

Supporting Information

**Au-Catalyzed Synthesis of 2-Alkylinoles from
N-Arylhydroxylamines and Terminal Alkynes**

Yanzhao Wang, Longwu Ye and Liming Zhang

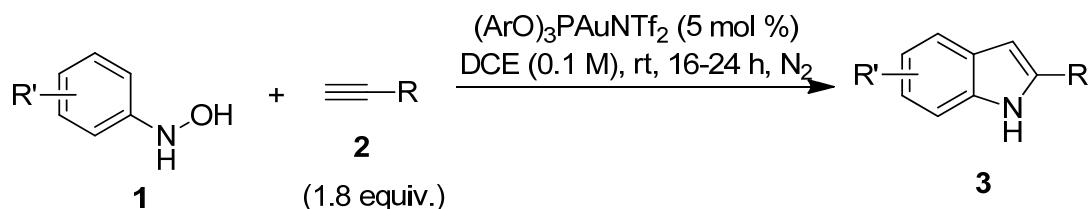
Department of Chemistry and Biochemistry, University of California, Santa Barbara,
California, 93106

Content	Page Number
General	1
General Procedure: Gold-Catalyzed Synthesis of 2-Alkyl indoles	2
References	10
^1H and ^{13}C NMR spectra	12

General. Ethyl acetate (ACS grade), hexanes (ACS grade), diethyl ether (ACS grade), NH₄OH (29.4% in H₂O, ACS reagent) were purchased from Fisher Scientific and used without further purification. Anhydrous DCE, toluene and commercially available reagents were used without further purification. Reactions were monitored by thin layer chromatography (TLC) using Silicycle precoated silica gel plates. Flash column chromatography was performed over Silicycle silica gel (230-400 mesh). ¹H NMR and ¹³C NMR spectra were recorded on a Varian 500 MHz Unity plus spectrometer and a Varian 400 MHz spectrometer using residue solvent peaks as internal standards. Infrared spectra were recorded with a Perkin Elmer FT-IR spectrum 2000 spectrometer and are reported in reciprocal centimeter (cm⁻¹). Mass spectra were recorded with Waters micromass ZQ detector using electrospray method.

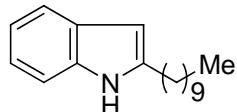
N-aryl hydroxylamines were prepared according to the literature procedure (D. A. Evans, H.-J. Song, K. R. Fandrick, *Org. Lett.* **2006**, 8, 3351-3354).

General Procedure: Gold-Catalyzed Synthesis of 2-Alkyl indoles



An oven-dried vial was charged with *N*-aryloxyamine **1** (0.3 mmol, 1 equiv), alkyne **2** (0.54 mmol, 1.8 equiv) and anhydrous DCE (3 mL, 0.1 M). The reaction was commenced by the addition of (ArO)₃PAuNTf₂ (Ar = 2,4-di-*tert*-butylphenyl, 16.8 mg, 5 mol %). After being stirred at room temperature for 16 – 24 h until the alkyne was completely consumed, the reaction mixture was concentrated under *vacuum*. The residue was purified via silica gel flash chromatography (eluents: ethyl acetate: hexanes = 1: 100) to give the desired indole **3**.

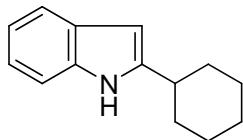
2-Decyl-1*H*-indole



3a

Compound **3a** was prepared in 84 % yield according to the general procedure (eluents: ethyl acetate: hexanes = 1: 100). ^1H NMR (400 MHz, CDCl_3) δ 7.86 (bs, 1H), 7.53 (d, J = 7.6 Hz), 7.30 (d, 1H, J = 7.6 Hz), 7.12 (td, 1H, J_1 = 7.6 Hz, J_2 = 1.2 Hz), 7.07 (td, 1H, J_1 = 7.2 Hz, J_2 = 1.2 Hz), 6.24 (d, 1H, J = 0.8 Hz), 2.75 (t, 2H, J = 8 Hz), 1.68 – 1.76 (m, 2H), 1.20 – 1.41 (m, 14H), 0.887 (t, 3H, J = 6.8 Hz); ^{13}C NMR (125 MHz, CDCl_3) δ 140.0, 135.8, 128.8, 120.9, 119.7, 119.5, 110.2, 99.4, 31.9, 29.6, 29.5, 29.4, 29.3, 29.2, 28.2, 22.7, 14.1; IR (neat): 3387, 3377, 3052, 2953, 2919, 2849, 1457; MS (ES $^+$) Calculated for $[\text{C}_{18}\text{H}_{28}\text{N}]^+$: 258.22; Found: 258.16.

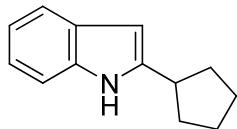
2-Cyclohexyl-1*H*-indole



3b

Compound **3b** was prepared in 77 % yield according to the general procedure (eluents: ethyl acetate: hexanes = 1: 100). ^1H NMR (500 MHz, CDCl_3) δ 7.89 (bs, 1H), 7.56 (dd, 1H, J_1 = 7.5 Hz, J_2 = 1 Hz), 7.31 (d, 1H, J = 8.5 Hz), 7.14 (td, 1H, J_1 = 7.5 Hz, J_2 = 1.5 Hz), 7.09 (td, 1H, J_1 = 7.5 Hz, J_2 = 1 Hz), 6.25 – 6.26 (m, 1H), 2.72 (tt, 1H, J_1 = 11 Hz, J_2 = 3.5 Hz), 2.08 – 2.11 (m, 2H), 1.86 – 1.90 (m, 2H), 1.76 – 1.81 (m, 1H), 1.39 – 1.55 (m, 4H), 1.29 – 1.35 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 145.1, 135.5, 28.6, 120.9, 119.8, 119.5, 110.3, 97.4, 37.3, 32.9, 26.2, 26.1; IR (neat): 3392, 2929, 2851, 1597, 1557, 1444, 1414; MS (ES $^+$) Calculated for $[\text{C}_{14}\text{H}_{18}\text{N}]^+$: 200.14; Found: 200.16.

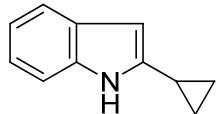
2-Cyclopentyl-1*H*-indole



3c

Compound **3c** was prepared in 62 % yield according to the general procedure (eluents: ethyl acetate: hexanes = 1: 100). ^1H NMR (400 MHz, CDCl_3) δ 7.89 (bs, 1H), 7.53 (dd, 1H, $J_1 = 7.6\text{Hz}$, $J_2 = 0.8\text{Hz}$), 7.30 (d, 1H, $J = 7.6\text{Hz}$), 7.12 (td, 1H, $J_1 = 7.2\text{Hz}$, $J_2 = 1.2\text{Hz}$), 7.04 – 7.09 (m, 1H), 6.24 – 6.2(m, 1H), 3.15 – 3.23 (m, 1H), 2.10 – 2.16 (m, 2H), 1.65 – 1.85 (m, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 143.9, 135.8, 128.6, 120.9, 119.8, 119.5, 110.2, 97.9, 38.8, 32.8, 25.2; IR (neat): 3584, 3054, 2954, 2868, 1547, 1458, 1289; MS (ES^+) Calculated for $[\text{C}_{13}\text{H}_{16}\text{N}]^+$: 186.13; Found: 186.15.

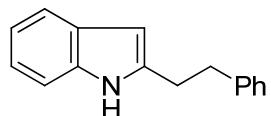
2-Cyclopropyl-1*H*-indole



3d

Compound **3d** was prepared in 70 % yield according to the general procedure (eluents: ethyl acetate: hexanes = 1: 100). ^1H NMR (500 MHz, CDCl_3) δ 7.90 (bs, 1H), 7.53 (d, 1H, $J = 7.5\text{ Hz}$), 7.28 (d, 1H, $J = 8\text{ Hz}$), 7.14 (td, 1H, $J_1 = 7.5\text{ Hz}$, $J_2 = 1\text{ Hz}$), 7.09 (td, 1H, $J_1 = 7.5\text{ Hz}$, $J_2 = 1\text{ Hz}$), 6.18 (d, 1H, $J = 1\text{ Hz}$), 1.94 – 1.99 (m, 1H), 0.96 – 1.00 (m, 2H), 0.78 – 0.81 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 147.1, 135.7, 128.6, 120.9, 119.67, 119.62, 110.2, 97.6, 8.80, 7.29; IR (neat): 3584, 3396, 3086, 3054, 3008, 2916, 2848, 1556, 1458, 1415; MS (ES^+) Calculated for $[\text{C}_{11}\text{H}_{11}\text{NNa}]^+$: 180.08; Found: 180.18

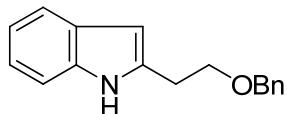
2-Phenethyl-1*H*-indole



3e

Compound **3e** was prepared in 89 % yield according to the general procedure (eluents: ethyl acetate: hexanes = 1: 100). ^1H NMR (400 MHz, CDCl_3) δ 7.74 (bs, 1H), 7.54 (d, 1H, J = 8 Hz), 7.32 (tt, 2H, J_1 = 6.8 Hz, J_2 = 2 Hz), 7.22 – 7.38 (m, 3H), 7.13 (td, 1H, J_1 = 8 Hz, J_2 = 1.6 Hz), 7.08 (td, 1H, J_1 = 7.2 Hz, J_2 = 1.2 Hz), 6.29 (m, 1H), 3.03 – 3.12 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3) δ 141.2, 140.0, 135.7, 128.6, 128.5, 128.4, 126.8, 121.1, 119.8, 119.6, 110.3, 99.8, 35.6, 30.1; IR (neat): 3584, 3395, 3058, 3021, 2915, 2852, 1553, 1456, 1416; MS (ES^+) Calculated for $[\text{C}_{16}\text{H}_{16}\text{N}]^+$: 222.13; Found: 222.15.

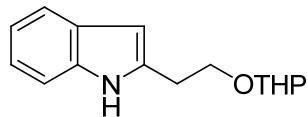
2-(2-(BenzylOxy)ethyl)-1*H*-indole



3f

Compound **3f** was prepared in 84 % yield according to the general procedure (eluents: ethyl acetate: hexanes = 1: 100). ^1H NMR (400 MHz, CDCl_3) δ 8.58 (bs, 1H), 7.54 (d, 1H, J = 7.6 Hz), 7.26 – 7.41 (m, 5H), 7.13 (t, 1H, J = 7.6 Hz), 7.07 (t, 1H, J = 7.6 Hz), 6.26 (s, 1H), 4.60 (s, 2H), 3.81 (t, 2H, J = 6 Hz), 3.07 (t, 2H, J = 6 Hz); ^{13}C NMR (100 MHz, CDCl_3) δ 137.9, 137.7, 135.9, 128.5, 128.3, 127.85, 127.78, 121.0, 119.8, 119.4, 110.5, 99.8, 73.3, 69.9, 28.6; IR (neat): 3584, 3407, 3056, 3029, 2914, 2861, 1553, 1456, 1287, 1096; MS (ES^+) Calculated for $[\text{C}_{17}\text{H}_{17}\text{NNaO}]^+$: 274.12; Found: 274.15.

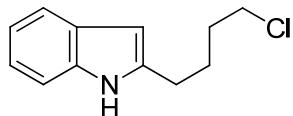
2-(2-(Tetrahydro-2H-pyran-2-yloxy)ethyl)-1*H*-indole



3g

Compound **3g** was prepared in 67 % yield according to the general procedure (eluents: ethyl acetate: hexanes = 1: 100). ^1H NMR (500 MHz, CDCl_3) δ 8.58 (bs, 1H), 7.54 (d, 1H, J = 7.5 Hz), 7.31 (d, 1H, J = 8 Hz), 7.12 (t, 1H, J = 7.5 Hz), 7.07 (t, 1H, J = 7 Hz), 6.27(s, 1H), 4.66 (t, 1H, J = 8.5 Hz), 4.06 – 4.11 (m, 1H), 3.82 – 3.87 (m, 1H), 3.73 (dt, 1H, J_1 = 9.5 Hz, J_2 = 6 Hz), 3.50 – 3.54 (m, 1H), 3.07 (t, 2H, J = 6 Hz), 1.85 – 1.90 (m, 1H), 1.76 – 1.82 (m, 1H), 1.52 – 1.70 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3) δ 137.7, 135.9, 128.4, 120.9, 119.8, 119.4, 110.4, 99.9, 99.3, 67.2, 62.6, 30.8, 28.6, 25.3, 19.8; IR (neat): 3401, 3316, 3055, 2943, 2869, 1553, 1457, 1134, 1030; MS (ES^+) Calculated for $[\text{C}_{15}\text{H}_{19}\text{NNaO}_2]^+$: 268.13; Found: 268.15.

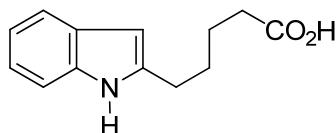
2-(4-Chlorobutyl)-1*H*-indole



3h

Compound **3c** was prepared in 62 % yield according to the general procedure (eluents: ethyl acetate: hexanes = 1: 100). ^1H NMR (400 MHz, CDCl_3) δ 7.87 (bs, 1H), 7.54 (dd, 1H, J_1 = 7.6 Hz, J_2 = 0.8 Hz), 7.31 (d, 1H, J = 8 Hz), 7.14 (td, 1H, J_1 = 7.6 Hz, J_2 = 1.2 Hz), 7.09 (td, 1H, J_1 = 7.6 Hz, J_2 = 1.2 Hz), 6.27 (d, 1H, J = 0.8 Hz), 3.58 (t, 2H, J = 6 Hz), 2.81 (t, 2H, J = 6.8 Hz), 1.87 – 1.90 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 138.8, 135.8, 128.7, 121.1, 119.8, 119.7, 110.3, 99.8, 44.8, 31.9, 27.4, 26.3; IR (neat): 3402, 3056, 2941, 2864, 1551, 1457, 1415, 1286; MS (ES^+) Calculated for $[\text{C}_{12}\text{H}_{15}\text{ClN}]^+$: 208.09; Found: 208.11.

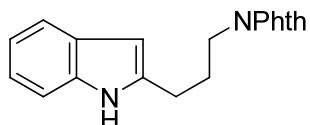
5-(1*H*-indol-2-yl)pentanoic acid



3i

Compound **3i** was prepared in 73 % yield according to the general procedure (eluents: ethyl acetate: hexanes = 1: 100). ^1H NMR (400 MHz, CDCl_3) δ 7.93 (bs, 1H), 7.5 (d, 1H, J = 7.6 Hz), 7.30 (d, 1H, J = 8 Hz), 7.05 – 7.14 (m, 2H), 6.25 (s, 1H), 2.80 (t, 2H, J = 7 Hz), 2.42 (t, 2H, J = 6.8 Hz), 1.70 – 1.83 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3) δ 178.5, 140.0, 135.8, 128.7, 121.1, 119.8, 119.6, 110.3, 99.7, 33.4, 28.4, 27.8, 24.1; IR (neat): 3584, 3390, 3045, 2939, 2861, 1700, 1457, 1412; MS (ES^+) Calculated for $[\text{C}_{13}\text{H}_{15}\text{NNaO}_2]^+$: 240.10; Found: 240.10.

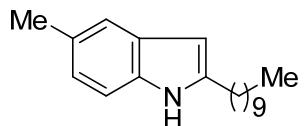
2-(3-(1*H*-indol-2-yl)propyl)isoindoline-1,3-dione



3j

Compound **3j** was prepared in 72 % yield according to the general procedure (eluents: ethyl acetate: hexanes = 1: 100). ^1H NMR (500 MHz, CDCl_3) δ 8.76 (bs, 1H), 7.82 – 7.87 (m, 2H), 7.71 – 7.73 (m, 2H), 7.50 (d, 1H, J = 7.5 Hz), 7.35 (d, 1H, J = 8 Hz), 7.11 (td, 1H, J_1 = 7.5 Hz, J_2 = 1 Hz), 7.04 (td, 1H, J_1 = 7.5 Hz, J_2 = 1 Hz), 6.27 (d, 1H, J = 1 Hz), 3.81 (t, 2H, J = 6.5 Hz), 2.80 (t, 2H, J = 7 Hz), 2.07 – 2.13 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 168.9, 138.5, 135.9, 134.1, 131.9, 128.7, 123.3, 121.0, 119.7, 119.5, 110.6, 99.8, 37.2, 28.8, 25.1; IR (neat): 3584, 3393, 3058, 2922, 2851, 1769, 1703, 1398; MS (ES^+) Calculated for $[\text{C}_{19}\text{H}_{16}\text{N}_2\text{NaO}_2]^+$: 327.11; Found: 327.11.

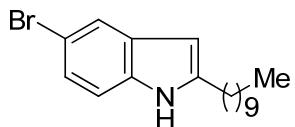
2-Decyl-5-methyl-1*H*-indole



3k

Compound **3k** was prepared in 64 % yield according to the general procedure (eluents: ethyl acetate: hexanes = 1: 100). ^1H NMR (400 MHz, CDCl_3) δ 7.76 (bs, 1H), 7.32 (d, 1H, J = 0.8 Hz), 7.18 (d, 1H, J = 8.4 Hz), 6.94 (dd, 1H, J_1 = 8.4 Hz, J_2 = 0.8 Hz), 6.14 – 6.16 (m, 1H), 2.73 (t, 2H, J = 7.6 Hz), 2.43 (s, 3H), 1.75 – 1.66 (m, 2H), 1.20 – 1.40 (m, 14H), 0.89 (t, 3H, J = 7.2 Hz); ^{13}C NMR (100 MHz, CDCl_3) δ 140.1, 134.0, 129.1, 128.7, 122.3, 119.5, 109.9, 98.9, 31.9, 29.59, 29.55, 29.4, 29.3, 29.2, 28.3, 22.7, 21.4, 14.1; IR (neat): 3376, 2953, 2918, 2850, 1470, 1412; MS (ES^+) Calculated for $[\text{C}_{19}\text{H}_{30}\text{N}]^+$: 272.24; Found: 272.27.

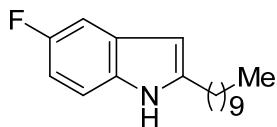
5-Bromo-2-decyl-1*H*-indole



3l

Compound **3l** was prepared in 86 % yield according to the general procedure (eluents: ethyl acetate: hexanes = 1: 100). ^1H NMR (400 MHz, CDCl_3) δ 7.89 (bs, 1H), 7.63 – 7.64 (m, 1H), 7.14 – 7.20 (m, 2H), 2.73 (t, 2H, J = 7.6 Hz), 1.66 – 1.74 (m, 2H), 1.22-1.40 (m, 14H), 0.89 (t, 3H, J = 6.4 Hz); ^{13}C NMR (100 MHz, CDCl_3) δ 141.4, 134.4, 130.6, 123.6, 122.2, 112.7, 111.6, 99.1, 31.9, 29.7, 29.6, 29.6, 29.4, 29.30, 29.27, 29.0, 28.2, 22.7, 14.2; IR (neat): 3403, 3315, 3055, 2943, 2870, 1457, 1418, 1134, 1030; MS (ES^+) Calculated for $[\text{C}_{18}\text{H}_{27}\text{BrN}]^+$: 336.13; Found: 336.08.

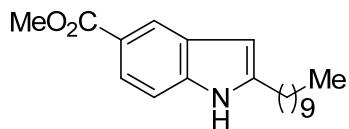
2-Decyl-5-fluoro-1*H*-indole



3m

Compound **3m** was prepared in 82 % yield according to the general procedure (eluents: ethyl acetate: hexanes = 1: 100). ^1H NMR (400 MHz, CDCl_3) δ 7.85 (bs, 1H), 7.15 – 7.20 (m, 2H), 6.82 – 6.88 (m, 1H), 6.19 – 6.21 (m, 1H), 2.74 (t, 2H, J = 7.6 Hz), 1.67 – 1.75 (m, 2H), 1.22 – 1.40 (m, 14H), 0.89 (t, 3H, J = 6.8 Hz); ^{13}C NMR (100 MHz, CDCl_3) δ 157.9(d, J = 231 Hz), 142.0, 132.2, 129.2 (d, J = 9 Hz), 110.6 (d, J = 10 Hz), 108.9 (d, J = 26 Hz), 104.6 (d, J = 24 Hz), 99.7 (d, J = 4 Hz), 31.9, 29.6, 29.5, 29.4, 29.3, 29.1, 28.3, 22.7, 14.1; IR (neat): 3465, 3417, 2954, 2926, 2854, 1585, 1486, 1452, 1169, 852; MS (ES^+) Calculated for $[\text{C}_{18}\text{H}_{26}\text{FNNa}]^+$: 298.19; Found: 298.16.

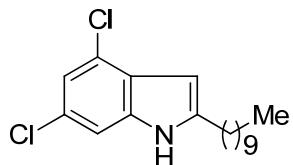
Methyl 2-decyl-1*H*-indole-5-carboxylate



3n

Compound **3n** was prepared in 76 % yield according to the general procedure (eluents: ethyl acetate: hexanes = 1: 100). ^1H NMR (400 MHz, CDCl_3) δ 8.30 (s, 1H), 8.27 (bs, 1H), 7.84 (dd, 1H, J_1 = 8.4 Hz, J_2 = 1.2 Hz), 7.29 (d, 1H, J = 8.4 Hz), 6.32 (s, 1H), 3.93 (s, 3H), 2.75 (t, 2H, 8 Hz), 1.68 – 1.76 (m, 2H), 1.20 – 1.40 (m, 14H), 0.89 (t, 3H, J = 6.8 Hz); ^{13}C NMR (100 MHz, CDCl_3) δ 168.4, 141.6, 138.5, 128.4, 122.6, 112.4, 121.4, 109.9, 100.6, 51.8, 31.9, 29.6, 29.5, 29.4, 29.3, 29.0, 28.2, 22.6, 14.1.

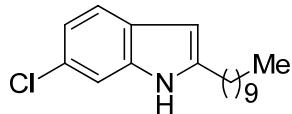
4 ,6-Dichloro-2-decyl-1*H*-indole



3o

Compound **3o** was prepared in 63 % yield according to the general procedure (eluents: ethyl acetate: hexanes = 1: 100). ^1H NMR (400 MHz, CDCl_3) δ 7.96 (bs, 1H), 7.17 (dd, 1H, J_1 = 1.6 Hz, J_2 = 1.2 Hz), 7.09 (d, 1H, J = 1.2 Hz), 6.30 – 6.32 (m, 1H), 2.73 (t, 2H, J = 7.6 Hz), 1.68 - 1.75 (m, 2H), 1.22 – 1.40 (m, 14H), 0.89 (t, 3H, J = 7.2 Hz); ^{13}C NMR (100 MHz, CDCl_3) δ 141.5, 136.2, 126.4, 126.4, 125.2, 119.7, 109.0, 98.2, 31.9, 29.6, 29.5, 29.4, 29.3, 29.2, 28.9, 28.2, 22.7, 14.1; IR (neat): 2953, 2927, 2854, 1614, 1577, 1468, 1328; MS (ES^+) Calculated for $[\text{C}_{18}\text{H}_{25}\text{Cl}_2\text{NNa}]^+$: 348.13; Found: 348.16.

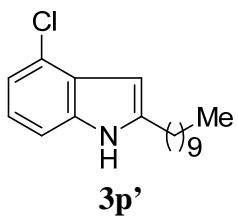
6-Chloro-2-decyl-1*H*-indole



3p

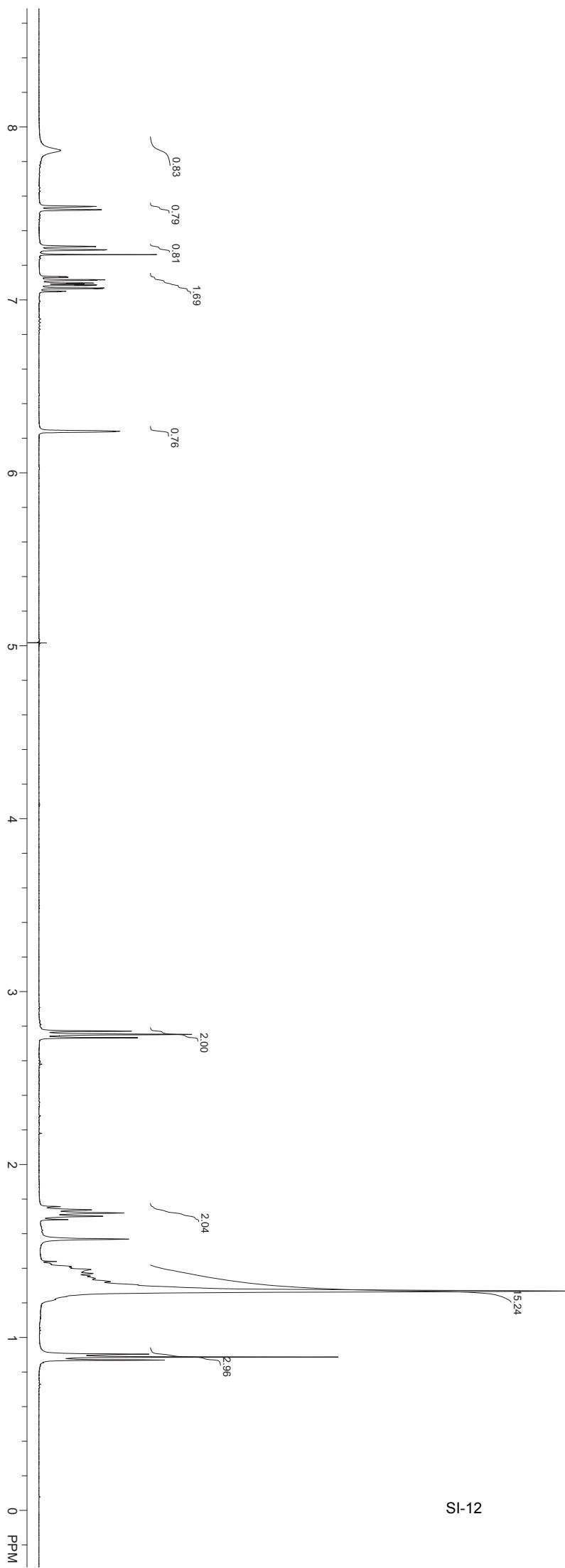
Compound **3p** and **3p'** was prepared in 85 % yield (1.3: 1) according to the general procedure (eluents: ethyl acetate: hexanes = 1: 100). **3p:** ^1H NMR (500 MHz, CDCl_3) δ 7.84 (bs, 1H), 7.41 (d, 1H, J = 9 Hz), 7.27 (t, 1H, J = 0.8 Hz), 7.02 – 7.05 (m, 1H), 6.20 – 6.21 (m, 1H), 2.73 (t, 2H, J = 7.5 Hz), 1.68 – 1.72 (m, 1H), 1.20 – 1.40 (m, 14H), 0.89 (t, 3H, J = 6.8 Hz); ^{13}C NMR (100 MHz, CDCl_3) δ 140.8, 136.1, 127.4, 126.6, 120.4, 120.2, 110.2, 99.5, 31.9, 29.6, 29.5, 29.4, 29.31, 29.28, 29.0, 28.2, 22.7, 14.1; IR (neat): 3584, 3403, 2954, 2924, 1543, 1467, 1397; MS (ES^+) Calculated for $[\text{C}_{18}\text{H}_{27}\text{ClN}]^+$: 292.18; Found: 292.18.

4-Chloro-2-decyl-1*H*-indole



3p': ^1H NMR (400 MHz, CDCl_3) δ 7.99 (bs, 1H), 7.19 (dt, 1H, $J_1 = 8\text{Hz}$, $J_2 = 0.8\text{Hz}$), 7.02 – 7.08 (m, 2H), 6.34 – 6.35 (m, 1H), 2.76 (t, 2H, $J = 8\text{ Hz}$), 1.69 – 1.77 (m, 2H), 1.23 – 1.43 (m, 14H), 0.88 (t, 3H, $J = 6.8\text{ Hz}$); ^{13}C NMR (100 MHz, CDCl_3) δ 140.8, 136.4, 127.6, 125.0, 121.5, 119.3, 108.8, 98.1, 31.9, 29.6, 29.5, 29.4, 29.30, 29.28, 29.1, 28.2, 22.7, 14.1; IR (neat): 3584, 3410, 2922, 2851, 1608, 1433; MS (ES^+) Calculated for $[\text{C}_{18}\text{H}_{27}\text{ClN}]^+$: 292.18; Found: 292.19.

D:\Greenware\Ntuus\20060723\1\DATA\\$wy23-60-pro.h1.fid
new experiment
Apr 1 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usc
Relaxation delay = 2.000 sec
NA = 16
Solvent = cdcl3
FD PTS Id = 20006
PTS Id = 32788
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt1SD = 0.24 Hz
SW2 = 1.00 Hz
Hz per Pt2ndD = 1.00 Hz
O1 = 2006.7504 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -46.58
B = -35.68
C = 0.00



3a



D:\Greenware\Ntu\20060731\DATA\\$wy2-30-pro-c13.fid
Standard c13 run using qcp probe
Mar 31 2011

USER:

SOLVENT: cdcl3

Experiment = s2pul

Pulse length = 9.500 usec

Relaxation delay = 5.000 sec

NA = 108

Solvent = cdcl3

FD PTS Id = 16000

PTSD = 16384

F1 = 100.576706 MHz

F2 = 399.949585 MHz

SW1 = 25000.00 Hz

AT1 = 0.04 sec

Hz per P1 1sID = 1.53 Hz

SW2 = 1.00 Hz

Hz per P1 2ndD = 1.00 Hz

O1 = 9529.8223 Hz

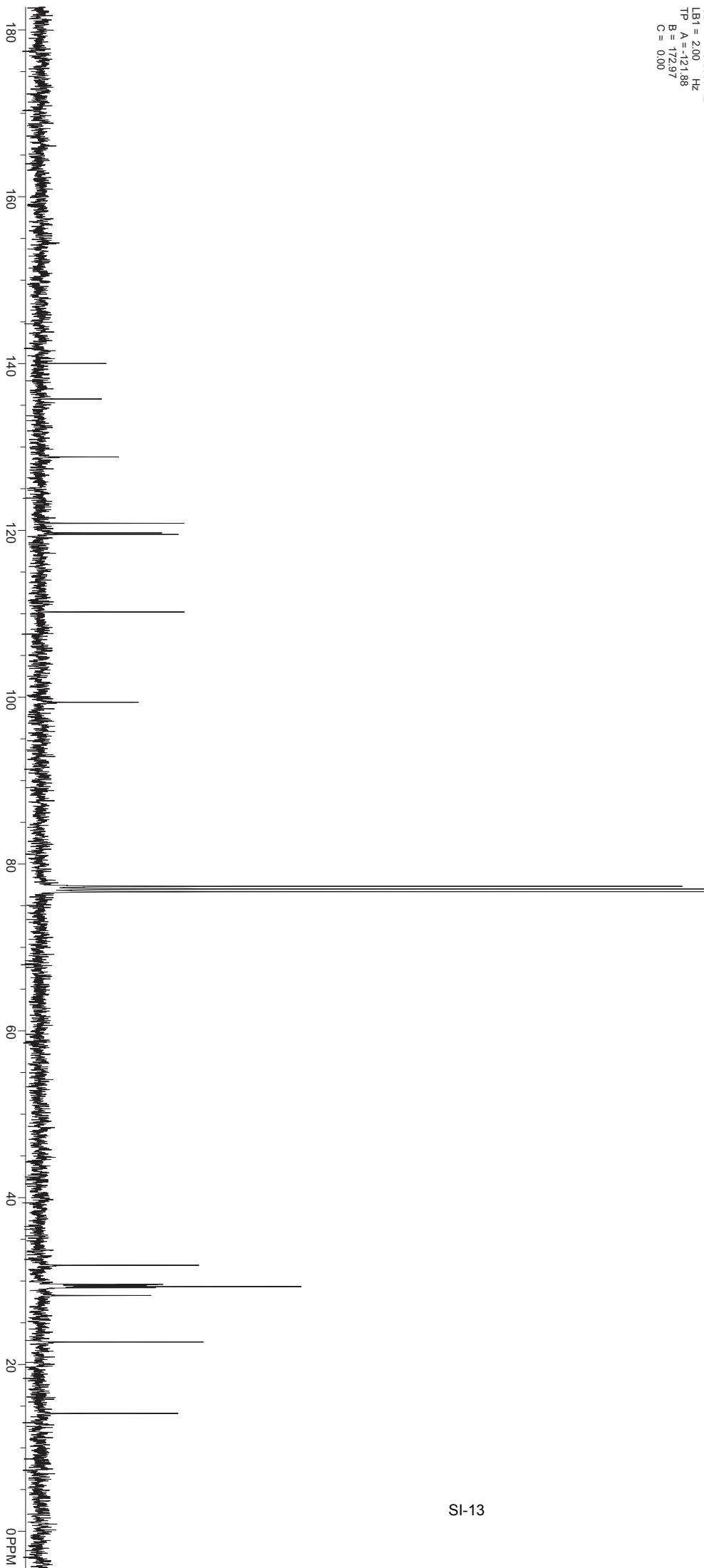
O2 = -0.5000 Hz

LB1 = 2.00 Hz

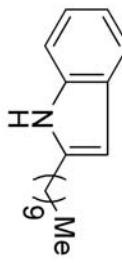
TP A = -121.88

B = 172.97

C = 0.00



3a



USER:

SOLVENT: cdcl₃

Experiment = s2pul

Pulse length = 7.075 usec

Relaxation delay = 4.800 sec

NA = 16

Solvent = cdcl₃

FD PTS Id = 20006

PT1 Id = 32788

F1 = 498.85851 MHz

F2 = 128.700813 MHz

SW1 = 8002.40 Hz

AT1 = 2.50 sec

Hz per Pt1sID = 0.24 Hz

SW2 = 1.00 Hz

Hz per Pt2ndD = 1.00 Hz

O1 = 2496.1272 Hz

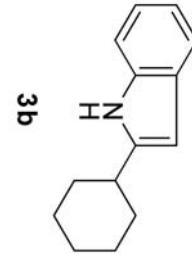
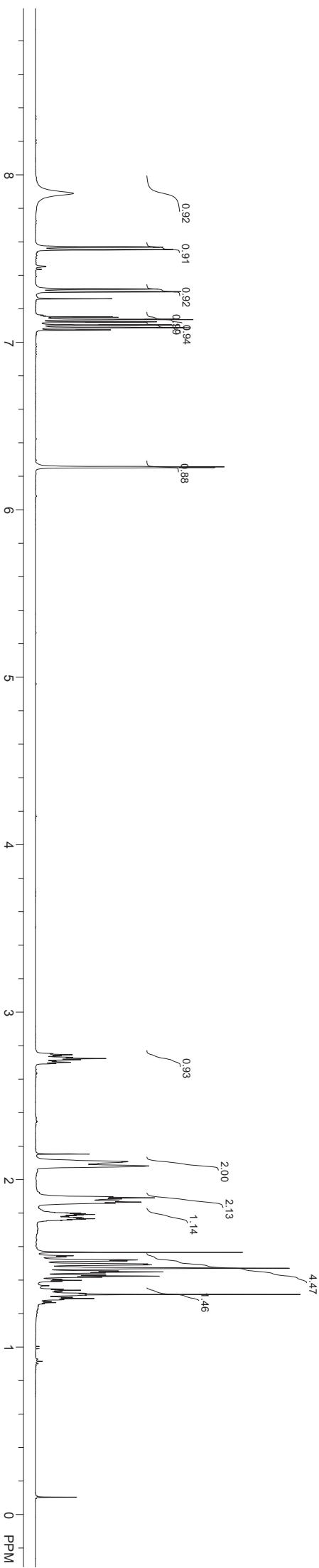
O2 = -5000.00 Hz

LB1 = 0.00 Hz

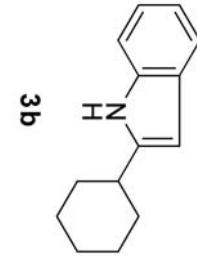
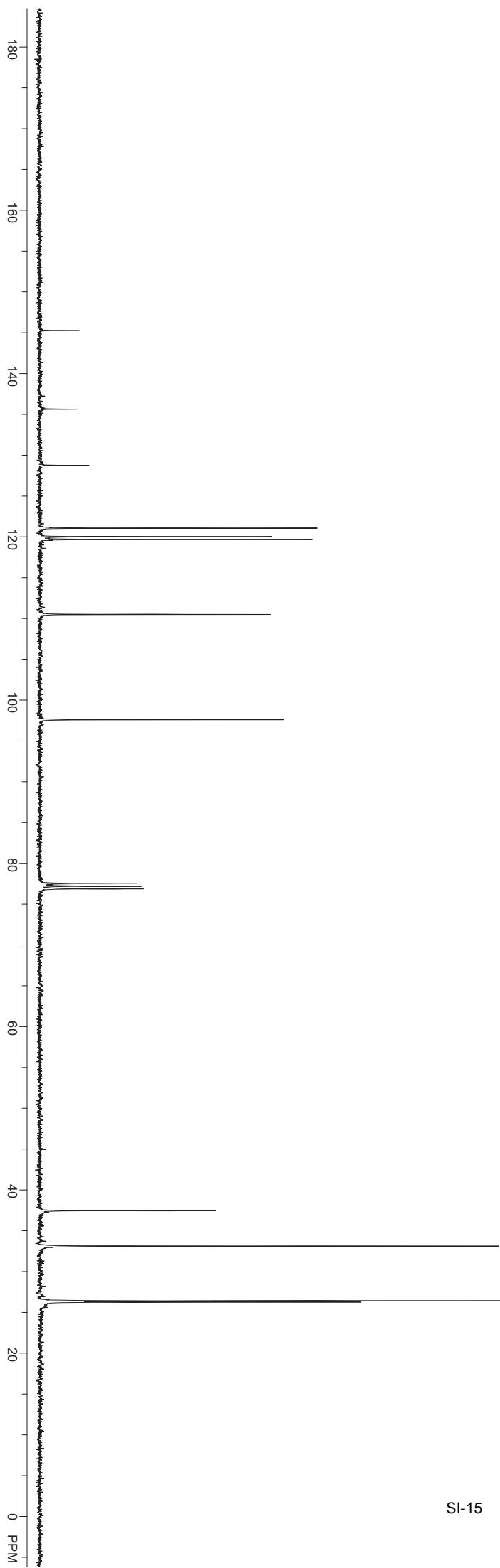
TP A = -128.44

B = 2.81

C = 0.00



D:\Greenware\NtuS 20060731\DATA\\$J\w-5-17-0ring-c-22.fid
Standard c13 run using qcp probe
Jan 25 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 934
Solvent = cdcl3
FD PTS Id = 28040
PTS Id = 32788
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 28940.66 Hz
AT1 = 1.00 sec
Hz per P1SID = 0.86 Hz
SW2 = 1.00 Hz
Hz per P12ndD = 1.00 Hz
O1 = 10071.4883 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -34.81
B = 2.63
C = 0.00



D:\Greenware\Ntu\20060731\DATA\\$J\w-5-1-9.fid
new experiment
Jan 5 2011

USER:

SOLVENT: cdcl₃

Experiment: s2pul

Pulse length = 11.663 usc

Relaxation delay = 4.800 sec

NA = 16

Solvent = cdcl₃

FID PTS Id = 20008

PTS Id = 32788

F1 = 399.950684 MHz

F2 = 100.575279 MHz

SW1 = 8003.20 Hz

AT1 = 2.50 sec

Hz per P1 1sID = 0.24 Hz

SW2 = 1.00 Hz

Hz per P1 2ndD = 1.00 Hz

O1 = 2006.3970 Hz

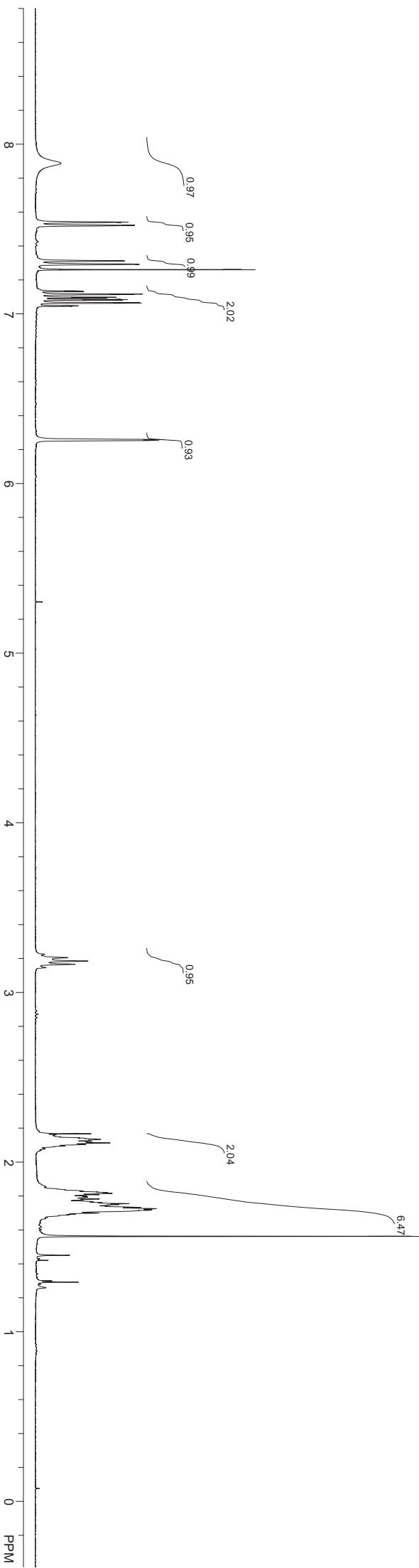
O2 = -0.5000 Hz

LB1 = 0.00 Hz

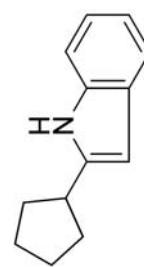
TP A = -57.50

B = -3.37

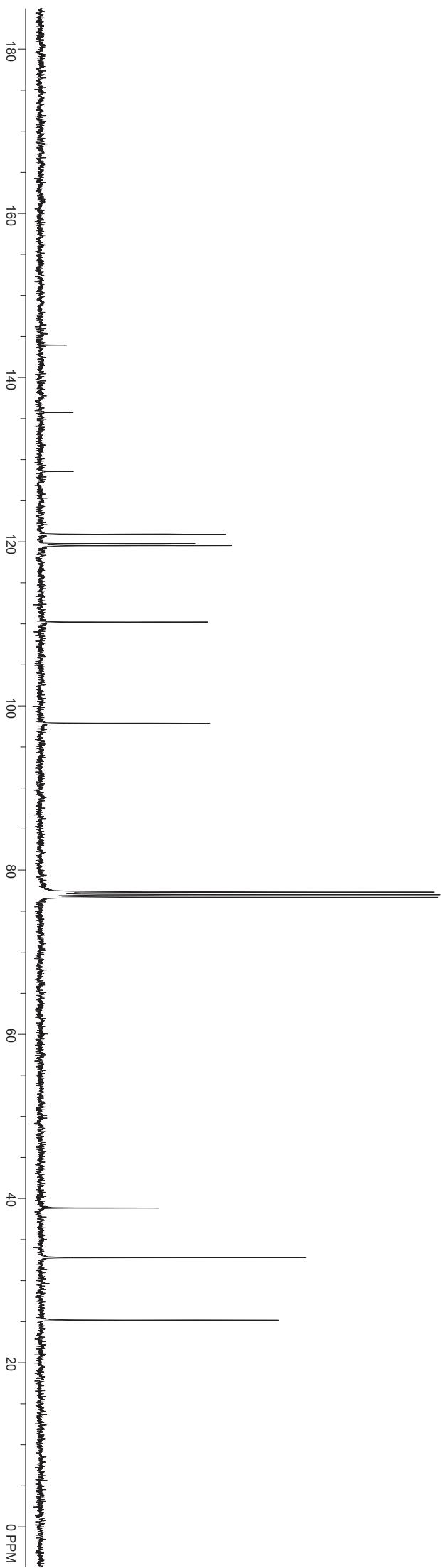
C = 0.00



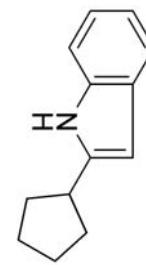
3c



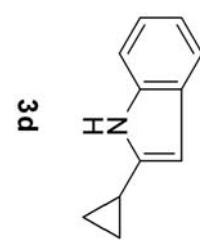
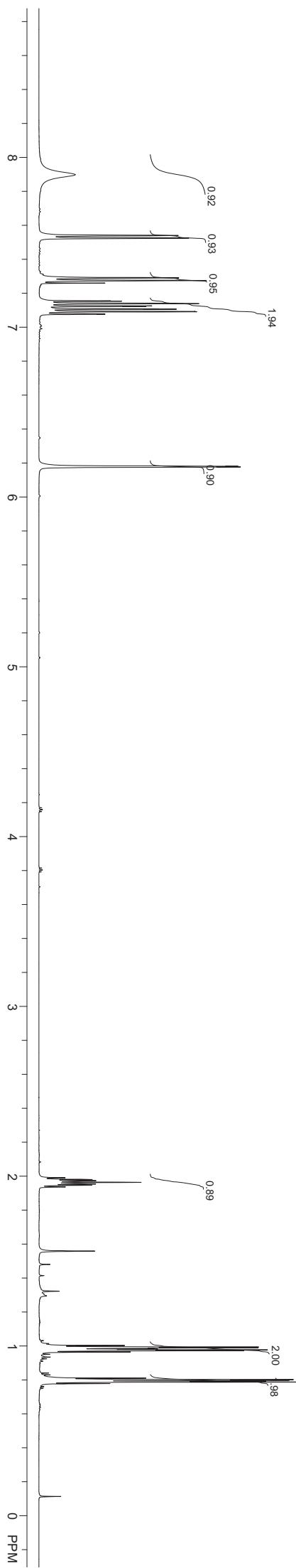
D:\Greenware\Ntuus\20060731\DATA\\$J\w-5-1-9-cc.fid
yw-5-1-5mmem-c
Jan 5 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.000 usec
Relaxation delay = 1.300 sec
NA = 1888
Solvent = cdcl3
FD PTS Id = 19608
PTS Id = 32788
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 27972.03 Hz
AT1 = 0.70 sec
Hz per Pt1SD = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt2ndD = 1.00 Hz
O1 = 10054.9897 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -29.53
B = 30.94
C = 0.00



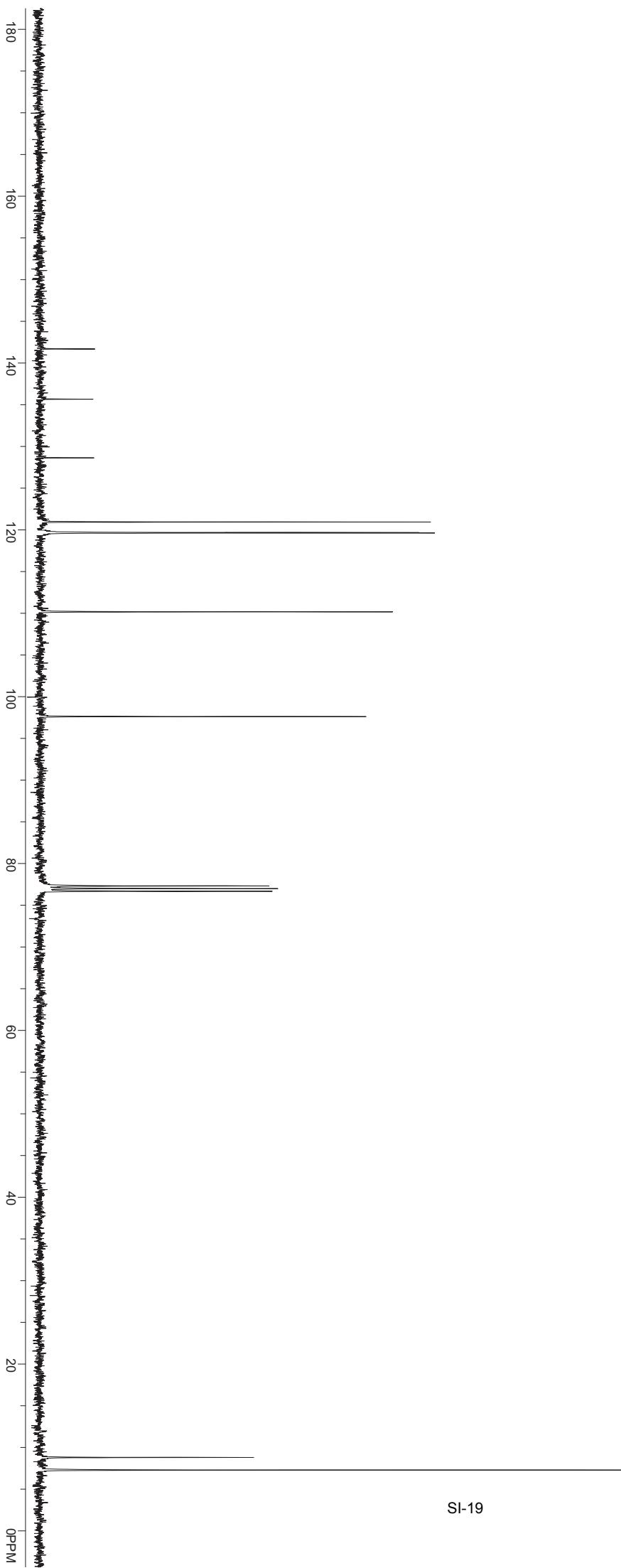
3c



D:\Greenware\Ntu\us.20060731\DATA\\$J\w-5-1-3mem-h.fid
5mm IDP
Jan 6 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.075 usec
Relaxation delay = 4.800 sec
NA = 8
Solvent = cdcl3
FD PTS Id = 20006
PTS Id = 32788
F1 = 498.85851 MHz
F2 = 128.700813 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt1SID = 0.24 Hz
SW2 = 1.00 Hz
Hz per Pt2ndD = 1.00 Hz
O1 = 2495.8831 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -82.97
B = 1.41
C = 0.00



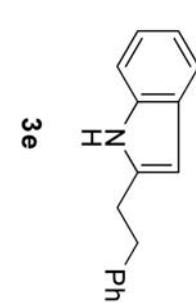
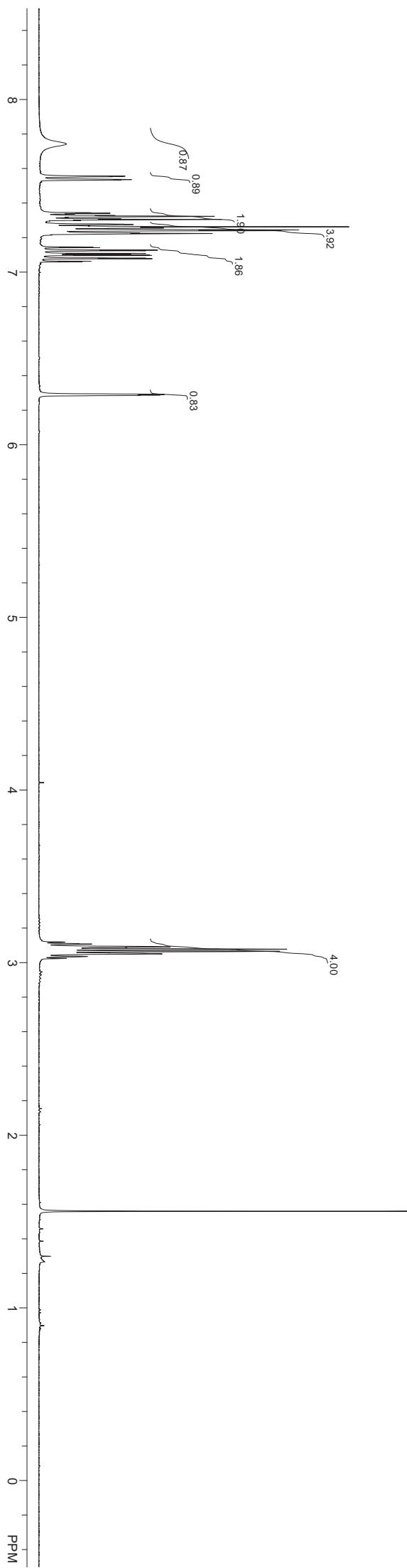
D:\Greenware\Ntu\$20060731\DATA\\$JW-5-3-1-3member-cc.fid
Standard c13 run using qcp probe
Jan 6 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.000 usec
Relaxation delay = 1.300 sec
NA = 50.4
Solvent = cdcl3
FD PTS Id = 19608
PTS Id = 32788
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 27972.03 Hz
AT1 = 0.70 sec
Hz per Pt1SD = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt2ndD = 1.00 Hz
O1 = 10050.7012 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -17.81
B = 9.84
C = 0.00



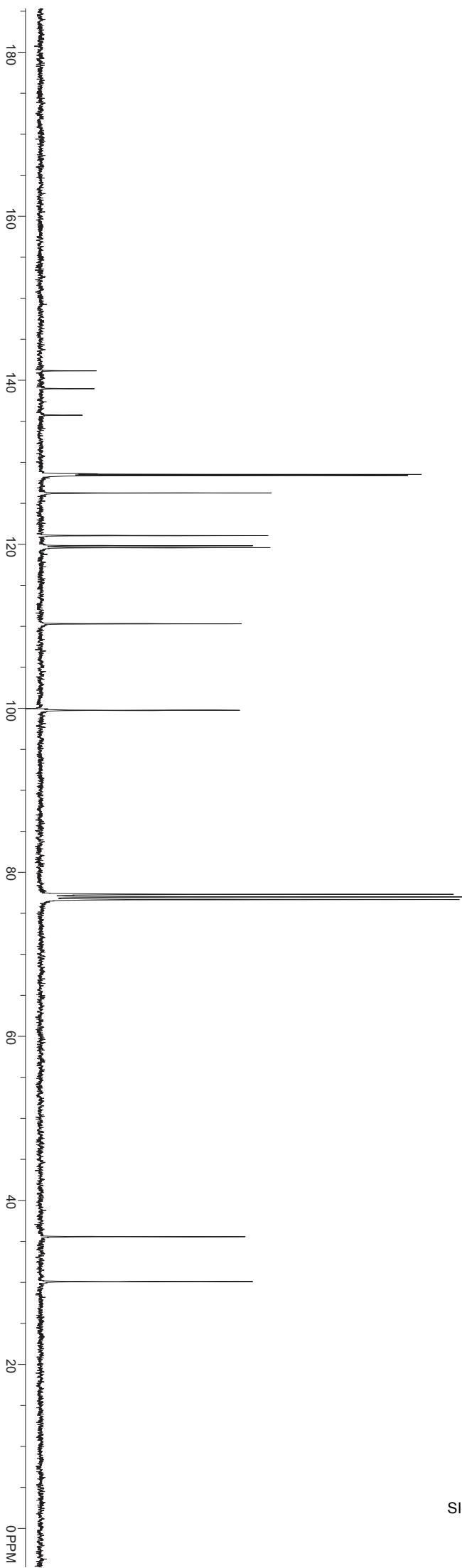
3d



D:\Greenware\Ntu\20060731\DATA\\$J\w-5-13-Ph-h.fid
new experiment
Jan 12 2011
USER:
SOLVENT: cdc13
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 12
Solvent = cdc13
FD PTS Id = 2008
PTS Id = 32788
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 800.020 Hz
AT1 = 2.50 sec
Hz per P1 1sID = 0.24 Hz
SW2 = 1.00 Hz
Hz per P1 2ndD = 1.00 Hz
O1 = 2007.1505 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -70.03
B = -13.98
C = 0.00



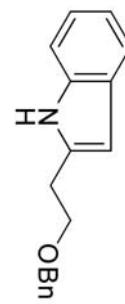
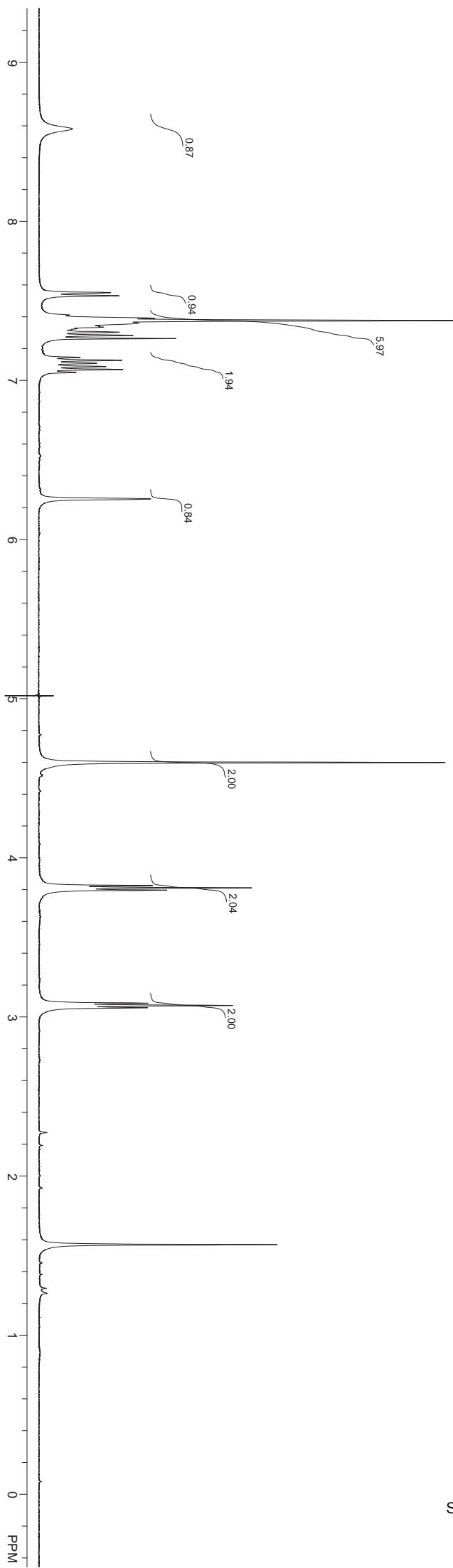
D:\Greenware\Ntus\20060731\DATA\\$J\w-5-13-Ph-cc.fid
Standard c13 run using qcp probe
Jan 12 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.000 usec
Relaxation delay = 1.300 sec
NA = 2016
Solvent = cdcl3
FD PTS Id = 19608
PTS Id = 32788
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 27972.03 Hz
AT1 = 0.70 sec
Hz per Pt1SD = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt2ndD = 1.00 Hz
O1 = 10053.2837 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -30.91
B = -0.75
C = 0.00



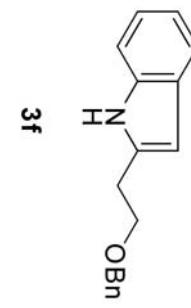
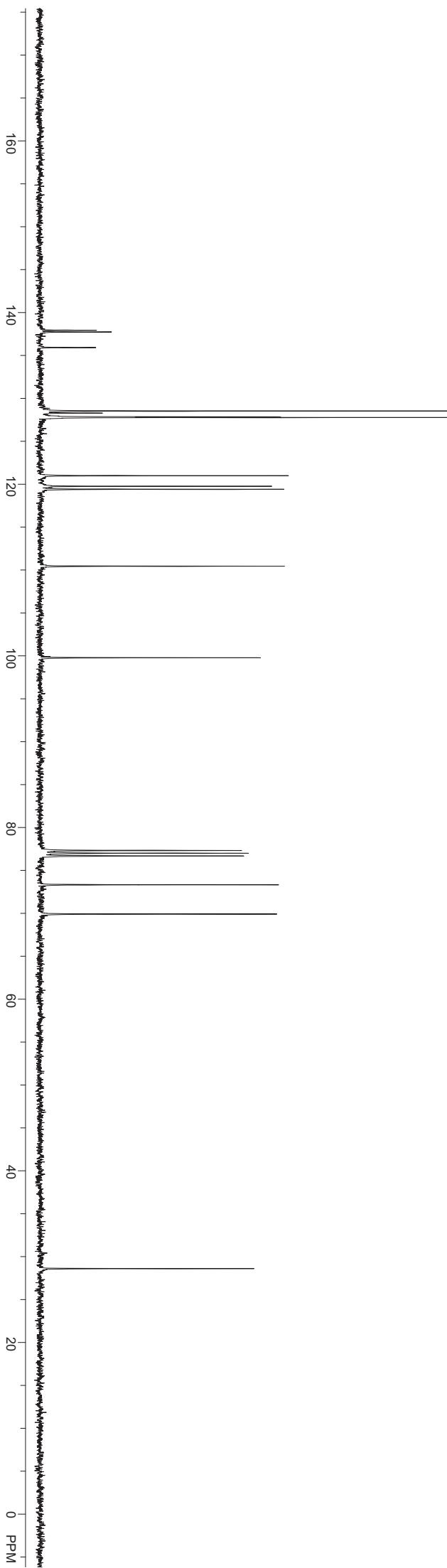
3e

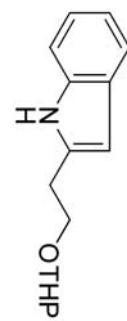
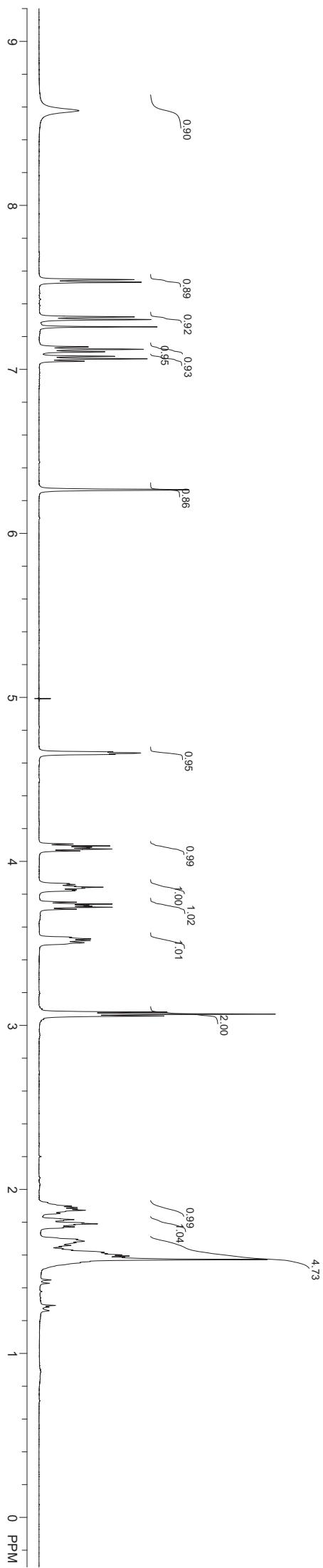


D:\Greenware\Ntu\20060731\DATA\\$J\w-5-14-2.fid
new experiment
Jan 12 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usc
Relaxation delay = 4.800 sec
NA = 14
Solvent = cdcl3
FD PTS Id = 20008
PTS Id = 32788
F1 = 398.950684 MHz
F2 = 100.575279 MHz
SW1 = 8003.20 Hz
AT1 = 2.50 sec
Hz per P1 1sID = 0.24 Hz
SW2 = 1.00 Hz
Hz per P1 2ndD = 1.00 Hz
O1 = 2007.1505 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -74.10
B = -8.96
C = 0.00

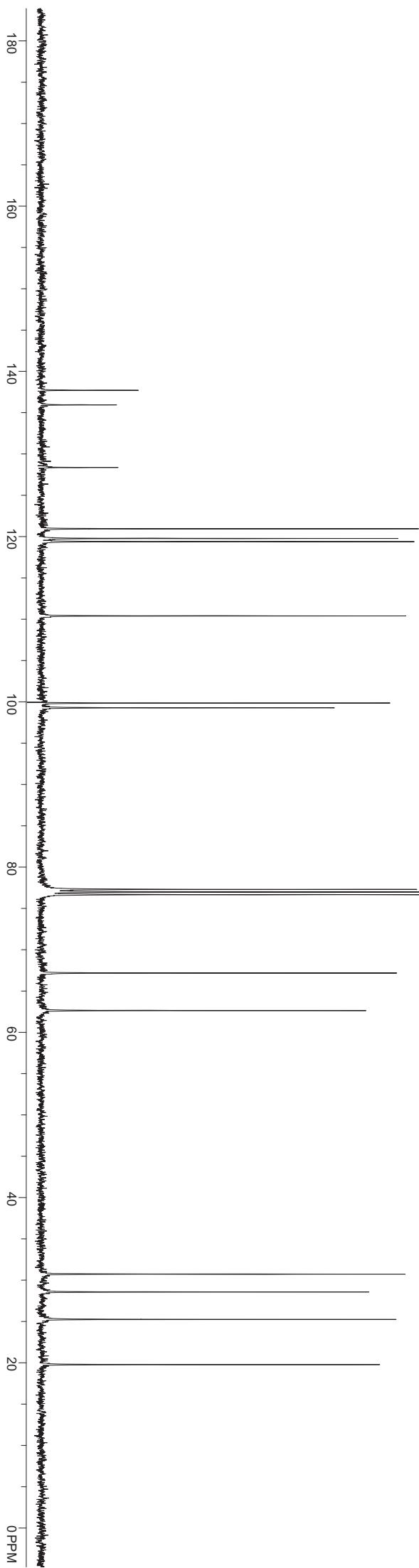


D:\Greenware\Ntu\20060731\DATA\\$J\w-5-14-OBn-cc.fid
Standard c13 run using qcp probe
Jan 12 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.000 usec
Relaxation delay = 1.300 sec
NA = 372
Solvent = cdcl3
FD PTS Id = 19608
PTS Id = 32788
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 27972.03 Hz
AT1 = 0.70 sec
Hz per Pt1SD = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt2ndD = 1.00 Hz
O1 = 100.08.1416 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -30.47
B = -4.22
C = 0.00





D:\Greenware\NtuS\20060731\DATA\\$J\w-5-17-THP-c
yw-5-17-THP-c
Jan 15 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.000 usec
Relaxation delay = 1.300 sec
NA = 1562
Solvent = cdcl3
FD PTS Id = 19608
PTS Id = 32788
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 27972.03 Hz
AT1 = 0.70 sec
Hz per Pt1SD = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt2ndD = 1.00 Hz
O1 = 10051.9111 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -1.02
B = 9.75
C = 0.00



D:\Greenware\Ntuus\20060731\DATA\\$J\w-5-3-1.fid
new experiment
Jan 6 2011

USER:

SOLVENT: cdcl₃

Experiment = s2pul

Pulse length = 11.663 usc

Relaxation delay = 4.800 sec

NA = 16

Solvent = cdcl₃

FID PTS Id = 20008

PTS Id = 32788

F1 = 399.950684 MHz

F2 = 100.575279 MHz

SW1 = 8003.20 Hz

AT1 = 2.50 sec

Hz per P1 1SD = 0.24 Hz

SW2 = 1.00 Hz

Hz per P1 2ndD = 1.00 Hz

O1 = 2007.1505 Hz

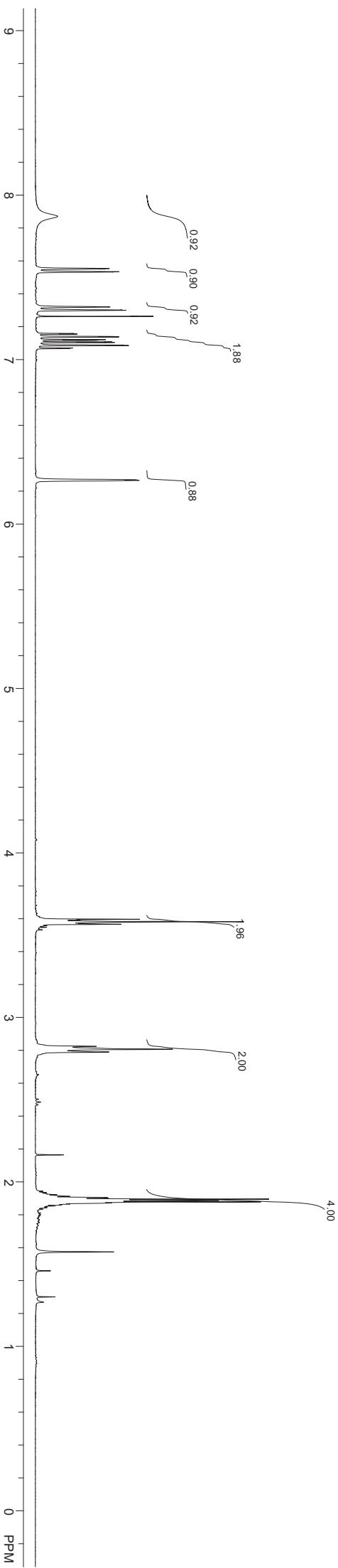
O2 = -0.5000 Hz

LB1 = 0.00 Hz

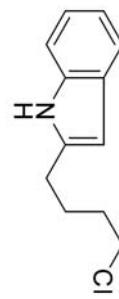
TP A = -51.23

B = -0.13

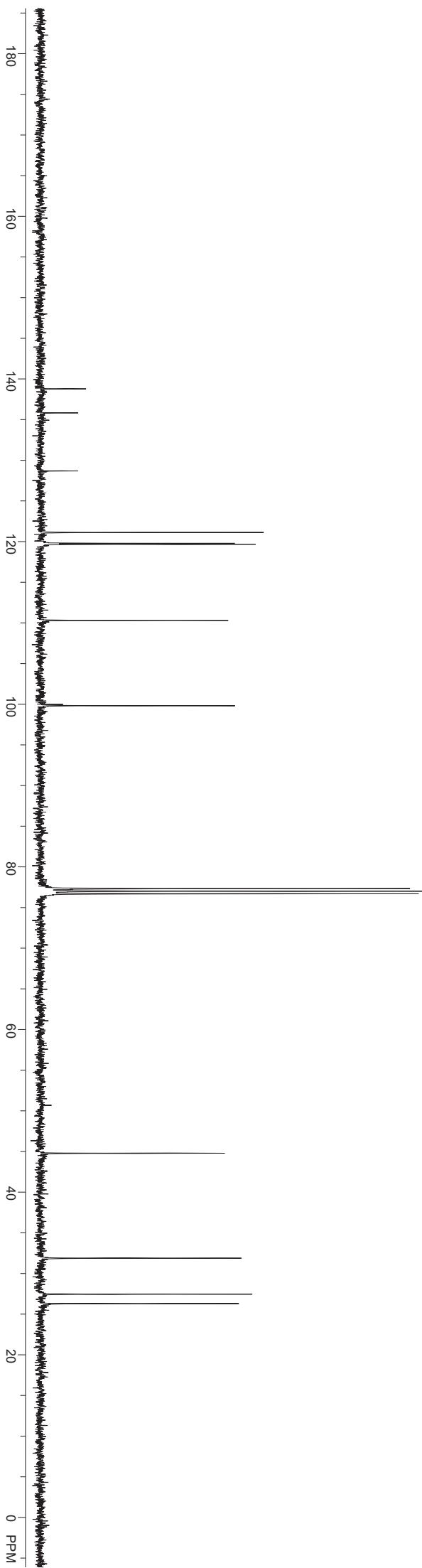
C = 0.00



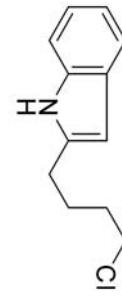
3h



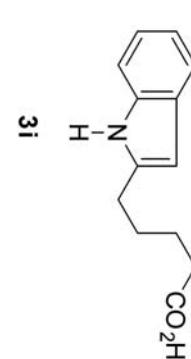
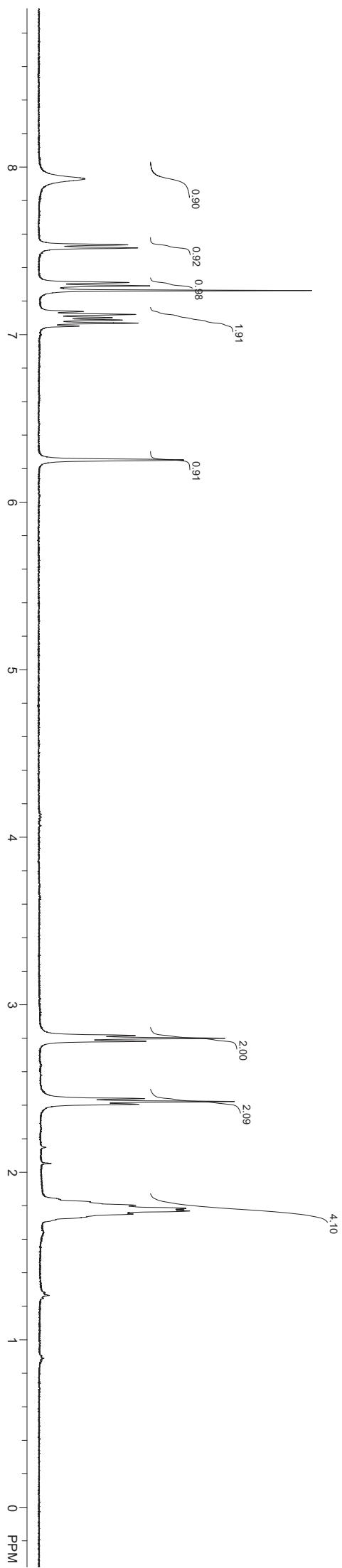
D:\Greenware\Ntus\20060731\DATA\\$J\w-5-3-1-Cl.cc.fid
yw-5-3-1-c
Jan 6 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.000 usec
Relaxation delay = 1.300 sec
NA = 986
Solvent = cdcl3
FD PTS Id = 19608
PTS Id = 32788
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 27972.03 Hz
AT1 = 0.70 sec
Hz per Pt1SID = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt2ndD = 1.00 Hz
O1 = 10054.9897 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -4.22
B = -11.25
C = 0.00



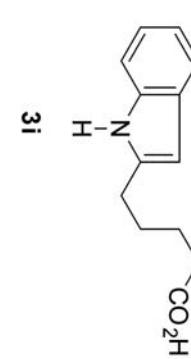
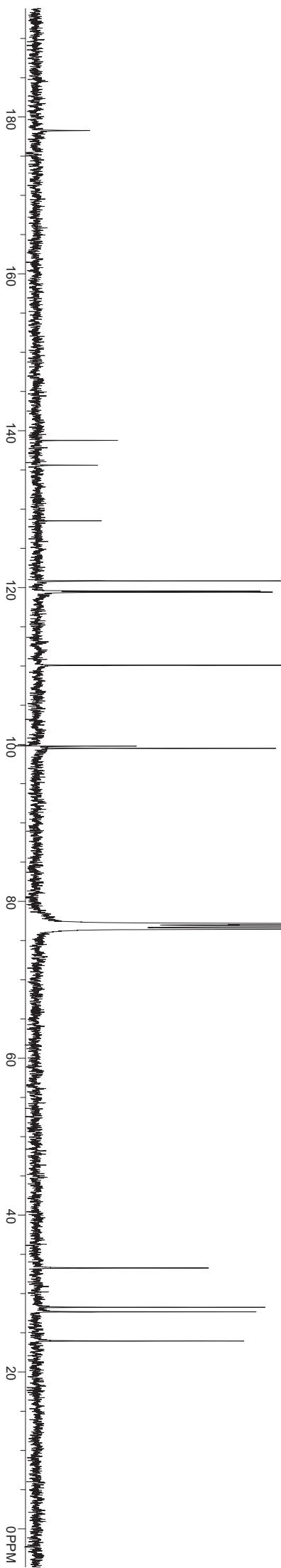
3h

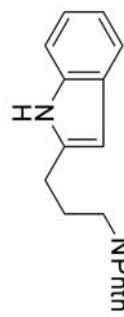
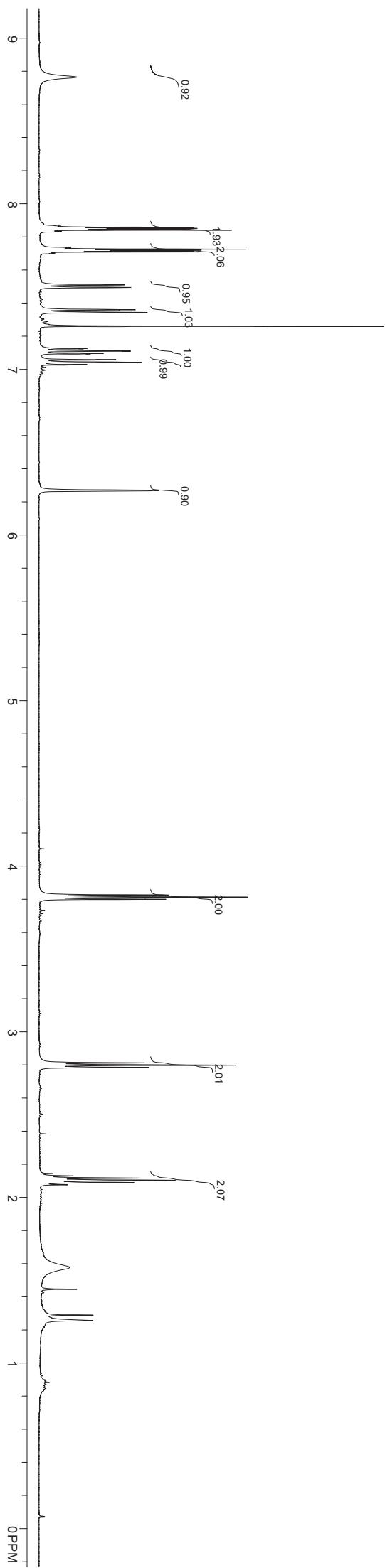


D:\Greenware\NtuS\20060731\DATA\\$J\w-5-7-CO2H-4h.h1d
new experiment
Jan 11 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usc
Relaxation delay = 4.800 sec
NA = 16
Solvent = cdcl3
FD PTS Id = 2008
PTS Id = 32788
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8003.20 Hz
AT1 = 2.50 sec
Hz per Pt1SD = 0.24 Hz
SW2 = 1.00 Hz
Hz per Pt2ndD = 1.00 Hz
O1 = 2007.1505 Hz
O2 = -5000.00 Hz
LB1 = 0.00 Hz
TP A = -52.51
B = 2.85
C = 0.00

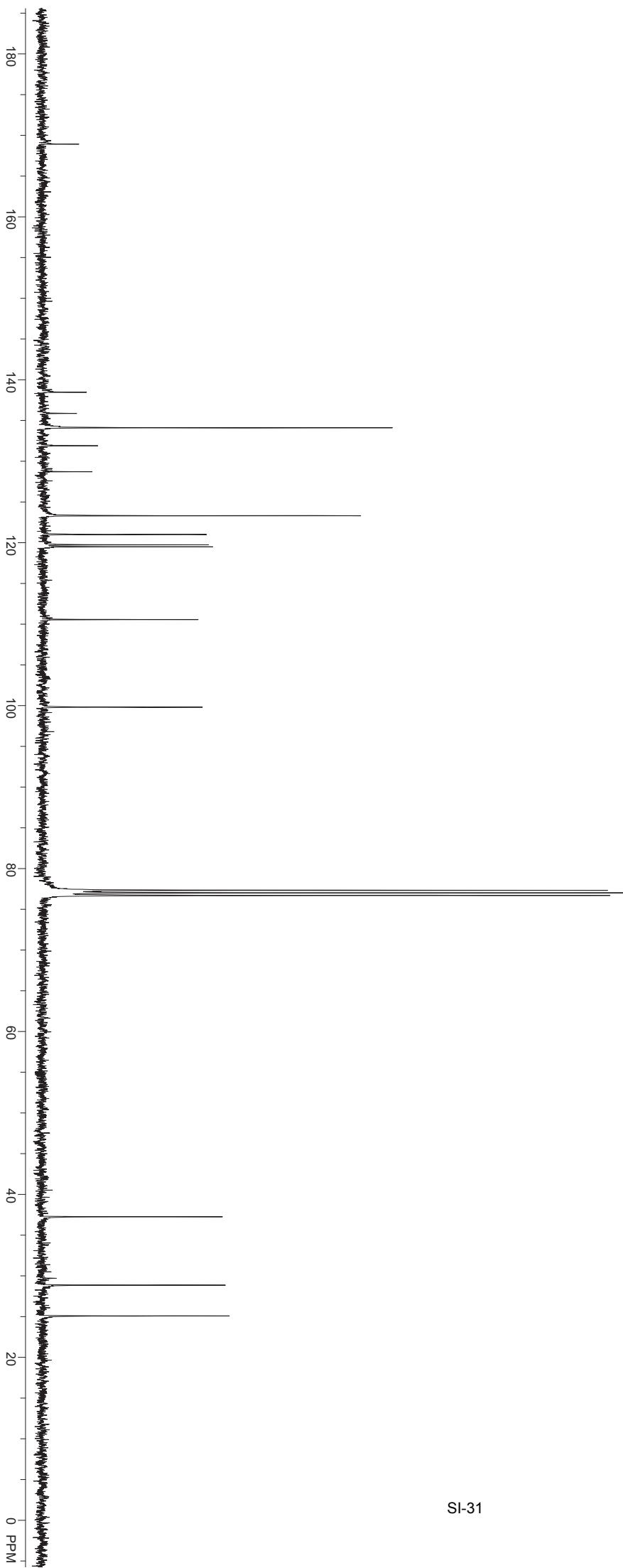


D:\Greenware\Ntu\$ 20060731\DATA\\$J\w-5-7-CO2H-cc.fid
Standard c13 run using qcp probe
Jan 12 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.000 usec
Relaxation delay = 1.300 sec
NA = 194.64
Solvent = cdcl3
FD PTS Id = 19608
PTS Id = 32788
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 27972.03 Hz
AT1 = 0.70 sec
Hz per Pt1SD = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt2ndD = 1.00 Hz
O1 = 10037.1719 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -68.20
B = 61.88
C = 0.00





D:\Greenware\Ntuus\20060731\DATA\\$J\w-5-46-cc.fid
yw-5-46-c
Feb 3 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 2562
Solvent = cdcl3
FD PTS Id = 20040
PTS Id = 32788
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 28040.66 Hz
AT1 = 1.00 sec
Hz per P1SID = 0.86 Hz
SW2 = 1.00 Hz
Hz per P12ndD = 1.00 Hz
O1 = 10056.3613 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -13.59
B = -39.38
C = 0.00



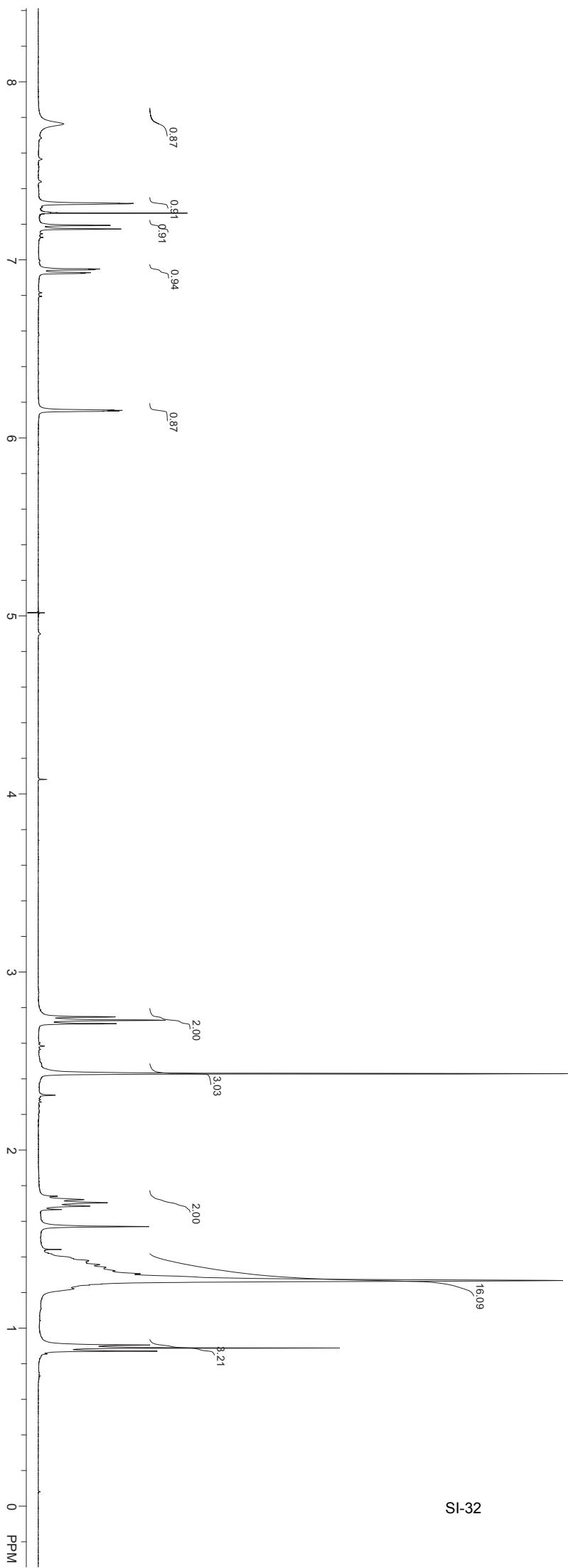
3j



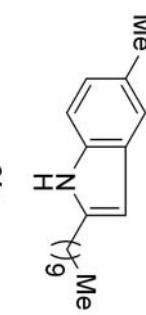
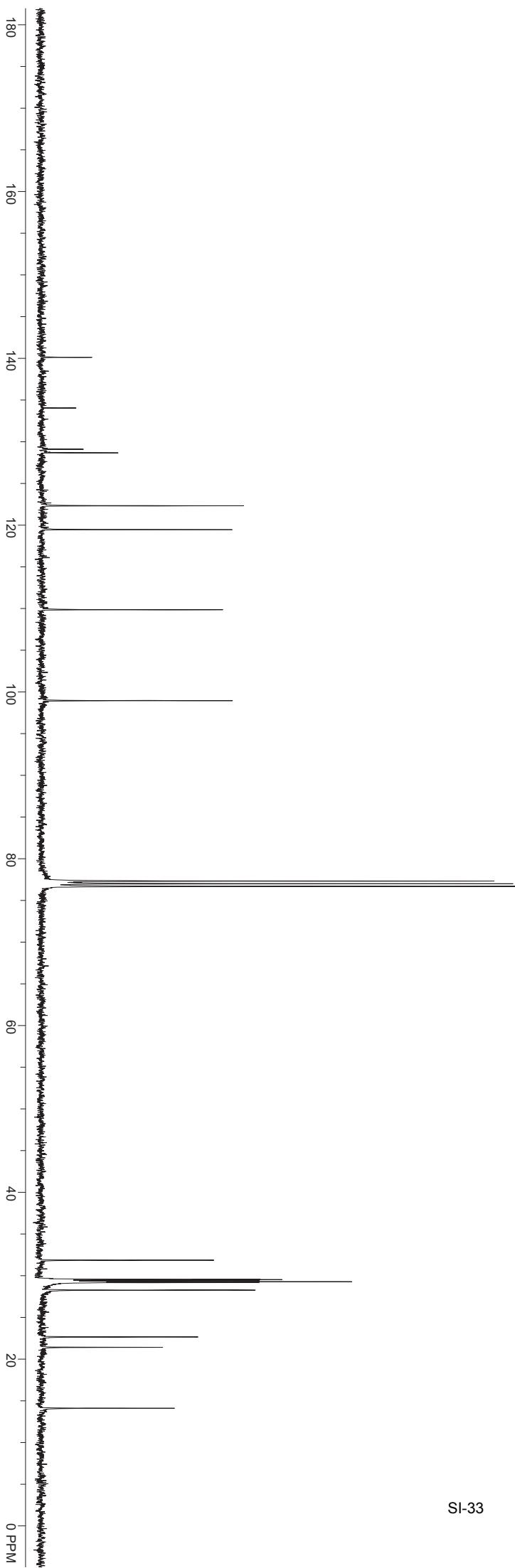
D:\Greenware\Ntu\20060731\DATA\\$J\w-5-29-Me-hh.fid
new experiment
Jan 24 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usc
Relaxation delay = 4.800 sec
NA = 14
Solvent = cdcl3
FD PTS Id = 20008
PTS Id = 32788
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8003.20 Hz
AT1 = 2.50 sec
Hz per Pt1SD = 0.24 Hz
SW2 = 1.00 Hz
Hz per Pt2ndD = 1.00 Hz
O1 = 2007.1505 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -65.43
B = 0.07
C = 0.00



3k



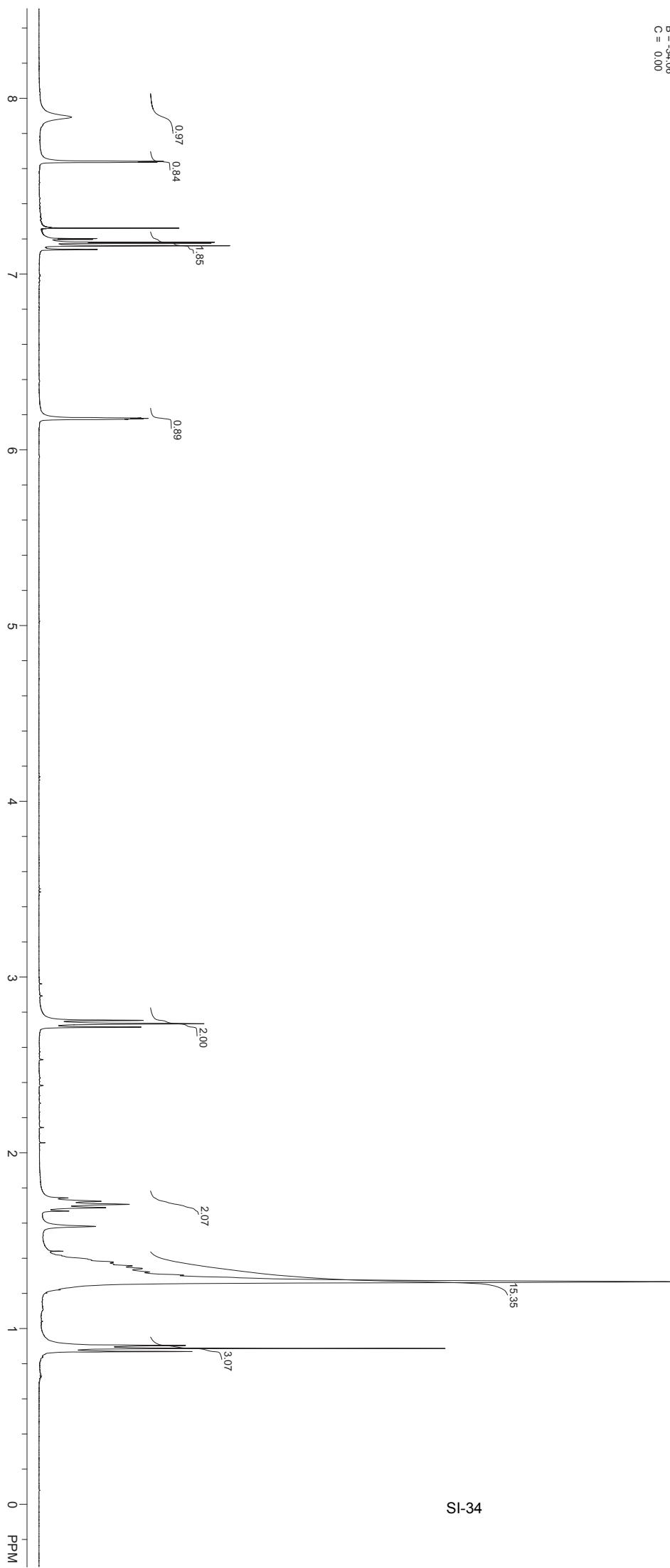
D:\Greenware\Ntuus\20060731\DATA\\$J\w-5-29-Me-c
yw-5-29-Me-c
Jan 24 2011
USER:
SOLVENT: cdcl3
Experiment: s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 2034
Solvent = cdcl3
FD PTS Id = 20040
PTS Id = 32788
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 28040.66 Hz
AT1 = 100 sec
Hz per Pt1SID = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt2ndD = 1.00 Hz
O1 = 10056.3613 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -59.53
B = -29.53
C = 0.00



D:\Greenware\Ntu\20060731\DATA\\$J\w-5-36-Br-f1.fid
new experiment
Jan 27 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usc
Relaxation delay = 4.800 sec
NA = 16
Solvent = cdcl3
FD PTS Id = 20006
PTS Id = 32788
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per P1 1SD = 0.24 Hz
SW2 = 1.00 Hz
Hz per P1 2ndD = 1.00 Hz
O1 = 2006.7504 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -40.58
B = -34.06
C = 0.00



3l



D:\Greenware\Ntu\$20060731\DATA\\$JW-5-36-Br-C.fid
Standard c13 run using qcp probe
Jan 27 2011

USER:

SOLVENT: cdcl3

Experiment = s2pul

Pulse length = 7.775 usec

Relaxation delay = 1.300 sec

NA = 1574

Solvent = cdcl3

FD PTS Id = 28040

PTS Id = 32788

F1 = 100.577232 MHz

F2 = 399.950684 MHz

SW1 = 28940.66 Hz

AT1 = 1.00 sec

Hz per P1 1sID = 0.86 Hz

SW2 = 1.00 Hz

Hz per P1 2ndD = 1.00 Hz

O1 = 10056.3604 Hz

O2 = -0.5000 Hz

LB1 = 2.00 Hz

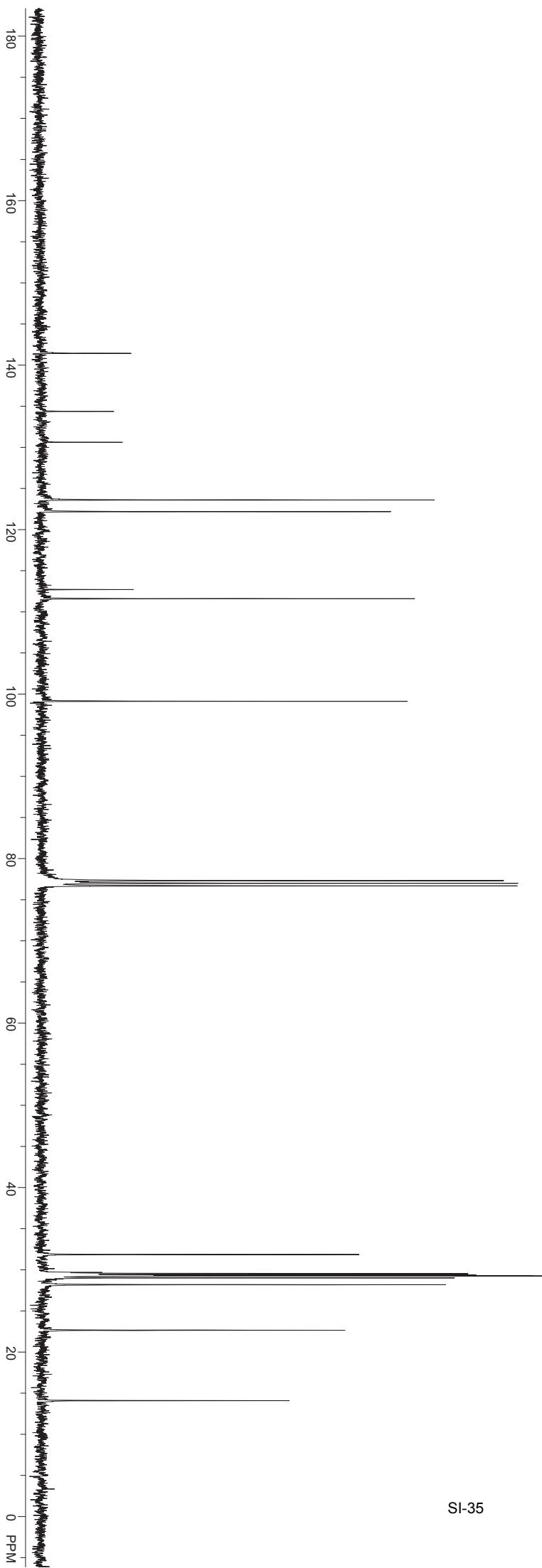
TP A = 20.63

B = -14.06

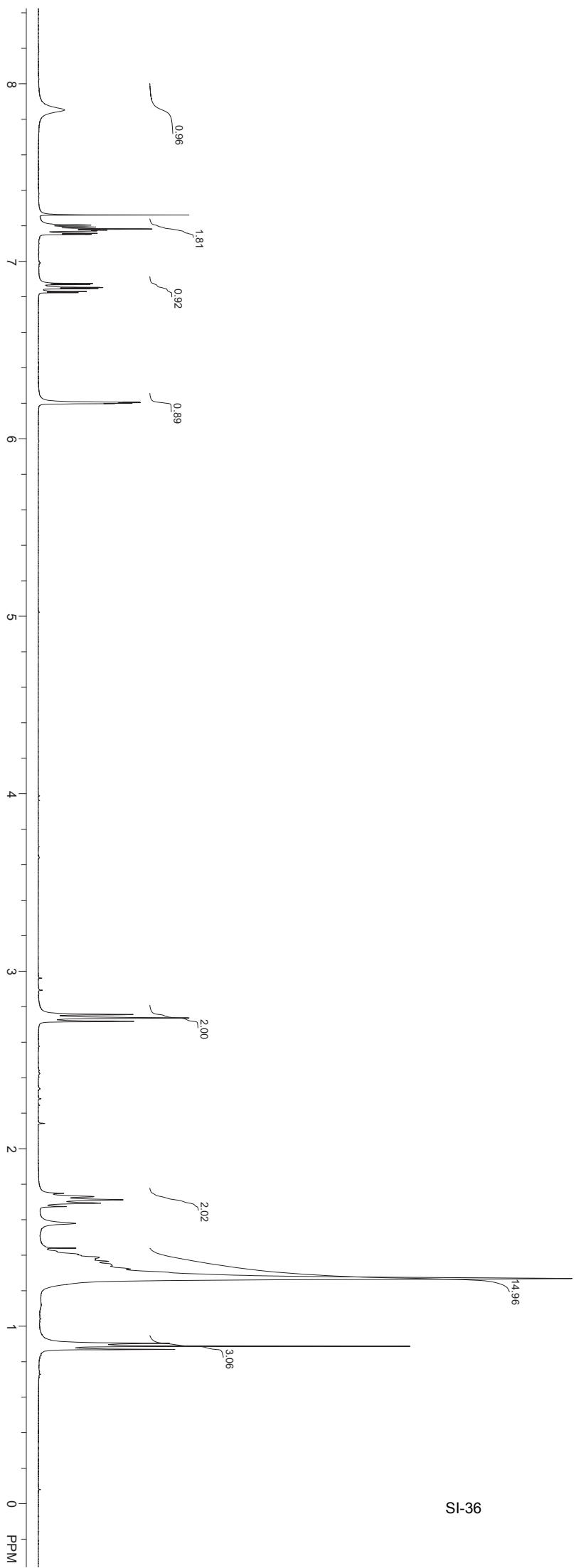
C = 0.00



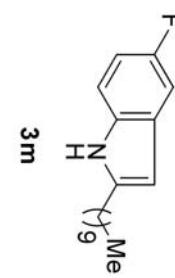
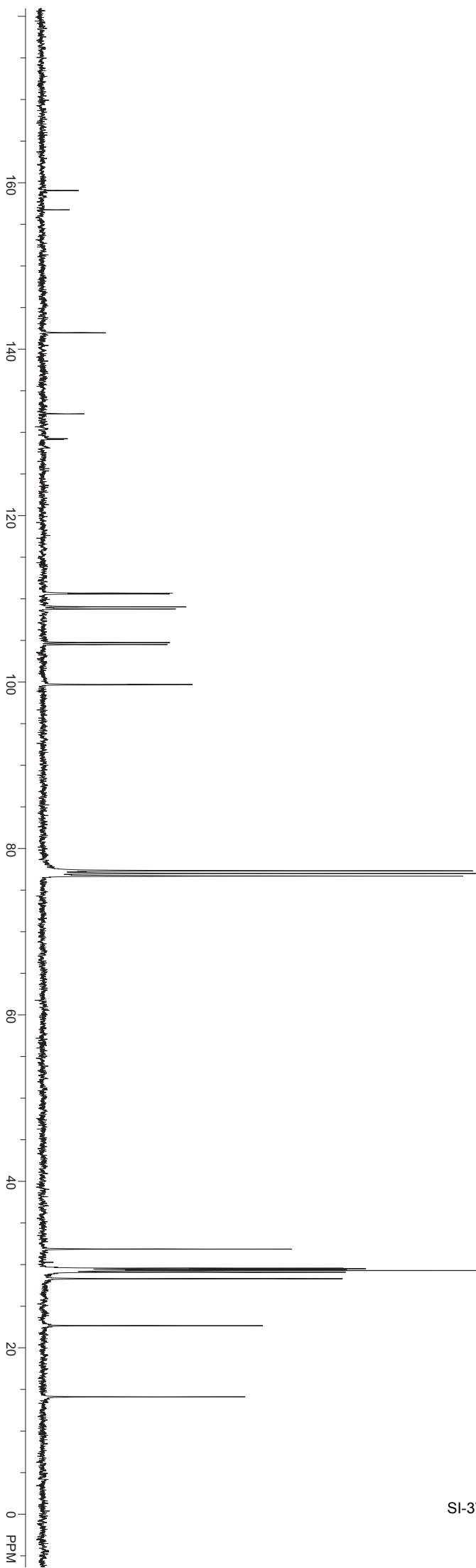
31



D:\Greenware\Ntu\20060731\DATA\\$J\w-5-36-F-h.fid
new experiment
Jan 26 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usc
Relaxation delay = 4.800 sec
NA = 12
Solvent = cdcl3
FD PTS Id = 20006
PTS Id = 32788
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per P1,1SD = 0.24 Hz
SW2 = 1.00 Hz
Hz per P1,2ndD = 1.00 Hz
O1 = 2006.7504 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -38.07
B = -36.95
C = 0.00



D:\Greenware\Ntus\20060731\DATA\\$J\w-5-36-F-c.fid
Standard c13 run using qcp probe
Jan 26 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 2486
Solvent = cdcl3
FD PTS Id = 28040
PTS Id = 32788
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 28940.66 Hz
AT1 = 1.00 sec
Hz per Pt1SD = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt2ndD = 1.00 Hz
O1 = 10056.3604 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -16.88
B = -9.84
C = 0.00



new experiment

Jan 20 2011

USER:

SOLVENT: cdcl_3

Experiment = $\text{32}\mu\text{J}$

Pulse length = 1.1663 usc

Relaxation delay = 4.8000 sec

NA = 12

Solvent = cdcl_3

FID PTS Id = 20008

PTS Id = 32768

F1 = 399.950684 MHz

F2 = 100.576279 MHz

SW1 = 8003.320 Hz

A11 = 2.50 sec

Hz per P1 1stD = 0.24 Hz

SW2 = 1.00 Hz

Hz per P2 1ndD = 1.00 Hz

O1 = 2007.1505 Hz

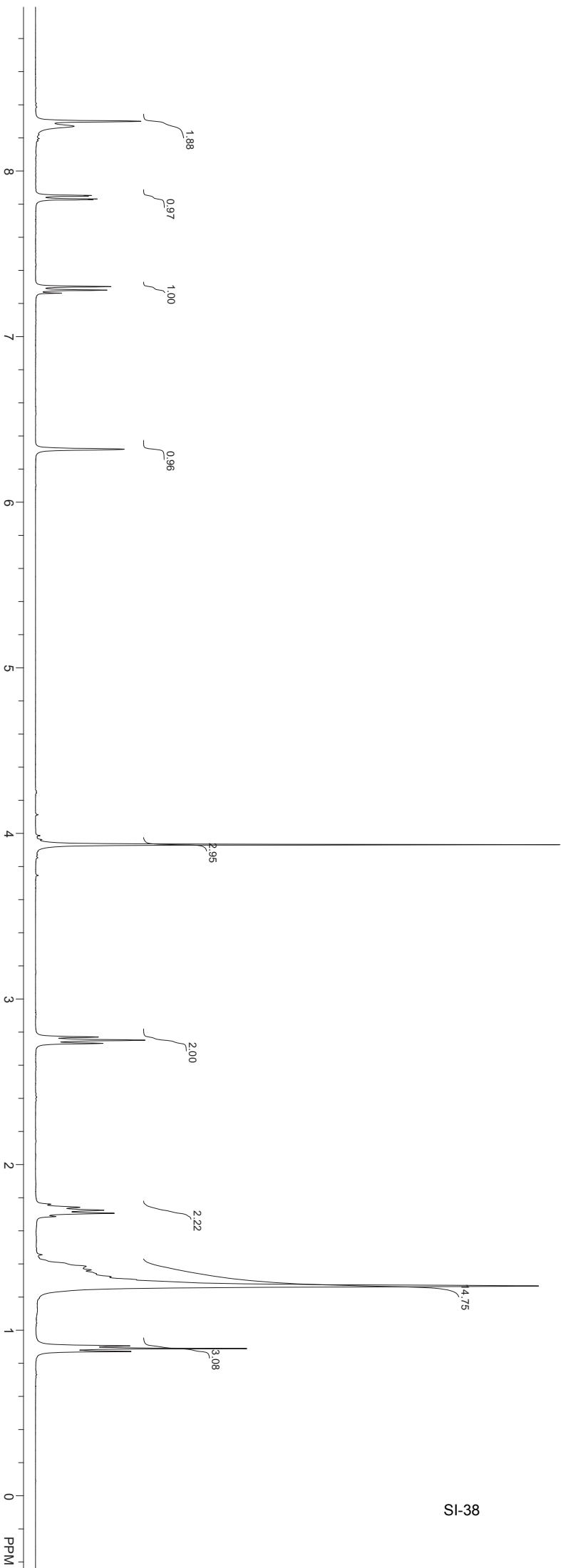
O2 = -0.5000 Hz

LB1 = 0.00 Hz

TP A = -63.06

B = -2.72

C = 0.00



C:\Users\zhang\laptop\Desktop\NMR\nuts\DATA\\$wyzz-247-nosy&d
H1_CDCL3
May 3 2011

USER:

SOLVENT: CDCl3

Experiment = NOESY1D

Pulse length = 9.000 usec

Relaxation delay = 1.000 sec

NA = 244

Solvent = CDCl3

FID PTS1d = 17012

PTS1d = 32768

F1 = 499.858551 MHz

F2 = 1.000000 MHz

SW1 = 8506.11 Hz

AT1 = 2.00 sec

Hz per Pt 1stD = 0.26 Hz

SW2 = 1.00 Hz

Hz per Pt 2ndD = 1.00 Hz

O1 = 2497.2578 Hz

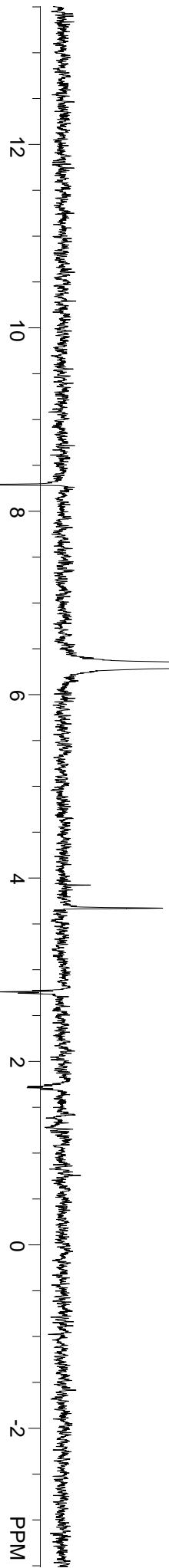
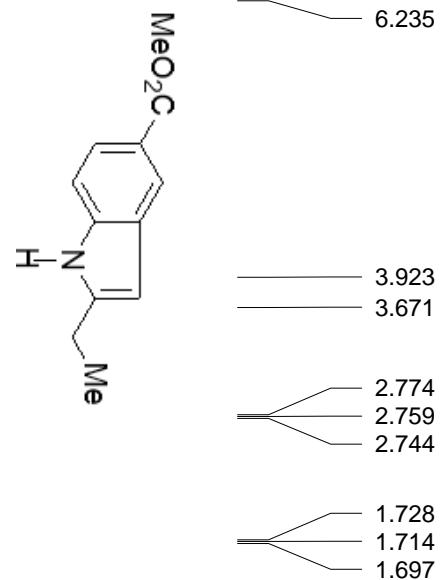
O2 = -0.5000 Hz

LB1 = 2.00 Hz

TP A = -16.69

B = -60.75

C = 0.00



D:\Greenware\NtuS 20060731\DATA\\$J\w-5-27-E.c.fid
Standard c13 run using qcp probe
Jan 20 2011

USER:

SOLVENT:

Experiment = cdcl3

Pulse length = 7.000 usec

Relaxation delay = 1.000 sec

NA = 84

Solvent = cdcl3

FID PTS Id = 19608

PTS Id = 32788

F1 = 100.577232 MHz

F2 = 399.950684 MHz

SW1 = 27972.03 Hz

AT1 = 0.70 sec

Hz per P1 1sID = 0.86 Hz

SW2 = 1.00 Hz

Hz per P1 2ndD = 1.00 Hz

O1 = 10054.1162 Hz

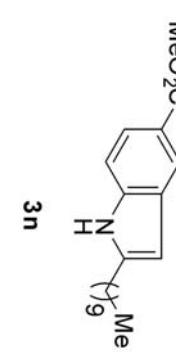
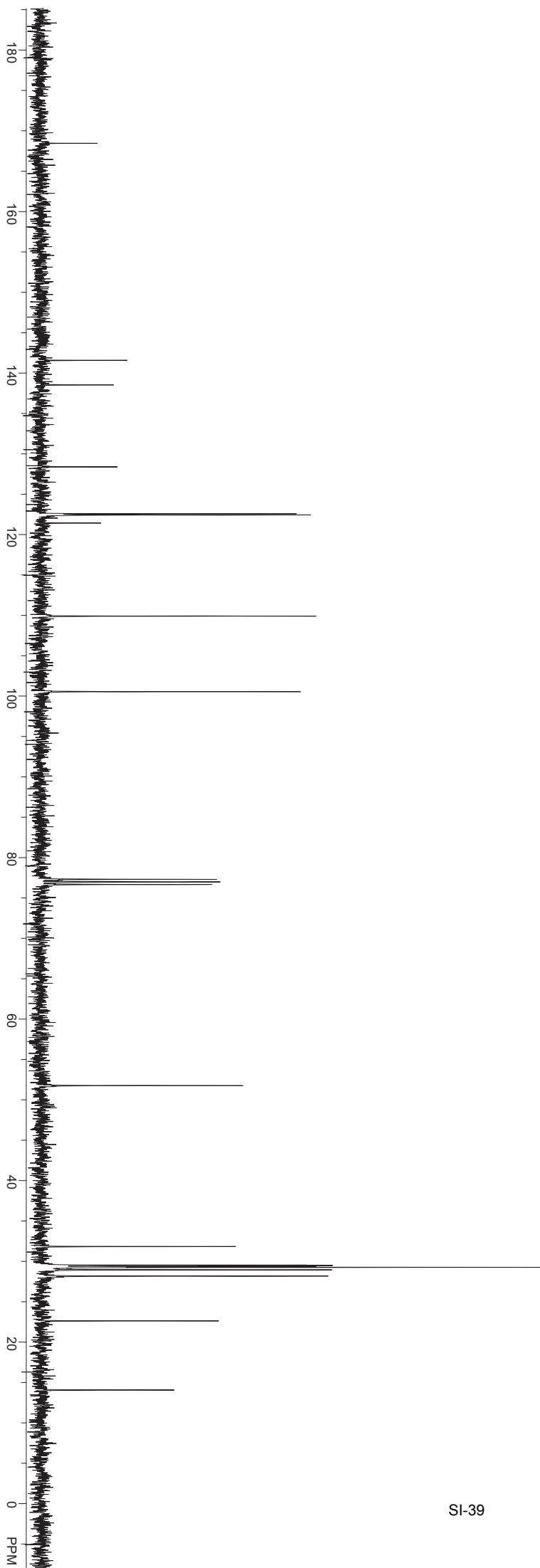
O2 = -0.5000 Hz

LB1 = 2.00 Hz

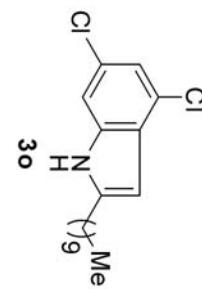
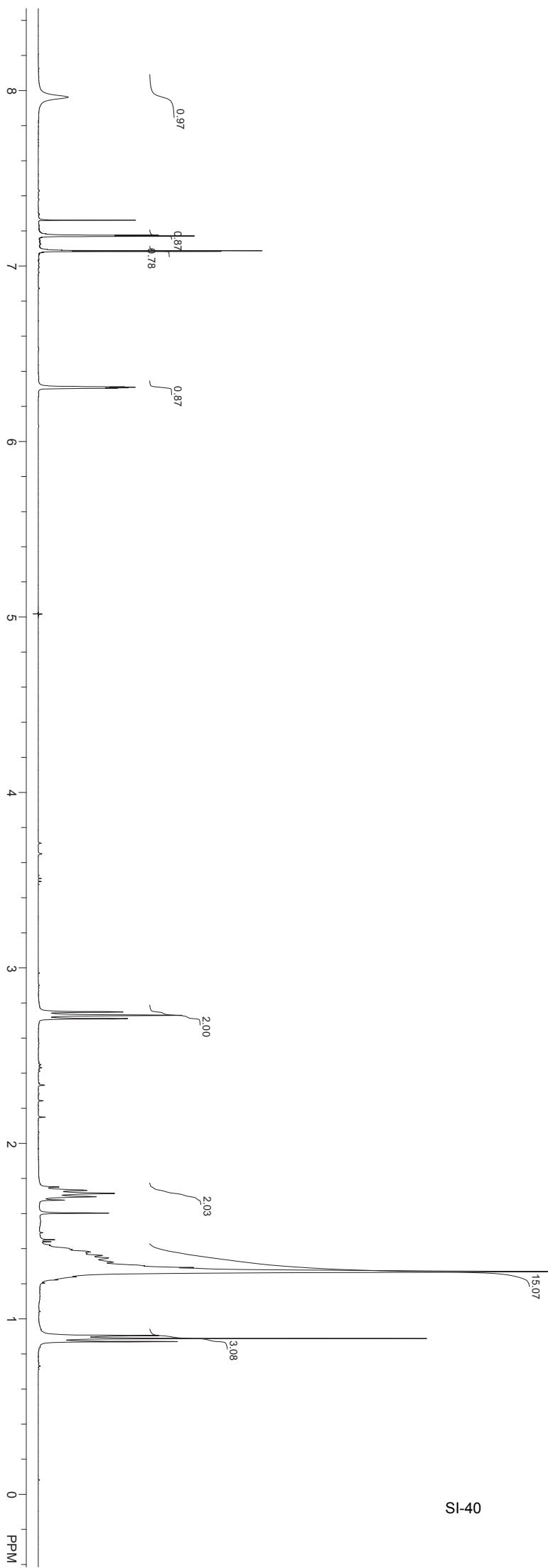
TP A = -5.63

B = 14.06

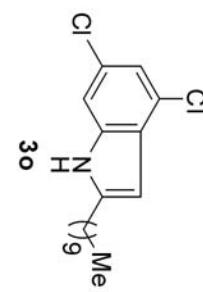
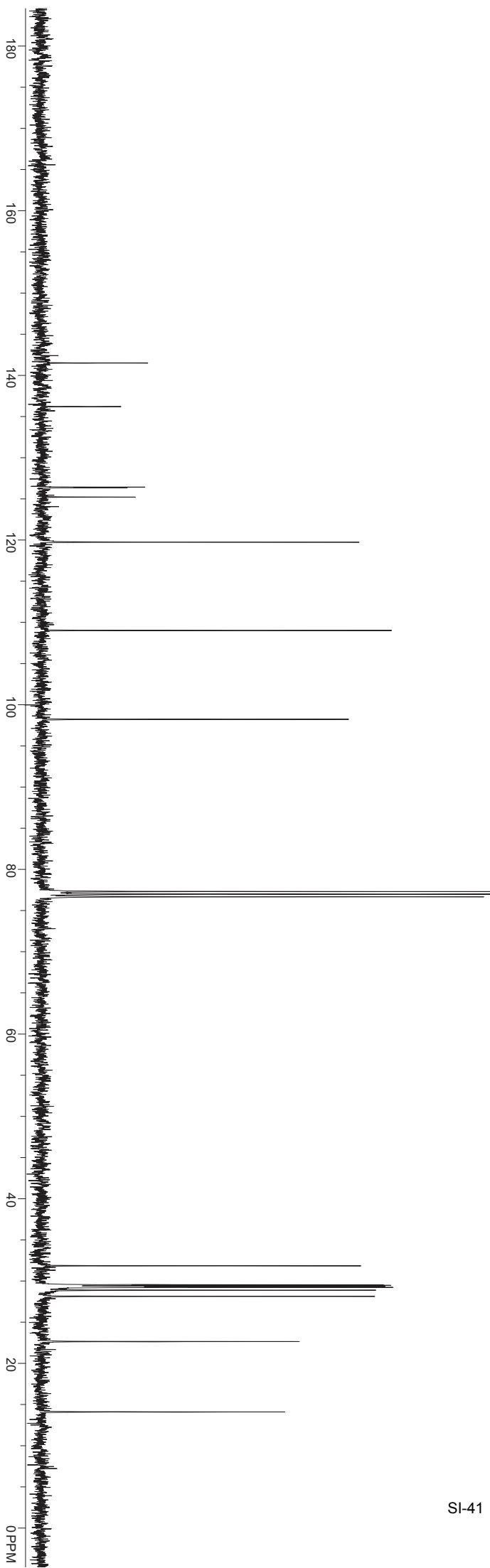
C = 0.00



D:\Greenware\Ntu\20060731\DATA\\$J\w-5-40-Ch.fid
new experiment
Jan 30 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usc
Relaxation delay = 4.800 sec
NA = 10
Solvent = cdcl3
FD PTS Id = 20006
PTS Id = 32788
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per P1SID = 0.24 Hz
SW2 = 1.00 Hz
Hz per P12ndD = 1.00 Hz
O1 = 2006.7504 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -39.94
B = -33.79
C = 0.00



D:\Greenware\Ntus\20060731\DATA\\$J\w-5-40-Clc.fid
yw-5-40-Clc
Jan 30 2011
USER:
SOLVENT: cdcl3
Experiment: s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 226
Solvent = cdcl3
FD PTS Id = 28040
PTS Id = 32788
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 28940.66 Hz
AT1 = 1.00 sec
Hz per P1SID = 0.86 Hz
SW2 = 1.00 Hz
Hz per P12ndD = 1.00 Hz
O1 = 10055.5137 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -76.41
B = 9.84
C = 0.00



5mm IDP

Jan 19 2011

USER:

SOLVENT: cdcl₃

Experiment = s2pul

Pulse length = 7.075 usec

Relaxation delay = 4.800 sec

NA = 16

Solvent = cdcl₃

FD PTS Id = 20006

PTS Id = 32788

F1 = 498.85851 MHz

F2 = 128.700813 MHz

SW1 = 8002.40 Hz

AT1 = 2.50 sec

Hz per P1,1SD = 0.24 Hz

SW2 = 1.00 Hz

Hz per P1,2ndD = 1.00 Hz

O1 = 2496.3250 Hz

O2 = -0.5000 Hz

LB1 = 0.00 Hz

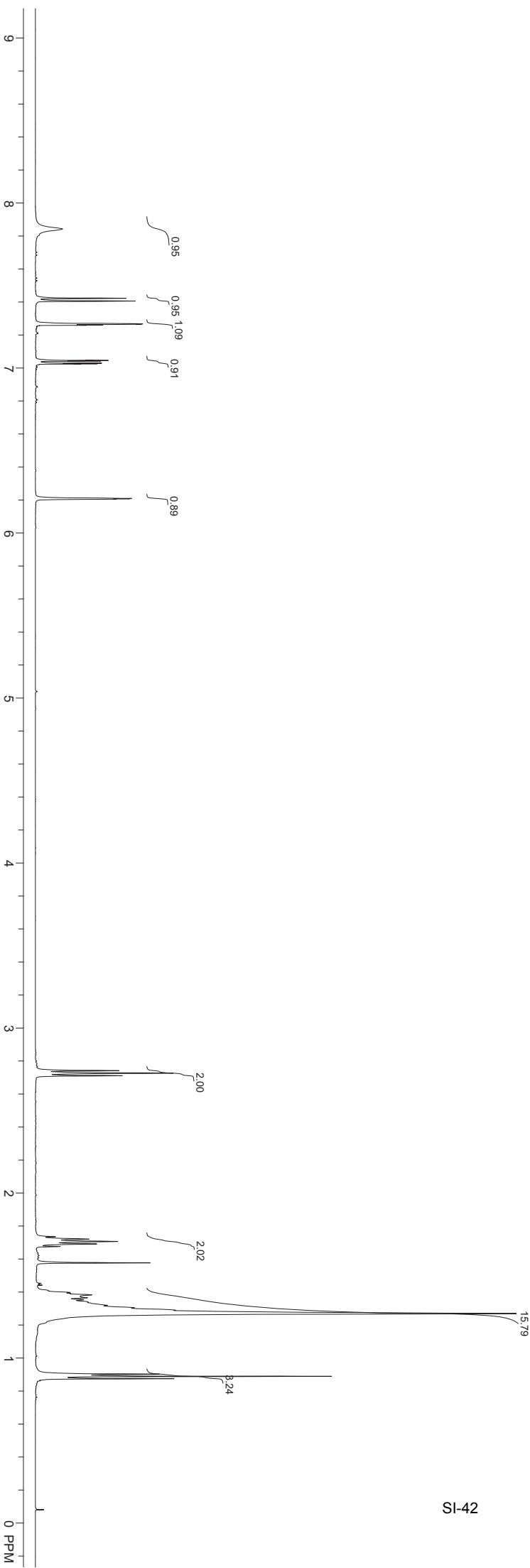
TP A = -128.46

B = 5.41

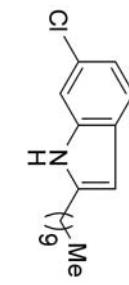
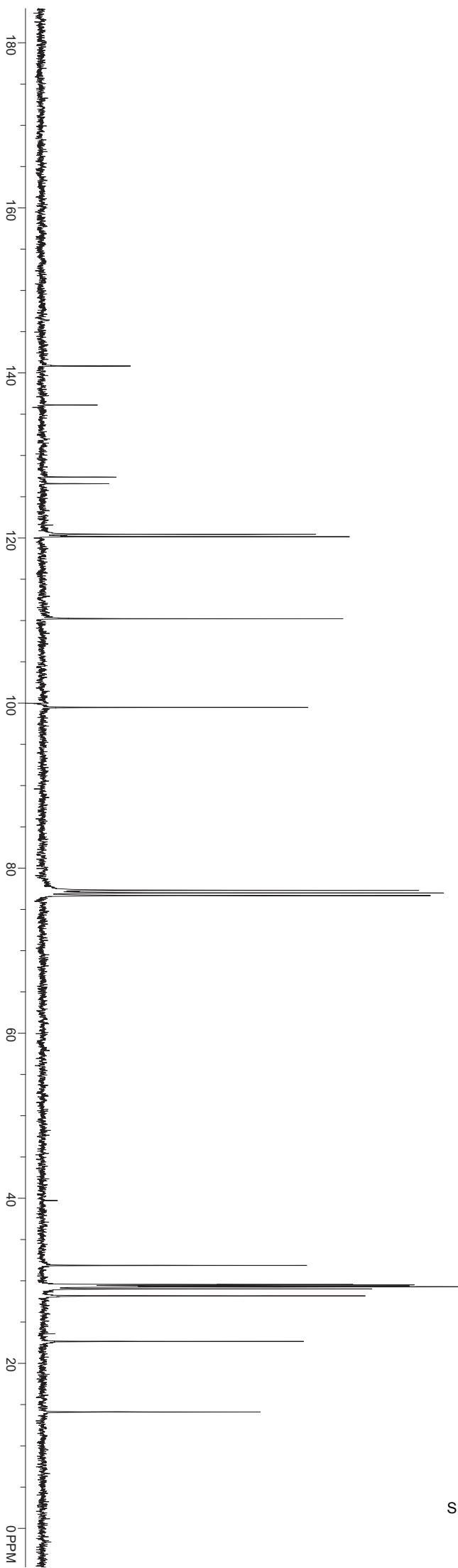
C = 0.00



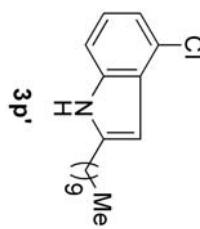
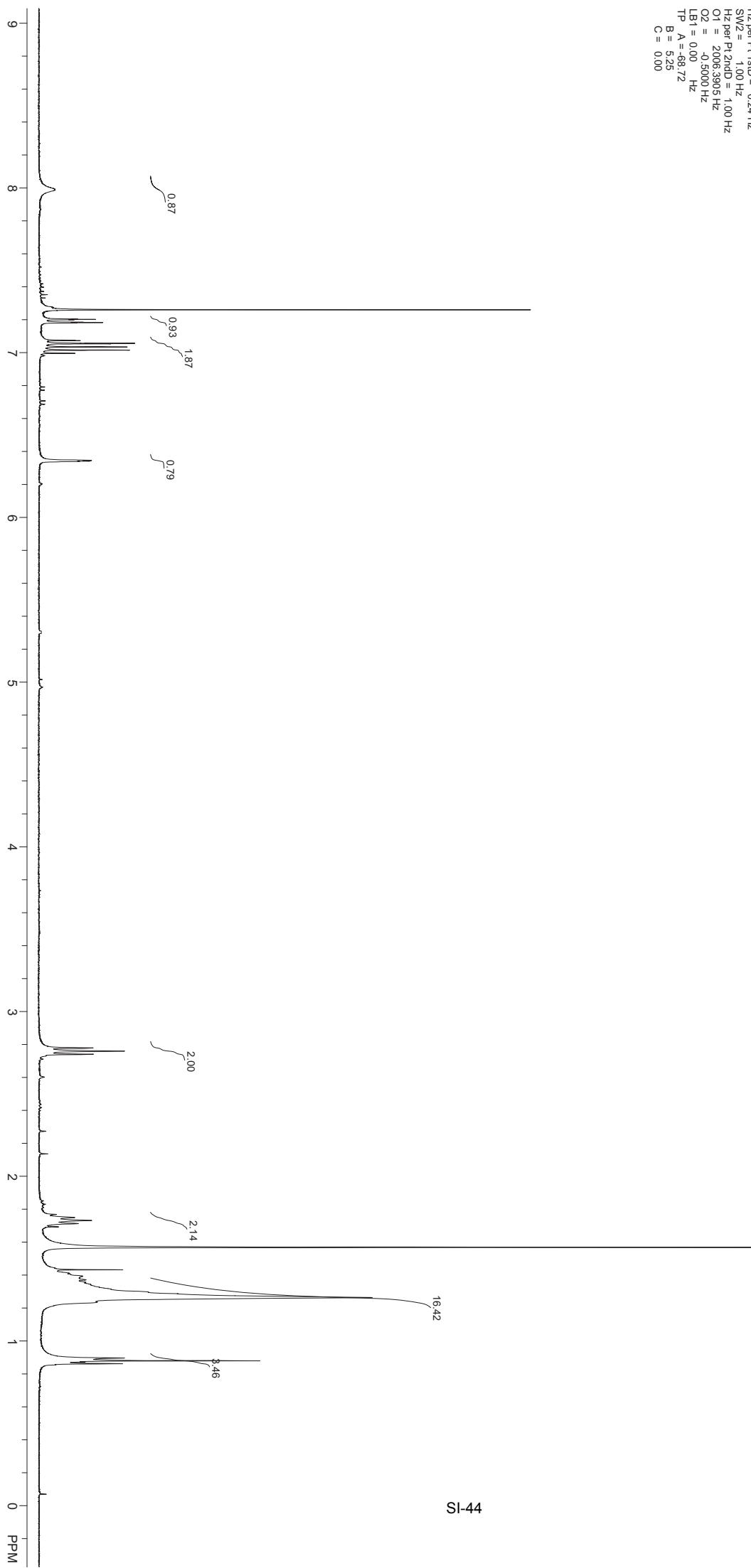
3p



D:\Greenware\Ntu\20060731\DATA\\$J\w-5-25-1-01.fid
yw-5-25-1.c
Jan 19 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.000 usec
Relaxation delay = 1.000 sec
NA = 1432
Solvent = cdcl3
FD PTS Id = 19608
PTS Id = 32788
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 27972.03 Hz
AT1 = 0.70 sec
Hz per Pt1SID = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt2ndD = 1.00 Hz
O1 = 100.053.3262 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -24.84
B = -26.72
C = 0.00



D:\Greenware\Ntu\us.20060731\DATA\\$J\w-5-25-2-h-400.fid
new experiment
Jan 19 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 16
Solvent = cdcl3
FD PTS Id = 20008
PTS Id = 32788
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8003.20 Hz
AT1 = 2.50 sec
Hz per P1,1SD = 0.24 Hz
SW2 = 1.00 Hz
Hz per P1,2ndD = 1.00 Hz
O1 = 2006.39051 Hz
O2 = -0.50000 Hz
LB1 = 0.00 Hz
TP A = -68.72
B = 5.25
C = 0.00



D:\Greenware\NtuS 20060731\DATA\\$J\w-5-25-2-Cl-cc.fid
Standard c13 run using qcp probe
Jan 21 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.000 usec
Relaxation delay = 1.000 sec
NA = 268.10
Solvent = cdcl3
FD PTS Id = 19581
PTS Id = 32788
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 27972.03 Hz
AT1 = 0.70 sec
Hz per Pt1SD = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt2ndD = 1.00 Hz
O1 = 10056.1797 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -7.29
B = -39.59
C = 0.00

