

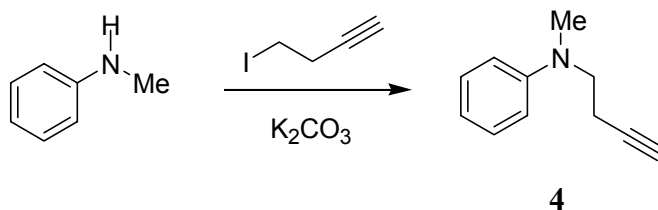
Supporting Information

**Gold or No Gold: One-Pot Synthesis of Tetrahydrobenz[b]azepin-4-ones from  
tertiary *N*-(But-3-ynyl)anilines**

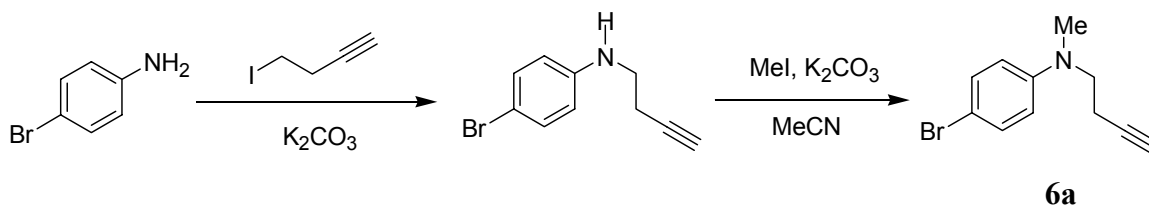
Li Cui, Guozhu Zhang, Yu Peng and Liming Zhang

Department of Chemistry/216, University of Nevada, Reno  
1664 North Virginia Street, Reno, Nevada 89557

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

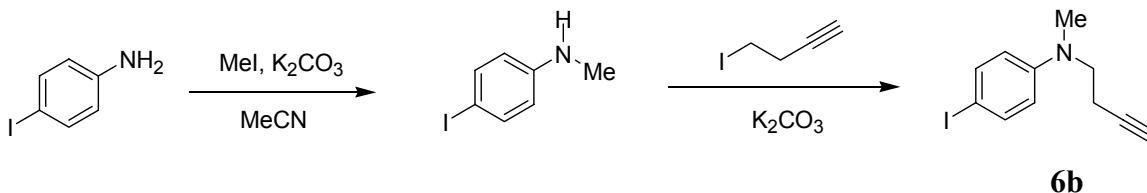


4-Iodobut-1-yne (1 mmol) was added to a mixture of *N*-methylaniline (2 mmol) and K<sub>2</sub>CO<sub>3</sub> (2 mmol) without solvents. The reaction was heated at 80 °C for 6 h and then cooled to room temperature. The reaction mixture was diluted with CH<sub>2</sub>Cl<sub>2</sub> (10 mL/mmol), and the solid was filtered off. The filtrate was concentrated under *vacuum*, and the residue was purified through silica gel flash column chromatography (eluent: hexanes: ethyl acetate = 25:1, then hexanes: ethyl acetate = 10:1) to afford compound **4** in 72 % yield. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.22 – 7.26 (m, 2H), 6.70 – 6.73 (m, 3H), 3.56 (t, 2H, *J* = 7.2 Hz), 2.96 (s, 3H), 2.69 (td, 2H, *J* = 7.2, 2.8 Hz), 1.99 (t, 1H, *J* = 2.8 Hz); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 148.4, 129.3, 116.6, 112.2, 82.2, 69.6, 51.8, 38.4, 16.4; IR (neat): 3289, 2911, 2115, 1601, 1501, 1356, 1282, 1228, 1356, 1193, 1115, 1037, 991; MS (ES<sup>+</sup>) Calculated for [C<sub>11</sub>H<sub>14</sub>N]<sup>+</sup>: 160.1; Found: 160.0.



4-Iodobut-1-yne (1 mmol) was added to a mixture of 4-bromophenylamine (2 mmol) and  $K_2CO_3$  (2 mmol) without solvents. The reaction was heated at 80 °C overnight and then cooled to room temperature. The reaction mixture was diluted with  $CH_2Cl_2$  (10 mL/ mmol), and the solid was filtered off. The filtrate was concentrated under *vacuum*, and the residue was purified through silica gel flash column chromatography (eluent: hexanes: ethyl acetate = 15:1) to afford (4-bromophenyl)but-3-ynylamine.

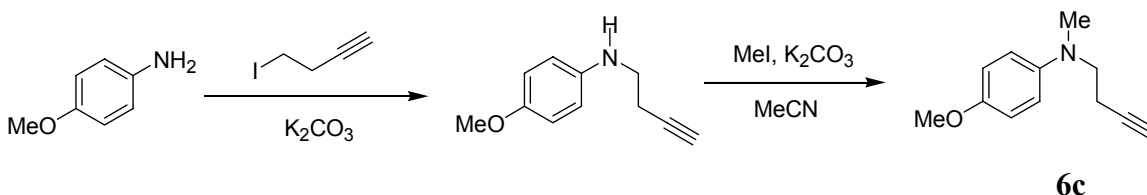
Iodomethane (2 mmol) was added to a mixture of (4-bromophenyl)but-3-ynylamine (1 mmol) and  $K_2CO_3$  (1 mmol) in anhydrous acetonitrile (5 mL/ mmol). The reaction was heated at 60 °C overnight and then cooled to room temperature. The reaction mixture was diluted with  $CH_2Cl_2$  (10 mL/ mmol), and the solid was filtered off. The filtrate was concentrated under *vacuum*, and the residue was purified through silica gel flash column chromatography (eluent: hexanes: ethyl acetate = 15:1) to afford compound **6a** in 45 % yield in 2 steps.  $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  7.30 (d, 2H,  $J$  = 9 Hz), 6.57 (d, 2H,  $J$  = 9 Hz), 3.53 (t, 2H,  $J$  = 7 Hz), 2.95 (s, 3H), 2.41 (td, 2H,  $J$  = 7.5, 2.5 Hz), 2.00 (t, 1H,  $J$  = 2.5 Hz);  $^{13}C$  NMR (125 MHz,  $CDCl_3$ )  $\delta$  147.4, 131.9, 113.8, 108.5, 81.8, 69.9, 51.7, 38.5, 16.4; IR (neat): 3293, 2914, 2360, 1590, 1497, 1365, 1189, 1113; MS ( $ES^+$ ) Calculated for  $[C_{11}H_{13}BrN]^+$ : 238.0; Found: 237.8.



Iodomethane (1 mmol) was added to a mixture of 4-iodophenylamine (1 mmol) and  $K_2CO_3$  (1 mmol) in anhydrous acetonitrile (5 mL/ mmol). The reaction was heated at 80 °C overnight and then cooled to room temperature. The reaction mixture was diluted with

CH<sub>2</sub>Cl<sub>2</sub> (10 mL/ mmol), and the solid was filtered off. The filtrate was concentrated under *vacuum*, and the residue was purified through silica gel flash column chromatography (eluent: hexanes: ethyl acetate = 15:1) to afford (4-iodophenyl)methylamine.

4-Iodobut-1-yne (1 mmol) was added to a mixture of (4-iodo-phenyl)-methylamine (1 mmol) and K<sub>2</sub>CO<sub>3</sub> (1 mmol) without solvents. The reaction was heated at 80 °C for 2d and then cooled to room temperature. The reaction mixture was diluted with CH<sub>2</sub>Cl<sub>2</sub> (10 mL/ mmol), and the solid was filtered off. The filtrate was concentrated under *vacuum*, and the residue was purified through silica gel flash column chromatography (eluent: hexanes: ethyl acetate = 15:1) to afford compound 6b in 35 % yield in 2 steps. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.45 (d, 2H, *J* = 9.2 Hz), 6.46 (d, 2H, *J* = 9.2 Hz), 3.51 (t, 2H, *J* = 7.2 Hz), 2.94 (s, 3H), 2.40 (td, 2H, *J* = 7.2, 2.8 Hz), 2.00 (t, 1H, *J* = 2.8 Hz); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 147.8, 137.7, 114.3, 81.8, 77.4, 69.9, 51.5, 38.4, 16.3; IR (neat): 3294, 2927, 2347, 2117, 1589, 1495, 1374, 1194, 1114, 963, 875, 824; MS (ES<sup>+</sup>) Calculated for [C<sub>11</sub>H<sub>13</sub>IN]<sup>+</sup>: 286.0; Found: 285.9.

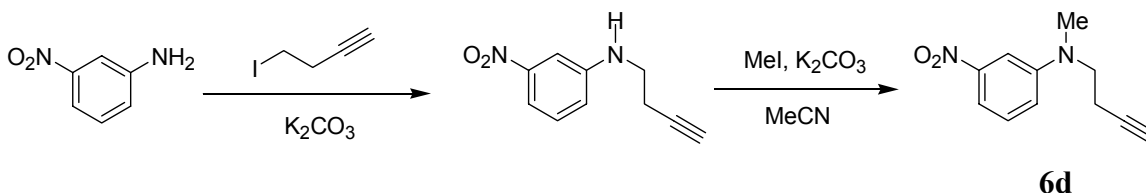


4-Iodobut-1-yne (1 mmol) was added to a mixture of 4-methoxyphenylamine (2 mmol) and K<sub>2</sub>CO<sub>3</sub> (2 mmol) without solvents. The reaction was heated at 80 °C for 5 h and then cooled to room temperature. The reaction mixture was diluted with CH<sub>2</sub>Cl<sub>2</sub> (10 mL/ mmol), and the solid was filtered off. The filtrate was concentrated under *vacuum*, and the residue was purified through silica gel flash column chromatography (eluent: hexanes: ethyl acetate = 25:1) to afford but-3-ynyl(4-methoxyphenyl)amine.

Iodomethane (1.2 mmol) was added to a mixture of but-3-ynyl-(4-methoxyphenyl)-amine (1 mmol) and K<sub>2</sub>CO<sub>3</sub> (1 mmol) in anhydrous acetonitrile (5 mL/ mmol). The reaction was heated at 60 °C overnight and then cooled to room temperature. The reaction mixture was

diluted with CH<sub>2</sub>Cl<sub>2</sub> (10 mL/ mmol), and the solid was filtered off. The filtrate was concentrated under *vacuum*, and the residue was purified through silica gel flash column chromatography (eluent: hexanes: ethyl acetate = 15:1) to afford compound **6c** in 28 % yield in 2 steps.

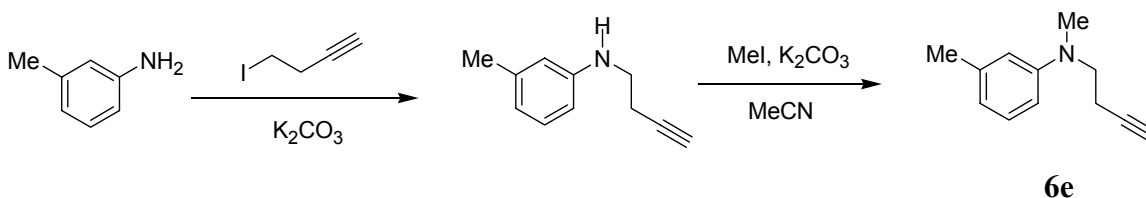
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 6.84 (d, 2H, *J* = 9 Hz), 6.71 (d, 2H, *J* = 9 Hz), 3.76 (s, 3H), 3.48 (t, 2H, *J* = 7.5 Hz), 2.90 (s, 3H), 2.39 (td, 2H, *J* = 7.5, 2.5 Hz), 1.99 (t, 1H, *J* = 2.5 Hz); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 151.9, 143.4, 114.8, 114.5, 82.4, 69.5, 55.8, 52.9, 38.9, 16.2; IR (neat): 3296, 2926, 2862, 1605, 1496, 1450, 1403, 1246, 1051; MS (ES<sup>+</sup>) Calculated for [C<sub>12</sub>H<sub>16</sub>NO]<sup>+</sup>: 190.1; Found: 190.0.



4-Iodobut-1-yne (1 mmol) was added to a mixture of 3-nitrophenylamine (2 mmol) and K<sub>2</sub>CO<sub>3</sub> (2 mmol) without solvents. The reaction was heated at 90 °C for 2 d and then cooled to room temperature. The reaction mixture was diluted with CH<sub>2</sub>Cl<sub>2</sub> (10 mL/ mmol), and the solid was filtered off. The filtrate was concentrated under *vacuum*, and the residue was purified through silica gel flash column chromatography (eluent: hexanes: ethyl acetate = 25:1, then hexanes: ethyl acetate = 15:1) to afford but-3-ynyl(3-nitrophenyl)amine.

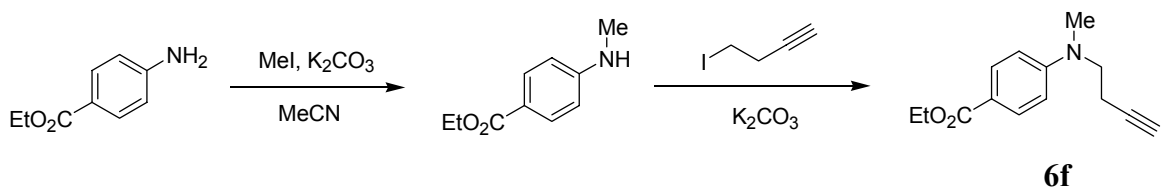
Iodomethane (4mmol) was added to a mixture of but-3-ynyl-(3-nitrophenyl)amine (1 mmol) and K<sub>2</sub>CO<sub>3</sub> (1 mmol) in anhydrous acetonitrile (5 mL/ mmol). The reaction was heated at 80 °C for 1 d and then cooled to room temperature. The reaction mixture was diluted with CH<sub>2</sub>Cl<sub>2</sub> (10 mL/ mmol), and the solid was filtered off. The filtrate was concentrated under *vacuum*, and the residue was purified through silica gel flash column chromatography (eluent: hexanes: ethyl acetate = 15:1) to afford compound **6d** in 62 % yield in 2 steps. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.49- 7.53 (m, 2H), 7.33 (t, 1H, *J* = 8.5

Hz), 6.97 (dd, 1H,  $J = 8, 2.5$  Hz), 3.63 (t, 2H,  $J = 7$  Hz), 3.07 (s, 3H), 2.47 (td, 2H,  $J = 7, 2.5$  Hz), 2.02 (t, 1H,  $J = 2.5$  Hz);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  149.7, 149.0, 129.7, 117.4, 110.9, 106.0, 81.4, 70.2, 51.4, 38.7, 16.6; IR (neat): 3293, 2910, 2360, 2118, 1617, 1525, 1345, 1228, 1198, 1122, 991, 846; MS ( $\text{ES}^+$ ) Calculated for  $[\text{C}_{11}\text{H}_{12}\text{N}_2\text{O}_2\text{Na}]^+$ : 227.1; Found: 226.9.



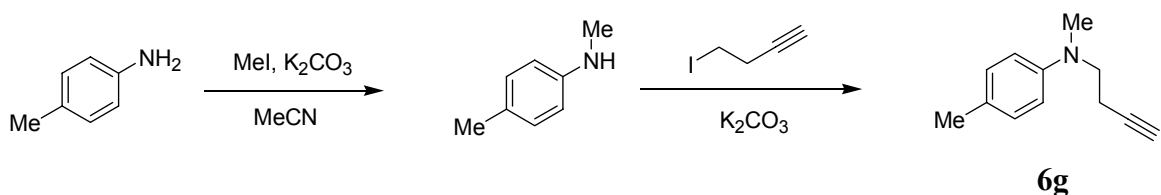
4-Iodobut-1-yne (1 mmol) was added to a mixture of *m*-toluidine (3 mmol) and  $\text{K}_2\text{CO}_3$  (3 mmol) without solvents. The reaction was heated at 60 °C for 4 h and then cooled to room temperature. The reaction mixture was diluted with  $\text{CH}_2\text{Cl}_2$  (10 mL/ mmol), and the solid was filtered off. The filtrate was concentrated under *vacuum*, and the residue was purified through silica gel flash column chromatography (eluent: hexanes: ethyl acetate = 15:1) to afford but-3-ynyl-*m*-tolylamine.

Iodomethane (1.2 mmol) was added to a mixture of but-3-ynyl-*m*-tolylamine (1 mmol) and  $\text{K}_2\text{CO}_3$  (1 mmol) in anhydrous acetonitrile (5 mL/ mmol). The reaction was stirred at room temperature for 1 d. The reaction mixture was diluted with  $\text{CH}_2\text{Cl}_2$  (10 mL/ mmol), and the solid was filtered off. The filtrate was concentrated under *vacuum*, and the residue was purified through silica gel flash column chromatography (eluent: hexanes: ethyl acetate = 15:1) to afford compound **6e** in 45 % yield in 2 steps.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.13 (t, 1H,  $J = 9.0$  Hz), 6.53- 6.56 (m, 3H), 3.55 (t, 2H,  $J = 7.2$  Hz), 2.97 (s, 3H), 2.43 (td, 2H,  $J = 7.6, 2.8$  Hz), 2.32 (s, 3H), 2.00 (t, 1H,  $J = 2.8$  Hz);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  148.5, 139.0, 129.1, 117.6, 113.0, 109.4, 82.3, 69.6, 51.8, 38.5, 21.9, 16.4; IR (neat): 3289, 2910, 2360, 2115, 1601, 1495, 1358, 1172, 1089, 1042, 998 ; MS ( $\text{ES}^+$ ) Calculated for  $[\text{C}_{12}\text{H}_{16}\text{N}]^+$ : 174.1; Found: 174.0.



Iodomethane (1.2 mmol) was added to a mixture of 4-aminobenzoic acid ethylester (1 mmol) and  $K_2CO_3$  (1 mmol) in anhydrous acetonitrile (5 mL/ mmol). The reaction was heated at 80 °C for 6 h and then cooled to room temperature. The reaction mixture was diluted with  $CH_2Cl_2$  (10 mL/ mmol), and the solid was filtered off. The filtrate was concentrated under *vacuum*, and the residue was purified through silica gel flash column chromatography (eluent: hexanes: ethyl acetate = 25:1, then hexanes: ethyl acetate = 10:1) to afford ethyl 4-methylaminobenzoate.

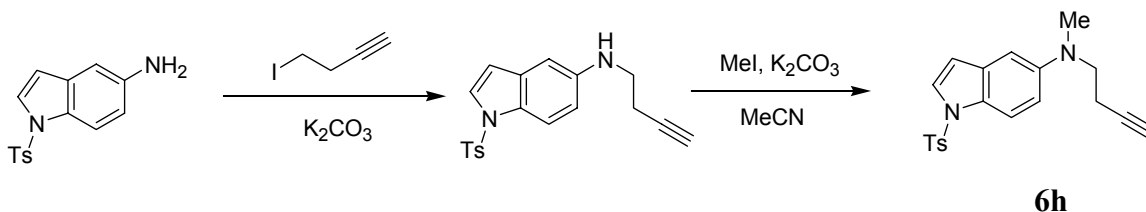
4-Iodobut-1-yne (1.2 mmol) was added to a mixture of 4-methylamino-benzoic acid ethylester (1 mmol) and  $K_2CO_3$  (2 mmol) without solvents. The reaction was heated at 90 °C for 4 h and then cooled to room temperature. The reaction mixture was diluted with  $CH_2Cl_2$  (10 mL/ mmol), and the solid was filtered off. The filtrate was concentrated under *vacuum*, and the residue was purified through silica gel flash column chromatography (eluent: hexanes: ethyl acetate = 25:1, then hexanes: ethyl acetate = 10:1) to afford compound **6f** in 31 % yield in 2 steps.  $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  7.91 (d, 2H,  $J = 9$  Hz), 6.65 (d, 2H,  $J = 9$  Hz), 4.32 (q, 2H,  $J = 7$  Hz), 3.61 (t, 2H,  $J = 7$  Hz), 3.06 (s, 3H), 2.46 (td, 2H,  $J = 7, 3$  Hz), 2.01 (t, 1H,  $J = 3$  Hz), 1.36 (t, 3H,  $J = 7$  Hz);  $^{13}C$  NMR (125 MHz,  $CDCl_3$ )  $\delta$  166.8, 151.5, 131.4, 117.8, 110.6, 81.5, 70.1, 60.1, 51.2, 38.6, 16.7, 14.1; IR (neat): 3289, 2977, 2368, 2114, 1699, 1604, 1523, 1384, 1276, 1183, 1106, 1026, 961, 827; MS ( $ES^+$ ) Calculated for  $[C_{14}H_{17}NO_2Na]^+$ : 254.1; Found: 253.9.



Iodomethane (1.2 mmol) was added to a mixture of *p*-toluidine (1 mmol) and  $K_2CO_3$  (1 mmol) in anhydrous acetonitrile (5 mL/ mmol). The reaction was stirred at room temperature overnight. The reaction mixture was diluted with  $CH_2Cl_2$  (10 mL/ mmol),

and the solid was filtered off. The filtrate was concentrated under *vacuum*, and the residue was purified through silica gel flash column chromatography (eluents: hexanes: ethyl acetate = 25:1, then hexanes: ethyl acetate = 10:1) to afford methyl-*p*-tolylamine.

4-Iodobut-1-yne (1.2 mmol) was added to a mixture of methyl-*p*-tolylamine (1 mmol) and K<sub>2</sub>CO<sub>3</sub> (2 mmol) without solvents. The reaction was heated at 90 °C for 4 h and then cooled to room temperature. The reaction mixture was diluted with CH<sub>2</sub>Cl<sub>2</sub> (10 mL/ mmol), and the solid was filtered off. The filtrate was concentrated under *vacuum*, and the residue was purified through silica gel flash column chromatography (eluents: hexanes: ethyl acetate = 50:1, then hexanes: ethyl acetate = 25:1) to afford compound **6g** in 49 % yield in 2 steps. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.04 (d, 2H, *J* = 7.2 Hz), 6.64 (d, 2H, *J* = 7.2 Hz), 3.52 (t, 2H, *J* = 7.2 Hz), 2.93 (s, 3H), 2.41 (td, 2H, *J* = 7.2, 2.8 Hz), 2.25 (s, 3H), 1.98 (t, 1H, *J* = 2.8 Hz); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 146.4, 129.8, 125.9, 112.6, 82.3, 69.5, 52.1, 38.5, 20.2, 16.2; IR (neat): 3301, 2914, 2368, 2113, 1617, 1519, 1356, 1185, 1111, 1039; MS (ES<sup>+</sup>) Calculated for [C<sub>12</sub>H<sub>16</sub>N]<sup>+</sup>: 174.1; Found: 174.0.

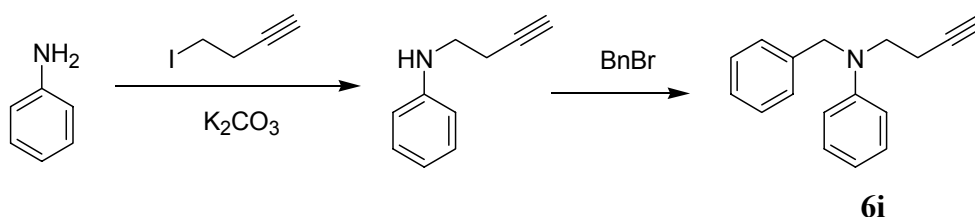


4-Iodobut-1-yne (1.2 mmol) was added to a mixture of 1-(toluene-4-sulfonyl)-1*H*-indol-5-ylamine (1 mmol) and K<sub>2</sub>CO<sub>3</sub> (1 mmol) without solvents. The reaction was heated at 60 °C overnight and then cooled to room temperature. The reaction mixture was diluted with CH<sub>2</sub>Cl<sub>2</sub> (10 mL/ mmol), and the solid was filtered off. The filtrate was concentrated under *vacuum*, and the residue was purified through silica gel flash column chromatography (eluents: hexanes: ethyl acetate = 7:1) to afford but-3-ynyl[1-(toluene-4-sulfonyl)-1*H*-indol-5-yl]amine.

Iodomethane (1.2 mmol) was added to a mixture of but-3-ynyl-[1-(toluene-4-sulfonyl)-1*H*-indol-5-yl]-amine (1 mmol) and K<sub>2</sub>CO<sub>3</sub> (1 mmol) in anhydrous acetonitrile (5 mL/ mmol). The reaction was stirred at 60 °C overnight and then cooled to room temperature.



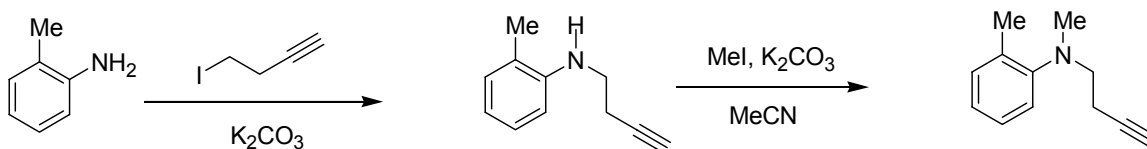
The reaction mixture was diluted with CH<sub>2</sub>Cl<sub>2</sub> (10 mL/ mmol), and the solid was filtered off. The filtrate was concentrated under *vacuum*, and the residue was purified through silica gel flash column chromatography (eluents: hexanes: ethyl acetate = 5:1) to afford compound **6h** in 50 % yield in 2 steps. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.82 (d, 1H, *J* = 9.2 Hz), 7.71 (d, 2H, *J* = 8 Hz), 7.43 (d, 1H, *J* = 3.6 Hz), 7.18 (d, 2H, *J* = 8 Hz), 6.82 (dd, 1H, *J* = 9.2, 2.4 Hz), 6.75 (d, 2H, *J* = 2.4 Hz), 6.51 (d, 1H, *J* = 3.6 Hz), 3.54 (t, 2H, *J* = 7.2 Hz), 2.95 (s, 3H), 2.40 (td, 2H, *J* = 7.2, 2.4 Hz), 2.32 (s, 3H), 1.98 (t, 1H, *J* = 2.4 Hz); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 145.7, 144.6, 135.4, 132.2, 129.8, 127.0, 126.8, 126.7, 114.3, 112.0, 109.3, 103.7, 82.2, 69.7, 52.8, 39.0, 21.5, 16.4; IR (neat): 3294, 2925, 2861, 2345, 2115, 1612, 1558, 1495, 1366, 1259, 1132, 1050, 876, 824; MS (ES<sup>+</sup>) Calculated for [C<sub>20</sub>H<sub>21</sub>N<sub>2</sub>O<sub>2</sub>S]<sup>+</sup>: 353.1; Found: 353.4.



4-Iodobut-1-yne (1 mmol) was added to a mixture of aniline (2 mmol) and K<sub>2</sub>CO<sub>3</sub> (2 mmol) without solvents. The reaction was heated at 80 °C for 6 h and then cooled to room temperature. The reaction mixture was diluted with CH<sub>2</sub>Cl<sub>2</sub> (10 mL/ mmol), and the solid was filtered off. The filtrate was concentrated under *vacuum*, and the residue was purified through silica gel flash column chromatography (eluents: hexanes: ethyl acetate = 15:1) to afford but-3-ynylphenylamine.

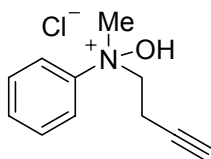
Benzyl bromide (1.2 mmol) was added to a mixture of but-3-ynylphenylamine (2 mmol) without solvents. The reaction was heated at 60 °C for 20 min. The reaction mixture was diluted with CH<sub>2</sub>Cl<sub>2</sub> (10 mL/ mmol), and the solid was filtered off. The filtrate was concentrated under *vacuum*, and the residue was purified through silica gel flash column chromatography (eluents: hexanes: ethyl acetate = 50:1) to afford compound **6i** in 43 % yield in 2 steps. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.18 – 7.31 (m, 7H), 6.69– 6.72 (m, 3H), 4.60 (s, 2H), 3.65 (t, 2H, *J* = 7.6 Hz), 2.52 (td, 2H, *J* = 7.6, 2.8 Hz), 2.00 (t, 1H, *J* = 2.8 Hz); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 147.7, 138.6, 129.3, 128.6, 126.9, 126.5, 116.7,

112.2, 82.0, 69.8, 54.5, 50.2, 29.7, 17.0; IR (neat): 3278, 2918, 2360, 1595, 1504, 1449, 1360, 1246, 1213, 1165, 1026, 996; MS (ES<sup>+</sup>) Calculated for [C<sub>17</sub>H<sub>18</sub>N]<sup>+</sup>: 236.1; Found: 235.9.



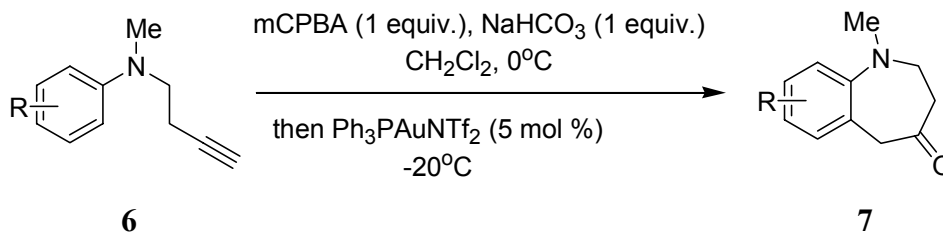
4-Iodobut-1-yne (1 mmol) was added to a mixture of *o*-toluidine (2 mmol) and K<sub>2</sub>CO<sub>3</sub> (2 mmol) without solvents. The reaction was heated at 60 °C for 2 d and then cooled to room temperature. The reaction mixture was diluted with CH<sub>2</sub>Cl<sub>2</sub> (10 mL/ mmol), and the solid was filtered off. The filtrate was concentrated under *vacuum*, and the residue was purified through silica gel flash column chromatography (eluent: hexanes: ethyl acetate = 25:1, then hexanes: ethyl acetate = 15:1) to afford but-3-ynyl-*o*-tolylamine.

Iodomethane (1.2 mmol) was added to a mixture of but-3-ynyl-*o*-tolylamine (1 mmol) and K<sub>2</sub>CO<sub>3</sub> (1 mmol) in anhydrous acetonitrile (5 mL/ mmol). The reaction was heated at 80 °C overnight and then cooled to room temperature. The reaction mixture was diluted with CH<sub>2</sub>Cl<sub>2</sub> (10 mL/ mmol), and the solid was filtered off. The filtrate was concentrated under *vacuum*, and the residue was purified through silica gel flash column chromatography (eluent: hexanes: ethyl acetate = 15:1) to afford desired product in 53 % yield in 2 steps. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.16- 7.21 (m, 2H), 7.07 (d, 1H, *J* = 7.5), 7.00 (t, 1H, *J* = 7), 3.14 (t, 2H, *J* = 7.5 Hz), 2.74 (s, 3H), 2.40 (td, 2H, *J* = 7.5, 2.5 Hz), 2.35 (s, 3H), 1.98 (t, 1H, *J* = 2.5 Hz); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 151.1, 133.4, 131.1, 126.3, 123.3, 120.2, 82.6, 69.1, 54.8, 41.6, 18.2, 17.3; IR (neat): 3297, 2936, 2115, 1599, 1493, 1369, 1169, 1094, 1037, 944; MS (ES<sup>+</sup>) Calculated for [C<sub>12</sub>H<sub>16</sub>N]<sup>+</sup>: 174.1; Found: 174.0.

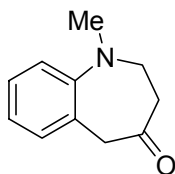


*m*CPBA (1 equiv.) was added into a solution of a *N*-(but-3-ynyl)aniline (1 equiv.) and NaHCO<sub>3</sub> (1 equiv.) in CH<sub>2</sub>Cl<sub>2</sub> (0.05 M) under N<sub>2</sub> at 0 °C. The reaction was stirred at 0 °C for 0.5 h. The N-oxide purified directly through silica gel flash column chromatography (eluent: DCM: MeOH = 2: 1). The anhydrous hydrogen chloride gas was bubbled into the eluent containing N-oxide then concentrated under vacuum to afford the desired product in 80 % yield. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.94- 7.92 (m, 2H), 7.67- 7.57 (m, 3H), 4.71- 4.63 (m, 1H), 4.44-4.36 (m, 1H), 4.21 (s, 3H), 2.92- 2.85 (m, 1H), 2.41- 2.34 (m, 1H), 2.03 (t, 1H, *J* = 2.8 Hz); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 145.8, 131.1, 130.4, 120.0, 77.1, 72.0, 69.2, 60.2, 13.9; IR (neat): 2923, 2859, 2253, 1713, 1605, 1555, 1497, 1452, 1401; MS (ES<sup>+</sup>) Calculated for [C<sub>11</sub>H<sub>14</sub>NO]<sup>+</sup>: 176.1; Found: 176.1.

#### General procedure A: Preparation of tetrahydrobenz[*b*]azepin-4-ones

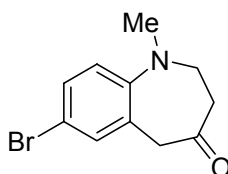


*m*CPBA (0.2 mmol) was added into a solution of a *N*-(but-3-ynyl)aniline (0.2 mmol) and NaHCO<sub>3</sub> (0.2 mmol) in CH<sub>2</sub>Cl<sub>2</sub> (0.05 M) under N<sub>2</sub> at 0 °C. The N-oxide formation was monitored by TLC. After completion of the N-oxide formation, Ph<sub>3</sub>PAuNTf<sub>2</sub> (5 mol %) was added into the reaction at -20 °C. Upon completion, the reaction was diluted with CH<sub>2</sub>Cl<sub>2</sub> (25 mL) and washed with 5 % aqueous Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> (10 mL), 10 % aqueous NaHCO<sub>3</sub> (10 mL) and water. The organic layer was washed with brine, dried with MgSO<sub>4</sub>, and concentrated under *vacuum*. The residue was purified through silica gel flash column (eluent: hexanes: ethyl acetate = 15:1).



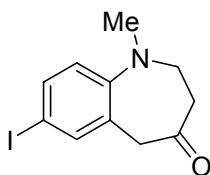
**5**

Compound **5** was prepared in 79 % yield according to the general procedure A. The reaction time is 30 min for the formation of N-oxide and 30 min for Au catalysis.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.27 (t, 1H,  $J$  = 6 Hz), 7.08 (d, 1H,  $J$  = 7.5 Hz), 7.01 (d, 1H,  $J$  = 8 Hz), 7.00 (t, 1H,  $J$  = 6.5 Hz), 3.68 (s, 2H), 3.26 (t, 2H,  $J$  = 6.5 Hz), 2.87 (s, 3H), 2.55 (t, 2H,  $J$  = 6.5 Hz);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  208.8, 149.3, 129.6, 129.4, 128.3, 122.2, 118.2, 53.9, 48.7, 41.6, 41.5; IR (neat): 2940, 2806, 2360, 1716, 1651, 1554, 1495, 1465, 1323, 1183, 1052; MS ( $\text{ES}^+$ ) Calculated for  $[\text{C}_{11}\text{H}_{13}\text{ONa}]^+$ : 198.1; Found: 198.0.



**7a**

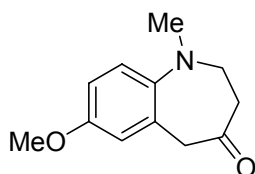
Compound **7a** was prepared in 73 % yield according to the general procedure A. The reaction time is 30 min for the formation of N-oxide and 30 min for Au catalysis.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.36 (dd, 1H,  $J$  = 8.8, 2.4 Hz), 7.21 (d, 1H,  $J$  = 2.4 Hz), 6.86 (d, 1H,  $J$  = 8.4 Hz), 3.64 (s, 2H), 3.26 (t, 2H,  $J$  = 6.8 Hz), 2.85 (s, 3H), 2.55 (t, 2H,  $J$  = 6.8 Hz);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  207.5, 148.3, 132.3, 131.3, 131.1, 119.8, 114.5, 53.6, 48.3, 41.6, 41.3; IR (neat): 2951, 2810, 2364, 2334, 1718, 1491, 1324, 1271, 1098; MS ( $\text{ES}^+$ ) Calculated for  $[\text{C}_{11}\text{H}_{12}\text{BrNONa}]^+$ : 276.0; Found: 275.9.



**7b**

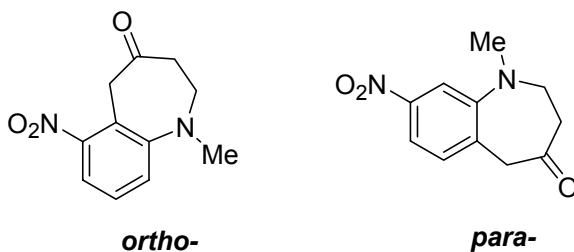
Compound **7b** was prepared in 68 % yield according to the general procedure A. The reaction time is 2 h for the formation of N-oxide and 30 min for Au catalysis.  $^1\text{H}$  NMR

(400 MHz, CDCl<sub>3</sub>)  $\delta$  7.36 (d, 1H,  $J$  = 8.4 Hz), 7.38 (s, 1H), 6.74 (d, 1H,  $J$  = 8.4 Hz), 3.63 (s, 2H), 3.28 (t, 2H,  $J$  = 7.2 Hz), 2.85 (s, 3H), 2.56 (t, 2H,  $J$  = 7.2 Hz); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  207.4, 149.0, 138.1, 137.2, 131.3, 120.2, 84.6, 53.5, 48.1, 41.5, 41.4; IR (neat): 2934, 2856, 2364, 2334, 1717, 1491, 1322, 1269, 1093; MS (ES<sup>+</sup>) Calculated for [C<sub>11</sub>H<sub>13</sub>INO]<sup>+</sup>: 302.0; Found: 301.7.



**7c**

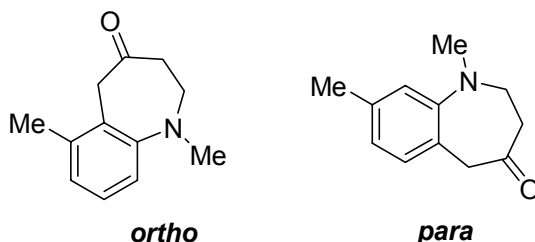
Compound **7c** was prepared in 73 % yield according to the general procedure A. The reaction time is 15 min for the formation of N-oxide and 15 min for Au catalysis. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  6.98 (d, 1H,  $J$  = 6 Hz), 6.81 (dd, 1H,  $J$  = 8.8, 3.2 Hz), 6.69 (d, 1H,  $J$  = 2.8 Hz), 3.78 (s, 3H), 3.62 (s, 2H), 3.15 (t, 2H,  $J$  = 6.4 Hz), 2.81 (s, 3H), 2.51 (t, 2H,  $J$  = 6.4 Hz); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  209.2, 155.2, 142.7, 131.9, 119.3, 115.5, 112.7, 55.5, 54.9, 48.6, 41.9, 41.4; IR (neat): 2940, 2799, 1716, 1608, 1501, 1252, 1124, 1042; MS (ES<sup>+</sup>) Calculated for [C<sub>12</sub>H<sub>15</sub>NO<sub>2</sub>Na]<sup>+</sup>: 228.1; Found: 227.9.



**7d**

Compound **7d** was prepared in 58 % yield (*ortho*: *para* = 1.35 :1) according to the general procedure A. The reaction time is 2 h for the formation of N-oxide and 30 min for Au catalysis. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  7.79 (d, 1H, *para*,  $J$  = 2 Hz), 7.77 (dd, 1H, *para*,  $J$  = 8, 2 Hz), 7.44 (d, 1H, *ortho*,  $J$  = 8 Hz), 7.37 (t, 1H, *ortho*,  $J$  = 8 Hz), 7.23 (d, 1H, *para*,  $J$  = 7.5 Hz), 7.20 (d, 1H, *ortho*,  $J$  = 8 Hz), 3.83 (s, 3H, *ortho*), 3.81 (s, 3H, *para*), 3.41 (t, 2H, *para*,  $J$  = 6 Hz), 3.35 (t, 2H, *ortho*,  $J$  = 6.8 Hz), 2.99 (s, 3H, *para*), 2.93 (s, 3H, *ortho*),

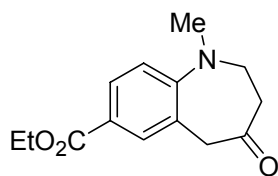
2.61 (t, 2H, *para*,  $J = 6.4$ ), 2.59 (t, 2H, *ortho*,  $J = 6.8$  Hz);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  205.7, 204.7, 151.0, 150.5, 150.1, 148.4, 135.2, 130.3, 128.4, 123.6, 122.4, 1117.3, 116.4, 112.5, 53.2, 52.9, 48.8, 43.7, 41.7, 41.6, 41.5, 40.8; IR (neat): 2914, 2855, 2360, 1718, 1525, 1345, 1109; MS ( $\text{ES}^+$ ) Calculated for  $[\text{C}_{12}\text{H}_{15}\text{NO}_2\text{Na}]^+$ : 228.1; Found: 227.9.



**7e**

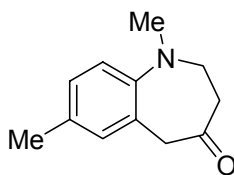
Compound **7e** was prepared in 70 % yield (*ortho*: *para* = 1:1) according to the general procedure A. The reaction time is 30 min for the formation of N-oxide and 30 min for Au catalysis.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.17 (t, 1H, *ortho*,  $J = 7.6$  Hz), 6.96 (d, 1H, *para*,  $J = 7.6$  Hz), 6.91 (d, 1H,  $J = 8$  Hz), 6.88 (d, 1H,  $J = 7.6$  Hz), 6.83 (s, 3H, *para*), 6.76 (d, 1H, *para*,  $J = 7.6$  Hz), 3.71 (s, 2H), 3.64 (s, 2H, *para*), 3.25 (t, 2H, *para*,  $J = 6.8$  Hz), 3.21 (t, 2H,  $J = 6$  Hz), 2.86 (s, 3H, *para*), 2.85 (s, 3H), 2.55 (t, 2H, *para*,  $J = 6.8$  Hz), 2.50 (t, 2H,  $J = 6$  Hz), 2.34 (s, 3H, *para*), 2.29 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  209.2, 208.8, 149.5, 149.1, 138.1, 136.2, 129.4, 128.7, 126.3, 124.7, 122.8, 119.0, 116.3, 54.0, 48.3, 44.3, 41.9, 41.6, 41.5, 40.9, 21.4, 20.4; IR (neat): 2925, 2806, 2360, 1718, 1577, 1454, 1324, 1174; MS ( $\text{ES}^+$ ) Calculated for  $[\text{C}_{12}\text{H}_{15}\text{NONa}]^+$ : 212.1; Found: 211.9.

Compound *Para*- **7e**:  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.17 (t, 1H,  $J = 7.6$  Hz), 6.91 (d, 1H,  $J = 8$  Hz), 6.88 (d, 1H,  $J = 7.6$  Hz), 3.71 (s, 2H), 3.21 (t, 2H,  $J = 6$  Hz), 2.85 (s, 3H), 2.50 (t, 2H,  $J = 6$  Hz), 2.29 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  208.8, 149.5, 136.2, 128.7, 127.5, 124.7, 116.3, 54.0, 44.3, 41.9, 40.9, 20.4; IR (neat): 2925, 2806, 2360, 1718, 1577, 1454, 1324, 1174; MS ( $\text{ES}^+$ ) Calculated for  $[\text{C}_{12}\text{H}_{15}\text{NONa}]^+$ : 212.1; Found: 211.9.



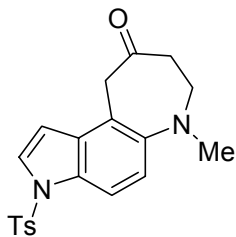
**7f**

Compound **7f** was prepared in 40 % yield according to the general procedure A. The reaction time is 30 min for the formation of N-oxide and 30 min for Au catalysis.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.90 (dd, 1H,  $J = 8.4, 2.4$  Hz), 7.72 (d, 1H,  $J = 2$  Hz), 6.89 (d, 1H,  $J = 8.4$  Hz), 4.34 (q, 2H,  $J = 7.2$  Hz) 3.80 (s, 2H), 3.50 (t, 2H,  $J = 6$  Hz), 2.99 (s, 3H), 2.64 (t, 2H,  $J = 6.4$  Hz), 1.37 (t, 3H,  $J = 7.2$  Hz);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  207.1, 166.4, 152.9, 131.7, 130.2, 125.3, 122.2, 116.4, 60.6, 52.2, 48.9, 41.7, 41.4, 14.4; IR (neat): 2914, 2360, 2338, 1705, 1603, 1508, 1363, 1274, 1183, 1113, 1029; MS ( $\text{ES}^+$ ) Calculated for  $[\text{C}_{14}\text{H}_{17}\text{NO}_3\text{Na}]^+$ : 270.1; Found: 269.9.

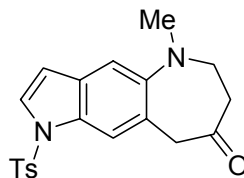


**7g**

Compound **7g** was prepared in 70 % yield according to the general procedure A. The reaction time is 30 min for the formation of N-oxide and 30 min for Au catalysis.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.07 (dd, 1H,  $J = 8.4, 1.6$  Hz), 6.91- 6.94 (m, 2H), 3.63 (s, 2H), 3.20 (t, 2H,  $J = 6.8$  Hz), 2.83 (s, 3H), 2.53 (t, 2H,  $J = 6.8$  Hz), 2.28 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  209.2, 146.9, 131.8, 130.3, 129.7, 128.7, 118.1, 54.4, 48.6, 41.7, 41.5, 20.5; IR (neat): 2940, 2364, 2323, 1718, 1504, 1326, 1274, 1178, 1089, 1035; MS ( $\text{ES}^+$ ) Calculated for  $[\text{C}_{12}\text{H}_{15}\text{NONa}]^+$ : 212.1; Found: 211.9.

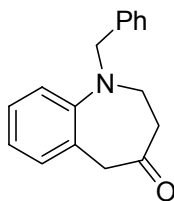


*ortho-7h*



*para-7h'*

Compound *ortho*-**7h** and *para*-**7h** was prepared in 65 % yield in a 1:1 separable mixture according to the general procedure A. The reaction time is 30 min for the formation of N-oxide and 30 min for Au catalysis. For compound *ortho*-**7h** :  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.86 (d, 2H,  $J = 8.8$  Hz), 7.74 (d, 2H,  $J = 8.8$  Hz), 7.54 (d, 2H,  $J = 3.6$  Hz), 7.21 (d, 2H,  $J = 8.8$  Hz), 7.05 (d, 2H,  $J = 5.2$  Hz), 6.58 (d, 2H,  $J = 3.6$  Hz), 3.78 (s, 2H), 3.23 (t, 2H,  $J = 6.8$  Hz), 2.86 (s, 3H), 2.50 (t, 2H,  $J = 6.8$  Hz), 2.34 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  208.6, 144.9, 135.3, 130.8, 130.6, 129.9, 127.0, 126.8, 121.6, 116.1, 112.7, 107.1, 54.7, 44.3, 42.0, 41.6, 21.6; IR (neat): 2926, 2861, 2381, 2345, 2327, 1714, 1597, 1558, 1495, 1451, 1369, 1272, 1172, 1142, 1050, 876, 824; MS ( $\text{ES}^+$ ) Calculated for  $[\text{C}_{20}\text{H}_{20}\text{N}_2\text{O}_3\text{SNa}]^+$ : 391.1; Found: 391.4. For compound *para*-**7h**:  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.74 (d, 2H,  $J = 8.4$  Hz), 7.71 (s, 1H), 7.49 (d, 1H,  $J = 3.6$  Hz), 7.22 (d, 2H,  $J = 8.8$  Hz), 7.17 (s, 1H), 6.57 (d, 1H,  $J = 3.6$  Hz), 3.73 (s, 2H), 3.14 (t, 2H,  $J = 6.8$  Hz), 2.84 (s, 3H), 2.47 (t, 2H,  $J = 6.8$  Hz), 2.34 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  209.1, 145.8, 144.9, 135.4, 130.8, 129.9, 128.7, 126.8, 126.4, 114.0, 110.8, 108.8, 54.7, 49.1, 42.1, 41.1, 21.6; IR (neat): 2925, 2861, 2382, 2347, 2081, 1713, 1607, 1557, 1495, 1451, 1371, 1260, 1172, 1120, 1092, 105, 875, 824; MS ( $\text{ES}^+$ ) Calculated for  $[\text{C}_{20}\text{H}_{20}\text{N}_2\text{O}_3\text{SNa}]^+$ : 391.1; Found: 391.2.

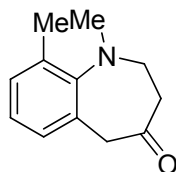


**7i**

Compound **7i** was prepared in 69 % yield according to the general procedure A. The reaction time is 2h for the formation of N-oxide and 30 min for Au catalysis.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.31- 7.36 (m, 4H), 7.23- 7.27 (m, 2H), 7.12 (d, 1H,  $J = 7.5$  Hz), 7.07 (d, 1H,  $J = 8.0$  Hz), 6.97 (td, 1H,  $J = 7.5$ , 1 Hz), 4.34 (s, 2H), 3.29 (s, 2H), 3.23 (t, 2H,  $J = 7$  Hz), 2.53 (s, 3H), 2.53 (t, 2H,  $J = 7$  Hz);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  208.6, 149.1, 138.4, 129.8, 129.4, 128.6, 128.4, 128.0, 127.3, 122.5, 119.4, 58.2, 50.9, 48.9, 41.6;

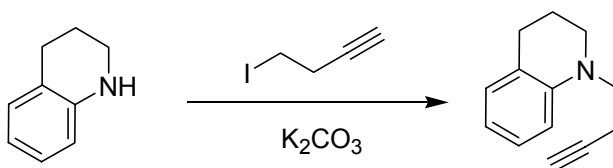


IR (neat): 2918, 2843, 2360, 2334, 1716, 1495, 1365, 1224; MS ( $\text{ES}^+$ ) Calculated for  $[\text{C}_{17}\text{H}_{17}\text{NONa}]^+$ : 274.1; Found: 273.9.



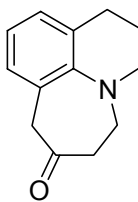
**9**

Compound **9** was prepared in 20 % yield according to the general procedure A. The reaction time is 1 h for the formation of N-oxide and 30 min for Au catalysis. For compound **8**:  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.16- 7.23 (m, 2H), 7.05 (s, 1H), 7.03 (s, 1H), 3.22 (t, 4H,  $J = 6$  Hz), 2.61 (t, 2H,  $J = 6$  Hz), 2.39 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  208.9, 147.0, 135.5, 131.7, 131.1, 130.8, 124.2, 51.0, 49.2, 41.3, 40.9, 19.2.



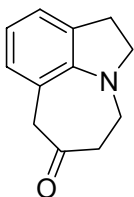
**10**

4-Iodobut-1-yne (1 mmol) was added to a mixture of 1,2,3,4-Tetrahydro-quinoline (2 mmol) and  $\text{K}_2\text{CO}_3$  (2 mmol) without solvents. The reaction was heated at 60 °C for 4 h and then cooled to room temperature. The reaction mixture was diluted with  $\text{CH}_2\text{Cl}_2$  (10 mL/ mmol), and the solid was filtered off. The filtrate was concentrated under *vacuum*, and the residue was purified through silica gel flash column chromatography (eluent: hexanes: ethyl acetate = 25:1, then hexanes: ethyl acetate = 15:1) to afford compound in 72 % yield.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.03 (t, 1H,  $J = 7.2$  Hz), 7.03 (d, 1H,  $J = 7.2$  Hz), 6.60– 6.56 (m, 2H), 3.48 (t, 2H,  $J = 7.6$  Hz), 3.33 (t, 2H,  $J = 5.6$  Hz), 2.74 (t, 2H,  $J = 6.4$  Hz), 2.45 (td, 2H,  $J = 8.4$  Hz,  $J = 2.4$  Hz), 1.99 (t, 1H,  $J = 2.4$  Hz), 1.97–1.92 (m, 2H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  144.3, 129.3, 127.2, 122.5, 116.0, 110.3, 82.4, 69.5, 50.4, 49.6, 28.0, 22.1, 15.9; IR (neat): 3288, 2926, 1600, 1450, 1344; MS ( $\text{ES}^+$ ) Calculated for  $[\text{C}_{13}\text{H}_{16}\text{N}]^+$ : 186.1; Found: 186.0.

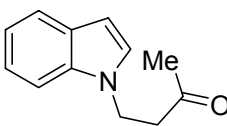


**11**

Compound **11** was prepared in 57 % yield according to the general procedure A, (2-biphenyl)<sup>t</sup>Bu<sub>2</sub>PAuNTf<sub>2</sub> was used. The reaction temperature for Au-catalysis was room temperature and the reaction time was 40 min. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 6.97 (d, 1H, *J* = 7.2 Hz), 6.87 (d, 1H, *J* = 6.4 Hz), 6.80-6.76 (m, 1H), 3.73 (s, 2H), 3.43 (t, 2H, *J* = 6.4 Hz), 3.20 (t, 2H, *J* = 5.6 Hz), 2.77 (t, 2H, *J* = 6.4 Hz), 2.63 (t, 2H, *J* = 6.4 Hz), 1.90–1.84(m, 2H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 208.6, 144.8, 128.6, 128.5, 128.0, 126.3, 120.5, 52.0, 51.7, 49.1, 42.0, 27.8, 19.4; IR (neat): 2936, 2855, 1718, 1595, 1491, 1450, 1317; MS (ES<sup>+</sup>) Calculated for [C<sub>13</sub>H<sub>15</sub>NNaO]<sup>+</sup>: 224.1; Found: 224.1.



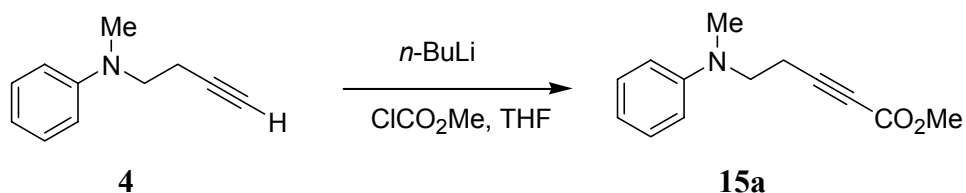
**13**



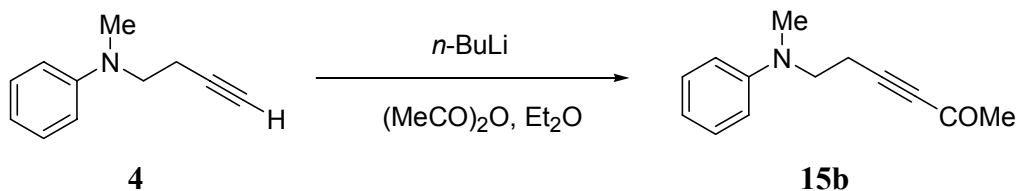
**14**

Compound **13** was isolated in 40 % yield along with **14** (26 % yield) according to the general procedure A, (2-biphenyl)<sup>t</sup>Bu<sub>2</sub>PAuNTf<sub>2</sub> was used. The reaction temperature for Au-catalysis was room temperature and the reaction time was 30 min. From compound **13**: <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.00 (d, 1H, *J* = 7.2 Hz), 6.78 (d, 1H, *J* = 7.6 Hz), 6.67-6.63 (m, 1H), 3.90 (s, 2H), 3.43-3.39 (m, 4H), 2.93 (t, 2H, *J* = 8.4 Hz), 2.83 (t, 2H, *J* = 5.6 Hz); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 207.1, 150.1, 131.0, 128.8, 123.4, 119.2, 114.2, 56.0, 47.9, 45.8, 44.6, 28.7; IR (neat): 2926, 2855, 1713, 1602, 1558, 1494, 1452; MS (ES<sup>+</sup>) Calculated for [C<sub>12</sub>H<sub>13</sub>NNaO]<sup>+</sup>: 210.1; Found: 209.9. For compound **14** was isolated in 26 % yield when making the compound **13** according to the general procedure A. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.62 (d, 1H, *J* = 8 Hz), 7.33 (d, 1H, *J* = 8.4 Hz), 7.25-7.19 (m, 1H), 7.13-7.08 (m, 2H), 6.47 (d, 1H, *J* = 2.8 Hz), 4.42 (t, 2H, *J* = 6.4 Hz), 2.94 (t, 2H, *J* = 6.4 Hz), 2.10 (s, 3H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 206.2, 135.5, 128.7, 128.2,

121.5, 121.1, 119.4, 109.0, 101.4, 43.4, 40.5, 30.4; IR (neat): 2923, 2855, 1711, 1607, 1489, 1453, 1399; MS (ES<sup>+</sup>) Calculated for [C<sub>12</sub>H<sub>13</sub>NNaO]<sup>+</sup>: 210.1; Found: 209.9.

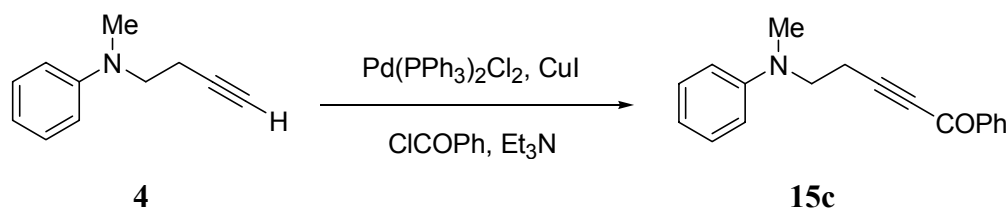


Compound **4** (1 mmol) was dissolved in THF (5 mL), and the resulting solution was cooled to -78 °C in a dry ice-acetone bath. *n*-BuLi (1.2 mmol) was added drop-wise over 3 minutes. After stirring at -78 °C for 0.5 h, The resulting mixture was stirred at -78 °C for another 0.5 h. Methyl chloroformate (1.2 mmol) was added in one portion. The reaction was allowed to warm to room temperature and stirred for 1 h. The reaction mixture was then quenched with sat. aqueous NH<sub>4</sub>Cl. The organic layer was separated. The aqueous layer was extracted with diethyl ether (2 x 10 mL). The combined organic layers was washed with brine (25 mL), dried upon MgSO<sub>4</sub>, filtered and concentrated. The residue was purified through silica gel flash column chromatography (eluent: hexanes: ethyl acetate = 2:1) to yield the desired compound **15a** in 60 % yield. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.27– 7.23 (m, 2H), 6.76– 6.70 (m, 3H), 3.77 (s, 3H), 3.63 (t, 2H, *J* = 7.2 Hz), 2.99 (s, 3H), 2.58 (t, 2H, *J* = 7.2 Hz); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 154.0, 148.0, 129.4, 117.0, 112.3, 87.2, 74.0, 52.6, 50.8, 38.5, 16.6; IR (neat): 3028, 2926, 2236, 1715, 1598, 1502, 1433, 1356, 1258; MS (ES<sup>+</sup>) Calculated for [C<sub>13</sub>H<sub>15</sub>NNaO<sub>2</sub>]<sup>+</sup>: 240.1; Found: 240.1.

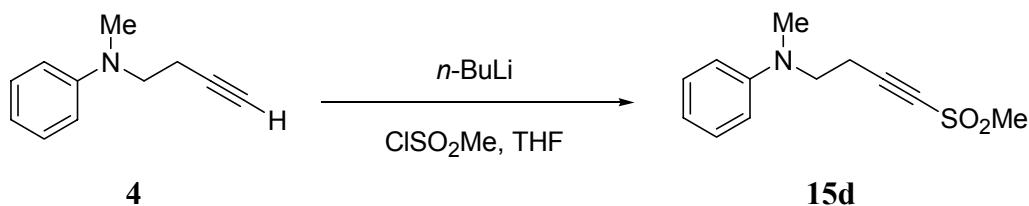


Compound **4**(1 mmol) was dissolved in Et<sub>2</sub>O (5 mL), and the resulting solution was cooled down to -78°C in a dry ice-acetone bath. *n*-BuLi (1.1 mmol) was added drop-wise over 5 minutes. After stirring at -78 °C for 0.5 h. The resulting mixture was stirred at -

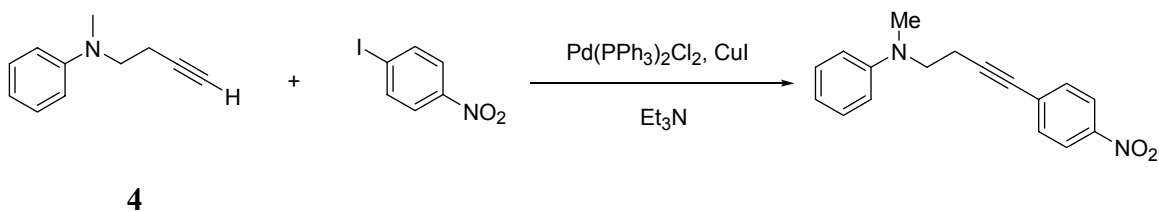
78°C for another 0.5 h. Acetyl chloride (12 mmol) was added in one portion. The reaction was allowed to warm to room temperature and stirred for 6 hours. The reaction mixture was then quenched with sat. aqueous NH<sub>4</sub>Cl. The organic layer was separated. The aqueous layer was extracted with diethyl ether (2 x 10 mL). The combined organic layers was washed with brine (25 mL), dried upon MgSO<sub>4</sub>, filtered and concentrated. The residue was purified through silica gel flash column chromatography (eluent: hexanes: ethyl acetate = 2:1) to yield the desired compound **15b** in 60 % yield. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.27– 7.23 (m, 2H), 6.76– 6.71 (m, 3H), 3.63 (t, 2H, *J* = 7.2 Hz), 2.99 (s, 3H), 2.61 (t, 2H, *J* = 7.2 Hz), 2.29 (s, 3H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 184.6, 148.1, 129.4, 117.0, 112.3, 91.2, 82.3, 50.9, 38.4, 32.6, 16.9; IR (neat): 2923, 2859, 2209, 1674, 1602, 1499, 1356, 1229; MS (ES<sup>+</sup>) Calculated for [C<sub>13</sub>H<sub>15</sub>NNaO]<sup>+</sup>: 224.1; Found: 224.1.



To a solution of anhydrous Et<sub>3</sub>N (2 mL) was successively added copper iodide (0.05 mmol), dichlorobis(triphenylphosphine)palladium (0.05 mmol). Under nitrogen, compound **4** (1.32 mmol) and benzoyl chloride (1.5 mmol) were added in succession. The resulting mixture was stirred at room temperature for 8 h. The reaction was quenched by filtration through a pad of silica gel using ethyl acetate as eluent. The filtrate was concentrated, and the residue was purified through silica gel flash column chromatography (eluent: hexanes: ethyl acetate = 2:1) to yield the desired compound **15c** in 52 % yield. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.10 (d, 2H, *J* = 6.8 Hz), 7.59 (t, 1H, *J* = 7.2 Hz), 7.45 (t, 2H, *J* = 7.6 Hz), 7.27 (t, 2H, *J* = 8.8 Hz), 6.77– 6.33 (m, 3H), 3.72 (t, 2H, *J* = 6.8 Hz), 3.02 (s, 3H), 2.75 (t, 2H, *J* = 6.8 Hz); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 177.9, 148.1, 136.6, 134.0, 129.5, 129.4, 128.5, 117.0, 112.4, 93.9, 80.7, 50.9, 38.4, 17.3; IR (neat): 3058, 2920, 2196, 1642, 1598, 1502, 1452, 1263; MS (ES<sup>+</sup>) Calculated for [C<sub>18</sub>H<sub>17</sub>NNaO]<sup>+</sup>: 286.1; Found: 286.1.

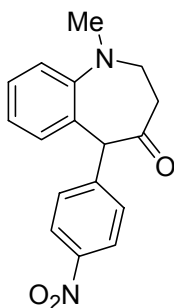


Compound **4** (2 mmol) was dissolved in THF (7 mL), and the resulting solution was cooled down to  $-78^\circ\text{C}$  in a dry ice-acetone bath. *n*-BuLi (3 mmol) was added drop-wise over 3 minutes. After stirring at  $-78^\circ\text{C}$  for 1 h. Methanesulfonyl chloride (2.4 mmol) was added in dropwise. The reaction was allowed to warm to room temperature and stirred for overnight. The reaction mixture was then quenched with sat. aqueous  $\text{NH}_4\text{Cl}$ . The organic layer was separated. The aqueous layer was extracted with diethyl ether (2 x 10 mL). The combined organic layers was washed with brine (25 mL), dried upon  $\text{MgSO}_4$ , filtered and concentrated. The residue was purified through silica gel flash column chromatography (eluent: hexanes: ethyl acetate = 2:1) to yield the desired compound **15d** in 18 % yield.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.28- 7.24 (m, 2H), 6.77- 6.71 (m, 3H), 3.67 (t, 2H,  $J = 6.8$  Hz), 3.08 (s, 3H), 2.99 (s, 3H), 2.67 (t, 2H,  $J = 6.8$  Hz);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  184.6, 148.1, 129.4, 117.0, 112.3, 91.2, 82.3, 50.9, 38.4, 32.6, 16.9; IR (neat): 3018, 2923, 2862, 2202, 1600, 1502, 1450, 1322, 1148; MS ( $\text{ES}^+$ ) Calculated for  $[\text{C}_{12}\text{H}_{15}\text{NNaO}_2\text{S}]^+$ : 260.1; Found: 260.0.



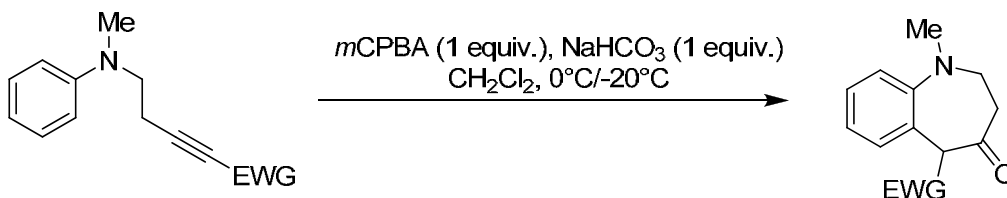
To a solution of anhydrous  $\text{Et}_3\text{N}$  (2 mL) was successively added copper iodide (0.03 mmol), dichlorobis(triphenylphosphine)palladium (0.015 mmol). Under nitrogen, compound **4** (0.3 mmol) and 1-iodo-4-nitro-benzene (0.3 mmol) were added in succession. The resulting mixture was stirred at  $80^\circ\text{C}$  for 10 min. The reaction was cooled down to room temperature and quenched by filtration through a pad of silica gel using ethyl acetate as eluent. The filtrate was concentrated, and the residue was purified through silica gel flash column chromatography (eluent: hexanes: ethyl acetate = 2:1) to yield the desired compound in 71 % yield.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.15 (d, 2H,  $J =$

7.2 Hz), 7.47 (d, 2H,  $J = 7.2$  Hz), 7.28– 7.24 (m, 2H), 6.78– 6.72 (m, 3H), 3.68 (t, 2H,  $J = 7.2$  Hz), 3.03 (s, 3H), 2.71 (t, 2H,  $J = 7.2$  Hz);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  148.4, 146.8, 132.2, 130.7, 129.3, 123.5, 116.8, 112.3, 94.0, 80.6, 51.5, 38.4, 17.7; IR (neat): 2923, 2855, 2219, 1593, 1506, 1342; MS ( $\text{ES}^+$ ) Calculated for  $[\text{C}_{17}\text{H}_{16}\text{N}_2\text{O}_2\text{H}]^+$ : 281.1; Found: 281.1.

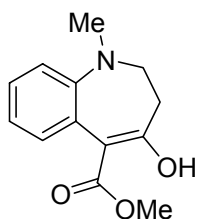


The above compound was prepared in 44 % yield according to the general procedure A. The reaction time is 30 min for the formation of N-oxide and 30 min for Au catalysis.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.13 (d, 2H,  $J = 9.2$  Hz), 7.38-7.33 (m, 3H), 7.20 (d, 1H,  $J = 7.6$  Hz), 7.08-7.04 (m, 2H), 4.75 (s, 1H), 3.42–3.35 (m, 1H), 3.18-3.13 (m, 1H), 2.96–2.89(m, 1H), 2.84 (s, 3H), 2.56–2.51 (m, 1H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  207.8, 148.2, 146.2, 133.8, 130.4, 130.0, 129.4, 124.0, 123.4, 120.1, 63.5, 56.0, 41.7, 39.9; IR (neat): 2933, 2859, 1716, 1600, 1517, 1491, 1447, 1346; MS ( $\text{ES}^+$ ) Calculated for  $[\text{C}_{17}\text{H}_{16}\text{N}_2\text{NaO}_3]^+$ : 319.1; Found: 319.0.

**General procedure B: Preparation of EWG substituted tetrahydrobenz[*b*]azepin-4-ones**

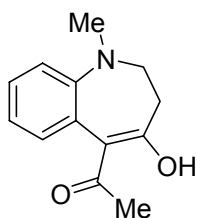


*m*CPBA (0.2 mmol) was added into a solution of a *N*-(but-3-ynyl)aniline (0.2 mmol) and NaHCO<sub>3</sub> (0.2 mmol) in CH<sub>2</sub>Cl<sub>2</sub> (0.05 M) under N<sub>2</sub> at 0 °C. The product formation was monitored by TLC. Upon completion, the reaction mixture was diluted with CH<sub>2</sub>Cl<sub>2</sub> (25 mL) and washed with 5 % aqueous Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> (10 mL), 10 % aqueous NaHCO<sub>3</sub> (10 mL), water and brine. The organic layer was dried with MgSO<sub>4</sub>, and concentrated under *vacuum*. The residue was purified through silica gel flash column chromatography (eluent: hexanes: ethyl acetate= 2:1).



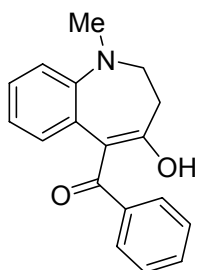
**16a**

Compound **16a** was prepared in 73% yield according to the general procedure B, reaction time is 30 min. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 13.01(s, 1H), 7.29 (d, 1H, *J* = 7.5 Hz), 7.26-7.22 (m, 1H), 7.06-7.01 (m, 2H), 3.76(s, 3H), 3.48-3.45 (m, 1H), 2.80 (s, 3H), 2.34 (t, 2H, *J* = 7 Hz); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 177.1, 171.8, 147.6, 131.2, 128.9, 127.5, 121.6, 118.8, 100.3, 62.2, 52.0, 41.4, 32.2; IR (neat): 2936, 2859, 1646, 1612, 1491, 1443, 1341, 1224; MS (ES<sup>+</sup>) Calculated for [C<sub>13</sub>H<sub>15</sub>NNaO<sub>3</sub>]<sup>+</sup>: 256.1; Found: 256.0.



**16b**

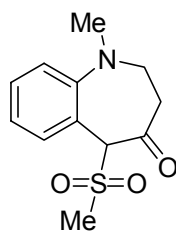
Compound **16b** was prepared in 76% yield according to the general procedure B, the reaction time was 60 min.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.29-7.26(m, 1H), 7.11-7.03(m, 3H), 3.67-3.55(m, 1H), 3.05-2.99 (m, 1H), 2.79(s, 3H), 2.65-2.55 (m, 1H), 2.29-2.23 (m, 1H), 2.10 (s, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  197.6, 184.7, 148.3, 131.0, 130.6, 128.1, 122.3, 118.9, 112.5, 59.1, 41.4, 37.6, 22.3; IR (neat): 2926, 2859, 1602, 1494, 1450, 1405, 1268; MS ( $\text{ES}^+$ ) Calculated for  $[\text{C}_{13}\text{H}_{15}\text{NNaO}_2]^+$ : 240.1; Found: 240.0.



**16c**

Compound **16c** was prepared in 82 % yield according to the general procedure B, the reaction time was 1 h.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.32-7.27 (m, 1H), 7.22-7.16 (m, 5H), 7.08 (d, 1H,  $J = 8$  Hz), 6.71-6.67 (m, 1H), 6.62 (d, 1H,  $J = 7.6$ Hz), 3.91-3.86 (m, 1H), 3.15-3.11 (m, 1H), 2.89 (s, 3H), 2.78-2.71 (m, 1H), 2.44-2.41 (m, 1H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  198.8, 180.4, 148.2, 135.5, 132.1, 131.4, 130.4, 129.5, 128.1, 127.6, 122.2, 118.5, 111.7, 58.9, 41.3, 37.9; IR (neat): 2930, 2808, 1725, 1600, 1560, 1494, 1455, 1403, 1334; MS ( $\text{ES}^+$ ) Calculated for  $[\text{C}_{18}\text{H}_{17}\text{NNaO}_2]^+$ : 302.1; Found: 302.0.





**16d**

Compound **16d** was prepared in 63 % yield according to the general procedure B, the reaction temperature was -20 °C and reaction time was 4 h.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.47-7.43(m, 1H), 7.39(d, 1H,  $J = 8$  Hz), 7.19-7.15(m, 2H), 4.65(s, 1H), 3.52-3.45(m, 1H), 3.07-3.02 (m, 1H), 2.99(s, 3H), 2.89-2.83 (m, 1H), 2.79(s, 3H), 2.57-2.52 (m, 1H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  201.6, 148.8, 133.8, 131.5, 125.4, 124.4, 120.3, 79.1, 55.9, 41.4, 40.8, 40.5; IR (neat): 2930, 2862, 1720, 1600, 1556, 1492, 1453, 1403; MS ( $\text{ES}^+$ ) Calculated for  $[\text{C}_{12}\text{H}_{15}\text{NNaO}_3\text{S}]^+$ : 276.1; Found: 276.0.

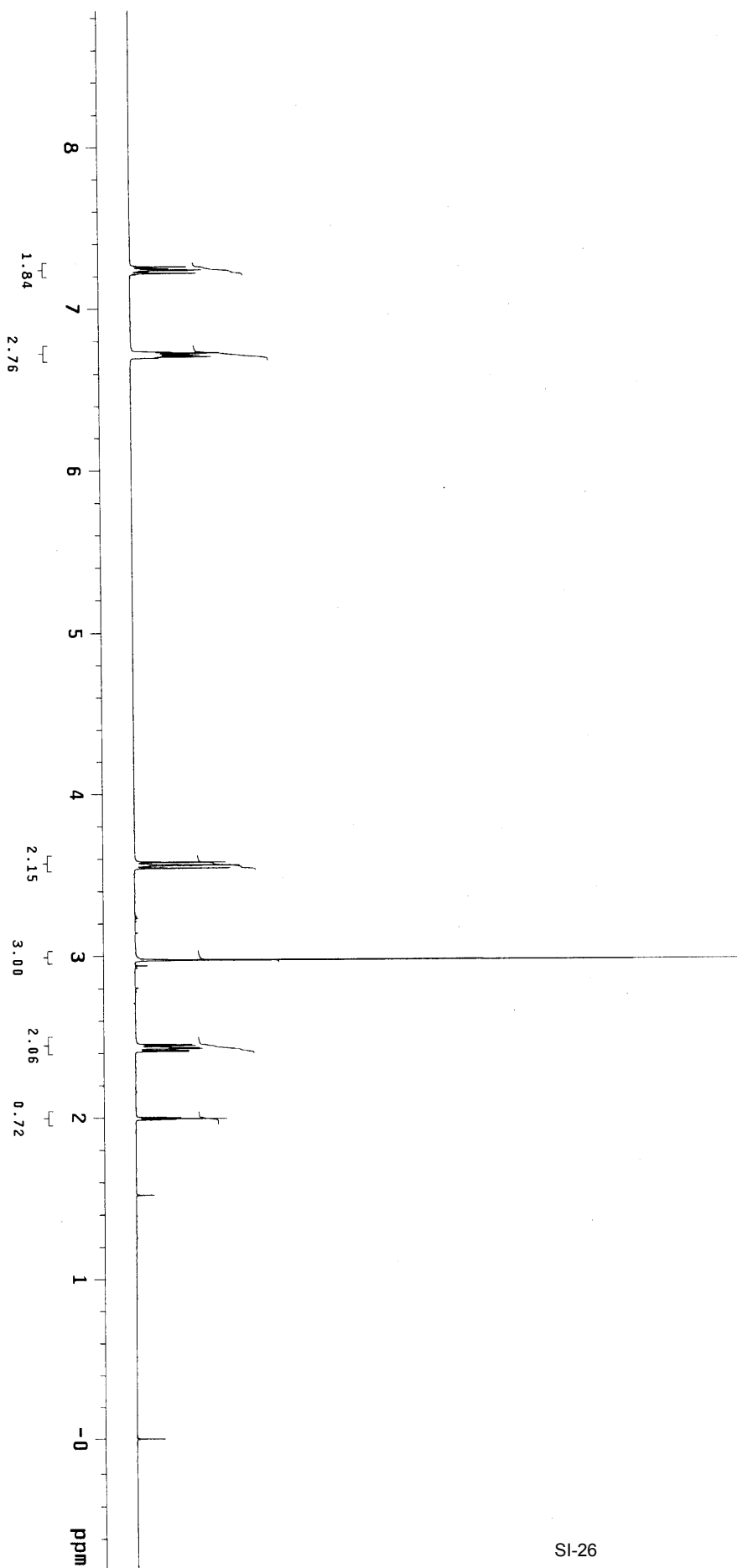
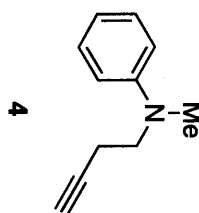
cut11-1-165-2-1H

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Sample ID: s\_20081209\_13  
File: 1301.fid

Pulse Sequence: s2pu1

Solvent: cdcl3  
Temp: 25.0 C / 298.1 K  
Sample #13, Operator: jicui  
File: 1301  
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Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.049 sec  
Width 6410.3 Hz  
8 repetitions  
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DATA PROCESSING  
Resol. enhancement -0.0 Hz  
FT size 65536  
Total time 0 min, 31 sec



cut11-methylamine

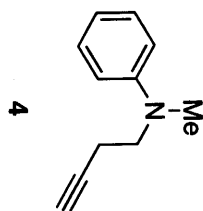
Automation directory: /home/walkup/vnmrSYS/data/auto\_2008.11.15

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  
19456 repetitions  
OBSERVE C13, 125.6732818 MHz  
DECOUPLE H1, 499.7964114 MHz  
Power 39 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 131072  
Total time 16 hr, 2 min, 14 sec



cut11-138-2-1H

File: cut11-138-2-1H

Pulse Sequence: szpul

Solvent: cdcl3

Temp: 25.0 C / 298.1 K

Operator: wai kup

File: cut11-138-2-1H

INOVA-500 "mesquite"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.049 sec

Width 8012.8 Hz

24 repetitions

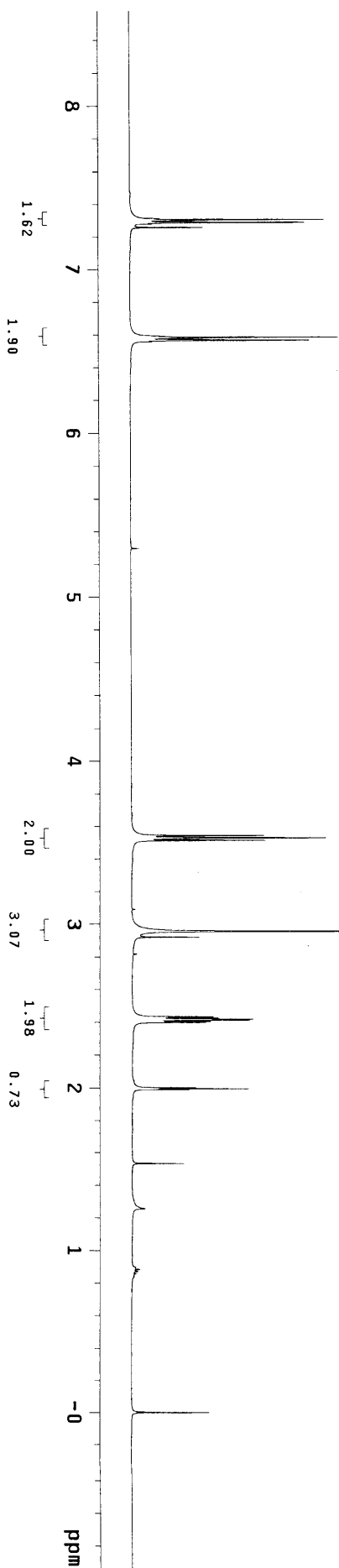
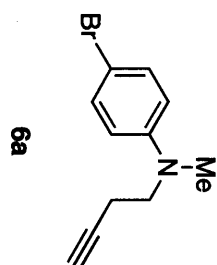
OBSERVE H1, 499.7939144 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 6 min, 31 sec



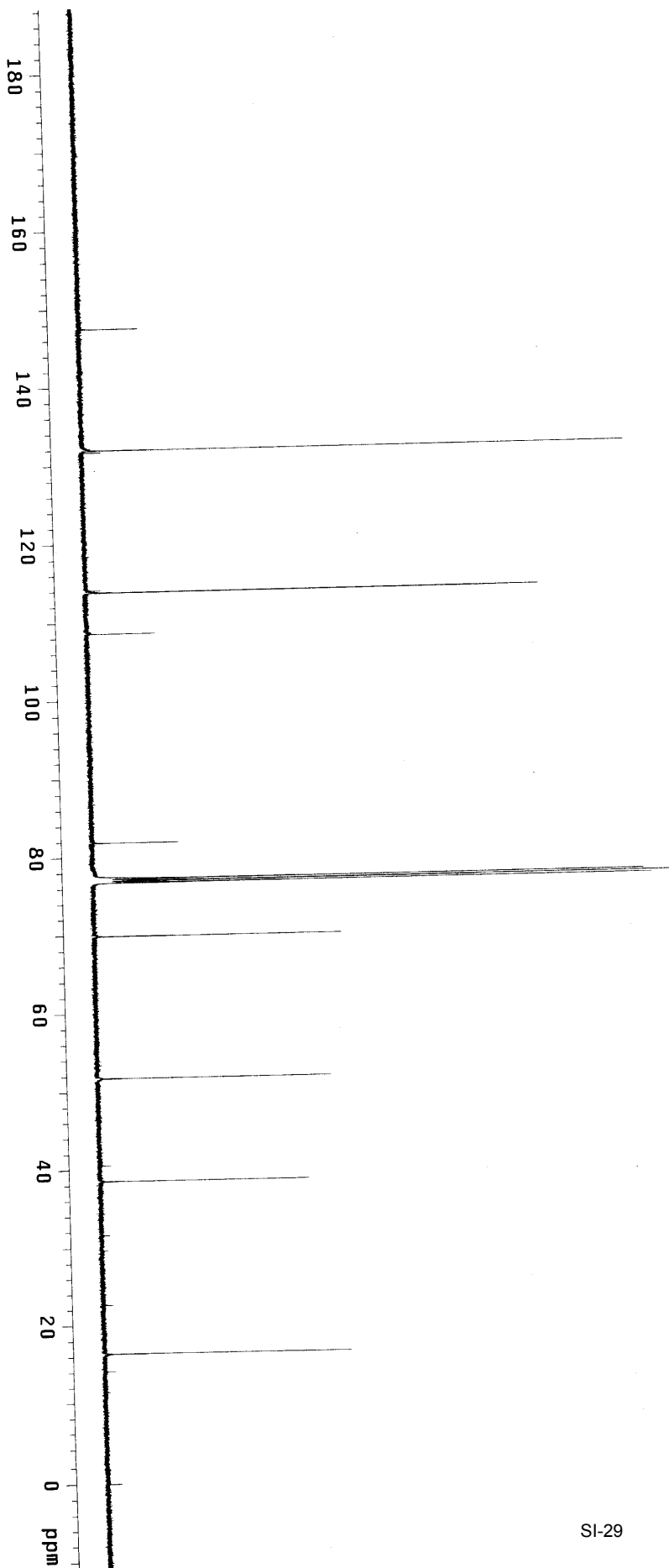
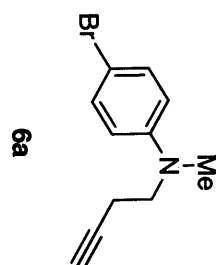
cut11-138-2-1H

Automation directory: /home/walakup/vnmr-sys/data/auto\_2008.11.20.02  
File: /mnt/argenta/nmr500/data/zhang/ticui/cut11-138-2-13C.fid  
Sample id: tmpstudy

Pulse Sequence: szpul

Solvent: cdcl3  
Temp: 25.0 C / 298.1 K  
Operator: walakup  
File: cut11-138-2-13C  
VNMRS-500 "nmr500"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 30487.8 Hz  
6912 repetitions  
OBSERVE C13, 125.6732795 MHz  
DECOUPLE H1, 499.7964114 MHz  
Power 39 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 131072  
Total time 160 hr, 22 min, 28 sec



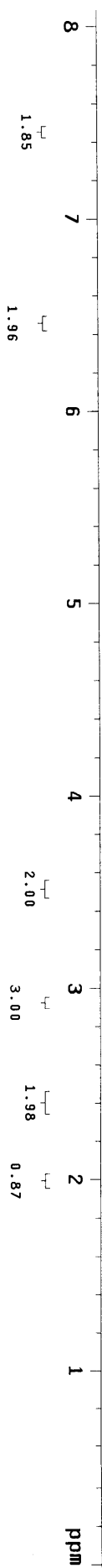
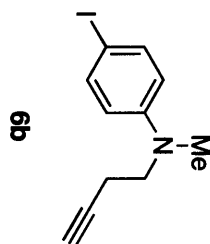
cu11-149-1

Automation directory: /home/walkup/vnmrsvs/data/auto 2008.11.27\_04  
File: /mnt/argenta/mr400/data/zhang/yupengl/2008-11-27-H-1.fid  
Sample id : tmpstudy

Pulse Sequence: s2pul

Solvent: cdcl3  
Temp: 25.0 C / 298.1 K  
Operator: walkup  
File: 2008-11-27-H-1  
VNMRS-400 "mr400"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.049 sec  
Width 6410.3 Hz  
8 repetitions  
OBSERVE H1, 400.0565585 MHz  
DATA PROCESSING  
Resol. enhancement -0.0 Hz  
F1 size 65356  
Total time 0 min, 24 sec

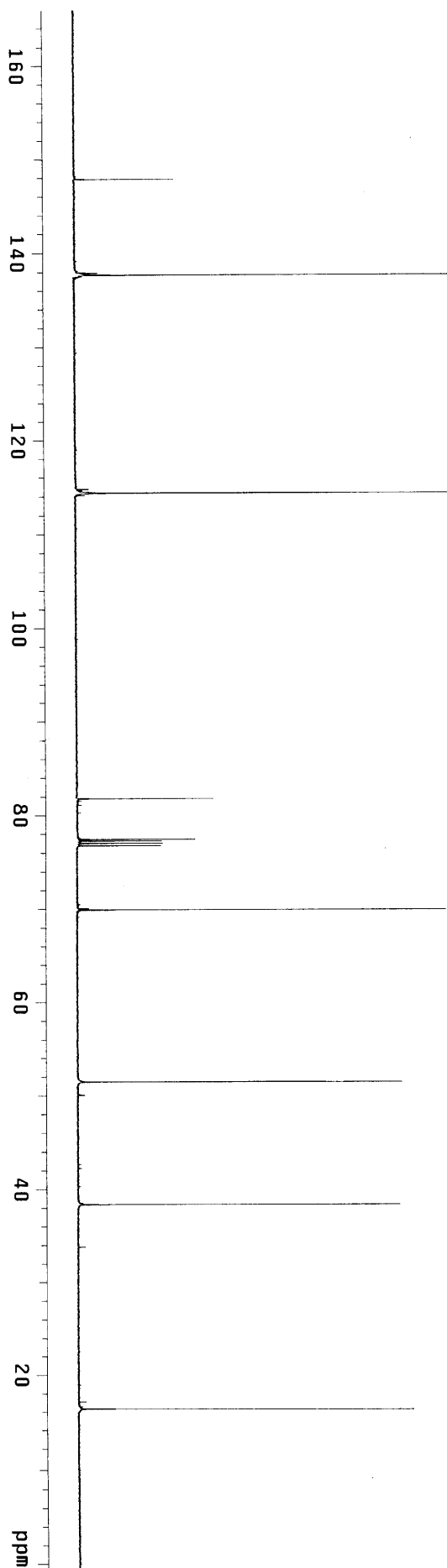
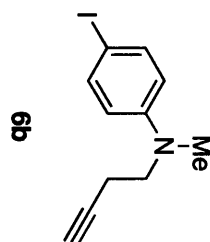


Automation directory: /home/walkup/vnmrsvs/data/auto.2008.11.30.03  
File: /mnt/argenta/nmr500/data/Zhang/yupeng2/2008-11-30-C13-1.fid  
Sample id: tmpstudy

Pulse Sequence: s2pul

Solvent: cdcl3  
Temp: 25.0 C / 298.1 K  
Operator: walkup  
File: 2008-11-30-C13-1  
Vnmrs-500 "nmr500"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 30487.8 Hz  
552 repetitions  
OBSERVE C13, 125.6732930 MHz  
DECOUPLE H1, 499.7964114 MHz  
Power 39 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 131072  
Total time 46 min, 11 sec



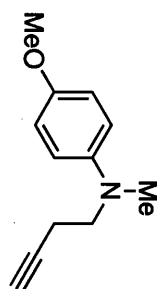
cu111-138-1-1H

Automation directory: /home/waikup/vnmrsvs/data/auto\_2008.12.09  
File: /mnt/argenta/nmr500/data/Zhang/11cu11-138-1-1H.fid  
Sample id: tmpstudy  
Sample: 4-hydroxy

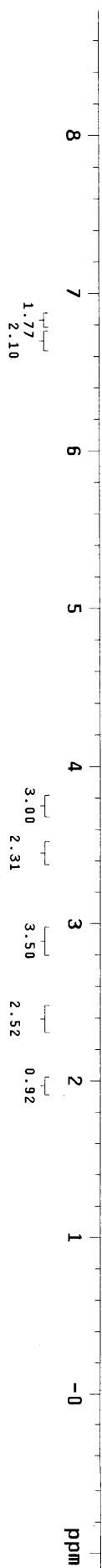
Pulse Sequence: s2pul

Solvent: cdcl3  
Temp: 25.0 C / 298.1 K  
Operator: waikup  
File: cu111-138-1-1H  
Vnmrs-500 "nmr500"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.049 sec  
Width 8012.8 Hz  
44 repetitions  
OBSERVE H1, 499.7939153 MHz  
DATA PROCESSING  
Line broadening 0.2 Hz  
F1 size 65536  
Total time 6 min, 31 sec



6c





cu111-138-1-13C

File: cu111-138-1-13C

Pulse Sequence: szpul

Solvent: cdc13

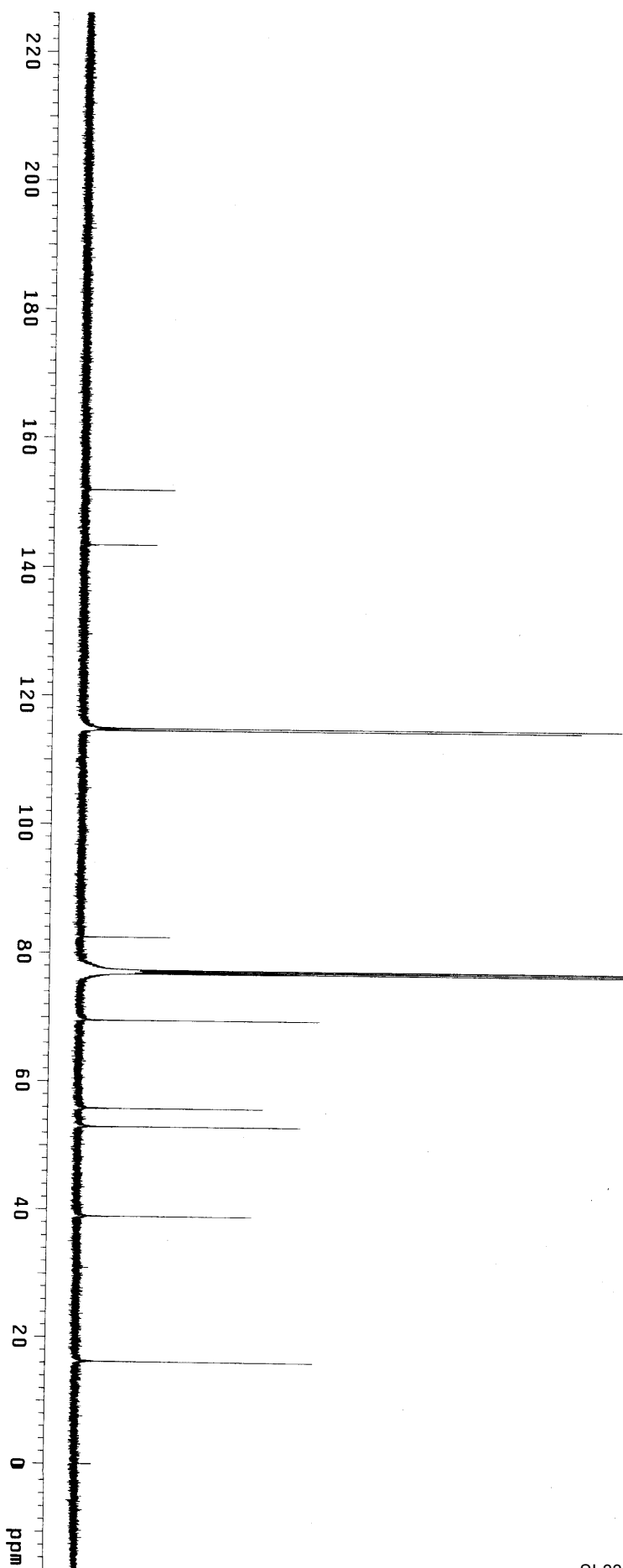
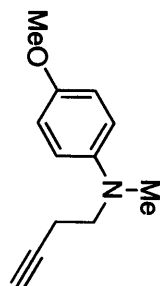
Temp: 25.0 C / 298.1 K

Operator: walkup

File: cu111-138-1-13C

INOVA-500 "mesquite"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 30487.8 Hz  
11200 repetitions  
OBSERVE C13, 125.673279 MHz  
DECOUPLE H1, 499.7964114 MHz  
Power 39 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 131072  
Total time 25 hr, 39 min, 35 sec



cu111-11242008-mn02-1h

Automation directory: /home/walkup/vnmrSYS/data/auto\_2008.11.24\_17

File : exp

Sample id : tmpstudy

Pulse Sequence: s2pu1

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 2.049 sec

Width 8012.8 Hz

28 repetitions

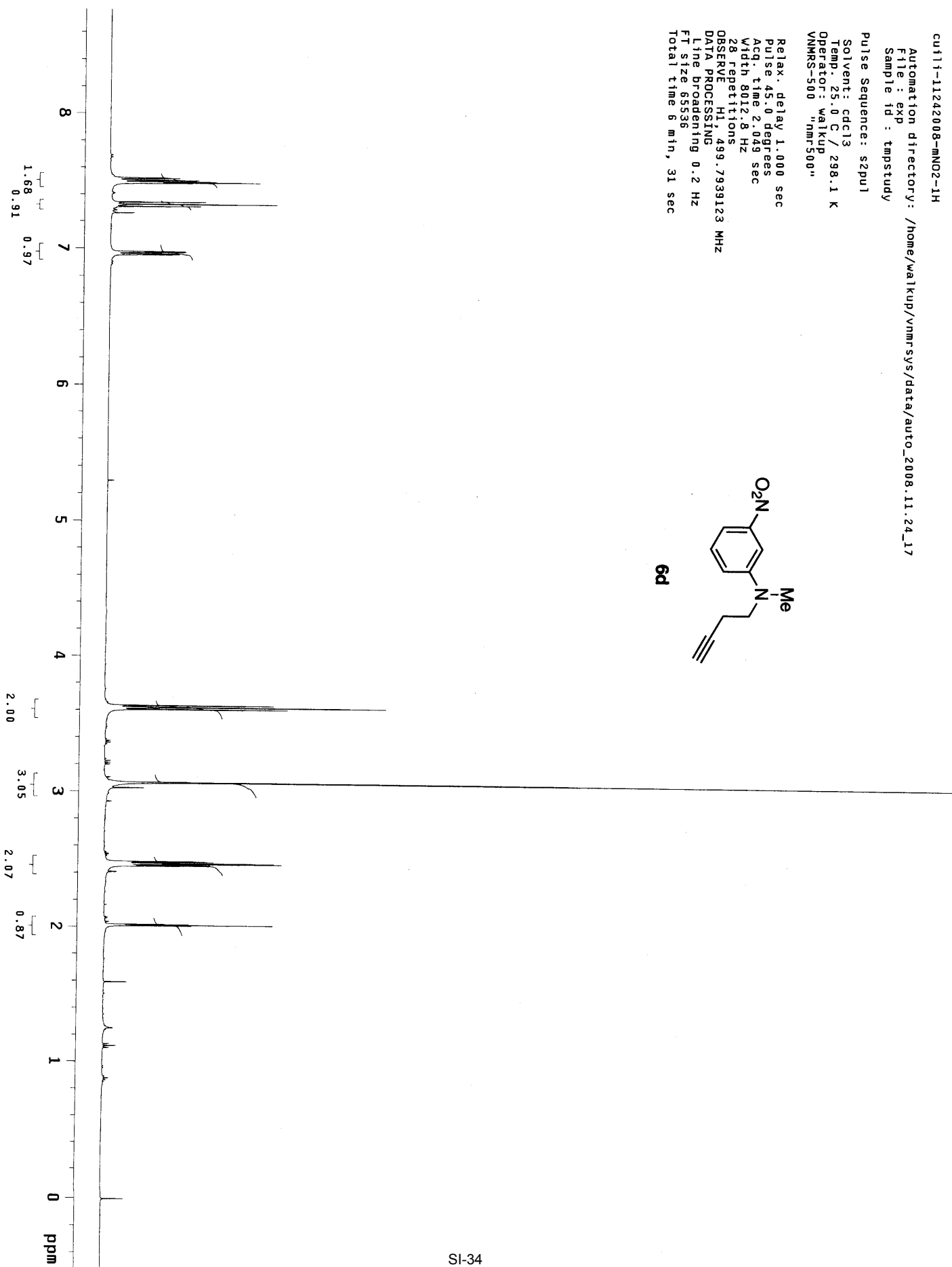
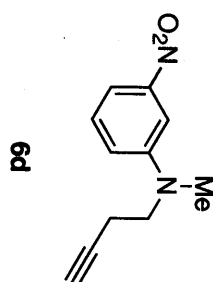
OBSERVE H1, 499.793123 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 6 min, 31 sec



cu111-11242008-mn02-1h

Automation directory: /home/walkup/vnmrSYS/data/auto\_2008.11.24\_17

File : exp

Sample id : tmpstudy

Pulse Sequence: s2pul

Solvent: cdcl3

Temp: 25.0 C / 298.1 K

Operator: walkup

VNMR5-500 "hmr500"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 30487.8 Hz

16640 repetitions

OBSERVE C13, 125.6732841 MHz

DECOUPLE H1, 499.7964114 MHz

Power 39 dB

continuously on

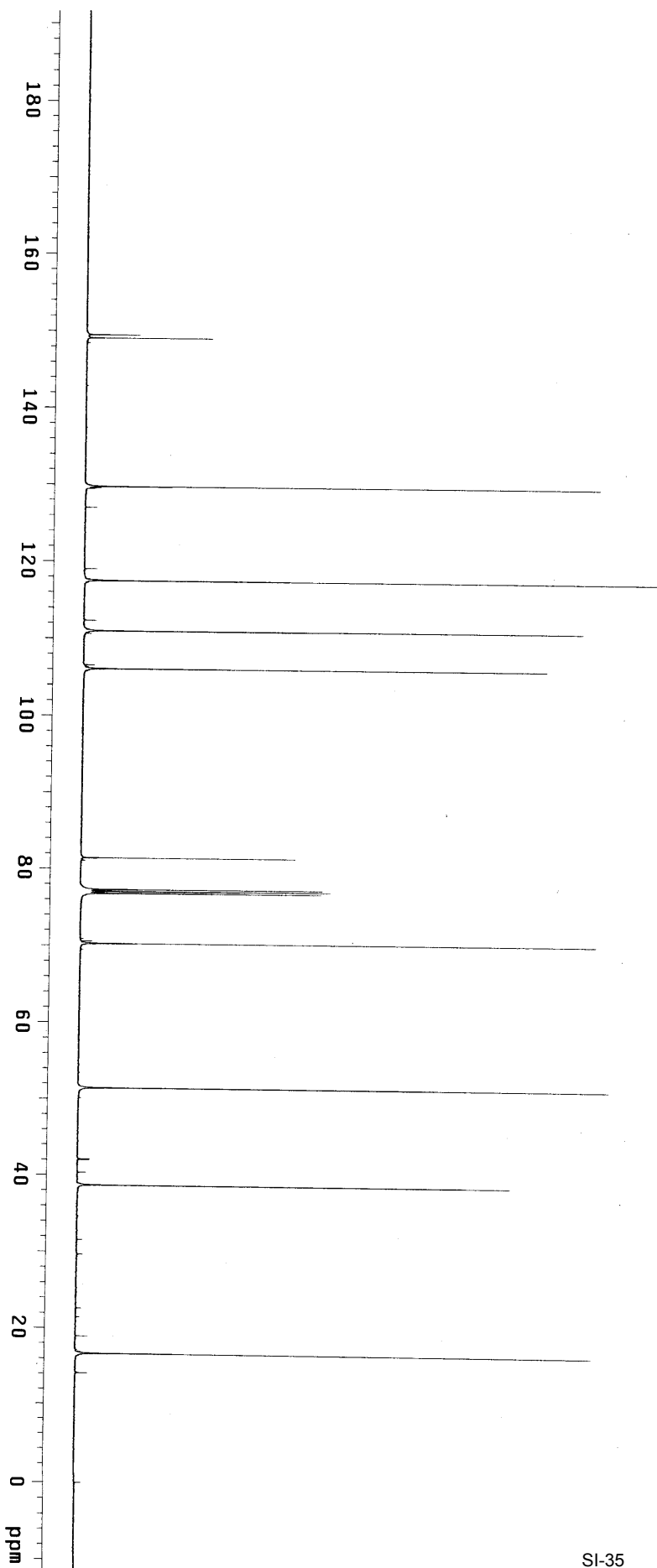
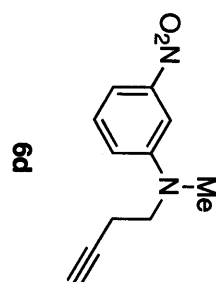
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 131072

Total time 12 hr, 49 min, 47 sec

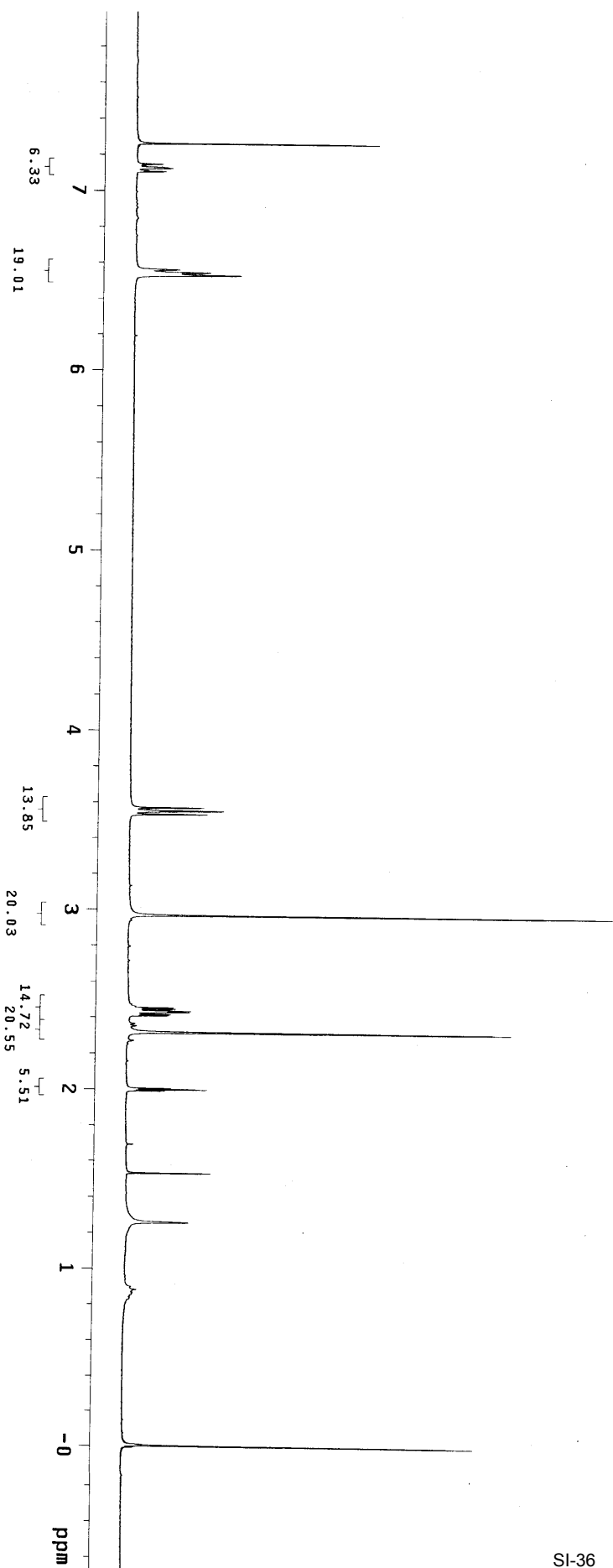
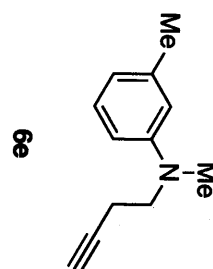


cu111-139-1

Automation directory: /home/walakup/vnmrSYS/data/auto-2008.12.09\_16  
File : /mnt/argenta/mr400/data/Zhang/11cu1/cu111-139-1-1H.f1d  
Sample id : tmpstudy

Pulse Sequence: s2pul  
Solvent: cdcl3  
Temp: 25.0 C / 298.1 K  
Operator: walakup  
File: cu111-139-1-1H  
Vnmrs-400 "mr400"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.049 sec  
Width 6410.3 Hz  
40 repetitions  
OBSERVE H1, 400.055508 MHz  
DATA PROCESSING  
Resol. enhancement -0.0 Hz  
FT size 65536  
Total time 6 min, 31 sec



cu111-139-1-13C

File: cu111-139-1-13Ca

Pulse Sequence: s2pu1

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: walkup

File: cu111-139-1-13Ca

INOVA-500 "mesquite"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 30487.8 Hz

17856 repetitions

OBSERVE C13, 125.6732781 MHz

DECOUPLE H1, 499.7964114 MHz

Power 39 dB

continuously on

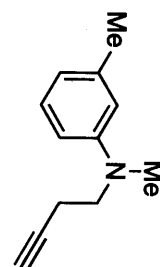
WALTZ-16 modulated

DATA PROCESSING

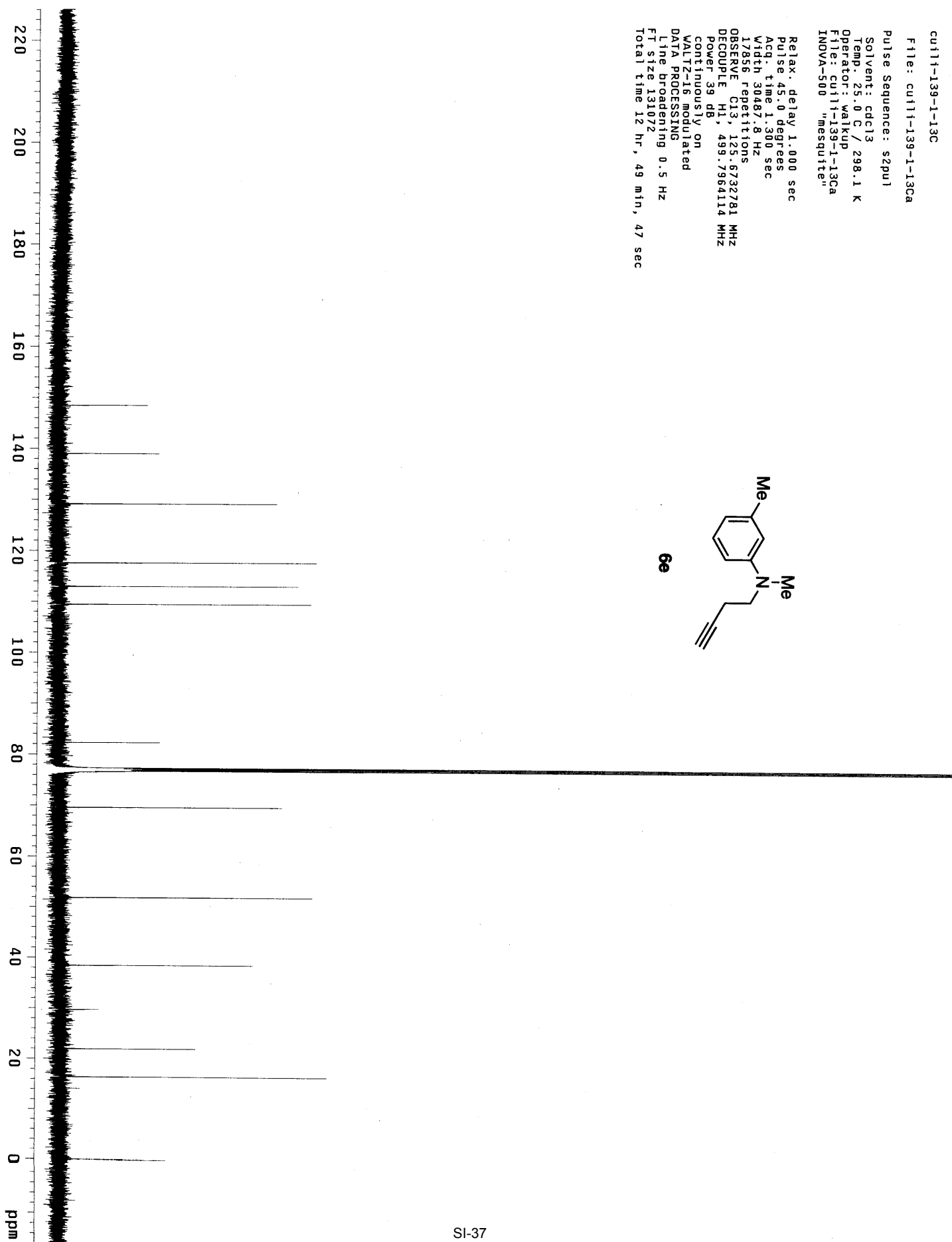
Line broadening 0.5 Hz

File size 131072

Total time 12 hr, 49 min, 47 sec



6e



cu111-155-1-1H

Automation directory: /home/walkup/vnmrSYS/data/auto\_2008.11.30\_04

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 2.049 sec

Width: 8012.8 Hz

28 repetitions

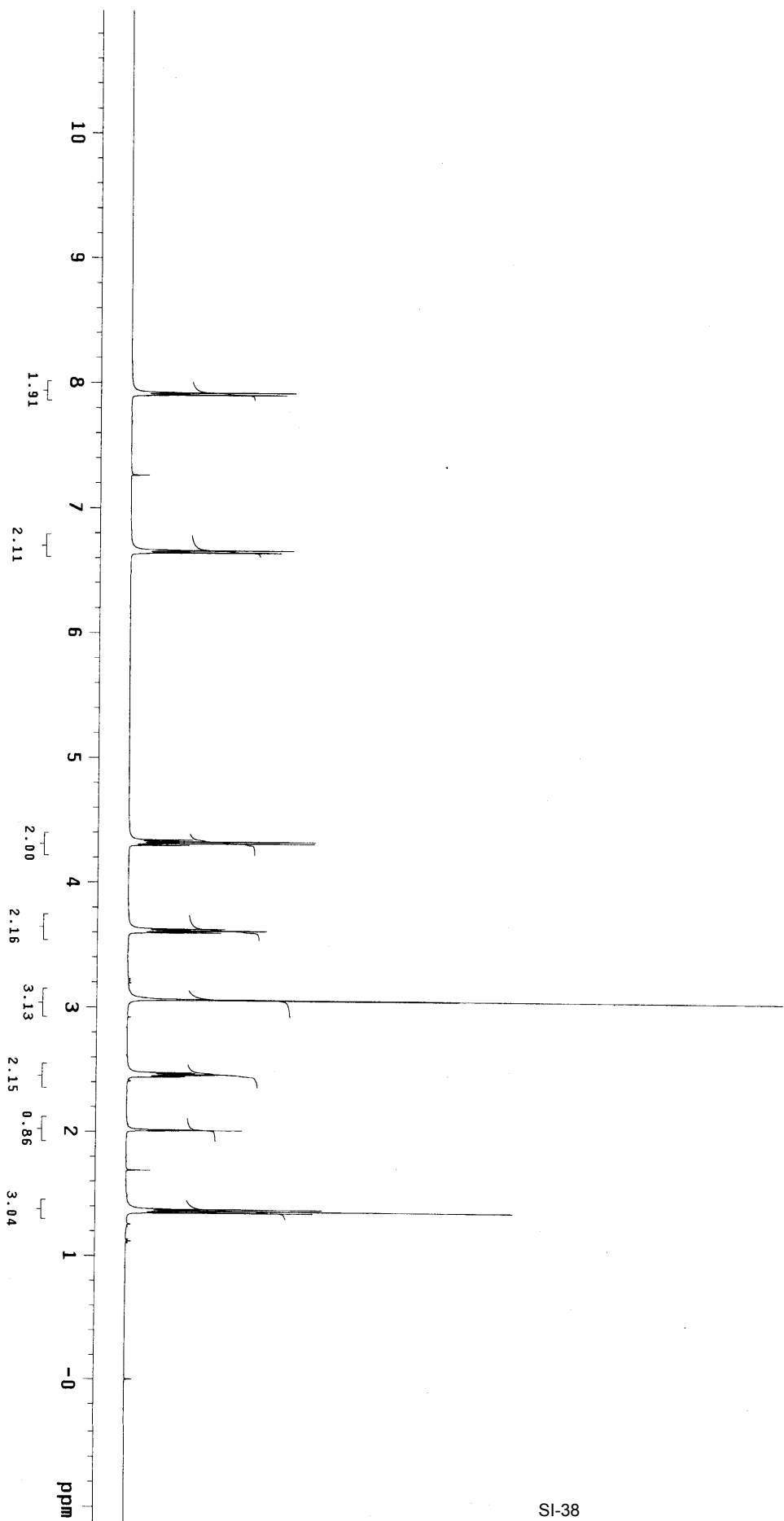
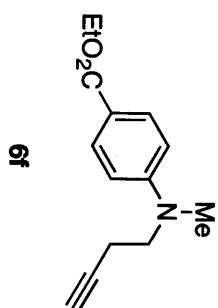
OBSERVE: H1, 499.7939127 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 6 min, 31 sec



cu111-155-1-13C

Automation directory: /home/waikup/vnmrSYS/data/2008.12.02

File: exp

Sample id: tmpstudy

Sample: PMBr in CDCl3

Pulse Sequence: szpul

Solvent: cdcl3

Temp: 25.0 C / 298.1 K

Operator: waikup

VNMR-500 "hmr500"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 30487.8 Hz

378 repetitions

OBSERVE C13, 125.6732846 MHz

DECOUPLE H1, 499.7964114 MHz

Power 39 dB

continuously on

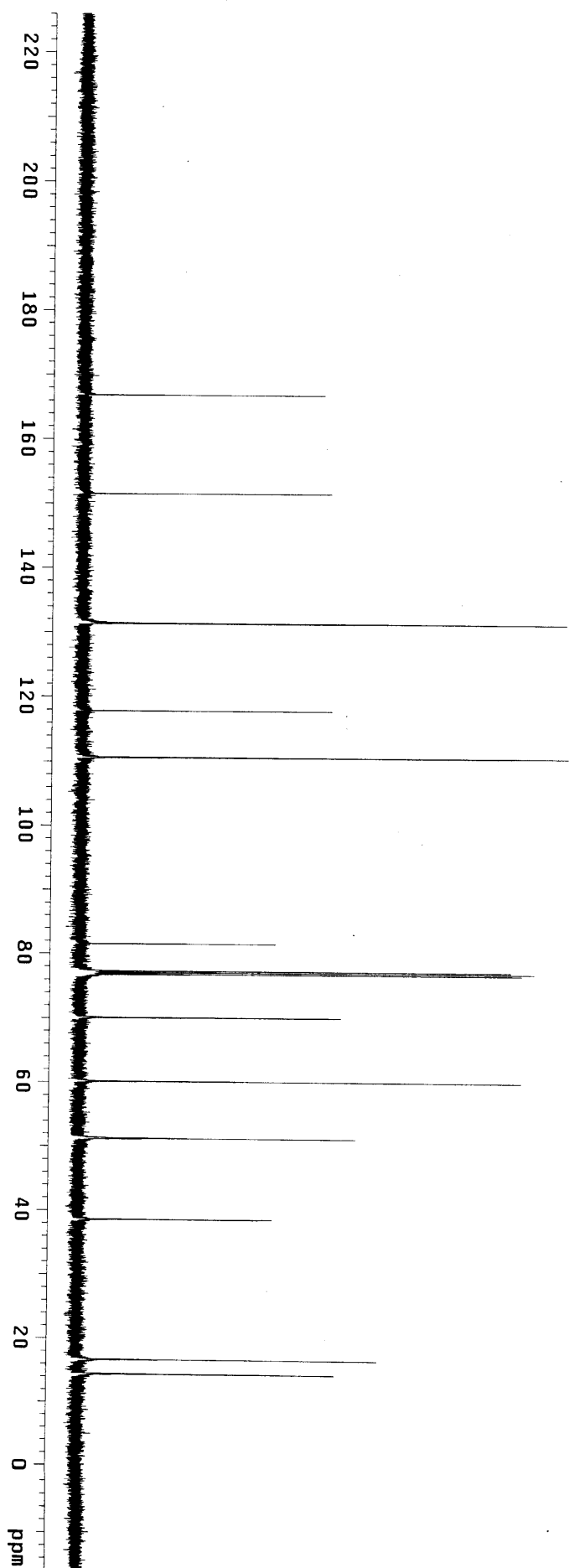
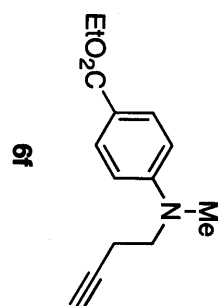
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 131072

Total time 38 min, 29 sec



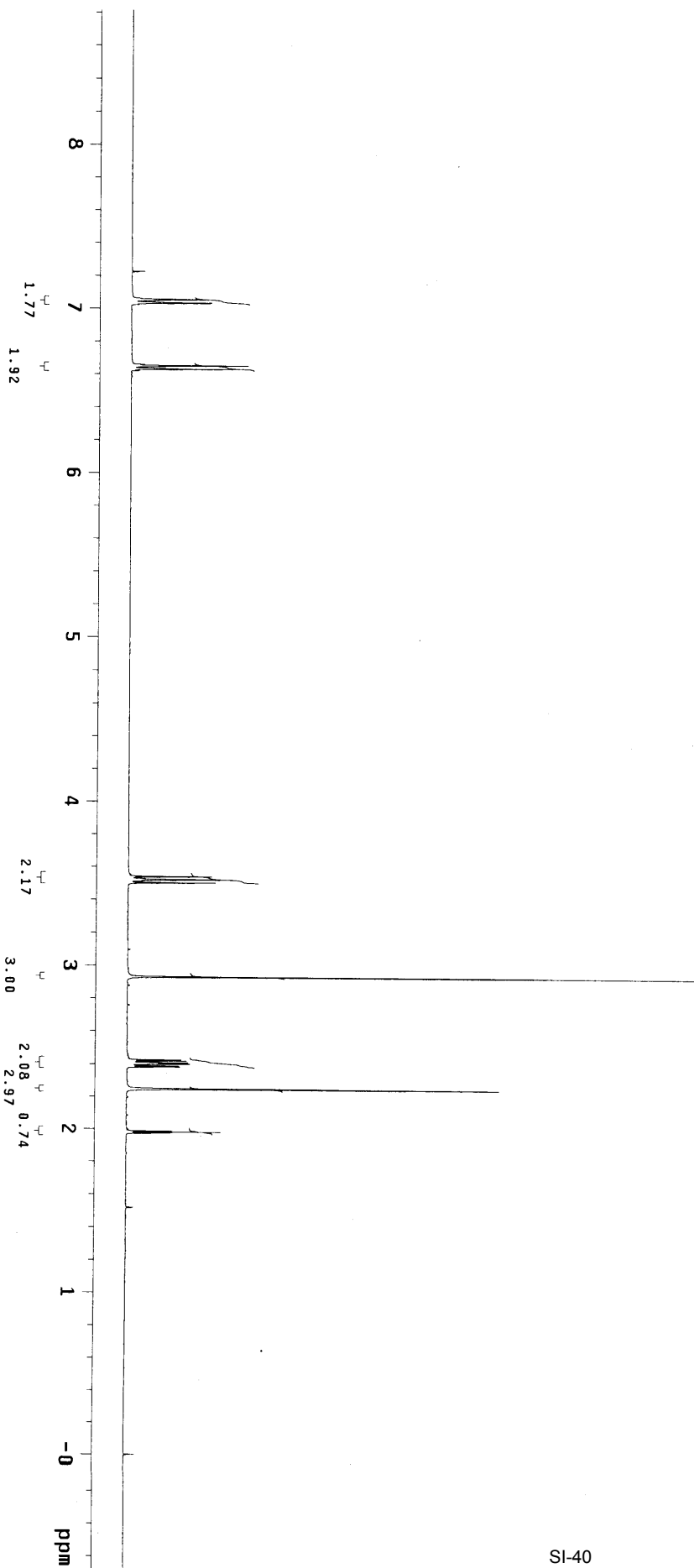
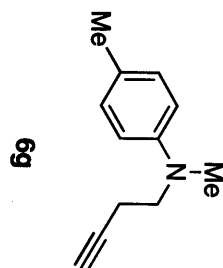
cu111-164-2-1H

Sample: cu111-146-2-1H  
Sample ID: s.20081208\_05  
File: 0501.fid

Pulse Sequence: szpul

Solvent: cdcl3  
Temp: 25.0 C / 298.1 K  
Sample #5, Operator: jfcu  
File: 0501  
VNMRS-400 "nmr400.localdomain"

Relax. delay: 1.000 sec  
Pulse: 45.0 degrees  
Acq. time: 2.083 sec  
Width: 6410.3 Hz  
8 repetitions  
OBSERVE: H1, 399.8626975 MHz  
DATA PROCESSING  
Resol. enhancement: -0.0 Hz  
FT size: 65536  
Total time: 0 min, 31 sec





cu111-1-164-1-13C

Automation directory: /home/walkup/vnmr5ys/data/auto\_2008.12.08\_01

File : exp

Sample id : tmpstudy

Pulse Sequence: s2pu1

Solvent: cdc13

Temp: 25.0 C / 298.1 K

Operator: walkup

VNMR5-500 "hmr500"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 30487.8 Hz

5824 repetitions

OBSERVE C13, 125.6732855 MHz

DECOUPLE H1, 499.7964114 MHz

Power 39 dB

continously on

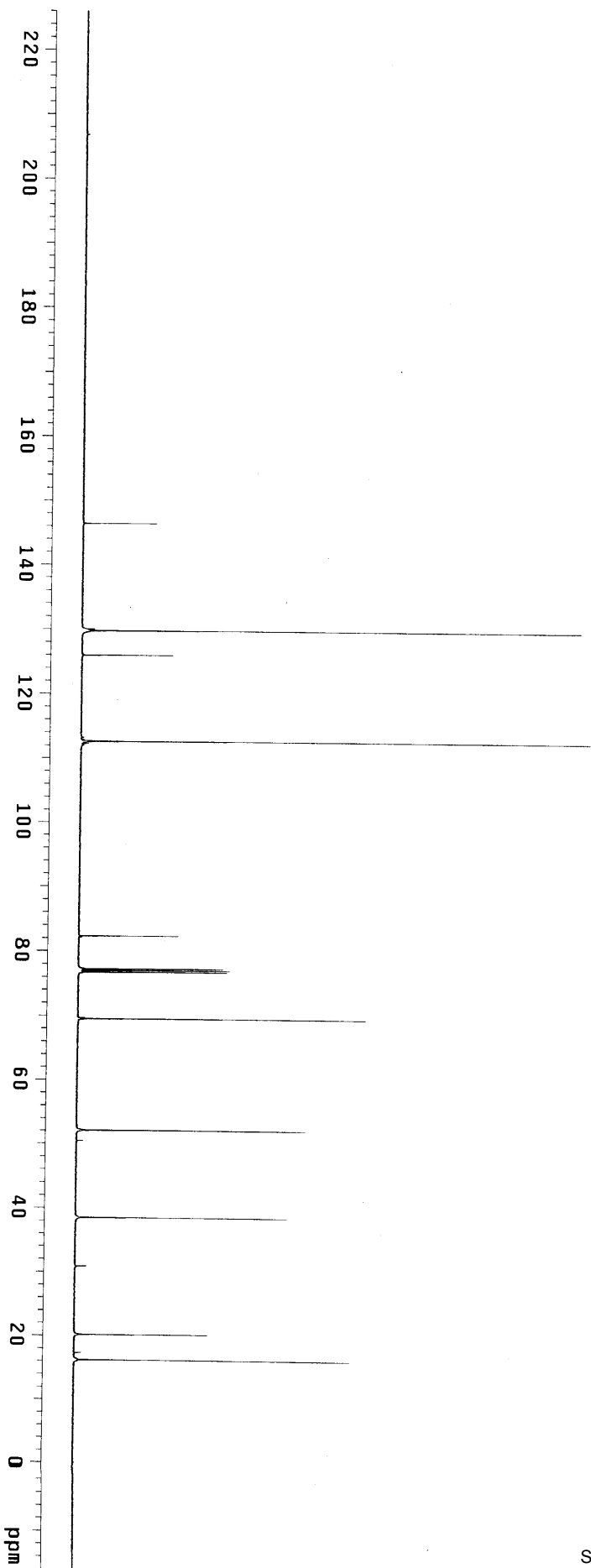
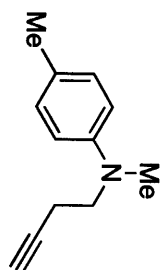
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 131072

Total time 12 hr, 49 min, 47 sec



pengyu-2008-12-05-H-3

Automation directory: /home/walkup/vnmrSYS/data/auto\_2008.12.05\_07

File : exp

Sample id : tmpstudy

Pulse Sequence: s2pu1

Solvent: cdcl3

Temp: 25.0 C / 298.1 K

Operator: walkup

VNMR-400 "mr400"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.043 sec

Width 6410.3 Hz

64 repetitions

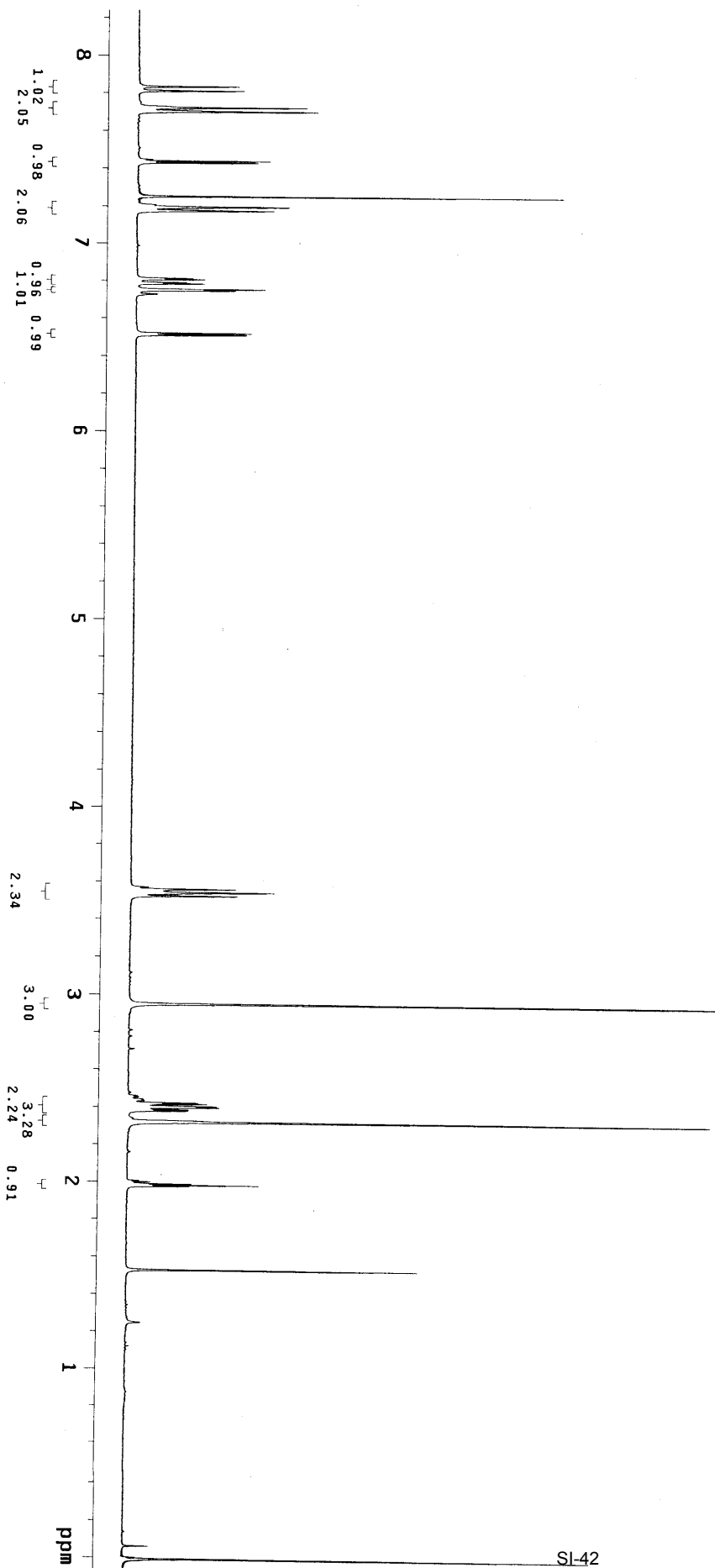
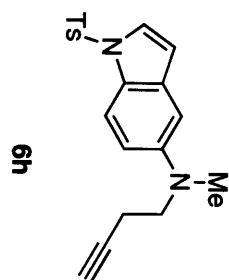
OBSERVE H1, 400.0565537 MHz

DATA PROCESSING

Resol. enhancement -0.0 Hz

FT size 65536

Total time 3 min, 15 sec



pengyu-12-5-C13-1

Automation directory: /home/walkup/vnmrSYS/data/auto\_2008.12.05

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

18000 repetitions

OBSERVE C13, 125.6732785 MHz

DECOUPLE H1, 499.7964114 MHz

Power 39 dB

continuously on

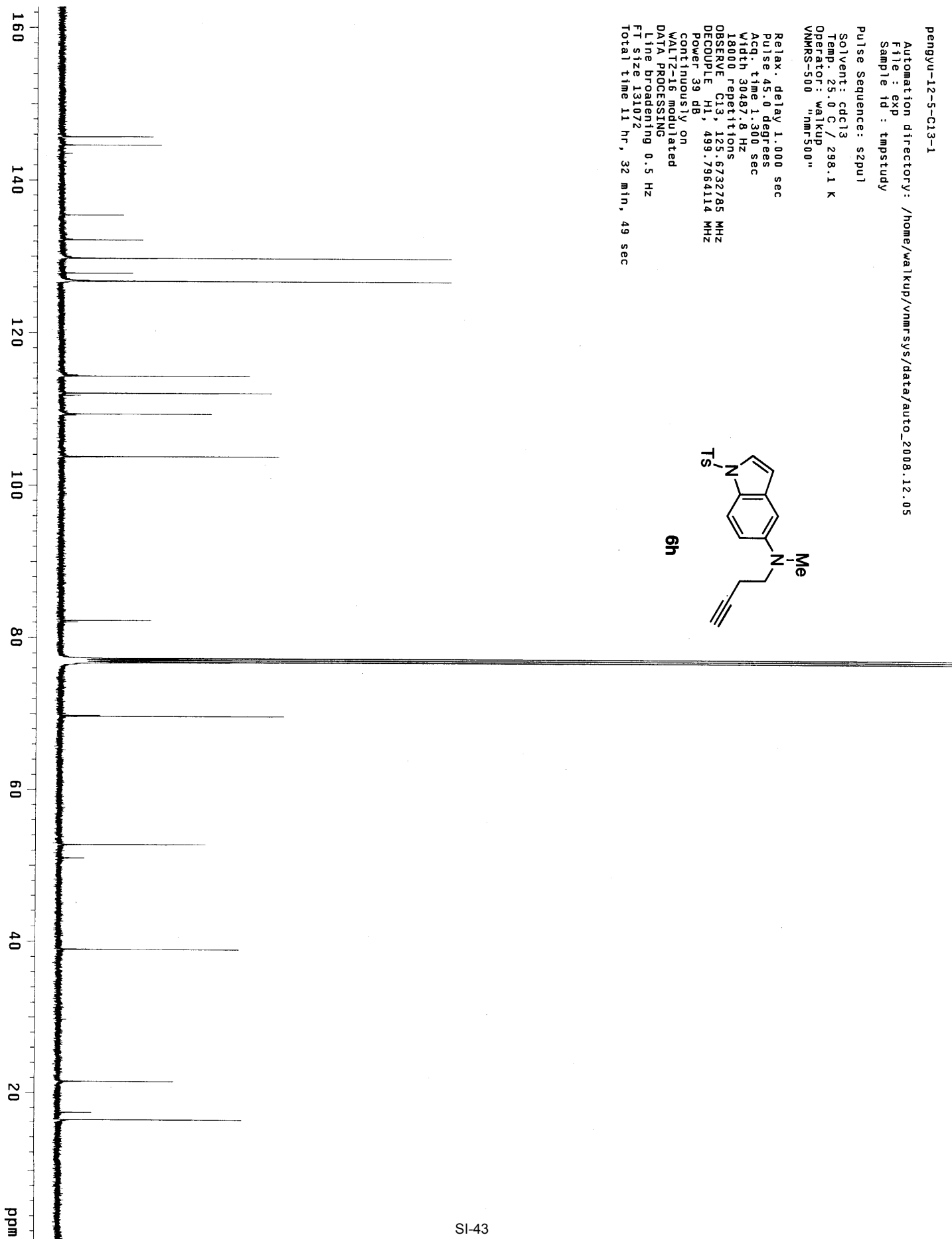
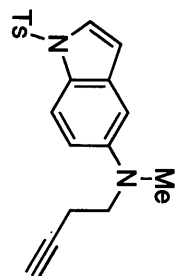
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 131072

Total time 11 hr, 32 min, 49 sec



cu111-130-1-1H

Automation directory: /home/walakup/vnmrsvs/data/auto 2008.12.09\_16  
File : /mnt/argenta/mr400/data/Zhang/11cu1/cu111-130-1-1H.fid  
Sample id : tmpstudy

Pulse Sequence: s2pul1

Solvent: cdcl3

Temp: 25.0 C / 298.1 K

Operator: walakup

File: cu111-130-1-1H

VNMR-400 "mr400"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.049 sec

Width 6410.3 Hz

60 repetitions

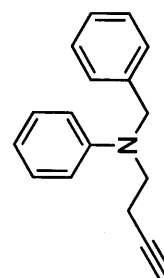
OBSERVE H1, 400.0565491 MHz

DATA PROCESSING

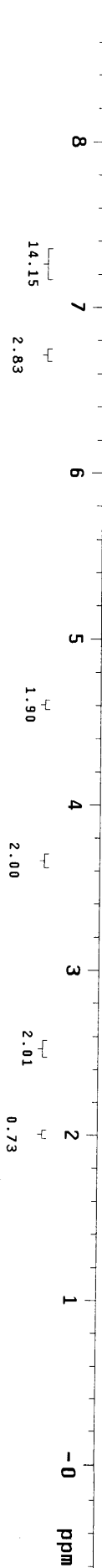
Resol. enhancement -0.0 Hz

FI size 65536

Total time 6 min, 37 sec



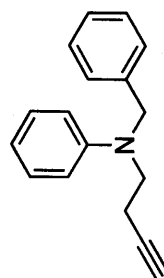
61



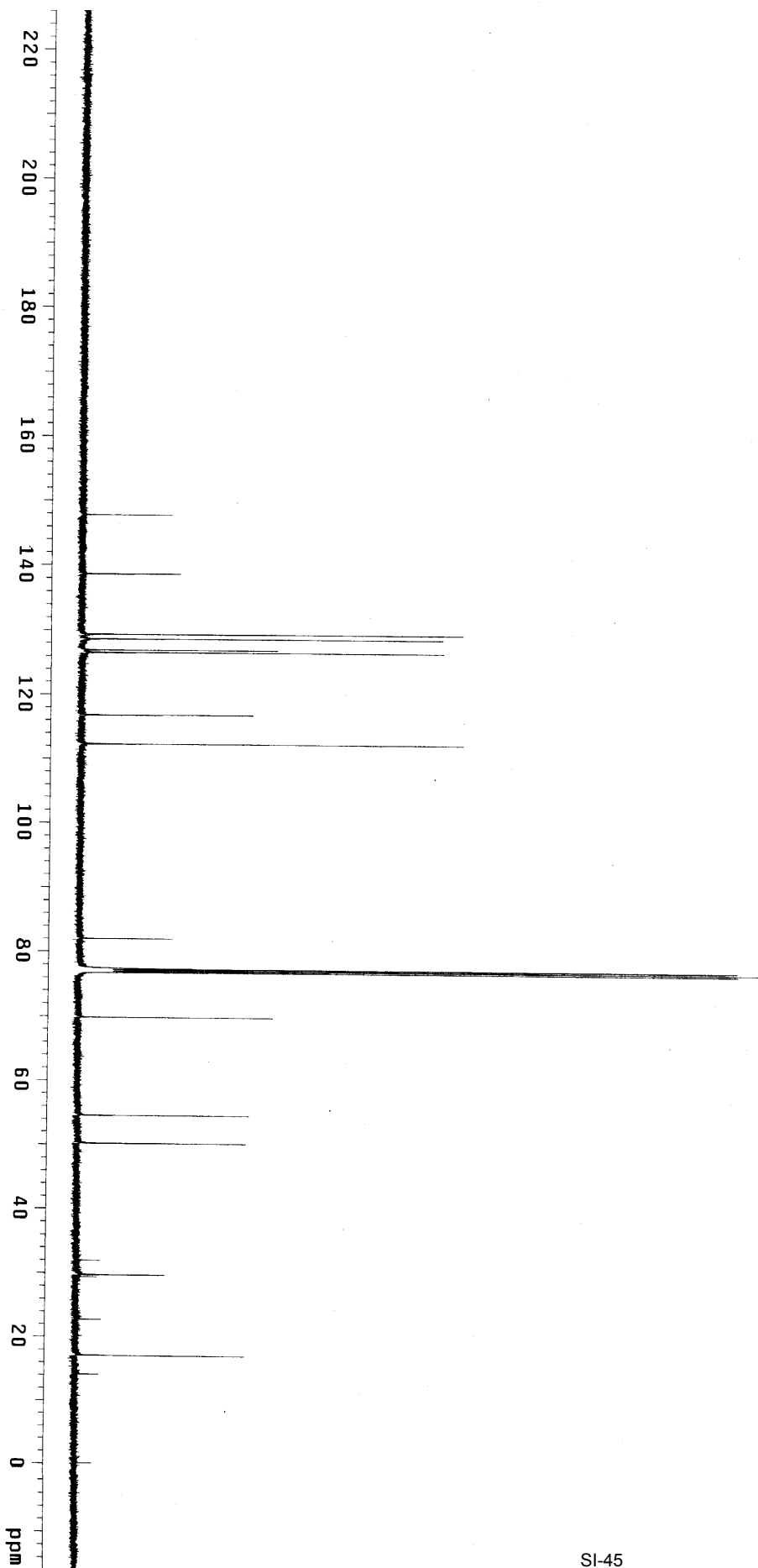
Automation directory: /home/walkup/vnmr500/data/aut\_2008.12.09  
File: /mnt/ergeta/nmr500/data/Zhang/ticut/cut11-130-1-13C.fid  
Sample id: tmpstudy

Pulse Sequence: szpu1  
Solvent: cdcl3  
Temp: 25.0 C / 298.1 K  
Operator: walkup  
File: cut11-130-1-13C  
VNMRS-500 "nmr500"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 30487.8 Hz  
4032 repetitions  
OBSERVE C13, 125.6732804 MHz  
DECOUPLE H1, 499.7964114 MHz  
Power 39 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 131072  
Total time 6 hr, 24 min, 53 sec



6i



cu11f-128-1-1H

File: cu11f-128-1-1H

Pulse Sequence: szpu1

Solvent: cdc13

Temp: 25.0 C / 298.1 K

Operator: waikup

File: cu11f-128-1-1H

INOVA-500 "mesquite"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.049 sec

Width 8012.8 Hz

40 repetitions

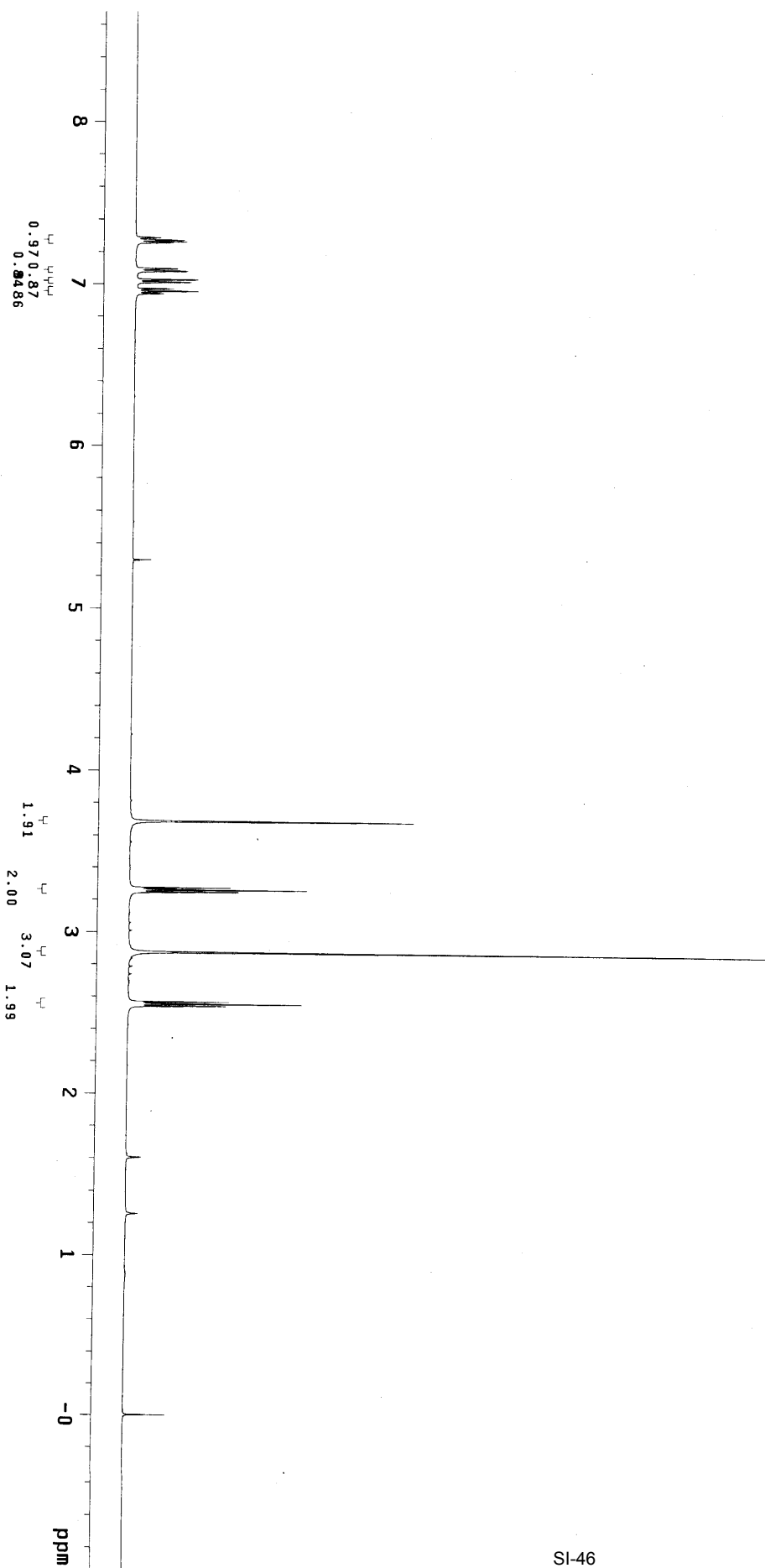
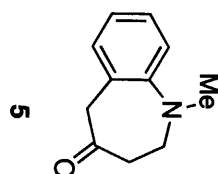
OBSERVE H1, 499.7939104 MHz

DATA PROCESSING

Line broadening 0.2 Hz

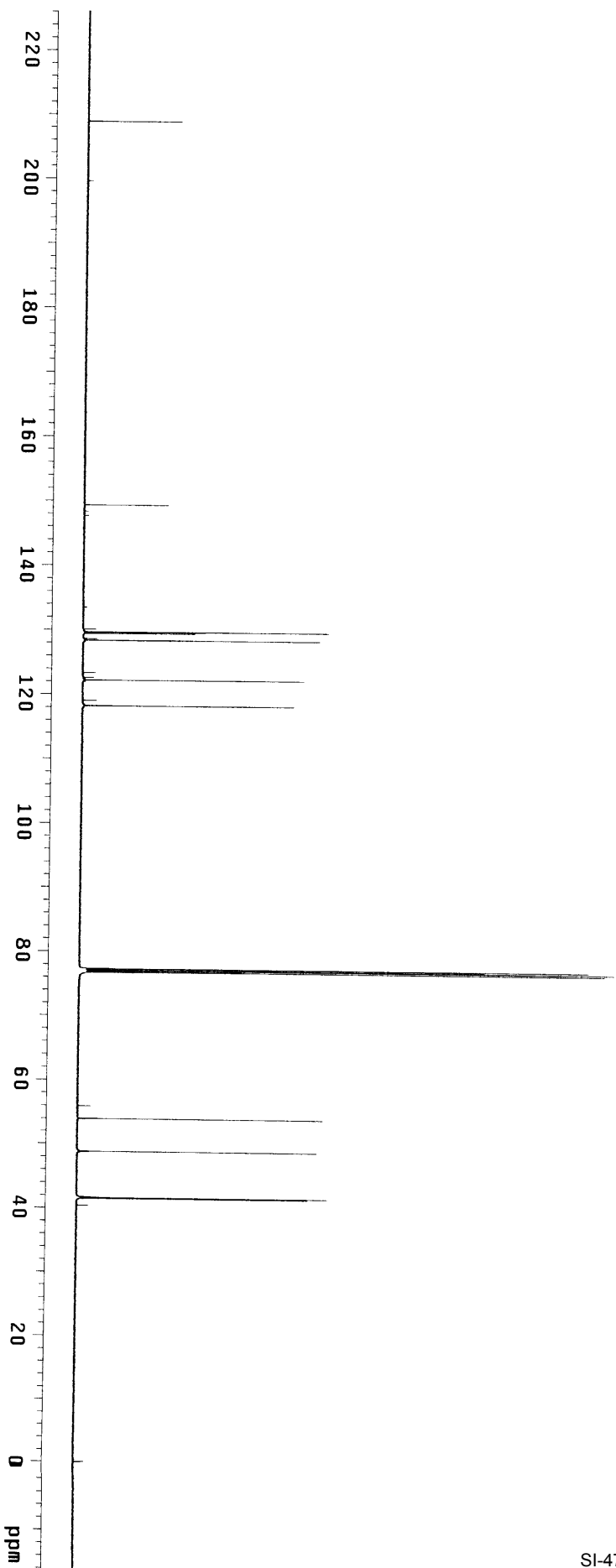
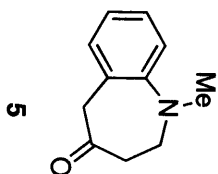
FT size 65536

Total time 6 min, 31 sec



```
Pulse Sequence: szpu1
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: walakup
VNMRS-500 "nmr500"
```

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 30467.8 Hz  
18560 repetitions  
OBSERVE C13, 125.6732809 MHz  
DECOUPLE H1, 429.7964114 MHz  
Power 39.0 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line frequency 0.5 Hz  
FT size 131072  
Total time 16 hr, 2 min, 14 sec



cu111-146-1-1H

Sample: 11-146-1-1H

Sample ID: s\_6\_01

File: guozhu/11-146-1-1H/Proton01.fid

Pulse Sequence: szpul

Solvent: cdcl3

Temp: 25.0 C / 298.1 K

Sample #6, Operator: guozhu

File: Proton01

VNMR-400 "nmr400.localdomain"

Relax. delay: 1.000 sec

Pulse: 45.0 degrees

Acq. time: 2.009 sec

Width: 6410.3 Hz

16 repetitions

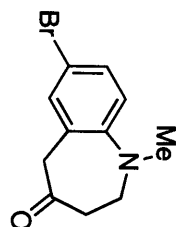
OBSERVE: H1, 399.8626810 MHz

DATA PROCESSING

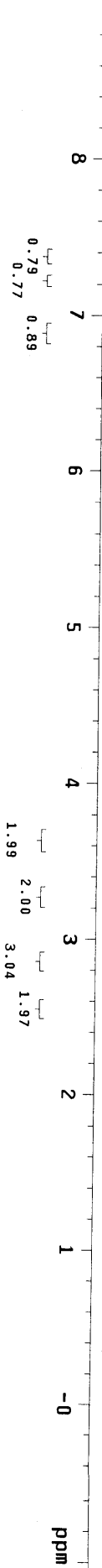
Resol. enhancement: -0.0 Hz

FT size: 65536

Total time: 0 min, 55 sec



7a





cu111-146-1-13C

File: cu111-146-1-13C

Pulse Sequence: szpul

Solvent: cdcl3

Temp: 25.0 C / 298.1 K

Operator: walkup

File: cu111-146-1-13C

INOVA-500 "redjacket"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 30487.8 Hz

17408 repetitions

OBSERVE C13, 125.6732804 MHz

DECOUPLE H1, 499.7964114 MHz

Power 39 dB

continuously on

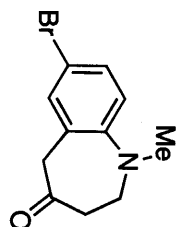
WALTZ-16 modulated

DATA PROCESSING

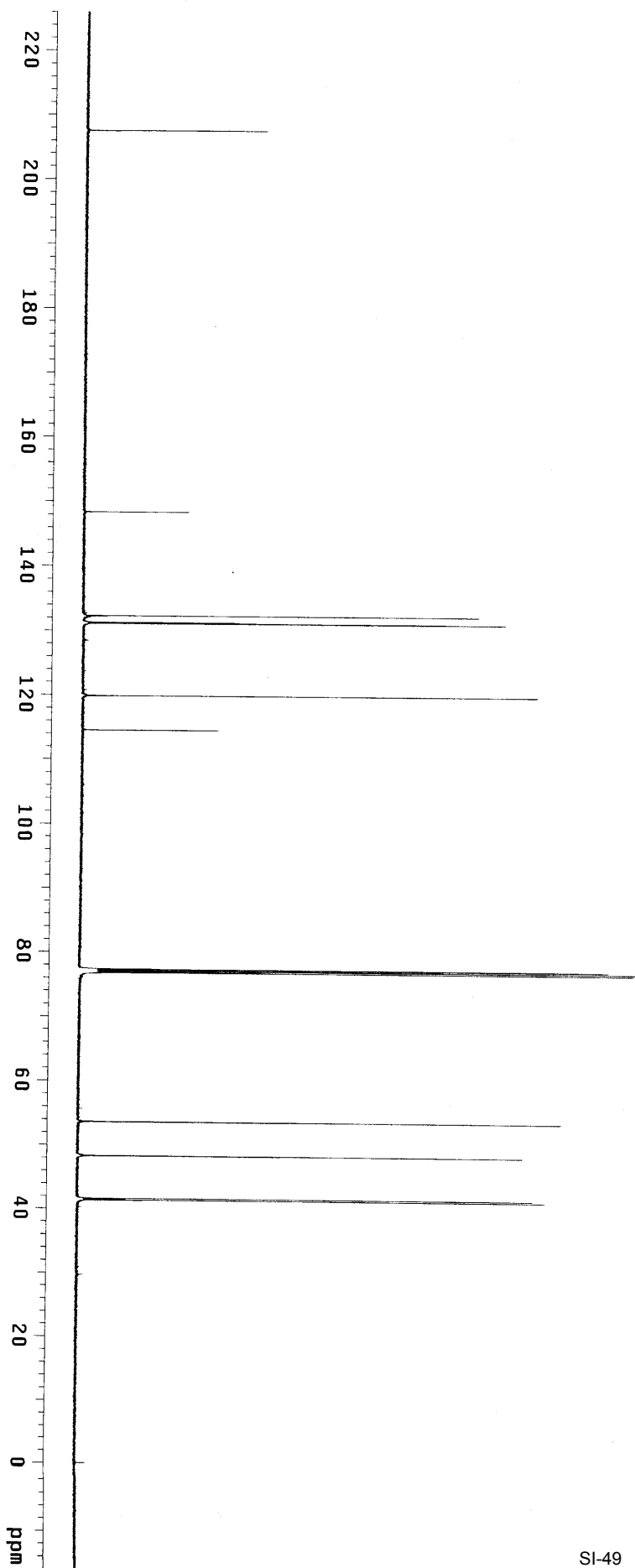
Line broadening 0.5 Hz

FT size 131072

Total time 12 hr, 49 min, 47 sec



7a



Automation directory: /home/walkup/vnmrSYS/data/auto 2008.12.01\_12  
File : /mnt/argenta/mr400/data/Zhang/yupeng1/2008-12-1-H-1.fid  
Sample id : tmpstudy

Pulse Sequence: s2pul

Solvent: cdc13

Temp: 25.0 C / 298.1 K

Operator: walkup

File: 2008-12-1-H-1  
VNMRS-400 "mr400"

Relax. delay 1.000 sec  
Pulse 45.0 degrees

Acq. time 2.049 sec  
Width 6410.3 Hz

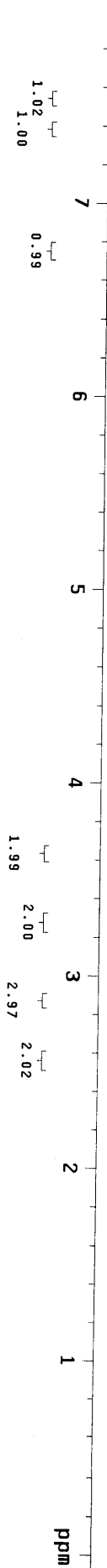
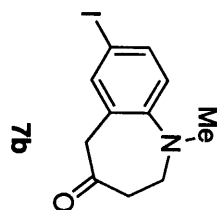
Single scan

OBSERVE H1, 400.0565469 MHz

DATA PROCESSING

Resol. enhancement -0.0 Hz  
FT size 65536

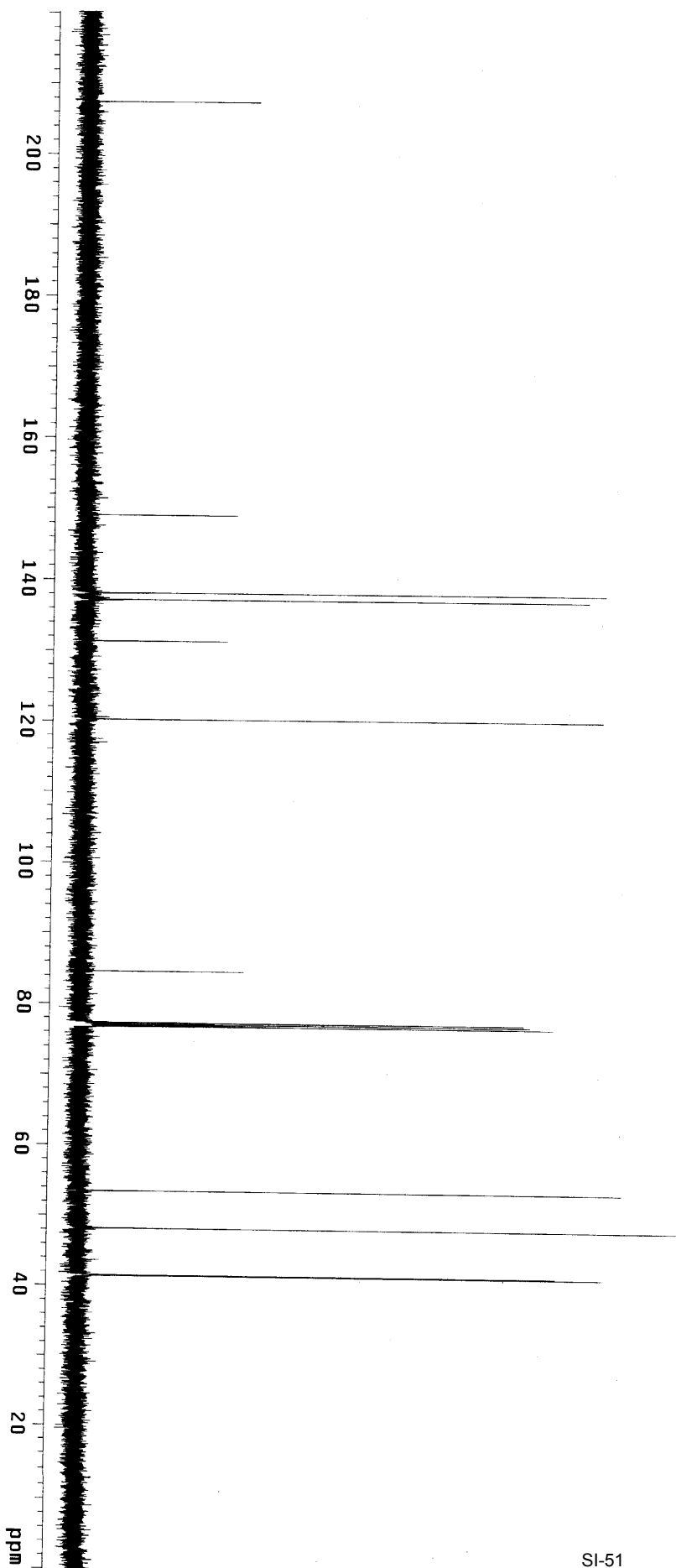
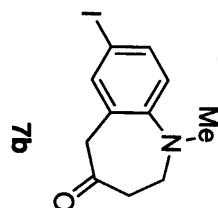
Total time 0 min, 3 sec



Automation directory: /home/waikup/vnmr500/data/auto\_2008.11.30.04  
File : /mnt/argenta/nmr500/data/zhang/yupengz/2008-12-1-C13-1.f1d  
Sample id : tmpstudy  
Sample : Diimide

Pulse Sequence: s2pul  
Solvent: cdcl3  
Temp: 25.0 C / 298.1 K  
Operator: waikup  
File: 2008-12-1-C13-1  
VNMRS-500 "nmr500"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 30487.8 Hz  
168 repetitions  
OBSERVE C13, 125.6732818 MHz  
DECOUPLE H1, 499.7964114 MHz  
Power 39 dB  
Continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 131072  
Total time 1 hr, 32 min, 22 sec



cu111-162-1-1H

Automation directory: /home/walkup/vnmrSYS/data/auto\_2008.12.04\_13

File : exp

Sample id : tmpstudy

Pulse Sequence: s2pu1

Solvent: cdc13

Temp: 25.0 C / 298.1 K

Operator: walkup

VNMRS-400 "mr400"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.049 sec

Width 6410.3 Hz

36 repetitions

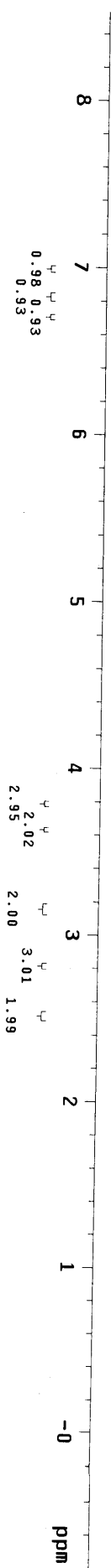
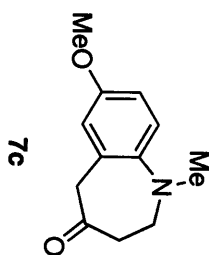
OBSERVE H1, 400.0565489 MHz

DATA PROCESSING

Resol. enhancement -0.0 Hz

FT size 65536

Total time 6 min, 31 sec



cu111-158-1-13C

Automation directory: /home/walkup/vnmrsvs/data/auto\_2008.12.05

File : exp

Sample id : tmpstudy

Pulse Sequence: s2pul

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

8000 repetitions

OBSERVE C13, 125.6732827 MHz

DECOUPLE H1, 499.7964114 MHz

Power 39 dB

continuously on

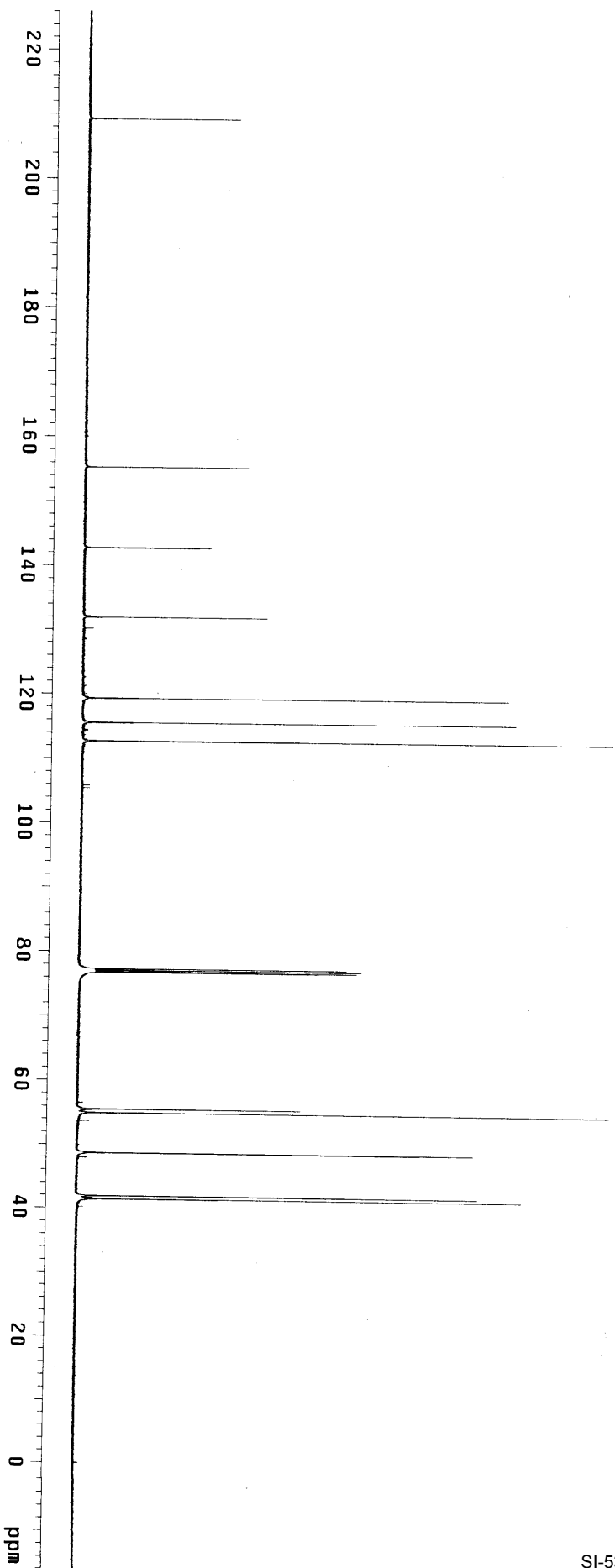
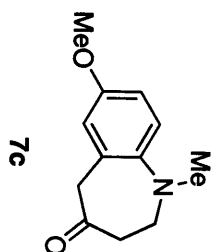
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 131072

Total time 25 hr, 39 min, 35 sec





cu111-151-1-1H

File: cu111-151-1-13C

Pulse Sequence: szpul

Solvent: cdcl3

Temp: 25.0 C / 298.1 K

Operator: walkup

File: cu111-151-1-13C

INOVA-500 "mesquite"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 30487.8 Hz

30000 repetitions

OBSERVE C13, 125.6732799 MHz

DECOUPLE H1, 499.7964114 MHz

Power 39 dB

continuously on

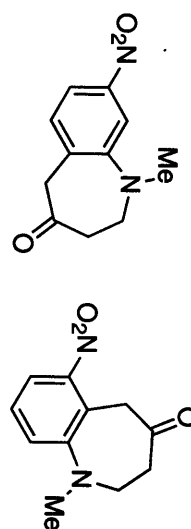
WALTZ-16 modulated

DATA PROCESSING

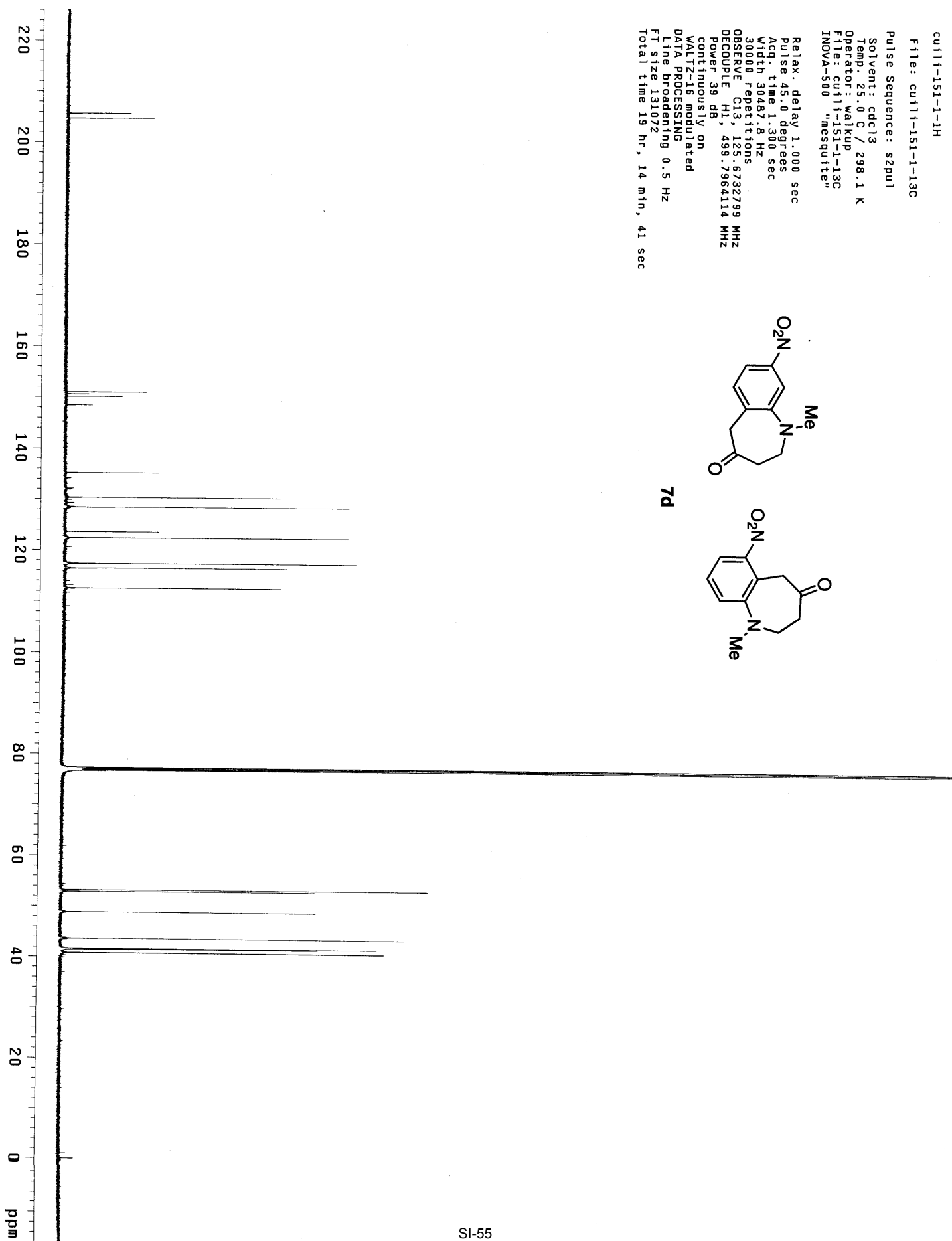
Line broadening 0.5 Hz

FT size 131072

Total time 19 hr, 14 min, 41 sec



7d



11cu1-159-1-1H

File: cu11i-159-1-1H

Pulse Sequence: szpu1

Solvent: cdcl3

Temp: 25.0 C / 298.1 K

Sample #17, Operator: 11cu1

File: cu11i-159-1-1H

INDVA-500 "mesquite"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.049 sec

Width 6410.3 Hz

8 repetitions

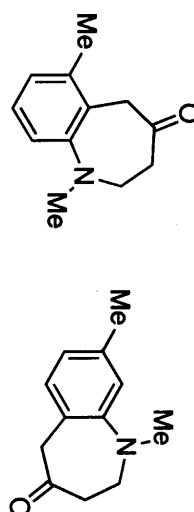
OBSERVE H1, 399.8626810 MHz

DATA PROCESSING

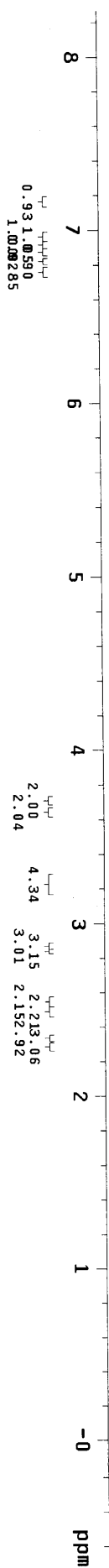
Resol. enhancement -0.0 Hz

FT size 65536

Total time 0 min, 30 sec



7e





cu11i-159-1-13C

Automation directory: /home/walkup/vnmrSYS/data/auto\_2008.12.03\_01

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

20976 repetitions

OBSERVE C13, 125.6732809 MHz

DECOUPLE H1, 499.7964114 MHz

Power 39 db

continuously on

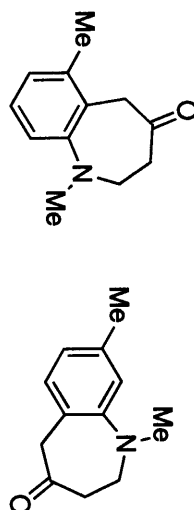
WALTZ-16 modulated

DATA PROCESSING

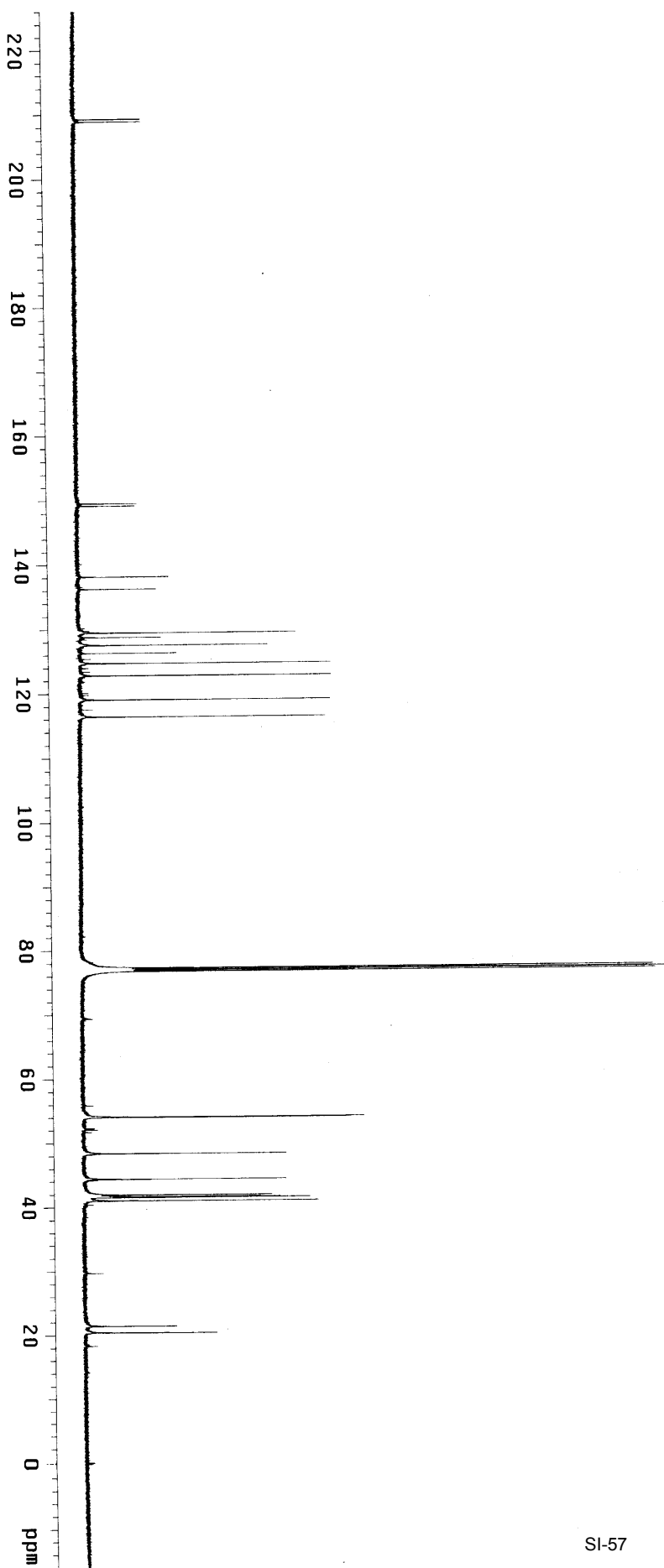
Line broadening 0.5 Hz

FT size 131072

Total time 19 hr, 14 min, 41 sec



7e



cu11i-158-1-1H

File: cu11i-158-1-1H

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: walkup

File: cu11i-158-1-1H

INOVA-500 "mesquite"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.049 sec

Width 6410.3 Hz

52 repetitions

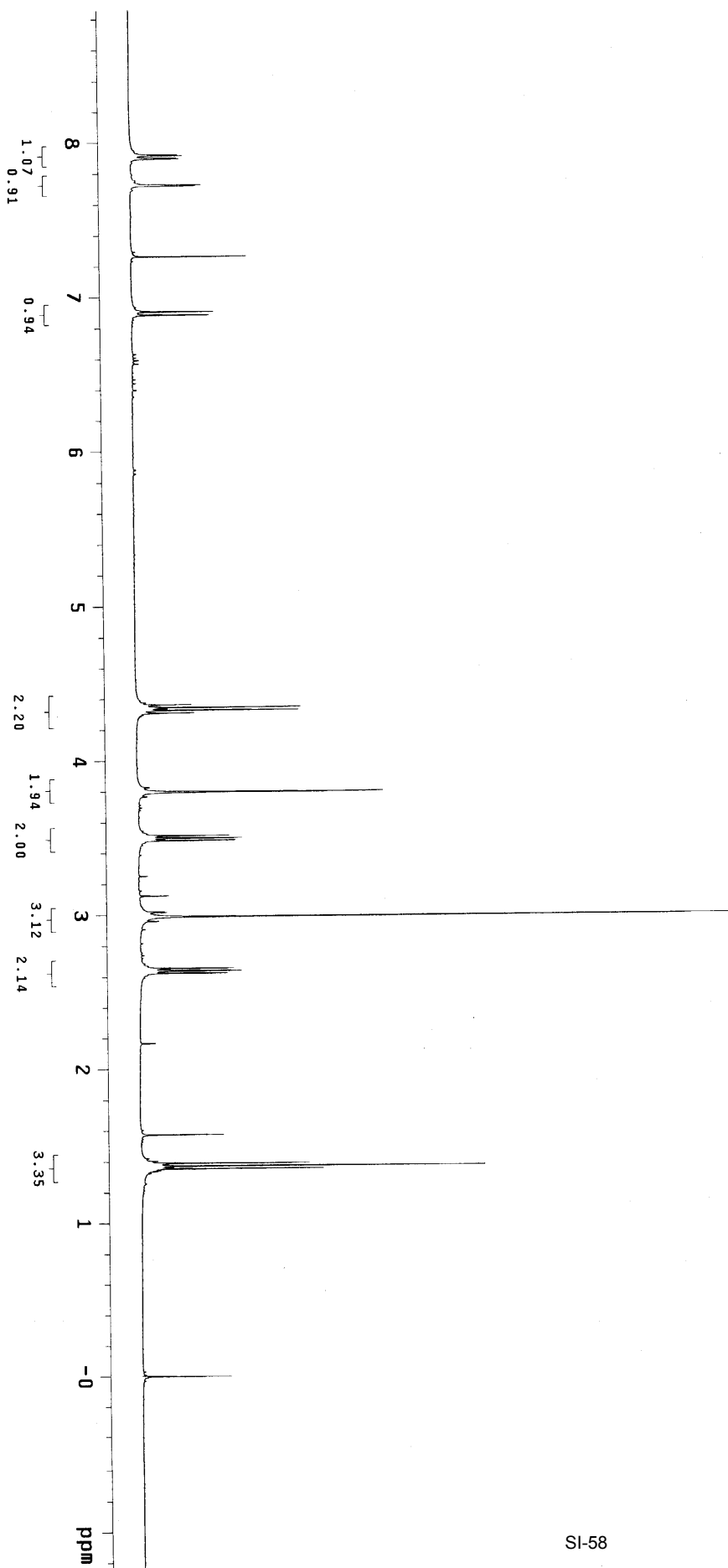
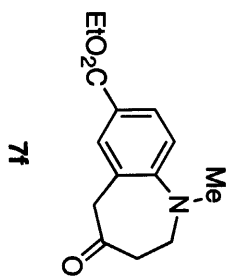
OBSERVE H1, 400.0565483 MHz

DATA PROCESSING

Resol. enhancement -0.0 Hz

FT size 65536

Total time 6 min, 31 sec



cut11-158-1-13Cb

Automation directory: /home/walkup/vnmrSYS/data/auto\_2008.12.06

File : exp

Sample id : tmpstudy

Pulse Sequence: s2pu1

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

22400 repetitions

OBSERVE C13, 125.6732804 MHz

DECOUPLE H1, 499.7964114 MHz

Power 39 dB

continuously ON

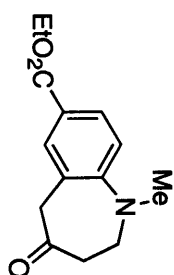
WALTZ-16 modulated

DATA PROCESSING

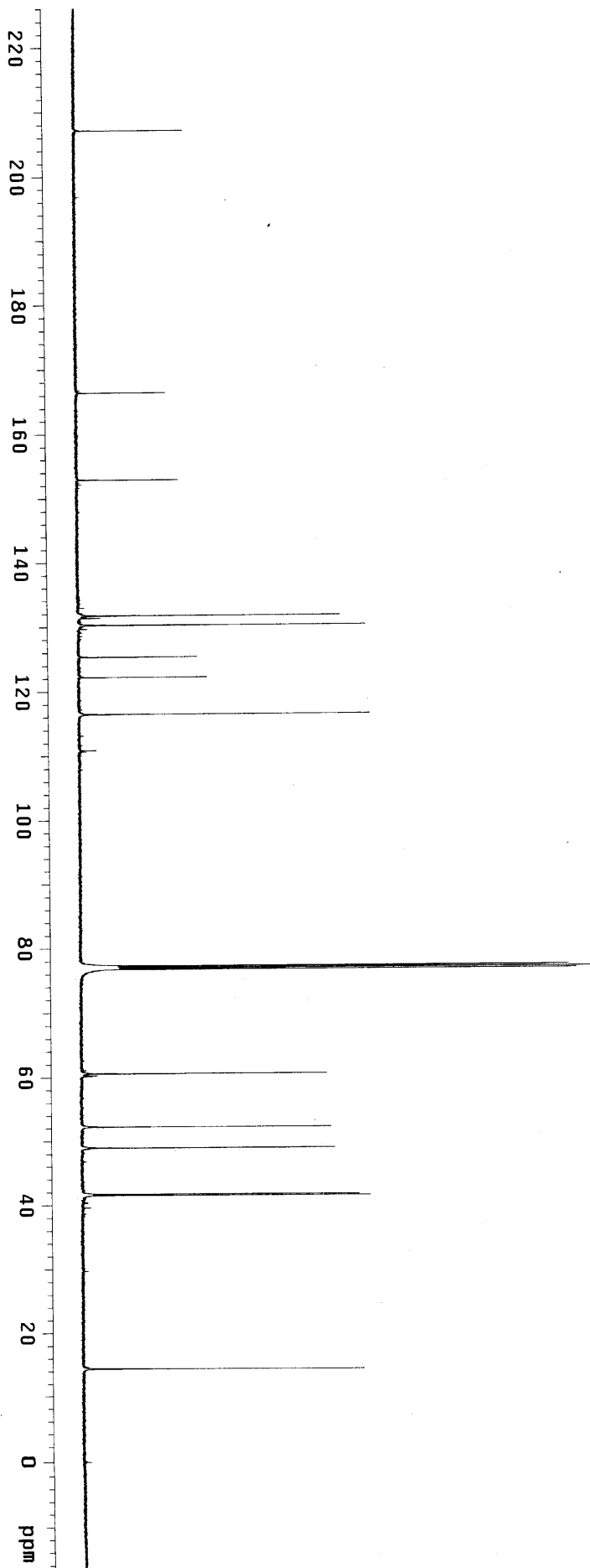
Line broadening 0.5 Hz

FT size 131072

Total time 19 hr, 14 min, 41 sec



7f



cu11f-167-1-1H

Automation directory: /home/walkup/vnmrsvs/data/auto\_2008.12.08\_10

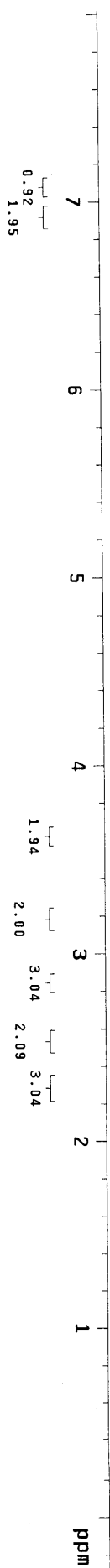
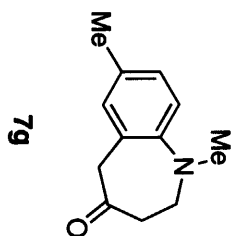
File : exp  
Sample id : tmpstudy

Pulse Sequence: s2pu1

Solvent: cdcl3  
Temp: 25.0 C / 298.1 K

Operator: walkup  
VNMRS-400 "mr400"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.049 sec  
Width 6410.3 Hz  
36 repetitions  
OBSERVE H1, 400.0565506 MHz  
DATA PROCESSING  
Resol. enhancement -0.0 Hz  
FT size 65536  
Total time 6 min, 31 sec



cu11-167-2-13C

Automation directory: /home/walkup/vnmrSYS/data/auto\_2008.12.08\_01

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

17856 repetitions

OBSERVE C13, 125.6732832 MHz

DECOUPLE H1, 499.7964114 MHz

Power 39 dB

continuously on

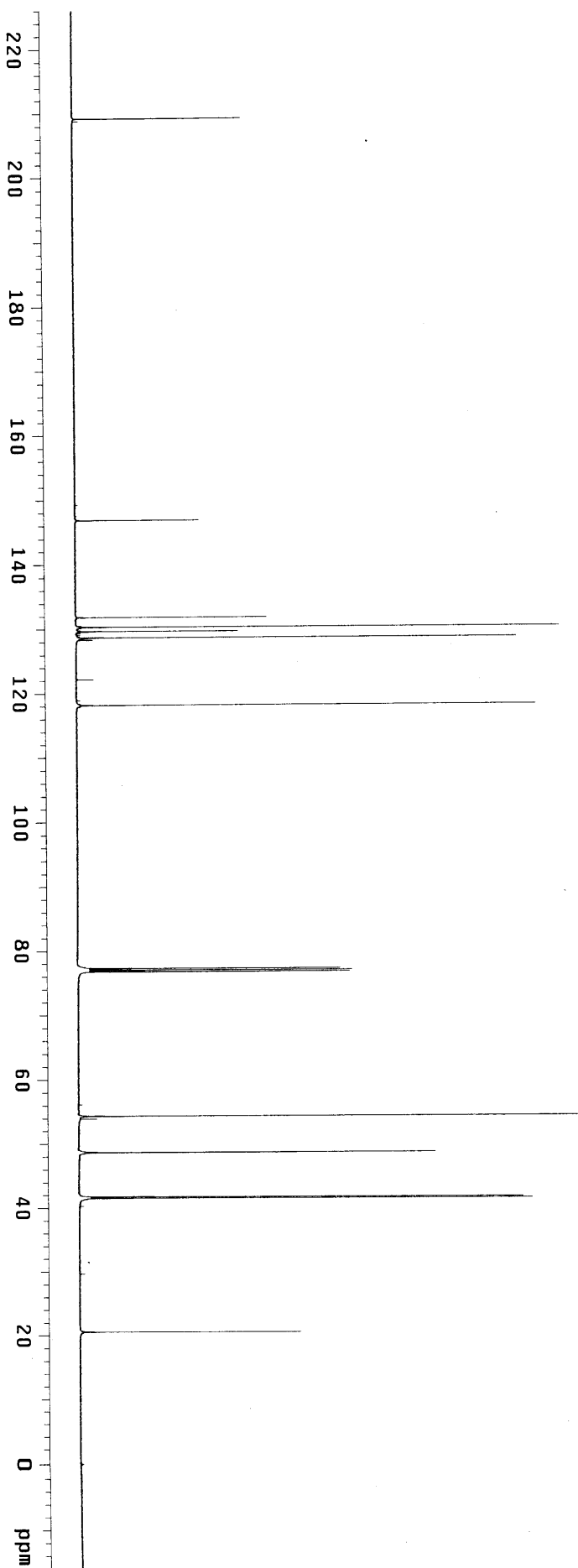
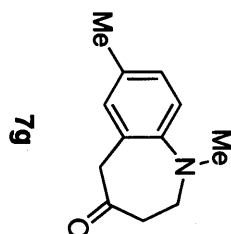
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 131072

Total time 19 hr, 14 min, 41 sec



pengyu-2008-12-9-H-3

Automation directory: /home/walkup/vnmrsvs/data/auto\_2008.12.09\_06

File : exp

Sample id : tmpstudy

Pulse Sequence: s2pul

Solvent: cdcl3

Temp: 25.0 C / 298.1 K

Operator: walkup

VNMR-400 "mr400"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.049 sec

Width 6410.3 Hz

64 repetitions

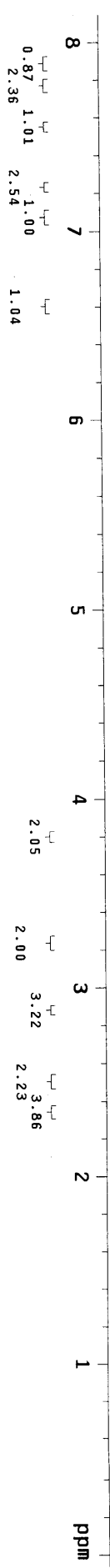
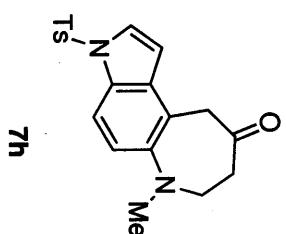
OBSERVE H1, 400.0565460 MHz

DATA PROCESSING

Resol. enhancement -0.0 Hz

FT size 65536

Total time 3 min, 15 sec



pengyu-12-10-C13-1aph

Automation directory: /home/walkup/vnmrSYS/data/auto\_2008.12.09

File: exp

Sample id: tmpstudy

Pulse Sequence: s2pul

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

5696 repetitions

OBSERVE C13, 125.6732799 MHz

DECOUPLE H1, 499.7964114 MHz

Power 39 dB

continuously on

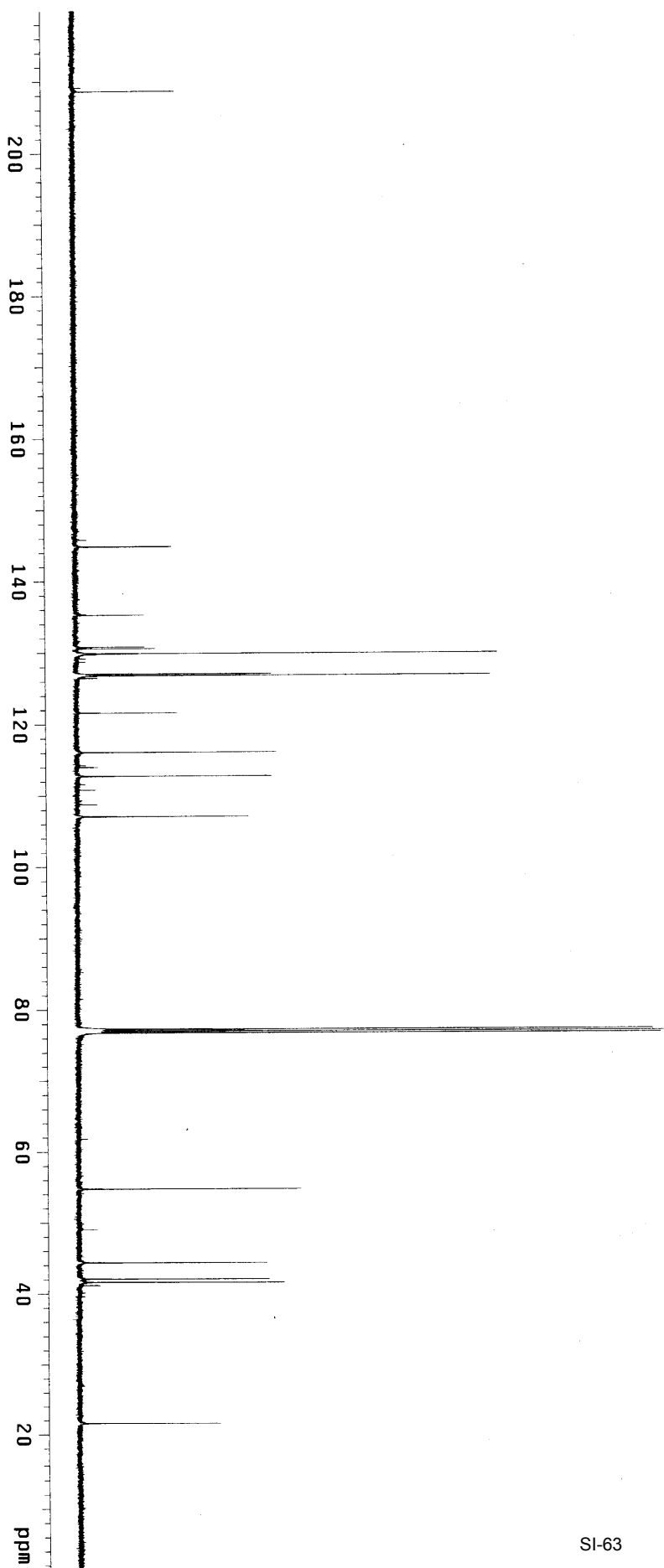
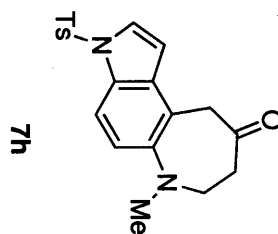
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 131072

Total time 9 hr, 14 min, 15 sec



pengyu-2008-12-9-H-1

Automation directory: /home/walkup/vnmrsvs/data/auto\_2008.12.09\_02

File : exp  
Sample id : tmpstudy

Pulse Sequence: s2pu1

Solvent: cdcl3

Temp: 25.0 C / 298.1 K

Operator: walkup  
VNMRS-400 "mr400"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.049 sec

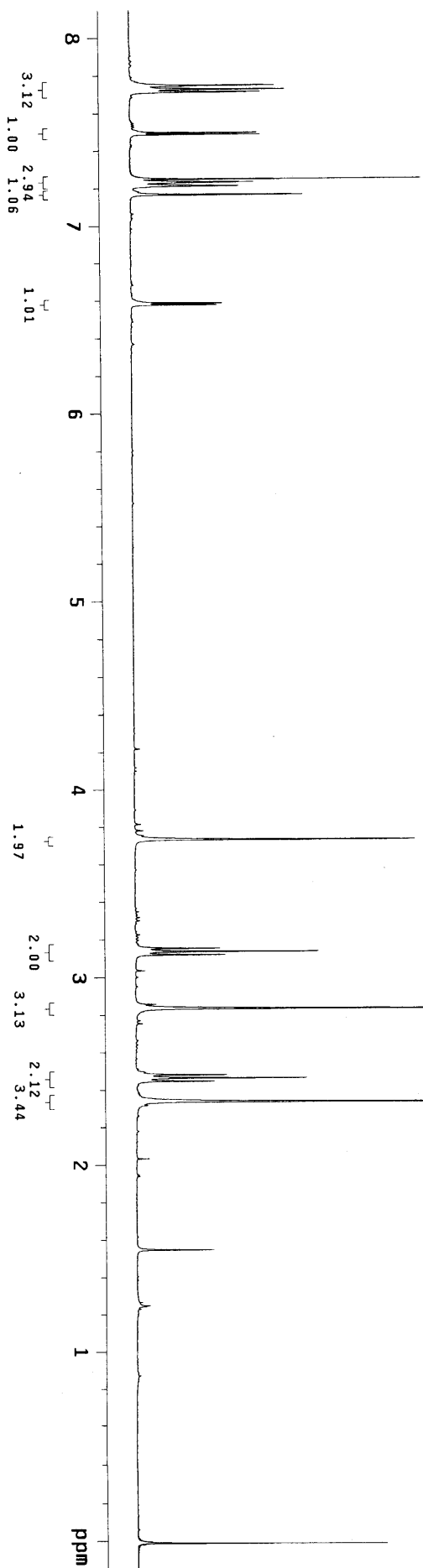
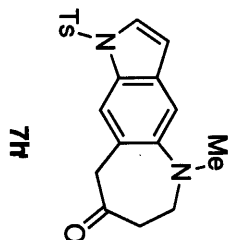
Width 6410.3 Hz

64 repetitions

OBSERVE H1, 400.0565537 MHz

DATA PROCESSING

Resol. enhancement -0.0 Hz  
F1 size 65536  
Total time 3 min, 15 sec



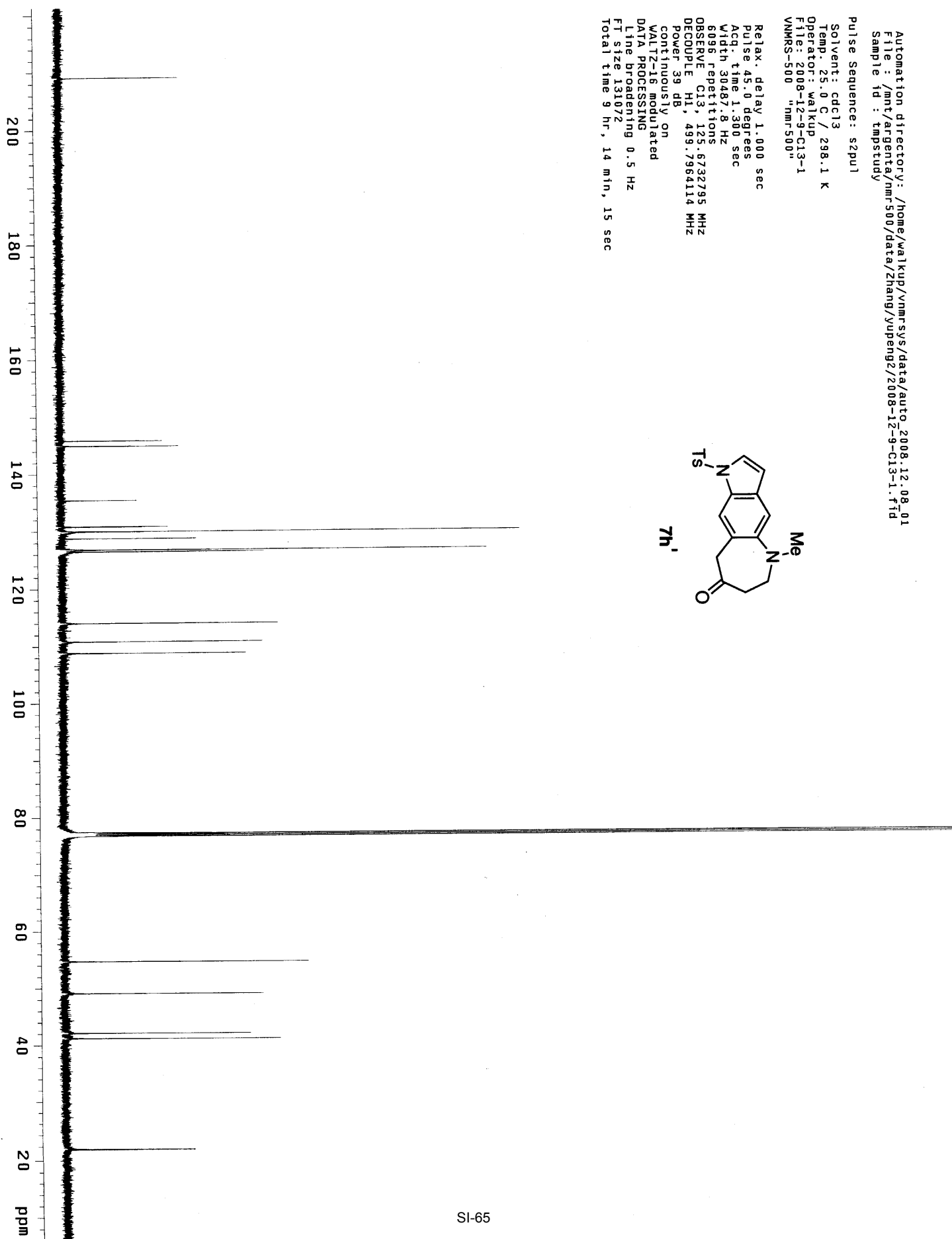
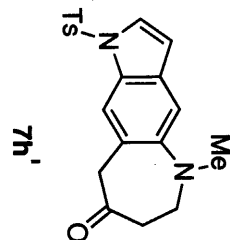


Automation directory: /home/walkup/vnmrsvs/data/auto\_2008.12.08\_01  
File: /mnt/argenta/nmr-500/data/Zhang/yupeng2/2008-12-9-C13-1.fid  
Sample id: tmpstudy

Pulse Sequence: szpul

Solvent: cdcl3  
Temp: 25.0 C / 298.1 K  
Operator: walkup  
File: 2008-12-9-C13-1  
Vnmrs-500 "nmr-500"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 30487.8 Hz  
6096 repetitions  
OBSERVE C13, 125.6732795 MHz  
DECOUPLE H1, 499.7964114 MHz  
Power 39 dB  
Continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 131072  
Total time 9 hr, 14 min, 15 sec



cu11-133-1-1H

File: cu11-133-1-1H

Pulse Sequence: szpul

Solvent: cdcl3

Temp: 25.0 C / 298.1 K

Operator: waiyup

File: cu11-133-1-1H

INOVA-500 "mesquite"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.049 sec

Width 8012.8 Hz

24 repetitions

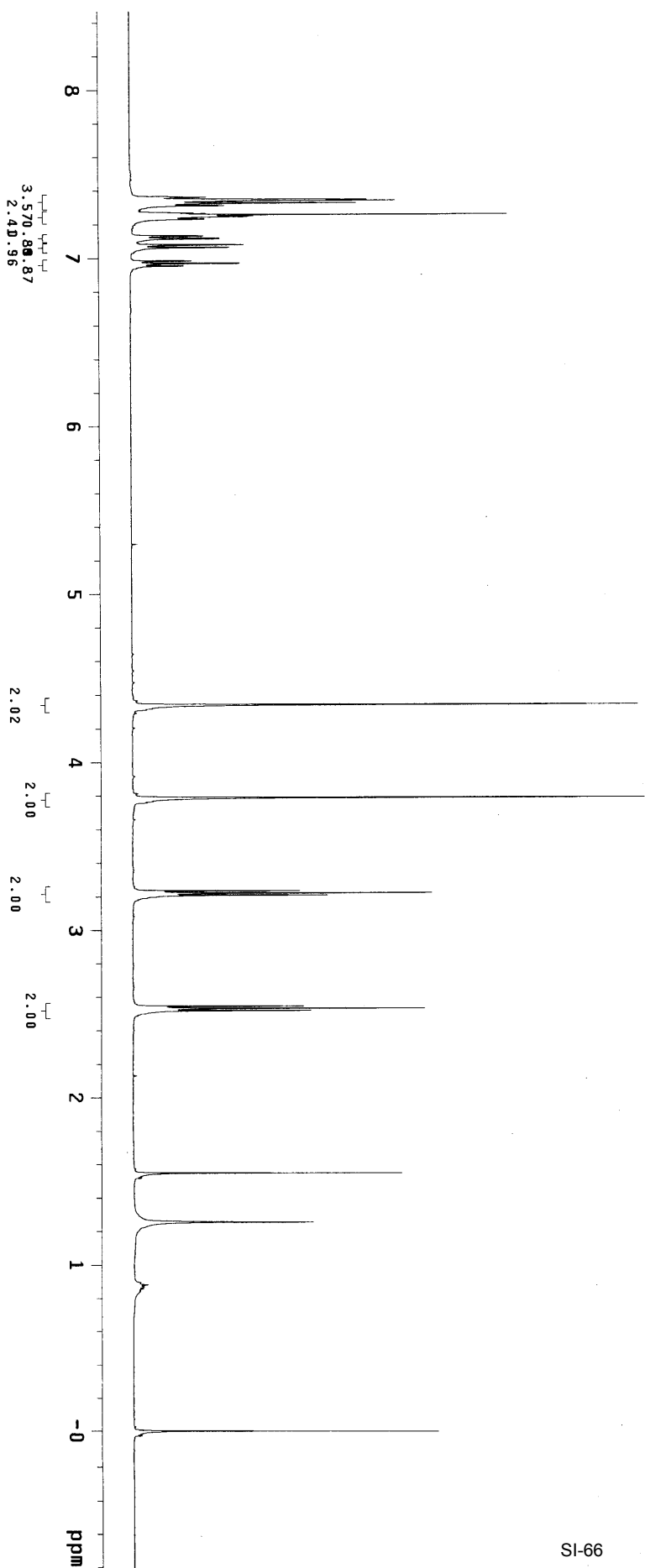
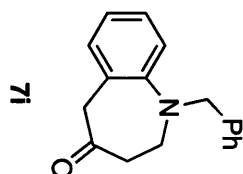
OBSERVE H1, 499.793139 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 6 min, 31 sec



cut11-133-1-13C

File: cut11-133-1-13Ca

Pulse Sequence: szpul

Solvent: cdcl3

Temp: 25.0 C / 298.1 K

Operator: walikup

File: cut11-133-1-13Ca

INOVA-500 "mesquite"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.380 sec

Width 30467.8 Hz

18560 repetitions

OBSERVE C13, 125.6732790 MHz

DECOUPLE H1, 499.7964114 MHz

Power 39 dB

continuously on

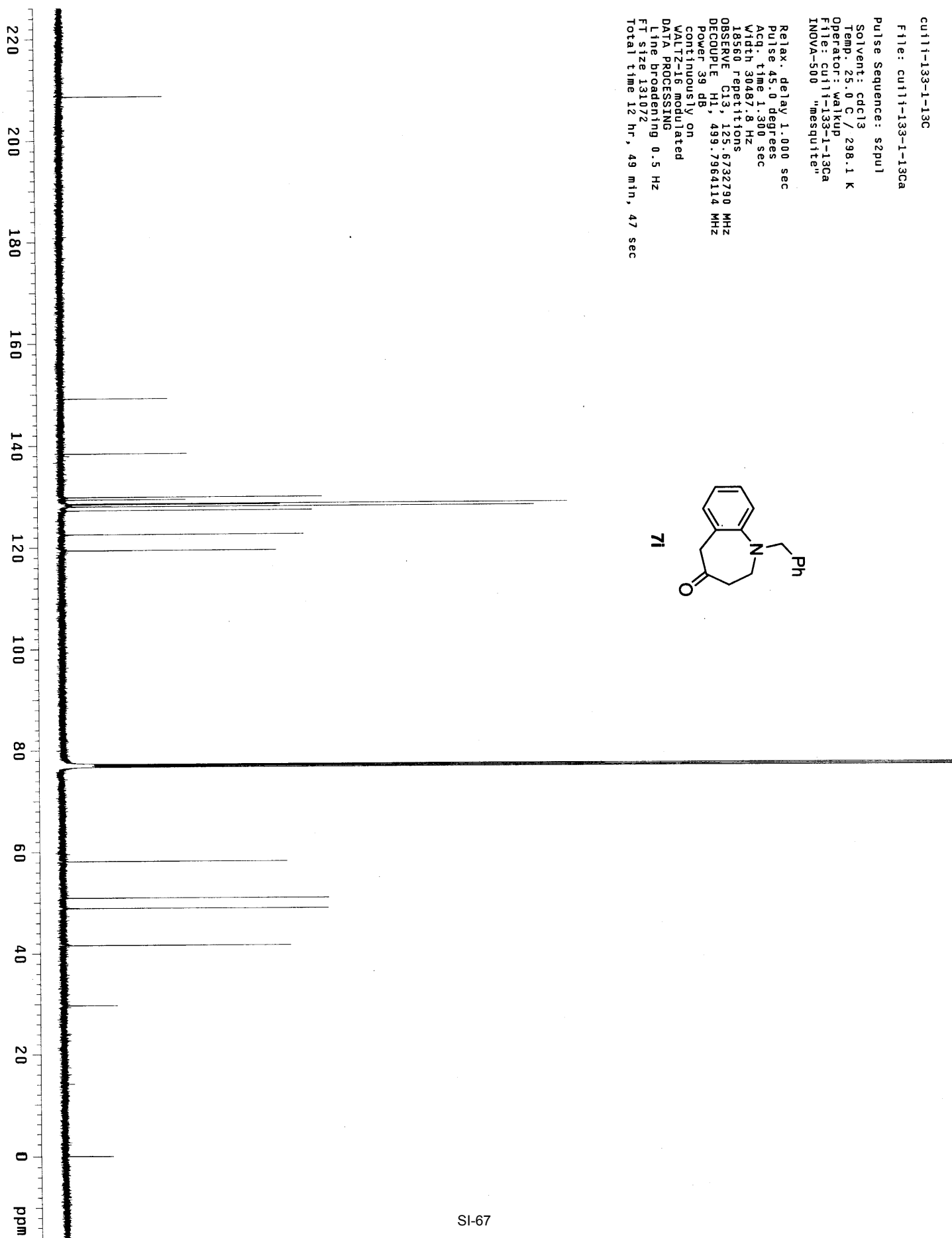
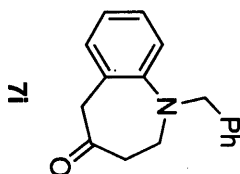
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

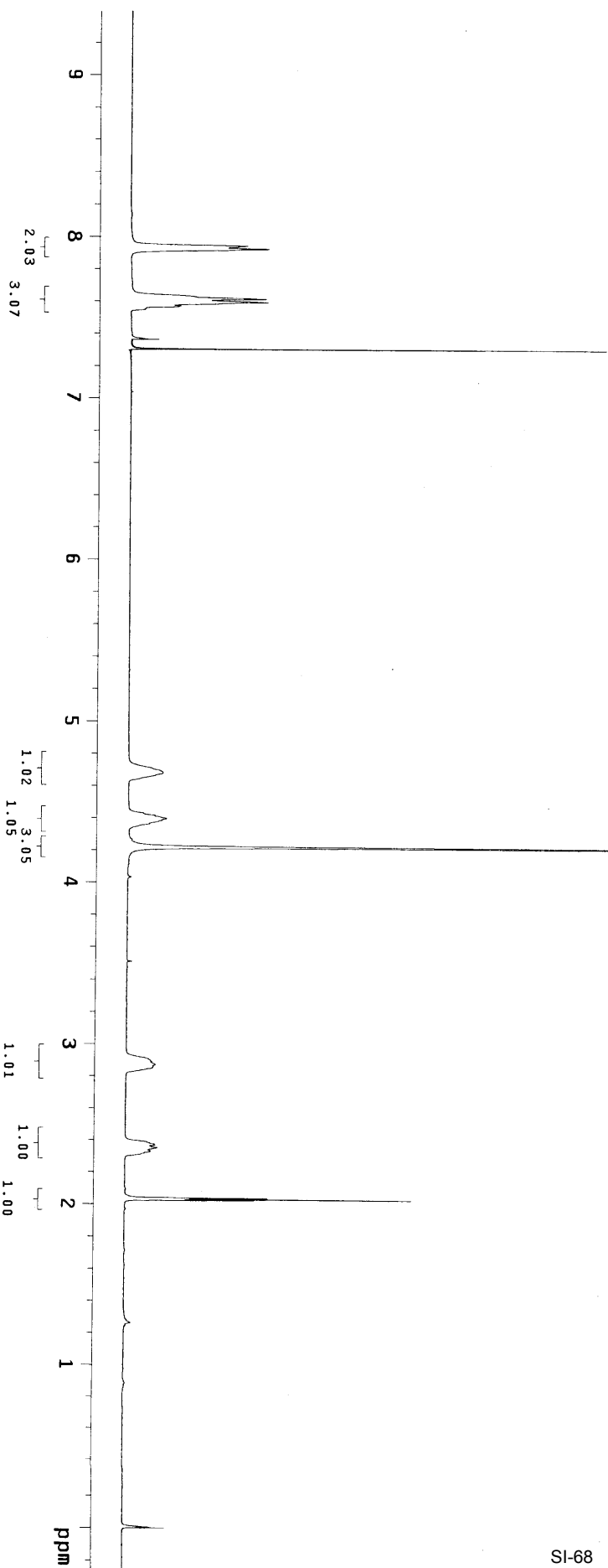
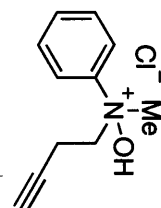
FT size 131072

Total time 12 hr, 49 min, 47 sec



expl Proton

SAMPLE SPECIAL  
date Dec 9 2008 temp 25.0  
solvent cdcl3 gain 30  
file /mnt/argenta/~ hst not used  
mr400/data/Zhang/g~ pw90 0.008  
uozhu/guozhu-20081~ 13.900  
209-2.fid alfa 6.600  
ACQUISITION  
sw 6410.3 f1  
at 2.049 f2  
np 26264 dp  
fb 4000 hs  
bs 32  
di 1.000 fn  
nt 8  
ct 8  
tn TRANSMITTER 8 SP  
sfreq 400.059 rf1  
tof 399.7 rfp  
tpwr 58 tp  
pw 6.950  
DECOUPLER WC  
dn C13 SC  
dof 0 VS  
dm nnn th  
dmm C  
dpwr 36  
dmf 29412  
ai cdc ph



expt1 Carbon

SAMPLE		SPECIAL	
date	Dec 9 2008	temp	25.0
solvent	cdcl3	gain	30
file	/mnt/argenta/~	spin	not used
nmr500/data/zhang/~	hst	0.008	
guozhu/C13-2008120~	pw90	9.600	
9-2.fid	atfa	10.000	

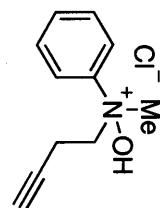
ACQUISITION		FLAGS	
sw	30487.8	11	n
at	1.300	1n	n
np	79298	dp	y
fb	17000	hs	nm
bs	12		
dl	1.000	1b	0.50
nt	12000	fn	not used
ct	5100		

TRANSMITTER		DISPLAY	
tn	C13	wp	24410.8
stfq	125.666	rfl	11757.6
tof	1255.2	rfl	9676.8
tpwr	52	rp	-146.6
pw	4.800	lp	-226.1

DECOUPLER		PLOT	
dn	H1	wc	250
dof	0	sc	0
dm	yyv	vs	54947
dmm	w	th	15
dpwr	39	at	
dmf	11900	cdc	ph



exp91 Proton

SAMPLE		SPECIAL	
date	Nov 30 2008	temp	25.0
solvent	cdcl3	gain	30
file	/mnt/argenta/~	spin	not used
mr400	/data/Zhang/g*	hst	0.008
uoznu	guoznu-20081*	py90	13.900
130-2.fid	alfa	6.600	

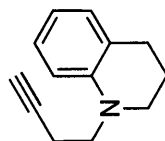
ACQUISITION		PROCESSING	
sw	6410.3	fl	n
at	2.049	in	n
np	25264	dp	y
fb	4000	hs	nn
bs	32		
dl	1.000	fn	65536
nt	8		
ct	8		

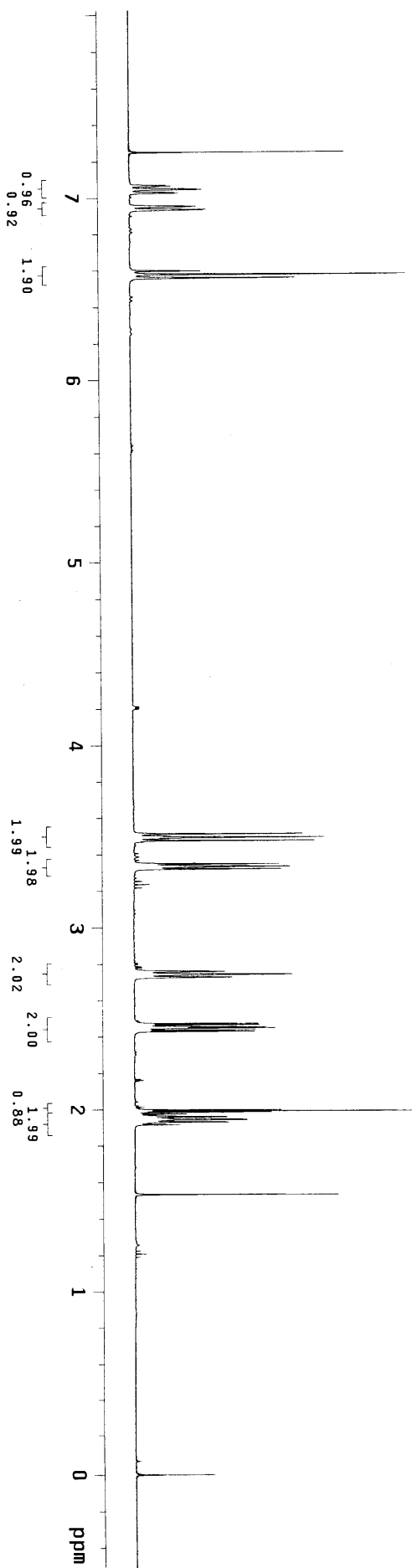
TRANSMITTER		DISPLAY	
tn	H1	sp	-210.7
stfrq	400.059	wp	3421.7
tof	399.8	rfl	804.4
tpwr	58	fp	67.0
	1p		4.3

DECOUPLER		PLOT	
dn	C13	wc	250
dof	0	sc	0
dm	nnn	th	381
dmm	c	at	3
dpwr	36		
dmf	29412		

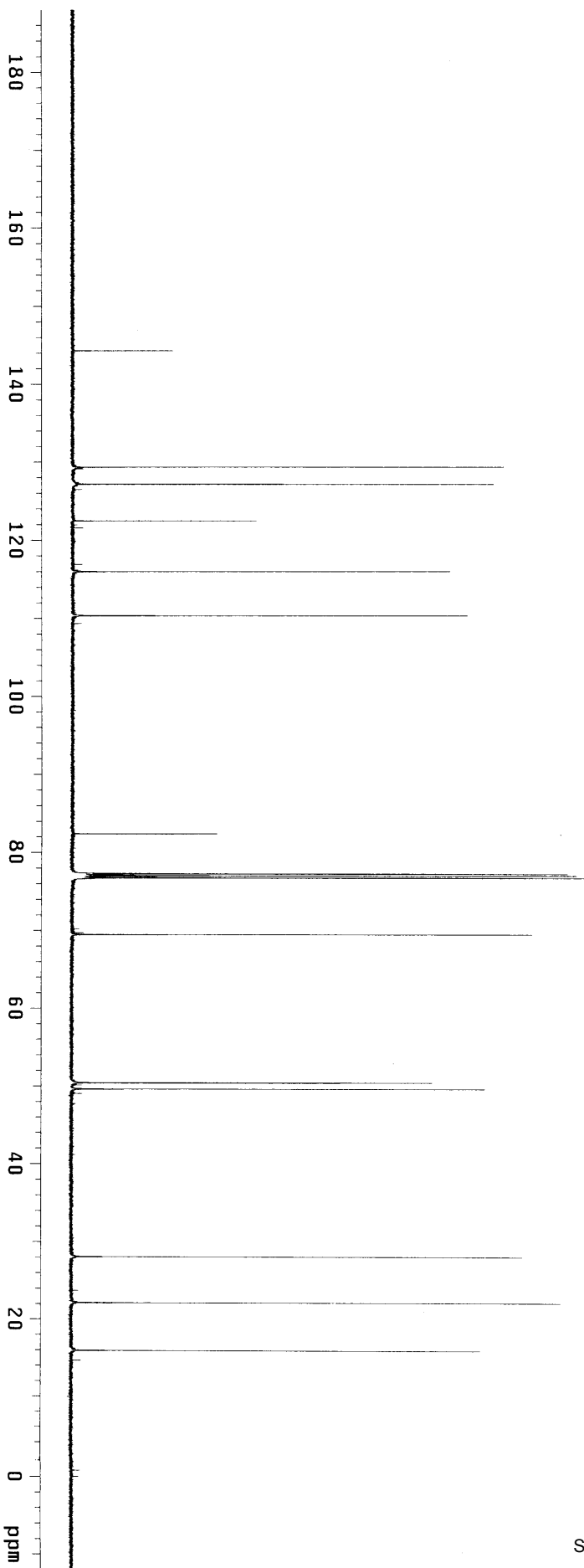
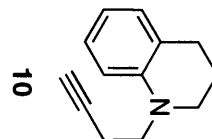


10



expt Carbon

SAMPLE			SPECIAL		
date	Dec 1 2008	temp	25.0		
solvent	cdcl3	gain	30		
file	/mnt/argenta/~	spin	not used		
nmr500/data/zhang/~	hst		0.008		
guozhu/C13-2008113-	pw90		9.500		
0-2.fid	alfa		10.000		
ACQUISITION			FLAGS		
sw	30487.8	11	n		
at	1.300	in	n		
np	79298	dp	y		
fb	17000	hs	n		
bs	12				
dl	1.000	lb	0.50		
nt	12000	fn	not used		
ct	7608				
TRANSMITTER			DISPLAY		
tn	C13	sp	-1520.7		
stfq	125.686	wp	25144.0		
tof	1255.2	rfl	11756.7		
tpwr	52	rfd	9676.8		
pw	4.800	lp	-52.1		
DECOUPLER			PLOT		
dn	H1	wc	250		
dof	0	sc	0		
dm	yyv	vs	37168		
dmm	w	th	8		
dpwr	39	at			
dmf	11900				

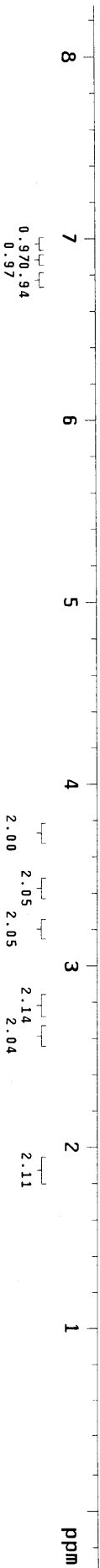
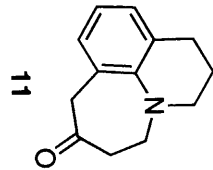


exp93 Proton

SAMPLE		SPECIAL	
date	Dec 1 2008	temp	25.0
solvent	cdcl3	gain	30
file	/mnt/argenta/~	spin	not used
mr400/data/Zhang/g	hst	0.008	
uozhu/guozhu-20081	pw90	13.900	
201-4.11d	alfa	6.600	

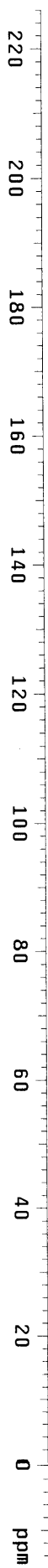
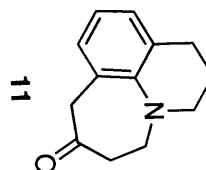
ACQUISITION		FLAGS	
sw	6410.3	11	n
at	2.049	in	n
np	25264	dp	y
fb	4000	hs	nn
bs	32		
dl	1.000	fn	65536
nt	8		
ct	8	sp	-134.2
TRANSMITTER		wp	3448.3
tn	H1	rfl	801.3
sfrq	400.059	rtp	0
tof	339.8	lp	-113.4
tpwr	58		12.5
pw	6.950	PLOT	
DECOUPLER		wc	250
dn	C13	sc	0
dof	0	vs	451
dm	nnn	th	
dmm	c	at	cdc ph
dpwr	36		
dmf	29412		





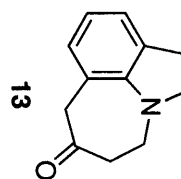
expt Carbon

SAMPLE SPECIAL  
date Dec 2 2008 temp 25.0  
solvent cdc13 gain 30  
file /mnt/argenta/~ hst not used  
nmr500/data/Zhang/~ hst 0.008  
guozhu/C13-2008120~ pw90 9.600  
1-4.fid alfa 10.000  
ACQUISITION  
sw 30487.8 i1 n  
at 1.300 tn n  
np 79298 dp y  
fb 17000 hs nn  
bs 12  
d1 1.000 lb  
nt 12000 fn  
ct 6648 not used  
TRANSMITTER C13 SP -2079.4  
tn wp 30487.3  
strq 125.686 rfp 11756.7  
tof 1255.2 rfp 9676.8  
tpwr 52 rfp -39.1  
pw 4.800 tp -256.3  
DECOUPLER H1 WC PLOT  
dn 0 SC 250  
dof 0 VS 0  
dm yyy th 46358  
dmm w 7  
dpwr 39 at cdc ph  
dmf 11900

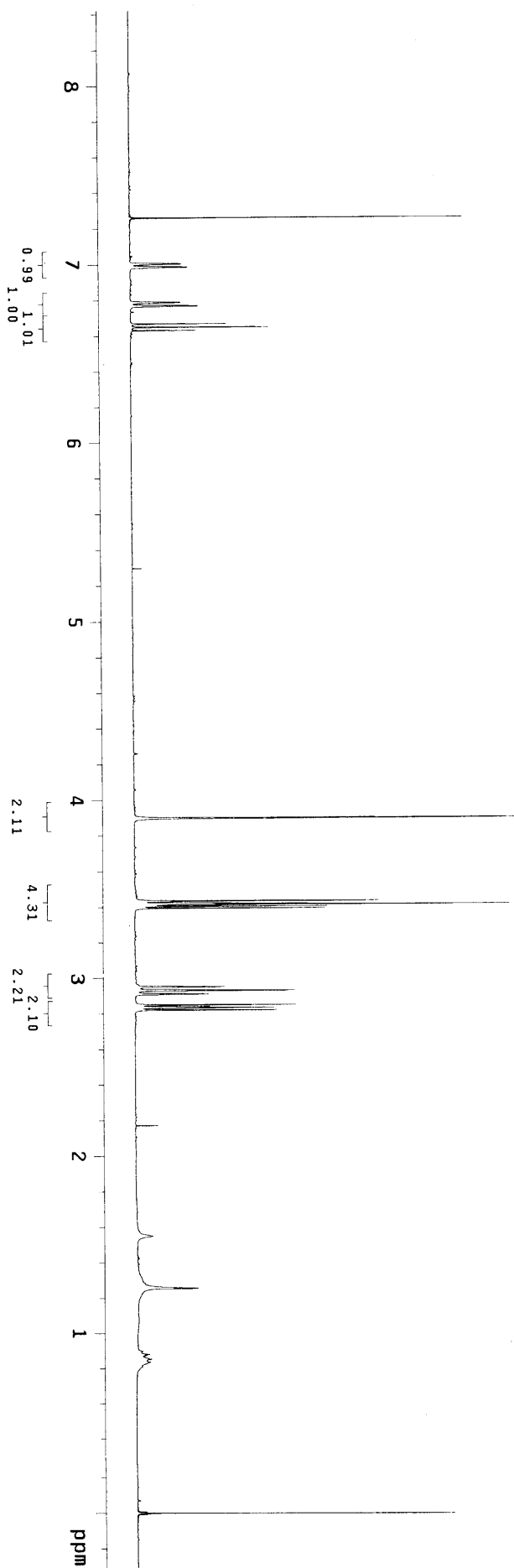


expl Proton

SAMPLE 7 2008 temp 25.0  
date Dec cdc13 gain 30  
solvent cdc13 not used  
title /mnt/argenta/~ spin 0.008  
mr400/data/2hang/g~ hst 13.900  
uozhu/guozhu-20081~ pw90 6.600  
207-1.fid alfa  
ACQUISITION  
sw 6410.3 f1  
at 2.049 in  
np 26264 dp  
fb 4000 hs  
bs 4 fn  
d1 1.000  
nt 120  
ct 120  
TRANSMITTER  
tn H1  
stfq 400.059 sp  
tof 399.8 rfp  
tpwr 58 lp  
pw 6.950  
DECOUPLER WC  
dn C13  
dof 0 vs  
dm nn th  
dmm c  
dpwr 36  
dmf 29412

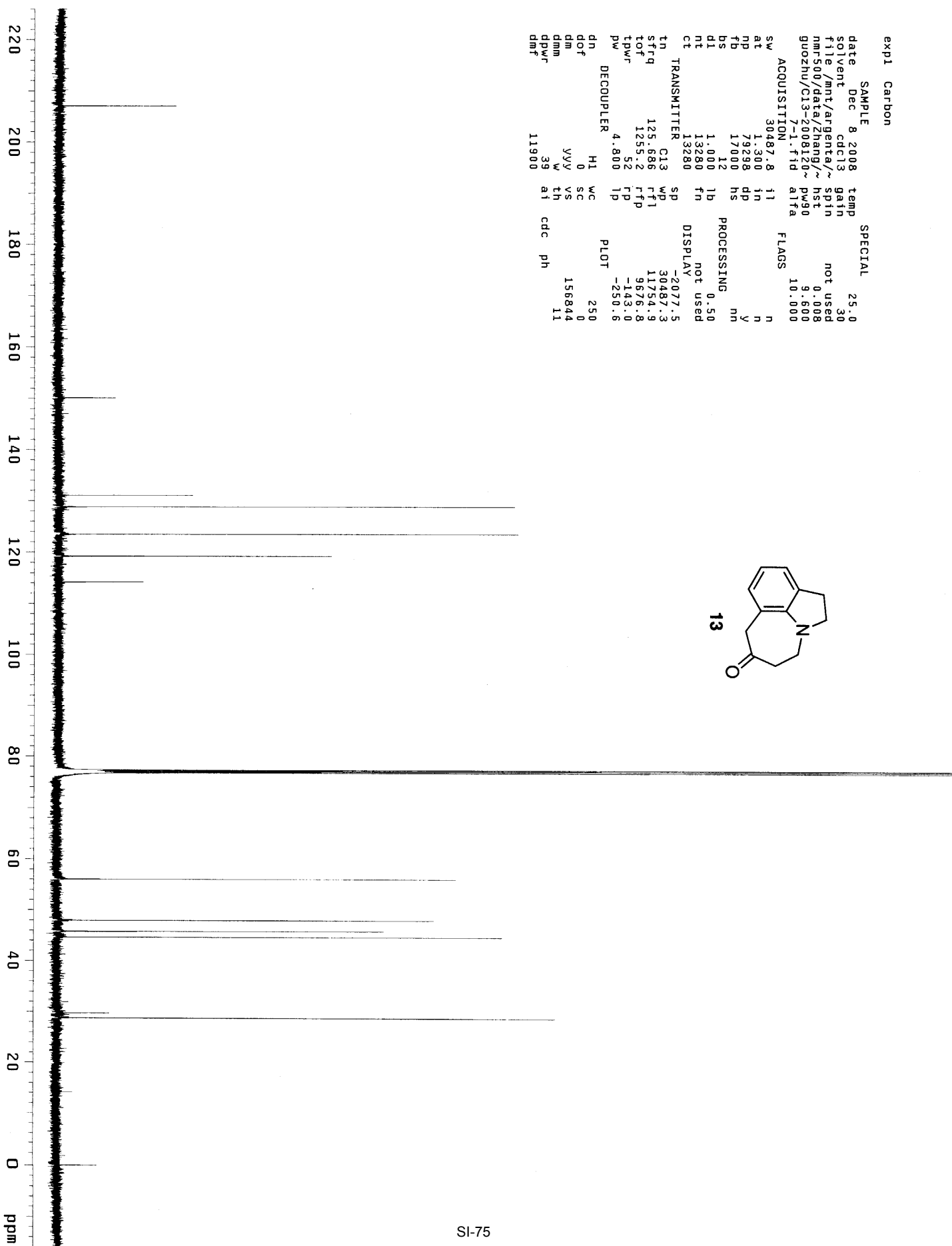
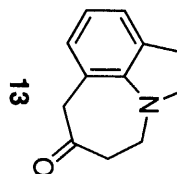


13



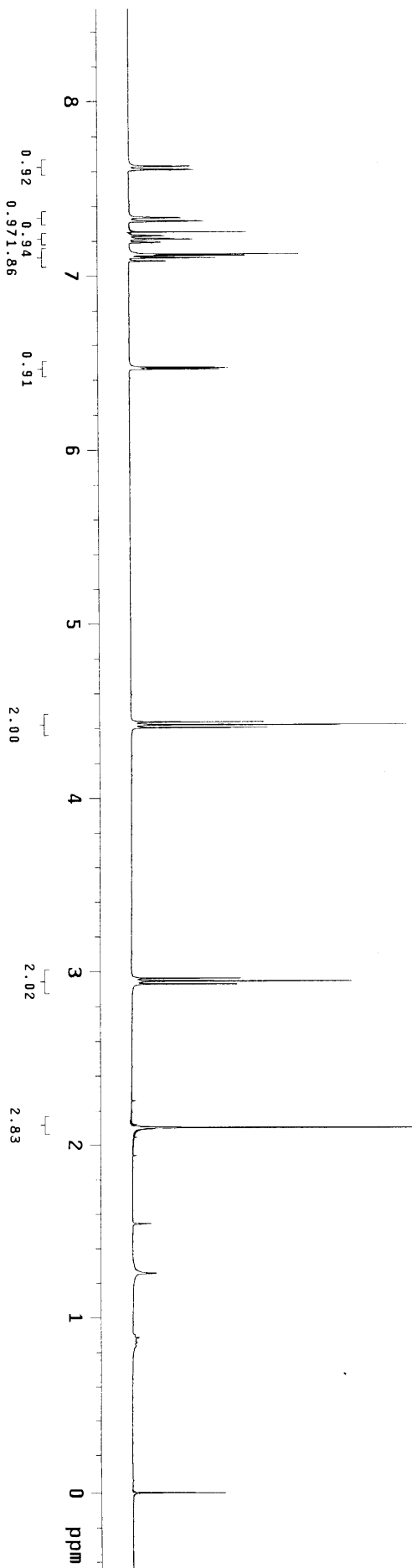
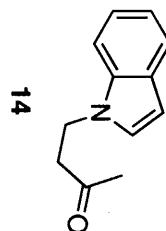
exptl Carbon

SAMPLE			SPECIAL		
date	Dec 8 2008	temp	25.0		
solvent	cdcl3	gain	30		
file	/mnt/argenta/~	spin	not used		
nmr500/data/Zhang/~	hst	0.008			
guozhu/c13-2008120~	pw90	9.600			
7-1.fid	atfa	10.000			
ACQUISITION			FLAGS		
sw	30487.8	i1	n		
at	1.300	in	n		
np	79298	dp	y		
fb	17000	hs	nn		
bs	12				
dl	1.000	lb			
nt	13280	fn	not used		
ct	13280	sp	DISPLAY		
TRANSMITTER			PLOT		
tn	C13	wp	-2077.5		
sfrq	125.686	rfl	30487.3		
tof	1255.2	rfl	11754.9		
tpwr	52	rp	9676.8		
pw	4.800	lp	-143.0		
DECOUPLER			PLOT		
dn	H1	wc	250		
dof	0	sc	0		
dm	yyy	vs	156844		
dmm	w	th	11		
dpwr	39	at			
dmf	11900	cdc	ph		



expi Proton

SAMPLE			SPECIAL		
date	Dec	7 2008	temp	25.0	
solvent	cdcl3	gain	30		
file	/mnt/argenta/~	spin	not used		
mr400/data/2hang/g~	hst	0.008			
nozhu/guozhu-20081~	pv90	13.900			
207-3.fid	alfa	6.600			
ACQUISITION			FLAGS		
sw	6410.3	il	n		
at	2.049	in	n		
np	26264	dp	y		
fb	4000	hs	nn		
bs	32				
d1	1.000	fn	65536		
nt	8				
ct	8	sp	-180.2		
TRANSMITTER			DISPLAY		
tn	H1	wd	3593.8		
sfreq	400.059	rfl	803.8		
tof	399.8	rtp	-35.6		
tpwr	58	lp	28.4		
pw	6.950				
DECOUPLER			PLOT		
dn	C13	wc	250		
dof	0	vs	0		
dm	nnn	th	260		
dmm	c	ai	2		
dpwr	36				
dmt	29412				



expl Carbon

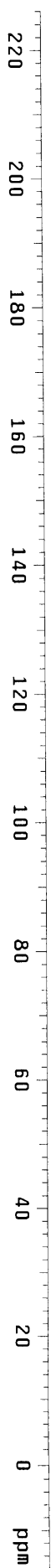
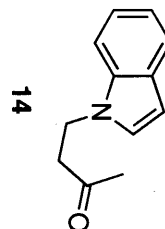
SAMPLE Dec 14 2008 temp 25.0  
date  
solvent cdc13 gain 30  
file /mnt/argenta/~ spin not used  
nmr500/data/2hang/~ hst 0.008  
guozhu/C13-2008120~ pw90 9.500  
7-3.fid alfa 10.000

ACQUISITION  
sw 30487.8 f1 11 n  
at 1.300 in n  
np 79298 dp y  
fb 17000 hs nn  
bs 12  
d1 1.000 fb 0.50  
nt 12000 fn not used  
ct 1464

TRANSMITTER  
tn C13 sp -2079.4  
stfq 125.686 rfi 30487.3  
tof 1255.2 rfp 11756.7  
tpwr 52 rfp 9676.8  
pw 4.800 ip 132.8  
-299.2

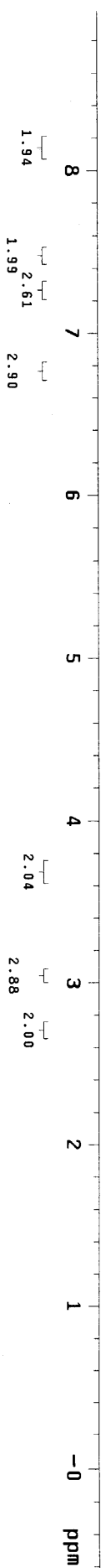
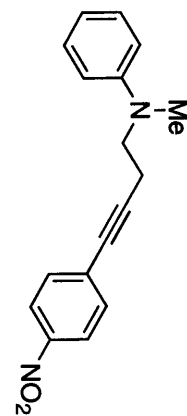
DECOUPLER  
dn H1 wc 250  
dof 0 sc 0  
dm yyv vs 52948  
dmm w th 8  
dpwr 39 ai cdc ph  
dmf 11900

PROCESSING 0.50  
DISPLAY not used



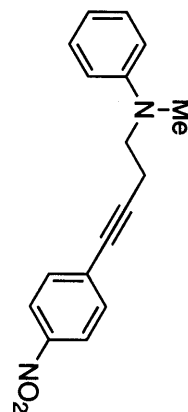
expt Proton

SAMPLE		SPECIAL	
date	Nov 18 2008	temp	25.0
solvent	cdcl3	gain	30
file	/mnt/argenta/~	spin	not used
mr400/data/Zhang/g*	hst	0.008	
wozhu/guozhu-20081~	pw90	13.900	
118-2.fid	atfa	6.600	
ACQUISITION			
sw	6410.3	f1	n
at	2.049	in	n
np	26264	dp	y
fb	4000	hs	nn
bs	4	fn	65536
dl	1.000	DISPLAY	-255.5
nt	8	SP	3849.7
ct	8	WD	800.9
TRANSMITTER			
tn	H1	rfl	0
strq	400.059	rtp	92.2
tof	399.8	tp	11.7
tpwr	58	WC	250
pw	6.950	SC	0
DECOUPLER			
dn	C13	VS	1317
dof	0	th	5
dm	nmn	at	cdc
dmm	c	ph	
dpwr	36		
dmf	29412		



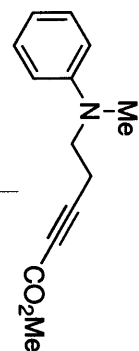
exp2 Carbon

SAMPLE SPECIAL  
date Nov 27 2008 temp 25.0  
solvent cdcl3 gain 30  
file /mnt/argenta/~ not used  
nmr500/data/Zhang/~ hst 0.008  
guozhu/C13-200811~ pw90 9.600  
8-2.fid alfa 10.000  
ACQUISITION FLAGS  
sw 30487.8 11 n  
at 1.300 11 n  
np 79298 dp y  
fb 17000 hs nn  
bs 12  
di 1.000 1b not used  
nt 12000 fn 0.50  
ct 4284 DISPLAY  
tn C13 SP -369.8  
stfq 125.686 rfi 21927.5  
tof 1255.2 rfp 11755.3  
tpwr 52 rp 9676.8  
pw 4.800 1p -53.1  
DECOUPLER H1 WC PLOT -236.3  
dn 0 SC 250  
dof 0 SC 0  
dm 0 SC 0  
dmm YVY VS 92209  
dpwr W th 7  
dmf 11900 ai cdc ph

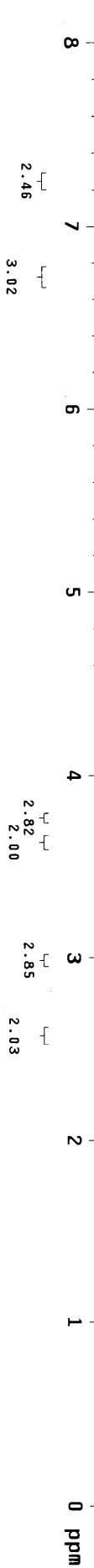


expt1 Proton

SAMPLE SPECIAL  
date Nov 16 2008 temp 25.0  
solvent cdcl3 gain 30  
file /mnt/argenta/~ spin not used  
mr400/data/Zhang/g~ hst 0.008  
uozhu/guozhu-20081~ pw90 13.900  
116-3.fid alfa 6.600  
ACQUISITION  
sw 6410.3 11 n  
at 2.049 1n n  
np 26264 dp y  
fb 4000 hs nn  
bs 32  
d1 1.000 fn 65536  
nt 1  
ct 1  
TRANSMITTER 1 SD  
tn H1 WP -146.9  
stfq 400.059 rfp 3419.9  
tof 399.8 rfp 801.5  
tpwr 58 1p -176.8  
pw 6.950 PLOT 12.6  
DECOUPLER WC 250  
dn C13 SC 0  
dof 0 VS 351  
dm nnm th 3  
dmm C at cdc ph  
dpwr 36  
dmf 29412



15a





expt Carbon

SAMPLE		SPECIAL	
date	Nov 17 2008	temp	25.0
solvent	cdcl3	gain	30
file	/mnt/argenta/~	spin	not used
nmr500/data/Zhang/~	hst	0.008	
guozhu/C13-200811~	pw90	9.600	
7-2.fid	atfa	10.000	

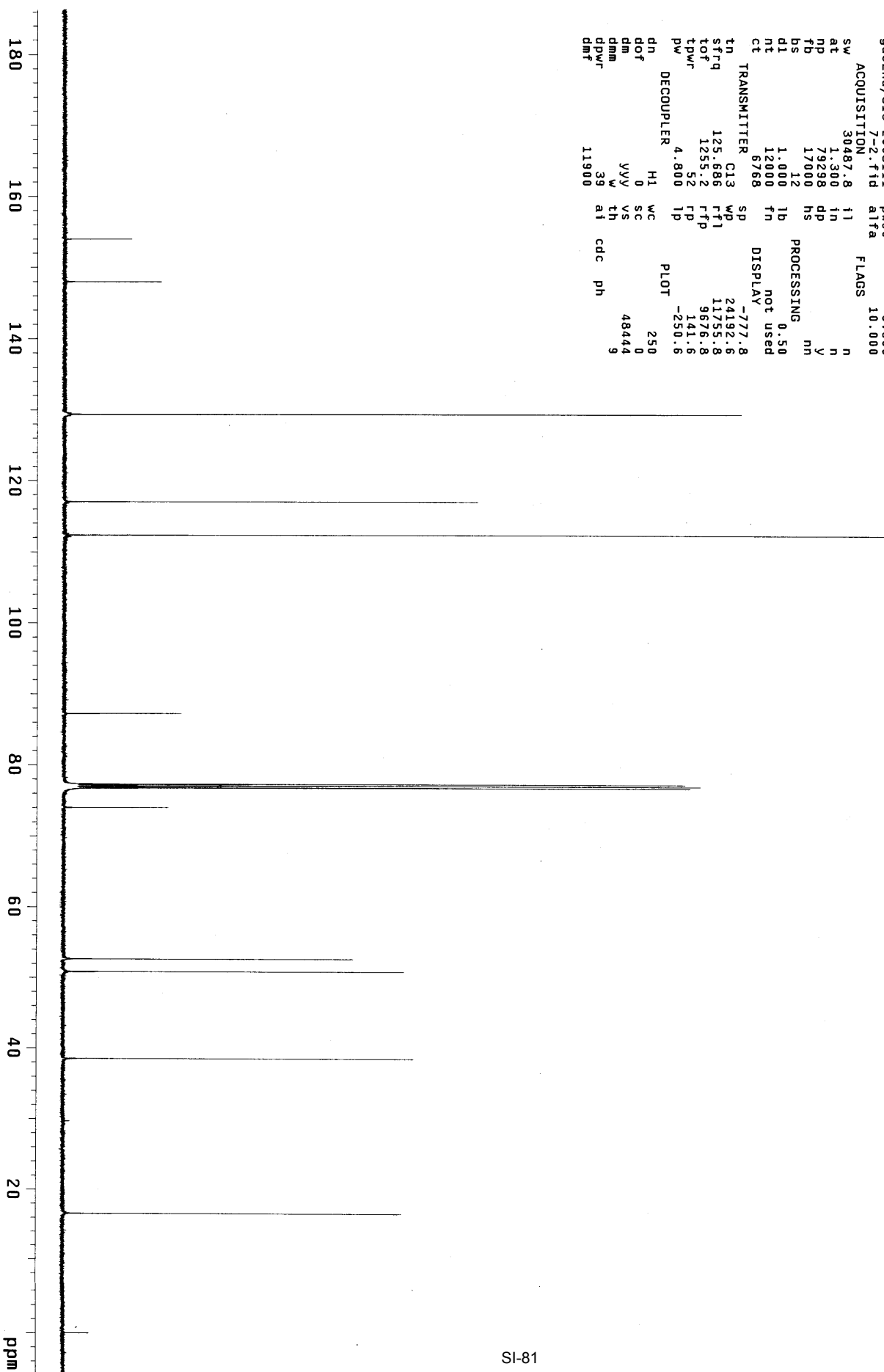
ACQUISITION		FLAGS	
sw	30467.8	i1	n
at	1.300	in	y
np	79298	dp	n
fb	17000	hs	nn
bs	12		
d1	1.000	lb	0.50
nt	12000	fn	not used
ct	6768	td	not used

TRANSMITTER		DISPLAY	
tn	C13	wd	-777.8
strq	125.686	rfl	24192.6
tof	1255.2	rfl	11755.8
tpwr	52	fp	9676.8
pw	4.800	lp	141.6
			-250.6

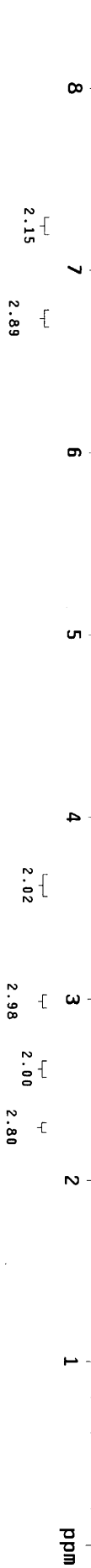
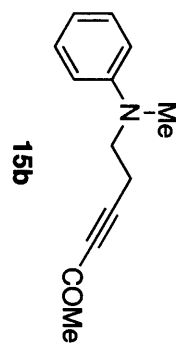
  

DECOUPLER		PLOT	
dn	H1	wc	250
dof	0	sc	0
dm	yyv	vs	48444
dmm	w	th	9
dpwr	39	at	cdc
dmt	11900		ph



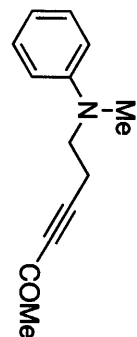
expt Proton

SAMPLE SPECIAL  
date Nov 25 2008 temp 25.0  
solvent cdc13 gain 30  
file /mnt/argenta/~ spin not used  
mr400/data/zhang/g~ hst 0.008  
nozhu/guozhu-20081~ pw90 13.900  
125-1.fid alfa 6.600  
ACQUISITION FLAGS  
sw 6410.3 11 n  
at 2.049 1n n  
np 26264 dp y  
fb 4000 hs nn  
bs 32  
di 1.000 fn  
nt 8  
ct 8  
TRANSMITTER 8 SP -60.6  
tn H1 rf1 3435.0  
strq 400.059 rfp 801.1  
tof 399.8 rfp -114.8  
tpwr 58 1p 4.3  
pw 6.950  
DECOUPLER WC 250  
dn C13 SC 0  
dof 0 VS 170  
dm nnn th 2  
dmm C at cdc ph  
dpwr 36  
dmf 29412



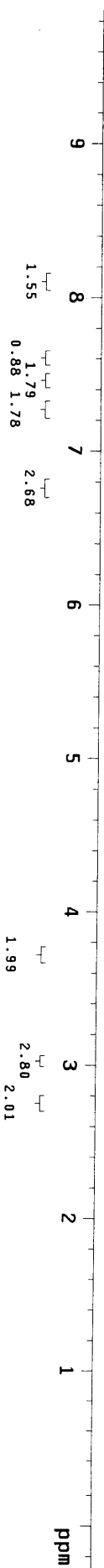
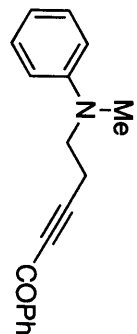
exp2 Carbon

SAMPLE SPECIAL  
date Nov 27 2008 temp 25.0  
solvent cdc13 gain 30  
file /mnt/argenta/~ spin not used  
nmr500/data/Zhang/~ hst 0.008  
guozhu/C13-2008112~ pw90 9.600  
5-1.fid a1fa 10.000  
ACQUISITION FLAGS  
sw 30487.8 11 n  
at 1.300 1n n  
np 79298 dp y  
fb 17000 hs nn  
bs 12  
d1 1.000 1b  
nt 12000 fn not used  
ct 2196 DISPLAY -682.9  
TRANSMITTER C13 SP WP 28426.5  
sfreq 125.686 rf1 11756.7  
tof 1255.2 rfp 9676.8  
tpwr 52 rfp -49.5  
pw 4.800 1p -241.5  
DECOUPLER H1 WC PLOT  
dn H1 WC 250  
dof 0 SC 0  
dm VVY VS 51596  
dmm W th 11  
dpwr 39 at cdc ph  
dmf 11900

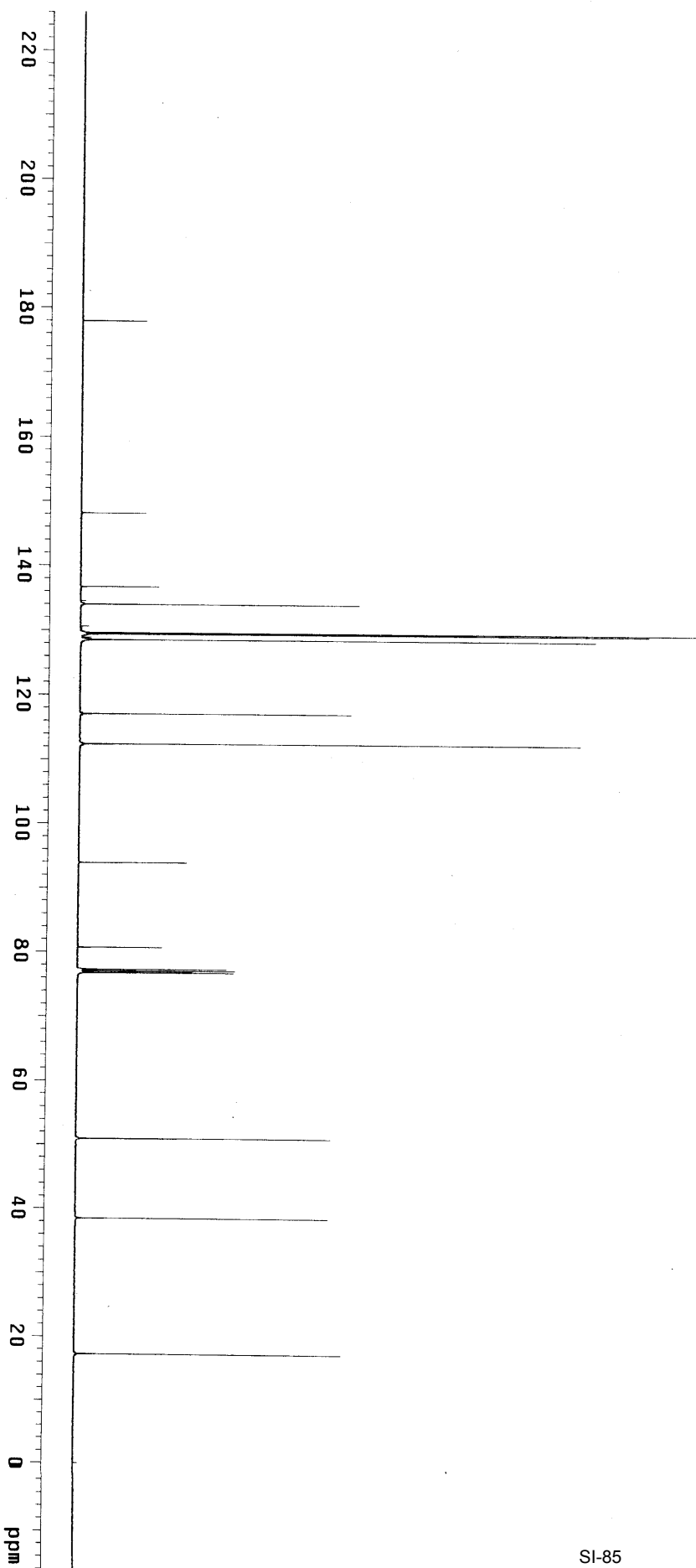
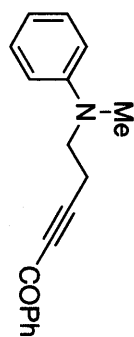


exp12 Proton

SAMPLE		SPECIAL	
date	Nov 23 2008	temp	25.0
solvent	cdcl3	gain	not used
file	/home/walkup/~	spin	not used
vmr/sys	/data/auto/~	hst	0.008
2008.11.23/guozhu/~		pw90	13.700
Guozhu-20081123-5-~		ai fa	10.000
1/Proton01.fid		FLAGS	
ACQUISITION			
sw	6410.3	in	n
at	2.049	dp	y
np	26264	hs	nn
fb	4000		
bs	32	fn	65536
ss	2		
dl	1.000	sp	-122.5
nt	8	wp	4070.2
ct	8	rf1	804.2
TRANSMITTER		rfp	105.2
tn	H1	tp	5.6
strq	399.865	ip	
tof	399.9		
tpwr	60	WC	250
pw	6.850	vs	0
DECOUPLER		th	261
dn	C13	at	cdc
dof	0	ph	3
dm	nmn		
dmm	c		
dpwr	33		
dmf	29412		



Automation directory: /home/walkup/vnmr5ys/data/auto\_2008.11.23\_04  
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  
4416 repetitions  
OBSERVE C13, 125.6732869 MHz  
DECOUPLE H1, 499.7964114 MHz  
Power 39 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 131072  
Total time 7 hr, 41 min, 52 sec



pengyu-2008-12-9-H-4

expi Proton

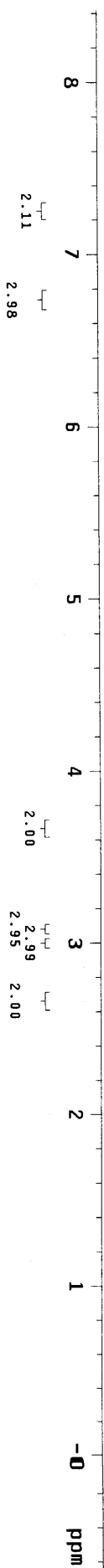
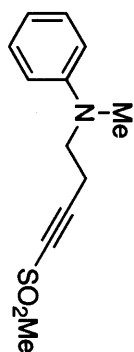
SAMPLE		SPECIAL	
date	Dec 9 2008	temp	25.0
solvent	cdcl3	gain	30
file	/mnt/argenta/~	spin	not used
mr400/data/zhang/g	hst	0.008	
uozhu/guozhu-20081	pw90	13.900	
209-1.fid	alpha	6.600	

ACQUISITION		FLAGS	
sw	6410.3	11	n
at	2.049	in	n
np	26264	dp	y
fb	4000	hs	nn
bs	32		
dl	1.000	fn	65536
nt	8	display	
ct	8	sp	-265.5
tn	TRANSMITTER	wp	3634.1
in	H1	rfl	802.1
sfrq	400.059	rtp	0
tof	399.8	fp	-17.7
tpwr	58	lp	-0.6
pw	6.950		

DECOUPLER		PLOT	
dn	C13	wc	250
dof	0	vs	0
dm	nnn	th	104
dmm	c	at	2
dpwr		cdc	ph
dmf	29412		



expt Carbon

SAMPLE SPECIAL 25.0  
date Dec 11 2008 temp 30  
solvent cdc13 gain 30  
file /mnt/argenta/~ spin not used  
nmr500/data/zhang/~ hst 0.008  
guozhu/C13-2008120~ pw90 9.600  
9-1.fid alfa 10.000  
ACQUISITION  
sw 30487.8 f1 n  
at 1.300 in n  
np 79298 dd y  
fb 17000 hs nn  
bs 12 f1  
di 1.000 1b 0.50  
nt 1200 f1 not used  
ct 4716  
TRANSMITTER  
tn C13 sp -1068.4  
sfreq 125.686 rf1 24839.7  
tof 1255.2 rfp 11759.5  
tpwr 52 rfp 9676.8  
pw 4.800 1p -148.6  
-238.0  
DECOUPLER H1 WC PLOT  
dn H1 WC 250  
dof 0 SC 0  
dm 0 SC 0  
dmm yvv vs 29542  
w th 10  
dpwr 39 at cdc ph  
dmf 11900



exp1 Proton

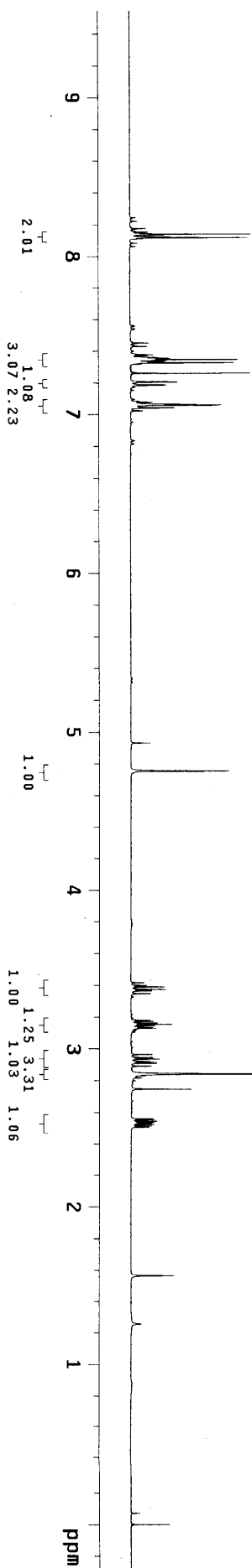
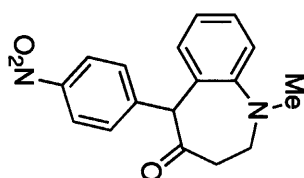
SAMPLE		SPECIAL	
date	Nov 27 2008	temp	25.0
solvent	cdcl3	gain	30
file	/mnt/argenta/~	spin	not used
mr400	/data/zhang/g-	hst	0.008
nozhu	/guozhu-20081-	pw90	13.900
	127-1.fid	alpha	6.600

ACQUISITION		FLAGS	
sw	6410.3	11	n
at	2.049	in	n
np	26264	dp	y
fb	4000	hs	nn
bs	32	fn	
dl	1.000	tn	
ct	8	sp	-123.2
tn	8	wp	3943.4
trf1		rf1	800.1
stfq	400.059	rfp	0
tof	399.8	fp	62.1
tpwr	58	ip	15.1
pw	6.950		

DECOUPLER		PLOT	
dn	C13	wc	250
dof	0	vs	0
dm	nn	th	222
dmm	c	ai	2
dpwr	36	cdc	ph
dmf	29412		





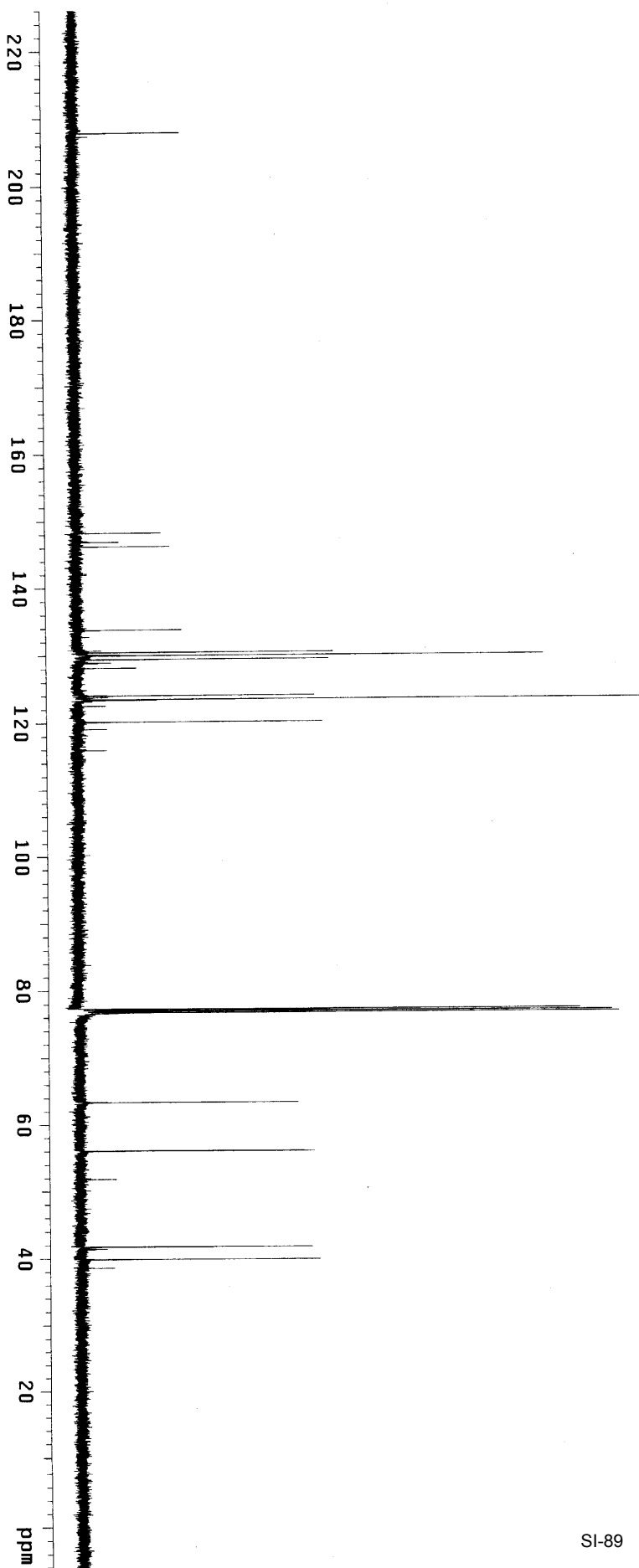
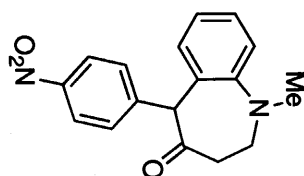
expl Carbon

SAMPLE SPECIAL 25.0  
date Nov 27 2008 temp  
solvent cdc13 gain 30  
file /mnt/argenta/~ hst not used  
nmr500/data/Zhang/~ pw90 0.008  
guozhu/C13-2008112~ 9.600  
7-1.fid alfa 10.000

ACQUISITION  
sw 30487.8 f1 n  
at 1300 in y  
np 79298 dp nm  
fb 17000 hs  
bs 12  
d1 1.000 lb 0.50  
nt 12000 fn not used  
ct 1128 DISPLAY

TRANSMITTER C13  
tn wp -821.9  
strq 125.686 rf1 29229.9  
tof 1255.2 rfp 11756.2  
tpwr 52 fp 9675.8  
pw 4.800 tp -208.0

DECOUPLER  
dn H1 WC 250  
dof 0 SC 0  
dm yyv vs 47509  
dmm yv th 13  
dpwr 39 at cdc ph  
dmf 11900



expt proton

SAMPLE Nov 24 2008 SPECIAL 25.0  
date  
solvent cdcl3 gain 30  
title /mnt/argenta/~ spin not used  
nmr500/data/Zhang/~ hst 0.008  
guozhu/H1-20081124~ pw90 13.400  
-1.fid alfa 6.600

ACQUISITION  
sw 8012.8 11  
at 2.049 1n  
np 32830 dd  
fb 4000 hs  
bs 8  
di 1.000 8  
nt 8  
ct 8

TRANSMITTER  
tn H1 sp  
sfrq 499.797 rfi  
tof 499.7 rfp  
tpwr 55 fp  
pw 6.700 1p

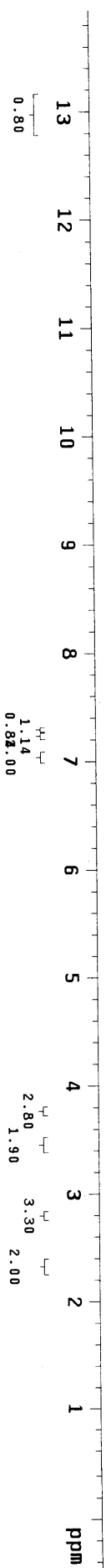
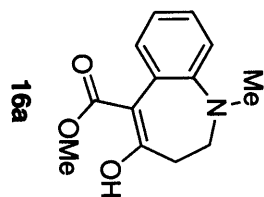
DECOUPLER  
dn C13 wc  
dof 0 sc  
dm nn vs  
dmm c th  
dpwr 33 ai  
dmf 32258

PROCESSING  
0.20  
65536

DISPLAY  
-243.8  
7210.3  
1009.9  
0  
-82.5  
-33.8

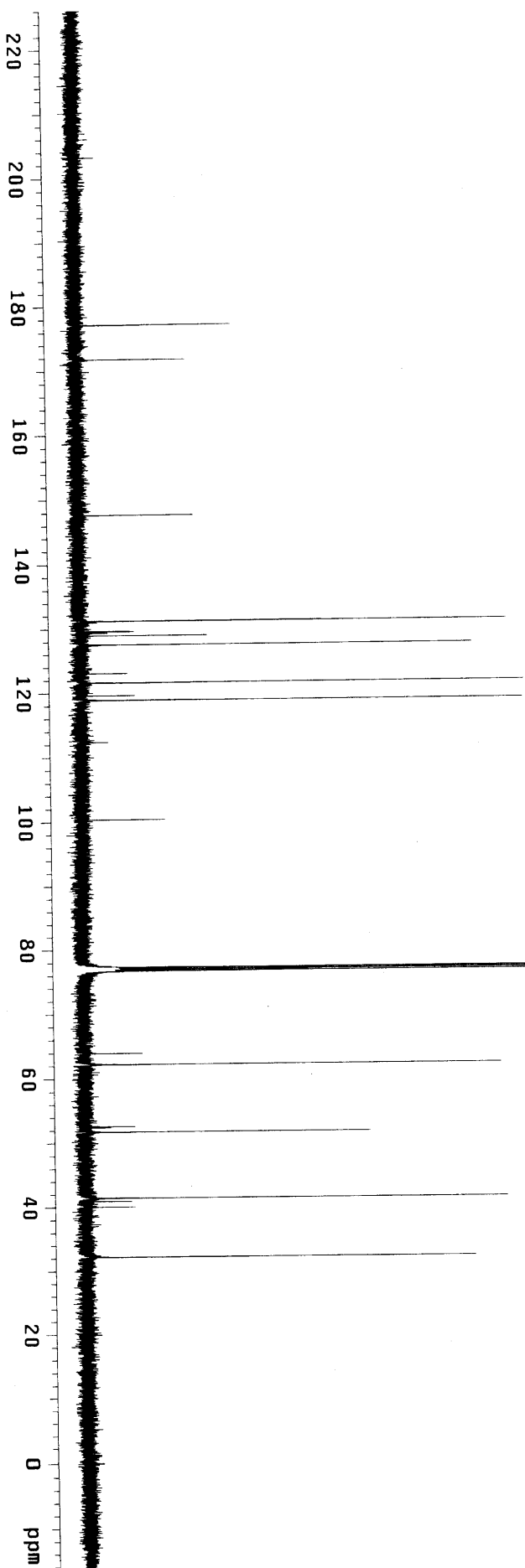
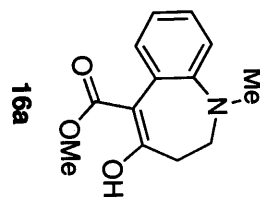
PLOT  
250  
0  
115  
2

cds ph



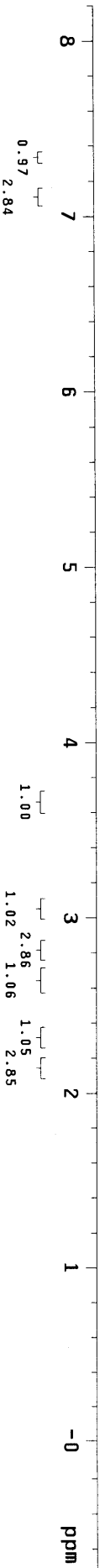
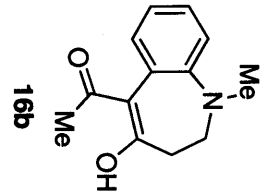
exp2 Carbon

SAMPLE Nov 27 2008 SPECIAL 25.0  
date  
solvent cdcl3 gain 30  
file /mnt/argenta/~ hst not used  
nmr500/data/Zhang/~ pw90 0.008  
guozhu/C13-2008112~ 9.600  
4-1.fid alfa 10.000  
ACQUISITION  
SW 30487.8 11 n  
at 1.300 in n  
np 79298 dp y  
fb 17000 ns nm  
bs 12  
d1 1.000 lb 0.50  
nt 12000 fn not used  
ct 1104  
TRANSMITTER SP -2078.5  
tn C13 WP 30487.3  
sfreq 125.686 rf1 11755.8  
tof 1255.2 rfp 9676.8  
tpwr 52 tp -47.1  
pw 4.800 1p -261.7  
DECOUPLER H1 WC PLOT  
dn H1 WC 250  
dof 0 SC 0  
dm YV VS 62108  
dmm W TH 12  
dpwr 39 ai cdc ph  
dmf 11900



expi Proton

SAMPLE  
date Dec 11 2008 temp -40.0  
solvent cdc13 gain 20  
file /mnt/argenta/~ not used  
nmr500/data/Zhang/~ hst 0.008  
guozhu/H1-20081211~ pw90 13.400  
-40degree.fid alfa 6.600  
ACQUISITION  
sw 8012.8 11  
at 2.049 in n  
np 32830 dp y  
fb 4000 hs nn  
bs 32  
dl 1.000 lb  
nt 8 fn  
ct 8  
TRANSMITTER  
tn H1 sp  
stfq 499.797 rfp  
tof 499.7 rfp  
tpwr 55 rp  
pw 6.700 lp  
DECOUPLER  
dn C13 wc  
dof 0 sc  
dm nnh vs  
dmm c th  
dpwr 33 at  
dmf 32258 cdc ph

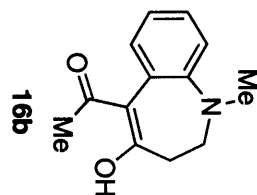


expt Carbon

SAMPLE SPECIAL  
date Nov 26 2008 temp 25.0  
solvent cdcl3 gain 30  
file /mnt/argenta/~ not used  
nmr500/data/Zhang/~ hst 0.008  
guozhu/C13-2008112~ pw90 9.600  
6-7.fid alfa 10.000

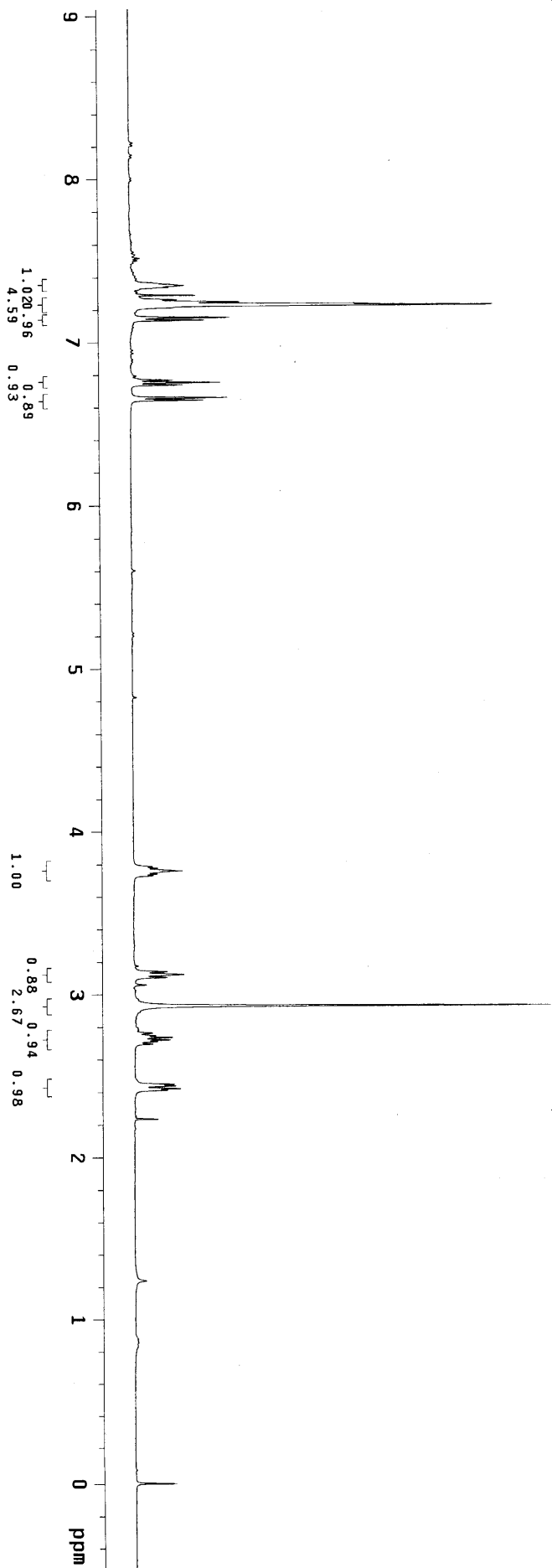
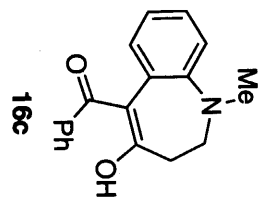
ACQUISITION  
sw 30487.8 f1 11 n  
at 1300 f2 11 y  
np 79298 dp 11 y  
fb 17000 ns nm  
bs 12  
d1 1.000 lb 0.50  
nt 12480 fn not used  
ct 12480

TRANSMITTER C13  
tn 30487.3 sp -2078.0  
sfreq 125.686 wf 30487.3  
tot 1255.2 rfi 11755.3  
tpwr 32 rfp 9676.8  
pw 4.800 tp -47.2  
DECOUPLER H1 PLOT  
dn H1 wc 250  
dof 0 sc 0  
dm yyv vs 54886  
w th 7  
dpwr 39 ai cdc ph  
dmf 11900



exp2 Proton

SAMPLE		SPECIAL	
date	Dec 11 2008	temp	-40.0
solvent	cdcl3	gain	20
file	/mnt/argenta/~	spin	not used
nmr500	/data/Zhang/~	hst	0.008
guozhu/H1-20081211~		pw90	13.400
-3-40degree.fid		alpha	6.600
ACQUISITION		FLAGS	
sw	8012.8	11	n
at	2.049	in	n
np	32830	dp	y
fb	4000	hs	nm
bs	32	PROCESSING	
d1	1.000	1b	0.20
nt	8	fn	65536
ct	8	DISPLAY	
TRANSMITTER		sp	-270.5
tn	H1	wp	4790.9
stfq	499.797	rfl	995.7
tof	499.7	rtp	-112.8
tpwr	55	tp	-27.7
pw	6.700	lp	
DECOUPLER		PLOT	
dn	C13	wc	250
dof	0	sc	0
dm	nm	vs	711
dmm	c	th	2
dpwr	33	ai	cdc ph
dmt	32258		



exp2 Carbon

SAMPLE SPECIAL  
date Nov 24 2008 temp 25.0  
solvent cdcl3 gain 30  
file /mnt/argenta/~ spin not used  
nmr500/data/Zhang/~ hst 0.008  
guozhu/C13-2008112~ pw90 9.600  
4-3.fid alfa 10.000

ACQUISITION  
sw 30487.8 11 n  
at 1.300 11 n  
np 79298 11 y  
fb 17000 11 nm  
bs 12 12  
d1 1.000 1b 0.50  
nt 12000 fm not used  
ct 348 348

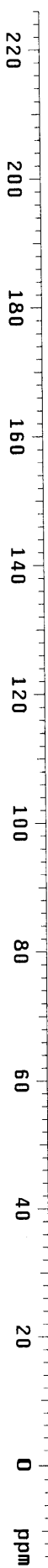
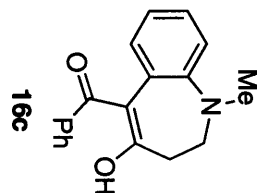
TRANSMITTER  
tn C13 wd -2078.9  
sfreq 125.686 rfi 30487.3  
tof 1255.2 rfp 11756.2  
tpwr 52 138.3  
pw 4.800 1p -235.8

DECOUPLER  
dn H1 wc 250  
dof 0 sc 0  
dm yyv vs 29114  
dmm w th 7  
dpwr 39 at cdc ph  
dmf 11900

PROCESSING  
not used  
nm

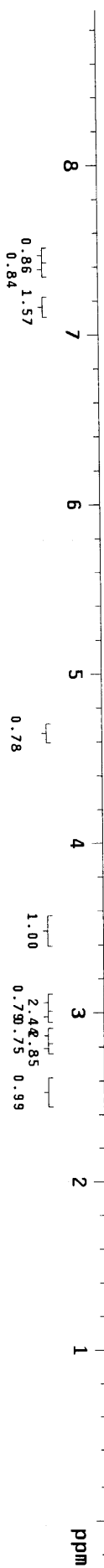
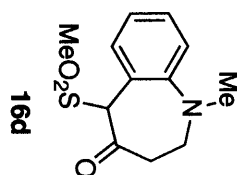
DISPLAY  
-2078.9  
30487.3  
11756.2  
9676.8  
138.3  
-235.8

PLOT



exp20 Proton

SAMPLE		SPECIAL	
date	Dec 10 2008	temp	30.0
solvent	cdcl3	gain	30
file	/mnt/argenta/~	spin	not used
mr400/data/Zhang/g~	hst	0.008	
uozhu/guozhu-20081~	pw90	13.900	
210-2.fid	alfa	6.600	
ACQUISITION		FLAGS	
sw	6410.3	il	n
at	2.049	in	n
np	26264	dp	y
fb	4000	hs	nm
bs	32	fn	65536
d1	1.000	sp	-123.2
nt	48	wd	3690.9
ct	48	ft1	799.9
TRANSMITTER		DISPLAY	
tn	H1	rf1	-21.8
stfq	400.059	rfp	29.5
tof	399.8	tp	250
tpwr	58	ip	0
pw	6.950	WC	765
DECOUPLER		SC	2
dn	C13	vs	
dof	0	th	
dmm	nmn	at	
dmm	c	cdc	
dpwr	36	ph	
dmf	29412		





exptl Carbon

SAMPLE SPECIAL  
date Dec 12 2008 temp 25.0  
solvent cdcl3 gain 30  
file /mnt/argenta/~ hst not used  
nmr500/data/Zhang/~ pw90 0.008  
guozhu/C13-2008121~ 9.600  
0-2.fid alfa 10.000

ACQUISITION  
sw 30487.8 11  
at 1300 in n  
np 79298 dp y  
fb 17000 ns nm  
bs 12  
d1 1.000 lb 0.50  
nt 12000 fn not used  
ct 12000 DISPLAY  
TRANSMITTER  
td -2078.0  
sfreq 30487.3  
tof 11755.3  
tpwr 9676.8  
pw 4.800 tp -148.6  
DECOUPLER 1P -237.2  
dn H1 WC PLOT  
dof 0 SC 250  
dm YV VS 0  
dmm W th 58826  
dpwr 39 ai cdc ph 9  
dmf 11900

