold pentane afforded **2c** as a white solid (0.067 g, 0.138 mmol, 68% yield). mp = 185-187 °C (decomp.) ^{1}H NMR (C_6D_6, 399.68 MHz): δ 0.19-0.28 (m, 2H, cy-*H*), 0.43-0.47 (m, 2H, cy-*H*), 0.75-0.90 (m, 3H, cy-*H*), 1.08-1.12 (m, 3H, cy-*H*), 1.74 (m overlapping singlet, 4H, cy-*H* and C(C*H*$_3$)), 1.90 (s, 6H, Ar-C*H*$_3$), 2.03 (s, 3H, C(C*H*$_3$)), 2.04 (s, 6H, Ar-C*H*$_3$), 2.35 (s, 6H, Ar-C*H*$_3$), 6.64 (s, 2H, Ar-*H*), 6.70 (s, 2H, Ar-*H*), 6.83 (s, 1H, *H*C=C). ^{13}C NMR (C_6D_6, 100.50 MHz): δ 19.12, 19.32, 20.79, 21.63, 24.34, 24.78, 25.86, 30.36, 33.70, 48.37, 59.95, 109.90, 129.26, 129.33, 131.14, 134.05, 137.11, 137.59, 137.67, 171.90. IR (KBr): ν = 3124.0, 3088.5, 2978.5, 2927.9, 2854.4, 1678.6, 1647.0, 1413.1, 1356.4, 1221.9, 1173.8, 1042.5, 851.8, 797.1 cm^{-1}. HRMS (CI): $[M+H]^+$ calcd. for $C_{32}H_{41}N_2O_2$: 485.3168; Found: 485.3164. Anal. calcd. for $C_{32}H_{40}N_2O_2$: C, 79.30; H, 8.32; N, 5.78; Found: C, 79.44; H, 8.18; N, 5.52.

Synthesis of 2d. An 8 mL vial was charged with **1** (0.075 g, 0.199 mmol, 1 eq), benzene (1 mL), and a stir bar. To this vial, 1-hexyne (0.016 g, 23 μL, 0.199 mmol, 1 eq) was added and the resultant mixture heated to 60 °C. After 16 h, the reaction was cooled to ambient temperature, and the volatiles were removed under reduced pressure. Washing the residue with a minimum amount of cold diethyl ether followed by drying under reduced pressure afforded **2d** as a white solid (0.085 g, 0.185 mmol, 93% yield). mp = 158-160 °C (decomp.) ^{1}H NMR (C_6D_6, 400.27 MHz): δ 0.41 (t, ^{3}J = 6.8 Hz, 3H, CH_2CH_3), 0.50-0.59 (m, 4H, $CH_2CH_2CH_3$), 1.46 (t, ^{3}J = 6.4 Hz, 2H, C=CCH_2CH_2), 1.76 (s, 3H, Ar-C*H*$_3$), 1.92 (s, 6H, Ar-C*H*$_3$), 1.99 (s, 3H, Ar-C*H*$_3$), 2.04 (s, 6H, Ar-C*H*$_3$), 2.31 (s, 6H, Ar-C*H*$_3$), 6.64 (s, 2H, Ar-*H*), 6.67 (s, 2H, Ar-*H*), 6.82 (s, 1H, *H*C=C). ^{13}C NMR (C_6D_6, 100.50 MHz): δ 13.42, 19.02, 19.10, 20.81, 21.39, 21.83, 23.49, 24.51, 28.39, 48.24, 59.20, 109.34, 128.35, 129.29, 129.35, 133.62, 137.03, 137.07, 137.60, 171.80. IR (KBr): ν = 3083.7, 2964.9, 2929.6, 2861.1, 1682.9, 1646.0, 1465.2, 1409.9, 1359.5, 1217.4, 1174.7, 1042.6, 849.0, 830.1, 801.3 cm^{-1}. HRMS (CI): $[M+H]^+$ calcd. for $C_{30}H_{39}N_2O_2$: 459.3012; Found: 459.3017. Anal. calcd. for $C_{30}H_{38}N_2O_2$: C, 78.56; H,8.35 ; N, 6.11; Found: C, 78.76; H, 8.19; N, 5.85.

Synthesis of 2e. An 8 mL vial was charged with **1** (0.075 g, 0.199 mmol, 1 eq), benzene (1 mL), and a stir bar. To this vial, 2-hexyne (0.033 g, 44.8 μL, 0.398 mmol, 2 eq) was added and the resultant mixture heated to 60 °C. After 16 h, the reaction was cooled to ambient temperature and the volatiles removed under reduced pressure. Washing the residue with a minimum amount of cold diethyl ether followed by drying under reduced pressure afforded **2e** as a white solid (0.081 g, 0.177 mmol, 89% yield). mp = 146-147 °C (decomp.) ^{1}H NMR (C_6D_6, 399.68 MHz): δ 0.28 (t, ^{3}J = 7.6 Hz, 3H, CH_2CH_3), 0.79 (sextet, ^{3}J = 7.2 Hz, 2H, $CH_2CH_2CH_3$), 1.44 (t, ^{3}J = 1.4 Hz, 3H, CH_3C=CCH_2), 1.68 (m, 2H, CH_3C=CCH_2CH_2), 1.91 (s, 3H, C(C*H*$_3$)), 1.97 (s, 3H, C(C*H*$_3$)), 2.03 (s, 6H, Ar-C*H*$_3$), 2.11 (s, 6H, Ar-C*H*$_3$), 2.21 (s, 6H, Ar-C*H*$_3$), 6.64 (overlapping singlets, 4H, Ar-*H*). ^{13}C NMR (C_6D_6, 100.50 MHz): δ 9.87, 13.19, 18.98, 19.24, 20.34, 20.80, 23.12, 24.36, 26.72, 48.20, 61.74, 118.17, 122.31, 129.23, 129.26, 134.02, 137.17, 137.20, 137.25,

172.00. IR (KBr): ν = 2992.9, 2978.9, 2952.6, 2924.6, 2872.0, 1837.1, 1685.7, 1648.0, 1607.7, 1461.2, 1410.7, 1216.1, 1172.7, 861.3 cm^{-1}. HRMS (CI): $[M+H]^+$ calcd. for $C_{30}H_{39}N_2O_2$: 459.3012; Found: 459.3009. Anal. calcd. for $C_{30}H_{38}N_2O_2$: C, 78.56; H, 8.35; N, 6.11; Found: C, 78.66; H, 8.19 ; N, 5.98.

Synthesis of 2f. An 8 mL vial was charged with **1** (0.075 g, 0.199 mmol, 1 eq), benzene (1 mL), and a stir bar. To this vial, 1-phenyl-1-butyne (0.052 g, 56.6 μL, 0.199 mmol, 1 eq) was added and the resultant mixture stirred at 23 °C. After 16 h, the volatiles were removed under reduced pressure. Washing the residue with a minimum amount of cold diethyl ether followed by drying under reduced pressure afforded **2f** as a white solid (0.098 g, 0.192 mmol, 97% yield). mp = 169-171 °C (decomp.) ^{1}H NMR (C_6D_6, 399.68 MHz): δ 0.36 (t, ^{3}J = 7.40 Hz, 3H, CH_2CH_3), 1.76 (q, ^{3}J = 7.40 Hz, 2H, CH_2CH_3), 1.95 (s, 6H, Ar-CH_3), 1.99 (s, 6H, Ar-CH_3), 2.11 (s, 3H, C(CH_3)), 2.12 (s, 3H, C(CH_3)), 2.36 (s, 6H, Ar-CH_3), 6.48 (s, 2H, Ar-*H*), 6.68 (s, 2H, Ar-*H*), 6.95-6.98 (m, 3H, Ar-*H*), 7.24-7.27 (m, 2H, Ar-*H*). ^{13}C NMR (C_6D_6, 100.49 MHz): δ 11.63, 18.50, 19.33, 19.50, 20.74, 23.07, 25.03, 47.82, 62.75, 121.80, 123.97, 128.75, 129.11, 129.26, 129.44, 129.74, 134.28, 136.99, 137.24, 138.33, 172.19. IR (KBr): ν = 3046.3, 2977.6, 2858.1, 1679.7, 1643.6, 1408.3, 1353.5, 1215.0, 1173.8, 774.5, 732.4, 695.5 cm^{-1}. HRMS (CI): $[M+H]^+$ calcd. for $C_{34}H_{39}N_2O_2$: 507.3012; Found: 507.3009. Anal. calcd. for $C_{34}H_{38}N_2O_2$: C, 80.60; H, 7.56; N, 5.53; Found: C, 80.69; H, 7.59; N, 5.55.

Synthesis of 2g. An 8 mL vial was charged with **1** (0.075 g, 0.199 mmol, 1 eq), diphenylacetylene (0.071 g, 0.398 mmol, 2 eq), benzene (1 mL), and a stir bar. The resultant mixture was then stirred at 60 °C for 16 h. Upon cooling to ambient temperature, the volatiles were removed under reduced pressure. Washing the residue with pentane followed by drying under reduced pressure afforded **2g** as a white solid (0.102 g, 0.184 mmol, 92% yield). mp = 184-186 °C (decomp.) ^{1}H NMR (C_6D_6, 399.68 MHz): δ 1.97 (s, 6H, C(CH_3)$_2$), 2.13 (s, 12H, Ar-CH_3), 2.16 (s, 6H, Ar-CH_3), 6.53 (s, 4H, Ar-*H*), 6.89-6.97 (bm, 10H, Ar-*H*). ^{13}C NMR (C_6D_6, 100.50 MHz): δ 19.68, 20.71, 24.26, 47.92, 64.44, 122.93, 128.49, 128.97, 129.47, 129.57, 134.46, 137.45, 138.04, 172.41. IR (KBr): ν = 3059.9, 2984.6, 2923.5, 2859.0, 1801.2, 1685.0, 1648.5, 1607.6, 1458.4, 1401.7, 1212.9, 1171.2, 778.8, 761.1, 692.6, 611.1 cm^{-1}. HRMS (CI): $[M+H]^+$ calcd. for $C_{38}H_{39}N_2O_2$: 555.3012; Found: 555.3006. Anal. calcd. for $C_{38}H_{38}N_2O_2$: C, 82.28; H, 6.90; N, 5.05; Found: C, 82.09; H, 7.07; N, 4.92.

Synthesis of 2h. A 25 mL Schlenk flask was charged with **1** (0.075 g, 0.199 mmol, 1 eq), benzene (1 mL), and a stir bar. To this vial, 1-(trimethylsilyl)-1-propyne (0.076 g, 56.4 μL, 0.398 mmol, 2 eq) was added and the resultant mixture heated to 60 °C. After 16 h, the reaction was then cooled to ambient temperature, and the volatiles were removed under reduced pressure. Washing the residue with a minimum amount of cold diethyl ether followed by drying under reduced pressure afforded **2h** as a white solid (0.090 g, 0.184 mmol, 93% yield). mp = 166-167 °C (decomp.) ^{1}H NMR (C_6D_6, 399.68 MHz): δ -0.29 (s, 9H, Si(CH_3)$_3$), 1.54 (s, 3H, C=CCH_3), 1.92 (s, 3H, (C(CH_3)), 2.00 (s, 3H, C(CH_3)), 2.04 (s, 6H, Ar-CH_3), 2.08 (s, 6H, Ar-CH_3), 2.22 (s, 6H, Ar-CH_3), 6.64 (s, 4H, Ar-*H*). ^{13}C NMR (C_6D_6, 100.50 MHz): δ -1.11, 11.52, 19.09, 19.98, 20.79, 23.25, 23.36, 48.34, 62.33, 123.41, 129.19, 129.24, 133.88, 137.06, 137.38, 137.57, 140.70, 172.00. IR (KBr): ν = 2995.8, 2981.1, 2962.4, 1922.6, 2861.5, 1750.8, 1683.1, 1648.1, 1607.1, 1461.9, 1404.5, 1353.9, 1251.8, 1215.2, 1031.9, 846.0, 774.7 cm^{-1}. HRMS (CI): $[M+H]^+$

calcd. for $C_{30}H_{41}N_2O_2Si$: 489.2937; Found: 489.2931. Anal. calcd. for $C_{30}H_{40}N_2O_2Si$: C, 73.73; H, 8.25; N, 5.73; Found: C, 73.61; H, 8.12; N, 5.43.

Synthesis of 2i. A 25 mL Schlenk flask was charged with **1** (0.075 g, 0.199 mmol, 1 eq), benzene (5 mL), and a stir bar. To this flask, dimethyl acetylenedicarboxylate (0.028 g, 24.5 µL, 0.199 mmol, 1 eq) was added and the resultant mixture stirred at 23 °C. After 5 min, the volatiles were removed under reduced pressure. Washing the residue with minimal pentane followed by drying under reduced pressure afforded **2i** as a white solid (0.100 g, 0.193 mmol, 97% yield). mp = 97-99 °C (decomp.) ^{1}H NMR (C_6D_6, 400.27 MHz): δ 1.96 (s, 6H, C(C*H*$_3$)$_2$), 2.06 (s, 6H, Ar-C*H*$_3$), 2.34 (s, 12H, Ar-C*H*$_3$), 2.98 (s, 6H, OC*H*$_3$), 6.65 (s, 4H, Ar-*H*). ^{13}C NMR (C_6D_6, 75.47 MHz): δ 18.84, 20.78, 23.24, 46.67, 52.43, 63.83, 125.78, 129.60, 132.17, 138.06, 138.35, 156.88, 171.59. IR (KBr): ν = 2954.6, 2926.0, 1813.2, 1723.0, 1696.5, 1665.3, 1406.4, 1247.3 cm^{-1}. HRMS (CI): $[M+H]^+$ calcd. for $C_{30}H_{35}N_2O_6$: 519.2495; Found: 519.2491. Anal. calcd. for $C_{30}H_{34}N_2O_6$: C, 69.48; H, 6.61; N, 5.40; Found: C, 69.63; H, 6.60; N, 5.34.

Synthesis of 3. An 8 mL vial was charged with **1** (0.075 g, 0.199 mmol, 1 eq), benzene (1 mL), and a stir bar. To this vial, dimethyl acetylenedicarboxylate (0.028 g, 24.5 µL, 0.199 mmol, 1 eq) was added and the resultant mixture stirred at 23 °C. After 48 h, the volatiles were removed under reduced pressure and the residue was purified by silica gel column chromatography using 1:1 hexanes/ethyl acetate as the eluent (R_f = 0.73). Removal of the volatiles under reduced pressure afforded **3** as a white solid (0.042 g, 0.081 mmol, 41% yield). mp = 156-158 °C (decomp.) ^{1}H NMR (C_6D_6, 400.27 MHz): δ 1.42 (s, 3H, C=CC*H*$_3$), 1.63 (s, 3H, C=CC*H*$_3$), 1.89 (overlapping singlets, 6H, C(C*H*$_3$)$_2$), 2.00 (s, 3H, C=CC*H*$_3$), 2.13 (s, 3H, Ar-C*H*$_3$), 2.23 (s, 3H, Ar-C*H*$_3$), 2.32 (s, 3H, Ar-C*H*$_3$), 2.85 (3H, OC*H*$_3$), 3.29 (s, 3H, OC*H*$_3$), 5.98 (s, 1H, C=C*H*), 6.14 (s, 1H, C=C*H*), 6.57 (s, 1H, Ar-*H*), 6.67 (s, 1H, Ar-*H*). ^{13}C NMR (C_6D_6, 74.47 MHz): δ 17.55, 18.53, 20.81, 21.30, 21.80, 22.15, 24.47, 25.28, 48.81, 51.21, 51.97, 62.22, 101.42, 119.58, 121.05, 127.12, 129.03, 129.17, 130.13, 132.74, 135.26, 138.07, 138.12, 143.28, 163.33, 167.52, 170.10, 170.62. IR (KBr): ν = 2981.2, 1937.6, 1737.9, 1720.1, 1698.3, 1664.6, 1640.0, 1447.3, 1387.8, 1351.3, 1233.8, 1150.7, 1018.7, 850.9, 840.6 cm^{-1}. HRMS (CI): $[M+H]^+$ calcd. for $C_{30}H_{35}N_2O_6$:519.2495; Found: 519.2496. Anal. calcd. for $C_{30}H_{34}N_2O_6$: C, 69.48; H, 6.61; N, 5.40; Found: C, 69.48; H, 6.58; N, 5.38.

Synthesis of 4. An 8 mL vial was charged with **1** (0.075 g, 0.199 mmol, 1 eq), benzene (1 mL), and a stir bar. To this vial, dimethyl acetylenedicarboxylate (0.028 g, 24.5 µL, 0.199 mmol, 1 eq) was added and the resultant mixture heated to 60 °C. After 12 h, the reaction mixture was cooled to ambient temperature and the volatiles were removed under reduced pressure. The residue was purified by silica gel column chromatography using 1:1 hexanes/ethyl acetate as the eluent (R_f = 0.68). Removal of the volatiles under reduced pressure afforded **4** as a white solid (0.083 g, 0.160 mmol, 80% yield). mp = 189-190 °C (decomp.) ^{1}H NMR (C_6D_6, 399.68 MHz): δ 1.46 (s, 6H, Ar-C*H*$_3$), 1.71 (s, 6H, Ar-C*H*$_3$), 1.99 (s, 3H, C(C*H*$_3$)), 2.01, (s, 3H, C(C*H*$_3$)), 2.32 (s, 6H, Ar-C*H*$_3$), 3.17 (s, 3H, OC*H*$_3$), 3.20 (s, 3H, OC*H*$_3$), 6.54 (s, 2H, Ar-*H*), 6.62 (s, 2H, Ar-*H*). ^{13}C NMR (C_6D_6, 100.50 MHz): δ 17.79, 20.85, 20.89, 21.25, 22.01, 51.36, 52.16, 52.26, 128.68, 128.95, 129.89, 130.66, 130.75, 137.95, 138.14, 138.95, 139.61, 159.42, 164.56, 167.01, 174.71, 182.58. IR (KBr): ν = 2992.9, 2948.3, 2925.3, 1732.5, 1708.9, 1576.7, 1436.8, 1251.9, 1232.6 cm^{-1}. HRMS (CI): $[M+H]^+$ calcd. for $C_{30}H_{35}N_2O_6$:519.2495; Found: 514.2495. Anal. calcd. for $C_{30}H_{34}N_2O_6$: C, 69.48; H, 6.61; N, 5.40; Found: C, 69.46; H, 6.59; N, 5.37.

In situ generation of 5a-c. An 8 mL vial was charged with **1** (0.025 g, 0.066 mmol, 1 eq), C_6D_6 (0.8 mL), and a stir bar. To this vial, aryl nitrile (2 eq), was added and then stirred at 23 °C for 2 h prior to spectroscopic analysis.

Spectroscopic data for 5a. ^{1}H NMR (C_6D_6, 399.68 MHz): δ 1.80 (s, 6H, Ar-C*H*$_3$), 2.03 (s, 3H, C(C*H*$_3$)), 2.15 (s, 3H, C(C*H*$_3$)), 2.25 (s, 6H, Ar-C*H*$_3$), 2.40 (s, 6H, Ar-C*H*$_3$), 6.46 (s 2H, Ar-*H*), 6.52 (s, 2H, Ar-*H*), 6.57-6.67 (m, 3H, Ar-*H*), 6.93-6.99 (m, 2H, Ar-*H*). ^{13}C NMR (C_6D_6, 100.50 MHz): δ 19.09, 19.30, 20.65, 21.11, 25.68, 49.54, 123.83, 127.11, 128.51, 129.34, 129.85, 132.16, 132.67, 136.64, 137.79, 138.50, 167.62, 172.17. IR (CH_2Cl_2): ν = 3061.6, 3029.5, 2979.8, 2923.6, 2860.0, 2229.9, 1740.2, 1712.3, 1699.9, 1666.0, 1608.8, 1490.7, 1447.9, 1411.3, 1384.6, 1329.2 cm^{-1}. HRMS (CI): $[M+H]^+$ calcd. for $C_{31}H_{34}N_3O_2$: 480.2651; Found: 480.2650.

Spectroscopic data for 5b. ^{1}H NMR (C_6D_6, 399.68 MHz): δ 1.83 (s, 6H, Ar-C*H*$_3$), 1.97 (s, 3H, C(C*H*$_3$)), 2.10 (s, 3H, C(C*H*$_3$)), 2.18 (s, 6H, Ar-C*H*$_3$), 2.32 (s, 6H, Ar-C*H*$_3$), 6.48 (s, 2H, Ar-*H*), 6.52 (s, 2H, Ar-*H*), 6.66-6.69 (overlapping m, 2H), 7.29-7.32 (m, 2H). ^{13}C NMR (C_6D_6, 100.50 MHz): δ 18.95, 19.19, 20.66, 20.94, 25.65, 49.61, 69.65, 127.54, 128.81, 129.44, 129.95, 132.14, 136.63, 137.92, 139.05, 149.81, 161.74, 171.98. IR (CH_2Cl_2): ν = 3110.4, 3062.0, 298.9, 2926.2, 2867.7, 2236.7, 1701.9, 1671.9, 1605.2, 1532.5, 1402.2, 1346.5 cm^{-1}. HRMS (CI): $[M]^+$ calcd. for $C_{31}H_{32}N_4O_4$: 524.2424; Found: 524.2419.

Spectroscopic data for 5c. ^{1}H NMR (C_6D_6, 399.68 MHz): δ 1.80 (s, 6H, Ar-C*H*$_3$), 2.00 (s, 3H, C(C*H*$_3$)), 2.16 (s, 3H, C(C*H*$_3$)), 2.27 (s, 6H, Ar-C*H*$_3$), 2.48 (s, 6H, Ar-C*H*$_3$), 2.84 (s, 3H, Ar-C*H*$_3$), 6.21 (d, ^{3}J = 8.8 Hz, 2H, Ar-*H*), 6.48 (s, 2H, Ar-*H*), 6.59 (s, 2H, Ar-*H*), 7.05 (overlapping d, 2H, Ar-*H*). ^{13}C NMR (C_6D_6, 100.50 MHz): δ 19.17, 19.36, 20.70, 21.16, 25.70, 49.50, 54.58, 68.95, 114.31, 115.77, 119.19, 129.33, 129.86, 132.69, 136.57, 137.85, 138.43, 163.35, 165.87, 172.30. IR (CH_2Cl_2): ν = 3060.3, 3013.0, 2971.6, 2938.8, 2842.6, 2226.0, 1712.3, 1698.5, 1663.8, 1606.7, 1509.5, 1407.7, 1303.6, 1172.1 cm^{-1}. HRMS (CI): $[M+H]^+$ calcd. for $C_{32}H_{36}N_3O_3$: 510.2757; Found: 510.2745.

In situ generation of 5d. An 8 mL vial was charged with **1** (0.015 g, 0.04 mmol, 1 eq), C_6D_6 (0.8 mL), and a stir bar. To this vial, acetonitrile (0.016 g, 20.8 μL, 0.40 mmol, 10 eq) was added and then stirred at 23 °C for 2 h prior to spectroscopic analysis.

Spectroscopic data for 5d. ^{1}H NMR (C_6D_6, 400.27 MHz): δ 0.95 (s, 3H, N=CC*H*$_3$), 1.85 (s, 3H, C(C*H*$_3$)), 1.97 (s, 3H, C(C*H*$_3$)), 2.03 (s, 6H, Ar-C*H*$_3$), 2.13 (s, 6H, Ar-C*H*$_3$), 2.19 (s, 6H, Ar-C*H*$_3$), 6.60 (s, 2H, Ar-*H*), 6.66 (s, 2H, Ar-*H*). ^{13}C NMR (C_6D_6, 75.47 MHz): δ 11.36, 18.71, 19.09, 20.80, 20.86, 25.99, 49.21, 65.11, 129.27, 129.96, 132.12, 136.35, 138.25, 138.52, 169.93, 171.92. IR (CH_2Cl_2): ν = 3164.7, 3058.8, 2998.5, 2939.9, 2924.5, 2290.9, 2253.9, 1740.6, 1712.3, 1698.4, 1663.5, 1608.6, 1461.7, 1442.7, 1410.8, 1373.0, 1328.9 cm^{-1}. HRMS (CI): $[M+H]^+$ calcd. for $C_{26}H_{32}N_3O_2$: 418.2495; Found: 418.2491.

Synthesis of 6. An 8 mL vial was charged with **1** (0.500 g, 1.33 mmol, 1 eq), tetracyanoethylene (0.170 g, 0.199 mmol, 1 eq), $CHCl_3$ (6 mL), and a stir bar. The resultant mixture was stirred at 23 °C. After 1 h, the volatiles were removed under reduced pressure which afforded a dark red residue. The residue was dissolved in CH_2Cl_2 and filtered through a six inch silica gel plug with copious amounts of CH_2Cl_2. The residual solvent volatiles were then removed under reduced

pressure, and the residue was washed with toluene until it became colorless. Drying under reduced pressure afforded **6** as an off-white solid (0.107 g, 0.0.212 mmol, 16% yield). mp = 169-170 °C. ^{1}H NMR ($CDCl_3$, 400.27 MHz): δ 1.73 (s, 6H, C(C*H*$_3$)$_2$), 1.81 (s, 3H, C(C*H*$_3$)), 1.87 (d, ^{3}J = 1.2 Hz, 6H, HC=CC*H*$_3$), 2.06 (s, 6H, Ar-C*H*$_3$), 2.32 (s, 3H, Ar-C*H*$_3$), 5.78 (d, ^{3}J = 1.2 Hz, C=C*H*), 6.97 (s, 2H, Ar-*H*). ^{13}C NMR ($CDCl_3$, 100.50 MHz): δ 16.88, 17.53, 21.16, 24.32, 24.97, 41.43, 45.19, 48.57, 73.41, 83.91, 111.33, 114.51, 125.71, 128.79, 129.89, 134.13, 140.27, 145.74, 157.19, 167.60, 167.77, 170.62. IR (KBr): ν = 2955.6, 2921.5, 2215.8, 1744.4, 1711.6, 1541.7, 1447.0, 1390.7, 1354.2, 1249.6, 1104.8, 975.7, 855.2 cm^{-1}. HRMS (ESI): [M+H]$^{+}$ calcd. for $C_{30}H_{29}N_6O_2$: 505.2347; Found: 505.2346.

Hydrolysis of 2g to 2,3-diphenylcyclopropenone. An 8 mL vial was charged with **1** (0.500 g, 1.33 mmol, 1 eq), diphenylacetylene (0.473 g, 2.66 mmol, 2 eq), benzene (6 mL), and a stir bar. After the resultant mixture was stirred at 60 °C for 16 h, the volatiles were removed under reduced pressure. Glacial acetic acid (3 mL) and concentrated hydrochloric acid (3 mL) were added to the reaction flask and the mixture was heated at 80 °C. After 2 h, the reaction mixture was cooled to ambient temperature, and the volatiles were removed under reduced pressure. The residue was purified via silica gel column chromatography using 1:1 hexanes/ethyl acetate (R_f = 0.34) followed by 100% ethyl acetate (R_f = 0.68) as the eluent. Removal of the volatiles under reduced pressure afforded 2,3-diphenylcycloprop-2-enone as a white solid (178 mg, 0.863 mmol, 66% yield). In agreement with literature values[2]: mp = 114-116 °C. ^{1}H NMR ($CDCl_3$, 399.68 MHz): δ 7.53-7.61 (m, 6H, Ar-*H*), 7.96-7.98 (m, 4H, Ar-*H*). ^{13}C NMR ($CDCl_3$, 100.50 MHz): δ 123.95, 129.31, 131.42, 132.65, 148.28, 155.74. IR (KBr): ν = 2923.3, 1839.1, 1618.8, 1440.8, 1338.4, 782.3, 759.1, 684.0, 511.8, 471.3 cm^{-1}. HRMS (CI): [M+H]$^{+}$ calcd. for $C_{15}H_{11}O$: 207.0810; Found: 207.0813.

Hydrolysis of 2g to trans-α-phenylcinnamic acid. An 8 mL vial was charged with **2g** (0.200 g, 0.361 mmol), glacial acetic acid (1.5 mL), concentrated hydrochloric acid (1.5 mL), and a stir bar. After stirring the resultant mixture at 100 °C for 48 h, the reaction mixture was cooled to ambient temperature and the volatiles were removed under reduced pressure. The residue was dissolved in diethyl ether (20 mL) and extracted with an aqueous solution saturated with $NaHCO_3$ (3 × 20 mL). The aqueous layer was acidified with 10 mol % HCl, and extracted with diethyl ether (3 × 50 mL). The organic layer from the acidic extract was then dried over Na_2SO_4 and filtered. The volatiles from the filtrate were removed under reduced pressure. Washing of the residue with a minimal quantity of pentane followed by drying under reduced pressure afforded trans-α-phenylcinnamic acid as a white solid (26 mg, 0.116 mmol, 32% yield). In agreement with literature values[3]: mp = 173-174 °C. ^{1}H NMR ($CDCl_3$, 399.68 MHz): δ 7.04-7.06 (m, 2H, Ar-*H*), 7.13-7.17 (m, 2H, Ar-*H*), 7.20-7.24 (m, 3H, Ar-*H*), 7.32-7.39 (m, 3H, Ar-*H*), 7.94 (s, 1H, C=C*H*), 11.6 (bs, 1H, CO_2*H*). ^{13}C NMR ($CDCl_3$, 100.50 MHz): δ 128.06, 128.26, 128.72, 129.49, 129.74, 130.84, 131.52, 134.25, 135.25, 142.46, 172.67. IR (KBr): ν = 3053.9, 3023.9, 2954.9, 2841.0, 2799.0, 2631.9, 1678.3, 1429.2, 1273.9, 707.4, 690.1 cm^{-1}. HRMS (CI): [M+H]$^{+}$ calcd. for $C_{15}H_{12}O_2$: 224.0837. Found: 224.0837.

Hydrolysis of 2e to 2-methyl-3-propylcycloprop-2-enone. An 8 mL vial was charged with **1** (0.500 g, 1.33 mmol, 1 eq), benzene (6 mL), and a stir bar. To this vial, 2-hexyne (0.218 g, 299 μL, 2.66 mmol, 2 eq) was added and the resultant mixture was stirred at 60 °C. After 16 h, the volatiles were removed under reduced pressure. Glacial acetic acid (3 mL) and concentrated

hydrochloric acid (3 mL) were added and the resultant mixture heated to 80 °C for 2 h. Upon cooling to ambient temperature, the volatiles were removed under reduced pressure. The residue was triturated with pentane and filtered. The filtrate was concentrated under reduced pressure. Vacuum distillation (20 mtorr) with heating (90 °C) of the crude residue afforded 2-methyl-3-propylcycloprop-2-enone as a clear liquid (103 mg, 0.935 mmol, 70% yield). In agreement with literature values[4]: ^{1}H NMR: ($CDCl_3$, 399.68 MHz): δ 0.92 (t, ^{3}J = 7.6 Hz, 3H, C*H*$_3$CH$_2$), 1.62 (sextet, ^{3}J = 7.2 Hz, 2H, CH$_2$C*H*$_2$CH$_3$), 2.15 (t, ^{3}J = 0.8 Hz, 3H, C=CC*H*$_3$), 2.47 (dt, ^{3}J = 4.0 Hz, 2H, C=CCH$_2$CH$_2$). ^{13}C NMR ($CDCl_3$, 100.50 MHz): δ 11.02, 13.56, 19.31, 27.91, 156.81, 159.67, 161.17. IR (CH_2Cl_2): 3054.1, 2966.6, 2936.4, 2876.0, 1846.4, 1633.4 cm^{-1}. HRMS (CI):[M+H]$^+$ calcd. for $C_7H_{11}O$: 111.0810. Found: 111.0811.

Hydrolysis of 2e to trans-2-methylhex-2-enoic acid and trans-2-ethylidenepentanoic acid. An 8 mL vial was charged with **2e** (0.150 g, 0.327 mmol, 1 eq), glacial acetic acid (1 mL), concentrated hydrochloric acid (1 mL), and a stir bar. The resultant mixture was then stirred at 100 °C for 48 h. Upon cooling to ambient temperature, the solution was basified with 1 M NaOH and extracted with diethyl ether (3 × 20 mL). The aqueous layer was acidified with 10% HCl and extracted with diethyl ether (3 × 50 mL). The organic layer from the acidic extract was dried over Na_2SO_4, filtered, and the volatiles removed under reduced pressure. The resultant residue was triturated with pentane and filtered. Removal of the volatiles from the filtrate under reduced pressure afforded a mixture of trans-2-methylhex-2-enoic acid and trans-2-ethylidenepentanoic acid (53:47) as a viscous clear liquid (18 mg, 0.140 mmol, 43% yield). In agreement with literature values[5,6]: ^{1}H NMR: ($CDCl_3$, 399.68 MHz): δ 0.90 (t, ^{3}J = 7.4 Hz, 3H, CH$_2$C*H*$_3$), 0.92 (t, ^{3}J = 7.4 Hz, 3H, CH$_2$CH$_2$C*H*$_3$), 1.44 (overlapping multiplets, 4H, CH$_2$C*H*$_2$CH$_3$), 1.82 (overlapping m, 6H, C=CC*H*$_3$), 2.16 (q, ^{3}J = 7.4 Hz, 2H, C=CHC*H*$_2$CH$_2$), 2.26 (t, ^{3}J = 7.8 Hz, 2H, C=CC*H*$_2$CH$_2$), 6.90 (dt, ^{3}J = 4.5 Hz, 1H, C=C*H*), 7.00 (q, ^{3}J = 7.2 Hz, 1H, C=C*H*). ^{13}C NMR ($CDCl_3$, 75.47 MHz): δ 11.96, 13.84, 13.88, 14.52, 21.70, 22.12, 27.96, 30.87, 127.06, 132.59, 140.31, 145.31, 173.31, 173.59. IR (CH_2Cl_2): 3505.9, 2962.1, 2932.7, 2872.9, 1715.8, 1685.2, 1641.3 cm^{-1}. HRMS (CI): [M+H]$^+$ calcd. for $C_7H_{13}O_2$: 129.0916. Found: 129.0917.

Evaluation of the Reactions Involving 1 and Various Nitriles. For **5a-c**: An 8 mL vial was charged with **1** (0.025 g, 0.066 mmol, 1 eq), C_7D_8 (0.6 mL), and a stir bar. To this vial, an aryl nitrile (1 eq) was added. **For 5d**: An 8 mL vial was charged with **1** (0.015 g, 0.066 mmol, 1 eq), C_7D_8 (1.6 mL), a stir bar, followed by acetonitrile (10 eq). In all cases, the resultant mixture was stirred for 45 min at 23 °C prior to being transferred to an NMR tube. The sample was then inserted into the NMR spectrometer and equilibrated at 0 °C. A ^{1}H NMR spectrum was taken at 10 °C intervals from 0-60 °C. The percent conversion was determined by the ratio of the methyl singlet of **1** at 1.34-1.49 ppm with the methyl singlet of **5a-d** at 2.25-2.46 ppm. The equilibrium constant K_{eq} was then calculated using the equation:

$$K_{eq} = \frac{[\mathbf{5}]}{[\mathbf{1}][RCN]}$$

The K_{eq} values calculated for **5a-d** at each 10 °C interval from 0-60 °C were used to generate a van't Hoff plot by plotting ln K_{eq} versus 1/T and fit to a linear regression (Figures S1-4). Using the following equations, ΔH and ΔS were calculated for each reaction investigated. The standard deviations are calculated from the linear regression fit.

$$slope = \frac{-\Delta H}{R} \qquad y - intercept = \frac{\Delta S}{R}$$

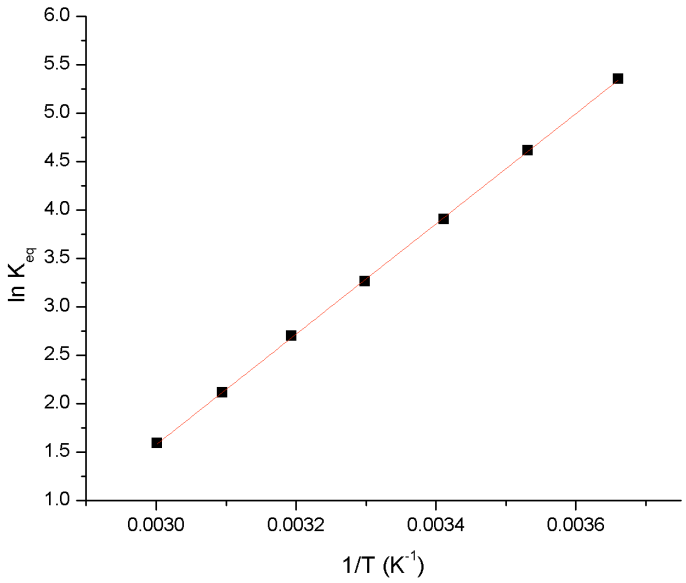


Figure S1. Plot of ln K_{eq} versus 1/T for the reaction **1** + benzonitrile → **5a**. The equation for the best fit line shown in red is as follows: y = mx + b, where m = 5700 ± 30 K^{-1} and b = -15.52 ± 0.1.

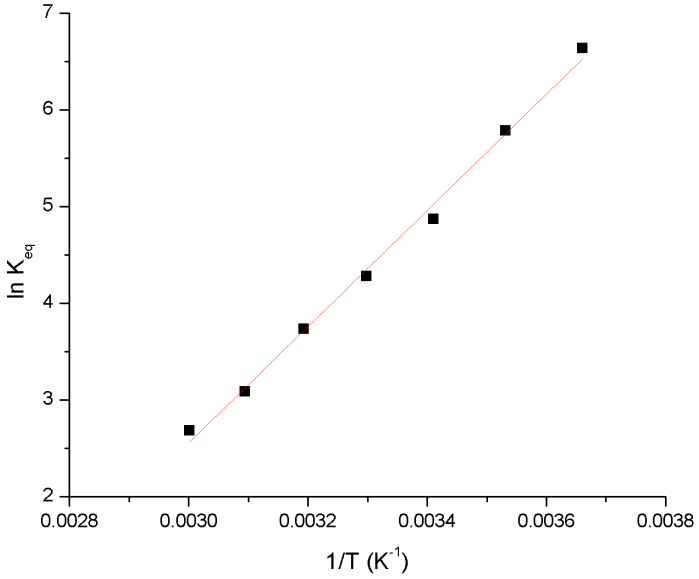


Figure S2. Plot of ln K_{eq} versus 1/T for the reaction **1** + 4-nitrobenzonitrile → **5b**. The equation for the best fit line shown in red is as follows: y = mx + b, where m = 6010 ± 190 K^{-1} and b = -15.5 ± 0.6.

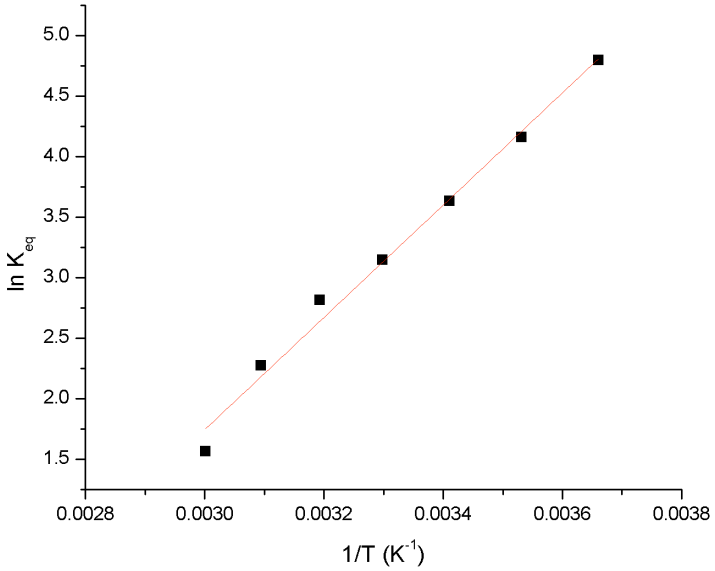


Figure S3. Plot of ln K_{eq} versus 1/T for the reaction **1** + 4-methoxybenzonitrile → **5c**. The equation for the best fit line shown in red is as follows: y = mx + b, where m = 4600 ± 200 K^{-1} and b = -12.2 ± 0.7.

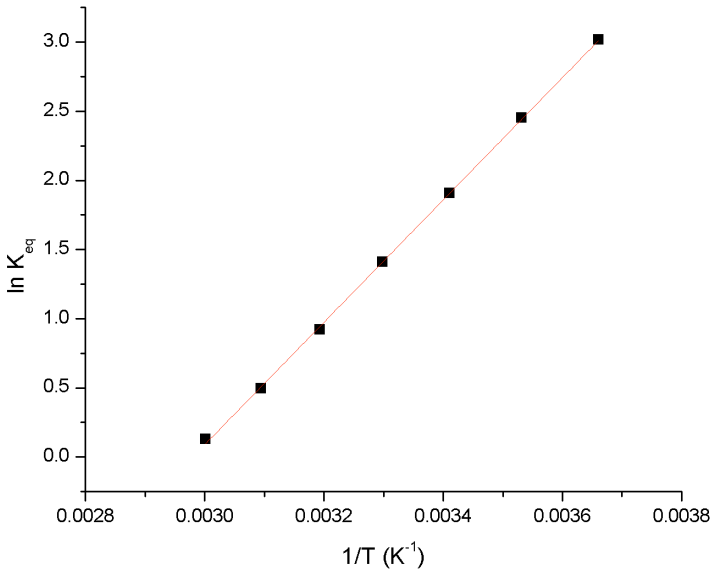


Figure S4. Plot of ln K_{eq} versus 1/T for the reaction **1** + acetonitrile → **5d**. The equation for the best fit line shown in red is as follows: y = mx + b, where m = 4420 ± 34 K^{-1} and b = -13.2 ± 0.11.

Evaluation of the Reactions Involving 1 and Various Alkynes. A 0.089 M stock solution of **1** was prepared by dissolving **1** (0.120 g, 0.319 mmol) in C_6D_6 (3.6 mL). An NMR tube equipped with a screw-cap septum was then charged inside of a glove box with the stock solution of **1** (0.6 mL, 0.053 mmol) and a sufficient quantity of C_6D_6 such that the total volume equaled 0.8 mL upon the addition of 10 eq of the alkyne analyzed. The sample was then equilibrated in an NMR probe at 50 °C. Upon equilibration, the sample was ejected from the instrument and 0.53 mmol (10 eq) of an alkyne was added via syringe. The NMR tube was then vigorously shaken to ensure proper mixing, and the sample reinserted into the NMR probe. After shimming, spectra (four scans each) were run every 30 sec for 1 h. The conversion to the cyclopropene product (**2b**,**d-f**, Figure S5) was measured by comparing the ratio of the ^{1}H NMR integrals assigned to the aryl protons of **1** (δ = 6.78 ppm; s, 4H) with the corresponding aryl protons attributed to the respective product (**2b**: 6.50 ppm, s, 2H; **2d**: 6.63 ppm, s, 2H; **2e**: 6.65 ppm; overlapping singlets, 4H; **2f**: 6.48 ppm, s, 2H). To account for the differing number of hydrogen atoms in each compound, the integrals for **2b**, **2d** and **2f** were doubled prior to calculating the integral ratio. Pseudo-first order rate constants were determined for these reactions by plotting the ln [**1**] versus time (Figures S6-S8). Linear fits of all data points collected for conversions < 90% were used to calculate the observed rate constants from the corresponding slopes.

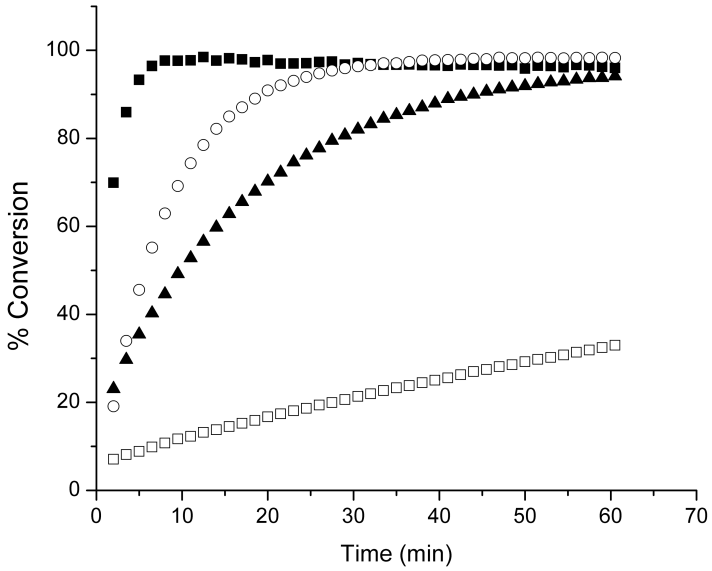


Figure S5. Plot of percent conversion versus time for the [2+1] cycloaddition of **1** with 2-hexyne (open squares), 1-phenyl-1-butyne (solid triangles), 1-hexyne (open circles), or 4-tert-butylphenylacetylene (solid squares). Conditions: $[\mathbf{1}]_0$ = 0.066 M, 10 eq of alkyne, 50 °C, C_6D_6. Every third data point is plotted for visual clarity.

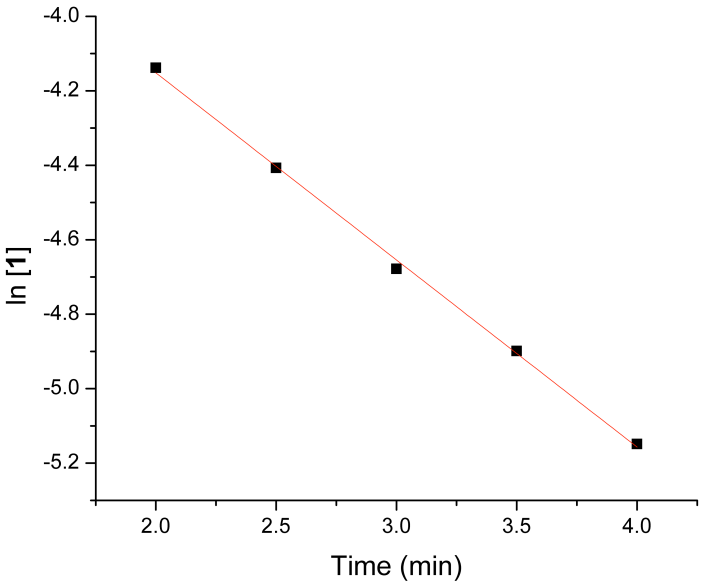


Figure S6. Plot of ln [**1**] versus time. Conditions: $[\mathbf{1}]_o$ = 0.066 M, $[\text{4-tert-butylphenylacetylene}]_o$ = 0.66 M (10 eq), C_6D_6, 50 °C. The equation for the best fit line is as follows: y = mx + b, where m = –0.502 ± 0.011 min^{-1} and b = –3.15 ± 0.03.

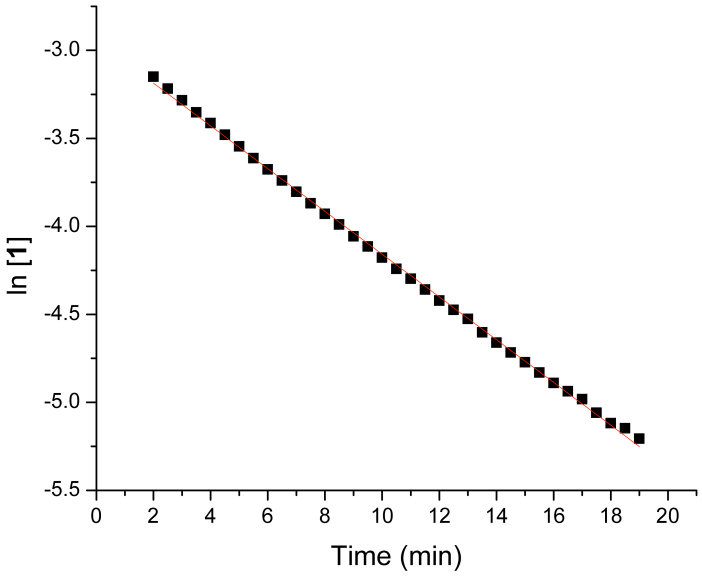


Figure S7. Plot of ln [**1**] versus time. Conditions: $[\mathbf{1}]_o$ = 0.066 M, $[\text{1-hexyne}]_o$ = 0.66 M (10 eq), C_6D_6, 50 °C. The equation for the best fit line is as follows: y = mx + b, where m = –0.1215 ± 0.0007 min^{-1} and b = –2.943 ± 0.008.

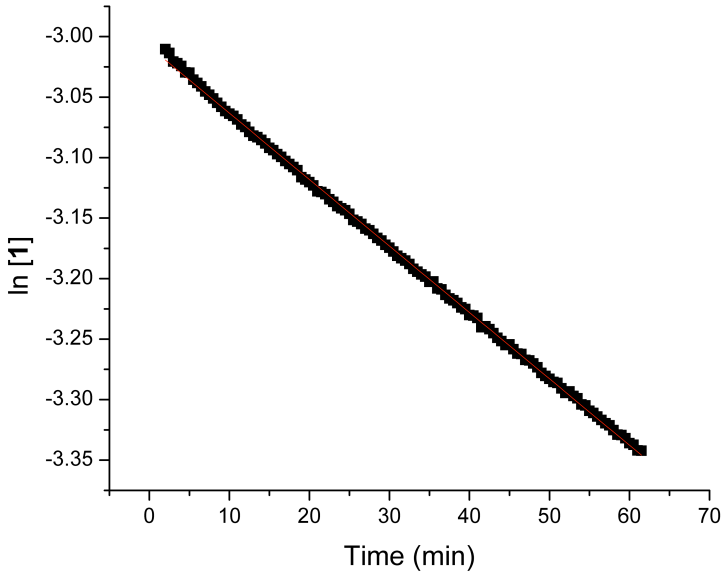


Figure S8. Plot of ln [**1**] versus time. Conditions: $[\mathbf{1}]_o$ = 0.066 M, $[\text{2-hexyne}]_o$ = 0.66 M (10 eq), C_6D_6, 50 °C. The equation for the best fit line is as follows: y = mx + b, where m = –0.00549 ± 0.00001 min^{-1} and b = –3.0083 ± 0.0004.

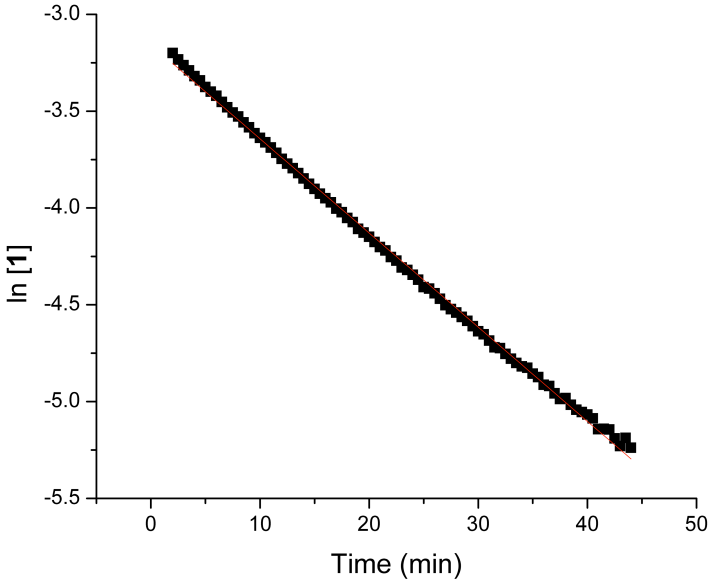


Figure S9. Plot of ln [**1**] versus time. Conditions: $[\mathbf{1}]_o$ = 0.066 M, $[\text{1-phenyl-1-butyne}]_o$ = 0.66 M (10 eq), C_6D_6, 50 °C. The equation for the best fit line is as follows: y = mx + b, where m = –0.0487 ± 0.0002 min^{-1} and b = –3.156 ± 0.005.

X-Ray Crystallography. Colorless, single crystals of **2a** were obtained by the slow diffusion of pentane into a saturated benzene solution; this compound crystallized in the monoclinic space group $P2_1/c$. Colorless single crystals of **2b** were grown by the slow evaporation of a benzene solution; this compound co-crystallized with a molecule of benzene in the monoclinic space group $P2_1/n$. Colorless, single crystals of **2c** were obtained by the slow evaporation of a benzene solution; this compound co-crystallized with a molecule of benzene in the monoclinic $P2_1/c$ space group. Colorless single crystals of **3** were obtained by the slow diffusion of pentane into a saturated benzene solution; this compound crystallized in the triclinic *P*-1 space group. Colorless, single crystals of **4** were obtained by the slow diffusion of pentane into a saturated benzene solution; this compound crystallized in the monoclinic I_2/a space group. Colorless, single crystals of **5c** were obtained by the slow diffusion of pentane into a benzene solution; this compound crystallized in the monoclinic $P2_1/n$ space group. Colorless, single crystals of **6** were obtained by the slow evaporation of a saturated chloroform solution; this compound co-crystallized with a molecule of chloroform in the triclinic *P*-1 space group. Crystallographic measurements were carried out on a Rigaku Mini CCD, Enraf-Nonius Kappa CCD, or Rigaku AFC-12 with Saturn 724+ CCD area detector diffractometer using graphite-monochromated Mo-K_α radiation (λ = 0.71073 Å) at 120 K or 140 K using an Oxford Cryostream low temperature device. A sample of suitable size and quality was selected and mounted onto a nylon loop. Data reductions were performed using DENZO-SMN.[7] The structures were solved by direct methods which successfully located most of the non-hydrogen atoms. Subsequent refinements on F_2 using the SHELXTL/PC package (version 5.1)[8] allowed the location of the remaining non-hydrogen atoms. Key details of the crystal and structure refinement data are summarized in Table S1 Further crystallographic details may be found in the respective CIFs which were deposited at the Cambridge Crystallographic Data Centre, Cambridge, UK. The CCDC reference numbers for **2a**, **2b**, **2c**, **3**, **4**, **5c** and **6** were assigned as 859318, 859319, 859320, 859321, 859322, 859323, and 859324, respectively.

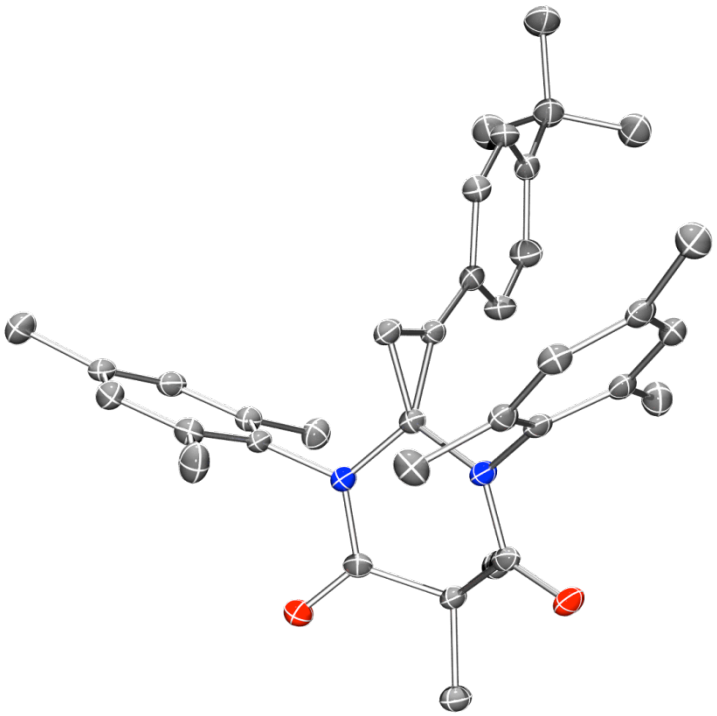


Figure S10. ORTEP diagram of **2b** with thermal ellipsoids drawn at 50% probability and H-atoms omitted for clarity.

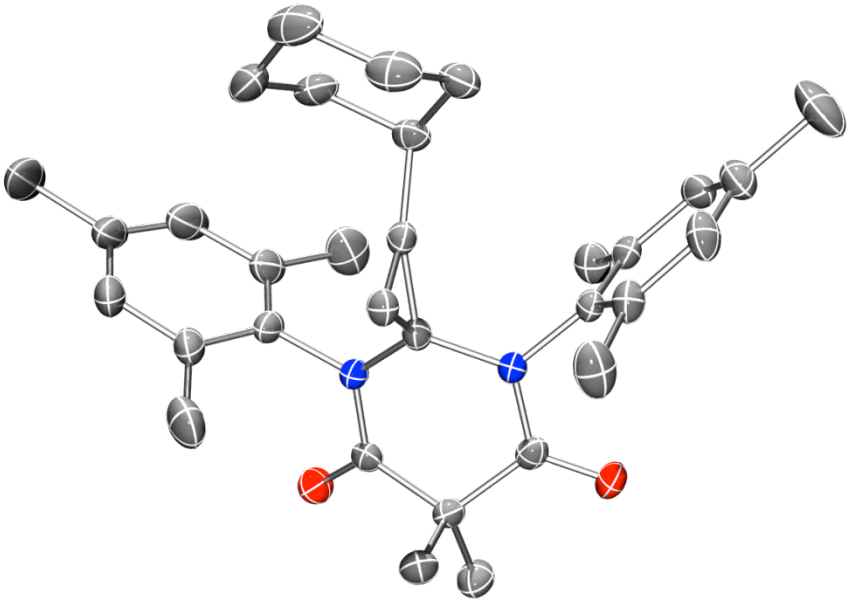


Figure S11. ORTEP diagram of **2c** with thermal ellipsoids drawn at 50% probability and H-atoms omitted for clarity.

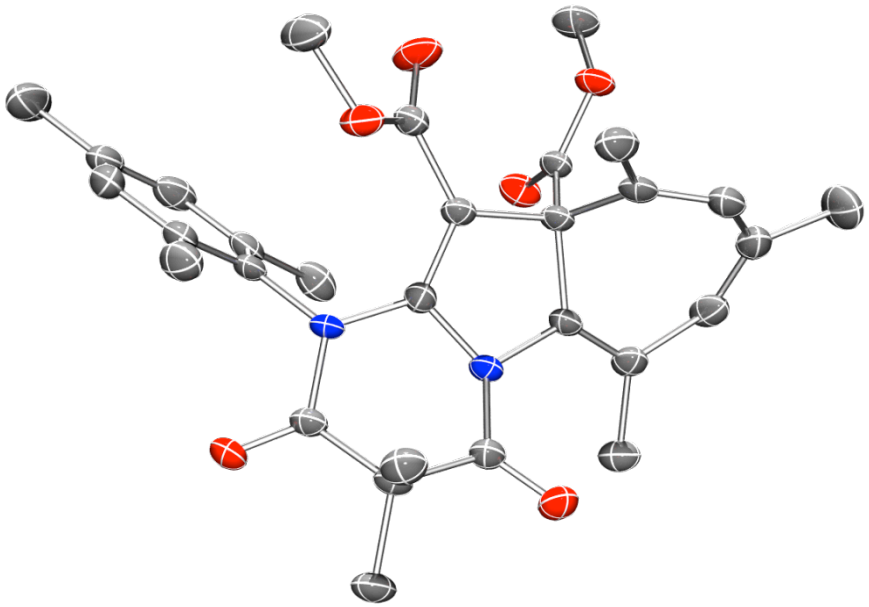


Figure S12. ORTEP diagram of **3** with thermal ellipsoids drawn at 50% probability and H-atoms omitted for clarity.

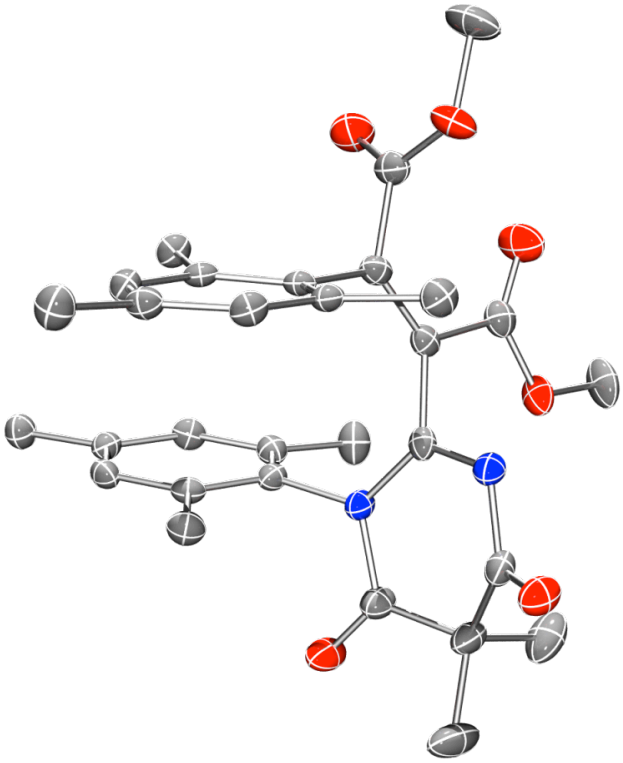


Figure S13. ORTEP diagram of **4** with thermal ellipsoids drawn at 50% probability and H-atoms omitted for clarity.

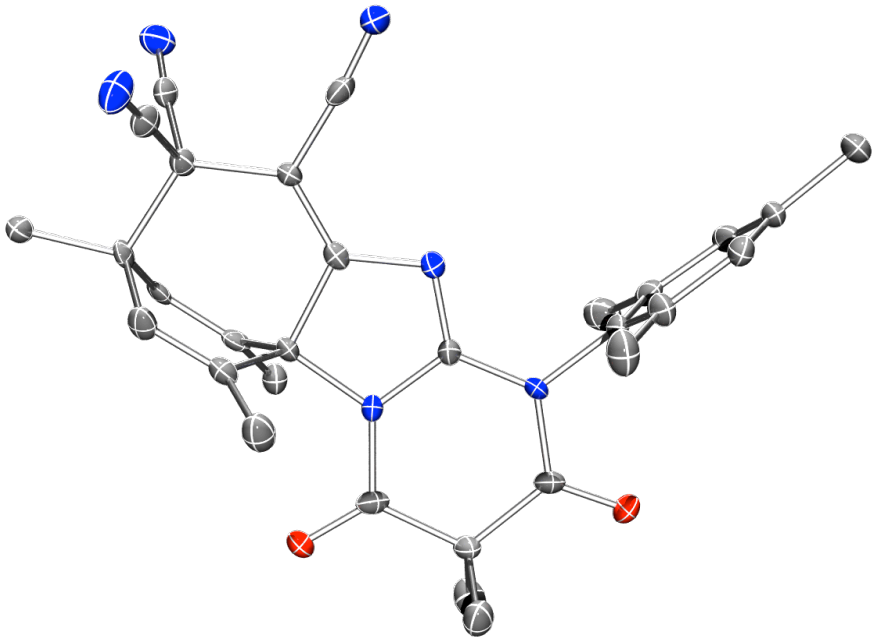
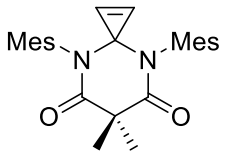


Figure S14. ORTEP diagram of **6** with thermal ellipsoids drawn at 50% probability and H-atoms omitted for clarity.

Table S1. Summary of crystal data, data collection, and structure refinement details.

	2[a]	**2b**·C_6H_6	**2c**·C_6H_6	**3**	**4**	**5c**	**6**·$CHCl_3$
Formula	$C_{26}H_{30}N_2O_2$	$C_{42}H_{48}N_2O_2$	$C_{38}H_{46}N_2O_2$	$C_{30}H_{34}N_2O_6$	$C_{30}H_{34}N_2O_6$	$C_{32}H_{35}N_3O_3$	$C_{30}H_{28}N_6O_2 \cdot CHCl_3$
M_r	402.52	612.82	562.77	518.59	518.59	509.63	623.95
crystal size (mm^3)	0.19 × 0.16 × 0.04	0.18 × 0.14 × 0.03	0.38 × 0.20 × 0.07	0.14 × 0.10 × 0.09	0.20 × 0.09 × 0.02	0.19 × 0.06 × 0.05	0.08 × 0.08 × 0.02
crystal	Monoclinic	Monoclinic	Monoclinic	Triclinic	Monoclinic	Monoclinic	Triclinic
space group	$P2_1/c$	$P2_1/n$	$P2_1/c$	P-1	$I2/a$	$P2_1/n$	P-1
a (Å)	8.3627(3)	16.8334(16)	12.0444(9)	9.2245(14)	20.1337(10)	8.7238(3)	11.880(3)
b (Å)	16.4334(6)	8.7348(8)	23.2835(17)	11.6531(18)	8.1571(4)	17.0451(7)	12.278(3)
c (Å)	15.9457(6)	24.305(2)	11.9648(9)	14.266(2)	33.9244(17)	18.8797(7)	12.464(3)
α (°)	90	90	90	97.528(4)	90	90	70.128(5)
β (°)	99.6680(10)	100.763(2)	103.659(2)	104.301(4)	93.899(3)	95.1970(10)	61.921(4)
γ (°)	90	90	90	108.506(3)	90	90	73.727(5)
V (Å^3)	2160.26(14)	3510.9(6)	3260.5(4)	1372.1(4)	5558.6(5)	2795.83(18)	1492.6(6)
Z	4	4	4	2	8	4	2
ρ_{calc} (g cm^{-3})	1.238	1.159	1.146	1.255	1.239	1.211	1.388
μ (mm^{-1})	0.078	0.070	0.070	0.088	0.086	0.078	0.347
F(000)	864	1320	1216	552	2208	1088	648
T (K)	120(2)	120(2)	150(2)	150(2)	120(2)	120(2)	150(2)
scan mode	ω	ω	ω	ω	ω	ω	ω
hkl range	-9 → 9	-20 → 20	-14 → 13	-10 → 10	-23 → 23	-10 → 10	-20 → 20
	-19 → 19	-10 → 10	-27 → 27	-13 → 13	-9 → 9	-20 → 20	-10 → 10
	-18 → 18	-28 → 28	-14 → 14	-16 → 16	-40 → 40	-22 → 22	-28 → 28
measd reflns	42443	67264	34255	19559	38508	55292	21392
unique reflns	3787 [0.0524]	6176 [0.0726]	5739 [0.1303]	4810 [0.0990]	4882 [0.0903]	4909[0.0621]	5161 [0.1077]
refinement	3787	6176	5739	4810	4882	4909	5161
refined	279	426	387	353	353	352	387
GOF on F^2	1.006	1.006	1.006	1.006	1.006	1.006	1.006
R1[a] (all data)	0.0419	0.0561	0.0647	0.0642	0.0563	0.0398	0.0863 (0.1580)
wR2 (all	0.1141	0.1446	0.1534	0.1400	0.1178	0.1033	0.1811 (0.2205)
ρ_{fin}	0.311	0.312	0.232	0.241	0.225	0.280	1.653
(max/min) (e Å^{-3})	-0.197	-0.287	-0.389	-0.306	-0.228	-0.169	-0.820

[a] $R1 = \sum||Fo| - |Fc||/\sum|Fo|$. [b] $wR2 = \{[\sum w(Fo^2 - Fc^2)^2]/[\sum w(Fo^2)^2]\}^{1/2}$.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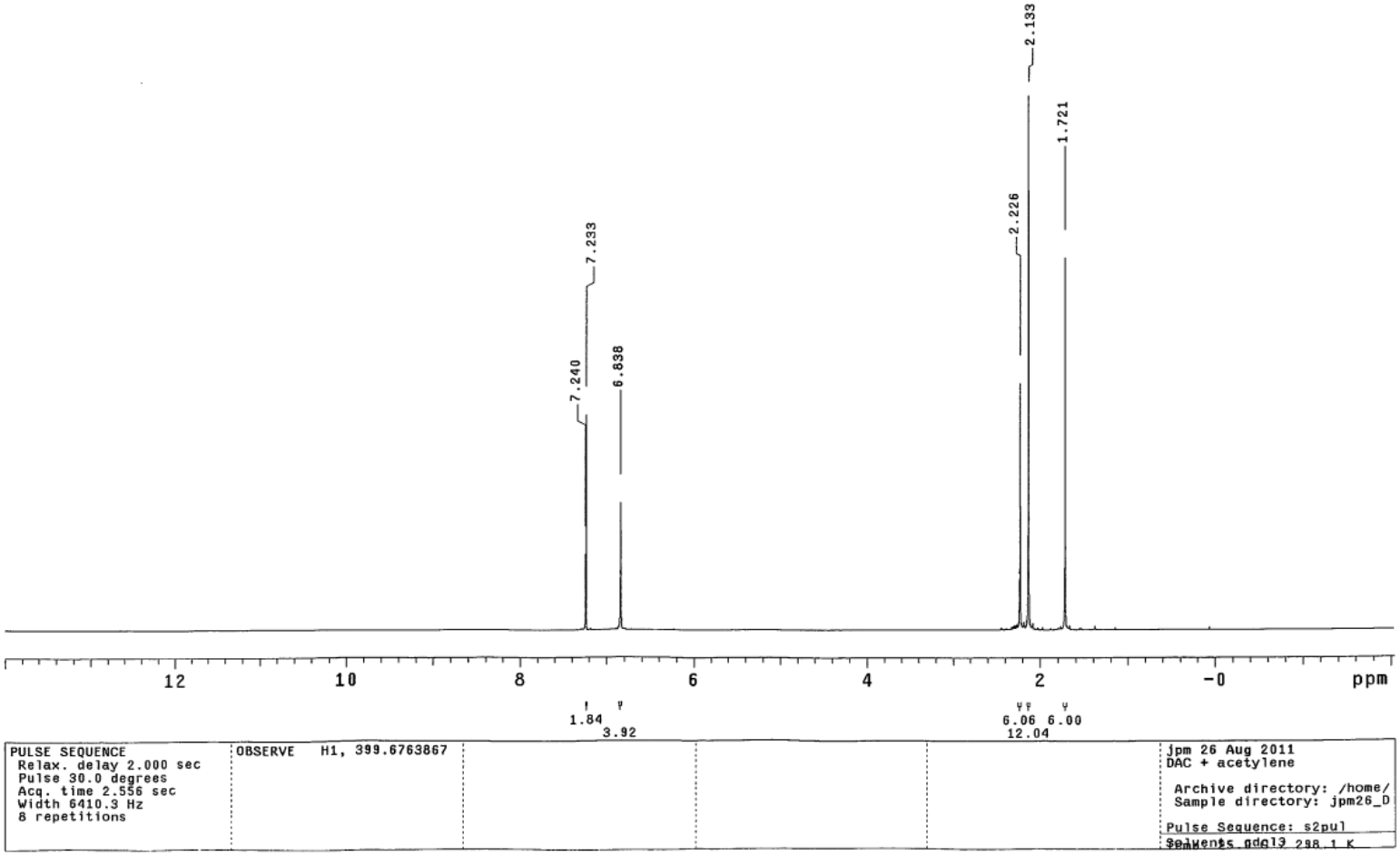
N
N
Mes
O
O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10
8
6
4
2
-0
ppm
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3.92
6.06
6.00
12.04
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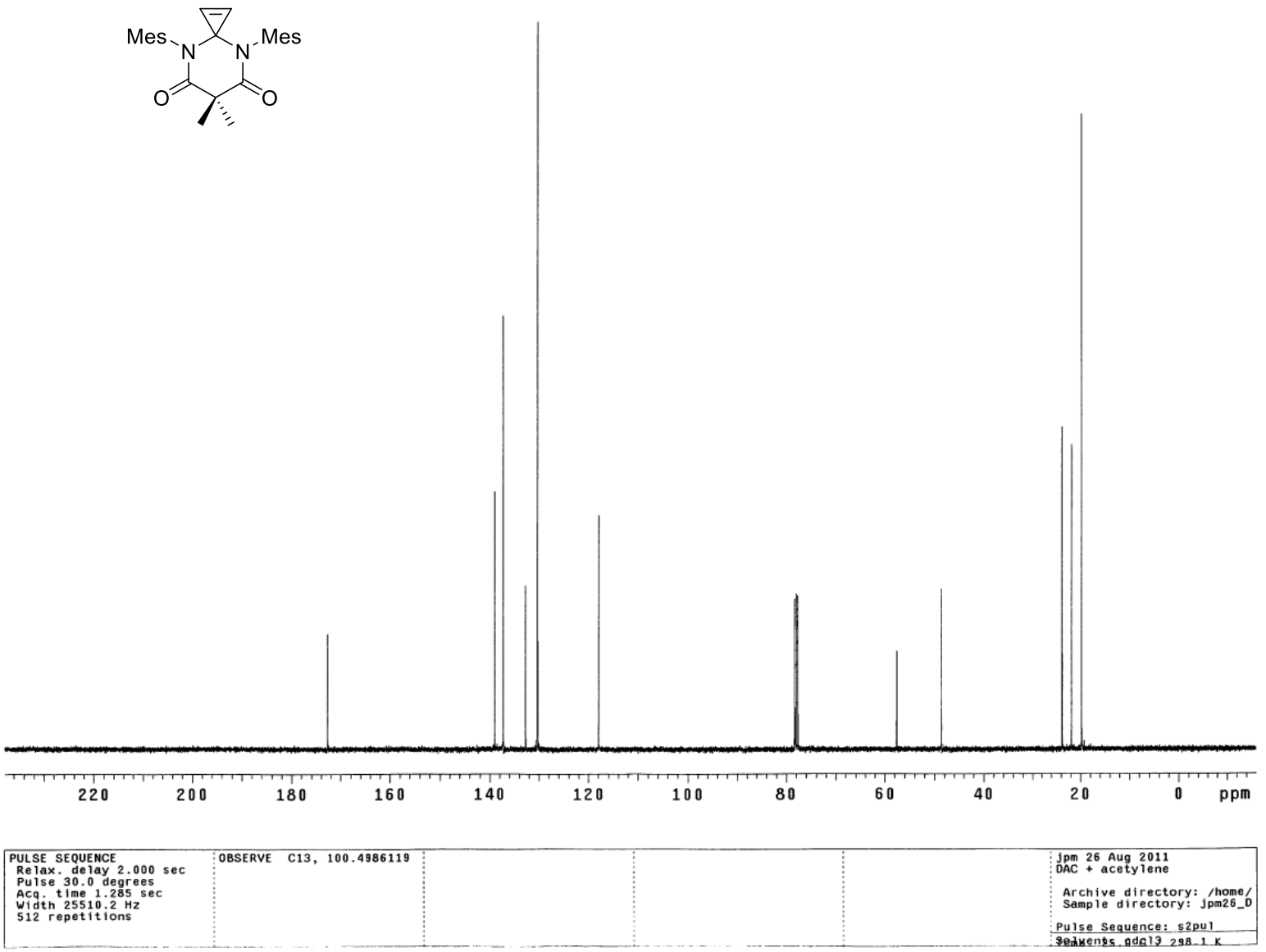
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 2.556 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 399.6763867
jpm 26 Aug 2011
DAC + acetylene
Archive directory: /home/
Sample directory: jpm26_D
Pulse Sequence: s2pul
Solvent: cdcl3 298.1 K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Mes
O
O
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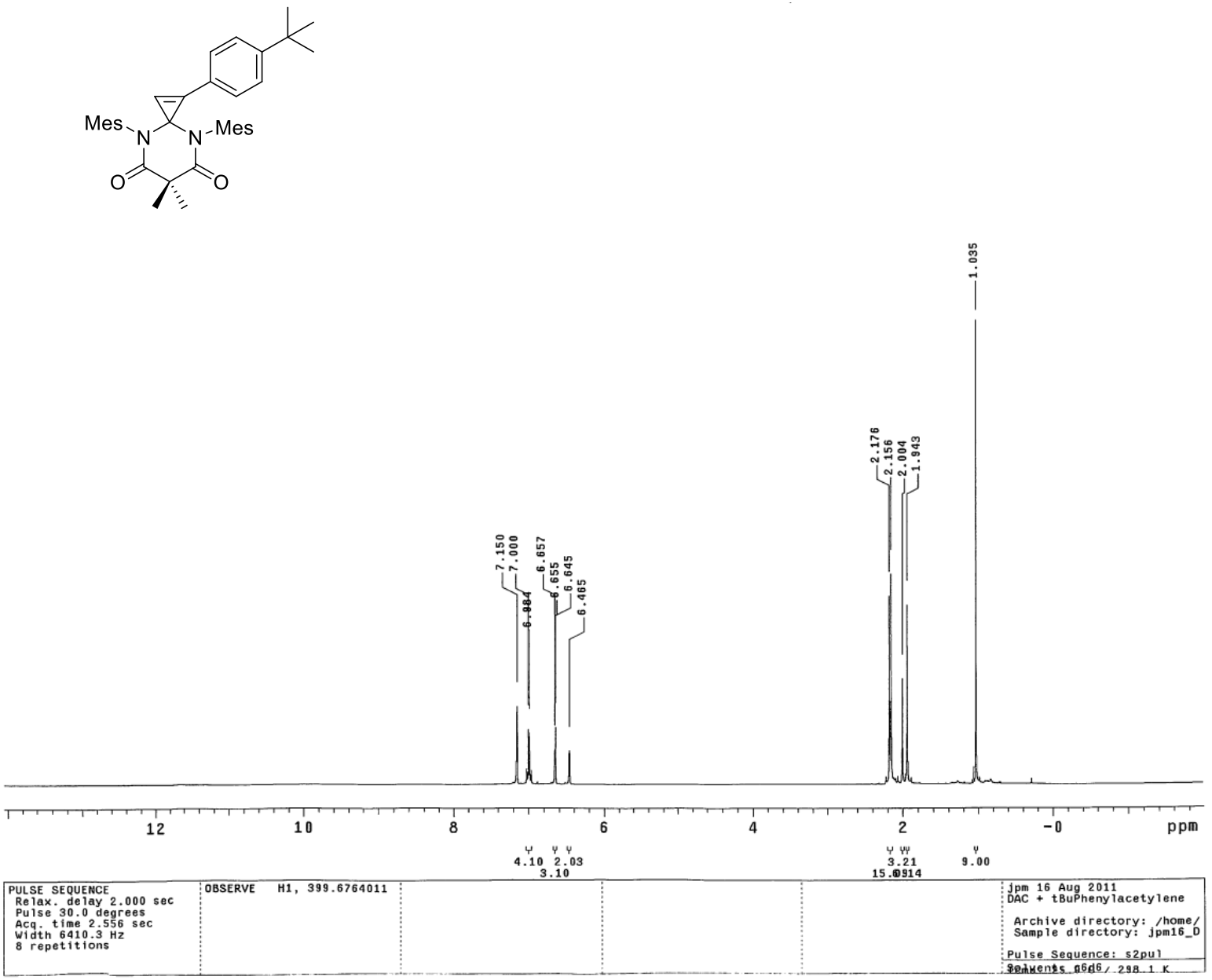
200
180
160
140
120
100
80
60
40
20
0
ppm
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.285 sec
Width 25510.2 Hz
512 repetitions
OBSERVE C13, 100.4986119
jpm 26 Aug 2011
DAC + acetylene
Archive directory: /home/
Sample directory: jpm26_D
Pulse Sequence: s2pul
Solvent: cdcl3 298.1 K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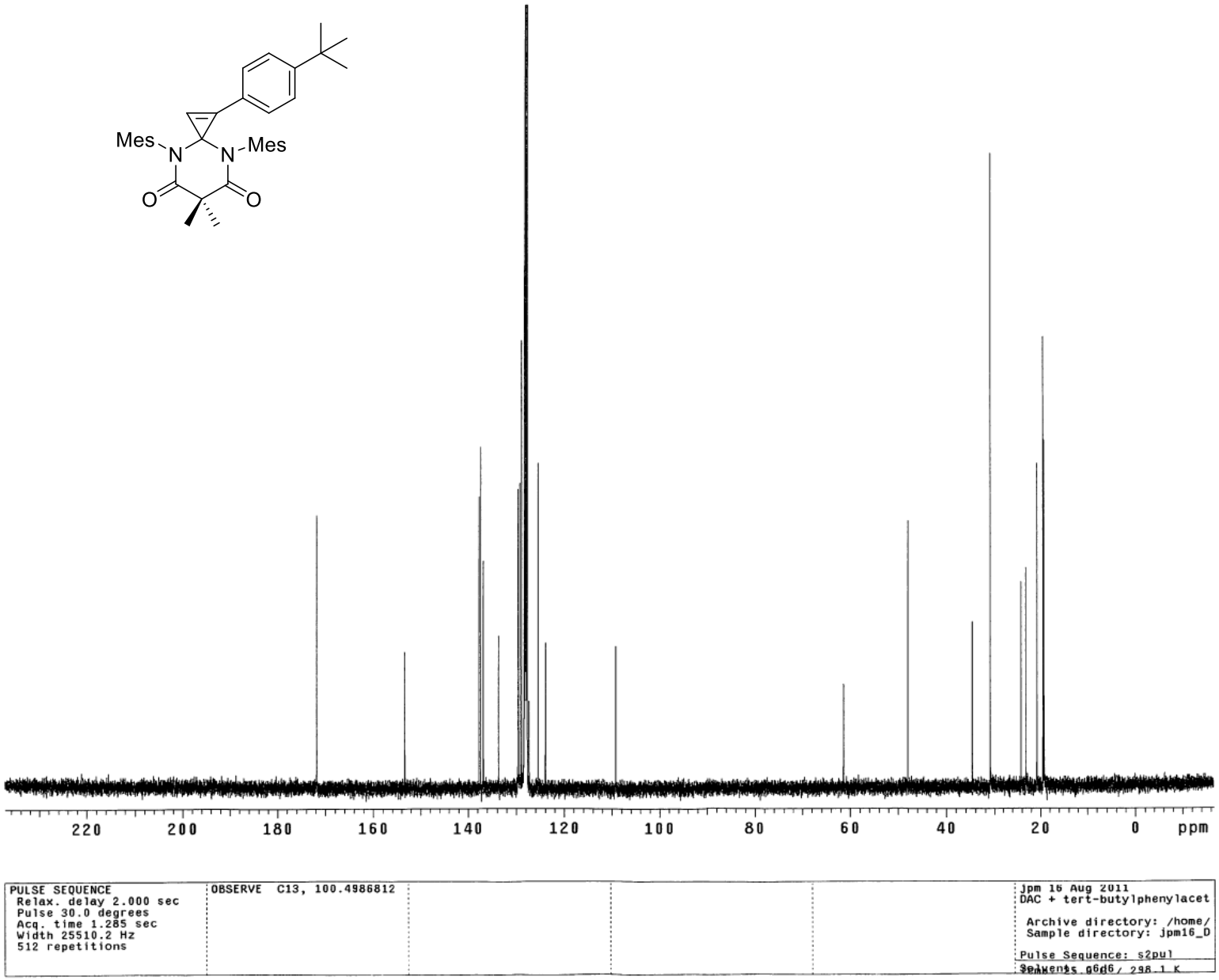
2.156
2.004
1.943
1.035
12
10
8
6
4
2
-0
ppm
4.10
2.03
3.10
3.21
15.09
14
9.00
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 2.556 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 399.6764011
jpm 16 Aug 2011
DAC + tBuPhenylacetylene
Archive directory: /home/
Sample directory: jpm16_D
Pulse Sequence: s2pul
Solvent: c6d6
Temp. 298.1 K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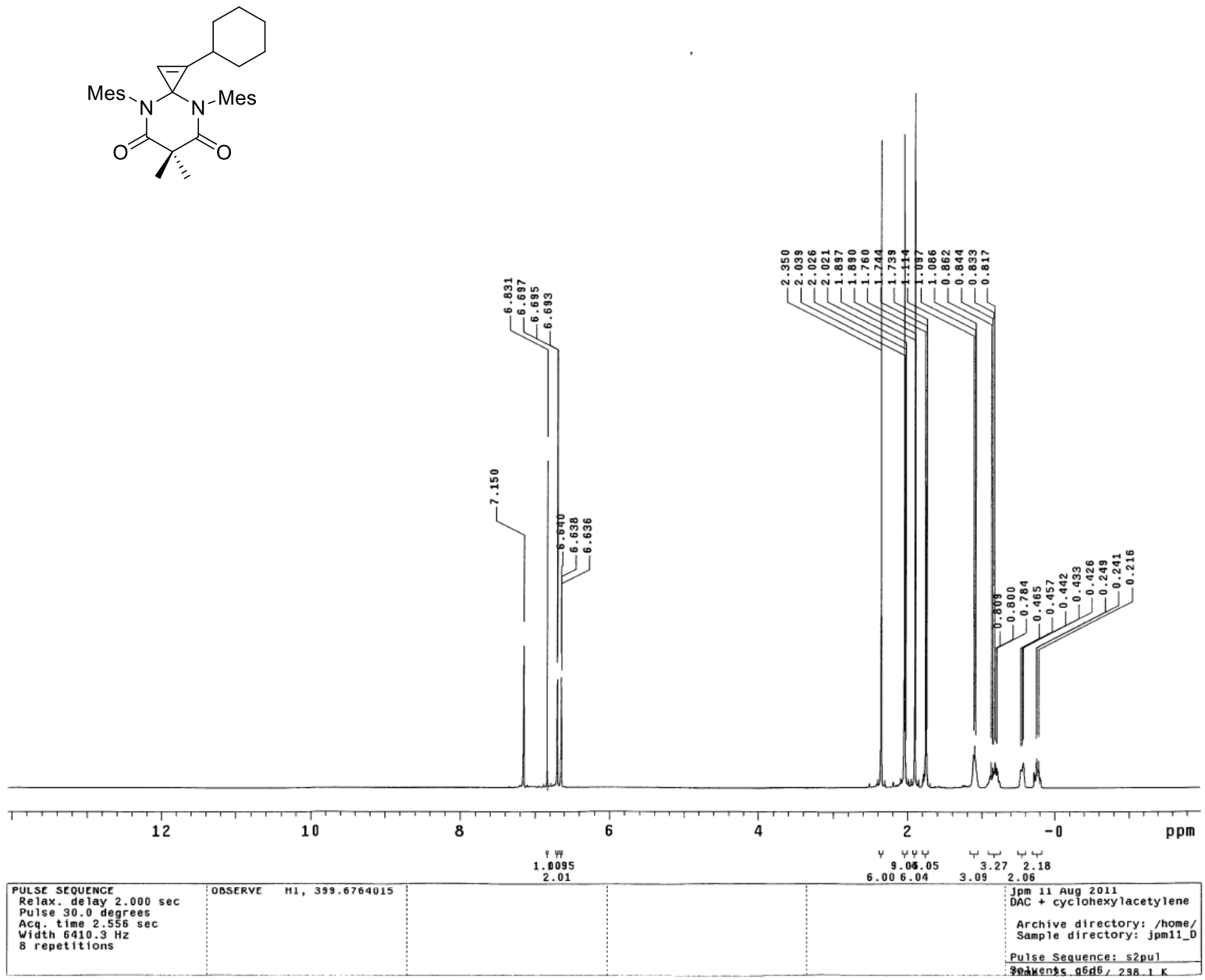
N
N
Mes
O
O
220
200
180
160
140
120
100
80
60
40
20
0
ppm
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.285 sec
Width 25510.2 Hz
512 repetitions
OBSERVE C13, 100.4986812
jpm 16 Aug 2011
DAC + tert-butylphenylacet
Archive directory: /home/
Sample directory: jpm16_D
Pulse Sequence: s2pul
Solvent: c6d6
Temp. 298.1 K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6.640
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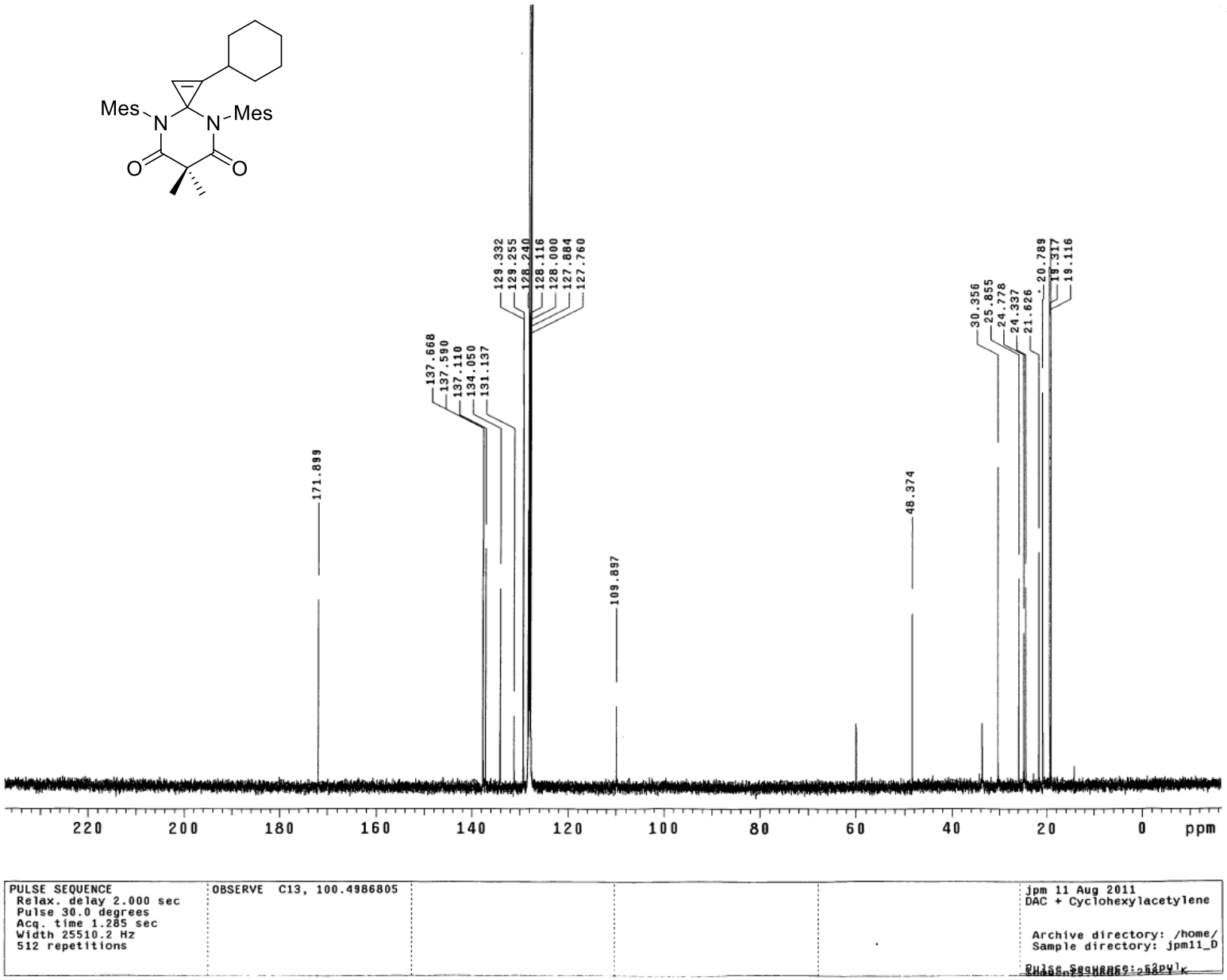
2.039
2.026
2.021
1.897
1.890
1.760
1.744
1.739
1.114
1.097
1.086
0.862
0.844
0.833
0.817
0.809
0.800
0.784
0.465
0.457
0.442
0.433
0.426
0.249
0.241
0.216
12
10
8
6
4
2
-0
ppm
1.00 2.01
6.00 6.04
3.09
3.27
2.06
2.18
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 2.556 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 399.6764015
jpm 11 Aug 2011
DAC + cyclohexylacetylene
Archive directory: /home/
Sample directory: jpm11_D
Pulse Sequence: s2pul
Solvent: c6d6 / 298.1 K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Mes
O
O
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131.137
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128.240
128.116
128.000
127.884
127.760
109.897
48.374
30.356
25.855
24.778
24.337
21.626
20.789
19.317
19.116
220
200
180
160
140
120
100
80
60
40
20
0
ppm
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.285 sec
Width 25510.2 Hz
512 repetitions
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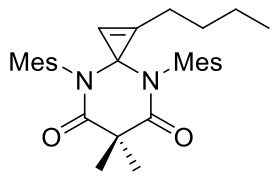
jpm 11 Aug 2011
DAC + Cyclohexylacetylene
Archive directory: /home/
Sample directory: jpm11_D

v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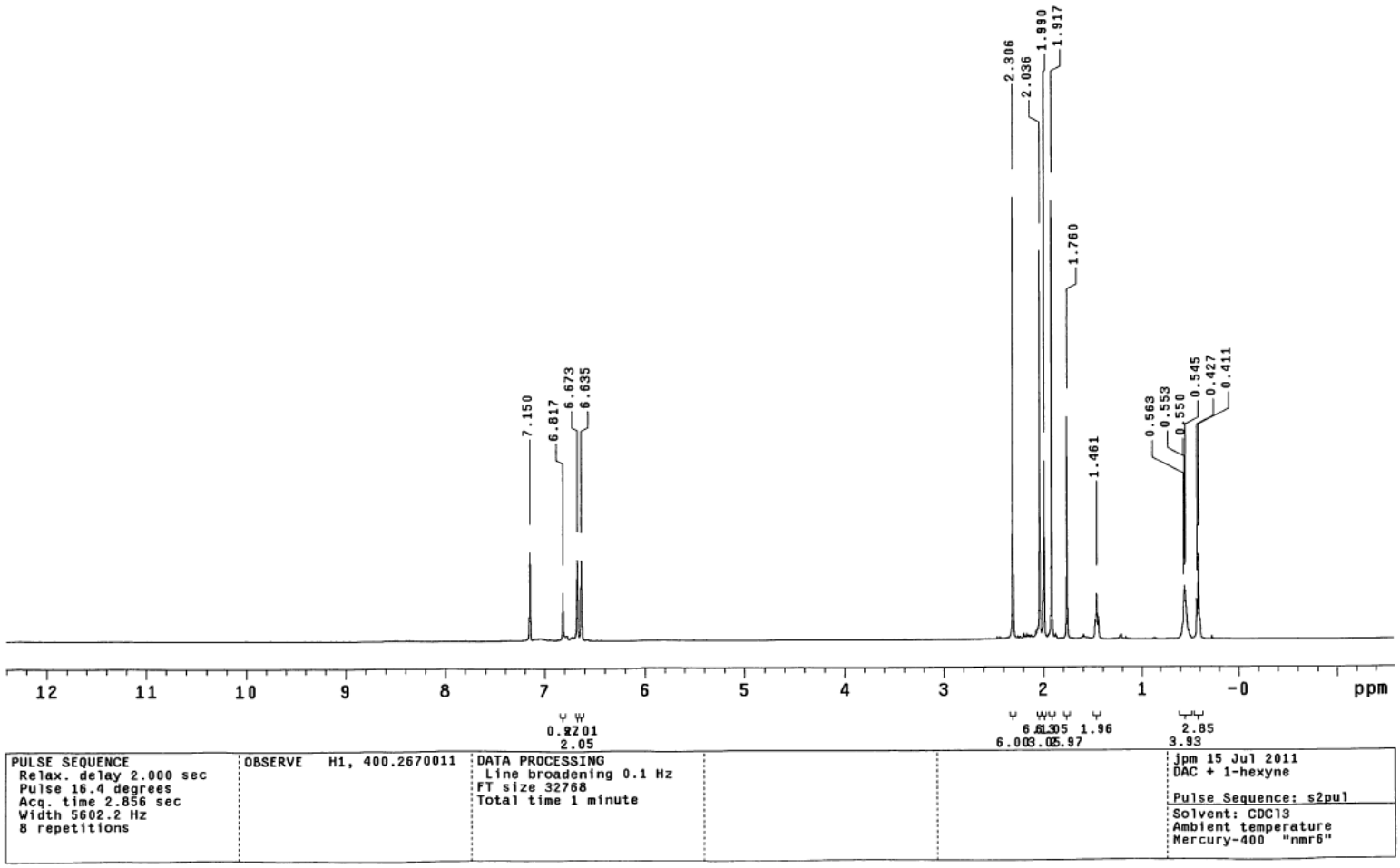
N
Mes
O
O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6.673
6.635
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1.990
1.917
1.760
1.461
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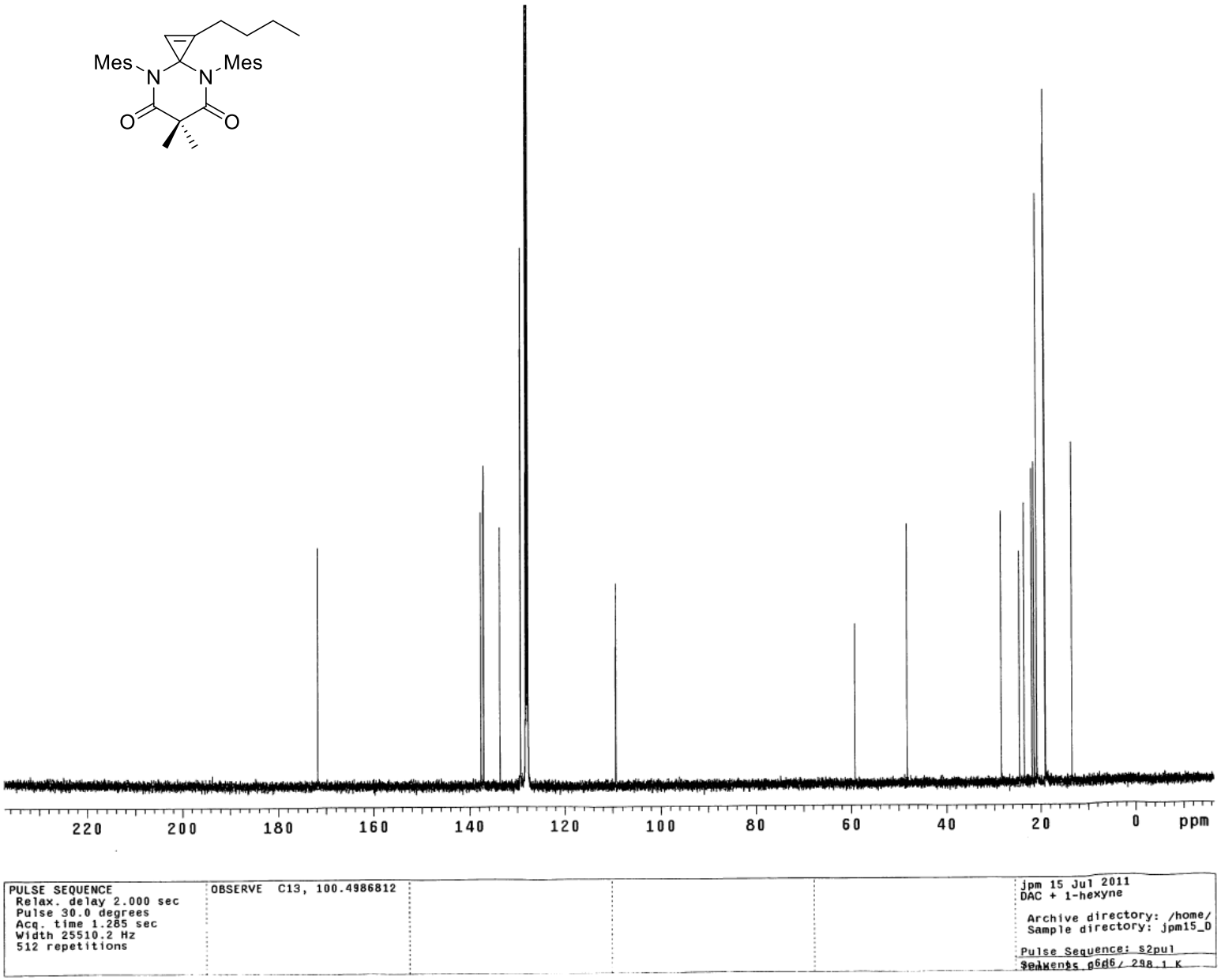
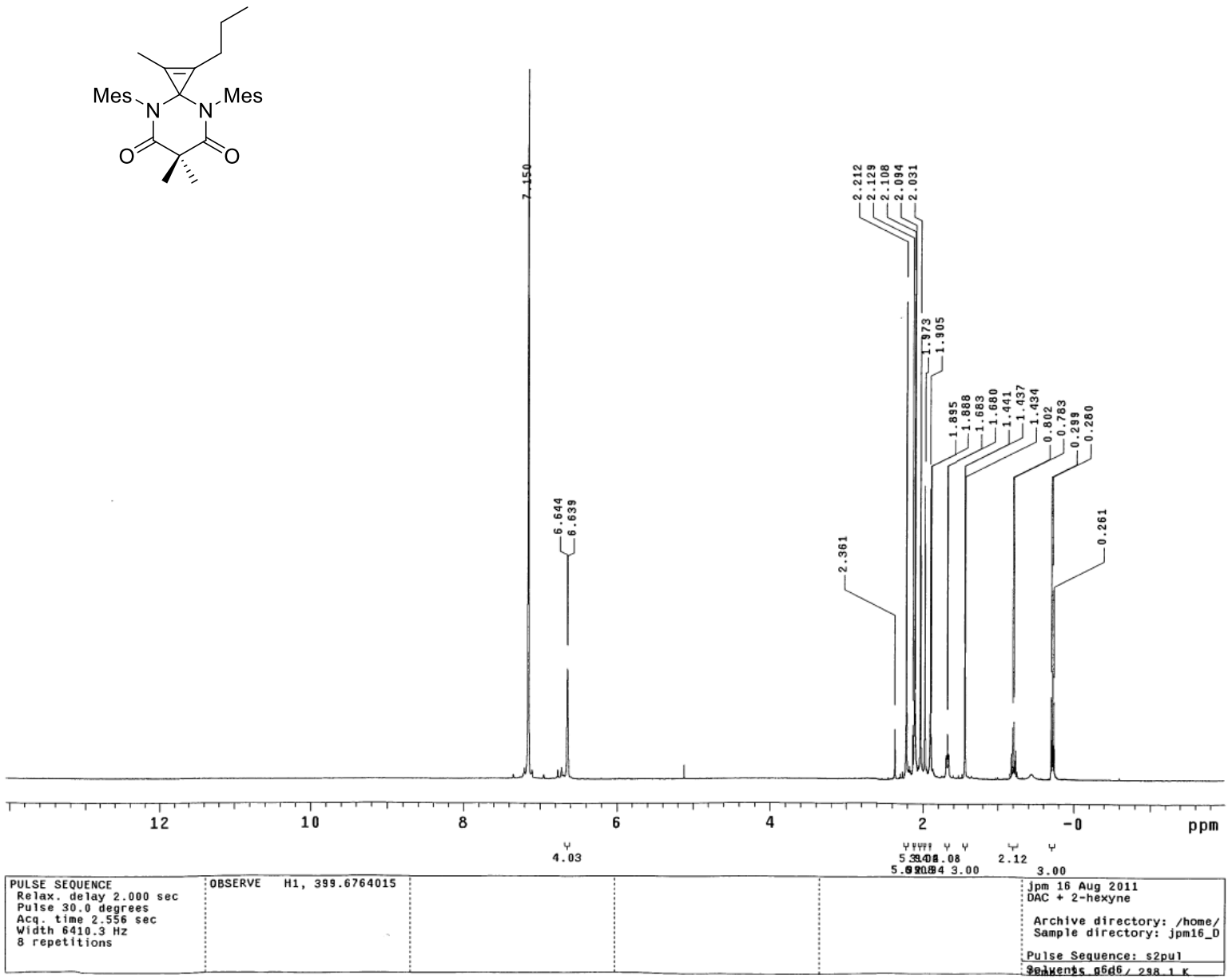
0.553
0.550
0.545
0.427
0.411
12
11
10
9
8
7
6
5
4
3
2
1
-0
ppm
0.92
2.01
2.05
6.00
3.05
5.97
1.96
2.85
3.93
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 16.4 degrees
Acq. time 2.856 sec
Width 5602.2 Hz
8 repetitions
OBSERVE H1, 400.2670011
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 1 minute
jpm 15 Jul 2011
DAC + 1-hexyne
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400 "nmr6"


Mes
N
N
Mes
O
O
220
200
180
160
140
120
100
80
60
40
20
0
ppm
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.285 sec
Width 25510.2 Hz
512 repetitions
OBSERVE C13, 100.4986812
jpm 15 Jul 2011
DAC + 1-hexyne
Archive directory: /home/
Sample directory: jpm15_D
Pulse Sequence: s2pul
Solvent: c6d6 / 298.1 K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N
Mes
O
O
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6.639
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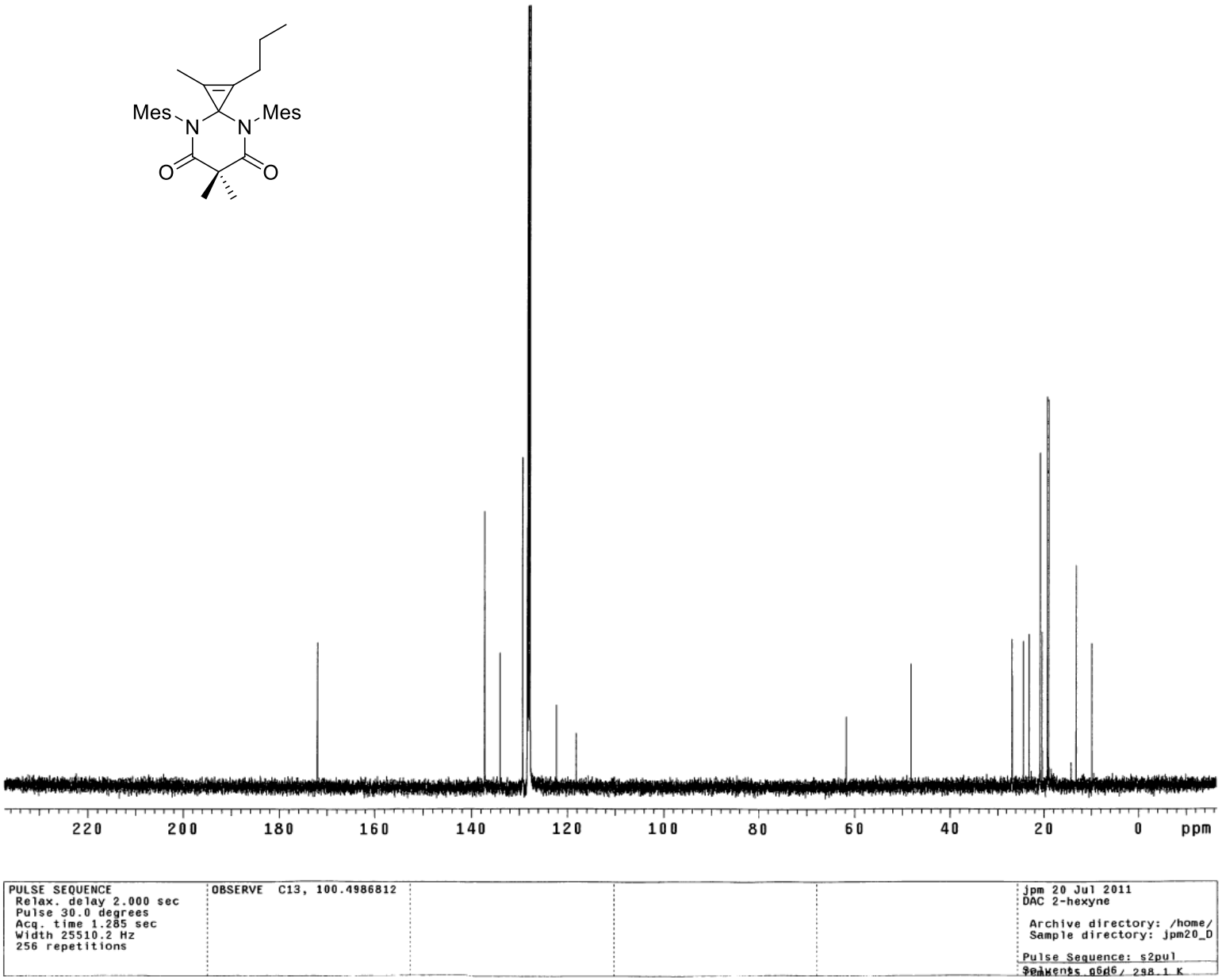
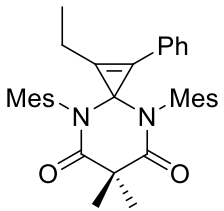
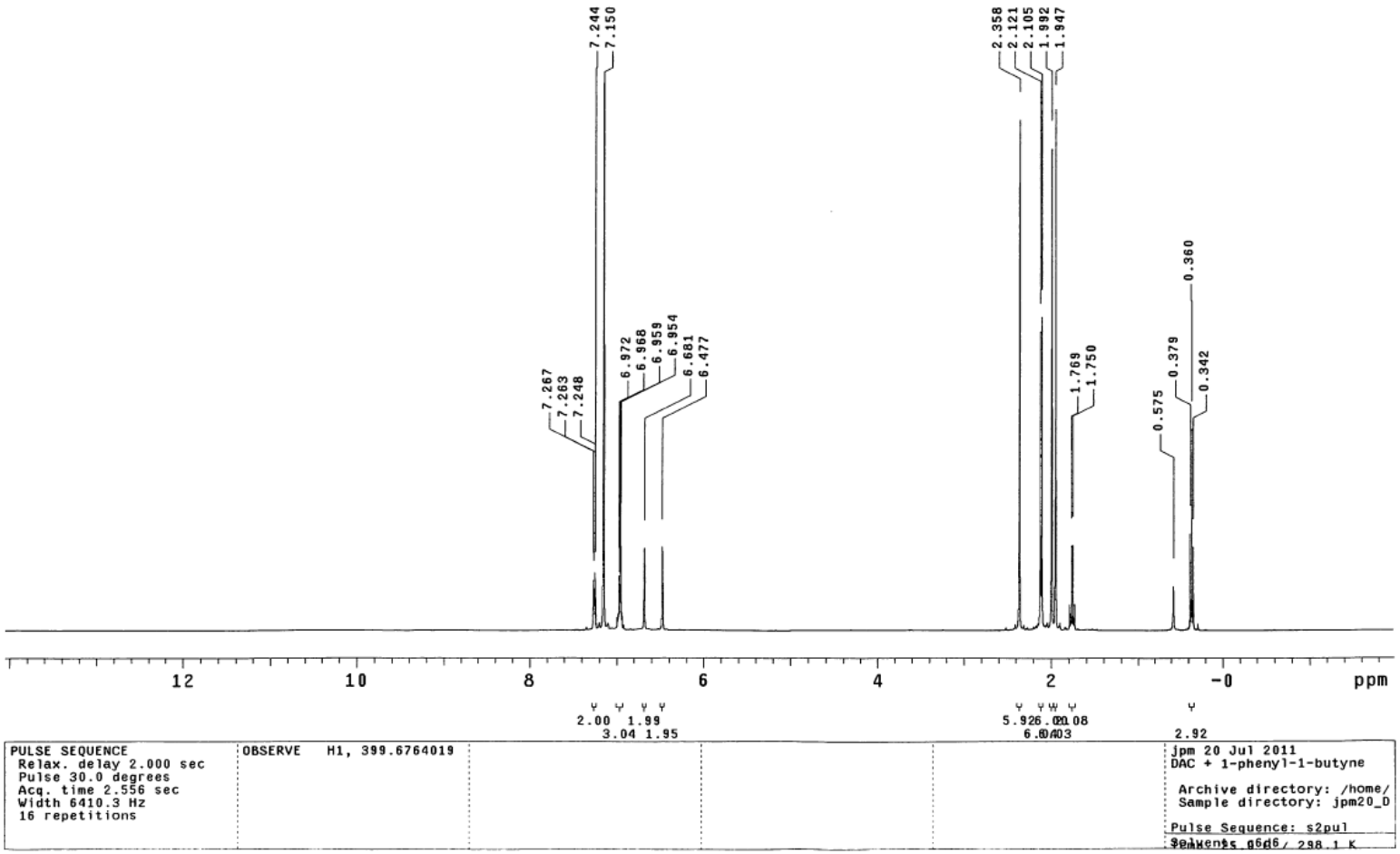
2.212
2.129
2.108
2.094
2.031
1.973
1.905
1.895
1.888
1.683
1.660
1.441
1.437
1.434
0.802
0.783
0.299
0.280
0.261
12
10
8
6
4
2
-0
ppm
4.03
2.12
3.00
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 2.556 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 399.6764015
jpm 16 Aug 2011
DAC + 2-hexyne
Archive directory: /home/
Sample directory: jpm16_D
Pulse Sequence: s2pul
Solvent: c6d6 / 298.1 K


Mes
N
N
Mes
O
O
220
200
180
160
140
120
100
80
60
40
20
0
ppm
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.285 sec
Width 25510.2 Hz
256 repetitions
OBSERVE C13, 100.4986812
jpm 20 Jul 2011
DAC 2-hexyne
Archive directory: /home/
Sample directory: jpm20_D
Pulse Sequence: s2pul
Solvent: c6d6
Temp. 298.1 K


Ph
Mes
N
N
Mes
O
O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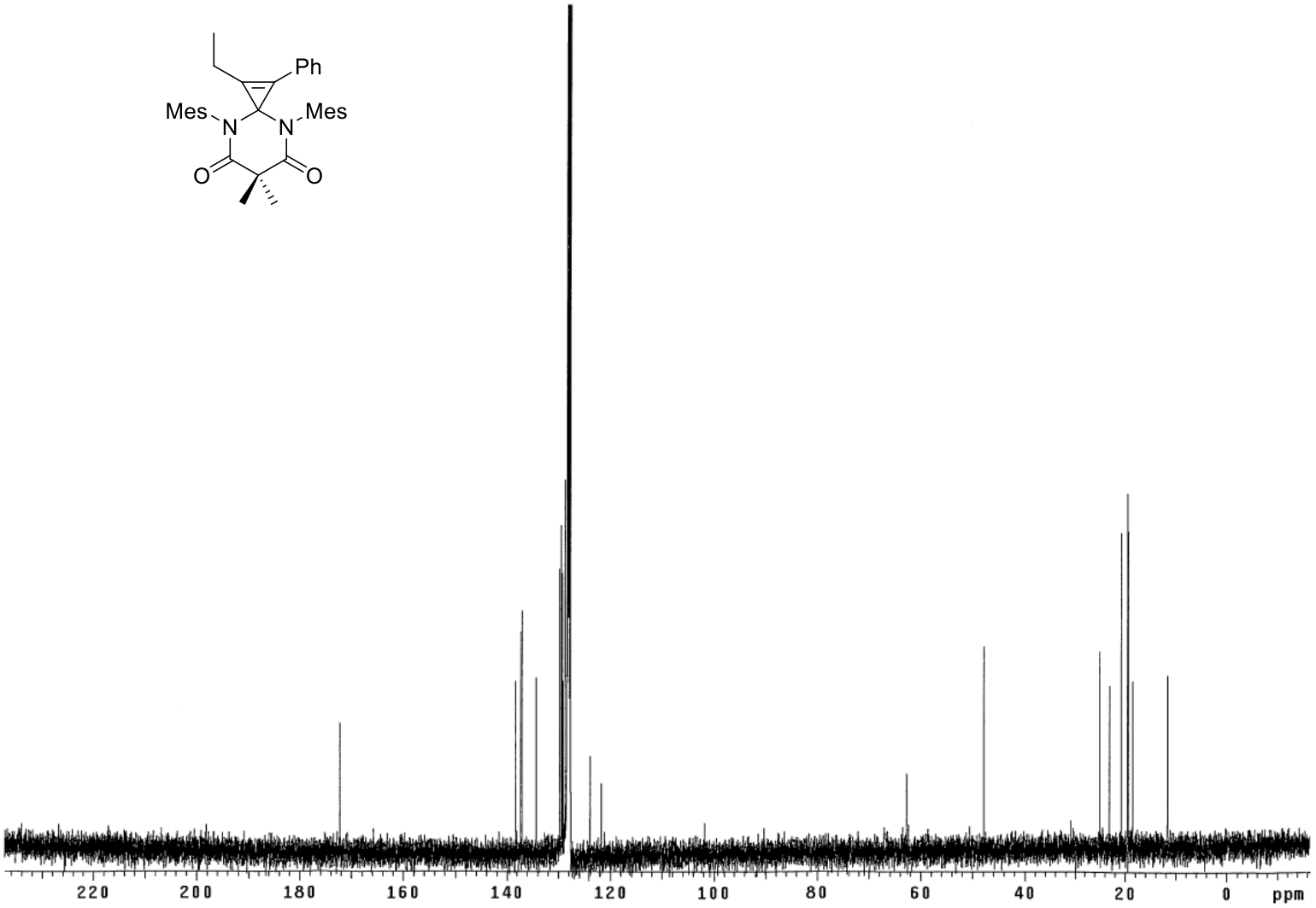
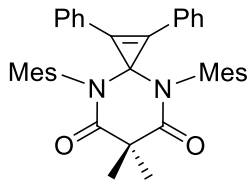
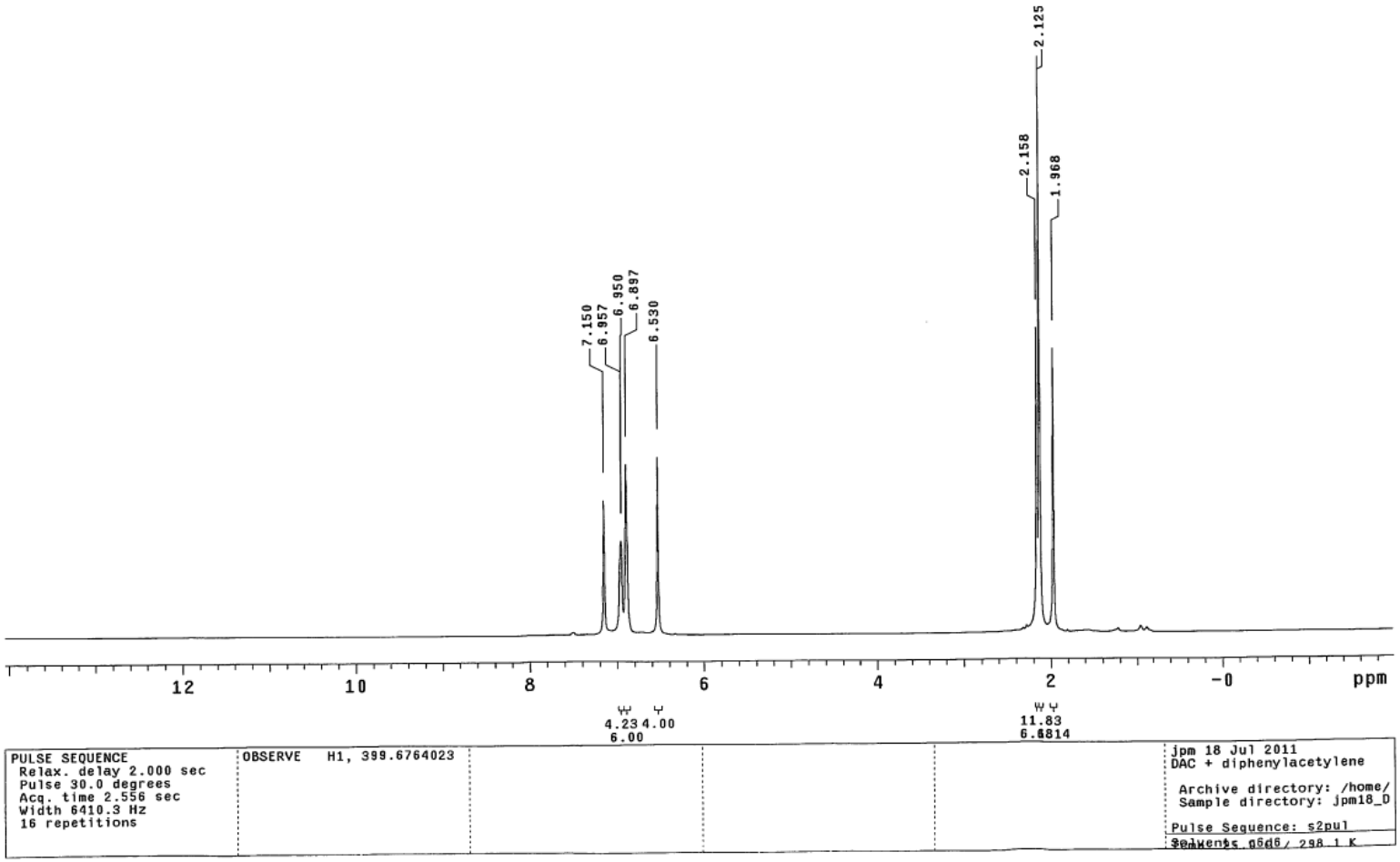
6.968
6.959
6.954
6.681
6.477
1.769
1.750
0.379
0.342
0.575
12
10
8
6
4
2
-0
ppm
2.00
1.99
3.04
1.95
5.92
6.00
2.92
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 2.556 sec
Width 6410.3 Hz
16 repetitions
OBSERVE H1, 399.6764019
jpm 20 Jul 2011
DAC + 1-phenyl-1-butyne
Archive directory: /home/
Sample directory: jpm20_D
Pulse Sequence: s2pul
Solvent: c6d6 / 298.1 K


Ph
Mes
N
N
Mes
O
O
220
200
180
160
140
120
100
80
60
40
20
0
ppm
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.285 sec
Width 25510.2 Hz
512 repetitions
OBSERVE C13, 100.4986812
jpm 22 Jul 2011
DAC + 1-phenyl-1-butyne
Archive directory: /home/
Sample directory: jpm22_D
Pulse Sequence: s2pul
Solvent: c6d6
298.1 K


Ph
Ph
Mes
N
N
Mes
O
O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10
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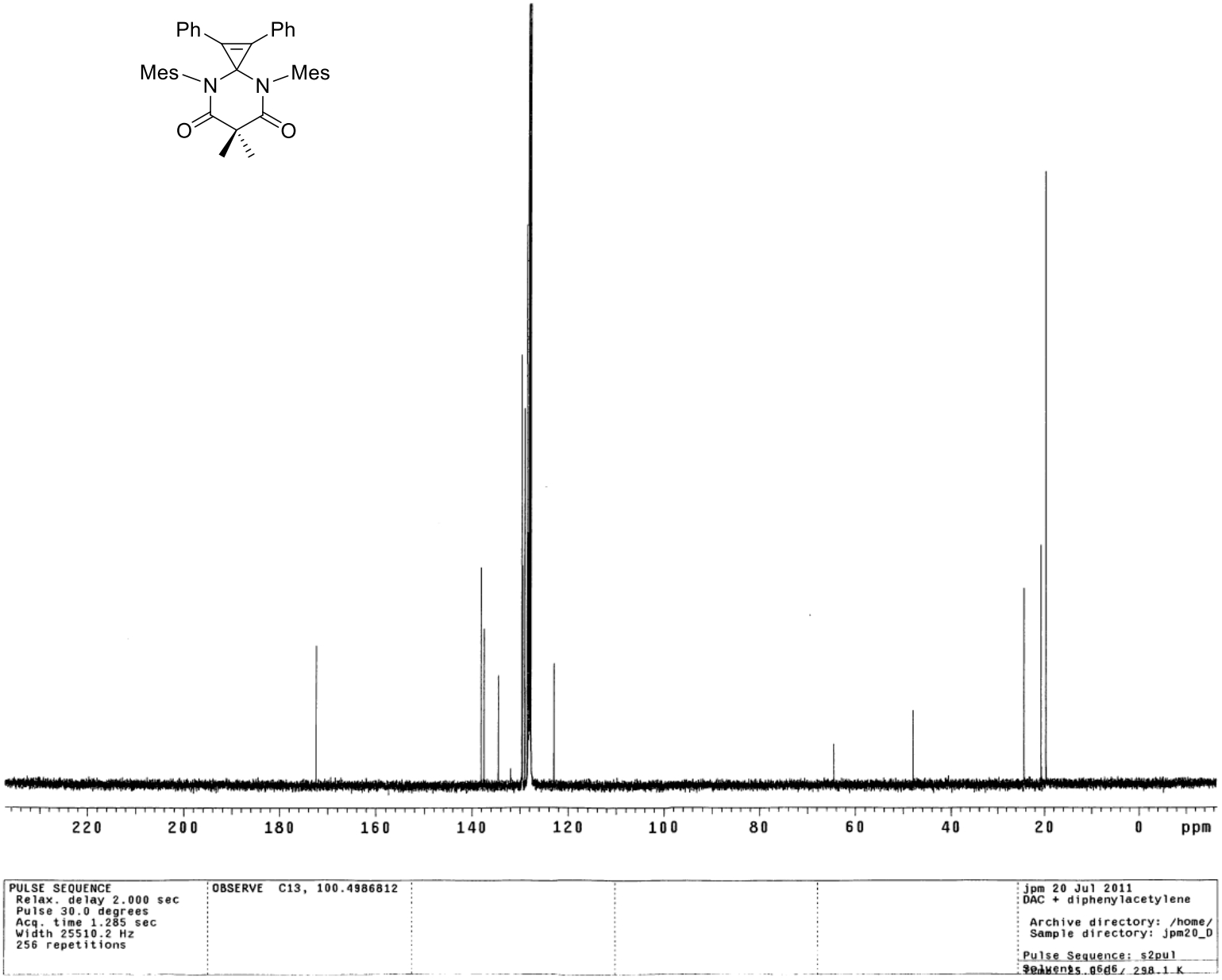
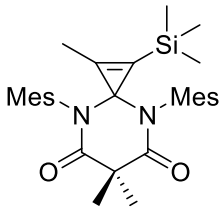
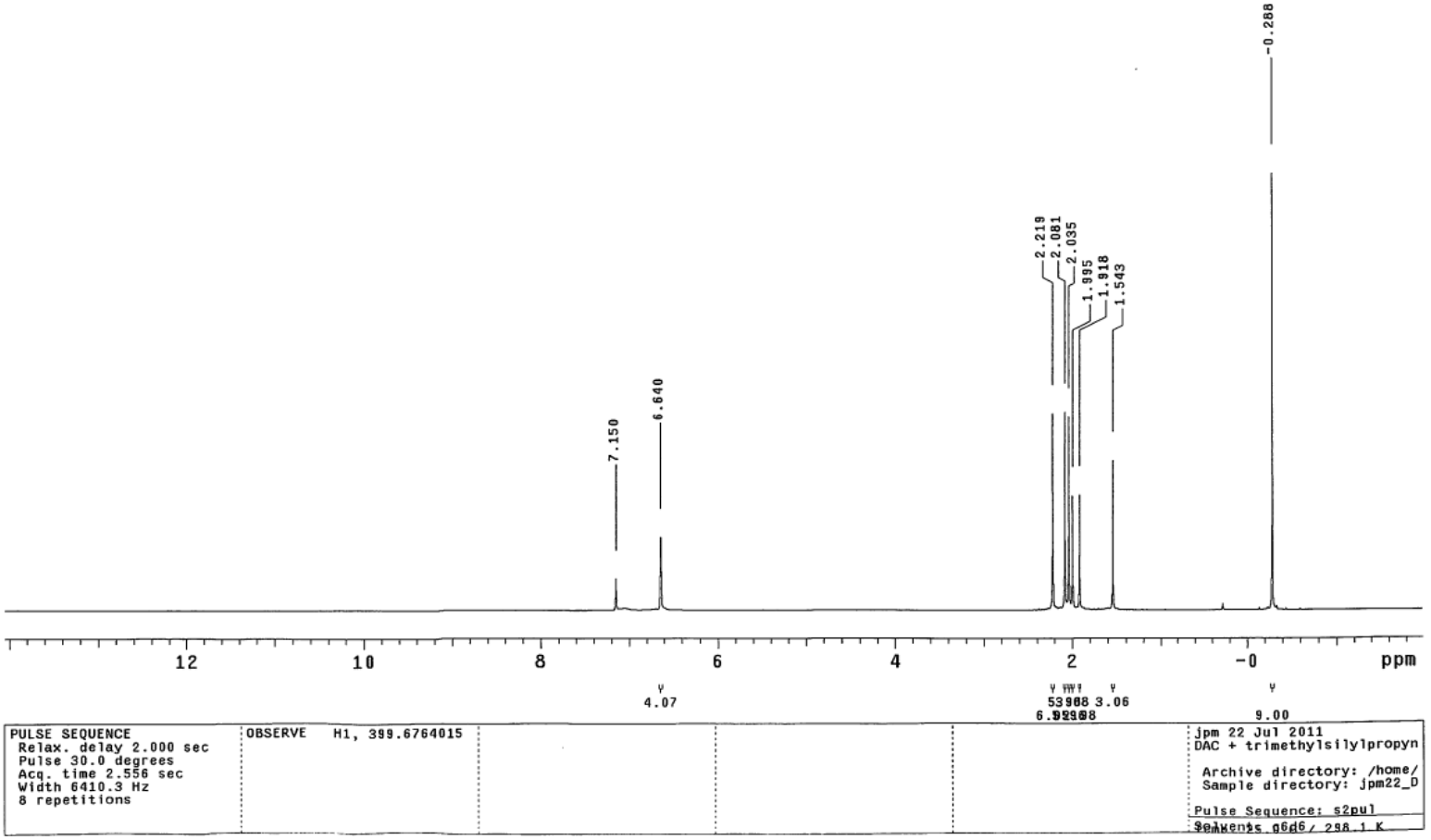
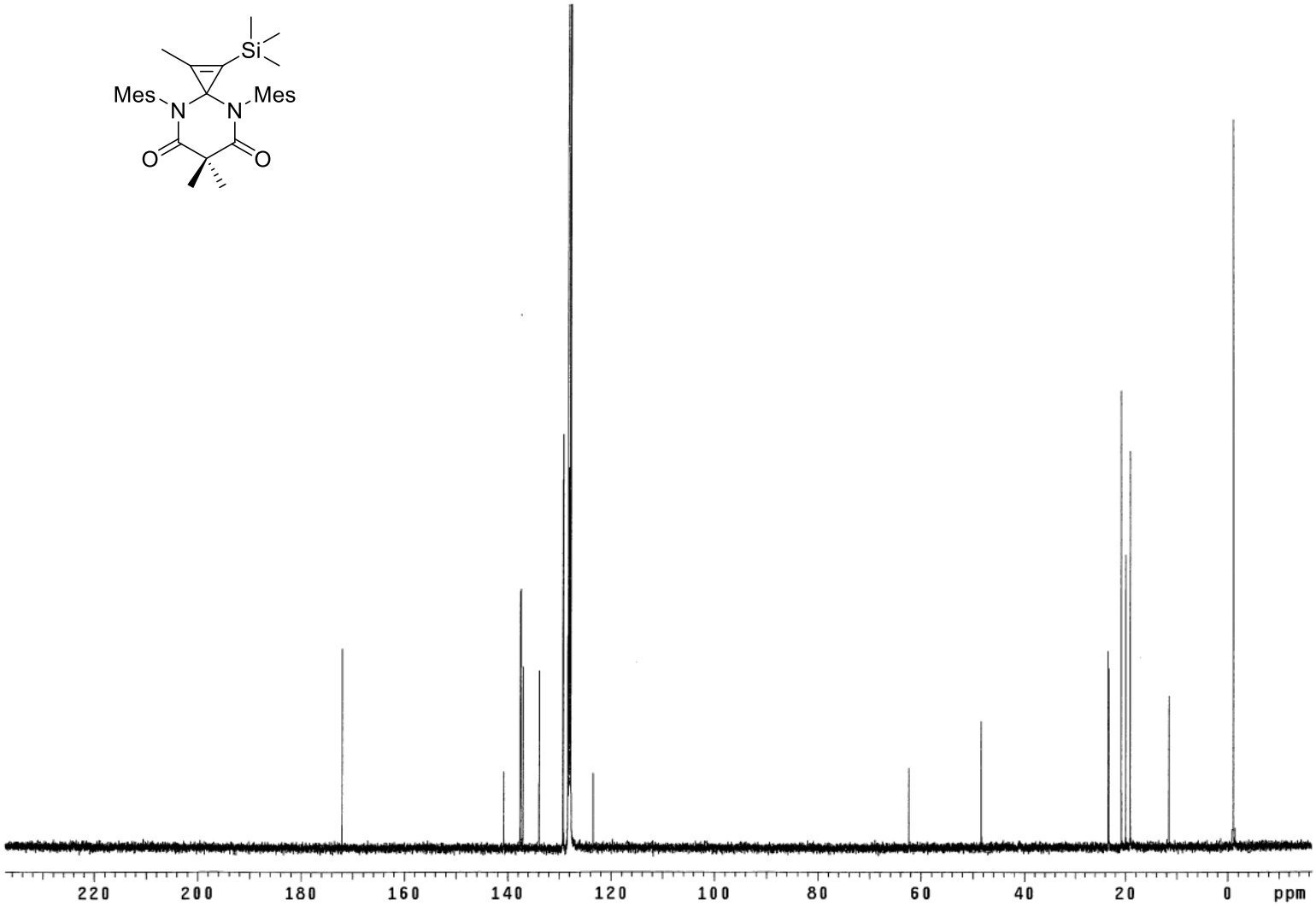
6
4
2
-0
ppm
4.23 4.00
6.00
11.83
6.6814
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 2.556 sec
Width 6410.3 Hz
16 repetitions
OBSERVE H1, 399.6764023
jpm 18 Jul 2011
DAC + diphenylacetylene
Archive directory: /home/
Sample directory: jpm18_D
Pulse Sequence: s2pul
Solvents: c6d6 / 298.1 K

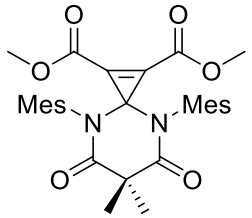

Ph
Ph
Mes
N
N
Mes
O
O
220
200
180
160
140
120
100
80
60
40
20
0
ppm
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.285 sec
Width 25510.2 Hz
256 repetitions
OBSERVE C13, 100.4986812
jpm 20 Jul 2011
DAC + diphenylacetylene
Archive directory: /home/
Sample directory: jpm20_D
Pulse Sequence: s2pul
Solvent: c6d6 / 298.1 K

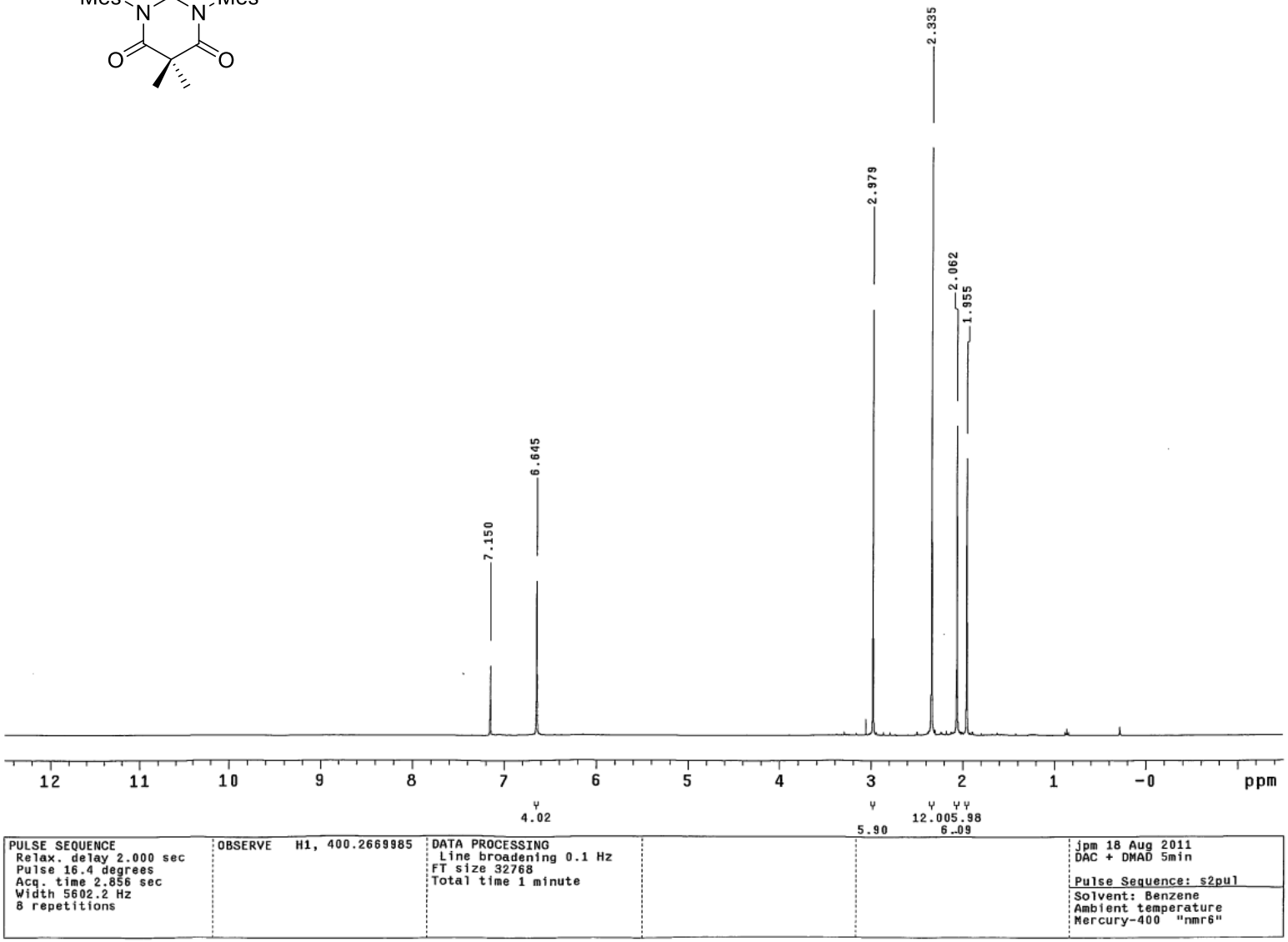

Si
Mes
N
N
Mes
O
O

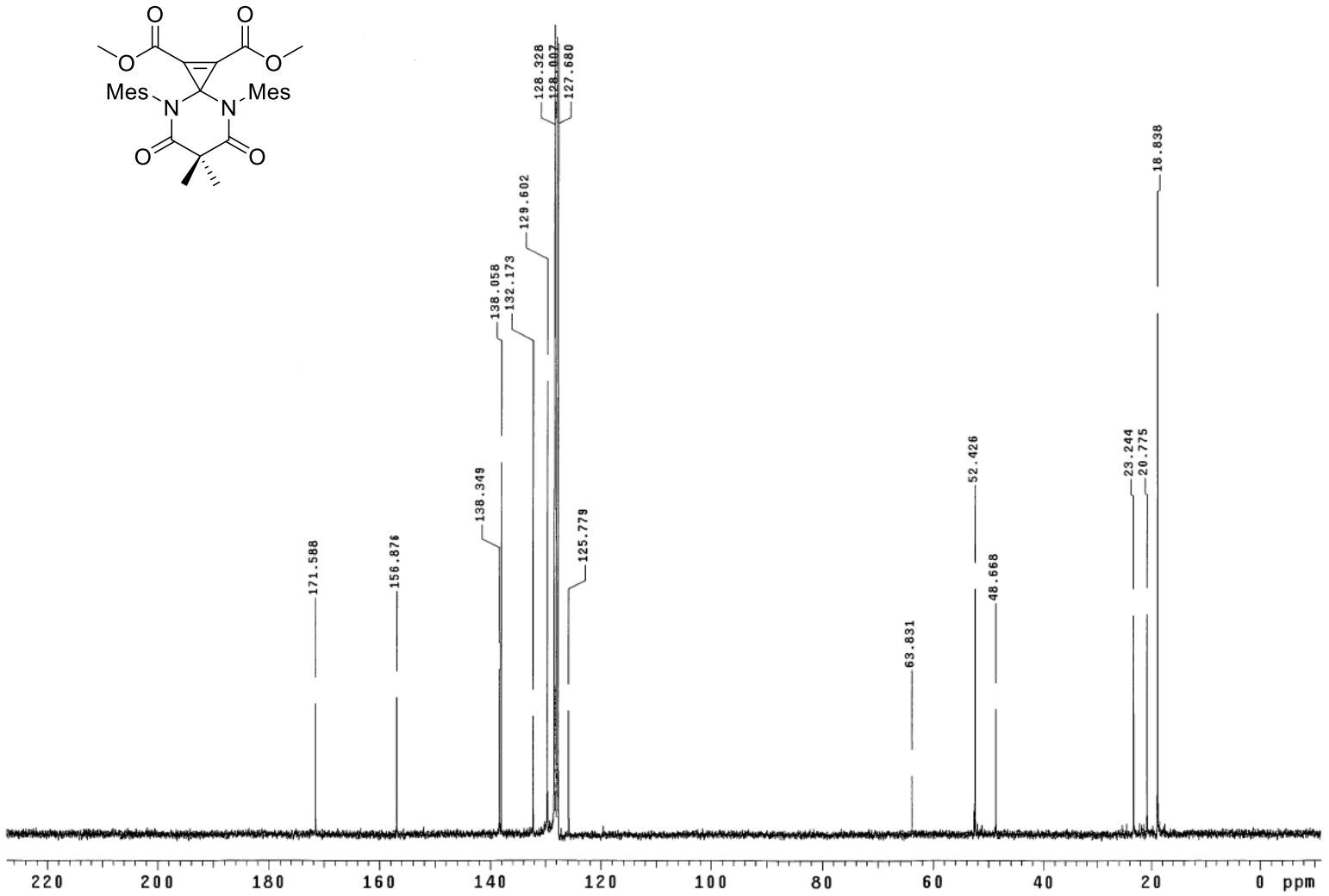

-0.288
2.219
2.081
2.035
1.995
1.918
1.543
7.150
6.640
12
10
8
6
4
2
-0
ppm
4.07
3.06
9.00
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 2.556 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 399.6764015
jpm 22 Jul 2011
DAC + trimethylsilylpropyn
Archive directory: /home/
Sample directory: jpm22_D
Pulse Sequence: s2pul
Solvent: c6d6 / 298.1 K



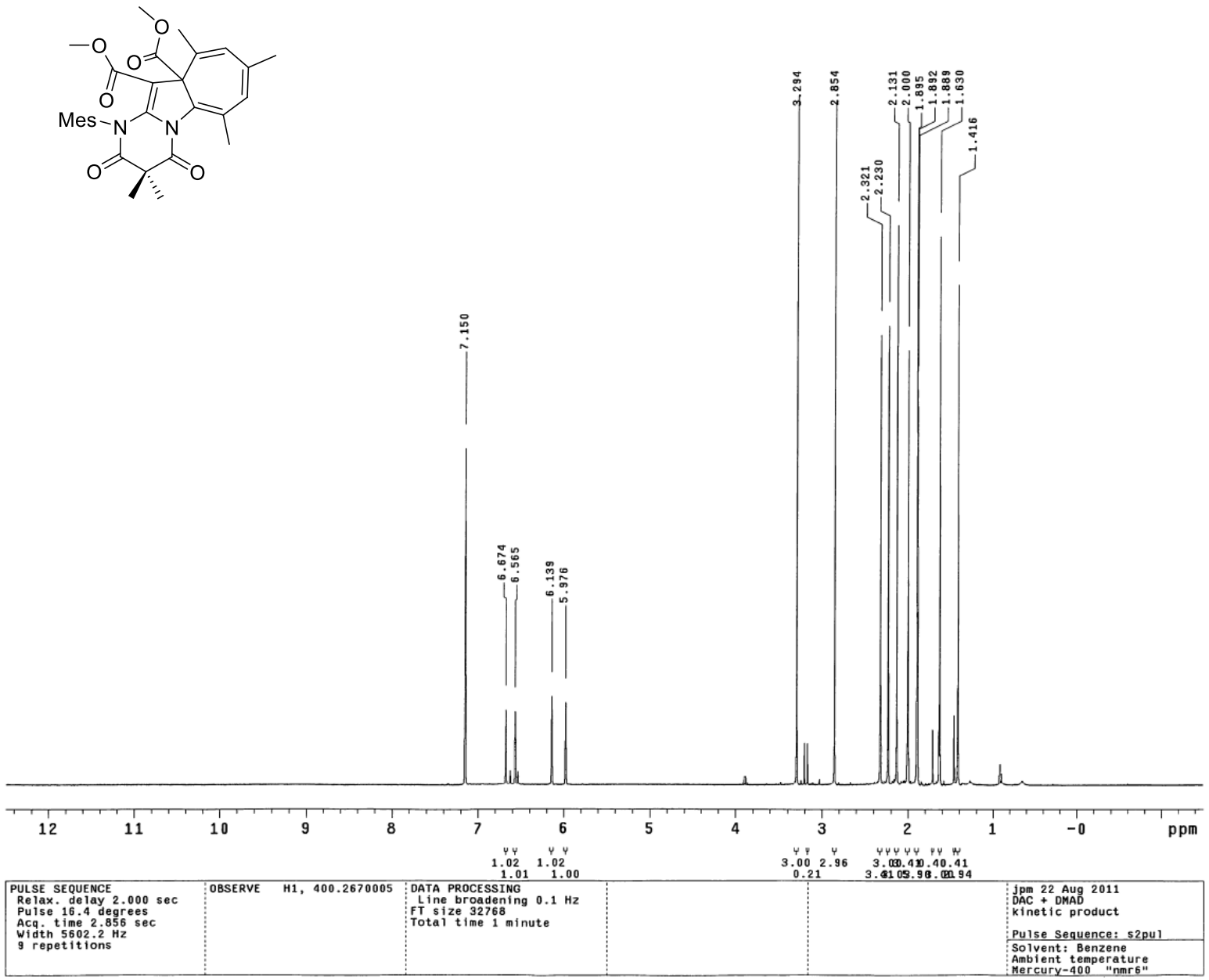
PULSE SEQUENCE Relax. delay 2.000 sec Pulse 30.0 degrees Acq. time 1.285 sec Width 25510.2 Hz 512 repetitions	OBSERVE C13, 100.4986805			jpm 22 Jul 2011 DAC + trimethylsilylpropyn Archive directory: /home/ Sample directory: jpm22_D Pulse Sequence: s2pul Solvent: c6d6 / 298.1 K

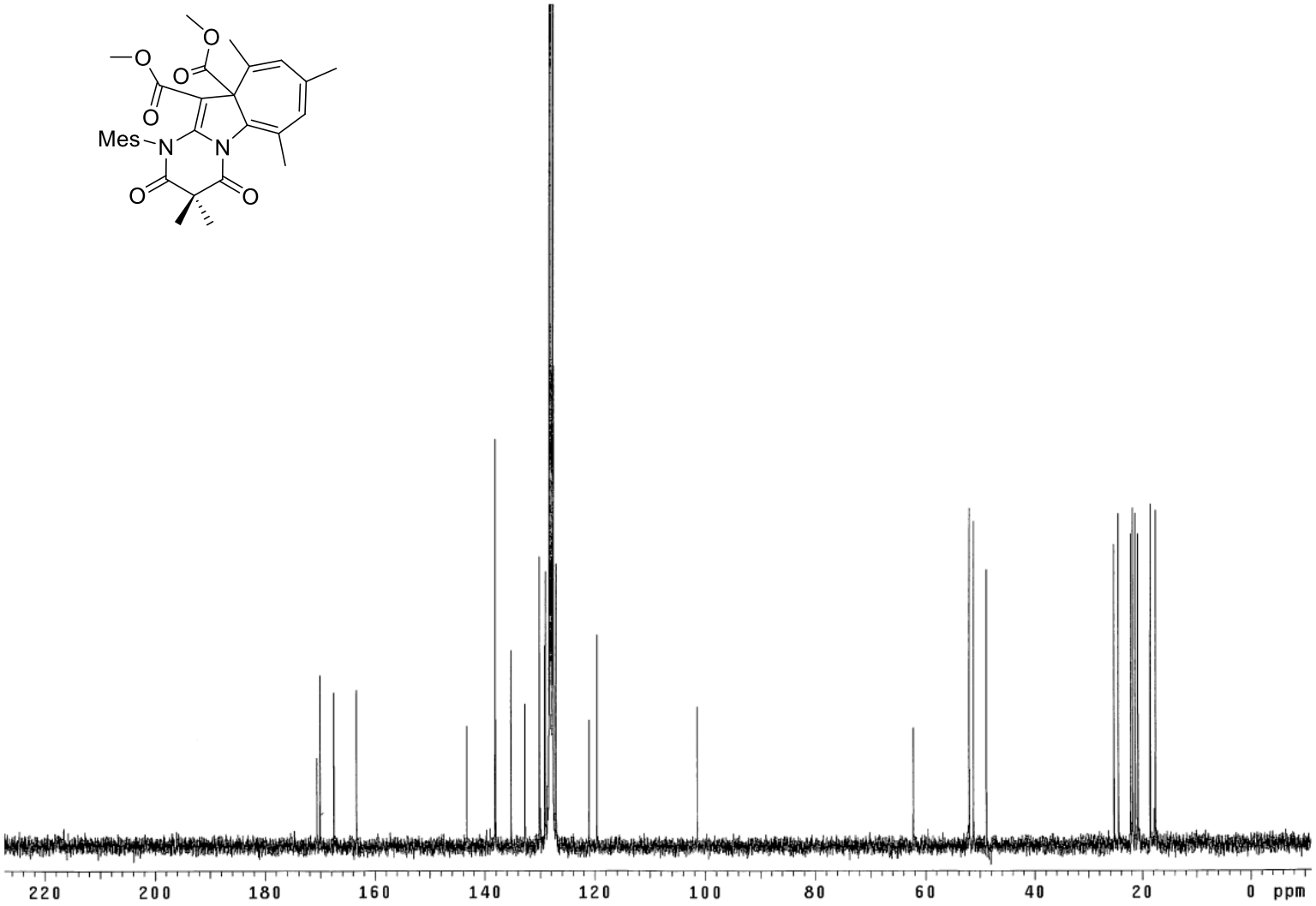

O
O
O
O
Mes
N
N
Mes
O
O


2.335
2.979
2.062
1.955
7.150
6.645
12
11
10
9
8
7
6
5
4
3
2
1
-0
ppm
4.02
5.90
12.00
5.98
6.09
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 16.4 degrees
Acq. time 2.856 sec
Width 5602.2 Hz
8 repetitions
OBSERVE H1, 400.2669985
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 1 minute
jpm 18 Aug 2011
DAC + DMAD 5min
Pulse Sequence: s2pul
Solvent: Benzene
Ambient temperature
Mercury-400 "nmr6"

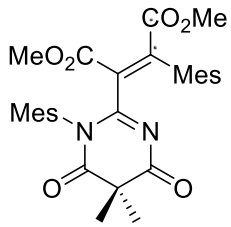


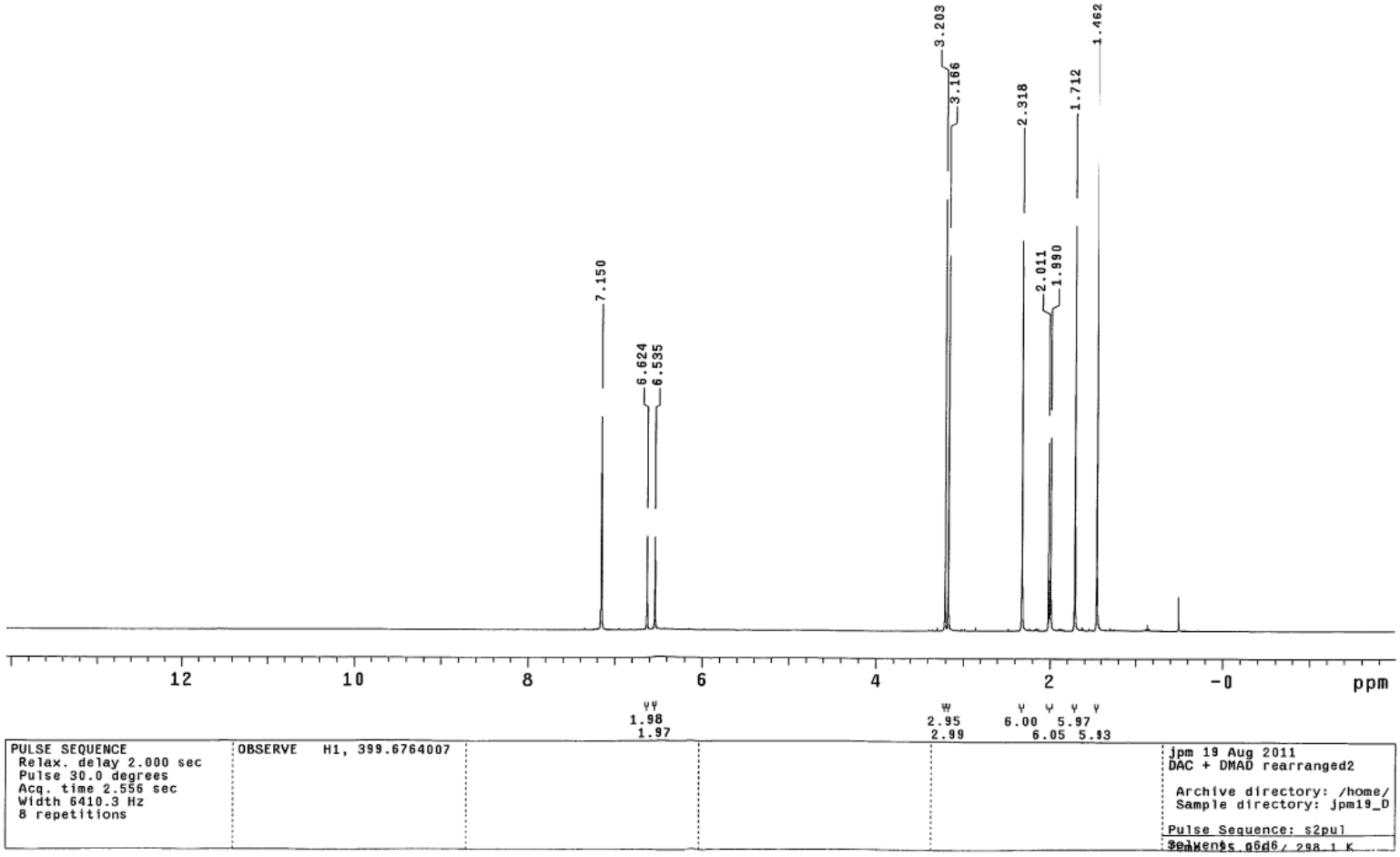
PULSE SEQUENCE Relax. delay 2.000 sec Pulse 36.0 degrees Acq. time 1.777 sec Width 18009.9 Hz 291 repetitions	OBSERVE C13, 75.4700005 DECOUPLE H1, 300.1409529 Power 40 dB continuously on WALTZ-16 modulated Single precision data	DATA PROCESSING Line broadening 1.0 Hz FT size 65536 Total time 18 minutes			13C OBSERVE Pulse Sequence: s2pul Solvent: Benzene Ambient temperature UNITYplus-300 "nmr2"

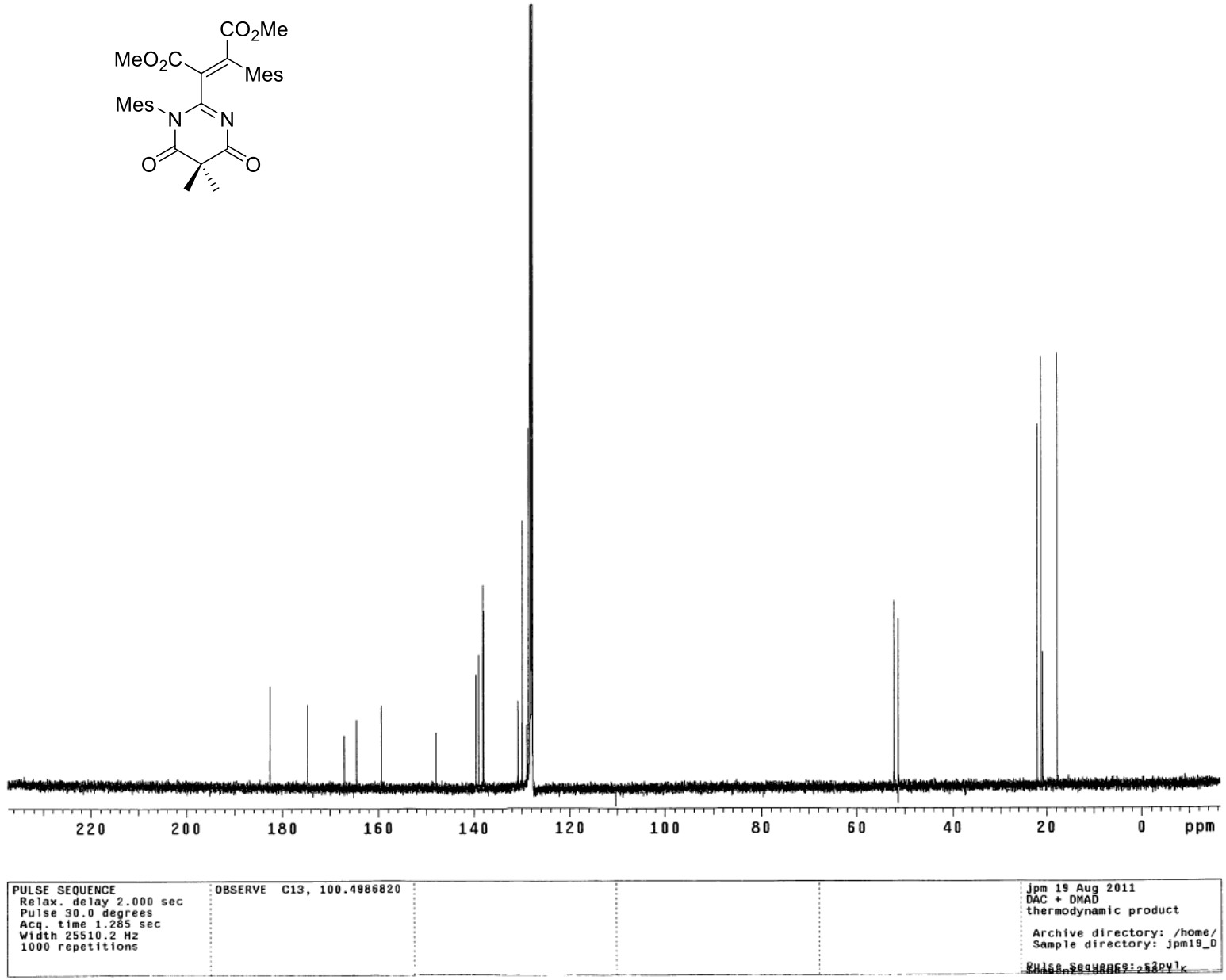

Mes
N
N
O
7.150
6.674
6.565
6.139
5.976
3.294
2.854
2.321
2.230
2.131
2.000
1.895
1.892
1.889
1.630
1.416
12
11
10
9
8
7
6
5
4
3
2
1
-0
ppm
1.02
1.01
1.02
1.00
3.00
0.21
2.96
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 16.4 degrees
Acq. time 2.856 sec
Width 5602.2 Hz
9 repetitions
OBSERVE H1, 400.2670005
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 1 minute
jpm 22 Aug 2011
DAC + DMAD
kinetic product
Pulse Sequence: s2pul
Solvent: Benzene
Ambient temperature
Mercury-400 "nmr6"

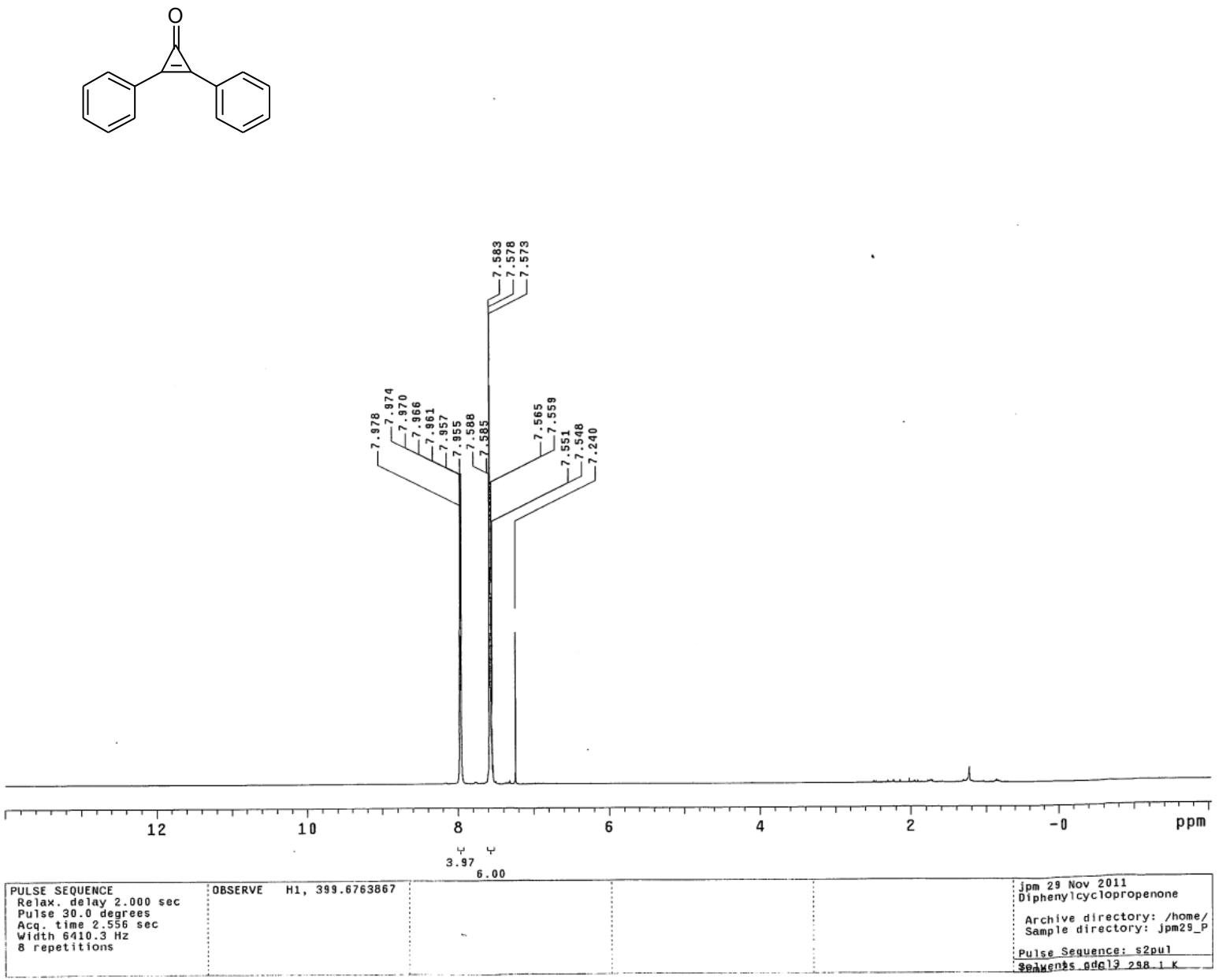


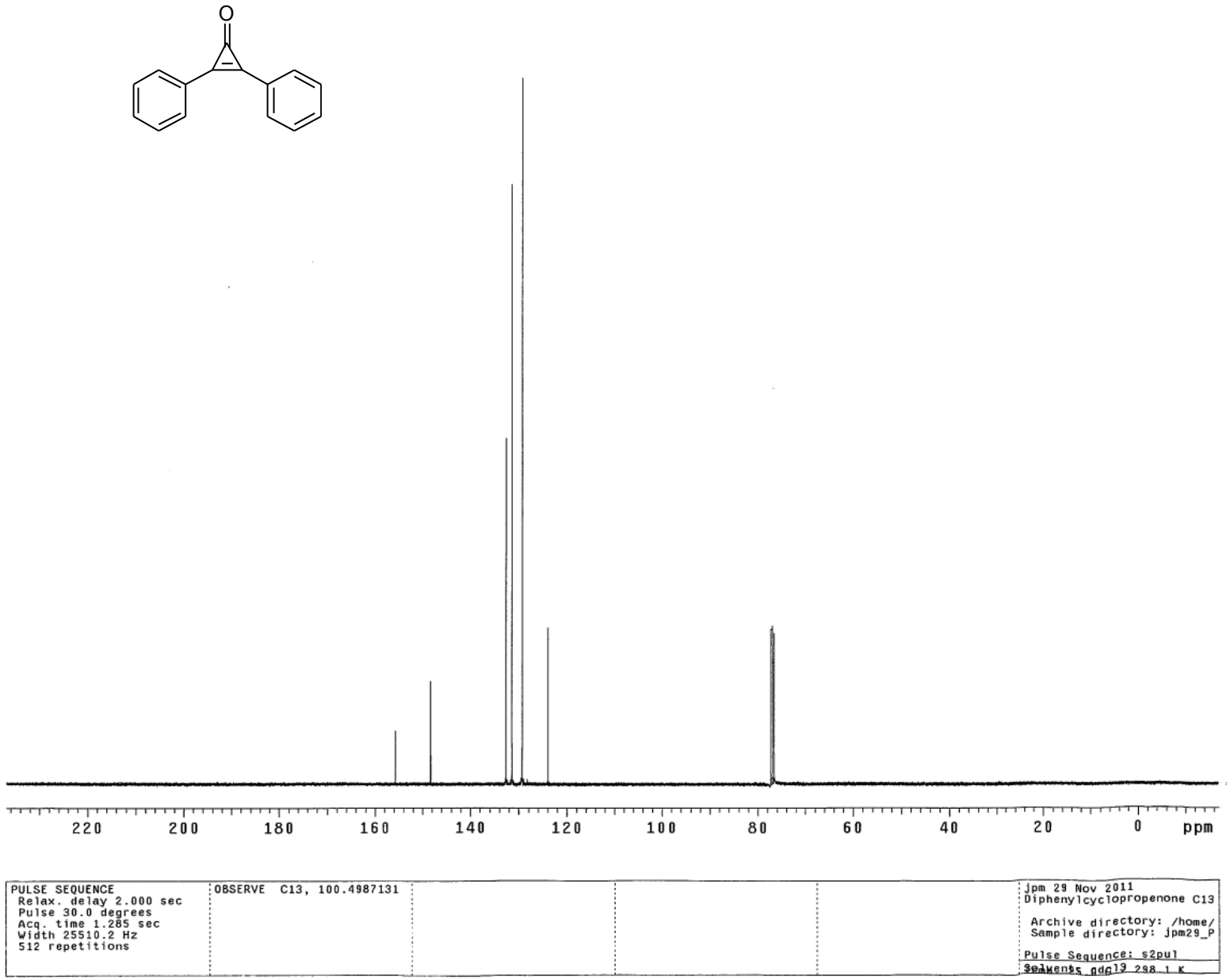
PULSE SEQUENCE Relax. delay 2.000 sec Pulse 36.0 degrees Acq. time 1.777 sec Width 18009.9 Hz 832 repetitions	OBSERVE C13, 75.4700011 DECOUPLE H1, 300.1409529 Power 40 dB continuously on WALTZ-16 modulated Single precision data	DATA PROCESSING Line broadening 1.0 Hz FT size 65536 Total time 52 minutes			jpm 23 Aug 2011 DAC + DMAD Kinetic product Pulse Sequence: s2pul Solvent: Benzene Ambient temperature UNITYplus-300 "nmr2"

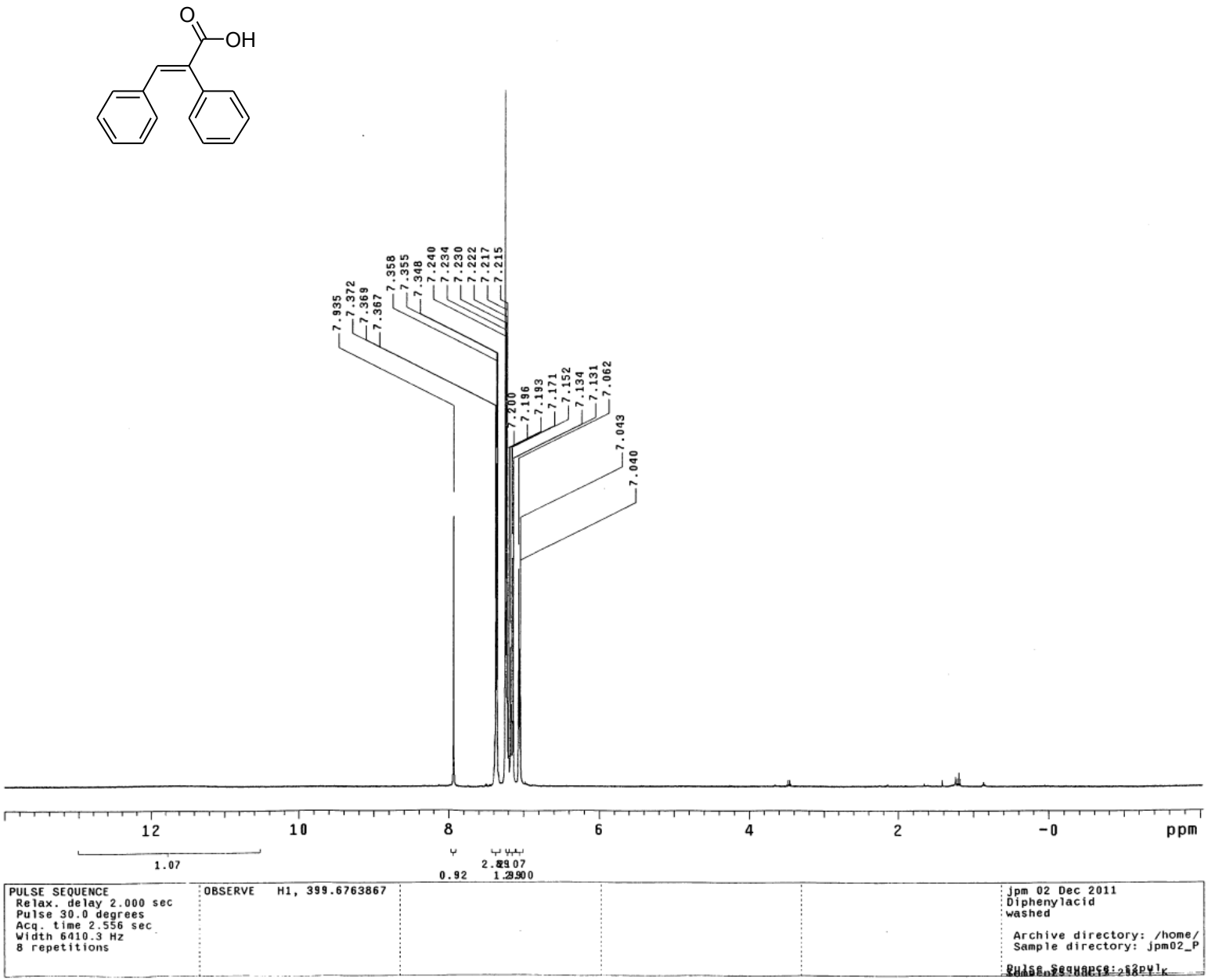

CO2Me
MeO2C
Mes
Mes
N
N
O
O

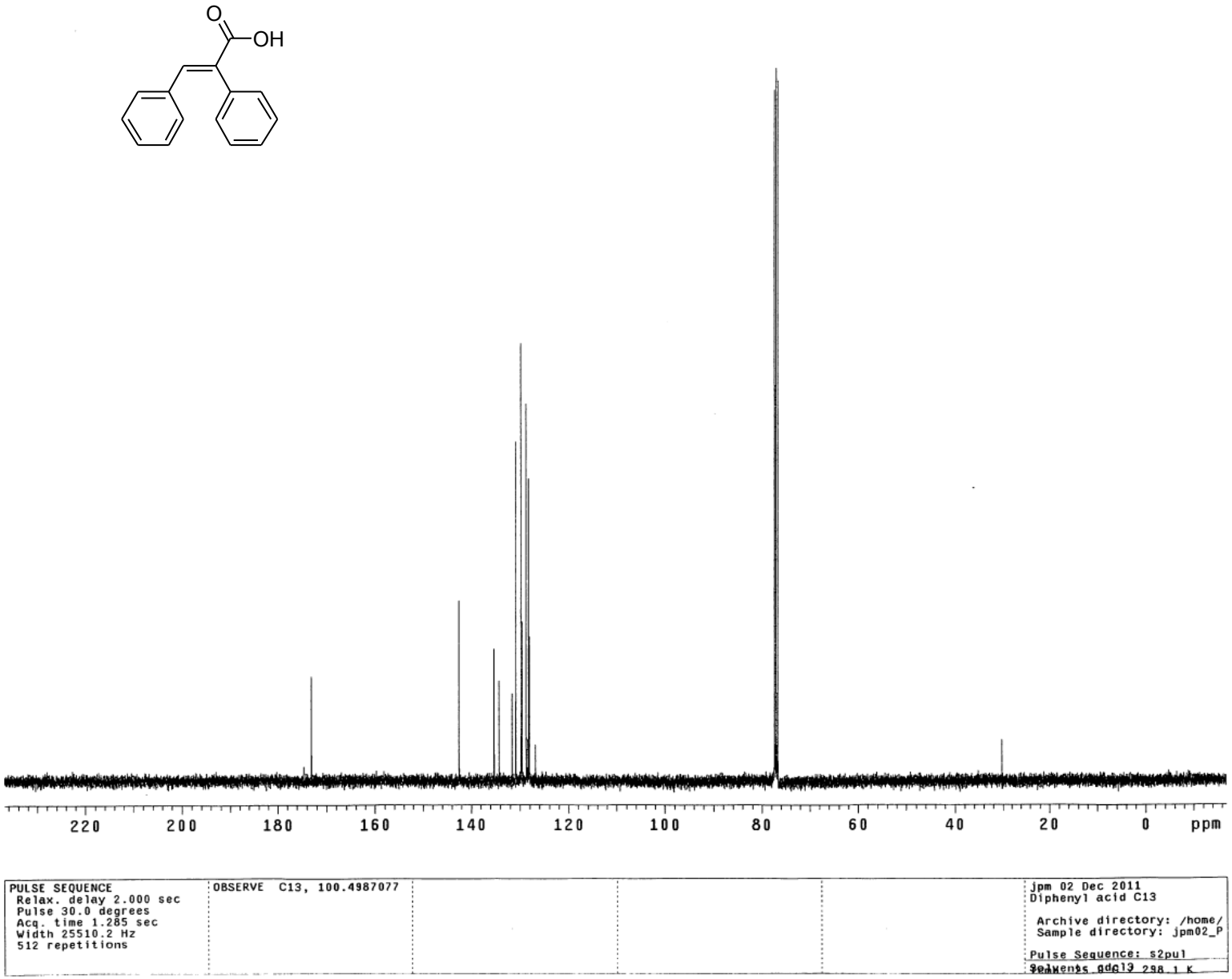

7.150
6.624
6.535
3.203
3.166
2.318
2.011
1.990
1.712
1.462
12
10
8
6
4
2
-0
ppm
1.98
1.97
2.95
2.99
6.00
5.97
6.05
5.93
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 2.556 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 399.6764007
jpm 19 Aug 2011
DAC + DMAD rearranged2
Archive directory: /home/
Sample directory: jpm19_D
Pulse Sequence: s2pul
Solvent: cdcl3
Temp: 298.1 K

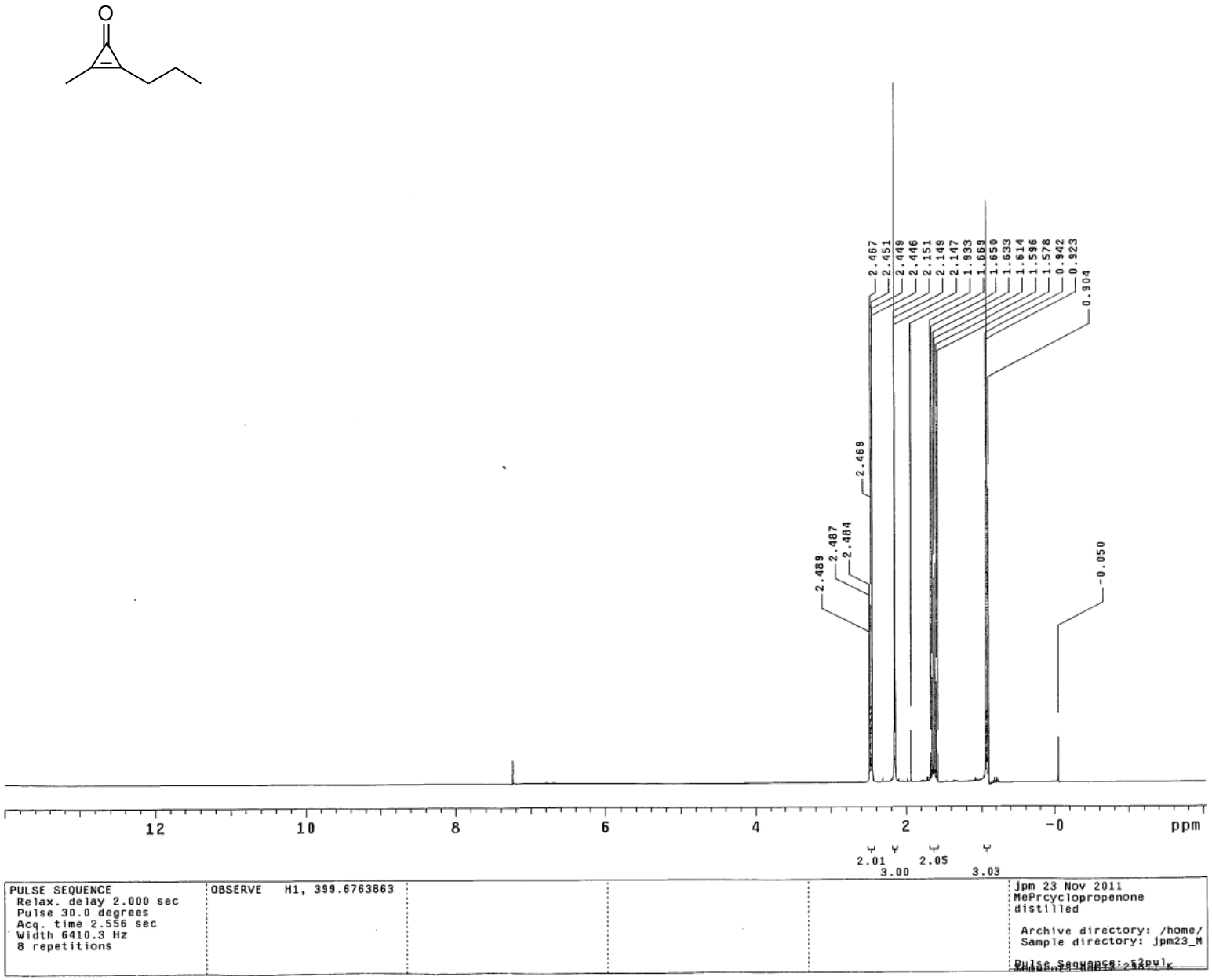

CO2Me
MeO2C
Mes
Mes
N
N
O
O
220
200
180
160
140
120
100
80
60
40
20
0
ppm
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.285 sec
Width 25510.2 Hz
1000 repetitions
OBSERVE C13, 100.4986820
jpm 19 Aug 2011
DAC + DMAD
thermodynamic product
Archive directory: /home/
Sample directory: jpm19_D

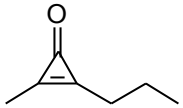

7.978
7.974
7.970
7.966
7.961
7.957
7.955
7.588
7.585
7.583
7.578
7.573
7.565
7.559
7.551
7.548
7.240
12
10
8
6
4
2
-0
ppm
3.97
6.00
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 2.556 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 399.6763867
jpm 29 Nov 2011
Diphenylcyclopropenone
Archive directory: /home/
Sample directory: jpm29_P
Pulse Sequence: s2pul
Solvents: cdcl3 298.1 K

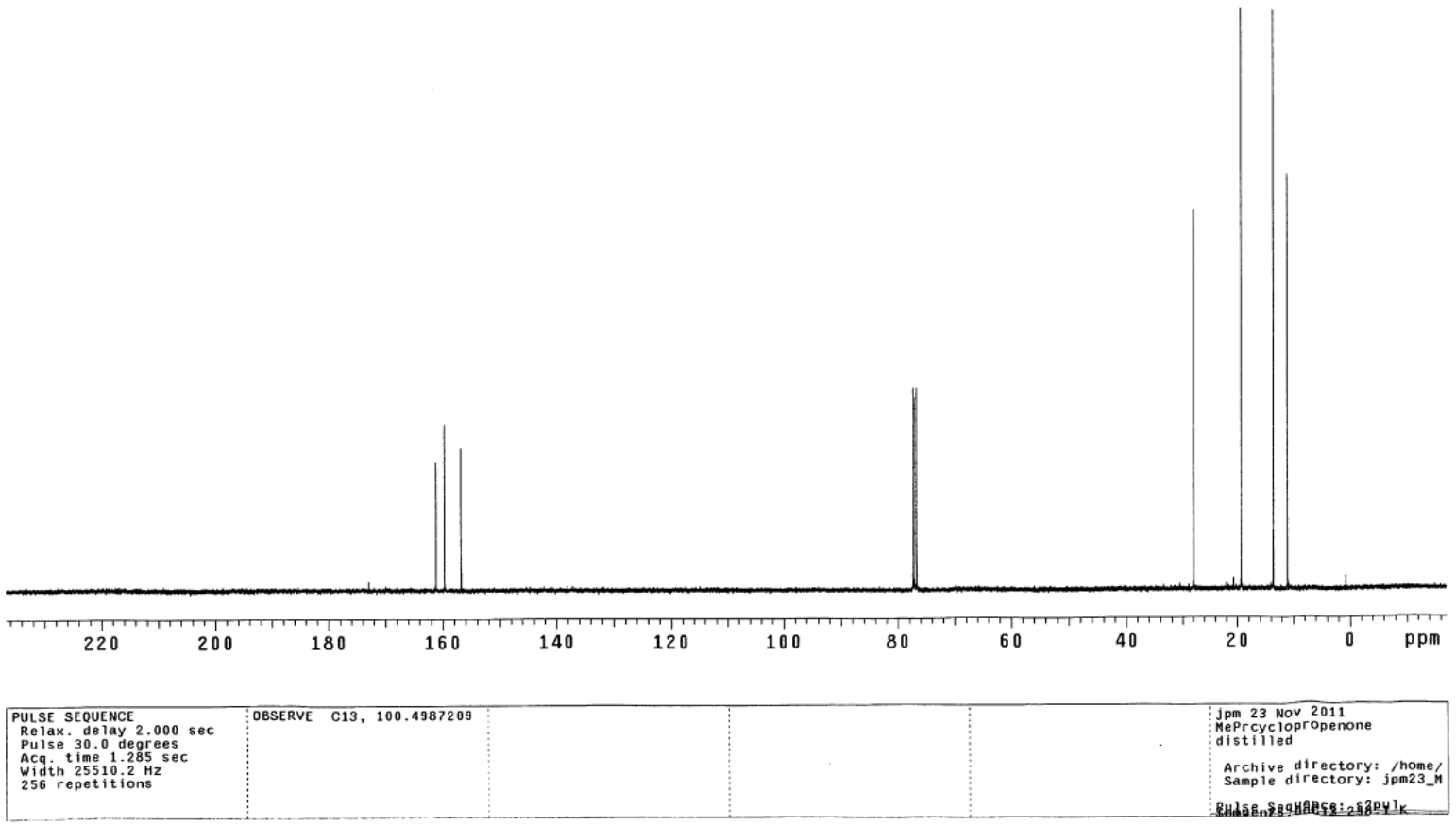

O
220
200
180
160
140
120
100
80
60
40
20
0
ppm
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.285 sec
Width 25510.2 Hz
512 repetitions
OBSERVE C13, 100.4987131
jpm 29 Nov 2011
Diphenylcyclopropenone C13
Archive directory: /home/
Sample directory: jpm29_P
Pulse Sequence: s2pul
Solvents: cdcl3 298.1 K

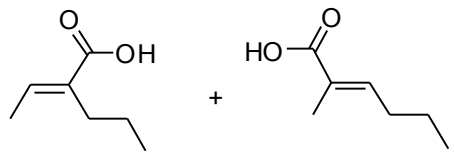

O
OH
7.935
7.372
7.369
7.367
7.358
7.355
7.348
7.240
7.234
7.230
7.222
7.217
7.215
7.200
7.196
7.193
7.171
7.152
7.134
7.131
7.062
7.043
7.040
12
10
8
6
4
2
-0
ppm
1.07
0.92
2.89
1.00
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 2.556 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 399.6763867
jpm 02 Dec 2011
Diphenylacid
washed
Archive directory: /home/
Sample directory: jpm02_P

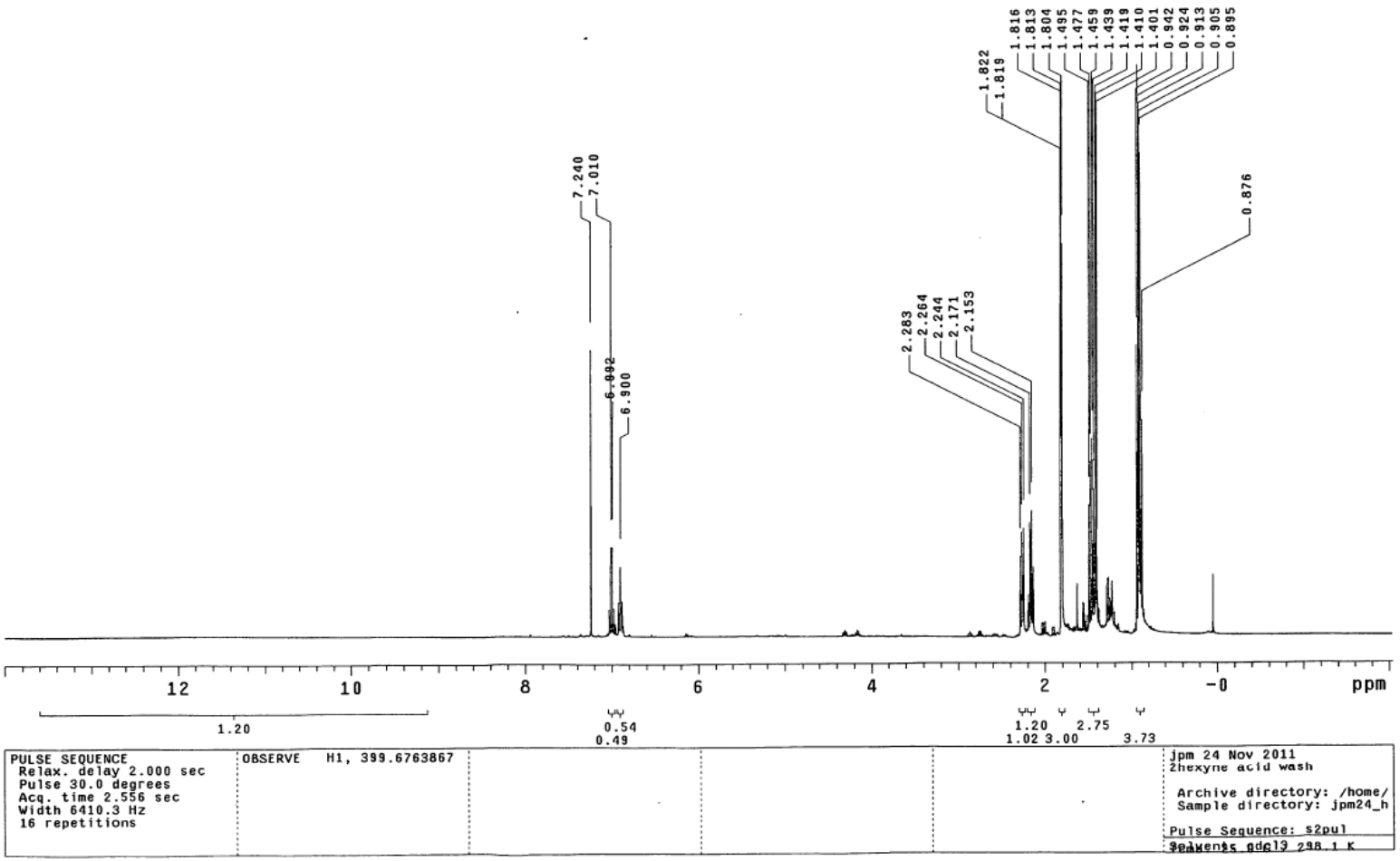

O
OH
220
200
180
160
140
120
100
80
60
40
20
0
ppm
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.285 sec
Width 25510.2 Hz
512 repetitions
OBSERVE C13, 100.4987077
jpm 02 Dec 2011
Diphenyl acid C13
Archive directory: /home/
Sample directory: jpm02_P
Pulse Sequence: s2pul
Solvents: cdcl3 298.1 K

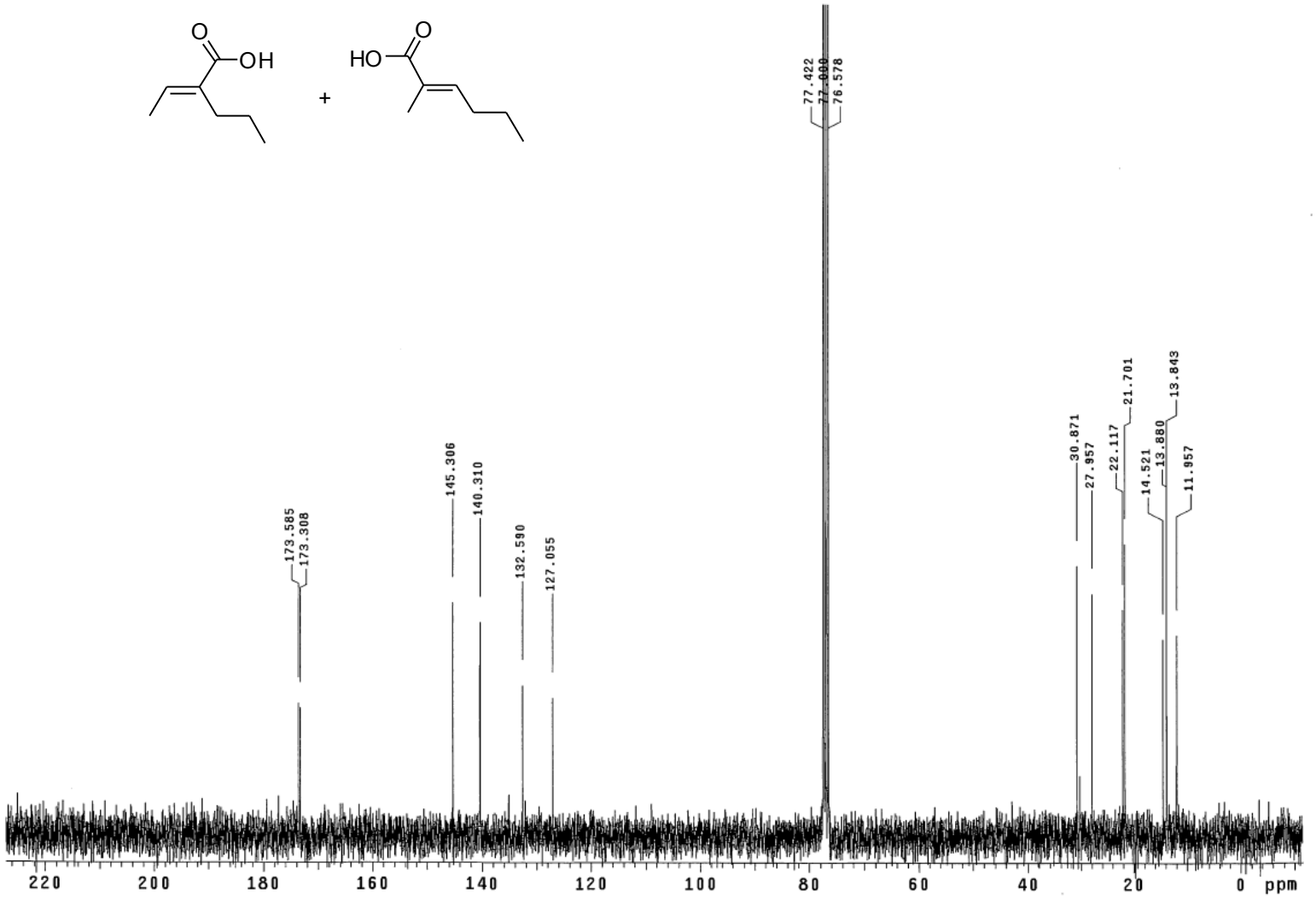

O
2.467
2.451
2.449
2.446
2.151
2.149
2.147
1.933
1.669
1.650
1.633
1.614
1.596
1.578
0.942
0.923
0.904
2.469
2.489
2.487
2.484
-0.050
12
10
8
6
4
2
-0
ppm
2.01
3.00
2.05
3.03
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 2.556 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 399.6763863
jpm 23 Nov 2011
MePrcyclopropenone
distilled
Archive directory: /home/
Sample directory: jpm23_M



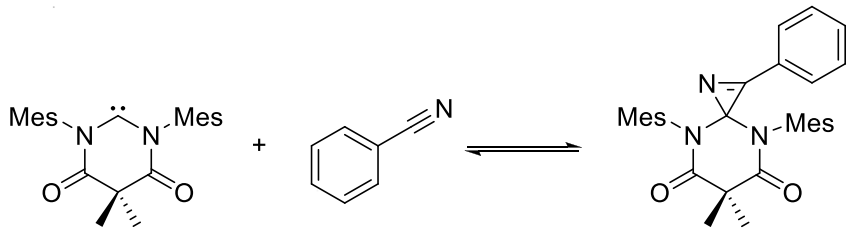

220
200
180
160
140
120
100
80
60
40
20
0
ppm
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.285 sec
Width 25510.2 Hz
256 repetitions
OBSERVE C13, 100.4987209
jpm 23 Nov 2011
MePrcyclopropenone
distilled
Archive directory: /home/
Sample directory: jpm23_M

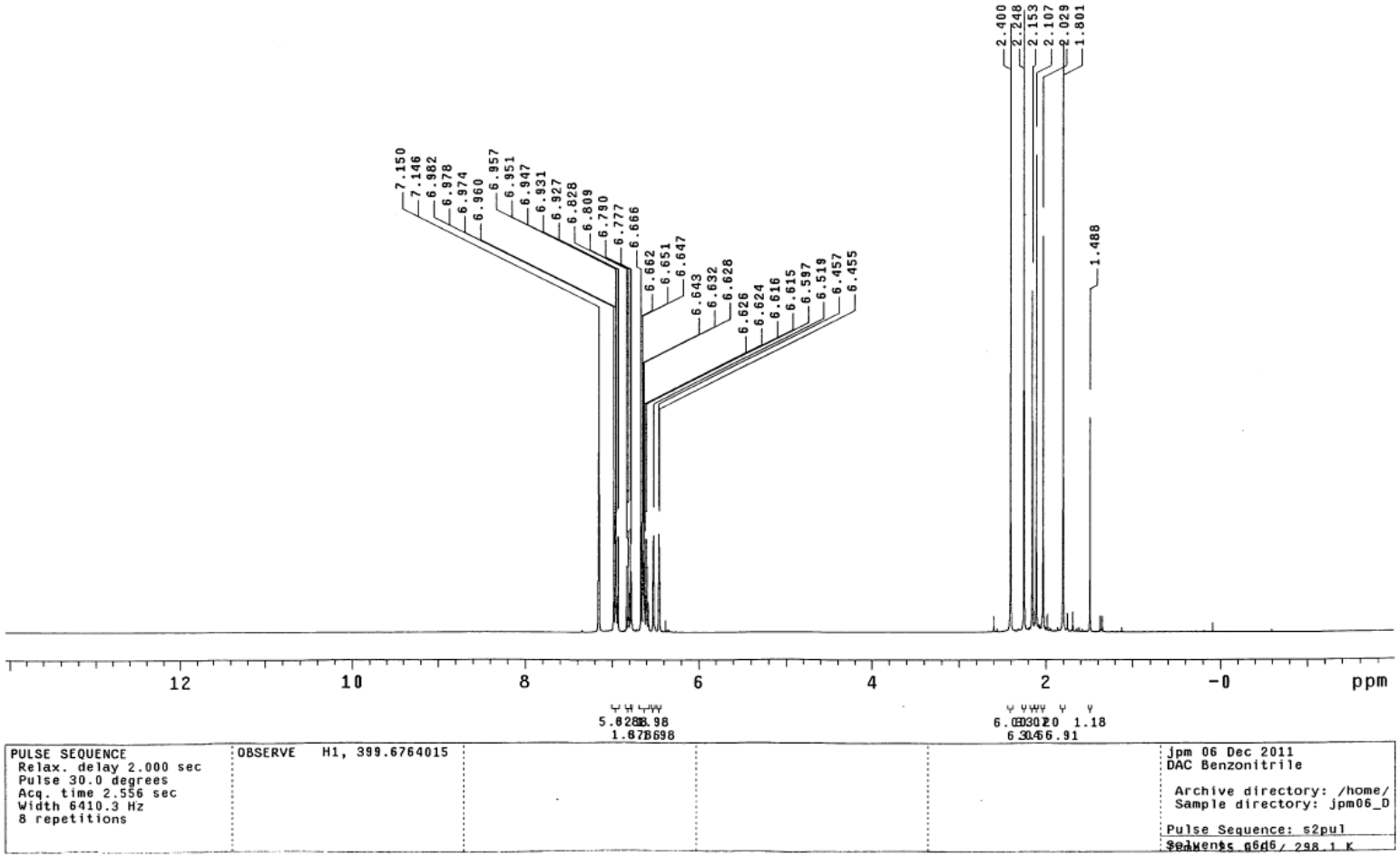

O
OH
+
HO
O

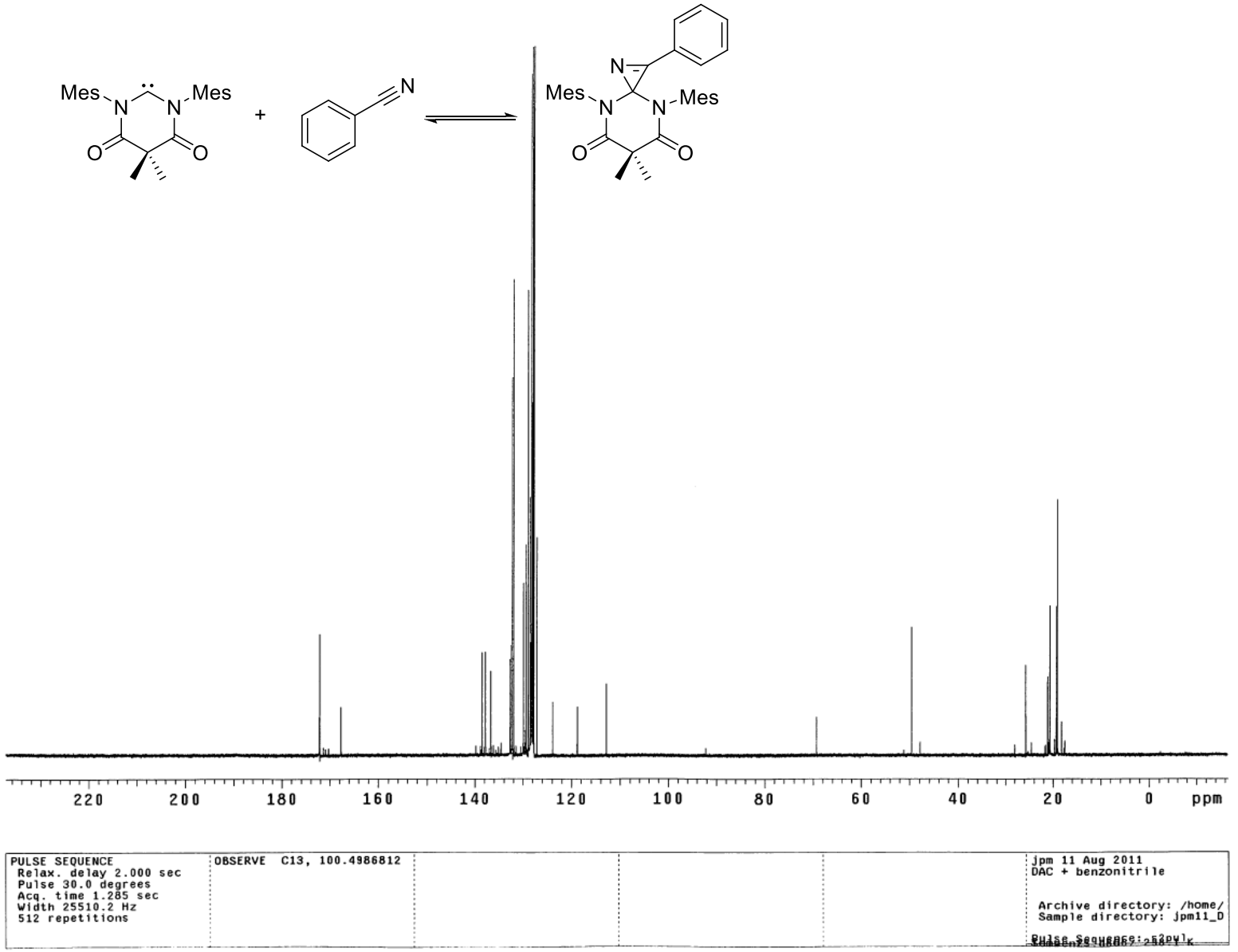

7.240
7.010
6.902
6.900
2.283
2.264
2.244
2.171
2.153
1.822
1.819
1.816
1.813
1.804
1.495
1.477
1.459
1.439
1.419
1.410
1.401
0.942
0.924
0.913
0.905
0.895
0.876
12
10
8
6
4
2
-0
ppm
1.20
0.54
0.49
1.20
1.02
2.75
3.00
3.73
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 2.556 sec
Width 6410.3 Hz
16 repetitions
OBSERVE H1, 399.6763867
jpm 24 Nov 2011
2hexyne acid wash
Archive directory: /home/
Sample directory: jpm24_h
Pulse Sequence: s2pul
Solvent: cdcl3 298.1 K

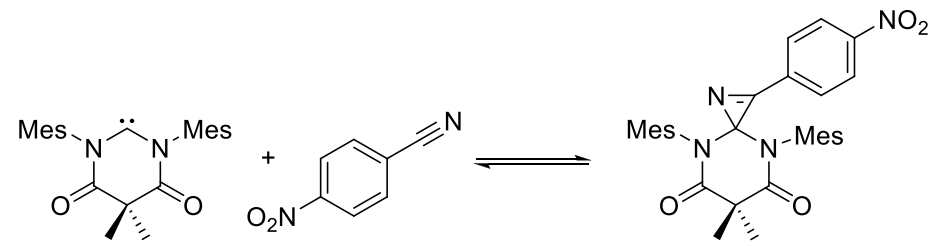


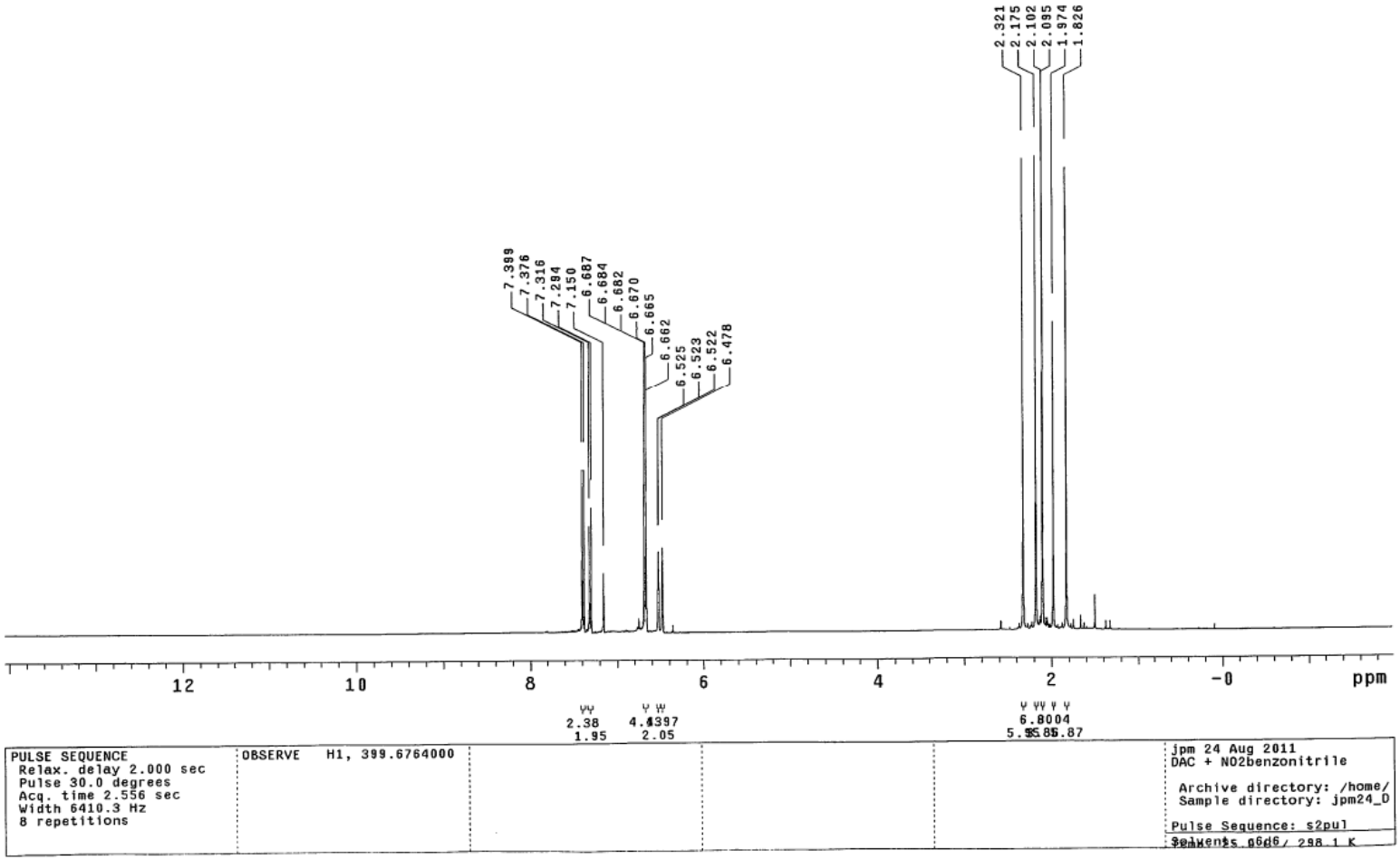
PULSE SEQUENCE Relax. delay 2.000 sec Pulse 36.0 degrees Acq. time 1.777 sec Width 18009.9 Hz 1248 repetitions	OBSERVE C13, 75.4700194 DECOUPLE H1, 300.1409259 Power 40 dB continuously on WALTZ-16 modulated Single precision data	DATA PROCESSING Line broadening 1.0 Hz FT size 65536 Total time 78 minutes			jpm 30 Nov 2011 2-hexyne acid C13 Pulse Sequence: s2pul Solvent: CDCl3 Ambient temperature UNITYplus-300 "nmr2"

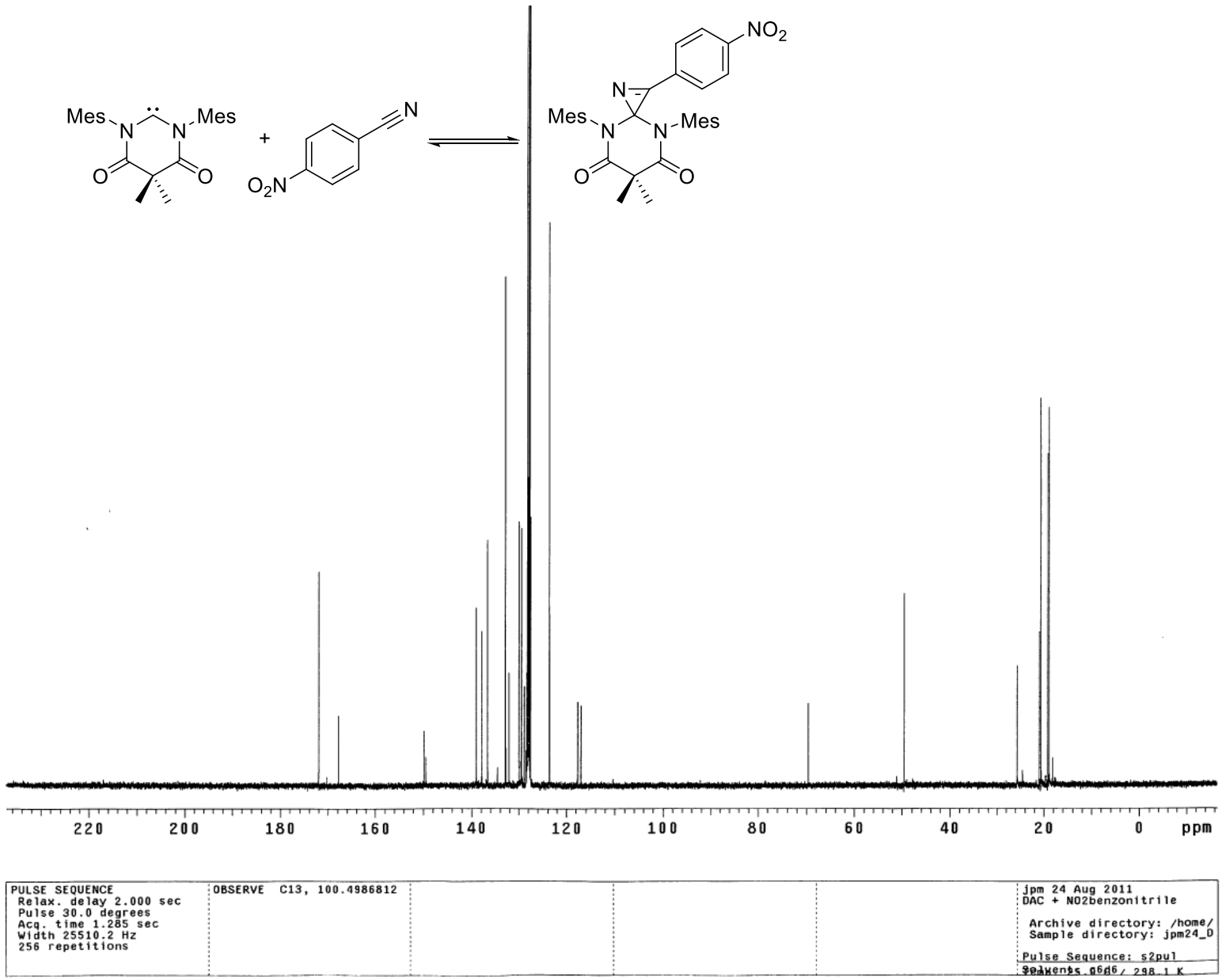

Mes
N
N
Mes
O
O
+
N
N
Mes
N
N
Mes
O
O

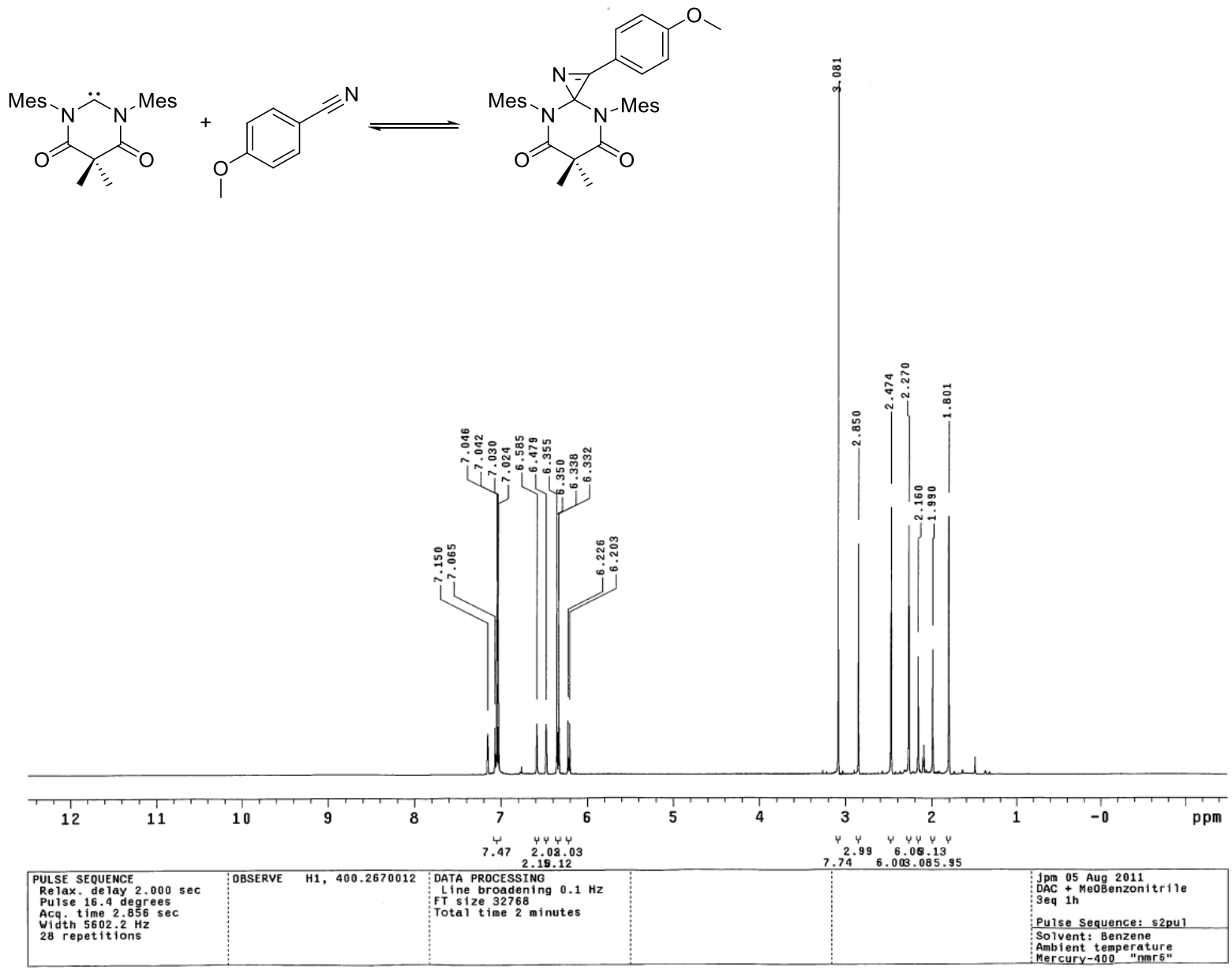

7.150
7.146
6.982
6.978
6.974
6.960
6.957
6.951
6.947
6.931
6.927
6.828
6.809
6.790
6.777
6.666
6.662
6.651
6.647
6.643
6.632
6.628
6.626
6.624
6.616
6.615
6.597
6.519
6.457
6.455
2.400
2.248
2.153
2.107
2.029
1.801
1.488
12
10
8
6
4
2
-0
ppm
1.18
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 2.556 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 399.6764015
jpm 06 Dec 2011
DAC Benzonitrile
Archive directory: /home/
Sample directory: jpm06_D
Pulse Sequence: s2pul
Solvent: c6d6 / 298.1 K

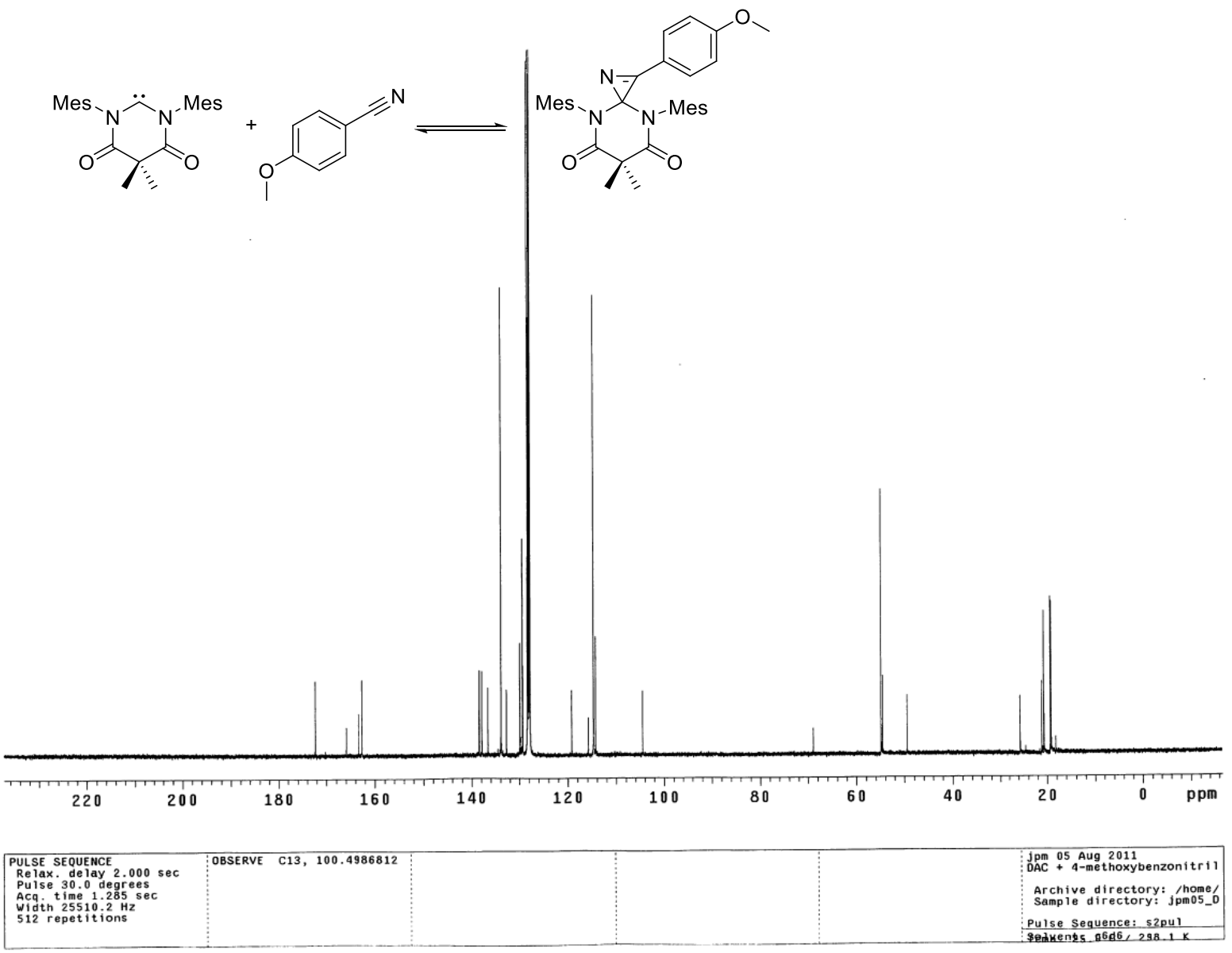

Mes
N
N
Mes
O
O
+
N
N
Mes
N
N
Mes
O
O
220
200
180
160
140
120
100
80
60
40
20
0
ppm
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.285 sec
Width 25510.2 Hz
512 repetitions
OBSERVE C13, 100.4986812
jpm 11 Aug 2011
DAC + benzonitrile
Archive directory: /home/
Sample directory: jpm11_D

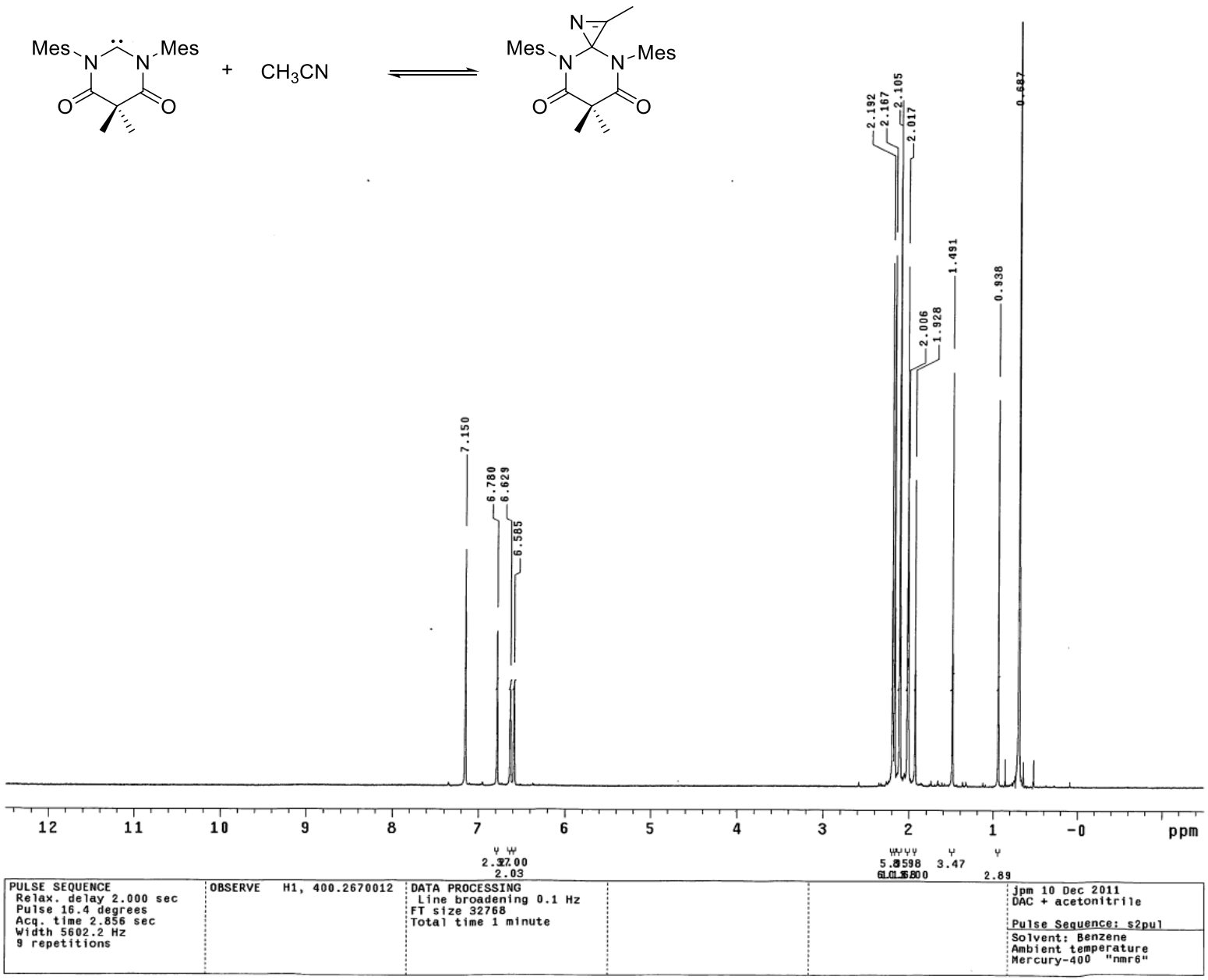

Mes
N
N
Mes
O
O
+
O_2N
N
NO_2
N
Mes
N
N
Mes
O
O

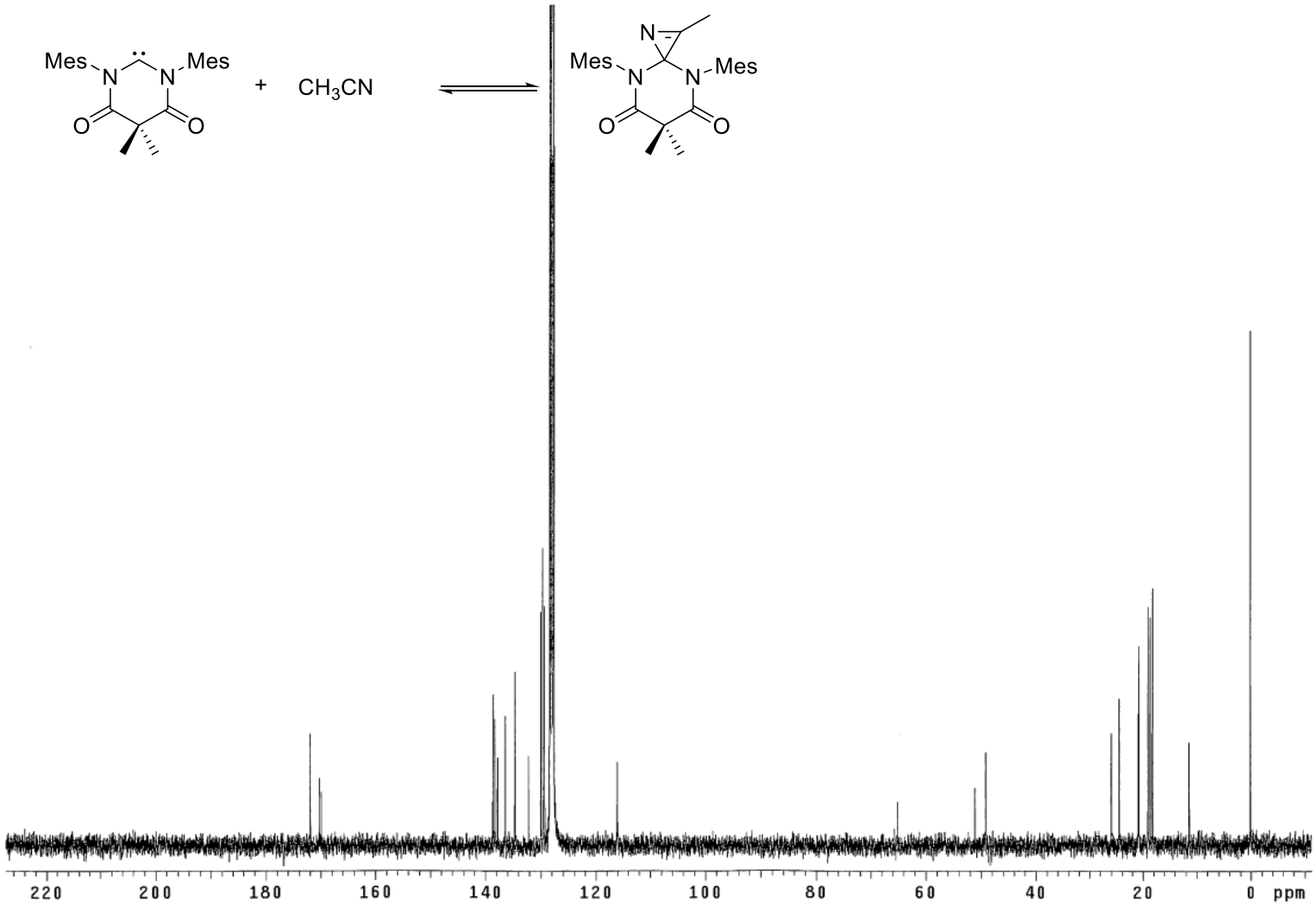

2.321
2.175
2.102
2.095
1.974
1.826
7.389
7.376
7.316
7.284
7.150
6.687
6.684
6.682
6.670
6.665
6.662
6.525
6.523
6.522
6.478
12
10
8
6
4
2
-0
ppm
2.38
1.95
4.4397
2.05
6.8004
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 2.556 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 399.6764000
jpm 24 Aug 2011
DAC + NO2benzonitrile
Archive directory: /home/
Sample directory: jpm24_D
Pulse Sequence: s2pul
Solvents: d6d6 / 298.1 K


Mes
N
N
Mes
O
O
+
N
O_2N
NO_2
N
Mes
N
N
Mes
O
O
220
200
180
160
140
120
100
80
60
40
20
0
ppm
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.285 sec
Width 25510.2 Hz
256 repetitions
OBSERVE C13, 100.4986812
jpm 24 Aug 2011
DAC + NO2benzonitrile
Archive directory: /home/
Sample directory: jpm24_D
Pulse Sequence: s2pul
Solvent: d6d6 / 298.1 K

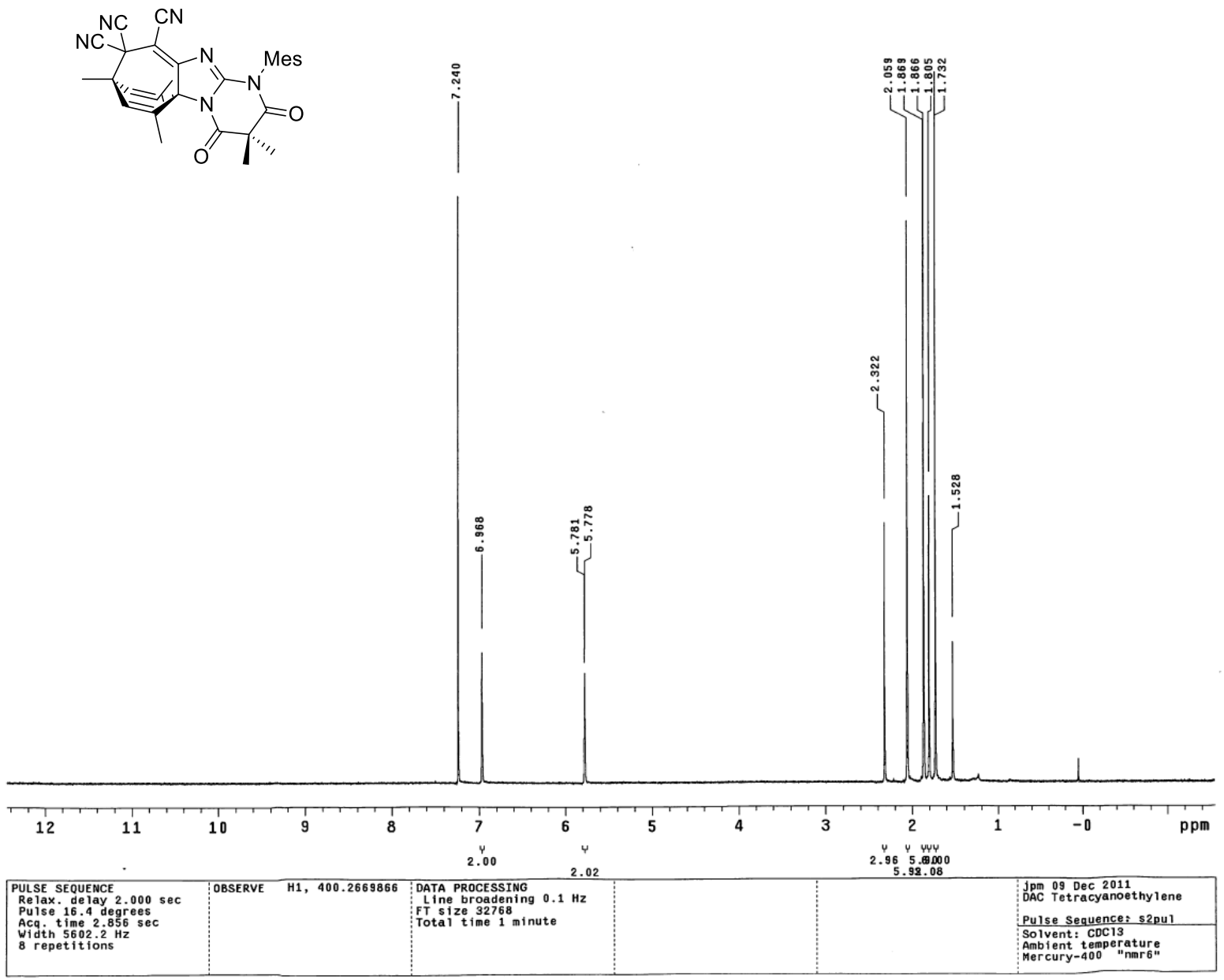

Mes
N
N
Mes
O
O
+
O
N
Mes
N
N
Mes
O
O
O
N
3.081
2.850
2.474
2.270
2.160
1.990
1.801
7.046
7.042
7.030
7.024
6.585
6.479
6.355
6.350
6.338
6.332
7.150
7.065
6.226
6.203
12
11
10
9
8
7
6
5
4
3
2
1
-0
ppm
7.47
2.03
3.03
2.19
9.12
2.99
6.00
6.06
3.08
6.13
5.95
7.74
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 16.4 degrees
Acq. time 2.856 sec
Width 5602.2 Hz
28 repetitions
OBSERVE H1, 400.2670012
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 2 minutes
jpm 05 Aug 2011
DAC + MeOBenzonitrile
3eq 1h
Pulse Sequence: s2pul
Solvent: Benzene
Ambient temperature
Mercury-400 "nmr6"

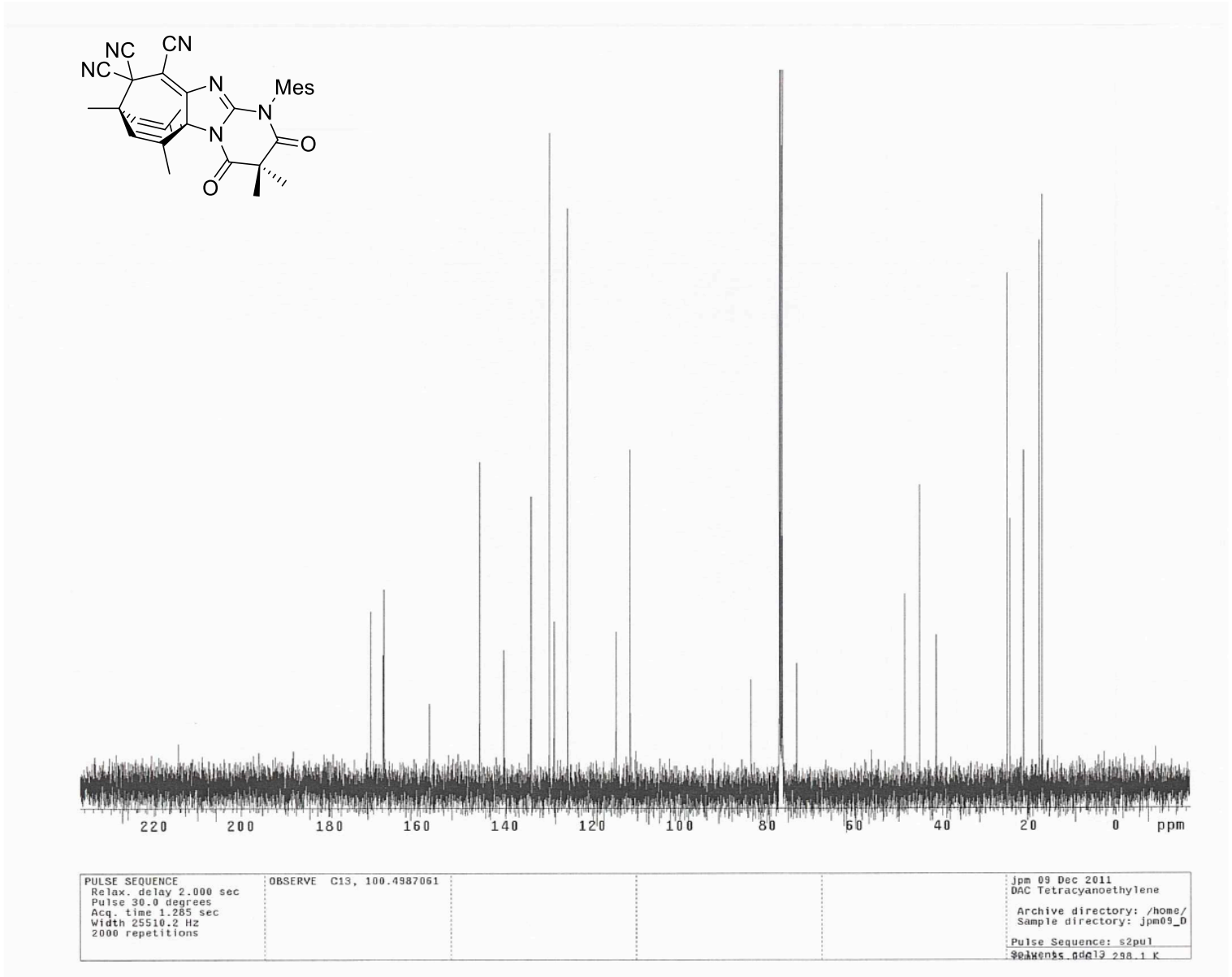

Mes
N
N
Mes
O
O
+
N
O
N
Mes
N
N
Mes
O
O
O
220
200
180
160
140
120
100
80
60
40
20
0
ppm
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.285 sec
Width 25510.2 Hz
512 repetitions
OBSERVE C13, 100.4986812
jpm 05 Aug 2011
DAC + 4-methoxybenzonitril
Archive directory: /home/
Sample directory: jpm05_D
Pulse Sequence: s2pul
Solvent: d6
Temp. 298.1 K


Mes
N
N
Mes
O
O
+
CH3CN
Mes
N
N
Mes
O
O
7.150
6.780
6.629
6.585
2.192
2.167
2.105
2.017
2.006
1.928
1.491
0.938
0.687
12
11
10
9
8
7
6
5
4
3
2
1
-0
ppm
2.03
3.47
2.89
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 16.4 degrees
Acq. time 2.856 sec
Width 5602.2 Hz
9 repetitions
OBSERVE H1, 400.2670012
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 1 minute
jpm 10 Dec 2011
DAC + acetonitrile
Pulse Sequence: s2pul
Solvent: Benzene
Ambient temperature
Mercury-400 "nmr6"



PULSE SEQUENCE Relax. delay 2.000 sec Pulse 36.0 degrees Acq. time 1.777 sec Width 18009.9 Hz 1296 repetitions	OBSERVE C13, 75.4700000 DECOUPLE H1, 300.1409529 Power 40 dB continuously on WALTZ-16 modulated Single precision data	DATA PROCESSING Line broadening 1.0 Hz FT size 65536 Total time 81 minutes			jpm 10 Dec 2011 DAC Acetonitrile C13 Pulse Sequence: s2pul Solvent: Benzene Ambient temperature UNITYplus-300 "nmr2"


NC
NC
CN
N
Mes
N
N
O
O
7.240
6.968
5.781
5.778
2.322
2.059
1.869
1.866
1.805
1.732
1.528
12
11
10
9
8
7
6
5
4
3
2
1
-0
ppm
2.00
2.02
2.96
5.92
2.08
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 16.4 degrees
Acq. time 2.856 sec
Width 5602.2 Hz
8 repetitions
OBSERVE H1, 400.2669866
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 1 minute
jpm 09 Dec 2011
DAC Tetracyanoethylene
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400 "nmr6"


NC
CN
NC
N
Mes
N
N
O
O
O
220
200
180
160
140
120
100
80
60
40
20
0
ppm
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.285 sec
Width 25510.2 Hz
2000 repetitions
OBSERVE C13, 100.4987061
jpm 09 Dec 2011
DAC Tetracyanoethylene
Archive directory: /home/
Sample directory: jpm09_D
Pulse Sequence: s2pul
Solvent: cdcl3 298.1 K

References

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