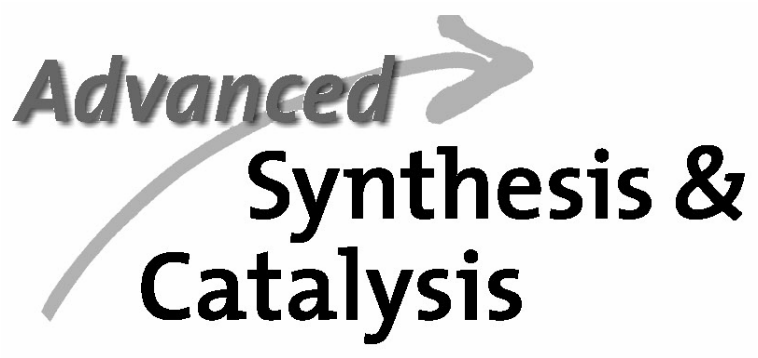

Supporting Information

Supporting Information

Gold-Catalyzed Efficient Formation of α, β-Unsaturated Ketones from Propargylic Acetates

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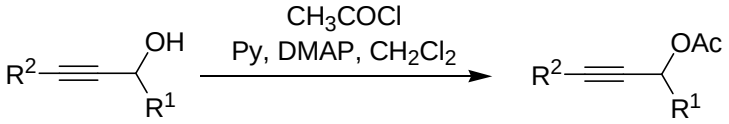
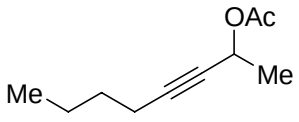
General. Ethyl acetate (ACS grade), hexanes (ACS grade) and diethyl ether (ACS grade) were purchased from Fisher Scientific and used without further purification. Anhydrous dichloromethane (HPLC grade) was purified by distillation over calcium hydride. Anhydrous tetrahydrofuran in Pure–Pac™ from Aldrich was used directly without further purification. Commercially available reagents were used without further purification. Reactions were monitored by thin layer chromatography(TLC) using whatman precoated silica gel plates. Flash column chromatography was performed over silacycle silica gel (230–400 mesh). ^{1}H NMR and ^{13}C 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 acetate

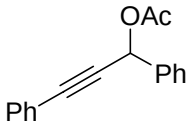


To a solution of propargylic alcohol (2.0 mmol), pyridine (1.65 mL, 20.0 mmol) and catalytic amount of DMAP in anhydrous CH_2Cl_2 (6.0 mL) at 0^{o}C, was slowly added acetyl chloride (0.29 mL, 4.0 mmol). The reaction was stirred at the same temperature for 30 min before being diluted with hexanes (30 mL). The solid precipitates were filtered off and the filtrate obtained was concentrated. The residue was purified through silica gel flash column chromatography (hexanes/ethyl acetate = 20/1) to yield the desired acetate.



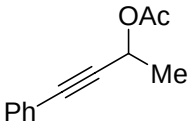
1

Compound **1** was prepared in 86% yield according to the general procedure A. ^{1}H 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 $[C_{10}H_{16}NaO_2]^{+}$: 191.1; Found: 191.0.



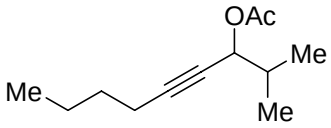
3a

Compound **3a** was prepared in 95% yield according to the general procedure A. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62–7.58 (m, 2H), 7.50–7.47 (m, 2H), 7.43–7.28 (m, 6H), 6.70 (s, 1H), 2.13 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.8, 137.2, 131.9, 128.9, 128.8, 128.3, 127.8, 122.1, 87.0, 85.6, 66.1, 21.1; IR (neat): 3065, 3035, 2936, 2230, 1742, 1599, 1491, 1370; MS (ES$^+$) Calculated for $[C_{17}H_{14}NaO_2]^+$: 273.2; Found: 273.1.



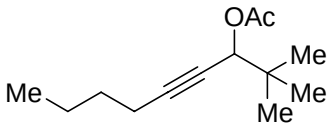
3b

Compound **3b** was prepared in 86% yield according to the general procedure A. ^{1}H NMR (400 MHz, $CDCl_3$) 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); ^{13}C NMR (100 MHz, $CDCl_3$) 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 $[C_{12}H_{12}NaO_2]^+$: 211.1; Found: 210.9.



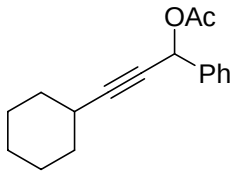
3c

Compound **3c** was prepared in 92% yield according to the general procedure A. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.21 (dt, 1H, *J* = 5.6, 2.0 Hz), 2.22 (td, 2H, *J* = 6.8, 2.0 Hz), 2.08 (s, 3H), 2.00–1.92 (m, 1H), 1.53–1.46 (m, 2H), 1.45–1.36 (m, 2H), 1.00 (d, 3H, *J* = 6.8 Hz), 0.97 (d, 3H, *J* = 6.8 Hz), 0.91 (t, 3H, *J* = 7.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.2, 86.7, 76.1, 69.5, 32.5, 30.6, 21.9, 21.1, 18.4, 18.2, 17.5, 13.5; IR (neat): 2964, 2935, 2876, 2234, 1743, 1468, 1371; MS (ES$^+$) Calculated for $[C_{12}H_{20}NaO_2]^+$: 219.1; Found: 219.0.



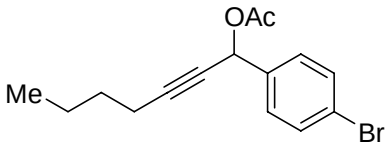
3d

Compound **3d** was prepared in 87% yield according to the general procedure A. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.10–5.09 (t, 1H, *J* = 2.0 Hz), 2.23–2.19 (dt, 2H, *J* = 2.0, 6.8 Hz), 2.09 (s, 3H), 1.51–1.46 (m, 2H), 1.45–1.36 (m, 2H), 0.989 (s, 9H), 0.92–0.89 (t, 3H, *J* = 7.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.3, 86.4, 76.3, 72.3, 35.1, 30.6, 25.5, 21.9, 21.0, 18.4, 13.5; IR (neat): 2961, 2936, 2873, 2236, 1744, 1592, 1466, 1370, 1238; MS (ES^+) Calculated for $[C_{13}H_{22}NaO_2]^+$: 233.2; Found: 233.1.



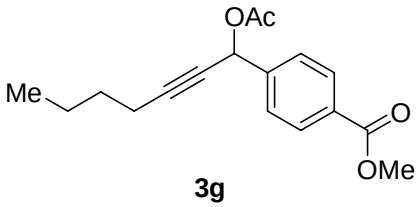
3e

Compound **3e** was prepared in 94% yield according to the general procedure A. ^{1}H NMR (400 MHz, $CDCl_3$) 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 $[C_{17}H_{20}NaO_2]^+$: 279.1; Found: 279.1.



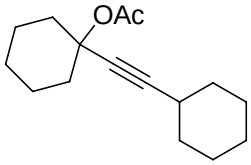
3f

Compound **3f** was prepared in 98% yield according to the general procedure A. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51–7.48 (m, 2H), 7.41–7.38 (m, 2H), 6.40 (t, 1H, *J* = 2.0 Hz), 2.26 (dt, 2H, *J* = 2.0, 7.2 Hz), 2.09 (s, 3H), 1.56–1.48 (m, 2H), 1.44–1.35 (m, 2H), 0.91 (t, 3H, *J* = 7.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.7, 136.8, 131.7, 129.4, 122.8, 88.8, 76.2, 65.4, 30.4, 21.9, 21.1, 18.5, 13.5; IR (neat): 3584, 3363, 2959, 2934, 2873, 2234, 1743, 1592, 1487, 1369, 1225, 1012, 953; MS (ES^+) Calculated for $[C_{15}H_{17}BrNaO_2]^+$: 331.0; Found: 331.0.



3g

Compound **3g** was prepared in 92% yield according to the general procedure A. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06–8.03 (m, 2H), 7.59–7.56 (m, 2H), 6.48 (t, 1H, *J* = 2.0 Hz), 3.92 (s, 3H), 2.27 (dt, 2H, *J* = 2.0, 7.2 Hz), 2.11 (s, 3H), 1.57–1.49 (m, 2H), 1.45–1.35 (m, 2H), 0.91 (t, 3H, *J* = 7.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.7, 166.6, 142.5, 130.4, 129.9, 127.5, 89.0, 76.1, 65.4, 52.2, 30.4, 21.9, 21.1, 18.5, 13.5; IR (neat): 3584, 3421, 2958, 2935, 2874, 2235, 1739, 1729, 1614, 1436, 1371, 1281, 1225, 1111, 1018, 958; MS (ES^+) Calculated for $[C_{17}H_{20}NaO_4]^+$: 311.1; Found: 311.1.

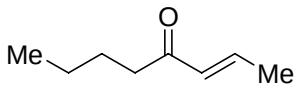


5f

Compound **5f** was prepared in 91% yield according to the general procedure A. ^{1}H 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 $[C_{16}H_{24}NaO_2]^+$: 271.2; Found: 271.1.

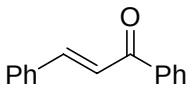
General procedure B: Preparation of *β*–monosubstituted enones

To a solution of propargylic acetate (0.2 mmol) in 2–butanone (4 mL) was added $Au(PPh_3)NTf_2$ (2.7 mg, 0.004 mmol) at room temperature. The reaction was stirred for the indicated time before quenched with NEt_3. The reaction mixture was concentrated, and the resulting residue was purified through silica gel flash column chromatography (hexanes/ethyl acetate = 20/1) to yield the desired *α,β*–unsaturated ketones.



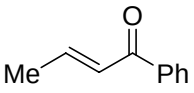
2

Compound **2** was prepared in 95% yield according to the general procedure B (reaction time: 16 h). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.84 (dq, 1H, *J* = 6.8, 16.0 Hz), 6.12 (dq, 1H, *J* = 1.2, 16.0 Hz), 2.52 (t, 2H, *J* = 7.2 Hz), 1.90 (dd, 3H, *J* = 1.2, 6.8 Hz), 1.59 (p, 2H, *J* = 7.2 Hz), 1.33 (sextet, 2H, *J* = 7.2 Hz), 0.91 (t, 3H, *J* = 7.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.8, 142.2, 132.0, 39.8, 26.4, 22.4, 18.2, 13.9; IR (neat): 2959, 2922, 2873, 1729, 1595, 1433, 1317; MS (ES^+) Calculated for $[C_8H_{14}NaO]^+$: 149.1; Found: 149.0.



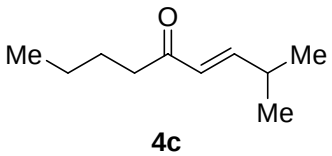
4a

Compound **4a** was prepared in 82% yield according to the general procedure B (reaction time: 16 h). This is a known compound and its spectra match the reported (Kryshtal, G. V.; Zhdankina, G. M.; Zlotin, S. G.; *Eur. J. Org. Chem.* **2005**, *13*, 2822-2827).



4b

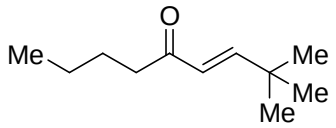
Compound **4b** was prepared in 78% yield according to the general procedure B (reaction time: 24 h). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94–7.91 (m, 2H), 7.58–7.53 (m, 1H), 7.49–7.44 (m, 2H), 7.07 (dq, 1H, *J* = 6.8, 15.2 Hz), 6.91 (dq, 1H, *J* = 1.6, 15.2 Hz), 2.01 (dd, 3H, *J* = 1.6, 7.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.8, 145.0, 137.9, 132.6, 128.5, 127.6, 77.2, 18.6; IR (neat): 3584, 3391, 3056, 2974, 2918, 2851, 1674, 1625, 1598, 1580, 1449, 1298, 1220, 1039, 1024, 966, 918; MS (ES^+) Calculated for $[C_{10}H_{10}NaO]^+$: 169.1; Found: 169.0.



4c

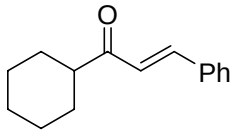
Compound **4c** was prepared in 92% yield according to the general procedure B (reaction time: 16 h). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.80 (dd, 1H, *J* = 6.8, 16 Hz), 6.04 (dd, 1H, *J* = 1.6, 16 Hz), 2.54 (t, 2H, *J* = 7.6 Hz), 2.46 (do, 1H, *J* = 1.6, 6.8 Hz), 1.59 (p, 2H, *J* = 7.6 Hz), 1.34 (sextet, 2H, *J* = 7.6 Hz), 1.07 (d, 6H, *J* = 6.8 Hz), 0.92 (t, 3H, *J* = 7.6 Hz); ^{13}C NMR (100 MHz,

$CDCl_3$) δ 201.3, 153.2, 127.5, 39.9, 31.1, 26.4, 22.4, 21.3, 13.9; IR (neat): 2959, 2924, 2855, 1731, 1597, 1436, 1316, 1262, 1156, 1121, 1045; MS (ES^+) Calculated for $[C_{10}H_{18}NaO]^+$: 177.1; Found: 177.1.



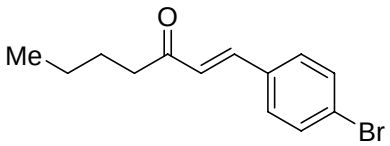
4d

Compound **4d** was prepared in 90% yield according to the general procedure B (reaction time: 16 h). ^1H NMR (400 MHz, $CDCl_3$) δ 6.81 (d, 1H, *J* = 16.4 Hz), 6.01 (d, 1H, *J* = 16.4 Hz), 2.55 (t, 2H, *J* = 7.6 Hz), 1.60 (p, 2H, *J* = 7.6 Hz), 1.34 (sextet, 2H, *J* = 7.6 Hz), 1.09 (s, 9H), 0.92 (t, 3H, *J* = 7.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.5, 156.8, 125.4, 40.0, 33.7, 28.7, 26.4, 22.4, 13.9; IR (neat): 2961, 2935, 2872, 1743, 1674, 1626, 1464, 1367, 1237, 1072; MS (ES^+) Calculated for $[C_{11}H_{20}NaO]^+$: 191.1; Found: 191.0.



4e

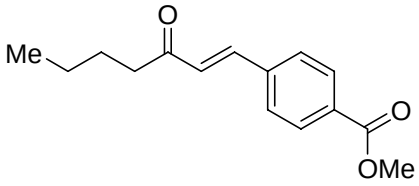
Compound **4e** was isolated as an *E*/*Z* (8/1) mixture in 88% yield according to the general procedure B (reaction time: 16 h). ^1H NMR (400 MHz, $CDCl_3$) (major isomer) δ 7.59 (d, 1H, *J* = 16 Hz), 7.57–7.54 (m, 2H), 7.38–7.37 (m, 3H), 6.81 (d, 1H, *J* = 16 Hz), 2.69–2.62 (m, 1H), 1.91–1.19 (m, 10H); ^{13}C NMR (100 MHz, $CDCl_3$) (major isomer) δ 203.1, 142.2, 134.8, 130.3, 128.9, 128.3, 124.7, 49.4, 28.7, 25.9, 25.8; IR (neat): 3080, 3057, 3026, 2949, 2929, 2915, 2849, 1683, 1613, 1575, 1449, 1370, 1146, 1067, 992; MS (GC–MS) Calculated for $[C_{15}H_{19}O]^+$: 215; Found: 215.



4f

Compound **4f** was prepared in 88% yield according to the general procedure B (reaction time: 12 h). ^1H NMR (400 MHz, $CDCl_3$) δ 7.54–7.51 (m, 2H), 7.48 (d, 1H, *J* = 16 Hz), 7.42–7.40 (m, 2H), 6.72 (d, 1H, *J* = 16 Hz), 2.65 (t, 2H, *J* = 7.6 Hz), 1.66 (p, 2H, *J* = 7.6 Hz), 1.38 (sextet, 2H, *J* = 7.6 Hz), 0.94 (t, 3H, *J* = 7.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.3, 140.8, 133.5,

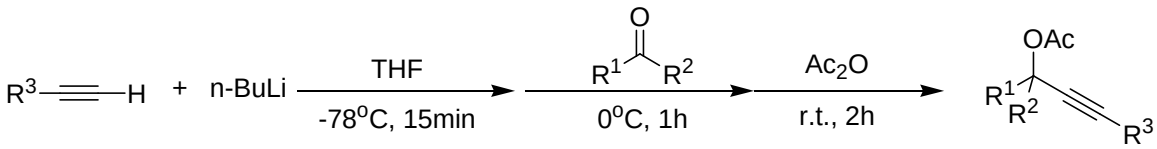
132.2, 129.6, 126.7, 124.6, 40.9, 26.38, 22.42, 13.9; IR (neat): 3065, 3031, 2951, 2932, 2895, 2870, 2354, 2321, 1687, 1684, 1616, 1487, 1404, 1068, 1057, 988, 810; MS (ES^+) Calculated for $[C_{13}H_{16}BrO]^+$: 267; Found: 267.



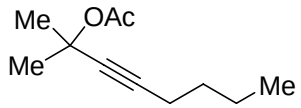
4g

Compound **4g** was prepared in 90% yield according to the general procedure B (reaction time: 12 h). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07–8.04 (m, 2H), 7.62–7.60 (m, 2H), 7.56 (d, 1H, *J* = 16 Hz), 6.81 54 (d, 1H, *J* = 16 Hz), 3.93 (s, 3H), 2.68 (t, 2H, *J* = 7.6 Hz), 1.67 (p, 2H, *J* = 7.6 Hz), 1.39 (sextet, 2H, *J* = 7.6 Hz), 0.95 (t, 3H, *J* = 7.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.3, 166.4, 140.7, 138.9, 131.4, 130.1, 128.1, 128.0, 52.3, 41.0, 26.3, 22.4, 13.9; IR (neat): 3016, 2956, 2932, 2868, 2354, 2320, 1722, 1651, 1433, 1412, 1283, 1110, 985, 977, 881; MS (ES^+) Calculated for $[C_{15}H_{18}NaO_3]^+$: 269.1; Found: 269.1.

General procedure C: Preparation of propargylic acetates

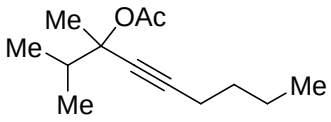


To a solution of alkyne (11 mmol) in anhydrous THF (42 mL) at –78^{o}C under N_2 was added *n*-BuLi (2.5 M solution in hexanes, 4.2 mL, 10.5 mmol). The reaction was stirred at the same temperature for 15 min before addition of ketone/aldehyde (10 mmol). The resulting mixture was allowed to warm to 0 °C gradually and stirred for an additional hour. Upon the addition of acetate anhydrous (2.4 mL, 25 mmol), the reaction mixture was stirred at room temperature for 2 h before quenched with aqueous $NaHCO_3$. The mixture was extracted with Et_2O (3 x 30 mL). 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.



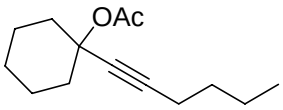
5a

Compound **5a** was prepared in 74% yield according to the general procedure C. ^{1}H 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 $[C_{11}H_{18}NaO_2]^+$: 205.1; Found: 205.1.



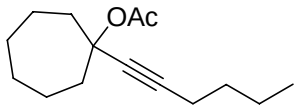
5b

Compound **5b** was prepared in 80% yield according to the general procedure C. ^{1}H 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 $[C_{13}H_{22}NaO_2]^+$: 233.2; Found: 233.2.



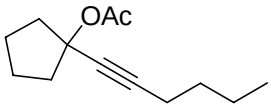
5c

Compound **5c** was prepared in 84% yield according to the general procedure C. ^{1}H 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 $[C_{14}H_{22}NaO_2]^+$: 245.2; Found: 245.1.



5d

Compound **5d** was prepared in 70% yield according to the general procedure C. ^{1}H 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 $[C_{15}H_{24}NaO_2]^+$: 257.2; Found: 259.2.

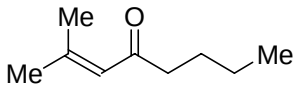


. **5e**

Compound **5e** was prepared in 70% yield according to the general procedure C. ^{1}H 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 $[C_{13}H_{20}NaO_2]^+$: 231.1; Found: 231.1.

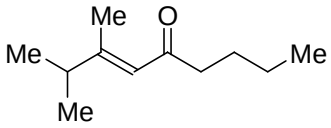
General procedure D: Preparation of *β,β*–disubstituted ketones

To a solution of propargylic acetate (0.2 mmol) in acetonitrile (4 mL) cooled in ice-water bath was added $Au(PPh_3)NTf_2$ (0.001 mmol, 0.2 mL of 0.05 M solution in acetone). The reaction mixture was stirred at the same temperature for 0.5 h before warming to room temperature. The reaction was quenched with NEt_3 after stirred for the indicated time. The reaction mixture was concentrated. The residue was purified through silica gel flash column chromatography (hexanes/ethyl acetate = 20/1) to yield the desired *β,β*–disubstituted ketones.



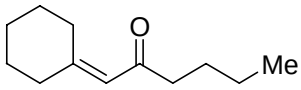
6a

Compound **6a** was prepared in 98% yield according to the general procedure D (reaction time: 16 h). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.08–6.06 (m, 1H), 2.40 (t, 2H, *J* = 7.6 Hz), 2.14 (d, 3H, *J* = 0.8 Hz), 1.88 (d, 3H, *J* = 1.2 Hz), 1.57 (p, 2H, *J* = 7.6 Hz), 1.32 (sextet, 2H, *J* = 7.6 Hz), 0.91 (t, 3H, *J* = 7.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.4, 154.6, 123.8, 44.0, 27.6, 26.4, 22.4, 20.6, 13.9; IR (neat): 2955, 2922, 2874, 2349, 2316, 1735, 1594, 1430, 1316, 1154, 1119, 1043, 874; MS (ES$^+$) Calculated for $[C_9H_{17}O]^+$: 141.1; Found: 141.1.



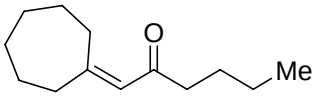
6b

Compound **6b** was isolated as a mixture of geometrical isomers (*E*/*Z* = 4/1) in 88% yield according to the general procedure D (reaction time: 24h). ^{1}H NMR (400 MHz, $CDCl_3$) (major isomer) δ 6.06–6.05 (m, 1H), 2.42 (t, 2H, *J* = 7.6 Hz), 2.33 (heptet, 1H, *J* = 6.8 Hz), 2.09 (d, 3H, *J* = 1.2 Hz), 1.61–1.53 (m, 2H), 1.37–1.25 (m, 2H), 1.06 (d, 6H, *J* = 6.7 Hz), 0.91 (t, 3H, *J* = 7.3 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) (major isomer) δ 202.0, 163.6, 121.1, 44.2, 38.2, 26.4, 22.4, 20.9, 16.8, 13.9; IR (neat): 3363, 2962, 2933, 2874, 1755, 1688, 1616, 1464, 1381, 1224, 1132, 1058, 925, 852; MS (GC–MS) Calculated for $[C_{11}H_{21}O]^+$: 169; Found: 169.



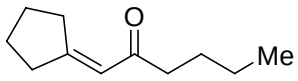
6c

Compound **6c** was prepared in 97% yield according to the general procedure D (reaction time: 16 h). ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.97 (t, 1H, *J* = 1.2 Hz), 2.01–2.78 (m, 2H), 2.41 (t, 2H, *J* = 7.6 Hz), 2.18–2.12 (m, 2H), 1.67–1.62 (m, 2H), 1.61–1.53 (m, 6H), 1.37–1.28 (m, 2H), 0.91 (t, 3H, *J* = 7.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.1, 161.5, 121.0, 44.2, 38.1, 29.9, 28.8, 27.9, 26.4, 26.3, 22.4, 13.9; IR (neat): 3367, 2932, 2859, 2354, 1685, 1622, 1448, 1137, 1064, 936; MS (ES$^+$) Calculated for $[C_{12}H_{20}NaO]^+$: 203.1; Found: 203.1.



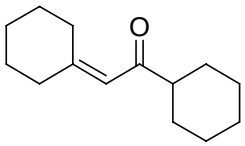
6d

Compound **6d** was prepared in 83% yield according to the general procedure D (reaction time: 16 h). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.06 (t, 1H, *J* = 0.9 Hz), 2.85 (dt, 2H, *J* = 0.9, 6.4 Hz), 2.40 (t, 2H, *J* = 7.6 Hz), 2.33 (dt, 2H, *J* = 0.9, 6.4 Hz), 1.68–1.51 (m, 10H), 1.33 (sextet, 2H, *J* = 7.2 Hz), 0.91 (t, 3H, *J* = 7.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.5, 165.6, 123.5, 44.3, 39.4, 33.1, 30.1, 29.4, 28.4, 26.7, 26.7, 22.7, 14.1; IR (neat): 3349, 3015, 2955, 2928, 2856, 1755, 1685, 1608, 1454, 1444, 1385, 1131, 1071, 956; MS (ES^+) Calculated for $[C_{13}H_{22}NaO]^+$: 217.2; Found: 216.9.



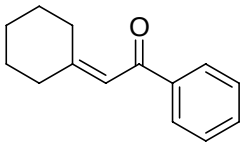
6e

Compound **6e** was prepared in 82% yield according to the general procedure D (reaction time: 16 h). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.24 (t, 1H, *J* = 1.2 Hz), 2.76 (t, 2H, *J* = 7.3 Hz), 2.41 (t, 2H, *J* = 7.5 Hz), 1.74 (p, 2H, *J* = 7.5 Hz), 1.64 (p, 2H, *J* = 7.5 Hz), 1.57 (p, 2H, *J* = 7.3 Hz), 1.32 (sextet, 2H, *J* = 7.3 Hz), 0.90 (t, 3H, *J* = 7.3 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.7, 168.0, 119.3, 43.7, 36.2, 33.4, 26.6, 26.4, 25.3, 22.4, 13.9; IR (neat): 3013, 2958, 2935, 2872, 2358, 1689, 1622, 1457, 1373, 1167, 1065, 855; MS (GC–MS) Calculated for $[C_{11}H_{19}O]^+$: 167; Found: 167.



6f

Compound **6f** was prepared in 93% yield according to the general procedure D (reaction time: 20 h). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.01 (d, 1H, *J* = 1.0 Hz), 2.79–2.77 (t, 2H, *J* = 4.6 Hz), 2.34–2.28 (m, 1H), 2.19–2.16 (t, 2H, *J* = 6.1 Hz), 1.85–1.57 (m, 12H), 1.38–1.18 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.3, 162.1, 120.5, 51.9, 38.4, 30.2, 29.1, 28.9, 28.2, 26.5, 26.2, 26.0; IR (neat): 3023, 2929, 2854, 1738, 1683, 1619, 1449, 1146, 1066, 982; MS (GC–MS) Calculated for $[C_{14}H_{23}O]^+$: 207; Found: 207.



Compound showed above was prepared in 22% yield according to the general procedure D (reaction time: 20 h). ^{1}H NMR (400MHz, $CDCl_3$) δ 7.96–7.93 (m, 2H), 7.55–7.51 (m, 1H), 7.47–7.43 (m, 2H), 6.60 (t, 1H, *J* = 1.1 Hz), 2.77 (t, 2H, *J* = 5.7 Hz), 2.32 (dt, 2H, *J* = 1.0, 6.3 Hz), 1.76–1.70 (m, 2H), 1.68–1.61 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.4, 162.8, 139.3, 132.3, 128.4, 128.3, 118.7, 38.4, 30.7, 28.9, 28.0, 26.3; IR (neat): 3080, 3060, 3030, 2930, 2854, 1995, 1660, 1609, 1578, 1447, 1391, 1384, 1240, 1219, 1042, 1021, 979, 834; MS (GC–MS) Calculated for $[C_{14}H_{16}O]^{+}$: 200; Found: 200.

exp2 Proton

SAMPLE		SPECIAL	
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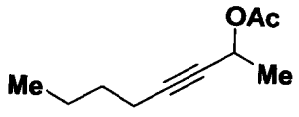
solvent	cdcl3	gain	40
file	exp	spin	not used
ACQUISITION		hst	0.008
sw	6410.3	pw90	13.900
at	2.049	alfa	6.600
np	26264	**FLAGS**	
fb	4000	il	n
bs	32	in	n
ss	2	dp	y
d1	1.000	hs	nn
nt	1	**PROCESSING**	
ct	1	lb	0.20
TRANSMITTER		fn	65536
tn	H1	**DISPLAY**	
sfrq	399.782	sp	-166.1
tof	399.5	wp	3752.9
tpwr	59	rfl	804.8
pw	6.950	rfp	0
DECOUPLER		rp	87.1
dn	C13	lp	-44.8
dof	0	**PLOT**	
dm	nnn	wc	250
dmm	c	sc	0
dpwr	34	vs	62
dmf	29412	th	2
		ai cdc ph	



exp1 Carbon

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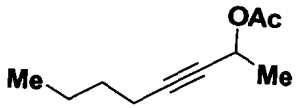
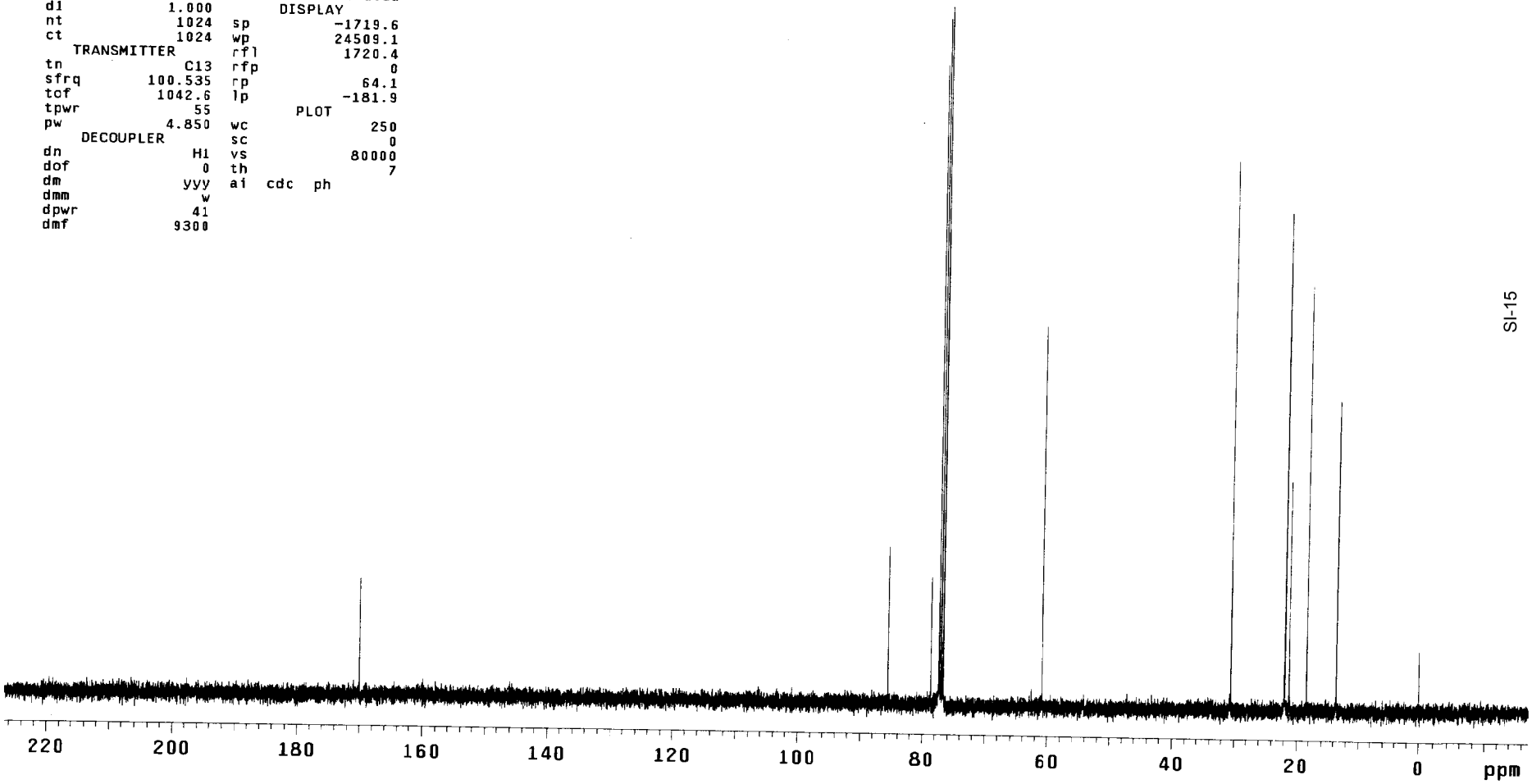
	.02_04/s_20060402_~	alfa	10.000
	001/data/cdcl3_02.~	FLAGS	
	fid	il	n
ACQUISITION		in	n
sw	24509.8	dp	y
at	1.300	hs	nn
np	63750	PROCESSING	
fb	17000	lb	0.50
bs	64	fn	not used
d1	1.000	DISPLAY	
nt	1024	sp	-1719.6
ct	1024	wp	24509.1
TRANSMITTER		rfl	1720.4
tn	C13	rfp	0
sfrq	100.535	rp	64.1
tof	1042.6	lp	-181.9
tpwr	55	PLOT	
pw	4.850	wc	250
DECOUPLER		sc	0
dn	H1	vs	80000
dof	0	th	7
dm	yyy	ai	cdc ph
dmm	w		
dpwr	41		
dmf	9300		





STANDARD 1H OBSERVE - profile

exp1 Proton

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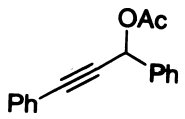
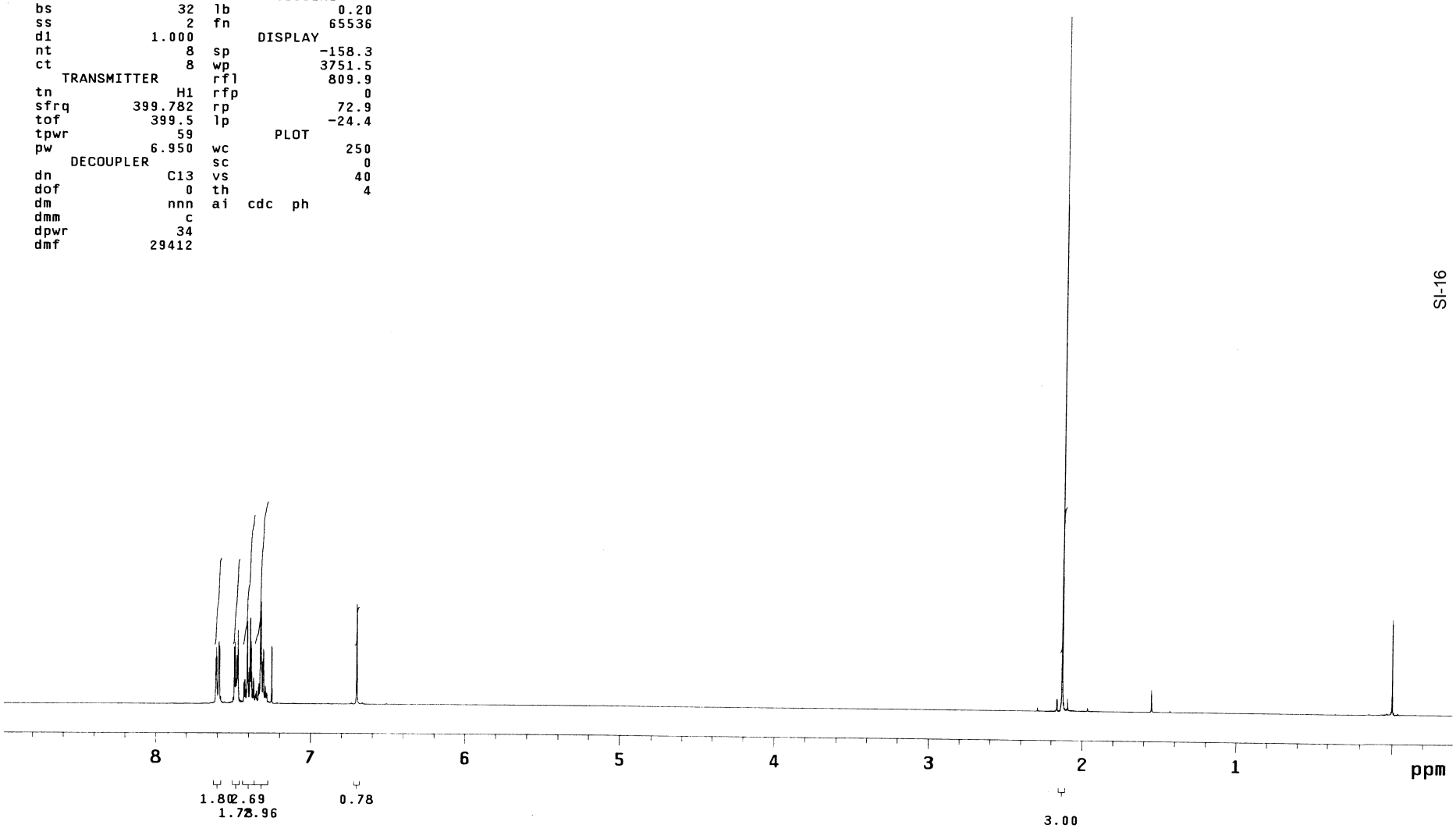
3/s_0_01/data/cdcl~		alfa	6.600
3_01.fid		FLAGS	
ACQUISITION		il	n
sw	6410.3	in	n
at	2.049	dp	y
np	26264	hs	nn
fb	4000	PROCESSING	
bs	32	lb	0.20
ss	2	fn	65536
d1	1.000	DISPLAY	
nt	8	sp	-158.3
ct	8	wp	3751.5
TRANSMITTER		rfl	809.9
tn	H1	rfp	0
sfrq	399.782	rp	72.9
tof	399.5	lp	-24.4
tpwr	59	PLOT	
pw	6.950	wc	250
DECOUPLER		sc	0
dn	C13	vs	40
dof	0	th	4
dm	nnn	ai	cdc ph
dmm	c		
dpwr	34		
dmf	29412		



3a



exp1 Carbon

SAMPLE		SPECIAL	
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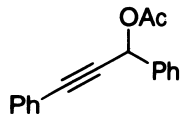
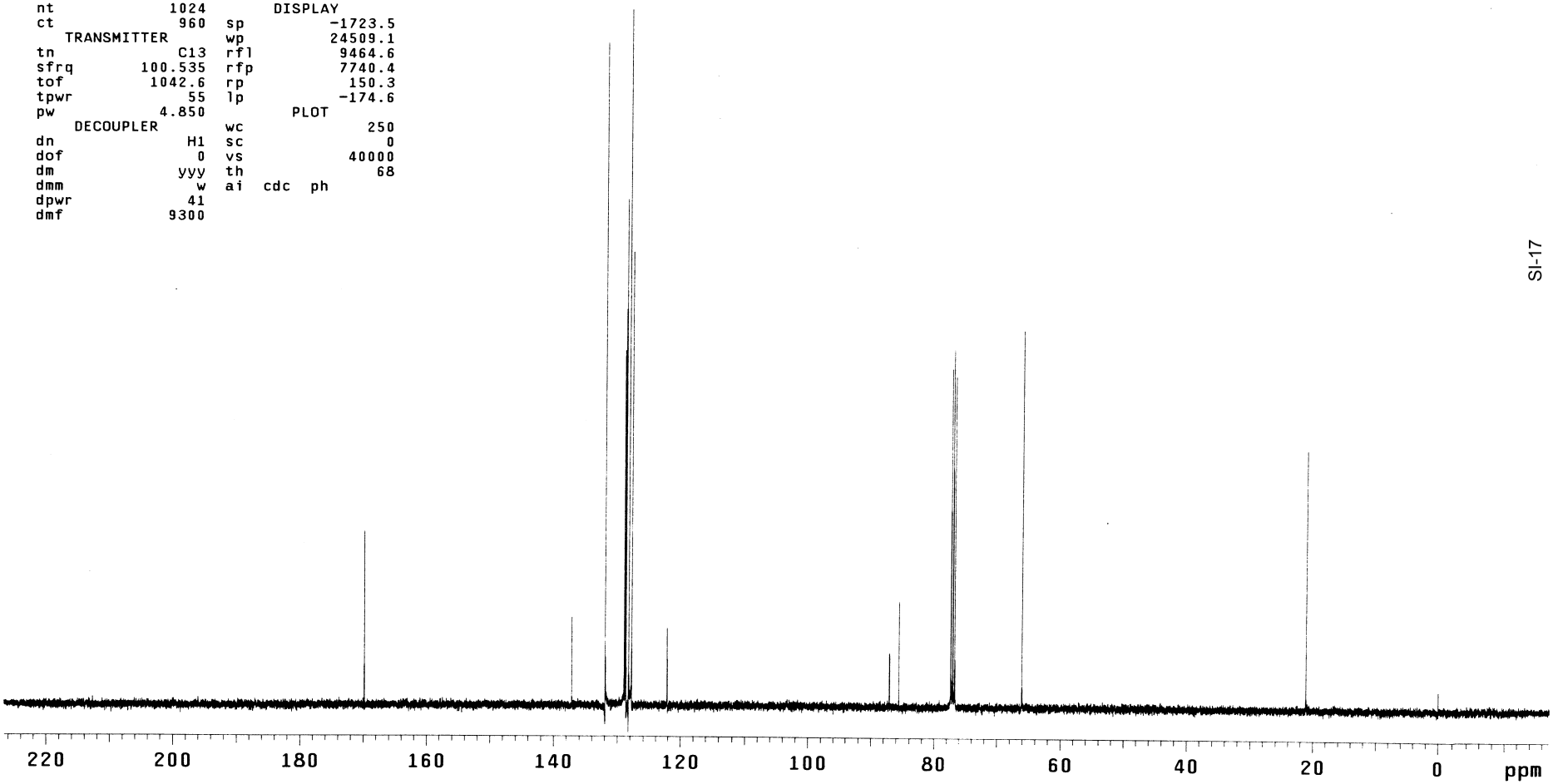
	3/s_0_01/data/cdcl~	alfa	10.000
	3_02.fid	FLAGS	
ACQUISITION		il	n
sw	24509.8	in	n
at	1.300	dp	y
np	63750	hs	nn
fb	17000	PROCESSING	
bs	64	lb	0.50
d1	1.000	fn	not used
nt	1024	DISPLAY	
ct	960	sp	-1723.5
TRANSMITTER		wp	24509.1
tn	C13	rfl	9464.6
sfrq	100.535	rfp	7740.4
tof	1042.6	rp	150.3
tpwr	55	lp	-174.6
pw	4.850	PLOT	
DECOUPLER		wc	250
dn	H1	sc	0
dof	0	vs	40000
dm	yyy	th	68
dmm	w	ai cdc ph	
dpwr	41		
dmf	9300		



3a



STANDARD 1H OBSERVE - profile

exp2 Proton

SAMPLE		SPECIAL	
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solvent	cdcl3	gain	not used
file	/home/walkup/~	spin	not used
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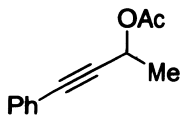
Volet/auto_2006.04~		pw90	13.900
.09_06/s_0_01/data~		alfa	6.600
/cdcl3_01.fid		FLAGS	
ACQUISITION		il	n
sw	6410.3	in	n
at	2.049	dp	y
np	26264	hs	nn
fb	4000	PROCESSING	
bs	32	lb	0.20
ss	2	fn	65536
d1	1.000	DISPLAY	
nt	8	sp	-169.8
ct	8	wp	3766.6
TRANSMITTER		rfl	806.4
tn	H1	rfp	0
sfrq	399.782	rp	72.5
tof	399.5	lp	-26.7
tpwr	59	PLOT	
pw	6.950	wc	250
DECOUPLER		sc	0
dn	C13	vs	55
dof	0	th	2
dm	nnn	ai	cdc ph
dmm	c		
dpwr	34		
dmf	29412		

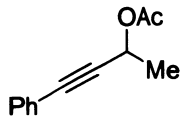


3b

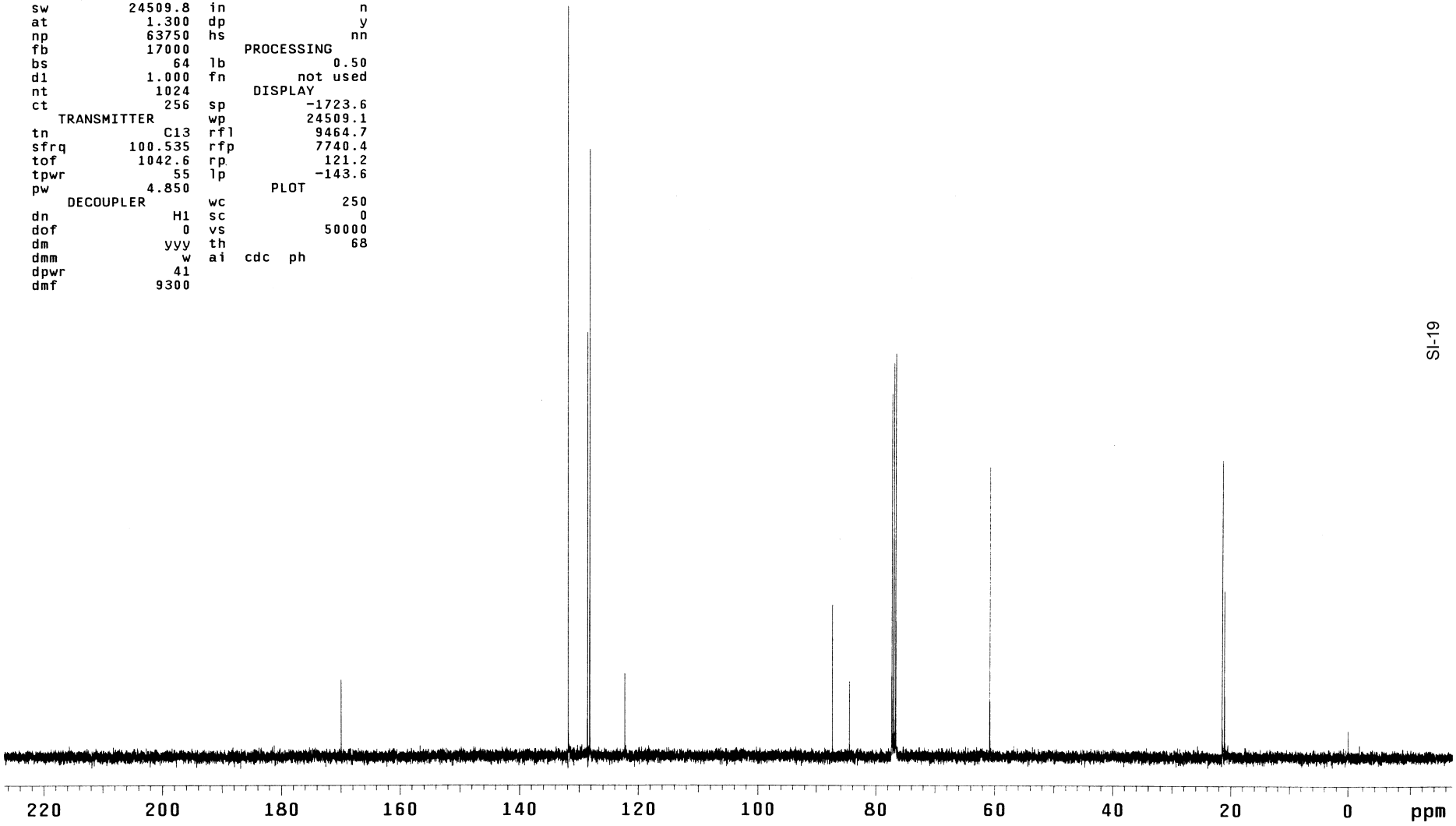
STANDARD 1H OBSERVE - profile

exp2 Carbon

SAMPLE		SPECIAL	
date	Apr 9 2006	temp	25.0
solvent	cdcl3	gain	30
file	/home/walkup/~	spin	not used
vnmrsys/data/Bell/~		hst	0.008
Volet/auto_2006.04~		pw90	9.700
.09_06/s_0_02/data~		alfa	10.000
/cdcl3_01.fid		FLAGS	
ACQUISITION		il	n
sw	24509.8	in	n
at	1.300	dp	y
np	63750	hs	nn
fb	17000	PROCESSING	
bs	64	lb	0.50
d1	1.000	fn	not used
nt	1024	DISPLAY	
ct	256	sp	-1723.6
TRANSMITTER		wp	24509.1
tn	C13	rfl	9464.7
sfrq	100.535	rfp	7740.4
tof	1042.6	rp	121.2
tpwr	55	lp	-143.6
pw	4.850	PLOT	
DECOUPLER		wc	250
dn	H1	sc	0
dof	0	vs	50000
dm	yyy	th	68
dmm	w	ai	cdc ph
dpwr	41		
dmf	9300		



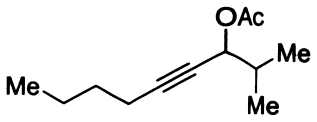
3b



STANDARD 1H OBSERVE - profile

exp1 Proton

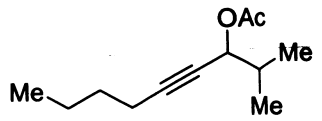
SAMPLE		SPECIAL	
date	Apr 10 2006	temp	25.0
solvent	cdcl3	gain	not used
file	/home/walkup/~	spin	not used
vnmrsys/data/Frost~		hst	0.008
/auto_2006.04.10_1~		pw90	13.900
5/s_0_01/data/cdcl~		alfa	6.600
3_01.fid		FLAGS	
ACQUISITION		il	n
sw	6410.3	in	n
at	2.049	dp	y
np	26264	hs	nn
fb	4000	PROCESSING	
bs	32	lb	0.20
ss	2	fn	65536
d1	1.000	DISPLAY	
nt	8	sp	-160.8
ct	8	wp	3751.5
TRANSMITTER		rfl	805.0
tn	H1	rfp	0
sfrq	399.782	rp	73.9
tof	399.5	lp	-19.8
tpwr	59	PLOT	
pw	6.950	wc	250
DECOUPLER		sc	0
dn	C13	vs	92
dof	0	th	2
dm	nnn	ai cdc ph	
dmm	c		
dpwr	34		
dmf	29412		



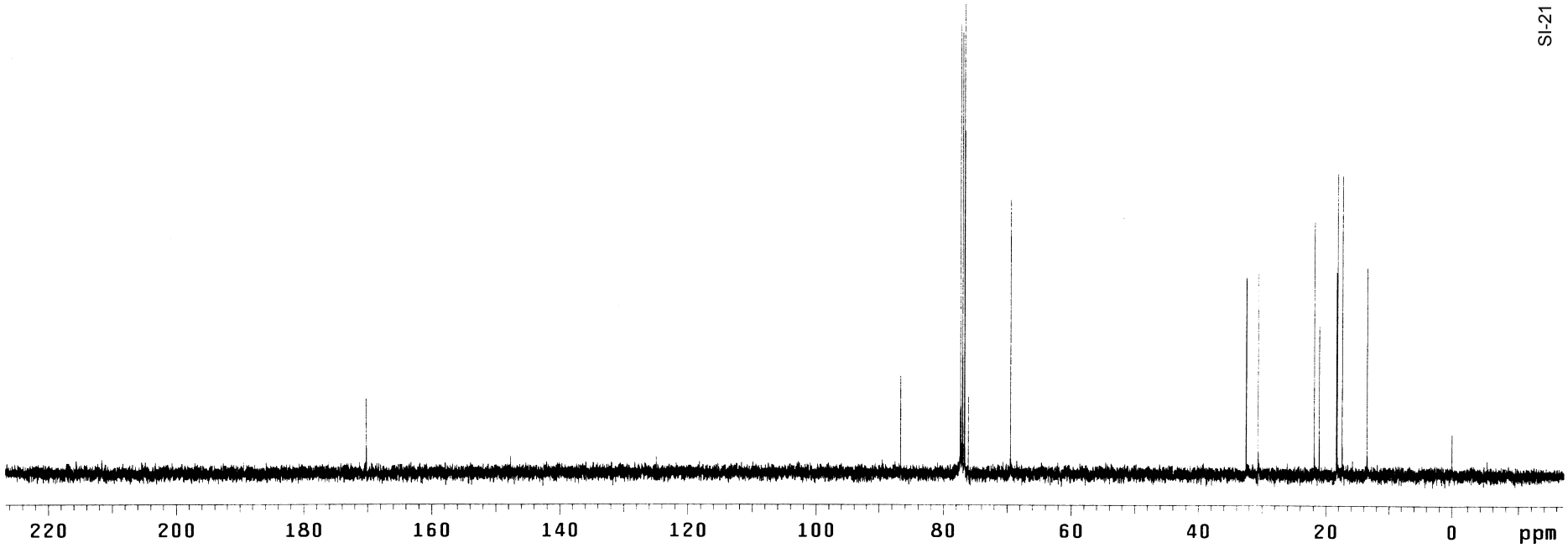
3c

exp1 Carbon

SAMPLE		SPECIAL	
date	Apr 10 2006	temp	25.0
solvent	cdcl3	gain	30
file	/home/walkup/~	spin	not used
	vnmrsys/data/Frost~	hst	0.008
	/auto_2006.04.10_1~	pw90	9.700
	5/s_0_01/data/cdcl~	alfa	10.000
	3_02.fid	FLAGS	
ACQUISITION		il	n
sw	24509.8	in	n
at	1.300	dp	y
np	63750	hs	nn
fb	17000	PROCESSING	
bs	64	lb	0.50
d1	1.000	fn	not used
nt	1024	DISPLAY	
ct	448	sp	-1722.9
TRANSMITTER		wp	24509.1
tn	C13	rfl	9464.1
sfrq	100.535	rfp	7740.4
tof	1042.6	rp	127.9
tpwr	55	lp	-133.3
pw	4.850	PLOT	
DECOUPLER		wc	250
dn	H1	sc	0
dof	0	vs	50000
dm	yyy	th	7
dmm	w	ai cdc ph	
dpwr	41		
dmf	9300		



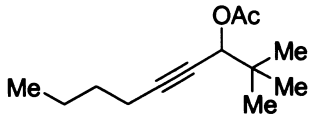
3c



STANDARD 1H OBSERVE - profile

exp1 Proton

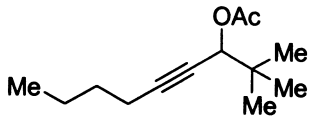
SAMPLE		SPECIAL	
date	May 3 2006	temp	25.0
solvent	cdcl3	gain	not used
file	/home/walkup/~	spin	not used
vnmrsys/data/Bell/~		hst	0.008
Rio/auto_2006.05.0~		pw90	13.900
3_10/s_20060503_00~		alfa	6.600
1/data/cdcl3_01.fi~		FLAGS	
	d	il	n
ACQUISITION		in	n
sw	6410.3	dp	y
at	2.049	hs	nn
np	26264	PROCESSING	
fb	4000	lb	0.20
bs	32	fn	65536
ss	2	DISPLAY	
d1	1.000	sp	-156.9
nt	8	wp	3753.5
ct	8	rfl	807.3
TRANSMITTER		rfp	0
tn	H1	rp	81.4
sfrq	399.782	lp	-59.4
tof	399.5	PLOT	
tpwr	59	wc	250
pw	6.950	sc	0
DECOUPLER		vs	40
dn	C13	th	2
dof	0	ai cdc ph	
dm	nnn		
dmm	c		
dpwr	34		
dmf	29412		



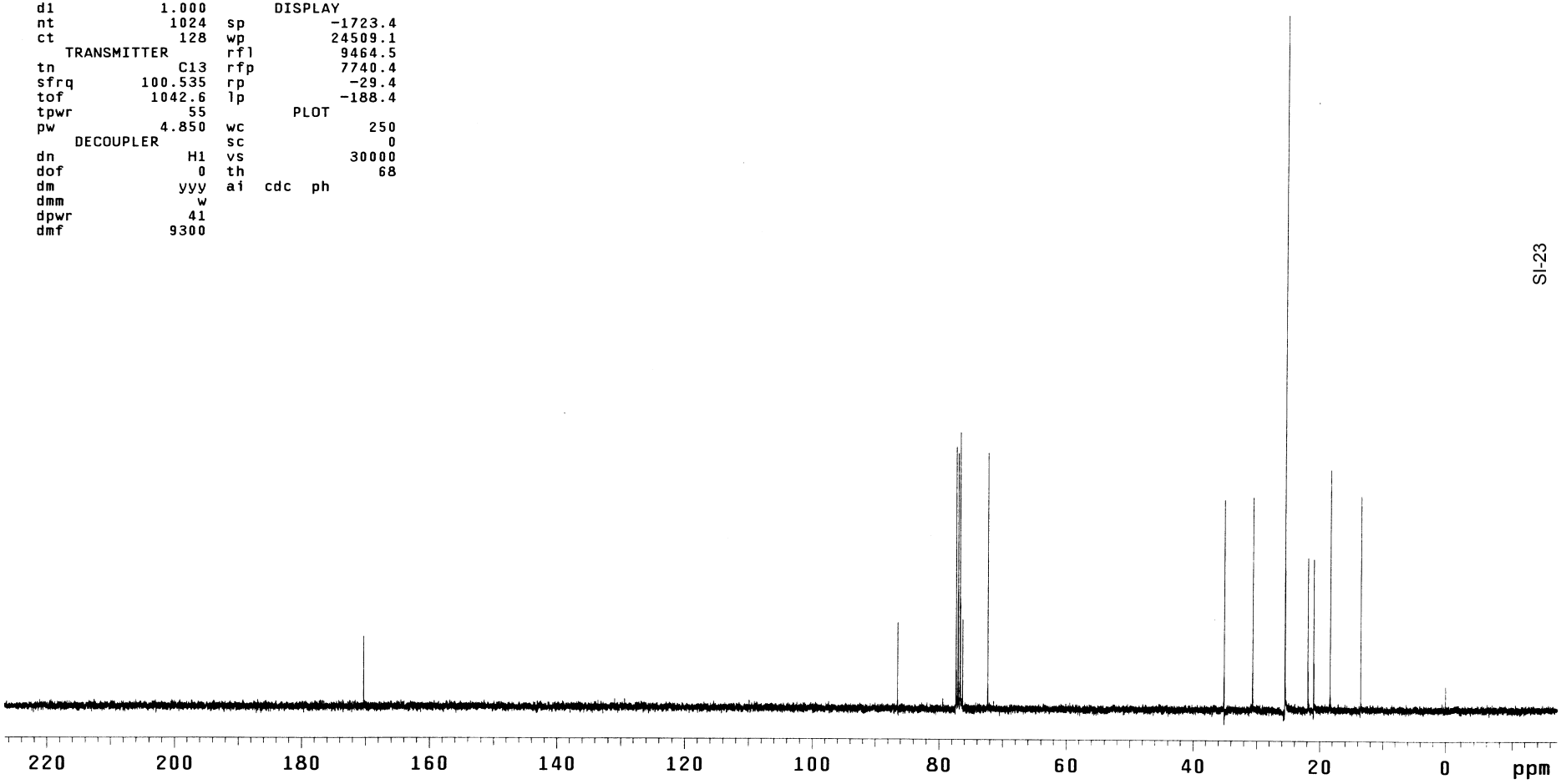
3d

exp1 Carbon

SAMPLE		SPECIAL	
date	May 3 2006	temp	25.0
solvent	cdcl3	gain	30
file	/home/walkup/~	spin	not used
	vnmrsys/data/Bell/~	hst	0.008
	Rio/auto_2006.05.0~	pw90	9.700
	3_10/s_20060503_00~	alfa	10.000
	1/data/cdcl3_02.fi~	FLAGS	
	d	il	n
ACQUISITION		in	n
sw	24509.8	dp	y
at	1.300	hs	nn
np	63750	PROCESSING	
fb	17000	lb	0.50
bs	64	fn	not used
d1	1.000	DISPLAY	
nt	1024	sp	-1723.4
ct	128	wp	24509.1
TRANSMITTER		rfl	9464.5
tn	C13	rfp	7740.4
sfrq	100.535	rp	-29.4
tof	1042.6	lp	-188.4
tpwr	55	PLOT	
pw	4.850	wc	250
DECOUPLER		sc	0
dn	H1	vs	30000
dof	0	th	68
dm	yyy	ai cdc ph	
dmm	w		
dpwr	41		
dmf	9300		



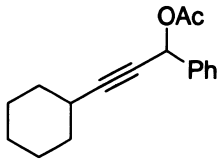
3d



STANDARD 1H OBSERVE - profile

exp1 Proton

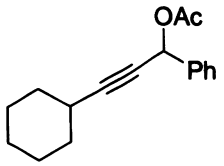
SAMPLE		SPECIAL	
date	Apr 10 2006	temp	25.0
solvent	cdcl3	gain	not used
file	/home/walkup/~	spin	not used
	vnmrsys/data/Frost~	hst	0.008
	/auto_2006.04.10_1~	pw90	13.900
	4/s_0_01/data/cdcl~	alfa	6.600
	3_01.fid	FLAGS	
ACQUISITION		il	n
sw	6410.3	in	n
at	2.049	dp	y
np	26264	hs	nn
fb	4000	PROCESSING	
bs	32	lb	0.20
ss	2	fn	65536
d1	1.000	DISPLAY	
nt	8	sp	-163.5
ct	8	wp	3751.5
TRANSMITTER		rfl	807.7
tn	H1	rfp	0
sfrq	399.782	rp	69.3
tof	399.5	lp	-13.7
tpwr	59	PLOT	
pw	6.950	wc	250
DECOUPLER		sc	0
dn	C13	vs	100
dof	0	th	2
dm	nnn	ai	cdc ph
dmm	c		
dpwr	34		
dmf	29412		



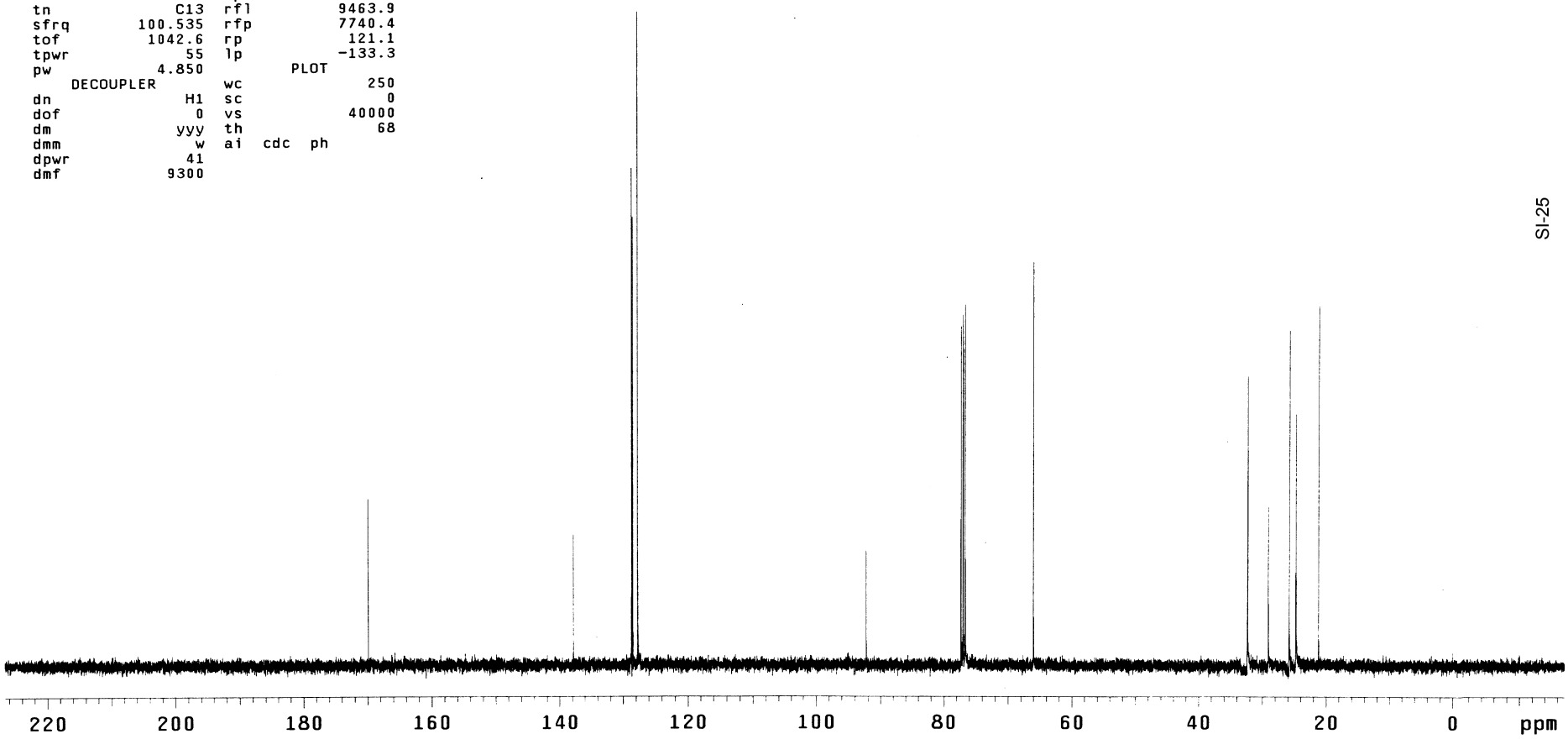
3e

exp1 Carbon

SAMPLE		SPECIAL	
date	Apr 10 2006	temp	25.0
solvent	cdcl3	gain	30
file	/home/walkup/~	spin	not used
	vnmrsys/data/Frost~	hst	0.008
	/auto_2006.04.10_1~	pw90	9.700
	4/s_0_01/data/cdcl~	alfa	10.000
	3_02.fid	FLAGS	
ACQUISITION		il	n
sw	24509.8	in	n
at	1.300	dp	y
np	63750	hs	nn
fb	17000	PROCESSING	
bs	64	lb	0.50
d1	1.000	fn	not used
nt	1024	DISPLAY	
ct	448	sp	-1722.8
TRANSMITTER		wp	24509.1
tn	C13	rfl	9463.9
sfrq	100.535	rfp	7740.4
tof	1042.6	rp	121.1
tpwr	55	lp	-133.3
pw	4.850	PLOT	
DECOUPLER		wc	250
dn	H1	sc	0
dof	0	vs	40000
dm	yyy	th	68
dmm	w	ai cdc ph	
dpwr	41		
dmf	9300		



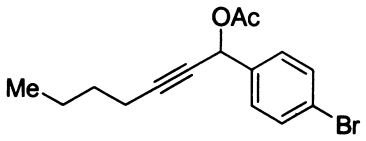
3e



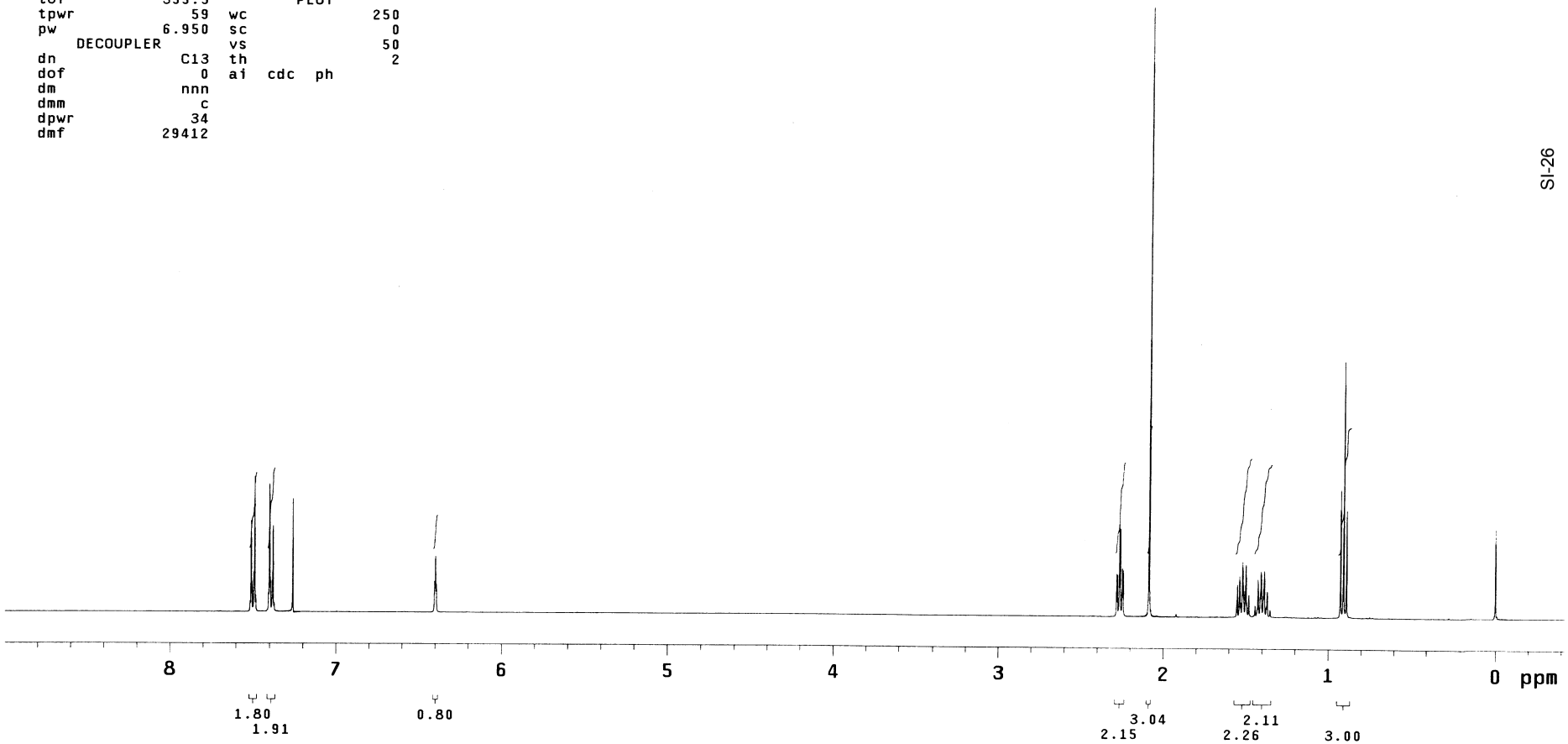
STANDARD 1H OBSERVE - profile

exp1 Proton

SAMPLE		SPECIAL	
date	May 7 2006	temp	25.0
solvent	cdcl3	gain	not used
file	/home/walkup/~	spin	not used
vnmrsys/data/Frost~		hst	0.008
/Wong/auto_2006.05~		pw90	13.900
.07_01/s_20060507_~		alfa	6.600
001/data/cdcl3_01.~		FLAGS	
	fid	il	n
ACQUISITION		in	n
sw	6410.3	dp	y
at	2.049	hs	nn
np	26264	PROCESSING	
fb	4000	lb	0.20
bs	32	fn	65536
ss	2	DISPLAY	
d1	1.000	sp	-169.4
nt	8	wp	3766.4
ct	8	rfl	809.1
TRANSMITTER		rfp	0
tn	H1	rp	65.7
sfrq	399.782	lp	-27.5
tof	399.5	PLOT	
tpwr	59	wc	250
pw	6.950	sc	0
DECOUPLER		vs	50
dn	C13	th	2
dof	0	ai	cdc ph
dm	nnn		
dmm	c		
dpwr	34		
dmf	29412		



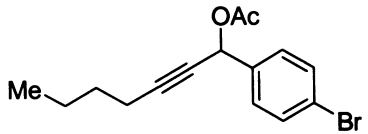
3f



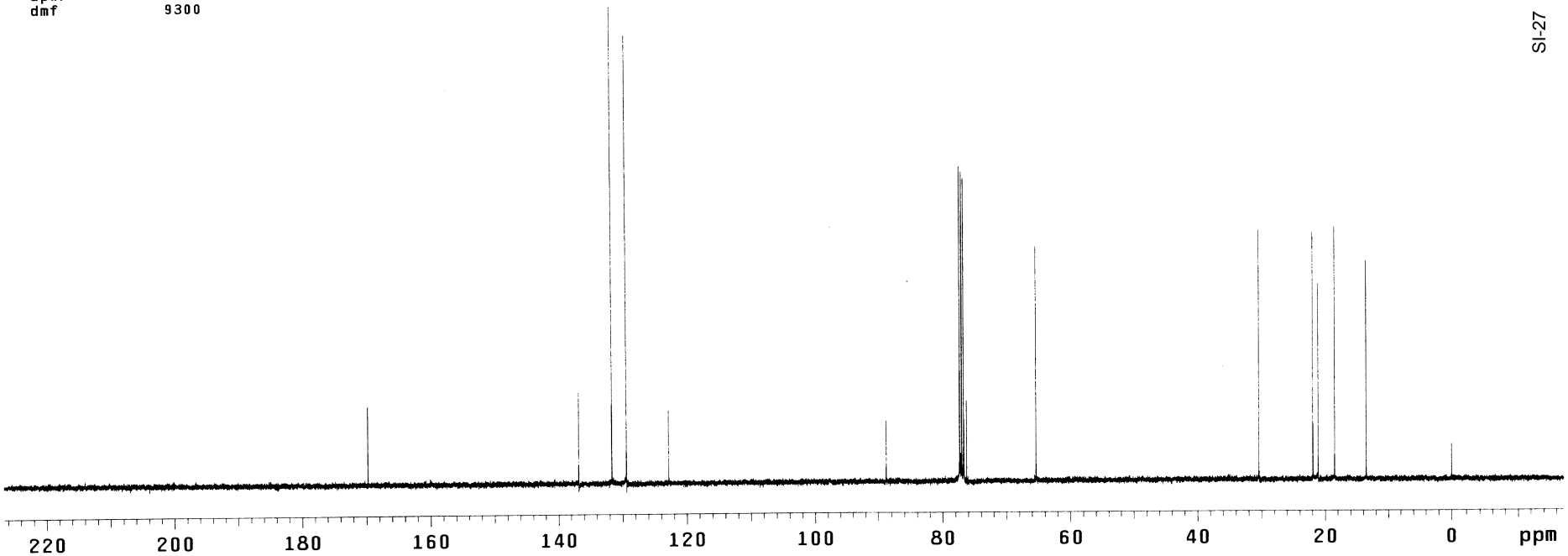
STANDARD 1H OBSERVE - profile
STANDARD 1H OBSERVE - profile

exp1 Carbon

SAMPLE		SPECIAL	
date	May 7 2006	temp	25.0
solvent	cdcl3	gain	30
file	/home/walkup/~	spin	not used
	vnmrsys/data/Frost~	hst	0.008
	/Wong/auto_2006.05~	pw90	9.700
	.07_01/s_20060507_~	alfa	10.000
	001/data/cdcl3_02.~	FLAGS	
	fid	il	n
ACQUISITION		in	n
sw	24509.8	dp	y
at	1.300	hs	nn
np	63750	PROCESSING	
fb	17000	lb	0.50
bs	64	fn	not used
d1	1.000	DISPLAY	
nt	2000	sp	-1724.0
ct	64	wp	24509.1
TRANSMITTER		rfl	9465.2
tn	C13	rfp	7740.4
sfrq	100.535	rp	-21.8
tof	1042.6	lp	-178.2
tpwr	55	PLOT	
pw	4.850	wc	250
DECOUPLER		sc	0
dn	H1	vs	40000
dof	0	th	68
dm	yyy	ai cdc ph	
dmm	w		
dpwr	41		
dmf	9300		



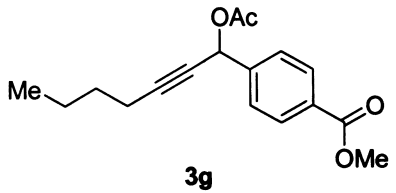
3f



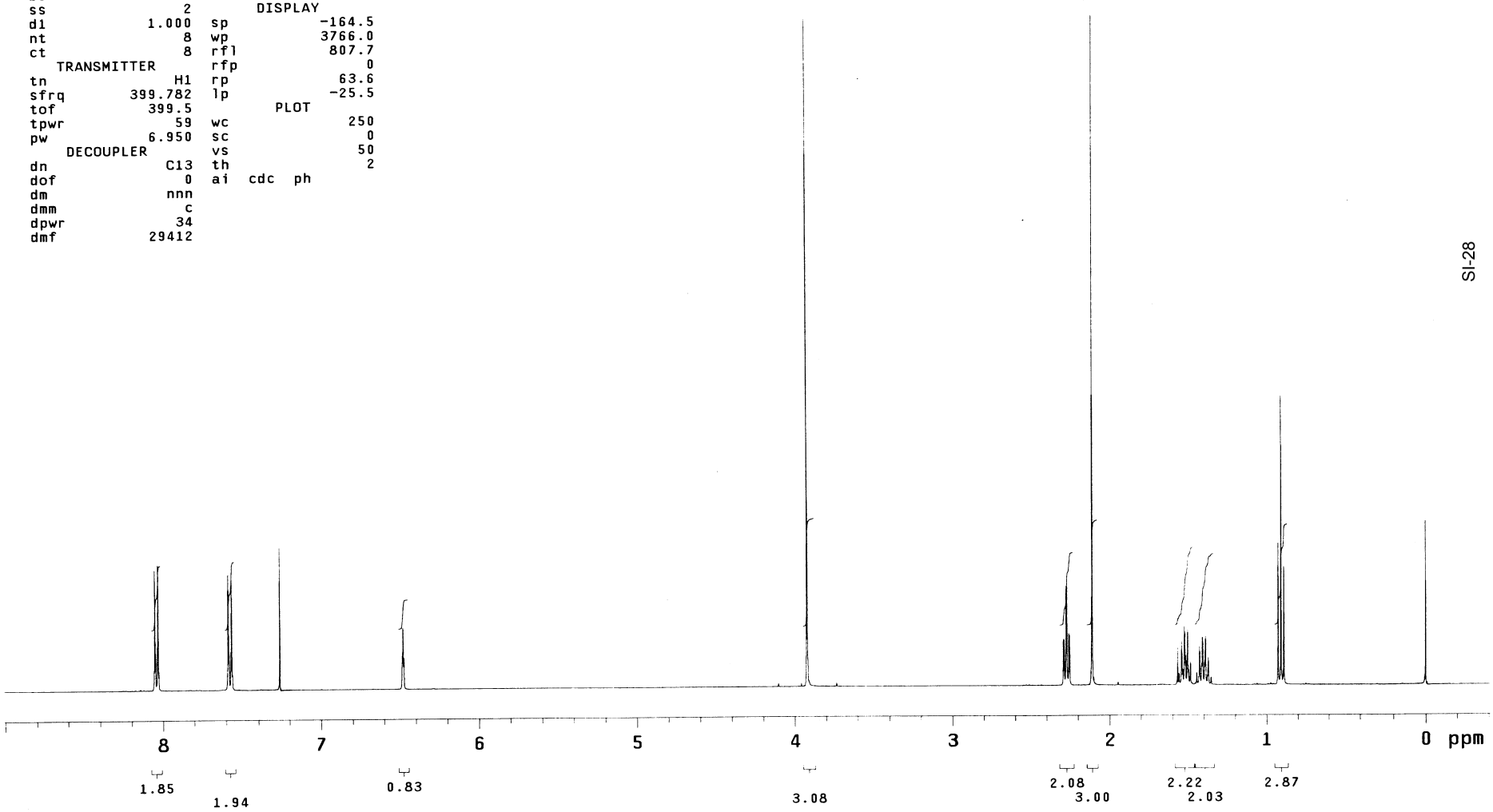
STANDARD 1H OBSERVE - profile

exp1 Proton

SAMPLE		SPECIAL	
date	May 5 2006	temp	25.0
solvent	cdcl3	gain	not used
file	/home/walkup/~	spin	not used
vnmrsys/data/Frost~		hst	0.008
/Harkreader/auto_2~		pw90	13.900
006.05.05_03/s_200~		alfa	6.600
60505_001/data/cdc~		FLAGS	
13_01.fid		il	n
ACQUISITION		in	n
sw	6410.3	dp	y
at	2.049	hs	nn
np	26264	PROCESSING	
fb	4000	lb	0.20
bs	32	fn	65536
ss	2	DISPLAY	
d1	1.000	sp	-164.5
nt	8	wp	3766.0
ct	8	rfl	807.7
TRANSMITTER		rfp	0
tn	H1	rp	63.6
sfrq	399.782	lp	-25.5
tof	399.5	PLOT	
tpwr	59	wc	250
pw	6.950	sc	0
DECOUPLER		vs	50
dn	C13	th	2
dof	0	ai	cdc ph
dm	nnn		
dmm	c		
dpwr	34		
dmf	29412		

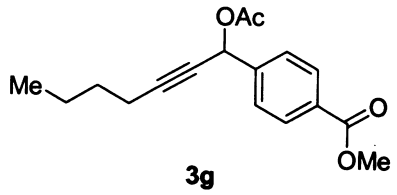


3g

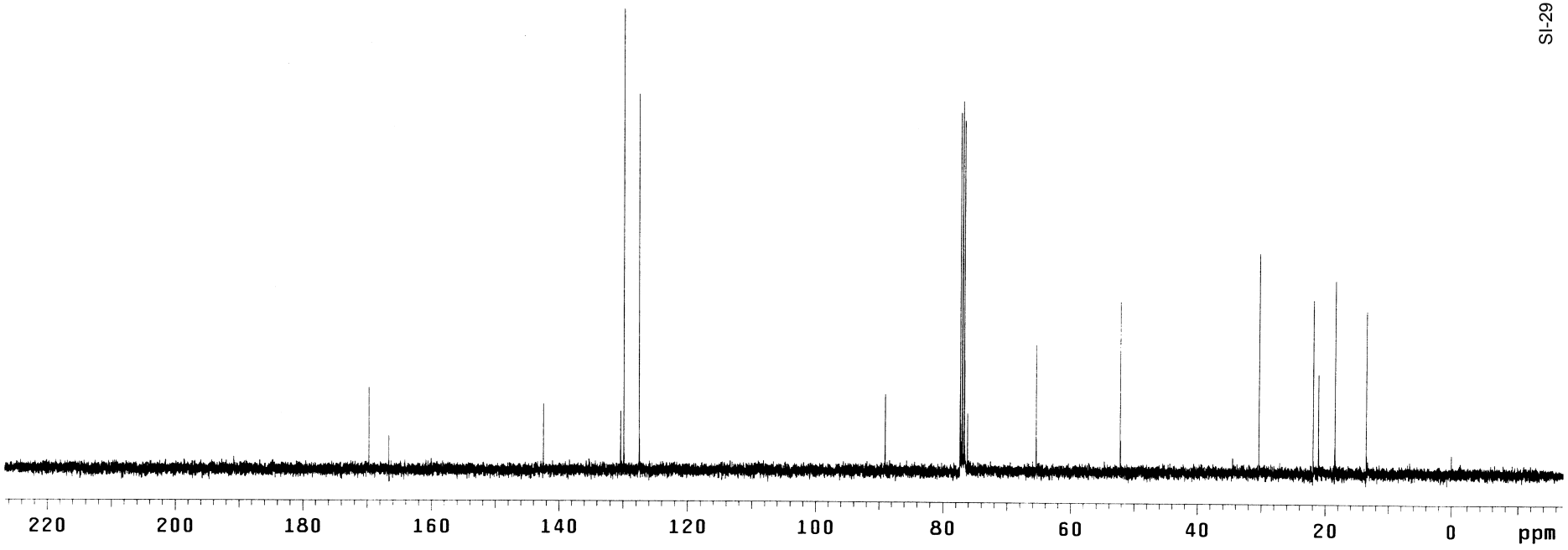


exp1 Carbon

SAMPLE		SPECIAL	
date	May 5 2006	temp	25.0
solvent	cdcl3	gain	30
file	/home/walkup/~	spin	not used
vnmrsys/data/Frost~		hst	0.008
/Harkreader/auto_2~		pw90	9.700
006.05.05_03/s_200~		alfa	10.000
60505_001/data/cdc~		FLAGS	
l3_02.fid		il	n
ACQUISITION		in	n
sw	24509.8	dp	y
at	1.300	hs	nn
np	63750	PROCESSING	
fb	17000	lb	0.50
bs	64	fn	not used
d1	1.000	DISPLAY	
nt	2000	sp	-1722.5
ct	64	wp	24509.1
TRANSMITTER		rfl	9463.7
tn	C13	rfp	7740.4
sfrq	100.535	rp	-49.6
tof	1042.6	lp	-133.3
tpwr	55	PLOT	
pw	4.850	wc	250
DECOUPLER		sc	0
dn	H1	vs	40000
dof	0	th	68
dm	yyy	ai cdc ph	
dmm	w		
dpwr	41		
dmf	9300		



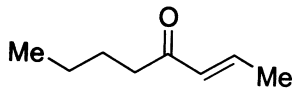
3g



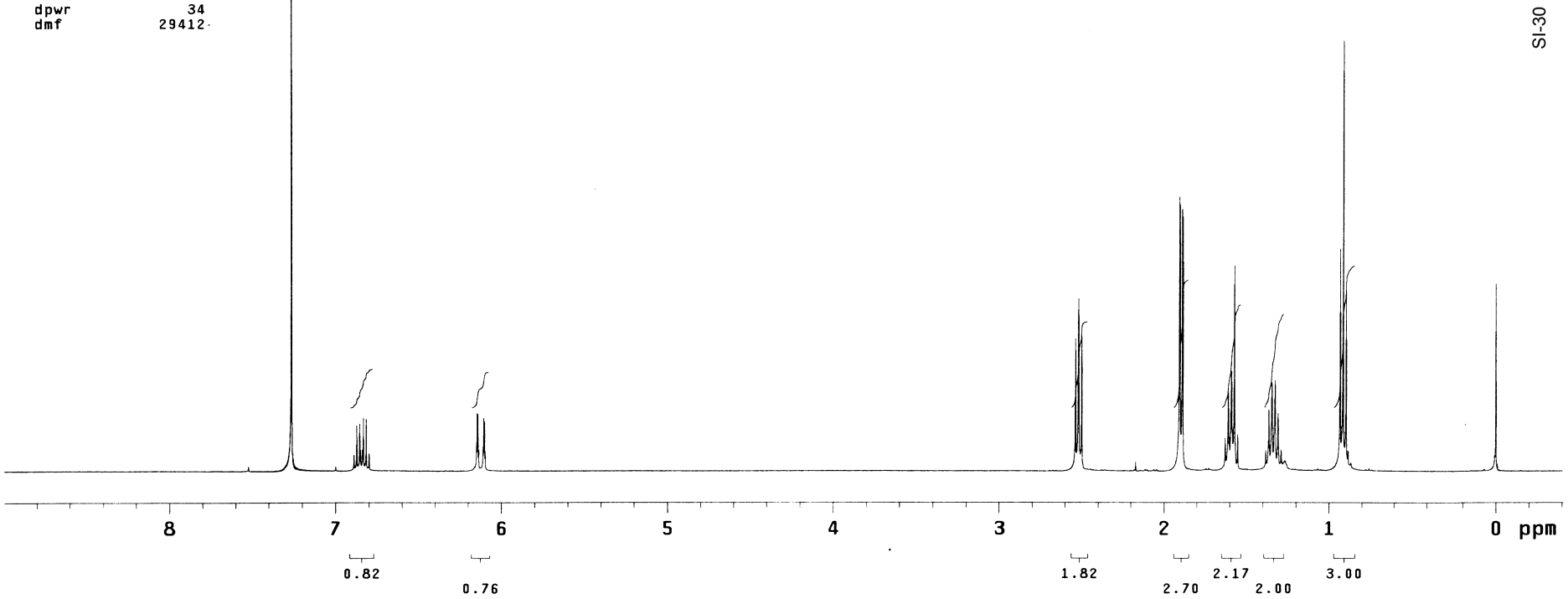
STANDARD 1H OBSERVE - profile
STANDARD 1H OBSERVE - profile
STANDARD 1H OBSERVE - profile
STANDARD 1H OBSERVE - profile

expl Proton

SAMPLE		SPECIAL	
date	May 4 2006	temp	25.0
solvent	cdcl3	gain	not used
file	/home/walkup/~	spin	not used
vnmrsys/data/Frost~		hst	0.008
/auto_2006.05.04_1~		pw90	13.900
5/s_20060504_001/d~		alfa	6.600
ata/cdcl3_01.fid		FLAGS	
ACQUISITION		il	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	-164.1
ct	8	wp	3761.1
TRANSMITTER		rfl	807.5
tn	H1	rfp	0
sfrq	399.782	rp	64.4
tof	399.5	lp	-35.3
tpwr	59	PLOT	
pw	6.950	wc	250
DECOUPLER		sc	0
dn	C13	vs	100
dof	0	th	3
dm	nnn	ai cdc ph	
dmm	c		
dpwr	34		
dmf	29412		

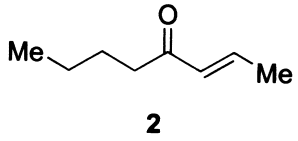


2

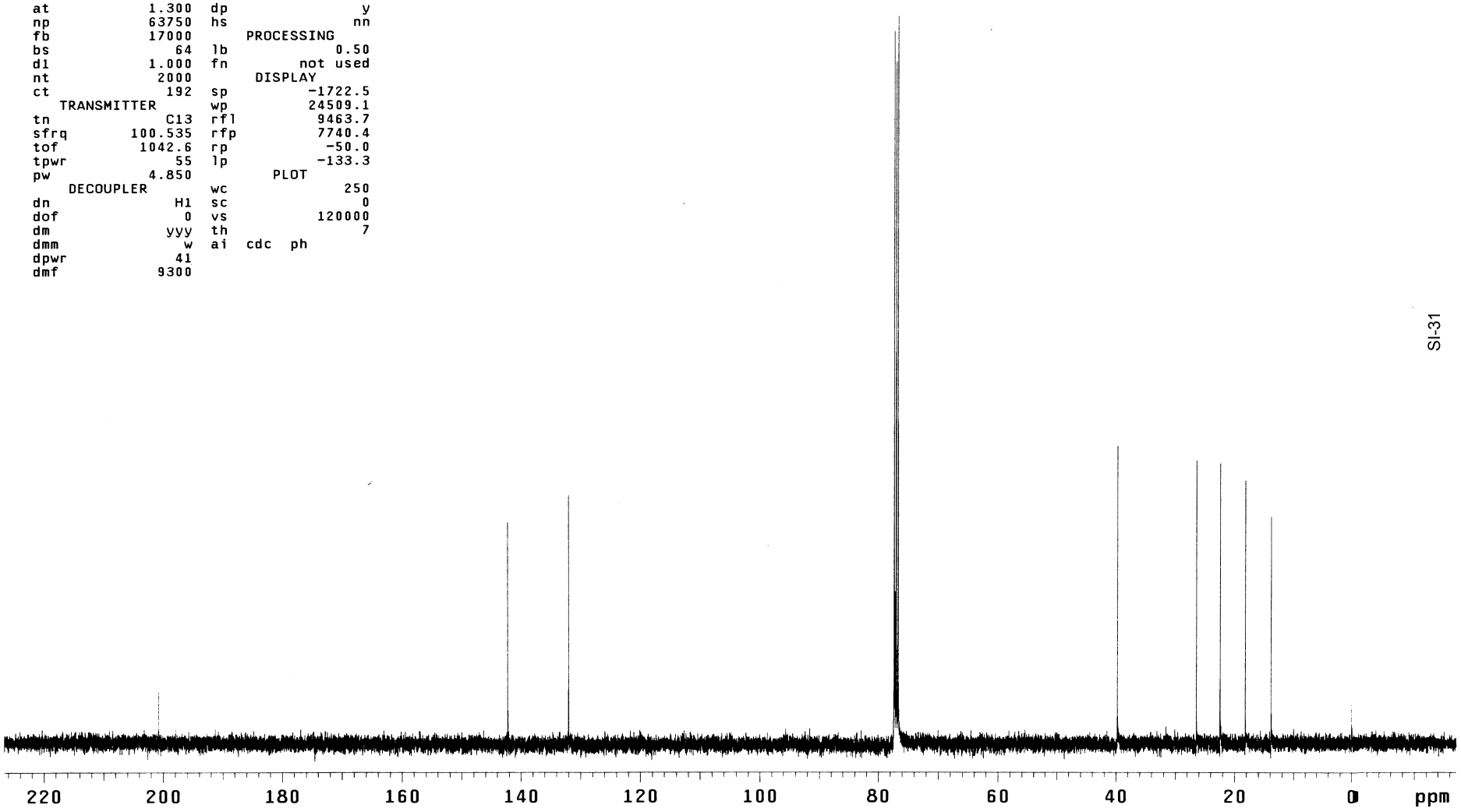


exp1 Carbon

SAMPLE		SPECIAL	
date	May 4 2006	temp	25.0
solvent	cdcl3	gain	30
file	/home/walkup/~	spin	not used
	vnmrsys/data/Frost~	hst	0.008
	/auto_2006.05.04_1~	pw90	9.700
	5/s_20060504_001/d~	alfa	10.000
	ata/cdcl3_02.fid	FLAGS	
ACQUISITION		il	n
sw	24509.8	in	n
at	1.300	dp	y
np	63750	hs	nn
fb	17000	PROCESSING	
bs	64	lb	0.50
d1	1.000	fn	not used
nt	2000	DISPLAY	
ct	192	sp	-1722.5
TRANSMITTER		wp	24509.1
tn	C13	rfl	9463.7
sfrq	100.535	rfp	7740.4
tof	1042.6	rp	-50.0
tpwr	55	lp	-133.3
pw	4.850	PLOT	
DECOUPLER		wc	250
dn	H1	sc	0
dof	0	vs	120000
dm	yyy	th	7
dmm	w	ai	cdc ph
dpwr	41		
dmf	9300		



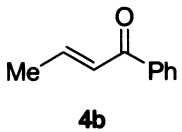
2



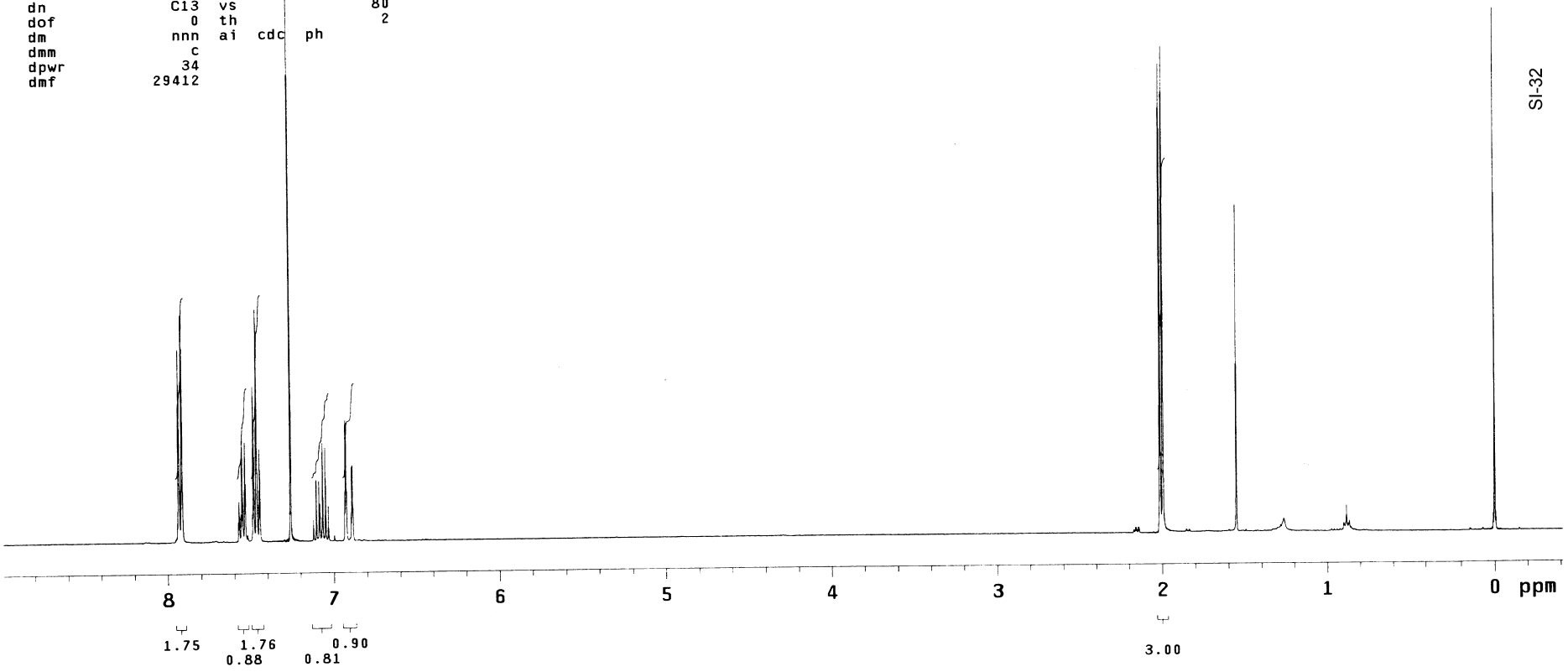
STANDARD 1H OBSERVE - profile
STANDARD 1H OBSERVE - profile
STANDARD 1H OBSERVE - profile

exp1 Proton

SAMPLE		SPECIAL	
date	May 4 2006	temp	25.0
solvent	cdcl3	gain	not used
file	/home/walkup/~	spin	not used
	vnmrsys/data/Frost~	hst	0.008
	/auto_2006.05.04_1~	pw90	13.900
	5/s_20060504_001/d~	alfa	6.600
	ata/cdcl3_01.fid	FLAGS	
ACQUISITION		il	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	-165.7
ct	8	wp	3761.1
TRANSMITTER		rfl	809.1
tn	H1	rfp	0
sfrq	399.782	rp	61.4
tof	399.5	lp	-24.9
tpwr	59	PLOT	
pw	6.950	wc	250
DECOUPLER		sc	0
dn	C13	vs	80
dof	0	th	2
dm	nnn	ai cdc ph	
dmm	c		
dpwr	34		
dmf	29412		



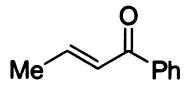
4b



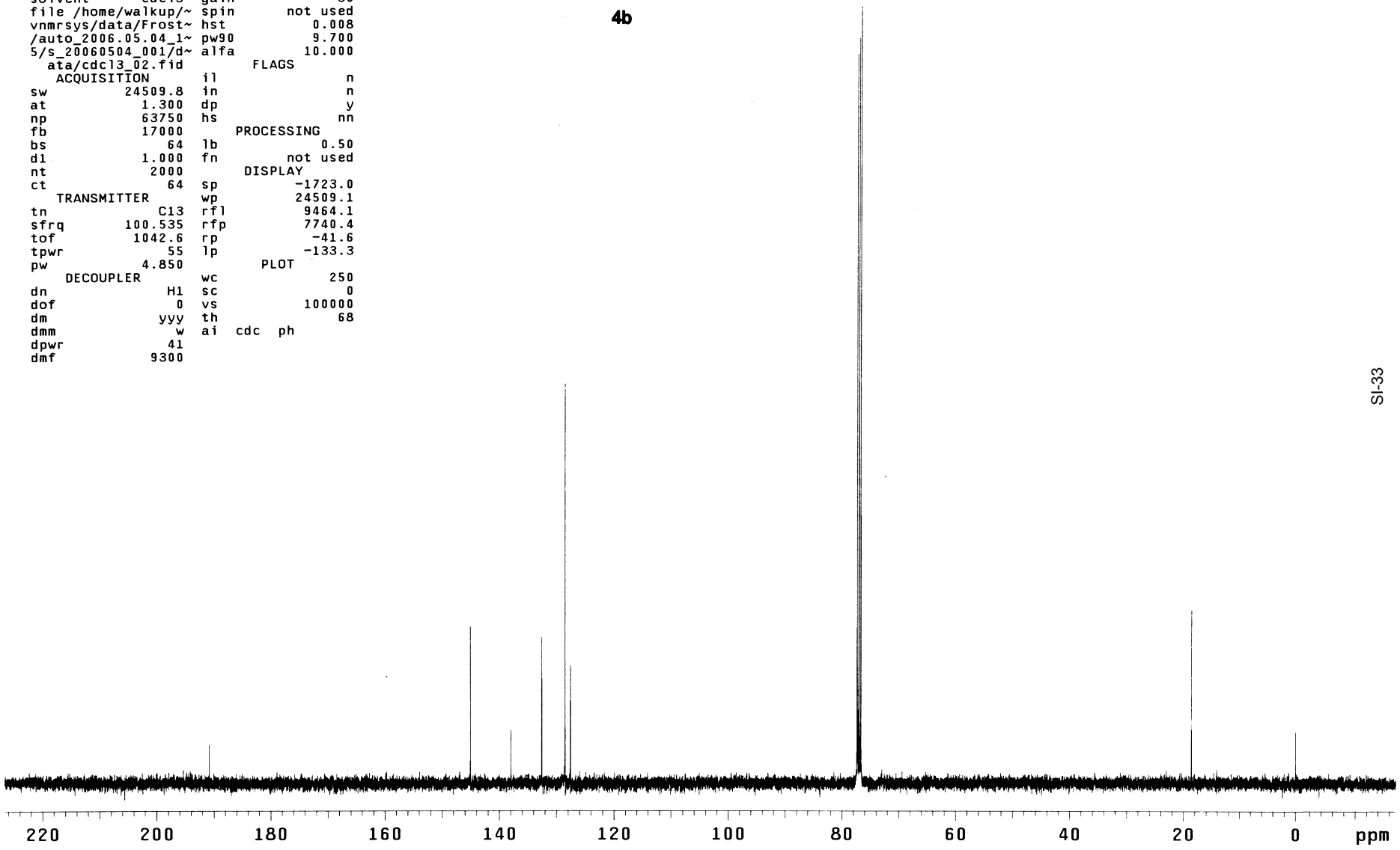
STANDARD 1H OBSERVE - profile
STANDARD 1H OBSERVE - profile
STANDARD 1H OBSERVE - profile

exp1 Carbon

SAMPLE		SPECIAL	
date	May 4 2006	temp	25.0
solvent	cdcl3	gain	30
file	/home/walkup/~	spin	not used
	vnmrsys/data/Frost~	hst	0.008
	/auto_2006.05.04_1~	pw90	9.700
	5/s_20060504_001/d~	alfa	10.000
	ata/cdcl3_02.fid	FLAGS	
ACQUISITION		il	n
sw	24509.8	in	n
at	1.300	dp	y
np	63750	hs	nn
fb	17000	PROCESSING	
bs	64	lb	0.50
d1	1.000	fn	not used
nt	2000	DISPLAY	
ct	64	sp	-1723.0
TRANSMITTER		wp	24509.1
tn	C13	rfl	9464.1
sfrq	100.535	rfp	7740.4
tof	1042.6	rp	-41.6
tpwr	55	lp	-133.3
pw	4.850	PLOT	
DECOUPLER		wc	250
dn	H1	sc	0
dof	0	vs	100000
dm	yyy	th	68
dmm	w	ai	cdc ph
dpwr	41		
dmf	9300		



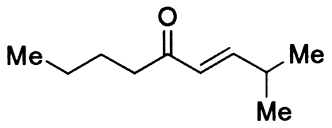
4b



STANDARD 1H OBSERVE - profile

exp1 Proton

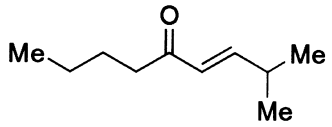
SAMPLE		SPECIAL	
date	May 4 2006	temp	25.0
solvent	cdcl3	gain	not used
file	/home/walkup/~	spin	not used
vnmrsys/data/Frost~		hst	0.008
/auto_2006.05.04_1~		pw90	13.900
6/s_20060504_001/d~		alfa	6.600
ata/cdcl3_01.fid		FLAGS	
ACQUISITION		il	n
sw	6410.3	in	n
at	2.049	dp	y
np	26264	hs	nn
fb	4000	PROCESSING	
bs	32	lb	0.20
ss	2	fn	65536
d1	1.000	DISPLAY	
nt	8	sp	-167.5
ct	8	wp	3758.4
TRANSMITTER		rfl	807.2
tn	H1	rfp	0
sfrq	399.782	rp	64.5
tof	399.5	lp	-20.2
tpwr	59	PLOT	
pw	6.950	wc	250
DECOUPLER		sc	0
dn	C13	vs	78
dof	0	th	21
dm	nnn	ai	cdc ph
dmm	c		
dpwr	34		
dmf	29412		



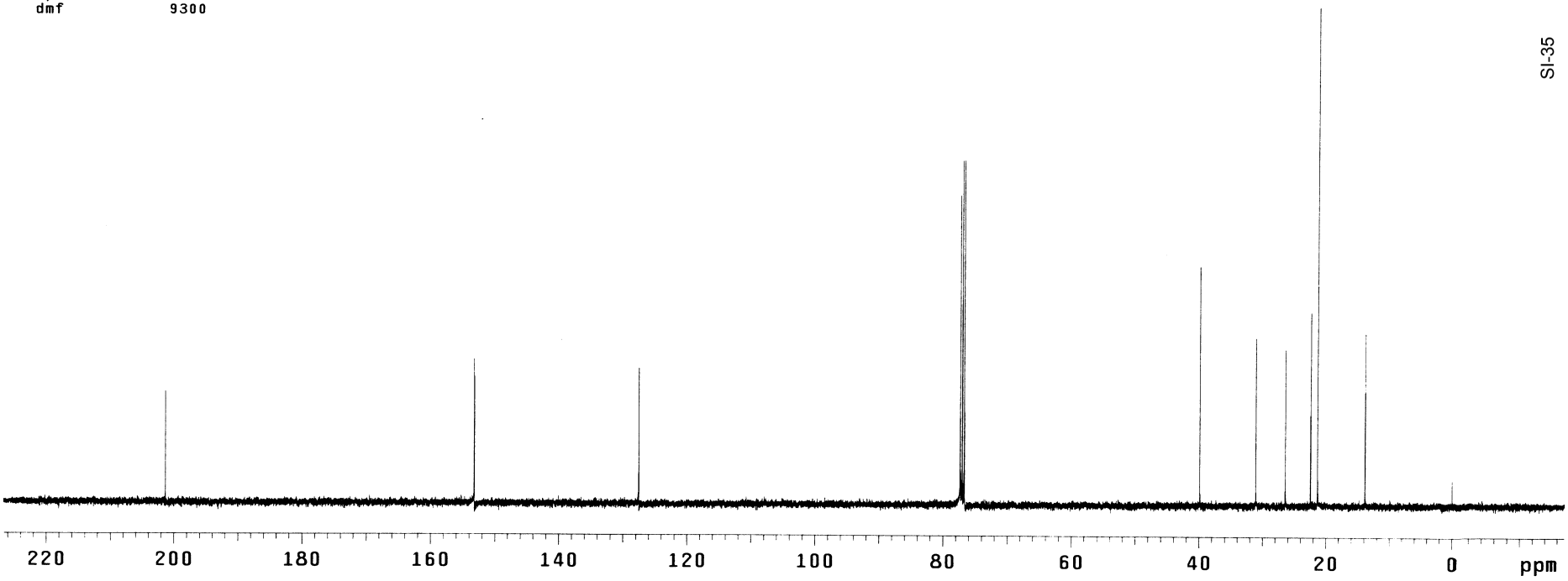
4c

exp1 Carbon

SAMPLE		SPECIAL	
date	May 4 2006	temp	25.0
solvent	cdcl3	gain	30
file	/home/walkup/~	spin	not used
	vnmrsys/data/Frost~	hst	0.008
	/auto_2006.05.04_1~	pw90	9.700
	6/s_20060504_001/d~	alfa	10.000
	ata/cdcl3_02.fid	FLAGS	
ACQUISITION		il	n
sw	24509.8	in	n
at	1.300	dp	y
np	63750	hs	nn
fb	17000	PROCESSING	
bs	64	lb	0.50
d1	1.000	fn	not used
nt	2000	DISPLAY	
ct	128	sp	-1722.8
TRANSMITTER		wp	24509.1
tn	C13	rfl	9464.0
sfrq	100.535	rfp	7740.4
tof	1042.6	rp	-31.4
tpwr	55	lp	-133.3
pw	4.850	PLOT	
DECOUPLER		wc	250
dn	H1	sc	0
dof	0	vs	40000
dm	yyy	th	68
dmm	w	ai cdc ph	
dpwr	41		
dmf	9300		



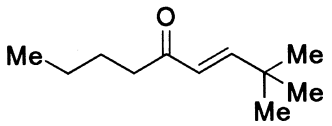
4c



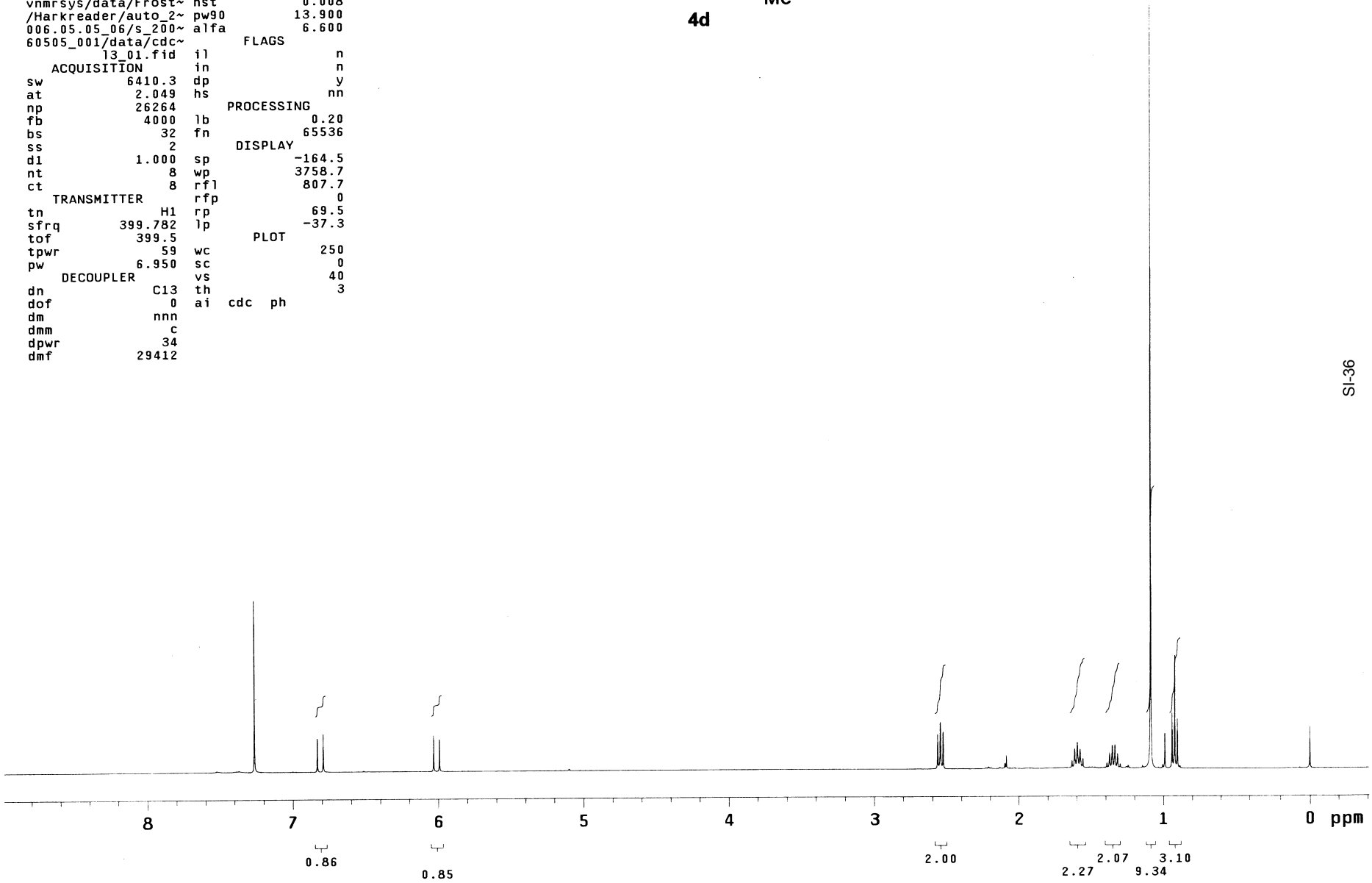
STANDARD 1H OBSERVE - profile

exp1 Proton

SAMPLE		SPECIAL	
date	May 5 2006	temp	25.0
solvent	cdcl3	gain	not used
file	/home/walkup/~	spin	not used
vnmrsys/data/Frost~		hst	0.008
/Harkreader/auto_2~		pw90	13.900
006.05.05_06/s_200~		alfa	6.600
60505_001/data/cdc~		FLAGS	
13_01.fid		il	n
ACQUISITION		in	n
sw	6410.3	dp	y
at	2.049	hs	nn
np	26264	PROCESSING	
fb	4000	lb	0.20
bs	32	fn	65536
ss	2	DISPLAY	
d1	1.000	sp	-164.5
nt	8	wp	3758.7
ct	8	rfl	807.7
TRANSMITTER		rfp	0
tn	H1	rp	69.5
sfrq	399.782	lp	-37.3
tof	399.5	PLOT	
tpwr	59	wc	250
pw	6.950	sc	0
DECOUPLER		vs	40
dn	C13	th	3
dof	0	ai	cdc ph
dm	nnn		
dmm	c		
dpwr	34		
dmf	29412		

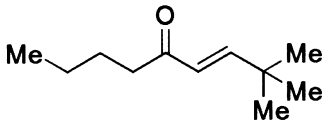


4d

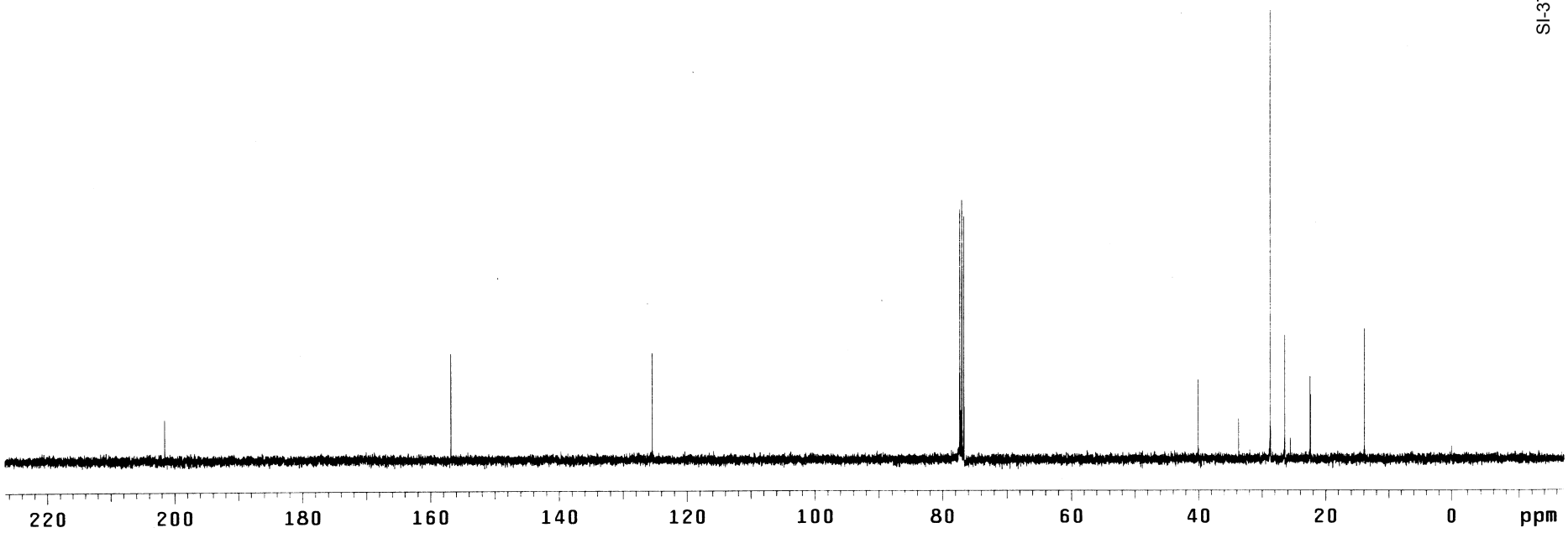


exp1 Carbon

SAMPLE		SPECIAL	
date	May 5 2006	temp	25.0
solvent	cdcl3	gain	30
file	/home/walkup/~	spin	not used
	vnmrsys/data/Frost~	hst	0.008
	/Harkreader/auto_2~	pw90	9.700
	006.05.05_06/s_200~	alfa	10.000
	60505_001/data/cdc~	FLAGS	
	13_02.fid	il	n
ACQUISITION		in	n
sw	24509.8	dp	y
at	1.300	hs	nn
np	63750	PROCESSING	
fb	17000	lb	0.50
bs	64	fn	not used
d1	1.000	DISPLAY	
nt	2000	sp	-1723.1
ct	128	wp	24509.1
TRANSMITTER		rfl	9464.2
tn	C13	rfp	7740.4
sfrq	100.535	rp	-4.1
tof	1042.6	lp	-200.6
tpwr	55	PLOT	
pw	4.850	wc	250
DECOUPLER		sc	0
dn	H1	vs	30000
dof	0	th	68
dm	yyy	ai cdc ph	
dmm	w		
dpwr	41		
dmf	9300		

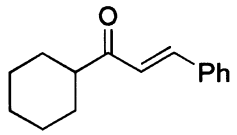


4d

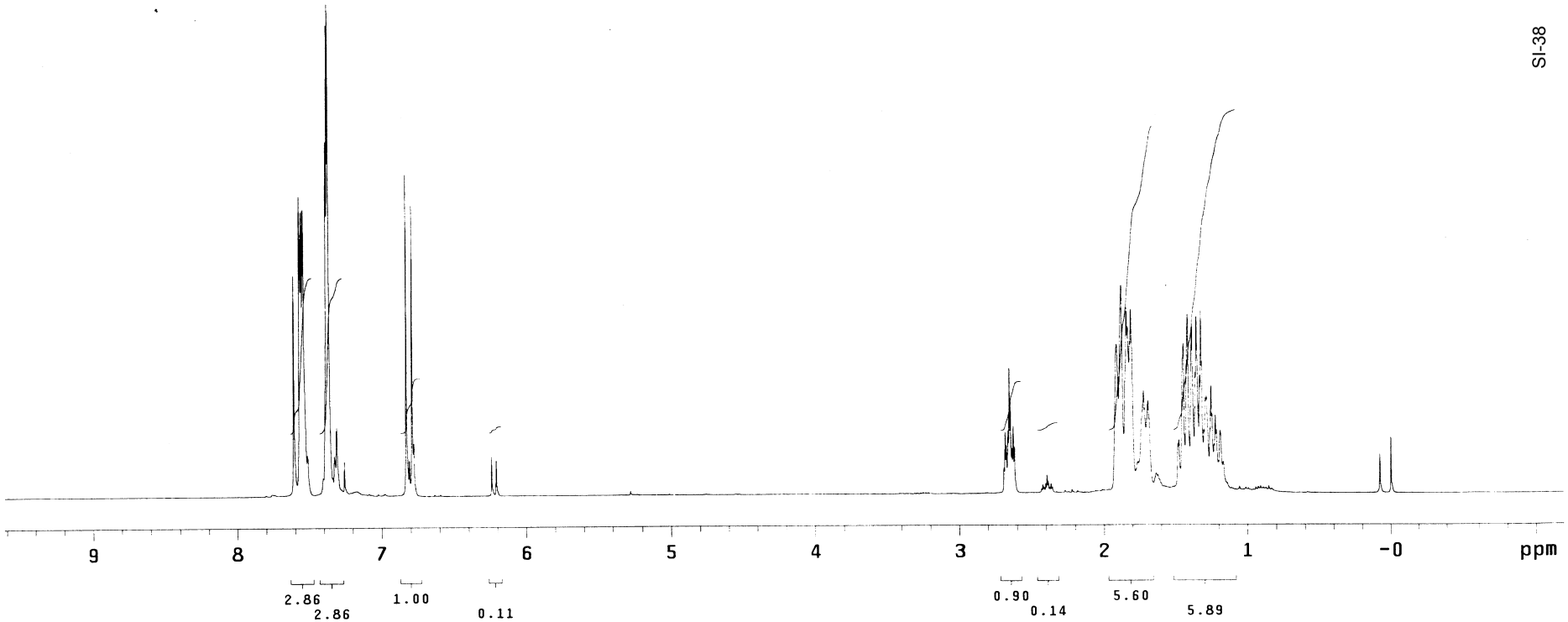


exp1 Proton

SAMPLE		SPECIAL	
date	Oct 2 2006	temp	25.0
solvent	cdcl3	gain	not used
file	/home/walkup/~	spin	not used
data/Zhang/GuotaoL~		hst	0.008
	i/255-1.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	
d1	1.000	lb	0.20
nt	8	fn	65536
ct	8	DISPLAY	
TRANSMITTER		sp	-478.3
tn	H1	wp	4323.9
sfrq	399.782	rfl	806.2
tof	399.5	rfp	0
tpwr	59	rp	119.6
pw	6.950	lp	-25.5
DECOUPLER		PLOT	
dn	C13	wc	250
dof	0	sc	0
dm	nnn	vs	425
dmm	c	th	2
dpwr	34	ai cdc ph	
dmf	29412		

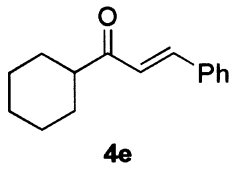


4e

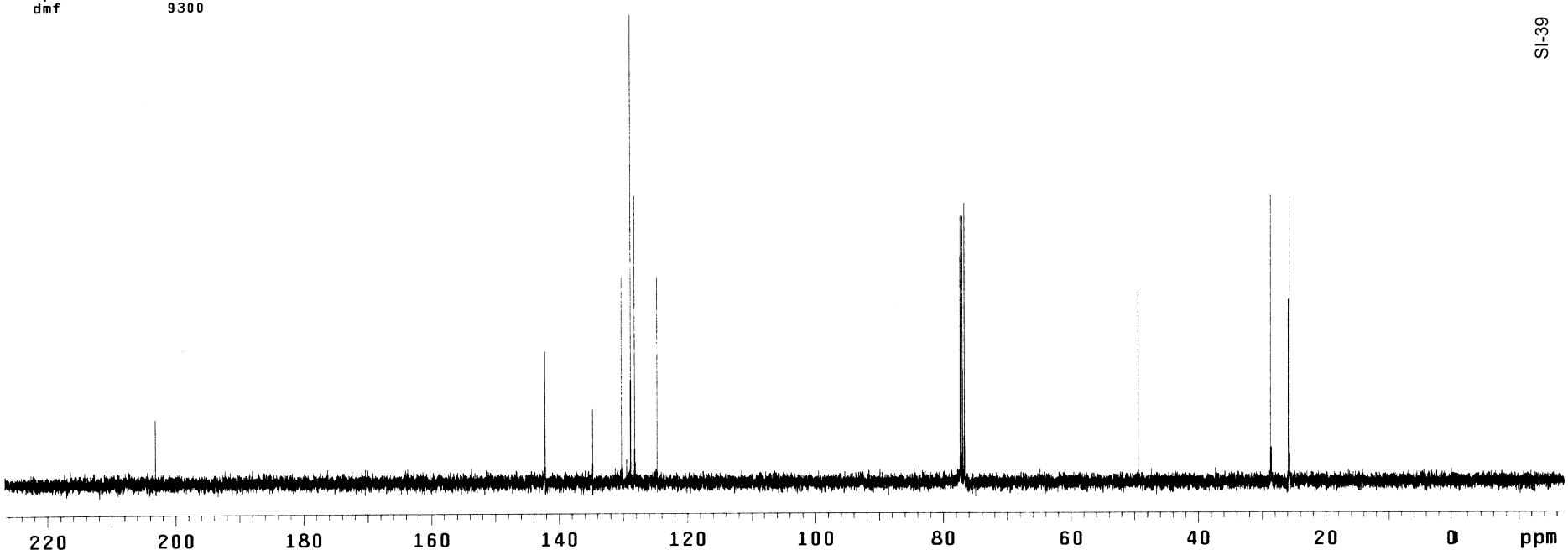


exp1 Carbon

SAMPLE		SPECIAL	
date	May 2 2006	temp	25.0
solvent	cdcl3	gain	30
file	/home/walkup/~	spin	not used
	vnmrsys/data/catal~	hst	0.008
	ano/samin/auto_200~	pw90	9.700
	6.05.02_05/s_20060~	alfa	10.000
	502_001/data/cdcl3~	FLAGS	
	02.fid	il	n
ACQUISITION		in	n
sw	24509.8	dp	y
at	1.300	hs	nn
np	63750	PROCESSING	
fb	17000	lb	0.50
bs	64	fn	not used
d1	1.000	DISPLAY	
nt	1024	sp	-1724.0
ct	128	wp	24509.1
TRANSMITTER		rfl	9465.1
tn	C13	rfp	7740.4
sfrq	100.535	rp	-30.3
tof	1042.6	lp	-133.3
tpwr	55	PLOT	
pw	4.850	wc	250
DECOUPLER		sc	0
dn	H1	vs	25000
dof	0	th	68
dm	yyy	ai cdc ph	
dmm	w		
dpwr	41		
dmf	9300		



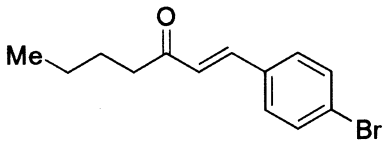
4e



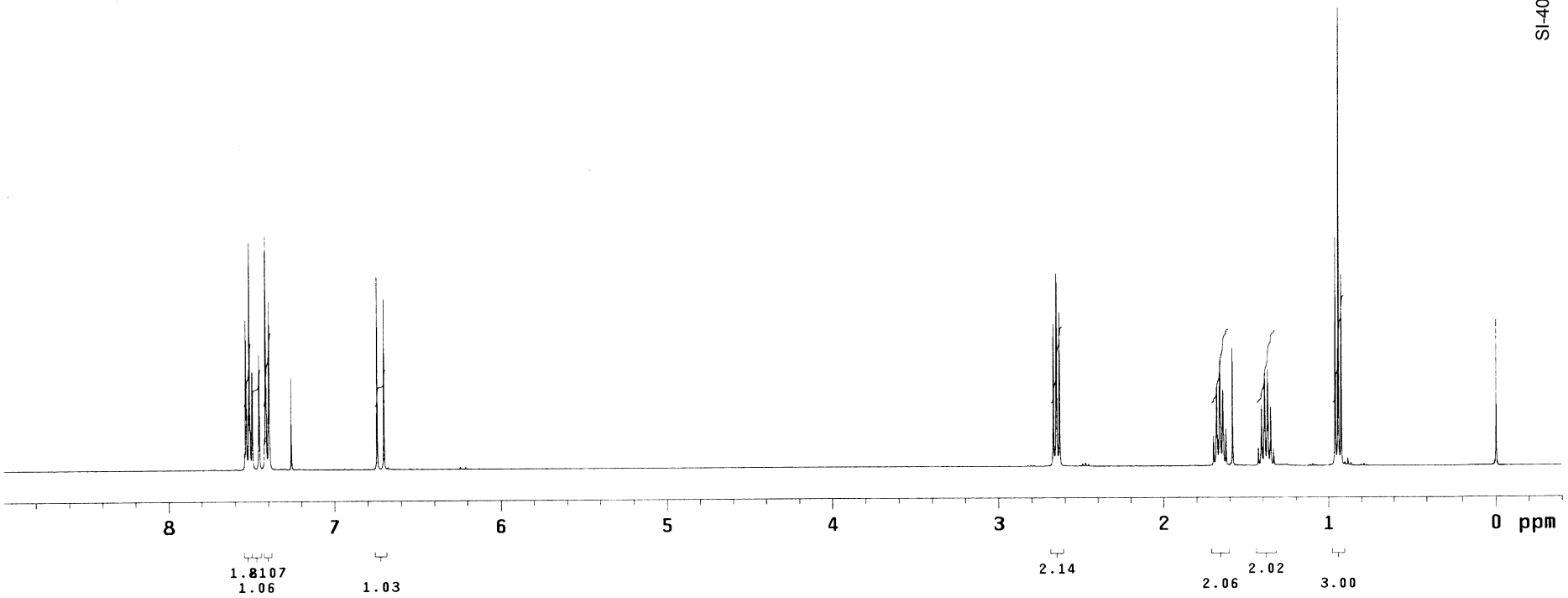
STANDARD 1H OBSERVE - profile

exp1 Proton

SAMPLE		SPECIAL	
date	May 7 2006	temp	25.0
solvent	cdcl3	gain	not used
file	/home/walkup/~	spin	not used
vnmrsys/data/Frost~		hst	0.008
/Wong/auto_2006.05~		pw90	13.900
.07_02/s_20060507_~		alfa	6.600
001/data/cdcl3_01.~		FLAGS	
	fid	il	n
ACQUISITION		in	n
sw	6410.3	dp	y
at	2.049	hs	nn
np	26264	PROCESSING	
fb	4000	lb	0.20
bs	32	fn	65536
ss	2	DISPLAY	
d1	1.000	sp	-162.0
nt	8	wp	3759.3
ct	8	rfl	808.7
TRANSMITTER		rfp	0
tn	H1	rp	66.4
sfrq	399.782	lp	-28.3
tof	399.5	PLOT	
tpwr	59	wc	250
pw	6.950	sc	0
DECOUPLER		vs	80
dn	C13	th	2
dof	0	ai cdc ph	
dm	nnn		
dmm	c		
dpwr	34		
dmf	29412		

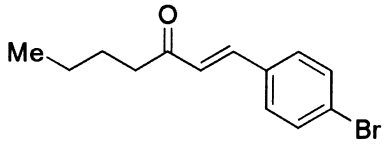


4f

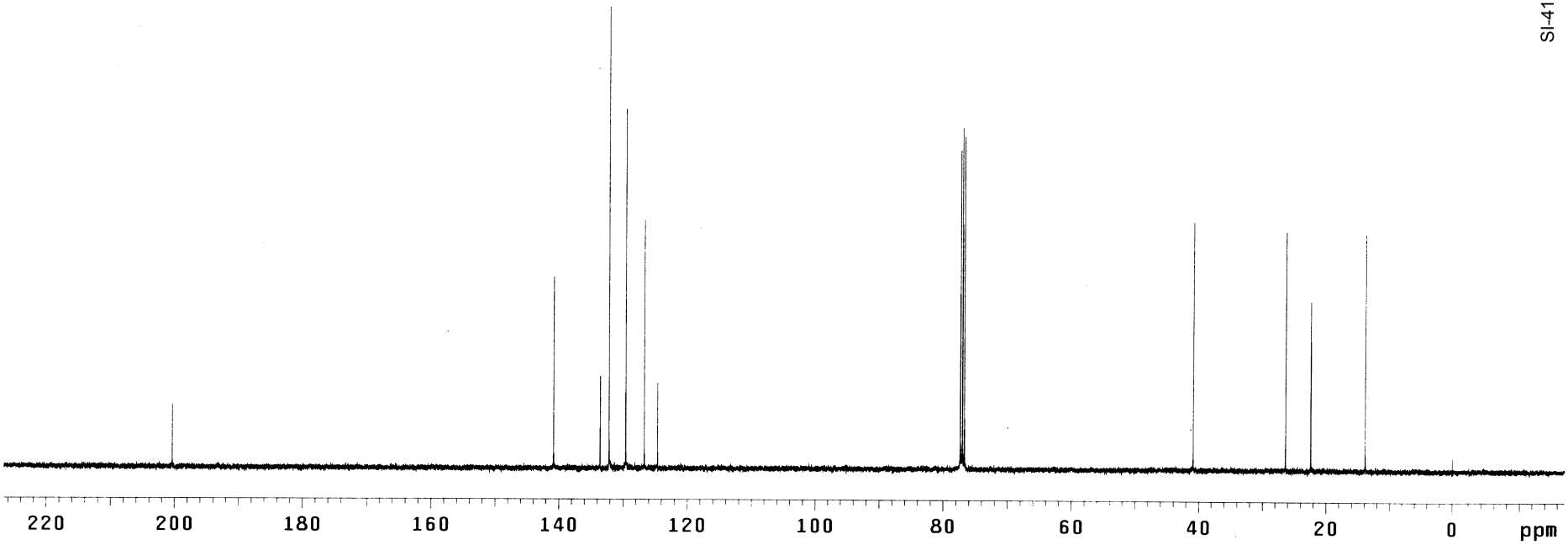


exp43 Carbon

SAMPLE		SPECIAL	
date	May 7 2006	temp	25.0
solvent	cdcl3	gain	30
file	/home/walkup/~	spin	not used
data/Zhang/Shaozho~		hst	0.008
	ng/1-c.fid	pw90	9.700
ACQUISITION		alfa	10.000
sw	24509.8	FLAGS	
at	1.300	il	n
np	63750	in	n
fb	17000	dp	y
bs	64	hs	nn
d1	1.000	PROCESSING	
nt	2000	lb	0.50
ct	2000	fn	not used
TRANSMITTER		DISPLAY	
tn	C13	sp	-1724.1
sfrq	100.535	wp	24509.1
tof	1042.6	rfl	9465.2
tpwr	55	rfp	7740.4
pw	4.850	rp	-22.1
DECOUPLER		lp	-194.5
dn	H1	PLOT	
dof	0	wc	250
dm	yyy	sc	0
dmm	w	vs	40000
dpwr	41	th	5
dmf	9300	ai cdc ph	



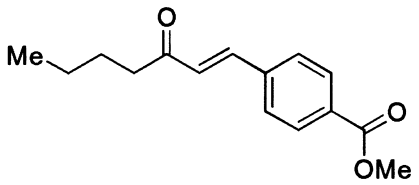
4f



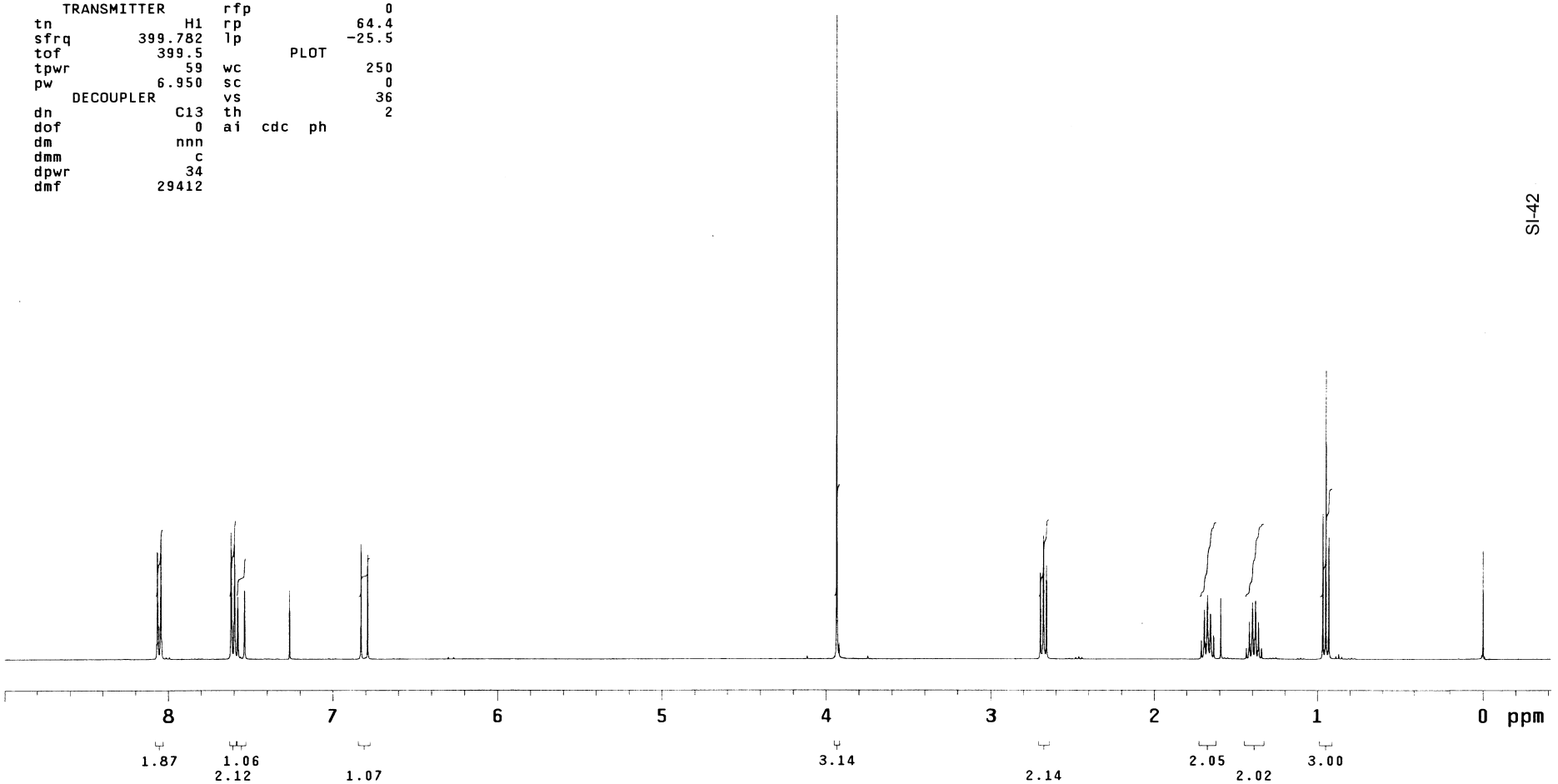
STANDARD 1H OBSERVE - profile

exp1 Proton

SAMPLE		SPECIAL	
date	May 7 2006	temp	25.0
solvent	cdcl3	gain	not used
file	/home/walkup/~	spin	not used
vnmrsys/data/Frost~		hst	0.008
/Wong/auto_2006.05~		pw90	13.900
.07_01/s_20060507_~		alfa	6.600
001/data/cdcl3_01.~		FLAGS	
	fid	il	n
ACQUISITION		in	n
sw	6410.3	dp	y
at	2.049	hs	nn
np	26264	PROCESSING	
fb	4000	lb	0.20
bs	32	fn	65536
ss	2	DISPLAY	
d1	1.000	sp	-167.8
nt	8	wp	3766.4
ct	8	rfl	807.5
TRANSMITTER		rfp	0
tn	H1	rp	64.4
sfrq	399.782	lp	-25.5
tof	399.5	PLOT	
tpwr	59	wc	250
pw	6.950	sc	0
DECOUPLER		vs	36
dn	C13	th	2
dof	0	ai cdc ph	
dm	nnn		
dmm	c		
dpwr	34		
dmf	29412		



4g



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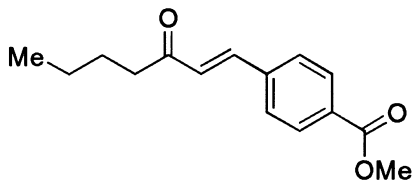
STANDARD 1H OBSERVE - profile
STANDARD 1H OBSERVE - profile
STANDARD 1H OBSERVE - profile

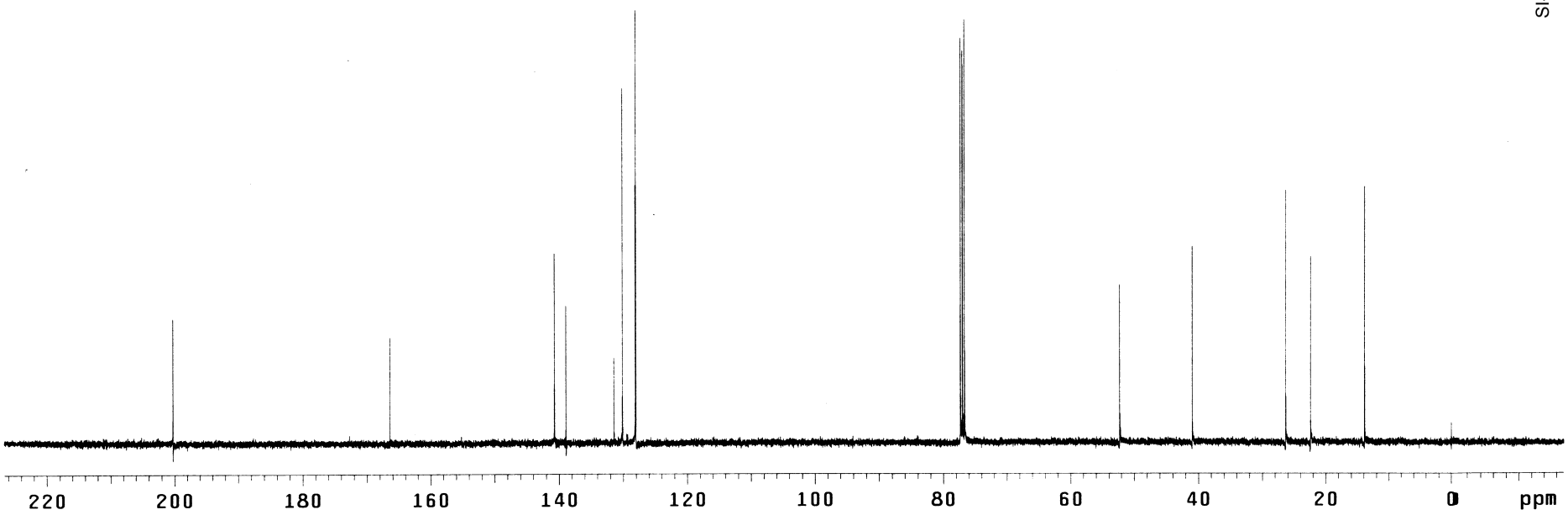
exp1  Carbon

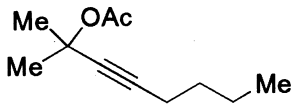
      SAMPLE
date    May  7 2006
solvent       cdcl3
file /home/walkup/~
vnmrsys/data/Frost~
/Wong/auto_2006.05~
.07_01/s_20060507_~
001/data/cdcl3_02.~
                fid
   ACQUISITION
sw          24509.8
at            1.300
np            63750
fb            17000
bs               64
d1            1.000
nt             2000
ct              128
   TRANSMITTER
tn              C13
sfrq        100.535
tof          1042.6
tpwr             55
pw            4.850
    DECOUPLER
dn                H1
dof                0
dm               yyy
dmm                w
dpwr              41
dmf             9300

      SPECIAL
temp           25.0
gain             30
spin       not used
hst             0.008
pw90            9.700
alfa           10.000
       FLAGS
il                 n
in                 n
dp                 y
hs                nn
    PROCESSING
lb              0.50
fn         not used
     DISPLAY
sp          -1723.3
wp          24509.1
rfl          9464.4
rfp          7740.4
rp            -50.7
lp           -133.3
        PLOT
wc               250
sc                 0
vs             50000
th                10
ai  cdc  ph
```



4g



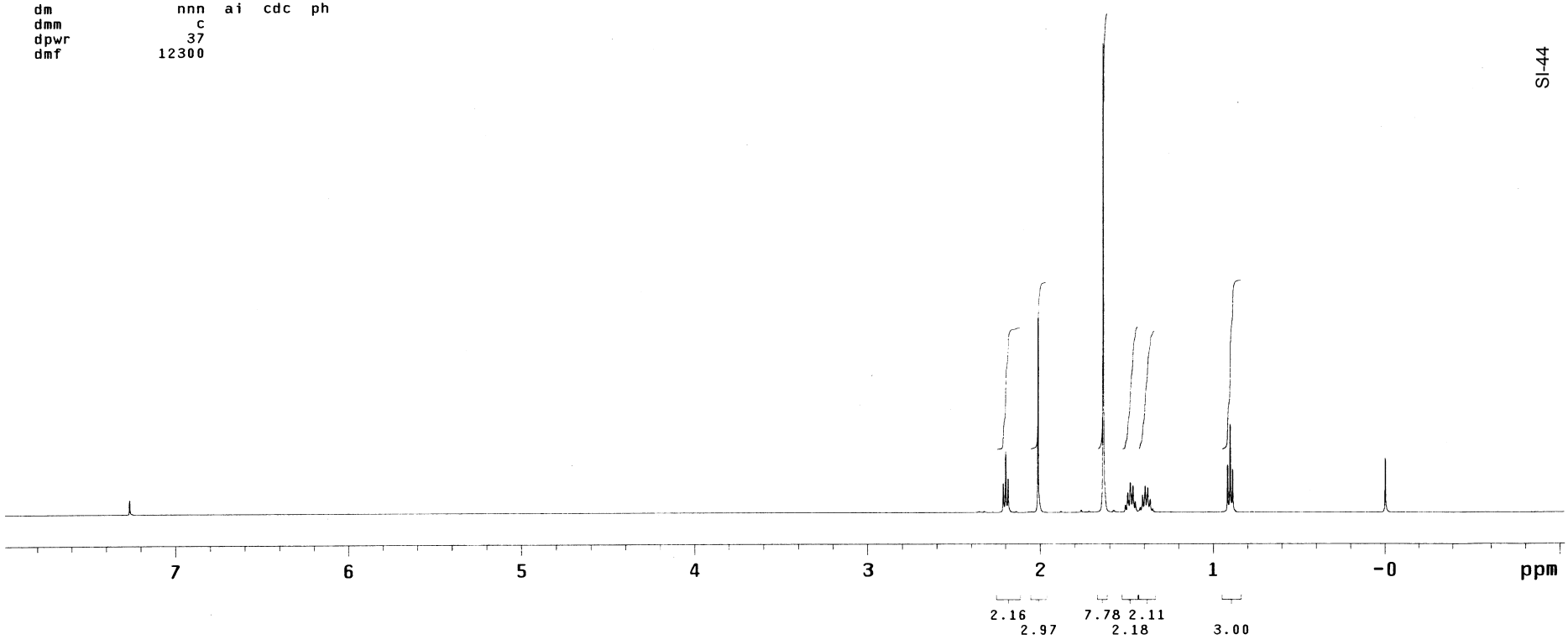


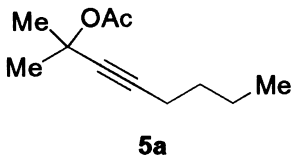
5a

```
exp1  Proton

      SAMPLE
date   Sep 23 2006
solvent      cdcl3
file /home/walkup/~
vnmrsys/data/auto_~
2006.09.23_05/Aug.~
01/data/cdcl3_01.f~
                id
   ACQUISITION
sw           8012.8
at            2.049
np            32830
fb             4000
bs               32
ss                2
d1            1.000
nt                8
ct                8
   TRANSMITTER
tn               H1
sfrq        499.809
tof           499.7
tpwr             54
pw            9.900
    DECOUPLER
dn              C13
dof               0
dm              nnn
dmm               c
dpwr             37
dmf           12300

      SPECIAL
temp             6.0
gain       not used
spin       not used
hst             0.008
pw90           19.800
alfa            6.600
      FLAGS
il                  n
in                  n
dp                  y
hs                 nn
   PROCESSING
lb              0.20
fn             65536
   DISPLAY
sp            -514.5
wp            4506.5
rfl           1000.9
rfp                0
rp              12.1
lp             -41.4
      PLOT
wc               250
sc                 0
vs                40
th                 2
ai  cdc  ph
```





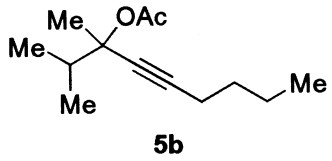
5a

exp1 Carbon

SAMPLE		SPECIAL	
date	Sep 23 2006	temp	6.0
solvent	cdcl3	gain	30
file	/home/walkup/~	spin	not used
	vnmrsys/data/auto_~	hst	0.008
	2006.09.23_05/Aug.~	pw90	13.500
	02/data/cdcl3_01.f~	alfa	10.000
id		FLAGS	
ACQUISITION		il	n
sw	30487.8	in	n
at	1.300	dp	y
np	79298	hs	nn
fb	17000	PROCESSING	
bs	64	lb	0.50
d1	1.000	fn	not used
nt	3200	DISPLAY	
ct	3200	sp	-405.8
TRANSMITTER		wp	23692.5
tn	C13	rfl	11755.3
sfrq	125.689	rfp	9677.1
tof	1255.3	rp	17.0
tpwr	46	lp	-325.6
pw	6.750	PLOT	
DECOUPLER		wc	250
dn	H1	sc	0
dof	0	vs	192980
dm	yyy	th	7
dmm	w	ai cdc ph	
dpwr	36		
dmf	7200		

exp1 Proton

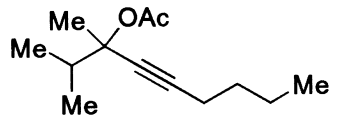
SAMPLE		SPECIAL	
date	Sep 22 2006	temp	25.0
solvent	cdcl3	gain	not used
file	/home/walkup/~	spin	not used
	vnmrsys/data/auto_~	hst	0.008
	2006.09.22_25/s_20~	pw90	13.900
	060922_001/data/cd~	alfa	6.600
	cl3_01.fid	FLAGS	
ACQUISITION		il	n
sw	6410.3	in	n
at	2.049	dp	y
np	26264	hs	nn
fb	4000	PROCESSING	
bs	4	lb	0.20
ss	2	fn	65536
d1	1.000	DISPLAY	
nt	32	sp	-87.8
ct	32	wp	3295.5
TRANSMITTER		rfl	805.0
tn	H1	rfp	0
sfrq	399.782	rp	18.8
tof	399.5	lp	44.0
tpwr	59	PLOT	
pw	6.950	wc	250
DECOUPLER		sc	0
dn	C13	vs	250
dof	0	th	2
dm	nnn	ai	cdc ph
dmm	c		
dpwr	34		
dmf	29412		



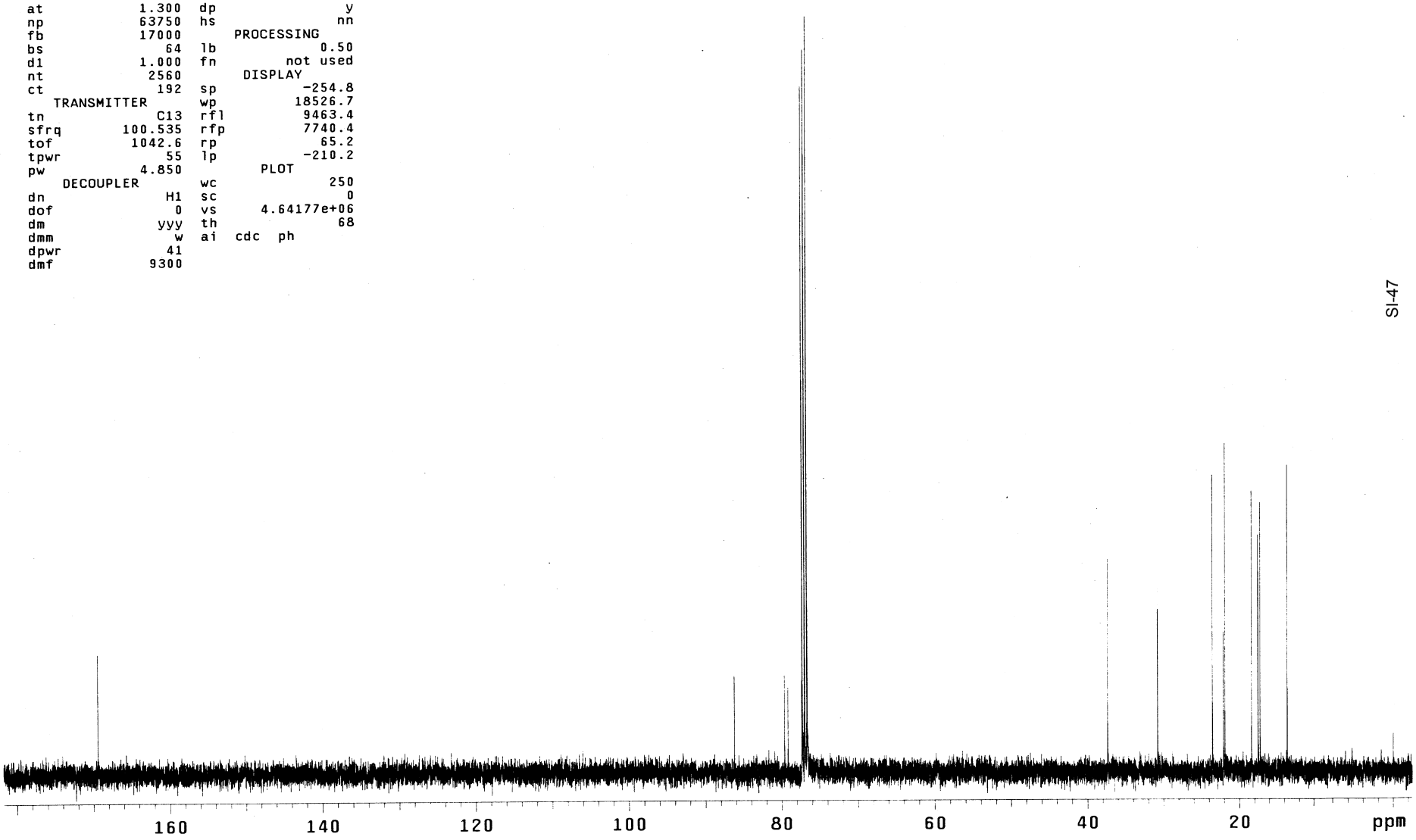
5b

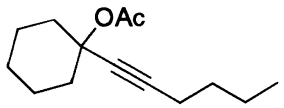
exp1 Carbon

SAMPLE		SPECIAL	
date	Sep 22 2006	temp	25.0
solvent	cdcl3	gain	30
file	/home/walkup/~	spin	not used
	vnmrsys/data/auto_~	hst	0.008
	2006.09.22_25/s_20~	pw90	9.700
	060922_001/data/cd~	alfa	10.000
	cl3_02.fid	FLAGS	
ACQUISITION		il	n
sw	24509.8	in	n
at	1.300	dp	y
np	63750	hs	nn
fb	17000	PROCESSING	
bs	64	lb	0.50
d1	1.000	fn	not used
nt	2560	DISPLAY	
ct	192	sp	-254.8
TRANSMITTER		wp	18526.7
tn	C13	rfl	9463.4
sfrq	100.535	rfp	7740.4
tof	1042.6	rp	65.2
tpwr	55	lp	-210.2
pw	4.850	PLOT	
DECOUPLER		wc	250
dn	H1	sc	0
dof	0	vs	4.64177e+06
dm	yyy	th	68
dmm	w	ai	cdc ph
dpwr	41		
dmf	9300		



5b

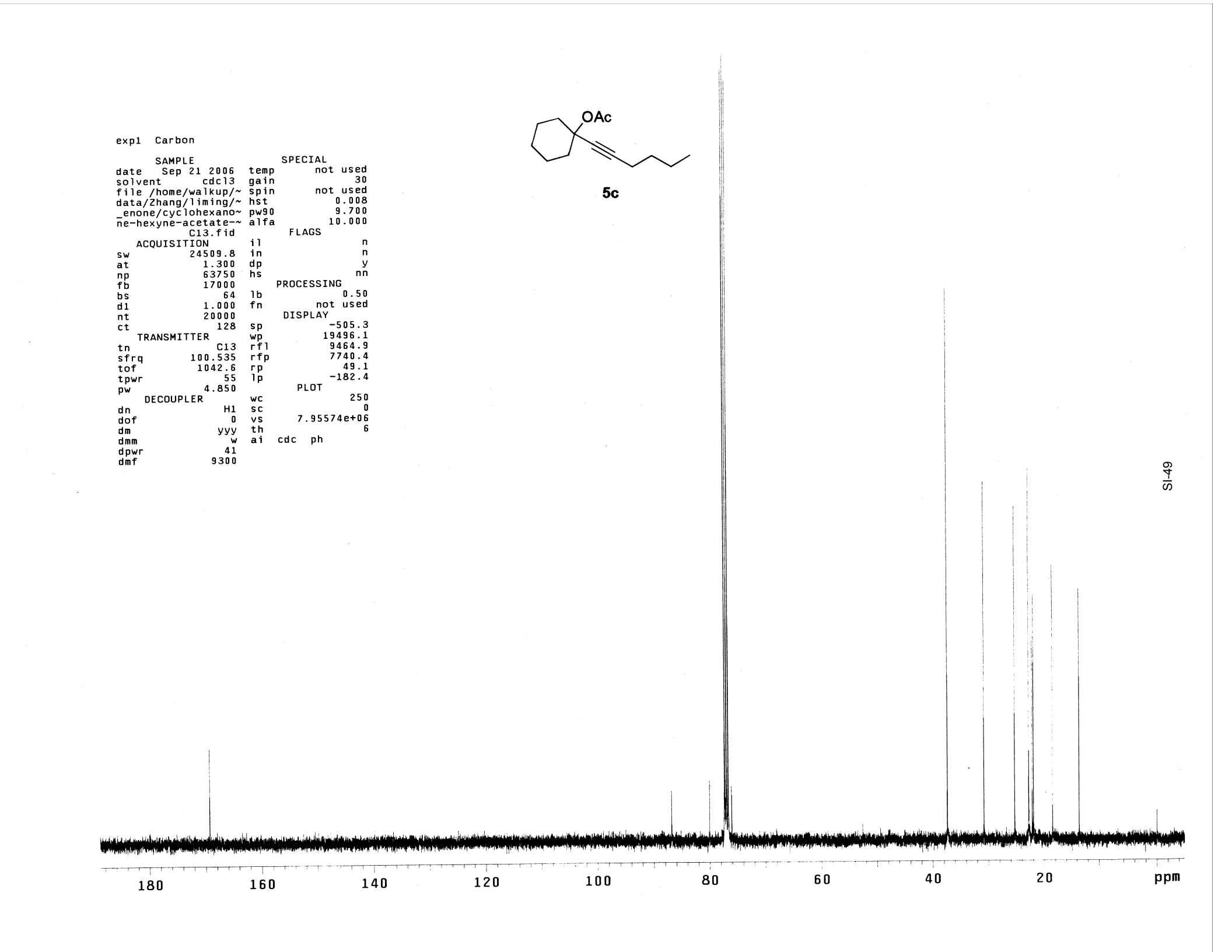




5c

exp1 Proton

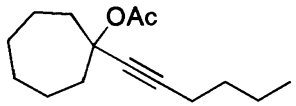
SAMPLE		SPECIAL	
date	Sep 21 2006	temp	not used
solvent	cdcl3	gain	20
file	/home/walkup/~	spin	not used
data/Zhang/liming/~		hst	0.008
_enone/cyclohexano~		pw90	13.900
ne-hexyne-acetate.~		alfa	6.600
	fid	FLAGS	
ACQUISITION		il	n
sw	6410.3	in	n
at	2.049	dp	y
np	26264	hs	nn
fb	4000	PROCESSING	
bs	32	lb	0.20
d1	1.000	fn	65536
nt	32	DISPLAY	
ct	32	sp	-181.0
TRANSMITTER		wp	3252.1
tn	H1	rfl	804.0
sfrq	399.782	rfp	0
tof	399.5	rp	41.7
tpwr	59	lp	-62.0
pw	6.950	PLOT	
DECOUPLER		wc	250
dn	C13	sc	0
dof	0	vs	24849
dm	nnn	th	3
dmm	c	ai cdc ph	
dpwr	34		
dmf	29412		


exp1 Carbon
SAMPLE
date Sep 21 2006
solvent cdcl3
file /home/walkup/~
data/Zhang/liming/~
_enone/cyclohexano~
ne-hexyne-acetate-~
C13.fid
ACQUISITION
sw 24509.8
at 1.300
np 63750
fb 17000
bs 64
d1 1.000
nt 20000
ct 128
TRANSMITTER
tn C13
sfrq 100.535
tof 1042.6
tpwr 55
pw 4.850
DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 41
dmf 9300
SPECIAL
temp not used
gain 30
spin not used
hst 0.008
pw90 9.700
alfa 10.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 0.50
fn not used
DISPLAY
sp -505.3
wp 19496.1
rfl 9464.9
rfp 7740.4
rp 49.1
lp -182.4
PLOT
wc 250
sc 0
vs 7.95574e+06
th 6
ai cdc ph
OAc
5c
S1-49
180
160
140
120
100
80
60
40
20
ppm

STANDARD 1H OBSERVE - profile

exp2 Proton

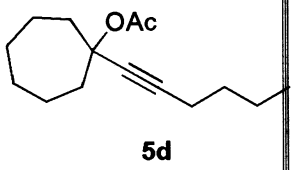
SAMPLE		SPECIAL	
date	Jun 29 2006	temp	25.0
solvent	cdcl3	gain	not used
file	/home/walkup/~	spin	not used
	vnmrsys/data/auto_~	hst	0.008
	2006.06.29_30/s_20~	pw90	14.000
	060629_001/data/cd~	alfa	6.600
	cl3_01.fid	FLAGS	
ACQUISITION		il	n
sw	6410.3	in	n
at	2.049	dp	y
np	26264	hs	nn
fb	4000	PROCESSING	
bs	32	lb	0.20
ss	2	fn	65536
d1	1.000	DISPLAY	
nt	8	sp	-94.0
ct	8	wp	3289.2
TRANSMITTER		rfl	3707.1
tn	H1	rfp	2902.4
sfrq	399.782	rp	151.9
tof	399.5	lp	-29.5
tpwr	58	PLOT	
pw	7.000	wc	250
DECOUPLER		sc	0
dn	C13	vs	717
dof	0	th	3
dm	nnn	ai	cdc ph
dmm	c		
dpwr	0		
dmf	200		



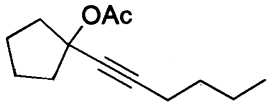
5d

exp1 Carbon

SAMPLE		SPECIAL	
date	Sep 24 2006	temp	6.0
solvent	cdcl3	gain	30
file	/home/walkup/~	spin	not used
	vnmrsys/data/auto_~	hst	0.008
	2006.09.24/Aug.01/~	pw90	13.500
	data/cdcl3_01.fid	alfa	10.000
ACQUISITION		**FLAGS**	
sw	30487.8	il	n
at	1.300	in	n
np	79298	dp	y
fb	17000	hs	nn
bs	64	**PROCESSING**	
d1	1.000	lb	0.50
nt	25600	fn	not used
ct	1216	**DISPLAY**	
TRANSMITTER		sp	-799.0
tn	C13	wp	24759.7
sfrq	125.689	rfl	11756.8
tof	1255.3	rfp	9677.1
tpwr	46	rp	-25.2
pw	6.750	lp	-212.8
DECOUPLER		**PLOT**	
dn	H1	wc	250
dof	0	sc	0
dm	yyy	vs	400000
dmm	w	th	15
dpwr	36	ai	cdc ph
dmf	7200		



5d

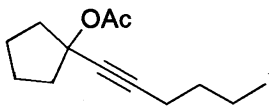


5e

```
exp1  Proton

      SAMPLE
date    Sep 21 2006
solvent       cdcl3
file /home/walkup/~
vnmrsys/data/auto_~
2006.09.21_17/s_20~
060921_001/data/cd~
        cl3_01.fid
   ACQUISITION
sw            6410.3
at             2.049
np             26264
fb              4000
bs                 4
ss                 2
d1             1.000
nt                32
ct                32
   TRANSMITTER
tn                H1
sfrq         399.782
tof            399.5
tpwr              59
pw             6.950
    DECOUPLER
dn              C13
dof               0
dm              nnn
dmm               c
dpwr             34
dmf           29412

      SPECIAL
temp        not used
gain        not used
spin        not used
hst            0.008
pw90          13.900
alfa           6.600
      FLAGS
il                n
in                n
dp                y
hs               nn
   PROCESSING
lb             0.20
fn            65536
    DISPLAY
sp           -135.0
wp           3248.6
rfl           803.6
rfp               0
rp             42.8
lp            -44.2
      PLOT
wc              250
sc                0
vs              220
th                2
ai  cdc  ph
```

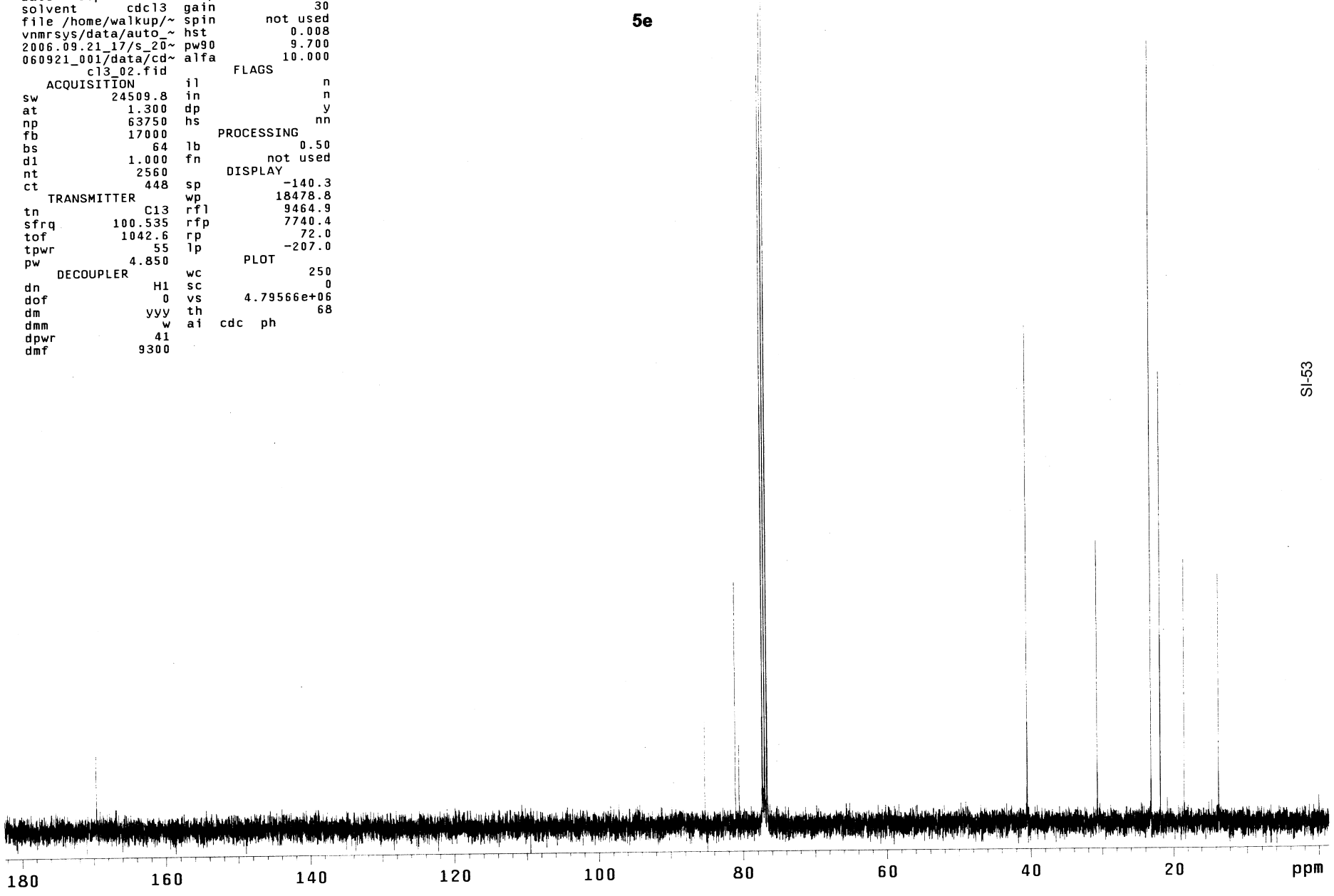


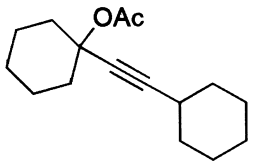
5e

```
exp1  Carbon

      SAMPLE
date    Sep 21 2006
solvent       cdcl3
file /home/walkup/~
vnmrsys/data/auto_~
2006.09.21_17/s_20~
060921_001/data/cd~
        cl3_02.fid
   ACQUISITION
sw          24509.8
at            1.300
np            63750
fb            17000
bs               64
d1            1.000
nt             2560
ct              448
   TRANSMITTER
tn              C13
sfrq        100.535
tof          1042.6
tpwr             55
pw            4.850
    DECOUPLER
dn               H1
dof               0
dm              yyy
dmm               w
dpwr             41
dmf            9300

      SPECIAL
temp        not used
gain              30
spin        not used
hst            0.008
pw90           9.700
alfa          10.000
      FLAGS
il                n
in                n
dp                y
hs               nn
   PROCESSING
lb             0.50
fn         not used
    DISPLAY
sp           -140.3
wp          18478.8
rfl          9464.9
rfp          7740.4
rp             72.0
lp           -207.0
       PLOT
wc              250
sc                0
vs      4.79566e+06
th               68
ai  cdc  ph
```

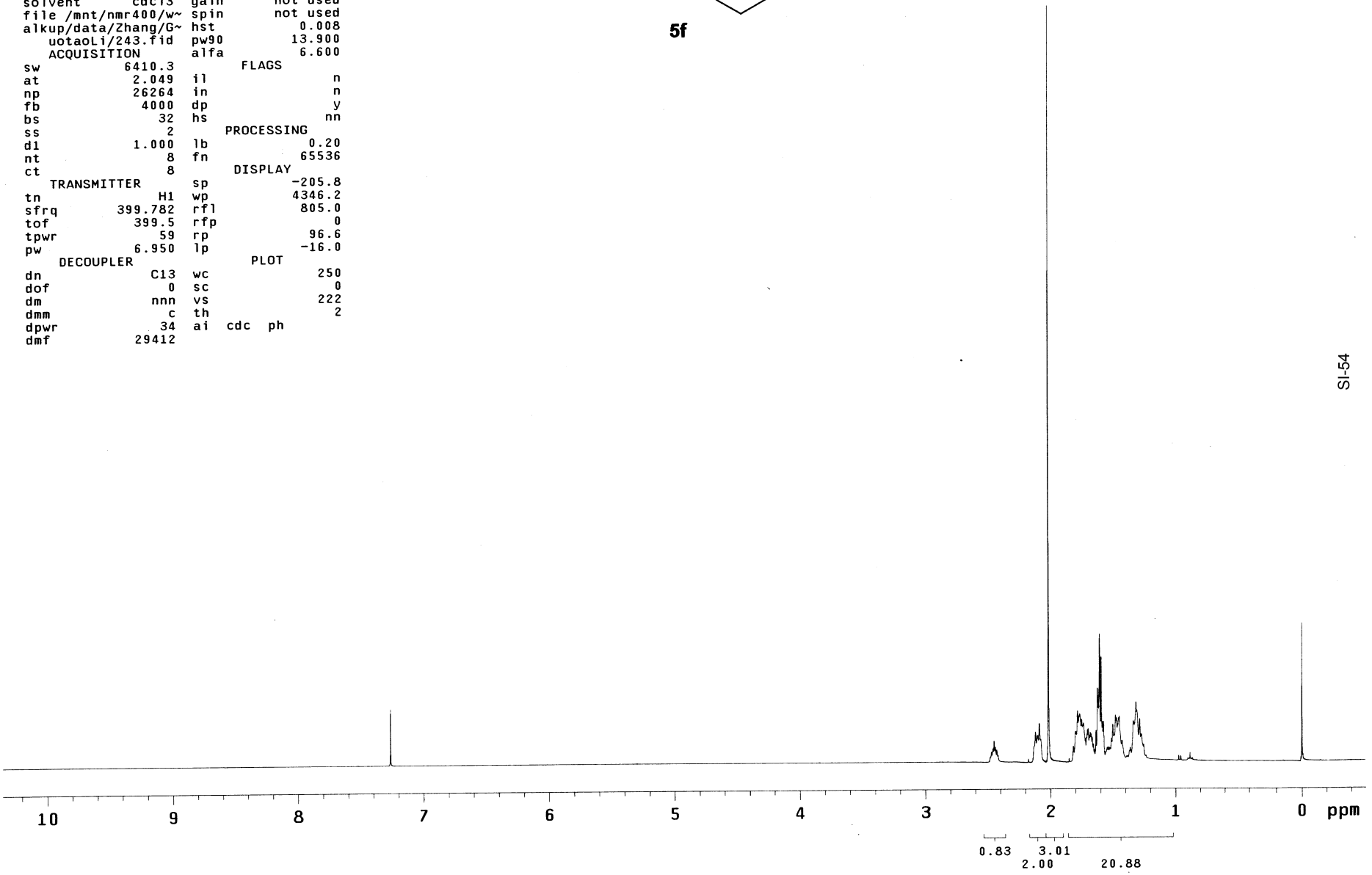


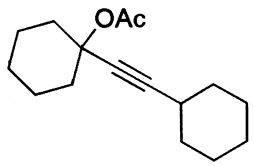


5f

exp1 Proton

SAMPLE		SPECIAL	
date	Sep 30 2006	temp	25.0
solvent	cdcl3	gain	not used
file	/mnt/nmr400/w~	spin	not used
alkup/data/Zhang/G~		hst	0.008
	uotaoLi/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	
d1	1.000	lb	0.20
nt	8	fn	65536
ct	8	DISPLAY	
TRANSMITTER		sp	-205.8
tn	H1	wp	4346.2
sfrq	399.782	rfl	805.0
tof	399.5	rfp	0
tpwr	59	rp	96.6
pw	6.950	lp	-16.0
DECOUPLER		PLOT	
dn	C13	wc	250
dof	0	sc	0
dm	nnn	vs	222
dmm	c	th	2
dpwr	34	ai cdc ph	
dmf	29412		

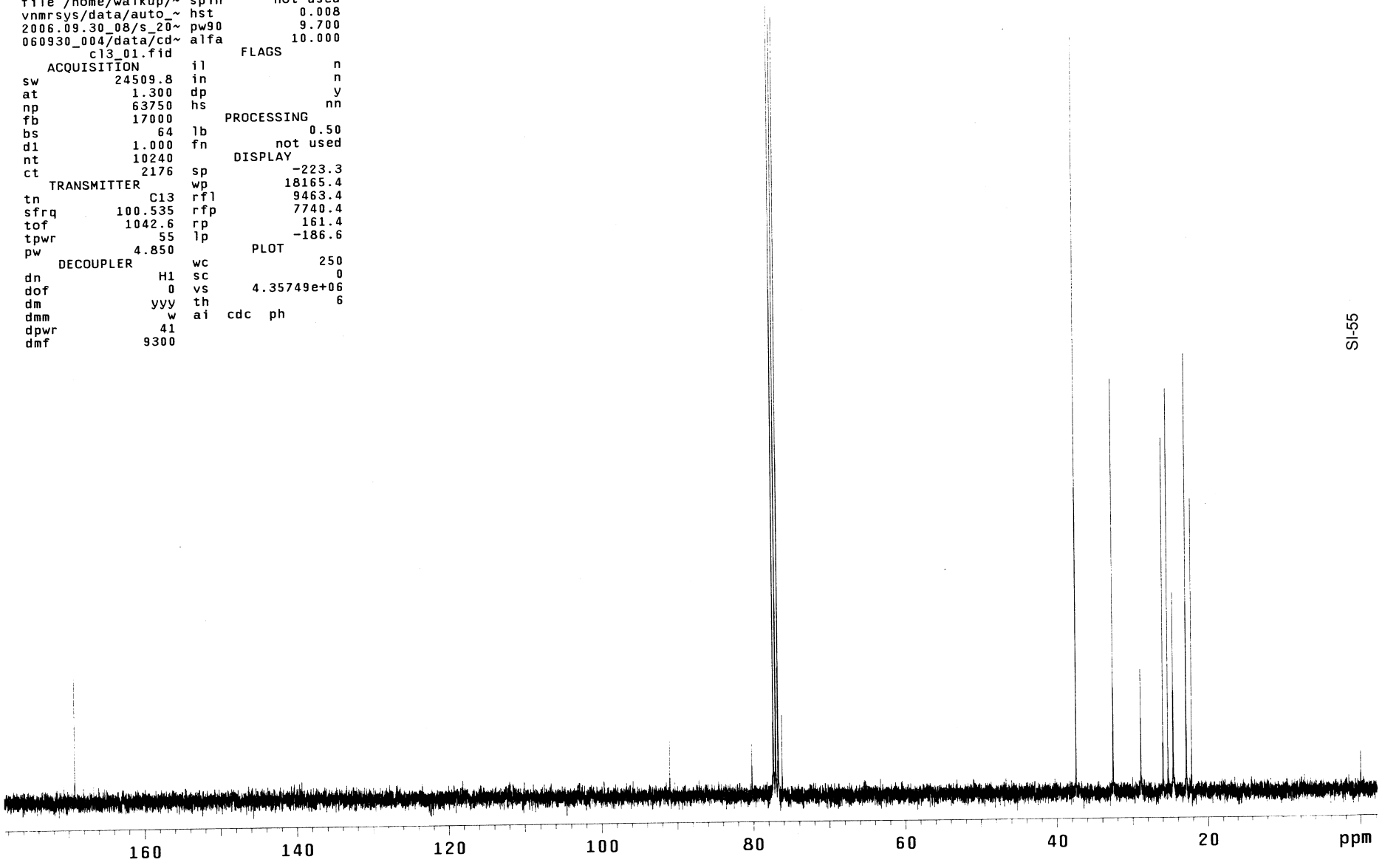


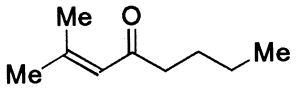


5f

exp1 Carbon

SAMPLE		SPECIAL	
date	Sep 30 2006	temp	25.0
solvent	cdcl3	gain	30
file	/home/walkup/~	spin	not used
	vnmrsys/data/auto_~	hst	0.008
	2006.09.30_08/s_20~	pw90	9.700
	060930_004/data/cd~	alfa	10.000
	cl3_01.fid	FLAGS	
ACQUISITION		il	n
sw	24509.8	in	n
at	1.300	dp	y
np	63750	hs	nn
fb	17000	PROCESSING	
bs	64	lb	0.50
d1	1.000	fn	not used
nt	10240	DISPLAY	
ct	2176	sp	-223.3
TRANSMITTER		wp	18165.4
tn	C13	rfl	9463.4
sfrq	100.535	rfp	7740.4
tof	1042.6	rp	161.4
tpwr	55	lp	-186.6
pw	4.850	PLOT	
DECOUPLER		wc	250
dn	H1	sc	0
dof	0	vs	4.35749e+06
dm	yyy	th	6
dmm	w	ai	cdc ph
dpwr	41		
dmf	9300		

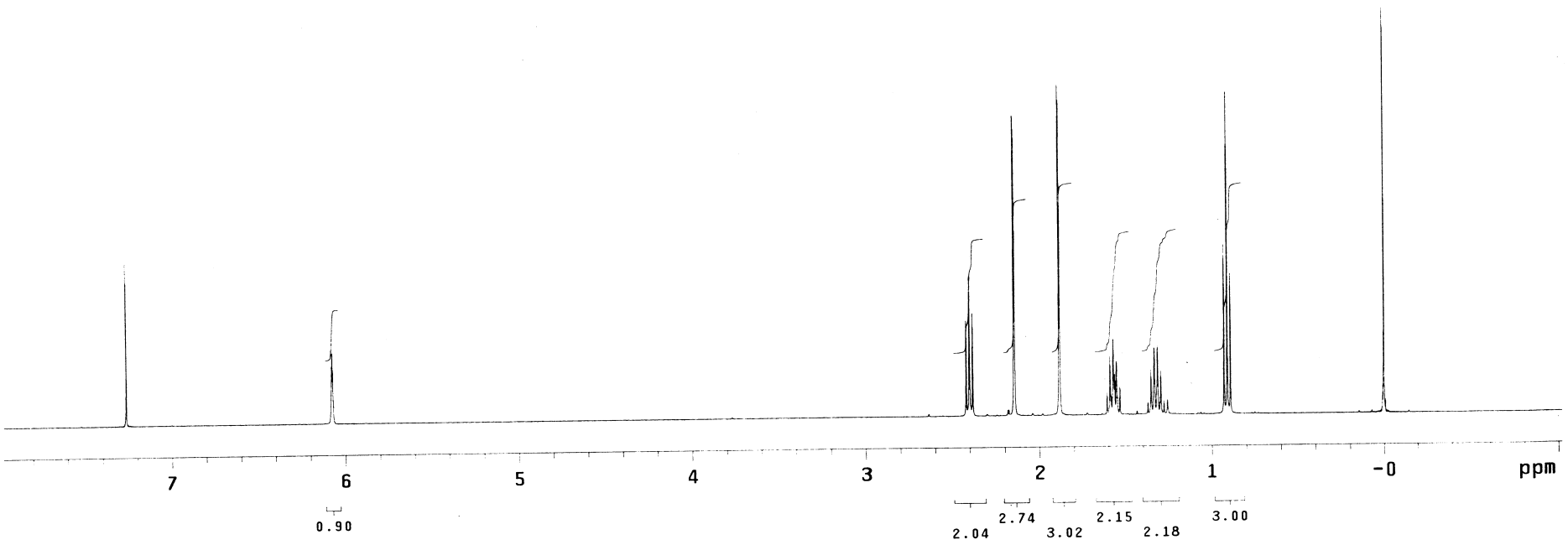


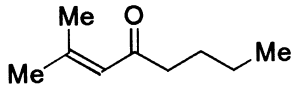


6a

```
exp1  Proton

      SAMPLE                    SPECIAL
date    Sep 24 2006   temp        not used
solvent       cdcl3   gain        not used
file /home/walkup/~   spin        not used
vnmrsys/data/auto_~   hst            0.008
2006.09.24_07/s_20~   pw90          13.900
060924_001/data/cd~   alfa           6.600
         cl3_01.fid          FLAGS
   ACQUISITION          il                 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           -409.1
ct                  8     wp           3596.8
   TRANSMITTER            rfl           804.8
tn                 H1     rfp               0
sfrq          399.782     rp               32.6
tof             399.5     lp            -25.1
tpwr               59           PLOT
pw              6.950     wc              250
     DECOUPLER            sc                0
dn                C13     vs              500
dof                 0     th                2
dm                nnn     ai  cdc  ph
dmm                 c
dpwr               34
dmf             29412
```

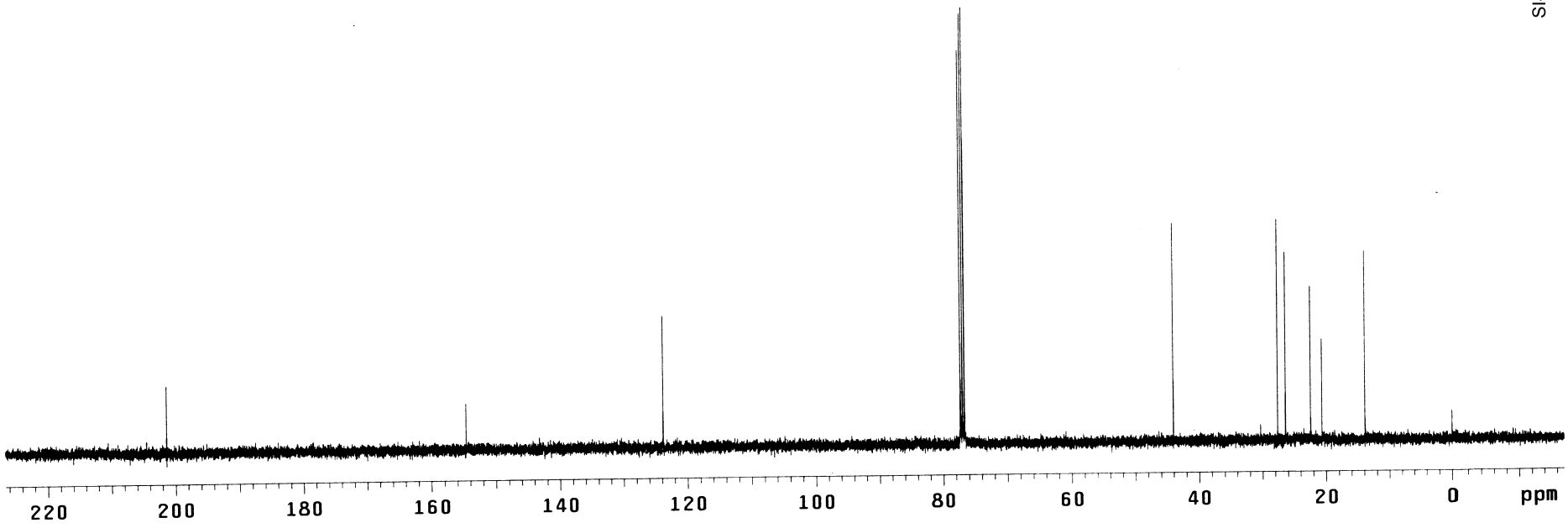




6a

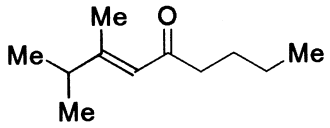
```
exp1  Carbon

      SAMPLE                SPECIAL
date    May 10 2006   temp          25.0
solvent       cdcl3   gain            30
file /home/walkup/~   spin      not used
vnmrsys/data/catal~   hst           0.008
ano/samin/auto_200~   pw90          9.700
6.05.10_01/s_20060~   alfa         10.000
510_001/data/cdcl3~         FLAGS
             _02.fid  il                n
   ACQUISITION        in                n
sw          24509.8   dp                y
at            1.300   hs               nn
np            63750        PROCESSING
fb            17000   lb             0.50
bs               64   fn         not used
d1            1.000        DISPLAY
nt             2000   sp          -1722.2
ct              128   wp          24509.1
   TRANSMITTER        rfl          9463.3
tn               C13  rfp          7740.4
sfrq         100.535   rp            -45.8
tof           1042.6   lp           -133.3
tpwr              55           PLOT
pw             4.850   wc             250
    DECOUPLER         sc               0
dn               H1   vs           50000
dof               0   th              68
dm              yyy   ai  cdc  ph
dmm               w
dpwr             41
dmf            9300
```



exp1 Proton

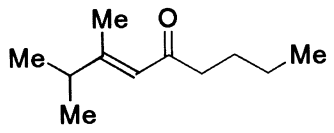
SAMPLE		SPECIAL	
date	Sep 28 2006	temp	25.0
solvent	cdcl3	gain	not used
file	/home/walkup/~	spin	not used
	vnmrsys/data/auto_~	hst	0.008
	2006.09.28_01/s_20~	pw90	13.900
	060928_001/data/cd~	alfa	6.600
	cl3_01.fid	FLAGS	
ACQUISITION		il	n
sw	6410.3	in	n
at	2.049	dp	y
np	26264	hs	nn
fb	4000	PROCESSING	
bs	4	lb	0.20
ss	2	fn	65536
d1	1.000	DISPLAY	
nt	32	sp	-132.2
ct	32	wp	3320.5
TRANSMITTER		rfl	804.0
tn	H1	rfp	0
sfrq	399.782	rp	124.7
tof	399.5	lp	-41.2
tpwr	59	PLOT	
pw	6.950	wc	250
DECOUPLER		sc	0
dn	C13	vs	248
dof	0	th	3
dm	nnn	ai cdc ph	
dmm	c		
dpwr	34		
dmf	29412		



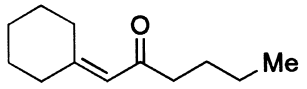
6b

exp1 Carbon

SAMPLE		SPECIAL	
date	Sep 28 2006	temp	25.0
solvent	cdcl3	gain	30
file	/home/walkup/~	spin	not used
data	/Zhang/Meng/en~	hst	0.008
one-linear-C13.fid		pw90	9.700
ACQUISITION		alfa	10.000
sw	24509.8	**FLAGS**	
at	1.300	il	n
np	63750	in	n
fb	17000	dp	y
bs	64	hs	nn
d1	1.000	**PROCESSING**	
nt	25600	lb	0.50
ct	64	fn	not used
TRANSMITTER		**DISPLAY**	
tn	C13	sp	-1722.3
sfrq	100.535	wp	24509.1
tof	1042.6	rfl	9463.4
tpwr	55	rfp	7740.4
pw	4.850	rp	154.4
DECOUPLER		lp	-214.1
dn	H1	**PLOT**	
dof	0	wc	250
dm	yyy	sc	0
dmm	w	vs	8.1328e+06
dpwr	41	th	4
dmf	9300	ai cdc ph	



6b



6c

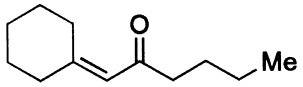
```
exp1  Proton

      SAMPLE                SPECIAL
date   Sep 24 2006   temp          25.0
solvent      cdcl3   gain            20
file /mnt/nmr400/w~  spin      not used
alkup/data/Zhang/l~  hst           0.008
iming/_enone/enone~  pw90         13.900
-cyclohexanone.fid   alfa          6.600
   ACQUISITION            FLAGS
sw           6410.3   il              n
at            2.049   in              n
np            26264   dp              y
fb             4000   hs             nn
bs                4       PROCESSING
d1            1.000   lb           0.20
nt               32   fn          65536
ct               32        DISPLAY
   TRANSMITTER        sp         -121.9
tn               H1   wp         3182.8
sfrq       399.782   rfl          804.8
tof            399.5   rfp            0
tpwr              59   rp          41.9
pw             6.950   lp         -26.2
    DECOUPLER             PLOT
dn               C13   wc           250
dof                0   sc             0
dm               nnn   vs         75748
dmm                c   th             2
dpwr              34   ai  cdc  ph
dmf            29412
```

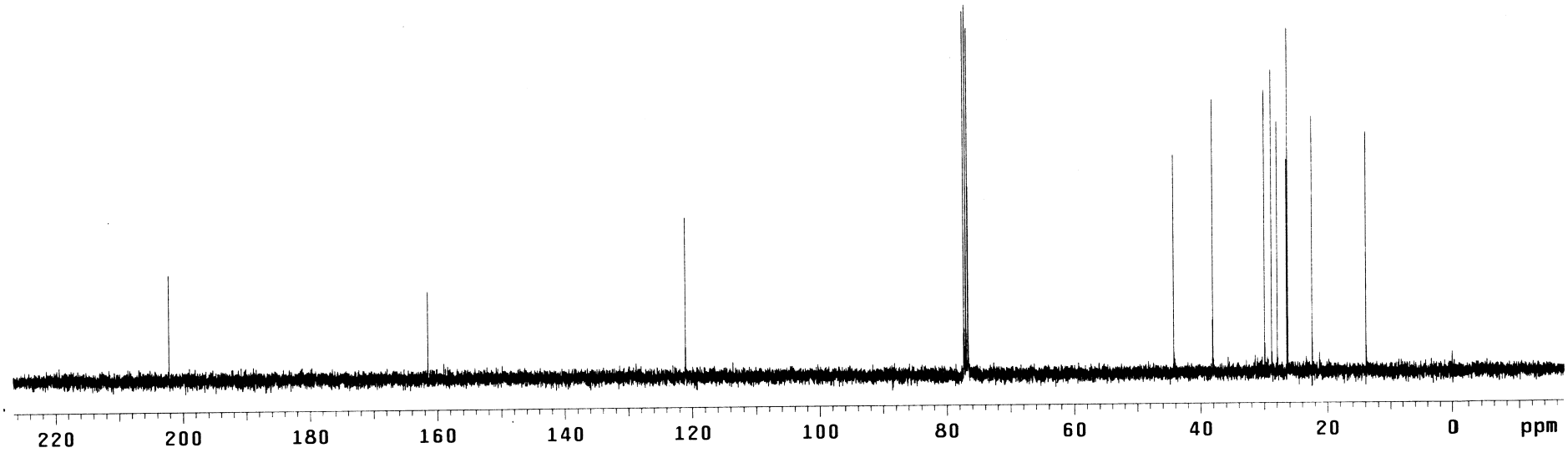
STANDARD 1H OBSERVE - profile
STANDARD 1H OBSERVE - profile

exp1 Carbon

SAMPLE		SPECIAL	
date	May 10 2006	temp	25.0
solvent	cdcl3	gain	30
file	/home/walkup/~	spin	not used
	vnmrsys/data/catal~	hst	0.008
	ano/samin/auto_200~	pw90	9.700
	6.05.10_01/s_20060~	alfa	10.000
	510_002/data/cdcl3~	FLAGS	
	_02.fid	il	n
ACQUISITION		in	n
sw	24509.8	dp	y
at	1.300	hs	nn
np	63750	PROCESSING	
fb	17000	lb	0.50
bs	64	fn	not used
d1	1.000	DISPLAY	
nt	2000	sp	-1722.8
ct	128	wp	24509.1
TRANSMITTER		rfl	9464.0
tn	C13	rfp	7740.4
sfrq	100.535	rp	-23.1
tof	1042.6	lp	-189.4
tpwr	55	PLOT	
pw	4.850	wc	250
DECOUPLER		sc	0
dn	H1	vs	40000
dof	0	th	14
dm	yyy	ai cdc ph	
dmm	w		
dpwr	41		
dmf	9300		



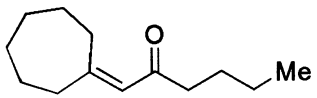
6c



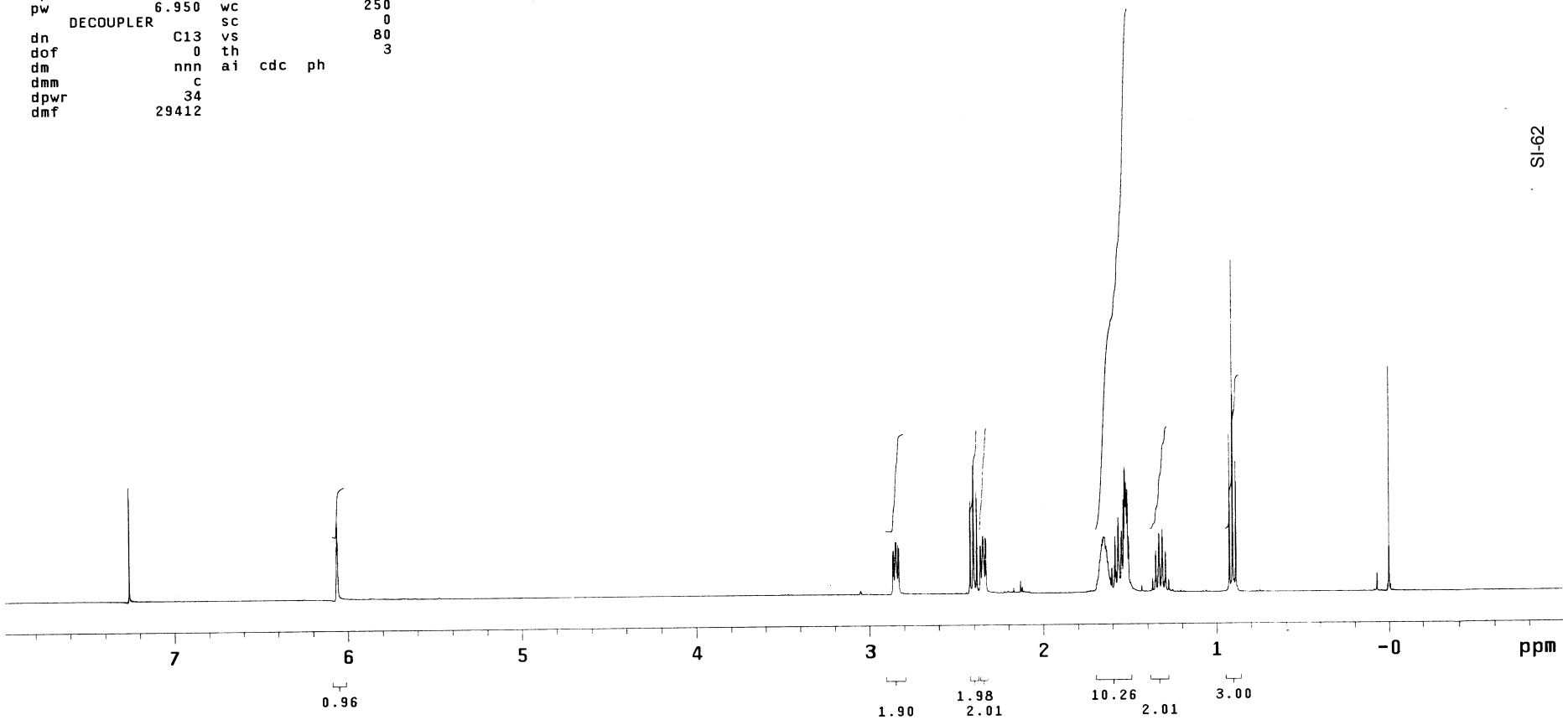
STANDARD 1H OBSERVE - profile

exp1 Proton

SAMPLE		SPECIAL	
date	Jul 21 2006	temp	25.0
solvent	cdcl3	gain	not used
file	/home/walkup/~	spin	not used
	vnmrsys/data/auto_~	hst	0.008
	2006.07.21_29/s_20~	pw90	13.900
	060721_001/data/cd~	alfa	6.600
	c13_01.fid	FLAGS	
ACQUISITION		il	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	-398.3
ct	8	wp	3586.8
TRANSMITTER		rfl	804.8
tn	H1	rfp	0
sfrq	399.782	rp	-1.6
tof	399.5	lp	-55.0
tpwr	59	PLOT	
pw	6.950	wc	250
DECOUPLER		sc	0
dn	C13	vs	80
dof	0	th	3
dm	nnn	ai cdc ph	
dmm	c		
dpwr	34		
dmf	29412		



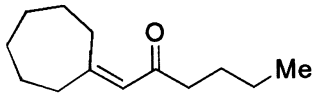
6d



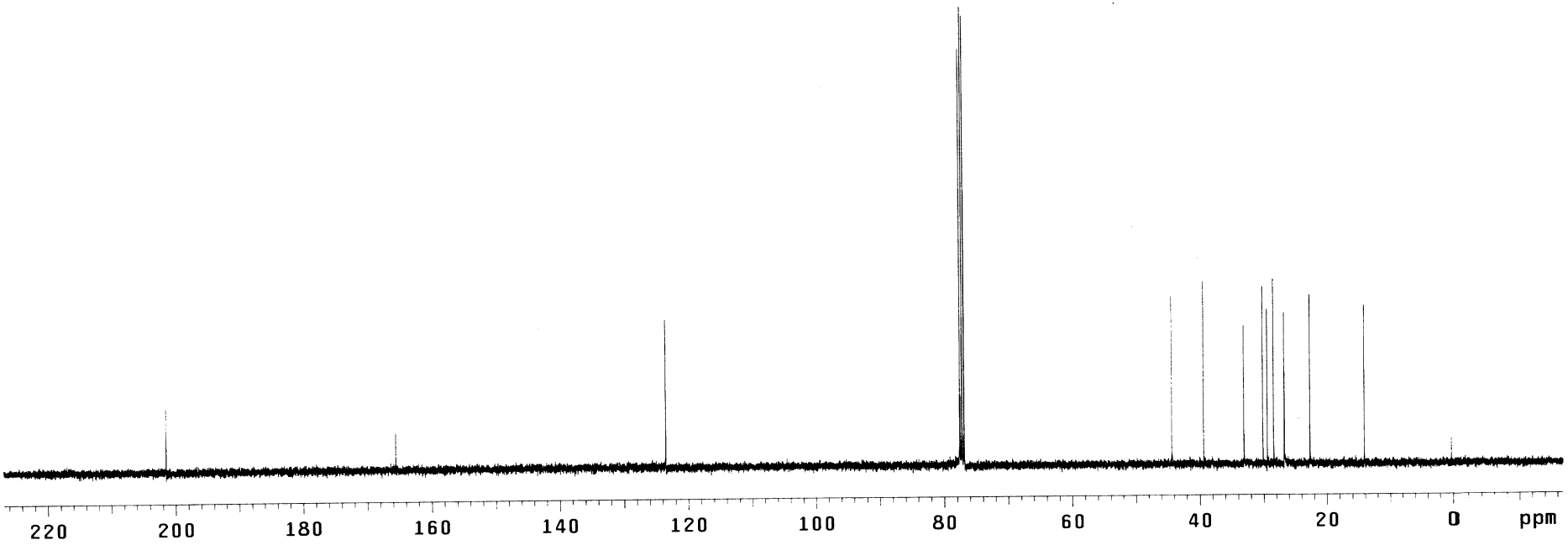
STANDARD 1H OBSERVE - profile

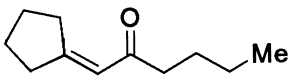
exp1 Carbon

SAMPLE		SPECIAL	
date	Jul 23 2006	temp	25.0
solvent	cdcl3	gain	30
file	/home/walkup/~	spin	not used
	vnmrsys/data/auto_~	hst	0.008
	2006.07.23_04/s_20~	pw90	9.700
	060723_001/data/cd~	alfa	10.000
	c13_01.fid	FLAGS	
ACQUISITION		il	n
sw	24509.8	in	n
at	1.300	dp	y
np	63750	hs	nn
fb	17000	PROCESSING	
bs	64	lb	0.50
d1	1.000	fn	not used
nt	50000	DISPLAY	
ct	4352	sp	-1699.1
TRANSMITTER		wp	24509.1
tn	C13	rfl	1699.8
sfrq	100.535	rfp	0
tof	1042.6	rp	-41.4
tpwr	55	lp	-133.3
pw	4.850	PLOT	
DECOUPLER		wc	250
dn	H1	sc	0
dof	0	vs	2e+06
dm	yyy	th	68
dmm	w	ai	cdc ph
dpwr	41		
dmf	9300		



6d

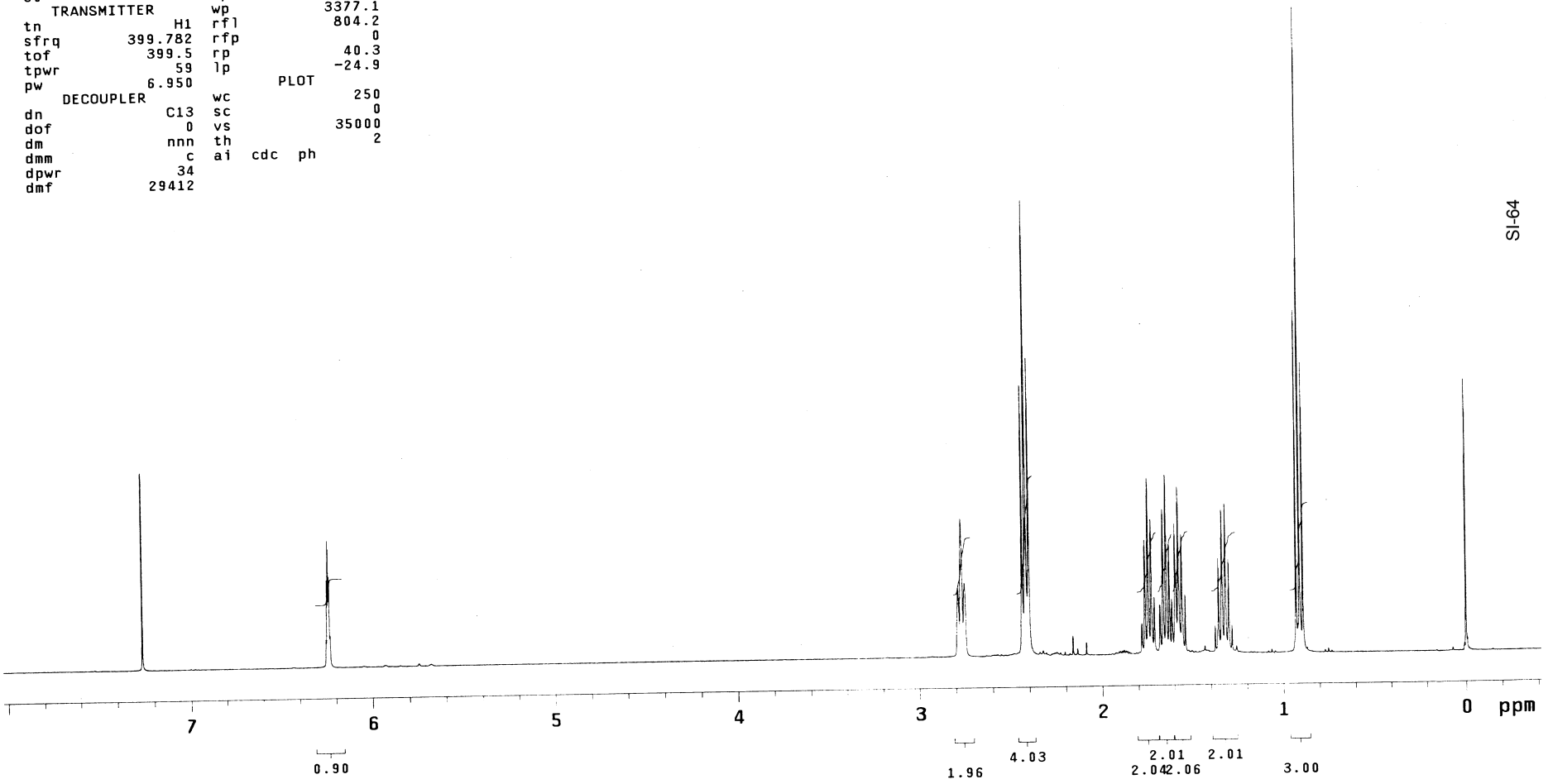


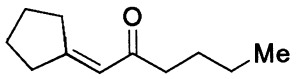


6e

```
expl  Proton

      SAMPLE                SPECIAL
date   Sep 24 2006  temp          25.0
solvent      cdcl3  gain            20
file /home/walkup/~ spin      not used
vnmrsys/data/auto_~ hst           0.008
2006.09.24/s_20060~ pw90         13.900
924_001/data/cdcl3~ alfa          6.600
          _01.fid          FLAGS
   ACQUISITION          il              n
sw           6410.3      in              n
at            2.049      dp              y
np            26264      hs             nn
fb             4000          PROCESSING
bs                4      lb           0.20
d1            1.000      fn          65536
nt               32          DISPLAY
ct               32      sp         -166.9
   TRANSMITTER           wp         3377.1
tn                H1     rfl         804.2
sfrq         399.782     rfp             0
tof            399.5     rp           40.3
tpwr              59     lp          -24.9
pw            6.950           PLOT
     DECOUPLER           wc            250
dn               C13     sc              0
dof                0     vs          35000
dm               nnn     th              2
dmm                c     ai  cdc  ph
dpwr              34
dmf            29412
```





6e

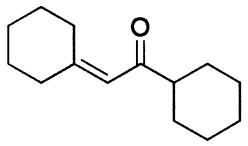
exp1 Carbon

SAMPLE		SPECIAL	
date	Sep 23 2006	temp	6.0
solvent	cdcl3	gain	30
file	/home/walkup/~	spin	not used
	vnmrsys/data/auto_~	hst	0.008
	2006.09.23_07/Aug.~	pw90	13.500
	02/data/cdcl3_01.f~	alfa	10.000
	id	FLAGS	
ACQUISITION		il	n
sw	30487.8	in	n
at	1.300	dp	y
np	79298	hs	nn
fb	17000	PROCESSING	
bs	64	lb	0.50
d1	1.000	fn	not used
nt	2560	DISPLAY	
ct	2432	sp	-123.0
TRANSMITTER		wp	26929.4
tn	C13	rfl	11756.7
sfrq	125.689	rfp	9677.1
tof	1255.3	rp	13.5
tpwr	46	lp	-307.1
pw	6.750	PLOT	
DECOUPLER		wc	250
dn	H1	sc	0
dof	0	vs	80000
dm	yyy	th	68
dmm	w	ai	cdc ph
dpwr	36		
dmf	7200		

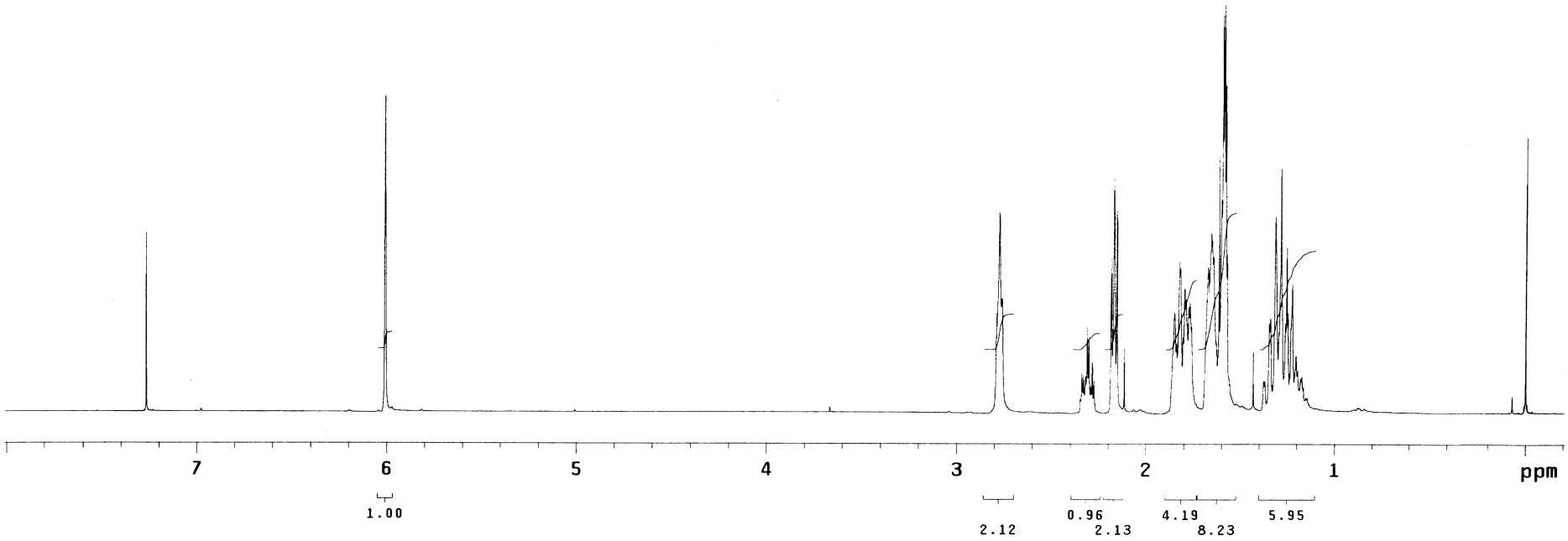
STANDARD 1H OBSERVE - profile
STANDARD 1H OBSERVE - profile

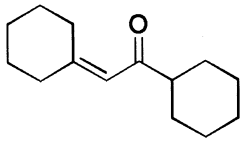
exp1 Proton

SAMPLE		SPECIAL	
date	Oct 4 2006	temp	25.0
solvent	cdcl3	gain	60
file	/mnt/nmr400/w~	spin	not used
alkup/data/Zhang/G~		hst	0.008
uotaoLi/enone-dicy~		pw90	13.900
clohexyl.fid		alfa	6.600
ACQUISITION		**FLAGS**	
sw	6410.3	il	n
at	2.049	in	n
np	26264	dp	y
fb	4000	hs	nn
bs	4	**PROCESSING**	
d1	1.000	lb	0.10
nt	32	fn	65536
ct	32	**DISPLAY**	
TRANSMITTER		sp	-84.9
tn	H1	wp	3287.9
sfrq	399.782	rfl	803.6
tof	399.5	rfp	0
tpwr	59	rp	23.7
pw	6.950	lp	-29.2
DECOUPLER		**PLOT**	
dn	C13	wc	250
dof	0	sc	0
dm	nnn	vs	400
dmm	c	th	3
dpwr	34	ai cdc ph	
dmf	29412		



6f

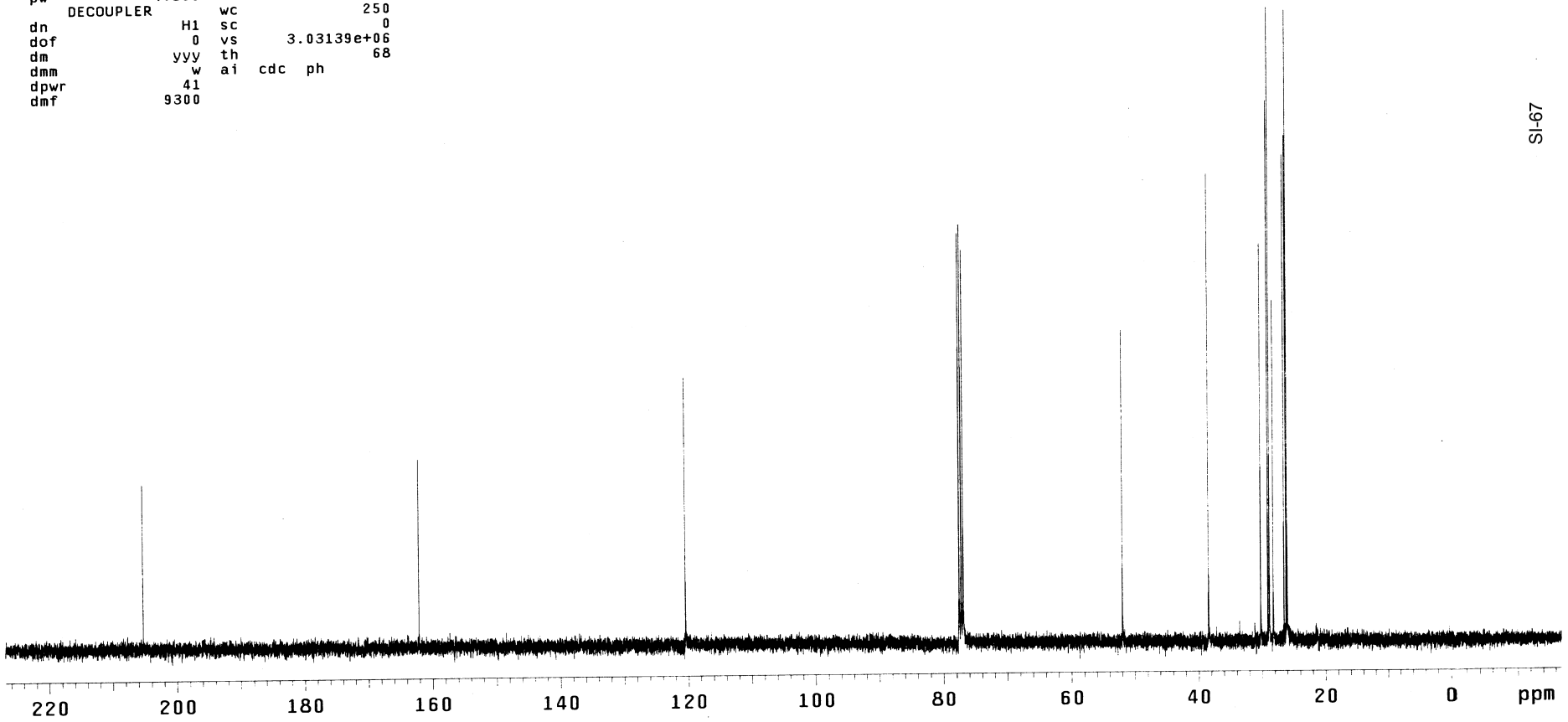




6f

exp1 Carbon

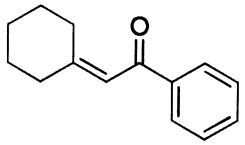
SAMPLE		SPECIAL	
date	Oct 2 2006	temp	25.0
solvent	cdcl3	gain	30
file	/home/walkup/~	spin	not used
	vnmrsys/data/auto_~	hst	0.008
	2006.10.02_22/s_20~	pw90	9.700
	061002_002/data/cd~	alfa	10.000
	cl3_01.fid	FLAGS	
ACQUISITION		il	n
sw	24509.8	in	n
at	1.300	dp	y
np	63750	hs	nn
fb	17000	PROCESSING	
bs	64	lb	0.50
d1	1.000	fn	not used
nt	10240	DISPLAY	
ct	320	sp	-1699.1
TRANSMITTER		wp	24509.1
tn	C13	rfl	1699.8
sfrq	100.535	rfp	0
tof	1042.6	rp	161.7
tpwr	55	lp	-205.7
pw	4.850	PLOT	
DECOUPLER		wc	250
dn	H1	sc	0
dof	0	vs	3.03139e+06
dm	yyy	th	68
dmm	w	ai	cdc ph
dpwr	41		
dmf	9300		



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

exp1 Proton

SAMPLE		SPECIAL	
date	Oct 4 2006	temp	25.0
solvent	cdcl3	gain	60
file	/mnt/nmr400/w~	spin	not used
	alkup/data/Zhang/G~	hst	0.008
	uotaoLi/LM1c-enone~	pw90	13.900
	-from-hexanone-phe~	alfa	6.600
	nylacetylene.fid	FLAGS	
ACQUISITION		il	n
sw	6410.3	in	n
at	2.049	dp	y
np	26264	hs	nn
fb	4000	PROCESSING	
bs	4	lb	0.10
d1	1.000	fn	65536
nt	32	DISPLAY	
ct	32	sp	-187.6
TRANSMITTER		wp	4070.4
tn	H1	rfl	806.0
sfrq	399.782	rfp	0
tof	399.5	rp	25.0
tpwr	59	lp	-33.3
pw	6.950	PLOT	
DECOUPLER		wc	250
dn	C13	sc	0
dof	0	vs	1559
dm	nnn	th	2
dmm	c	ai cdc ph	
dpwr	34		
dmf	29412		



Std proton

exp2 Carbon

SAMPLE		SPECIAL	
date	Oct 4 2006	temp	25.0
solvent	cdcl3	gain	30
file	exp	spin	not used
ACQUISITION		hst	0.008
sw	30487.8	pw90	15.300
at	1.300	alfa	10.000
np	79298	**FLAGS**	
fb	17000	il	n
bs	64	in	n
d1	1.000	dp	y
nt	20480	hs	nn
ct	1088	**PROCESSING**	
TRANSMITTER		lb	0.50
tn	C13	fn	not used
sfrq	125.689	**DISPLAY**	
tof	1255.3	sp	-2076.8
tpwr	49	wp	30487.3
pw	7.650	rfl	11754.4
DECOUPLER		rfp	9677.1
dn	H1	rp	-18.5
dof	0	lp	-312.4
dm	yyy	**PLOT**	
dmm	w	wc	250
dpwr	39	sc	0
dmf	12200	vs	46778
		th	7
		ai cdc ph