Efficient Nucleophilic Aromatic Substitution between Aryl Nitrofluorides and Alkynes

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General: All reactions were run under inert atmosphere using anhydrous solvents. Unless otherwise noted, materials were obtained from commercial sources and used without further purification. Reactions were followed by HPLC and TLC. The purity of each inhibitor was determined by high-performance liquid chromatography (HPLC) and was >95% unless otherwise noted. ^1H NMR and ^{13}C NMR spectra were obtained on a Bruker AMX 400 spectrometer. ^1H assignment abbreviations are the following: singlet (s), doublet (d), triplet (t), quartet (q), pentet (p), broad singlet (bs), broad multiplet (bm), broad quartet (bq), doublet of doublets (dd), doublet of triplets (dt), and multiplet (m). Electrospray mass spectrum (ES-MS) were recorded on a Micromass-Quattro-II mass spectrometer. FTIR spectra were taken on a Perkin-Elmer 241 polarimeter. Purification was performed using flash column chromatography (FCC) on silica gel (10-40 μm or 230-400 mesh, Silicycle).

Typical Procedure: A rt solution of nitro-fluoroaryl (1.0 eq) and alkyne (1.1 eq) in THF (0.3 M) was treated dropwise with sodium hexamethyldisilazane (NaHMDS, 1.0 M in THF, 1.5 eq) then stirred for 1-5h at 60°C. On completion of the reaction, the mixture was diluted with Et_2O , washed with water and brine, dried over MgSO_4 , filtered, concentrated and purified by flash chromatography using Et_2O /hexanes or EtOAc /hexanes to afford the desired product.

1-[(4-methoxyphenyl)ethynyl]-2-nitrobenzene (Table 1, entry 1): orange solid; R_f = 0.21 (20% Et_2O /hexanes); ^1H NMR (CDCl_3 , 400 MHz) δ 8.09 (d, J = 8.2 Hz, 1H), 7.71 (d, J = 7.8 Hz, 1H), 7.60 (t, J = 7.6 Hz, 1H), 7.56 (d, J = 8.6 Hz, 2H), 7.44 (t, J = 7.8 Hz, 1H), 7.92 (d, J = 8.4 Hz, 2H), 3.86 (s, 3H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 160.6, 149.6, 134.5, 133.9, 133.0, 128.2, 124.9, 119.4, 114.6, 114.3, 97.8, 84.1, 55.6; MS (EI, $\text{M}+\bullet$) 253; HRMS for $\text{C}_{15}\text{H}_{11}\text{NO}_3$ calc 253.0739, found 253.0732; FTIR 3001, 2214, 1601, 1567, 1523, 1332, 1287, 1136, 1026, 835, 684 cm^{-1} .

1-nitro-2-(phenylethynyl)benzene (Table 2, entry 1): All data are consistent with literature: Li, J.-H.; Zhang, X.-D., Xie, Y.-X. *Eur. J. Org. Chem.* **2005**, 4256.

1-[(4-methylphenyl)ethynyl]-2-nitrobenzene (Table 2, entry 2): orange solid; R_f = 0.37 (20% Et_2O /hexanes); ^1H NMR (CDCl_3 , 400 MHz) δ 8.09 (d, J = 8.2 Hz, 1H), 7.72 (d, J = 7.8 Hz, 1H), 7.60 (t, J = 7.4 Hz, 1H), 7.50 (d, J = 8.0 Hz, 2H), 7.46 (t, J = 8.2 Hz, 1H), 7.20 (d, J = 7.6 Hz, 2H), 2.39 (s, 3H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 149.5, 139.6, 134.5, 132.7, 131.9, 129.2, 128.3, 124.7, 119.3, 119.0, 97.5, 84.3, 21.6; MS (EI, $\text{M}+\bullet$) 237; HRMS for $\text{C}_{15}\text{H}_{11}\text{NO}_2$ calc 237.0790, found 237.0786; FTIR 2218, 1604, 1524, 1342, 1291, 817, 744 cm^{-1} .

1-nitro-2-[[4-(trifluoromethyl)phenyl]ethynyl]benzene (Table 2, Entry 3): yellow solid; $R_f = 0.34$ (20% Et₂O/hexanes); ¹H NMR (CDCl₃, 400 MHz) δ 8.14 (d, $J = 8.2$ Hz, 1H), 7.78 (t, $J = 8.3$ Hz, 2H), 7.73 (d, $J = 7.6$ Hz, 1H), 7.65 (t, $J = 7.6$ Hz, 1H), 7.58 (t, $J = 7.6$ Hz, 1H), 7.52 (m, 2H); ¹³C NMR (CDCl₃, 100 MHz) δ 149.2, 135.0, 134.5, 133.0, 131.6, 129.2, 129.0, 126.0, 124.7, 122.1, 120.6, 118.2, 92.6, 89.9; MS (EI, M+•) 291; HRMS for C₁₅H₈NO₂F₃ calc 291.0507, found 291.0500.

N,N-dimethyl-4-[(2-nitrophenyl)ethynyl]aniline (Table 2, entry 4): red solid; $R_f = 0.18$ (20% Et₂O/hexanes); ¹H NMR (CDCl₃, 400 MHz) δ 8.07 (d, $J = 8.2$ Hz, 1H), 7.68 (d, $J = 7.8$ Hz, 1H), 7.56 (t, $J = 7.6$ Hz, 1H), 7.49 (d, $J = 8.4$ Hz, 2H), 7.38 (t, $J = 7.8$ Hz, 1H), 6.67 (d, $J = 8.4$ Hz, 2H), 3.03 (s, 6H); ¹³C NMR (CDCl₃, 100 MHz) δ 150.7, 148.9, 134.1, 133.4, 132.6, 127.3, 124.7, 119.9, 111.6, 108.7, 99.5, 83.7, 40.1; MS (EI, M+•) 266; HRMS for C₁₆H₁₄N₂O₂ calc 266.1055, found 266.1048; FTIR 2904, 2209, 1600, 1519, 1339, 1228, 821, 740 cm⁻¹.

4-[(2-nitrophenyl)ethynyl]benzonitrile (Table 2, entry 5): yellow solid; $R_f = 0.13$ (20% Et₂O/hexanes); ¹H NMR (CDCl₃, 400 MHz) δ 8.15 (d, $J = 8.2$ Hz, 1H), 7.75 (d, $J = 7.8$ Hz, 1H), 7.69 (s, 4H), 7.66 (t, $J = 7.6$ Hz, 1H), 7.55 (t, $J = 8.0$ Hz, 1H); ¹³C NMR (CDCl₃, 100 MHz) δ 149.6, 134.7, 133.0, 132.4, 132.3, 129.5, 127.2, 124.9, 118.3, 117.7, 112.4, 94.7, 88.7; MS (EI, M+•) 248; HRMS for C₁₅H₈N₂O₂ calc 248.0586, found 248.0589; FTIR 2225, 1607, 1567, 1522, 1339, 1295, 909, 837, 743, 554 cm⁻¹.

1-[(3-methoxyphenyl)ethynyl]-2-nitrobenzene (Table 2, entry 6): orange oil; $R_f = 0.24$ (20% Et₂O/hexanes); ¹H NMR (CDCl₃, 400 MHz) δ 8.10 (d, $J = 8.2$ Hz, 1H), 7.74 (d, $J = 7.8$ Hz, 1H), 7.62 (t, $J = 7.6$ Hz, 1H), 7.48 (t, $J = 8.1$ Hz, 1H), 7.30 (t, $J = 8.2$ Hz, 1H), 7.21 (d, $J = 7.4$ Hz, 1H), 7.12 (s, 1H), 6.96 (d, $J = 8.2$ Hz, 1H), 3.85 (s, 3H); ¹³C NMR (CDCl₃, 100 MHz) δ 159.4, 149.6, 134.6, 132.8, 129.5, 128.6, 124.7, 124.6, 123.3, 118.7, 116.5, 116.0, 97.0, 84.5, 55.3; MS (EI, M+•) 253; HRMS for C₁₅H₁₁NO₃ calc 253.0379, found 253.0732; FTIR 2210, 1608, 1573, 1524, 1491, 1342, 1226, 1043, 783, 744, 685 cm⁻¹.

1-methoxy-2-[(2-nitrophenyl)ethynyl]benzene (Table 2, entry 7): yellow solid; $R_f = 0.19$ (20% Et₂O/hexanes); ¹H NMR (CDCl₃, 400

MHz) δ 8.10 (d, J = 8.2 Hz, 1H), 7.77 (d, J = 7.6 Hz, 1H), 7.59 (m, 2H), 7.46 (t, J = 8.2 Hz, 1H), 7.37 (t, J = 7.6 Hz, 1H), 6.98 (t, J = 7.4 Hz, 1H), 6.94, (d, J = 7.4 Hz, 1H), 3.96 (s, 3H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 160.4, 149.3, 134.7, 134.0, 132.7, 130.8, 128.3, 124.6, 120.5, 119.1, 111.6, 110.8, 93.9, 88.7, 55.9; MS (EI, $\text{M}^+\bullet$) 253; HRMS for $\text{C}_{15}\text{H}_{11}\text{NO}_3$ calc 253.0739, found 253.0732; FTIR 2215, 1607, 1565, 1517, 1461, 1338, 1250, 1022, 746 cm^{-1} .

1-bromo-2-[(2-nitrophenyl)ethynyl]benzene (Table 2, entry 8): yellow solid; R_f = 0.32 (10% EtOAc/hexanes); ^1H NMR (CDCl_3 , 400 MHz) δ 8.11 (d, J = 7.4 Hz, 1H), 7.80 (dd, J = 7.6, 1.2 Hz, 1H), 7.62 (m, 3H), 7.50 (dt, J = 7.8, 1.4 Hz, 1H), 7.34 (dt, J = 7.5, 0.8 Hz, 1H), 7.24 (dt J = 7.8, 1.8, 1H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 149.2, 134.9, 134.0, 132.9, 132.5, 130.3, 128.9, 127.1, 125.7, 124.7, 124.6, 118.4, 95.4, 88.9; MS (EI, $\text{M}^+\bullet$) 301; HRMS for $\text{C}_{14}\text{H}_8\text{NO}_2\text{Br}$ calc 300.9738, found 300.9744.

1-[(3-bromophenyl)ethynyl]-2-nitrobenzene (Table 2, entry 9): yellow solid; R_f = 0.25 (20% Et₂O/hexanes); ^1H NMR (CDCl_3 , 400 MHz) δ 8.12 (d, J = 8.3 Hz, 1H), 7.74 (m, 2H), 7.64 (t, J = 7.6 Hz, 1H), 7.53 (m, 3H), 7.27 (m, 1H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 149.6, 134.59, 134.57, 132.9, 132.3, 130.5, 129.9, 128.9, 124.8, 124.3, 122.2, 118.2, 95.2, 85.9; MS (EI, $\text{M}^+\bullet$) 301, 303; HRMS for $\text{C}_{14}\text{H}_8\text{NO}_2\text{Br}$ calc 300.9738, found 300.9744; FTIR 2223, 1608, 1524, 1343, 881, 782, 743, 678 cm^{-1} .

3-[(2-nitrophenyl)ethynyl]pyridine (Table 2, entry 10): yellow solid; R_f = 0.13 (50% Et₂O/hexanes); ^1H NMR (CDCl_3 , 400 MHz) δ 8.84 (s, 1H), 8.62 (dd, J = 4.9, 1.8 Hz, 1H), 8.14 (d, J = 8.2 Hz, 1H), 7.89 (m, 1H), 7.74 (d, J = 7.6 Hz, 1H), 7.65 (t, J = 7.65 Hz, 1H), 7.53 (m, 1H), 7.33 (m, 1H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 152.4, 149.5, 149.4, 138.8, 134.6, 133.0, 129.1, 124.8, 123.1, 119.6, 118.0, 93.3, 87.8; MS (EI, $\text{M}^+\bullet$) 224; HRMS for $\text{C}_{13}\text{H}_8\text{NO}_2$ calc 224.0586, found 224.0591; FTIR 2222, 1520, 1484, 1340, 788, 744, 700 cm^{-1} .

2-[(2-nitrophenyl)ethynyl]thiophene (Table 2, entry 11): red oil; R_f = 0.29 (20% EtOAc/hexanes); ^1H NMR (CDCl_3 , 400 MHz) δ 8.12 (d, J = 8.2 Hz, 1H), 7.71 (d, J = 6.8 Hz, 1H), 7.62 (t, J = 7.6 Hz, 1H), 7.47 (t, J = 8.2 Hz, 1H), 7.41 (m, 2H), 7.07 (dd, J = 5.1, 3.9 Hz, 1H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 148.9, 134.2, 133.4, 132.9, 128.9, 128.5, 127.3, 124.8, 122.2, 118.5, 90.5, 88.8; MS (EI, $\text{M}^+\bullet$) 229; HRMS for $\text{C}_{12}\text{H}_7\text{NO}_2\text{S}$ calc 229.0197, found 229.0202; FTIR 3106, 2203, 1607, 1524, 1342, 1216, 852, 743, 706 cm^{-1} .

1-nitro-2-(4-phenylbut-1-yn-1-yl)benzene (Table 2, entry 12): red oil; $R_f = 0.24$ (20% Et₂O/hexanes); ¹H NMR (CDCl₃, 400 MHz) δ 7.95 (d, $J = 8.0$ Hz, 1H), 7.49 (m, 2H), 7.37 (m, 1H), 7.32–7.19 (m, 5H), 2.94 (t, $J = 7.5$ Hz, 2H), 2.76 (t, $J = 7.5$ Hz, 2H); ¹³C NMR (CDCl₃, 100 MHz) δ 150.0, 140.3, 134.8, 132.5, 128.5, 128.4, 128.0, 126.4, 124.4, 119.1, 98.3, 76.6, 34.6, 22.0; MS (EI, M⁺•) 251; HRMS for C₁₆H₁₃NO₂ calc 251.0946, found 251.0950; FTIR 2929, 2229, 1607, 1526, 1344, 849, 784, 745, 699 cm⁻¹.

N-benzyl-N-methyl-3-(2-nitrophenyl)prop-2-yn-1-amine (Table 2, entry 13): red oil; $R_f = 0.17$ (20% EtOAc/hexanes); ¹H NMR (CDCl₃, 400 MHz) δ 8.05 (d, $J = 8.2$ Hz, 1H), 7.66 (d, $J = 7.4$ Hz, 1H), 7.58 (t, $J = 7.6$ Hz, 1H), 7.46 (t, $J = 7.8$ Hz, 1H), 7.35 (m, 5H), 3.70 (s, 2H), 3.60 (s, 2H), 2.46 (s, 3H); ¹³C NMR (CDCl₃, 100 MHz) δ 149.8, 138.3, 134.9, 132.7, 129.2, 128.4, 128.3, 127.2, 124.4, 118.5, 93.4, 80.9, 60.0, 45.7, 42.0; MS (EI, M⁺•) 280; HRMS for C₁₇H₁₆N₂O₂ calc 280.1212, found 280.1207; FTIR 2794, 1608, 1526, 1344, 1026, 852, 743, 699 cm⁻¹.

1-(cyclohexylethynyl)-2-nitrobenzene (Table 2, entry 14): yellow oil; $R_f = 0.42$ (20% Et₂O/hexanes); ¹H NMR (CDCl₃, 400 MHz) δ 7.98 (d, $J = 8.2$ Hz, 1H), 7.59 (m, 1H), 7.52 (t, $J = 7.5$ Hz, 1H), 7.39 (t, $J = 7.39$ Hz, 1H), 2.69 (m, 1H), 1.89 (m, 2H), 1.78 (m, 2H), 1.62 (m, 2H), 1.54 (m, 1H), 1.39 (m, 3H); ¹³C NMR (CDCl₃, 100 MHz) δ 150.1, 134.7, 132.4, 127.7, 124.3, 119.4, 103.2, 76.0, 32.1, 29.9, 25.8, 24.6; MS (EI, M⁺•) 229; HRMS for C₁₄H₁₅NO₂ calc 229.1103, found 229.1098; FTIR 2931, 2855, 2230, 1607, 1526, 1449, 1346, 856, 783, 745 cm⁻¹.

1-(cyclopropylethynyl)-2-nitrobenzene (Table 2, entry 15): yellow oil; $R_f = 0.35$ (20% Et₂O/hexanes); ¹H NMR (CDCl₃, 400 MHz) δ 7.98 (d, $J = 8.0$ Hz, 1H), 7.55 (dt, $J = 7.6, 1.4$ Hz, 1H), 7.51 (dt, $J = 8.0, 1.0$ Hz, 1H), 7.38 (dt, $J = 8.4, 1.6$ Hz, 1H), 1.55 (m, 1H), 0.94 (m, 4H); ¹³C NMR (CDCl₃, 100 MHz) δ 149.9, 134.6, 132.5, 127.6, 124.4, 119.4, 102.7, 9.1, 0.6; MS (EI, M⁺•) 187; HRMS for C₁₁H₉NO₂ calc 187.0633, found 187.0624; FTIR 2231, 1607, 1525, 1344, 955, 858, 745 cm⁻¹.

Triethyl-(2-nitro-phenylethynyl)-silane (Table 2, entry 16): yellow oil; $R_f = 0.38$ (20% Et₂O/hexanes); ¹H NMR (CDCl₃, 400 MHz) δ 8.02 (d, $J = 8.2$ Hz, 1H), 7.68 (d, $J = 7.6$ Hz, 1H), 7.56 (t, $J = 7.6$ Hz, 1H), 7.45 (t, $J = 7.8$ Hz, 1H), 1.07 (t, $J = 7.8$ Hz, 9H), 0.72 (q, $J = 7.8$ Hz, 6H); ¹³C NMR (CDCl₃, 100 MHz) δ 150.1, 153.3, 132.6, 128.7, 124.4, 118.5, 101.6, 100.4, 7.4, 4.2; MS (ESI, Pos) 262.1; MS (EI, M⁺•) 261; HRMS for C₁₄H₁₉NO₂Si calc 261.1185, found 261.1180; FTIR 2956, 2912, 2876, 1606, 1530, 1346, 1008, 865, 820, 727 cm⁻¹.

1-bromo-2-[(4-methoxyphenyl)ethynyl]-3-nitrobenzene (Table 3, entry 1): orange solid; R_f = 0.17 (20% Et₂O/hexanes); ¹H NMR (CDCl₃, 400 MHz) δ 7.98 (d, J = 8.2 Hz, 1H), 7.90 (d, J = 8.0 Hz, 1H), 7.60 (d, J = 8.8 Hz, 2H), 7.28 (t, J = 8.1 Hz, 1H), 6.93 (d, J = 8.8 Hz, 2), 3.86 (s, 3H); ¹³C NMR (CDCl₃, 100 MHz) δ 160.8, 150.8, 136.7, 133.8, 128.0, 127.9, 123.4, 120.9, 114.2, 114.1, 103.3, 82.9, 55.4; MS (EI, M+•) 331; HRMS for C₁₅H₁₀NO₃Br calc 330.9844, found 330.9838; FTIR 2213, 1589, 1510, 1247, 1145, 825, 740 cm⁻¹.

2-[(4-methoxyphenyl)ethynyl]-1-methyl-3-nitrobenzene (Table 3, entry 2): orange solid; R_f = 0.19 (10% EtOAc/hexanes); ¹H NMR (CDCl₃, 400 MHz) δ 7.86 (d, J = 8.0 Hz, 1H), 7.55 (d, J = 8.6 Hz, 2H), 7.50 (d, J = 7.7 Hz, 1H), 7.31 (t, J = 8.0 Hz, 1H), 6.91 (d, J = 8.6 Hz, 2H), 3.86 (s, 3H), 2.62 (s, 3H); ¹³C NMR (CDCl₃, 100 MHz) δ 160.4, 150.2, 142.8, 133.7, 133.5, 127.2, 122.0, 118.5, 114.6, 114.1, 102.2, 82.2, 55.3, 21.3; MS (EI, M+•) 267; HRMS for C₁₆H₁₃NO₃ calc 267.0895, found 267.0888; FTIR 2837, 2209, 1600, 1524, 1510, 1336, 1287, 1251, 1165, 1030, 828, 802, 748 cm⁻¹.

1-[(4-methoxyphenyl)ethynyl]-2-nitro-4-(trifluoromethyl)benzene (Table 3, entry 3): orange solid; R_f = 0.24 (10% EtOAc/hexanes); ¹H NMR (CDCl₃, 400 MHz) δ 8.36 (s, 1H), 7.83 (s, 2H), 7.58 (d, J = 8.8 Hz, 2H), 6.93 (d, J = 8.8 Hz, 2H), 3.87 (s, 3H); ¹³C NMR (CDCl₃, 100 MHz) δ 160.9, 149.0, 135.0, 134.0, 129.17, 122.2, 122.1, 114.2, 113.6, 101.1, 83.3, 55.4; MS (EI, M+•) 321; HRMS for C₁₆H₁₀NO₃F₃ calc 321.0613, found 321.0609; FTIR (neat) 2210, 1605, 1536, 1326, 1250, 1121, 1090, 829 cm⁻¹.

4-[(4-bromo-2-nitrophenyl)ethynyl]phenyl methyl ether (Table 3, entry 4): orange solid; R_f = 0.26 (20% Et₂O/hexanes); ¹H NMR (CDCl₃, 400 MHz) δ 8.24 (d, J = 2.0 Hz, 1H), 7.72 (dd, J = 8.3, 2.0 Hz, 1H), 7.56 (d, J = 8.3 Hz, 1H), 7.55 (d, J = 8.8 Hz, 2H), 6.91 (d, J = 8.8 Hz, 2H), 3.86 (s, 3H); ¹³C NMR (CDCl₃, 100 MHz) δ 160.6, 149.5, 135.9, 135.3, 133.7, 127.8, 121.2, 118.2, 114.2, 114.1, 99.0, 83.2, 55.3; MS (EI, M+•) 331, 333; HRMS for C₁₅H₁₁NO₂ calc 330.9844, found 330.9838; FTIR 2967, 2216, 1603, 1549, 1517, 1340, 1249, 1140, 1031, 827 cm⁻¹.

1-chloro-3-[(4-methoxyphenyl)ethynyl]-2-nitrobenzene (Table 3, entry 5): off-white solid; R_f = 0.17 (20% Et₂O/hexanes); ¹H

NMR (CDCl₃, 400 MHz) δ 7.53 (dd, J = 7.4, 1.0 Hz, 1H), 7.46 (d, J = 8.6 Hz, 2H), 7.42 (m, 2H), 6.89 (d, J = 8.8 Hz, 1H), 3.85 (s, 3H); ¹³C NMR (CDCl₃, 100 MHz) δ 160.6, 133.6, 130.9, 130.6, 129.6, 125.3, 118.8, 114.1, 113.4, 97.4, 80.5, 55.3; MS (EI, M+•) 287; HRMS for C₁₅H₁₀NO₃Cl calc 287.0349, found 287.0345; FTIR 2958, 2836, 2232, 2203, 1602, 1590, 1543, 1508, 1371, 1292, 1251, 1165, 1029, 831, 792 cm⁻¹.

MBL-4077-0139PA1

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File Name	1LAVFS01Nmrdata\Dalamiaperle\1nmr\MBL-4077-0139PA1	010001r		Frequency (MHz)	400.13
Nucleus	1H	Number of Transients	128	Original Points Count	32768
Owner	chemistry	Points Count	32768	Receiver Gain	1448.20
SW(cyclical) (Hz)	6410.26	Pulse Sequence	zgpg0	Spectrum Offset (Hz)	2661.5767
Sweep Width (Hz)	6410.06	Solvent	CHLOROFORM-d		

05/18/2006 09:54

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[3.78 .. 3.93]	3.000	3.18835e+9	3.000
2	[6.85 .. 6.96]	1.880	1.99849e+9	1.880
3	[7.40 .. 7.49]	0.927	9.85276e+8	0.927
4	[7.51 .. 7.64]	2.810	2.98676e+9	2.810
5	[7.66 .. 7.74]	0.951	1.01079e+9	0.951
6	[8.04 .. 8.13]	0.840	8.92617e+8	0.840

No.	Annotation	(ppm)
1	CHLOROFORM-d	7.27

No.	(ppm)	Height	(Hz)
1	3.86	1543.1	0.5073
2	6.90	2762.6	0.1274
3	6.93	2771.0	0.1474
4	7.27	2908.9	0.4650
5	7.43	2971.2	0.0323
6	7.44	2978.8	0.0674
7	7.46	2986.6	0.0429
8	7.55	3019.1	0.1315

Jan 18 mai 2006

MBL-4077-0139
Exploratoire
CDCl₃ 1D proton
3913-140 10/1
23 May 2006

MBL-4077-0158PA1

06/01/2006 10:07

Acquisition Time (sec)	5.1120	Comment	1Dproton CDC13 D: mlaperle 12	Date	01 Jun 2006 13:56:16
File Name	\\LAVFS01\Nmrdata\Data\mlaperle\Nmr\MBL-4077-0158PA1_010001r			Frequency (MHz)	400.13
Nucleus	¹ H	Number of Transients	16	Original Points Count	32768
Owner	chemistry	Points Count	32768	Receiver Gain	1448.20
SW(cyclical) (Hz)	6410.26	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2467.1252
Sweep Width (Hz)	6410.06

No.	(ppm)	Height	(Hz)	No.	Annotation	(ppm)
1	7.27	0.4910	2908.9	1	CHLOROFORM-d	7.27

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[2.34 .. 2.46]	3.000	3.16559e+9	3.000
2	[7.16 .. 7.24]	1.918	2.02363e+9	1.918
3	[7.42 .. 7.55]	2.810	2.96499e+9	2.810
4	[7.57 .. 7.65]	0.967	1.02087e+9	0.967
5	[7.68 .. 7.77]	0.925	9.76480e+8	0.925
6	[8.04 .. 8.14]	0.862	9.09244e+8	0.862

16 Jun 2006.

MBL-4077-0158PA1

06/05/2006 10:02

Acquisition Time (sec)	1.3566	Comment	1Dcarbon CDCl3 D: mlaperle 22	Date	03 Jun 2006 00:44:48
File Name	\\LAVFS01\Nmr\data\mlaperle\NMR-4077-0158PA1_030001r			Frequency (MHz)	100.61
Nucleus	13C	Number of Transients	5120	Original Points Count	32768
Owner	chemistry	Points Count	32768	Receiver Gain	20642.50
SW(cyclical) (Hz)	24154.59	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10015.7305
Sweep Width (Hz)	24153.85

No.	Annotation	(ppm)
1	CHLOROFORM-d	77.00

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	21.59	2172.2	0.4017	9	124.67	12543.0	0.6468
2	76.68	7714.7	0.3855	10	128.25	12903.5	0.7243
3	77.00	7747.2	0.3850	11	129.20	12999.3	0.9585
4	77.32	7778.9	0.3858	12	131.91	13272.0	1.0000
5	84.25	8477.0	0.1161	13	132.74	13355.3	0.5739
6	97.50	9809.7	0.1068	14	134.46	13528.6	0.6283
7	118.97	11969.5	0.0890	15	139.56	14041.6	0.1675
8	119.27	12000.5	0.1165	16	149.48	15039.7	0.0392

MBL-4077-0168PA1

06/09/2006 16:26

Acquisition Time (sec)	5.1120	Comment	1Dproton CDCl3 D: mlapierte 62	Date	09 Jun 2006 17:29:36
File Name	\\LAVF5011\Nmrdata\Datam\apierte\hnm\MBL-4077-0168PA1_0300001r			Frequency (MHz)	400.13
Nucleus	¹ H	Number of Transients	16	Original Points Count	32768
Owner	chemistry	Points Count	32768	Receiver Gain	1290.20
SW(cyclical) (Hz)	6410.26	Pulse Sequence	zgpg	Spectrum Offset (Hz)	2661.3811
Sweep Width (Hz)	6410.06	Solvent	CHLOROFORM-d

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[7.45 .. 7.62]	3.334	9.11452e+9	3.334
2	[7.62 .. 7.69]	1.141	3.12008e+9	1.141
3	[7.69 .. 7.84]	3.235	8.84370e+9	3.235
4	[8.10 .. 8.19]	1.000	2.73486e+9	1.000

No.	Annotation	(ppm)
1	CHLOROFORM-d	7.27

No.	(ppm)	Hz	Height
1	7.27	2908.9	0.5000
2	7.48	2991.9	0.0438
3	7.50	2999.7	0.1163
4	7.52	3007.1	0.1041
5	7.52	3010.9	0.1347
6	7.55	3019.3	0.0780
7	7.56	3026.1	0.0743
8	7.58	3033.8	0.1209
9	7.60	3041.2	0.0569
10	7.63	3054.1	0.0664

APu 12 jun 2006

MBL-4077-0168PA1

06/09/2006 08:49

Acquisition Time (sec)	1.3566	Comment	13Carbon CDC13 D: mlaperte 41	Date	09 Jun 2006 11:24:48
File Name	\\LAVFS01\Nmr\data\mlaperte\mbl-4077-0168PA1_020001r			Frequency (MHz)	100.61
Nucleus	13C	Number of Transients	2364	Original Points Count	32768
Owner	chemistry	Points Count	32768	Receiver Gain	20642.50
SW(cyclical) (Hz)	24154.59	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10067.3262
Sweep Width (Hz)	24153.85				

VerticalScaleFactor = 1

No.	Annotation	(ppm)
1	CHLOROFORM-d	77.00

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	77.00	7747.2	0.7007	10	125.90	12667.6	0.3100
2	89.87	9042.3	0.0945	11	125.95	12672.0	0.3218
3	92.63	9320.2	0.1189	12	126.00	12677.2	0.1336
4	118.23	11895.8	0.1087	13	128.94	12972.8	0.9668
5	120.56	12130.2	0.0626	14	129.15	12994.1	1.0000
6	122.10	12285.0	0.0630	15	131.56	13236.7	0.6031
7	124.74	12550.4	0.8496	16	133.00	13381.9	0.8281
8	124.81	12557.8	0.1041	17	134.45	13527.8	0.8353
9	125.85	12662.4	0.1266	18	134.99	13581.6	0.7943

1/b 9 juin 2006.

MBL-4077-0171PA1

06/09/2006 16:33

Acquisition Time (sec)	5.1120	Comment	1Dproton CDCl3 D: mlaperle 73	Date	09 Jun 2006 19:39:44
File Name	\\LAVFS01\Nmrdata\Datam\mlaperle\mbl-4077-0171PA1_010001r			Frequency (MHz)	400.13
Nucleus	1H	Number of Transients	16	Original Points Count	32768
Owner	chemistry	Points Count	32768	Receiver Gain	1149.40
SW(cyclical) (Hz)	6410.26	Pulse Sequence	zgpg0	Spectrum Offset (Hz)	2659.4250
Sweep Width (Hz)	6410.06	Solvent	CHLOROFORM-d

No.	(ppm)	Height	(Hz)	No.	(ppm)	Height	(Hz)
1	3.03	1211.9	1.0000	9	7.50	3001.1	0.1388
2	6.66	2666.8	0.1335	10	7.54	3017.7	0.0385
3	6.69	2675.2	0.1536	11	7.56	3025.5	0.0776
4	7.27	2908.9	0.3579	12	7.58	3033.0	0.0439
5	7.37	2947.1	0.0338	13	7.67	3068.4	0.0841
6	7.38	2954.9	0.0703	14	7.69	3076.2	0.0614
7	7.40	2962.5	0.0447	15	8.06	3226.1	0.0706
8	7.48	2992.7	0.1307	16	8.08	3234.3	0.0669

No.	Annotation	(ppm)
1	CHLOROFORM-d	7.27

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[2.97 .. 3.08]	6.000	7.10885e+9	6.000
2	[6.60 .. 6.72]	2.051	2.43008e+9	2.051
3	[7.34 .. 7.43]	0.996	1.17959e+9	0.996
4	[7.45 .. 7.52]	1.902	2.25406e+9	1.902
5	[7.53 .. 7.61]	1.021	1.20992e+9	1.021
6	[7.63 .. 7.72]	0.956	1.13254e+9	0.956
7	[8.02 .. 8.11]	0.883	1.04663e+9	0.883

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MBL-4077-0171PA1

06/12/2006 09:57

Acquisition Time (sec)	1.3566	Comment	1Dcarbon CDC13 D: mlaperle 74	Date	10 Jun 2006 07:38:40
File Name	\\LAVFS01\Nmr\data\mlaperle\mbl-4077-0171PA1_020001r			Frequency (MHz)	100.61
Nucleus	13C	Number of Transients	5120	Original Points Count	32768
Owner	chemistry	Points Count	32768	Receiver Gain	20642.50
SW/cyclical (Hz)	24154.59	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10065.1152
Sweep Width (Hz)	24153.85

No.	Annotation	(ppm)
1	CHLOROFORM-d	77.00

No.	(ppm)	(Hz)	Height
1	40.07	4032.0	0.6061
2	76.68	7714.7	0.3754
3	77.00	7747.2	0.3687
4	77.32	7778.9	0.3710
5	83.72	8423.1	0.0975
6	99.54	10015.4	0.1046
7	108.73	10939.7	0.1042
8	111.61	11229.4	1.0000
9	119.85	12058.7	0.0834
10	124.66	12542.3	0.5114
11	127.27	12804.7	0.5898
12	132.64	13345.8	0.5167
13	133.39	13420.9	0.9511
14	134.07	13488.8	0.5201
15	148.92	14983.7	0.0389
16	150.66	15158.4	0.0983

MBL-4077-0143PA1

05/19/2006 16:32

Acquisition Time (sec)	5.1120	Comment	1Dproton CDCl3 D: mlaperis 64	Date	19 May 2006 19:46:08
File Name	\\LAVFS01\Nmr\data\1D\mlaperis\MBL-4077-0143PA1_010001r			Frequency (MHz)	400.13
Nucleus	¹ H	Number of Transients	16	Original Points Count	32768
Owner	chemistry	Points Count	32768	Receiver Gain	1625.50
SW(cyclical) (Hz)	6410.26	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2657.6636
Sweep Width (Hz)	6410.06

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[7.50 .. 7.60]	1.056	1.21456e+9	1.056
2	[7.62 .. 7.67]	0.867	9.97091e+8	0.867
3	[7.67 .. 7.72]	4.384	5.04217e+9	4.384
4	[7.72 .. 7.79]	1.183	1.36008e+9	1.183
5	[8.09 .. 8.19]	1.000	1.15014e+9	1.000

No.	Annotation	(ppm)
1	CHLOROFORM-d	7.27

No.	(ppm)	Height
1	7.27	2908.9
2	7.53	3014.8
3	7.55	3022.4
4	7.57	3030.4
5	7.64	3058.6
6	7.66	3066.2
7	7.69	3076.6
8	7.74	3098.3
9	7.76	3106.1
10	8.14	3255.2
11	8.16	3263.4

19 mai 2006.

MBL-4077-0143PA1

05/23/2006 14:18

Acquisition Time (sec)	1.3566	Comment	1Dcarbon CDC13 D: mlaferle 79	Date	20 May 2006 21:26:24
File Name	\\LAVFS01\Nmrdata\Data\mlaferle\Nmr\MBL-4077-0143PA1_020001r			Frequency (MHz)	100.61
Nucleus	13C	Number of Transients	5120	Origin	spect
Owner	chemistry	Points Count	32768	Pulse Sequence	zgpg60
SW(cyclical) (Hz)	24154.59	Solvent	CHLOROFORM-d	Receiver Gain	16384.00
Sweep Width (Hz)	24153.85			Spectrum Offset (Hz)	10062.9043

No.	Annotation	(ppm)
1	CHLOROFORM-d	77.00

No.	(ppm)	(Hz)	Height
1	77.00	7747.2	0.3907
2	88.63	8917.8	0.1202
3	94.67	9525.2	0.1284
4	112.40	11309.0	0.1243
5	117.66	11838.3	0.0958
6	118.29	11901.7	0.1997
7	124.90	12566.6	0.6443
8	127.19	12797.3	0.1282
9	129.49	13028.0	0.7523
10	132.10	13290.5	1.0000
11	132.28	13308.9	0.0343
12	132.42	13322.9	0.9368
13	133.03	13384.8	0.6534
14	134.67	13549.2	0.6484
15	149.62	15053.7	0.0447

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MBL-4077-0144PA1

Acquisition Time (sec)	5.1120	Comment	1Dproton CDCl3 D: mlaparte 64	Date	18 May 2006 21:09:20
File Name	ILAVFS01Nmrdata\Datamlaparte\mlm\MBL-4077-0144PA1	Origin	010001r	Frequency (MHz)	400.13
Nucleus	¹ H	Number of Transients	16	Original Points Count	32768
Owner	chemistry	Points Count	32768	Receiver Gain	1024.00
SW(cyclical) (Hz)	6410.26	Pulse Sequence	CHLOROFORM-d	Spectrum Offset (Hz)	2656.0891
Sweep Width (Hz)	6410.06				

VerticalScaleFactor = 1

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	3.85	1541.3	1.0000	11	7.46	2986.4	0.0560	1	[3.79 .. 3.93]	3.000	6.23810e+9	3.000
2	6.95	2781.8	0.0838	12	7.48	2994.0	0.1200	2	[6.92 .. 7.01]	0.922	1.91754e+9	0.922
3	6.97	2790.0	0.0932	13	7.50	3002.1	0.0764	3	[7.09 .. 7.16]	0.900	1.87076e+9	0.900
4	7.12	2850.6	0.1655	14	7.60	3040.6	0.0684	4	[7.17 .. 7.25]	0.953	1.98161e+9	0.953
5	7.20	2881.4	0.0954	15	7.62	3048.2	0.1354	5	[7.29 .. 7.34]	0.711	1.47815e+9	0.711
6	7.22	2888.8	0.1461	16	7.64	3055.7	0.0728	6	[7.44 .. 7.52]	0.941	1.95731e+9	0.941
7	7.27	2908.9	0.3810	17	7.73	3091.9	0.1431	7	[7.58 .. 7.66]	0.954	1.98371e+9	0.954
8	7.28	2912.3	0.1354	18	7.75	3099.7	0.1047	8	[7.69 .. 7.78]	0.925	1.92391e+9	0.925
9	7.30	2920.5	0.1487	19	8.09	3238.0	0.1254	9	[8.05 .. 8.15]	0.864	1.79756e+9	0.864
10	7.32	2928.3	0.0645	20	8.11	3246.2	0.1177					

19 mai 2006.

MBL-4077-0144PA1

05/23/2006 14:20

Acquisition Time (sec)	1.3566	Comment	1Dcarbon CDCl3 D: mlaperle 68	Date	20 May 2006 18:35:44
File Name	\\LAVFS01\Nmrdata\Datam\laperle\m\MBL-4077-0144PA1_020001r	Origin	spect	Frequency (MHz)	100.61
Nucleus	13C	Number of Transients	5120	Original Points Count	32768
Owner	chemistry	Points Count	32768	Receiver Gain	20642.50
SW(cyclical) (Hz)	24154.59	Pulse Sequence	zgpg60	Spectrum Offset (Hz)	10064.3779
Sweep Width (Hz)	24153.85	Solvent	CHLOROFORM-d		

VerticalScaleFactor = 1

No.	(ppm)	Height
1	55.32	0.8509
2	76.68	0.5396
3	77.00	0.5561
4	77.20	0.0441
5	77.32	0.5427
6	84.51	0.1501
7	97.01	0.1502
8	115.99	1.0000
9	116.48	0.7468
10	118.67	1.1939.3

No.	(ppm)	Height
11	123.30	0.1748
12	124.57	0.8664
13	124.71	0.8563
14	128.55	0.9524
15	129.50	0.8444
16	132.81	0.7937
17	134.59	0.8328
18	149.55	0.0486
19	159.35	0.1560

No.	Annotation	(ppm)
1	CHLOROFORM-d	77.00

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[54.86 .. 55.54]	0.071	2.30238e+9	0.071
2	[75.86 .. 78.06]	0.222	7.24650e+9	0.222
3	[84.33 .. 84.70]	0.012	3.78114e+8	0.012
4	[96.82 .. 97.19]	0.013	4.10994e+8	0.013
5	[115.63 .. 117.01]	0.166	5.41577e+9	0.166
6	[118.49 .. 118.87]	0.009	2.99073e+8	0.009
7	[123.08 .. 123.53]	0.014	4.64375e+8	0.014

No.	(ppm)
8	[124.20 .. 125.40]
9	[128.07 .. 129.05]
10	[129.19 .. 130.07]
11	[132.49 .. 133.33]
12	[134.29 .. 135.35]
13	[149.34 .. 149.80]
14	[159.17 .. 159.66]

Bu 23 mai 2006.

MBL-4077-0145PA1

Acquisition Time (sec) 5.1120		Comment		Date	
File Name	\\LAVFS01\Nmd\al\Data\lapier\hnm\MBL-4077-0145PA1	1Dproton CDC13 D: mlapierle 65		19 May 2006 19:50:24	
Nucleus	¹ H	Number of Transients	16	Frequency (MHz)	400.13
Owner	chemistry	Points Count	32768	Original Points Count	32768
SW(cyclical) (Hz)	6410.26	Solvent	CHLOROFORM-d	Receiver Gain	1625.50
Sweep Width (Hz)	6410.06	Pulse Sequence	zgpg0	Spectrum Offset (Hz)	2654.9253

05/19/2006 16:35

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[3.90 .. 4.01]	3.000	2.76316e+9	3.000
2	[6.89 .. 7.03]	1.911	1.76022e+9	1.911
3	[7.33 .. 7.41]	0.983	9.05793e+8	0.983
4	[7.41 .. 7.51]	0.966	8.89814e+8	0.966
5	[7.51 .. 7.65]	1.903	1.76309e+9	1.903
6	[7.70 .. 7.82]	0.932	8.58747e+8	0.932
7	[8.04 .. 8.15]	0.849	7.81911e+8	0.849

No.	Annotation	(ppm)
1	CHLOROFORM-d	7.27

No.	(ppm)	Height	(Hz)
1	3.96	1584.2	0.3528
2	6.93	2771.0	0.0469
3	6.95	2779.4	0.0524
4	6.96	2783.9	0.0276
5	6.98	2792.0	0.0496
6	7.00	2799.4	0.0275
7	7.27	2908.9	0.4727
8	7.35	2942.6	0.0256
9	7.37	2950.2	0.0424
10	7.39	2957.1	0.0195
11	7.39	2958.4	0.0219
12	7.44	2976.6	0.0205
13	7.46	2984.1	0.0433
14	7.48	2992.3	0.0279
15	7.57	3027.9	0.0447
16	7.59	3035.1	0.0626
17	7.60	3042.4	0.0479
18	7.62	3049.8	0.0244
19	7.76	3104.8	0.0485
20	7.78	3112.4	0.0391
21	8.09	3236.6	0.0429
22	8.11	3244.8	0.0407

16h 23 mai 2006

05/26/2006 08:32

Acquisition Time (sec)	Comment	Date
File Name 13C	1Dcarbon CDCIS D: mlaperfe 65 \\LAVFS01\Nmr\data\Data\mlaperfe\nmr\MBL-4077-0145PA1_030001r	24 May 2006 05:49:52
Nucleus	Number of Transients 5120 Origin spect	Frequency (MHz) 100.61
Owner	Points Count Pulse Sequence	Original Points Count 32768
SW/cyclical (Hz)	Solvent CHLOROFORM-d	Receiver Gain 18390.40
Sweep Width (Hz)		Spectrum Offset (Hz) 10056.2695

VerticalScaleFactor = 1

No.	Annotation	(ppm)
1	CHLOROFORM-d	77.00

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	55.88	5622.0	0.8222	11	120.52	12125.8	0.8351
2	76.68	7715.5	0.5117	12	124.62	12538.6	0.8371
3	77.00	7747.2	0.5224	13	128.27	12905.7	1.0000
4	77.21	7767.8	0.4057	14	130.82	13162.2	0.9931
5	77.32	7778.9	0.5026	15	132.70	13365.9	0.8325
6	88.72	8925.9	0.1329	16	133.67	13449.0	0.0266
7	93.92	9450.0	0.1315	17	133.97	13479.2	0.8750
8	110.75	11143.2	0.8276	18	134.69	13551.4	0.8429
9	111.61	11229.4	0.1123	19	149.29	15020.5	0.5556
10	119.10	11982.8	0.1155	20	160.42	16143.3	0.1388

Ab 26 mai 2006.

SS-4084-0674PA1

Acquisition Time (sec)	2.5559	Comment	1Dproton CDCl3 D: ssurpren 51	Date	12 Mar 2007 18:33:36	03/13/2007 1:42:08 PM
Date Stamp	12 Mar 2007 18:33:36	Nucleus	1H	File Name	\\navs01.am.boehringer.com\Nmrdata\Data\ssurpren\Nmr\SS-4084-0674PA1_011001r	
Frequency (MHz)	400.13	Owner	chemistry	Number of Transients	16	
Original Points Count	16384	SW(cyclical) (Hz)	6410.26	Points Count	32768	spec
Receiver Gain	1448.20	Sweep Width (Hz)	6410.06	Solvent	CHLOROFORM-d	zg60
Spectrum Offset (Hz)	2465.5598					

1.5 SS-4084-0674PA1_011001r VerticalScaleFactor = 1

*See last
13 mhrs 2007*

No.	(ppm)	Value	Absolute Value	Non-Negative Value	No.	(ppm)	Height	(Hz)	No.	(ppm)	Height	(Hz)
1	7.20	7.30	3.294	3.294	1	7.23	2892.7	0.0645	11	7.53	3014.6	0.0960
2	7.30	7.38	1.184	1.184	2	7.23	2894.1	0.0748	12	7.62	3050.4	0.1271
3	7.48	7.55	1.140	1.140	3	7.25	2901.9	0.1854	13	7.64	3057.0	0.3729
4	7.59	7.69	3.284	3.284	4	7.27	2908.9	1.0000	14	7.66	3064.5	0.2903
5	7.77	7.85	1.093	1.093	5	7.33	2931.1	0.1088	15	7.81	3123.5	0.1671
6	8.08	8.17	1.000	1.000	6	7.34	2938.5	0.1689	16	7.82	3130.4	0.1296
					7	7.36	2946.1	0.0781	17	7.83	3131.4	0.1317
					8	7.49	2998.9	0.0803	18	8.12	3247.6	0.1547
					9	7.51	3006.2	0.1508	19	8.14	3255.8	0.1397
					10	7.53	3013.2	0.0949				

SS-4084-0674PA1

Acquisition Time (sec)	0.6783	Comment	13Carbon CDC13 D: ssurpren 80	Date	12 Mar 2007 22:36:48	03/13/2007 12:00:34 PM
Date Stamp	12 Mar 2007 22:36:48	Nucleus	13C	File Name	\\lavs01.am.boehringer.com\Nmrdata\Dat\ssurpren\m1SS-4084-0674PA1_0200001r	
Frequency (MHz)	100.61	Owner	chemistry	Number of Transients	640	spec
Original Points Count	16384	SW(cyclical) (Hz)	24154.59	Points Count	32768	zgpg60
Receiver Gain	16384.00	Sweep Width (Hz)	24153.85	Solvent	CHLOROFORM-d	
Spectrum Offset (Hz)	10015.7275	VerticalScaleFactor	= 1	Pulse Sequence		

See Post
13 mvs 2007

MBL-4077-0174PA1

06/14/2006 09:02

Acquisition Time (sec)	5.1120	Comment	1Dproton CDC13 D: mlaperle 3	Date	14 Jun 2006 12:48:00
File Name	\\LAVFS01\Nmr\data\mlaperle\hnmr\MBL-4077-0174PA1	010001r		Frequency (MHz)	400.13
Nucleus	1H			Original Points Count	32768
Owner	chemistry		Origin	Receiver Gain	1290.20
SW(cyclical) (Hz)	6410.26		Pulse Sequence	Spectrum Offset (Hz)	2466.7336
Sweep Width (Hz)	6410.06		Solvent		
			CHLOROFORM-d		

VerticalScaleFactor = 1

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[7.22 .. 7.26]	0.365	3.32573e+8	0.365
2	[7.47 .. 7.59]	3.231	2.94096e+9	3.231
3	[7.59 .. 7.68]	1.172	1.06733e+9	1.172
4	[7.69 .. 7.79]	2.053	1.86920e+9	2.053
5	[8.08 .. 8.16]	1.000	9.10671e+8	1.000

No.	Annotation	(ppm)
1	CHLOROFORM-d	7.27

No.	(ppm)	Height	(Hz)	Height
1	7.24	2898.8	0.0453	0.0856
2	7.27	2908.9	0.5710	0.0489
3	7.28	2914.4	0.0854	0.0958
4	7.49	2997.6	0.0373	0.0666
5	7.51	3005.6	0.0794	0.1198
6	7.53	3012.0	0.1712	0.1090
7	7.55	3019.5	0.1291	0.0771
8	7.62	3047.4	0.0429	0.0723

JPB 17 Jun 2006

MBL-4077-0174PA1

06/15/2006 08:45

Acquisition Time (sec)	1.3566	Comment	1Dcarbon CDC13 D: mlaperte 36	Date	15 Jun 2006 00:44:48
File Name	\\LAVFS01\Nmr\data\Datamiaperte\Nmr\MBL-4077-0174PA1_0200001r			Frequency (MHz)	100.61
Nucleus	13C	Number of Transients	5120	Origin	spect
Owner	chemistry	Points Count	32768	Pulse Sequence	zgpg50
SW(cyclical) (Hz)	24154.59	Solvent	CHLOROFORM-d	Receiver Gain	16384.00
Sweep Width (Hz)	24153.85			Spectrum Offset (Hz)	10016.4678

No.	Annotation	(ppm)
1	CHLOROFORM-d	77.00

No.	(ppm)	(Hz)	Height
1	76.68	7715.5	0.5256
2	77.00	7747.2	0.5146
3	77.32	7779.6	0.5148
4	85.87	8639.1	0.1394
5	95.22	9580.4	0.1475
6	118.20	11892.9	0.1444
7	122.23	12297.5	0.1997
8	124.32	12508.4	0.1699
9	124.78	12554.8	0.8747
10	128.92	12971.3	0.9735
11	129.87	13066.4	0.8212
12	130.53	13132.7	0.7827
13	132.31	13311.8	0.9725
14	132.90	13371.6	0.8427
15	134.57	13539.6	0.9543
16	134.59	13541.8	1.0000
17	149.56	15047.8	0.0518

JPW 15 juin 2006

MBL-4077-0165PA1

Acquisition Time (sec)	5.1120	Comment	1Dproton CDC13 D: mlaperle 1	Date	06 Jun 2006 17:44:32
File Name	\\LAVFS01\Nmr\data\mlaperle\mbl-4077-0165PA1	Origin	010001r	Frequency (MHz)	400.13
Nucleus	1H	Number of Transients	16	Original Points Count	32768
Owner	chemistry	Points Count	32768	Receiver Gain	1625.50
SW(cyclical) (Hz)	6410.26	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2466.7336
Sweep Width (Hz)	6410.06				

06/06/2006 15:45

Chemical Shift (ppm)												
No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	Annotation	(ppm)		
1	7.27	2908.9	0.4987	12	7.63	3054.9	0.0233	23	7.91	3163.6	0.0371	
2	7.28	2911.3	0.2887	13	7.65	3062.5	0.0457	24	7.91	3165.4	0.0325	1
3	7.32	2930.1	0.0252	14	7.67	3069.0	0.0230	25	8.13	3251.7	0.0414	CHLOROFORM-d
4	7.34	2935.0	0.0299	15	7.67	3070.1	0.0258	26	8.15	3259.9	0.0390	
5	7.34	2937.1	0.0373	16	7.75	3101.8	0.0496	27	8.61	3444.6	0.0313	
6	7.35	2942.8	0.0296	17	7.77	3108.1	0.0311	28	8.61	3446.1	0.0411	
7	7.51	3005.0	0.0145	18	7.77	3109.5	0.0360	29	8.62	3449.3	0.0432	
8	7.51	3006.4	0.0193	19	7.88	3153.9	0.0192	30	8.62	3451.0	0.0426	
9	7.53	3013.8	0.0416	20	7.89	3155.8	0.0380	31	8.64	3453.7	0.0426	
10	7.55	3020.6	0.0239	21	7.89	3157.6	0.0346	32	8.64	3455.4	0.0426	
11	7.55	3022.0	0.0283	22	7.90	3161.7	0.0236	33	8.64	3457.1	0.0426	
12	7.55	3023.4	0.0327	23	7.91	3163.6	0.0371	34	8.64	3458.8	0.0426	
13	7.55	3024.8	0.0371	24	7.91	3165.4	0.0325	35	8.64	3460.4	0.0426	
14	7.55	3026.2	0.0414	25	8.13	3251.7	0.0414	36	8.64	3462.0	0.0426	
15	7.55	3027.6	0.0457	26	8.15	3259.9	0.0390	37	8.64	3463.6	0.0426	
16	7.55	3029.0	0.0496	27	8.61	3444.6	0.0313	38	8.64	3465.2	0.0426	
17	7.55	3030.4	0.0496	28	8.61	3446.1	0.0411	39	8.64	3466.8	0.0426	
18	7.55	3031.8	0.0496	29	8.62	3449.3	0.0432	40	8.64	3468.4	0.0426	
19	7.55	3033.2	0.0496	30	8.62	3451.0	0.0426	41	8.64	3470.0	0.0426	
20	7.55	3034.6	0.0496	31	8.64	3453.7	0.0426	42	8.64	3471.6	0.0426	
21	7.55	3036.0	0.0496	32	8.64	3455.4	0.0426	43	8.64	3473.2	0.0426	
22	7.55	3037.4	0.0496	33	8.64	3457.1	0.0426	44	8.64	3474.8	0.0426	
23	7.55	3038.8	0.0496	34	8.64	3458.8	0.0426	45	8.64	3476.4	0.0426	
24	7.55	3040.2	0.0496	35	8.64	3478.0	0.0426	46	8.64	3478.0	0.0426	
25	7.55	3041.6	0.0496	36	8.64	3479.6	0.0426	47	8.64	3480.0	0.0426	
26	7.55	3043.0	0.0496	37	8.64	3481.2	0.0426	48	8.64	3481.6	0.0426	
27	7.55	3044.4	0.0496	38	8.64	3483.2	0.0426	49	8.64	3483.6	0.0426	
28	7.55	3045.8	0.0496	39	8.64	3485.2	0.0426	50	8.64	3485.6	0.0426	
29	7.55	3047.2	0.0496	40	8.64	3487.2	0.0426	51	8.64	3487.6	0.0426	
30	7.55	3048.6	0.0496	41	8.64	3489.2	0.0426	52	8.64	3489.6	0.0426	
31	7.55	3050.0	0.0496	42	8.64	3491.2	0.0426	53	8.64	3491.6	0.0426	
32	7.55	3051.4	0.0496	43	8.64	3493.2	0.0426	54	8.64	3493.6	0.0426	
33	7.55	3052.8	0.0496	44	8.64	3495.2	0.0426	55	8.64	3495.6	0.0426	
34	7.55	3054.2	0.0496	45	8.64	3497.2	0.0426	56	8.64	3497.6	0.0426	
35	7.55	3055.6	0.0496	46	8.64	3499.2	0.0426	57	8.64	3499.6	0.0426	
36	7.55	3057.0	0.0496	47	8.64	3501.2	0.0426	58	8.64	3501.6	0.0426	
37	7.55	3058.4	0.0496	48	8.64	3503.2	0.0426	59	8.64	3503.6	0.0426	
38	7.55	3059.8	0.0496	49	8.64	3505.2	0.0426	60	8.64	3505.6	0.0426	
39	7.55	3061.2	0.0496	50	8.64	3507.2	0.0426	61	8.64	3507.6	0.0426	
40	7.55	3062.6	0.0496	51	8.64	3509.2	0.0426	62	8.64	3509.6	0.0426	
41	7.55	3064.0	0.0496	52	8.64	3511.2	0.0426	63	8.64	3511.6	0.0426	
42	7.55	3065.4	0.0496	53	8.64	3513.2	0.0426	64	8.64	3513.6	0.0426	
43	7.55	3066.8	0.0496	54	8.64	3515.2	0.0426	65	8.64	3515.6	0.0426	
44	7.55	3068.2	0.0496	55	8.64	3517.2	0.0426	66	8.64	3517.6	0.0426	
45	7.55	3069.6	0.0496	56	8.64	3519.2	0.0426	67	8.64	3519.6	0.0426	
46	7.55	3071.0	0.0496	57	8.64	3521.2	0.0426	68	8.64	3521.6	0.0426	
47	7.55	3072.4	0.0496	58	8.64	3523.2	0.0426	69	8.64	3523.6	0.0426	
48	7.55	3073.8	0.0496	59	8.64	3525.2	0.0426	70	8.64	3525.6	0.0426	
49	7.55	3075.2	0.0496	60	8.64	3527.2	0.0426	71	8.64	3527.6	0.0426	
50	7.55	3076.6	0.0496	61	8.64	3529.2	0.0426	72	8.64	3529.6	0.0426	
51	7.55	3078.0	0.0496	62	8.64	3531.2	0.0426	73	8.64	3531.6	0.0426	
52	7.55	3079.4	0.0496	63	8.64	3533.2	0.0426	74	8.64	3533.6	0.0426	
53	7.55	3080.8	0.0496	64	8.64	3535.2	0.0426	75	8.64	3535.6	0.0426	
54	7.55	3082.2	0.0496	65	8.64	3537.2	0.0426	76	8.64	3537.6	0.0426	
55	7.55	3083.6	0.0496	66	8.64	3539.2	0.0426	77	8.64	3539.6	0.0426	
56	7.55	3085.0	0.0496	67	8.64	3541.2	0.0426	78	8.64	3541.6	0.0426	
57	7.55	3086.4	0.0496	68	8.64	3543.2	0.0426	79	8.64	3543.6	0.0426	
58	7.55	3087.8	0.0496	69	8.64	3545.2	0.0426	80	8.64	3545.6	0.0426	
59	7.55	3089.2	0.0496	70	8.64	3547.2	0.0426	81	8.64	3547.6	0.0426	
60	7.55	3090.6	0.0496	71	8.64	3549.2	0.0426	82	8.64	3549.6	0.0426	
61	7.55	3092.0	0.0496	72	8.64	3551.2	0.0426	83	8.64	3551.6	0.0426	
62	7.55	3093.4	0.0496	73	8.64	3553.2	0.0426	84	8.64	3553.6	0.0426	
63	7.55	3094.8	0.0496	74	8.64	3555.2	0.0426	85	8.64	3555.6	0.0426	
64	7.55	3096.2	0.0496	75	8.64	3557.2	0.0426	86	8.64	3557.6	0.0426	
65	7.55	3097.6	0.0496	76	8.64	3559.2	0.0426	87	8.64	3559.6	0.0426	
66	7.55	3099.0	0.0496	77	8.64	3561.2	0.0426	88	8.64	3561.6	0.0426	
67	7.55	3100.4	0.0496	78	8.64	3563.2	0.0426	89	8.64	3563.6	0.0426	
68	7.55	3101.8	0.0496	79	8.64	3565.2	0.0426	90	8.64	3565.6	0.0426	
69	7.55	3103.2	0.0496	80	8.64	3567.2	0.0426	91	8.64	3567.6	0.0426	
70	7.55	3104.6	0.0496	81	8.64	3569.2	0.0426	92	8.64	3569.6	0.0426	
71	7.55	3106.0	0.0496	82	8.64	3571.2	0.0426	93	8.64	3571.6	0.0426	
72	7.55	3107.4	0.0496	83	8.64	3573.2	0.0426	94	8.64	3573.6	0.0426	
73	7.55	3108.8	0.0496	84	8.64	3575.2	0.0426	95	8.64	3575.6	0.0426	
74	7.55	3110.2	0.0496	85	8.64	3577.2	0.0426	96	8.64	3577.6	0.0426	
75	7.55	3111.6	0.0496	86	8.64	3579.2	0.0426	97	8.64	3579.6	0.0426	
76	7.55	3113.0	0.0496	87	8.64	3581.2	0.0426	98	8.64	3581.6	0.0426	
77	7.55	3114.4	0.0496	88	8.64	3583.2	0.0426	99	8.64	3583.6	0.0426	
78	7.55	3115.8	0.0496	89	8.64	3585.2	0.0426	100	8.64	3585.6	0.0426	
79	7.55	3117.2	0.0496	90	8.64	3587.2	0.0426	101	8.64	3587.6	0.0426	
80	7.55	3118.6	0.0496	91	8.64	3589.2	0.0426	102	8.64	3589.6	0.0426	
81	7.55	3120.0	0.0496	92	8.64	3591.2	0.0426	103	8.64	3591.6	0.0426	
82	7.55	3121.4	0.0496	93	8.64	3593.2	0.0426	104	8.64	3593.6	0.0426	
83	7.55	3122.8	0.0496	94	8.64	3595.2	0.0426	105	8.64	3595.6	0.0426	
84	7.55	3124.2	0.0496	95	8.64	3597.2	0.0426	106	8.64	3597.6	0.0426	
85	7.55	3125.6	0.0496	96	8.64	3599.2	0.0426	107	8.64	3599.6	0.0426	
86	7.55	3127.0	0.0496	97	8.64	3601.2	0.0426	108	8.64	3601.6	0.0426	
87	7.55	3128.4	0.0496	98	8.64	3603.2	0.0426	109	8.64	3603.6	0.0426	
88	7.55	3129.8	0.0496	99	8.64	3605.2	0.0426	110	8.64	3605.6	0.0426	
89	7.55	3131.2	0.0496	100	8.64	3607.2	0.0426	111	8.64	3607.6	0.0426	
90	7.55	3132.6	0.0496	101	8.64	3609.2	0.0426	112	8.64	3609.6	0.0426	
91	7.55	3134.0	0.0496	102	8.64	3611.2	0.0426	113	8.64	3611.6	0.0426	
92	7.55	3135.4	0.0496	103	8.64	3613.2	0.0426	114	8.64	3613.6	0.0426	
93	7.55	3136.8	0.0496	104	8.64	3615.2	0.0426	115	8.64	3615.6	0.0426	
94	7.55	3138.2	0.0496	105	8.64	3617.2	0.0426	116	8.64	3617.6	0.0426	
95	7.55	3139.6	0.0496	106	8.64	3619.2	0.0426	117	8.64	3619.6	0.0426	
96	7.55	3141.0	0.0496	107	8.64	3621.2	0.0426	118	8.64	3621.6	0.0426	
97	7.55	3142.4	0.0496	108	8.64	3623.2	0.0426	119	8.64	3623.6	0.0426	
98	7.55	3143.8	0.0496	109	8.64	3625.2	0.0426	120	8.64	3625.6	0.0426	
99	7.55	3145.2	0.0496	110	8.64	3627.2	0.0426	121	8.64	3627.6	0.0426	
100	7.55	3146.6	0.0496	111	8.64	3629.2	0.0426	122	8.64	3629.6	0.0426	
101	7.55	3148.0	0.0496	112								

Yb 7 Jun 2006

MBL-4077-0165PA1

06/08/2006 12:55

Acquisition Time (sec)	1.3566	Comment	1Dcarbon CDCl3 D: mlaperle 47	Date	08 Jun 2006 10:48:32
File Name	\\LAVFS01\Nmr\data\mlaperle\mbl-4077-0165PA1_020001r			Frequency (MHz)	100.61
Nucleus	¹³ C	Number of Transients	5120	Origin	spect
Owner	chemistry	Points Count	32768	Pulse Sequence	zgpg60
SW(cyclical) (Hz)	24154.59	Solvent	CHLOROFORM-d	Receiver Gain	20642.50
Sweep Width (Hz)	24153.85			Spectrum Offset (Hz)	10014.2559

No.	Annotation	(ppm)
1	CHLOROFORM-d	77.00

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	77.00	7747.2	0.4402	8	129.12	12991.2	0.9929
2	87.82	8835.9	0.1580	9	132.96	13377.5	0.8424
3	93.32	9389.5	0.1538	10	134.61	13543.3	0.8291
4	117.95	11867.1	0.1223	11	138.84	13969.4	0.7004
5	119.57	12030.7	0.1492	12	149.36	15027.9	1.0000
6	123.09	12384.5	0.7203	13	149.51	15042.7	0.0708
7	124.81	12557.0	0.8784	14	152.39	15332.3	0.6551

100% 9 jun 2006

MBL-4077-0198PA1

Acquisition Time (sec)	2.5559	Comment	1Dproton CDCl3 D: mlaperle 22	Date	28 Jun 2006 16:06:24	06/28/2006 14:24:11
Date Stamp	28 Jun 2006 16:06:24	File Name	\\LAVFS01\Nmr\data\1\mlaperle\mnt\MBL-4077-0198PA1_010001r			
Frequency (MHz)	400.13	Nucleus	¹ H	Number of Transients	16	
Original Points Count	16384	Owner	chemistry	Points Count	32768	spect
Receiver Gain	574.70	SW(cyclical) (Hz)	6410.26	Solvent	CHLOROFORM-d	zg60
Spectrum Offset (Hz)	2465.7556	Sweep Width (Hz)	6410.06	Pulse Sequence		

MBL-4077-0198PA1_010001r Vertical Scale Factor = 1

flu 29 jun 2006.

MBL-4077-0198PA1

07/04/2006 10:21:47

Acquisition Time (sec)	0.6783	Comment	1Dcarbon CDC13 D. mlaperle 31	Date	04 Jul 2006 00:42:40
Date Stamp	04 Jul 2006 00:42:40	File Name	\\LAVFS01\Nmrdata\Data\mlaperle\hnmr\MBL-4077-0198PA1_020001r		
Frequency (MHz)	100.61	Nucleus	¹³ C	Number of Transients	5120
Original Points Count	16384	Owner	chemistry	Points Count	32768
Receiver Gain	18390.40	SW(cyclical) (Hz)	24154.59	Pulse Sequence	zgpg60
Spectrum Offset (Hz)	10010.5713	Sweep Width (Hz)	24153.85	Solvent	CHLOROFORM-d

No.	(ppm)	Height
1	77.00	7747.2
2	88.79	8933.2
3	90.48	9103.5
4	118.51	11923.8
5	122.20	12295.3
6	124.75	12551.1
7	127.30	12808.4
8	128.48	12927.1
9	128.90	12969.1
10	132.89	13370.8
11	133.40	13421.7
12	134.18	13499.8
13	148.88	14979.3

9 Jul 2006

MBL-4077-0203PA1

07/07/2006 14:14:56

Acquisition Time (sec)	2.5559	Comment	1Dproton CDC13 D: mlaperle 16	Date	07 Jul 2006 17:44:32
Date Stamp	07 Jul 2006 17:44:32				
Frequency (MHz)	400.13	Nucleus	1H	File Name	\\LAVFS01\Nmrdata\16\mlaperle\hnmr\MBL-4077-0203PA1_030001r
Original Points Count	16384	Owner	chemistry	Number of Transients	16
Receiver Gain	322.50	SW(cyclical) (Hz)	6410.26	Points Count	32768
Spectrum Offset (Hz)	2451.8665	Sweep Width (Hz)	6410.06	Solvent	CHLOROFORM-d
				Pulse Sequence	zgpg
				Origin	spect

MBL-4077-0203PA1

07/10/2006 08:43:29

Acquisition Time (sec)	0.6783	Comment	1Dcarbon CDCl3 D: mlaperle 16	Date	09 Jul 2006 02:08:00
Date Stamp	09 Jul 2006 02:08:00			File Name	\\LAVFS01\Nmr\data\data\mlaperle\mr\MBL-4077-0203PA1_031001r
Frequency (MHz)	100.61	Nucleus	¹³ C	Number of Transients	5120
Original Points Count	16384	Owner	chemistry	Points Count	32768
Receiver Gain	16384.00	SW(cyclical) (Hz)	24154.59	Pulse Sequence	zgpg80
Spectrum Offset (Hz)	10017.2041	Sweep Width (Hz)	24153.85	Solvent	CHLOROFORM-d

MBL-4077-0203PA1_031001r Vertical Scale Factor = 1

16 Jul 2006

06/28/2006 16:07:38

Acquisition Time (sec)	2.5559	Comment	1Dproton CDCl3 D: mlapierte 33	Date	28 Jun 2006 18:50:40
Date Stamp	28 Jun 2006 18:50:40			File Name	\\LAVFS01\Nmr\data\Delta\mlapierte\mr\MBL-4077-0199P1A_0100001r
Frequency (MHz)	400.13			Number of Transients	16
Original Points Count	16394			Owner	chemistry
Receiver Gain	574.70			Points Count	32768
				Pulse Sequence	zgpg
Spectrum Offset (Hz)	24665.7559			Solvent	CHLOROFORM-d
Sweep Width (Hz)	6410.06

1.0 0.5 0
Feb 29, in 2006

MBL-4077-0199PA1

07/04/2006 10:31:29

Acquisition Time (sec)	0.6783	Comment	1Dcarbon CDCl3 D: mlaperle 32	Date	04 Jul 2006 03:09:52
Date Stamp	04 Jul 2006 03:09:52	File Name	\\LAVFS01\Nmrdata\Data\mlaperle\mbl-4077-0199PA1_020001r	Origin	spect
Frequency (MHz)	100.61	Nucleus	¹³ C	Points Count	32768
Original Points Count	16384	Owner	chemistry	Pulse Sequence	zgpg80
Receiver Gain	9195.20	SW(cyclical) (Hz)	24154.59	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	10060.6924	Sweep Width (Hz)	24153.85		

MBL-4077-0199PA1_020001r Vertical Scale Factor = 1

No.	(ppm)	(Hz)	Height
1	42.00	4225.9	0.5734
2	45.66	4594.4	0.5654
3	59.99	6035.5	0.5643
4	76.68	7715.5	0.1535
5	77.00	7747.2	0.1577
6	77.32	7778.9	0.1502
7	80.91	8140.8	0.1126
8	93.41	9398.4	0.1272
9	118.54	11926.8	0.0687
10	124.44	12520.2	0.4547
11	127.18	12795.8	0.5090
12	128.28	12906.4	1.0000
13	128.36	12914.5	0.5657
14	129.21	13000.0	0.9889
15	132.65	13346.5	0.4436
16	134.89	13571.3	0.4508
17	138.28	13912.6	0.1319
18	149.83	15074.3	0.0328

Dec 4 jil 2006

MBL-4077-0206PA1

07/05/2006 16:53:42

Acquisition Time (sec)	2.5559	Comment	1Dproton CDCl3 D. mlaperte 35	Date	05 Jul 2006 19:35:28
Date Stamp	05 Jul 2006 19:35:28	File Name	\\lavfs01\mrd\data\mlaperte\mml\MBL-4077-0206PA1_010001r	Origin	spect
Frequency (MHz)	400.13	Nucleus	1H	Points Count	32768
Original Points Count	16384	Owner	chemistry	Pulse Sequence	zgpg0
Receiver Gain	574.70	SW(cyclical) (Hz)	6410.26	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	2466.1467	Sweep Width (Hz)	6410.06		

MBL-4077-0206PA1_010001r

ChemicalScaleFactor = 1

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	1.30 .. 1.46	3.303	1.05791e+10	3.303
2	1.48 .. 1.69	3.614	1.15771e+10	3.614
3	1.72 .. 1.94	2.248	7.19912e+9	2.248
4	1.84 .. 1.97	2.115	6.77464e+9	2.115
5	2.63 .. 2.76	0.943	3.02010e+9	0.943
6	7.34 .. 7.43	1.000	3.20359e+9	1.000
7	7.48 .. 7.55	0.986	3.15814e+9	0.986
8	7.56 .. 7.64	0.976	3.12565e+9	0.976
9	7.93 .. 8.02	0.898	2.87566e+9	0.898

CHLOROFORM-d

7.27

7.27 6 Jul 2006

MBL-4077-0206PA1

07/10/2006 08:51:22

Acquisition Time (sec)	0.6783	Comment	1Carbon CDCl3 D. mlapierle 19	Date	09 Jul 2006 07:02:24
Date Stamp	09 Jul 2006 07:02:24	File Name	\\LAVFS01\Nmr\data\1mlapierle\nt\MBL-4077-0206PA1_030001r	Origin	spect
Frequency (MHz)	100.61	Nucleus	13C	Points Count	32768
Original Points Count	16384	Owner	chemistry	Solvent	CHLOROFORM-d
Receiver Gain	10321.30	SW (Hz)	24154.59	Pulse Sequence	zgpg60
Spectrum Offset (Hz)	10017.2051	Sweep Width (Hz)	24153.85

MBL-4077-0205PA2

Acquisition Time (sec)	2.5559	Comment	1Dproton CDC13 D: mlaperife 61	Date	11 Jul 2006 14:15:28	07/11/2006 10:19:44
Date Stamp	11 Jul 2006 14:15:28	Nucleus	1H	File Name	\\LAVFS01\Nmr\data\mlaperife\hmt\MBL-4077-0205PA2_0100001r	
Frequency (MHz)	400.13	Owner	chemistry	Number of Transients	16	
Original Points Count	16384	SW(cyclical) (Hz)	6410.26	Points Count	32768	spect
Receiver Gain	1448.20	Sweep Width (Hz)	6410.06	Solvent	CHLOROFORM-d	zg80
Spectrum Offset (Hz)	2465.7556			Pulse Sequence		

MBL-4077-0205PA2_0100001r Vertical Scale Factor = 1

MBL-4077-0205PA2

07/12/2006 08:42:39

Acquisition Time (sec)	0.6783	Comment	13Carbon CDC13 D: mlaperle 82	Date	12 Jul 2006 05:39:12
Date Stamp	12 Jul 2006 05:39:12	File Name	\\LAVFS011\mirdat\mlaperle\mlaperle\mbl-4077-0205PA2_020001r	Origin	spect
Frequency (MHz)	100.61	Nucleus	13C	Number of Transients	5120
Original Points Count	16384	Owner	chemistry	Points Count	32768
Receiver Gain	20842.50	SW(cyclical) (Hz)	24154.59	Pulse Sequence	zgpg60
Spectrum Offset (Hz)	10017.2100	Sweep Width (Hz)	24153.85	Solvent	CHLOROFORM-d

MBL-4077-0205PA2_020001r Vertical Scale Factor = 1

No.	(ppm)	(Hz)	Height
1	0.62	62.5	0.2958
2	9.18	923.5	1.0000
3	71.19	7162.6	0.1081
4	77.00	7747.2	0.8044
5	102.72	10334.5	0.0834
6	119.37	12010.1	0.0678
7	124.43	12519.4	0.5577
8	127.58	12836.4	0.6318
9	132.52	13333.2	0.5112
10	134.62	13544.8	0.5237
11	149.92	15083.9	0.0220

MBL-4077-0166PA1

Acquisition Time (sec)	5.1120	Comment	1Dproton CDCl3 D: mlaperle 17	Date	07 Jun 2006 14:06:56
File Name	\\LAVFS01\Nmrdata\Datam\mlaperle\Nmr\MBL-4077-0166PA1	Origin	010001r	Frequency (MHz)	400.13
Nucleus	1H	Number of Transients	32	Original Points Count	32768
Owner	chemistry	Points Count	32768	Receiver Gain	574.70
SW(cyclical) (Hz)	6410.26	Pulse Sequence	zg30	Spectrum Offset (Hz)	2655.7085
Sweep Width (Hz)	6410.06	Solvent	CHLOROFORM-d		

06/07/2006 10:25

VerticalScaleFactor = 1

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[0.63 .. 0.77]	6.117	1.03136e+10	6.117
2	[0.99 .. 1.13]	9.000	1.51735e+10	9.000
3	[7.40 .. 7.50]	0.968	1.63163e+9	0.968
4	[7.50 .. 7.61]	0.996	1.67841e+9	0.996
5	[7.62 .. 7.72]	0.955	1.61025e+9	0.955
6	[7.96 .. 8.07]	0.887	1.49615e+9	0.887

No.	Annotation	(ppm)
1	CHLOROFORM-d	7.27

No.	(ppm)	Height	Area
1	0.69	274.8	0.1957
2	0.71	282.7	0.4913
3	0.73	290.7	0.4989
4	0.75	298.3	0.1884
5	1.06	422.2	0.6400
6	1.07	428.4	0.8340
7	1.07	430.0	1.0000
8	1.09	437.8	0.4227
9	7.27	2907.2	0.1507
10	7.27	2908.9	0.1660

Ylbw 9 jun 2006

MBL-4077-0166PA1

06/08/2006 12:58

Acquisition Time (sec)	1.3566	Comment	1Dcarbon CDC13 D: mlaperle 48	Date	08 Jun 2006 11:03:28
File Name	\\LAVFS01\Nmrdata\mlaperle\mr\MBL-4077-0166PA1_020001r			Frequency (MHz)	100.61
Nucleus	¹³ C	Number of Transients	1588	Original Points Count	32768
Owner	chemistry	Points Count	32768	Receiver Gain	20642.50
SW(cyclical) (Hz)	24154.59	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10017.2051
Sweep Width (Hz)	24153.85				

VerticalScaleFactor = 1

No.	Annotation	(ppm)
1	CHLOROFORM-d	77.00

No.	(ppm)	(Hz)	Height
1	4.18	420.8	1.0000
2	7.41	745.1	0.8546
3	76.68	7715.5	0.1837
4	77.00	7747.2	0.1842
5	77.32	7779.6	0.1843
6	100.40	10101.6	0.0816
7	101.63	10225.4	0.0636

Sp 9 jun 2006

MBL-4077-0220PA1_010004VerticalScaleFactor = 1

MBL-4077-0220PA1

07/17/2006 10:41:14

Acquisition Time (sec)	0.6783	Comment	13Carbon CDCl3 D: mlapierte 54	Date	15 Jul 2006 10:46:24
Date Stamp	15 Jul 2006 10:46:24	File Name	\\LAVFS01\Nmrdata\Data\mlapierte\mbl-4077-0220PA1_021001r	Origin	spect
Frequency (MHz)	100.61	Nucleus	13C	Pulse Sequence	zgpg60
Original Points Count	16384	Owner	chemistry		
Receiver Gain	18390.40	SW(cyclical) (Hz)	24154.59		
Spectrum Offset (Hz)	10016.4668	Sweep Width (Hz)	24153.85		

No.	(ppm)	(Hz)	Height
1	55.36	5569.7	0.4964
2	77.00	7747.2	0.4638
3	82.88	8338.4	0.0985
4	103.29	10392.0	0.0972
5	114.06	11476.4	0.1265
6	114.15	11485.2	1.0000
7	120.86	12159.7	0.0694
8	123.37	12412.5	0.5550
9	127.91	12869.6	0.1548
10	127.96	12874.0	0.6043
11	133.77	13459.3	0.9407
12	136.67	13751.2	0.5481
13	150.76	15168.7	0.0393
14	160.75	16173.4	0.1045

MBL-4077-0221PA1

07/14/2006 15:38:27

Acquisition Time (sec)	2.5559	Comment	1D proton CDCl3 D: mlaperte 30	Date	14 Jul 2006 19:18:24
Date Stamp	14 Jul 2006 19:18:24	File Name	11AVFS01NmrData\mlaperte\mbl-4077-0221PA1_010001r	Origin	spect
Frequency (MHz)	400.13	Nucleus	¹ H	Points Count	32768
Original Points Count	16384	Owner	chemistry	Solvent	CHLOROFORM-d
Receiver Gain	1024.00	SW(cyclical) (Hz)	6410.26	Pulse Sequence	zg30
Spectrum Offset (Hz)	2465.7559	Sweep Width (Hz)	6410.06		

No.	(ppm)	(Hz)	Height
1	2.62	1047.8	0.7482
2	3.86	1543.1	0.8850
3	6.90	2762.4	0.2129
4	6.93	2771.0	0.2255
5	7.27	2908.9	0.4932
6	7.29	2918.9	0.0620
7	7.31	2926.7	0.1264
8	7.33	2934.8	0.0783
9	7.49	2998.9	0.1095
10	7.51	3006.6	0.0928
11	7.54	3016.0	0.2215
12	7.56	3024.6	0.2053
13	7.85	3141.2	0.0988
14	7.87	3149.2	0.0915

MBL-4077-0221PA1_010001r Vertical Scale Factor = 1

11/17/17 Jul 2006

MBL-4077-0221PA1

07/17/2006 10:43:56

Acquisition Time (sec)	0.6783	Comment	1Dcarbon CDCl3 D: mlaperle 55	Date	15 Jul 2006 13:13:36
Date Stamp	15 Jul 2006 13:13:36	File Name	\\LAVFS01\Nmrdata\Data\mlaperle\mmr\MBL-4077-0221PA1_030001r	Origin	spect
Frequency (MHz)	100.61	Nucleus	13C	Number of Transients	5120
Original Points Count	16384	Owner	chemistry	Points Count	32768
Receiver Gain	18390.40	SW(cyclical) (Hz)	24154.59	Pulse Sequence	zgpg60
Spectrum Offset (Hz)	10016.4678	Sweep Width (Hz)	24153.85	Solvent	CHLOROFORM-d

No.	(ppm)	(Hz)	Height
1	21.29	2142.0	0.3551
2	55.33	5566.7	0.5080
3	77.00	7747.2	0.4668
4	82.22	8272.8	0.1085
5	102.20	10282.2	0.1103
6	114.10	11480.1	0.9504
7	114.64	11534.6	0.1064
8	118.45	11917.2	0.0767
9	121.97	12271.7	0.5403
10	127.23	12801.0	0.5969
11	133.45	13426.8	1.0000
12	133.71	13452.6	0.5237
13	142.78	14366.0	0.1236
14	150.23	15114.9	0.0434
15	160.35	16132.9	0.1049

MBL-4077-0222PA1

07/18/2006 09:08:41

Acquisition Time (sec)	2.5559	Comment	1D proton CDCl3 D: mlaperle 46	Date	17 Jul 2006 21:28:32
Date Stamp	17 Jul 2006 21:28:32	File Name	\\LAVFS01\Nmrdata\Data\mlaperle\nmr\MBL-4077-0222PA1_010001r	Origin	spect
Frequency (MHz)	400.13	Nucleus	¹ H	Points Count	32768
Original Points Count	16384	Owner	chemistry	Solvent	CHLOROFORM-d
Receiver Gain	1290.20	SW(cyclical) (Hz)	6410.26		
Spectrum Offset (Hz)	2466.1467	Sweep Width (Hz)	6410.06		

MBL-4077-0222PA1_010001r
VerticalScaleFactor = 1

No.	(ppm)	(Hz)	Height
1	3.87	1547.4	0.7923
2	6.92	2769.9	0.1868
3	6.94	2778.7	0.2173
4	7.27	2908.9	0.4865
5	7.57	3028.3	0.1933
6	7.59	3037.1	0.1985
7	7.83	3132.5	0.4026
8	8.36	3346.8	0.1533

MBL-4077-0222PA1

07/20/2006 08:31:56

Acquisition Time (sec)	0.6783	Comment	1Dcarbon CDCl3 D: mlapette 89	Date	20 Jul 2006 10:57:04
Date Stamp	20 Jul 2006 10:57:04	File Name	\\LAVFS011\Nmrdata\mlapette\mmr\MBL-4077-0222PA1_020001r	Origin	spect
Frequency (MHz)	100.61	Nucleus	13C	Pulse Sequence	zgpg60
Original Points Count	16384	Owner	chemistry		
Receiver Gain	2580.30	SW(cyclical) (Hz)	24154.59		
Spectrum Offset (Hz)	10017.2051	Sweep Width (Hz)	24153.85		

No.	(ppm)	(Hz)	Height
1	55.36	5570.4	0.5052
2	77.00	7747.2	0.3824
3	83.26	8377.4	0.0941
4	101.10	10172.4	0.1049
5	113.64	11433.6	0.1113
6	114.24	11494.1	1.0000
7	122.14	12286.7	0.2138
8	122.18	12292.4	0.2144
9	122.85	12360.2	0.0684
10	129.14	12892.7	0.2228
11	129.17	12896.4	0.2246
12	134.01	13482.9	0.9456
13	135.01	13583.9	0.5389
14	148.98	14888.8	0.0425
15	160.93	16191.9	0.1126

MBL-4077-0222PA1_020001r

VerticalScaleFactor = 1

MBL-4077-0191PA1

06/21/2006 11:57:38

Acquisition Time (sec)	2.5559	Comment	1D proton CDCl3 D: mlaperle 46	Date	21 Jun 2006 15:47:12
Date Stamp	21 Jun 2006 15:47:12	File Name	\\LAVFS01\Nmrdata\mlaperle\NMR\MBL-4077-0191PA1_010001r	Origin	spect
Frequency (MHz)	400.13	Nucleus	¹ H	Pulse Sequence	zgpg0
Original Points Count	16384	Owner	chemistry	Solvent	CHLOROFORM-d
Receiver Gain	1448.20	SW(cyclical) (Hz)	6410.26		
Spectrum Offset (Hz)	2465.7556	Sweep Width (Hz)	6410.06		

MBL-4077-0191PA1_010001r Vertical Scale Factor = 1

No.	(ppm)	(Hz)	Height
1	3.86	1542.9	0.5604
2	6.90	2762.0	0.1277
3	6.92	2770.8	0.1370
4	7.27	2908.9	0.5652
5	7.53	3014.6	0.1348
6	7.55	3021.2	0.1199
7	7.56	3023.4	0.1344
8	7.57	3029.5	0.1001
9	7.70	3080.7	0.0565
10	7.70	3082.7	0.0579
11	7.72	3089.1	0.0444
12	7.73	3091.1	0.0455
13	8.24	3295.7	0.0837
14	8.24	3297.7	0.0834

MBL-4077-0191PA1

06/28/2006 11:01:33

Acquisition Time (sec)	0.6783	Comment	1Carbon CDCl3 D: mlaperte 21	Date	27 Jun 2006 23:30:08
Date Stamp	27 Jun 2006 23:30:08	File Name	\\LAVFS01\Nmrdata\Data\mlaperte\mbL-4077-0191PA1_020001r		
Frequency (MHz)	100.61	Nucleus	13C	Number of Transients	2500
Original Points Count	16384	Owner	chemistry	Points Count	32768
Receiver Gain	16384.00	SW(cyclical) (Hz)	24154.59	Pulse Sequence	zgpg60
Spectrum Offset (Hz)	10015.7305	Sweep Width (Hz)	24153.85	Solvent	CHLOROFORM-d

MBL-4077-0191PA1_020001r Vertical Scale Factor = 1

No.	(ppm)	(Hz)	Height
1	55.34	5567.5	0.4728
2	76.68	7714.7	0.3728
3	77.00	7747.2	0.3729
4	77.32	7778.9	0.3725
5	83.24	8375.2	0.1144
6	98.99	9960.1	0.1242
7	114.06	11475.6	0.1348
8	114.15	11485.2	1.0000
9	118.15	11887.7	0.0845
10	121.16	12189.9	0.1279
11	127.77	12854.8	0.5297
12	133.69	13451.2	0.9598
13	135.25	13607.4	0.5336
14	135.88	13670.8	0.5321
15	149.45	15036.8	0.0447
16	160.57	16155.7	0.1247

AB 20 jun 2006

MBL-4077-0217PA1

07/13/2006 09:48:54

Acquisition Time (sec)	2.5559	Comment	1Dproton CDC13 D: mlaperie 15	Date	13 Jul 2006 13:37:04
Date Stamp	13 Jul 2006 13:37:04	File Name	\\LAVFS01\Nmrdata\Data\mlaperie\nmr\MBL-4077-0217PA1_010001r		
Frequency (MHz)	400.13	Nucleus	¹ H	Number of Transients	16
Original Points Count	16384	Owner	chemistry	Points Count	32768
Receiver Gain	1625.50	SW(cyclical) (Hz)	6410.26	Pulse Sequence	zg30
Spectrum Offset (Hz)	2465.9512	Sweep Width (Hz)	6410.06	Solvent	CHLOROFORM-d

MBL-4077-0217PA1_010001 Vertical Scale Factor = 1

No.	(ppm)	(Hz)	Height
1	3.85	1539.0	0.3759
2	6.88	2752.8	0.0886
3	6.90	2761.6	0.0971
4	7.27	2908.9	0.4875
5	7.38	2952.8	0.0175
6	7.40	2960.8	0.0507
7	7.42	2968.4	0.0540
8	7.44	2975.7	0.0634
9	7.45	2980.7	0.1004
10	7.47	2989.3	0.0888
11	7.52	3007.7	0.0444
12	7.52	3008.7	0.0434
13	7.54	3015.2	0.0332
14	7.54	3016.1	0.0328

Alu 17 Jul. 2006

MBL-4077-0217PA1

07/17/2006 10:35:04

Acquisition Time (sec)	0.6783	Comment	13Carbon CDCl3 D: mlaperle 35	Date	15 Jul 2006 00:42:40
Date Stamp	15 Jul 2006 00:42:40	File Name	\\AVFS01\Nmrdata\Data\mlaperle\hnm\MBL-4077-0217PA1_020001r	Origin	spect
Frequency (MHz)	100.61	Nucleus	13C	Points Count	5120
Original Points Count	16384	Owner	chemistry	Pulse Sequence	zgpg60
Receiver Gain	20642.50	SW(cyclical) (Hz)	24154.59	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	10017.2051	Sweep Width (Hz)	24153.85		

No.	(ppm)	(Hz)	Height
1	55.34	5567.5	0.5271
2	77.00	7747.2	0.5298
3	80.46	8095.1	0.1155
4	97.38	9797.9	0.1291
5	113.40	11409.3	0.1236
6	114.11	11480.8	0.9600
7	118.81	11953.3	0.0876
8	125.23	12599.8	0.0817
9	129.57	13036.9	0.6451
10	130.55	13134.9	0.5876
11	130.91	13171.1	0.5662
12	133.60	13442.3	1.0000
13	160.59	16157.2	0.1201

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