



Supporting Information

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**Platinum-Catalyzed Formation of Cyclic
Ketone-Fused Indoles from N-(2-Alkynylphenyl)lactams**

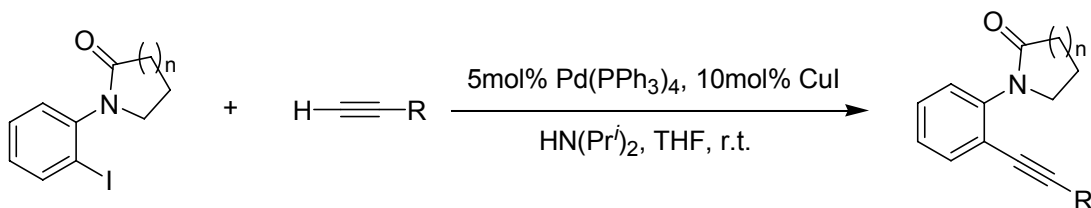
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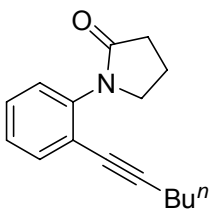
General: Ethyl acetate (ACS grade), hexanes (ACS grade) and diethyl ether (ACS grade) were purchased from Fisher Scientific and used without further purification. Anhydrous tetrahydrofuran and anhydrous dichloromethane in Pure-Pac™ from Aldrich were used directly without further treatment. Commercially available reagents were used without further purification. The NMR data were the same as reported. 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.

The Sonagashira reaction precursors for lactams **7k**, **7l**, and **7m** were prepared according to a known procedure (U. Ladziata, A. Y. Kuposov, K. Y. Lo, J. Willging, V. N. Nemykin, V. V. Zhdankin, *Angew. Chem., Int. Ed.*, **2005**, *44*, 7127) from the corresponding substituted 2-iodoanilines. 2-iodo-6-methoxyaniline (Y. Kondo, S. Kojima, T. Sakamoto, *J. Org. Chem.* **1997**, *62*, 6507), 4-bromo-2-iodoaniline (D. Roche, K. Prasad, O. Repic, T. J. Blacklock, *Tetrahedron Let.*, **2000**, *41*, 2083, and ethyl 4-amino-3-iodobenzate (M. M. Slutsky, T. V. Jones, G. N. Tew, *J. Org. Chem.* **2007**, *72*, 342) were prepared according to literature procedures.

General procedure A: preparation of *N*-(2-Alkynylphenyl) Lactams

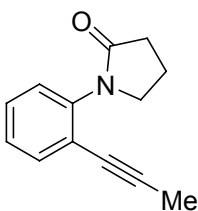


To a solution of the lactam in THF were added sequentially the alkyne (2.0~3.0 eq.), a catalyst [Pd(PPh₃)₄ or PdCl₂(PPh₃)₂, 5 mol %], CuI (10 mol %), and HN(*i*Pr)₂ (4 eq.) at room temperature. The resulting mixture was stirred at room temperature for the time indicated. After all the lactam was consumed, the mixture was concentrated under vacuum, and the resulting residue was purified through silica gel flash column chromatography with hexanes/ethyl acetate (1:1).



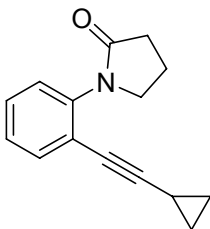
3

Compound **3** was isolated in 97% yield following the general procedure A using $\text{Pd}(\text{PPh}_3)_4$ as catalyst and 2 eq. of 1-hexyne. Reaction time: 2.5 h. ^1H NMR (400MHz, CDCl_3) δ : 7.46 (dd, 1H, $J = 1.6, 7.6$ Hz), 7.33-7.20 (m, 3H), 3.87 (t, 2H, $J = 7.0$ Hz), 2.56 (t, 2H, $J = 8.1$ Hz), 2.43 (t, 2H, $J = 6.1$ Hz), 2.19 (quintet, 2H, $J = 7.5$ Hz), 1.62-1.55 (m, 2H), 1.52-1.43 (m, 2H), 0.95 (t, 3H, $J = 7.3$ Hz); ^{13}C NMR (125 MHz, CDCl_3) δ : 174.7, 140.1, 133.4, 128.4, 127.6, 127.3, 122.1, 95.4, 50.1, 31.4, 30.7, 22.0, 19.2, 19.1, 13.6; IR (neat): 3063, 2928, 2862, 2230, 1699, 1494, 1451, 1404, 1050, 875, 824; MS (ES^+) Calculated for $[\text{C}_{16}\text{H}_{19}\text{NONa}]^+$ 264.1; Found: 263.9.



7a

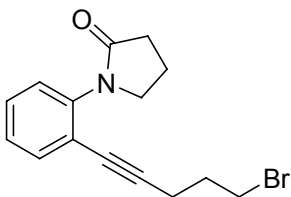
Compound **7a** was isolated in 70% yield following the general procedure A using $\text{Pd}(\text{PPh}_3)_4$ as catalyst and excess of propyne. Reaction time: 12 h. ^1H NMR (500MHz, CDCl_3) δ : 7.46 (dd, 1H, $J = 1.5, 8.0$ Hz), 7.33-7.21 (m, 3H), 3.87 (t, 2H, $J = 7.0$ Hz), 2.57 (t, 2H, $J = 7.0$ Hz), 2.18 (quintet, 2H, $J = 7.0$ Hz), 2.08 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ : 174.8, 140.2, 133.4, 128.5, 127.6, 127.3, 121.9, 90.8, 76.4, 50.2, 31.5, 19.3, 4.5; IR (neat): 2925, 2253, 1688, 1607, 1493, 1451, 1050, 824; MS (ES^+) Calculated for $[\text{C}_{13}\text{H}_{13}\text{NONa}]^+$: 222.0; Found: 221.8.



7b

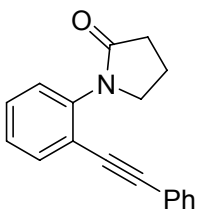
Compound **7b** was isolated in 85% yield following the general procedure A using $\text{Pd}(\text{PPh}_3)_4$ as catalyst and 2 eq. of ethynylcyclopropane. Reaction time: 3 h. ^1H NMR

(400MHz, CDCl₃) δ : 7.44 (dd, 1H, J = 1.2, 7.6 Hz), 7.32~7.18 (m, 3H), 3.85 (t, 2H, J = 7.2 Hz), 2.56 (t, 2H, J = 7.6 Hz), 2.23~2.15 (m, 2H), 1.48~1.42 (m, 1H), 0.91~0.86 (m, 2H), 0.79~0.75 (m, 2H); ¹³C NMR (125 MHz, CDCl₃) δ : 174.7, 140.2, 133.2, 128.4, 127.5, 127.2, 121.8, 98.6, 72.3, 50.1, 31.5, 19.2, 8.7, 0.26; IR (neat): 2926, 2229, 1700, 1596, 1493, 1450, 1403, 1304, 1257, 1050, 957, 874, 824; MS (ES⁺) Calculated for [C₁₅H₁₅NONa]⁺ 248.1; Found: 248.1.



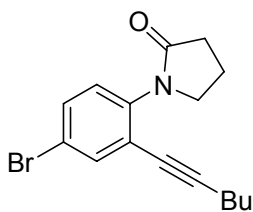
7c

Compound **7c** was isolated in quantitative yield following the general procedure A using Pd(PPh₃)₄ as catalyst and 3 eq. of 5-bromo-1-pentyne. Reaction time: 3 h. ¹H NMR (400MHz, CDCl₃) δ : 7.46 (dd, 1H, J = 7.6, 1.6 Hz), 7.35~7.31 (m, 1H), 7.26~7.21 (m, 2H), 3.86 (t, 2H, J = 6.8 Hz), 3.59 (t, 2H, J = 6.4 Hz), 2.64 (t, 2H, J = 6.8 Hz), 2.59 (t, 2H, J = 8.4 Hz), 2.26~2.21 (m, 2H), 2.15~2.08 (m, 2H); ¹³C NMR (125 MHz, CDCl₃) δ : 174.7, 140.3, 133.5, 128.8, 127.5, 127.4, 121.6, 92.8, 78.4, 50.3, 32.4, 31.4, 31.3, 19.2, 18.2; IR (neat): 3016, 2925, 1699, 1607, 1494, 1451, 1050, 875, 824; MS (ES⁺) Calculated for [C₁₅H₁₆BrNONa]⁺ 328.0; Found: 328.0.



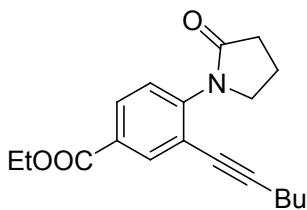
7e

Compound **7e** was isolated in 71% yield following the general procedure A using Pd(PPh₃)₂Cl₂ as catalyst and 2 eq. of phenylacetylene. Reaction time: 4h. ¹H NMR (400MHz, CDCl₃) δ : 7.60 (dd, 1H, J = 1.6, 7.6 Hz), 7.51~7.47 (m, 2H), 7.41~7.27 (m, 6H), 3.95 (t, 2H, J = 6.9 Hz), 2.60 (t, 2H, J = 8.0 Hz), 2.27~2.19 (m, 2H); ¹³C NMR (125 MHz, CDCl₃) δ : 174.8, 140.3, 133.3, 131.4, 129.3, 128.6, 128.4, 127.7, 127.4, 123.0, 121.2, 94.2, 86.0, 50.3, 31.5, 19.3; IR (neat): 3063, 2926, 2861, 1698, 1497, 1448, 1404, 1050, 875, 824; MS (ES⁺) Calculated for [C₁₈H₁₅NONa]⁺ 284.1; Found: 283.9.



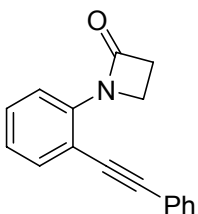
7l

Compound **7l** was isolated in 77% yield following the general procedure A using $\text{Pd}(\text{PPh}_3)_2\text{Cl}_2$ as catalyst and 2 eq. of 1-hexyne. Reaction time: 2h. ^1H NMR (400MHz, CDCl_3) δ : 7.59 (d, 1H, $J = 2.4$ Hz), 7.20 (dd, 1H, $J = 8.4, 2.4$ Hz), 7.13 (d, 1H, $J = 8.4$ Hz), 3.85 (t, 2H, $J = 6.8$ Hz), 2.55 (t, 2H, $J = 8.0$ Hz), 2.43 (t, 2H, $J = 7.2$ Hz), 2.19 (quintet, 2H, $J = 7.6$ Hz), 1.61-1.54 (m, 2H), 1.51-1.42 (m, 2H), 0.95 (t, 3H, $J = 7.2$ Hz); ^{13}C NMR (125 MHz, CDCl_3) δ : 174.8, 139.1, 136.0, 131.6, 129.0, 123.9, 120.5, 97.1, 76.1, 49.9, 31.3, 30.6, 22.0, 19.2, 19.1, 13.6; IR (neat): 2928, 2862, 2226, 1699, 1489, 1455, 1404, 1304, 1050, 876, 824; MS (ES^+) Calculated for $[\text{C}_{16}\text{H}_{18}\text{BrNONa}]^+$ 342.1; Found: 341.8.

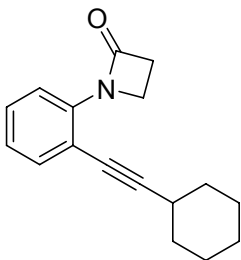


7m

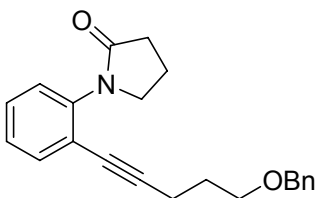
Compound **7m** was isolated in 80% yield following the general procedure A using $\text{Pd}(\text{PPh}_3)_2\text{Cl}_2$ as catalyst and 2 eq. of 1-hexyne. Reaction time: 2h. ^1H NMR (400MHz, CDCl_3) δ : 8.13 (d, 1H, $J = 2.0$ Hz), 7.96 (dd, 1H, $J = 8.4, 1.6$ Hz), 7.37 (d, 1H, $J = 8.4$ Hz), 4.37 (q, 2H, $J = 7.2$ Hz), 3.93 (t, 2H, $J = 7.2$ Hz), 2.58 (t, 2H, $J = 8.0$ Hz), 2.45 (t, 2H, $J = 7.2$ Hz), 2.21 (quintet, 2H, $J = 7.6$ Hz), 1.63-1.56 (m, 2H), 1.52-1.45 (m, 2H), 1.40 (t, 3H, $J = 7.2$ Hz), 0.95 (t, 3H, $J = 7.2$ Hz); ^{13}C NMR (100 MHz, CDCl_3) δ : 174.7, 165.5, 143.9, 134.9, 129.4, 129.2, 127.3, 121.7, 96.7, 76.8, 61.2, 49.8, 31.5, 30.6, 22.0, 19.3, 14.3, 13.6; IR (neat): 2927, 1715, 1604, 1495, 1452, 1229, 1097, 1050, 875, 824; MS (ES^+) Calculated for $[\text{C}_{19}\text{H}_{23}\text{NO}_3\text{Na}]^+$ 336.2; Found: 335.8.



This compound was isolated in quantitative yield following the general procedure A using $\text{Pd}(\text{PPh}_3)_4$ as catalyst and 2 eq. of phenylacetylene. Reaction time: 3 h. ^1H NMR (500MHz, CDCl_3) δ : 8.09 (d, 1H, $J = 8.5$ Hz), 7.51~7.47 (m, 3H), 7.38~7.35 (m, 3H), 7.30 (t, 1H, $J = 7.5$ Hz), 7.07 (t, 1H, $J = 7.5$ Hz), 4.25 (t, 2H, $J = 4.5$ Hz), 3.13 (t, 2H, $J = 4.5$ Hz); ^{13}C NMR (125 MHz, CDCl_3) δ : 166.1, 139.1, 134.0, 131.1, 129.4, 128.6, 128.5, 123.9, 123.0, 120.9, 111.4, 93.7, 86.8, 42.3, 37.4; IR (neat): 2926, 2253, 1746, 1607, 1494, 1451, 1050, 824; MS (ES^+) Calculated for $[\text{C}_{17}\text{H}_{13}\text{NONa}]^+$ 270.1; Found: 270.3.



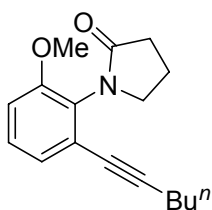
This compound was isolated in 75% yield following the general procedure A using $\text{Pd}(\text{PPh}_3)_4$ as catalyst and 2 eq. of cyclohexylacetylene. Reaction time: 3 h. ^1H NMR (400MHz, CDCl_3) δ : 8.01 (d, 1H, $J = 8.0$ Hz), 7.49 (d, 1H, $J = 8.0$ Hz), 7.22 (t, 1H, $J = 8.0$ Hz), 6.99 (t, 1H, $J = 8.0$ Hz), 4.15 (t, 2H, $J = 4.4$ Hz), 3.09 (t, 2H, $J = 4.4$ Hz), 2.60~2.50 (m, 1H), 1.96~1.87 (m, 2H), 1.80~1.70 (m, 2H), 1.62~1.46 (m, 3H), 1.42~1.30 (m, 3H). ^{13}C NMR (125 MHz, CDCl_3) δ : 166.1, 138.8, 134.3, 128.4, 123.9, 120.9, 112.6, 98.9, 77.7, 42.2, 37.2, 32.4, 30.0, 25.8, 25.0. IR (neat): 2927, 2253, 1738, 1607, 1494, 1451, 1050, 907, 824, 732; MS (ES^+) Calculated for $[\text{C}_{17}\text{H}_{19}\text{NONa}]^+$ 276.1; Found: 276.1.



7d

A solution of *N*-(2-iodophenyl)- γ -lactam (0.143g, 0.5 mmol) and 5-benzyloxy-1-pentyne (0.174g, 1 mmol) in piperidines (2 mL) was added $\text{Pd}(\text{PPh}_3)_2\text{Cl}_2$ (11 mg, 0.015 mmol) and CuI (6 mg, 0.03 mmol). The resulting mixture was heated to 70°C, and the reaction

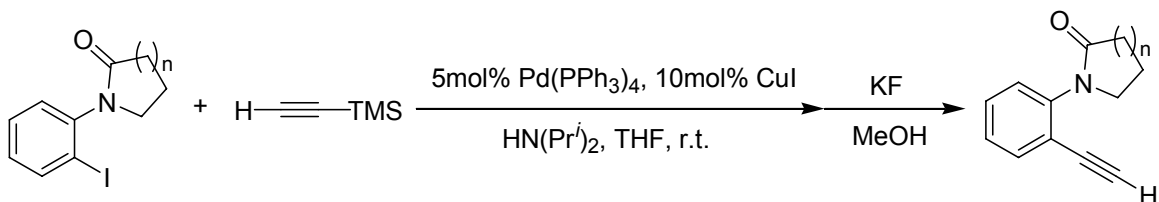
finished in 30 min. The resulting mixture was concentrated, and the residue was purified via silica gel flash column chromatography to give compound **7d** in 96% yield. ^1H NMR (500MHz, CDCl_3) δ : 7.43 (dd, 1H, $J = 7.7, 1.3$ Hz), 7.34~7.19 (m, 8H), 4.52 (s, 2H), 3.83 (t, 2H, $J = 7.0$ Hz), 3.61 (t, 2H, $J = 6.3$ Hz), 2.56~2.52 (m, 4H), 2.17~2.11 (m, 2H), 1.92~1.87 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ : 174.6, 140.0, 138.3, 133.3, 128.5, 128.3, 127.5, 127.5, 127.5, 127.5, 127.2, 121.8, 94.6, 77.5, 72.9, 68.7, 50.1, 31.4, 28.9, 19.1, 16.4; IR (neat): 3020, 1686, 1494, 1451, 1216, 1050, 875, 824; MS (ES^+) Calculated for $[\text{C}_{22}\text{H}_{33}\text{NO}_2\text{Na}]^+$ 356.2; Found: 356.1.



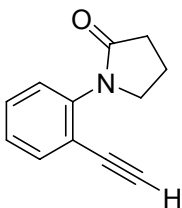
7k

A solution of *N*-(6-methoxy-2-iodophenyl)- γ -lactam (0.200g, 0.63 mmol) and 1-hexyne (0.103g, 1.26 mmol) in piperidines (2 mL) was added $\text{Pd}(\text{PPh}_3)_2\text{Cl}_2$ (13 mg, 0.019 mmol) and CuI (12 mg, 0.063 mmol) under N_2 . The resulting mixture was heated to 70°C , and the reaction finished in 30 min. The resulting mixture was concentrated, and the residue was purified via silica gel flash column chromatography to give compound **7k** in 68% yield. ^1H NMR (400MHz, CDCl_3) δ : 7.19 (t, 1H, $J = 8.0$ Hz), 7.04 (dd, 1H, $J = 7.6, 1.2$ Hz), 6.87 (dd, 1H, $J = 8.4, 0.8$ Hz), 3.80 (s, 3H), 3.75-3.61 (m, 2H), 2.61-2.45 (m, 2H), 2.40 (t, 2H, $J = 7.2$ Hz), 2.27-2.12 (m, 2H), 1.60-1.42 (m, 4H), 0.94 (t, 3H, $J = 7.2$ Hz); ^{13}C NMR (100 MHz, CDCl_3) δ : 174.6, 155.6, 128.5, 128.4, 124.5, 124.5, 111.3, 94.4, 76.8, 55.7, 48.8, 30.9, 30.6, 21.8, 19.2, 19.0, 13.4; IR (neat): 2932, 2862, 2230, 1704, 1574, 1472, 1296, 1100, 1051, 1015, 875, 824; MS (ES^+) Calculated for $[\text{C}_{17}\text{H}_{21}\text{NO}_2\text{Na}]^+$ 294.2; Found: 294.2.

General procedure B: preparation of ethynyl lactams

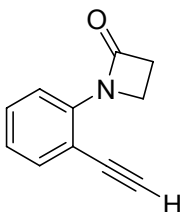


To a solution of the lactam and (trimethylsilyl)acetylene (1.5 eq.) in THF were added $\text{PdCl}_2(\text{PPh}_3)_2$ (0.05 eq.), CuI (0.1 eq.), and $\text{HN}(\text{iPr})_2$ (5.0 eq.). The resulting mixture was stirred at room temperature for 2.5 h. When the lactam was consumed, the mixture was concentrated under vacuum. The resulting residue was dissolved in MeOH and treated with $\text{KF}\cdot\text{H}_2\text{O}$ (3eq.) at room temperature for 10h. The reaction mixture was concentrated under vacuum, and the residue was purified through silica gel flash column chromatography with hexanes/ethyl acetate (1:1).



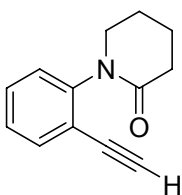
7j

Compound **7j** was isolated in 73% yield following the general procedure B. ^1H NMR (400MHz, CDCl_3) δ : 7.56 (dd, 1H, J = 1.4, 7.6 Hz), 7.42-7.38 (m, 1H), 7.30-7.24 (m, 2H), 3.88 (t, 2H, J = 7.0 Hz), 3.28 (s, 1H), 2.57 (t, 2H, J = 8.0 Hz), 2.24-2.17 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ : 174.8, 140.8, 134.0, 129.8, 127.6, 127.3, 82.0, 80.3, 50.2, 31.4, 19.1; IR (neat): 3220, 3063, 2926, 2103, 1699, 1491, 1449, 1405, 1306, 1119, 1050, 875, 824; MS (ES^+) Calculated for $[\text{C}_{12}\text{H}_{11}\text{NONa}]^+$ 208.1; Found: 208.0.



10

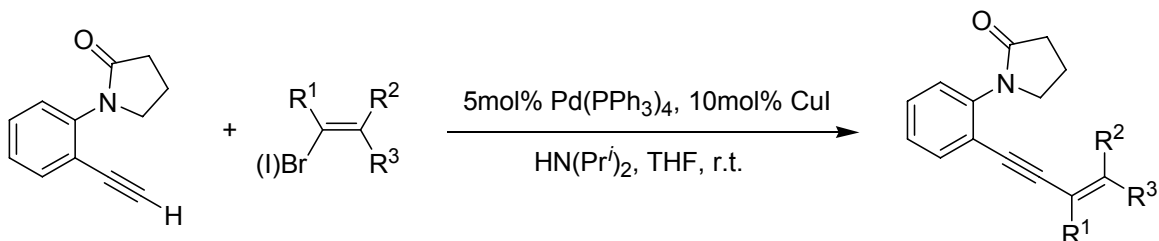
Compound **9** was isolated in 80% yield following the general procedure B. ^1H NMR (400MHz, CDCl_3) δ : 8.05 (d, 1H, J = 8.4 Hz), 7.44 (d, 1H, J = 7.6 Hz), 7.32 (t, 1H, J = 7.2 Hz), 7.04 (t, 1H, J = 7.6 Hz), 4.17 (t, 2H, J = 4.8 Hz), 3.28 (s, 1H), 3.11 (t, 2H, J = 4.8 Hz); ^{13}C NMR (125 MHz, CDCl_3) δ : 166.1, 139.7, 134.8, 129.8, 123.9, 120.9, 110.3, 82.2, 81.1, 42.2, 37.2; IR (neat): 2253, 1746, 1596, 1492, 1446, 1363, 1050, 907, 730; MS (ES^+) Calculated for $[\text{C}_{11}\text{H}_9\text{NONa}]^+$ 194.1; Found 194.0.



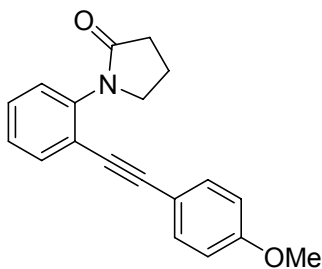
12

Compound **12** was isolated in 53% yield following the general procedure B. ^1H NMR (500MHz, CDCl_3) δ : 7.58 (d, 1H, $J = 7.5$ Hz), 7.40 (t, 1H, $J = 7.5$ Hz), 7.28 (t, 1H, $J = 7.5$ Hz), 7.22 (d, 1H, $J = 7.5$ Hz), 3.61 (bs, 2H), 3.22 (s, 1H), 2.57 (t, 2H, $J = 6.5$ Hz), 1.99~1.92 (m, 4H); ^{13}C NMR (125 MHz, CDCl_3) δ : 169.9, 145.4, 133.9, 130.1, 128.1, 127.4, 120.9, 81.2, 80.2, 51.2, 32.7, 23.5, 21.4; IR (neat): 2926, 2253, 1607, 1494, 1451, 1050, 907, 732; MS (ES^+) Calculated for $[\text{C}_{13}\text{H}_{13}\text{NONa}]^+$:222.0; Found: 221.7.

General procedure C: preparation of lactam with alkenyl or aryl substituents at its alkyne terminus



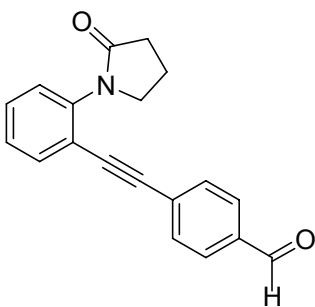
To a solution of alkyne **7j** (1.0 eq.) and an alkenyl/aryl halide (2.0eq.) were added a catalyst $[\text{Pd}(\text{PPh}_3)_4$ or $\text{PdCl}_2(\text{PPh}_3)_2$, 5 mol %), CuI (10 mol %), and $\text{HN}(\text{iPr})_2$ (3.0~5.0 eq.). The resulting mixture was stirred at room temperature for the indicated time. After **7j** was consumed, the reaction mixture was concentrated under vacuum. The residue was purified through silica gel flash column chromatography with hexanes/ethyl acetate (1:1).



7f

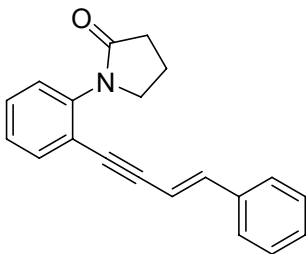
Compound **7f** was isolated in 97% yield following the general procedure C using $\text{Pd}(\text{PPh}_3)_4$ as catalyst and 2 eq. of 4-iodoanisole. Reaction time: 5 h. ^1H NMR (400MHz,

CDCl₃) δ : 7.57 (dd, 1H, J = 1.2, 8.0 Hz), 7.44~7.26 (m, 5H), 6.90~6.86 (m, 2H), 3.95 (t, 2H, J = 6.8 Hz), 3.83 (s, 3H), 2.59 (t, 2H, J = 7.6 Hz), 2.26~2.18 (m, 2H); ¹³C NMR (125 MHz, CDCl₃) δ : 174.8, 159.8, 140.1, 133.1, 132.9, 128.9, 127.7, 127.3, 121.5, 115.1, 114.1, 94.3, 84.8, 55.3, 50.3, 31.6, 19.3; IR (neat): 2926, 2212, 1699, 1606, 1512, 1494, 1451, 1403, 1250, 1050, 875, 824; MS (ES⁺) Calculated for [C₁₉H₁₇NONa]⁺ 314.1; Found: 314.1.



7g

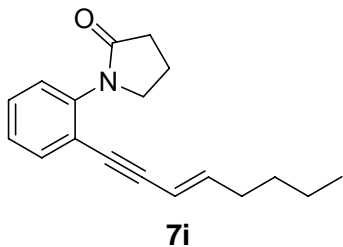
Compound **7g** was isolated in 80% yield following the general procedure C using Pd(PPh₃)₂Cl₂ as catalyst and 2 eq. of 4-bromobenzaldehyde. Reaction time: 2.5 h. ¹H NMR (400MHz, CDCl₃) δ : 10.03 (s, 1H), 7.88 (d, 2H, J = 8.8 Hz), 7.65~7.62 (m, 3H), 7.46~7.43 (m, 1H), 7.36~7.33 (m, 2H), 3.95 (t, 2H, J = 6.8 Hz), 2.62 (t, 2H, J = 8.0 Hz), 2.29~2.21 (m, 2H); ¹³C NMR (125 MHz, CDCl₃) δ : 191.3, 174.7, 140.6, 135.7, 133.5, 131.9, 130.0, 129.6, 129.2, 127.6, 127.5, 120.5, 93.1, 90.1, 50.5, 31.5, 19.4; IR (neat): 2925, 2216, 1699, 1601, 1494, 1451, 1403, 1050, 875, 824; MS (ES⁺) Calculated for [C₁₉H₁₅NONa]⁺ 312.1; Found: 311.9.



7h

Compound **7h** was isolated in 97% yield following the general procedure C using Pd(PPh₃)₄ as catalyst and 2 eq. of β -bromostyrene. Reaction time: 4h. ¹H NMR (400MHz, CDCl₃) δ : 7.54 (dd, 1H, J = 1.2, 7.6 Hz), 7.44~7.24 (m, 8H), 6.96 (d, 1H, J = 16.0 Hz), 6.38 (d, 1H, J = 16.0 Hz), 3.92 (t, 2H, J = 6.8 Hz), 2.61 (t, 2H, J = 8.0 Hz), 2.27~2.20 (m, 2H); ¹³C NMR (125 MHz, CDCl₃) δ : 174.8, 141.6, 140.2, 136.1, 133.3, 129.2, 128.8, 128.7, 127.6, 127.3, 126.4, 121.3, 107.8, 93.7, 88.3, 50.3, 31.5, 19.3; IR (neat): 2925,

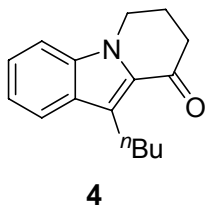
2195, 1699, 1607, 1492, 1451, 1403, 1050, 875, 824; MS (ES⁺) Calculated for [C₂₀H₁₇NONa]⁺ 310.1; Found: 310.0.



Compound **7i** was isolated in 99% yield following the general procedure C using Pd(PPh₃)₄ as catalyst and 2 eq. of 1-iodo-1-hexene. Reaction time: 2.5 h. ¹H NMR (400MHz, CDCl₃) δ: 7.48 (d, 1H, *J* = 7.6 Hz), 7.35~7.21 (m, 3H), 6.21 (dt, 1H, *J* = 7.2, 15.6 Hz), 5.68 (dt, 1H, *J* = 1.6, 15.6 Hz), 3.88 (t, 2H, *J* = 6.8 Hz), 2.57 (t, 2H, *J* = 6.8 Hz), 2.24~2.13 (m, 4H), 1.46~1.30 (m, 4H), 0.91 (t, 3H, *J* = 7.2 Hz); ¹³C NMR (125 MHz, CDCl₃) δ: 174.8, 145.7, 140.1, 133.2, 128.8, 127.6, 127.3, 121.5, 109.4, 93.3, 84.4, 50.2, 32.9, 31.5, 30.8, 22.2, 19.3, 13.8; IR (neat): 2926, 2253, 1681, 1607, 1493, 1451, 1050, 824; MS (ES⁺) Calculated for [C₁₃H₁₃NONa]⁺ 290.1; Found: 290.3.

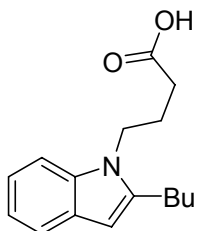
General procedure D: PtCl₄/PtCl₂-catalyzed reaction of lactams

To a 0.01 M solution of the lactam in anhydrous 1,2-dichloroethane was added 10 mol % of PtCl₄ or PtCl₂ (if specified) under an atmosphere of O₂. The resulting mixture was refluxing for the indicated time. Upon the completion of the reaction, the solvent was removed under vacuum, and the residue was purified via silica gel flash column chromatography (eluent: hexanes/ethyl acetate = 3:1) to yield the desired product.



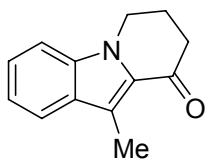
Compound **4** was isolated in 83% yield following the general procedure D. Reaction time: 1 h. ¹H NMR (400MHz, CDCl₃) δ: 7.73 (dt, 1H, *J* = 8.0, 0.8 Hz), 7.40~7.30 (m, 2H), 7.14 (dd, 1H, *J* = 6.8, 1.2 Hz), 4.22 (t, 2H, *J* = 6.0 Hz), 3.18 (t, 2H, *J* = 8.0 Hz), 2.72 (t, 2H, *J* = 6.4 Hz), 2.39~2.33 (m, 2H), 1.68~1.61 (m, 2H), 1.46~1.37 (m, 2H), 0.93 (t, 3H, *J* = 7.2 Hz); ¹³C NMR (125 MHz, CDCl₃) δ: 191.1, 136.3, 129.1, 126.9, 125.9, 125.2, 121.6,

120.1, 110.1, 41.5, 38.1, 32.9, 24.6, 23.1, 22.8, 14.0; IR (neat): 3016, 2926, 2860, 1669, 1495, 1050, 875, 824; MS (ES⁺) Calculated for [C₁₆H₁₉NONa]⁺ 264.1; Found: 264.3.



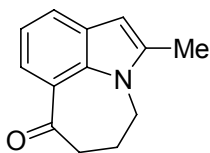
6

Compound **6** was isolated as the side product during the reaction of **3**. ¹H NMR (500MHz, CDCl₃) δ: 7.51 (d, 1H, *J* = 7.6 Hz), 7.27 (d, 1H, *J* = 8.0 Hz), 7.14-7.10 (m, 1H), 7.07-7.03 (m, 1H), 7.25 (d, 1H, *J* = 0.8 Hz), 4.14 (t, 2H, *J* = 7.6 Hz), 2.71 (t, 2H, *J* = 7.6 Hz), 2.41 (t, 2H, *J* = 7.2 Hz), 2.08 (quintet, 2H, *J* = 7.2 Hz), 1.76-1.69 (m, 2H), 1.46 (sextet, 2H, *J* = 7.6 Hz), 0.97 (t, 3H, *J* = 7.2 Hz); ¹³C NMR (100 MHz, CDCl₃) δ: 177.8, 140.9, 136.5, 128.2, 120.6, 119.8, 119.3, 108.9, 99.1, 41.9, 30.7, 30.7, 26.3, 24.9, 22.6, 13.9; IR (neat): 2926, 2861, 1706, 1699, 1608, 1495, 1452, 1258, 1232, 1050, 875, 824; MS (ES⁺) Calculated for [C₁₆H₂₁NONa]⁺ 282.2; Found: 282.0.



8a

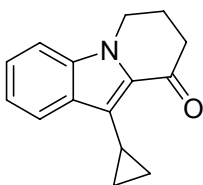
Compound **8a** was isolated in 83% yield following the general procedure D. Reaction time: 1.5 h. ¹H NMR (400MHz, CDCl₃) δ: 7.70 (d, 1H, *J* = 8.4 Hz), 7.40~7.25 (m, 2H), 7.15 (t, 1H, *J* = 6.8 Hz), 4.19 (t, 2H, *J* = 5.6 Hz), 2.72 (t, 2H, *J* = 6.4 Hz), 2.68 (s, 3H), 2.38~2.32 (m, 2H); ¹³C NMR (125 MHz, CDCl₃) δ: 191.4, 136.3, 129.4, 127.3, 125.9, 121.4, 120.1, 119.7, 110.0, 41.4, 37.9, 23.1, 120.3; IR (neat): 2926, 2253, 1661, 1539, 1494, 1452, 1376, 1332, 1234, 1107, 1050, 824; MS (ES⁺) Calculated for [C₁₃H₁₃NONa]⁺ 222.0; Found: 221.7.



9a

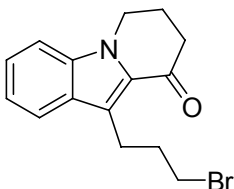
Compound **9a** was isolated as the side product during the reaction of **7a**. ¹H NMR (500MHz, CDCl₃) δ: 7.95 (dd, 1H, *J* = 1.0, 7.5 Hz), 7.72 (dd, 1H, *J* = 1.0, 7.5 Hz), 7.13 (t,

1H, $J = 7.5$ Hz), 6.39 (s, 1H), 4.24~4.22 (m, 2H), 3.12~3.09 (m, 2H), 2.45 (s, 3H), 2.37~2.32 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ : 198.9, 137.6, 134.6, 130.2, 125.7, 124.1, 120.6, 118.9, 101.5, 47.7, 44.6, 21.7, 13.6; IR (neat): 2925, 1660, 1607, 1494, 1451, 1261, 1050, 875, 824; MS (ES^+) Calculated for $[\text{C}_{13}\text{H}_{13}\text{NONa}]^+$ 222.1; Found: 222.0.



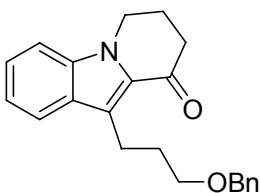
8b

Compound **8b** was isolated in 71% yield following the general procedure D. Reaction time: 14 h. ^1H NMR (400MHz, CDCl_3) δ : 7.66 (d, 1H, $J = 5.2$ Hz), 7.35~7.24 (m, 2H), 7.06 (dd, 1H, $J = 6.8, 1.6$ Hz), 4.16 (t, 2H, $J = 5.6$ Hz), 2.97~2.90 (m, 1H), 2.73 (t, 2H, $J = 6.4$ Hz), 2.36~2.30 (m, 2H), 1.16~1.06 (m, 4H); ^{13}C NMR (125 MHz, CDCl_3) δ : 190.9, 136.5, 130.4, 125.8, 125.7, 125.0, 122.4, 120.1, 110.3, 41.4, 38.1, 22.9, 8.9, 7.9; IR (neat): 3012, 2926, 1661, 1532, 1336, 1193, 1114, 1049, 1024, 875, 824; MS (ES^+) Calculated for $[\text{C}_{15}\text{H}_{15}\text{NONa}]^+$ 248.1; Found: 247.8.



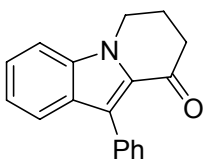
8c

Compound **8c** together with the corresponding chloride was isolated as an inseparable mixture in a combined 88% yield following the general procedure D. Reaction time: 11 h. ^1H NMR (500MHz, CDCl_3) δ : 7.79 (d, 1H, $J = 8.1$ Hz), 7.41~7.38 (m, 1H), 7.34~7.32 (m, 1H), 7.19~7.15 (m, 1H), 4.22 (t, 2H, $J = 5.9$ Hz), 3.44 (t, 2H, $J = 6.8$ Hz), 3.31 (t, 2H, $J = 7.2$ Hz), 2.72 (t, 2H, $J = 6.5$ Hz), 2.39~2.34 (m, 2H), 2.28~2.22 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ : 191.1, 136.2, 129.2, 126.9, 126.8, 126.1, 122.7, 122.6, 121.4, 121.4, 120.5, 120.5, 110.2, 110.2, 45.0, 41.5, 37.9, 33.9, 33.6, 33.3, 23.4, 23.0, 22.1; IR (neat): 2927, 2254, 1664, 1536, 1494, 1452, 1050, 908, 824; MS (ES^+) Calculated for $[\text{C}_{15}\text{H}_{16}\text{BrNONa}]^+$ 328.0; Found: 328.2; for $[\text{C}_{15}\text{H}_{16}\text{ClrNONa}]^+$ 284.1, Found: 283.8.



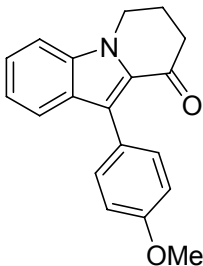
8d

Compound **8d** was isolated in 81% yield following the general procedure D. Reaction time: 2 h. ^1H NMR (400MHz, CDCl_3) δ : 7.75 (d, 1H, J = 8.4 Hz), 7.39~7.24 (m, 7H), 7.15~7.11 (m, 1H), 4.49 (s, 2H), 4.19 (t, 2H, J = 6.0 Hz), 3.53 (t, 2H, J = 6.4 Hz), 3.27 (t, 2H, J = 7.6 Hz), 2.70 (t, 2H, J = 6.4 Hz), 2.37~2.31 (m, 2H), 2.05~1.98 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ : 191.0, 138.8, 136.2, 129.1, 128.3, 127.6, 127.3, 127.0, 126.0, 124.2, 121.6, 120.3, 110.1, 72.7, 70.1, 41.4, 37.9, 30.4, 23.0, 21.4; IR (neat): 2927, 2253, 1663, 1536, 1495, 1453, 1108, 908, 824; MS (ES^+) Calculated for $[\text{C}_{22}\text{H}_{33}\text{NO}_2\text{Na}]^+$ 356.2; Found: 356.0.



8e

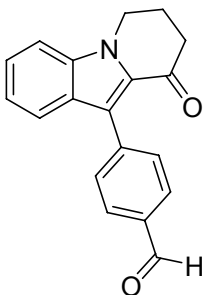
Compound **8e** was isolated in 64% yield following the general procedure D. Reaction time: 23 h. ^1H NMR (400MHz, CDCl_3) δ : 7.71 (d, 1H, J = 8.0 Hz), 7.60 (d, 2H, J = 7.2 Hz), 7.48~7.34 (m, 5H), 7.17 (dd, 1H, J = 1.2, 6.0 Hz), 4.32 (t, 2H, J = 5.6 Hz), 2.76 (t, 2H, J = 6.0 Hz), 2.48~2.38 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ : 189.7, 136.5, 133.5, 130.5, 128.3, 127.8, 127.3, 126.7, 126.2, 123.1, 122.5, 121.3, 110.2, 41.8, 38.1, 22.9; IR (neat): 2317, 1674, 1494, 1457, 1052, 874, 824; MS (ES^+) Calculated for $[\text{C}_{18}\text{H}_{15}\text{NONa}]^+$ 284.1; Found: 284.3.



8f

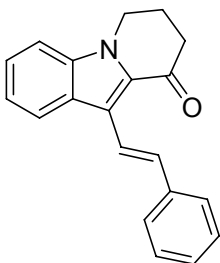
Compound **8f** was isolated in 73% yield following the general procedure D. Reaction time: 11 h. ^1H NMR (500MHz, CDCl_3) δ : 7.71 (d, 1H, J = 8.0 Hz), 7.56~7.53 (m, 2H),

7.42~7.37 (m, 2H), 7.16 (t, 1H, $J = 8.0$ Hz), 7.01~6.98 (m, 2H), 4.29 (t, 2H, $J = 6.0$ Hz), 3.87 (s, 3H), 2.74 (t, 2H, $J = 6.0$ Hz), 2.43~2.38 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ : 189.8, 158.8, 136.5, 131.6, 128.2, 126.7, 126.1, 125.7, 122.9, 122.5, 121.1, 113.4, 110.1, 55.2, 41.8, 38.1, 22.9; IR (neat): 2926, 2253, 1669, 1608, 1494, 1451, 1248, 1050, 824; MS (ES^+) Calculated for $[\text{C}_{19}\text{H}_{17}\text{NONa}]^+$ 314.1; Found: 314.0.



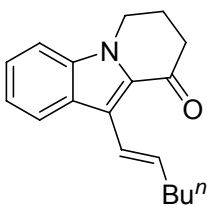
8g

Compound **8g** was isolated in 70% yield following the general procedure D. Reaction time: 34 h. ^1H NMR (400MHz, CDCl_3) δ : 10.06 (s, 1H), 7.96~7.94 (m, 2H), 7.77~7.75 (m, 2H), 7.69~7.68 (m, 2H), 7.47~7.41 (m, 2H), 7.23~7.19 (m, 1H), 4.33 (t, 2H, $J = 5.6$ Hz), 2.76 (t, 2H, $J = 6.0$ Hz), 2.47~2.41 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ : 192.1, 189.8, 140.3, 136.5, 135.0, 131.2, 129.3, 128.5, 126.4, 126.3, 121.9, 121.8, 121.3, 110.4, 41.9, 37.9, 22.8; IR (neat): 3049, 2925, 1694, 1673, 1602, 1495, 1451, 1403, 1331, 1208, 1094, 1050, 942, 875, 823; MS (ES^+) Calculated for $[\text{C}_{19}\text{H}_{15}\text{NONa}]^+$ 312.1; Found: 311.9.



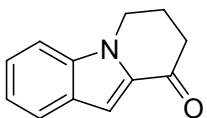
8h

Compound **8h** was isolated in 60% yield following the general procedure D. Reaction time: 14 h. ^1H NMR (400MHz, CDCl_3) δ : 8.27 (d, 1H, $J = 16.8$ Hz), 8.18 (d, 1H, $J = 8.0$ Hz), 7.62 (d, 1H, $J = 7.6$ Hz), 7.45~7.35 (m, 2H), 7.27~7.23 (m, 1H), 4.24 (t, 2H, $J = 5.6$ Hz), 2.77 (t, 2H, $J = 6.0$ Hz), 2.42~2.35 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ : 190.9, 138.2, 137.1, 131.6, 129.4, 128.6, 127.4, 126.5, 126.2, 124.6, 123.3, 122.5, 121.6, 120.2, 110.5, 41.6, 38.0, 22.8; IR (neat): 3055, 2927, 2246, 1661, 1596, 1510, 1494, 1448, 1408, 1367, 1336, 1303, 1276, 1247, 1194, 1109, 1010, 956, 909, 875, 824; MS (ES^+) Calculated for $[\text{C}_{20}\text{H}_{17}\text{NONa}]^+$ 310.1; Found: 310.0.



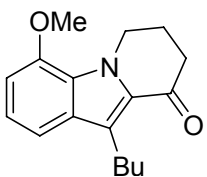
8i

Compound **8i** was isolated in 52% yield following the general procedure D. Reaction time: 48 h. ^1H NMR (400MHz, CDCl_3) δ : 8.02 (d, 1H, J = 8.4 Hz), 7.44~7.25 (m, 3H), 7.20~7.16 (m, 1H), 6.53 (dt, 1H, J = 7.2, 16.4 Hz), 4.21 (t, 2H, J = 6.0 Hz), 2.73 (t, 2H, J = 6.4 Hz), 2.39~2.31 (m, 4H), 1.56~1.51 (m, 2H), 1.47~1.38 (m, 2H), 0.95 (t, 3H, J = 7.2 Hz); ^{13}C NMR (125 MHz, CDCl_3) δ : 190.9, 136.9, 135.3, 128.4, 126.0, 124.8, 123.3, 123.0, 121.1, 120.8, 110.3, 41.5, 38.0, 33.6, 31.8, 29.7, 22.8, 22.4, 14.0; IR (neat): 2955, 2926, 1667, 1607, 1494, 1451, 1050, 874, 824; MS (ES^+) Calculated for $[\text{C}_{18}\text{H}_{21}\text{NONa}]^+$ 290.2; Found: 290.0.



8j

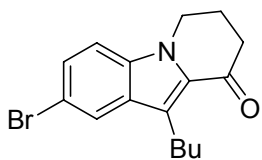
Compound **8j** was isolated in 73% yield using PtCl_4 as catalyst and in 95% yield using PtCl_2 following the general procedure D. Reaction time: 22 h. ^1H NMR (400MHz, CDCl_3) δ : 7.72 (d, 1H, J = 8.4 Hz), 7.39~7.33 (m, 2H), 7.31 (s, 1H), 7.16 (dd, 1H, J = 5.6, 1.6 Hz), 4.23 (t, 2H, J = 6.0 Hz), 2.74 (t, 2H, J = 7.2 Hz), 2.42~2.36 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ : 190.2, 137.3, 133.7, 126.6, 125.6, 123.4, 121.1, 110.3, 105.6, 41.3, 37.0, 23.2; IR (neat): 2925, 2348, 1671, 1472, 1050; MS (ES^+) Calculated for $[\text{C}_{12}\text{H}_{11}\text{NONa}]^+$ 208.1; Found: 208.0.



8k

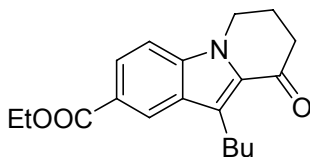
Compound **8k** was isolated in 89% yield following the general procedure D. Reaction time: 1 h. ^1H NMR (400MHz, CDCl_3) δ : 7.28 (d, 1H, J = 8.0 Hz), 7.00 (t, 1H, J = 8.0 Hz), 6.71 (t, 1H, J = 7.6 Hz), 4.68 (t, 2H, J = 6.0 Hz), 3.92 (s, 3H), 3.14 (t, 2H, J = 7.6 Hz), 2.66 (t, 2H, J = 6.8 Hz), 2.29 (quintet, 2H, J = 6.4 Hz), 1.66~1.58 (m, 2H), 1.45~1.36 (m, 2H), 0.93 (t, 3H, J = 7.6 Hz); ^{13}C NMR (100 MHz, CDCl_3) δ : 191.3, 148.2, 129.5, 128.7, 127.0, 125.5, 120.1, 113.8, 105.3, 55.4, 44.8, 37.9, 32.8, 24.8, 23.6, 22.9, 14.0; IR (neat):

2927, 2861, 1659, 1537, 1495, 1451, 1241, 1051, 1016, 874, 824; MS (ES⁺) Calculated for [C₁₇H₂₁NO₂Na]⁺ 294.2; Found: 294.0.



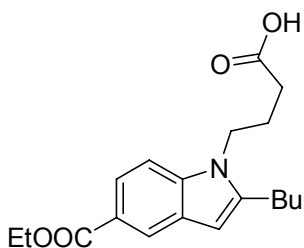
8l

Compound **8l** was isolated in 71% yield following the general procedure D. Reaction time: 1 h. ¹H NMR (400MHz, CDCl₃) δ: 7.84 (d, 1H, *J* = 1.6 Hz), 7.42 (dd, 1H, *J* = 8.8, 1.6 Hz), 7.19 (d, 1H, *J* = 8.8 Hz), 4.18 (t, 2H, *J* = 6.0 Hz), 3.11 (t, 2H, *J* = 7.6 Hz), 2.72 (t, 2H, *J* = 6.4 Hz), 2.36 (quintet, 2H, *J* = 6.4 Hz), 1.65-1.57 (m, 2H), 1.40 (quintet, 2H, *J* = 7.6 Hz), 0.94 (t, 3H, *J* = 7.6 Hz); ¹³C NMR (100 MHz, CDCl₃) δ: 190.9, 134.8, 129.7, 128.7, 128.4, 124.3, 123.9, 113.3, 111.7, 41.6, 37.9, 32.8, 24.5, 22.9, 22.8, 14.0; IR (neat): 2927, 2860, 1668, 1538, 1452, 1405, 1343, 1118, 1051, 904, 872, 824; MS (ES⁺) Calculated for [C₁₆H₁₈BrNONa]⁺ 242.1; Found: 241.6.

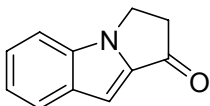


8m

Compound **8m** was isolated in 65% yield following the general procedure D. Reaction time: 1 h. ¹H NMR (400MHz, CDCl₃) δ: 8.50 (s, 1H), 8.04 (d, 1H, *J* = 8.8 Hz), 7.32 (d, 1H, *J* = 8.8 Hz), 4.42 (q, 2H, *J* = 7.6 Hz), 4.24 (t, 2H, *J* = 6.0 Hz), 3.20 (t, 2H, *J* = 7.6 Hz), 2.74 (t, 2H, *J* = 6.4 Hz), 2.38 (quintet, 2H, *J* = 6.0 Hz), 1.69-1.61 (m, 2H), 1.48-1.39 (m, 5H), 0.95 (t, 3H, *J* = 7.6 Hz); ¹³C NMR (100 MHz, CDCl₃) δ: 190.8, 167.2, 138.3, 130.1, 126.9, 126.6, 126.4, 124.8, 122.6, 109.8, 60.8, 41.8, 37.9, 33.0, 24.6, 22.8, 14.4, 14.0; IR (neat): 2928, 2860, 1691, 1665, 1540, 1495, 1452, 1385, 1312, 1250, 1122, 1050, 875, 824; MS (ES⁺) Calculated for [C₁₉H₂₃NO₃Na]⁺ 336.2; Found: 335.8.

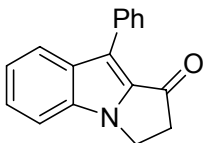


This compound was isolated as the side product during the reaction of **7m**. ^1H NMR (400MHz, CDCl_3) δ : 8.29 (d, 1H, $J = 1.6$ Hz), 7.86 (dd, 1H, $J = 8.8, 1.6$ Hz), 7.28 (d, 1H, $J = 8.8$ Hz), 6.35 (s, 1H), 4.38 (q, 2H, $J = 7.2$ Hz), 4.16 (t, 2H, $J = 7.6$ Hz), 2.72 (t, 2H, $J = 7.6$ Hz), 2.42 (t, 2H, $J = 6.8$ Hz), 2.08 (quintet, 2H, $J = 7.2$ Hz), 1.79-1.71 (m, 2H), 1.52-1.39 (m, 5H), 0.98 (t, 3H, $J = 7.2$ Hz); ^{13}C NMR (100 MHz, CDCl_3) δ : 178.2, 167.9, 142.5, 139.1, 127.6, 122.7, 122.2, 121.6, 108.4, 100.5, 60.5, 42.2, 30.7, 30.5, 26.3, 24.8, 22.6, 14.4, 13.9; IR (neat): 2928, 2861, 1699, 1611, 1494, 1452, 1309, 1299, 1256, 1230, 1096, 1050, 874, 824; MS (ES^+) Calculated for $[\text{C}_{19}\text{H}_{23}\text{NO}_3\text{Na}]^+$ 354.2; Found: 353.9.

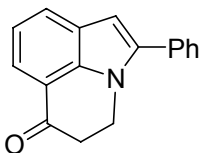


11

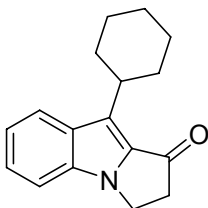
Compound **11** was isolated in 85% yield using PtCl_4 as catalyst and in 99% yield using PtCl_2 following the general procedure D. Reaction time: 8 h in the case of PtCl_4 ; 24 h in the case of PtCl_2 . ^1H NMR (500MHz, CDCl_3) δ : 7.75 (d, 1H, $J = 8.5$ Hz), 7.41 (d, 1H, $J = 8.5$ Hz), 7.35 (t, 1H, $J = 8.5$ Hz), 7.18 (t, 1H, $J = 8.5$ Hz), 6.99 (s, 1H), 4.39 (t, 2H, $J = 6.0$ Hz), 3.18 (t, 2H, $J = 6.0$ Hz); ^{13}C NMR (125 MHz, CDCl_3) δ : 192.8, 135.3, 135.2, 132.1, 125.1, 124.1, 121.5, 110.4, 98.8, 39.9, 39.4; IR (neat): 2253, 1713, 1540, 1494, 1451, 1050, 907, 824, 732; MS (ES^+) Calculated for $[\text{C}_{11}\text{H}_9\text{NONa}]^+$ 194.1; Found: 194.0.



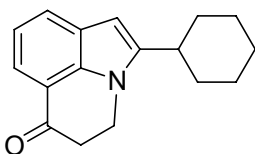
This compound was isolated in 67% yield along with 33% of the Friedel-Crafts acylation product (shown below) following the general procedure D. Reaction time: 4 h. ^1H NMR (400MHz, CDCl_3) δ : 8.01 (d, 1H, $J = 8.0$ Hz), 7.86 (d, 2H, $J = 8.0$ Hz), 7.48 (t, 2H, $J = 7.6$ Hz), 7.42~7.30 (m, 3H), 7.26~7.18 (m, 1H), 4.38 (t, 2H, $J = 6.0$ Hz), 3.21 (t, 2H, $J = 6.0$ Hz); ^{13}C NMR (125 MHz, CDCl_3) δ : 192.0, 135.2, 132.6, 130.8, 130.3, 129.2, 128.5, 127.2, 125.4, 123.2, 121.8, 116.9, 110.5, 39.8, 39.5; IR (neat): 2253, 1705, 1553, 1494, 1451, 1050, 907, 824, 730; MS (ES^+) Calculated for $[\text{C}_{17}\text{H}_{13}\text{NONa}]^+$ 270.1; Found: 270.1.



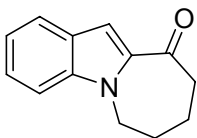
^1H NMR (400MHz, CDCl_3) δ : 7.83 (dd, 1H, J = 6.0, 0.8 Hz), 7.73 (dd, 1H, J = 6.4, 0.8 Hz), 7.56~7.42 (m, 5H), 7.22 (t, 1H, J = 6.0 Hz), 6.66 (s, 1H), 4.45 (t, 2H, J = 5.2 Hz), 3.10 (t, 2H, J = 5.2 Hz); ^{13}C NMR (125 MHz, CDCl_3) δ : 192.8, 141.9, 141.1, 131.6, 128.8, 128.7, 128.4, 127.9, 126.6, 120.5, 118.6, 118.2, 102.7, 42.8, 38.2; IR (neat): 2926, 2253, 1682, 1592, 1494, 1454, 1050, 907, 731; MS (ES^+) Calculated for $[\text{C}_{17}\text{H}_{13}\text{NONa}]^+$ 270.1; Found: 270.1.



This compound was isolated in 67% yield along with 33% of the Friedel-Crafts acylation product (shown below) following the general procedure D. Reaction time: 2 h. ^1H NMR (500MHz, CDCl_3) δ : 7.84 (d, 1H, J = 8.5 Hz), 7.37~7.32 (m, 2H), 7.14 (t, 1H, J = 6.5 Hz), 4.36 (t, 2H, J = 6.5 Hz), 3.20 (m, 1H), 3.18 (t, 2H, J = 6.5 Hz), 1.99~1.92 (m, 2H), 1.86~1.76 (m, 5H), 1.47~1.41 (m, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ : 192.6, 134.8, 131.2, 130.7, 125.1, 124.1, 123.1, 120.3, 110.4, 39.9, 39.4, 35.7, 33.2, 27.0, 26.0; IR (neat): 2928, 2253, 1699, 1558, 1494, 1450, 1307, 1050, 824; MS (ES^+) Calculated for $[\text{C}_{17}\text{H}_{19}\text{NONa}]^+$ 276.1; Found: 276.3.

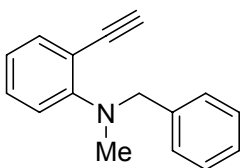


^1H NMR (500MHz, CDCl_3) δ : 7.72 (d, 1H, J = 7.6 Hz), 7.63 (d, 1H, J = 7.6 Hz), 7.13 (t, 1H, J = 7.6 Hz), 6.31 (s, 1H), 4.36 (t, 2H, J = 6.8 Hz), 3.07 (t, 2H, J = 6.8 Hz), 2.73~2.67 (m, 1H), 2.06~2.03 (m, 2H), 1.91~1.88 (m, 2H), 1.82~1.78 (m, 1H), 1.56~1.32 (m, 5H); ^{13}C NMR (125 MHz, CDCl_3) δ : 192.9, 147.7, 139.9, 127.9, 126.1, 119.8, 117.5, 117.4, 97.9, 41.5, 38.1, 35.8, 33.0, 26.5, 26.0; IR (neat): 2930, 2253, 1681, 1594, 1494, 1451, 1050, 907, 731, 650; MS (ES^+) Calculated for $[\text{C}_{17}\text{H}_{19}\text{NONa}]^+$ 276.1; Found: 276.1.



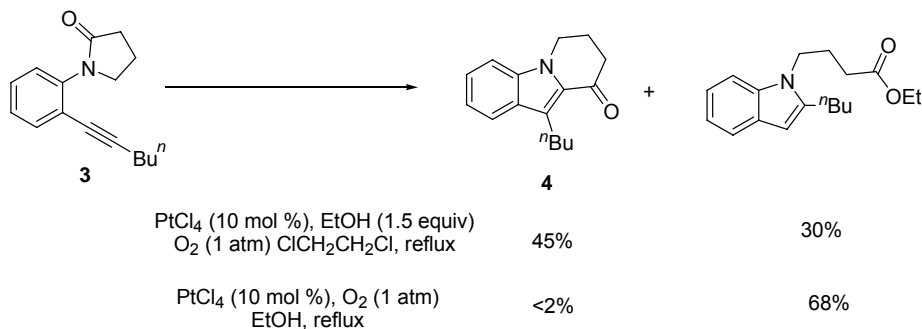
13

Compound **13** was isolated in 45% yield using PtCl_2 as catalyst following the general procedure D. Reaction time: 36 h. ^1H NMR (500MHz, CDCl_3) δ : 7.69 (d, 1H, $J = 8.0$ Hz), 7.38~7.25 (m, 1H), 7.26 (d, 1H, $J = 8.5$ Hz), 7.15~7.12 (m, 1H), 4.38 (t, 2H, $J = 6.0$ Hz), 2.89~2.86 (m, 2H), 2.16~2.11 (m, 2H), 2.00~1.97 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ : 194.7, 139.2, 138.8, 126.3, 125.3, 123.1, 120.6, 110.2, 108.8, 43.2, 40.5, 26.8, 20.7; IR (neat): 2928, 2253, 1699, 1558, 1494, 1450, 1050, 824; MS (ES^+) Calculated for $[\text{C}_{13}\text{H}_{13}\text{NONa}]^+$ 222.0; Found: 222.1.



^1H NMR (500MHz, CDCl_3) δ : 7.49 (dd, 1H, $J = 1.5, 7.5$ Hz), 7.37~7.23 (m, 6H), 6.92~6.88 (m, 2H), 4.47 (s, 2H), 3.34 (s, 1H), 2.74 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ : 154.7, 138.7, 135.0, 129.7, 128.3, 128.2, 126.9, 120.8, 118.3, 114.6, 82.8, 82.6, 60.2, 39.3; IR (neat): 2295, 1607, 1494, 1451, 1049, 907, 824; MS (ES^+) Calculated for $[\text{C}_{16}\text{H}_{16}\text{N}]^+$ 222.1; Found: 222.1.

Mechanism study: trapping acylium C and/or the preceding zwitterionic intermediate.



Experiment 1: Compound **3** was used as substrate, and the reaction was run according to the general procedure D except with the addition of 1,5 equiv. of EtOH. Reaction time: 1h. The ethyl ester was isolated in 30% yield along with product **4** (45% yield). For the ethyl ester: ^1H NMR (400MHz, CDCl_3) δ : 7.53 (d, 1H, $J = 7.6$ Hz), 7.29 (d, 1H, $J = 7.6$

Hz), 7.13 (dt, 1H, $J = 7.6, 1.2$ Hz), 7.06 (dt, 1H, $J = 7.6, 1.2$ Hz), 7.26 (s, 1H), 4.17-4.11 (m, 4H), 2.72 (t, 2H, $J = 7.6$ Hz), 2.34 (t, 2H, $J = 7.2$ Hz), 2.07 (quintet, 2H, $J = 7.2$ Hz), 1.78-1.70 (m, 2H), 1.48 (sextet, 2H, $J = 7.6$ Hz), 1.26 (t, 3H, $J = 7.2$ Hz), 0.98 (t, 3H, $J = 7.6$ Hz); ^{13}C NMR (100 MHz, CDCl_3) δ : 172.8, 141.0, 136.5, 128.1, 120.5, 119.7, 119.2, 109.0, 98.9, 60.6, 42.0, 31.2, 30.6, 26.3, 25.1, 22.6, 14.2, 14.0; IR (neat): 3056, 2958, 2932, 1733, 1464, 1315, 1161, 1033, 874; MS (ES^+) Calculated for $[\text{C}_{18}\text{H}_{25}\text{NO}_2\text{Na}]^+$ 310.2; Found: 310.1.

Experiment 2: Compound **3** was used as substrate, and the reaction was run according to the general procedure D except that EtOH was used as solvent. Reaction time: 1h. The ethyl ester was isolated in 68% yield.

File: hxg-gzmade

Pulse Sequence: szpul

Solvent: cdcl3

Temp: 25.0 C / 298.1 K

Operator: walkup

File: hxg-gzmade

INOVA-500 "redjacket"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.049 sec

Width 8012.8 Hz

8 repetitions

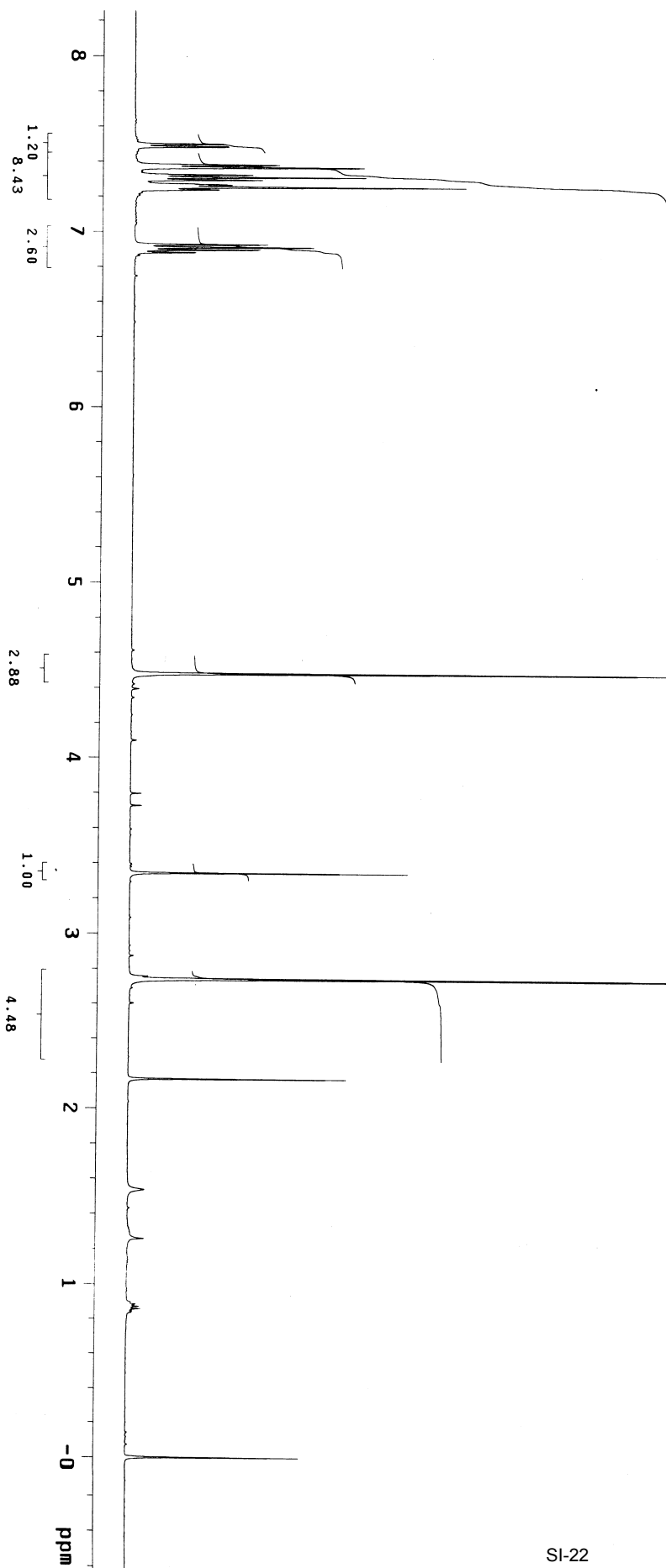
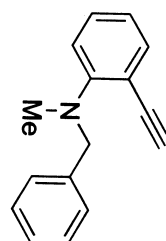
OBSERVE H1

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

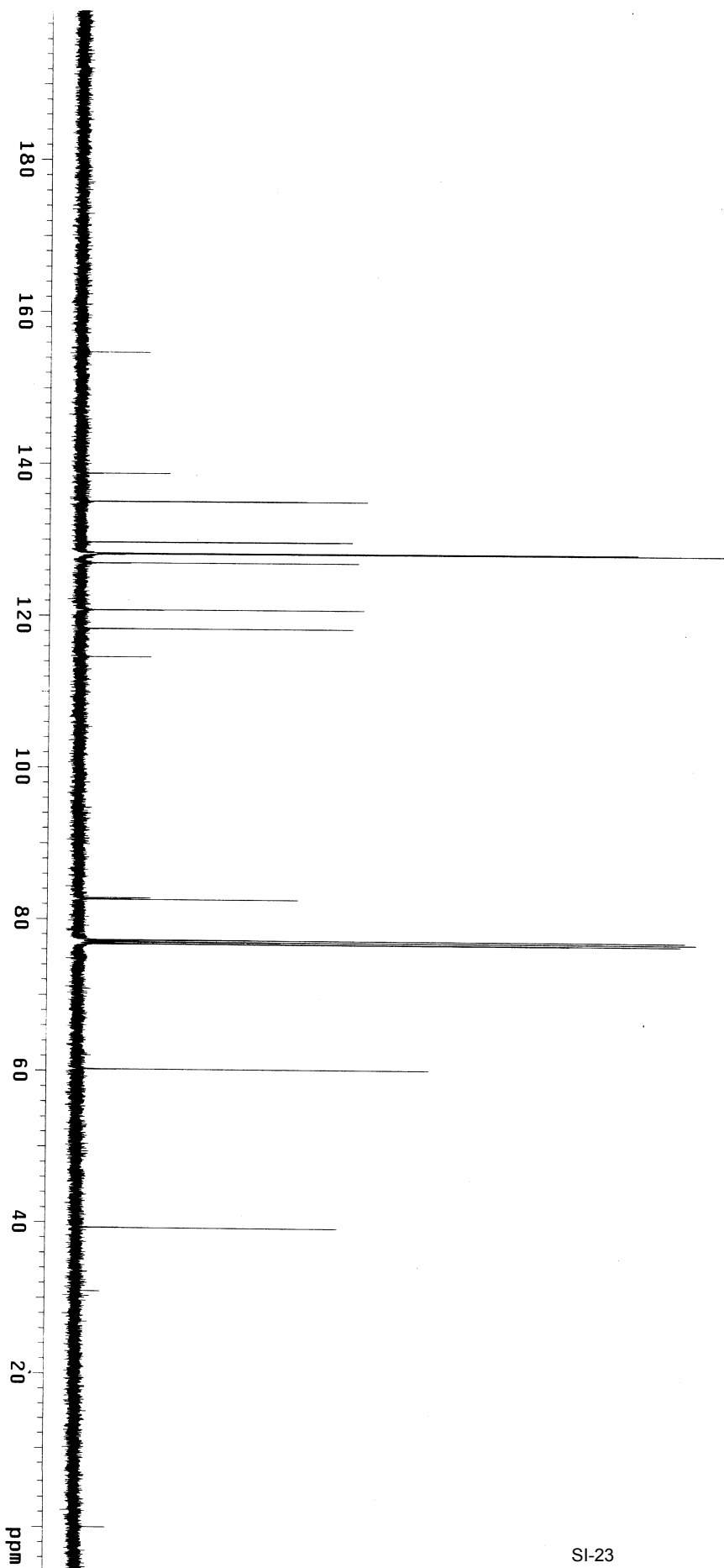
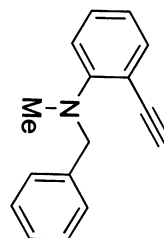
Total time 0 min, 30 sec



Automation directory: /home/walkup/vnmrSYS/data/auto_2007.06.25_11
File : exp
Sample id : tmpstudy

Pulse Sequence: s2pul
Solvent: cdcl3
Temp: 25.0 C / 298.1 K
Operator: walkup
VNMRS-500 "nmr500"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 30487.8 Hz
384 repetitions
OBSERVE C13, 125.6746044 MHz
DECOUPLE H1, 499.8016822 MHz
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 19 min, 42 sec

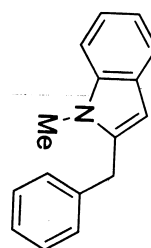


Automation directory: /home/walkup/vnmr-sys/data/auto_2007.07.01.07
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Sample id : s_20070701_002

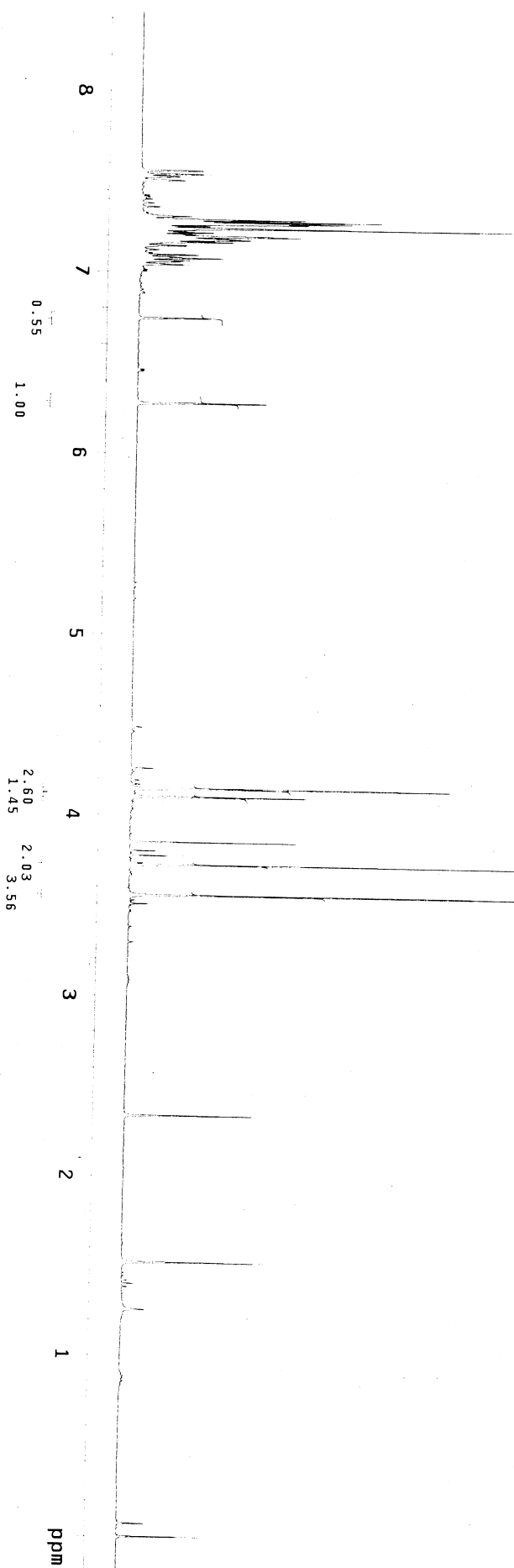
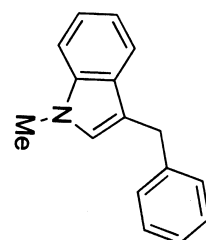
Pulse Sequence: s2pul1

Solvent: cdc13
Temp: 25.0 C / 298.1 K
Operator: walkup
File: cdc13_01
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, 399.8656793 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65356
Total time 0 min, 30 sec



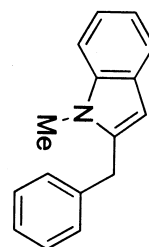
and



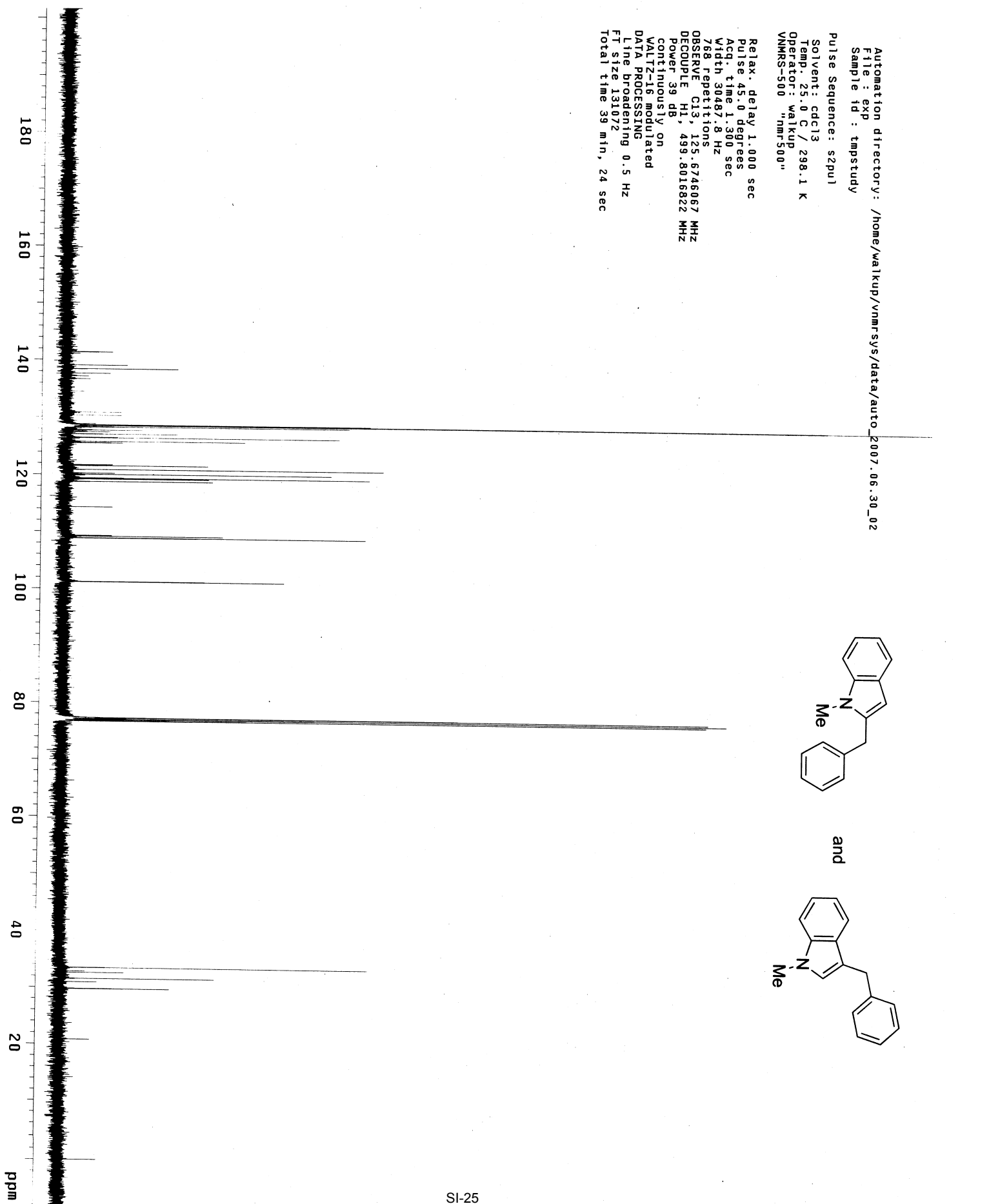
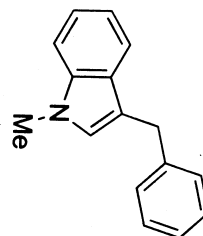
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File : exp
Sample id : tmpstudy

Pulse Sequence: s2pu1
Solvent: cdc13
Temp: 25.0 C / 298.1 K
Operator: walkup
VNMRS-500 "nmr500"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 30487.8 Hz
768 repetitions
OBSERVE C13, 125.6746067 MHz
DECOUPLE H1, 499.8016822 MHz
Power 39 db
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 39 min, 24 sec

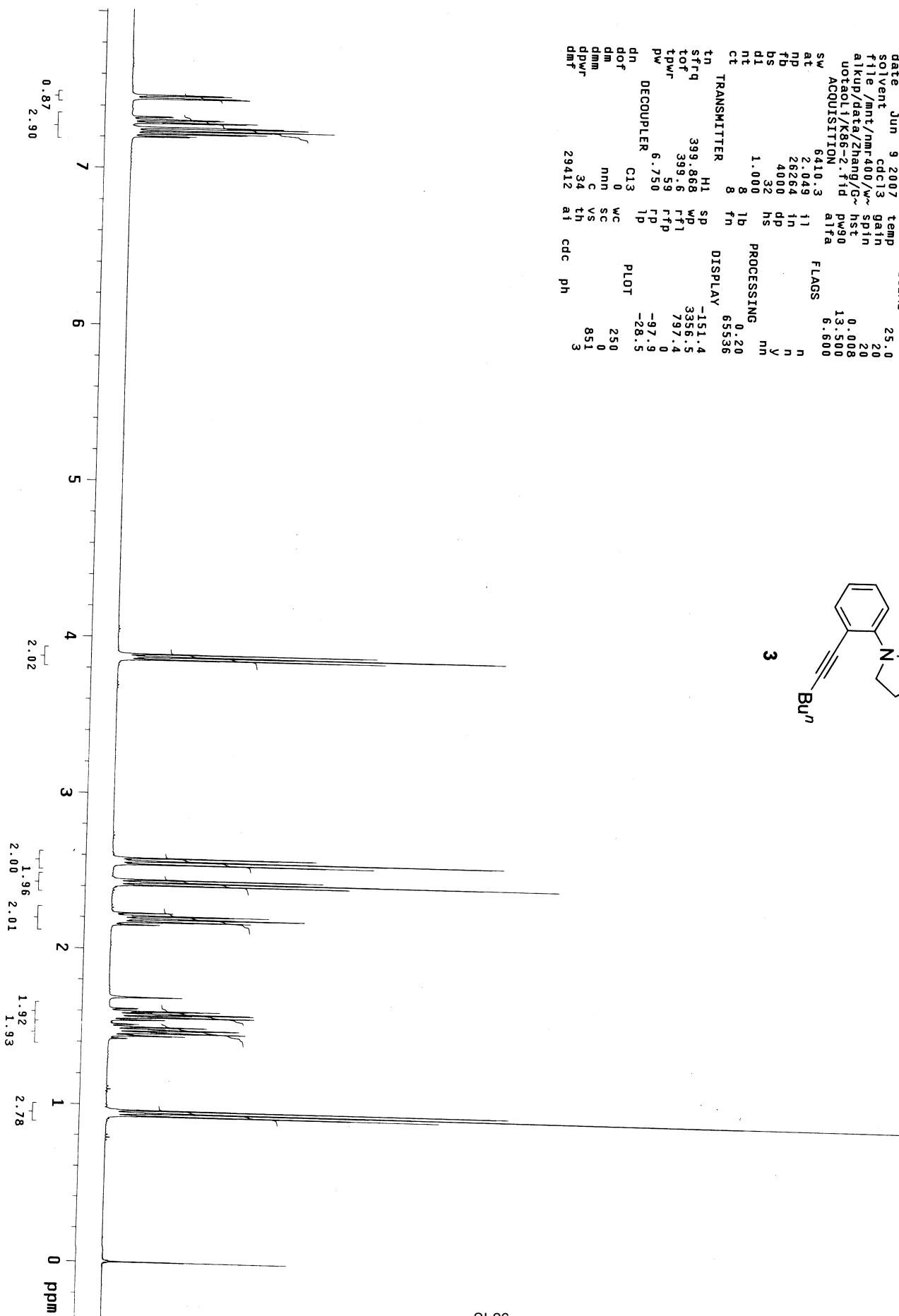
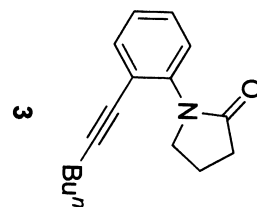


and



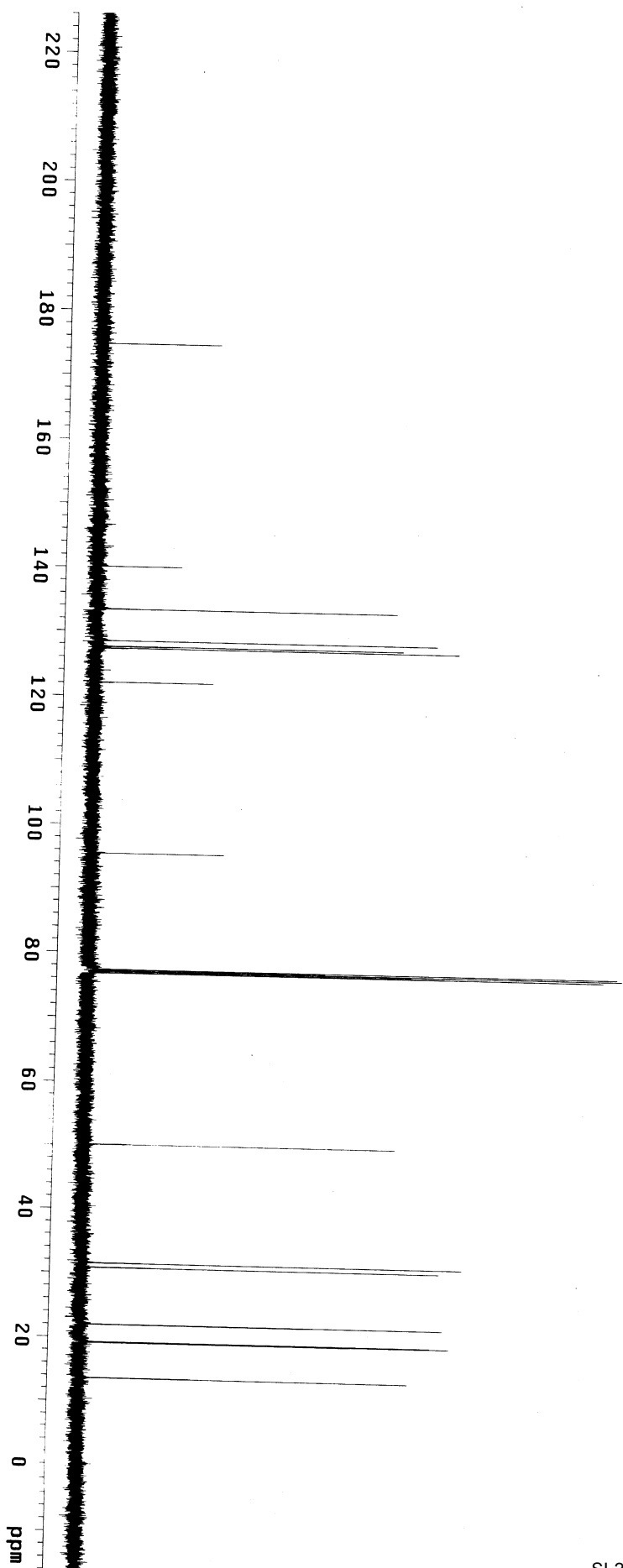
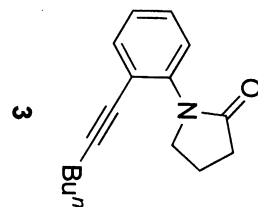
exp2 Proton

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alkup/data/Zhang/G~		hst	0.008
uotaoli/K86-2.fid		pw90	13.500
ACQUISITION		atfa	6.600
sw	6410.3	flags	
at	2.049	11	n
np	26264	in	n
fb	4000	dp	y
bs	32	hs	nm
d1	1.000	PROCESSING	0.20
nt	8	1b	65536
ct	8	fn	
TRANSMITTER		DISPLAY	
tn	H1	sp	-151.4
sfreq	399.868	wd	3356.5
tof	399.6	rfl	797.4
tpwr	59	rtp	-97.9
pw	6.750	tp	-28.5
DECOUPLER		PLOT	
dn	C13	wc	250
dof	0	sc	0
dm	nmn	vs	851
dmm	c	th	3
dpwr	34	ai	cdc
dnt	29412	ph	



expt Carbon

SAMPLE		SPECIAL	
date	Jun 9 2007	temp	25.0
solvent	cdcl3	gain	30
file	exp	spn	not used
ACQUISITION		hst	0.008
sw	30487.8	pw50	15.300
at	1.300	altfa	10.000
np	79298	FLAGS	
fb	17000	11	n
bs	64	in	n
dl	1.000	dp	y
nt	1024	hs	nm
ct	128	PROCESSING	0.50
tn	TRANSMITTER C13	fb	not used
sfreq	125.688	sp	-2080.2
tofr	1253.3	wp	30487.3
tpwr	49	rfl	11757.6
pw	7.650	rffp	9676.9
DECOUPLER		rfp	-38.6
dn	H1	lp	-250.8
dof	0	PLOT	
dmm	YVY	WC	250
dmm	YV	SC	0
dprf	39	VS	23094
dprf	12200	th	68
at	cdc	ph	



File: hxg-4-25H

Pulse Sequence: szpu1

Solvent: cdcl3

Temp: 25.0 C / 298.1 K

Operator: walkup

File: hxg-4-25H

INOVA-500 "sittingbul1"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.049 sec

Width 8012.8 Hz

8 repetitions

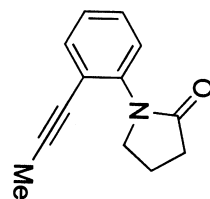
OBSERVE H1 499.7991817 MHz

DATA PROCESSING

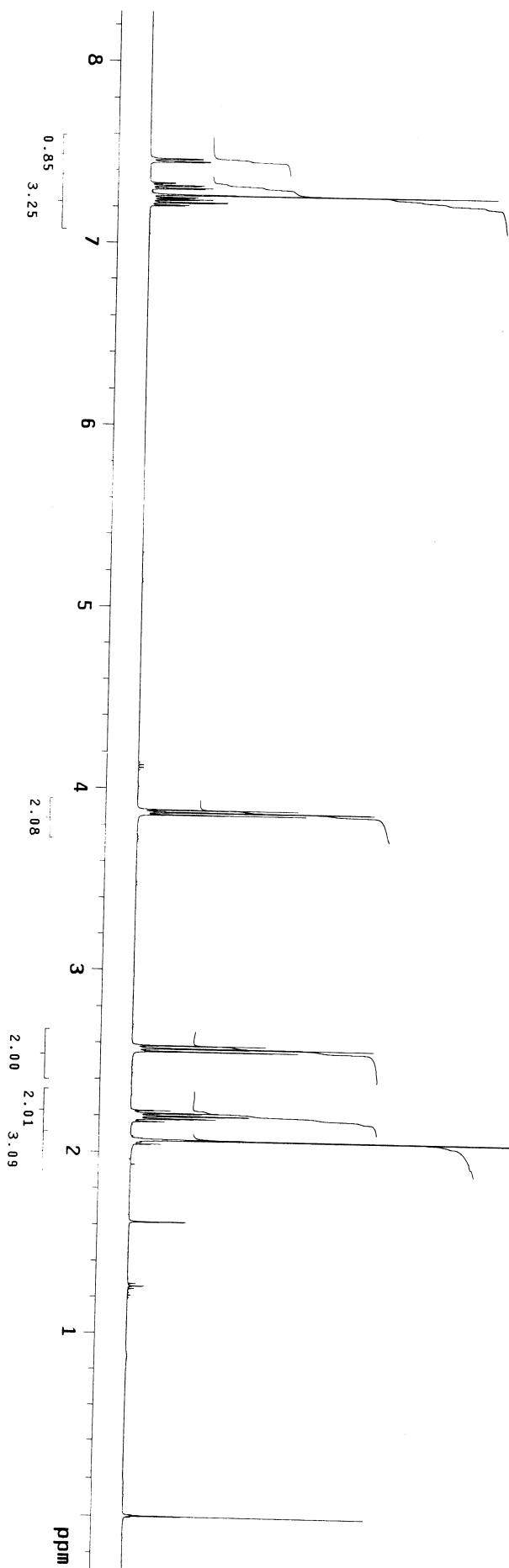
Line broadening 0.2 Hz

FT size 65536

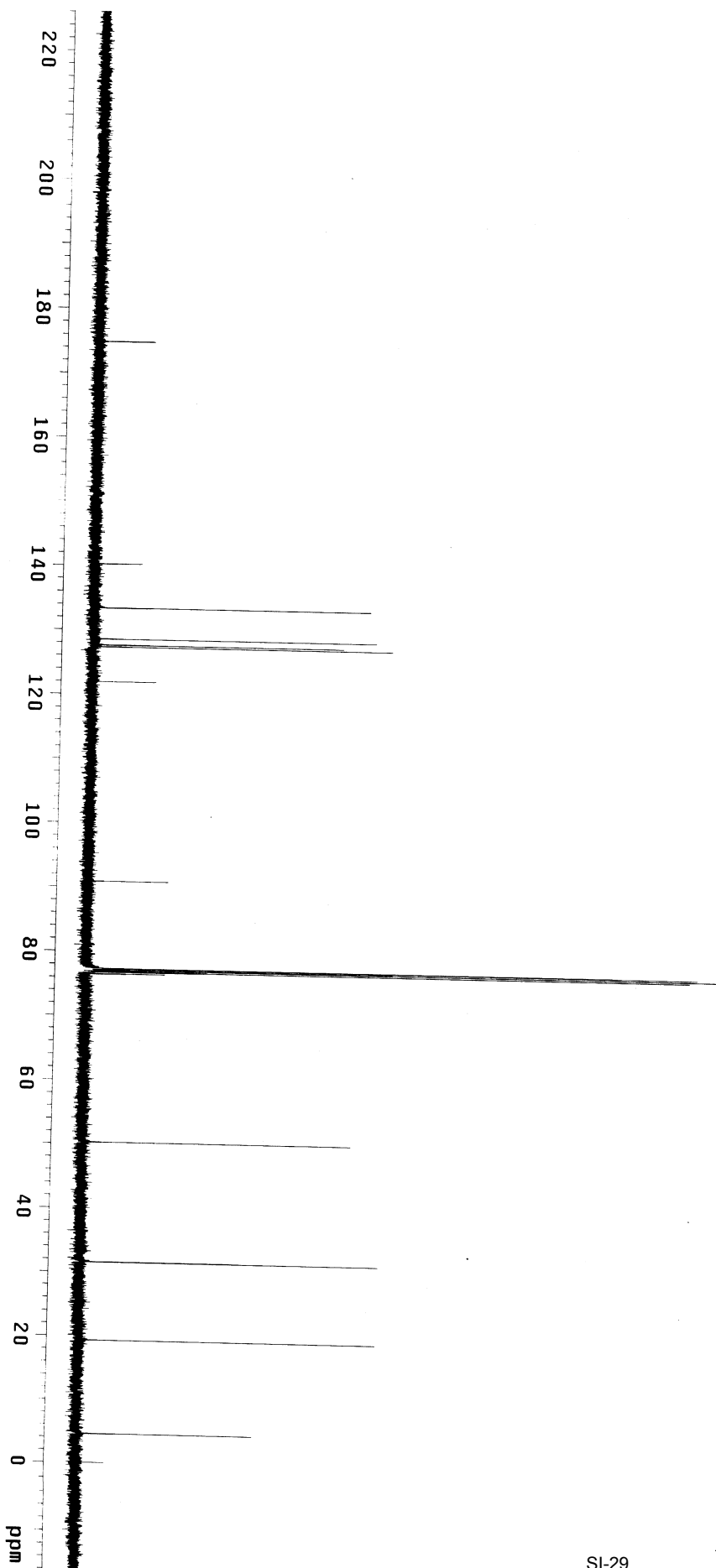
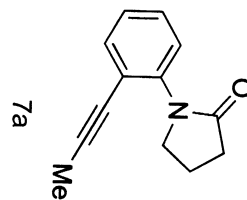
Total time 0 min, 30 sec



7a

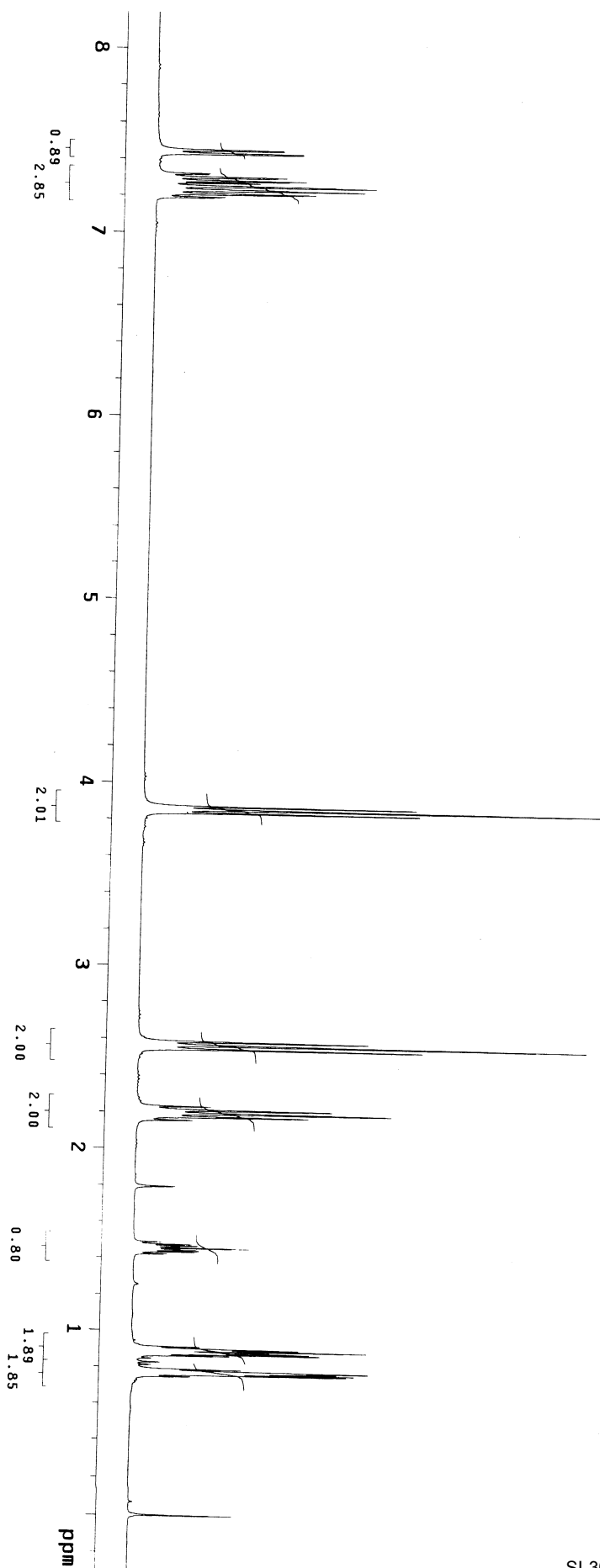
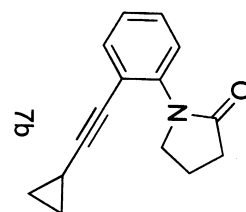


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Sample id : tmpstudy
Pulse Sequence: szpul
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: walkup
VNMRS-500 "nmr500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 30487.8 Hz
512 repetitions
OBSERVE C13, 125.6746053 MHz
DECOUPLE H1, 499.8016822 MHz
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 39 min, 24 sec



exp2 Proton

SAMPLE		SPECIAL	
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alkup/data/Zhang/G~	hst		0.008
uotaol/K157-2.fid	pw90		13.500
ACQUISITION		atfta	6.600
sw	6410.3	flags	
at	2.049	in	n
np	26264	in	n
fb	4000	dp	v
bs	32	hs	nn
dl	1.000	PROCESSING	
nt	8	lb	0.20
ct	8	fn	65356
TRANSMITTER		DISPLAY	
tn	HI	sp	-131.3
sfreq	399.868	wp	3409.2
tof	399.6	rftl	794.8
tpwr	59	rfd	0
pw	6.750	fp	-22.1
DECOUPLER		lp	-19.9
dn	C13	PLOT	
dof	0	wc	250
dm	nnn	sc	0
dmm	c	vs	1044
dpwr	34	th	2
dmt	29412	at	cdc
			ph



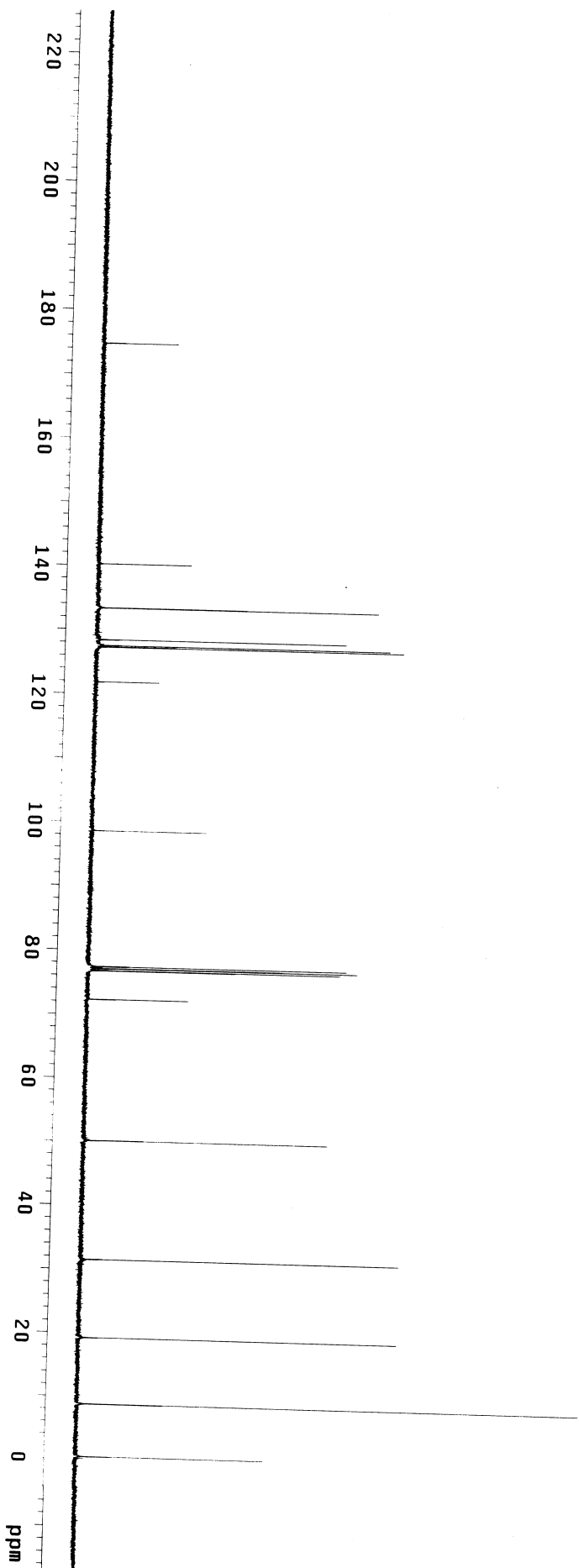
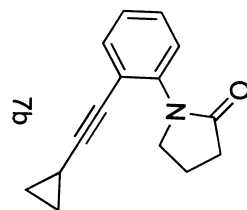
exps Carbon

SAMPLE		SPECIAL	
date	Jun 20 2007	temp	25.0
solvent	cdcl3	gain	30
file	/mnt/nmr400/w~	spin	20
alkup/data/Zhang/G~	hst	0.008	
uotaol/K157-2carb~	pw90	11.900	
on.fid	alfa	10.000	

ACQUISITION		FLAGS	
sw	24509.8	11	n
at	1.300	in	n
np	63750	dp	y
fb	17000	hs	nn
bs	64		
dl	1.000	lb	0.50
nt	3200	fn	not used
ct	3200		

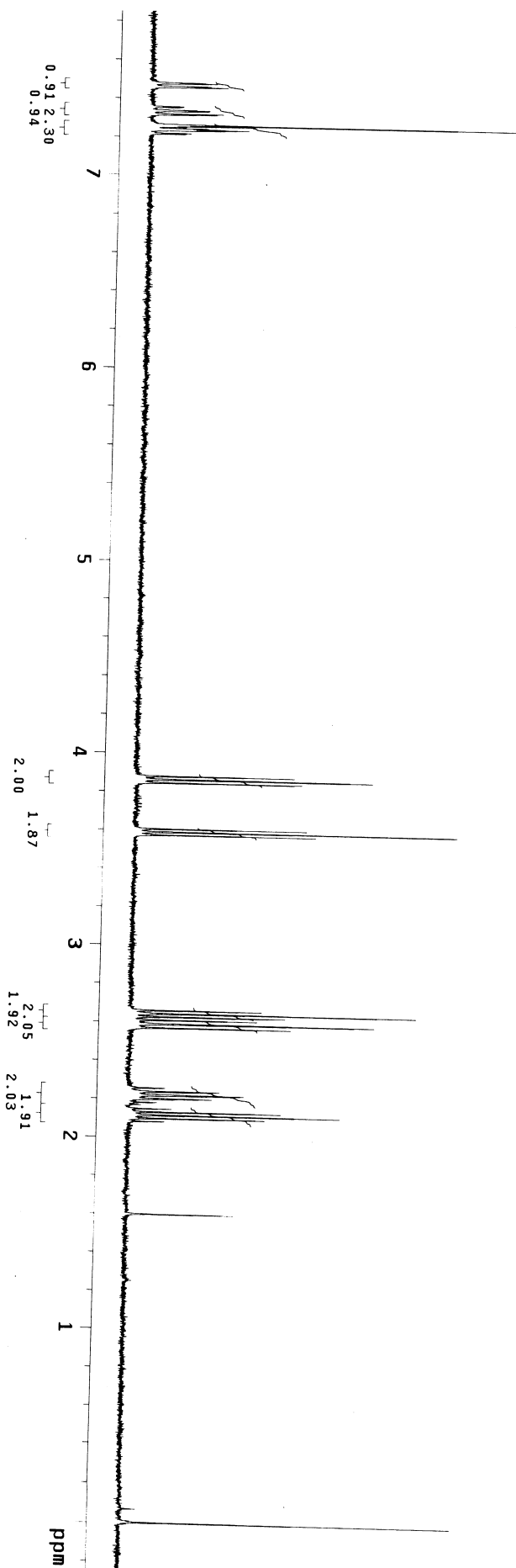
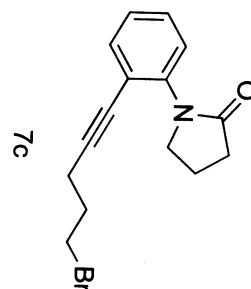
TRANSMITTER		DISPLAY	
tn	C13	sp	-1725.1
sfreq	100.557	wp	24509.1
tof	1042.8	rfl	9467.9
tpwr	53	rfl	7742.1
pw	5.950	lp	179.7
			-199.3

DECOUPLER		PLOT	
dn	H1	WC	250
dof	0	SC	0
dm	YVY	VS	53937
dmm	W	th	7
dpwr	41	at	cdc ph
dmf	9500		



exp5 Proton

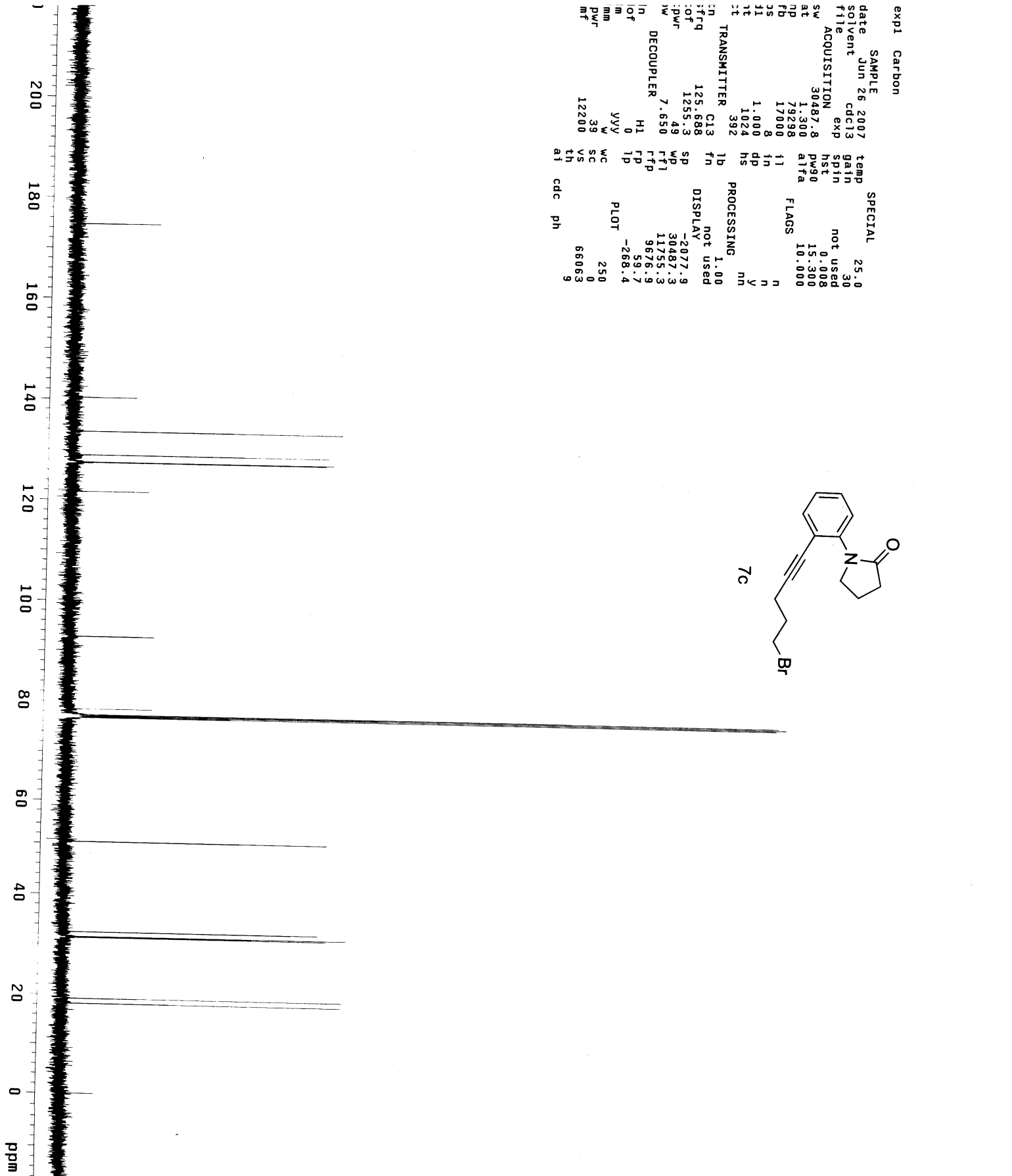
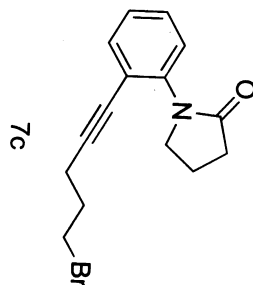
SAMPLE		SPECIAL	
date	Jun 25 2007	temp	25.0
solvent	cdcl3	gain	30
file	/mnt/nmr/400/w~	spin	not used
akup/date	Zhang/G~	hst	0.008
uotaol/K183-1.fid		pw90	13.500
ACQUISITION		atfa	6.600
sw	6410.3	flags	
at	2.049	i1	n
rp	26264	in	n
fb	4000	dp	v
bs	8	hs	nn
d1	1.000	nt	
ct	8	fb	0.20
tn	8	fn	65536
TRANSMITTER			
tn	H1	sp	DISPLAY
stfq	399.868	wp	-108.6
tof	399.6	rfl	3248.0
tpwr	59	rff	798.5
pw	6.750	fp	0
DECOUPLER			
dn	C13	tp	-109.2
dof	0	ip	-21.1
dm	nmn	WC	250
dmm	c	SC	0
dpwr	34	VS	54163
dmf	29412	tn	4
	at	cdc	ph



expt Carbon

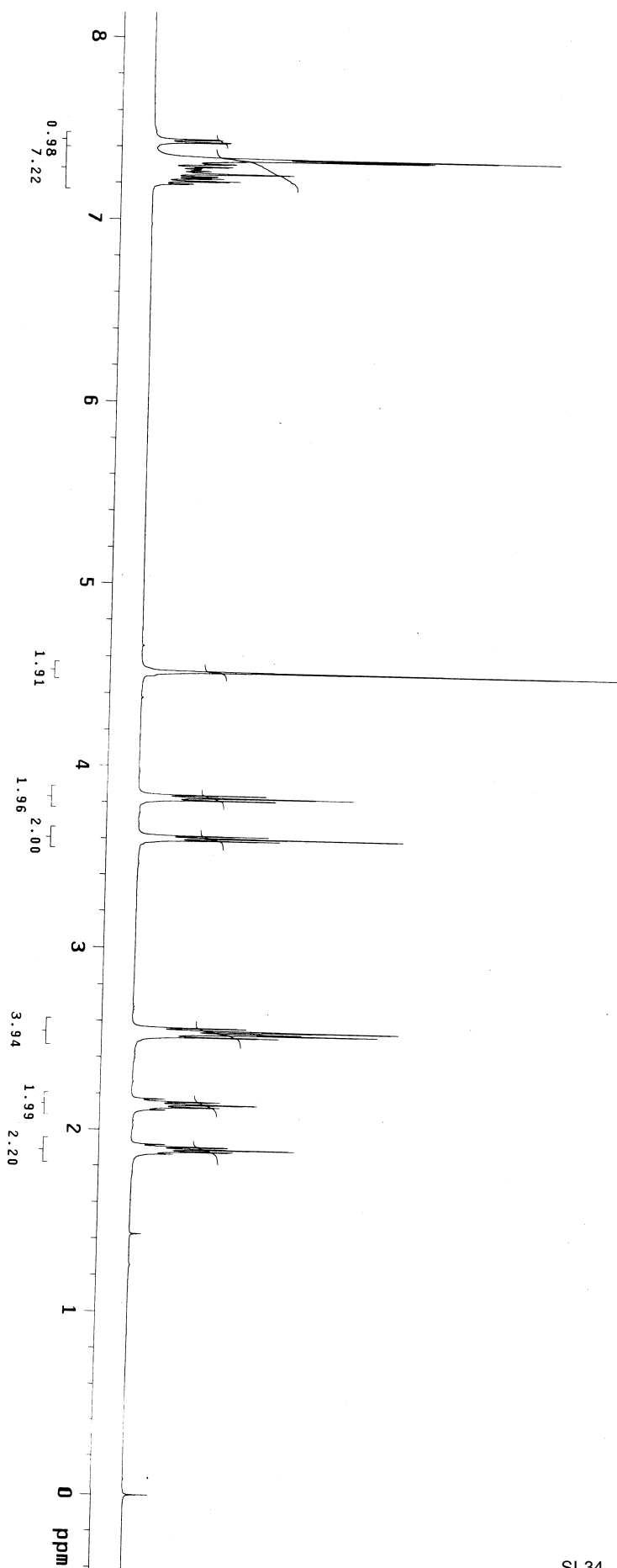
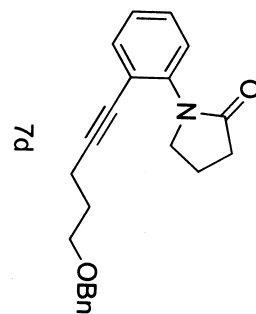
SAMPLE
date Jun 26 2007
solvent cdc13
file exp
ACQUISITION
sw 30487.8
at 1.300
np 79288
fb 17000
cs 8
st 1.000
1t 1024
392
TRANSMITTER
in c13
:frq 125.688
:ot 125.3
:pwr 49
w 7.650
DECOUPLER
in H1
:ot 0
:m vvy
mm w
pwr w
mf 12200
th vs
at cdc ph

SPECIAL
temp 25.0
gain 30
spin not used
hst 0.008
pw90 15.300
alfa 10.000
FLAGS
n
n
y
nn
1.00
not used
DISPLAY
-2077.9
30487.3
11755.3
9676.9
59.7
-268.4
PLOT
250
0
66063
9



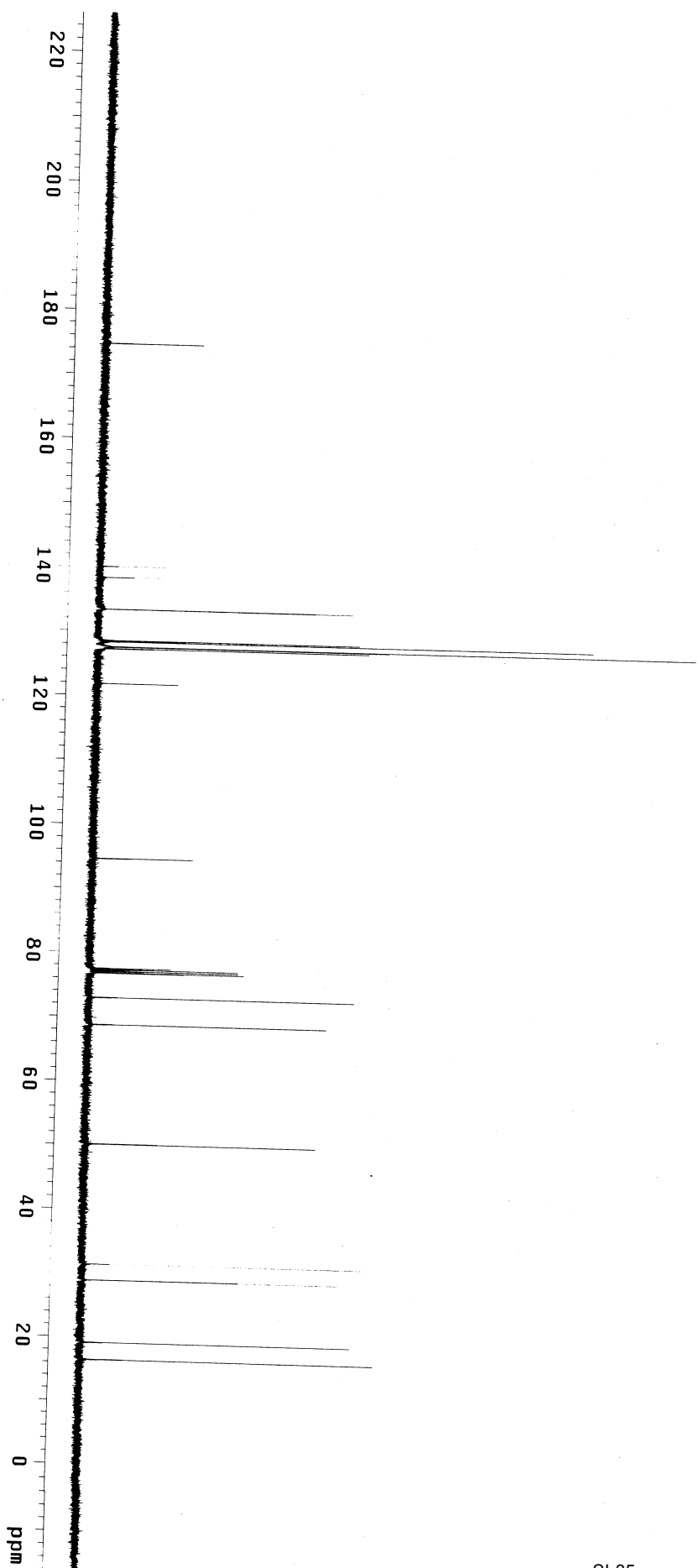
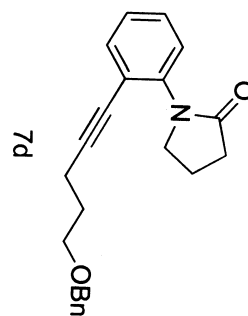
exp2 Proton

SAMPLE		SPECIAL	
date	Jun 30 2007	temp	25.0
solvent	cdcl3	gain	30
file	/mnt/nmr/500/W~	spin	not used
alkup/data/zhang/L~	1/K205.fid	hst	0.008
		pw90	14.700
		alfa	6.600
ACQUISITION			
sw	8012.8	flags	
at	2.049	11	n
np	32830	in	n
tb	4000	dp	y
bs	8	hs	nn
di	1.000	lb	nn
nt	8	fn	0.20
ct	8		65536
TRANSMITTER			
tn	H1	sp	-220.3
sfrq	499.802	wp	4286.9
tof	499.7	rfl	1011.4
tpwr	54	rfd	0
pw	7.350	fp	-174.5
DECOUPLER			
dn	C13	lp	-13.0
dof	0	wc	
dm	nnn	sc	250
dmm	c	vs	0
dpwr	34	th	38
dmf	32258	at	2
		cdc	ph



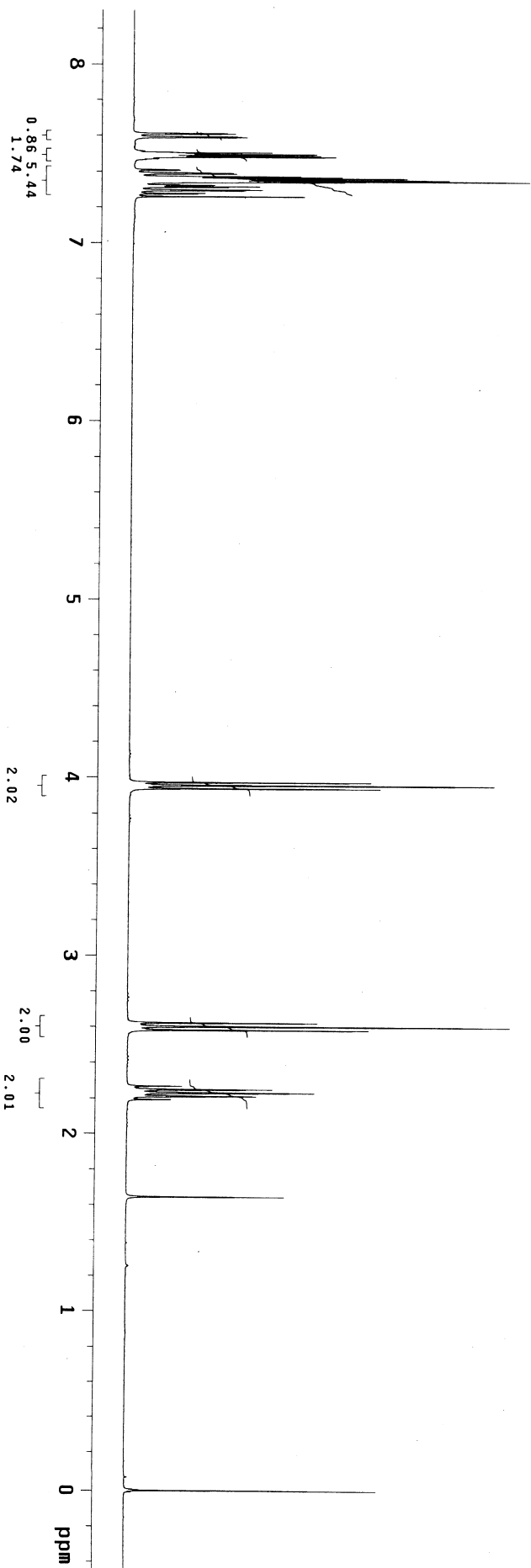
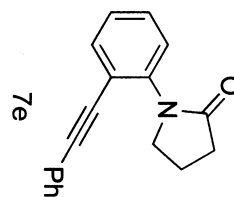
exp3 Carbon

SAMPLE		SPECIAL	
date	Jun 30 2007	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	atfa	10.000
np	79298	FLAGS	
fb	17000	i1	n
bs	16	in	n
dl	1.000	dp	v
nt	1024	hs	nn
ct	80	PROCESSING	0.50
tn	C13	lb	fn
sfrq	125.688	sp	not used
tof	1255.3	wp	DISPLAY
tpwr	49	rfl	-2092.3
pv	7.650	rfl	30487.3
DECOUPLER		rfl	11769.7
dn	H1	rfl	9676.9
dof	0	lp	150.5
dm	VVY	PLOT	-247.3
dmm	w	WC	250
dpwr	39	SC	0
dmf	12200	VS	8429
th	at	cdc	ph
			7

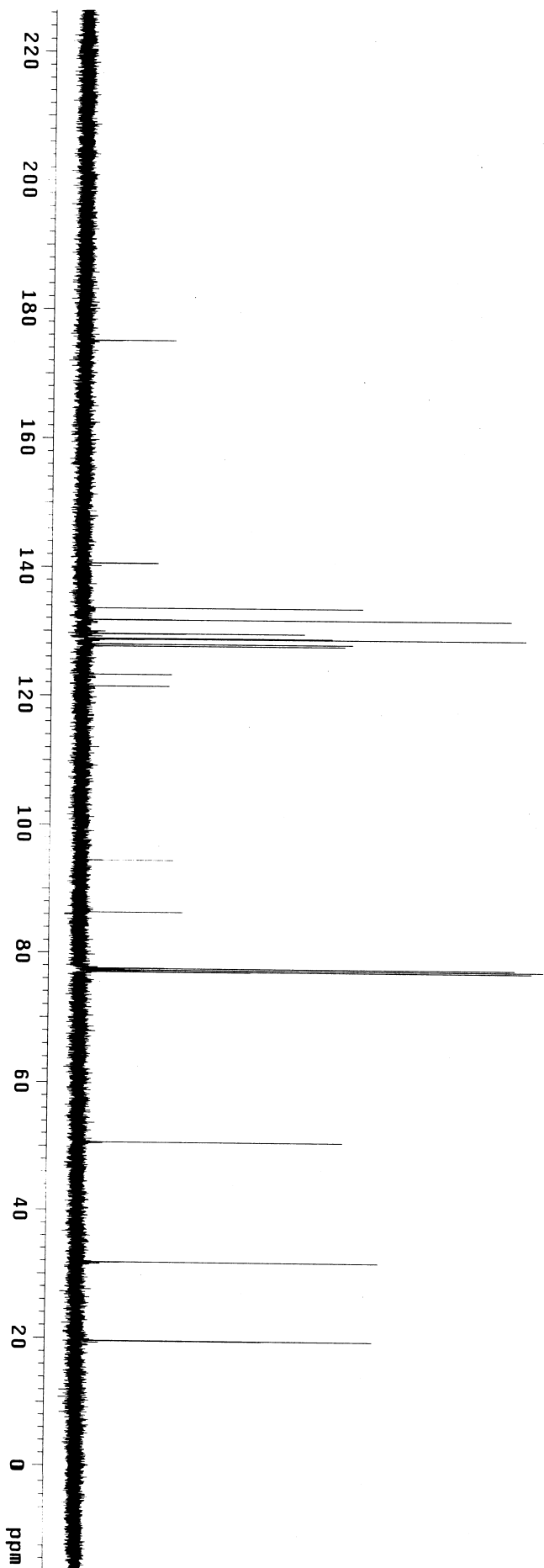
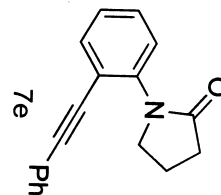


exp2 Proton

SAMPLE		SPECIAL	
date	Jun 10 2007	temp	25.0
solvent	cdcl3	gain	26
file	/mnt/nmr400/w-	spin	20
akup	data/Zhang/G-	nst	0.008
uotao	Li/K65-2.fid	pw90	13.500
ACQUISITION		alfta	6.600
sw	6410.3	flags	
at	2.049	11	n
np	25264	in	n
fb	4000	dp	y
bs	32	hs	nm
dl	1.000	1b	0.20
nt	8	fn	65536
ct	8	td	
TRANSMITTER		PROCESSING	
tn	H1	sp	-183.1
sfreq	399.868	wd	3503.5
tof	399.6	rf1	799.7
tpwr	59	rfp	-85.8
pw	6.750	fp	-29.2
DECOUPLER		PLOT	
dn	C13	1p	
dof	0	wc	250
dm	nmn	sc	0
dmm	c	vs	487
dpwr	34	th	3
dmf	29412	ai	cdc
			ph

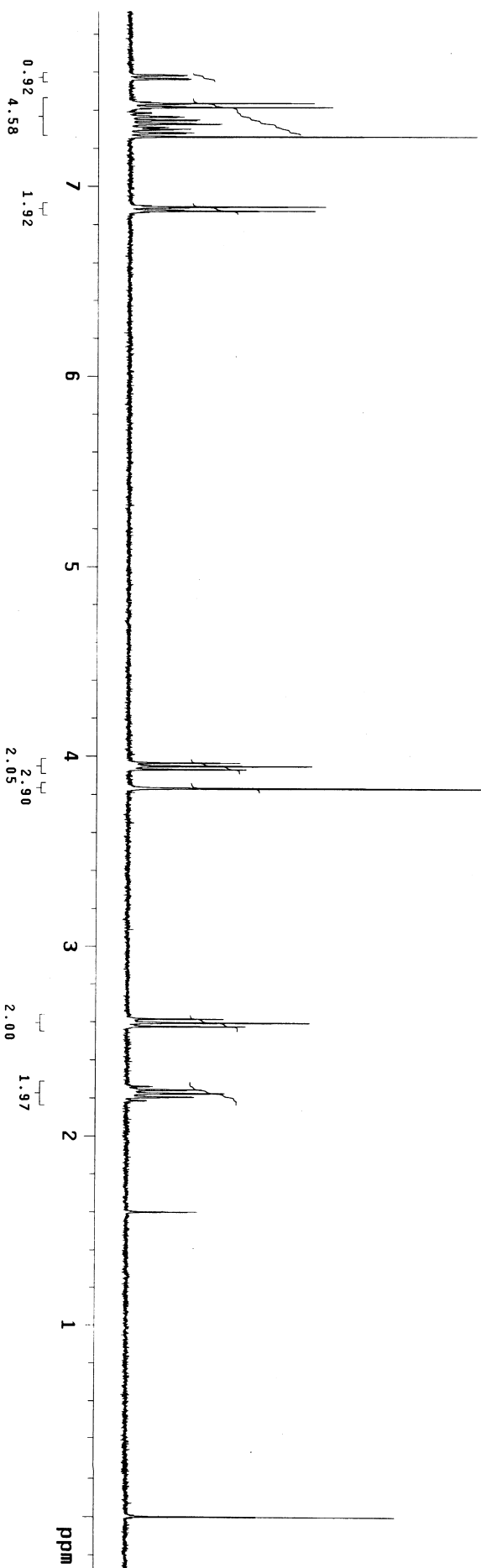
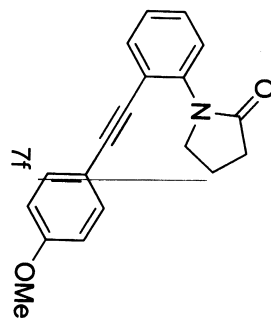


SAMPLE										SPECIAL	
date	Jun	9	2007	temp	25.0						
solvent	cdcl3	gain	30								
file	/home/walkup/~	spin	not used								
data	/zhang/li/633	hst	0.008								
	2carbon.tfid	pw90	15.3000								
		alfa	10.0000								
ACQUISITION				FLACS							
sw	30487.8										
at	1.300	11	n								
np	79298	in	n								
fb	17000	dp	n								
bs	64	hs	n								
d1	1.000		ny								
nt	1024	1b	not used								
ct	64	fn	0.50								
TRANSMITTER				DISPLAY							
tn	C13	sp	-2047.6								
sfreq	125.688	wd	30487.3								
tof	12553	rfl	2048.0								
tpwr	49	rtp	0								
dw	7.650	fp	-20.9								
		1p	-309.3								
DECOUPLER				PLOT							
dn	H1	wc	250								
dof	0	sc	0								
dm	yyv	vs	17188								
dmm	w	th	8								
dpwr	39										
dmf	12200	at	cdc	ph							



exp5 Proton

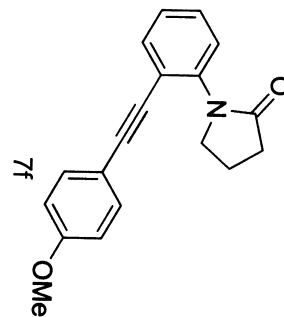
SAMPLE		SPECIAL	
date	Jun 25 2007	temp	25.0
solvent	cdcl3	gain	20
file	/mnt/nmr400/w-	spin	not used
akup	data/Zhang/G-	nst	0.008
uotaol	K184-1.fid	pw90	13.500
ACQUISITION		alpha	6.600
sw	6410.3	flags	
at	2.049	fl	n
np	25264	in	n
fb	4000	dp	y
bs	32	hs	nm
dl	1.000	PROCESSING	0.20
nt	8	lb	65536
ct	8	fn	
TRANSMITTER		DISPLAY	
tn	H1	sp	-116.4
sfreq	399.868	wd	3284.0
tof	399.6	rf1	799.1
tpwr	59	rfp	0
pw	6.750	fp	-104.0
DECOUPLER		lp	-30.0
dn	C13	plot	
dof	0	wc	250
dm	nmn	sc	0
dmm	c	vs	132518
dpwr	34	th	2
dmf	29412	ai	cdc
		ph	



```

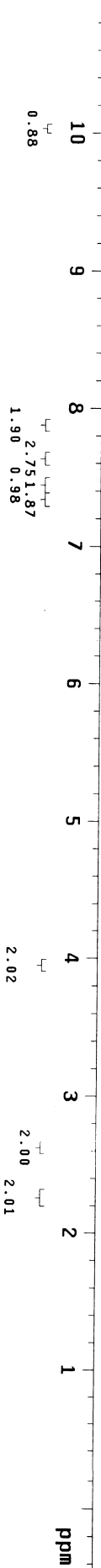
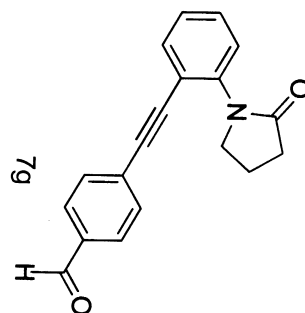
expt Carbon
SAMPLE
date Jun 26 2007 temp 25.0
solvent cdc13 gain 30
file exp not used
ACQUISITION
sw 30487.8 hst 0.008
at 1.300 pw50 15.300
np 79298 alfa 10.000
fb 17000 flags n
bs 8 in n
dl 1.000 dp y
nt 1024 hs nn
ct 456 PROCESSING 1.00
TRANSMITTER C13 fb fn not used
stfrq 125.688 sp DISPLAY
tof 1255.3 wp -2077.9
tpwr 49 rfp 30487.3
pw 7.650 rfp 11755.3
DECOUPLER H1 rf 9676.9
dn H1 fd 33.0
dof 0 lp -214.2
dm yyy PLOT
dmm w 250
dpwr w 39
dmf 12200 th 46606
at cdc ph 9

```



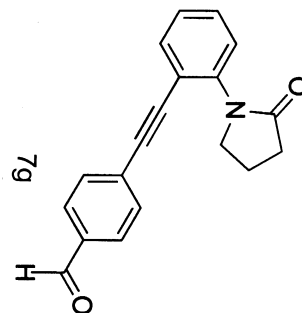
exp2 Proton

SAMPLE		SPECIAL	
date	Jun 21 2007	temp	not used
solvent	cdc13	gain	20
file	/mnt/nmr400/w-	spin	20
alkup/data/Zhang/G-	hst	0.008	
notao1/K171-2.fid	pw90	13.500	
ACQUISITION	alfa	6.600	
sw	6410.3	11	n
at	2.049	in	n
np	26264	dp	y
fb	4000	hs	nm
bs	32	fn	0.20
dl	1.000	PROCESSING	65536
nt	8	1b	0.20
ct	8	fn	65536
TRANSMITTER			
tn	H1	sp	-185.6
sfrq	399.868	wd	4542.0
tof	399.6	rfl	798.2
tdwr	59	rfl	-23.3
pw	6.750	tp	-26.0
DECOUPLER			
dn	C13	1p	
dof	0	WC	PLOT
dm	nn	sc	250
dmm	c	vs	0
dpwr	34	th	2419
dmf	29412	ai	2
	cdc	ph	



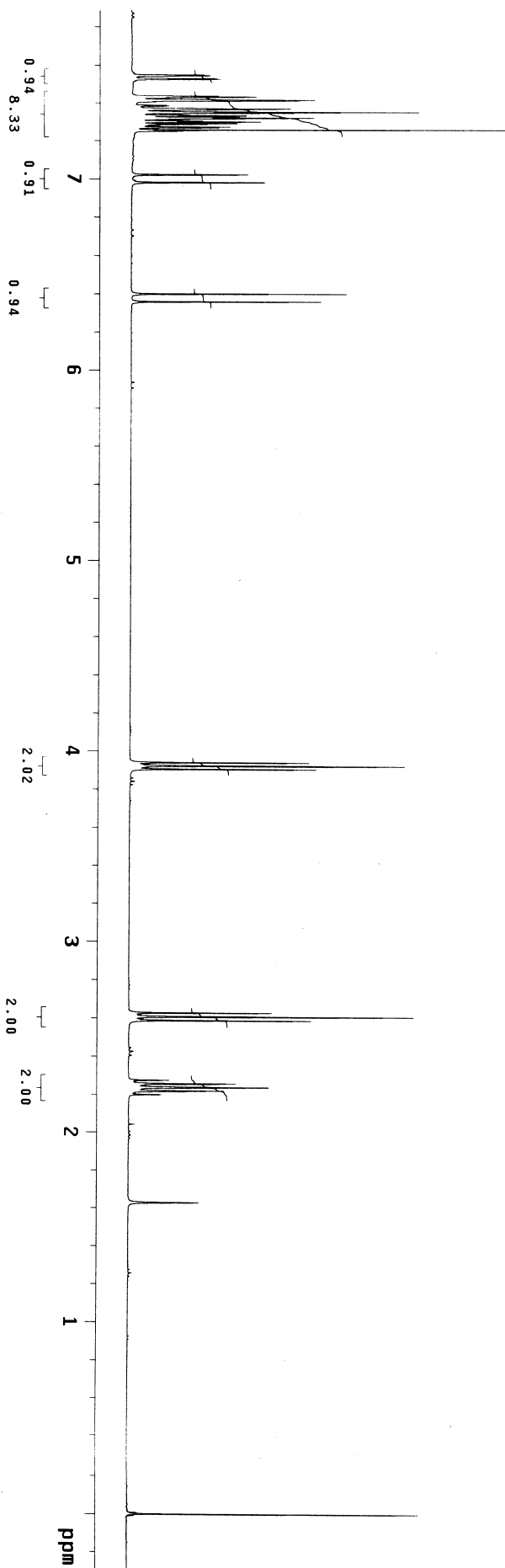
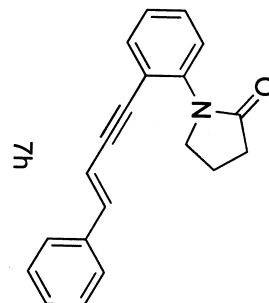
expi Carbon

SAMPLE SPECIAL
date Jun 21 2007 temp 25.0
solvent cdc13 gain 30
file /home/walkup/~ not used
vmr/sys/data/auto_~ hst 0.008
2007.06.21_03/Aug.~ pw90 15.300
01/data/cdc13_01.f~ alfa 10.000
id
ACQUISITION
sw 30487.8 f1 n
at 1.300 in y
np 79298 dp nm
fb 17000 hs PROCESSING 0.50
bs 64 lb not used
d1 1.000 fn DISPLAY
nt 1800 not used
ct 1800
TRANSMITTER
tn C13 sp -2077.4
sfq 125.688 wf 30487.3
tof 1255.3 rfp 11754.9
tpwr 7.650 fp 9676.9
pw 7.650 lp -17.8
DECOUPLER WC PLOT -237.7
dn H1 wc 250
dof H1 sc 0
dm 0 vs 69796
dmm yyv th 8
dpwr w al cdc ph
dmf 12200



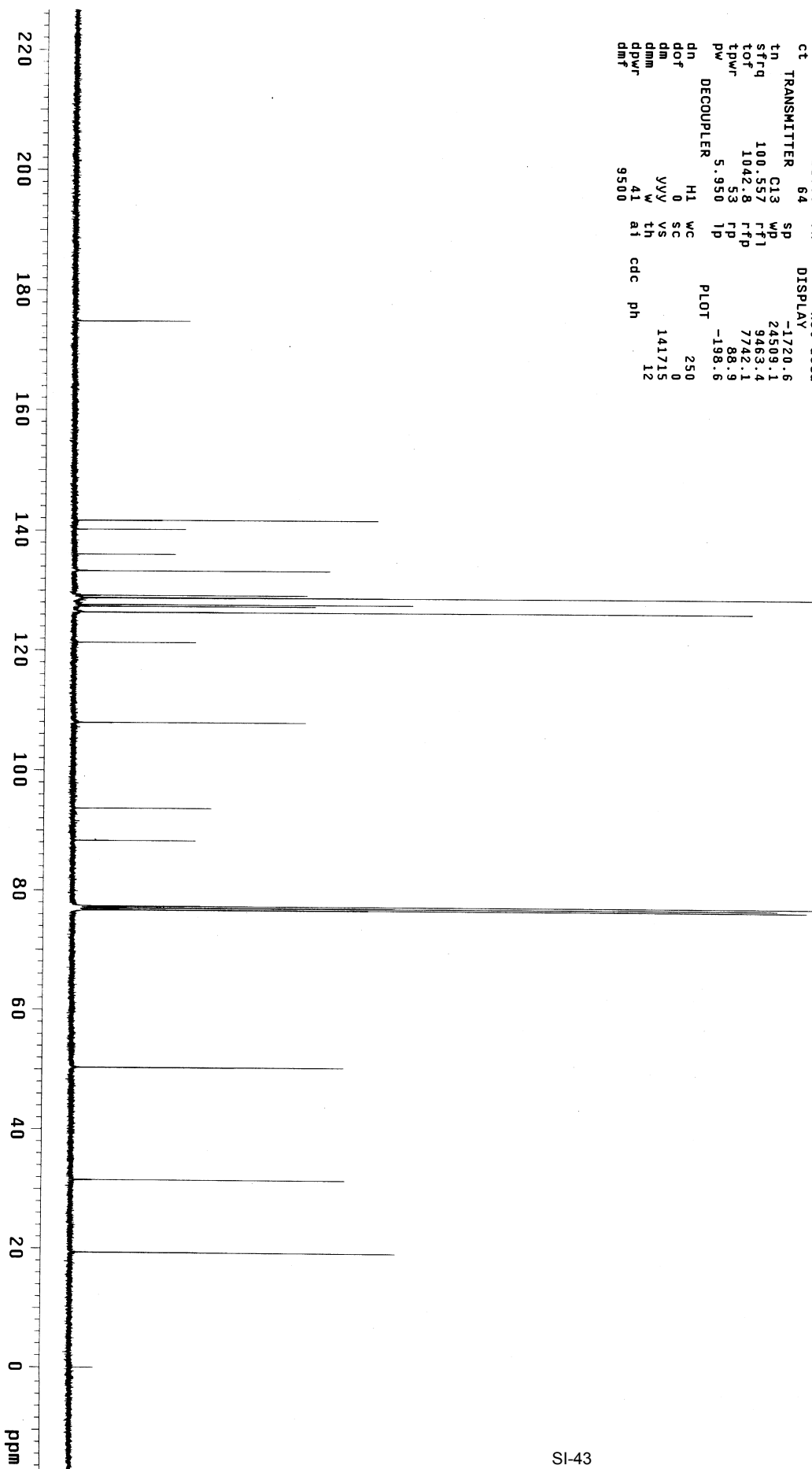
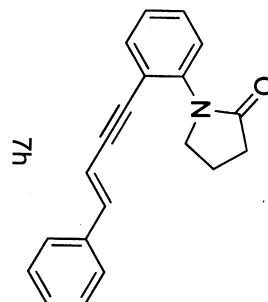
exp2 Proton

SAMPLE		SPECIAL	
date	Jun 11 2007	temp	25.0
solvent	cdcl3	gain	20
file	/mnt/nmr/400/w~	spin	20
alkup/data/zhang/G~	hst	0.008	
notatol/K114-2.fid	pw90	13.500	
ACQUISITION	alfa	6.500	
sw	6410.3	FLAGS	
at	2.049	11	n
np	25264	in	n
fd	4000	dp	y
bs	32	hs	nn
d1	1.000	PROCESSING	
nt	8	1b	0.20
ct	8	fn	65536
TRANSMITTER		DISPLAY	
tn	H1	sp	-124.8
sfrq	399.868	wd	3278.3
tof	399.6	rf1	800.1
tpwr	53	rfp	0
pw	6.750	fp	-98.4
DECOUPLER		1p	-27.5
dn	C13	PLOT	
dof	0	wc	250
dm	nn	sc	0
dmm	c	vs	1177
dpwr	34	th	3
dmf	29412	ai	cdc
		ph	



exp2 Carbon

SAMPLE		SPECIAL	
date	Jun 11 2007	temp	25.0
solvent	cdcl3	gain	30
file	/home/walkup/~	spin	20
mar400/walkup/data~	hst	0.008	
/Zhang/Guotaoli/K1~	pw90	11.900	
14-2carbon.fid	ai fa	10.000	
ACQUISITION		FLAGS	
sw	24509.8	fl	n
at	1.300	in	n
np	63750	dp	y
fb	17000	hs	nn
bs	64	PROCESSING	
d1	1.000	lb	0.50
nt	12000	fn	not used
ct	64	DISPLAY	
TRANSMITTER		sp	-1720.6
tn	C13	wp	24508.1
sfreq	100.557	rf1	9468.4
tor	1042.8	rfp	7742.1
tpwr	53	fp	88.9
pw	5.950	lp	-198.6
DECOUPLER		PLOT	
dn	H1	wc	250
dof	0	sc	0
dm	yyv	vs	141715
dmm	w	th	12
dpwr	41	ai	cdc
dnt	9500	ph	

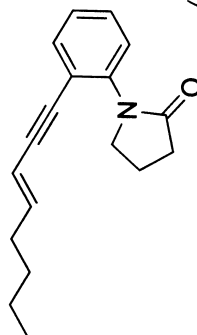


Automation directory: /home/walkup/vnmrsys/data/auto_2007.06.27
File: s_20070627_001/data/cdc13_01.fid
Sample id: s_20070627_001

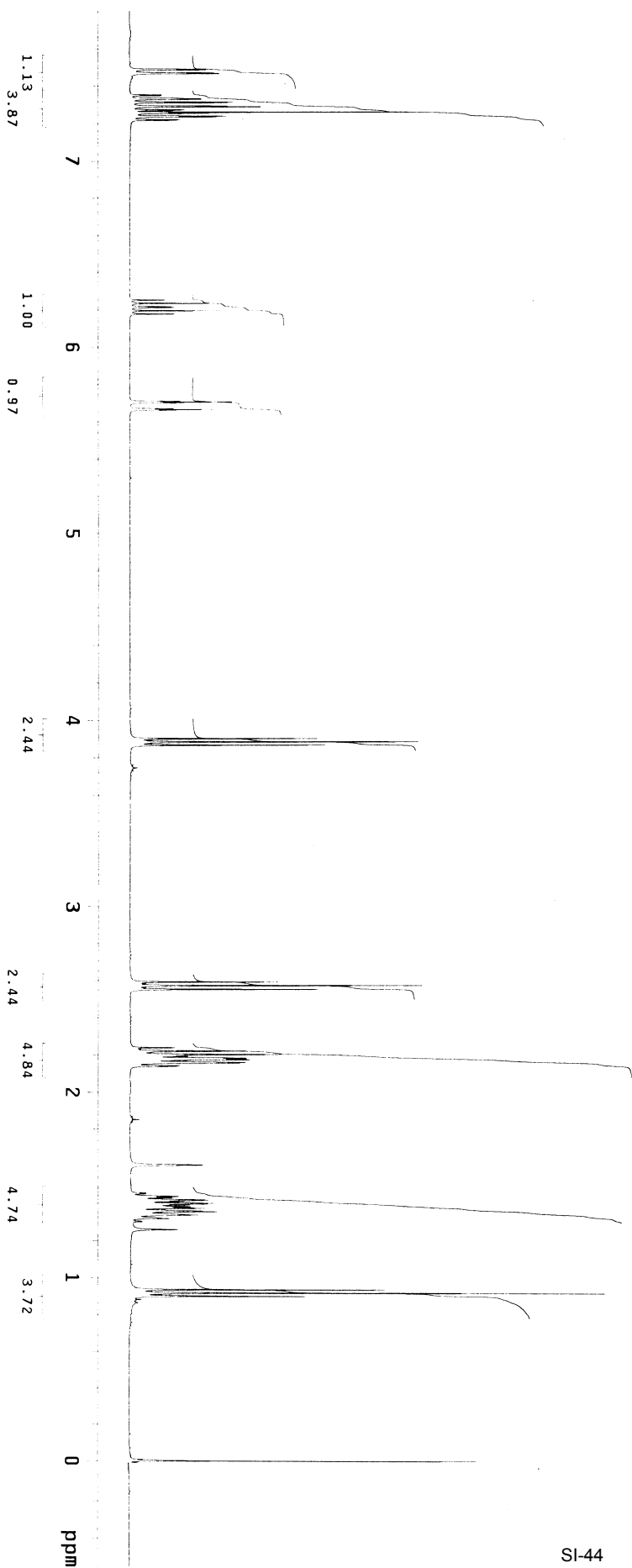
Pulse Sequence: szpul

Solvent: cdc13
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 399.8656721 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min, 30 sec



71



expi Carbon

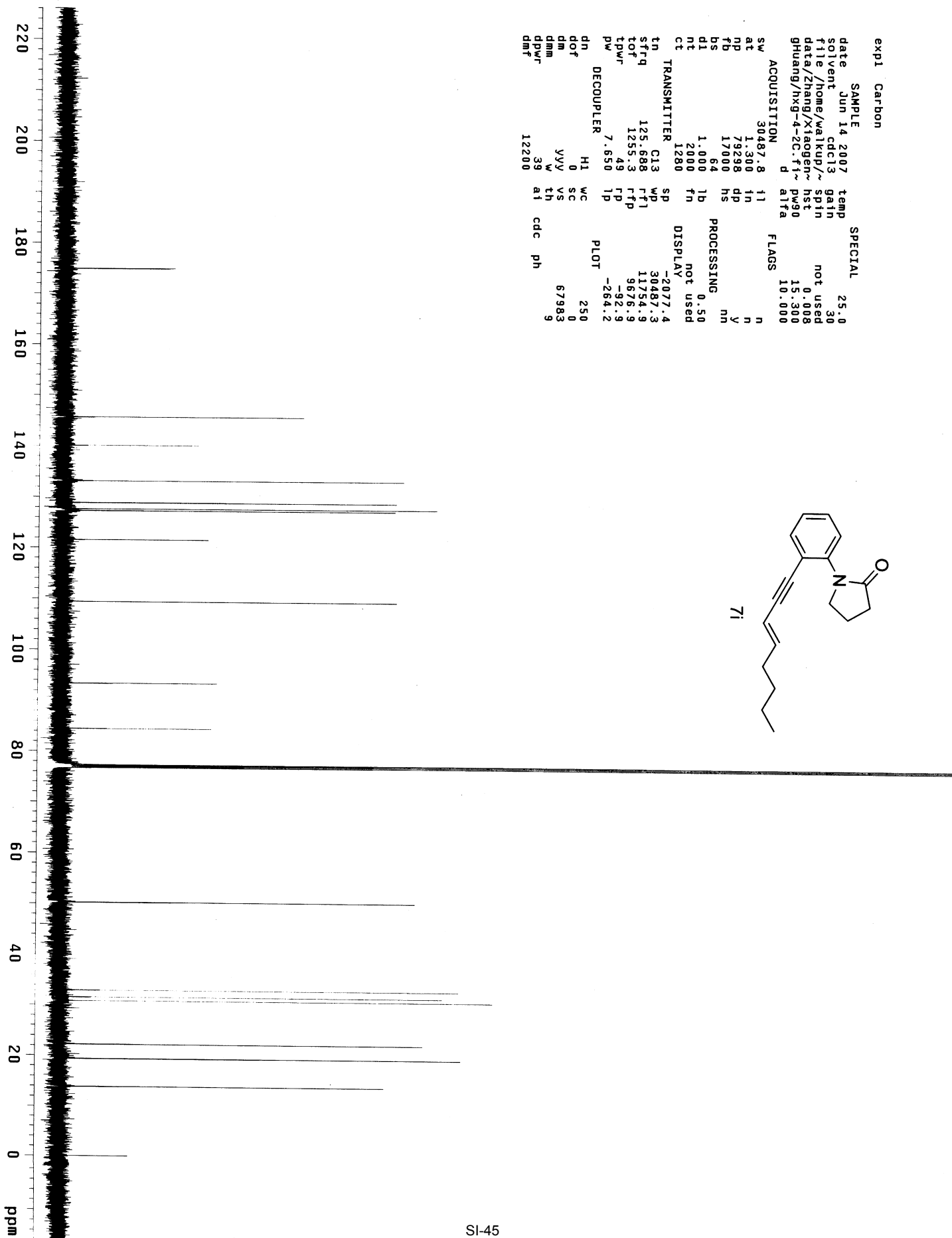
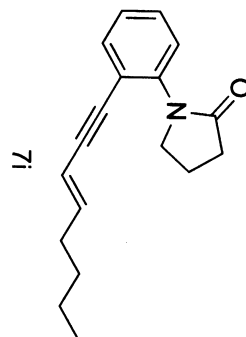
SAMPLE SPECIAL
date Jun 14 2007 temp 25.0
solvent cdc13 gain 30
file /home/walkup/~ not used
data/Zhang/X1aogen~ hst 0.008
ghuang/hxg-4-2C.f1~ pw90 15.300
d alfa 10.000

ACQUISITION
sw 30487.8 f1
at 1.300 f2
np 79298 dp
fb 17000 hs
bs 64
d1 1.000 lb
nt 2000 fn
ct 1280
TRANSMITTER
tn C13 sp -2077.4
sfreq 125.688 wf 30487.3
tof 1255.3 rfi 11754.9
tpwr 49 rfp 9676.9
pw 7.650 tp -92.9
-264.2

DECOUPLER
dn H1 wc
dof 0 sc 250
dm 0 vs
dmm VVV 67983
dpwr w th
dmf 39 at cdc ph
12200

PROCESSING
0.50
not used
nn
DISPLAY
not used

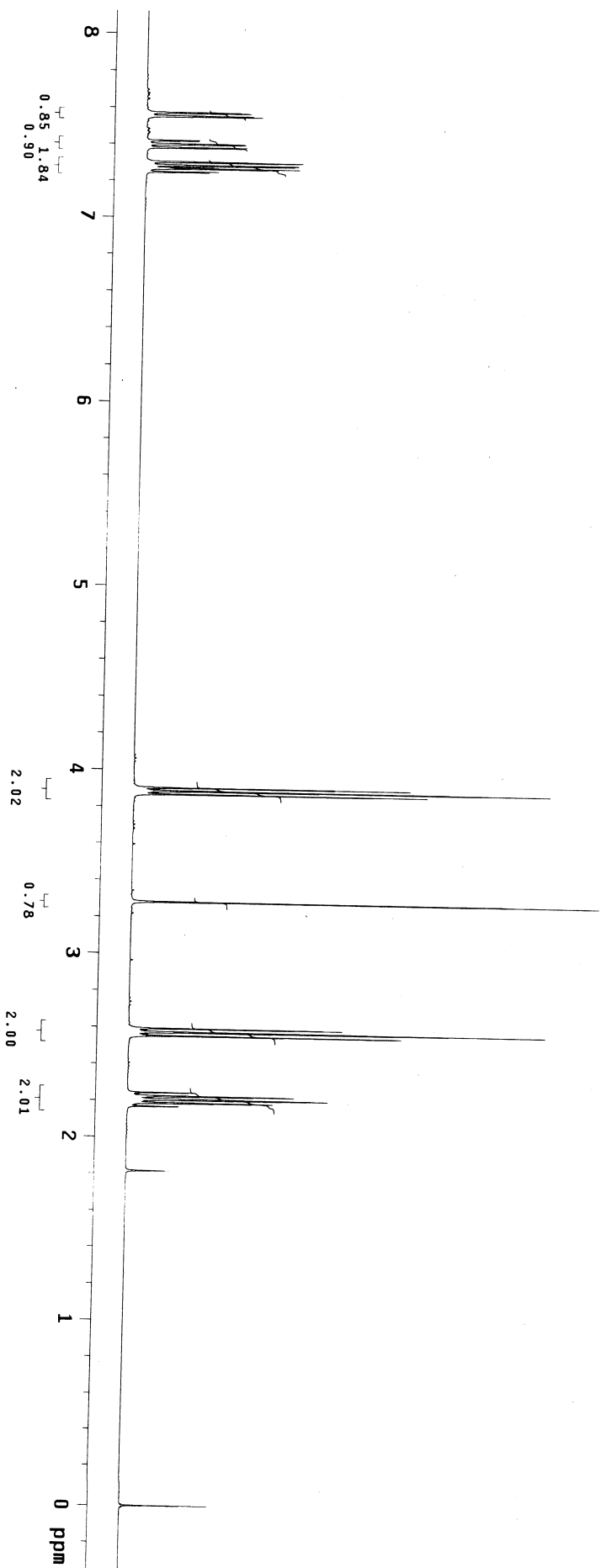
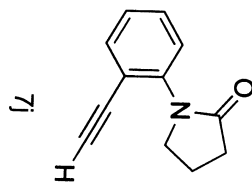
PLOT
250
0
67983
9



STANDARD 1H OBSERVE - profile

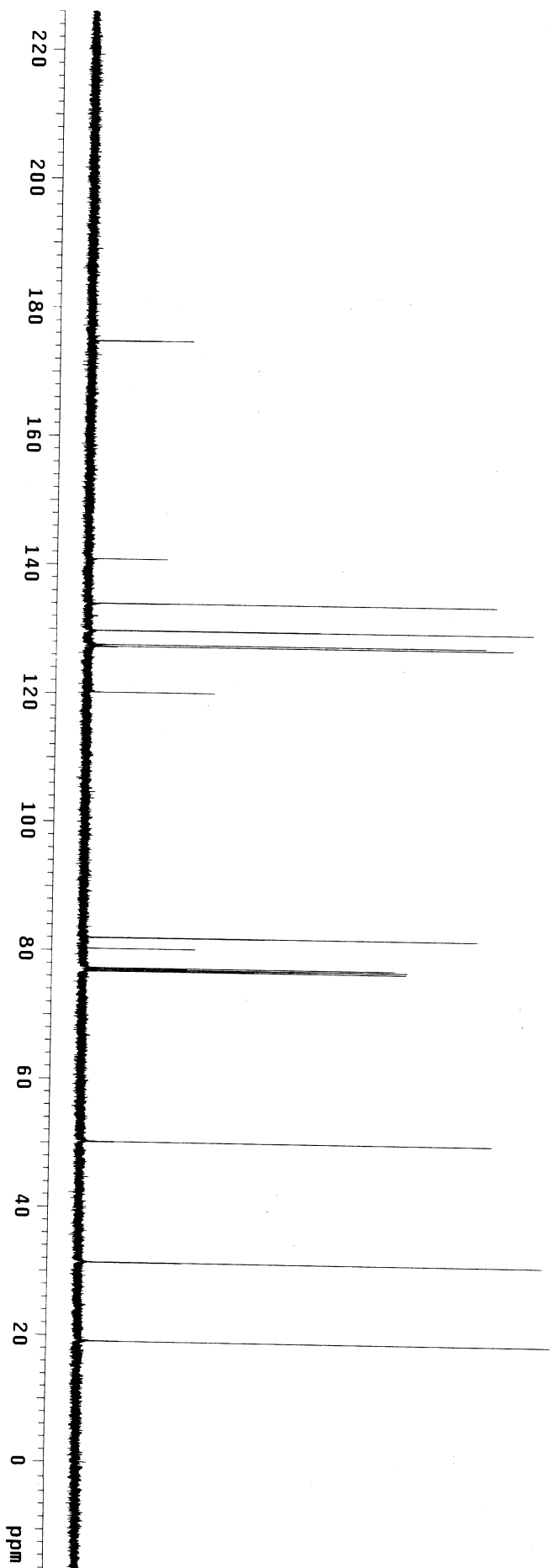
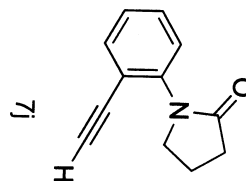
exp2 Proton

SAMPLE		SPECIAL	
date	Jun 9 2007	temp	25.0
solvent	cdcl3	gain	20
file	/mnt/nmr400/w~	spin	not used
akup/data	Zhang/G~	hst	0.008
uotaol/K94-2	.fid	pw90	13.500
ACQUISITION	alpha	6.600	
sw	6410.3	FLAGS	
at	2.049	11	n
np	26254	in	n
fb	4000	dp	y
bs	32	hs	nn
dl	1.000	hs	nn
nt	8	1b	0.20
ct	8	fn	65536
TRANSMITTER		PROCESSING	
tn	H1	sp	-148.9
stfrq	399.868	wp	3395.9
tof	399.6	rfl	794.8
tpwr	59	rtp	0
pw	6.750	tp	-97.6
DECOUPLER		PLOT	
dn	C13	1p	-26.3
dof	0	wc	250
dm	nnn	sc	0
dmm	c	vs	339
dpwr	34	th	2
dnt	29412	ai	cdc
		ph	



expt Carbon

SAMPLE 9 2007 SPECIAL 25.0
date Jun 9 2007 temp 25.0
solvent cdc13 gain 30
file exp hst not used
ACQUISITION 30487.8
sw 1.300 alfa 15.300
at 79298 n
np 17000 n
fb 64 n
bs 1.000 y
dl 1024 y
nt 128 nm
ct TRANSMITTER 128
tn 125.688 lb fn not used
strq 125.688 sp DISPLAY
tof 125.3 wp 30487.3
tpwr 49 rfi 11762.8
pw 7.650 rfp 9676.9
DECOUPLER H1 tp -28.3
dn 0 lp -287.0
dof 0 PLOT
dm yyy wc 250
dmw w 39
dmf 12200 vs 0
th 14226
aj cdc ph 11



STANDARD 1H OBSERVE - profile
 exp1 proton

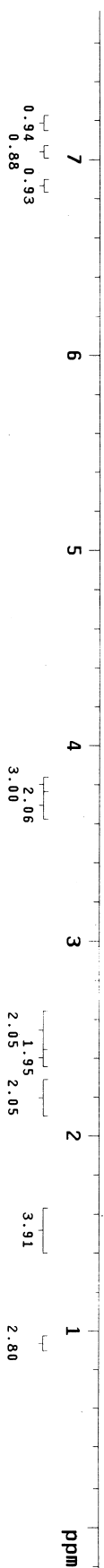
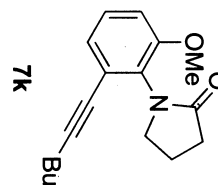
SAMPLE SPECIAL 24.0
 date Aug 4 2007 temp 30
 solvent cdc13 gain 30
 file /home/waikup/~ not used
 nmr400/waikup/data~ hst 0.008
 /Zhang/Guotaol1/K2~ pw90 13.500
 90-25.fid atfa 6.600

ACQUISITION 6410.3 f1
 sw 2.043 in n
 at 2.043 in n
 np 26264 dp y
 fb 4000 hs
 bs 8
 d1 1.000 lb 0.20
 nt 8 fn 65536

PROCESSING 0.20
 ct 8 fn 65536

TRANSMITTER 8
 tn H1 sp -96.4
 stfq 399.868 rfi 3201.4
 tof 399.6 rfp 788.8
 tpwr 59 fp 157.0
 pw 6.750 lp -21.6

DECOUPLER C13 wc 250
 dn 0 sc 0
 dof 0 sc 0
 dm mn vs 57
 dmm c th 2
 dpwr 34 ai cdc ph
 dmf 29412



expl Carbon

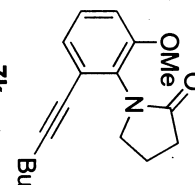
SAMPLE

SPECIAL

date Aug 4 2007 temp 24.0
solvent cdcl3 gain 30
file /home/walkup/~ not used
nmr sys/data6/autoc~ hsf 0.008
2007.08.04.06.3.20~ p990 11.900
070804_001/data/cd~ atfa 10.000

070804_001

FLAGS



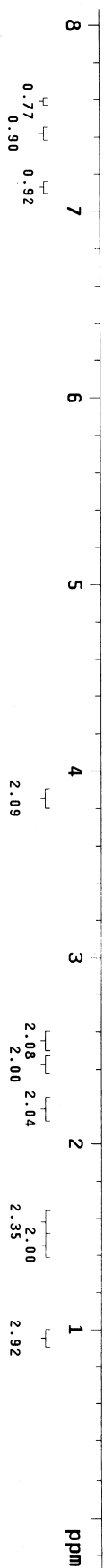
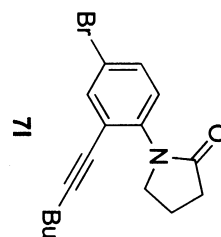
7k

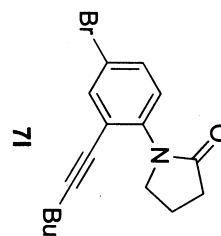
ACQUISITION
sw 24509.8 tn 11 n
at 1.300 dp 1 y
np 63750 hs
fb 17000
bs 64 lb
dl 1.000 fn not used
nt 3200
ct 64 sp
TRANSMITTER
tn C13 wp -1733.3
sfreq 100.557 rfi 24509.1
tof 1042.8 rfp 9476.2
tpwr 53 lp -152.2
pw 5.950
DECOUPLER
dn H1 wc 250
dof 0 sc 0
dm yyy th 17546
gmm ai cdc ph 68
gdwr 41
gnt 9500

220 200 180 160 140 120 100 80 60 40 20 0 ppm

expt Proton

SAMPLE		SPECIAL	
date	Jul 30 2007	temp	25.0
solvent	cdcl3	gain	60
file	/mnt/nmr400/w~	spin	not used
alkun/data/zhang/G~		hst	0.008
notaoi/K283-3.fid		pw30	13.500
ACQUISITION		atfa	6.600
sw	6410.3	flags	
at	2.049	n	n
np	26264	in	n
fb	4000	dp	y
bs	8	hs	nm
d1	1.000	PROCESSING	
nt	8	lb	0.20
ct	8	fn	6536
TRANSMITTER			
tn	H1	sp	DISPLAY
sfrq	399.868	wp	-120.1
tof	399.6	rfl	3352.8
tpwr	59	rfl	798.0
pw	6.750	rp	172.6
DECOUPLER	C13	lp	-33.4
dn	0	PLOT	
dof	0	wc	250
dm	nmn	sc	0
dmm	c	vs	21
dpr	34	th	3
dnt	29412	ai	cdc
		ph	

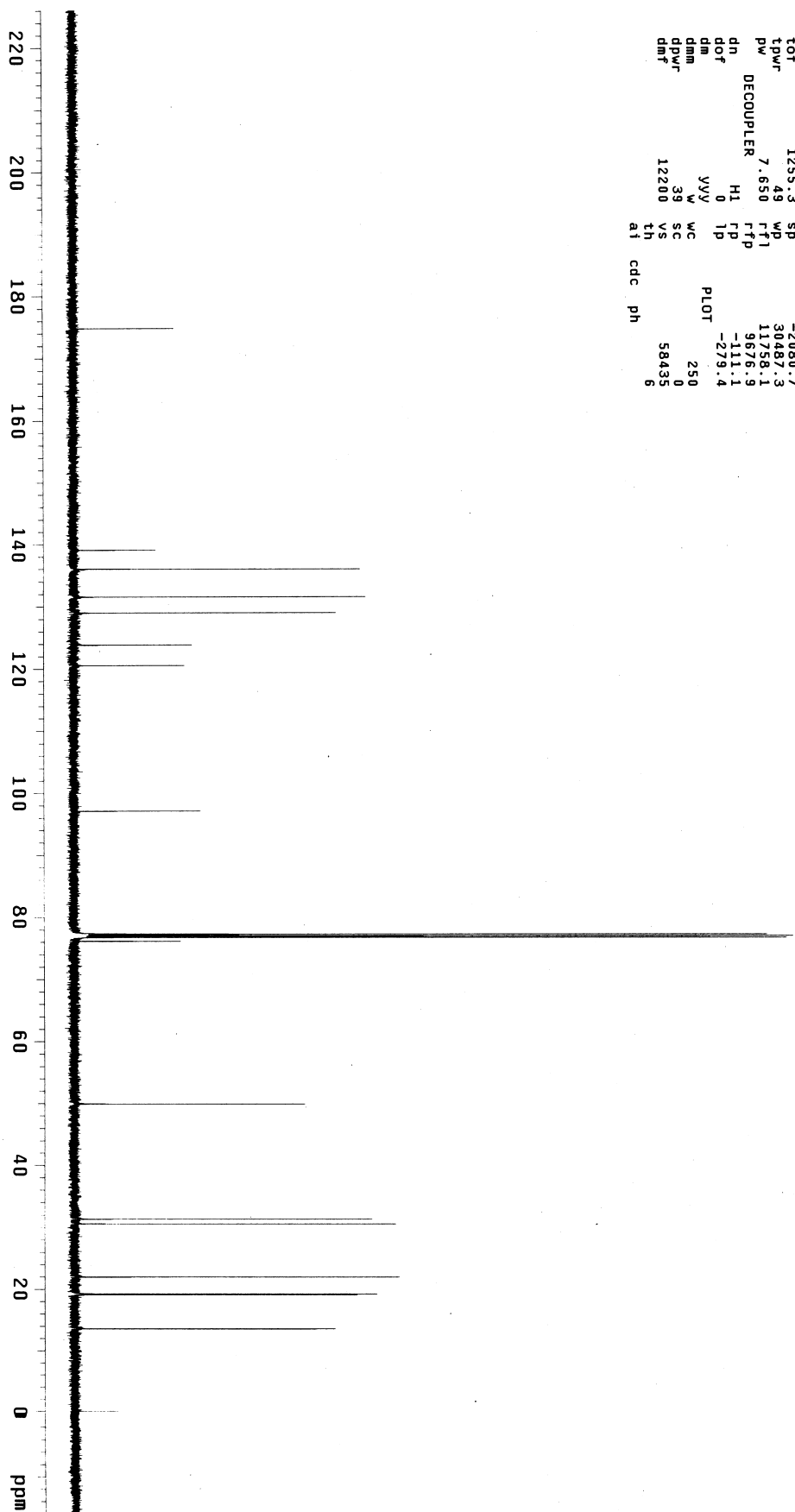




```

expt Carbon
SAMPLE
date Jul 31 2007 temp 25.0
solvent cdcl3 gain 30
file ACQUISITION exp hst not used
file ACQUISITION exp hst 0.008
sw 30487.8 pw90 15.300
at 1.300 atfa 10.000
np 79288
fb 17000
bs 64
d1 1.000 dp
nt 2000 hs
ct TRANSMITTER 1600 PROCESSING 0.50
tn tn 1b not used
sfreq 125.688 sp DISPLAY -2080.7
tof 1255.3 wp 30487.3
tpwr 49 rfi 11758.1
pw 7.650 rfp 9676.9
DECOUPLER H1 lp -111.1
dn 0 PLOT -279.4
dof 0
dm yvy 250
dmm w 39
dpmr sc 0
dmf 12200 vs 58435
th ai cdc ph 6

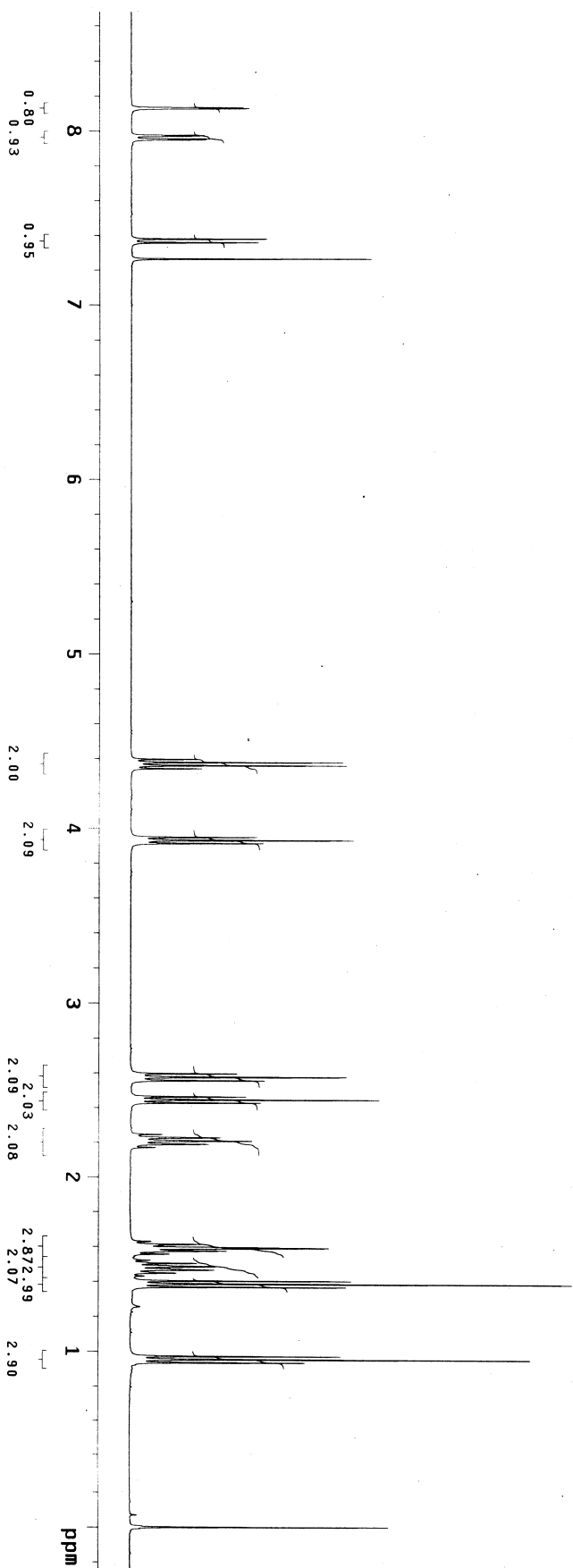
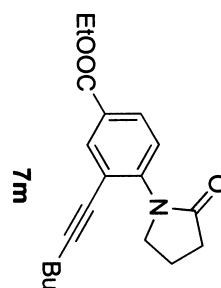
```



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

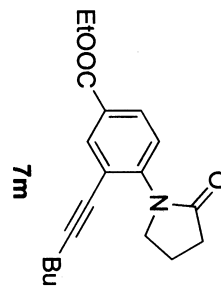
expt Proton

SAMPLE		SPECIAL	
date	Aug 3 2007	temp	25.0
solvent	cdcl3	gain	30
file	/home/walshp/~	spin	not used
nmr400	walshp/data/~	hst	13.500
/Zhang/Su03a01/K2~	pw90		6.600
532.110	atfa		
ACQUISITION		FLAGS	
sw	6410.3	f1	n
at	2.049	in	y
np	26264	dp	nn
fb	4000	hs	
bs	8		
d1	1.000	lb	0.20
nt	8	fn	65536
ct	8		
TRANSMITTER		DISPLAY	
tn	H1	sp	-105.4
sfrq	399.868	wp	3576.2
tof	399.6	rfl	797.8
tdwr	59	rpf	0
pw	6.750	lp	151.0
DECOUPLER		PLOT	
dn	C13	wc	250
dof	0	sc	0
dm	nmh	vs	699
dmm	c	th	3
ddwr	34	ai	cdc
dntf	29412	ph	



expt1 Carbon

SAMPLE SPECIAL 25.0
date Aug 3 2007 temp 30
solvent cdc13 gain 30
f1le /home/wai/kup/~ not used
vnmr/sys/data/autoc~ nst 0.008
2007.08.03/s-20070~ pw90 11.900
803_001/data/cdc13~ alfa 10.000
01.fid
ACQUISITION
sw 24509.8 in 11 n
at 1.300 dp hs y
np 63750 hs nh
fb 17000 lb
bs 64 fn not used
d1 1.000 not used
nt 12000
ct 64
TRANSMITTER
tn C13 sp -1719.1
stfq 100.557 wp 24509.1
tof 1042.8 rfp 9481.9
tpwr 53 lp -171.9
pw 5.950 PLOT -202.9
DECOUPLER
dn H1 WC 250
dof 0 SC 0
dm 0 VS 160246
dmm W yyy th 11
dpwr w at cdc ph
dmf 9500



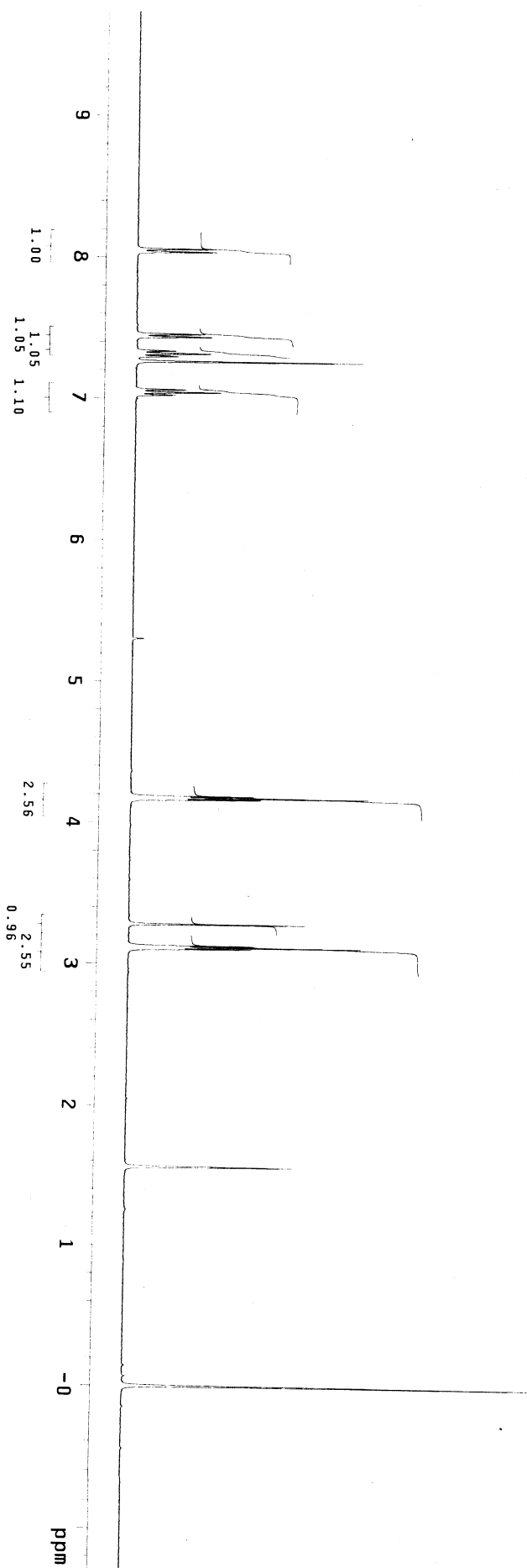
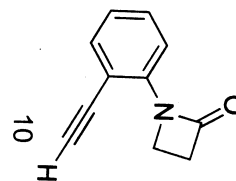
220 200 180 160 140 120 100 80 60 40 20 0 ppm

Automation directory: /home/walkup/vnmr/sys/data/auto_2007.06.01_34
File : s_20070601_001/data/cdc13_02.fid
Sample id : s_20070601_001

Pulse Sequence: s2pu1

Solvent: cdc13
Temp: 25.0 C / 298.1 K
Operator: walkup
File: cdc13_02
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, 399.8656717 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min, 30 sec

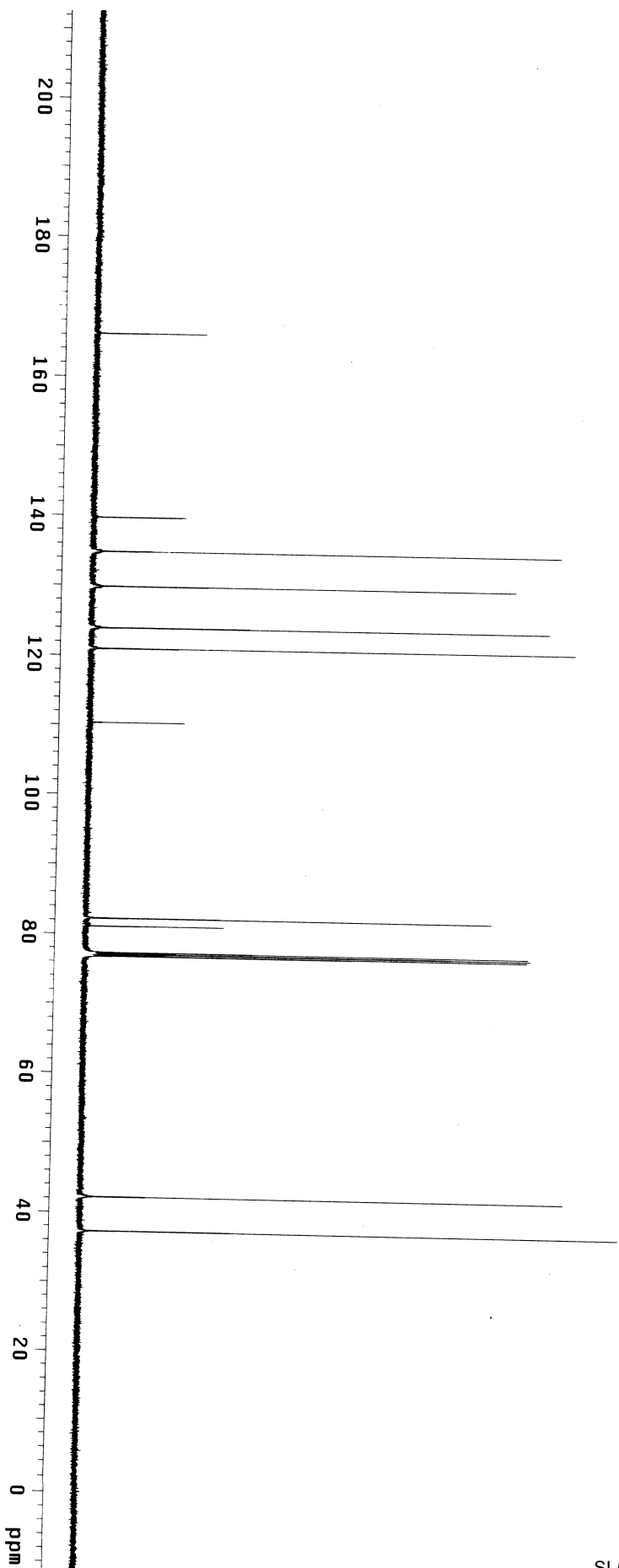
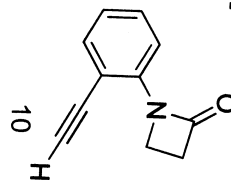


Automation directory: /home/walkup/vnmrSYS/data/auto_2007.06.10_01
File : Aug.02/data/cdc13_01.fid
Sample id : Aug.02

Pulse Sequence: szpu1

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
1728 repetitions
OBSERVE C13, 125.6746077 MHz
DECOUPLE H1, 499.8016622 MHz
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 1 hr, 18 min, 49 sec

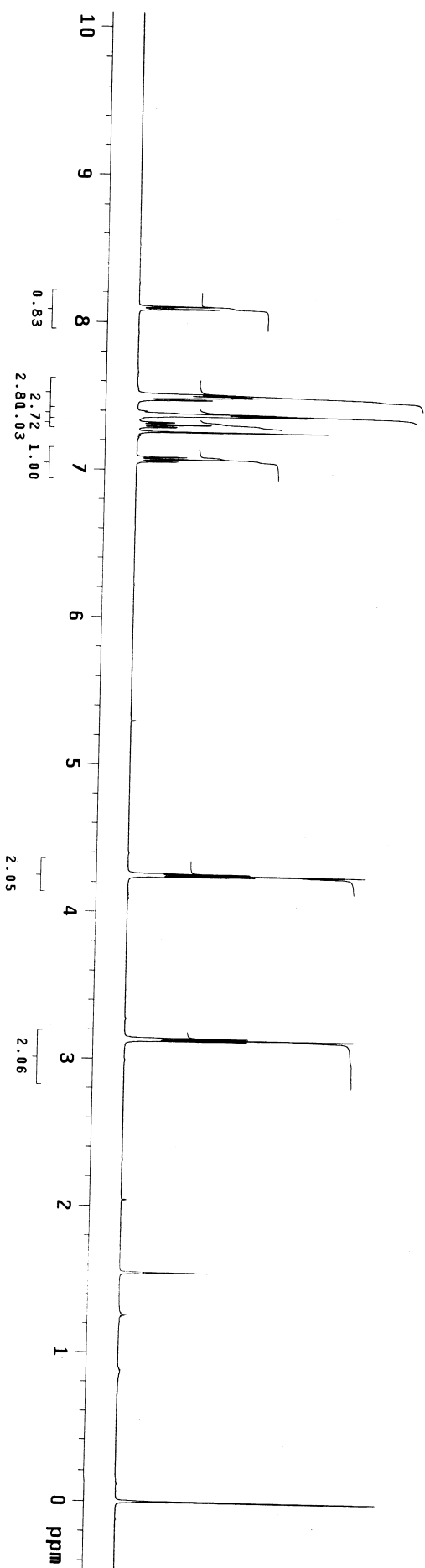
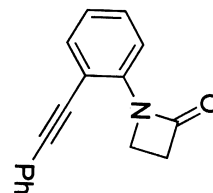


Automation directory: /home/walkup/vnmrsys/data/auto_2007.06.25_15
File : Aug.01/data/cdcl3_01.fid
Sample id : Aug.01

Pulse Sequence: szpu1

Solvent: cdcl3
Temp: 25.0 C / 298.1 K
Operator: walkup
File: cdcl3_01
VNMRS-500 "nmr500"

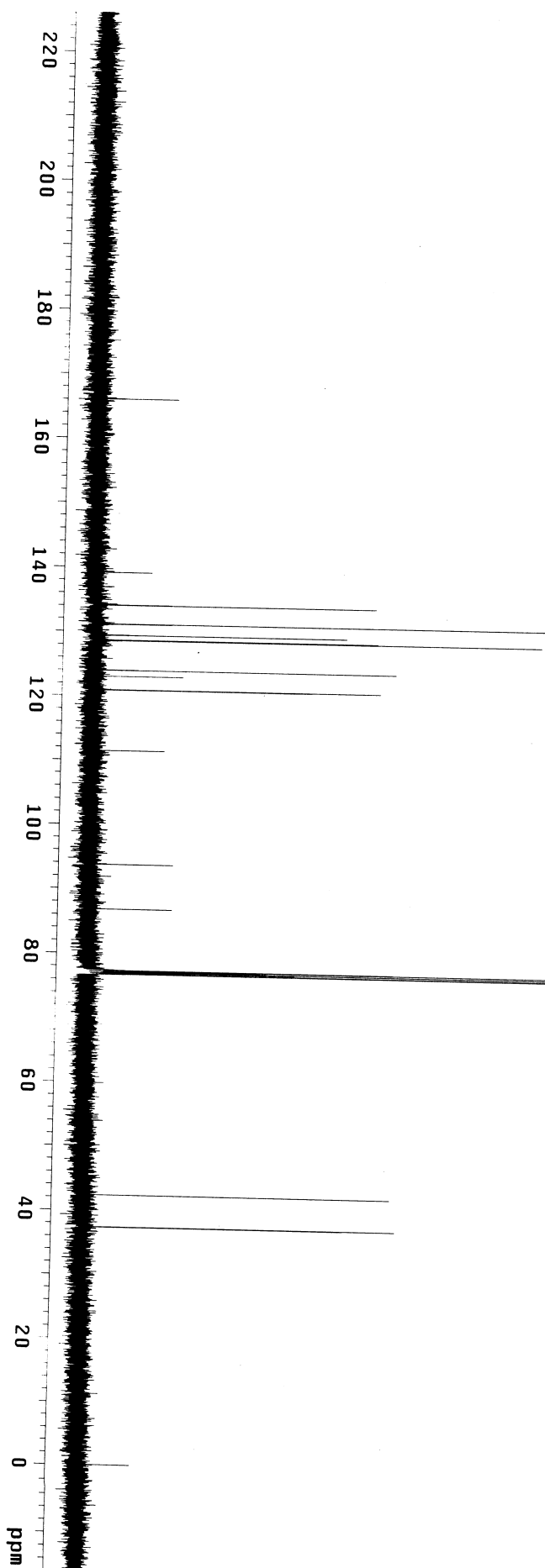
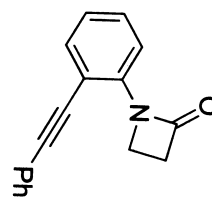
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.049 sec
Width 8012.8 Hz
8 repetitions
OBSERVE H1 499.791639 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min, 30 sec



Automation directory: /home/walkup/vnmrSYS/data/auto_2007.06.25_15
File : exp
Sample id : tmpstudy

Pulse Sequence: szpu1
Solvent: cdcl3
Temp: 25.0 C / 298.1 K
Operator: walkup
Vnmrs-500 "nmr500"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 30487.8 Hz
576 Repetitions
OBSERVE C13, 125.6746039 MHz
DECOUPLE H1, 499.8016822 MHz
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 39 min, 24 sec

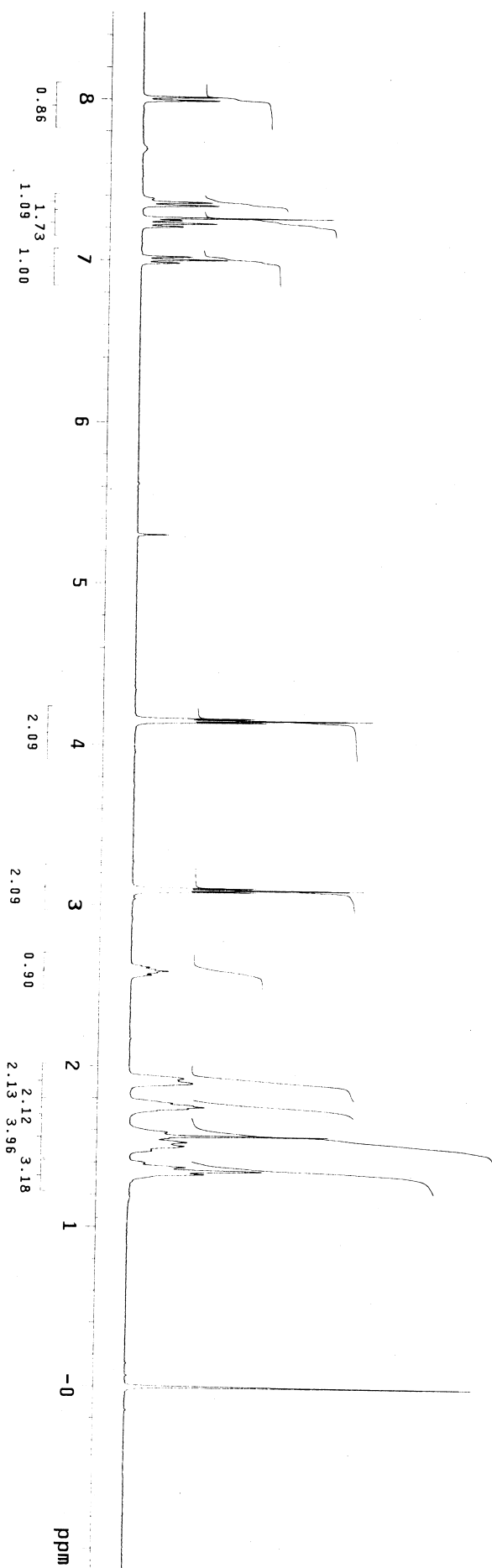
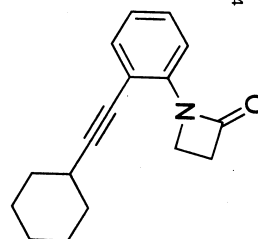


Automation directory: /home/walkup/vnmrsvs/data/auto_2007.06.01_34
File: s_20070601_003/data/cdc13_03.fid
Sample id: s_20070601_003

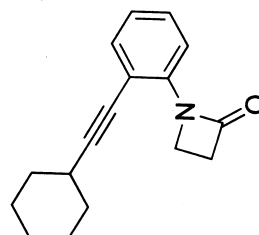
Pulse Sequence: szpul

Solvent: cdcl3
Temp: 25.0 C / 298.1 K
Operator: walkup
File: cdc13_03
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, 399.8656715 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min, 30 sec



File: hxg-3-145C
 Pulse Sequence: s2pu1
 Solvent: cdcl3
 Temp: 25.0 C / 298.1 K
 Operator: walkup
 File: hxg-3-145C
 INOVA-500 "sittingbu11"
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.300 sec
 Width 30487.8 Hz
 2240 repetitions
 OBSERVE C13, 125.6746013 MHz
 DECOUPLE H1, 499.8016822 MHz
 Power 39 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 131072
 Total time 2 hr, 33 min, 57 sec



File: hxg-3-159H

Pulse Sequence: szpu1

Solvent: cdcl3

Temp: 22.0 C / 295.1 K

Operator: wai kup

File: hxg-3-159H

INOVA-500 "redjacket"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.049 sec

Width 8012.8 Hz

8 repetitions

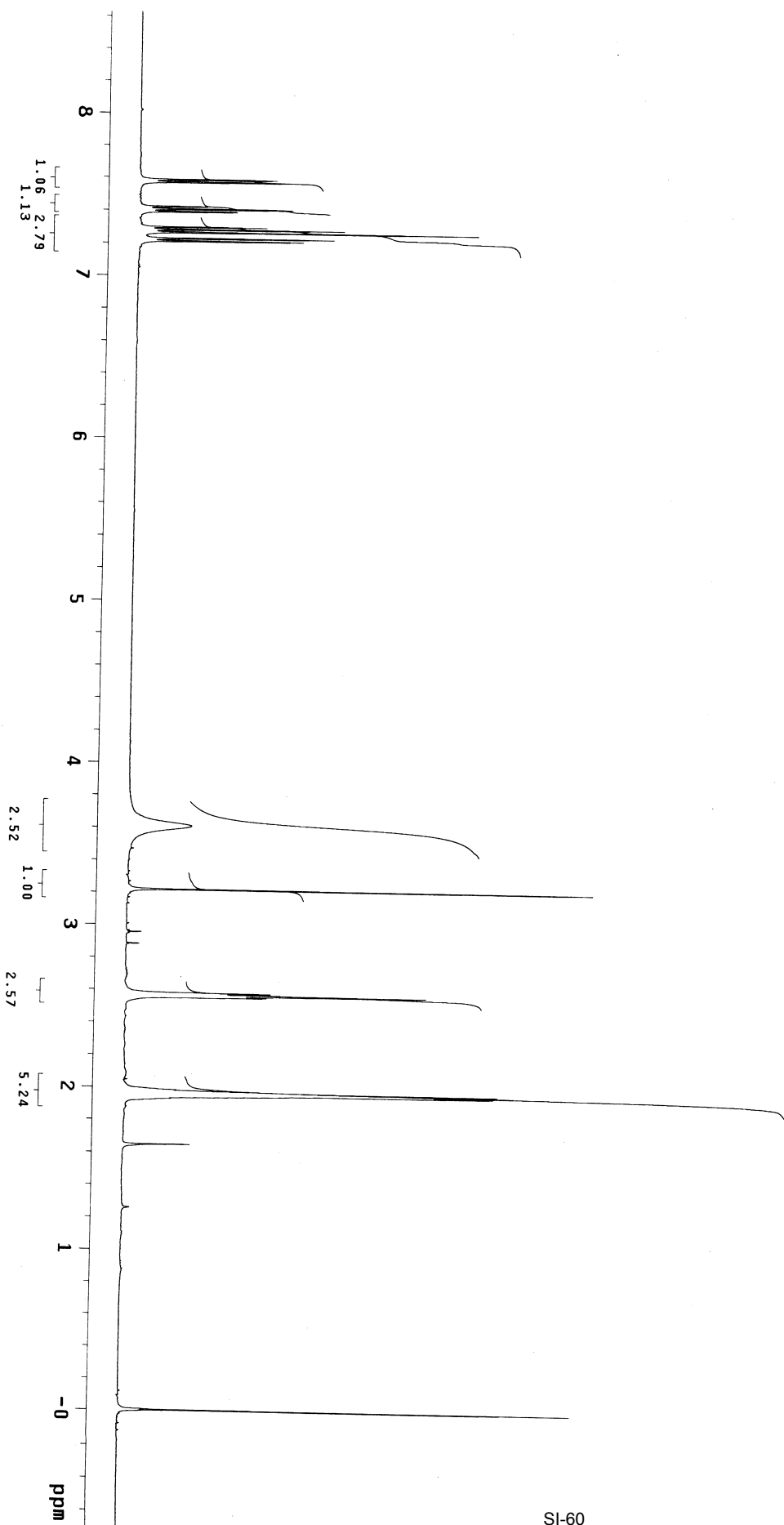
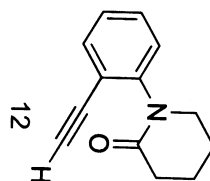
OBSERVE H1, 499.791815 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 0 min, 30 sec



File: hxg-3-159C

Pulse Sequence: szpu1

Solvent: cdcl3

Temp: 22.0 C / 295.1 K

Operator: wai kup

File: hxg-3-159C

INOVA-500 "redjacket"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 30487.8 Hz

S12 repetitions

OBSERVE C13, 125.6746067 MHz

DECOUPLE H1, 499.8016822 MHz

Power 39 dB

continuously on

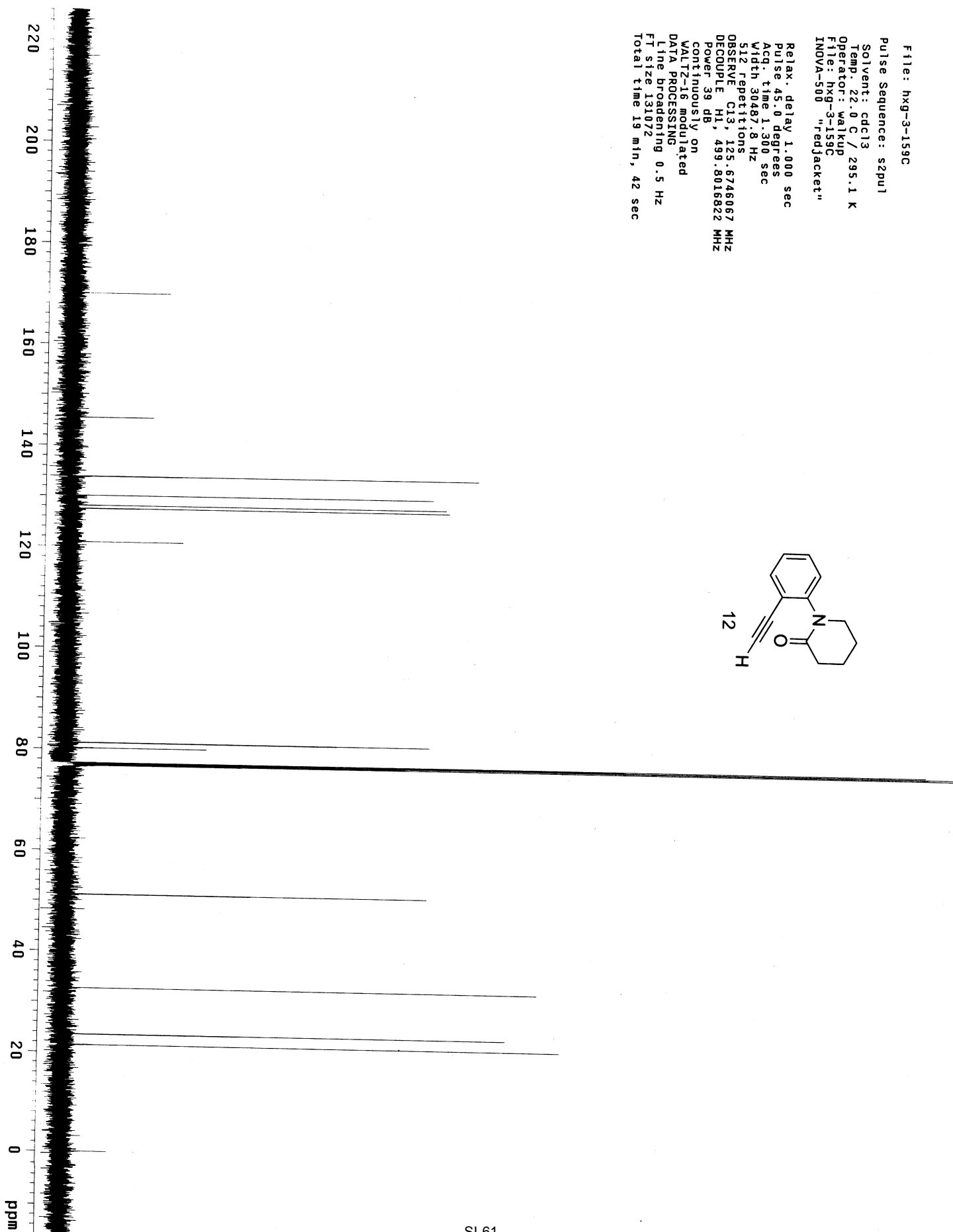
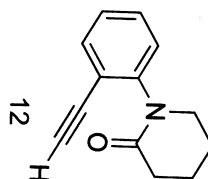
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

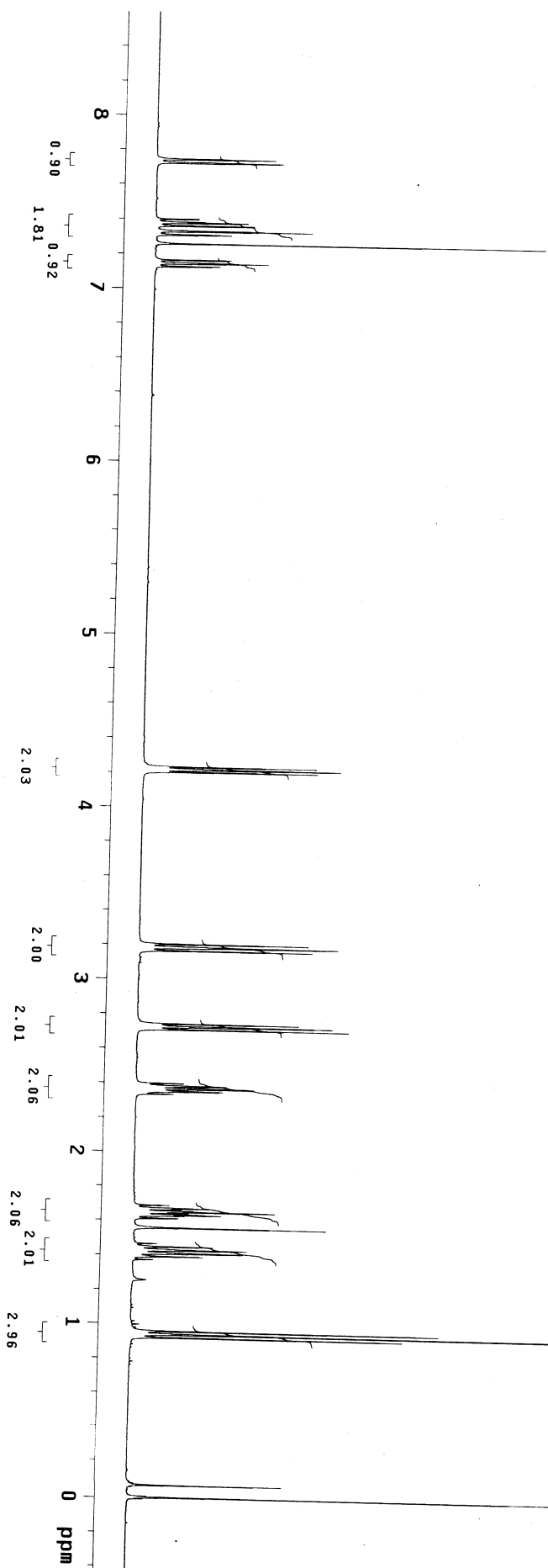
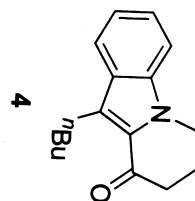
FT size 131072

Total time 19 min, 42 sec



exp2 Proton

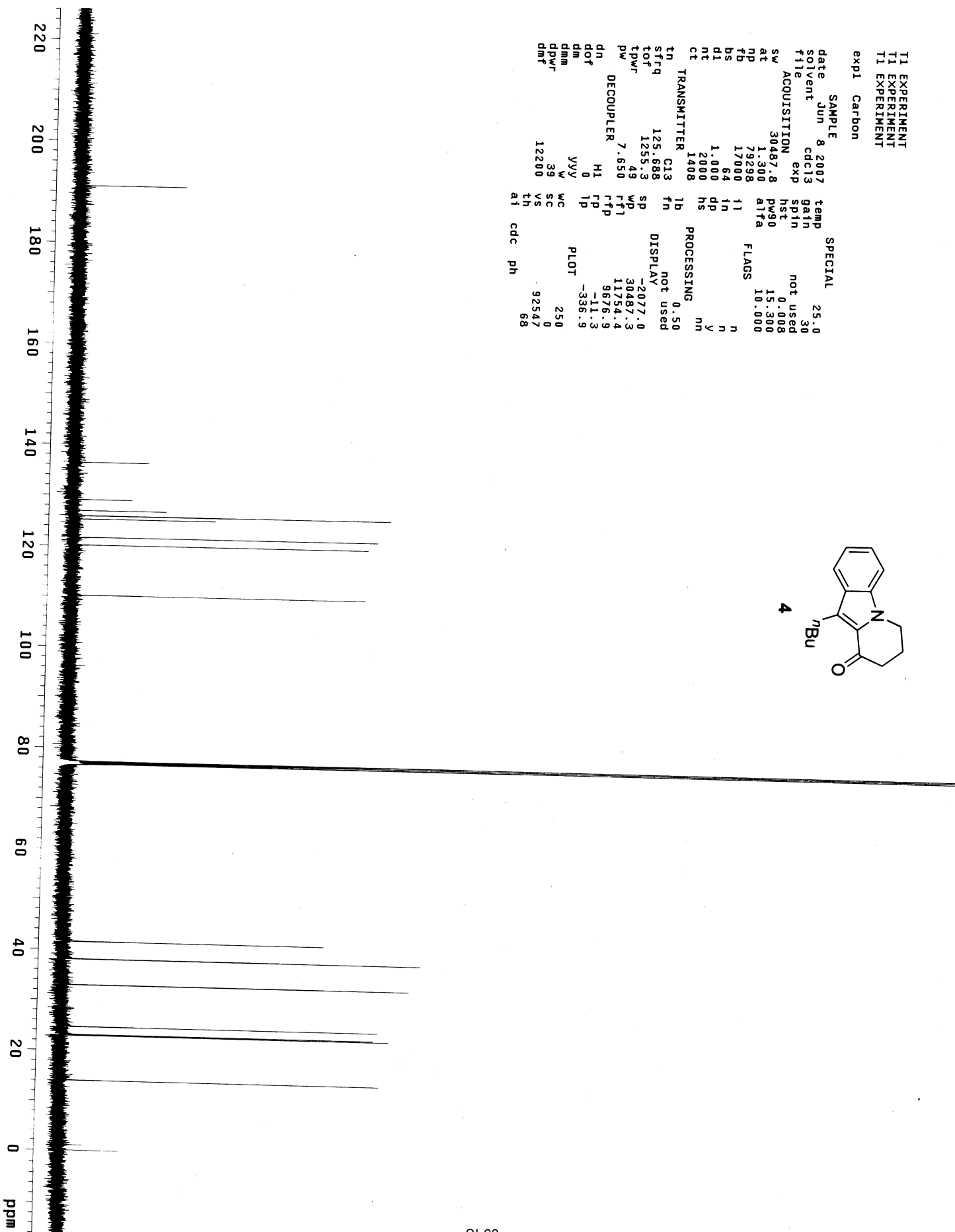
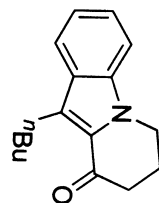
SAMPLE		SPECIAL	
date	Jun 8 2007	temp	25.0
solvent	cdcl3	gain	20
file	/mnt/nmr400/w-	spin	20
alkup/data/zhang/G-	nst	0.008	
uotaol/K102-1.fid	pw90	13.500	
ACQUISITION	alfta	6.600	
sw	6410.3	FLAGS	
at	2.049	11	n
np	26264	in	n
fb	4000	dp	y
bs	32	hs	nn
di	1.000	PROCESSING	
nt	8	lb	0.20
ct	8	tn	65536
TRANSMITTER		DISPLAY	
tn	H1	sp	-176.3
strq	399.868	wp	3614.2
tof	399.6	rfl	799.9
tpwr	59	rfd	0
pw	6.750	fd	-96.4
DECOUPLER		lp	-29.6
dn	C13	1p	
dof	0	WC	250
dm	nnn	SC	0
dmm	C	VS	2098
dpwr	34	th	3
dmt	29412	ai	cdc ph



T1 EXPERIMENT
T1 EXPERIMENT
T1 EXPERIMENT
expt Carbon

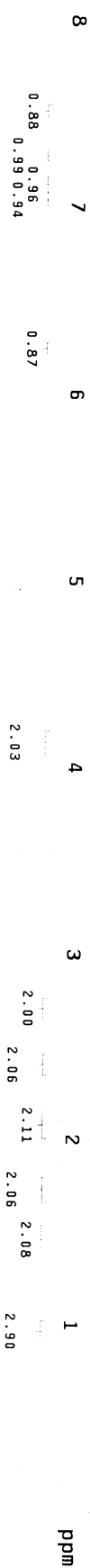
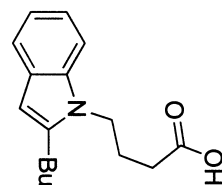
SAMPLE date Jun 8 2007 SPECIAL temp 25.0
solvent cdc13 gain 30
file exp not used
ACQUISITION hst 0.008
sw 30487.8 pw90 15.300
at 1.300 alfa 10.000
np 79298
fb 17000
bs 64
dl 1.000
nt 2000
ct 1408
TRANSMITTER C13
fn 1b
stfq 125.688
tof 1255.3
tpwr 49
pw 7.650
DECOUPLER H1
dn 0
dof 0
dm YVY
dmm W
dpwr 39
dmf 12200
th 68
at cdc ph

PROCESSING 0.50
not used
DISPLAY -2077.0
WD 30487.3
rf1 11754.4
rfp 9676.9
-11.3
-336.9
PLOT 250
0
92547
68




STANDARD 1H OBSERVE - profile
expt Proton

SAMPLE SPECIAL
date Aug 2 2007 temp 25.0
solvent cdc13 gain 30
file exp hst not used
ACQUISITION 6419.3 pps 13.500
sw 2.049 atfa 8.600
at 2.049
np 2.049
td 4000 i1 n
bs 8 tn n
dl 1.000 dp y
nt 8 hs nh
ct 8
TRANSMITTER 8 lb
tn H1 fn
sfrq 399.868 sp DISPLAY
tof 399.6 SP -132.2
tpwr 59 wp 3375.1
pw 6.750 rfi 805.9
DECOUPLER C13 rfd 0
dn 0 lp -76.7
dof 0 wc -24.8
dm c WC PLOT
dmm 34 250
dpwr 34 0
dmf 29412 VS 1296
ai cdc ph 12



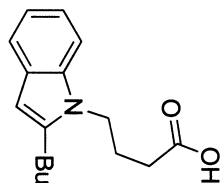
exp1 Noesy1d

6

CC1=C(C(=O)O)CCN1c2ccccc2

expt Carbon

SAMPLE SPECIAL
date Aug 2 2007 temp 25.0
solvent cdc13 gain 30
file /home/waikup/~ spin not used
vnmrsvs/data/auto~ hst 0.008
2007.08.02/5.20070~ pw90 11.900
802_001/data/cdc13~ atfa 10.000
06.fid
ACQUISITION
sw 24509.8 f1 n
at 1.350 dp n
fb 63750 hs y
bs 17000
dl 64 fb
d1 1.000 fn not used
nt 13200 DISPLAY 0.50
ct 13200 sp -1718.4
tn TRANSMITTER C13 wp 24509.1
sfrq 100.557 rfi 9461.2
tof 1042.8 rfp 7742.1
tpwr 53 lp 106.7
pw 5.950 PLOT -193.1
DECOUPLER WC 250
dn H1 sc 0
dof 0 vs 171899
dm yvy th
dmm w ai cdc ph 5
dpwr 41
dmf 9500

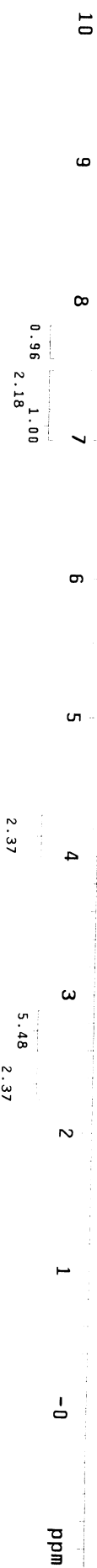
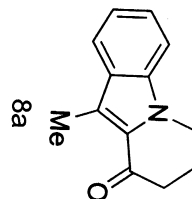


220 200 180 160 140 120 100 80 60 40 20 0 ppm

Automation directory: /home/walkup/vnmrSYS/data/auto_2007.06.24_08
File : s_20070624_001/data/cdc13_02.fid
Sample id : s_20070624_001

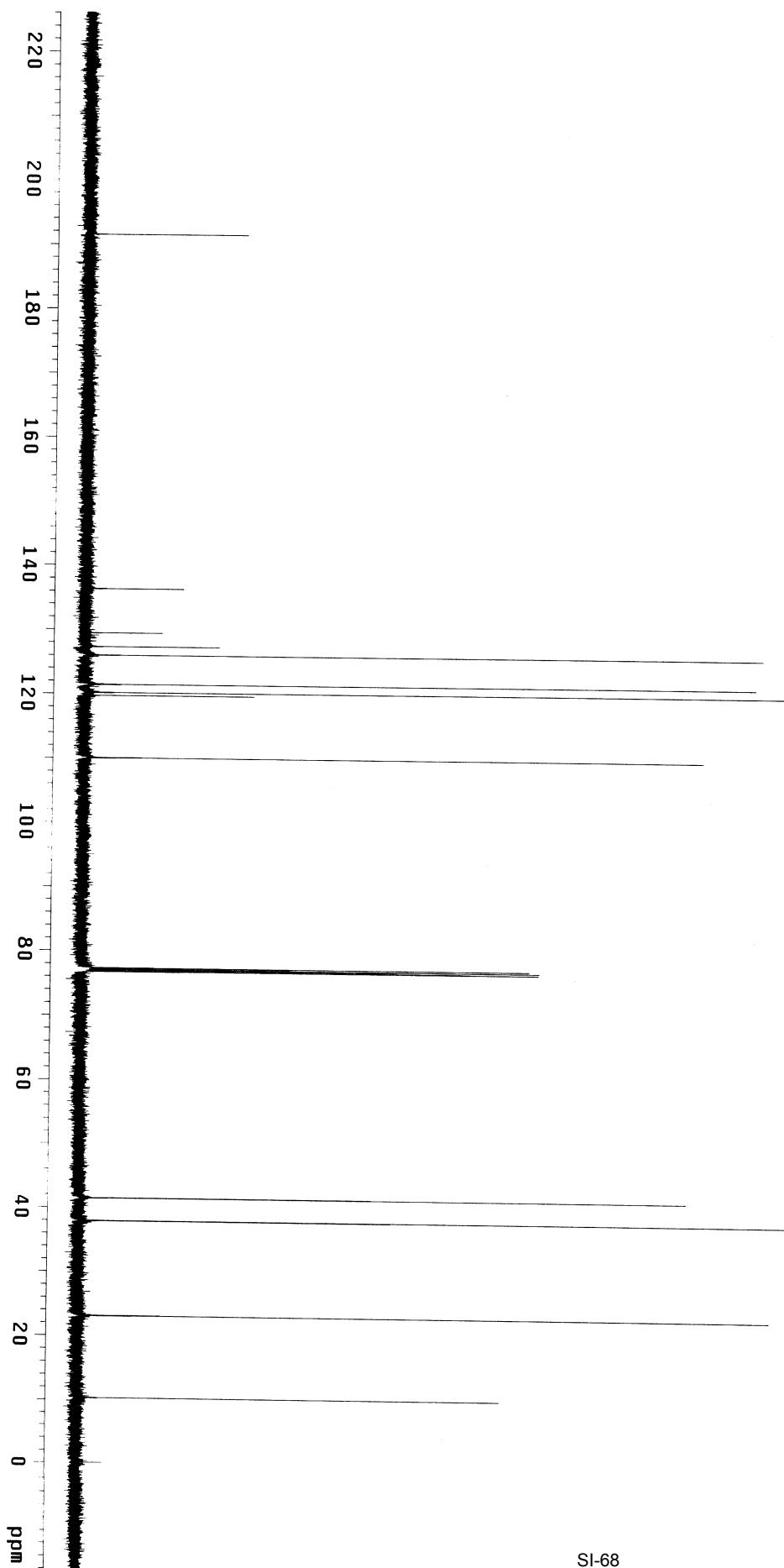
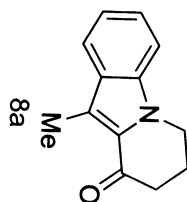
Pulse Sequence: s2pul
Solvent: cdc13
Temp: 25.0 C / 298.1 K
Operator: walkup
File: cdc13_02
VNMRS-400 "NMR400"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.009 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 399.8656762 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min, 30 sec



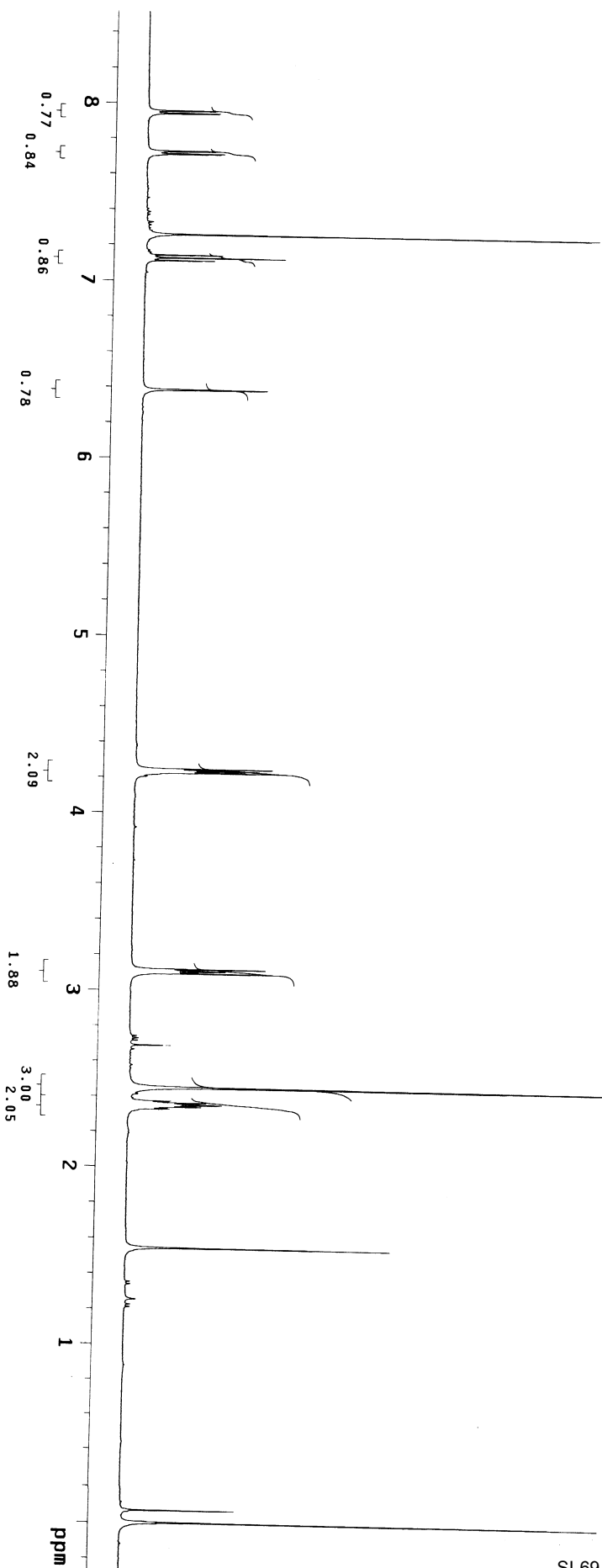
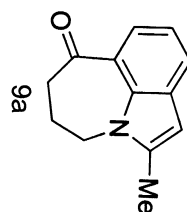
```
Pulse Sequence: s2pu1
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: walkup
File: hxg-4-27C
INOVIA-500 "redjacket"
```

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 30487.8 Hz
Sic repetitions
OBSERVE C13, 125.6746072 MHz
DECOUPLE H1, 499.8016822 MHz
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
Ft size 131072
Total time 33 min, 24 sec



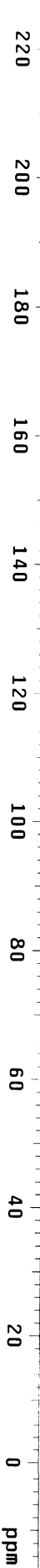
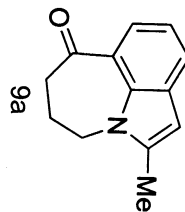
exp5 Proton

SAMPLE		SPECIAL	
date	Jun 26 2007	temp	25.0
solvent	cdcl3	gain	30
file	/mnt/nmr/500/w~	spin	not used
alkup/data/Zhang/L~		hst	0.006
1/K188-2.fid		pw90	14.700
ACQUISITION		atfa	6.600
sw	8012.8	flags	
at	2.049	in	n
np	32830	dp	y
fb	4000	hs	nn
bs	8	PROCESSING	0.20
d1	1.000	fn	65536
nt	8	DISPLAY	
ct	8	SP	-145.7
tn	TRANSMITTER	WP	4401.3
stfrq	499.802	rff1	1008.2
tot	499.8	rffp	0
tpwr	54	ip	-30.0
pw	7.350	PLOT	
dn	DECOUPLER		
dof	C13	WC	250
dm	0	SC	0
dmm	nmn	VS	520
dpwr	34	th	2
dmt	32258	ai	cdc ph



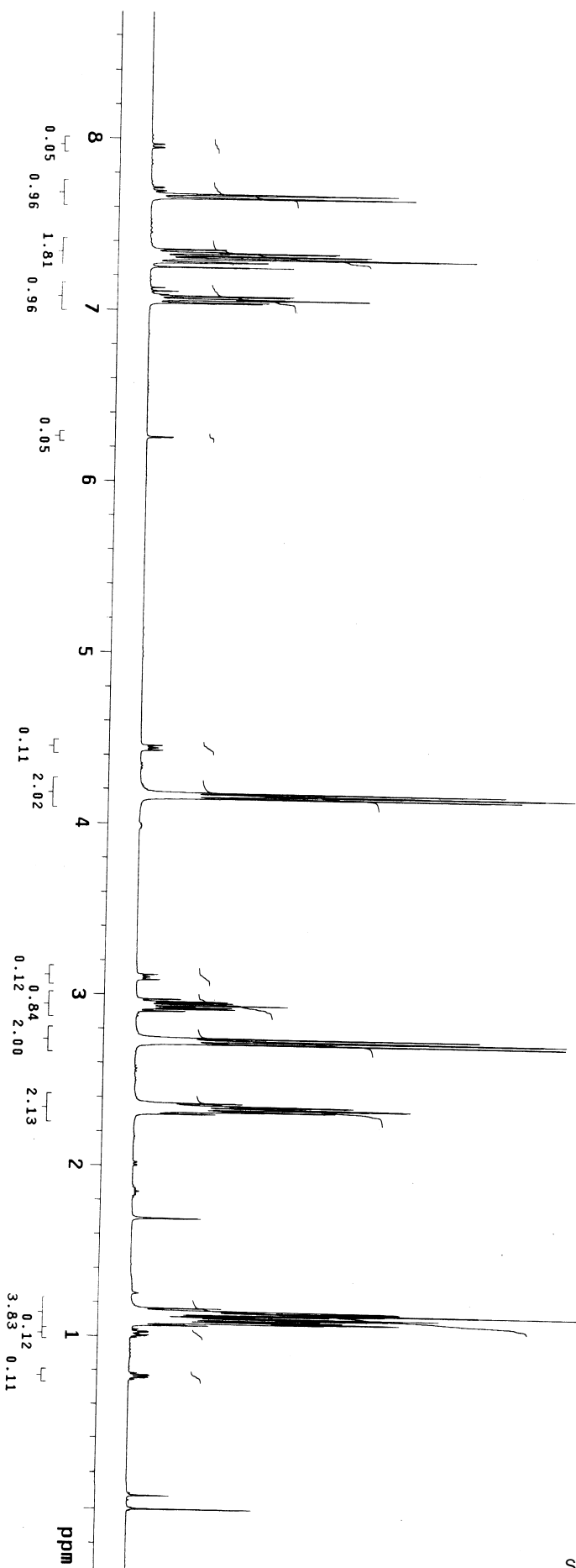
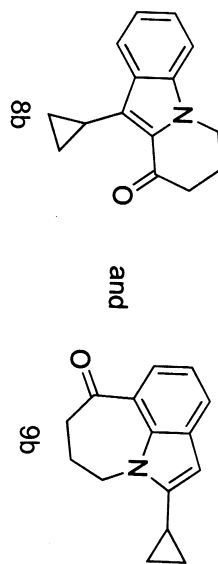
expi Carbon

SAMPLE				SPECIAL			
date	Jun 26 2007	temp	25.0				
solvent	cdcl3	gain	30				
file	exp	spin	not used				
ACQUISITION							
sw	30487.8	hst	0.008				
at	1.300	pw90	15.300				
np	79298	alpha	10.000				
fb	17000	flags					
bs	8	in	n				
d1	1.000	dp	n				
nt	3000	hs	y				
ct	2440	PROCESSING	nn				
TRANSMITTER							
tn	cl3	fb	0.50				
strq	125.688	tn	not used				
tof	1255.3	sp	DISPLAY				
tpwr	49	wp	-2076.5				
pw	7.650	rfl	30487.3				
DECOUPLER							
dn	H1	rtp	11753.9				
dof	0	rp	9676.9				
dm	yy	lp	63.7				
dmm	w	PLOT	-286.5				
dpwr	39	WC	250				
dmf	12200	SC	0				
	th	VS	124604				
	ai	cdc	4				
		ph					



exp2 Proton

SAMPLE			SPECIAL		
date	Jun 19 2007	temp	25.0		
solvent	cdcl3	gain	20		
file	/mnt/nmr400/w~	spin	20		
akup/data/Zhang/G~	hst		0.008		
notaoL1/K160-1.fid	pw90		13.500		
ACQUISITION	alfa		6.600		
sw	6410.3	FLAGS			
at	2.049	i1	n		
np	26264	in	n		
fb	4000	dp	y		
bs	32	hs	nn		
dl	1.000	PROCESSING	0.20		
nt	8	jb	65536		
ct	8	fn			
TRANSMITTER		DISPLAY			
tn	H1	sp	-149.8		
strq	399.868	wd	3643.9		
tof	399.6	rfl	803.2		
tpwr	59	rffp	0		
pw	6.750	fp	-19.5		
DECOUPLER		lp	-27.8		
dn	C13	1p			
dof	0	WC			
dm	nmh	SC	250		
dmm	c	VS	0		
dpwr	34	th	1084		
dmf	29412	ai	2		
		cdc	ph		



exp5 Carbon

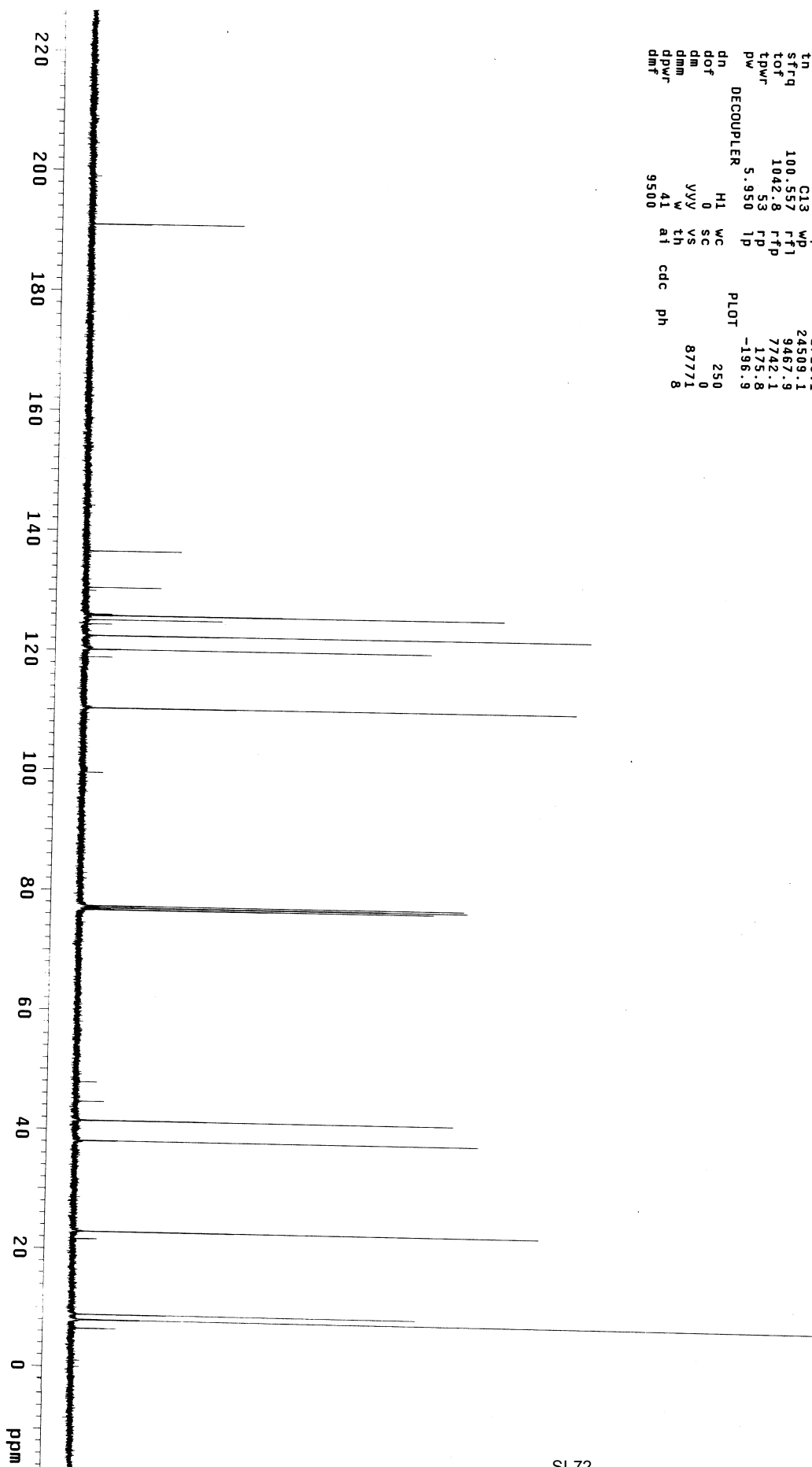
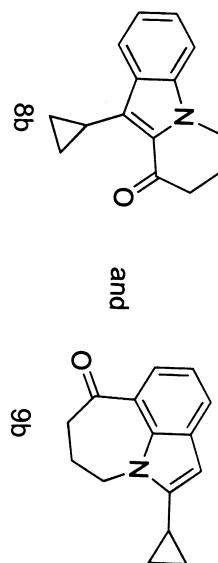
SAMPLE date Jun 19 2007 SPECIAL 25.0
solvent cdc13 gain 30
file /mnt/nmr400/w~ hst 20
alkup/data/Zhang/G~ pw90 0.008
notao1/K160-1carb~ pw90 11.900
on.fid alfa 10.000

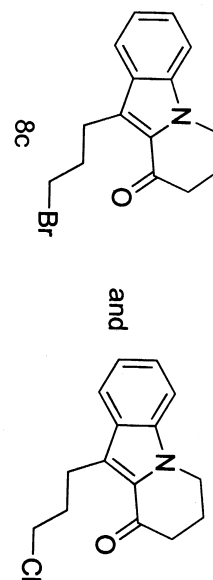
ACQUISITION
sw 24509.8 f1
at 1.300 in
np 63750 dp
fb 17000 hs
bs 32
dl 1.000 lb
nt 4000 fn
ct 1408

PROCESSING
not used
0.50
nn

TRANSMITTER
in C13 sp
sfreq 100.557 wf -1725.1
tof 1042.8 rfp 24509.1
tpwr 53 fp 9467.9
pw 5.950 ip 7742.1
-175.8
-196.9

DECOUPLER
dn H1 WC PLOT
dof 0
dm 0 SC 250
dmm 0 VS 0
dpwr 41 th 87771
dmf 9500 ai cdc ph 8





exp3 Proton

SAMPLE
date Jun 26 2007
solvent cdcl3
file /home/waikup/~
vnmrsvs/data/auto_~
2007.06.26-05/AUG_~
02/data/cdcl3_01.f
id

SPECIAL
temp 25.0
gain not used
spn not used
hst 0.008
pw90 14.700
atfa 6.600
flags

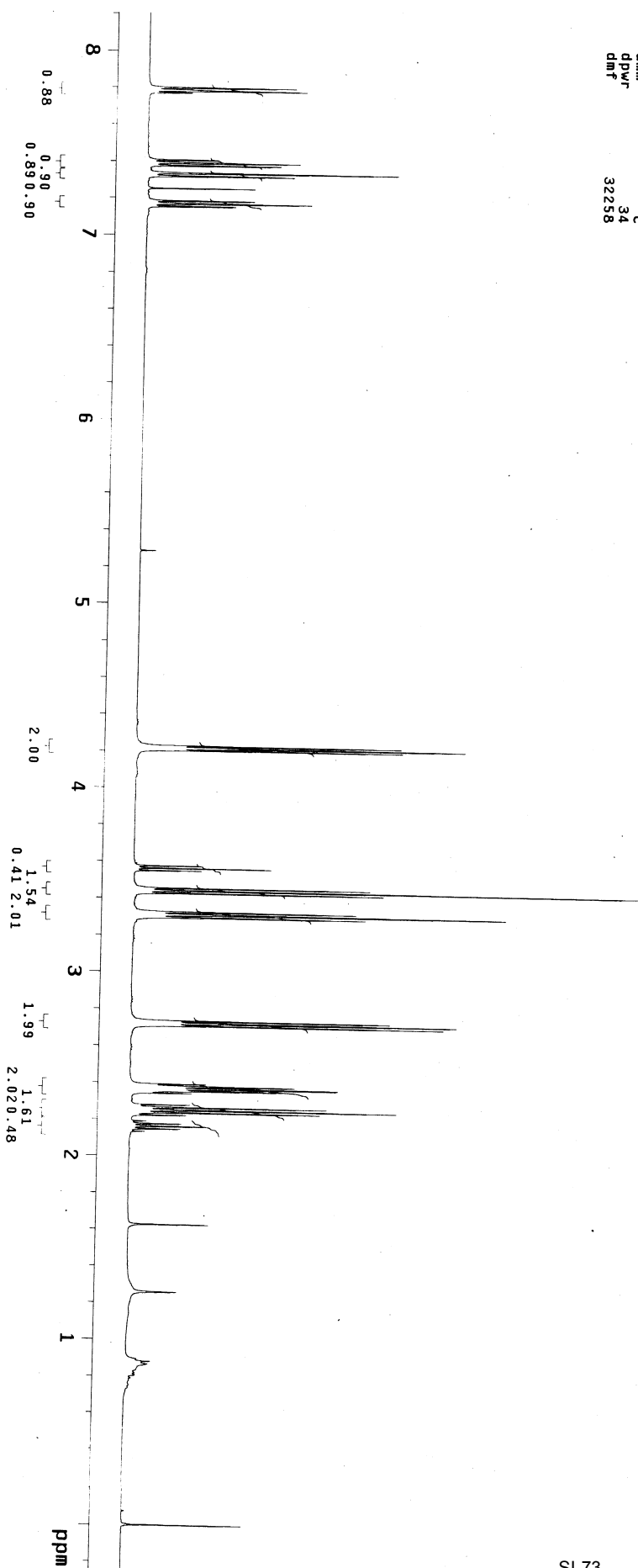
ACQUISITION
sw 8012.8
at 2.049
np 32830
fb 4000
bs 32
ss 2
dl 1.000
nt 8
ct 8
tn 8
sfreq 499.802
tof 499.7
tpwr 34
pw 7.350
DECOUPLER WC
dn C13
dof 0
dm 0
dmm nnn
dpwr c
dmf 34
32258

PROCESSING
hs y
nm
0.20
65536
fn
0.20
65536
fn

DISPLAY
-137.7
4238.5
1011.6
96.6
-32.9
250
0
308
2

TRANSMITTER
H1
f1
rfp
ip
PLOT

ph



exp3 Carbon

SAMPLE

SPECIAL

25.0

date Jul 1 2007

temp 25.0

solvent cdc13

gain 30

file /home/walkup/~

spin not used

vmrsvs/data/auto_~

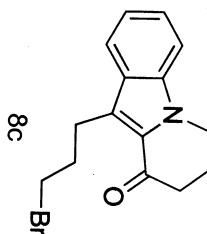
hst 0.008

2007.07.01/Aug.~

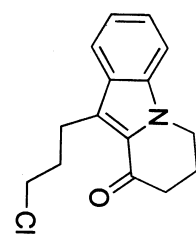
pw50 15.300

01/data/cdc13_01.f~

alfa 10.000



and



ACQUISITION

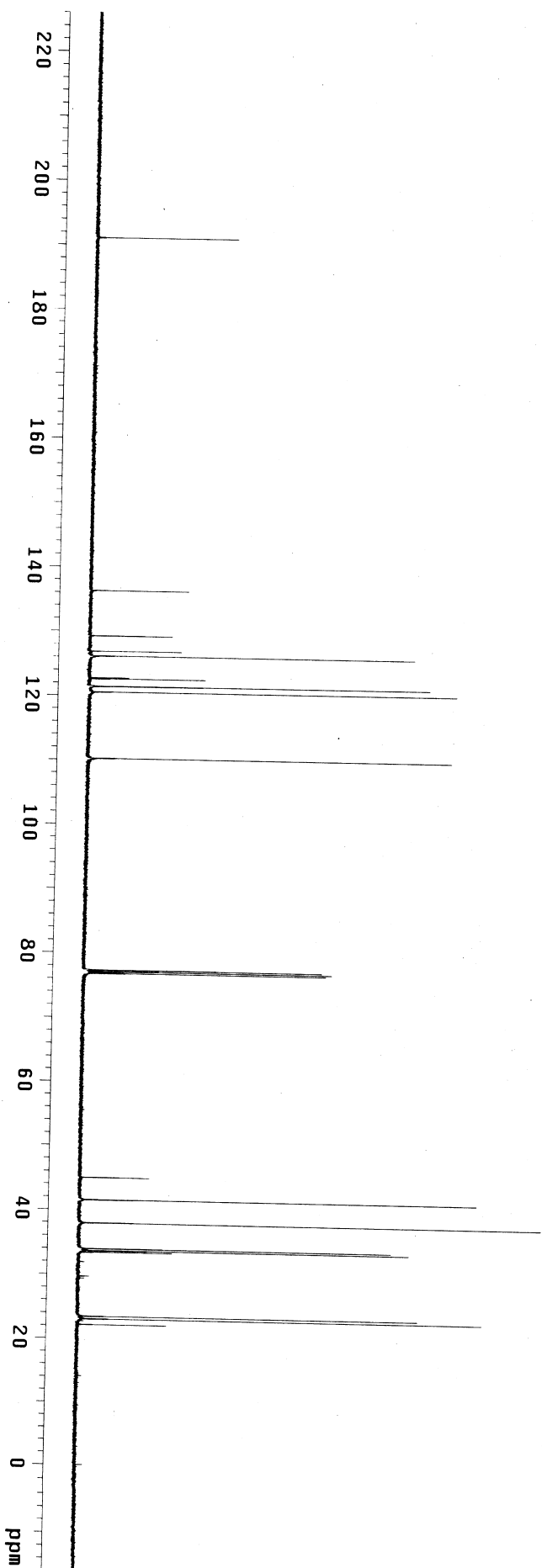
id	11	FLAGS	n
sw	30487.8	in	n
at	1.300	dp	y
np	79298	hs	nm
fb	17000	bs	nm
bs	64	fb	0.50
dl	1.000	fn	not used
nt	4000	sp	not used
ct	1536	display	-2083.0

TRANSMITTER

tn	C13	wd	30487.3
stfq	125.688	rf1	11760.4
tof	1255.3	rfp	9676.9
tpwr	49	lp	156.6
pw	7.650	plot	-279.7

DECOUPLER

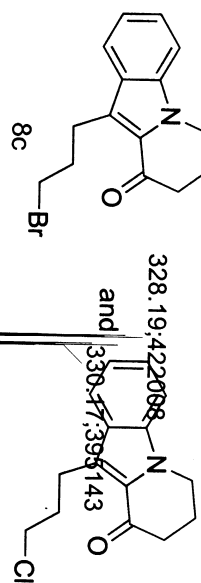
dn	H1	wc	250
dof	0	sc	0
dm	0	vs	17141
dmm	yyv	th	2
dpwr	w	ai	cdc
dmf	39	ph	
	12200		



K186 31 (0.573) Cm (2.44)

100

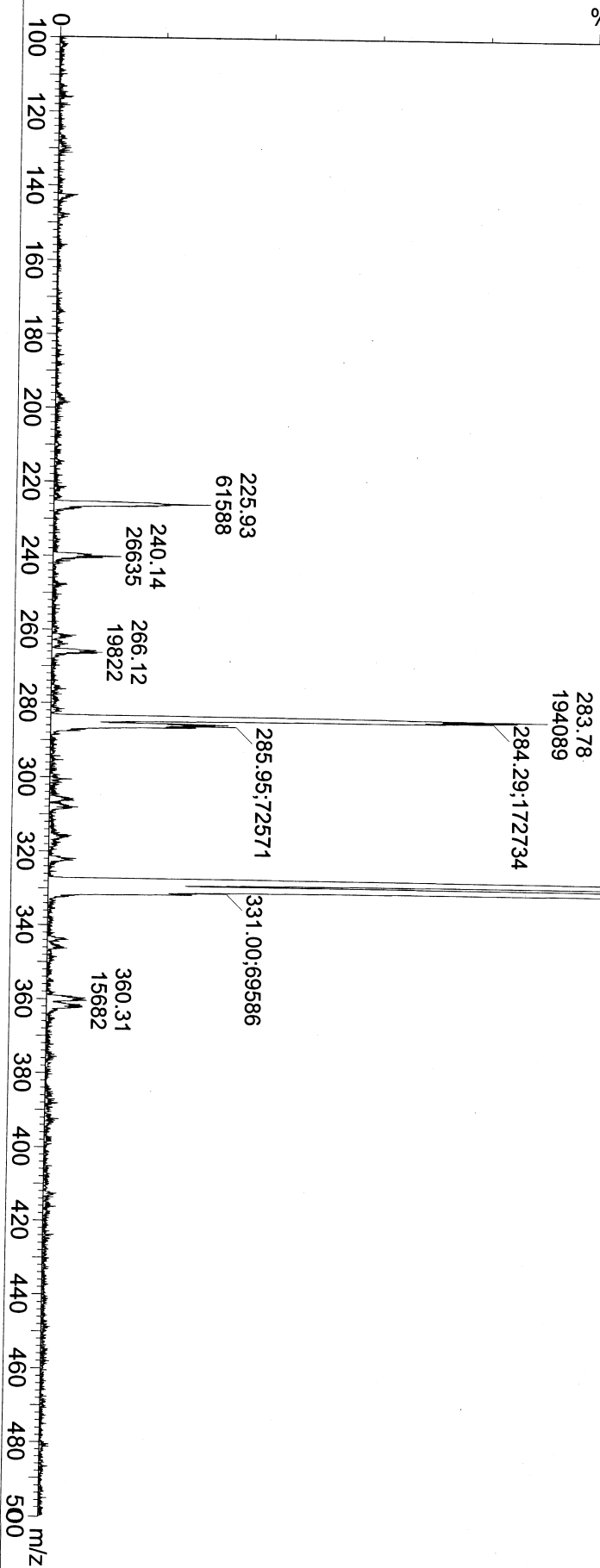
MAA266



27-Jun-2007

Scan ES+
4.22e5

%

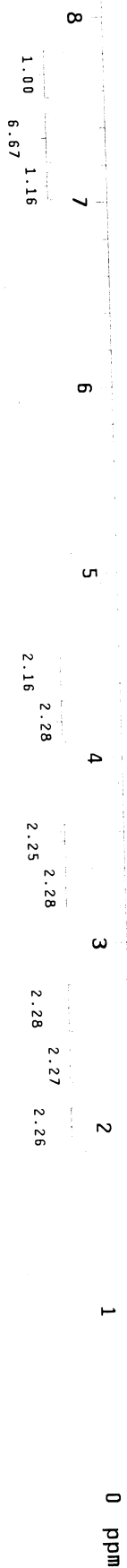
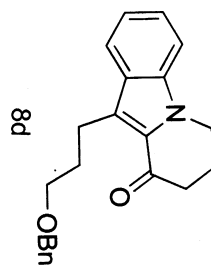


Automation directory: /home/walkup/vnmrsvs/data/auto_2007.07.01_07
File : s_20070701_001/data/cdc13_01.fid
Sample id : s_20070701_001

Pulse Sequence: s2pul

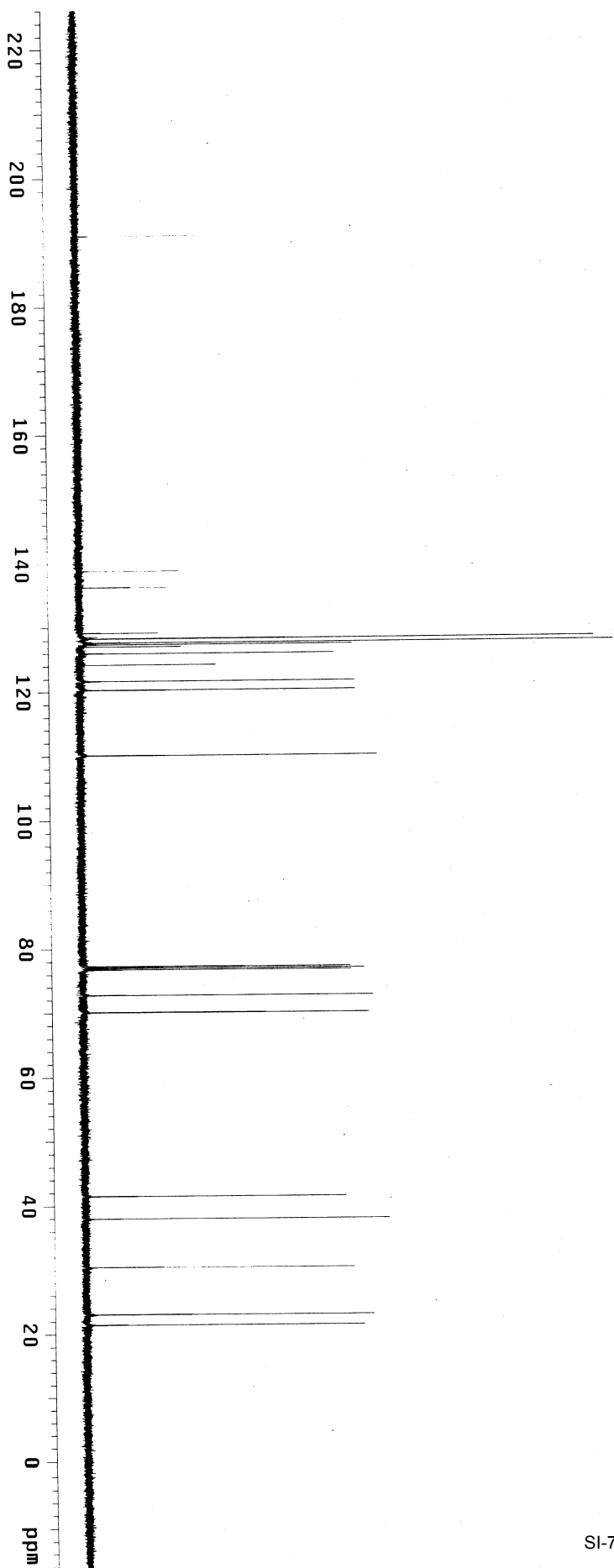
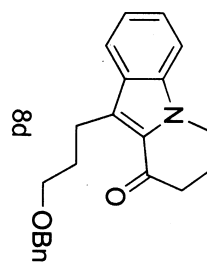
Solvent: cdcl3
Temp: 25.0 C / 298.1 K
Operator: walkup
File: cdc13_01
VNMR-400 "NMR400"

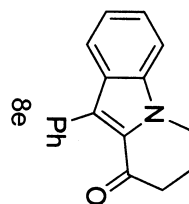
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.049 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 399.8656807 MHz
DATA PROCESSING
Line broadening 0.2 Hz
Ft size 65536
Total time 0 min, 30 sec



Automation directory: /home/walkup/vnmrSYS/data/auto_2007.07.01_06
 File : exp
 Sample id : tmpstudy
 Pulse Sequence: szpul
 Solvent: cdcl3
 Temp. 25.0 C / 298.1 K
 Operator: walkup
 VNMRS-500 "nmr500"

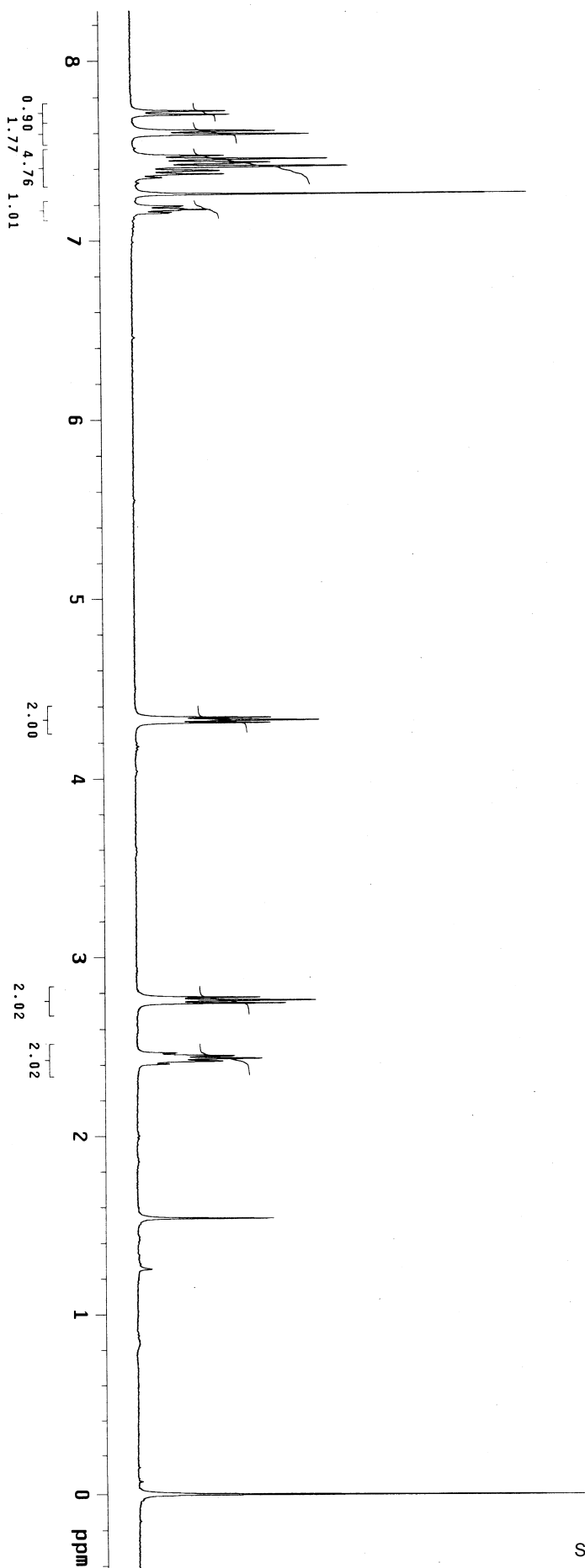
Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.300 sec
 Width 30487.8 Hz
 256 repetitions
 OBSERVE C13, 125.6746100 MHz
 DECOUPLE H1, 499.8016822 MHz
 power 39 db
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 131072
 Total time 39 min, 24 sec





exp2 Proton

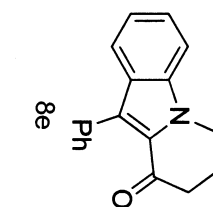
SAMPLE		SPECIAL	
date	Jun 4 2007	temp	25.0
solvent	cdcl3	gain	20
file	/mnt/nmr400/W~	spin	not used
akcup/data/2hang/G~	hst	0.008	
uotaoli/K33-2.fid	pw90	13.500	
ACQUISITION	alpha	6.600	
sw	6410.3	FLAGS	
at	2.049	11	n
np	26264	in	n
fb	4000	dp	y
bs	332	hs	nm
dl	1.000	PROCESSING	0.20
nt	8	1b	65536
ct	8	fn	
TRANSMITTER		DISPLAY	
tn	H1	SP	-176.5
stfq	399.868	WD	3487.2
tof	399.6	rfl	800.7
tpwr	59	rffp	0
pw	6.750	fp	163.2
DECOUPLER	1p	PLOT	-19.3
dh	C13	WC	250
dof	0	SC	0
dm	nm	VS	4555
dmm	C	th	2
dpwr	34	ai	cdcl3
dmf	29412	ph	



expl Carbon

SPECIAL

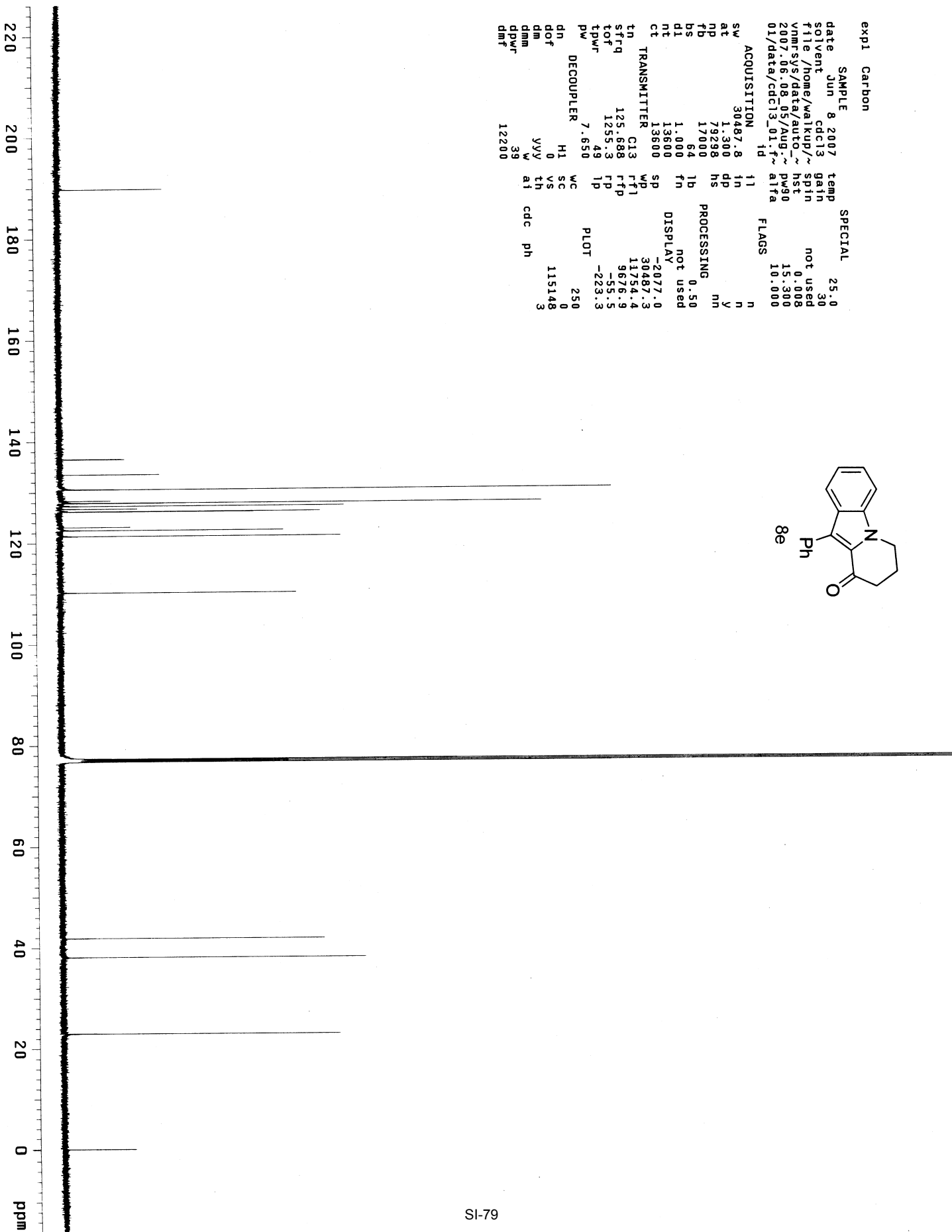
date Jun 8 2007 temp 25.0
solvent cdc13 gain 30
f1le /home/walkup/~ not used
vnmr/sys/data/auto_~ hst 0.008
2007.06.08_05/Aug.~ pw90 15.300
01/data/cdc13_01.f~ alfa 10.000



FLAGS

ACQUISITION

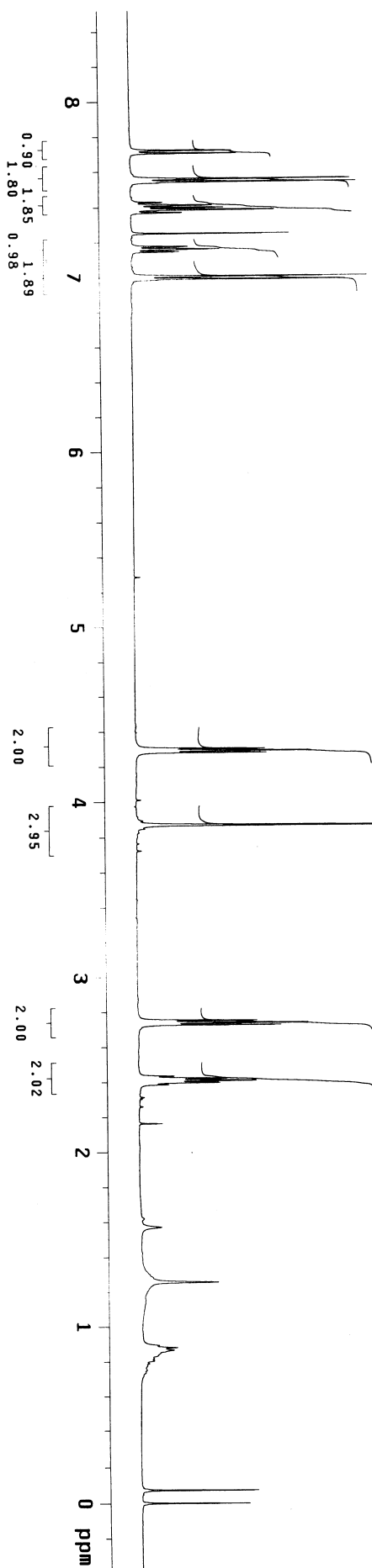
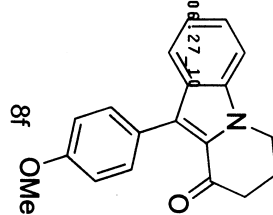
id i1 n
sw 30487.8 in
at 1300 y
np 79298 hs nm
fb 17000
bs 64 lb
d1 1.000 fn
nt 13600 not used
ct 13600 DISPLAY
tn TRANSMITTER C13 SP -2077.0
sfreq 125.688 rfi 30487.3
tot 1255.3 rfp 11754.4
tpwr 49 tp -55.5
pw 7.650 1p -223.3
DECOUPLER H1 WC 250
dn H1 SC 0
dof 0 VS 115148
dm 0 YVY th 3
w al cdc ph
dpm 39
dpr 12200

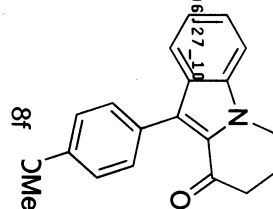


Automation directory: /home/walkup/vnmrSYS/data/auto_2007.08
File: Aug.02/data/cdcl3_01.fid
Sample id: Aug.02

Pulse Sequence: szpul
Solvent: cdcl3
Temp: 25.0 C / 298.1 K
Operator: walkup
File: cdcl3_01
Vnmrs-500 "nmr-500"

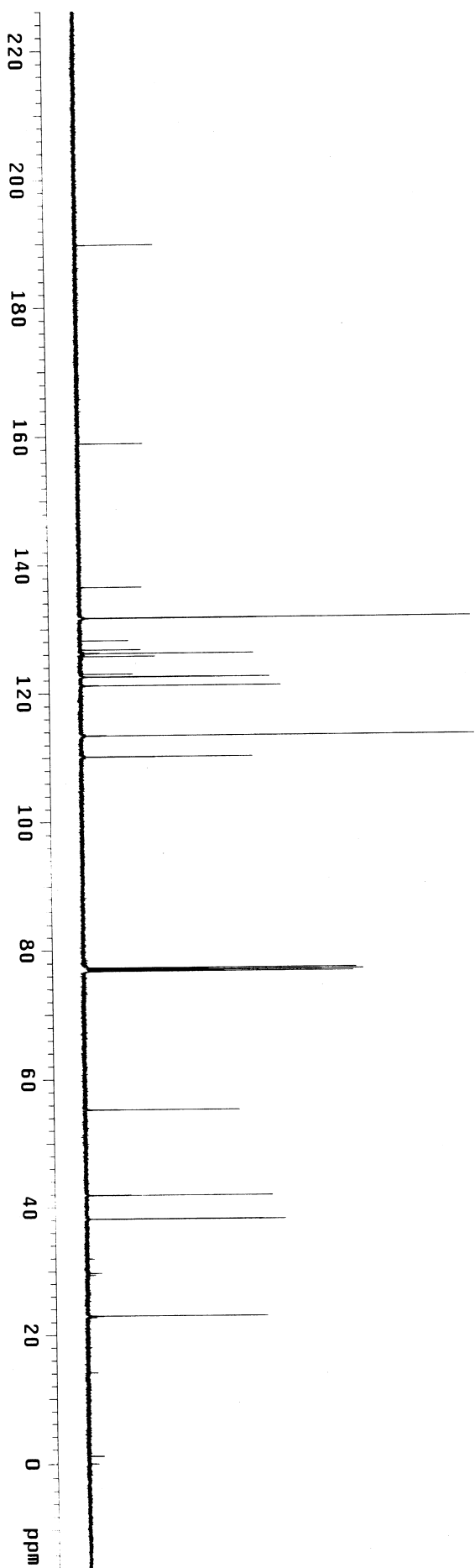
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.089 sec
Width 8012.8 Hz
8 repetitions
OBSERVE H1, 499.7991883 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min, 30 sec





Automation directory: /home/walkup/vnmr/sys/data/auto_2007.06/27-10
 File : exp
 Sample id : tmpstudy
 Pulse Sequence: szpul
 Solvent: cdcl3
 Temp: 25.0 C / 298.1 K
 Operator: walkup
 Vnmr-500 "nmr500"

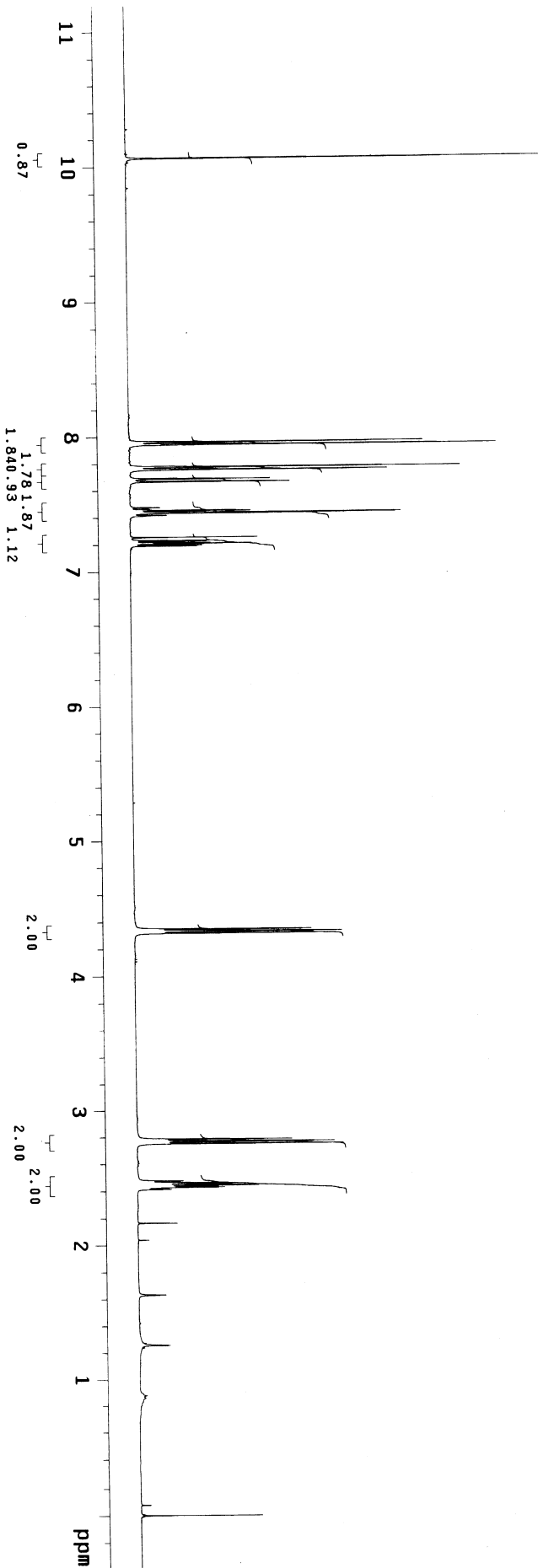
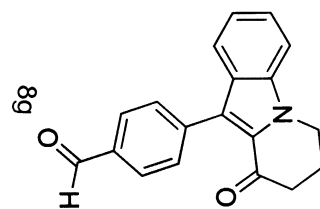
Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.300 sec
 Width 30487.8 Hz
 1024 repetitions
 OBSERVE C13, 125.6746067 MHz
 DECOUPLE H1, 499.8016822 MHz
 Power 39 db
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 131072
 Total time 39 min, 24 sec



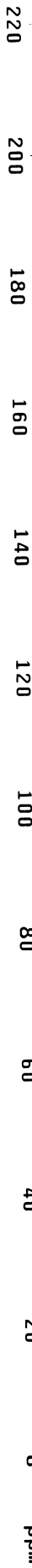
STANDARD 1H OBSERVE - profile

exp2 Proton

SAMPLE		SPECIAL	
date	Jun 25 2007	temp	25.0
solvent	cdcl3	gain	not used
file	/mnt/nmr400/w~	spin	not used
akup/data/zhang/G~	hst	0.008	
notool/K15-2.fid	pw90	13.500	
ACQUISITION	alfta	6.600	
sw	6410.3	FLAGS	
at	2.049	11	n
np	26264	1n	n
fb	4000	dp	y
bs	32	hs	n
ss	2	PROCESSING	
dl	1.000	1b	0.20
nt	8	fn	65536
ct	8	DISPLAY	
tn	TRANSMITTER	sp	-168.6
stf	399.868	wp	4644.1
tof	399.6	rfp	801.5
tpwr	59	rfp	-105.6
pw	6.750	1p	-32.0
DECOUPLER		PLOT	
dn	C13	WC	250
dof	0	SC	0
dm	nmn	VS	895
dmm	34	tn	2
dpwr	C	at	cdc
dmf	29412	ph	



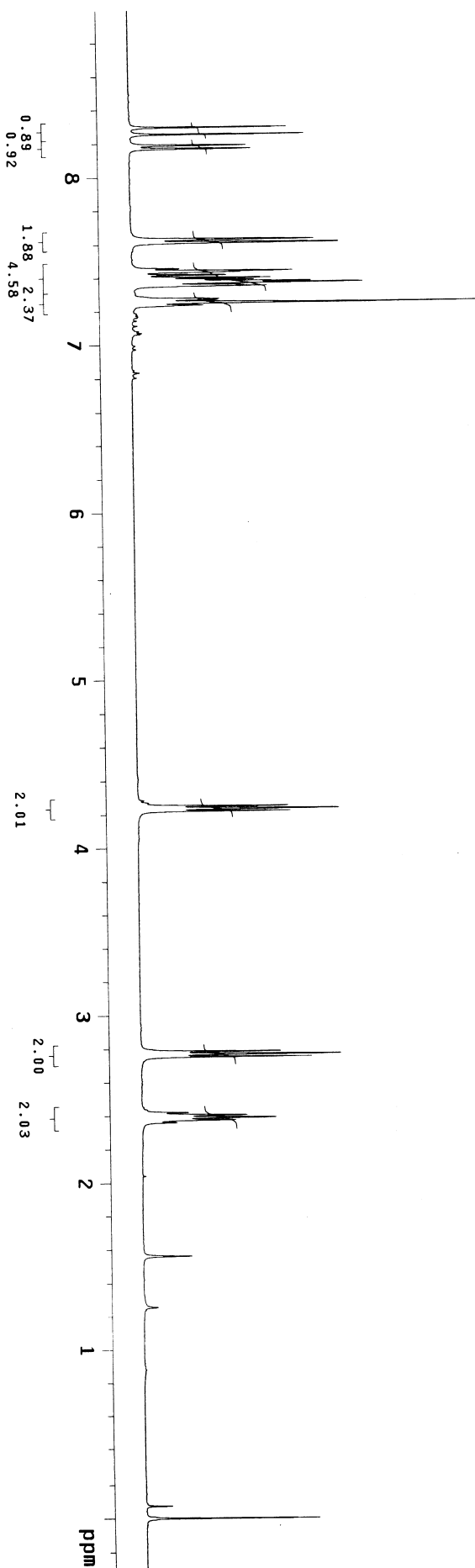
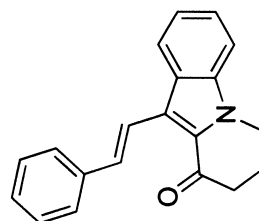
SPECIAL		25.0
temp	30	
gga	not used	
sp	0.008	
hst	15.300	
pw90	10.000	
alpha		
FLAGS		
l1	n	
in	n	
dp	y	
hs	nn	
PROCESSING		
l1b	1.00	
fn	not used	
DISPLAY		
sp	-2082.6	
wd	30487.3	
l1	11760.0	
r1	9676.9	
r1p	35.5	
r1p	35.5	
l1p	-252.5	
PLOT		
wc	250	
sc	0	
vs	18919	
th	7	
cdc	ph	

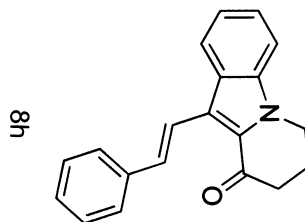


STANDARD 1H OBSERVE - profile

exp1 proton

SAMPLE		SPECIAL	
date	Jun 21 2007	temp	25.0
solvent	cdcl3	gain	20
file	/mnt/nmr400/w~	spin	not used
akup/data/zhang/G~	hst	0.008	
uotaol/K1672.fid	pw90	13.500	
ACQUISITION	alfa	6.600	
sw	6410.3	FLAGS	
at	2.049	11	n
np	26264	1n	n
fb	4000	dp	y
bs	32	hs	nn
di	1.000	PROCESSING	0.20
nt	8	1b	0.20
ct	8	fn	65536
TRANSMITTER		DISPLAY	
tn	H1	sp	-129.1
stfq	399.868	wp	3725.5
tof	399.6	rfl	802.8
tpwr	59	rtp	0
pw	6.750	tp	-20.7
DECOUPLER		PLOT	
dn	C13	1p	-22.2
dof	0	WC	250
dm	nmn	SC	0
dmm	C	VS	2325
dpwr	34	tn	2
dmf	29412	at	cdc
			ph

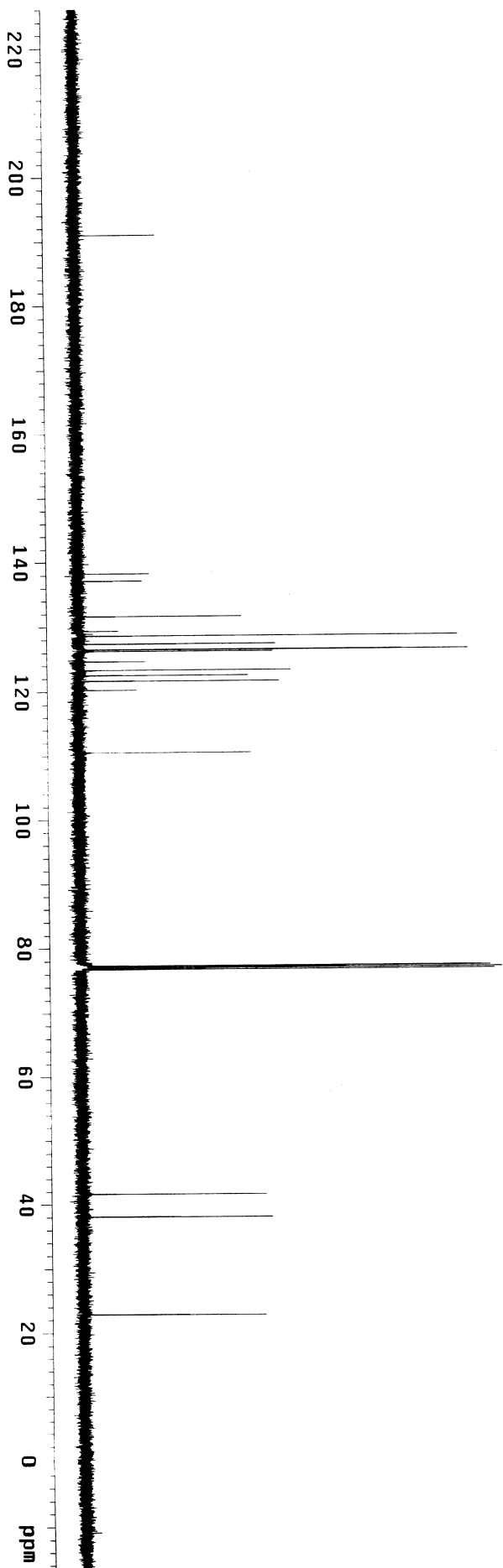




```

expt Carbon
SAMPLE
date Jun 21 2007
solvent cdcl3
file exp
ACQUISITION
sw 30487.8
at 1.300
np 79298
fb 17000
bs 32
di 1.000
nt 1024
ct 320
TRANSMITTER C13
tn 125.688
stfq 1255.3
tof 49
tpwr 7.650
pw DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 39
dmf 12200
SPECIAL
temp 25.0
gain 30
spn not used
nst 0.008
pw90 15.300
alfa 10.000
FLAGS
t1 n
t2 n
t3 y
t4 nn
t5 nn
t6 nn
t7 nn
t8 nn
t9 nn
t10 nn
t11 nn
t12 nn
t13 nn
t14 nn
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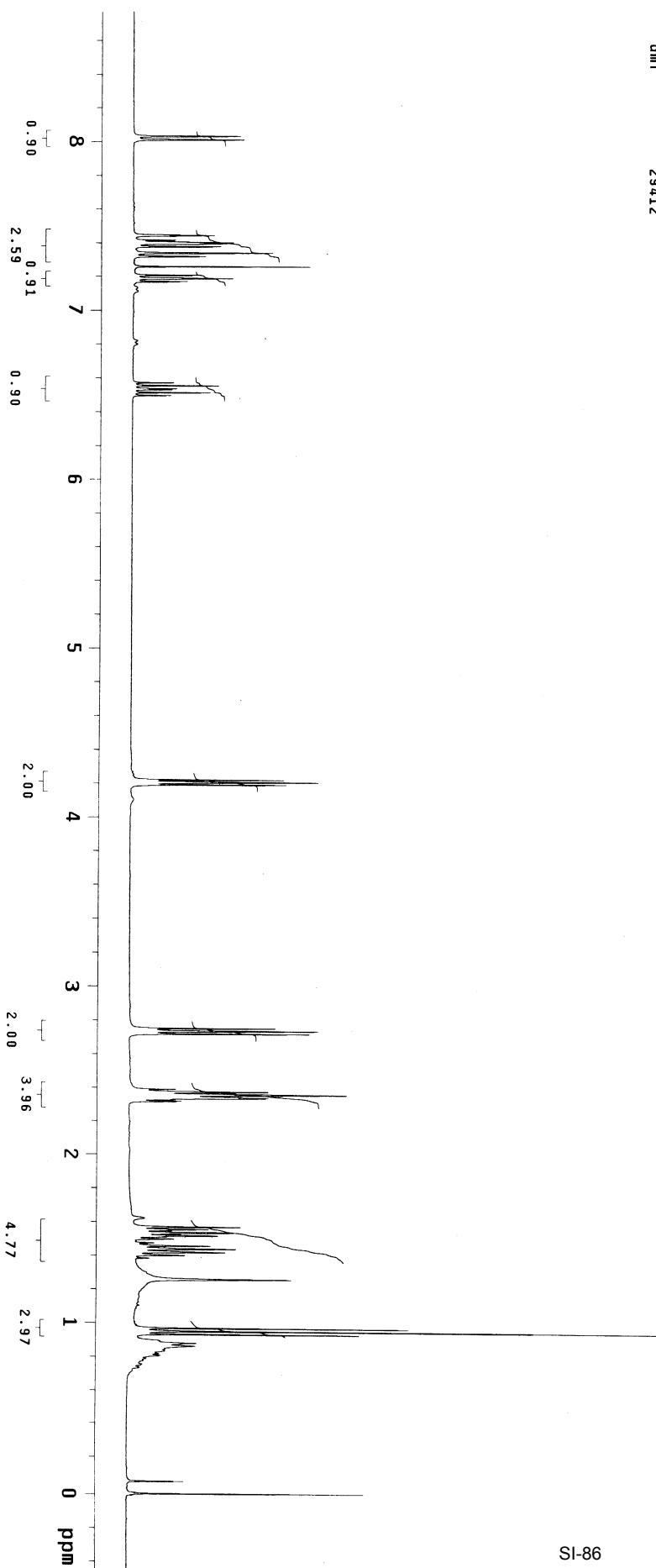
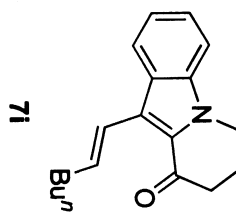
```



STANDARD 1H OBSERVE - profile

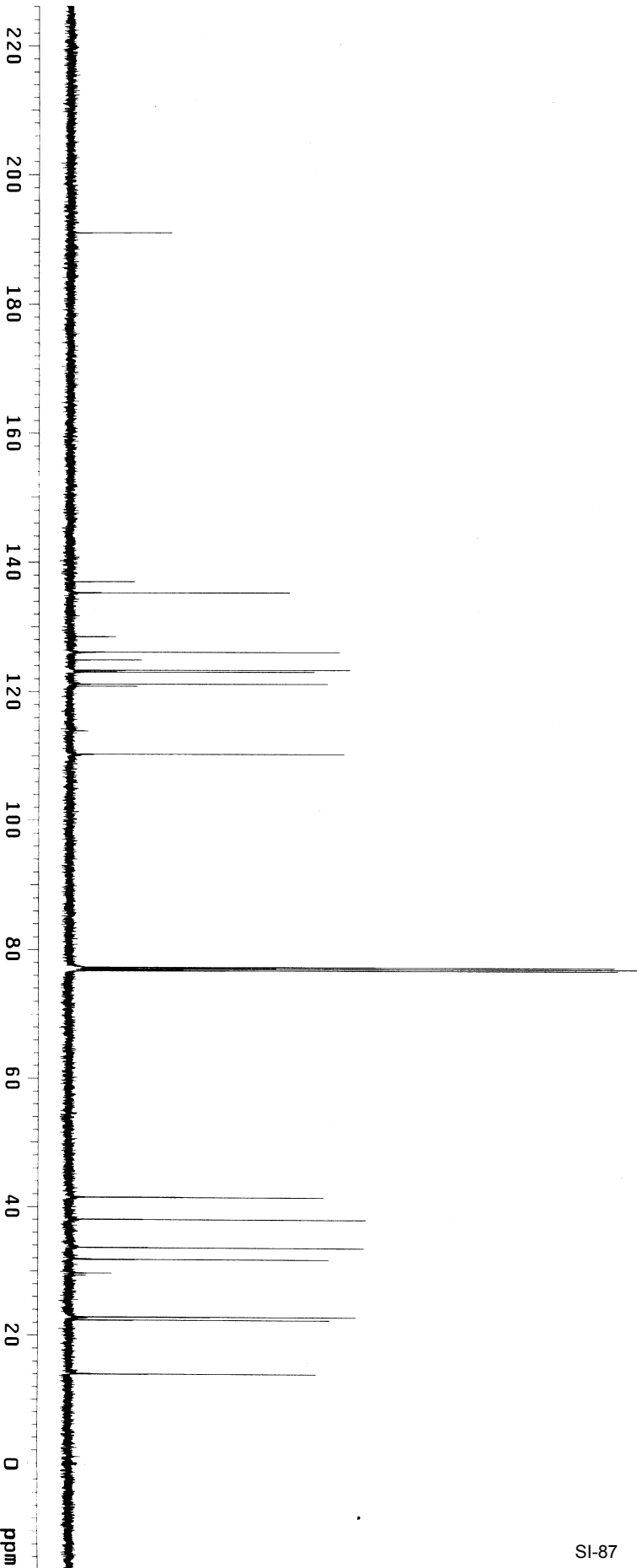
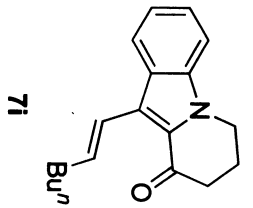
exp2 Proton

SAMPLE		SPECIAL	
date	Jun 25 2007	temp	25.0
solvent	cdc13	gain	not used
file	/mnt/nmr400/w~	spin	not used
akup/data	Zhang/G~	hsf	0.008
uotaol/K174-1.fid	pw50	13.500	
ACQUISITION	atfa	6.600	
sw	6410.3	FLAGS	
at	2.049	11	n
np	26264	in	n
fb	4000	dp	y
bs	32	hs	nn
ss	2	PROCESSING	
dl	1.000	1b	0.20
nt	8	fn	65356
ct	8	fn	65356
TRANSMITTER		DISPLAY	
tn	H1	sp	-188.0
sfrq	399.868	wp	3694.8
tof	399.6	rfl	800.5
tpwr	59	rfp	0
pw	6.750	lp	-106.1
DECOUPLER		PLOT	
dn	C13	wc	250
dof	0	sc	0
dm	nnn	vs	1902
dmm	c	th	3
dpwr	34	at	cdc
dmf	29412	ph	



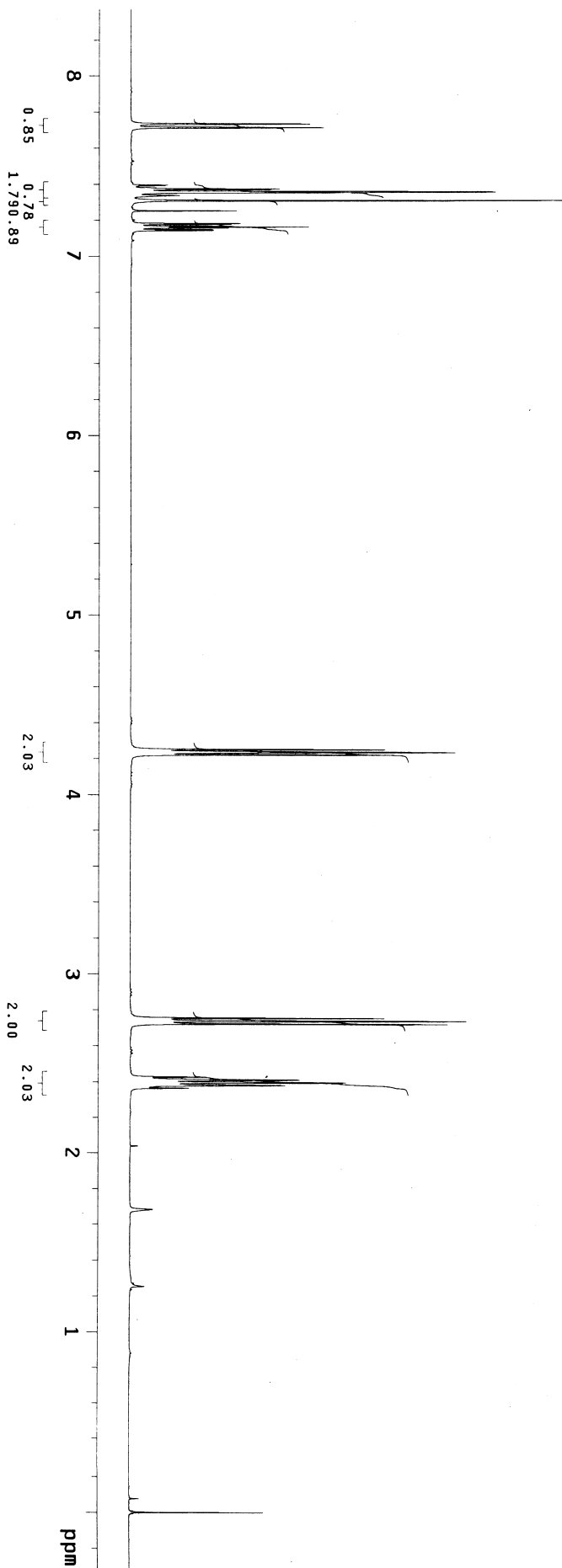
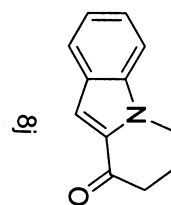
expi Carbon

SAMPLE		SPECIAL	
date	Jun 26 2007	temp	25.0
solvent	cdc13	gain	30
file	cdc13	not used	
ACQUISITION		hst	0.008
sw	30487.8	pw50	15.300
at	1.300	alpha	10.000
np	79298	FLAGS	
fb	17000	11	n
bs	8	in	n
dl	1.000	dp	y
nt	1024	hs	nn
ct	672	PROCESSING	1.00
tn	TRANSMITTER C13	fb	fn
strq	125.688	sp	not used
tof	1255.3	wp	DISP
tpwr	49	rfl	-2077.4
pw	7.650	rfl	30487.3
DECOUPLER		rfl	11754.9
dn	H1	rfl	9676.9
dn	0	lp	64.0
dn	0	lp	-273.7
dn	yyy	PLOT	
dmm	w	WC	250
dpwr	39	SC	0
dmt	12200	VS	46287
at	cdc	ph	68



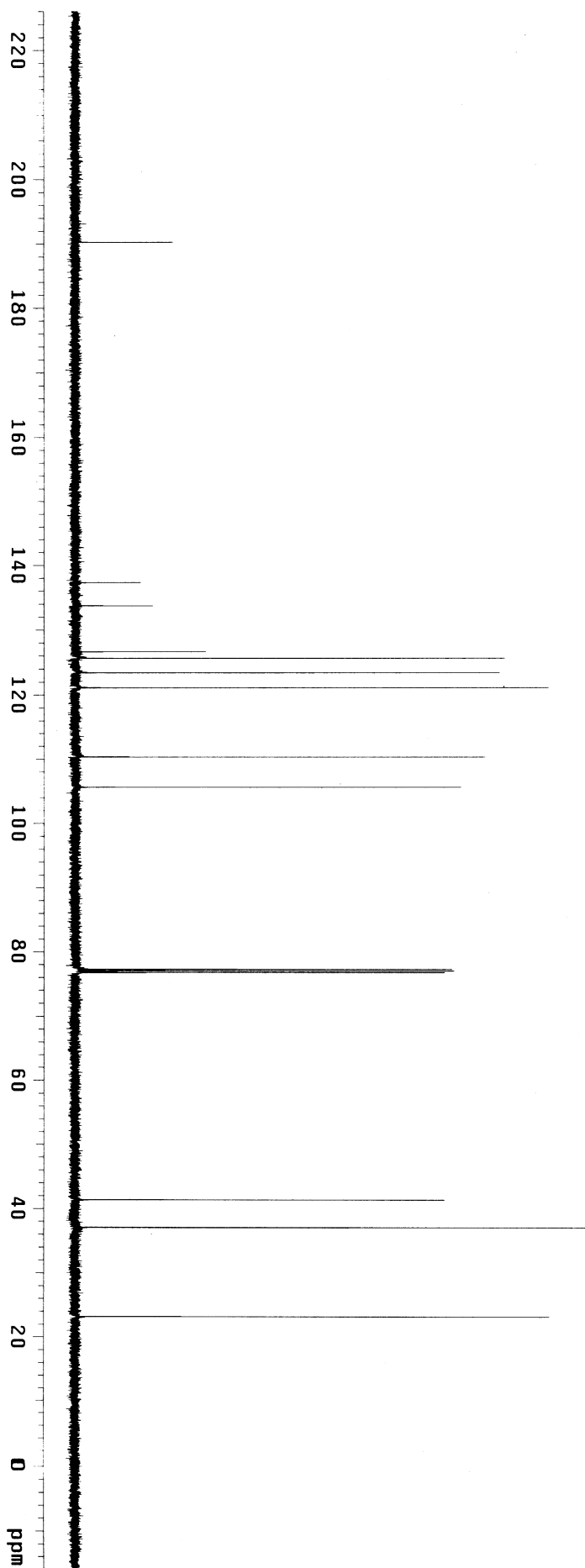
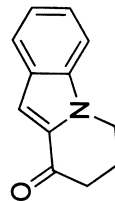
exp2 Proton

SAMPLE		SPECIAL	
date	Jun 8 2007	temp	25.0
solvent	cdcl3	gain	20
file	/mnt/nmr400/w~	spin	20
alkup/data/Zhang/G-	hst	0.008	
uotaol/K104-1.71d	pw90	13.500	
ACQUISITION	atfa	6.500	
sw	6410.3	FLAGS	
at	2.049	n	
np	26264	n	
fb	4000	dp	y
bs	32	hs	nn
d1	1.000	PROCESSING	
nt	8	0.20	
ct	8	65536	
TRANSMITTER		fn	DISPLAY
tn	H1	sp	-136.7
strq	399.868	wp	3483.9
tof	399.6	rfl	802.3
tpwr	59	rtp	0
pw	6.750	rp	-97.6
DECOUPLER		lp	-28.7
dn	C13	PLOT	
dof	0	WC	250
dm	nmh	SC	0
dmm	C	VS	637
dpwr	34	th	2
dmt	29412	at	cdc ph



T1 EXPERIMENT
T1 EXPERIMENT
T1 EXPERIMENT
expt Carbon

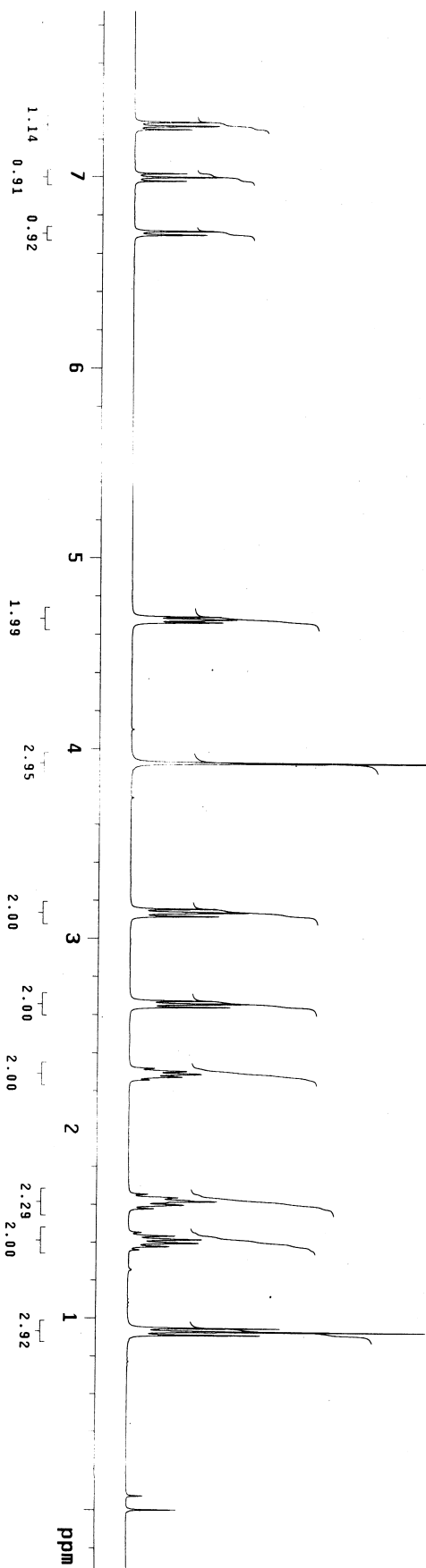
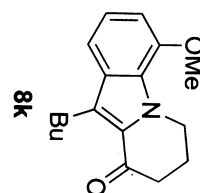
SAMPLE		SPECIAL	
date	Jun 8 2007	temp	25.0
solvent	cdcl3	gain	30
file	exp	sp1n	not used
ACQUISITION		hst	0.008
sw	30487.8	pw90	15.300
at	1.300	alfa	10.000
np	73298	FLAGS	
fb	17000	i1	n
bs	64	in	n
d1	1.000	dp	y
nt	2000	hs	nm
ct	192	PROCESSING	
tn	TRANSMITTER C13	lb	0.50
sfrq	125.688	fn	not used
tof	1255.3	DISPLAY	
tpwr	49	sp	-2082.6
pw	7.650	wd	30487.3
DECOUPLER		rfl	11760.0
dn	H1	rfd	9676.9
dof	0	tp	-48.7
dm	yyv	ip	-229.4
dmm	w	PLOT	
dpwr	39	wc	250
dmf	12200	sc	0
		vs	17176
		th	13
		ai	cdc ph



STANDARD 1H OBSERVE - profile

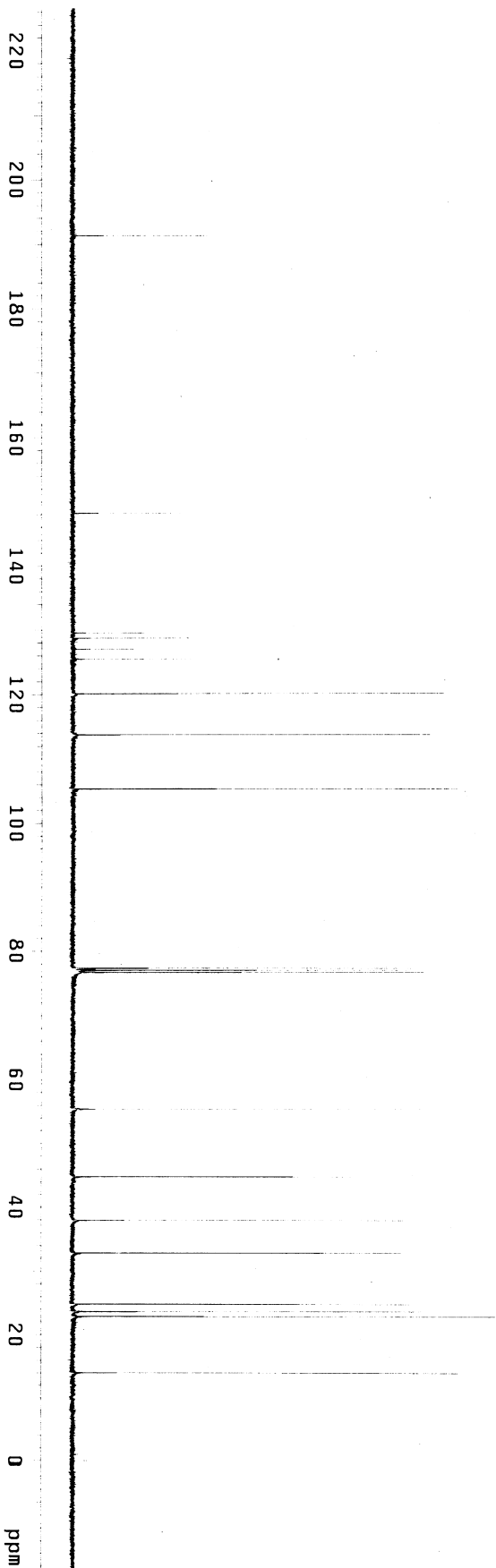
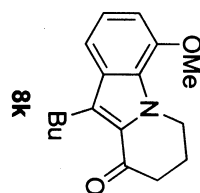
expt proton

SAMPLE		SPECIAL	
date	Aug 2 2007	temp	25.0
solvent	cdcl3	gain	30
file	/home/waikup/~	spin	not used
nmr-400	/waikup/data/~	hst	0.008
/Zhang/Guotaoli/K2~	pw90	13.500	
92-1.fid	alfa	6.500	
ACQUISITION		FLAGS	
sw	6410.3	11	n
at	2.049	in	y
np	26264	dp	nm
fb	4000	hs	nm
bs	8	lb	nm
dl	1.000	fb	nm
nt	8	tp	nm
ct	8	fp	nm
TRANSMITTER		DISPLAY	
tn	h1	sp	-132.2
strq	399.868	rf1	3280.6
tor	399.8	rfp	802.8
tpwr	59	rfp	154.2
pw	6.750	tp	-30.1
DECOUPLER		PLOT	
dn	C13	wc	250
dof	0	sc	0
dm	nmn	vs	179
dmm	c	th	3
dpwr	34	at	cdc
dnt	29412	ph	



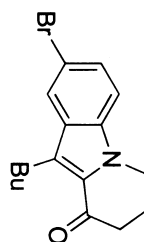
STANDARD 1H OBSERVE - profile
expt Carbon

SAMPLE 2 2007 temp 25.0
date Aug 2 2007 gain 30
solvent cdc13 not used
file ACQUISITION exp hsf 0.008
sw 24509.8 pps 11.900
at 1.3200 alfa 10.000
np 63750 i1 n
fb 17000 i1 n
bs 16 i1 n
dl 1.000 dp y
nt 3200 hs nm
ct 2960
TRANSMITTER lb fn PROCESSING 0.50
in C13 not used
sfreq 100.557 sp DISPLAY
iof 1042.8 wp -1721.4
tpwr 53 24509.1
pw 5.950 rfi 9464.2
DECOUPLER H1 rfp 7742.1
dn 0 tp -179.4
dof 0
dm yvy PLOT
dmm w 250
dpwr 41 0
dmf 9500 56722
th 5
ai cdc ph

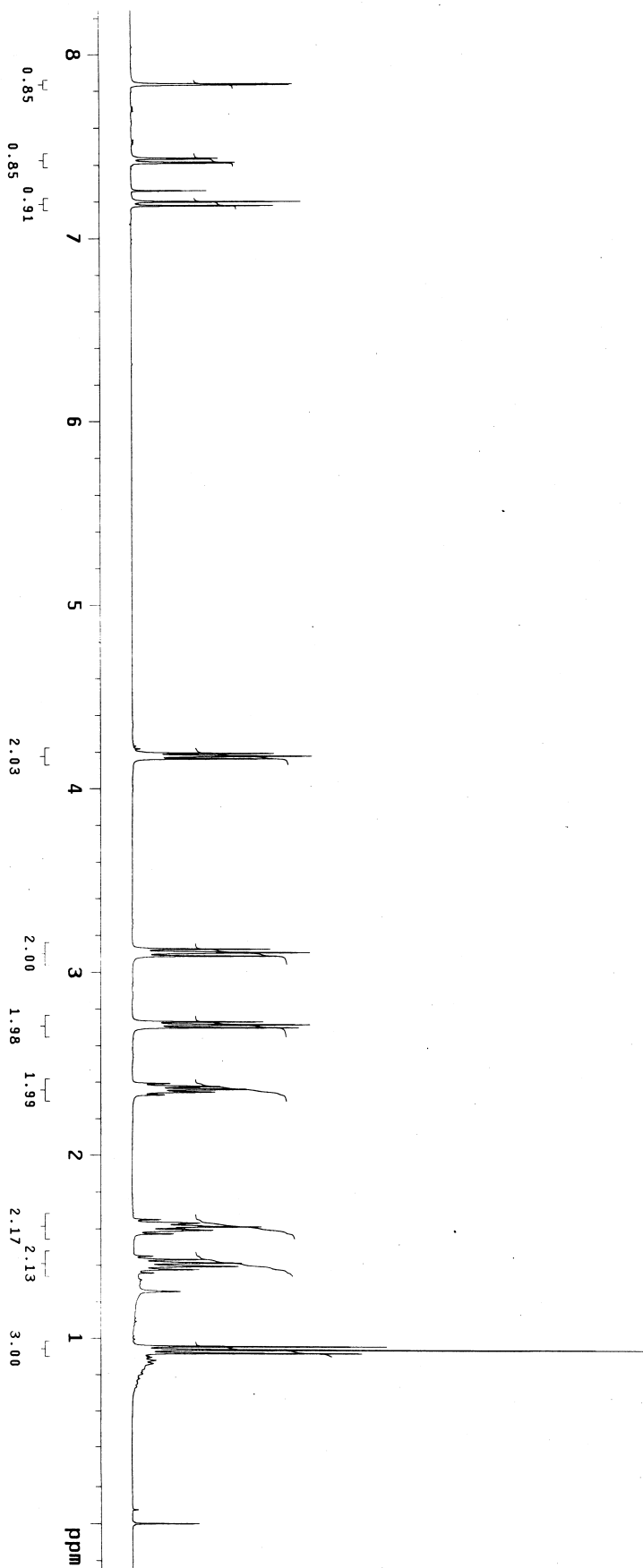


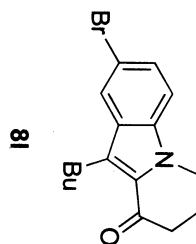
expt1 Proton

SAMPLE		SPECIAL	
date	Jul 31 2007	temp	25.0
solvent	cdcl3	gain	30
file	/mnt/nmr400/w~	spin	not used
alkup/data/Zhang/G~	hst	pw90	13.500
notaul/K284-1.fid	alpha	pw90	6.600
ACQUISITION			
sw	6410.3	fl	11
at	2.049	in	n
nd	26264	dp	y
fb	4000	hs	nn
bs	8	PROCESSING	
dl	1.000	0.20	65536
nt	8	fn	1b
ct	8	fn	1b
TRANSMITTER			
tn	H1	sp	DISPLAY
strq	399.868	wp	-106.6
tor	399.6	rf1	3405.3
tpwr	59	rfp	796.9
pw	6.750	tp	75.2
DECOUPLER			
dn	C13	tp	-13.5
dof	0	wc	PLOT
dm	nmn	sc	250
dmm	c	vs	0
dpr	34	th	183
dmf	29412	ai	cdc
		ph	6



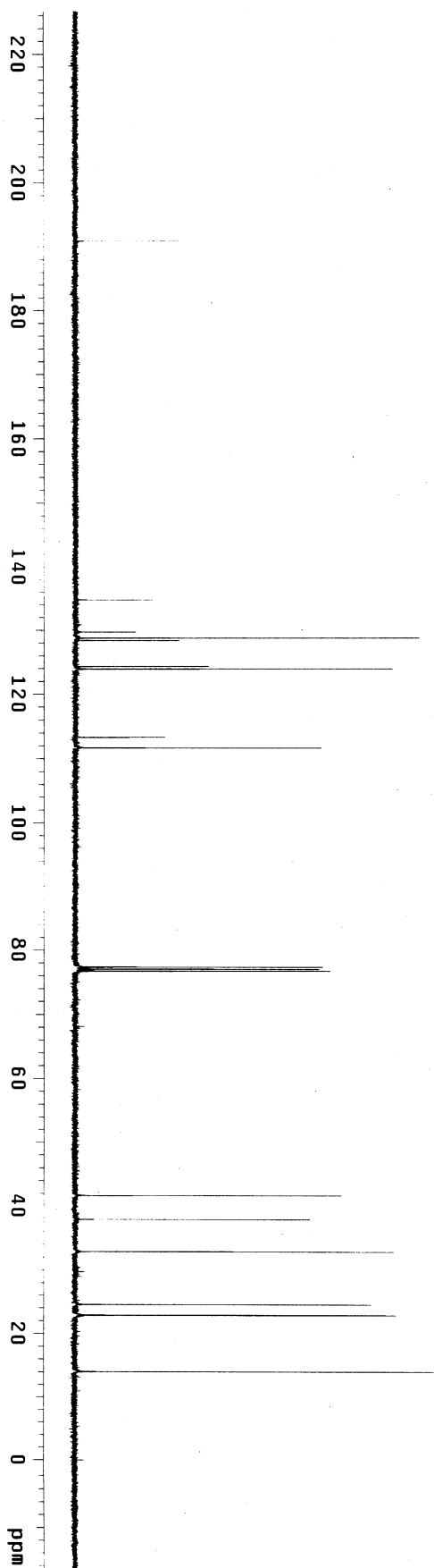
81





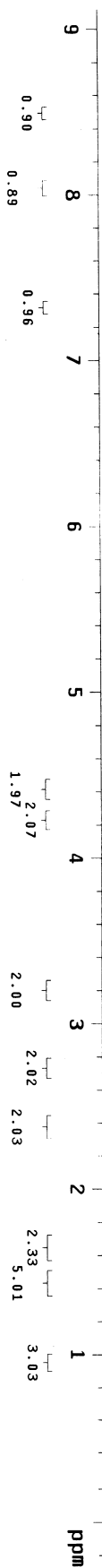
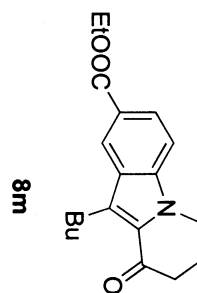
```

expt Carbon
SAMPLE
date Jul 31 2007 temp 25.0
solvent cdcl3 gain 60
file /mnt/nmr400/w~ spin not used
alkup/data/zhang/G~ hst 0.008
nutaol/K284-1carb~ pw30 11.900
on fid aifa 10.000
ACQUISITION
sw 24509.8 f1 n
at 1.300 f2 n
np 63750 dp y
fb 17000 hs mn
bs 64
d1 1.000 lb 0.50
nt 1200 fn not used
ct 1200
TRANSMITTER
tn C13 sp -1721.4
sfrq 100.557 wp 24509.1
tof 1042.8 rfi 9464.2
tdwr 53 rfp 7742.1
pw 5.950 lp -115.9
DECOUPLER
dn H1 WC PLOT 250
dof 0 SC 0
dm YVY VS 1417
dmm w th 6
dpwr ai ai cdc ph
dmf 9500
  
```



expt Proton

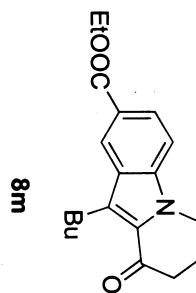
SAMPLE		SPECIAL	
date	Aug 1 2007	temp	25.0
solvent	cdcl3	gain	30
file	/mnt/nmr400/w~	spin	not used
akup/data/zhang/G~		hst	0.008
notatol/K286-1.fid		pw90	13.500
notatol/K286-1.fid		atfa	6.600
ACQUISITION			
sw	6410.3	flags	
at	20049	il	n
np	26254	in	n
fb	4000	dp	y
bs	8	hs	nn
dl	1.000	hs	nn
nt	8	lb	0.20
ct	8	fn	6536
TRANSMITTER			
tn	H1	sp	-125.4
sfrq	399.868	wp	3770.9
tof	399.6	rfl	796.0
tpwr	59	rfd	0
pw	6.750	rp	81.4
decoupler	C13	lp	-25.2
dn	0	plot	
dof	0	wc	250
dm	nnn	sc	0
dmm	c	vs	576
dpr	34	th	2
dnt	29412	ai	cdc
		ph	



```

expt Carbon
SAMPLE 1 2007 temp 25.0
date Aug 1 2007 gain 25.0
solvent cdc13 spin not used
f1le /home/walkup/~ hst 0.008
vnmr/sys/data/auto_~ pw90 11.900
2007.08.01/s-20070~ alfa 10.000
801_001/data/cdc13~
ACQUISITION 01.fid
sw 24509.8 11 n
at 1.300 1n y
np 63750 hs PROCESSING nm
fb 17000 not used
bs 64 1b 0.50
dl 1.000 fn not used
nt 2000 DISPLAY
ct 2000 SP -1720.6
tn TRANSMITTER C13 WP 24509.1
sfreq 100.557 rfl 9463.4
tof 1042.8 ffp 7742.1
tpwr 53 1p 111.3
pw 5.950 PLOT -185.6
DECOUPLER H1 WC 250
dn H1 SC 0
dof 0 VS 82640
dm 0 yvy W 5
dmm w at cdc ph
dpwr 41
dmf 9500

```

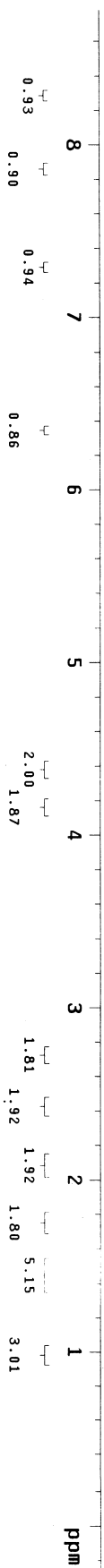
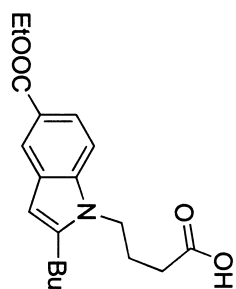


220 200 180 160 140 120 100 80 60 40 20 0 ppm

```

expt  Proton
SAMPLE
date Aug 3 2007 temp 25.0
solvent cdc13 gain 30
file/home/walkup/~ not used
nmr400/walkup/data/~ hst 13.500
/Zhang/buotaol/K2~ py20 6.600
36-3-110 atfa
ACQUISITION
sw 6410.3 f1 n
at 2.049 f2 n
np 26264 dp y
fb 4000 hs
bs 8
d1 1.000 lb 0.20
nt 1 fn 65536
ct 1
TRANSMITTER
tn H1 sp -108.2
sfrq 399.868 rfl 3619.5
tof 399.6 rfp 800.5
tdwr 59 rp 0
pw 6.750 lp 155.8
DECOUPLER C13 WC PLOT -33.1
dn C13 WC 250
dof 0 SC 0
dm nnn VS 300
dmm C th
dpuv 34 ai cdc ph 2
dmf 29412
SPECIAL

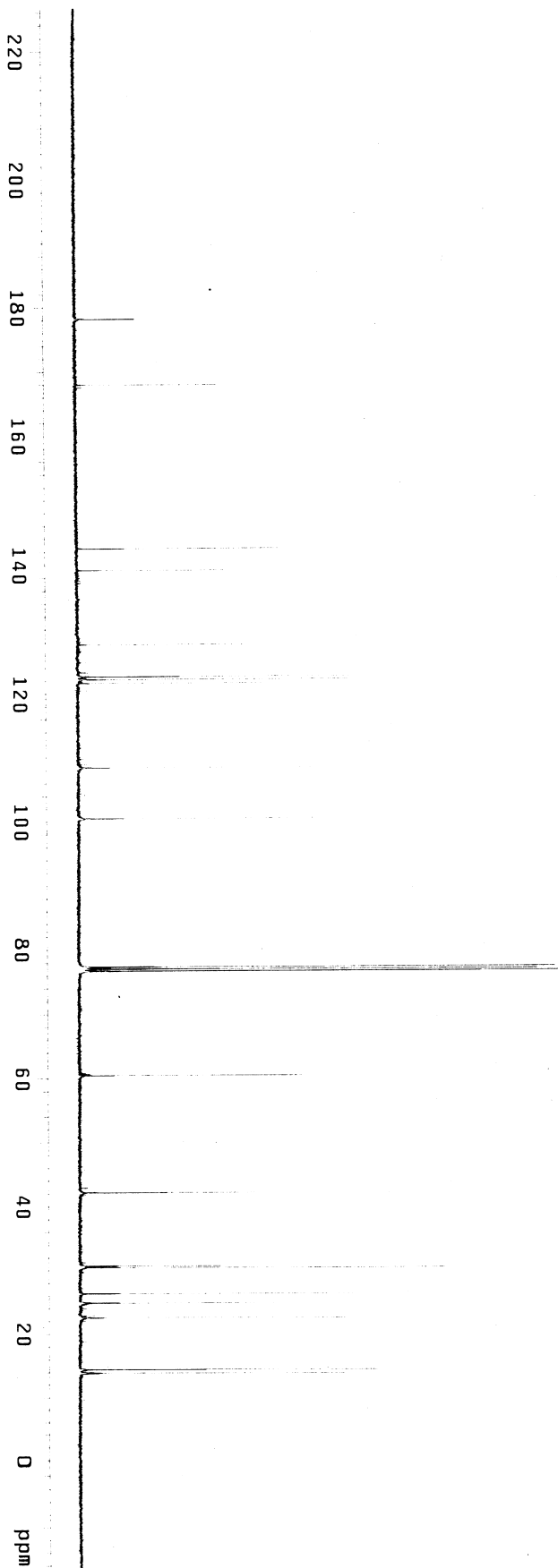
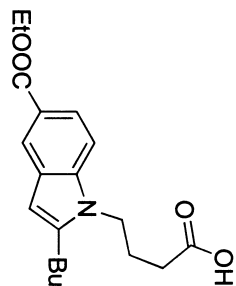
```



```

expt Carbon
SAMPLE
date Aug 3 2007 temp 25.0
solvent cdc13 gain 30
f1le /home/walrup/~ not used
vnmr/sys/data/autoc hst 0.006
2007.08.03.16/s_20~ pw90 11.900
070803_001/data/cd~ alfa 10.000
c13-01.f1d FLAGS
ACQUISITION 11 n
sw 24509.8 tn n
at 1.300 dp y
np 63750 hs n
fb 17000
bs 64 lb
dl 1.000 fn
nt 12000 not used
ct 12000 DISPLAY
TRANSMITTER SP -1719.9
tn wd 24509.1
sfreq rfl 9462.7
iof rfp 7742.1
tpwr fp -172.9
pw 5.950 lp -193.0
DECOUPLER WC PLOT
dn H1 250
dof 0
dm 0
dmm yvy 82807
dpwr w at cdc ph 8
dmt 41
9500

```

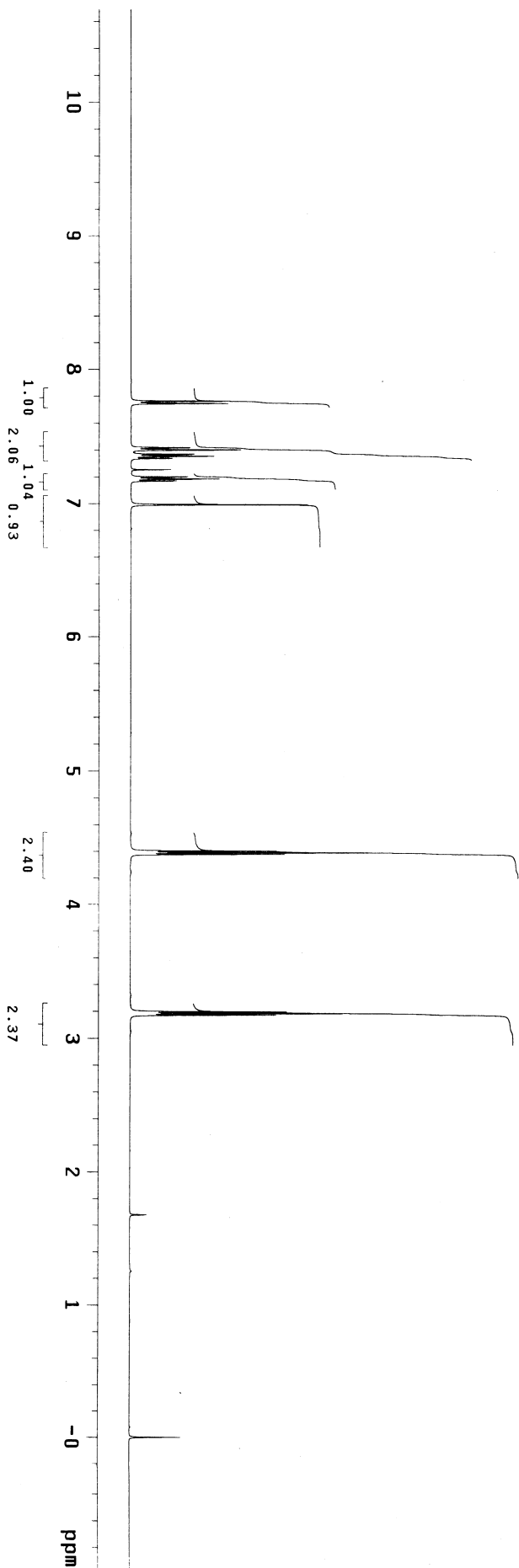
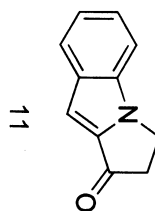


Automation directory: /home/waikup/vnmrSYS/data/auto_2007.06.12
File : Aug.01/data/cdc13_01.fid
Sample id : Aug.01

Pulse Sequence: szpul

Solvent: cdc13
Temp: 22.0 C / 295.1 K
Operator: waikup
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: 499.7991866 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min, 30 sec

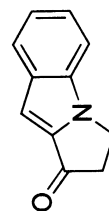


Automation directory: /home/walkup/vnmrSYS/data/auto 2007.06.12
File: /home/walkup/data/Zhang/XiaogengHuang/hxg-3-157C.fid
Sample id: tmpstudy

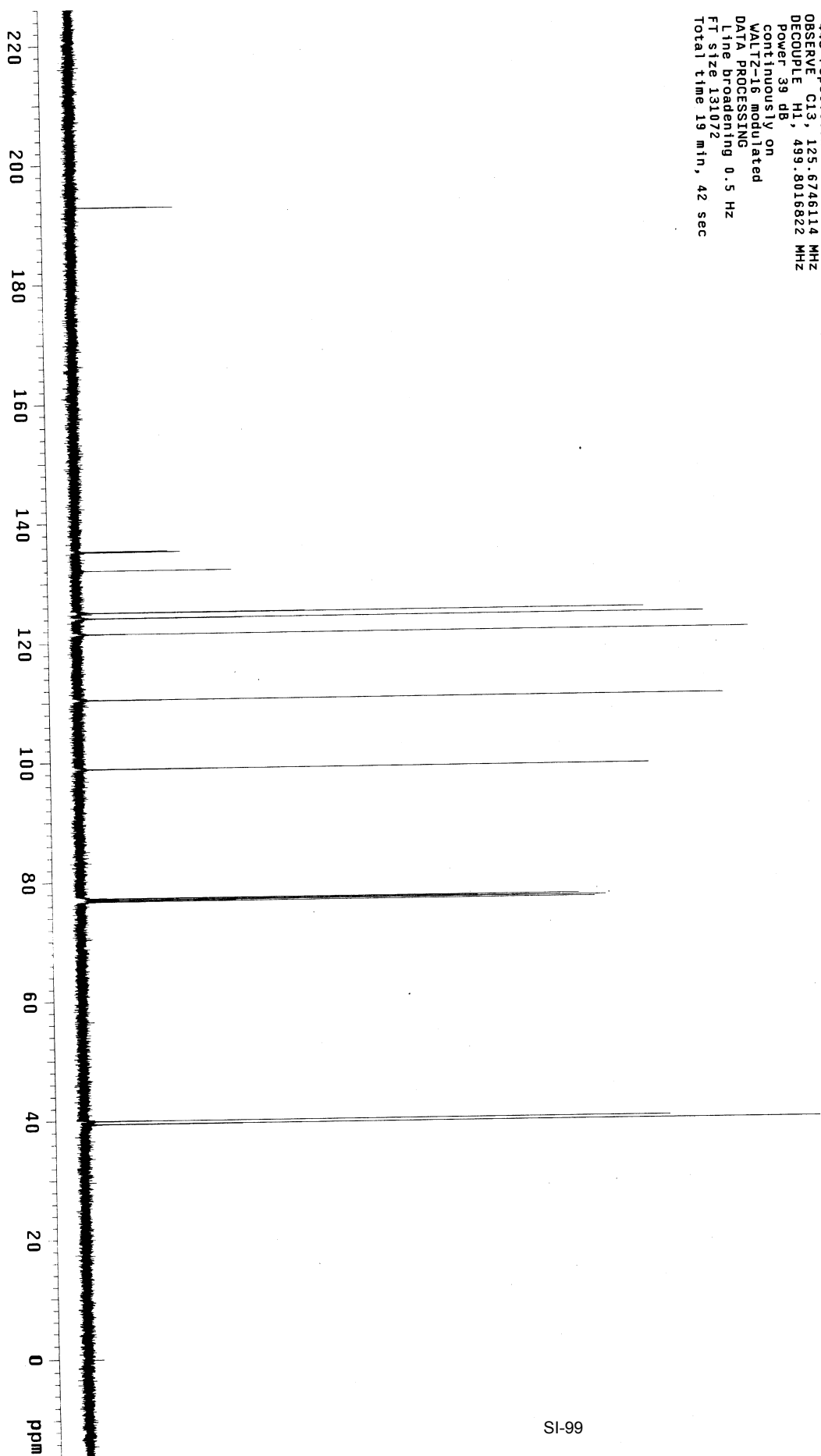
Pulse Sequence: szpul

Solvent: cdcl3
Temp: 22.0 C / 295.1 K
Operator: walkup
File: hxg-3-157C
VNMRS-500 "nmr-500"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 30487.8 Hz
448 repetitions
OBSERVE C13, 125.6746114 MHz
DECOUPLE H1, 499.8016822 MHz
Power 39 db
continuously on
WALTZ-16 modulated
DATA PROCESSING
line broadening 0.5 Hz
FT size 131072
Total time 19 min, 42 sec



11



File: hxg-3-155-2C

Pulse Sequence: s2pul

Solvent: cdcl3

Temp: 25.0 C / 298.1 K

Operator: Walkup

File: hxg-3-155-2C

INOVA-500 "redjacket"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 30487.8 Hz

600 repetitions

OBSERVE C13, 125.6746105 MHz

DECOUPLE H1, 499.8016822 MHz

Power 39 dB

continuously on

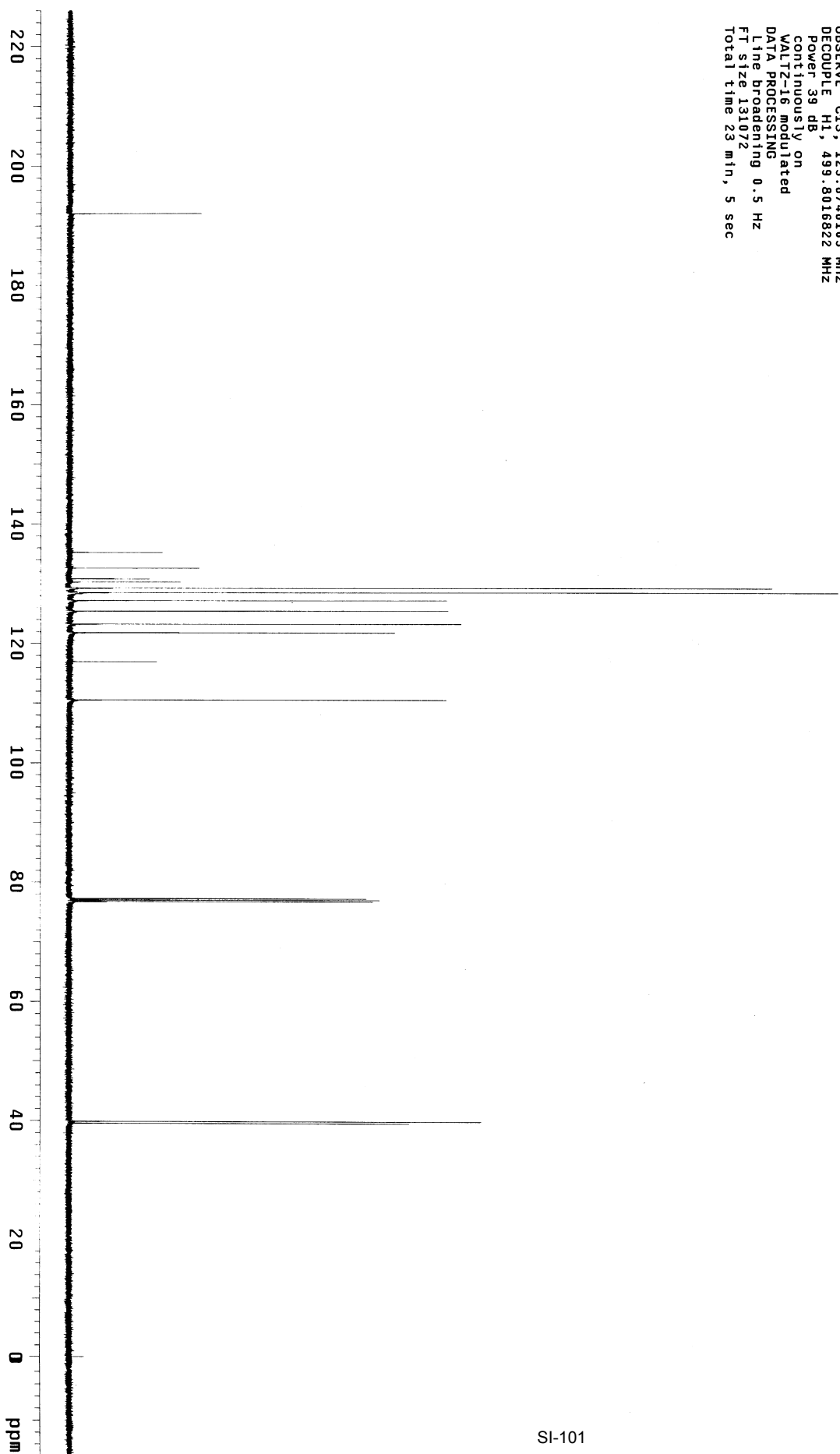
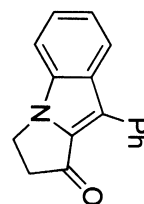
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 131072

Total time 23 min, 5 sec

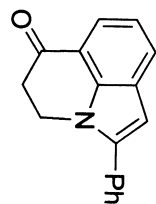


Automation directory: /home/walkup/vnmrSYS/data/auto_2007.06.11_26
File : s_20070611_002/data/cdc13_02.fid
Sample id : s_20070611_002

Pulse Sequence: szpul

Solvent: cdc13
Temp. 25.0 C / 298.1 K
Operator: walkup
File: cdc13_02
Vnmrs-400 "NMR400"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.009 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 399.8656747 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min, 30 sec

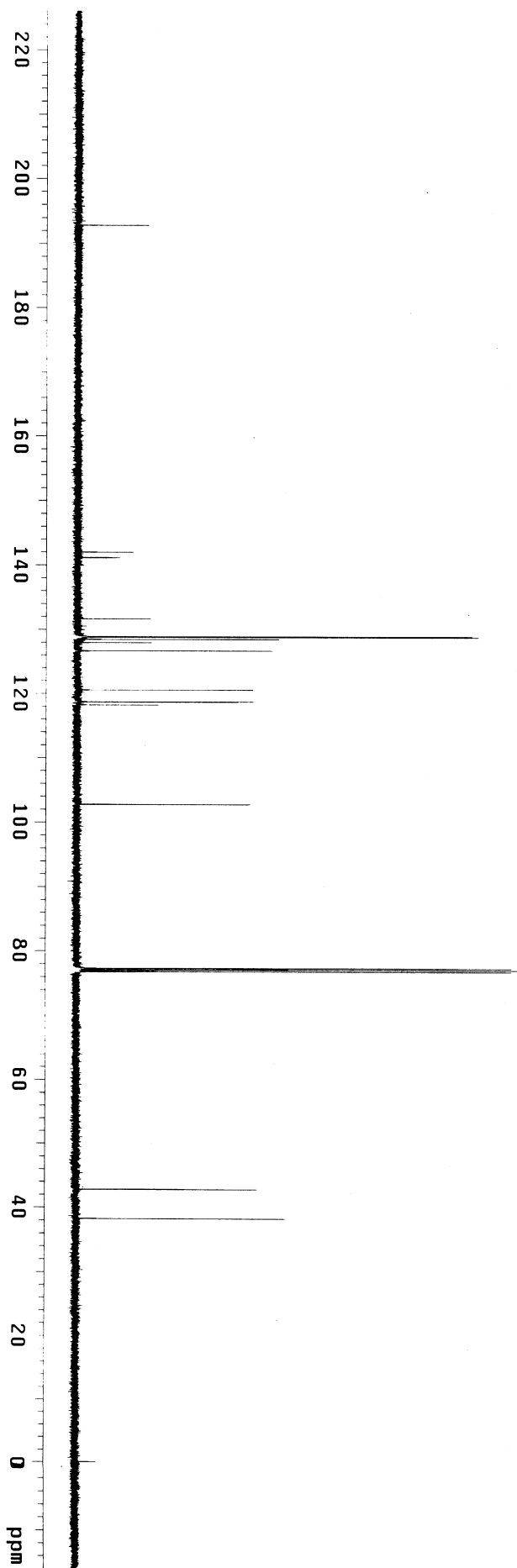
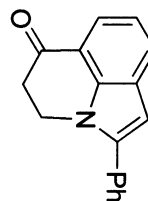


Automation directory: /home/walkup/vnmrSYS/data/auto_2007.06.11_10
File : exp
Sample id : tmpstudy

Pulse Sequence: szpul

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

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 30487.8 Hz
800 repetitions
OBSERVE C13, 125.6746053 MHz
DECOUPLE H1, 499.8016822 MHz
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 30 min, 47 sec



File: hxg-3-158-2H

Pulse Sequence: szpu1

Solvent: cdcl3

Temp: 25.0 C / 298.1 K

Operator: walkup

File: hxg-3-158-2H

INOVA-500 "redjacket"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.049 sec

Width 8012.8 Hz

8 repetitions

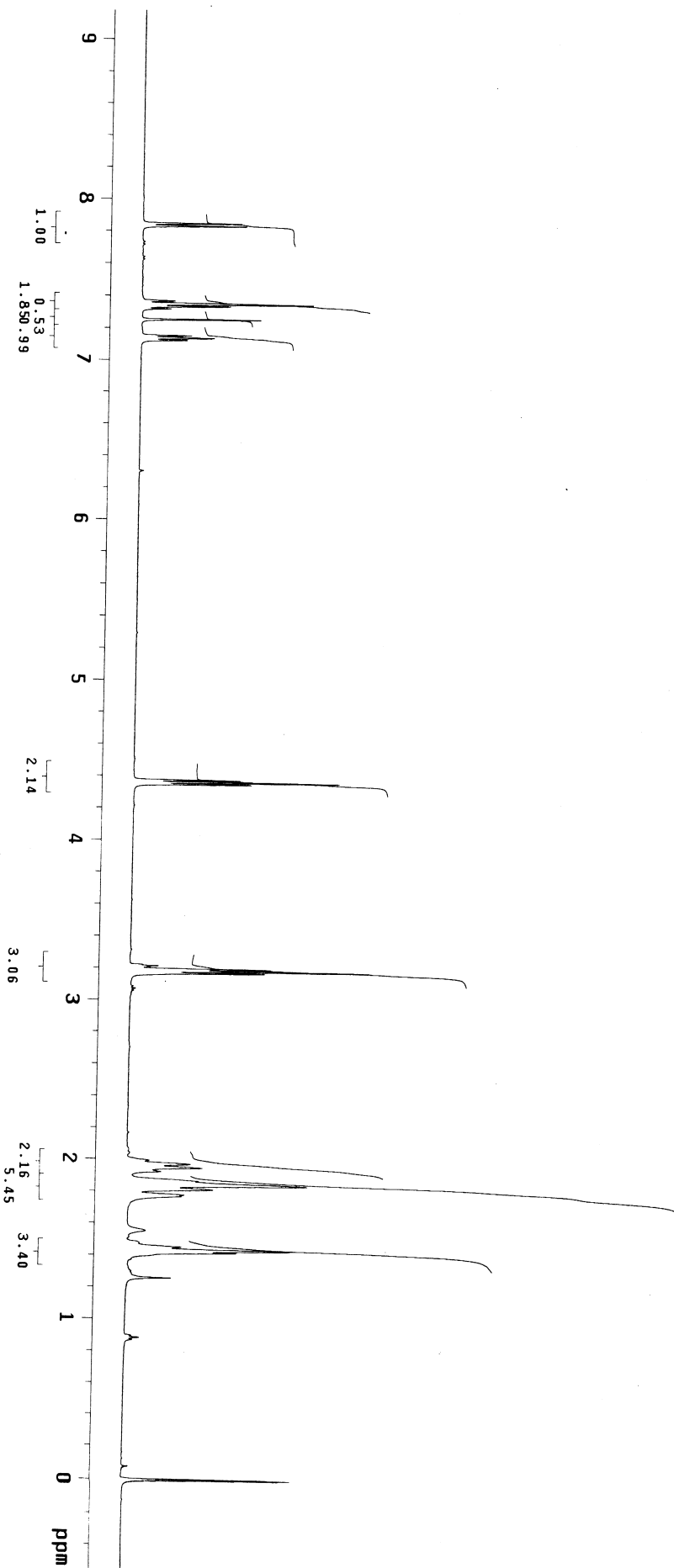
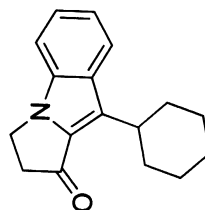
OBSERVE H1 499.791854 MHz

DATA PROCESSING

Line broadening 0.2 Hz

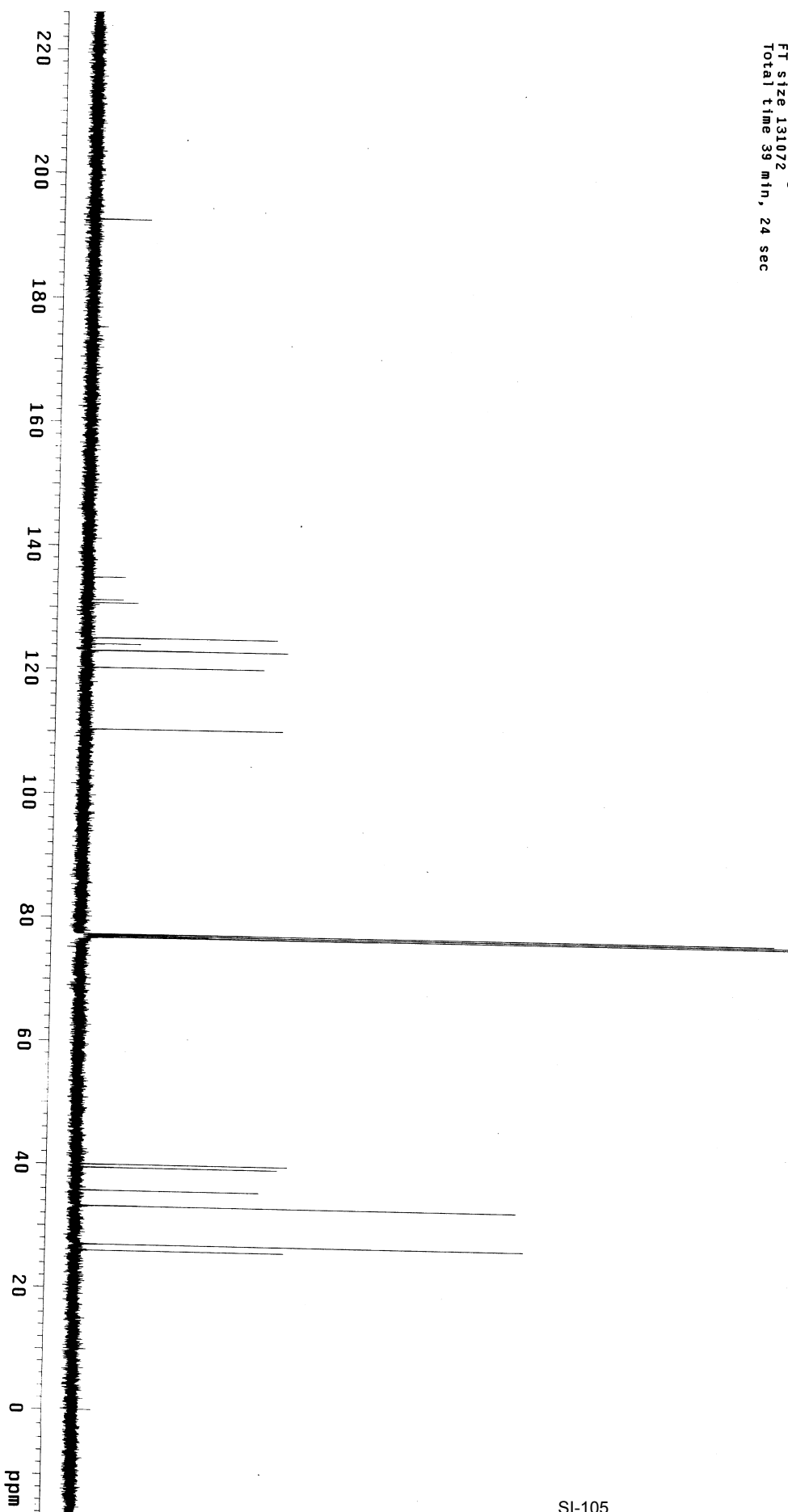
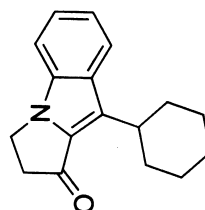
FT size 65536

Total time 0 min, 30 sec



Automation directory: /home/walkup/vnmrSYS/data/auto_2007.06.25_13
File : exp
Sample id : tmpstudy
Pulse Sequence: szpu1
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: walkup
VNMR-500 "nmr500"

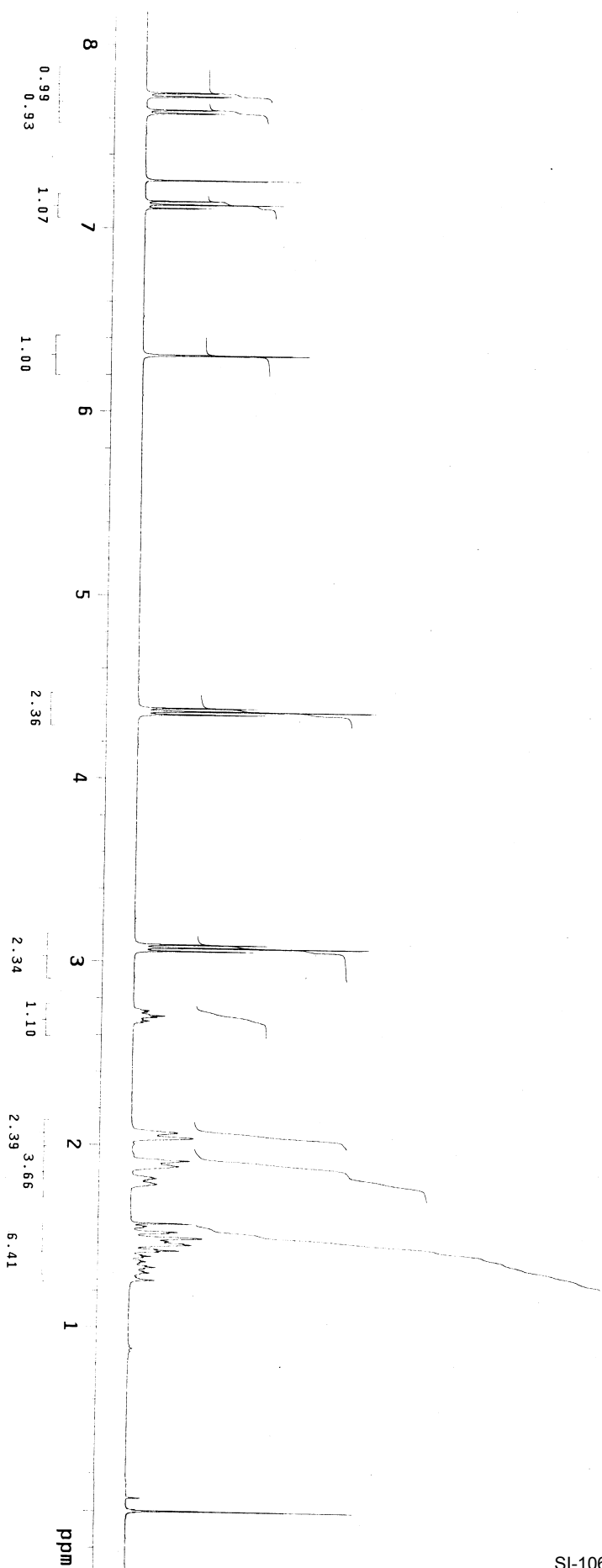
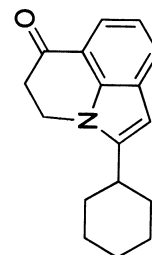
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 30487.8 Hz
384 repetitions
OBSERVE C13, 125.6746039 MHz
DECOUPLE H1, 499.5016822 MHz
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 39 min, 24 sec



Automation directory: /home/walrup/vnmrSYS/data/auto_2007.06.11_14
File : s_20070611_001/data/cdc13_02.fid
Sample id : s_20070611_001

Pulse Sequence: s2pu1
Solvent: cdc13
Temp: 25.0 C / 298.1 K
Operator: walrup
File: cdc13_02
VNMR-400 "NMR400"

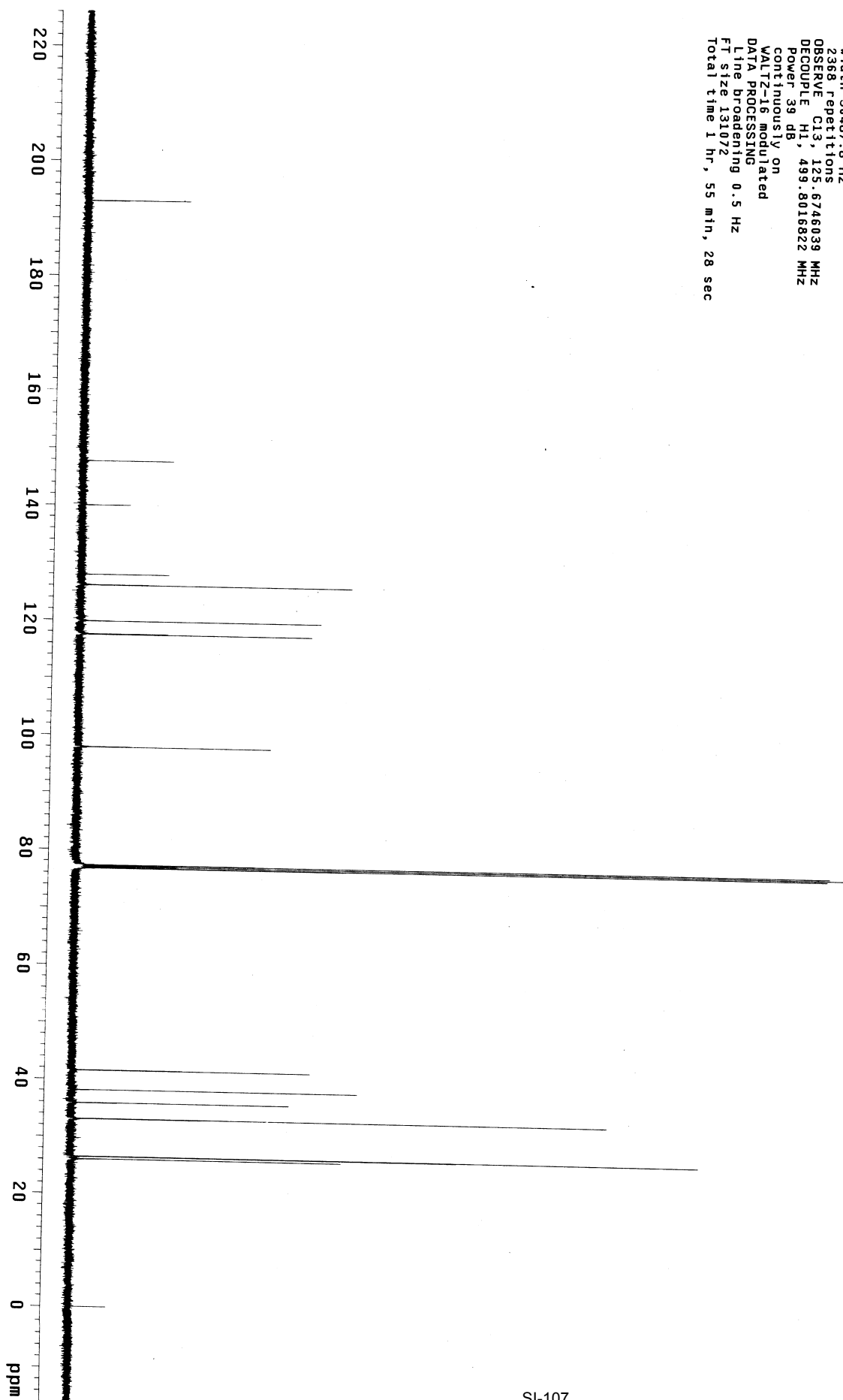
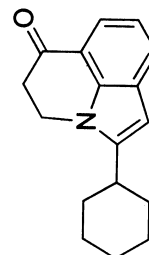
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.049 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 399.8656733 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min, 30 sec



Automation directory: /home/walkup/vnmrSYS/data/auto_2007.06.11_08
File : exp
Sample id : tmpstudy

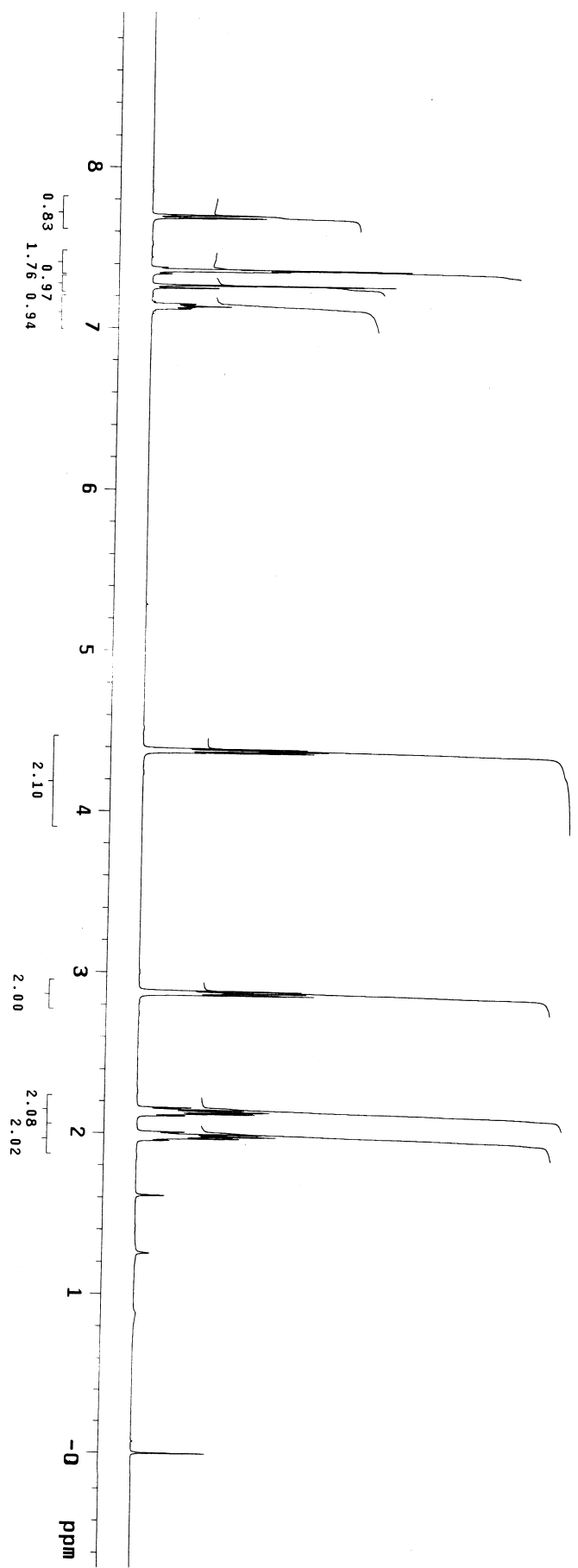
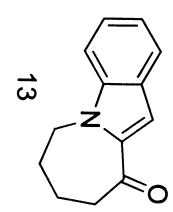
Pulse Sequence: s2pul
Solvent: cdc13
Temp: 25.0 C / 298.1 K
Operator: walkup
VNMRS-500 "nmr500"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 30487.8 Hz
2368 repetitions
OBSERVE C13, 125.6746039 MHz
DECOUPLE H1, 499.8016822 MHz
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 1 hr, 55 min, 28 sec



File: hxg-4-13H
 Pulse Sequence: szpul
 Solvent: cdcl3
 Temp: 25.0 C / 298.1 K
 Operator: walkup
 File: hxg-4-13H
 NOVA-500 "redjacket"

Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.049 sec
 Width 8012.8 Hz
 Repetitions
 NSERVE H1, 499.7991866 MHz
 FTA PROCESSING
 Line broadening 0.2 Hz
 Size 65536
 Total time 0 min, 30 sec



Automation directory: /home/walkup/vnmr sys/data/auto_2007.06.25_14
File : exp
Sample id : tmpstudy

Pulse Sequence: s2pu1

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: walkup

VNMR-500 "nmr-500"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 30487.8 Hz

640 repetitions

OBSERVE C13, 125.6746072 MHz

DECOUPLE H1, 499.8016822 MHz

Power 39 dB

continuously on

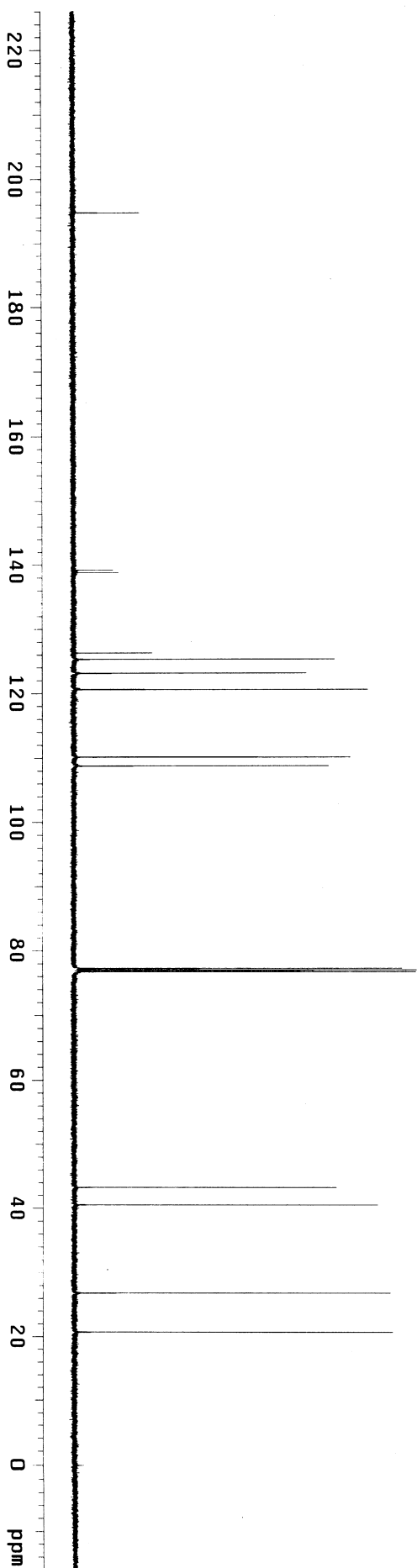
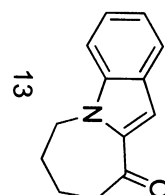
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 131072

Total time 39 min, 24 sec



Automation directory: /home/walkup/vnmr sys/data/auto_2007.06.25_14
File : exp
Sample id : tmpstudy

Pulse Sequence: s2pu1

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: walkup

VNMR-500 "nmr-500"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 30487.8 Hz

640 repetitions

OBSERVE C13, 125.6746072 MHz

DECOUPLE H1, 499.8016822 MHz

Power 39 dB

continuously on

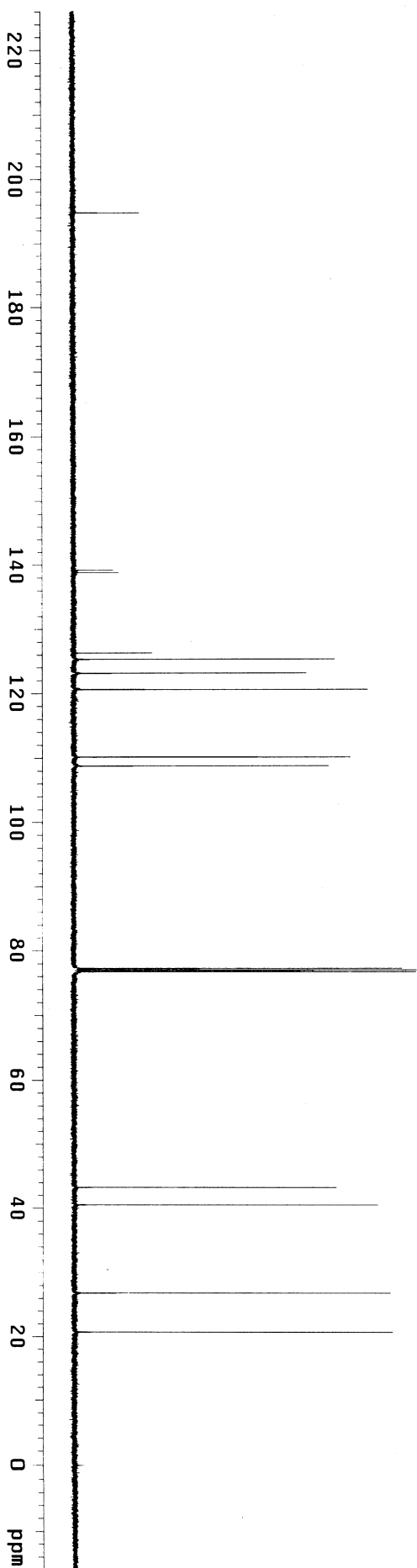
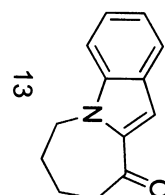
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

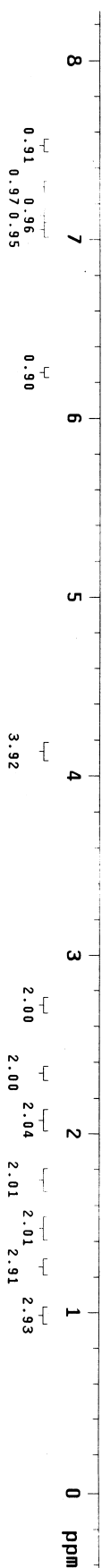
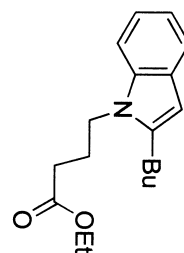
FT size 131072

Total time 39 min, 24 sec

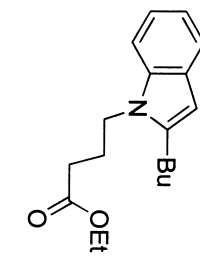


expt1 Proton

SAMPLE		SPECIAL	
date	Aug 31 2007	temp	25.0
solvent	cdcl3	gain	30
file	/home/walkup/~	spin	not used
nmr400/walkup/data/~	hst	0.008	
/Zhang/Guotaol i/K3~	pw90	13.400	
77-lb.fid	alfa	6.600	
ACQUISITION		FLAGS	
sw	6410.3	il	n
at	2.049	in	n
np	26264	dp	v
fb	4000	hs	nh
bs	8	PROCESSING	n
dl	1.000	lb	0.20
nt	8	fn	65536
ct	8	DISPLAY	-182.9
tn	HI	sp	3490.9
strq	399.866	rfl	805.9
tof	399.6	rfl	0
tpwr	59	rp	27.7
pw	6.700	lp	-27.0
DECOUPLER		PLOT	
dn	Cl3	wc	250
dof	0	sc	0
dm	nmh	vs	328
dmm	c	th	12
dpwr	34	ai	cdc
dmf	29412	ph	



expt Carbon



SAMPLE SPECIAL 25.0
date Aug 31 2007 temp 30
solvent cdcl3 gain 30
file /home/walkup/~ hst not used
nmrSYS/data/auto~ hst 0.008
2007.08.31.02/Aug~ pw90 15.300
01/data/cdcl3_02.f~ a1fa 10.000

ACQUISITION
id 11
SW 30487.8
at 1.300
np 79298
td 17000
bs 64
d1 1.000
nt 3000
ct 64

TRANSMITTER
in C13
sfrq 125.687
tof 1255.2
tpwr 49
pw 7.650

DECOUPLER
dn H1
dof 0
dm vs
dmm yvy
dpm w
dmf 12200

PROCESSING
hs
nm
0.50
not used
DISPLAY
-2081.2
30487.3
11758.6
9676.9
-56.9
-264.0

PLOT
wc 250
sc 0
vs 0
th 26406
at 14
cdc ph

