

Supporting Information

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

Yanzhao Wang, Longwu Ye and Liming Zhang

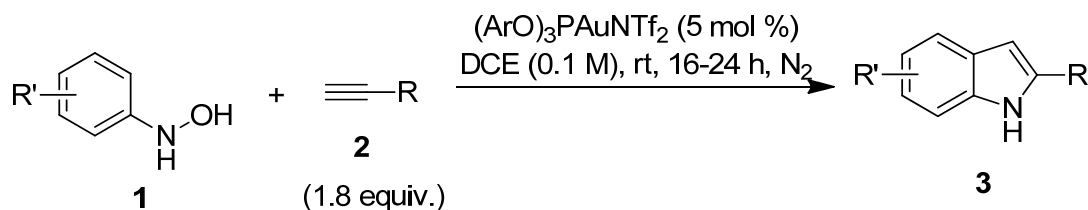
Department of Chemistry and Biochemistry, University of California, Santa Barbara,
California, 93106

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

General. Ethyl acetate (ACS grade), hexanes (ACS grade), diethyl ether (ACS grade), NH_4OH (29.4% in H_2O , 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 ^{13}C NMR spectra were recorded on a Varian 500 MHz Unity plus spectrometer and a Varian 400 MHz spectrometer using residue solvent peaks as internal standards. Infrared spectra were recorded with a Perkin Elmer FT-IR spectrum 2000 spectrometer and are reported in reciprocal centimeter (cm^{-1}). Mass spectra were recorded with Waters micromass ZQ detector using electrospray method.

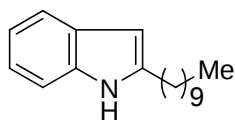
N-aryl hydroxylamines were prepared according to the literature procedure (D. A. Evans, H.-J. Song, K. R. Fandrick, *Org. Lett.* **2006**, 8, 3351-3354).

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



An oven-dried vial was charged with *N*-arylhydroxylamine **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 $(\text{ArO})_3\text{PAuNTf}_2$ (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 (eluent: ethyl acetate: hexanes = 1: 100) to give the desired indole **3**.

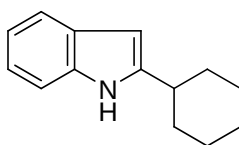
2-Decyl-1*H*-indole



3a

Compound **3a** was prepared in 84 % yield according to the general procedure (eluent: 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.

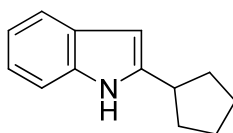
2-Cyclohexyl-1*H*-indole



3b

Compound **3b** was prepared in 77 % yield according to the general procedure (eluent: 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.

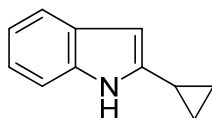
2-Cyclopentyl-1*H*-indole



3c

Compound **3c** was prepared in 62 % yield according to the general procedure (eluent: 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.

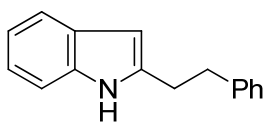
2-Cyclopropyl-1*H*-indole



3d

Compound **3d** was prepared in 70 % yield according to the general procedure (eluent: 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 $[\text{C}_{11}\text{H}_{11}\text{N}]^+$: 180.08; Found: 180.18

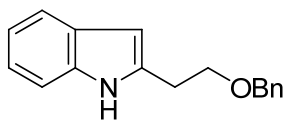
2-Phenethyl-1*H*-indole



3e

Compound **3e** was prepared in 89 % yield according to the general procedure (eluent: 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.

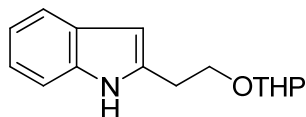
2-(2-(Benzyloxy)ethyl)-1*H*-indole



3f

Compound **3f** was prepared in 84 % yield according to the general procedure (eluent: 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.

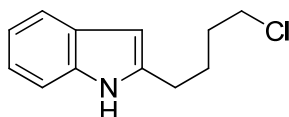
2-(2-(Tetrahydro-2H-pyran-2-yloxy)ethyl)-1H-indole



3g

Compound **3g** was prepared in 67 % yield according to the general procedure (eluent: 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.

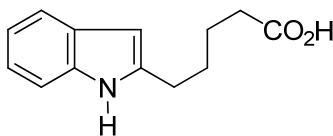
2-(4-Chlorobutyl)-1H-indole



3h

Compound **3c** was prepared in 62 % yield according to the general procedure (eluent: 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.

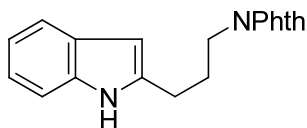
5-(1*H*-indol-2-yl)pentanoic acid



3i

Compound **3i** was prepared in 73 % yield according to the general procedure (eluent: 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.

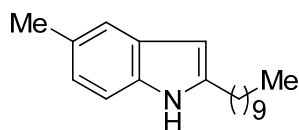
2-(3-(1*H*-indol-2-yl)propyl)isoindoline-1,3-dione



3j

Compound **3j** was prepared in 72 % yield according to the general procedure (eluent: 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.

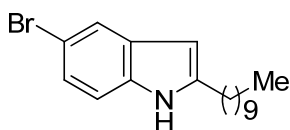
2-Decyl-5-methyl-1H-indole



3k

Compound **3k** was prepared in 64 % yield according to the general procedure (eluent: 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.

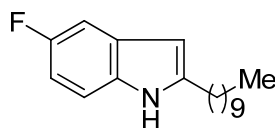
5-Bromo-2-decyl-1H-indole



3l

Compound **3l** was prepared in 86 % yield according to the general procedure (eluent: 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.

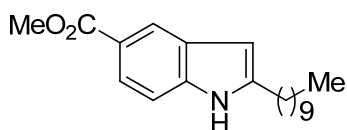
2-Decyl-5-fluoro-1*H*-indole



3m

Compound **3m** was prepared in 82 % yield according to the general procedure (eluent: ethyl acetate: hexanes = 1: 100). ¹H NMR (400 MHz, CDCl₃) 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); ¹³C NMR (100 MHz, CDCl₃) 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 [C₁₈H₂₆FNNa]⁺: 298.19; Found: 298.16.

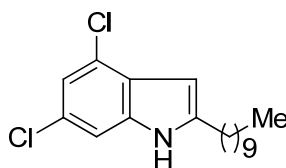
Methyl 2-decyl-1*H*-indole-5-carboxylate



3n

Compound **3n** was prepared in 76 % yield according to the general procedure (eluent: ethyl acetate: hexanes = 1: 100). ¹H NMR (400 MHz, CDCl₃) 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); ¹³C NMR (100 MHz, CDCl₃) 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.

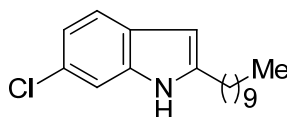
4,6-Dichloro-2-decyl-1H-indole



3o

Compound **3o** was prepared in 63 % yield according to the general procedure (eluent: 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.

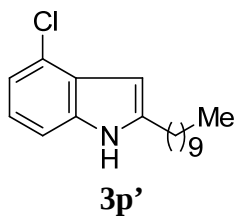
6-Chloro-2-decyl-1H-indole



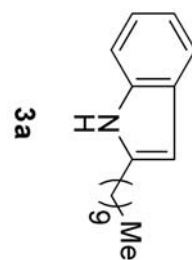
3p

Compound **3p** and **3p'** was prepared in 85 % yield (1.3: 1) according to the general procedure (eluent: 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.

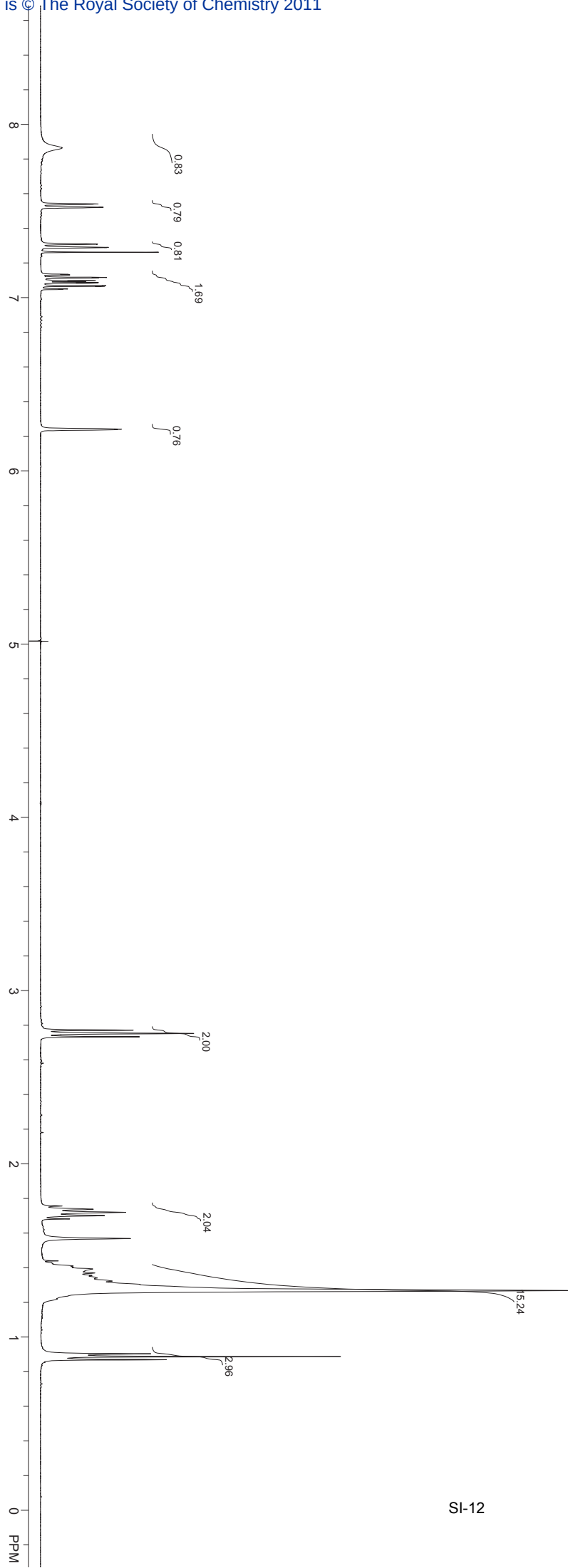
4-Chloro-2-decyl-1H-indole



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.

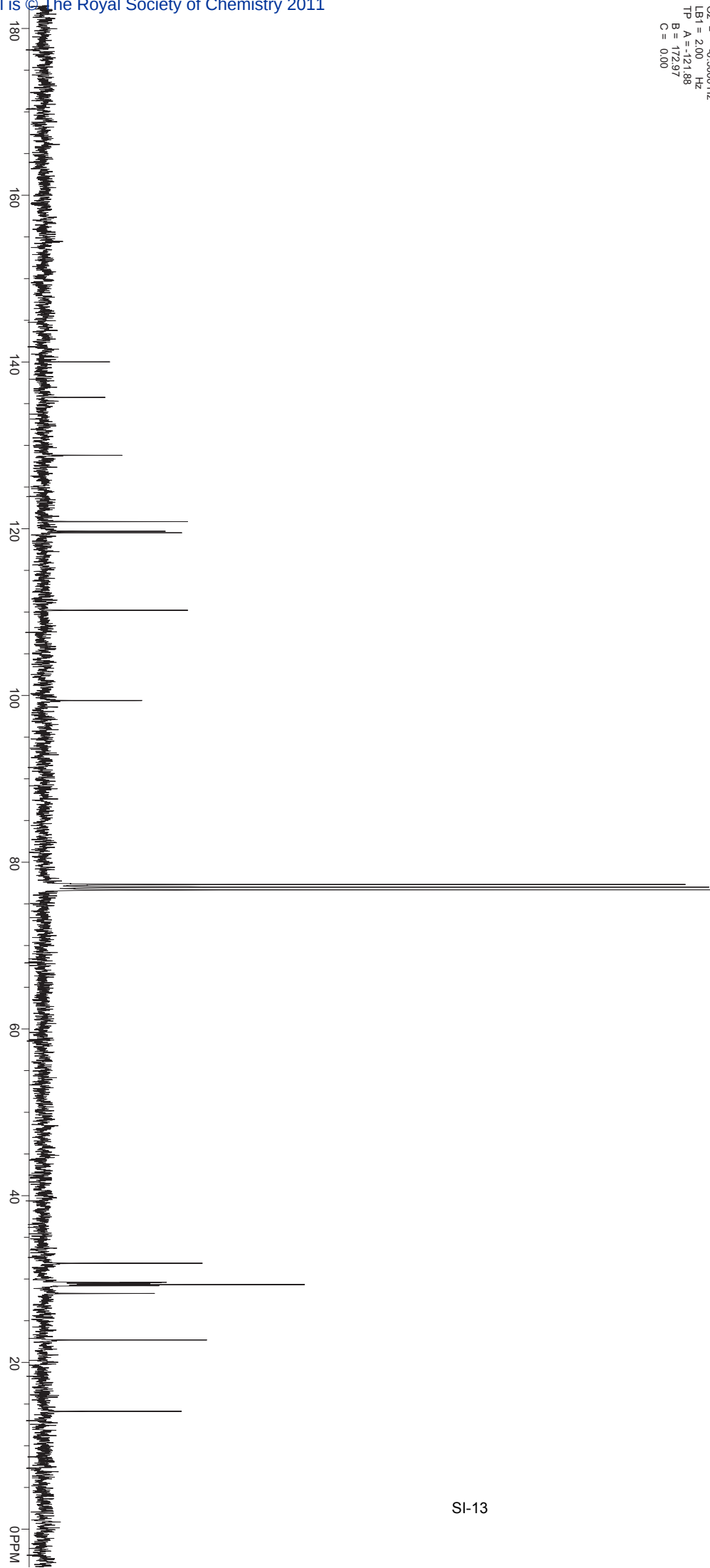
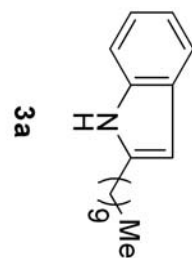


D:\Greenware\Nlus 20080731\DATA\Swy23-60-pro-h1.fid
new experiment
Apr 1 2011
USER:
SOLVENT: cdd3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 2.000 sec
NA = 16
Solvent = cdd3
FID P1S1d = 20006
PT1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt 1s1d = 0.24 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndd = 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

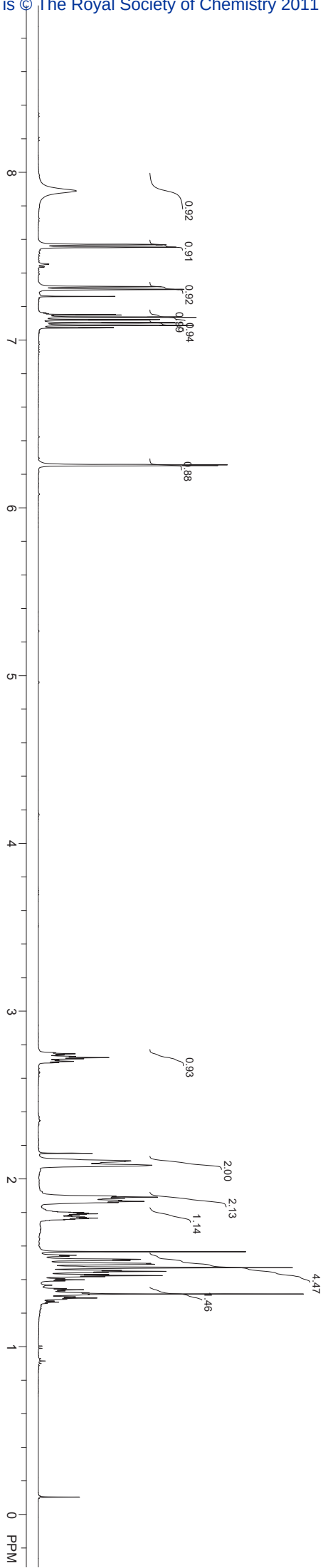
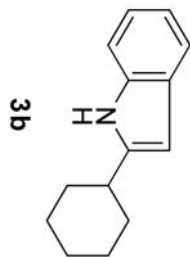


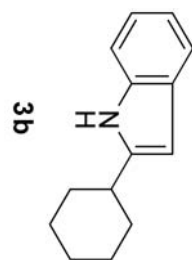
D:\Greenware\Nlus 20080731\DATA\Swy23-60-pro-c13.fid
Standard c13 run using qnp probe
Mar 31 2011

USER:
SOLVENT: cddc3
Experiment: s2pul
Pulse length = 9.500 usec
Relaxation delay = 5.000 sec
NA = 108
Solvent = cddc3
FID P1S1d = 16000
PT1S1d = 16384
F1 = 100.576706 MHz
F2 = 399.949585 MHz
SW1 = 25000.00 Hz
AT1 = 0.64 sec
Hz per Pt 1s1D = 1.53 Hz
SW2 = 1.00 Hz
Hz per Pt 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

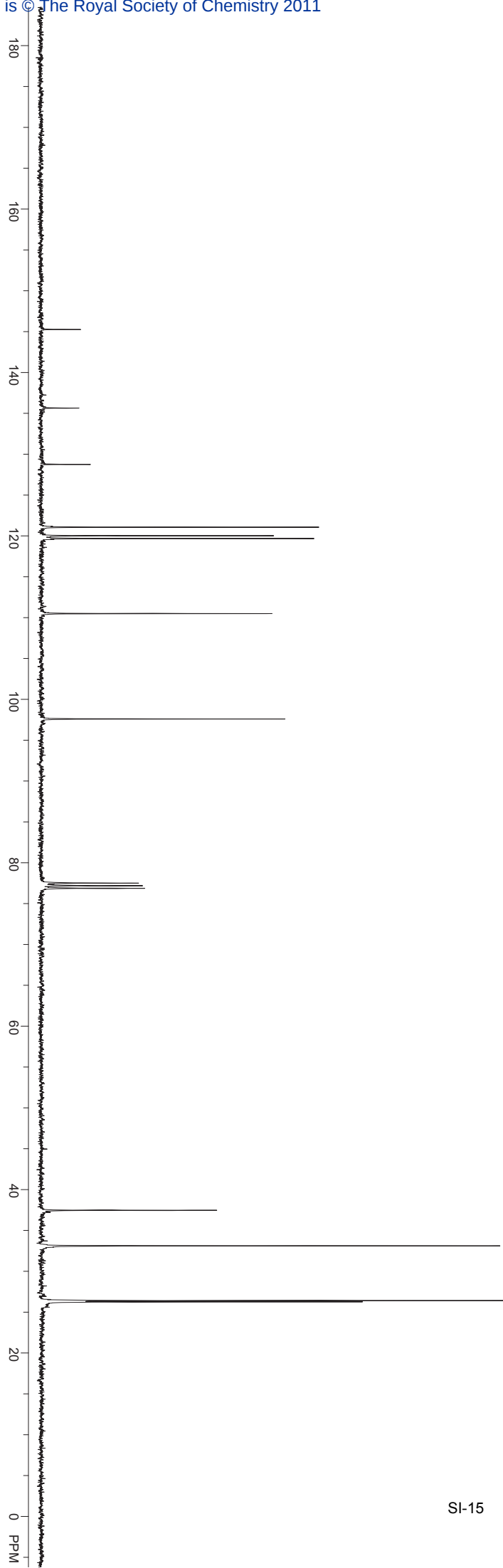


D:\Greenware\Nius 20080731\DATA\Sym-5-17-6ring-15-h.fid
Scan IDP
Jan 16 2011
USER:
SOLVENT: cdd3
Experiment = s2pul
Pulse length = 7.075 usec
Relaxation delay = 4.800 sec
NA = 16
Solvent = cdd3
FID P1S1d = 20006
PT1d = 32768
F1 = 499.858551 MHz
F2 = 125.700813 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per P1 1sID = 0.24 Hz
SW2 = 1.00 Hz
Hz per P1 2nd = 1.00 Hz
O1 = 2496.1272 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -128.44
B = 2.81
C = 0.00





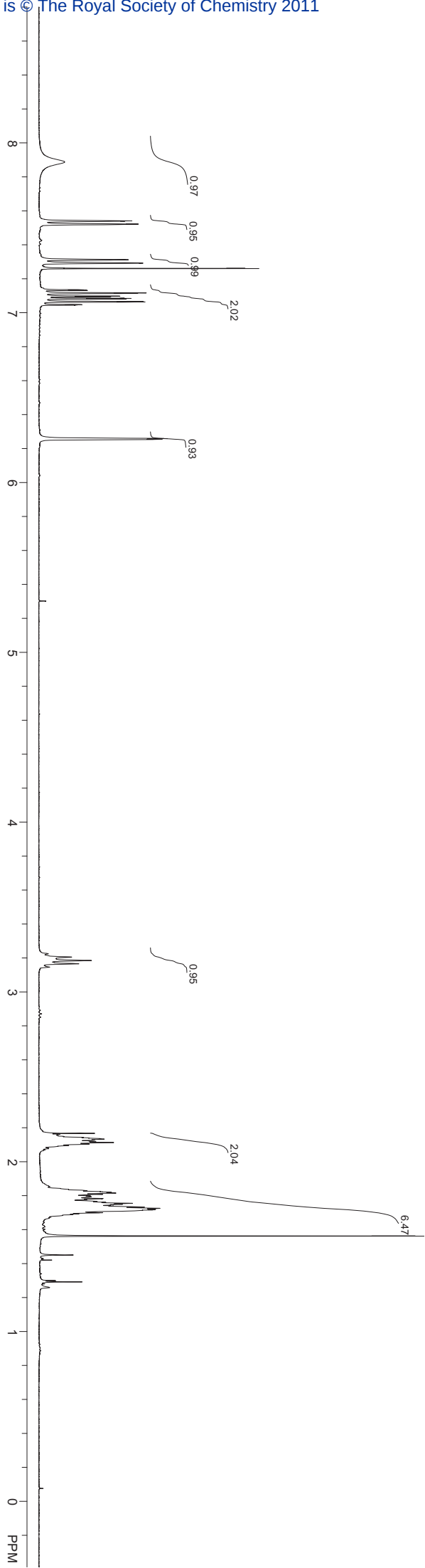
D:\Greenware\Nlus 20080731\DATA\5yw-5-17-6ring-cc2.fid
Standard c13 run using qnp probe
Jan 29 2011
USER:
SOLVENT: cdc13
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 934
Solvent = cdc13
FID P1SID = 28040
PTSID = 32768
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 28040.66 Hz
AT1 = 1.00 sec
Hz per P1 1SID = 0.86 Hz
SW2 = 1.00 Hz
Hz per P1 2nD = 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\Nlus 20080731\DATA\$\yw-5-1-9.fid
new experiment
Jan 5 2011
USER:
SOLVENT: cddc3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 16
Solvent = cddc3
FID P1S1d = 20008
PT1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8003.20 Hz
AT1 = 2.50 sec
Hz per Pt 1s1d = 0.24 Hz
SW2 = 1.00 Hz
Hz per Pt 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



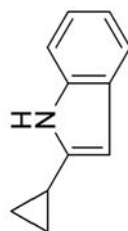
D:\Greenware\Nlus 20080731\DATA\yw-5-1-9-cc.fid
yw-5-1-9main-c
Jan 9 2011
USER:
SOLVENT: cdc13
Experiment = s2pul
Pulse length = 7.000 usec
Relaxation delay = 1.300 sec
NA = 1888
Solvent = cdc13
FID P1S1d = 19608
PT1S1d = 32768
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 27972.03 Hz
AT1 = 0.70 sec
Hz per Pt 1s1D = 0.85 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 10054.9697 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -29.53
B = 30.94
C = 0.00



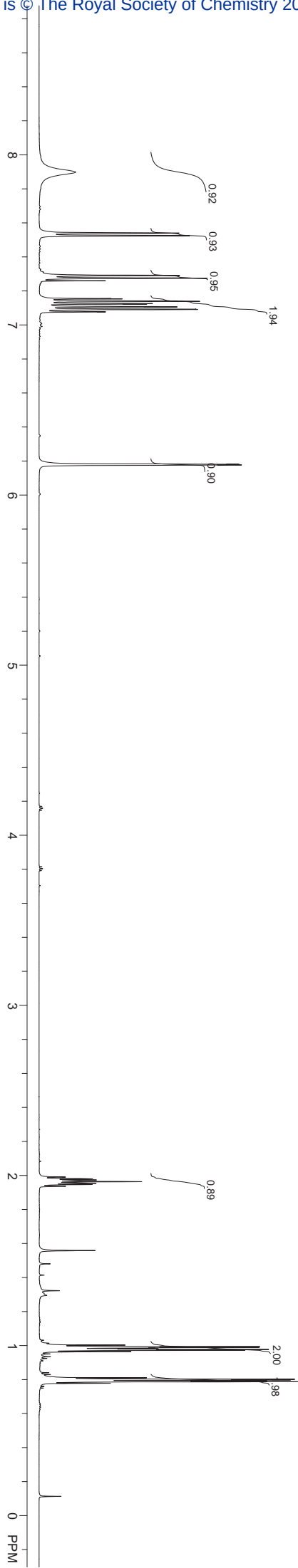
3c



D:\Greenware\Nlus 20080731\DATA\5yw-5-1-3mem-h.fid
5mm IDP
Jan 6 2011
USER:
SOLVENT: cdd3
Experiment = s2pul
Pulse length = 7.075 usec
Relaxation delay = 4.800 sec
NA = 8
Solvent = cdd3
FID P1S1d = 20006
PT1d = 32768
F1 = 499.858551 MHz
F2 = 125.700813 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt 1s1d = 0.24 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndd = 1.00 Hz
O1 = 2495.8831 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -82.97
B = 14.1
C = 0.00



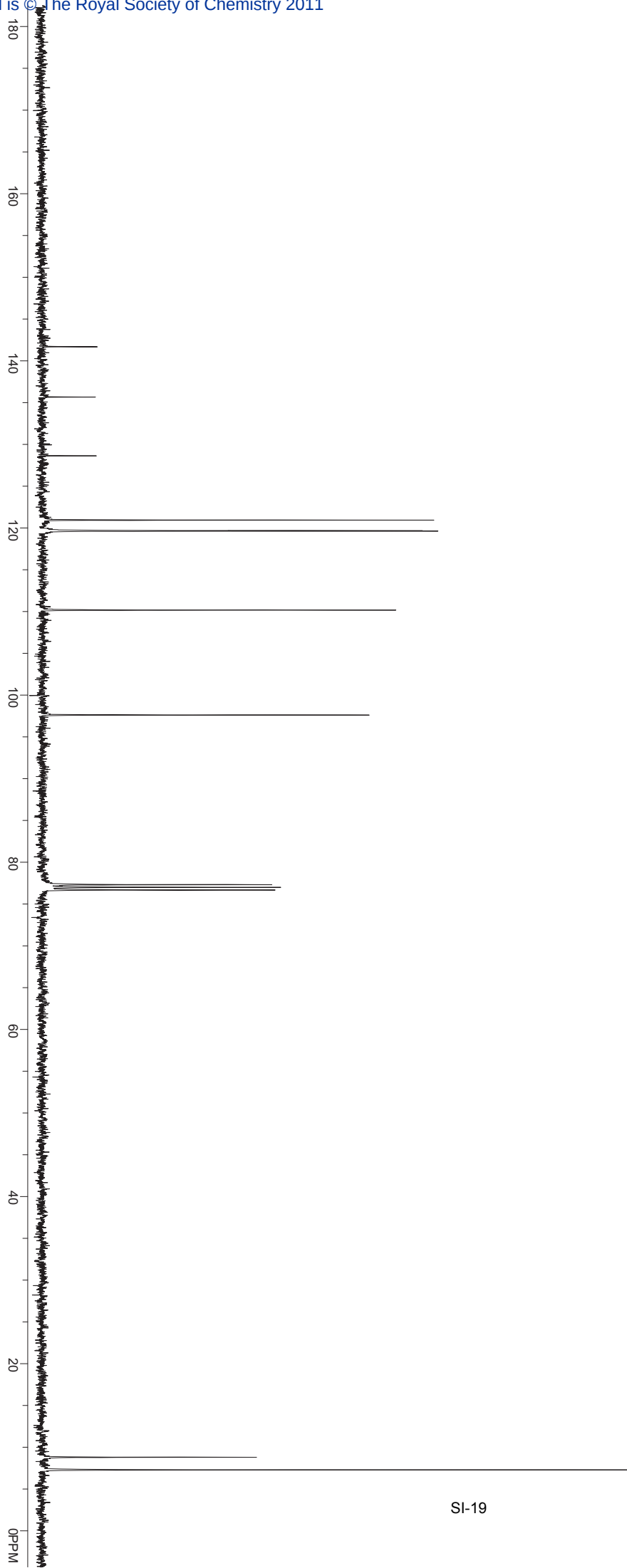
3d



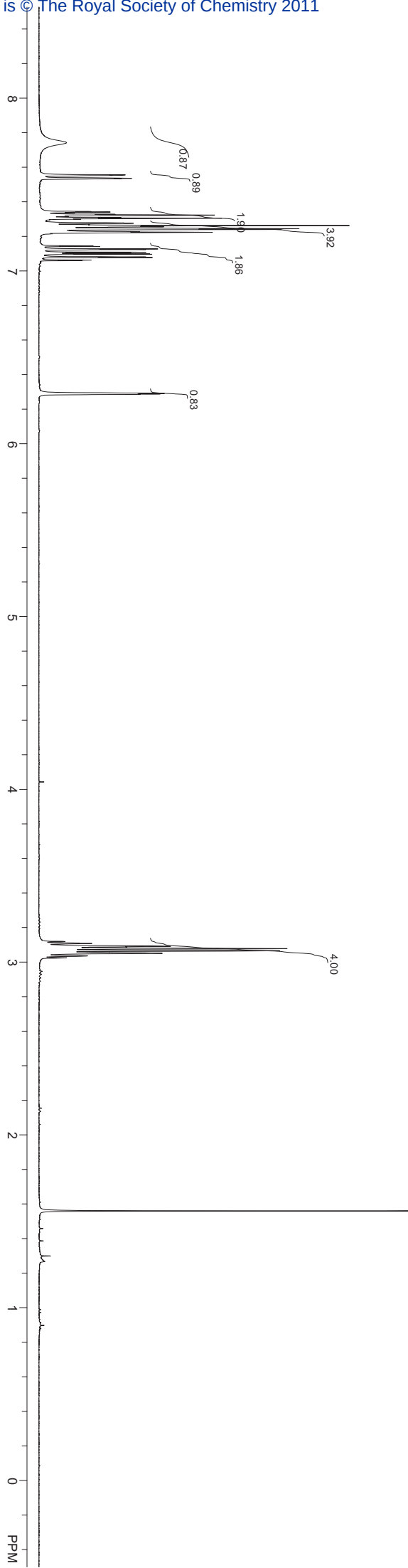
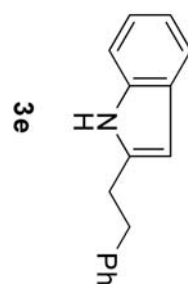
D:\Greenware\Nlus 20080731\DATA\5yw-5-3-1-3member-cc.fid
Standard c13 Run using qnp probe
Jan 6 2011
USER:
SOLVENT: cddc3
Experiment = s2pul
Pulse length = 7.000 usec
Relaxation delay = 1.300 sec
NA = 504
Solvent = cddc3
FID PTSid = 19608
PTSid = 32768
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 27972.03 Hz
AT1 = 0.70 sec
Hz per Pt 1sID = 0.85 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 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

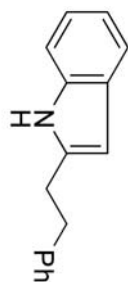


D:\Greenware\Nlus 20080731\DATA\5yw-5-13-Ph-h.fid
new experiment
Jan 12 2011
USER:
SOLVENT: cdd3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 12
Solvent = cdd3
FID P1S1d = 20008
PT1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8003.20 Hz
AT1 = 2.50 sec
Hz per Pt 1s1d = 0.24 Hz
SW2 = 1.00 Hz
Hz per Pt 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

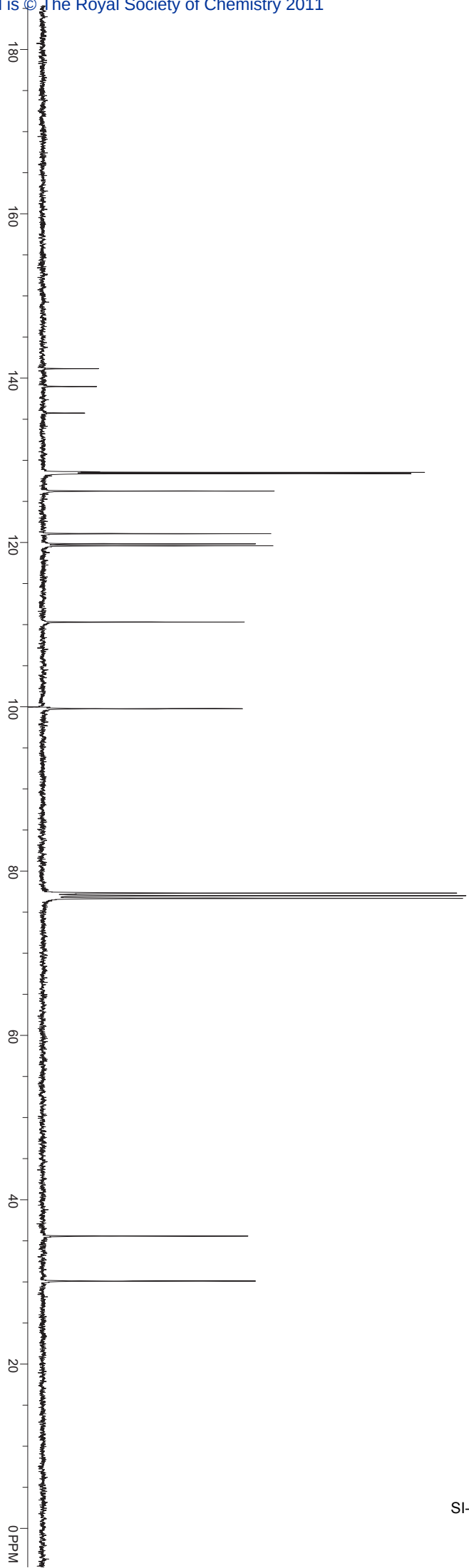


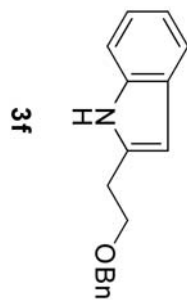
D:\Greenware\Nlus 20080731\DATA\5yw-5-13-Ph-cc.fid
Standard c13 run using qnp probe
Jan 12 2011

USER:
SOLVENT: cdd3
Experiment = s2pul
Pulse length = 7.000 usec
Relaxation delay = 1.300 sec
NA = 2016
Solvent = cdd3
FID P1SID = 19608
PTSID = 32768
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 27972.03 Hz
AT1 = 0.70 sec
Hz per P1 1SID = 0.85 Hz
SW2 = 1.00 Hz
Hz per P1 2nd = 1.00 Hz
O1 = 10053.2637 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -30.91
B = -0.75
C = 0.00

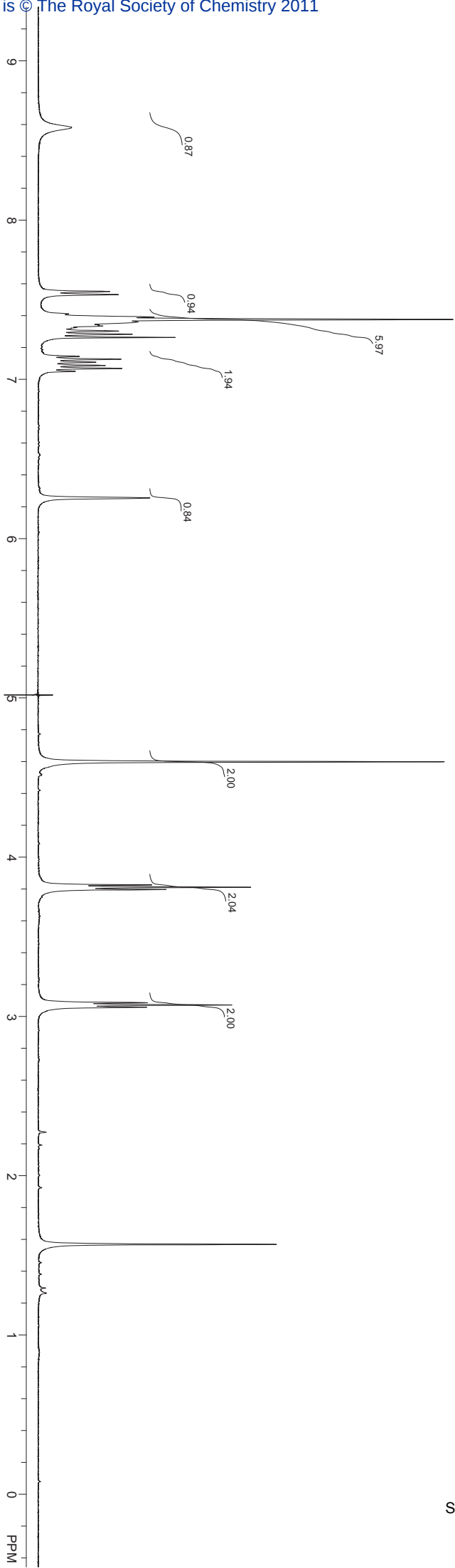


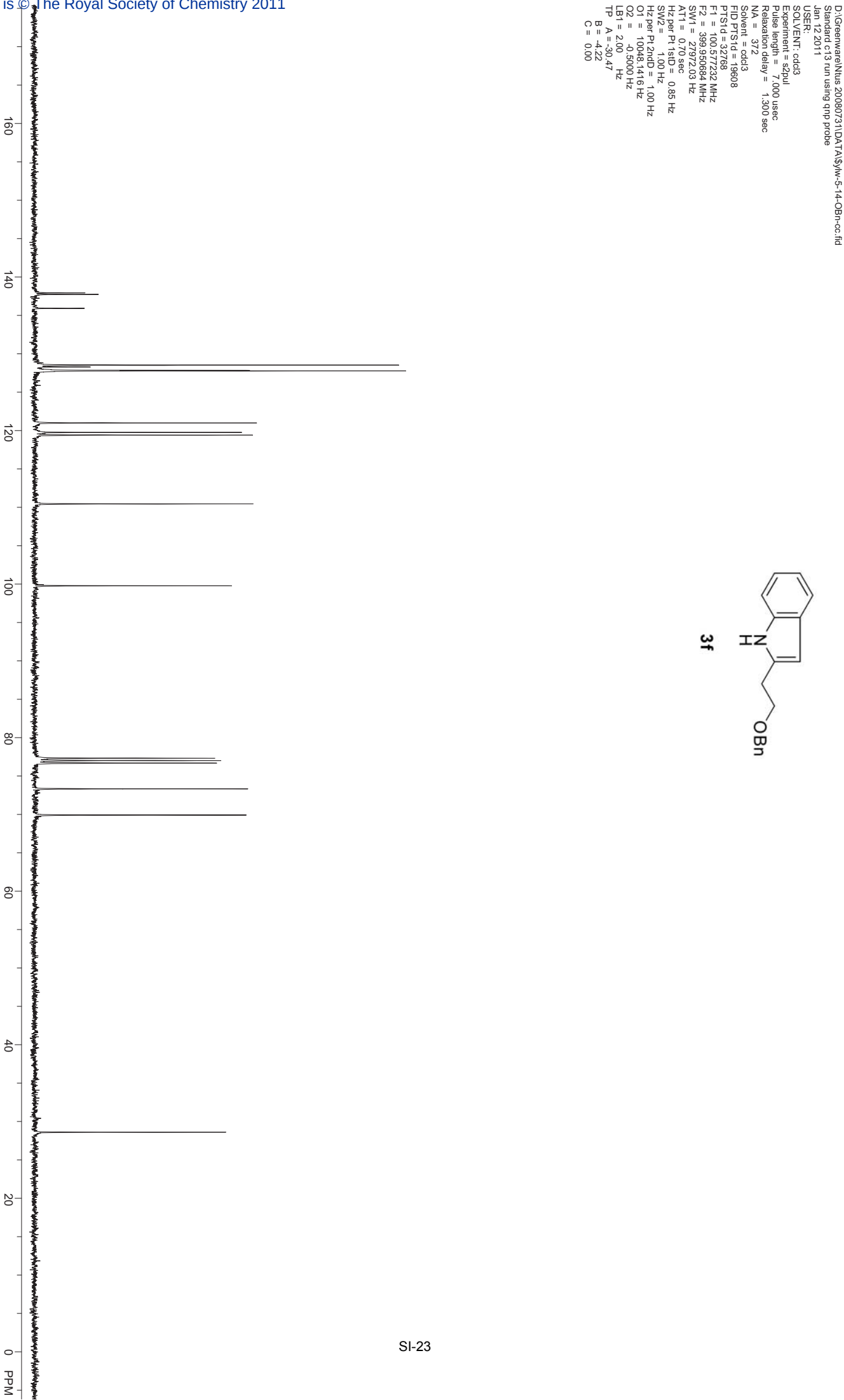
3e





D:\Greenware\Nlus 20080731\DATA\Syw-5-14-2.fid
new experiment
Jan 12 2011
USER:
SOLVENT: cddc3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 14
Solvent = cddc3
FID PTStid = 20008
PTStid = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8003.20 Hz
AT1 = 2.50 sec
Hz per Pt 1sID = 0.24 Hz
SW2 = 1.00 Hz
Hz per Pt 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

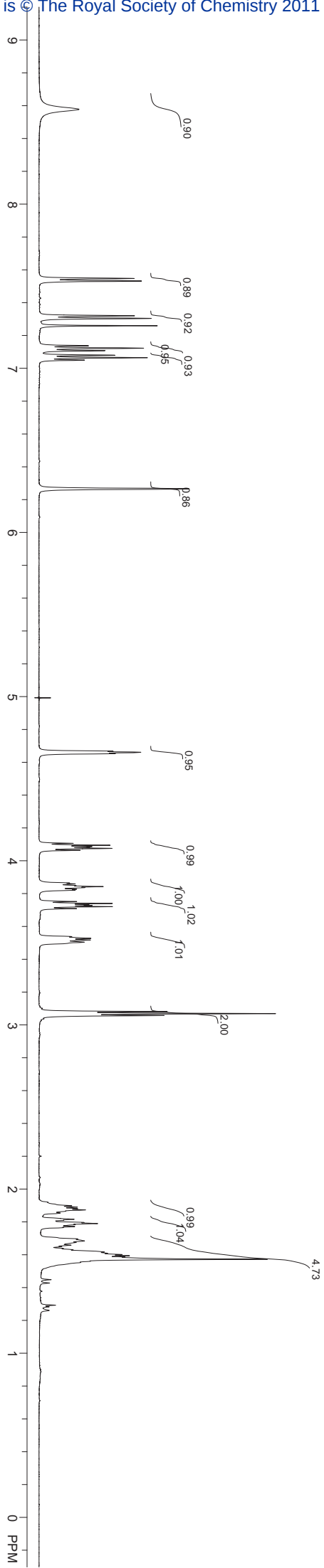


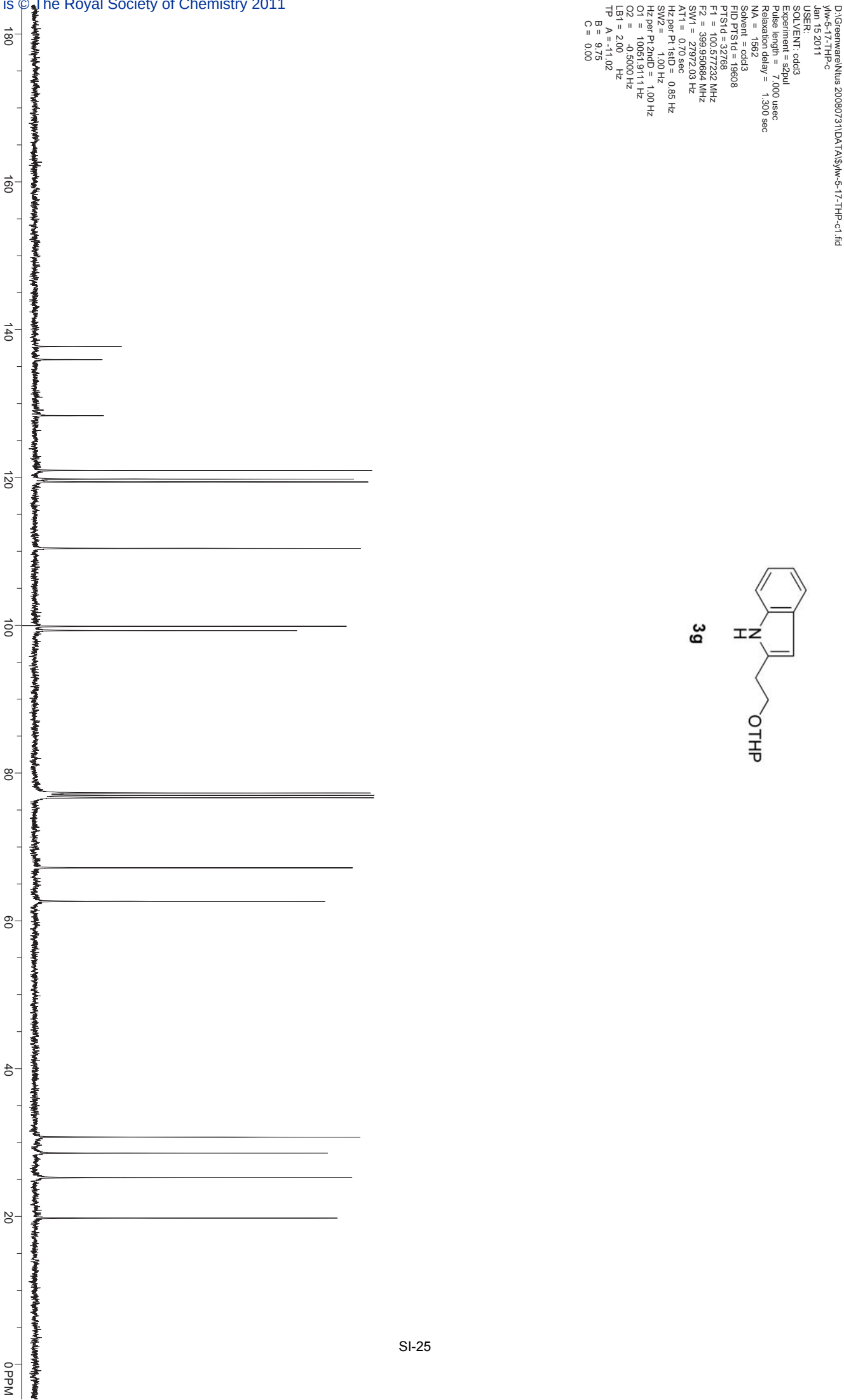


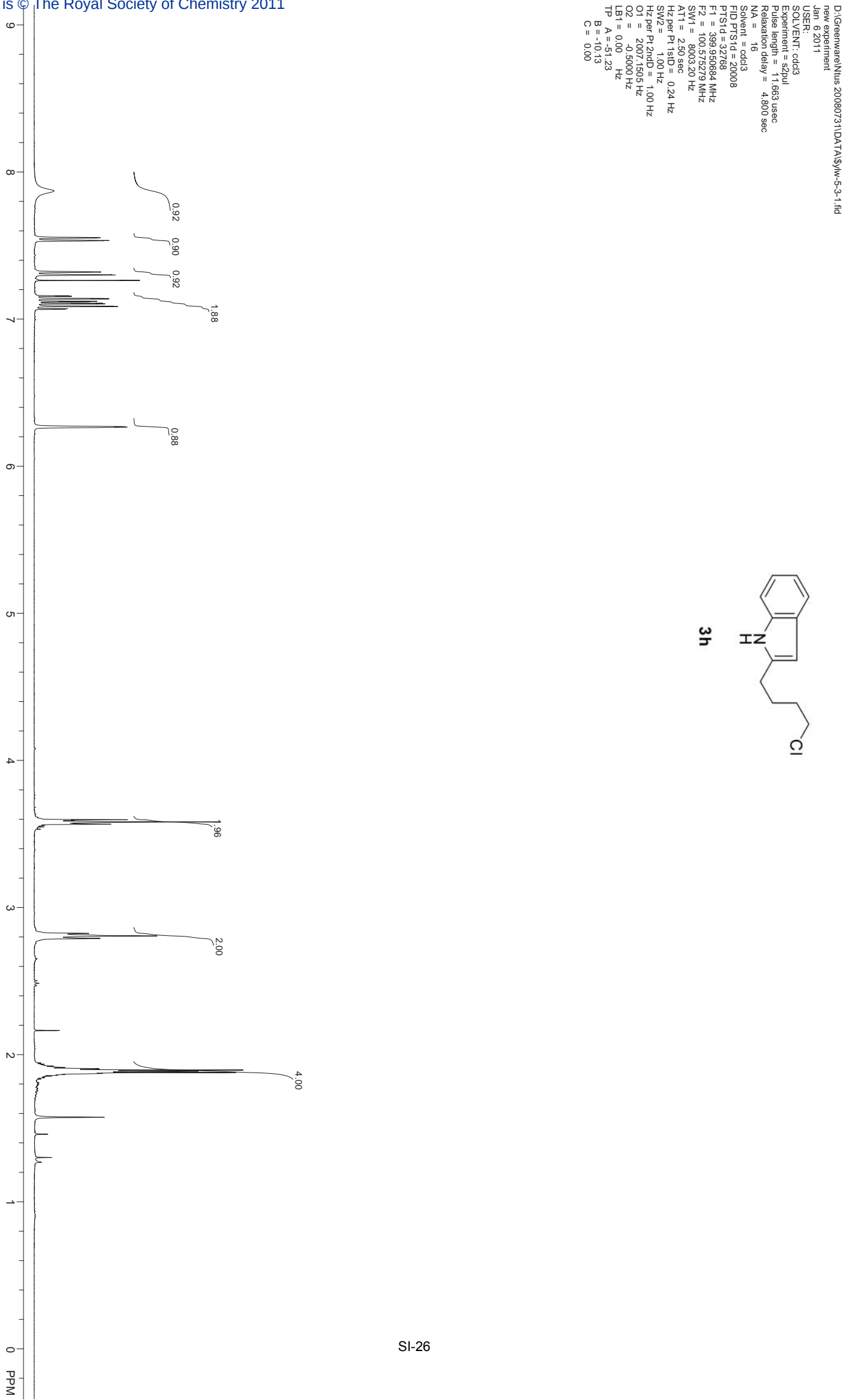
D:\Greenware\Nius 20080731\DATA\$yw-5-17-THP-hh.fid
Scan IDP
Jan 14 2011
USER:
SOLVENT: cdd3
Experiment = s2pul
Pulse length = 7.075 usec
Relaxation delay = 4.800 sec
NA = 14
Solvent = cdd3
FID PTStid = 20006
PTStid = 32768
F1 = 499.858551 MHz
F2 = 125.700813 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt1SID = 0.24 Hz
SW2 = 1.00 Hz
Hz per Pt2nd = 1.00 Hz
O1 = 2495.7266 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -123.90
B = -3.40
C = 0.00



3g



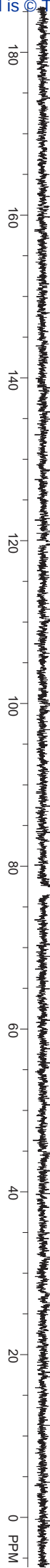


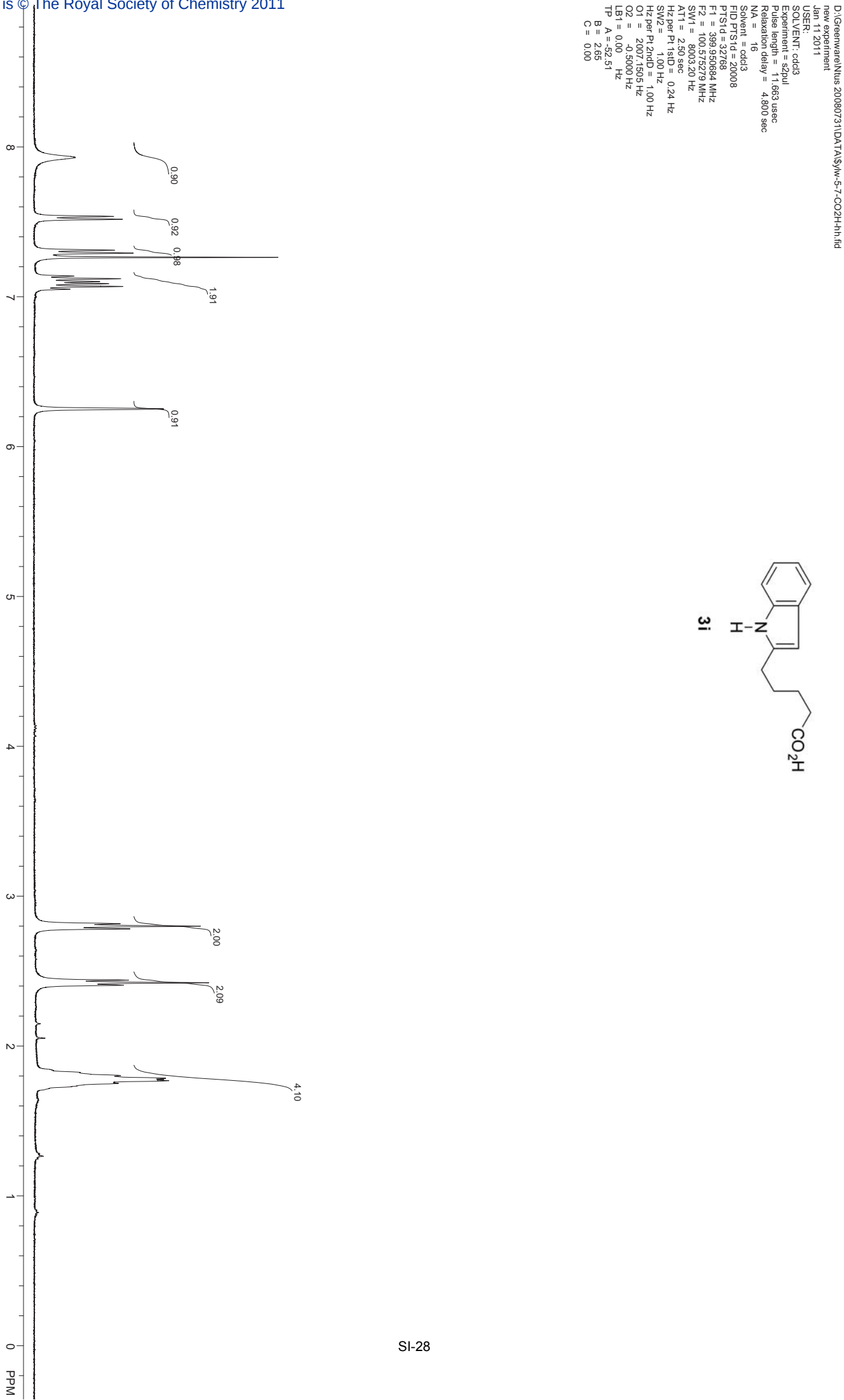


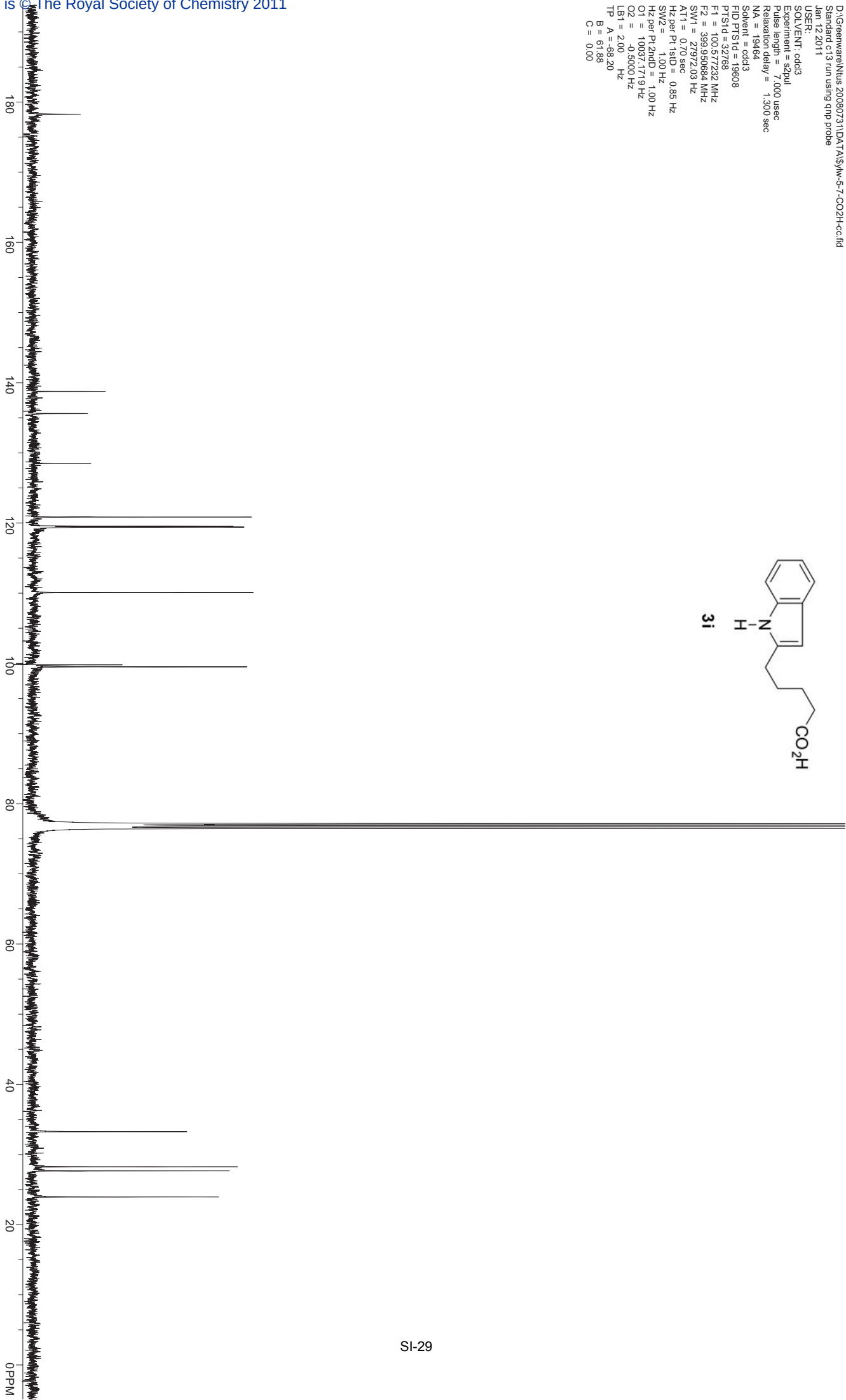
D:\Greenware\Nlus 20080731\DATA\5hw-5-3-1-Cl-cc.fid
5hw-5-3-1-cc
Jan 6 2011
USER:
SOLVENT: cdc13
Experiment = s2pul
Pulse length = 7.000 usec
Relaxation delay = 1.300 sec
NA = 986
Solvent = cdc13
FID P1SID = 19608
P1SID = 32768
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 27972.03 Hz
AT1 = 0.70 sec
Hz per P1 1SID = 0.85 Hz
SW2 = 1.00 Hz
Hz per P1 2nd = 1.00 Hz
O1 = 10054.9697 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -4.22
B = -11.25
C = 0.00



3h



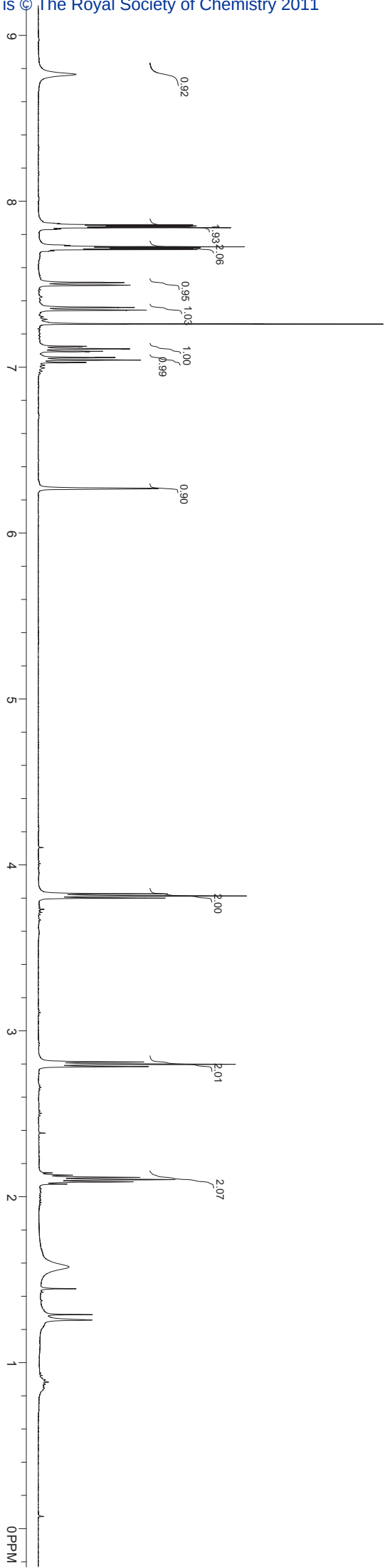




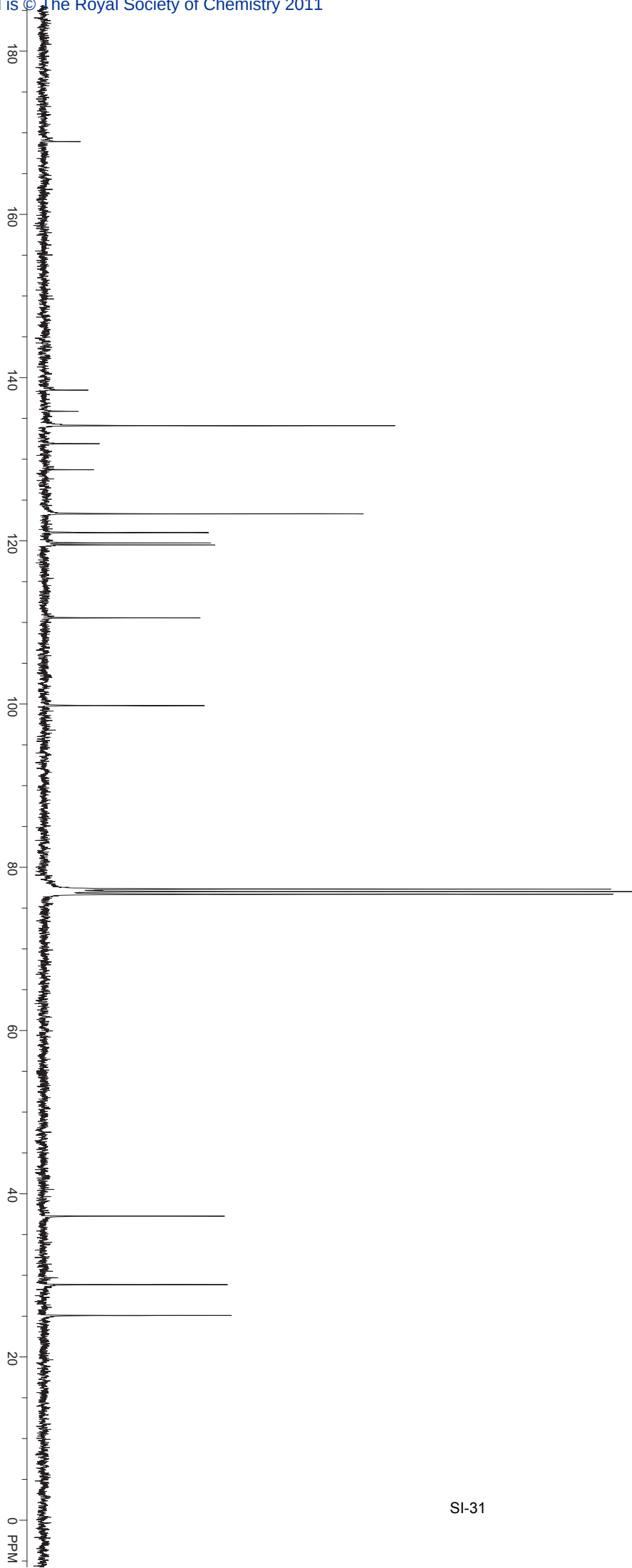
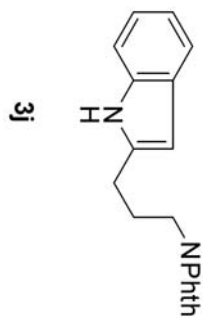
D:\Greenware\Nlus 20080731\DATA\5yw-5-46-1nph-h.fid
5nm IDP
Feb 3 2011
USER:
SOLVENT: cdd3
Experiment = s2pul
Pulse length = 7.075 usec
Relaxation delay = 4.800 sec
NA = 12
Solvent = cdd3
FID P1S1d = 20006
P1S1d = 32768
F1 = 499.858551 MHz
F2 = 125.700813 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per P1 1s1d = 0.24 Hz
SW2 = 1.00 Hz
Hz per P1 2ndd = 1.00 Hz
O1 = 2496.3713 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -121.20
B = 0.55
C = 0.00



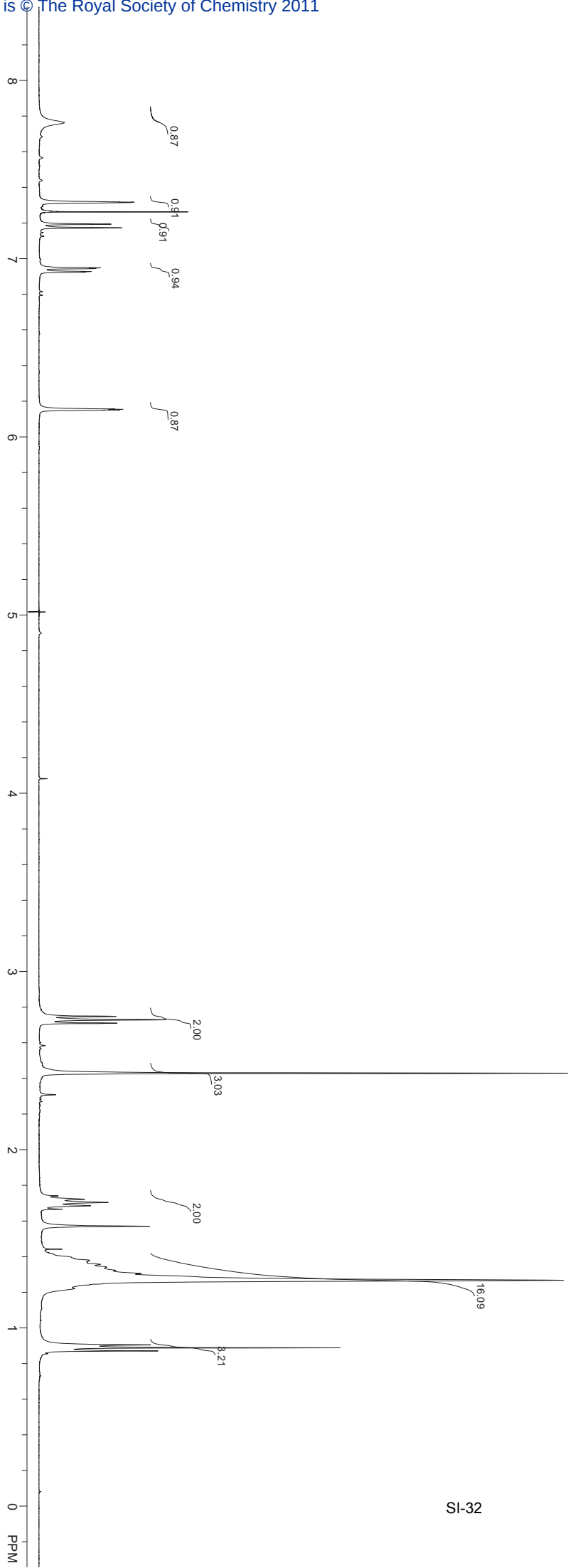
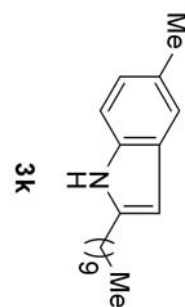
3j

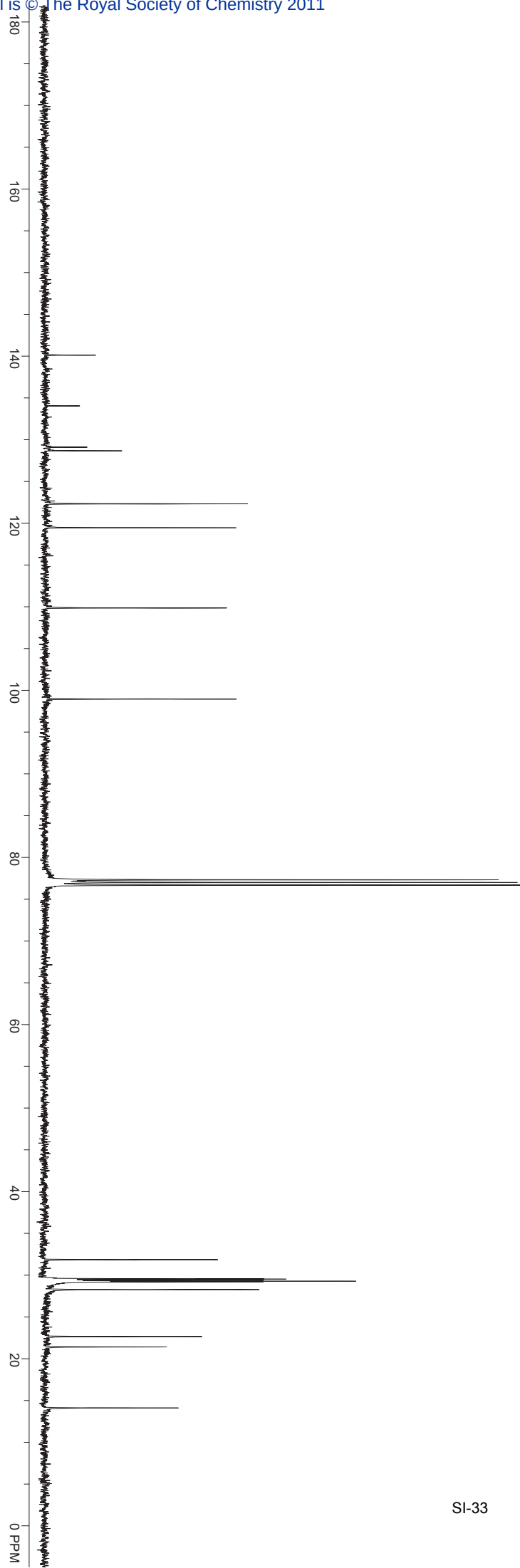
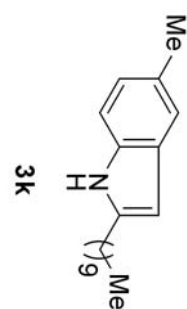


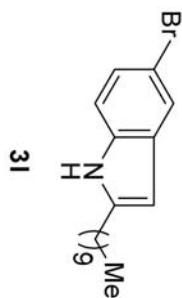
D:\Greenware\Nlus 20080731\DATA\$\yw-5-4b-cc.fid
yw-5-4b-cc
Feb 3 2011
USER:
SOLVENT: cddc3
Experiment: s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 2562
Solvent = cddc3
FID PTStid = 28040
PTStid = 32768
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 28040.66 Hz
AT1 = 1.00 sec
Hz per Pt1sID = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt2nd = 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



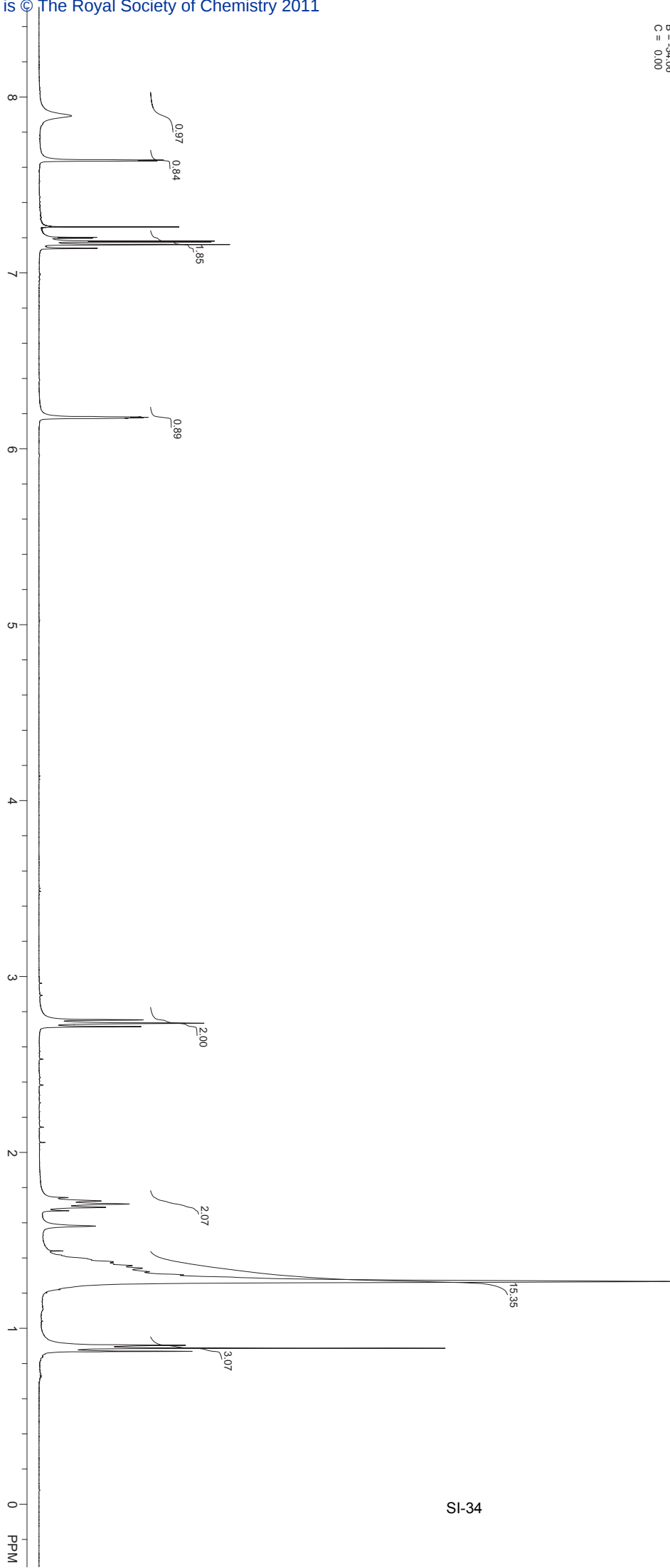
D:\Greenware\Nlus 20080731\DATA\S\yw-5-29-Me-hi.fid
new experiment
Jan 24 2011
USER:
SOLVENT: cdd3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 14
Solvent = cdd3
FID P1S1d = 20008
PT1S1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8003.20 Hz
AT1 = 2.50 sec
Hz per Pt1s1d = 0.24 Hz
SW2 = 1.00 Hz
Hz per Pt2nd = 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

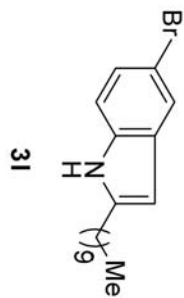




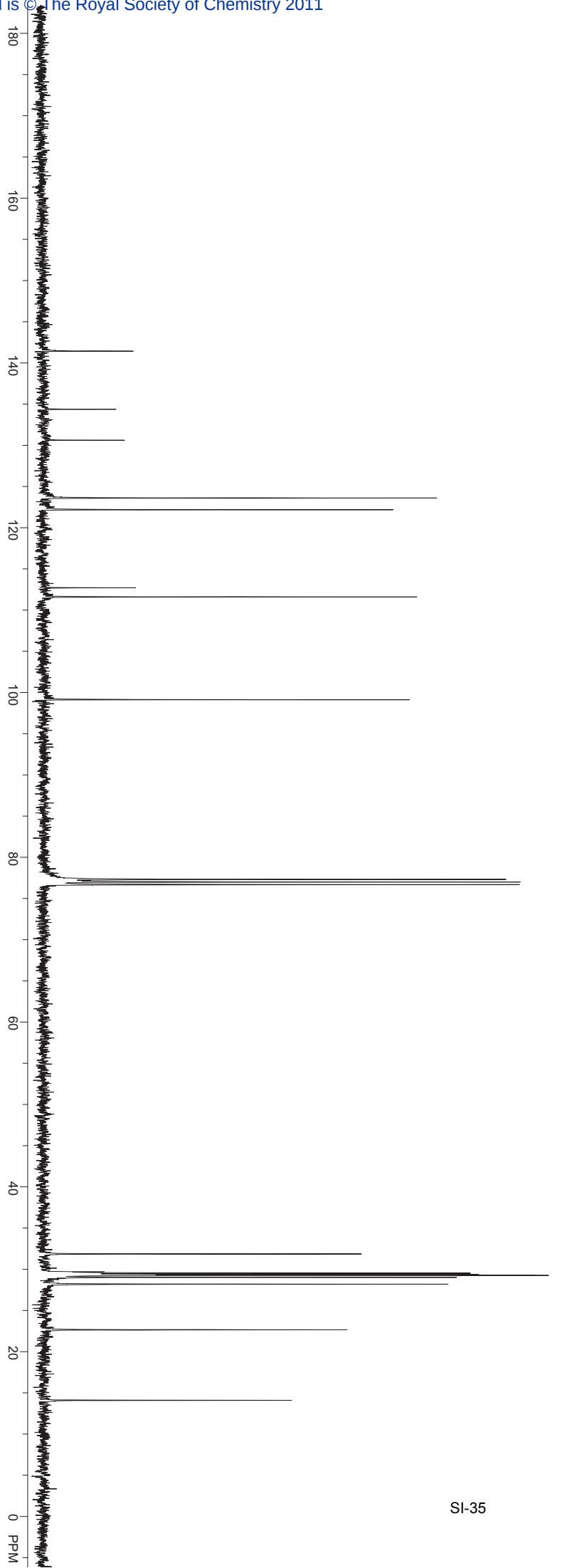


D:\Greenware\Nlus 20080731\DATA\5yw-5-36-B1-H.fid
new experiment
Jan 27 2011
USER:
SOLVENT: cddc3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 16
Solvent = cddc3
FID P1S1d = 20006
PT1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per P1 1sID = 0.24 Hz
SW2 = 1.00 Hz
Hz per P1 2nd = 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

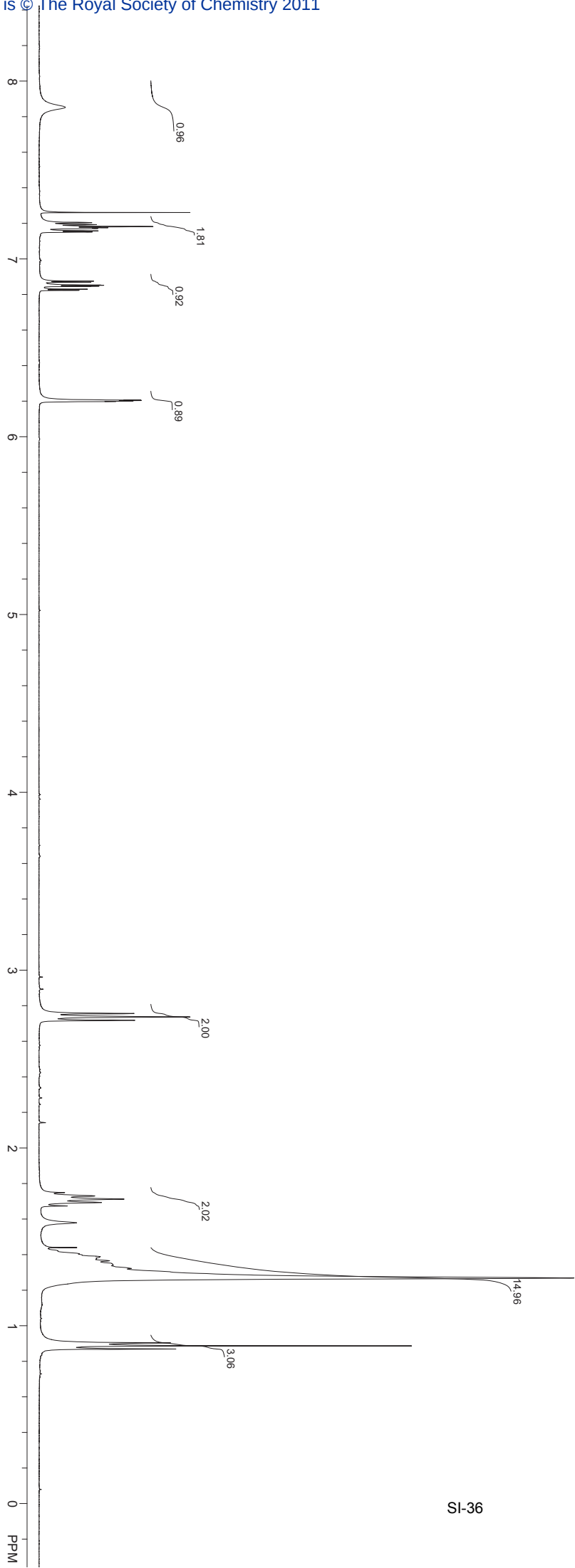
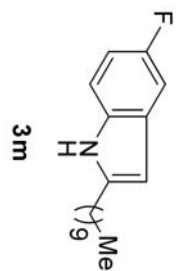


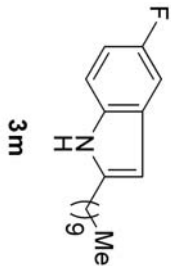
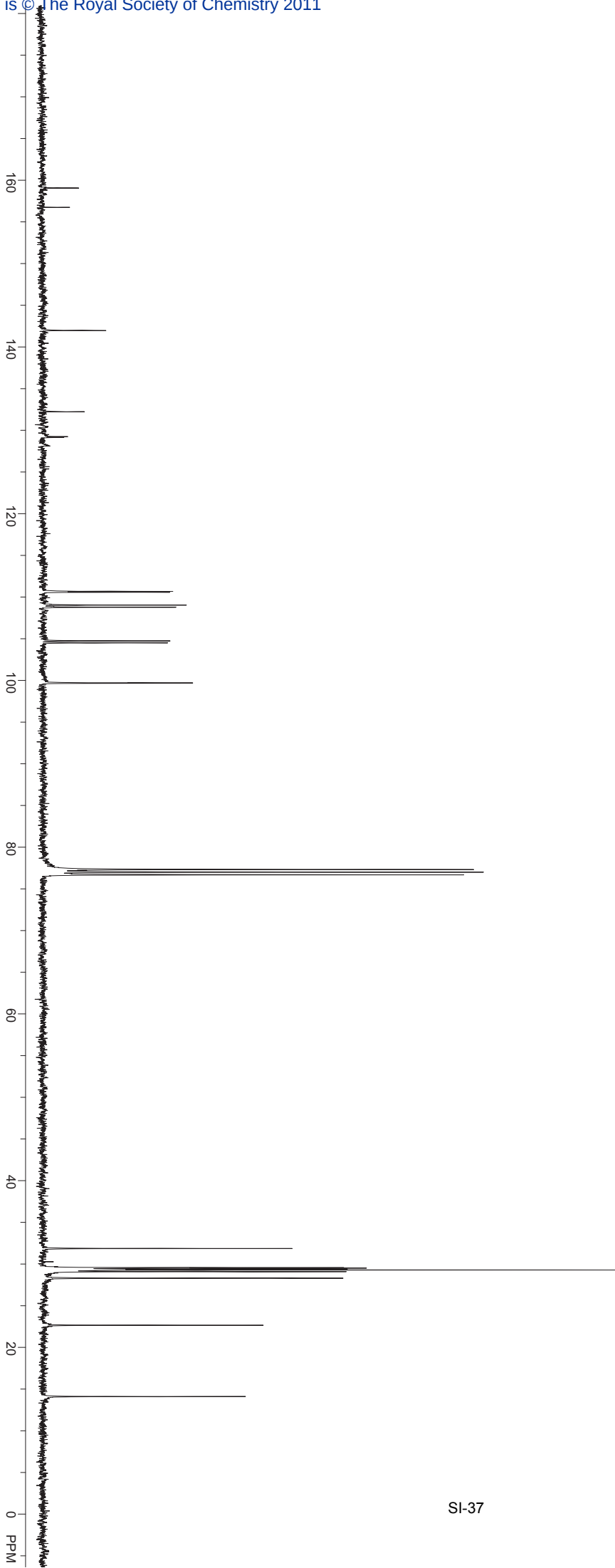


D:\Greenware\Nlus 20080731\DATA\5yw-5-36-Br-c.fid
Standard c13 run using qnp probe
Jan 27 2011
USER:
SOLVENT: cddc3
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 1574
Solvent = cddc3
FID P1S1d = 28040
PT1d = 32768
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 28040.66 Hz
AT1 = 1.00 sec
Hz per Pt 1s1d = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt 2nd = 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



D:\Greenware\Nlus 20080731\DATA\5yw-5-36-F-h.fid
new experiment
Jan 26 2011
USER:
SOLVENT: cdd3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 12
Solvent = cdd3
FID P1S1d = 20006
PT1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per P1 1s1d = 0.24 Hz
SW2 = 1.00 Hz
Hz per P1 2nd = 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

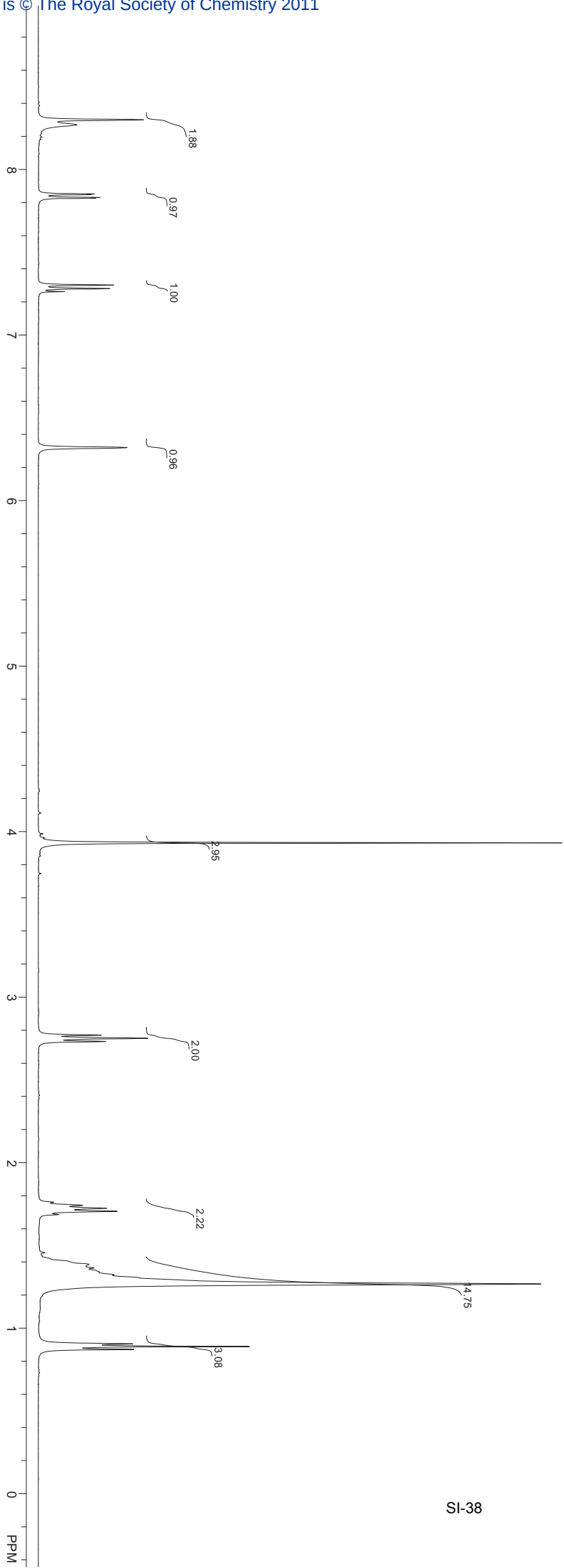
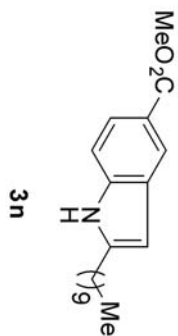




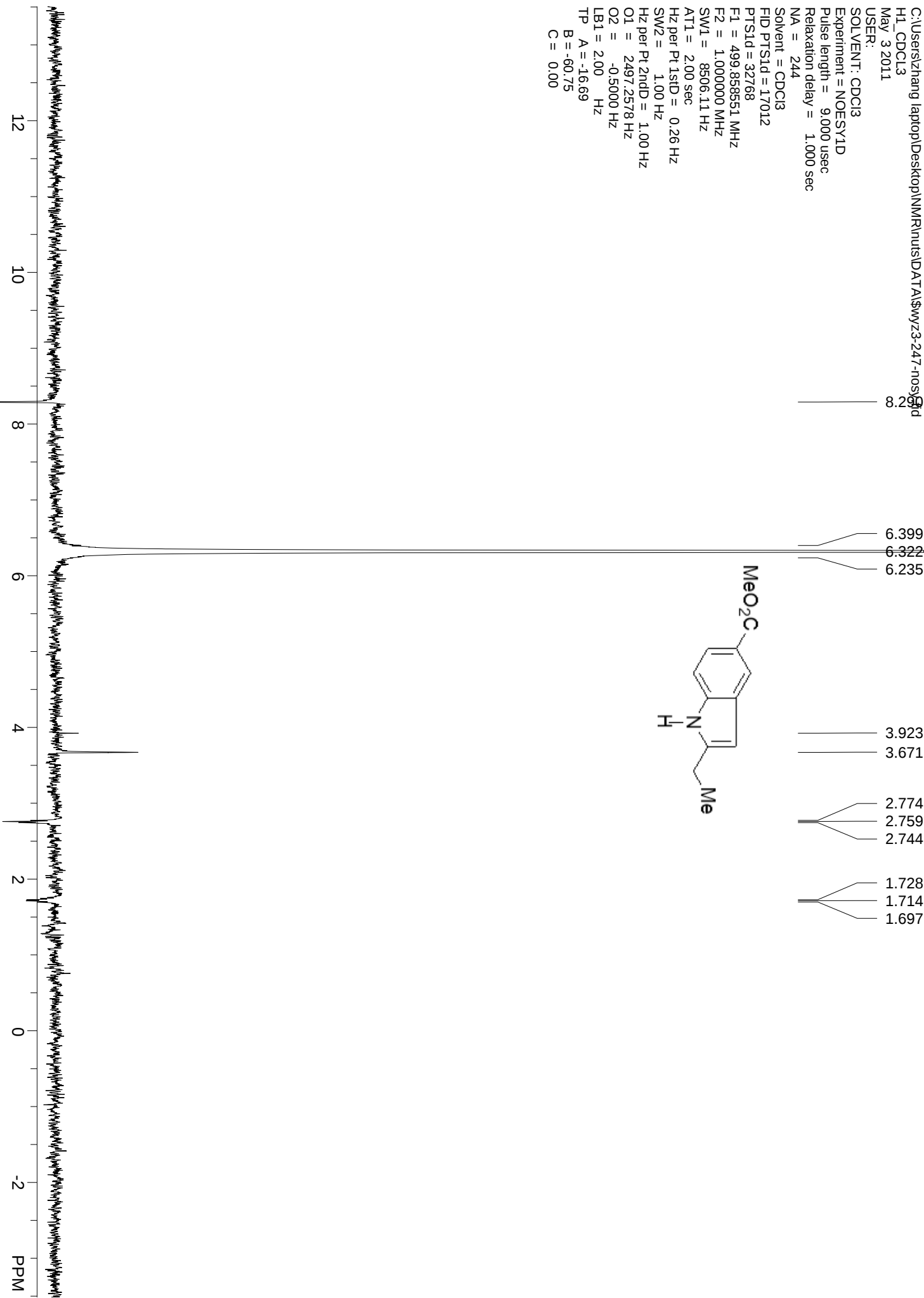
D:\Greenware\Nlus 20080731\DATA\5yw-5-36-F-c.fid
Standard c13 run using qnp probe
Jan 26 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 2486
Solvent = cdcl3
FID P1S1d = 28040
PT1d = 32768
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 28040.66 Hz
AT1 = 1.00 sec
Hz per Pt 1s1d = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt 2nd = 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

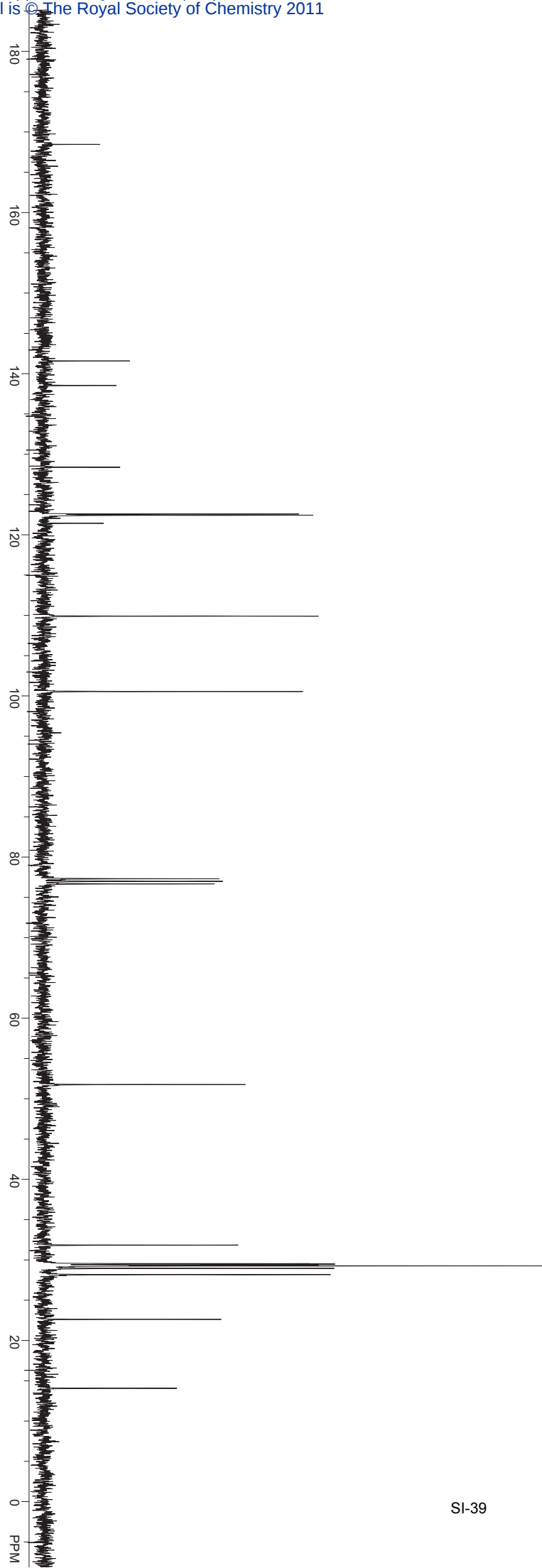
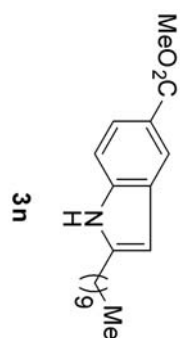
D:\Greenware\Nlus 20080731\DATA\5\w-5-27-E-hh.fid
new experiment
Jan 20 2011

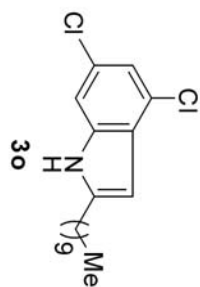
USER:
SOLVENT: cdd3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 12
Solvent = cdd3
FID PTStid = 20008
PTStid = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8003.20 Hz
AT1 = 2.50 sec
Hz per Pt1StD = 0.24 Hz
SW2 = 1.00 Hz
Hz per Pt2nd = 1.00 Hz
OT = 20071505 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -63.06
B = -2.72
C = 0.00



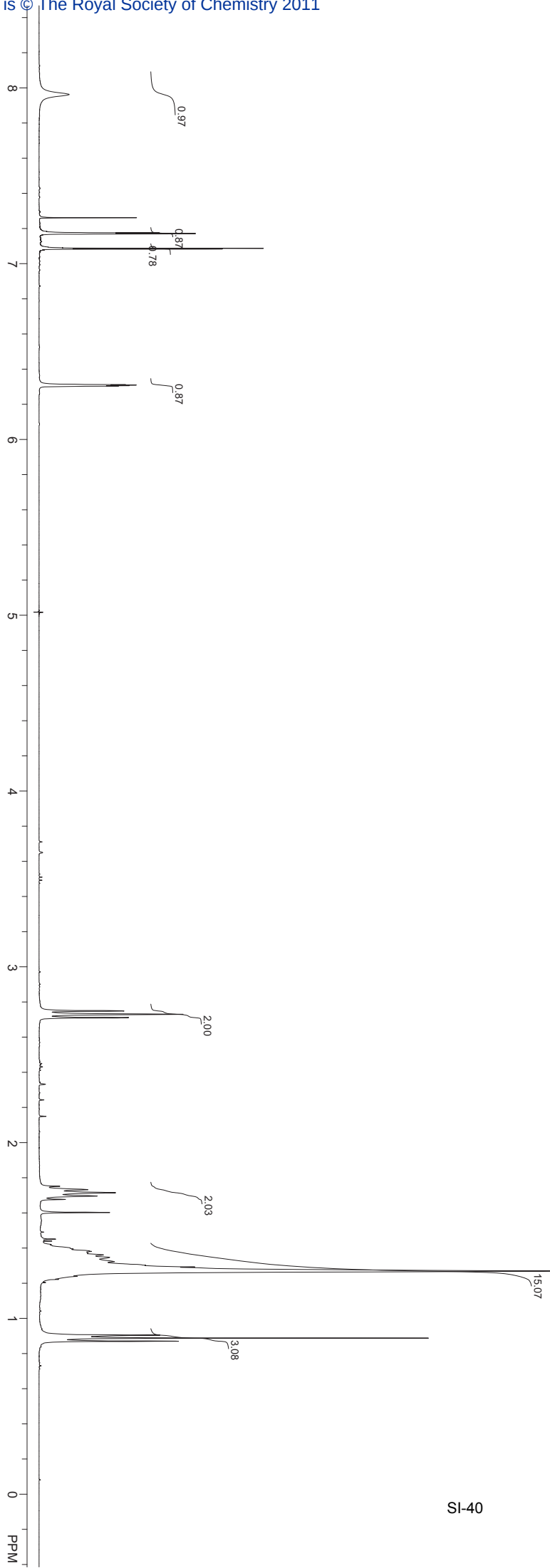
C:\Users\zhang\laptop\Desktop\NMR\ntuts\DATA\5wyz3-247-nosy-8d
H1_CDCL3
May 3 2011
USER:
SOLVENT: CDCl3
Experiment = NOESY1D
Pulse length = 9.000 usec
Relaxation delay = 1.000 sec
NA = 244
Solvent = CDCl3
FID PTSId = 17012
PTSId = 32768
F1 = 499.858551 MHz
F2 = 1.000000 MHz
SW1 = 8506.11 Hz
AT1 = 2.00 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

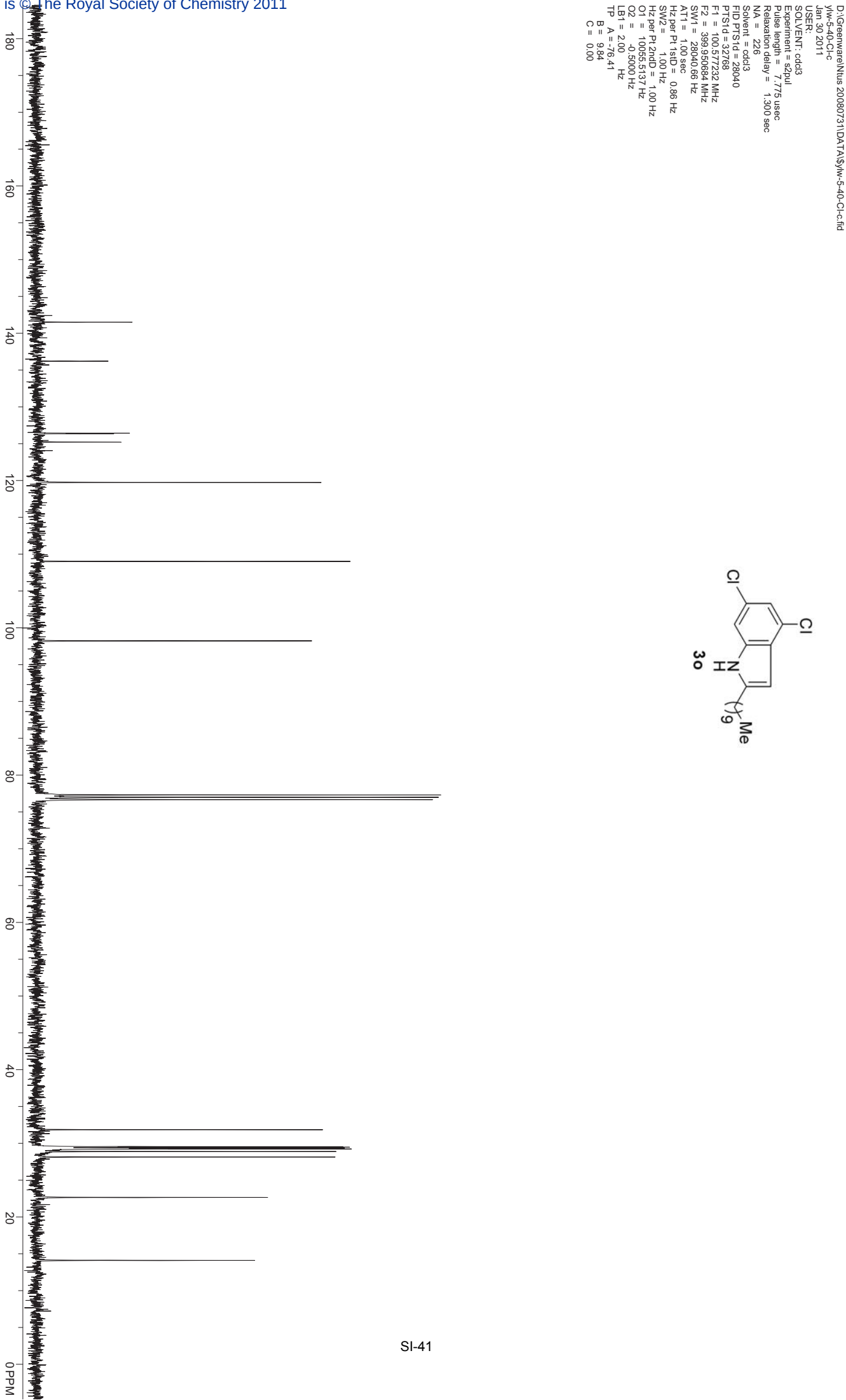




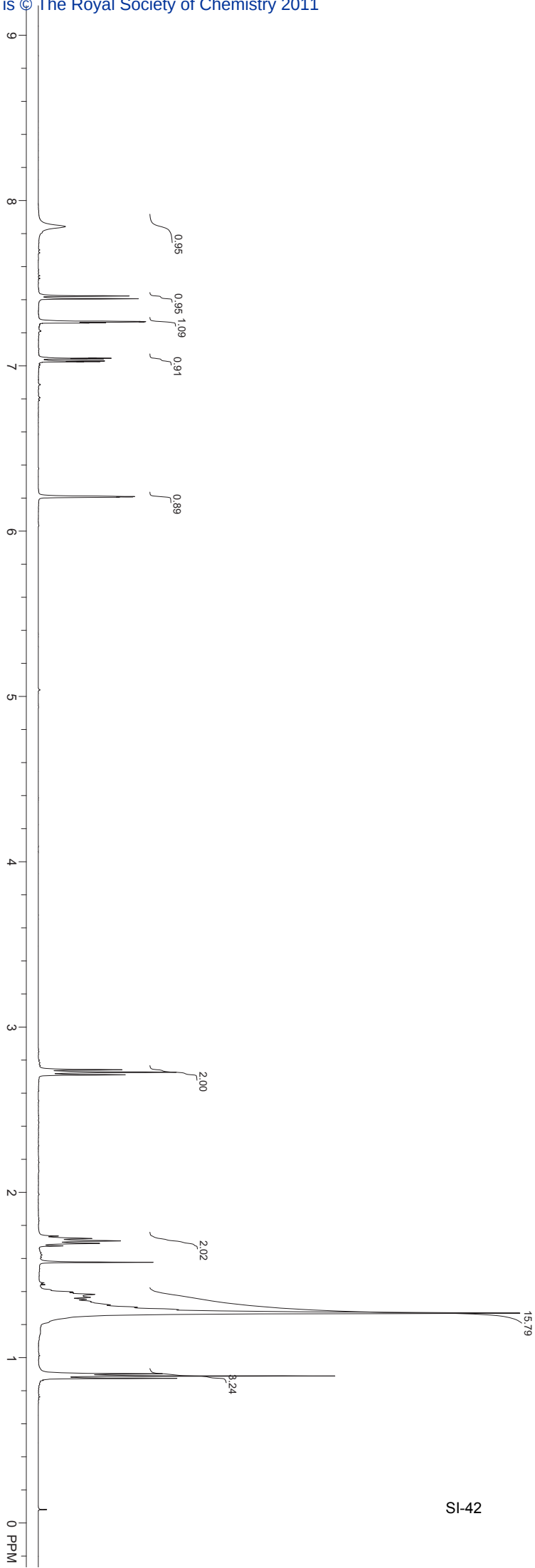
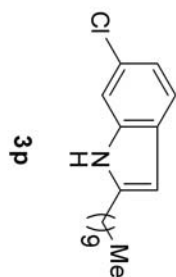


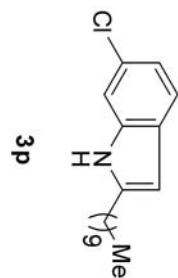
D:\Greenware\Nlus 20080731\DATA\Syw-5-40-Cl-h.fid
new experiment
Jan 30 2011
USER:
SOLVENT: cdd3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 10
Solvent = cdd3
FID P1S1d = 20006
PT1S1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt 1s1D = 0.24 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 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



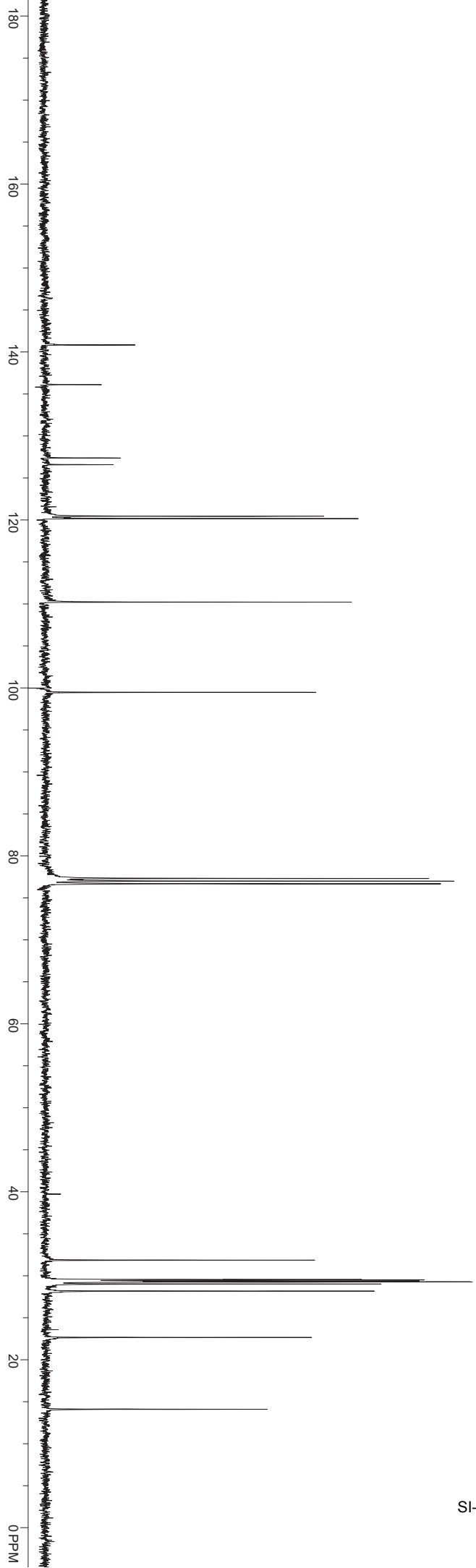


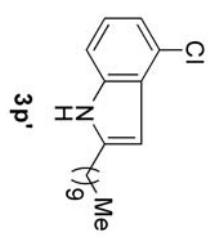
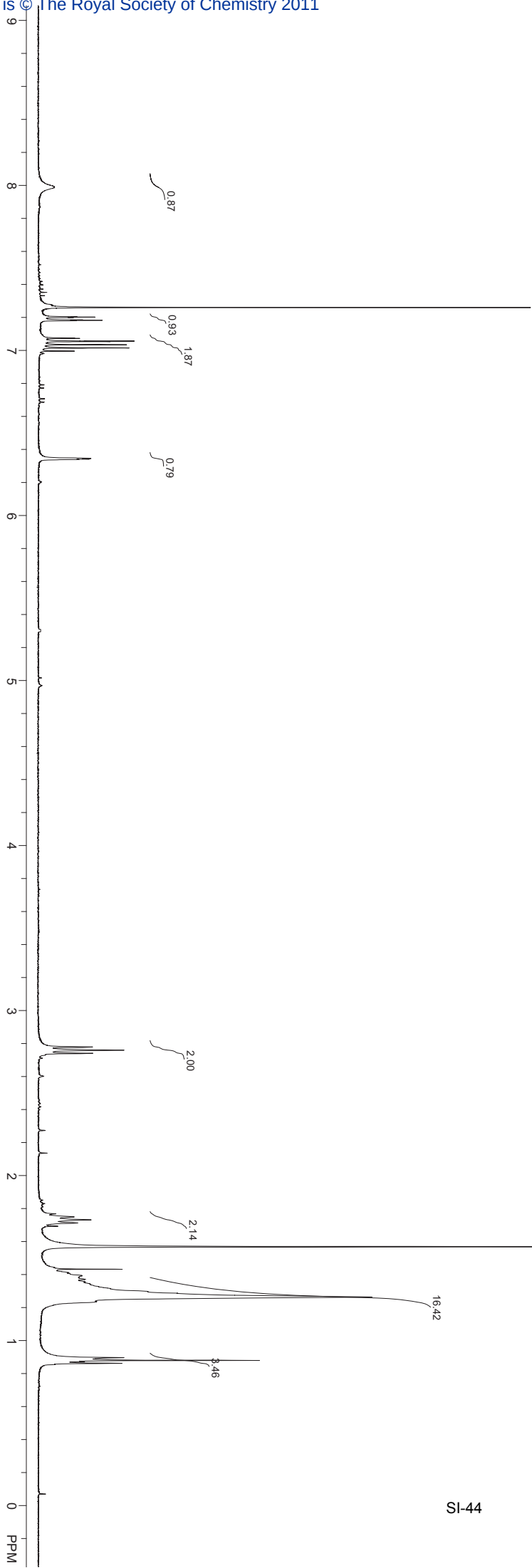
D:\Greenware\Nlus 20080731\DATA\\${yw-5-25-1}.fid
 Smn IDP
 Jan 19 2011
 USER:
 SOLVENT: cdd3
 Experiment = s2pul
 Pulse length = 7.075 usec
 Relaxation delay = 4.800 sec
 NA = 16
 Solvent = cdd3
 FID PTStid = 20006
 PTStid = 32768
 F1 = 499.858551 MHz
 F2 = 125.700813 MHz
 SW1 = 8002.40 Hz
 AT1 = 2.50 sec
 Hz per Pt1sID = 0.24 Hz
 SW2 = 1.00 Hz
 Hz per Pt2nd = 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





D:\Greenware\Nlus 20080731\DATA\$\yw-5-25-1-c1.fid
yw-5-25-1-c
Jan 19 2011
USER:
SOLVENT: cdd3
Experiment = s2pul
Pulse length = 7.000 usec
Relaxation delay = 1.000 sec
NA = 1432
Solvent = cdd3
FID P1S1d = 19608
PT1S1d = 32768
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 27972.03 Hz
AT1 = 0.70 sec
Hz per Pt 1s1D = 0.85 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 10055.3262 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -24.84
B = -26.72
C = 0.00





D:\Greenware\Nlus 20080731\DATA\5yw-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
FID P1S1d = 20008
PT1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8003.20 Hz
AT1 = 2.50 sec
Hz per P1 1s1d = 0.24 Hz
SW2 = 1.00 Hz
Hz per P1 2nd = 1.00 Hz
O1 = 2006.3905 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -68.72
B = 5.25
C = 0.00

