

Supporting Information

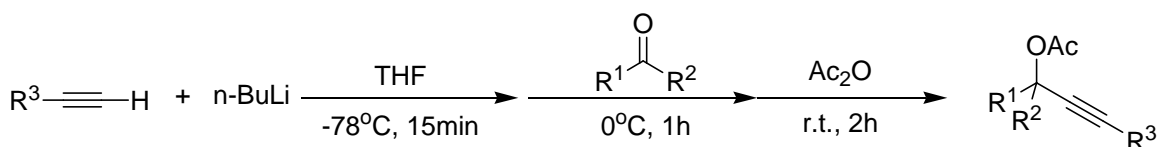
**Gold-Catalyzed Efficient Preparation of Linear α -Iodoenone from
Propargylic acetates**

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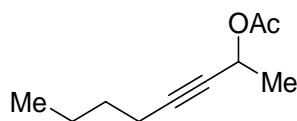
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General. Ethyl acetate (ACS grade), hexanes (ACS grade) and diethyl ether (ACS grade) were purchased from Fisher Scientific and used without further purification. Anhydrous Acetone (HPLC grade) was purchased from Acros Organics. Anhydrous tetrahydrofuran in Pure-Pac™ from Aldrich was used directly without further purification. N-bromosuccinimide was purchased from Acros Organics. N-Iodosuccinimide was purchased from Alfa Aesar. Commercially available reagents were used without further purification. Reactions were monitored by thin layer chromatography(TLC) using silicycle precoated silica gel plates. Flash column chromatography was performed over silicycle silica gel (230-400 mesh). ¹H NMR and ¹³C NMR spectra were recorded on a Varian 500 MHz Unity plus spectrometer and a Varian 400 MHz spectrometer using residue solvent peaks as internal standards. Infrared spectra were recorded with a Perkin Elmer FT-IR spectrum 2000 spectrometer and are reported in reciprocal centimeter (cm⁻¹). Mass spectra were recorded with Waters micromass ZQ detector using electron spray method.

General procedure A: Preparation of propargylic acetates

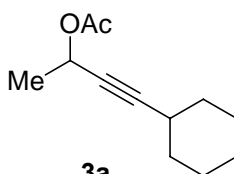


To a solution of alkyne (11 mmol) in anhydrous THF (42 mL) at $-78^{\circ}C$ under N_2 was added *n*-BuLi (2.5 M solution in hexanes, 4.2 mL, 10.5 mmol). The reaction was stirred at the same temperature for 15 min before the addition of ketone/aldehyde (10 mmol). The resulting mixture was allowed to warm to $0^{\circ}C$ gradually and stirred for an additional hour. Upon the addition of acetate anhydrous (2.4 mL, 25 mmol), the reaction mixture was warmed to room temperature and stirred for 2 h before quenched with aqueous $NaHCO_3$. The mixture was extracted with Et_2O (3 x 30 mL), and the combined organic phases were washed with water and brine, dried with anhydrous $MgSO_4$, and filtered. The filtrate was concentrated, and the residue was purified through silica gel flash column chromatography (hexanes/ethyl acetate = 20/1) to yield the desired acetate.



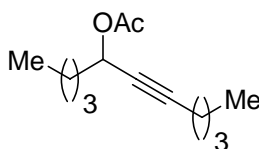
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Compound **1** was prepared in 86% yield according to the general procedure A. ^1H NMR (400MHz, CDCl_3) δ 5.44 (qt, 1H, $J = 6.8, 2.0$ Hz), 2.20 (td, 2H, $J = 7.0, 2.0$ Hz), 2.06 (s, 3H), 1.53 - 1.34 (m, 7H), 0.91 (t, 3H, $J = 7.2$ Hz); ^{13}C NMR (100 MHz, CDCl_3) δ 170.0, 85.6, 78.6, 60.9, 30.6, 21.9, 21.8, 21.2, 18.4, 13.6; IR (neat): 2989, 2960, 2937, 2874, 2249, 1744, 1467, 1453, 1371; MS (ES^+) Calculated for $[\text{C}_{10}\text{H}_{16}\text{NaO}_2]^+$: 191.1; Found: 191.0.



3a

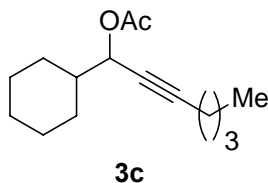
Compound **3a** was prepared in 83% yield according to the general procedure A. ^1H NMR (500MHz, CDCl_3) δ 5.47 (qt, 1H, $J = 6.5, 2.0$ Hz), 2.40 – 2.36 (m, 1H), 2.07 (s, 3H), 1.79 - 1.67 (m, 4H), 1.50 – 1.39 (m, 7H), 1.32 - 1.27 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 170.0, 89.5, 78.5, 60.9, 32.4, 28.9, 25.8, 24.8, 21.9, 21.2; IR (neat): 2988, 2933, 2856, 2244, 1741, 1592, 1450, 1317, 1340, 1309, 1224, 1170, 1592, 1450; MS (ES^+) Calculated for $[\text{C}_{12}\text{H}_{18}\text{NaO}_2]^+$: 217.3; Found: 217.2.



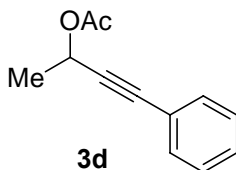
3b

Compound **3b** was prepared in 80% yield according to the general procedure A. ^1H NMR (500MHz, CDCl_3) δ 5.35 (t, 1H, $J = 6.5$ Hz), 2.21 (td, 2H, $J = 7.0, 1.7$ Hz), 2.07 (s, 3H), 1.77 - 1.69 (m, 2H), 1.49 (Quintet, 2H, $J = 7.2$ Hz), 1.43 - 1.31 (m, 6H), 0.93 – 0.89 (m, 6H); ^{13}C NMR (125 MHz, CDCl_3) δ 170.1, 86.1, 77.6, 64.6, 34.8, 30.6, 27.2, 22.2, 21.9, 21.2, 18.4, 13.9, 13.6; IR (neat): 2959, 2935, 2871, 2864, 2242, 1743, 1468,

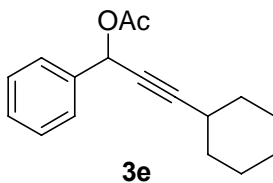
1433, 1371, 1351, 1234, 1161, 1108, 1019, 959; MS (ES⁺) Calculated for [C₁₃H₂₂NaO₂]⁺: 233.3; Found: 233.3.



Compound **3c** was prepared in 84% yield according to the general procedure A. ¹H NMR (500MHz, CDCl₃) δ 5.20 (d, 1H, *J* = 6.0 Hz), 2.21 (t, 2H, *J* = 7.0 Hz), 2.07 (s, 3H), 1.84 - 1.58 (m, 5H), 1.49 (Quintet, 2H, *J* = 7.2 Hz), 1.39 (Sextet, 2H, *J* = 7.2 Hz), 1.27 – 1.03 (m, 6H), 0.90 (t, 3H, *J* = 7.2 Hz); ¹³C NMR (125 MHz, CDCl₃) δ 170.2, 86.8, 76.4, 68.8, 42.0, 30.6, 28.6, 28.0, 26.2, 25.8, 25.7, 21.9, 21.1, 18.4, 13.6; IR (neat): 2960, 2931, 2856, 2239, 1742, 1593, 1452, 1432, 1370, 1231, 1119, 1018, 977; MS (ES⁺) Calculated for [C₁₅H₂₄NaO₂]⁺: 259.4; Found: 259.2.

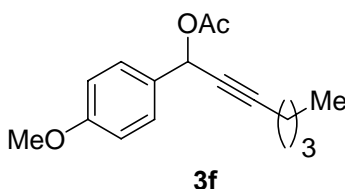


Compound **3d** was prepared in 86% yield according to the general procedure A. ¹H NMR (400 MHz, CDCl₃) δ 7.45–7.43 (m, 2H), 7.33–7.27 (m, 3H), 5.67 (q, 1H, *J* = 6.6 Hz), 2.11 (s, 3H), 1.58 (d, 3H, *J* = 6.6 Hz); ¹³C NMR (100 MHz, CDCl₃) δ 169.9, 131.8, 128.6, 128.2, 122.2, 87.4, 84.5, 60.8, 21.5, 21.1; IR (neat): 3058, 2990, 2939, 2247, 1743, 1599, 1491, 1444, 1372; MS (ES⁺) Calculated for [C₁₂H₁₂NaO₂]⁺: 211.1; Found: 210.9.

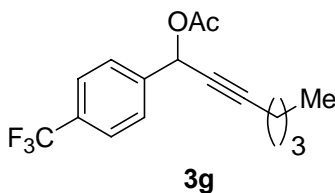


Compound **3e** was prepared in 94% yield according to the general procedure A. ¹H NMR (400 MHz, CDCl₃) δ 7.55–7.51 (m, 2H), 7.39–7.31 (m, 3H), 6.49 (d, 1H, *J* = 2.0

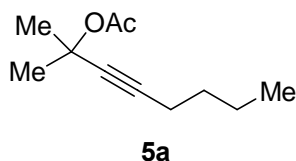
Hz), 2.49–2.44 (m, 1H), 2.09 (s, 3H), 1.82–1.79 (m, 2H), 1.73–1.66 (m, 2H), 1.54–1.43 (m, 3H), 1.36–1.26 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 169.9, 137.8, 128.7, 128.5, 127.7, 92.3, 76.6, 66.0, 32.37, 32.35, 29.1, 25.8, 24.8, 21.2; IR (neat): 3090, 3066, 3035, 2932, 2855, 2236, 1742, 1604, 1588, 1495, 1450, 1369; MS (ES^+) Calculated for $[\text{C}_{17}\text{H}_{20}\text{NaO}_2]^+$: 279.1; Found: 279.1.



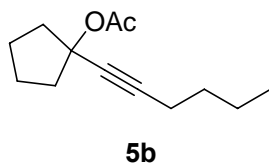
Compound **3f** was prepared in 87% yield according to the general procedure A. ^1H NMR (500MHz, CDCl_3) δ 7.46 (d, 2H, J = 8.5 Hz), 6.89 (d, 2H, J = 8.5 Hz), 6.42 (s, 1H), 3.81 (s, 3H), 2.27 (t, 2H, J = 7.0 Hz), 2.07 (s, 3H), 1.52 (Quintet, 2H, J = 7.2 Hz), 1.41 (Sextet, 2H, J = 7.2 Hz), 0.91 (t, 3H, J = 7.2 Hz); ^{13}C NMR (125 MHz, CDCl_3) δ 170.0, 159.9, 129.9, 129.3, 113.8, 88.1, 76.8, 65.8, 55.3, 30.5, 21.9, 21.2, 18.5, 13.6; IR (neat): 3072, 3037, 3003, 2959, 2935, 2873, 2838, 2292, 2234, 1741, 1611, 1587, 1514, 1465, 1443, 1428, 1369, 1343, 1305, 1279, 1251, 1229, 1175, 1144, 1110, 1034, 1015, 952, 909, 832; MS (ES^+) Calculated for $[\text{C}_{16}\text{H}_{20}\text{NaO}_3]^+$: 283.3; Found: 283.2.



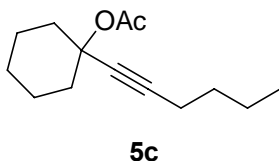
Compound **3g** was prepared in 85% yield according to the general procedure A. ^1H NMR (400MHz, CDCl_3) δ 7.63 (s, 1H), 6.48 (t, 1H, J = 2.0 Hz), 2.27 (td, 2H, J = 7.2, 2.4 Hz), 2.11 (s, 3H), 1.52 (Quintet, 2H, J = 7.2Hz), 1.40 (Sextet, 2H, J = 7.2 Hz), 0.91 (t, 3H, J = 7.2 Hz); ^{13}C NMR (100 MHz, CDCl_3) δ 169.7, 141.5, 130.8 (q, $J_{\text{C-F}}$ = 32 Hz), 127.9, 125.6 (q, $J_{\text{C-F}}$ = 3.7 Hz), 123.9 (q, $J_{\text{C-F}}$ = 270.0 Hz), 89.2, 76.0, 65.3, 30.4, 21.9, 21.0, 18.5, 13.5; IR (neat): 3067, 2962, 2935, 2876, 2295, 2236, 1928, 1746, 1622, 1590, 1468, 1422, 1371, 1327, 1227, 1168, 1129, 1109, 1068, 1018, 959, 922, 850, 836; MS (ES^+) Calculated for $[\text{C}_{16}\text{H}_{17}\text{NaO}_2]^+$: 321.3; Found: 321.2.



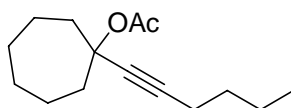
Compound **5a** was prepared in 74% yield according to the general procedure C. ^1H NMR (500MHz, CDCl_3) δ 2.20 (t, 2H, $J = 7.0$), 2.01 (s, 3H), 1.64 (s, 6H), 1.48 (p, 2H, $J = 7.6$ Hz), 1.39 (sextet, 2H, $J = 7.6$ Hz), 0.90 (t, 3H, $J = 7.6$); ^{13}C NMR (125 MHz, CDCl_3) δ 169.4, 84.6, 81.3, 72.6, 30.6, 29.3, 22.1, 21.9, 18.4, 13.6; IR (neat): 2987, 2960, 2936, 2875, 2245, 1747, 1586, 1468, 1434, 1368, 1329, 1266, 1245, 1196, 1016, 953, 822; MS (ES^+) Calculated for $[\text{C}_{11}\text{H}_{18}\text{NaO}_2]^+$: 205.1; Found: 205.1.



Compound **5b** was prepared in 70% yield according to the general procedure C. ^1H NMR (400 MHz, CDCl_3) δ 2.22–2.15 (m, 4H), 2.12–2.04 (m, 2H), 2.02 (s, 3H), 1.74–1.70 (m, 4H), 1.50–1.44 (m, 2H), 1.43–1.35 (m, 2H), 0.90 (t, 3H, $J = 7.6$ Hz); ^{13}C NMR (100 MHz, CDCl_3) δ 169.7, 85.3, 81.0, 80.5, 40.5, 30.7, 23.2, 21.9, 18.5, 13.6; IR (neat): 2960, 2933, 2875, 2246, 1746, 1593, 1453, 1435, 1367, 1334, 1241, 1124, 1016, 970; MS (ES^+) Calculated for $[\text{C}_{13}\text{H}_{20}\text{NaO}_2]^+$: 231.1; Found: 231.1.

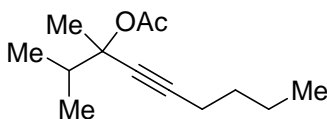


Compound **5c** was prepared in 84% yield according to the general procedure C. ^1H NMR (400 MHz, CDCl_3) δ 2.254 (t, 2H, $J = 7.2$ Hz), 2.11–2.06 (m, 2H), 2.03 (s, 3H), 1.84–1.77 (m, 2H), 1.63–1.29 (m, 10H), 0.91 (t, 3H, $J = 7.2$ Hz); ^{13}C NMR (100 MHz, CDCl_3) δ 169.3, 86.8, 80.0, 76.1, 37.4, 30.8, 25.3, 22.7, 22.1, 21.9, 18.5, 13.6; IR (neat): 2936, 2861, 2244, 1746, 1600, 1447, 1431, 1367, 1301, 1264, 1230, 1184, 1131, 1034, 1020, 965; MS (ES^+) Calculated for $[\text{C}_{14}\text{H}_{22}\text{NaO}_2]^+$: 245.2; Found: 245.1.



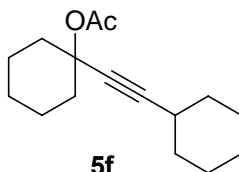
5d

Compound **5d** was prepared in 70% yield according to the general procedure C. ^1H NMR (400 MHz, CDCl_3) δ 2.24–2.17 (m, 4H), 2.06–2.04 (m, 2H), 2.01 (s, 3H), 1.57–1.37 (m, 12H), 0.90 (t, 3H, $J = 7.2$ Hz); ^{13}C NMR (100 MHz, CDCl_3) δ 169.4, 86.0, 81, 2, 79.5, 40.5, 30.7, 28.2, 22.2, 21.9, 18.5, 13.6; IR (neat): 2936, 2861, 2244, 1746, 1600, 1447, 1431, 1367, 1301, 1264, 1230, 1184, 1131, 1034, 1020, 965; MS (ES^+) Calculated for $[\text{C}_{15}\text{H}_{24}\text{NaO}_2]^+$: 257.2; Found: 259.2.



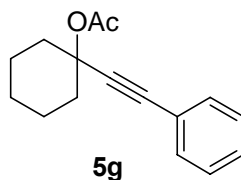
5e

Compound **5e** was prepared in 80% yield according to the general procedure C. ^1H NMR (400 MHz, CDCl_3) δ 2.23 (t, 2H, $J = 7.2$ Hz), 2.16 (heptet, 1H, $J = 6.6$ Hz), 2.01 (s, 3H), 1.61 (s, 3H), 1.53–1.43 (m, 2H), 1.42–1.37 (m, 2H), 1.01 (d, 3H, $J = 6.6$ Hz), 0.97 (d, 3H, $J = 6.6$ Hz), 0.90 (t, 3H, $J = 7.2$ Hz); ^{13}C NMR (100 MHz, CDCl_3) δ 169.4, 86.2, 79.6, 79.2, 37.4, 30.8, 23.5, 22.1, 21.9, 18.4, 17.5, 17.2, 13.6; IR (neat): 2965, 2936, 2876, 2244, 1746, 1559, 1458, 1436, 1371, 1336, 1243, 1129, 1060, 1014, 942; MS (ES^+) Calculated for $[\text{C}_{13}\text{H}_{22}\text{NaO}_2]^+$: 233.2; Found: 233.2.



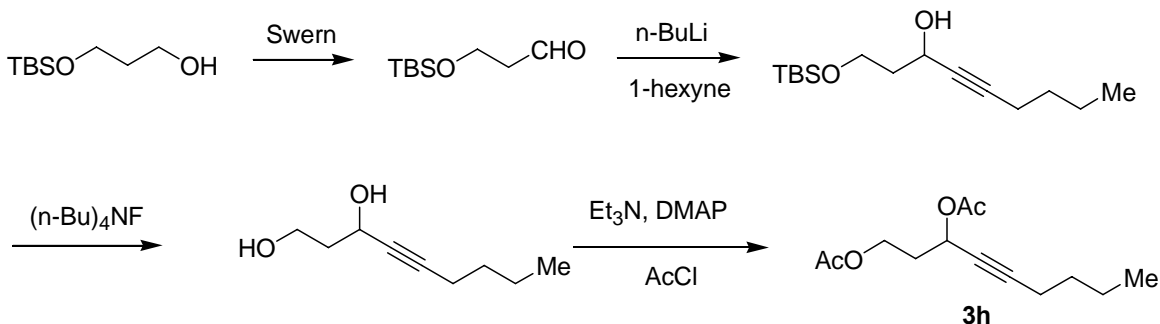
5f

Compound **5f** was prepared in 91% yield according to the general procedure A. ^1H NMR (400 MHz, CDCl_3) δ 2.47–2.43 (m, 1H), 2.13–2.08 (m, 2H), 2.02 (s, 3H), 1.82–1.24 (m, 18H); ^{13}C NMR (100 MHz, CDCl_3) δ 169.2, 91.0, 80.2, 76.2, 37.5, 32.6, 28.9, 26.0, 25.3, 24.6, 22.9, 22.2; IR (neat): 2933, 2857, 2663, 2237, 1746, 1615, 1447, 1367, 1229, 1184, 1022; MS (ES^+) Calculated for $[\text{C}_{16}\text{H}_{24}\text{NaO}_2]^+$: 271.2; Found: 271.1.



Compound **5g** was prepared in 88% yield according to the general procedure A. ^1H NMR (500 MHz, CDCl_3) δ 7.46 -7.44 (m, 2H), 7.29 -7.28 (m, 3H), 2.24 -2.19 (m, 2H), 2.07 (s, 3H), 1.93 -1.88 (m, 2H), 1.70 -1.65 (m, 4H), 1.59 - 1.53 (m, 1H), 1.39 -1.33 (m, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 169.2, 131.8, 128.2, 128.1, 122.8, 89.1, 86.2, 75.9, 37.1, 25.2, 22.7, 22.0; IR (neat): 3082, 3057, 3035, 3023, 2937, 2861, 2667, 2229, 2203, 1743, 1675, 1599, 1573, 1491, 1444, 1367, 1346, 1312, 1264, 1229, 1163, 1138, 1071, 1041, 1022, 959; MS (ES^+) Calculated for $[\text{C}_{16}\text{H}_{18}\text{NaO}_2]^+$: 265.3; Found: 265.2.

Preparation propargylic acetate **3h**



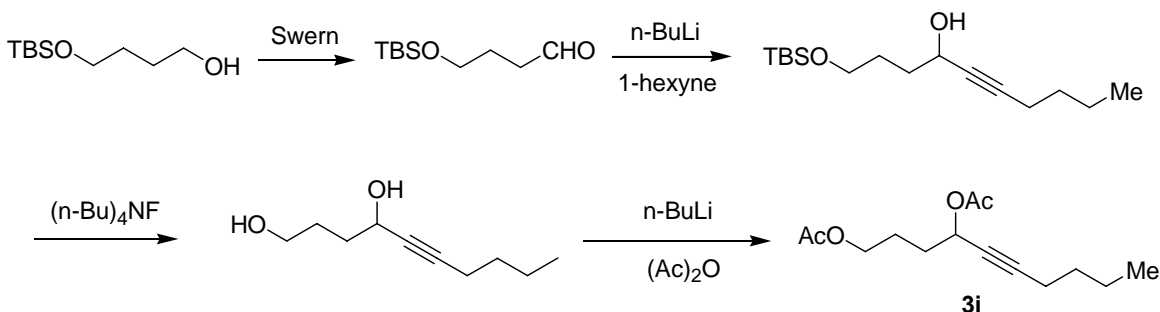
A solution oxalyl chloride (1.9 g, 10 mmol) in DCM (110 mL) was cooled in a dry ice-acetone bath under nitrogen. To the solution was added dropwise anhydrous DMSO (1.6 mL, 22 mmol). After the addition, the reaction was kept at -78°C for half an hour. A solution of mono-TBS protected propane-1,3-diol (1.9 g, 10 mmol) in DCM (20 mL) was added dropwise, and the reaction mixture was stirred at -78°C for 1 hour. The reaction was quenched by addition of Et_3N (6.9 mL, 50 mmol). The reaction was allowed to warm to room temperature. The organic layer was successively washed with saturated NH_4Cl (100 mL) and brine (100 mL). the resulting organic layer was dried upon anhydrous MgSO_4 , filtered, concentrated in vacuo to give the crude aldehyde (2.3 g) which could be used in the next step without further purification.

A solution of 1-hexyne (1.30 g, 15.8 mmol) in THF (50 ml) was cooled to -78°C in a dry ice-acetone bath under nitrogen, and n-BuLi (1.6M in Hexane, 9.17 mL, 14.64

mmol) was added dropwise in 15 mins. After the addition, a solution of the crude aldehyde (2.3 g, 12.2 mmol) in THF (10 mL) was added dropwise, the resulting reaction mixture was allowed to warm to room temperature gradually. The reaction was quenched by addition of saturated NH_4Cl (30 mL). The aqueous layer was extracted with Et_2O (3 x 50 mL). The combined organic layer was washed with brine (100 mL), dried with MgSO_4 , filtered, and concentrated to give an oil. The desired alcohol was purified by bulb-to-bulb distillation as a clear liquid (1.4 g, 50% yield two steps)

To a solution of the above alcohol (270 mg, 1 mmol) in THF (5 mL) was added TBAF (1M in THF, 1 mL). The resulting mixture was stirred at room temperature for 2 hours. The reaction was cooled down in an ice-water bath, and Et_3N (0.3 mL, 3 mmol) and DMAP (cat) were added followed by dropwise addition of CH_3COCl (0.18 mL, 2.5 mmol). The resulting mixture was allowed to rise to room temperature and stir for 4 hours. The reaction was quenched by addition of water (20 mL). The organic layer was extracted with Et_2O (3 x 15 mL). The combined organic layer was washed with brine (50 mL), dried upon MgSO_4 , filtered, and concentrated to give an oily residue, which was purified by flash-column to give diacetate **3h** (160 mg, 67% yield). ^1H NMR (400 MHz, CDCl_3) δ 5.47 (tt, 1H, $J = 6.8, 2.0$ Hz), 4.25–4.15 (m, 2H), 2.20 (td, 2H, $J = 6.8, 2.0$ Hz), 2.13–2.03 (m, 8H), 1.51–1.45 (m, 2H), 1.41–1.36 (m, 2H), 0.90 (t, 3H, $J = 6.8$ Hz); ^{13}C NMR (125 MHz, CDCl_3) δ 170.9, 170.0, 87.0, 76.5, 61.5, 60.4, 34.1, 30.4, 21.9, 21.0, 20.9, 18.3, 13.5; IR (neat): 2960, 2936, 2874, 2247, 1744, 1592, 1459, 1432, 1370, 1232, 1159, 1045, 960; MS (ES^+) Calculated for $[\text{C}_{13}\text{H}_{20}\text{NaO}_4]^+$: 263.1; Found: 263.2.

Preparation propargylic acetate **3i**



A solution oxalyl chloride (0.4 g, 2 mmol) in DCM (20 mL) was cooled to -78°C in a dry ice-acetone bath under nitrogen. To the solution was added dropwise anhydrous DMSO (0.32 mL, 4.4 mmol). After addition, the reaction was kept at -78°C for half an

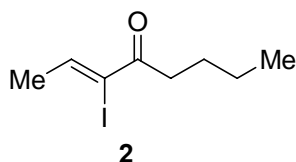
hour. A solution of mono-TBS protected butane-1,4-diol (0.38 g, 2 mmol) in DCM (4 mL) was added dropwise, and the resulting mixture was stirred at -78°C for 1 hour. The reaction was quenched by the addition of Et₃N (1.38 mL, 10 mmol). The reaction was allowed to warm to room temperature. The organic layer was successively washed with saturated NH₄Cl (20 mL) and brine (20 mL). The resulting organic layer was dried with anhydrous MgSO₄, filtered, and concentrated in *vacuo* to give the crude aldehyde, which was used in the next step without further purification.

A solution of 1-hexyne (0.13 g, 0.16 mmol) in THF (10 mL) was cooled to -78°C in a dry ice-acetone bath under nitrogen, and *n*-BuLi (1.6M in Hexane, 1 mL, 1.6 mmol) was added dropwise. The resulting mixture was stirred for 15 mins, and a solution of aldehyde (0.23 g, 1.2 mmol) in THF (10 mL) was added dropwise. Upon the addition, the reaction mixture was allowed to warm to room temperature and stirred for 15 min. The reaction was quenched by the addition of saturated NH₄Cl (10 mL). The aqueous layer was extracted with Et₂O (3 x 20 mL). The combined organic layer was washed with brine (50 mL), dried upon MgSO₄, filtered, and concentrated to give an oily residue, which was purified by flash-column to give the desired alcohol (0.2 g, 35% yield, two steps)

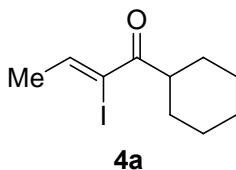
To a solution of the alcohol (90 mg, 0.3 mmol) in THF (5 mL) was added the TBAF (1M in THF, 0.3 mL, 0.3 mmol). The resulting mixture was stirred at room temperature for 2 hours. The reaction cooled down to -78°C in a dry ice-acetone bath under nitrogen, and *n*-BuLi (1.6M in Hexane, 0.37 mL, 0.6 mmol) was added dropwise. Upon the addition, the reaction mixture was stirred for 15 min, and a solution of acetic anhydride (0.12 g, 0.6 mmol) in THF (2 mL) was added dropwise. The reaction was allowed to warm to room temperature and kept stirring for half an hour. The reaction was quenched by addition of saturated NH₄Cl (10 mL). The aqueous layer was extracted with Et₂O (3 x 10 mL). The combined organic layer was washed with brine (50 mL), dried upon MgSO₄, filtered, and concentrated to give an oily residue, which was purified by flash-column to give diacetate **3i** (60 mg, 83% yield two steps). ¹H NMR (400 MHz, CDCl₃) δ 5.40–5.38 (m, 1H), 4.10 (t, 2H, *J* = 4.8 Hz), 2.21 (t, 2H, *J* = 6.8 Hz), 2.08 (s, 3H), 2.06 (s, 3H), 1.83–1.74 (m, 4H), 1.48 (sextet, 2H, *J* = 8 Hz), 1.39 (sextet, 2H, *J* = 8 Hz), 0.91 (t, 3H, *J* = 7.6 Hz); ¹³C NMR (100 MHz, CDCl₃) δ 171.1, 170.0, 86.7, 64.0, 63.9, 31.7, 30.5, 24.3, 21.9, 21.1, 21.0, 18.4, 13.6; IR (neat): 3308, 2960, 2935, 2337, 1741, 1592, 1430, 1370, 1232, 1023; MS (ES⁺) Calculated for [C₁₄H₂₂NaO₄]⁺: 277.1; Found: 277.2.

General procedure B: Preparation of α -iodoenone **4** and **6**

To a solution of propargylic acetate **3** or **5** (0.2 mmol) in anhydrous acetone (4 mL) cooled in ice-water bath were added H₂O (0.005 mL, 1.39 eq) and Au(PPh₃)NTf₂ (0.05 M in acetone, 0.08 mL). The solution was treated with NIS (0.24 mmol, 1.2 eq). The reaction was stirred for two hours before quenched with NEt₃ (1 drop) and aqueous Na₂S₂O₃ (5 mL). The mixture was extracted with Et₂O (3 x 8 mL). The combined organic phases were washed with H₂O (10 mL) and brine (10 mL), dried with anhydrous MgSO₄, and filtered. The filtrate was concentrated, and the residue was purified through silica gel flash column chromatography (hexanes/ethyl acetate = 50/1) to yield the desired α -iodo- α , β -unsaturated ketones **4** or **6**

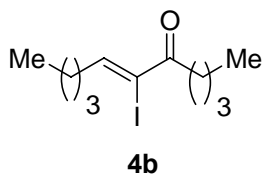


Compound **2** was prepared as a mixture of geometrical isomers (Z/E = 45/1) in 89% yield according to the general procedure B. ¹H NMR (400 MHz, CDCl₃) (major isomer) δ 7.11 (q, 1H, J = 6.8 Hz), 2.81 (t, 2H, J = 7.6 Hz), 2.07 (d, 3H, J = 6.8 Hz), 1.63 (Quintet, 2H, J = 7.6 Hz), 1.34 (Sextet, 2H, J = 7.6 Hz), 0.92 (t, 3H, J = 7.6 Hz); ¹³C NMR (125 MHz, CDCl₃) (major isomer) δ 194.9, 146.8, 114.3, 37.5, 30.3, 27.1, 23.9, 22.3, 13.8; IR (neat): 2958, 2932, 2871, 1702, 1683, 1611, 1464, 1413, 1373, 1288, 1262, 1238, 1288, 1262, 1238, 1171, 1113, 1072; MS (ES⁺) Calculated for [C₈H₁₃NaIO]⁺: 275.0; Found: 275.0.

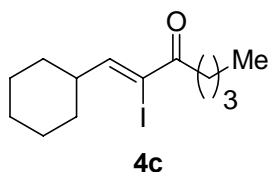


Compound **4a** was isolated as a mixture of geometrical isomers (Z/E = 12/1) in 82% yield according to the general procedure B. ¹H NMR (500 MHz, CDCl₃) (major isomer) δ 7.08 (q, 1H, J = 7.0 Hz), 3.14 (q, 1H, J = 7.0 Hz), 2.08 (d, 3H, J = 7.0 Hz), 1.80-1.78 (m, 4H), 1.48 – 1.22 (m, 6H); ¹³C NMR (125 MHz, CDCl₃) (major isomer) δ 198.2, 146.1, 113.9, 45.4, 29.9, 25.8, 25.7, 24.0; IR (neat): 3019, 2932, 2855, 2664, 1678, 1611, 1463,

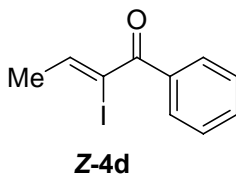
1450, 1372, 1287, 1264, 1241, 1188, 1163, 1131, 1109, 1081, 1071, 1030, 974, 895, 884, 824; MS (ES⁺) Calculated for [C₁₀H₁₅NaIO]⁺: 301.0; Found: 300.9.



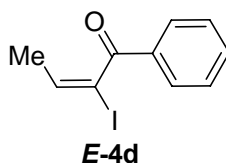
Compound **4b** was prepared as a mixture of geometrical isomers (*Z/E* = 10/1) in 94% yield according to the general procedure B. Compound **4b** (major isomer): ¹H NMR (400 MHz, CDCl₃) δ 6.99 (t, 1H, *J* = 6.8 Hz), 2.82 (t, 2H, *J* = 7.2 Hz), 2.42 (q, 2H, *J* = 7.6 Hz), 1.67–1.50 (m, 4H), 1.45–1.30 (m, 4H), 0.97–0.89 (m, 6H); ¹³C NMR (125 MHz, CDCl₃) δ 195.0, 151.2, 112.4, 37.7, 37.6, 29.7, 27.1, 22.4, 22.3, 13.8, 13.8; IR (neat): 3351, 2958, 2930, 2872, 2735, 1683, 1604, 1465, 1413, 1379, 1291, 1236, 1167, 1123, 1088, 934; MS (ES⁺) Calculated for [C₁₁H₁₉INaO]⁺: 317.0; Found: 317.0.



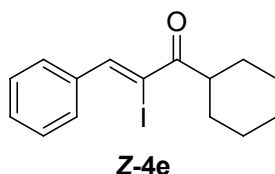
Compound **4c** was prepared as a mixture of geometrical isomers (*Z/E* = 19/1) in 91% yield according to the general procedure B with exceptions that 10 mol % of AgNTf₂ was added together with Au(PPh₃)NTf₂ and a column basified with Et₃N was used for purification. Compound **4c** (major isomer): ¹H NMR (500 MHz, CDCl₃) δ 6.74 (d, 1H, *J* = 9 Hz), 2.80 (t, 2H, *J* = 15 Hz), 2.60–2.52 (m, 1H), 1.82–1.68 (m, 5H), 1.60 (quintet, 2H, *J* = 7.5 Hz), 1.41–1.31 (m, 4H), 1.27–1.20 (m, 3H), 1.92 (t, 3H, *J* = 7.5 Hz); ¹³C NMR (125 MHz, CDCl₃) δ 195.3, 155.7, 109.9, 46.8, 37.6, 30.7, 27.2, 25.7, 25.2, 22.3, 13.8; IR (neat): 3351, 2928, 2852, 2662, 2351, 1683, 1601, 1448, 1278, 1224, 1169, 1128, 1089, 968; MS (ES⁺) Calculated for [C₁₃H₂₁INaO]⁺: 343.1; Found: 343.0.



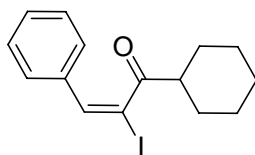
Compound **4d** was prepared in 75% yield in a 1.2:1 Z/E ratio of separable isomers according to the general procedure B. Compound **Z-4d**: ^1H NMR (400 MHz, CDCl_3) δ 7.69 (d, 2H, $J = 8$ Hz), 7.55 (t, 2H, $J = 8$ Hz), 7.44 (t, 2H, $J = 8$ Hz), 6.73 (q, 1H, $J = 8$ Hz), 2.09 (d, 3H, $J = 8$ Hz); ^{13}C NMR (125 MHz, CDCl_3) δ 191.9, 149.7, 135.8, 132.4, 129.6, 128.4, 110.5, 23.6; IR (neat): 3297, 3059, 2924, 2851, 2356, 1993, 1658, 1606, 1577, 1446, 1371, 1314, 1260, 1179, 1120, 1060, 1025, 965 $\text{MS (ES}^+)$ Calculated for $[\text{C}_{10}\text{H}_9\text{INaO}]^+$: 295.0; Found: 295.0.



Compound **E-4d**: ^1H NMR (400 MHz, CDCl_3) δ 7.98 (d, 2H, $J = 8$ Hz), 7.61 (t, 2H, $J = 8$ Hz), 7.49 (t, 2H, $J = 8$ Hz), 6.67 (q, 1H, $J = 8$ Hz), 1.67 (d, 3H, $J = 8$ Hz); ^{13}C NMR (125 MHz, CDCl_3) δ 192.7, 140.8, 134.0, 133.6, 129.9, 128.9, 90.4, 18.7; IR (neat): 3053, 2916, 2850, 2347, 1666, 1596, 1448, 1329, 1227, 1174, 1115, 1012; $\text{MS (ES}^+)$ Calculated for $[\text{C}_{10}\text{H}_9\text{INaO}]^+$: 295.0; Found: 295.0.

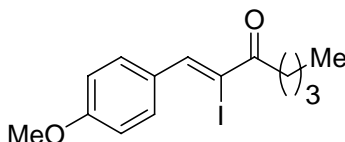


Compound **4e** was prepared in 97% yield in a 1:2 Z/E ratio of separable isomers according to the general procedure B. Compound **Z-4e**: ^1H NMR (500 MHz, CDCl_3) δ 7.96 (s, 1H), 7.75–7.70 (m, 2H), 7.46–7.43 (m, 3H), 3.33 (tt, 1H, $J = 11.5, 3$ Hz), 1.92–1.83 (m, 4H), 1.74–1.72 (m, 1H), 1.54–1.46 (m, 2H), 1.42–1.23 (m, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 199.5, 145.6, 135.9, 130.0, 129.5, 128.3, 107.2, 45.6, 30.0, 25.8; IR (neat): 3334, 3057, 3023, 2930, 2853, 2662, 1674, 1591, 1491, 1445, 1366, 1262, 1186, 1150, 1112, 1013, 925; $\text{MS (ES}^+)$ Calculated for $[\text{C}_{15}\text{H}_{17}\text{INaO}]^+$: 363.0; Found: 362.9.



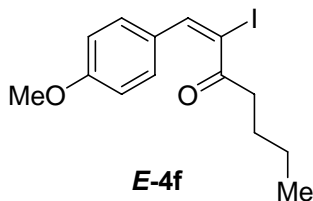
E-4e

Compound **E-4e**: ^1H NMR (500 MHz, CDCl_3) δ 7.46 (s, 1H), 7.32–7.31 (m, 3H), 7.19–7.17 (m, 2H), 2.47 (tt, 1H, $J = 11$, 3.5 Hz), 1.82 (d, 2H, $J = 11.5$ Hz), 1.68–1.54 (m, 2H), 1.58–1.54 (m, 1H), 1.39–1.32 (m, 2H), 1.16–1.02 (m, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 206.3, 143.0, 136.7, 129.0, 129.6, 128.1, 96.3, 49.5, 29.5, 25.6, 25.6; IR (neat): 3352, 3057, 3024, 2930, 2853, 2662, 1687, 1598, 1572, 1494, 1448, 1366, 1312, 1289, 1236, 1141, 1071, 1007, 926, 814; MS (ES^+) Calculated for $[\text{C}_{15}\text{H}_{17}\text{INaO}]^+$: 363.0; Found: 362.9.



Z-4f

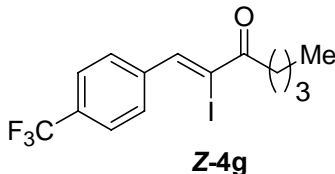
Compound **4f** was prepared in 84% yield in a 1.05:1 Z/E ratio of separable isomers according to the general procedure B. Compound **Z-4f**: ^1H NMR (400 MHz, CDCl_3) δ 8.02 (s, 1H), 7.90 (d, 2H, $J = 8.8$ Hz), 6.98 (d, 2H, $J = 8.8$ Hz), 3.87 (s, 3H), 2.97 (t, 2H, $J = 8$ Hz), 1.70 (quintet, 2H, $J = 7.2$ Hz), 1.39 (sextet, 2H, $J = 7.6$ Hz), 0.95 (t, 3H, $J = 7.2$ Hz); ^{13}C NMR (125 MHz, CDCl_3) δ 195.9, 161.4, 146.1, 132.0, 127.6, 113.8, 104.6, 55.4, 37.8, 27.4, 22.4, 13.9; IR (neat): 3003, 2957, 2932, 2871, 2838, 1674, 1604, 1587, 1568, 1509, 1463, 1255, 1148, 1029, 826; MS (ES^+) Calculated for $[\text{C}_{14}\text{H}_{17}\text{INaO}_2]^+$: 367.0; Found: 366.9.



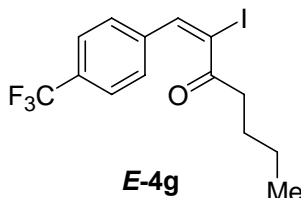
E-4f

Compound **E-4f**: ^1H NMR (400 MHz, CDCl_3) δ 7.36 (s, 1H), 7.13 (d, 2H, $J = 8.8$ Hz), 6.84 (d, 2H, $J = 8.8$ Hz), 3.81 (s, 3H), 2.54 (t, 2H, $J = 7.6$ Hz), 1.56 (quintet, 2H, $J = 7.2$ Hz), 1.24 (sextet, 2H, $J = 7.6$ Hz), 0.83 (t, 3H, $J = 7.2$ Hz); ^{13}C NMR (125 MHz, CDCl_3) δ

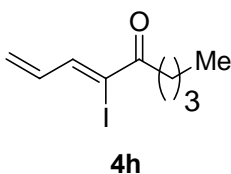
203.9, 160.2, 142.6, 129.7, 129.2, 114.0, 94.7, 55.3, 40.2, 26.4, 22.1, 13.7; IR (neat): 3271, 2957, 2930, 2870, 1685, 1604, 1509, 1456, 1293, 1255, 1178, 1122, 1032; MS (ES⁺) Calculated for [C₁₄H₁₇IO₂]⁺: 267.0; Found: 267.0.



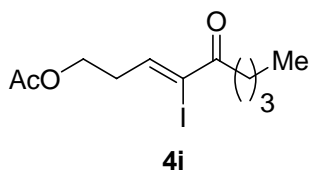
Compound **4g** was prepared in 96% yield in a 5:1 Z/E ratio of separable isomers according to the general procedure B. Compound **Z-4g**: ¹H NMR (400 MHz, CDCl₃) δ 8.00 (s, 1H), 7.81 (d, 2H, *J* = 8.4 Hz), 7.70 (d, 2H, *J* = 8.4 Hz), 2.99 (t, 2H, *J* = 7.2 Hz), 1.71 (Quintet, 2H, *J* = 7.2 Hz), 1.40 (Sextet, 2H, *J* = 7.2 Hz), 0.96 (t, 3H, *J* = 7.2 Hz); ¹³C NMR (125 MHz, CDCl₃) δ 196.2, 144.8, 139.8, 131.6 (q, *J*_{C-F} = 32.4 Hz), 129.8, 125.6 (q, *J*_{C-F} = 3.72 Hz), 124.0 (q, *J*_{C-F} = 270.8 Hz), 110.2, 38.4, 27.3, 22.5, 14.1; IR (neat): 3070, 2960, 2934, 2874, 1681, 1598, 1466, 1412, 1324, 1168, 1128, 1068, 1017, 885, 827; MS (ES⁺) Calculated for [C₁₄H₁₄NaF₃IO]⁺: 405.0; Found: 404.9.



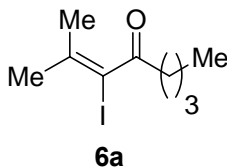
Compound **E-4g**: ¹H NMR (400 MHz, CDCl₃) δ 7.58 (d, 2H, *J* = 8.4 Hz), 7.38 (s, 1H), 7.31 (d, 2H, *J* = 8.4 Hz), 2.55 (t, 2H, *J* = 7.2 Hz), 1.56 (Quintet, 2H, *J* = 7.2 Hz), 1.24 (Sextet, 2H, *J* = 7.2 Hz), 0.83 (t, 3H, *J* = 7.2 Hz); ¹³C NMR (125 MHz, CDCl₃) δ 203.0, 140.7, 139.5, 130.7 (q, *J*_{C-F} = 32.4 Hz), 128.2, 125.7 (q, *J*_{C-F} = 3.75 Hz), 123.8 (q, *J*_{C-F} = 270.6 Hz), 99.68, 40.0, 26.0, 22.0, 13.7; IR (neat): 3070, 2960, 2923, 2870, 1699, 1597, 1459, 1421, 1324, 1168, 1126, 1068, 1017, 874, 830; MS (ES⁺) Calculated for [C₁₄H₁₄NaF₃IO]⁺: 405.0; Found: 404.9.



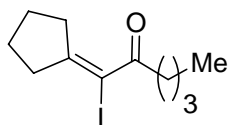
Compound **4h** was prepared in 80% yield according to the general procedure B. ^1H NMR (500 MHz, CDCl_3) δ 7.37 (d, 1H, $J = 10$ Hz), 6.78 (td, 1H, $J = 16.5, 10$ Hz), 5.88 (d, 1H, $J = 17$ Hz), 5.76 (d, 1H, $J = 10$ Hz), 2.87 (t, 2H, $J = 7.5$ Hz), 1.65 (Quintet, 2H, $J = 7.5$ Hz), 1.36 (sextet, 2H, $J = 7.5$ Hz), 0.93 (t, 3H, $J = 7.5$ Hz); ^{13}C NMR (125 MHz, CDCl_3) δ 195.4, 146.2, 139.3, 128.9, 110.6, 37.7, 27.1, 22.3, 13.9; IR (neat): 3274, 2958, 2331, 1682, 1597, 1456, 1597, 1457, 1261, 1123, 1042. MS (ES^+) Calculated for $[\text{C}_9\text{H}_{13}\text{INaO}]^+$: 286.9; Found: 286.6.



Compound **4i** was prepared in 83% yield according to the general procedure B. ^1H NMR (400 MHz, CDCl_3) δ 7.00 (t, 1H, $J = 6.8$ Hz), 4.13 (t, 2H, $J = 6.4$ Hz), 2.82 (t, 2H, $J = 7.2$ Hz), 2.50 (q, 2H, $J = 7.2$ Hz), 2.07 (s, 3H), 1.90 (quintet, 2H, $J = 7.2$ Hz), 1.63 (quintet, 2H, $J = 7.6$ Hz), 1.35 (sextet, 2H, $J = 7.6$ Hz), 0.93 (t, 3H, $J = 6.8$ Hz); ^{13}C NMR (125 MHz, CDCl_3) δ 194.9, 171.0, 149.8, 113.0, 63.5, 37.7, 34.6, 27.1, 26.7, 22.3, 21.0, 13.8; IR (neat): 3271, 2958, 2872, 1738, 1683, 1604, 1456, 1366, 1241, 1159, 1118, 1044; MS (ES^+) Calculated for $[\text{C}_{12}\text{H}_{19}\text{INaO}_3]^+$: 361.0; Found: 360.9.

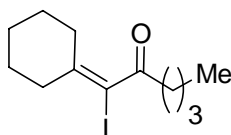


Compound **6a** was prepared in 96% yield according to the general procedure B. ^1H NMR (400 MHz, CDCl_3) δ 2.81 (t, 2H, $J = 7.2$ Hz), 2.03 (s, 3H), 1.96 (s, 3H), 1.61 (Quintet, 2H, $J = 7.2$ Hz), 1.35 (Sextet, 2H, $J = 7.2$ Hz), 0.93 (t, 3H, $J = 7.2$ Hz); ^{13}C NMR (125 MHz, CDCl_3) δ 202.3, 144.3, 95.5, 40.5, 30.3, 26.4, 22.3, 21.9, 13.8; IR (neat): 2958, 2932, 2873, 1688, 1601, 1464, 1441, 1406, 1380, 1368, 1258, 1238, 1155, 1105, 1044, 910, 842; MS (ES^+) Calculated for $[\text{C}_9\text{H}_{15}\text{NaIO}]^+$: 289.0; Found: 289.0.



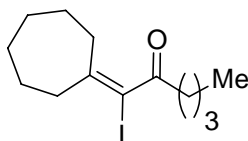
6b

Compound **6b** was prepared in 87% yield according to the general procedure B. ^1H NMR (400 MHz, CDCl_3) δ 2.85 (t, 2H, $J = 7.2$ Hz), 2.70 (tt, 2H, $J = 7.2$, 1.2 Hz), 2.47 (tt, 2H, $J = 7.2$, 1.2 Hz), 1.89 (Quintet, 2H, $J = 7.2$ Hz), 1.72 (Quintet, 2H, $J = 7.2$ Hz), 1.58 (Quintet, 2H, $J = 7.2$ Hz), 1.34 (Sextet, 2H, $J = 7.2$ Hz), 0.92 (t, 3H, $J = 7.2$ Hz); ^{13}C NMR (125 MHz, CDCl_3) δ 198.9, 166.4, 92.3, 44.4, 41.8, 36.1, 28.7, 26.9, 24.9, 22.3, 13.9; IR (neat): 2959, 2936, 2872, 1674, 1573, 1466, 1452, 1413, 1379, 1306, 1289, 1264, 1172, 1158, 1137, 1088, 911; MS (ES^+) Calculated for $[\text{C}_{11}\text{H}_{17}\text{NaIO}]^+$: 315.0; Found: 315.0.



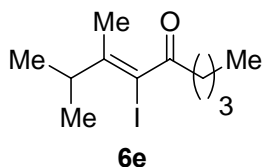
6c

Compound **6c** was prepared in 91% yield according to the general procedure B. ^1H NMR (400 MHz, CDCl_3) δ 2.79 (t, 2H, $J = 7.2$ Hz), 2.41 (t, 2H, $J = 5.6$ Hz), 2.33 (t, 2H, $J = 5.6$ Hz), 1.66 – 1.50 (m, 8H), 1.35 (Sextet, 2H, $J = 7.2$ Hz), 0.93 (t, 3H, $J = 7.2$ Hz); ^{13}C NMR (125 MHz, CDCl_3) δ 202.5, 149.2, 92.4, 40.3, 39.6, 32.9, 28.0, 27.4, 26.3, 25.9, 22.3, 13.8; IR (neat): 2957, 2932, 2857, 1694, 1606, 1464, 1448, 1404, 1350, 1260, 1221, 1145, 1077, 1069, 984, 854; MS (ES^+) Calculated for $[\text{C}_{12}\text{H}_{19}\text{NaIO}]^+$: 329.0; Found: 329.0.

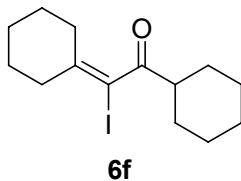


6d

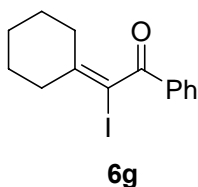
Compound **6d** was prepared in 99% yield according to the general procedure B. ^1H NMR (400 MHz, CDCl_3) δ 2.80 (t, 2H, $J = 7.2$ Hz), 2.47 – 2.42 (m, 4H), 1.69 – 1.49 (m, 10H), 1.35 (Sextet, 2H, $J = 7.2$ Hz), 0.93 (t, 3H, $J = 7.2$ Hz); ^{13}C NMR (125 MHz, CDCl_3) δ 202.4, 151.4, 96.1, 41.5, 40.4, 33.5, 29.2, 28.5, 28.0, 26.4, 26.1, 22.3, 13.8; IR (neat): 2956, 2927, 2857, 1688, 1599, 1464, 1457, 1404, 1351, 1266, 1160, 1132, 1081, 957, 909; MS (ES^+) Calculated for $[\text{C}_{13}\text{H}_{21}\text{NaIO}]^+$: 343.0; Found: 343.0.



Compound **6e** was isolated as a mixture of geometrical isomers ($Z/E = 1/2.31$) in 88% yield according to the general procedure B. ^1H NMR (500 MHz, CDCl_3) (major isomer) δ 2.83 (Quintet, 1H, $J = 7.0$ Hz), 2.79 (t, 2H, $J = 7.5$ Hz), 1.88 (s, 3H), 1.61 (Quintet, 2H, $J = 7.5$ Hz), 1.35 (Quintet, 2H, $J = 7.5$ Hz), 1.02 (d, 6H, $J = 7.0$ Hz), 0.93 (t, 3H, $J = 7.5$ Hz); ^1H NMR (500 MHz, CDCl_3) (minor isomer) δ 2.94 (Quintet, 1H, $J = 7.0$ Hz), 2.78 (t, 2H, $J = 7.5$ Hz), 1.77 (s, 3H), 1.61 (Quintet, 2H, $J = 7.5$ Hz), 1.35 (Quintet, 2H, $J = 7.5$ Hz), 1.02 (d, 6H, $J = 7.0$ Hz), 0.93 (t, 3H, $J = 7.5$ Hz) ^{13}C NMR (125 MHz, CDCl_3) (major isomer) δ 202.5, 150.6, 95.9, 40.3, 39.8, 33.5, 26.3, 22.3, 21.0, 19.7, 13.8; ^{13}C NMR (125 MHz, CDCl_3) (minor isomer) δ 202.7, 149.5, 93.9, 40.3, 39.8, 33.5, 26.3, 22.3, 21.6, 14.6, 13.8; IR (neat): 2962, 2932, 2872, 1695, 1620, 1615, 1464, 1404, 1385, 1363, 1342, 1225, 1151, 1101, 1062, 983, 900; MS (ES^+) Calculated for $[\text{C}_{11}\text{H}_{19}\text{NaIO}]^+$: 317.1; Found: 317.0.



Compound **6f** was prepared in 96% yield according to the general procedure B. ^1H NMR (500 MHz, CDCl_3) δ 3.03 (tt, 1H, $J = 11, 3.0$ Hz), 2.42 (t, 2H, $J = 7.5$ Hz), 2.30 (t, 2H, $J = 6$ Hz), 1.92 (d, 2H, $J = 12.5$ Hz), 1.80–1.77 (m, 2H), 1.69–1.50 (m, 7H), 1.41–1.10 (m, 5H); ^{13}C NMR (125 MHz, CDCl_3) δ 204.9, 149.4, 91.8, 47.5, 39.6, 33.4, 28.8, 28.0, 27.4, 25.9, 25.8, 25.7; IR (neat): 3351, 2930, 2853, 2609, 1684, 1616, 1448, 1350, 1309, 1219, 1149, 1084, 982; MS (ES^+) Calculated for $[\text{C}_{14}\text{H}_{21}\text{INaO}]^+$: 355.0; Found: 355.0.

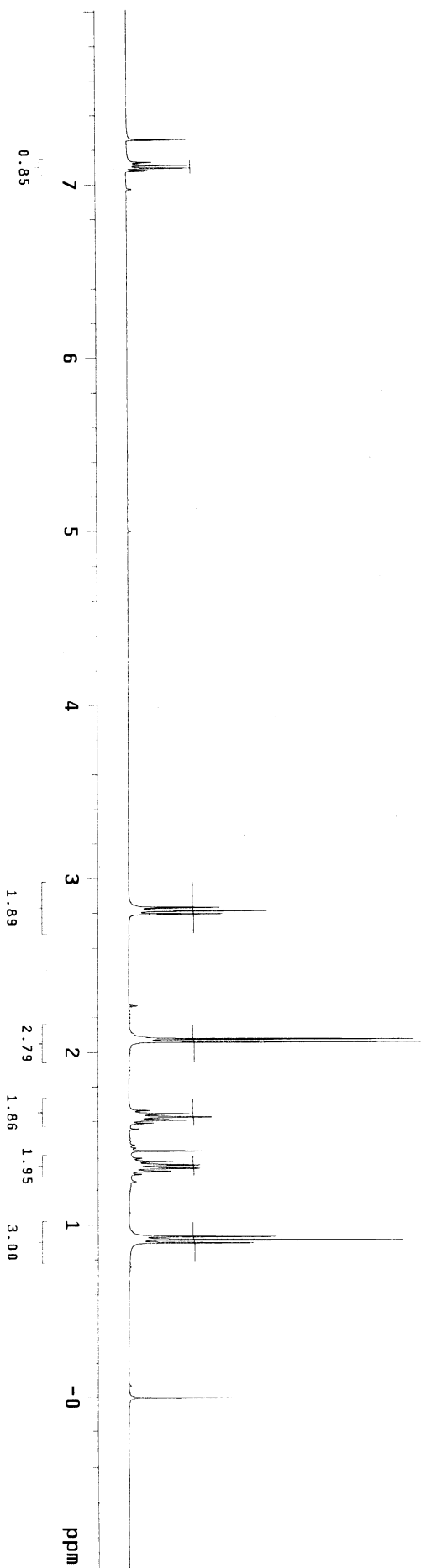
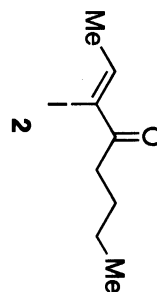


Compound **6g** was prepared in 83% yield according to the general procedure B. ^1H NMR (400 MHz, CDCl_3) δ 7.98 (d, 2H, $J = 8$ Hz), 7.50 (t, 1H, $J = 7.6$ Hz), 7.48 (t, 2H, $J = 7.6$ Hz), 2.55 (t, 2H, $J = 6$ Hz), 2.22 (t, 2H, $J = 6$ Hz), 1.75–1.69 (m, 2H), 1.60–1.54 (m, 2H), 1.47–1.42 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 193.1, 149.6, 134.0, 133.7, 130.0, 128.7, 87.7, 38.9, 33.2, 27.5, 27.4, 25.8; IR (neat): 3308, 3061, 2932, 2854, 2668, 2201, 1966, 1908, 1817, 1777, 1664, 1632, 1596, 1579, 1448, 1311, 1221, 1173, 1022, 982, 824; MS (ES^+) Calculated for $[\text{C}_{14}\text{H}_{15}\text{INaO}]^+$: 349.0; Found: 349.0.

Automation directory: /home/walkup/vnmr/sys/data/auto_2007.01.04_12
File: exp
Sample id: tmpstudy

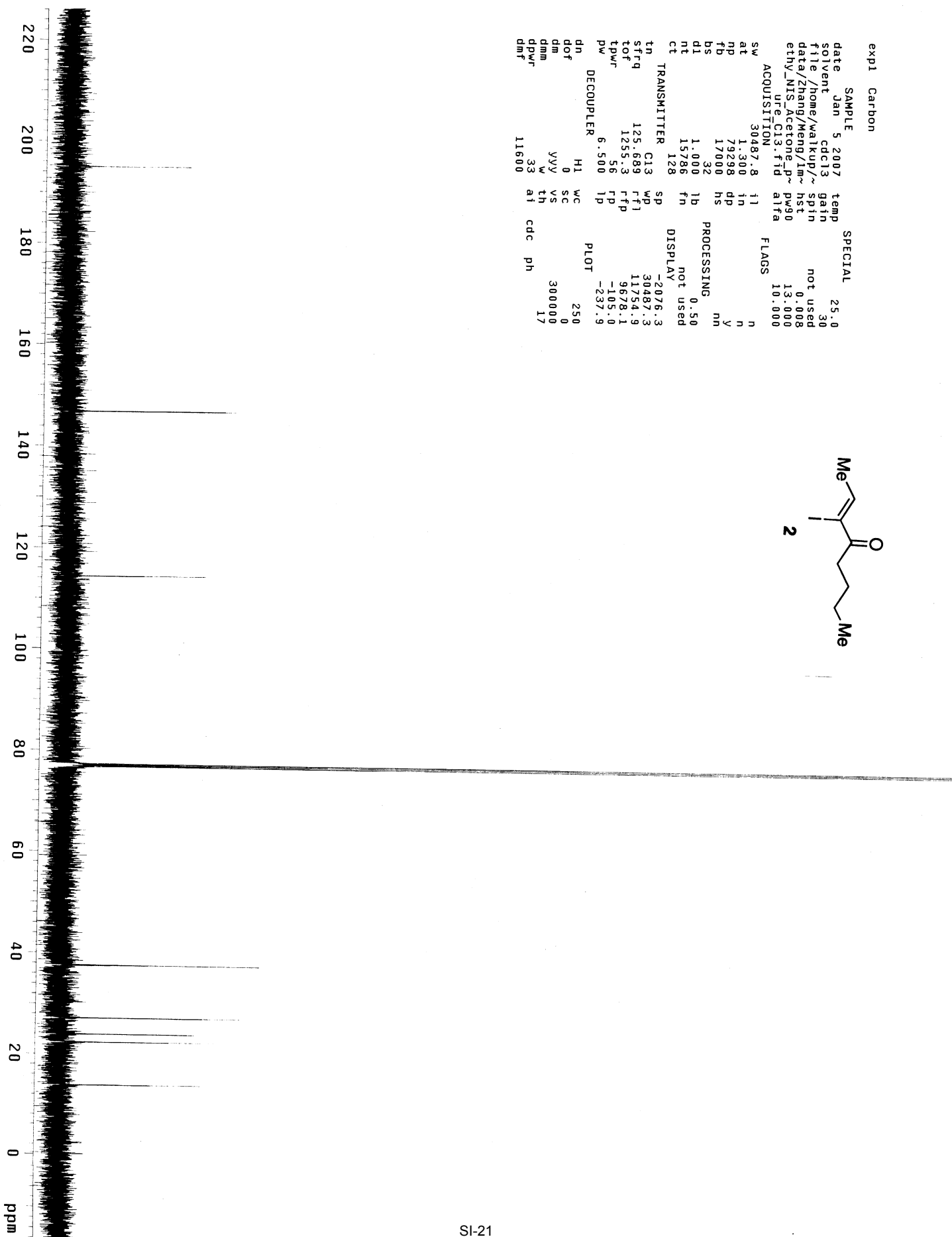
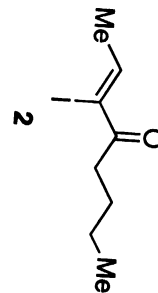
Pulse Sequence: szpul
Solvent: cdcl3
Temp: 25.0 C / 298.1 K
Operator: walkup
VNMRS-400 "NMR400"

Relax. delay: 1.000 sec
Pulse: 45.0 degrees
Acq. time: 2.049 sec
Width: 6410.3 Hz
8 repetitions
OBSERVE H1, 399.7793055 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min, 30 sec



exp1 Carbon

SAMPLE SPECIAL
date Jan 5 2007 temp 25.0
solvent cdc13 gain 30
file /home/walkup/~ not used
data/Zhang/Meng/1m~ hst 0.008
ethy_NIS_Acetone-P~ pw90 13.000
ure_C13.fid alfa 10.000
ACQUISITION
sw 30487.8 f1
at 1.300 n
np 79298 dp y
fb 17000 hs nm
bs 32
d1 1.000 lb
nt 15786 fn
ct 128
TRANSMITTER
tn C13 sp -2076.3
sfrq 125.689 wp 30487.3
tof 1255.3 rfp 11754.9
tpwr 56 rfp 9678.1
pw 6.500 ip -105.0
DECOUPLER
dn H1 wc
dof 0 sc 250
dm 0 vs 0
dmm YYY 300000
dpwr w th 17
dmf 33 ai cdc ph 11600

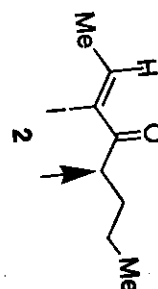


Automation directory: /home/walkup/vnmrSYS/data/2007.04.10_60
File: /home/walkup/data/Zhang/Meng/neozy_1me_NIS_2.fid
Sample id: tmpstudy

Pulse Sequence: NOESY1D

Solvent: cdcl3
Temp: 25.0 C / 298.1 K
Operator: walkup
File: neozy_1me_NIS_2
VNMRS-500 "nmr500"

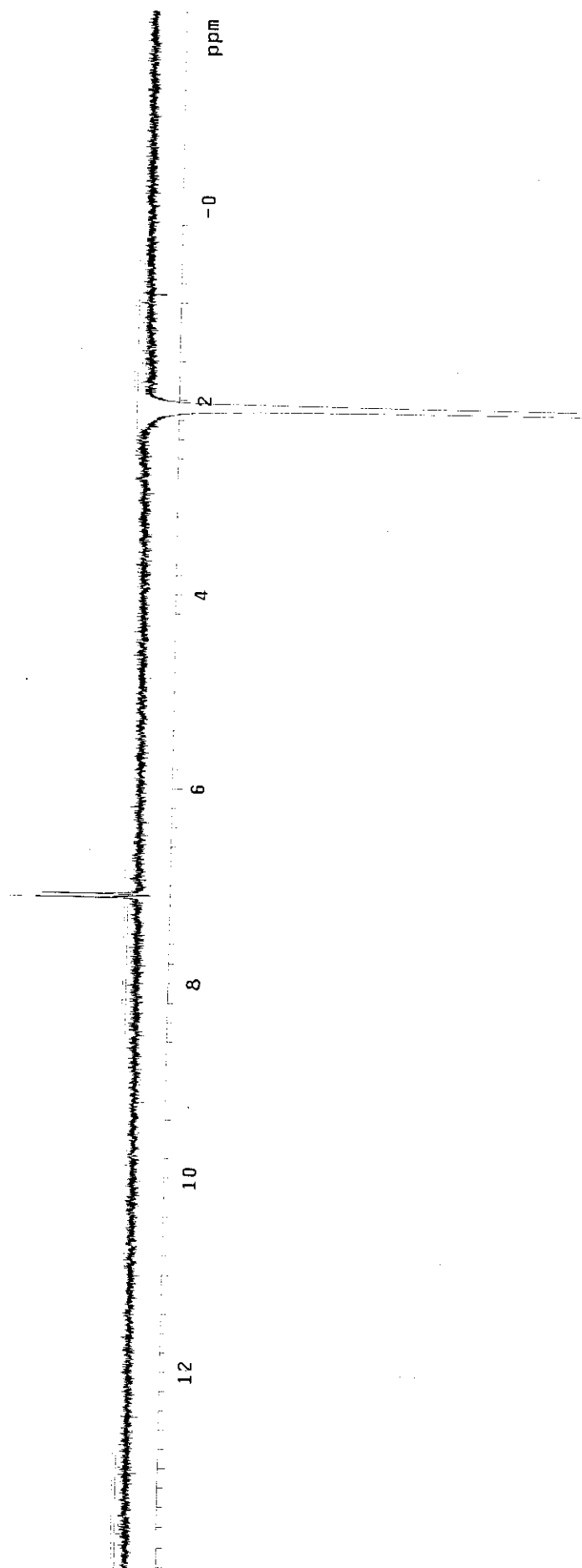
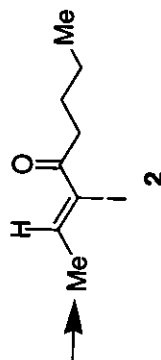
Relax. delay 1.000 sec
Pulse 90.0 degrees
Mixing 0.500 sec
Acq. time 1.998 sec
Width 8012.8 Hz
96 repetitions
OBSERVE H1, 499.8058870 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 10 hr, 36 min, 14 sec



Automation directory: /home/walkup/vnmrsys/data/auto_2007.04.10_60
File : /home/walkup/data/Zhang/Meng/neozy_1me_NIS_3.fid
Sample id : tmpstudy

Pulse Sequence: NOESY1D
Solvent: cdcl3
Temp: 25.0 C / 298.1 K
Operator: walkup
File: neozy_1me_NIS_3
VNMRS-500 "nmr500"

Relax. delay 1.000 sec
Pulse 90.0 degrees
Mixing 0.500 sec
Acq. time 1.998 sec
Width 8012.8 Hz
136 repetitions
OBSERVE H1, 499.8058870 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 10 hr, 50 min, 9 sec

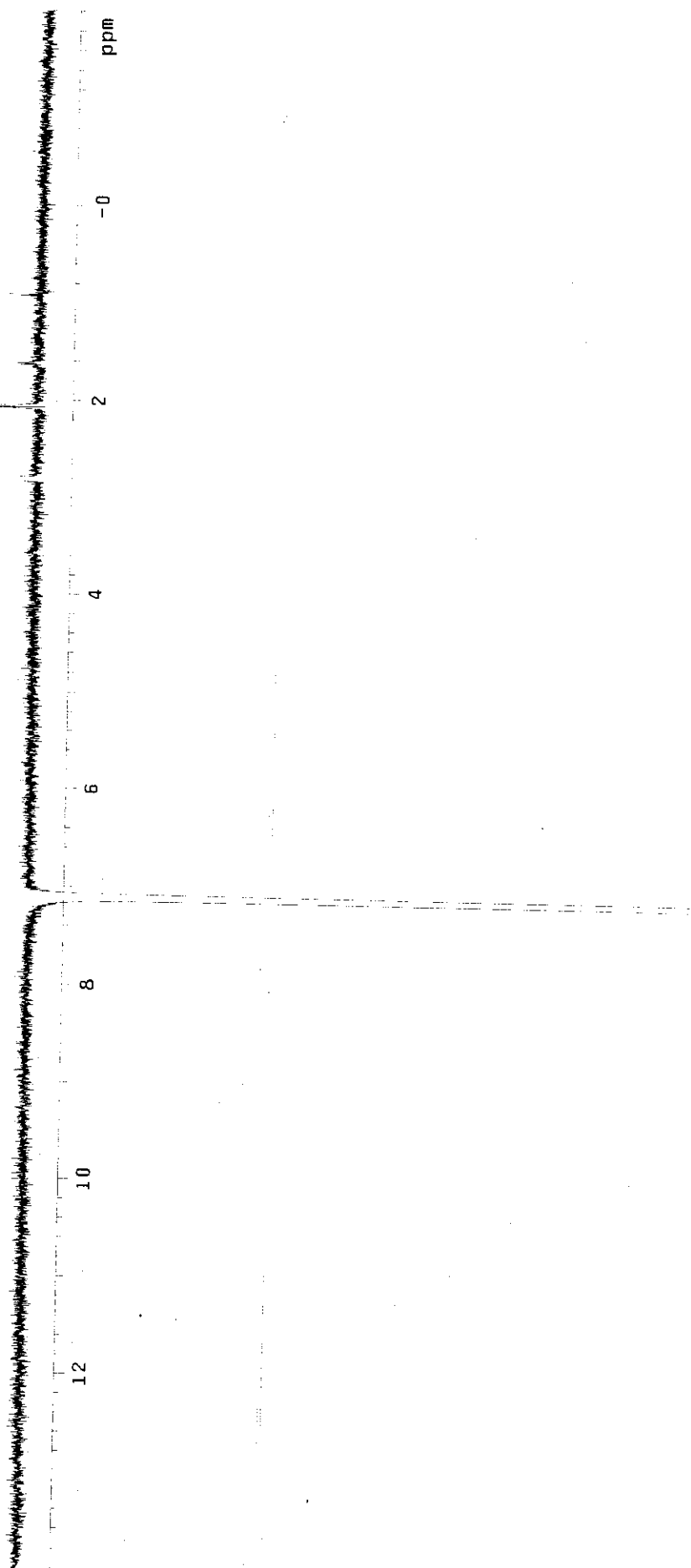
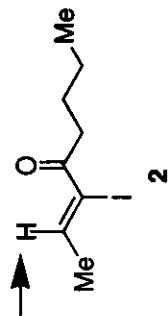


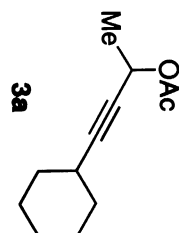
Automation directory: /home/walkup/vnmrSYS/data/auto.2007.04.10_60
File : /home/walkup/data/Zhang/Meng/neozy_ime_NIS_3.fid
Sample id : tmpstudy

Pulse Sequence: NOESY1D

Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: walkup_NIS_3
File: neozy_ime_NIS_3
VNMR-500 "nmr500"

Relax. delay 1.000 sec
Pulse 90.0 degrees
Mixing 0.500 sec
Acq. time 1.998 sec
Width 8012.8 Hz
136 repetitions
OBSERVE H1, 499.8058870 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 10 hr, 50 min, 9 sec





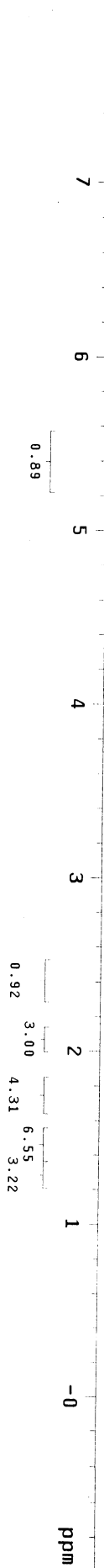
exptl Proton

SAMPLE		SPECIAL	
date	Feb 16 2007	temp	25.0
solvent	cdcl3	gain	not used
file	/home/walkup/~	spin	not used
data	/Zhang/Meng/JM~	hst	0.008
e_C6_acetate-SM-H1~		pw90	14.700
		alt	6.600

ACQUISITION		PROCESSING	
sw	8012.8	11	n
at	2.049	in	n
np	32830	dp	y
fb	4000	hs	n
bs	32		
ss	2		
dl	1.000	1b	fn
nt	8		65536

TRANSMITTER		DISPLAY	
ct	8	sp	-501.0
tn	H1	wp	4494.3
stfq	499.809	rfl	1003.8
tof	499.7	rtp	0
tpwr	54	lp	-155.6
pw	7.350		-36.5

DECOUPLER		PLOT	
dn	C13	wc	250
dof	0	sc	0
dm	nnn	th	100
dmm	c	at	cdc
dpwr	34		ph
dmf	32258		

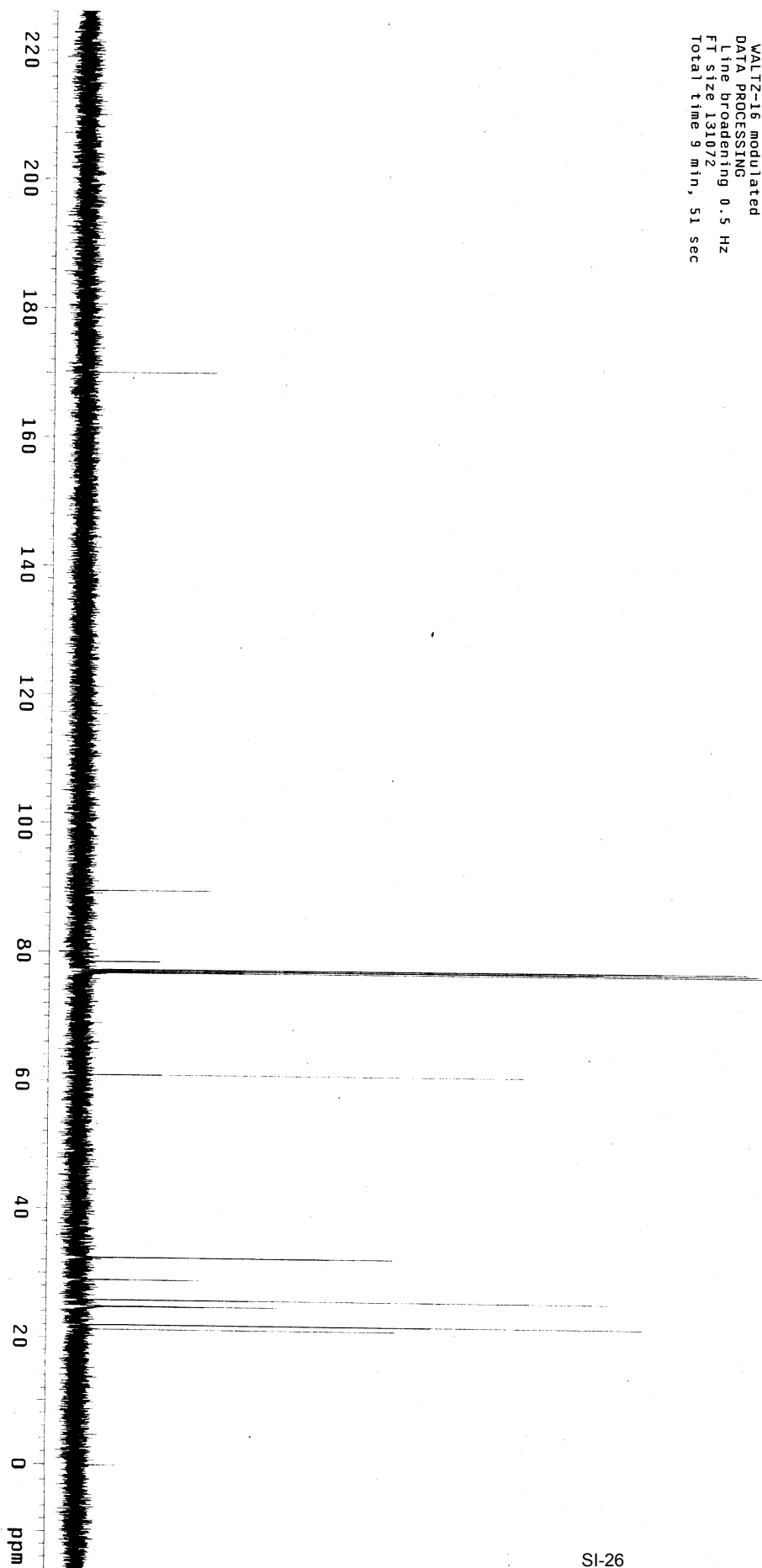
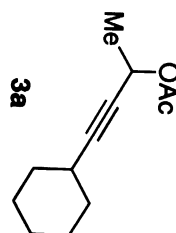


Automation directory: /home/walkup/vnmrsvs/data/auto_2007.02.16_10
File : Aug.04/data/cdc13_01.fid
Sample id : Aug.04

Pulse Sequence: s2pul

Solvent: cdc13
Temp.: 25.0 C / 298.1 K
Operator: walkup
File: cdc13_01
VNMRS-500 "nmr500"

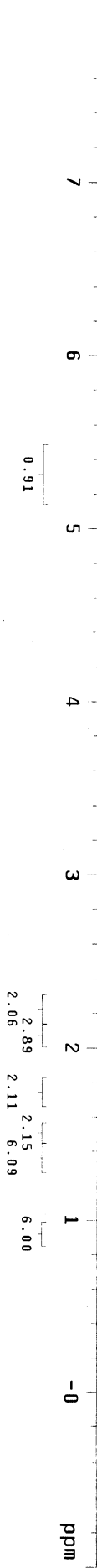
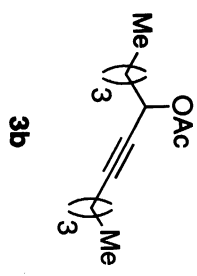
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 30487.8 Hz
64 repetitions
OBSERVE C13, 125.6762906 MHz
DECOUPLE H1, 499.8083861 MHz
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 9 min, 51 sec



Automation directory: /home/walkup/vnmrSYS/data/auto_2007.02.16_10
 File : Aug_02/data/cdc13_01.fid
 Sample id : Aug.02

Pulse Sequence: s2pul
 Solvent: cdc13
 Temp: 25.0 C / 298.1 K
 Operator: walkup
 File: cdc13_01
 VNMRS-500 "hmr500"

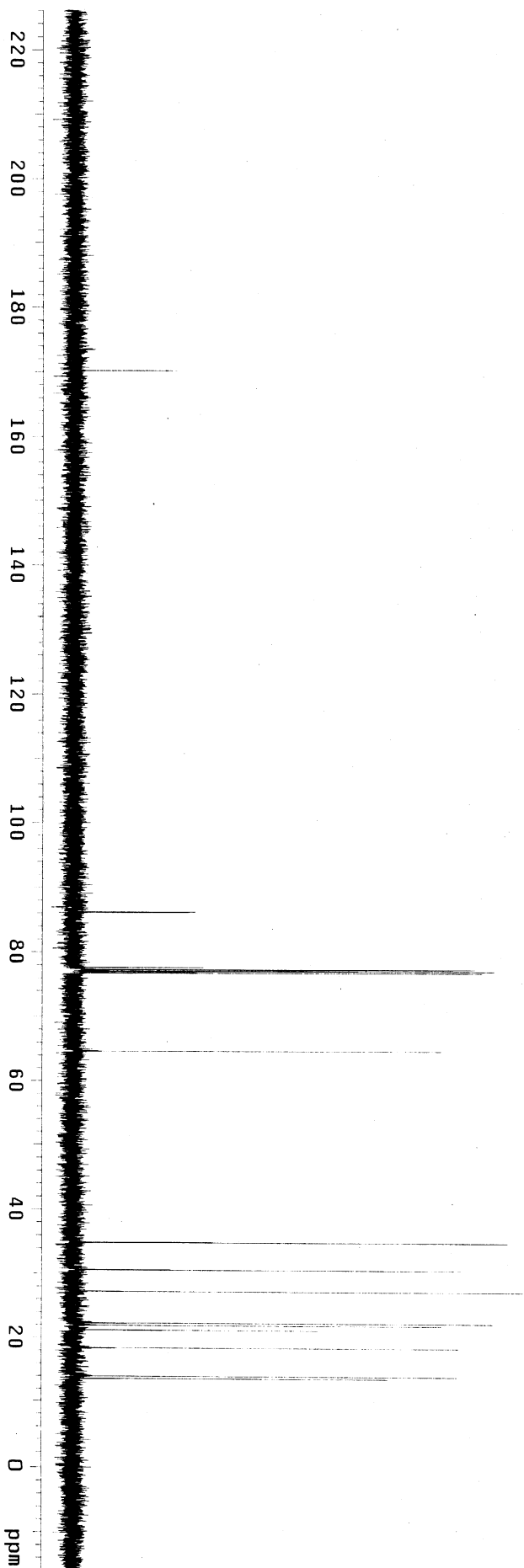
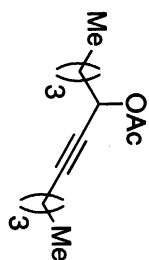
Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.049 sec
 Width 8012.8 Hz
 8 repetitions
 OBSERVE H1, 499.805822 MHz
 DATA PROCESSING
 Line broadening 0.2 Hz
 FT size 65536
 Total time 0 min, 30 sec

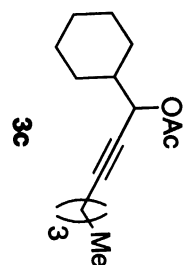


Automation directory: /home/waikup/vnmrSYS/data/auto_2007.02.16_10
File : Aug.03/data/cdc13_01.fid
Sample id : Aug.03

Pulse Sequence: szpul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: waikup
File: cdc13_01
VNMRS-500 "nmr500"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 30487.8 Hz
64 repetitions
OBSERVE C13, 125.6762906 MHz
DECOUPLE H1, 499.8083861 MHz
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 9 min, 51 sec





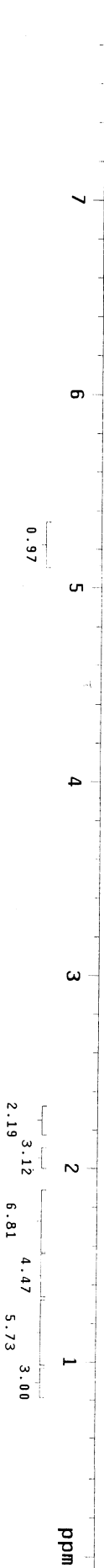
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expt Proton

SAMPLE
date Feb 16 2007 temp 25.0
solvent cdc13 gain not used
file /home/walkup/~ spin not used
vnmrsvs/data/auto_~ hsf 0.008
2007.02.16_10/AUG.~ pw90 14.700
01/data/cdc13_01.f~ alfa 6.600

SPECIAL
id 11 flags n
ACQUISITION
sw 8012.8 in n
at 2.049 dp y
np 32830 hs n
fb 4000
bs 32 lb
ss 2 fn
d1 1.000 DISPLAY -41.0
nt 8 sp 4030.4
ct 8 wp 1007.6
tn TRANSMITTER H1 rfp 0
sfreq 499.809 rf 154.2
tof 499.7 lp -39.2
tpwr 54 PLOT 250
pw 7.350 wc 0
DECOUPLER C13 sc 0
dn 0 vs 424
dof 0 th 50
dm nn ai cdc ph
dmm c
dpwr 34
dmf 32258

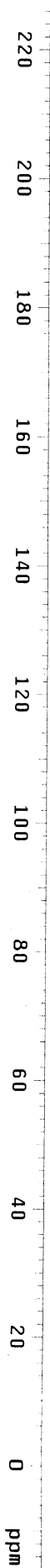
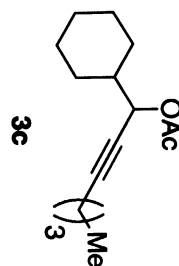
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expt Carbon

SAMPLE SPECIAL 25.0
date Feb 16 2007 temp 30
solvent cdc13 gain 30
file /home/walkup/~ not used
vnmr/sv/data/auto/~ hst 0.008
2007.02.16_10/AUG.~ pw90 15.300
02/data/cdc13_01.f~ alfa 10.000

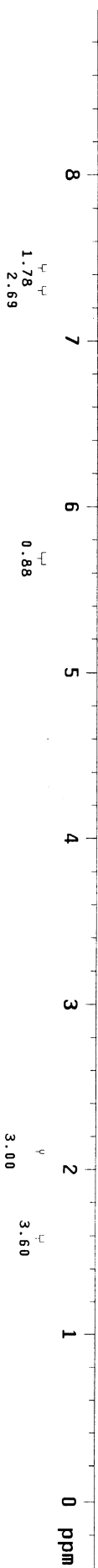
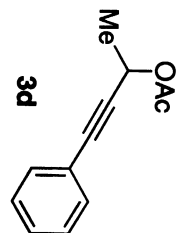
id id
ACQUISITION
sw 30487.8 f1 n
at 1.300 in n
np 79298 dp y
fb 17000 hs n
bs 32 lb PROCESSING 0.50
dl 1.000 fn not used
nt 500
ct 64 DISPLAY
TRANSMITTER
tn C13 sp -2077.7
sfrq 125.689 wp 30487.3
tof 1255.3 rfi 11756.2
tpwr 49 rp 9678.1
pw 7.650 lp 150.8
DECOUPLER PLOT -253.5
dn H1 WC 250
dof HI SC 0
dm 0 VS 24229
dmm YVY th 6
dpwr w ai cdc ph
dmf 12200



STANDARD 1H OBSERVE - profile

exp2 Proton

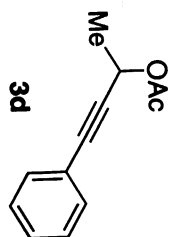
SAMPLE		SPECIAL	
date	Apr 9 2006	temp	25.0
solvent	cdcl3	gain	not used
file	/home/waikup/~	spin	not used
nmrsvs/data/Bel1/~	hst	0.008	
Violet/auto-2006.04~	pw90	13.900	
.09_06/s_0_01/data~	alpha	6.600	
ACQUISITION: f1d		FLAGS	n
sw	6410.3	in	n
at	2.049	dp	y
np	26264	hs	nn
fb	4000	PROCESSING	
bs	32	lb	0.20
ss	2	fn	65536
d1	1.000	DISPLAY	
nt	8	sp	-169.8
ct	8	wp	3766.6
TRANSMITTER		rf1	806.4
tn	H1	rfp	0
stfq	399.782	rp	72.5
tof	399.5	tp	-26.7
tpwr	59	PLOT	
pw	6.950	wc	250
DECOUPLER		sc	0
dn	C13	vs	55
dof	0	th	2
dm	nmn	at	cdc ph
dmm	C		
dpwr	34		
dmf	29412		



STANDARD 1H OBSERVE - profile

exp2 Carbon

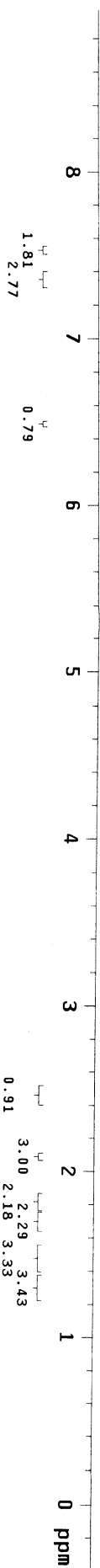
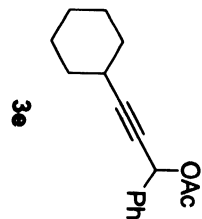
SAMPLE SPECIAL
date Apr 9 2006 temp 25.0
solvent cdc13 gain 30
file /home/waikup/~ hst not used
vnmrsvs/data/Be11/~ pw90 0.008
Voiet/auto_2006.04~ 9.700
.09_06/s_0_02/data~ alfa 10.000
/cdc13.01.fid
ACQUISITION
sw 24509.8 in n
at 1.300 dp y
np 63750 hs nn
fb 17000
bs 64 lb
d1 1.000 fn not used
nt 1024 DISPLAY
ct 256 SP -1723.6
TRANSMITTER C13 wp 24509.1
tn rf1 9468.7
strq 100.535 rfp 7740.4
tof 1042.6 rp 121.2
tpwr 55 1p -143.6
pw 4.850
DECOUPLER wc 250
dn H1 SC 0
dof 0 VS 50000
dm YVY th 68
dmm W
dpwr 41
dmf 9300



STANDARD 1H OBSERVE - profile

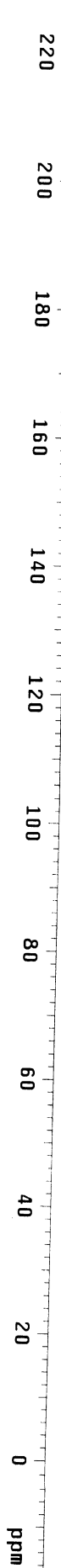
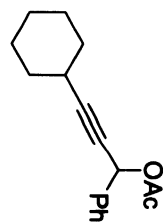
expt Proton

SAMPLE		SPECIAL	
date	Apr 10 2006	temp	25.0
solvent	cdcl3	gain	not used
file	/home/walkup/~	spin	not used
nmrSYS/data/Frost~	hst	pw90	13.900
/auto_2006.04.10_1~	alpha	6.600	
4/s_001/data/cdcl3	3.01.fid	FLAGS	
ACQUISITION		PROCESSING	
sw	6410.3	in	n
at	2.049	dp	y
np	26264	hs	nn
fb	4000	lb	0.20
bs	32	fn	65536
ss	2	sd	-163.5
di	1.000	wp	3751.5
nt	8	rf1	807.7
ct	8	rfp	69.3
tn	H1	rfp	-13.7
stfq	399.782	rfp	
tof	399.5	rfp	
tpwr	59	WC	250
pw	6.950	SC	0
DECOUPLER		VS	100
dh	C13	th	2
dof	0	at	cdc ph
dm	nmh		
dmm	c		
dpwr	34		
dmf	29412		



expi Carbon

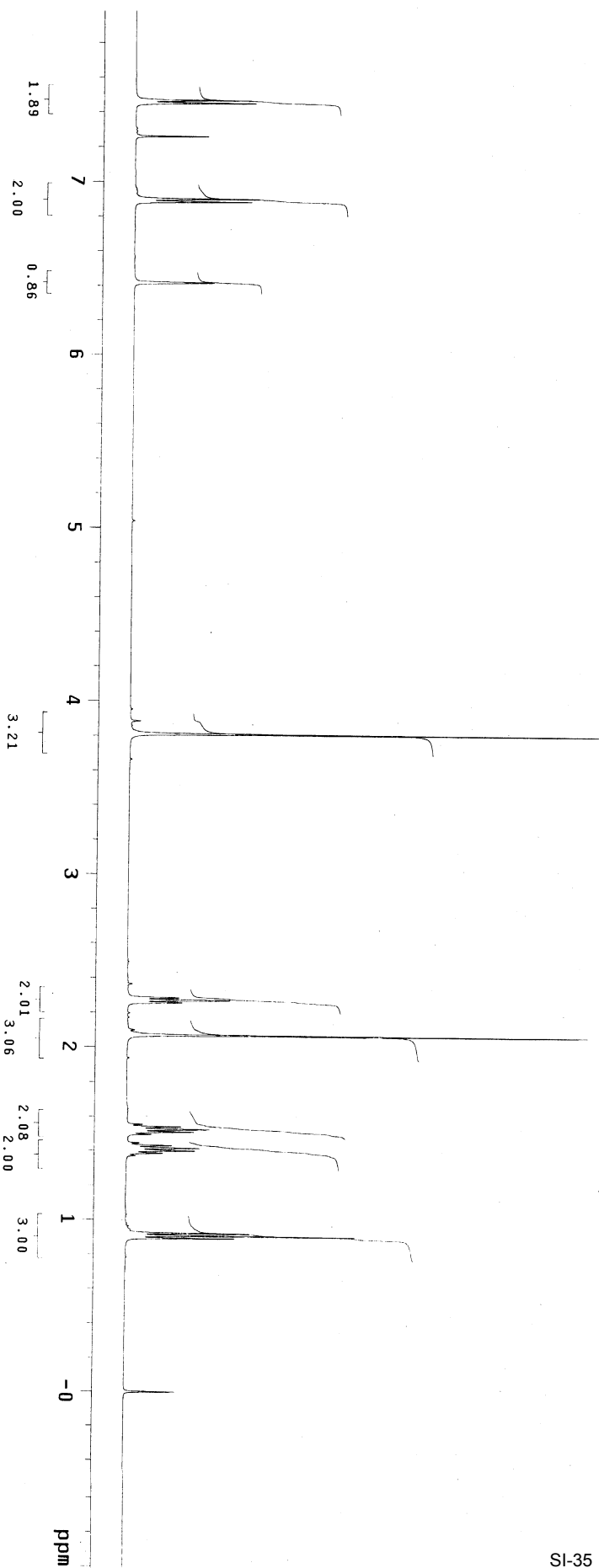
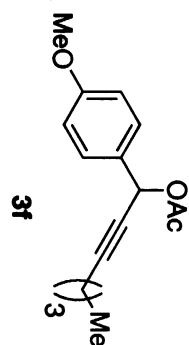
SAMPLE SPECIAL 25.0
date Apr 10 2006 temp
solvent cdc13 gain 30
file /home/walkup/~ spin
vmrsvs/data/frost~ hsf not used
/auto_2006.04.10_1~ pw90 0.008
4/s_01/data/cdc1~ alfa 9.700
3_02.fid 10.000
ACQUISITION
sw 24509.8 11 n
at 1.300 1n in n
np 63750 dp hs v
fb 17000 hs PROCESSING nm
bs 64 1b 0.50
dl 1.000 fn not used
nt 1024 1024 DISPLAY
ct 448 448 SP -1722.8
tn TRANSMITTER C13 WP 24509.1
stfq 100.535 rfi 9463.9
tof 1042.6 rfp 7740.4
tpwr 55 1p 121.1
pw 4.850 PLOT -133.3
DECOUPLER WC 250
dn H1 SC 0
dof 0 VS 40000
dm YYV th 68
dmm W ai cdc ph
dpwr 41
dmf 9300

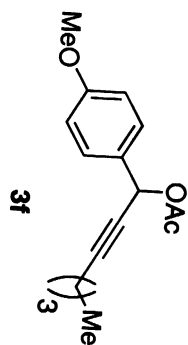


Automation directory: /home/walkup/vnmrSYS/data/auto_2007.02.16_10
 File : Aug.06/data/cdc13_01.fid
 Sample id : Aug.06

Pulse Sequence: s2pul
 Solvent: cdc13
 Temp: 25.0 C / 298.1 K
 Operator: walkup
 File: cdc13_01
 VNMRS-500 "nmr500"

Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.049 sec
 Width 8012.8 Hz
 8 repetitions
 OBSERVE H1, 499.805864 MHz
 DATA PROCESSING
 Line broadening 0.2 Hz
 FT size 65536
 Total time 0 min, 30 sec



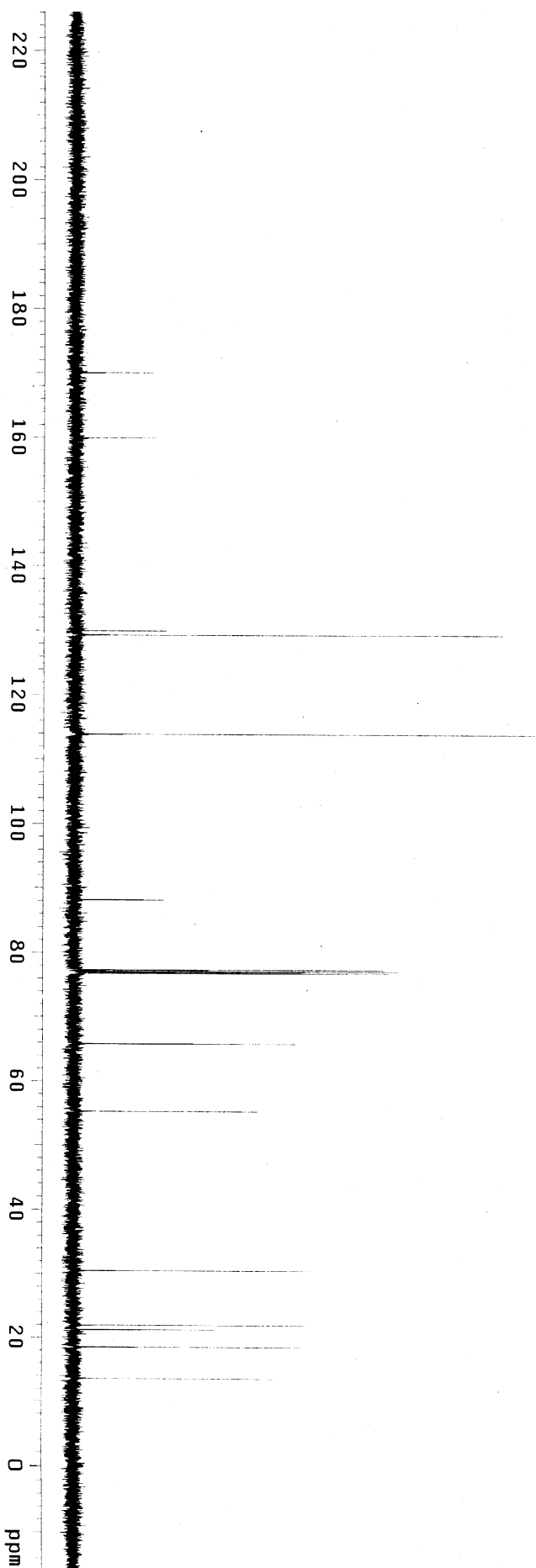


Automation directory: /home/walkup/vnmr/sys/data/auto_2007.02.16_10
 File : Aug.07/data/cdc13_01.fid
 Sample id : Aug.07

Pulse Sequence: s2pul

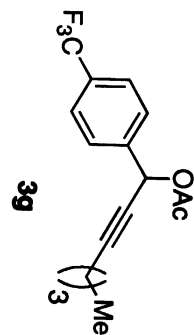
Solvent: cdc13
 Temp. 25.0 C / 298.1 K
 Operator: walkup
 File: cdc13_01
 VNMRS-500 "nmr500"

Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.300 sec
 Width 30487.8 Hz
 64 repetitions
 OBSERVE C13, 125.6762919 MHz
 DECOUPLE H1, 499.6083661 MHz
 Power 39 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 131072
 Total time 9 min, 51 sec



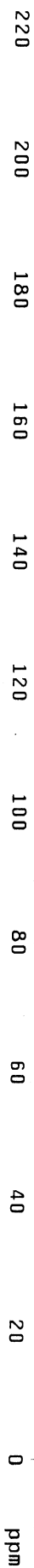
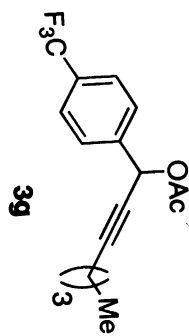
exp3 Proton

SAMPLE		SPECIAL	
date	Feb 16 2007	temp	25.0
solvent	cdcl3	gain	not used
file	/home/walkup/~	spin	not used
data	Zhang/Meng/CF~	hst	0.008
	3-acetate-H1.fid	pw90	13.900
ACQUISITION		ai	6.500
sw	6410.3	fl	6.500
at	2.049	in	n
np	26264	dp	n
fb	4000	ys	y
bs	32	hs	nn
ss	2	PROCESSING	
d1	1.000	lb	0.20
nt	8	fn	65536
ct	8	DISPLAY	
TRANSMITTER		sp	-400.1
tn	H1	wp	4000.7
sfreq	399.782	rf1	3707.9
tot	399.5	rtp	2902.4
tpwr	59	rp	-157.7
pw	6.950	lp	-34.0
DECOUPLER		PLOT	
dn	C13	wc	250
dof	0	sc	0
dm	nnn	vs	54
dmm	c	th	44
dpwr	34	ai	cdc ph
dnt	29412		



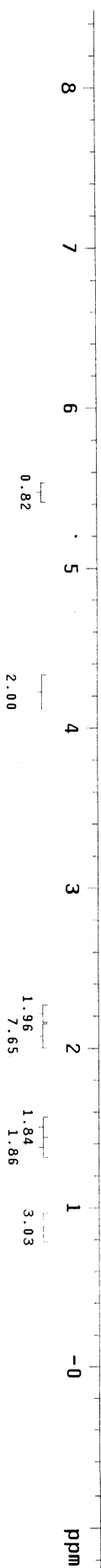
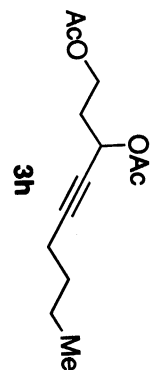
exp3 Carbon

SAMPLE SPECIAL 25.0
date Feb 18 2007 temp 30
solvent cdc13 gain 30
file /home/walkup/- spin not used
vnmr/sys/data/autoc-hst 0.008
2007.02.18.10/5.20- pw90 9.700
070218_002/data/cd- alfa 10.000
c13-01.fid
ACQUISITION
sw 24509.8 in n
at 1.300 dp y
np 63750 hs nm
fb 17000
bs 32 lb not used
d1 1.000 tn
nt 25600 DISPLAY
ct 2464 SP -1723.0
tn TRANSMITTER C13 WD 24509.1
sfreq 100.535 rfi 9464.9
tof 1042.6 rfp 7741.2
tpwr 1p 50.5
pw 4.850 PLOT -189.5
DECOUPLER WC 250
dn H1 SC 0
dof 0 VS 89494
dm YVY th 4
dmm w ai cdc ph
dpwr 41
dmf 9300



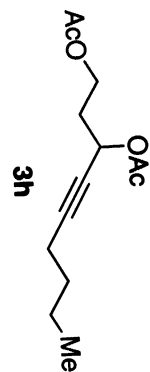
expt1 Proton

SAMPLE		SPECIAL	
date	Feb 1 2007	temp	25.0
solvent	cdcl3	gain	30
file	/home/vnmr1/~/mr400/waikup/data/~Zhang/GuoZhu/H1-20~070201-71.fid	not used	0.008
		pw90	13.900
		alpha	6.600
ACQUISITION		FLAGS	
sw	6410.3	11	n
at	2.049	in	n
np	26264	dp	y
fb	4000	hs	nn
bs	8	1b	nn
dl	1.000	1b	nn
nt	8	fn	65536
ct	8	fn	65536
TRANSMITTER		SP	DISP
tn	H1	wp	-512.9
sfrq	399.782	rfl	3906.4
tof	399.5	rfl	800.1
tpwr	59	rp	-44.7
pw	6.950	1p	-26.3
DECOUPLER		1p	PLOT
dn	C13	wc	250
dof	0	sc	0
dm	nnn	vs	1981
dmm	c	th	2
dpwr	34	ai	cdc
dmf	29412	ph	



expl Carbon

SAMPLE SPECIAL 25.0
date Feb 5 2007 temp 30
solvent cdc13 gain 30
file /home/vnmr1/nr not used
mr500/waikup/data/~nst 0.008
Zhang/Guozhu/C13-2- pw90 15.300
0070205-71-2.fid alfa 10.000
ACQUISITION
sw 30487.8 f1 n
at 1.300 in n
nd 79298 dp v
fb 17000 hs n
bs 12 h
d1 1.000 lb 0.50
nt 12000 fn not used
ct 912
TRANSMITTER
tn C13 sp -2080.1
sfrq 125.689 wp 30487.3
tof 1255.3 rfi 11757.6
tpwr 49 rfp 9677.1
pw 7.650 lp -33.4
DECOUPLER H1 PLOT -255.6
dn HI WC 250
dof 0 SC 0
dm YVY VS 14325
dmm W th ai cdc ph 9
dpwr 39
dmf 12200



expl Proton

SAMPLE date Feb 10 2007 temp 25.0
 solvent cdc13 gain 30
 file /home/vnmr1/n- not used
 mr400/waikup/data/~ hst 0.008
 Zhang/Guozhu/H1-20~ pw90 13.900
 070210-83.fid alpha 6.600

ACQUISITION
 sw 6410.3 f1
 at 2.049 in
 np 26264 dp
 fd 4000 hs
 bs 8
 d1 1.000 lb
 nt 8 fn
 ct 8

TRANSMITTER
 tn H1 sp
 stfq 399.782 rfi
 tof 399.5 rfd
 tpwr 59 fp
 pw 6.950 lp

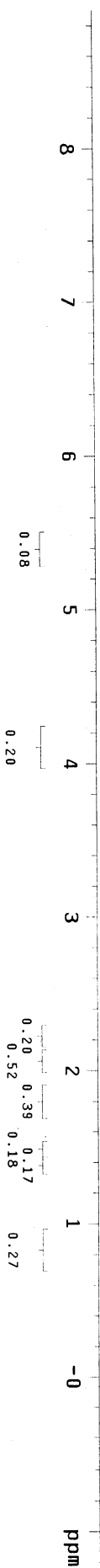
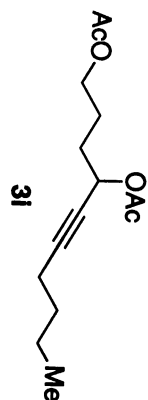
DECOUPLER
 dn C13 wc
 dof 0 sc
 dm nn vs
 dmm c th
 dpwr 34 ai
 dmf 29412

PROCESSING
 0.20
 65536

DISPLAY
 -510.4
 4068.0
 803.2
 0
 114.3
 -26.7

PLOT
 250
 0
 969
 2

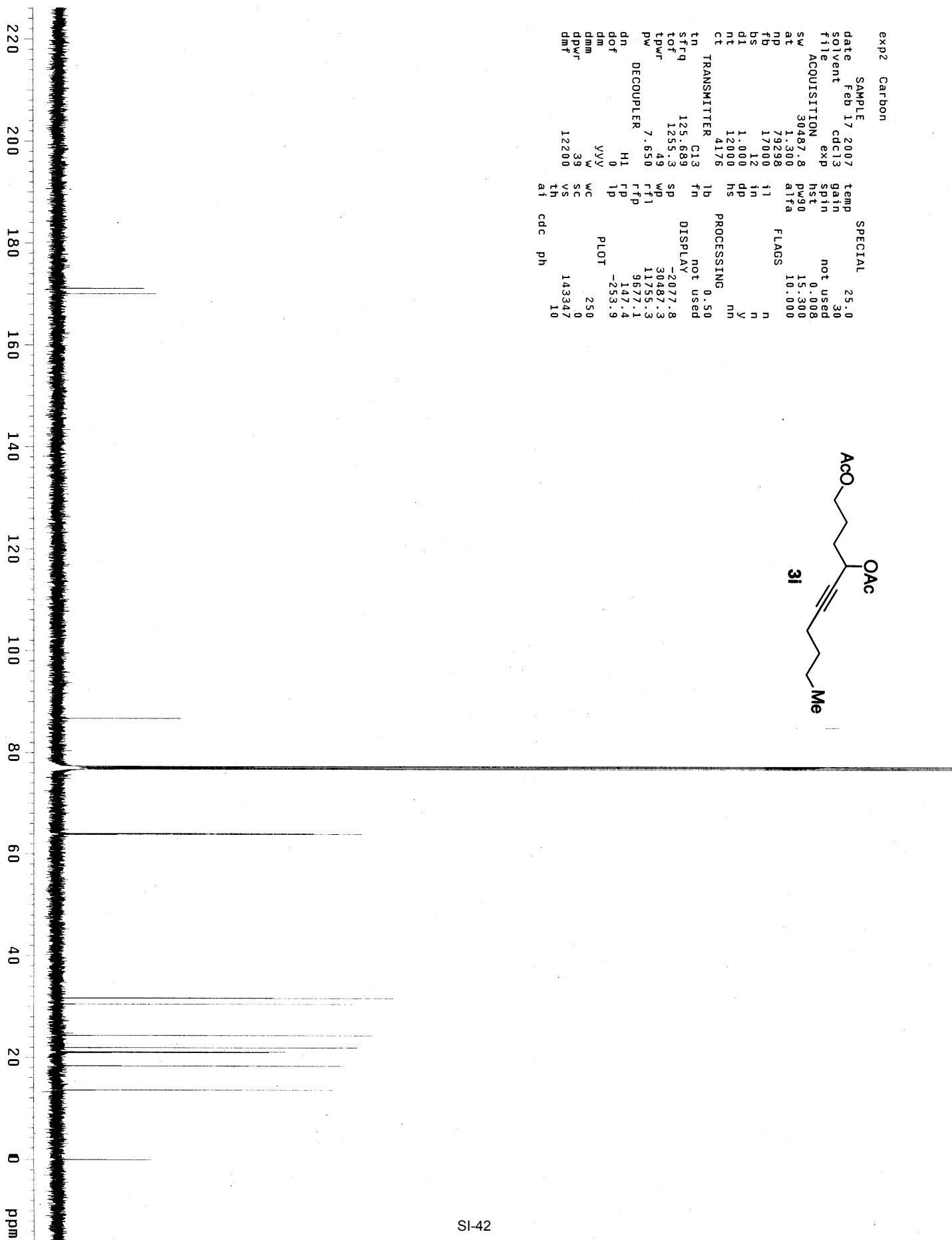
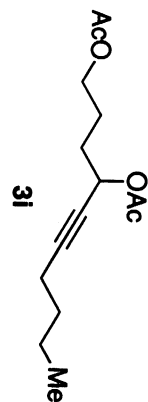
cds ph



exp2 Carbon

SAMPLE SPECIAL
date Feb 17 2007 temp 25.0
solvent cdc13 gain 30
title exp not used
ACQUISITION hst 0.008
sw 30487.8 pw90 15.300
at 1.300 alfa 10.000
np 79298
fb 17000
bs 12
dl 1.000
nt 12000
ct 4176
tn C13
sfrq 125.689
tof 1255.3
tpwr 49
pw 7.650
DECOUPLER H1
dn 0
dof 0
dm YYY
dmm W
dpwr 39
dmf 12200
ai cdc ph

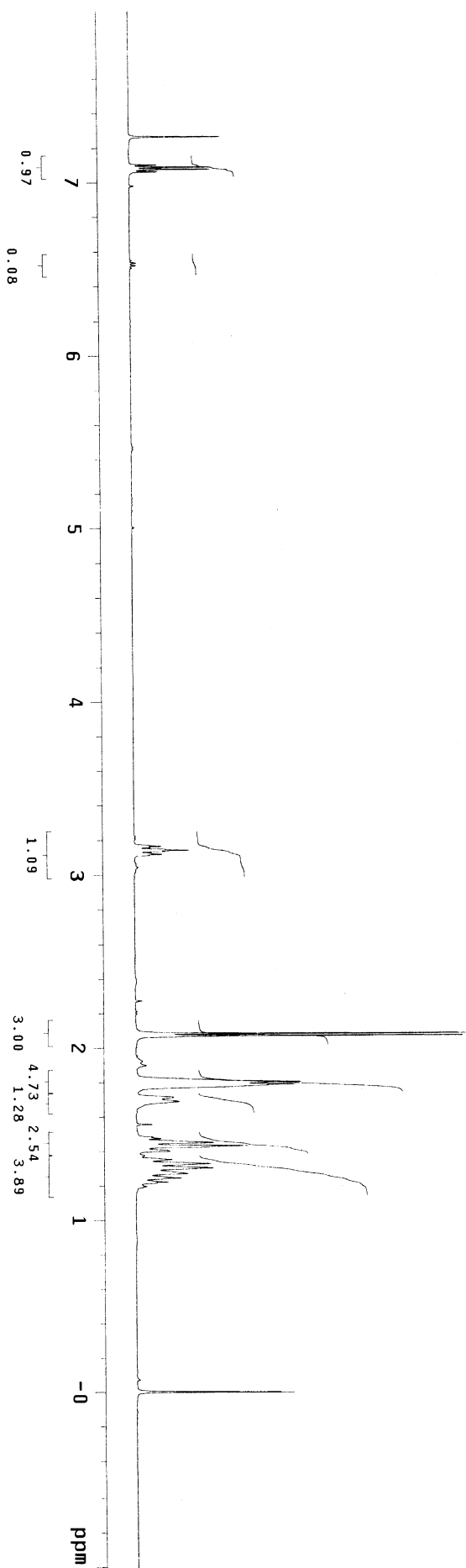
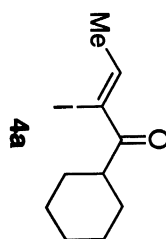
PROCESSING 0.50
not used
DISPLAY
-2077.8
30487.3
11755.3
9677.1
147.4
-253.9
PLOT 250
0
143347
10



STANDARD 1H OBSERVE - profile

expl Proton

SAMPLE		SPECIAL	
date	Jan 10 2007	temp	25.0
solvent	cdcl3	gain	not used
file	/home/wakup/~	spin	not used
data	zhang/meng/im	hst	0.008
ethy	Crting_NIS_AC	pw90	14.700
etone	pure_C13.fid	alpha	6.600
ACQUISITION		FLAGS	
sw	8012.8	il	n
at	2.049	in	n
np	32830	dp	y
fb	4000	hs	nn
bs	32	lb	nn
ss	2	fn	nn
dl	1.000	fn	nn
nt	8	fn	nn
ct	8	fn	nn
TRANSMITTER		DISPLAY	
tn	H1	sp	-512.0
sfrq	499.809	wp	4505.3
tof	499.7	rfl	1006.5
tpwr	54	rp	-160.4
pw	7.350	lp	-38.5
DECOUPLER		PLOT	
dn	C13	WC	250
dof	0	SC	0
dm	nn	VS	150
dmm	C	th	2
dpwr	34	ai	cdc
dmf	32258	ph	



STANDARD 1H OBSERVE - profile

expt Carbon

SAMPLE SPECIAL 25.0
date Jan 10 2007 temp 30
solvent cdc13 gain 30
file /home/walkup/~ not used
vnmrSYS/data/auto_~ hst 0.008
2007.01.10_04/Aug.~ pw90 15.300
05/data/cdc13_01.f~ alfa 10.000

ACQUISITION
id
sw 30487.8
at 1.300
np 79298
fb 17000
bs 64
d1 1.000
nt 256
ct 64

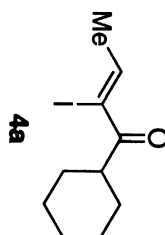
TRANSMITTER
tn C13
sfreq 125.689
tof 1255.3
tpwr 49
pw 7.650

DECOUPLER
dn H1
dof 0
dm YYY
dmm W
dpwr 39
dmf 12200

PROCESSING
hs
lb 0.50
fn not used

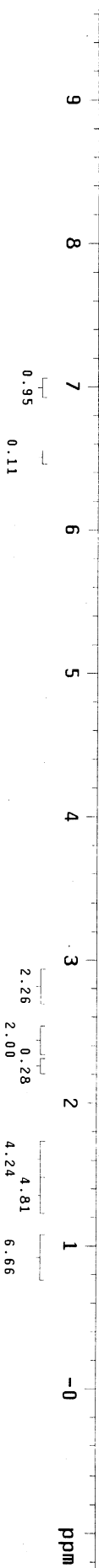
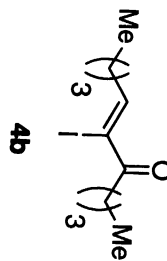
DISPLAY
sp -2075.4
wp 30487.3
rf1 11754.0
rfp 9678.1
rp -138.3
lp -228.6

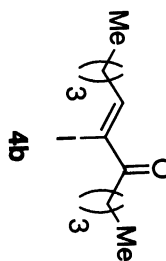
PLOT
wc 250
sc 0
vs 20000
th 6
ai cdc ph



expt Proton

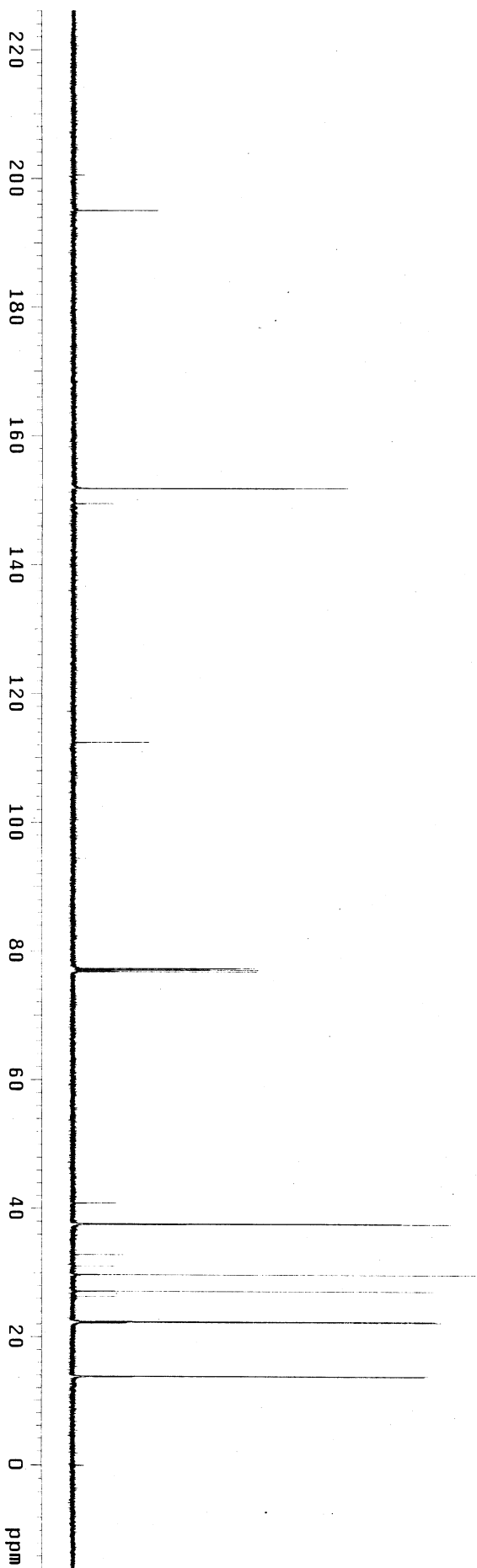
SAMPLE		SPECIAL	
date	Jan 18 2007	temp	25.0
solvent	cdcl3	gain	30
file	/home/vnmr1/n-	spin	not used
mr400	/waikup/data/~	hsc	0.008
Zhang/GuoZhu/H1-20~		pw90	13.900
070118-57.fid		alpha	6.600
ACQUISITION		FLAGS	
sw	6410.3	il	n
at	2.049	in	n
np	26264	dp	v
fb	4000	hs	nn
bs	8	ps	nn
dl	1.000	lb	0.20
nt	8	fn	65536
ct	8	fn	65536
TRANSMITTER		DISPLAY	
tn	H1	sp	-508.8
stfrq	399.782	wp	4360.7
tof	399.5	rfl	801.7
tpwr	59	rfd	0
pw	6.950	lp	141.3
DECOUPLER		PLOT	
dn	C13	wc	250
dof	0	sc	0
dm	nnn	vs	2431
dmm	c	th	3
dpwr	34	at	cdc ph
dmf	29412		





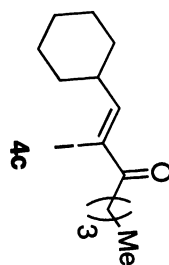
```

exp1 Carbon
SAMPLE
date Jan 18 2007 temp 25.0
solvent cdcl3 gain 30
file /home/vnmr1/n- spin not used
m500/waikup/data/~ nst 0.008
Zhang/Guozhu/C13-2~ pw90 15.500
0070118-59.fid alfa 10.000
ACQUISITION
sw 30487.8 f1 n
at 1.300 in n
np 79298 dp y
fb 17000 hs nn
bs 64
d1 1.000 lb not used
nt 1280 tn
ct 576 DISPLAY
TRANSMITTER
tn C13 sp -2078.7
sfrq 125.689 wf 30487.3
tof 1255.3 rfi 11756.2
tdwr 49 rfp 9677.1
pw 7.650 lp -109.7
DECOUPLER H1 PLOT -236.1
dn H1 WC 250
dof 0 SC 0
dm YVY VS 17864
dmm w th 9
dpwr 39 ai cdc ph
dmf 12200
  
```



expi Proton

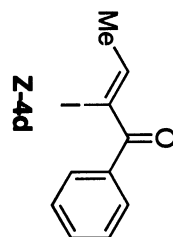
SAMPLE		SPECIAL	
date	Jan 25 2007	temp	25.0
solvent	cdcl3	gain	30
file	/home/vnmr1/n-	spin	not used
m500	walnut/data/~	hsc	0.008
Zhang/GuoZhu/H1-20~		pw90	14.700
070125-65.fid	alpha		6.600
ACQUISITION		FLAGS	
sw	8012.8	f1	n
at	2.049	in	n
np	32830	dp	y
fb	4000	hs	nn
bs	8		
dl	1.000	lb	0.20
nt	8	fn	65536
ct	8		
TRANSMITTER		DISPLAY	
tn	H1	sp	-298.1
sfrq	499.809	wp	4921.0
tof	499.7	rfl	1004.8
tpwr	54	rfp	57.5
pw	7.350	lp	-36.3
DECOUPLER		PLOT	
dn	C13	wc	250
dof	0	sc	0
dmm	nnn	vs	321
dmm	c	th	2
dpwr	34	ai	cdc ph
dmf	32258		





expl Proton

SAMPLE SPECIAL 25.0
date Jan 22 2007 temp
solvent Jan 22 2007 gain
file /home/vnmr1/n- spin
mr400/waikup/data/~ hst not used
Zhang/Guozhu/H1-20~ pw90 0.008
070122-63.fid alfa 13.500
6.500
ACQUISITION
sw 6410.3 f1
at 2.049 in n
np 26264 dp y
fb 4000 hs
bs 32 lb
dl 1.000 jb
nt 8 fn
ct 8
TRANSMITTER
tn H1 SP
sfrq 399.782 rf1
tof 399.5 rfi 4542.4
tpwr 59 fp 805.4
pw 6.950 lp 132.6
DECOUPLER PLOT -27.4
dh C13 WC 250
dof 0 SC 0
dm nn VS 46503
dmm C th
dpwr 34 ai
dmf 29412 cdc ph 3



expt Carbon

SAMPLE

SPECIAL

25.0

date Jan 21 2007

solvent cdcl3

gain 30

file /home/vnmr1/n-

not used

mf500/walkup/data/~

hst 0.008

Zhang/Guozhu/C13-2-

pv90 15.300

0070121-63-2.fid

alpha 10.000

FLAGS

n

ACQUISITION

sw 30487.8

at 1.300

in n

np 79298

dp y

fb 17000

hs nn

bs 64

hs nn

d1 1.000

lb 0.50

nt 10240

fn not used

ct 1088

fn not used

sp -2076.4

wp 30487.3

rf1 11753.9

rfp 9677.1

rfp -66.0

lp -302.4

pl 250

sc 0

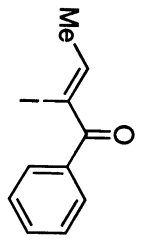
vs 58899

th 7

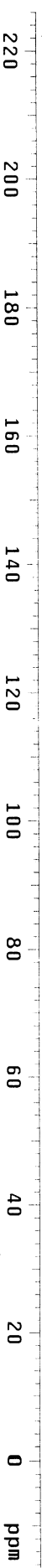
at cdc

ph

dmf 12200

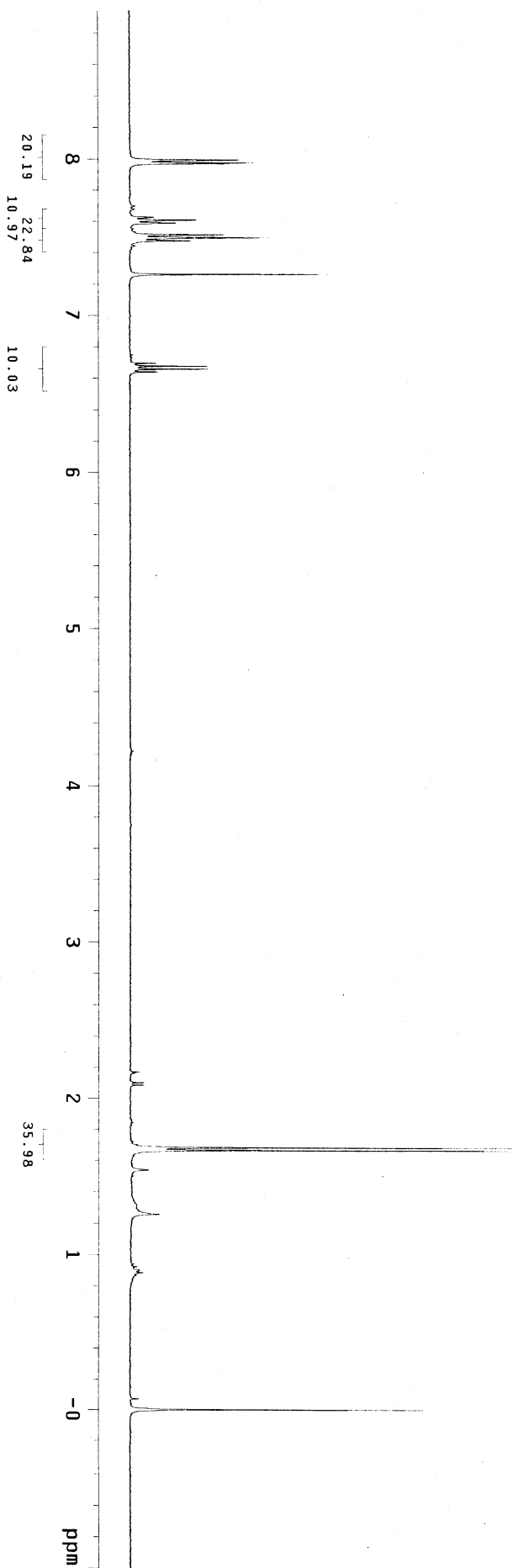
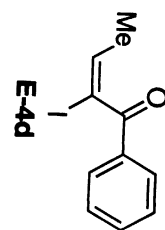


Z-4d



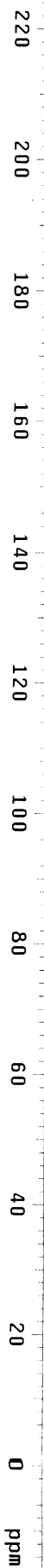
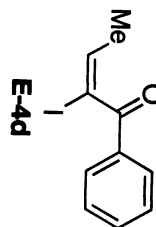
expi Proton

SAMPLE SPECIAL 25.0
date Jan 22 2007 temp 20
solvent cdc13 gain 20
file /home/vnmr1/n- not used
mr400/waikup/data/~ hsc 0.008
Zhang/GuoZhu/H1-20~ pw90 13.900
070122-62.fid alfa 6.600
ACQUISITION
SW 6410.3 f1 n
at 2.049 in n
np 26264 dp y
fb 4000 hs nn
bs 32 lb
dl 1.000 fn
nt 8
ct TRANSMITTER SP DISPLAY
tn H1 -412.2
sfrq 399.782 rfi 3987.2
tof 399.5 rfp 806.0
tpwr 59 rp 133.7
pw 6.950 lp -24.3
DECOUPLER PLOT
dn C13 WC 250
dof 0 SC 0
dm nn VS 72251
dmm C th
dpwr 34 ai cdc ph 2
dmf 29412



exp2 Carbon

SAMPLE		SPECIAL	
date	Feb 17 2007	temp	25.0
solvent	cdc13	gain	30
file	cdc13	spin	not used
ACQUISITION		nst	0.008
sw	30487.8	pw90	15.300
at	1.300	alfa	10.000
np	79298	FLAGS	
fb	17000	i1	n
bs	64	in	n
d1	1.000	dp	y
nt	24000	hs	nn
ct	896	PROCESSING	
tn	TRANSMITTER	lb	0.50
stfrq	125.689	fn	not used
tofr	1255.3	sp	DISPLAY
tdwr	49	wp	-2078.2
pw	7.650	rfl	30487.3
DECOUPLER		rfd	11755.8
dn	H1	rp	9677.1
dof	0	lp	141.5
dm	yyy	PLOT	
dmm	w	wc	-236.9
dpwr	39	sc	250
dnt	12200	vs	0
th		ai	52598
ai	cdc	ph	5



expl Proton

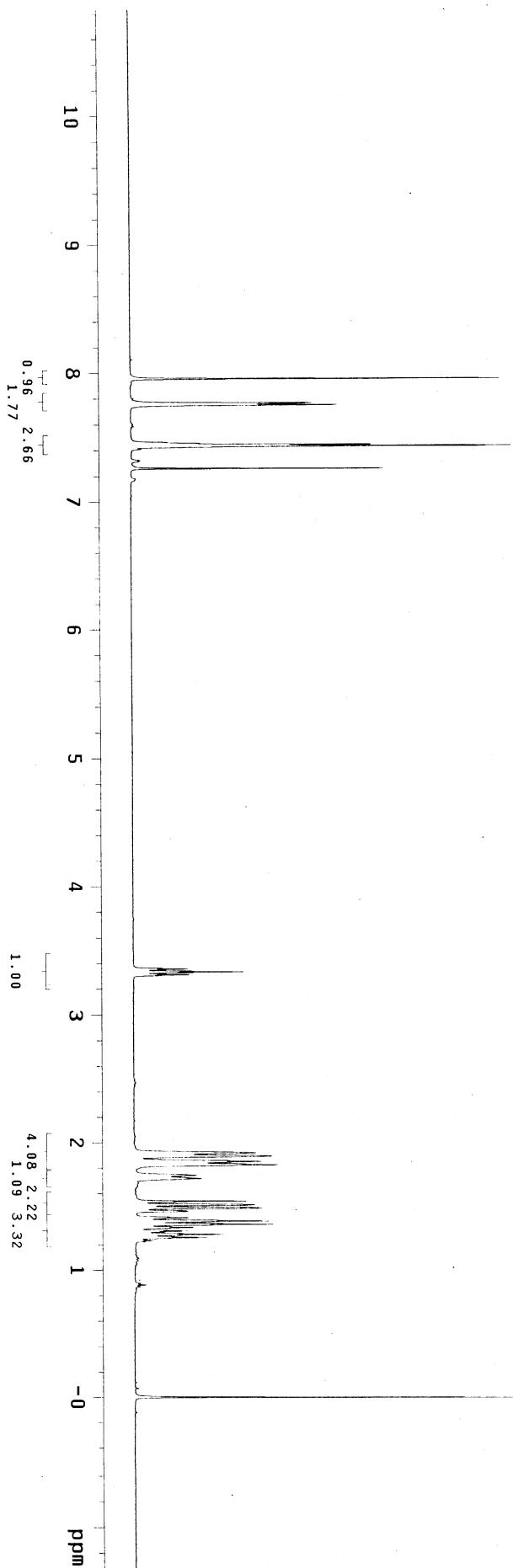
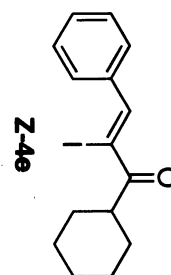
SAMPLE date Jan 28 2007 temp 25.0
SOLVENT cdc13 gain 30
FILE /home/vnmr1/nr spin not used
MR 500/waikup/data/~ hst 0.008
Zhang/Guozhu/H1-20~ pw90 14.700
070128-68-lower.f1~ alfa 6.600

ACQUISITION d
SW 8012.8 f1
AT 2.049 in
NP 32830 dp
FB 4000 hs
BS 8 lb
D1 1.000 fn
NT 8
CT 8
TRANSMITTER H1
TN 499.809 wp
STFQ 499.7 rfi
TOF 54 rfp
TPWR 7.350 lp
PW DECOUPLER C13
DN 0 WC
DOF 0 VS
DM 0 TH
DMM 34
DPWR 34
DMF 32258

PROCESSING
0.20
65536
DISPLAY
-678.8
6094.5
1007.0
-68.7
-33.5
PLOT
250
0
421
2

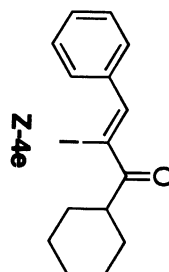
FLAGS
n
v
nn
nn

cds ph



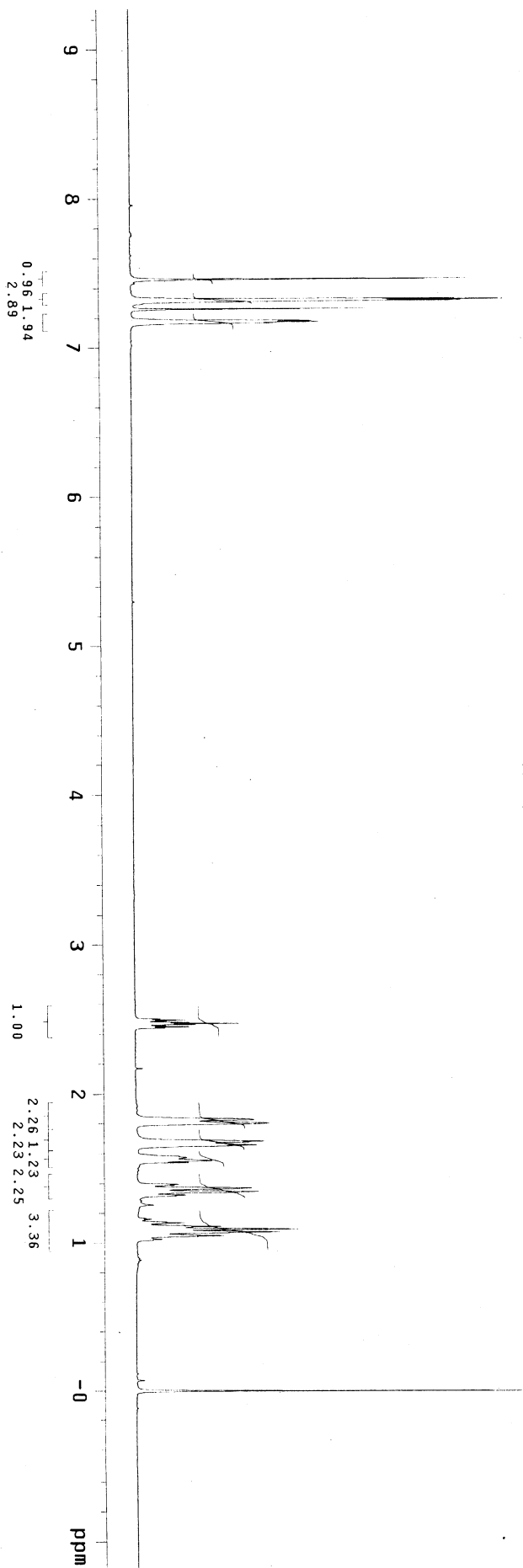
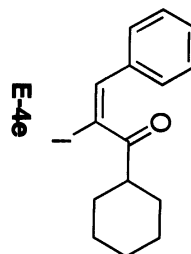
expi Carbon

SAMPLE SPECIAL 25.0
date Jan 28 2007 temp 25.0
solvent cdcl3 gain 30
file /mnt/nmr500/w* spin not used
akup/data/2hang/G- hst 0.008
uoznu/C13-20070128- pw90 15.300
-68-lower.fid alfa 10.000
ACQUISITION
sw 30487.8 f1 n
at 1.300 in n
np 79298 dp y
fb 17000 hs nn
bs 16
dl 1.000 lb
nl 12000 fn
ct 384
TRANSMITTER
tn C13 sp -2076.8
sfrq 125.689 wf 30487.3
tof 1255.3 rfi 11754.4
tpwr 49 rfp 9677.1
pw 7.650 lp -0.5
DECOUPLER H1 PLOT -282.3
dn H1 WC 250
dof 0 SC 0
dm YYY VS 30039
dmm w th
dpwr 39 at cdc ph 3
dmf 12200



expl Proton

SAMPLE		SPECIAL	
date	Jan 28 2007	temp	25.0
solvent	cdcl3	gain	30
file	/home/vnmr1/n~	spin	not used
mr500	/walkup/data/~	hst	0.008
Zhang	/Guozhu/H1-20~	pw90	14.700
070128-68.fid	alfa	6.600	
ACQUISITION		FLAGS	
sw	8012.8	il	n
at	2.049	in	n
np	32830	dp	y
fb	4000	hs	nn
bs	8	PROCESSING	
d1	1.000	lb	0.20
nt	8	fn	65536
ct	8	DISPLAY	
TRANSMITTER		sp	-603.0
tn	H1	wd	5236.4
sfrq	499.809	rfl	1007.0
tof	499.7	rfl	0
tpwr	54	rp	-74.1
pw	7.350	tp	-35.4
DECOUPLER		PLOT	
dn	C13	wc	250
dof	0	sc	0
dm	nnn	vs	370
dmm	c	th	2
dpwr	34	at	
dmf	32258	cdc	ph

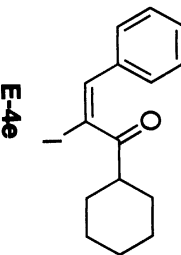


expl Carbon

SPECIAL

date Jan 28 2007 temp 25.0
solvent cdc13 gain 30
file /home/vnmr1/n- not used
mr500/walakup/data/~ hst 0.008
Zhang/Guozhu/C13-2~ pw90 15.300
0070128-68-upper.f~ alfa 10.000

E-4e



ACQUISITION

id il in n

FLAGS

n

sw 30487.8 in n

at 1.300 dp y

np 79298 hs nn

fb 17000 bs

bs 16 lb not used

d1 1.000 fn

nt 12220

ct 1360

tn TRANSMITTER

sfreq C13

tofr 125.689 rfp

tpwr 1255.3

pw 7.650

DECOUPLER

dn H1

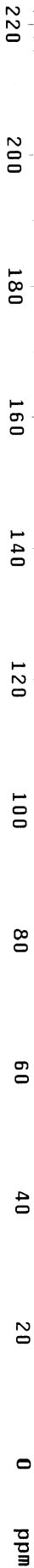
dof 0

dm YVY

dmm w

dpwr ai

dmf 12200



expl Proton

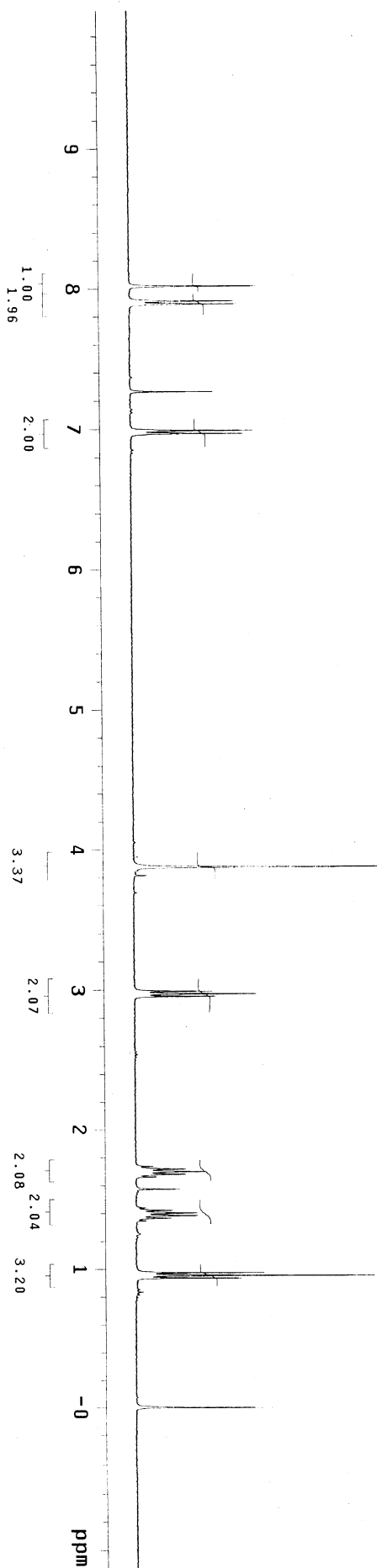
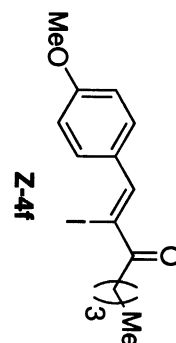
SPECIAL

date Feb 8 2007 temp 25.0
solvent cdcl3 gain 30
file /home/vnmr1/n~ not used
mr400/walakup/data/~ hst 0.008
Zhang/Guozhu/H1-20~ pw90 13.900
070208-81_lower-2.~ alfa 6.600

fid flags

ACQUISITION

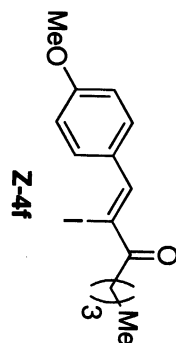
sw 6410.3 in n
at 2.049 dp v
np 26264 hs nn
fb 4000
bs 8 lb 0.20
d1 1.000 fn 65536
nt 24
ct 24
TRANSMITTER H1
tn 399.782 rfi -465.6
sfreq 399.5 rfp 4457.5
tof 399.5 tp 804.8
tpwr 39 ip 4.2
pw 6.950 plot -29.3
DECOUPLER WC 250
dn C13 SC 0
dof 0 VS 17371
dm nn th 2
dmm c ai cdc ph
dpwr 34
dmf 29412

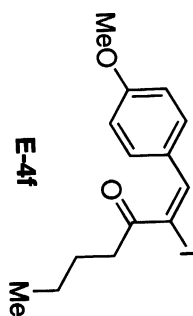


expl Carbon

SAMPLE SPECIAL 25.0
date Feb 13 2007 temp 30
solvent cdc13 gain 30
f1le /home/walkup/~ not used
nmr500/walkup/data nst 0.008
/Zhang/Guozhu/C13-~ pw90 15.500
20070213-81-lower.~ alfa 10.000

ACQUISITION
f1d
sw 30487.8 i1 n
at 1.300 in y
np 79298 hs n
fb 17000
bs 12 fn
d1 1.000 not used
nt 12000
ct 924 DISPLAY
tn TRANSMITTER 924 SP -2076.8
sfq C13 wp 30487.3
tof 125.689 rfi 11754.4
tpwr 1255.3 rfp 9677.1
pw 7.650 lp -82.3
DECOUPLER PLOT -289.8
dn H1 WC 250
dof 0 SC 0
dm 0 VS 23464
dmm YYY th
dpwr w ai cdc ph 6
dmf 12200

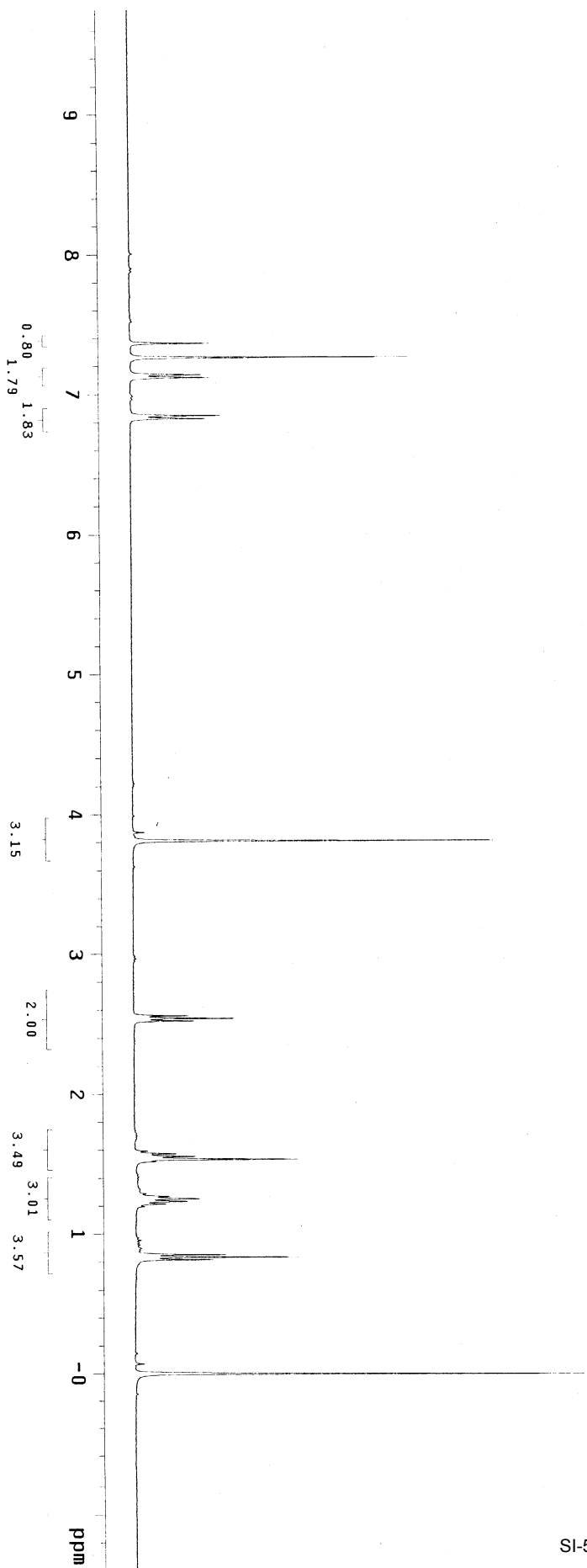




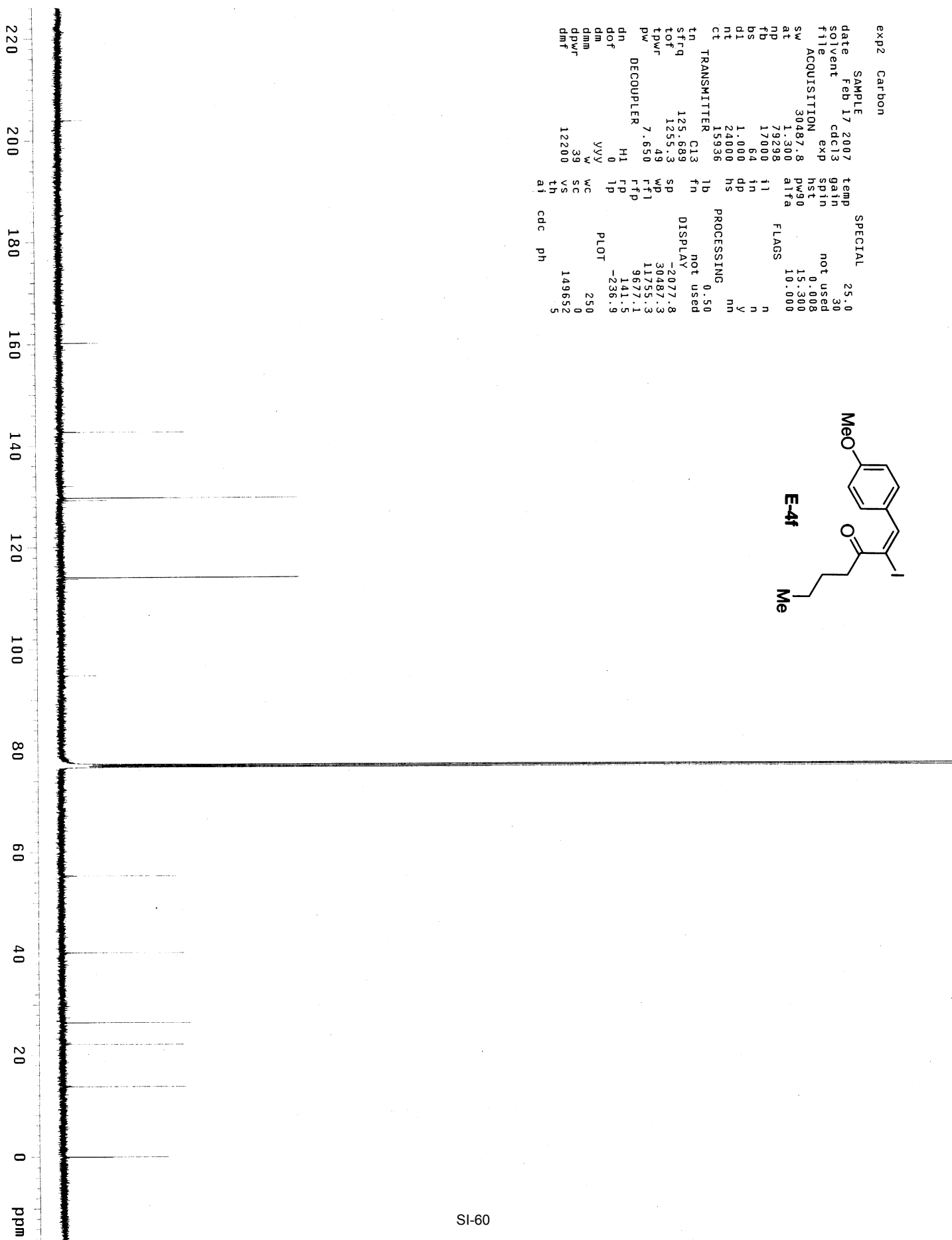
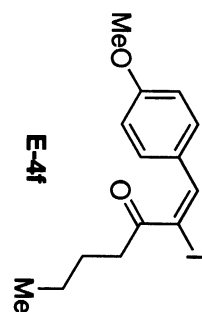
```

expt  proton
SAMPLE
date    Feb 12 2007
solvent  cdcl3
file    /home/vnmr1/n~
mr400/walkup/data/~
Zhang/Guozhu/H1-20~
070212-81-upper.fi~
SPECIAL
temp    25.0
gain    30
spin    not used
nst     0.008
pw90    13.900
alfa    6.500
ACQUISITION
d       1
f1      n
in      y
dp      nm
hs      0.20
PROCESSING
0.20
nm
65536
DISPLAY
-564.0
4461.6
806.4
25.2
-19.7
PLOT
250
0
1771
2
DECOUPLER
WC
SC
VS
TH
AI
CDC
PH
DMF
29412

```



SAMPLE						SPECIAL					
date	Feb 17 2007	temp	25.0								
solvent	cddc13	gain	30								
file	exp	spin	not used								
ACQUISITION											
sw	30487.8	pw90	0.008								
at	1.300	alfta	15.300								
np	79298		10.000								
fb	17000	i1	n								
bs	64	in	n								
di	1.000	dp	y								
nt	24000	hs	nm								
ct	15936										
TRANSMITTER						PROCESSING					
tn	C13	lb	f1	0.50							
sfrq	125.689		not used								
tof	1255.3	wd	-2077.8								
tpwr	49	sp	30487.3								
pw	7.650	rfl	11755.3								
DECOUPLER											
tn	H1	r1p	9677.1								
dof	0	lp	141.5								
dm	yyy		-236.9								
dmm		wc	PLOT								
dppr	39	sc	250								
dmf	12200	vs	0								
		th	149652								
		ai	.5								
		cdc	ph								



STANDARD 1H OBSERVE - profile

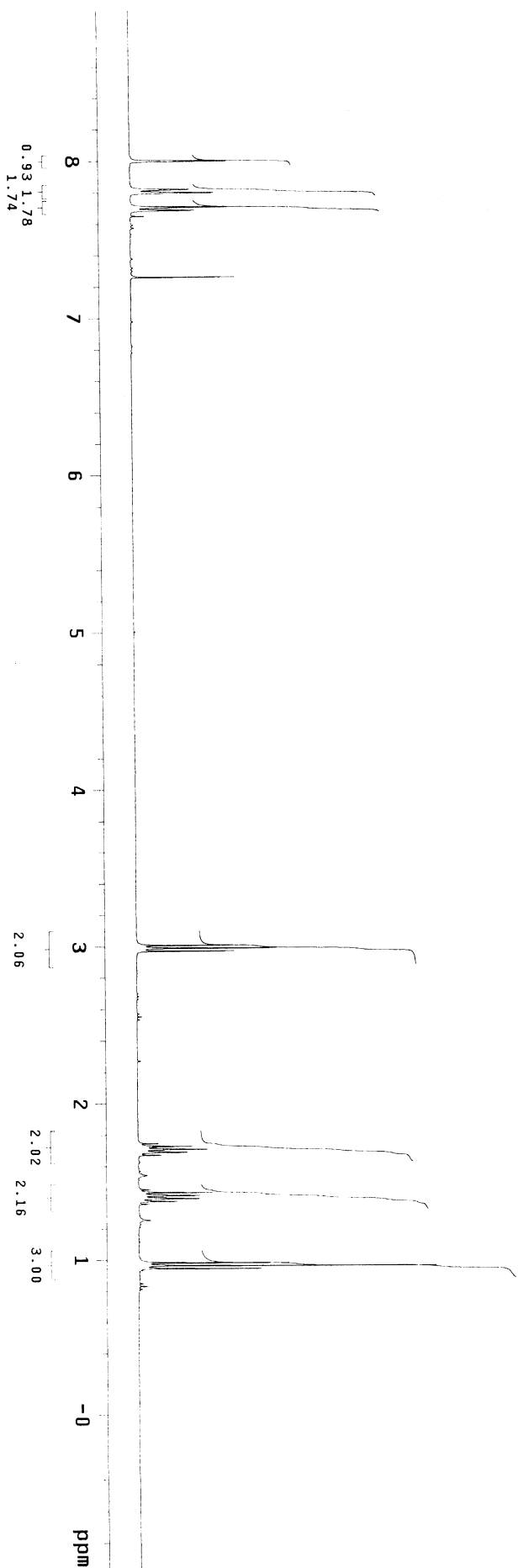
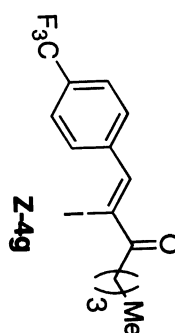
Automation directory: /home/walkup/vnmrsvs/data/auto_2007.02.09_19
 File: s_20070209_003/data/cdc13_01.fid
 Sample id: s_20070209_003

Pulse Sequence: szpul

Solvent: cdcl3
 Temp: 25.0 C / 298.1 K
 Operator: walkup
 File: cdc13_01
 VNMR-400 "NMR400"

Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.049 sec
 Width 6410.3 Hz
 8 repetitions

OBSERVE H1, 399.7793051 MHz
 DATA PROCESSING
 Line broadening 0.2 Hz
 FT size 65536
 Total time 0 min, 30 sec



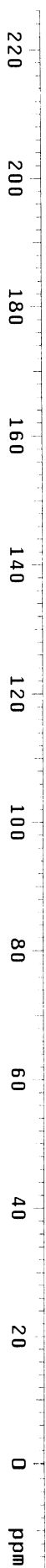
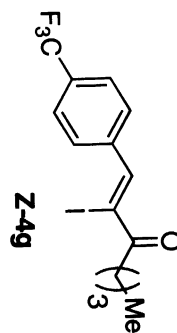
STANDARD 1H OBSERVE - profile

exp2 Carbon

SAMPLE SPECIAL 25.0
date Feb 10 2007 temp 30
solvent cdc13 gain 30
file /home/walakup/~ not used
vnmr/svs/data/auto_~ hst 0.008
2007.02.10_04/Aug.~ pw90 15.300
04/data/cdc13_01.f~ alfa 10.000

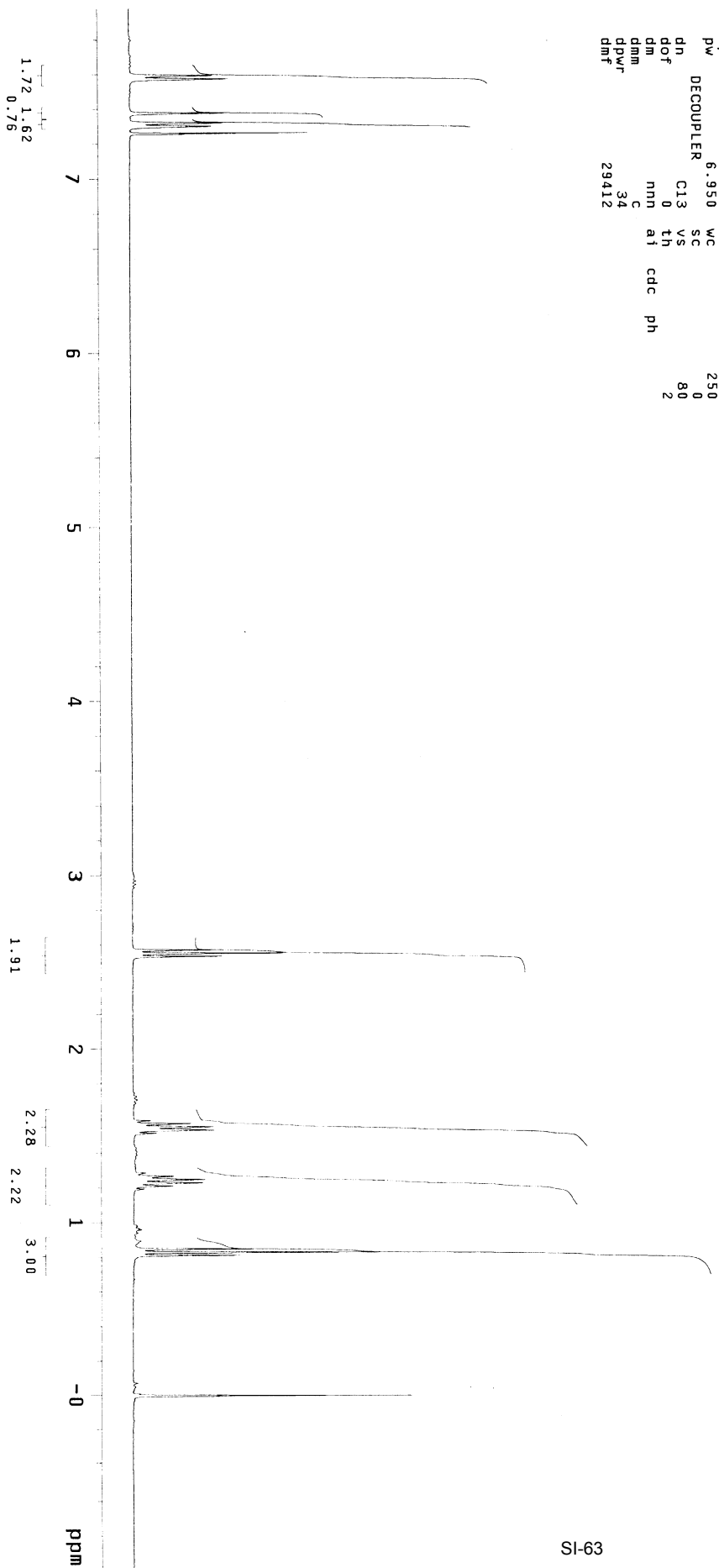
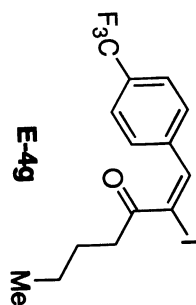
ACQUISITION
id i1 n
sw 30487.8 in y
at 1.300 dp y
np 79298 hs nm
fb 17000
bs 32 lb 0.50
d1 1.000 fn not used
nt 12800
ct 288
TRANSMITTER C13
in wp -2078.2
sfreq 125.689 rfi 30487.3
tot 1255.3 rfp 11755.8
tpwr 49 tp -37.6
pw 7.650 lp -231.6

DECOUPLER WC 250
dn H1 SC 0
dof 0 VS 30326
dm YVY th 3
dmm w ai cdc ph
dpwr 39
dmf 12200



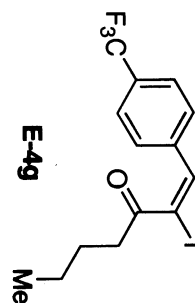
exp1 Proton

SAMPLE		SPECIAL	
date	Feb 12 2007	temp	25.0
solvent	cdcl3	gain	not used
file	/home/waikup/~	spin	not used
nmr	sys/data/auto_~	hst	0.008
2007.02.12_22/s_20~		pw90	13.900
070212_001/data/cd~		alfa	6.600
c13.02.fid		flags	
ACQUISITION		i1	n
sw	6410.3	in	y
at	2.049	dp	nm
np	26264	hs	
fb	4000	PROCESSING	0.20
bs	32	lb	65536
ss	2	fn	
di	1.000	DISPLAY	-404.6
nt	8	sp	3595.0
ct	8	wd	805.8
TRANSMITTER	H1	rfl	0
tn	399.782	rfp	119.0
strq	399.5	tp	-23.8
tof	59	PLOT	250
tpwr	6.950	WC	0
pw		SC	80
DECOUPLER	C13	VS	2
dn	0	th	
dof	nnn	ai	cdc ph
dm	34		
dmm	34		
dpwr	29412		
dmf			



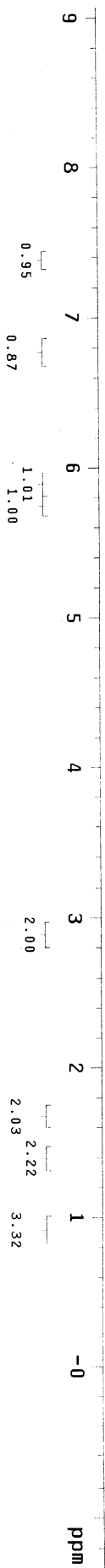
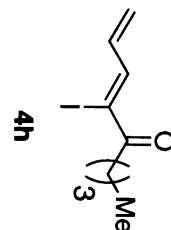
expt Carbon

SAMPLE SPECIAL
date Feb 12 2007 temp 25.0
solvent cdcl3 gain 30
file /home/walkup/~ hst not used
nmr500/walkup/data~ hst 0.008
/699-1carbon.fid pw90 15.300
ACQUISITION alfa 10.000
sw 30487.8
at 1.300 il
np 79298 in
fb 17000 dp
bs 64 hs
d1 1.000
nt 20480 lb
ct 128 fn
TRANSMITTER C13
tn 125.689 sp
sfreq 125.689 wd
tof 1255.3 rfi
tpwr 49 rfp
pw 7.650 tp
DECOUPLER H1 lp
dn H1
dof 0
dm 0
dmm YYY WC
dpwr W SC
dmf 39 VS
ai 3 TH
cdc ph
3



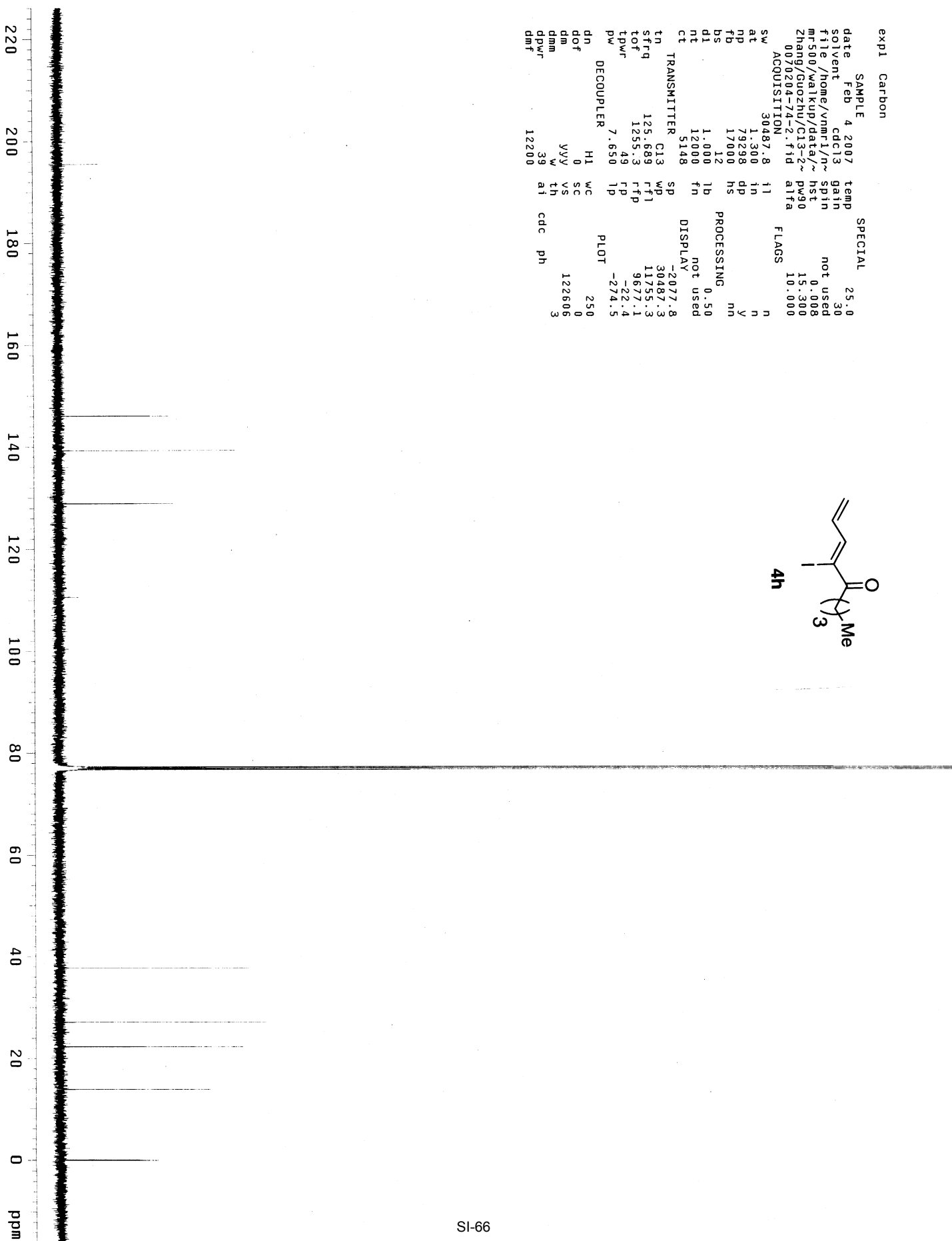
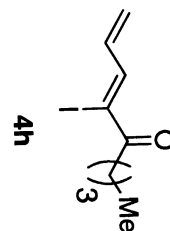
expl Proton

SAMPLE 4 2007 temp 25.0
date Feb 4 2007 gain 30
solvent cdcl3 not used
file /home/vnmr1/n- spt 0.908
mr500/walakup/data/~ hst 14.700
Zhang/Guozhu/H1-20~ pw90 6.600
070204-74.fid alfa
ACQUISITION
sw 8012.8 il n
at 2.049 in n
np 32830 dp v
fb 4000 hs nn
bs 8
d1 1.000 lb 0.20
nt 8 fn 65536
ct 8
TRANSMITTER
tn H1 sp -677.8
stfq 499.809 rfi 5211.2
tof 499.7 rfi 1006.0
tpwr 54 ffp -37.4
pw 7.350 lp -40.1
DECOUPLER
dn C13 wc 250
dof 0 sc 0
dm nn vs 763
dmm c th 2
dpwr 34 ai
dmf 32258
cdcl3 ph



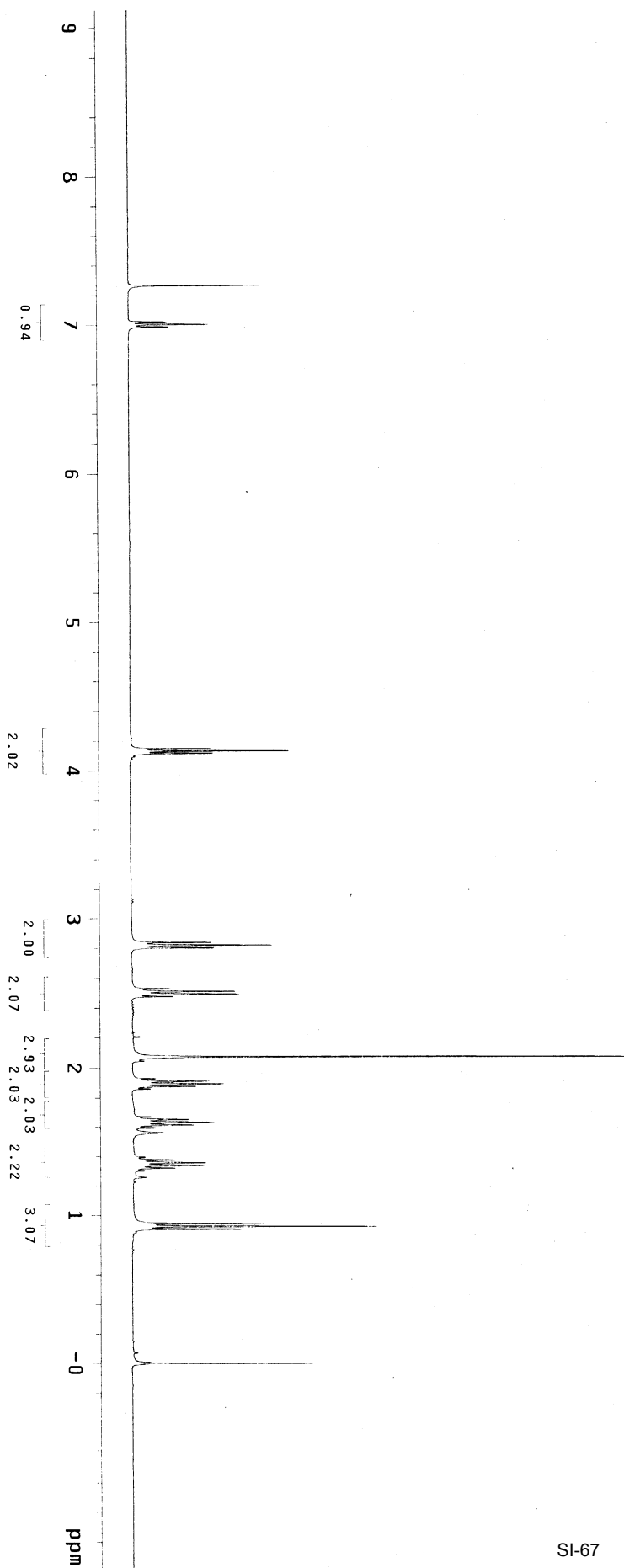
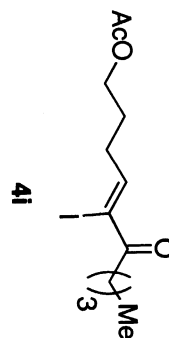
expl Carbon

SAMPLE 4 2007 SPECIAL 25.0
date Feb 4 2007 temp 25.0
solvent cdc13 gain 30
title /home/vnmr1/nst not used
mr500/waikup/data/~ 0.008
Zhang/Guozhu/C13-2- pw90 15.300
0070204-74-2.fid alfa 10.000
ACQUISITION
SW 30487.8 f1 n
at 1.300 in n
np 79298 dp y
fb 17000 hs n
bs 12
d1 1.000 lb
nt 12000 fn
ct 5148
TRANSMITTER SP
tn C13 wp -2077.8
sfrq 125.689 rfi 30487.3
tof 1255.3 rfp 11755.3
tpwr 49 rp 9677.1
pw 7.650 lp -22.4
DECOUPLER H1 WC PLOT -274.5
dn HI WC 250
dof 0 SC 0
dm YYY VS 122606
dmm w th
dpwr 39 ai cdc ph 3
dmf 12200



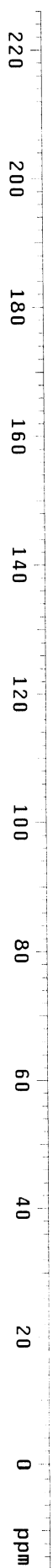
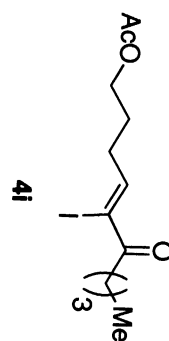
expl Proton

SAMPLE SPECIAL 25.0
date Feb 12 2007 temp 30
solvent cdc13 gain 30
file /home/vnmr1/n- not used
mr400/waikup/data/~ hst 0.008
Zhang/Guozhu/H1-20~ pw90 13.900
070212-84.fid alfa 6.600
ACQUISITION
SW 6410.3 il n
at 2.049 in n
np 26264 dp v
fb 4000 hs nn
bs 8
dl 1.000 lb 0.20
nt 8 fn 65536
ct 8
TRANSMITTER
tn H1 sp -562.8
sfrq 399.782 rf1 4209.3
tof 399.5 rfp 805.2
tpwr 59 fp 126.1
pw 6.950 lp -44.8
DECOUPLER
dn C13 wc 250
dof 0 sc 0
dm nn vs 543
dmm c th 2
dpwr 34 ai cdc ph
dmf 29412



expl Carbon

SAMPLE		SPECIAL	
date	Feb 12 2007	temp	25.0
solvent	cdcl3	gain	30
file	/home/waikup/~	spin	not used
nmr500/waikup/data~	hst	0.008	
/Zhang/Guozhu/C13~	pw90	15.300	
20070212-84.fid	alfa	10.000	
ACQUISITION		FLAGS	
sw	30487.8	il	n
at	1.300	in	y
np	79298	dp	n
fb	17000	hs	nm
bs	12	PROCESSING 0.50	
d1	1.000	lb	not used
nt	12000	fn	not used
ct	960	DISPLAY	
TRANSMITTER		sp	-2076.5
tn	C13	wp	30487.3
sfrq	125.689	rfl	11754.1
tof	1255.3	rtp	9677.1
tpwr	43	tp	-28.1
pw	7.650	tp	-280.5
DECOUPLER		PLOT	
dn	H1	wc	250
dof	0	sc	0
dm	yyv	vs	40671
dmm	w	th	6
dwr	39	ai	cdc ph
dntf	12200		



expl Proton

SPECIAL

date Sep 23 2006 temp 6.0
solvent cdc13 gain not used
title /home/walkup/~ not used
vnmr/sys/data/auto_~ hst 0.008
2006.09.23_05/Aug.~ pw90 19.800
01/data/cdc13_01.f~ alfa 6.600

FLAGS

ACQUISITION

id i1 n
sw 8012.8 in n
at 2.049 dp y
np 32830 hs nm
fb 4000
bs 32 lb 0.20
ss 2 fn 65536
d1 1.000
nt 8
ct 8

DISPLAY

sp -514.5
wp 4506.5
rf1 1000.9
rfp 0

TRANSMITTER

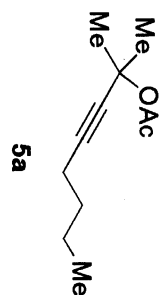
tn H1
sfreq 499.809
tofr 499.7
tpwr 54
pw 9.900

PLOT

WC 250
SC 0
VS 40
TH 2

DECOUPLER

dn C13
dof 0
dm nn
ddm ai
dpuw cdc ph
dmf 12300



expt Carbon

SAMPLE SPECIAL

date Sep 23 2006 temp 6.0
solvent cdc13 gain 30
file /home/walkup/~ not used
vnmrsvs/data/auto/~ hst 0.008
2006.09.23_05/Aug.~ pw90 13.500
02/data/cdc13_01.f~ alfa 10.000

FLAGS

id n

ACQUISITION

sw 30487.8 il n
at 1.500 dp y
np 79298 hs nm

PROCESSING

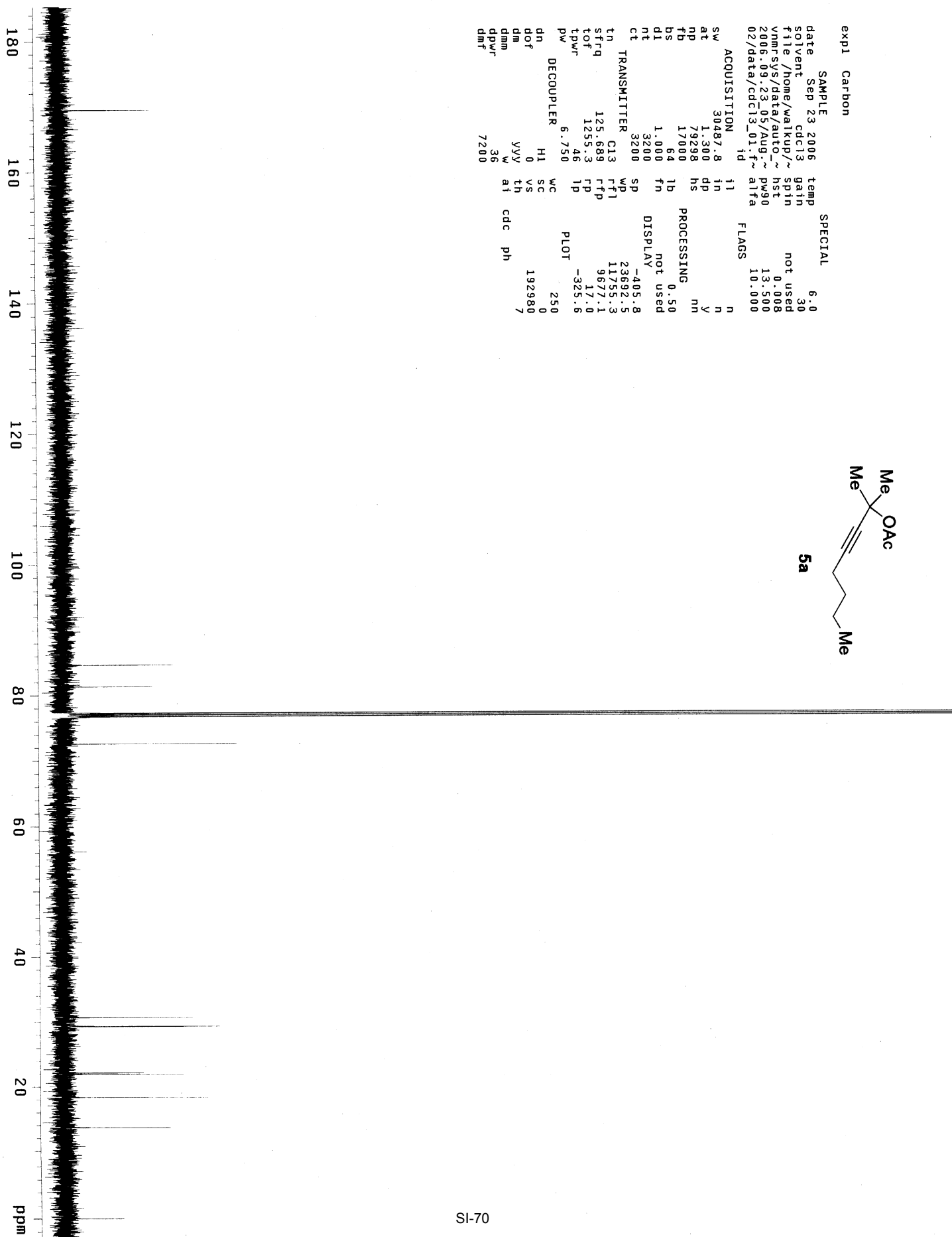
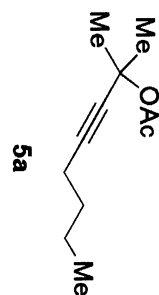
bs 64 lb 0.50
dl 1.000 fn not used

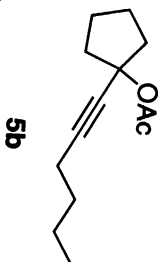
DISPLAY

ct 3200 sp -405.8
tn TRANSMITTER C13 wd 23692.5
stfrq 125.689 rfi 11755.3
tof 125.3 rfp 9677.1
tpwr 46 tp 17.0
pw 6.750 PLOT -325.6

DECOUPLER

dn H1 wc 250
dof 0 vs 0
dm yyv th 192980
dmm v ai cdc ph 7
dpwr 36
dmt 7200

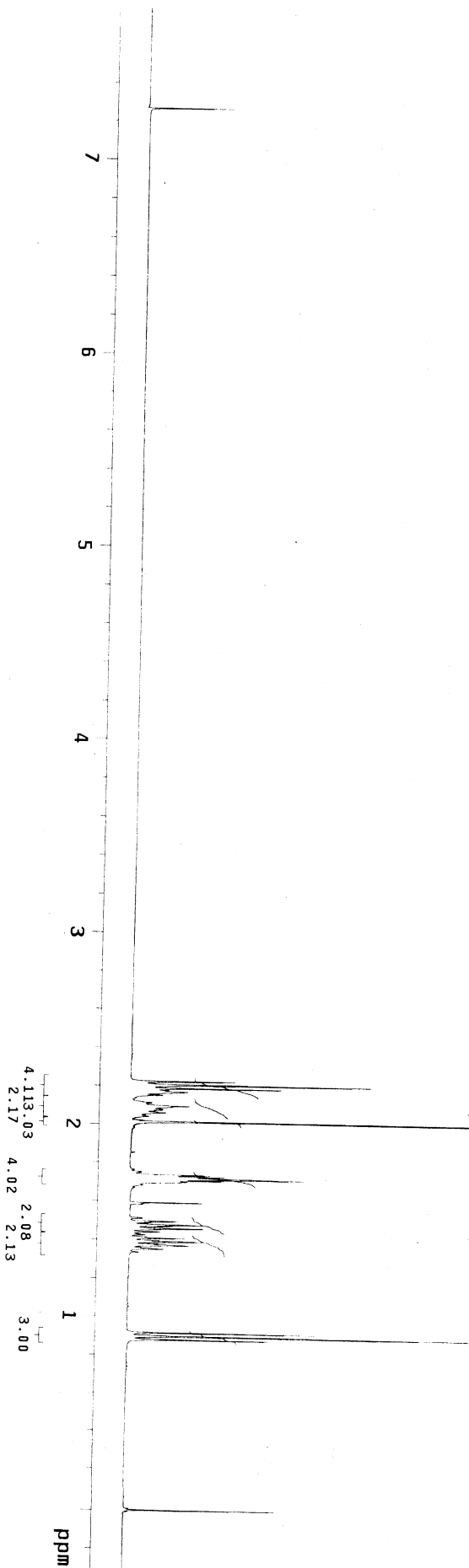




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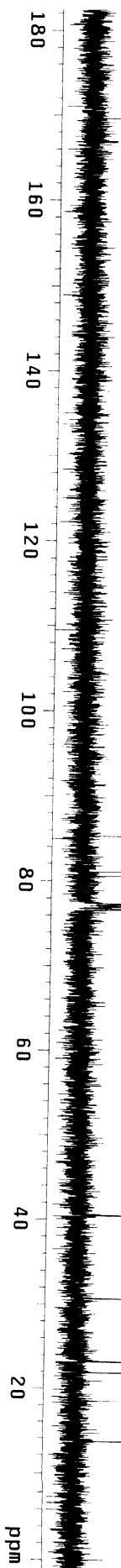
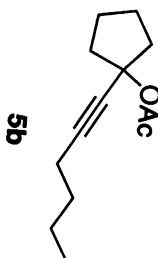
expt  Proton
SAMPLE
date   Sep 21 2006      temp  not used
solvent cdc13          gain   not used
file    /home/walkup/~  spm    not used
vnmrsws/data/autoc~   hst     0.008
2006.09.21_17/5-20~   pw90    13.900
060921_001/data/cd~   alpha   6.600
c13-01.fid
ACQUISITION
sw      6410.3          in      n
at      2.049          dd      y
np      26264          hs      nn
fb      4000           1b      0.20
bs      4             2       65536
ss      1.000          fn      DISPLAY
di      32            sp      -135.0
nt      32            wp      3248.6
ct      32            rfp     803.6
TRANSMITTER
tn      H1            rf      42.8
sfreq   399.782      lp      -44.2
tof      399.5       PLOT
tpwr     53          250
pw      6.950        0
DECOUPLER C13        220
dn      0            2
dof      th          ai      cdc   ph
dm      nn
dmm      c
dpwr     34
dmf      29412

```



expt Carbon

SAMPLE		SPECIAL	
date	Sep 21 2006	temp	not used
solvent	cdcl3	gain	30
file	/home/walkup/~	spin	not used
nmr	sys/data/auto_	hst	0.008
2006.09.21_17s-20~		pw90	9.700
060921_001/data/cd~		alfa	10.000
c13-02.fid		flags	
ACQUISITION			
sw	24509.8	il	n
at	1.300	in	n
np	63750	dp	y
fb	17000	hs	nn
bs	64	lb	0.50
d1	1.000	fn	not used
nt	2560	display	
ct	448	sp	-140.3
tn	TRANSMITTER	wd	18478.8
tn	c13	rfl	9464.9
sfrq	100.535	rff	7740.4
tof	1042.6	fp	72.0
tpwr	35	lp	-207.0
pw	4.850	plot	
DECOUPLER			
dn	H1	wc	250
dof	0	sc	0
dm	yyv	th	4.73566e+06
dmm	w	at	68
dpwr	41	cdc	ph
dmf	9300		



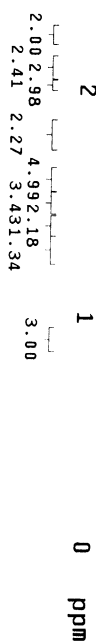
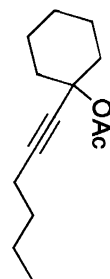
expt1 Proton

SAMPLE		SPECIAL	
date	Sep 21 2006	temp	not used
solvent	cdcl3	gain	20
file	/home/walkup/~	spin	not used
data	/Zhang/11ming/~	hst	0.008
-enone/cyclohexano-	pw90	13.900	
ne-hexyne-acetate-	alpha	6.600	

ACQUISITION		PROCESSING	
sw	6410.3	in	n
at	2.049	dp	y
np	26264	hs	nn
fb	4000		
bs	32	1b	0.20
d1	1.000	fn	65536
nt	32		
ct	32	sp	-181.0

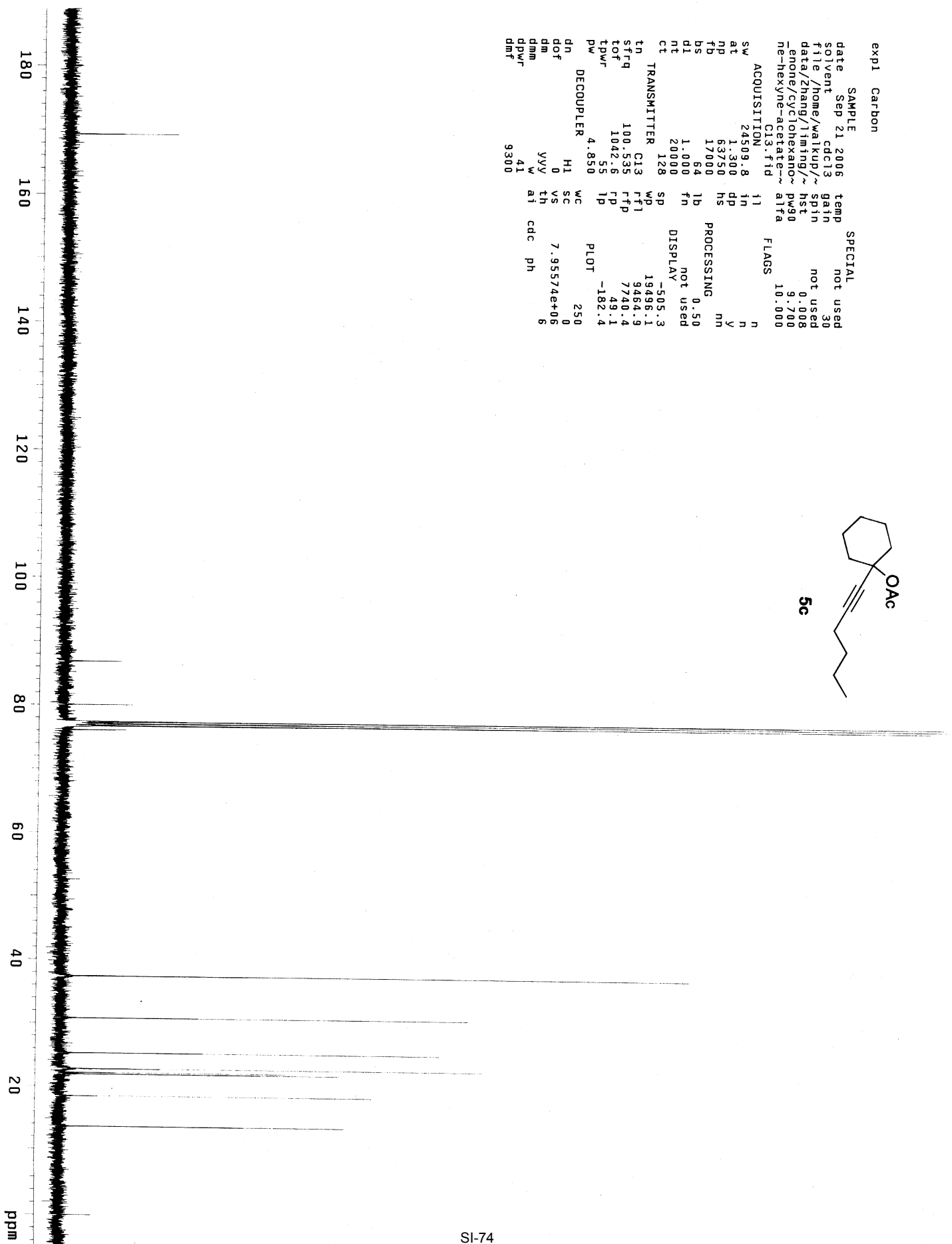
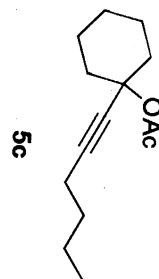
TRANSMITTER		DISPLAY	
tn	H1	wd	3252.1
sfrq	399.782	rfl	804.0
tof	399.5	rfl	41.7
tpwr	59	tp	-62.0
pw	6.950		

DECOUPLER		PLOT	
dn	C13	wc	250
dof	0	vs	0
dm	nmn	th	24849
dmm	c		
dpwr	34	ai	cdc ph
dmf	29412		



expt1 Carbon

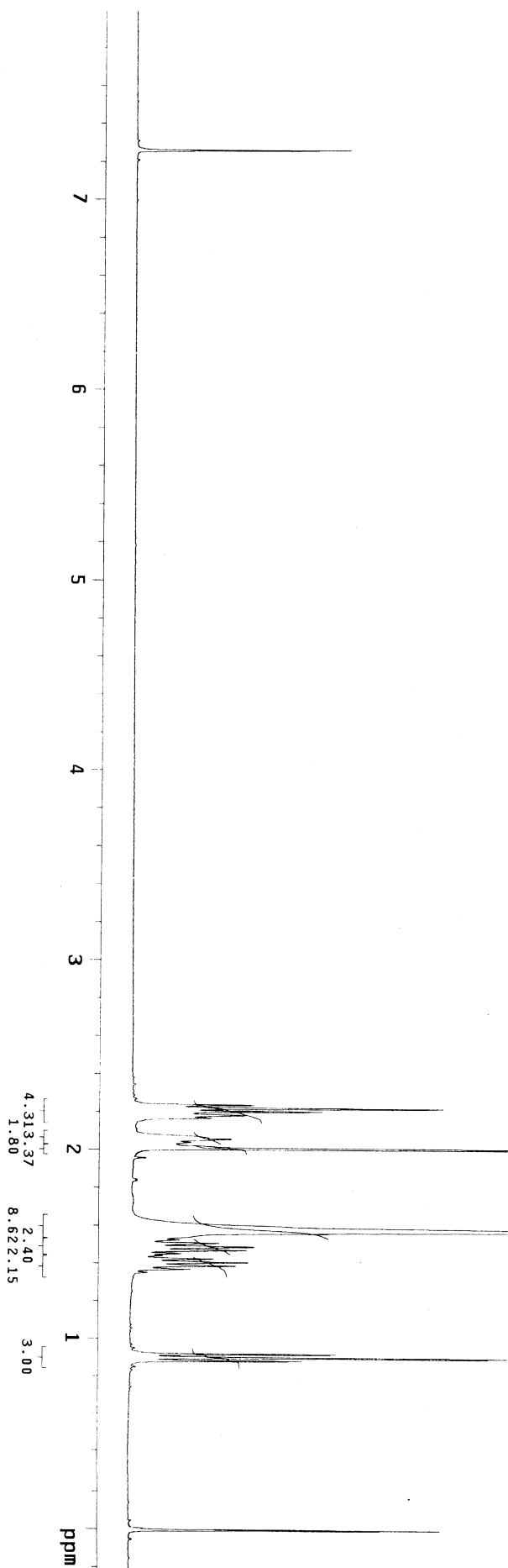
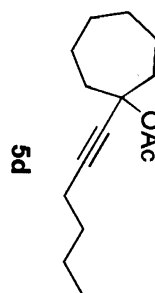
SAMPLE				SPECIAL			
date	sep 21 2006	temp	not used				
solvent	cdcl3	gain	30				
file	/home/walkup/~	spin					
data/	zhang/1hmq/	hst	not used				
-name	/cyclohexano-	pw30	0.008				
ne-hexyne-acetate-	~	alfa	9.700				
	C13.fid		10.000				
ACQUISITION				FLAGS			
sw	24509.8	f1	n				
at	1.300	in	n				
np	63750	dp	n				
fb	17000	hs	y				
bs	64	lb	n				
d1	1.000	fn	0.50				
nt	20000		not used				
ct	128	DISPLAY					
TRANSMITTER				-505.3			
tn	C13	wp	19496.1				
sfreq	100.535	rfl	9464.9				
tof	1042.6	rp	7740.4				
tpwr	55	tp	49.1				
pw	4.850	lp	-182.4				
DECOUPLER				PLOT			
dn	H1	wc	250				
dof	0	sc	0				
dm	yyv	vs	7.95574e+06				
dmm	yv	th	6				
dpmr	41	ai	cdc				
dmf	9300	ph					



STANDARD 1H OBSERVE - profile

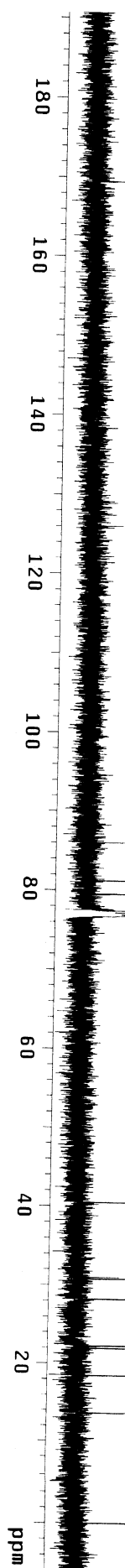
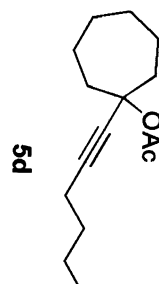
exp2 Proton

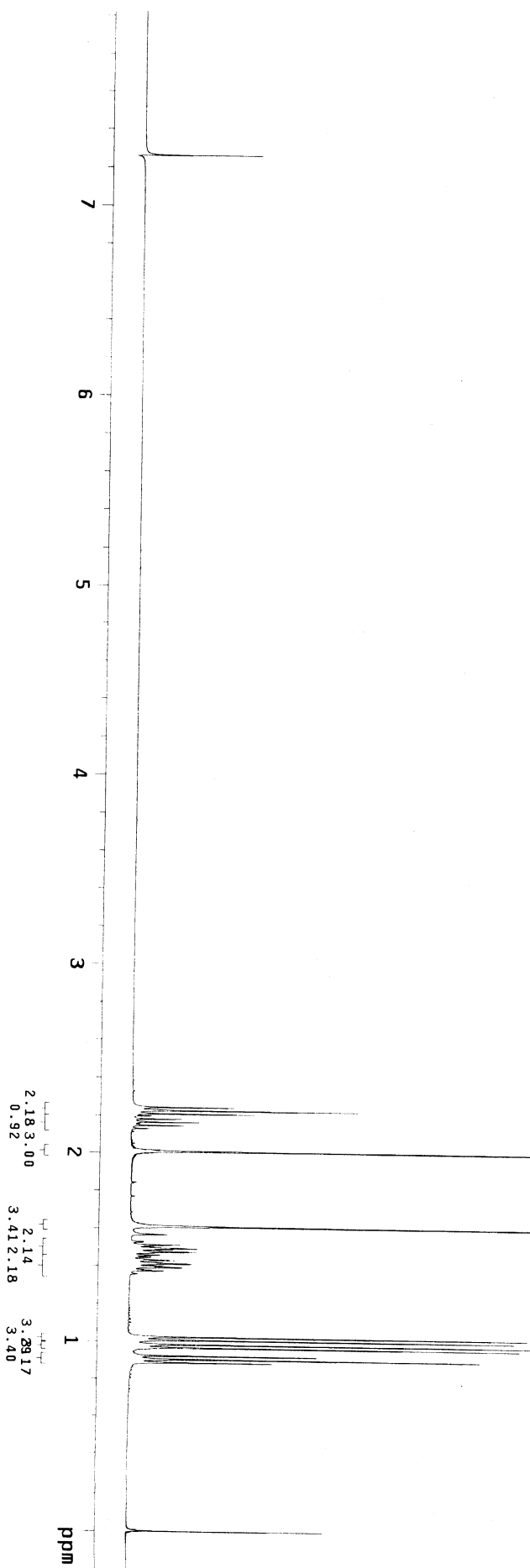
SAMPLE		SPECIAL	
date	Jun 29 2006	temp	25.0
solvent	cdcl3	gain	not used
file	/home/walkup/~	spin	not used
nmr	sys/data/autoc	hst	0.008
2006.06.29_30/5_20	pw90	14.000	
060629_001/data/cd	alfa	6.600	
c13.01.fid	flags		
ACQUISITION		PROCESSING	
sw	6410.3	in	n
at	2.049	dp	y
np	26264	hs	nn
fb	4000	lb	0.20
bs	32	fn	65536
ss	2	td	
d1	1.000	sp	-94.0
nt	8	wd	3289.2
ct	8	rfi	3707.1
td	TRANSMITTER	tp	2902.4
sfreq	H1	ip	151.9
tof	399.782	pl	-29.5
tpwr	399.5	plot	
pw	58	wc	250
DECOUPLER		sc	0
dn	C13	vs	717
dof	0	th	3
dm	nmn	at	
dmm	c	cdc	ph
dpmr	0		
dmt	200		



expt Carbon

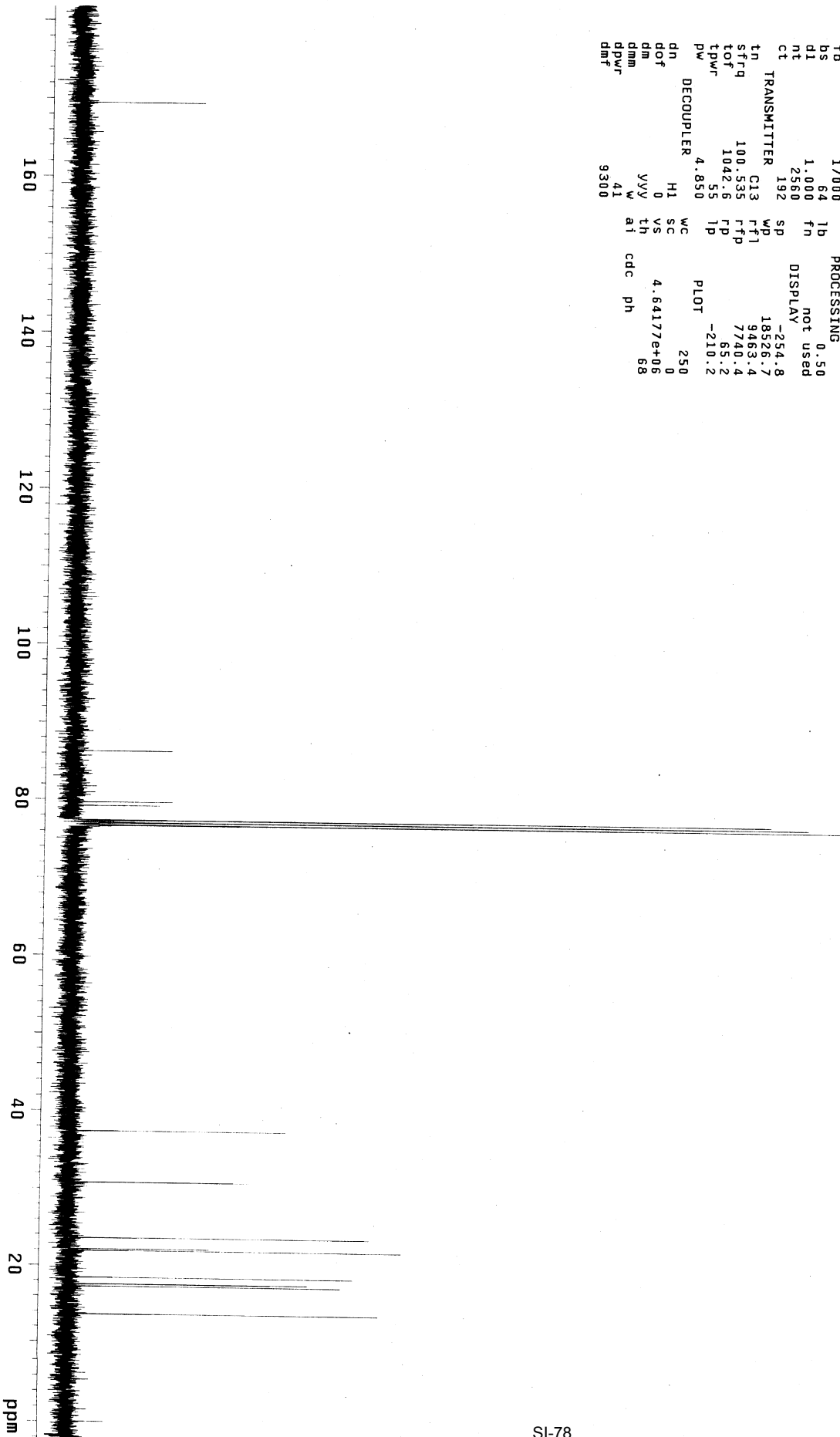
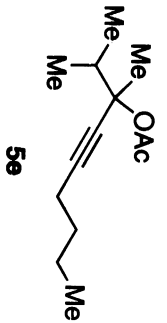
SAMPLE SPECIAL
date Sep 24 2006 temp 6.0
solvent cdc13 gain 30
file /home/waikup/~ not used
vnmr/s/data/auto/~ hst 0.008
2006.09.24/Aug.01/~ pw90 13.500
data/cdc13_01.fid alfa 10.000
ACQUISITION
sw 30487.8 f1
at 1.300 in n
np 79298 dp y
fb 17000 ns n
bs 64
dl 1.000 lb 0.50
nt 25600 fn not used
ct 1216
TRANSMITTER
tn C13 sp -799.0
sfrq 125.689 rfi 11756.8
tof 1255.3 rfp 9677.1
tdwr 46 tp -25.2
pw 6.750 tp -212.8
DECOUPLER
dn H1 WC PLOT
dof 0 SC 250
dm 0 VS 0
dmm YVY 400000
dpwr w th 15
dmf 36 ai cdc ph
7200

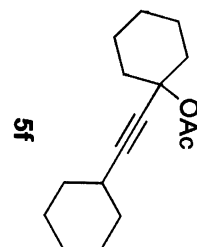


[illegible]

expi Carbon

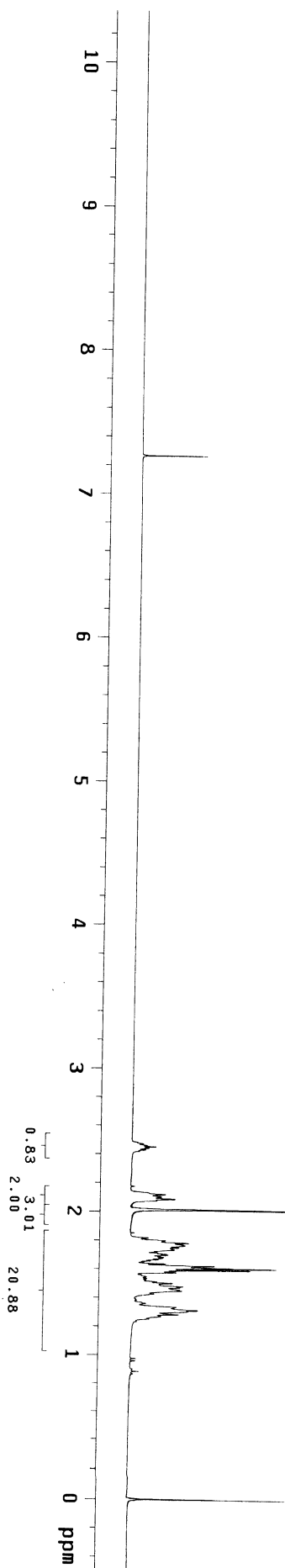
SAMPLE date Sep 22 2006 temp 25.0
solvent cdc13 gain 30
file /home/walkup/~ hst not used
vnmr.sys/data/autoc- hst 0.008
2006.09.22_25/S-20~ pw90 9.700
060922_001/data/cd~ alfa 10.000
c13-02.fid
ACQUISITION
sw 24509.8 i1 n
at 1.300 in n
np 63750 dp y
fb 17000 hs nm
bs 64 lb 0.50
dl 1.000 tn not used
nt 2560
ct 192
TRANSMITTER
tn C13 wp -254.8
sfreq 100.535 rfi 18526.7
tof 1042.6 rfp 9463.4
tpwr 1042.6 ip 7740.4
pw 4.850 ip 65.2
DECOUPLER WC PLOT -210.2
dn H1 WC 250
dof 0 SC 0
dm 0 VS 4.64177e+06
dmm yvy th 68
dpwr w ai cdc ph
dmf 9300





expt1 Proton

SAMPLE		SPECIAL	
date	Sep 30 2006	temp	25.0
solvent	cdcl3	gain	not used
file	/mnt/nmr400/w-	spn	not used
alkup/data/Zhang/G~	hst	pw90	0.008
uotaol1/243.fid	pw90	13.900	
ACQUISITION		alfa	6.600
sw	6410.3	FLAGS	
at	2.049	il	n
np	26264	in	n
fb	4000	dp	y
bs	32	hs	nn
ss	2	PROCESSING	
dl	1.000	lb	0.20
nt	8	fn	65536
ct	8	DISPLAY	
TRANSMITTER		sp	-205.8
tn	H1	wd	4346.2
sfrq	399.782	rfl	805.0
tof	399.5	rffp	0
tpwr	59	tp	96.6
pw	6.950	tp	-16.0
DECOUPLER		PLOT	
dn	C13	wc	250
dof	0	sc	0
dm	nn	vs	222
dmm	c	th	2
dpwr	34	ai	cdc
dmf	29412	ph	



expt Carbon

SAMPLE SPECIAL
date Sep 30 2006 temp 25.0
solvent cdcl3 gain 30
file /home/walakup/~ spin not used
vnmrsvs/data/auto/~ hst 0.008
2006_09_30_08/S_20~ pw90 9.700
060930_004/data/cd- alfa 10.000
c13_01.f1d

FLAGS

n

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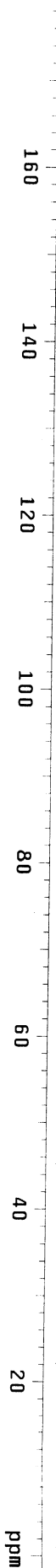
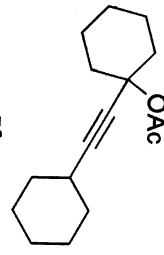
ACQUISITION
sw 24509.8
at 1.300
np 63750
fb 17000
bs 64
dl 1.000
nt 10240
ct 2176
tn TRANSMITTER
stf 100.535
tof 1042.6
tpwr 55
pw 4.850
dn DECOUPLER
dm H1
dm 0
dm yv 41
dm w
dm ai
dm cdc
dm ph
dm 9300

PROCESSING
0.50
not used

DISPLAY
-223.3
18165.4
9463.4
7740.4
161.4
-186.6

PLOT
250
0
4.35749e+06
6

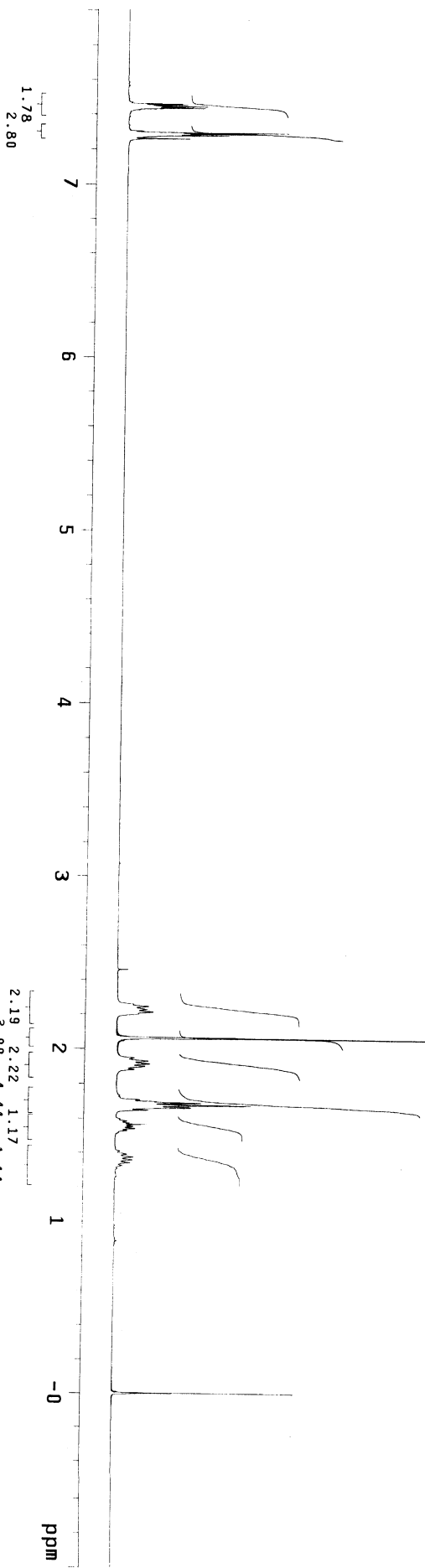
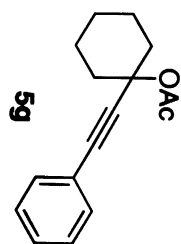
5f



STANDARD 1H OBSERVE - profile
STANDARD 1H OBSERVE - profile
STANDARD 1H OBSERVE - profile
STANDARD 1H OBSERVE - profile

expt1 Proton

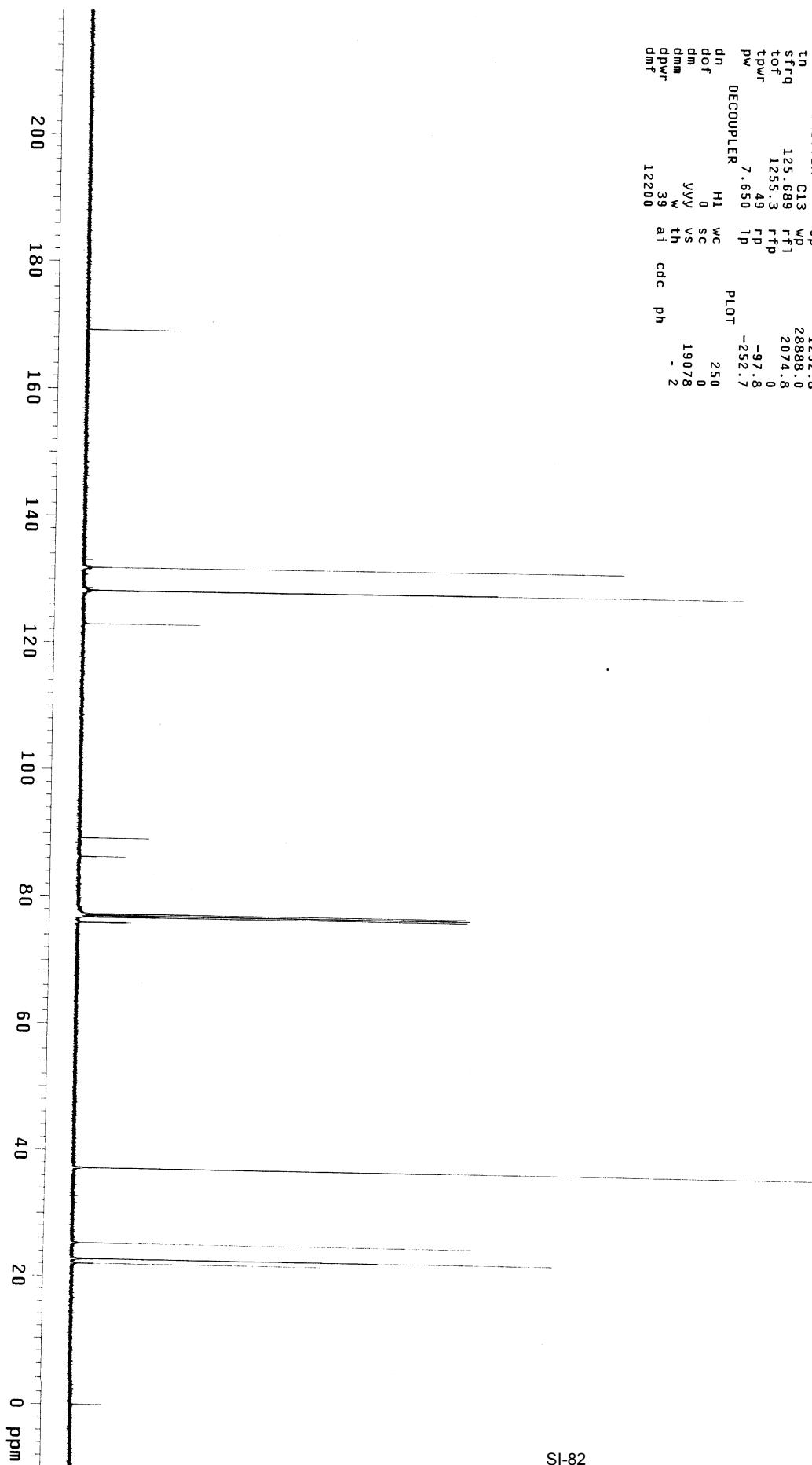
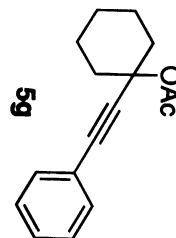
SAMPLE		SPECIAL	
date	Sep 26 2006	temp	25.0
solvent	cdcl3	gain	not used
file	/home/walkup/~	spin	not used
nmr	sys/data/autoc~	hst	0.008
2006.09.26_33/s-20~		pw90	13.900
060926_003/data/cd~		alpha	6.500
c13.01.fid		flags	
ACQUISITION			
sw	6410.3	in	n
at	2.049	dp	y
np	26264	hs	nn
fb	4000	PROCESSING	
bs	32	lb	0.20
ss	2	fn	65536
d1	1.000	DISPLAY	
nt	8	sp	-402.8
ct	8	wd	3604.2
TRANSMITTER			
tn	H1	rfp	805.8
sfreq	399.782	fp	117.9
tof	399.5	lp	-41.5
tpwr	59	PLOT	
pw	6.950	sc	250
DECOUPLER			
dn	C13	vs	0
dof	0	th	200
dmm	nmn	at	cdc
dpmr	c	ph	
dmt	29412		



STANDARD 1H OBSERVE - profile

expt Carbon

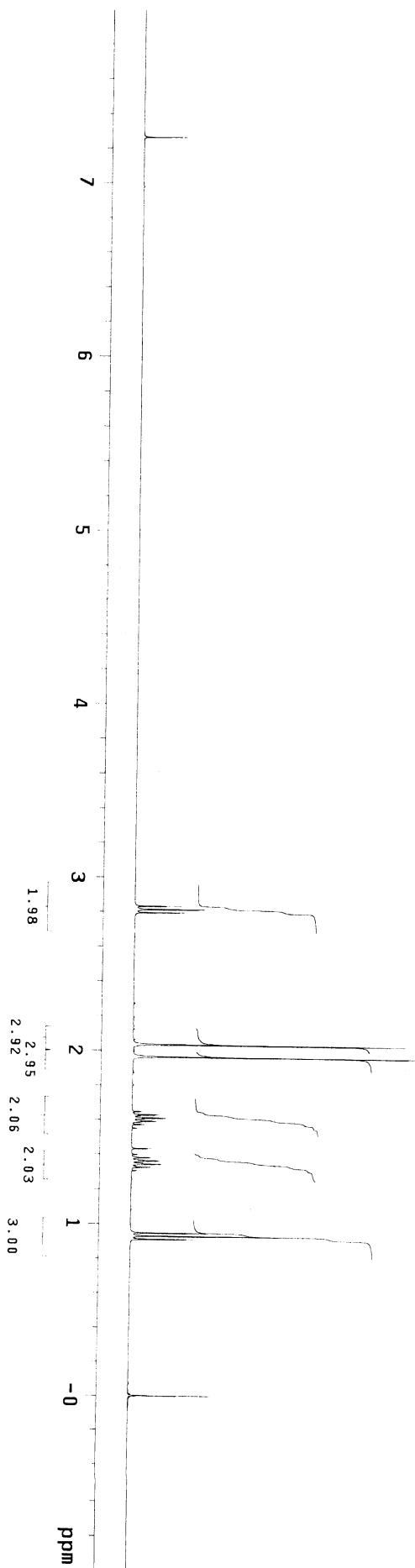
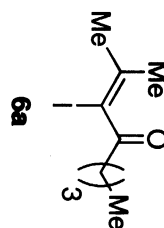
SAMPLE		SPECIAL	
date	Sep 28 2006	temp	25.0
solvent	cdcl3	gain	30
file	/home/waikup/~	spin	not used
nmrsvs	/data/auto/~	hst	0.008
2006.09.28/Aug.01/~	pw90	15.300	
data/cdcl3_01.fid	atfa	10.000	
ACQUISITION		FLAGS	
sw	30487.8	11	n
at	1.300	in	n
np	79298	dp	y
fb	17000	hs	n
bs	64		
dl	1.000	lb	0.50
nt	3300	fn	not used
ct	3264		
TRANSMITTER		DISPLAY	
tn	C13	sp	-1292.8
strq	125.689	wp	28888.0
tof	1255.3	rfl	2074.8
tpwr	49	rfd	0
pw	7.650	lp	-97.8
DECOUPLER		PLOT	
dn	H1	wc	250
dof	0	sc	0
dm	yyv	vs	19078
dmm	w	th	-2
dpwr	39	at	cdc
dmf	12200	ph	



STANDARD 1H OBSERVE - profile
STANDARD 1H OBSERVE - profile
STANDARD 1H OBSERVE - profile
STANDARD 1H OBSERVE - profile

exp2 Proton

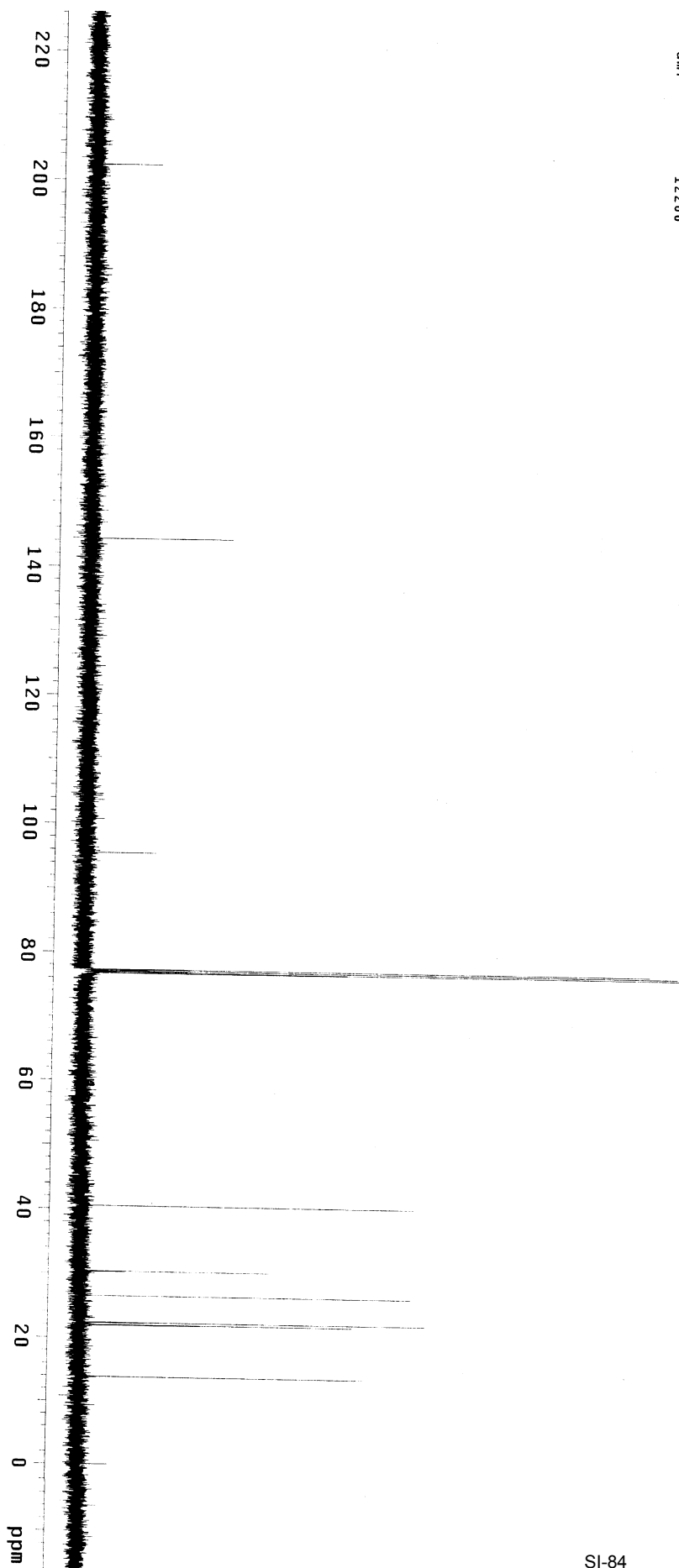
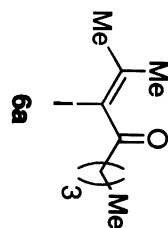
SAMPLE		SPECIAL	
date	Jan 5 2007	temp	25.0
solvent	cdcl3	gain	not used
file	/home/walkup/~	spin	not used
nmr	sys/data/autoc13	hst	0.008
2007.01.05_09/s-20~		pw90	13.900
070105_004/data/cd~		alfa	6.500
c13 01.fid		flags	
ACQUISITION			
sw	6410.3	il	n
at	2.049	dp	y
np	26264	hs	nn
fb	4000	PROCESSING	
bs	32	lb	0.20
ss	2	fn	65536
d1	1.000	DISPLAY	
nt	8	sp	-400.7
ct	8	wd	3601.5
TRANSMITTER			
tn	H1	rfp	805.0
stfq	399.782	tp	-47.5
tof	399.5	lp	-36.0
tpwr	59	PLOT	
pw	6.950	wc	250
DECOUPLER			
dn	C13	vs	0
dof	0	th	100
dm	nmn	ai	cdc
dmm	0	ph	3
dpwr	34		
dnt	29412		



STANDARD 1H OBSERVE - profile

exptl Carbon

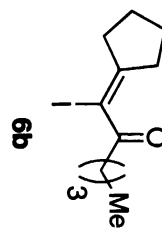
SAMPLE		SPECIAL	
date	Jan 8 2007	temp	25.0
solvent	cdcl3	gain	30
file	/home/walkup/~	spin	not used
nmrSYS/data/auto_~	hst	pw90	0.008
2007.01.08.11/Aug.~	pw90	15.300	
01/data/cdcl3_01.f~	alfta	10.000	
ACQUISITION		FLAGS	
sw	30487.8	in	n
at	1.300	dp	v
np	79298	hs	nn
fb	17000	PROCESSING	
bs	32	lb	0.50
dl	1.000	fn	not used
nt	2560	DISPLAY	
ct	224	sp	-2075.8
TRANSMITTER		wp	30487.3
tn	C13	rfl	11754.4
sfrq	125.689	rfd	9678.1
tof	1255.3	rp	154.2
tpwr	49	lp	-301.0
pw	7.650	PLOT	
DECOUPLER		wc	250
dn	H1	sc	0
dof	0	vs	20000
dm	yyy	th	8
dmm	w	at	cdc ph
dpwr	39		
dmf	12200		



STANDARD 1H OBSERVE - profile

exp4 Proton

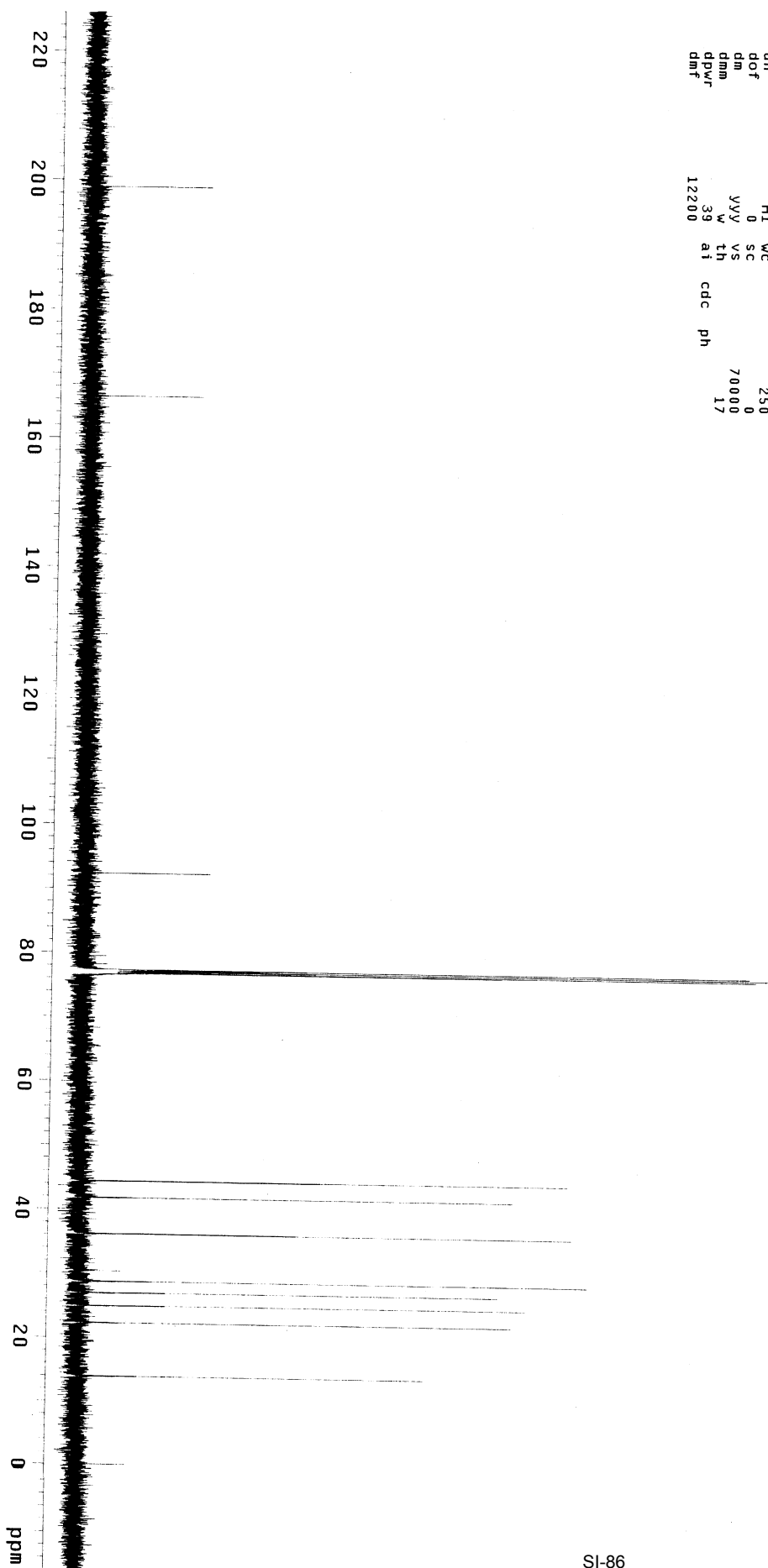
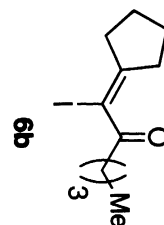
SAMPLE		SPECIAL	
date	Jan 9 2007	temp	25.0
solvent	cdc13	gain	not used
file	/home/walrup/~	spin	not used
nmrsvs	/data/autot~	hst	0.008
	2007.01.09/S_20070~	pw90	13.900
	109_001/data/cdc13~	alpha	6.600
ACQUISITION		FLAGS	
sw	6410.3	in	n
at	2.049	dp	y
np	26264	hs	nm
fb	4000	PROCESSING	0.20
bs	32	lb	65536
ss	2	fn	
dl	1.000	DISPLAY	
nt	8	sp	-393.2
ct	8	wd	3583.9
TRANSMITTER		rfl	805.4
tn	H1	rfd	0
sfrq	399.782	rfp	-71.8
tof	399.5	lp	-44.4
tpwr	59	PLOT	250
pw	6.950	WC	0
DECOUPLER		SC	280
dn	C13	VS	3
dof	0	th	
dm	nmn	ai	cdc
dmm	C	ph	
dpwr	34		
dmf	29412		



STANDARD 1H OBSERVE - profile

expt Carbon

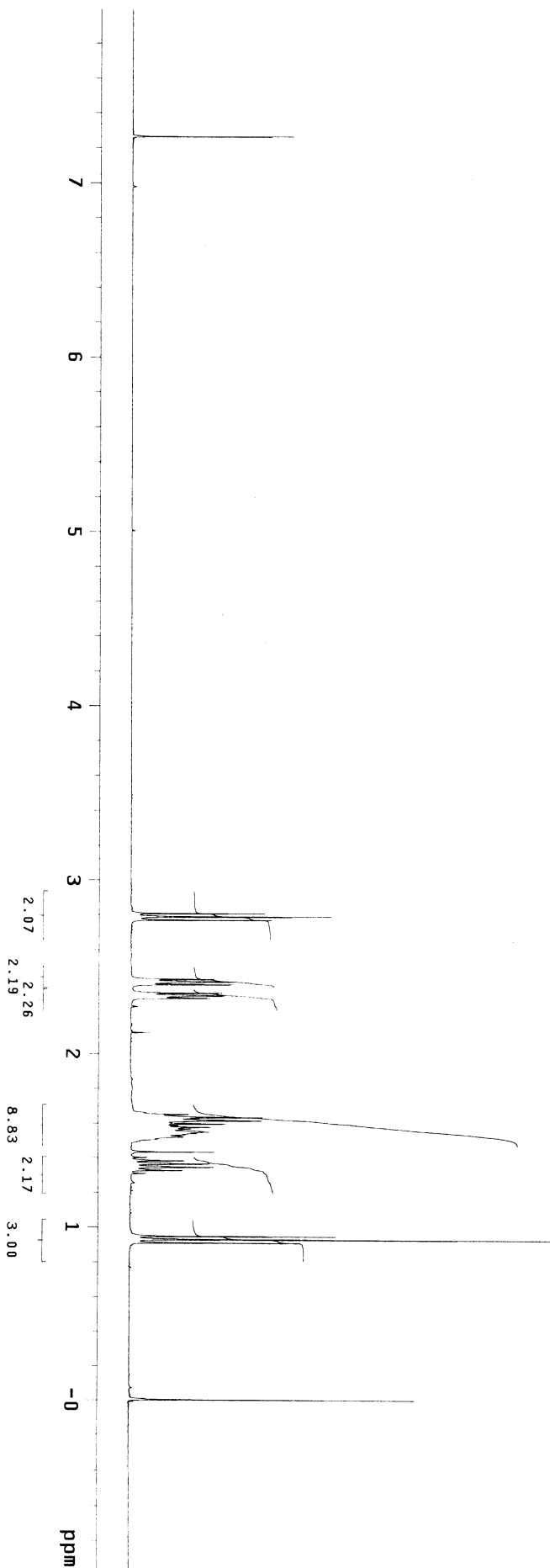
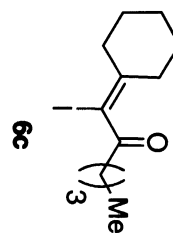
SAMPLE				SPECIAL			
date	Jan 9 2007	temp	25.0				
solvent	cdcl3	gain	30				
file	/home/walkup/~	not used					
data	/Zhang/Weng/C5~	hst	0.008				
ring_NIS	Acetone-p	pw90	15.300				
ue_C13	ftd	atfa	10.000				
ACQUISITION				FLAGS			
sw	30487.8	i1	n				
at	1.300	in	n				
np	79298	dp	y				
fb	17000	hs	nn				
bs	32						
d1	1.000	lb	0.50				
nt	2560	fn	not used				
ct	704						
TRANSMITTER				DISPLAY			
tn	C13	sp	-2075.4				
strq	125.689	wp	30487.3				
tof	1255.3	rfl	11753.9				
tpwr	49	rfd	9678.1				
pw	7.650	lp	-114.2				
DECOUPLER				PLOT			
dn	H1	wc	250				
dof	0	sc	0				
dm	yyy	vs	70000				
dmm	w	th	17				
dpwr	39	ai					
dmf	12200	cdc	ph				



STANDARD 1H OBSERVE - profile

exp2 Proton

SAMPLE		SPECIAL	
date	Jan 3 2007	temp	25.0
solvent	cdcl3	gain	not used
file	/home/walakup/~	spin	not used
nmrsvs/data/	auto~	hst	0.008
2007.01.03.11/	s-20~	pw90	13.900
070103_001/	data/cd~	alfa	6.600
c13	01.fid	FLAGS	
ACQUISITION			
sw	6410.3	in	n
at	2.049	dp	y
np	26264	hs	nn
fb	4000	PROCESSING	
ss	32	lb	0.20
dl	1.000	fn	65536
nt	8	sp	-397.3
ct	8	wp	3594.0
TRANSMITTER		rf1	805.0
tn	H1	rfp	0
stfq	399.782	fp	-39.4
tof	399.5	lp	-46.8
tpwr	59	PLOT	
pw	6.950	wc	250
DECOUPLER		sc	0
dn	C13	vs	300
dof	0	th	2
dm	nmn	at	cdc
dmm	c	ph	
dpwr	34		
dmf	29412		



STANDARD 1H OBSERVE - profile

expt Carbon

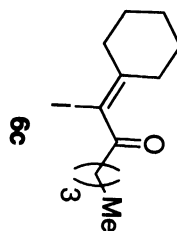
SAMPLE SPECIAL
 date Jan 10 2007 temp 25.0
 solvent cdc13 gain 30
 file /home/walkup/~ not used
 vnmf sys/data/auto_~ hst 0.008
 2007.01.10_01/Aug.~ pw90 15.300
 03/data/cdc13_01.f~ alfa 10.000
 id

ACQUISITION
 sw 30487.8 il n
 at 1.300 in y
 np 79298 hs nn
 fb 17000
 bs 64 lb 0.50
 dl 1.000 fn not used
 nt 256
 ct 64

TRANSMITTER
 tn C13 sp -2077.7
 sfrq 125.689 rfi 30487.3
 tof 1255.3 rfp 11756.2
 tpwr 49 tp -124.6
 pw 7.650 -259.1

DECOUPLER
 dn WC
 dof H1 250
 dm 0
 dmm VS 7000
 dpwr th 7
 dmf w ai cdc ph

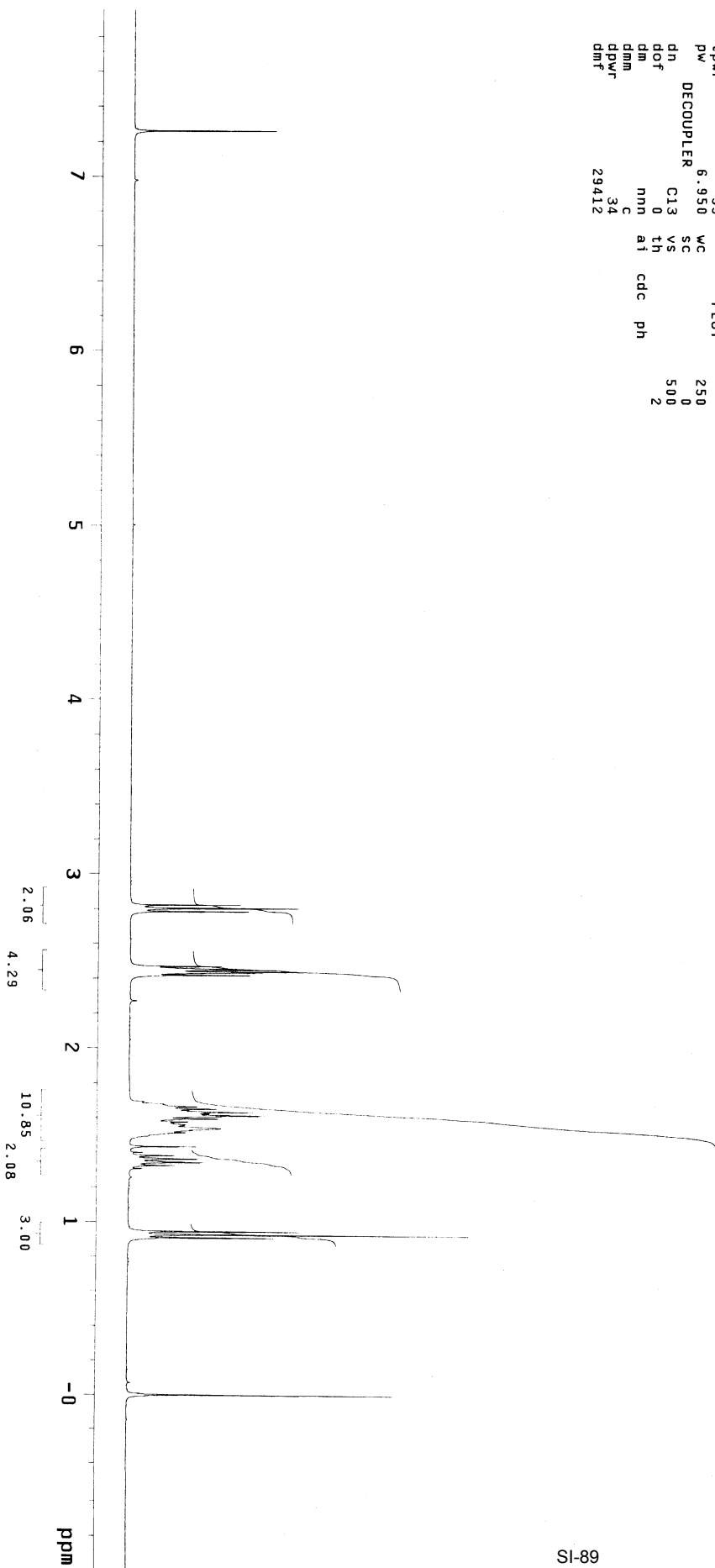
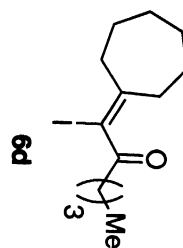
12200



STANDARD 1H OBSERVE - profile
STANDARD 1H OBSERVE - profile
STANDARD 1H OBSERVE - profile

exp2 Proton

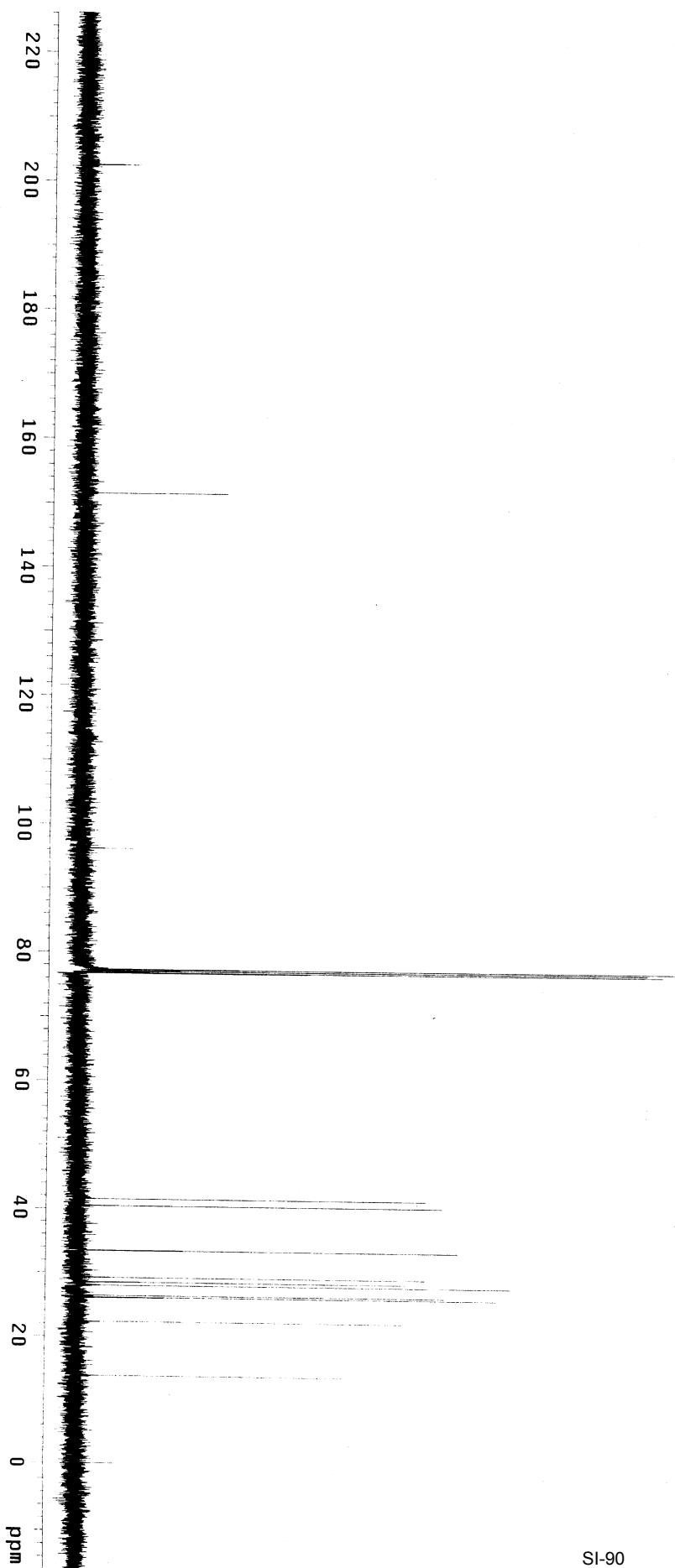
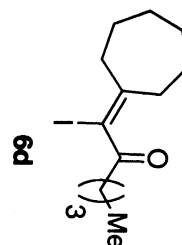
SAMPLE SPECIAL
date Jan 5 2007 temp 25.0
solvent cdcl3 gain not used
file /home/walkup/~ spin not used
vnmrsvs/data/auto ~ hst 0.008
2007.01.05.09/s-20~ pw90 13.900
070105_003/data/cd~ a1fa 6.600
C13 01.fid
ACQUISITION
sw 6410.3 in n
at 2.049 dp y
np 26264 hs nn
fb 4000
bs 32 lb
ss 2 fn
di 1.000 DISPLAY 65536
nt 8 SP -405.5
ct 8 WP 3586.6
TRANSMITTER H1 rfp 805.8
in 399.782 rfp 0
sfreq 399.5 lp -46.4
tof 399.5 1p -33.1
tpwr 59
pw 6.950 WC 250
DECOUPLER C13 VS 0
dn 0 tn ai cdc ph 500
dof 0
dm nnh
dmm c
dpwr 34
dmf 29412



STANDARD 1H OBSERVE - profile

expt Carbon

SAMPLE		SPECIAL	
date	Jan 9 2007	temp	25.0
solvent	cdcl3	gain	30
file	/home/walkup/~	spin	not used
nmr	sys/data/aut/~	hst	0.008
2007.01.09/Aug.01/~	pw90	15.300	
data/cdcl3_01.fid	alfa	10.000	
ACQUISITION		FLAGS	
sw	30487.8	i1	n
at	1.300	in	n
np	79298	dp	y
fb	17000	hs	nn
bs	64		
d1	1.000	lb	0.50
nt	256	fn	not used
ct	256		
TRANSMITTER		DISPLAY	
tn	C13	sp	-2075.8
sfrq	125.689	wp	30487.3
tof	1255.3	rfl	11754.4
tpwr	49	rfp	9678.1
pw	7.650	fp	141.7
DECOUPLER		lp	-232.2
dn	H1		
dof	0	WC	250
dm	0	SC	0
dmm	YVY	VS	23000
dpmr	W	th	7
dmf	39	ai	
	12200	cdc	ph



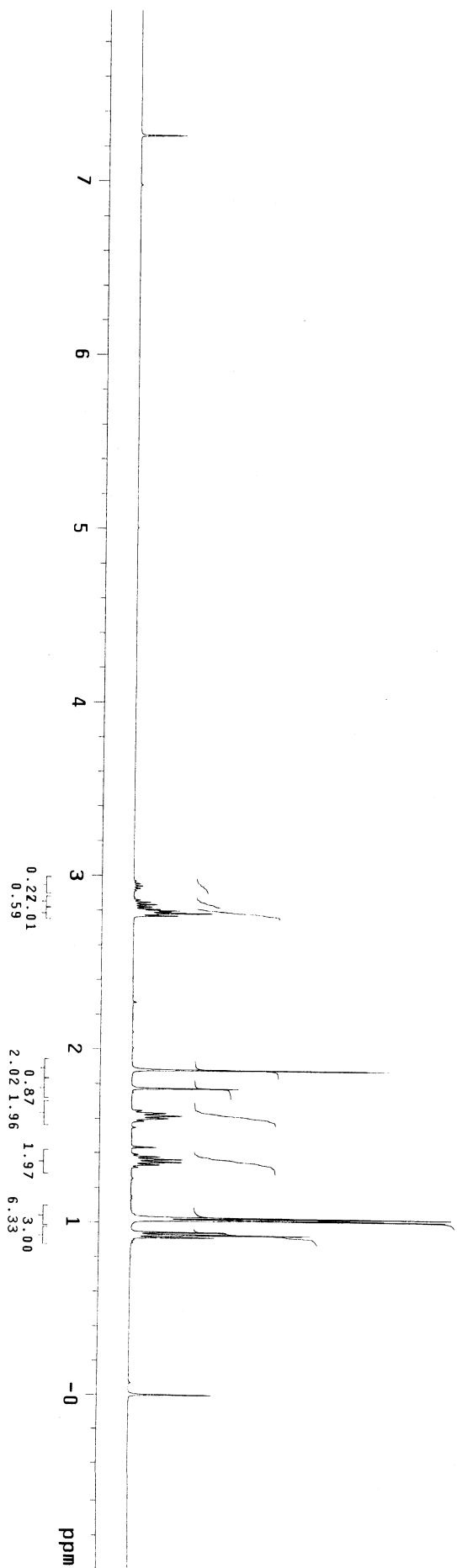
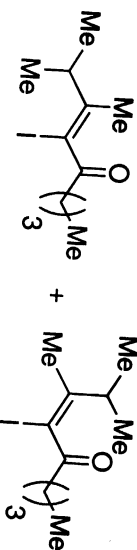
STANDARD 1H OBSERVE - profile

expt Proton

SAMPLE		SPECIAL	
date	Jan 9 2007	temp	25.0
solvent	cdc13	gain	not used
file	/home/walkup/~	spin	not used
vmr	sys/data/auto_~	hst	0.008
2007.01.09_04/AUG.~		pw90	14.700
01/data/cdc13_01.f~		alfa	6.600

ACQUISITION		FLAGS	
sw	8012.8	in	n
at	2.049	dp	y
np	32830	hs	nn
fb	4000		
bs	32	lb	0.20
ss	2	fn	65536
dl	1.000		
nt	8	sp	-509.6
ct	8	wd	4499.4
tn	8	rfl	1007.5
sfreq	499.809	rfp	0
tof	499.7	tp	-159.8
tpwr	54	ip	-32.4
pw	7.350	wc	250

DECOUPLER		PLOT	
dn	C13	sc	0
dof	0	th	80
dm	nnn	ai	cdc
dmm		ph	
dpwr	34		
dnt	32258		

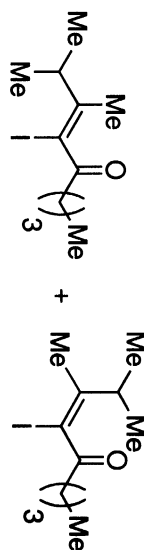


STANDARD 1H OBSERVE - profile
STANDARD 1H OBSERVE - profile

expt Carbon

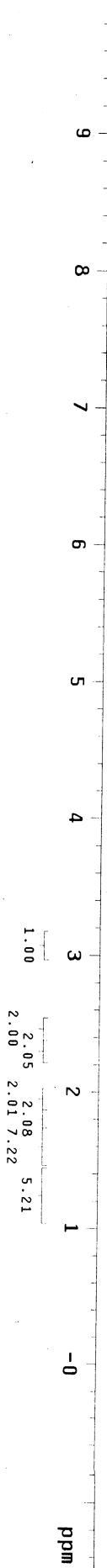
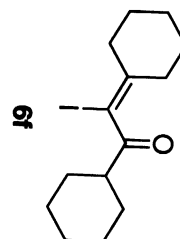
SAMPLE SPECIAL 25.0
date Jan 9 2007 temp
solvent cdc13 gain 30
file /home/walkup/~ not used
vmr/sys/data/auto_~ hst 0.008
2007.01.09.06/Aug.~ pw90 15.300
03/data/cdc13_01.f~ alfa 10.000

ACQUISITION id f1 FLAGS
sw 30487.8 in n
at 1.300 dp y
np 79298 hs
tb 17000
bs 32 lb
d1 1.000 fn
nt 500 not used
ct 256 DISPLAY
tn TRANSMITTER C13 SP -2075.8
sfreq 125.689 rf1 11734.4
tof 1255.3 rfp 9678.1
tpwr 49 tp -126.6
pw 7.650 PLOT -259.6
DECOUPLER WC 250
dn H1 SC 0
dof 0
dm yy th 40000
dmm w at
dpwr 39 cdc ph 4
dmf 12200



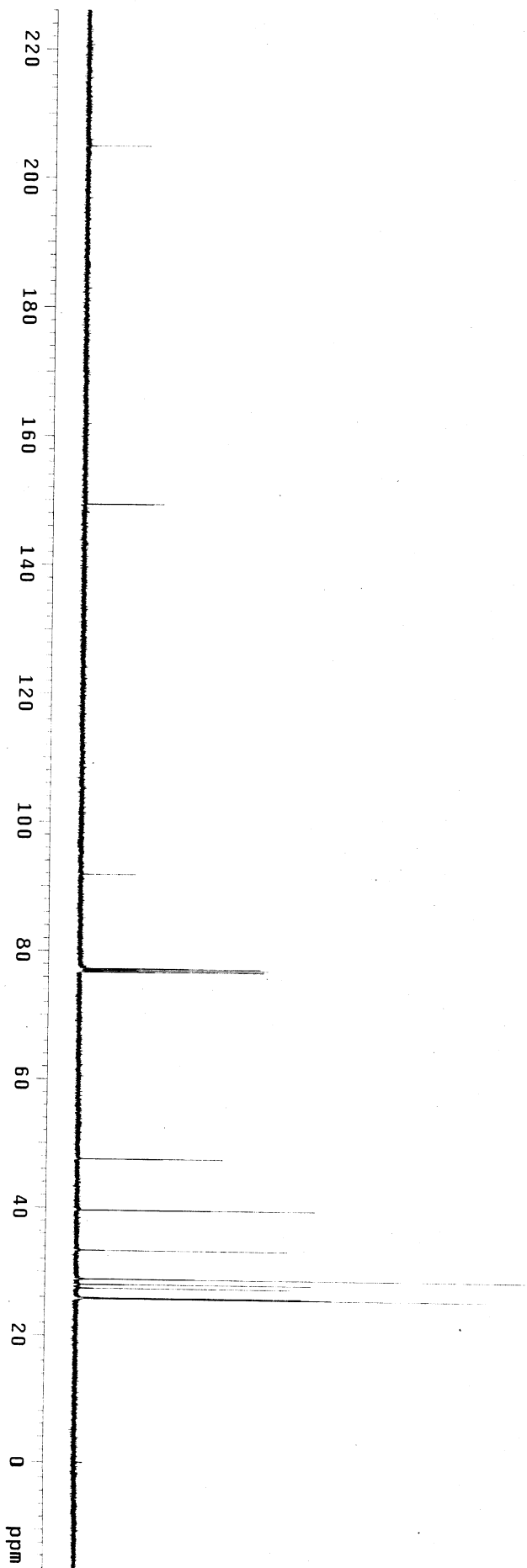
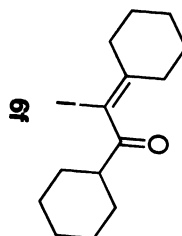
expt1 Proton

SAMPLE		SPECIAL	
date	Jan 18 2007	temp	25.0
solvent	cdcl3	gain	30
file	/home/vmr1/n~	spin	not used
mr500	waikup/data/~	hst	0.008
Zhang/Guozhu/H1-20~		pw90	14.700
070118-60.fid		alfa	6.600
ACQUISITION		FLAGS	
sw	8012.8	i1	n
at	2.049	in	n
np	32830	dp	y
fb	4000	hs	nn
bs	8		
d1	1.000	lb	0.20
nt	1	fn	65536
ct	1		
TRANSMITTER		DISPLAY	
tn	H1	sp	-751.4
sfrq	499.809	wd	5703.2
tof	499.7	rfl	1004.0
tpwr	54	rfp	0
pwr	7.350	tp	-170.4
DECOUPLER		PLOT	
dn	C13	wc	250
dof	0	sc	0
dm	nn	vs	185
dmm	c	th	2
dpwr	34	ai	cdc
dmf	32258	ph	



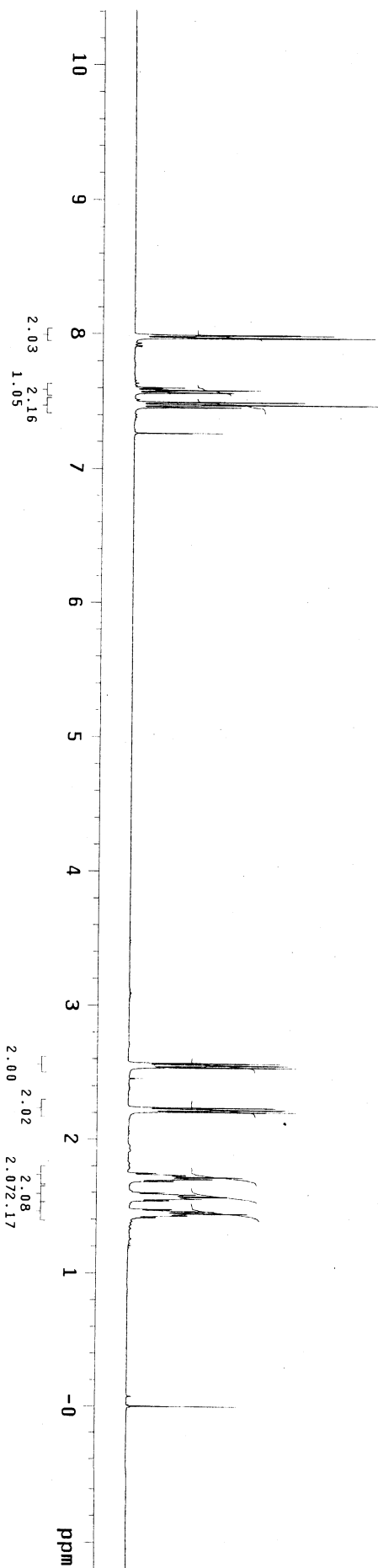
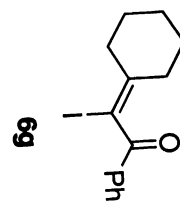
expt Carbon

SAMPLE SPECIAL
date Jan 18 2007 temp 25.0
solvent cdc13 gain 30
file /home/vmr1/n~ spin not used
mr500/waikup/data/~ hst 0.008
Zhang/Guozhu/C13-2~ pw90 15.300
0070118-61.fid alfa 10.000
ACQUISITION
sw 30487.8 f1 n
at 1.300 in n
np 79298 dp y
fb 17000 hs nn
bs 64
d1 1.000 lb
nt 1280 fn not used
ct 320
TRANSMITTER SP DISPLAY
tn C13 wd -2077.8
sfrq 125.689 rf1 30487.3
tof 1255.3 rfp 11755.3
tpwr 49 9677.1
pw 7.650 tp -102.1
DECOUPLER PLOT
dn H1 WC 250
dof 0 SC 0
dm 0 VS 12965
dmm VVV w th 6
dpwr 39 ai cdc ph
dmf 12200



expt1 Proton

SAMPLE		SPECIAL	
date	Jan 18 2007	temp	25.0
solvent	cdcl3	gain	30
file	/home/vnmr1/n~	spin	not used
mr400	wal kup/data/~	hst	0.008
Zhang/Guozhu/H1-20~		pw90	13.900
070117-56.fid	alfa		6.600
ACQUISITION		FLAGS	
sw	6410.3	i1	n
at	2.049	in	n
np	26264	dp	y
fb	4000	hs	nn
bs	8		
dl	1.000	lb	0.20
nt	1	fn	65536
ct	1		
TRANSMITTER		DISPLAY	
tn	H1	sp	-492.2
sfrq	399.782	wd	4653.5
tof	399.5	rfl	805.2
tpwr	53	rtp	139.3
pw	6.950	tp	-23.1
DECOUPLER		PLOT	
dn	C13	wc	250
dof	0	sc	0
dm	nnn	vs	2720
dmm	c	th	3
dpwr	34	ai	cdc
dmf	29412	ph	



expt Carbon

SAMPLE SPECIAL
date Jan 18 2007 temp 25.0
solvent cdc13 gain 30
file /home/vmr1/n~ spin not used
m:500/walkup/data/~ hst 0.008
Zhang/Guozhu/C13-2~ pw90 15.300
0070118-58.fid alfa 10.000
ACQUISITION
sw 30487.8 f1
at 1.300 in n
np 79298 dp y
fb 17000 hs nn
bs 64
dl 1.000 lb
nt 1280 fn not used
ct 768
TRANSMITTER
tn C13 sp -2081.0
sfreq 125.689 wf 30487.3
tof 1255.3 rfp 11758.6
tpwr 49 rfp 9677.1
pw 7.650 tp -101.7
DECOUPLER PLOT -263.1
dn H1 wc 250
dof 0 sc 0
dm 0 vs 0
dmm YVW 9090
dpwr 39 ai
dmf 12200 cdc ph 2

