Supporting Information

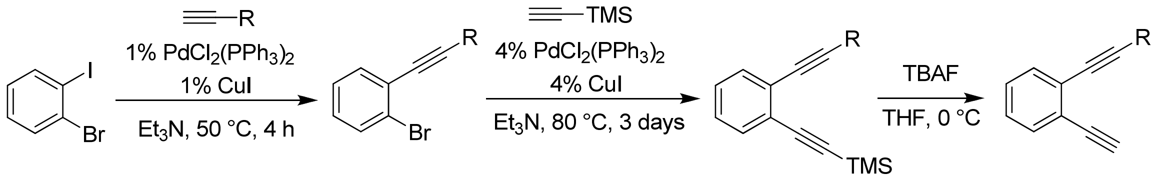
Experimental and Computational Evidence for Gold Vinylidenes: Generation from Terminal Alkynes via a Bifurcation Pathway and Facile C-H Insertions

Longwu Ye, Yanzhao Wang, Donald Aue* and Liming Zhang*

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

General. 1, 2-Dichloroethane (HPLC grade), ethyl acetate (ACS grade), hexanes (ACS grade) and diethyl ether (ACS grade) were purchased from Fisher Scientific and used without further purification. 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 silicycle pre-coated silica gel plates. Flash column chromatography was performed over silicycle silica gel (230-400 mesh). ^{1}H NMR and ^{13}C NMR spectra were recorded on a Varian 500 MHz Unity plus spectrometer and a Varian 400 MHz spectrometer using residue solvent peaks as internal standards. Infrared spectra were recorded with a Perkin Elmer FT-IR spectrum 2000 spectrometer and are reported in reciprocal centimeter (cm^{-1}). Mass spectra were recorded with Micromass QTOF2 Quadrupole/Time-of-Flight Tandem mass spectrometer using electron spray ionization.

General procedure A: preparation of benzene-1,2-diynes 1



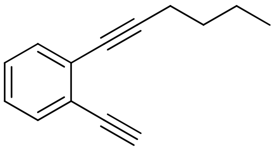
A **B** **1**

CuI (0.068 g, 0.36 mmol), $PdCl_2(PPh_3)_2$ (0.25 g, 0.36 mmol) and terminal alkyne (46.7 mmol) were added to the solution of 1-bromo-2-iodobenzene (4.5 mL, 35.5 mmol) in Et_3N (100 mL) at room temperature. Then, the whole was stirred at 50 °C for another 4 h. After the reaction was complete, the resulting mixture was filtered rapidly through a funnel with a thin layer of celite and was eluted with Et_2O. The filtrate was concentrated and the residue was purified by chromatography on silica gel to afford the product **A**.

CuI (0.054 g, 0.29 mmol), $PdCl_2(PPh_3)_2$ (0.21 g, 0.29 mmol) and ethynyltrimethylsilane (1.5 mL, 10.7 mmol) were added to the solution of **A** (7.1 mmol) in Et_3N (20 mL) at room temperature. Then, the whole was stirred at 80 °C for another 72 h. After the reaction was complete, the resulting mixture was filtered rapidly through a funnel with a thin layer of celite and was eluted with Et_2O. The filtrate was concentrated and the residue was purified by chromatography on silica gel to afford the product **B**.

A solution of tetrabutylammonium fluoride (1.0 M, 4.8 mL, 4.8 mmol) was added dropwise to a solution of **B** (4.0 mmol) in THF (35 mL) at 0 °C, and the mixture was stirred at 0 °C for 15 min. After addition of an aqueous NH_4Cl solution, the mixture was extracted three times with Et_2O. The combined organic layers were washed with brine, dried with anhydrous $MgSO_4$, and the solvents evaporated to dryness. The oily residue was purified by short-column chromatography on silica gel (eluent: hexanes/EtOAc) to yield benzene-1,2-diyne **1**.

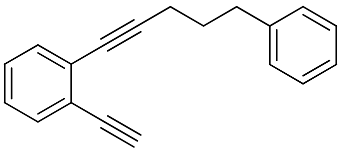
1-ethynyl-2-(hex-1-yn-1-yl)benzene (1a)



1a

Compound **1a** was prepared following the general procedure A. Its spectroscopic data match those reported.[1] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (dd, 1H, J_1 = 7.6 Hz, J_2 = 1.6 Hz), 7.42 (dd, 1H, J_1 = 7.6 Hz, J_2 = 1.6 Hz), 7.20 – 7.28 (m, 2H), 3.30 (s, 1H), 2.49 (t, 2H, J = 6.8 Hz), 1.50 – 1.67 (m, 4H), 0.97 (t, 3H, J = 7.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 132.4, 131.8, 128.4, 127.1, 124.3, 94.9, 82.4, 80.4, 79.0, 30.7, 21.8, 19.2, 13.6.

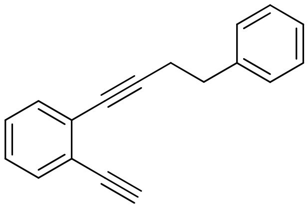
1-ethynyl-2-(5-phenylpent-1-yn-1-yl)benzene (1b)



1b

Compound **1b** was prepared following the general procedure A. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (dd, 1H, J_1 = 7.6 Hz, J_2 = 0.8 Hz), 7.46 (d, 1H, J = 7.6 Hz), 7.21 – 7.35 (m, 7H), 3.32 (s, 1H), 2.89 (t, 2H, J = 7.6 Hz), 2.52 (t, 2H, J = 7.2 Hz), 1.98 (p, 2H, J = 6.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.7, 132.5, 131.9, 128.6, 128.4, 128.3, 127.2, 127.0, 125.8, 124.3, 94.4, 82.5, 80.5, 79.6, 34.6, 30.2, 18.9; IR (neat): 3283, 3060, 3026, 2941, 2860, 2229, 2107, 1478, 1441, 759, 700; GCMS *m*/*z* 244 (M^+).

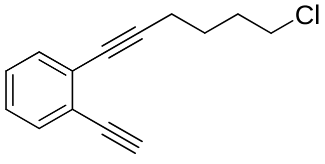
1-ethynyl-2-(4-phenylbut-1-yn-1-yl)benzene (1c)



1c

Compound **1c** was prepared following the general procedure A. ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.53 (d, 1H, J = 7.2 Hz), 7.44 (dd, 1H, J_1 = 7.2 Hz, J_2 = 1.6 Hz), 7.24 – 7.39 (m, 7H), 3.30 (s, 1H), 3.01 (t, 2H, J = 7.4 Hz), 2.82 (t, 2H, J = 7.6 Hz); ^{13}C NMR (100 MHz, CDCl$_3$) δ 140.6, 132.4, 131.9, 128.5, 128.4, 128.3, 127.3, 126.8, 126.2, 124.3, 94.0, 82.3, 80.6, 79.6, 35.0, 21.7; IR (neat): 3283, 3061, 3027, 2928, 2860, 2229, 2108, 1604, 1478, 1441, 759, 699; GCMS m/z 230 (M$^+$).

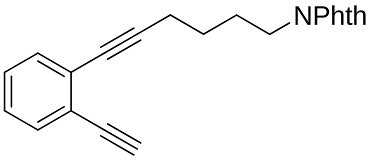
1-(6-chlorohex-1-yn-1-yl)-2-ethynylbenzene (1d)



1d

Compound **1d** was prepared following the general procedure A. ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.48 (dd, 1H, J_1 = 7.2 Hz, J_2 = 1.2 Hz), 7.41 (dd, 1H, J_1 = 7.2 Hz, J_2 = 1.6 Hz), 7.20 – 7.29 (m, 2H), 3.61 (t, 2H, J = 6.6 Hz), 3.31 (s, 1H), 2.53 (t, 2H, J = 6.8 Hz), 1.99 – 2.07 (m, 2H), 1.74 – 1.81 (m, 2H); ^{13}C NMR (100 MHz, CDCl$_3$) δ 132.4, 131.8, 128.4, 127.3, 126.7, 124.3, 93.7, 82.4, 80.6, 79.7, 44.6, 31.4, 25.6, 18.8; IR (neat): 3286, 3060, 2952, 2866, 2229, 2107, 1478, 1441, 759; GCMS m/z 216 (M$^+$).

2-(6-(2-ethynylphenyl)hex-5-yn-1-yl)isoindoline-1,3-dione (1e)

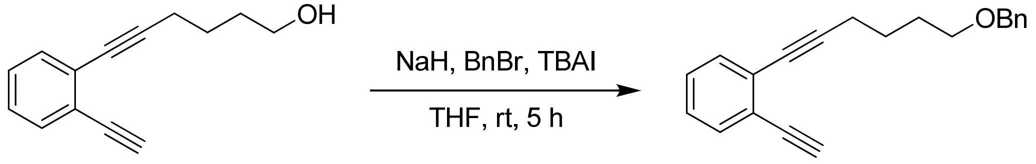


1e

Compound **1e** was prepared following the general procedure A. ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.82 – 7.85 (m, 2H), 7.69 – 7.72 (m, 2H), 7.45 (dd, 1H, J_1 = 8.0 Hz, J_2 = 1.6 Hz), 7.38 (dd, 1H, J_1 = 8.0 Hz, J_2

= 1.2 Hz), 7.18 – 7.27 (m, 2H), 3.74 (t, 2H, J = 7.2 Hz), 3.36 (s, 1H), 2.53 (t, 2H, J = 6.8 Hz), 1.88 – 1.96 (m, 2H), 1.64 – 1.72 (m, 2H); ^{13}C NMR (100 MHz, CDCl$_3$) δ 168.4, 133.9, 132.3, 132.0, 131.8, 128.3, 127.2, 126.8, 124.4, 123.1, 93.9, 82.3, 80.8, 79.6, 37.5, 27.8, 23.8, 19.1; IR (neat): 3272, 3060, 2941, 2864, 2232, 1770, 1710, 1397, 1372, 1038, 761, 719; MS (ES$^+$) Calculated for [C$_{22}$H$_{17}$NNaO$_2$]$^+$: 350.1; Found: 350.1.

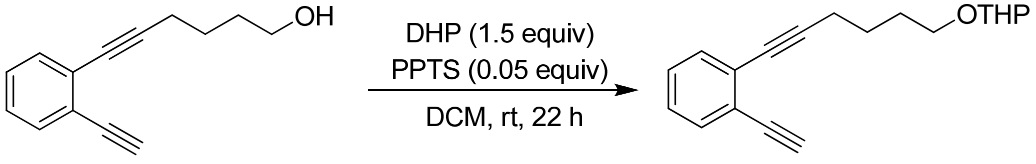
1-(6-(benzyloxy)hex-1-yn-1-yl)-2-ethynylbenzene (1f)



1f’ **1f**

Compound **1f’** was made according to the general procedure **A.** The corresponding benzyl ether **1f** was prepared according to the following procedure: to a solution of **1f’** (0.30 g, 1.5 mmol) in THF (5 mL) was added portionwise NaH (0.072 g, 1.8 mmol) at 0 °C. Upon the end of the H$_2$ formation, benzyl bromide (0.19 mL, 1.65 mmol) and TBAI (0.075 mmol) was added to the reaction. The resulting mixture was then stirred at room temperature for 5 h. The reaction mixture was quenched with a saturated solution of NH$_4$Cl, extracted with Et$_2$O (3 × 50 mL) and the combined organic layers were washed with water (2 × 20 mL), brine (20 mL), dried with MgSO$_4$, and concentrated. The crude product was purified with flash silica gel column chromatography (eluents: hexanes : ethyl acetate = 30:1) to get **1f** (0.39 g) in 90% yield. ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.52 (dd, 1H, J_1 = 7.6 Hz, J_2 = 1.6 Hz), 7.44 (d, 1H, J = 7.6 HZ), 7.39 (d, 4H, J =4.4 Hz), 7.22 – 7.36 (m, 3H), 4.55 (s, 2H), 3.57 (t, 2H, J = 6.4 Hz), 3.32 (s, 1H), 2.55 (t, 2H, J = 6.8 Hz), 1.87 – 1.94 (m, 2H), 1.75 – 1.82 (m, 2H); ^{13}C NMR (100 MHz, CDCl$_3$) δ 138.5, 132.3, 131.7, 128.3, 128.2, 127.5, 127.4, 127.1, 126.9, 124.3, 94.5, 82.4, 80.6, 79.3, 72.7, 69.7, 28.7, 25.5, 19.3; IR (neat): 3282, 3061, 3030, 2939, 2862, 2231, 2107, 1717, 1478, 1361, 1104; MS (ES$^+$) Calculated for [C$_{21}$H$_{20}$NaO]$^+$: 311.1; Found: 311.1.

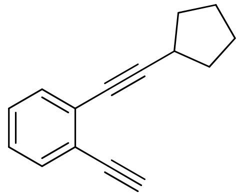
2-((6-(2-ethynylphenyl)hex-5-yn-1-yl)oxy)tetrahydro-2H-pyran (1g)



1f’ **1g**

The THP-protected diyne **1g** was prepared from **1f'** according to the following procedure: to a solution of **1f'** (0.60 g, 3.0 mmol) in DCM (30 mL) was added DHP (0.38 g, 4.5 mmol) and PPTS (0.038 g, 0.15 mmol) at room temperature. The resulting mixture was stirred for 22 h. DCM (30 mL) was added to the reaction mixture and it was washed with brine (30 mL), dried with $MgSO_4$, and concentrated. The crude product was purified with flash silica gel column chromatography (eluents: hexanes : ethyl acetate = 25:1) to give **1g** (0.72 g) in 85% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (d, 1H, *J* = 7.2 Hz), 7.37 (d, 1H, *J* = 8.0 Hz), 7.15 – 7.24 (m, 2H), 4.56 (t, 1H, *J* = 3.2 Hz), 3.74 – 3.86 (m, 2H), 3.39 – 3.49 (m, 2H), 3.29 (s, 1H), 2.48 (t, 2H, *J* = 6.8 Hz), 1.65 – 1.83 (m, 6H), 1.46 – 1.58 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 132.2, 131.7, 128.2, 127.0, 126.9, 124.3, 98.6, 94.4, 82.3, 80.5, 79.2, 66.8, 62.1, 30.6, 28.7, 25.3, 19.5, 19.2; IR (neat): 3283, 3060, 2942, 2868, 2231, 2106, 1725, 1478, 1119, 1034; MS (ES$^+$) Calculated for $[C_{19}H_{22}NaO_2]^+$: 305.2; Found: 305.2.

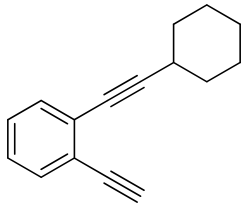
1-(cyclohexylethynyl)-2-ethynylbenzene (1h)



1h

Compound **1h** was prepared following the general procedure A. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (dd, 1H, J_1 = 7.6 Hz, J_2 = 0.8 Hz), 7.41 (dd, 1H, J_1 = 7.6 Hz, J_2 = 0.8 Hz), 7.18 – 7.28 (m, 2H), 3.30 (s, 1H), 2.88 – 2.95 (m, 1H), 1.97 – 2.02 (m, 2H), 1.75 – 1.84 (m, 4H), 1.61 – 1.64 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 132.3, 131.6, 128.3, 127.1, 127.0, 124.4, 99.3, 82.4, 80.4, 78.5, 33.8, 30.9, 24.9; IR (neat): 3286, 3060, 2960, 2870, 2224, 2108, 1477, 1450, 758; GCMS *m*/*z* 194 (M$^+$).

1-(cyclopentylethynyl)-2-ethynylbenzene (1i)

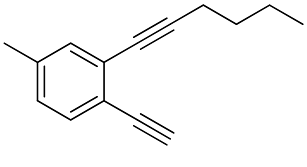


1i

Compound **1i** was prepared following the general procedure A. This compound is known and the spectroscopic data match those reported.[2] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (dd, 1H, J_1 = 7.6 Hz, J_2 =

1.6 Hz), 7.40 (dd, 1H, J_1 = 7.6 Hz, J_2 = 1.6 Hz), 7.19 – 7.28 (m, 2H), 3.27 (s, 1H), 2.65 – 2.71 (m, 1H), 1.77 – 1.90 (m, 4H), 1.52 – 1.64 (m, 3H), 1.35 – 1.41 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 132.3, 131.7, 128.3, 127.1, 127.0, 124.4, 98.9, 82.4, 80.4, 79.1, 32.5, 29.7, 25.9, 24.6; IR (neat): 3288, 3061, 2930, 2853, 2223, 2107, 1478, 1441, 758; GCMS *m*/*z* 208 (M^+).

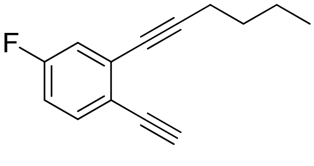
1-ethynyl-2-(hex-1-ynyl)-4-methylbenzene (1j)



1j

Compound **1j** was made according to the general procedure **A** except using with 1-bromo-2-iodo-4-methylbenzene as the starting material. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (d, 1H, *J* = 8.0 Hz), 7.23 (s, 1H), 7.02 (d, 1H, *J* = 7.6 Hz), 3.32 (s, 1H), 2.47 (t, 2H, *J* = 6.8 Hz), 2.31 (s, 3H), 1.48 – 1.66 (m, 4H), 0.95 (t, 3H, *J* = 7.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.6, 132.4, 132.3, 128.1, 126.9, 121.4, 94.5, 82.6, 79.6, 79.1, 30.7, 21.9, 19.2, 13.6; IR (neat): 3290, 3027, 2957, 2931, 2871, 2229, 2107, 1603, 1489, 1466, 821; GCMS *m*/*z* 196 (M^+).

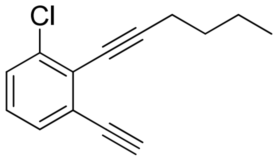
1-ethynyl-4-fluoro-2-(hex-1-yn-1-yl)benzene (1k)



1k

Compound **1k** was made according to the general procedure **A** except using with 1-bromo-4-fluoro-2-iodobenzene as the starting material. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.92 (td, 1H, J_1 = 8.8 Hz, J_2 = 5.6 Hz), 7.09 (dd, 1H, J_1 = 9.2 Hz, J_2 = 2.8 Hz), 6.92 (td, 1H, J_1 = 8 Hz, J_2 = 2.8 Hz), 3.24 (s, 1H), 2.47 (t, 2H, *J* = 7.0 Hz), 1.57 – 1.65 (m, 2H), 1.47 – 1.54 (m, 2H), 0.95 (t, 3H, *J* = 7.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.0 (d, *J* = 248.5 Hz), 134.2 (d, *J* = 8.5 Hz), 129.2 (d, *J* = 10.2 Hz), 120.6 (d, *J* = 3.4 Hz), 118.6 (d, *J* = 23.8 Hz), 114.9 (d, *J* = 22.1 Hz), 96.3, 81.5, 80.1, 78.2, 30.5, 21.9, 19.2, 13.5; IR (neat): 3304, 3073, 2958, 2933, 2872, 2232, 2110, 1602, 1568, 1478, 1290,1264, 1171, 872, 822; GCMS *m*/*z* 200 (M^+).

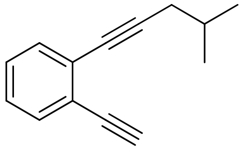
1-chloro-3-ethynyl-2-(hex-1-ynyl)benzene (1l)



1l

Compound **1l** was made according to the general procedure **A** except using with 1-bromo-3-chloro-2-iodobenzene as the starting material. ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.36 – 7.40 (m, 2H), 7.13 (t, 1H, *J* = 8.0 Hz), 3.31 (s, 1H), 2.55 (t, 2H, *J* = 6.8 Hz), 1.52 – 1.69 (m, 4H), 0.96 (t, 3H, *J* = 6.8 Hz); ^{13}C NMR (100 MHz, CDCl$_3$) δ 136.1, 130.7, 129.4, 127.5, 126.7, 126.3, 101.0, 81.7, 81.2, 76.2, 30.5, 21.8, 19.5, 13.6; IR (neat): 3298, 3068, 2957, 2932, 2871,2233, 2113, 1551, 1439, 1142, 852, 786, 733; GCMS *m*/*z* 216 (M$^+$).

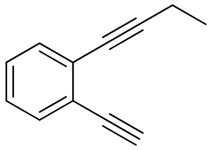
1-ethynyl-2-(4-methylpent-1-yn-1-yl)benzene (1m)



1m

Compound **1m** was made according to the general procedure **A**. ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.48 (dd, 1H, J_1 = 7.2 Hz, J_2 = 1.6 Hz), 7.42 (dd, 1H, J_1 = 8.0 Hz, J_2 = 1.6 Hz), 7.19 – 7.29 (m, 2H), 3.28 (s, 1H), 2.38 (d, 2H, *J* = 6.4 Hz), 1.90 – 2.00 (m, 1H), 1.08 (d, 6H, *J* = 6.8 Hz); ^{13}C NMR (100 MHz, CDCl$_3$) δ 132.4, 131.9, 128.4, 127.2, 127.1, 124.3, 93.9, 82.5, 80.4, 79.9, 28.7, 28.1, 22.0; IR (neat): 3288, 3062, 2958, 2926, 2870, 2235, 2108, 1478, 1441, 758; GCMS *m*/*z* 182 (M$^+$).

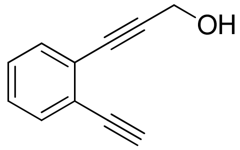
1-but-1-ynyl-2-ethynyl-benzene (1n)



1n

Compound **1n** was made according to the general procedure **A**. ^{1}H NMR (500 MHz, CDCl$_3$) δ 7.48 (dd, 1H, J_1 = 7.5 Hz, J_2 = 1.5 Hz), 7.41 (dd, 1H, J_1 = 8.0 Hz, J_2 = 1.0 Hz), 7.20 – 7.28 (m, 2H), 3.30 (s, 1H), 2.49 (q, 2H, J = 7.5 Hz), 1.27 (t, 3H, J = 7.5 Hz); ^{13}C NMR (125 MHz, $CDCl_3$) δ 132.4, 131.7, 128.3, 127.1, 126.9, 124.3, 96.2, 82.3, 80.4, 78.3, 13.9, 13.3; IR (neat): 3286, 3061, 2978, 2937, 2917, 2877, 2236, 2211, 1478, 1441, 1320; GCMS *m/z* 154 (M^+).

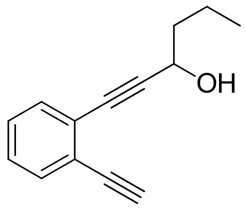
3-(2-ethynylphenyl)prop-2-yn-1-ol (1o)



1o

Compound **1o** was made according to the general procedure **A**. This compound is known and the spectroscopic data match those reported.[3]

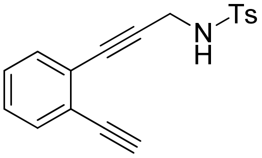
1-(2-ethynylphenyl)hex-1-yn-3-ol (1p)



1p

Compound **1p** was made according to the general procedure **A**. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.45 – 7.47 (m, 1H), 7.40 – 7.42 (m, 1H), 7.20 – 7.26 (m, 2H), 4.65 (dd, 1H, J_1 = 6.5 Hz, J_2 = 1.5 Hz), 3.32 (s, 1H), 2.85 (d, 1H, J = 5.5 Hz), 1.76 – 1.83 (m, 2H), 1.53 – 1.60 (m, 2H), 0.94 (t, 3H, J = 7.0 Hz); ^{13}C NMR (125 MHz, $CDCl_3$) δ 132.3, 131.8, 128.3, 127.8, 125.5, 124.4, 94.5, 82.9, 82.1, 81.0, 62.6, 39.7, 18.4, 13.7; IR (neat): 3289(bs), 3062, 2959, 2934, 2872, 2204, 2108, 1478, 1441, 1031, 759; GCMS *m/z* 198 (M^+).

N-(3-(2-ethynylphenyl)prop-2-yn-1-yl)-4-methylbenzenesulfonamide (1q)

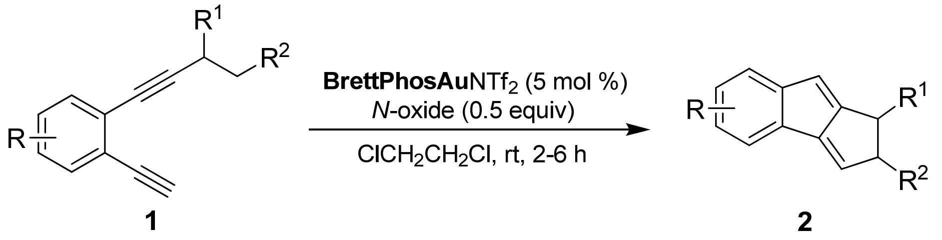


1q

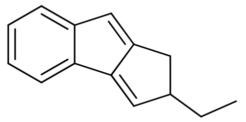
Compound **1q** was made according to the general procedure **A**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, 2H, *J* = 8.0 Hz), 7.42 – 7.45 (m, 1H), 7.19 – 7.26 (m, 4H), 7.07 – 7.10 (m, 1H), 4.98 (t, 1H, *J* = 6.0 Hz), 4.12 (d, 2H, *J* = 6.0 Hz), 3.26 (s, 1H), 2.29 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.7, 136.6, 132.4, 131.9, 129.6, 128.3, 128.2, 127.4, 125.0, 124.4, 87.2, 83.0, 81.7, 81.1, 33.4, 21.4; IR (neat): 3281, 3063, 2923, 2850, 1596, 1441, 1327, 1159, 1065, 813; MS (ES$^+$) Calculated for $[C_{18}H_{15}NNaO_2S]^+$: 332.1; Found: 332.1.

General procedure B: gold-catalyzed cycloisomerization of benzene-1,2-diynes.

2,6-dibromopyridine *N*-oxide **5** or lutidine *N*-oxide **6** (0.15 mmol) and BrettPhosAuNTf$_2$ (15.3 mg, 0.015 mmol) were added in this order to a solution of a benzene-1,2-diyne **1** (0.30 mmol) in DCE (3.0 mL) at room temperature. The reaction mixture was stirred at rt and the progress of the reaction was monitored by TLC. The reaction typically took 2 – 6 h. Upon completion, the mixture was concentrated and the residue was purified by chromatography on silica gel (eluent: hexanes/ethyl acetate) to afford the desired product **2**.



2-ethyl-1,2-dihydrocyclopenta[a]indene (2a)

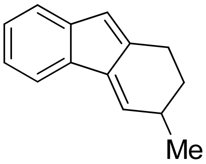


2a

Compound **2a** was prepared in 90% isolated yield using lutidine *N*-oxide (**6**) as the additive according to the general procedure B. The reaction time was 6 h. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, 1H, *J* = 7.6 Hz), 7.22 – 7.26 (m, 2H), 7.06 – 7.10 (m, 1H), 6.75 (dd, 1H, J_1 = 2.8 Hz, J_2 = 1.6 Hz), 6.25 – 6.27 (m, 1H), 3.34 – 3.39 (m, 1H), 2.94 (ddd, 1H, J_1 = 18.4 Hz, J_2 = 6.4 Hz, J_3 = 2.0 Hz), 2.36 (dt, 1H, J_1 = 18.4 Hz, J_2 = 2.0 Hz), 1.62 – 1.71 (m, 1H), 1.53 – 1.60 (m, 1H), 1.03 (t, 3H, *J* = 7.6 Hz); ^{13}C NMR (125 MHz,

$CDCl_3$) δ 154.1, 150.9, 149.0, 137.8, 129.7, 127.7, 122.9, 122.0, 120.1, 115.4, 54.6, 30.0, 28.4, 12.3; IR (neat): 3045, 2961, 2929, 2874, 1710, 1604, 1461, 1323, 1034, 966; GCMS *m*/*z* 182 (M^+).

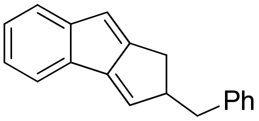
3-methyl-2,3-dihydro-1*H*-fluorene (3a)



3a

This title compound was formed as a minor product in the above reaction. When $IPrAuNTf_2$ was the catalyst, this minor product was formed in a sufficient yield to allow separation. ^1H NMR (600 MHz, $CDCl_3$) δ 7.48 (d, 1H, J = 7.8 Hz), 7.15 – 7.16 (m, 2H), 7.04 – 7.07 (m, 1H), 6.68 (t, 1H, J = 2.4 Hz), 6.38 (s, 1H), 2.81 (dt, 1H, J_1 = 16.2 Hz, J_2 = 4.8 Hz), 2.56 – 2.65 (m, 2H), 2.00 – 2.05 (m, 1H), 1.47 – 1.54 (m, 1H), 1.21 (d, 3H, J = 4.8 Hz)6.28 (s, 1H), 3.10 – 3.14 (m, 2H), 2.73 – 2.76 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154143.7, 139.7, 138.9, 135.3, 134.6, 127.4, 123.7, 123.0, 119.8, 119.1, 33.1, 31.5, 23.8, 20.9; IR (neat): 3052, 3011, 2957, 2928, 2871, 2855, 1719, 1700, 1649, 1458, 1016; GCMS *m*/*z* 182 (M^+).

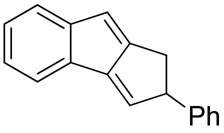
2-benzyl-1,2-dihydrocyclopenta[a]indene (2b)



2b

Compound **2b** was prepared in 91% yield using 2,6-dibromopyridine *N*-oxide (**5**) as the additive according to the general procedure B. The reaction time was 4 h. ^1H NMR (500 MHz, $CDCl_3$) δ 7.59 (d, 1H, J = 7.5 Hz), 7.35 – 7.39 (m, 2H), 7.25 – 7.30 (m, 5H), 7.10 – 7.14 (m, 1H), 6.69 (t, 1H, J = 2.0 Hz), 6.29 (s, 1H), 3.74 – 3.79 (m, 1H), 2.86 – 2.97 (m, 3H), 2.48 (dt, 1H, J_1 = 18.0 Hz, J_2= 2.0 Hz); ^{13}C NMR (125 MHz, $CDCl_3$) δ 153.5, 150.8, 149.2, 140.3, 136.9, 129.7, 128.8, 128.4, 127.9, 126.1, 123.0, 122.1, 120.1, 115.9, 54.5, 41.9, 30.2; IR (neat): 3060, 3026, 2921, 2850, 1709, 1603, 1495, 1453, 1324, 1030, 966, 910; GCMS *m*/*z* 244 (M^+).

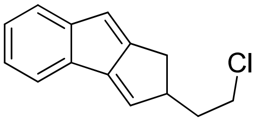
2-phenyl-1,2-dihydrocyclopenta[a]indene (2c)



2c

Compound **2c** was prepared in 95% yield using 2,6-dibromopyridine *N*-oxide (**5**) as the additive according to the general procedure B. The reaction time was 4 h. ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.64 (d, 1H, J = 7.6 Hz), 7.22 – 7.35 (m, 7H), 7.11 – 7.17 (m, 1H), 6.76 (dd, 1H, J_1 = 3.5 Hz, J_2 = 2.0 Hz), 6.36 (t, 1H, J = 0.8 Hz), 4.61 – 4.64 (m, 1H), 3.33 (ddd, 1H, J_1 = 18.4 Hz, J_2 = 6.8 Hz, J_3 = 2.0 Hz), 2.68 (dt, 1H, J_1= 18.4 Hz, J_2 = 2.0 Hz); ^{13}C NMR (100 MHz, CDCl$_3$) δ 153.9, 151.0, 150.1, 143.8, 136.1, 129.8, 128.7, 128.2, 127.4, 126.7, 123.3, 122.3, 120.3, 116.4, 57.9, 34.0; IR (neat): 3064, 3026, 2914, 2841, 1601, 1494, 1444, 1427, 1197, 942, 820; GCMS m/z 230 (M$^+$).

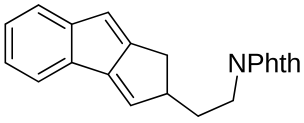
2-(2-chloroethyl)-1,2-dihydrocyclopenta[a]indene (2d)



2d

Compound **2d** was prepared in 82% yield using 2,6-dibromopyridine *N*-oxide (**5**) as the additive according to the general procedure B. The reaction time was 4 h. ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.58 (d, 1H, J = 7.6 Hz), 7.22 – 7.24 (m, 2H), 7.08 – 7.12 (m, 1H), 6.69 (t, 1H, J = 2.0 Hz), 6.28 (d, 1H, J = 1.2 Hz), 3.62 – 3.73 (m, 3H), 3.01 (ddd, 1H, J_1 = 18.4 Hz, J_2 = 6.4 Hz, J_3 = 2.0 Hz), 2.38 (dt, 1H, J_1 = 18.4 Hz, J_2 = 2.0 Hz), 2.08 – 2.16 (m, 1H), 1.95 – 2.04 (m, 1H); ^{13}C NMR (125 MHz, CDCl$_3$) δ 152.9, 150.8, 149.6, 135.6, 129.5, 128.0, 123.3, 122.1, 120.2, 116.2, 50.1, 43.3, 38.2, 29.9; IR (neat): 3066, 2998, 2926, 2865, 1707, 1602, 1444, 1285; GCMS m/z 216 (M$^+$).

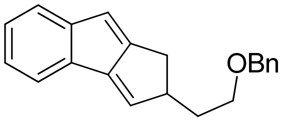
2-(2-(1,2-dihydrocyclopenta[a]inden-2-yl)ethyl)isoindoline-1,3-dione (2e)



2e

Compound **2e** was prepared in 93% yield using lutidine *N*-oxide (**6**) as the additive according to the general procedure B. The reaction time was 6 h. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 – 7.84 (m, 2H), 7.71 – 7.73 (m, 2H), 7.56 (d, 1H, J = 8.0 Hz), 7.21 – 7.22 (m, 2H), 7.05 – 7.09 (m, 1H), 6.74 (dd, 1H, J_1 = 2.8 Hz, J_2 = 1.6 Hz), 6.26 (t, 1H, J = 0.8 Hz), 3.81 – 3.86 (m, 2H), 3.41 – 3.46 (m, 1H), 3.02 (ddd, 1H, J_1 = 18.4 Hz, J_2 = 6.4 Hz, J_3 = 2.0 Hz), 2.47 (dt, 1H, J_1 = 18.4 Hz, J_2 = 2.0 Hz), 1.85 – 1.94 (m, 1H), 1.99 – 2.07 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 168.3, 153.2, 150.8, 149.6, 136.0, 133.9, 132.0, 129.6, 128.0, 123.2, 123.1, 122.1, 120.2, 116.1, 50.2, 36.6, 34.1, 30.2; IR (neat): 3063, 2926, 2853, 1769, 1710, 1605, 1399, 1372; MS (ES$^+$) Calculated for $[C_{22}H_{17}NNaO_2]^+$: 350.1; Found: 350.1.

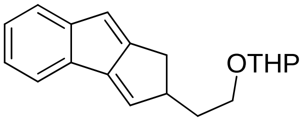
2-(2-(benzyloxy)ethyl)-1,2-dihydrocyclopenta[a]indene (2f)



2f

Compound **2f** was prepared in 89% yield using lutidine *N*-oxide (**6**) as the additive according to the general procedure B. The reaction time was 6 h. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58 (d, 1H, J = 8.0 Hz), 7.35 – 7.39 (m, 4H), 7.29 – 7.34 (m, 1H), 7.21 – 7.24 (m, 2H), 7.06 – 7.11 (m, 1H), 6.73 (dd, 1H, J_1 = 2.5 Hz, J_2 = 1.5 Hz), 6.26 (t, 1H, J = 1.0 Hz), 4.55 (s, 2H), 3.59 – 3.67 (m, 3H), 2.96 (ddd, 1H, J_1 = 18.0 Hz, J_2 = 6.5 Hz, J_3 = 2.0 Hz), 2.40 (dt, 1H, J_1 = 18.0 Hz, J_2 = 2.0 Hz), 1.95 – 2.02 (m, 1H), 1.81 – 1.88 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 153.7, 150.8, 149.0, 138.3, 137.5, 129.7, 128.3, 127.8, 127.6, 127.5, 123.0, 122.0, 120.1, 115.6, 73.1, 68.9, 50.0, 35.5, 30.4; IR (neat): 3064, 2925, 2857, 1601, 1445, 1363, 1204, 1028, 821; MS (ES$^+$) Calculated for $[C_{21}H_{20}NaO]^+$: 311.1; Found: 311.1.

2-(2-(1,2-dihydrocyclopenta[a]inden-2-yl)ethoxy)tetrahydro-2H-pyran (2g)

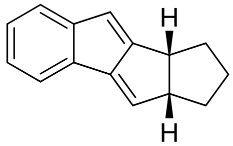


2g

Compound **2g** was prepared in 92% yield using lutidine *N*-oxide (**6**) as the additive according to the general procedure B. The reaction time was 6 h. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, 1H, J = 7.6 Hz), 7.23 (d, 2H, J = 4.0 Hz), 7.07 – 7.12 (m, 1H), 6.76 (d, 1H, J = 2.0 Hz), 6.27 (s, 1H), 4.62 (dd, 1H, J_1 =

6.8 Hz, J_2 = 3.2 Hz), 3.85 – 3.95 (m, 2H), 3.51 – 3.60 (m, 3H), 2.99 (dd, 1H, J_1 = 18.0 Hz, J_2 = 6.4 Hz), 2.43 (d, 1H, J = 18.4 Hz), 1.93 – 2.03 (m, 1H), 1.72 – 1.88 (m, 3H), 1.52 – 1.65 (m, 4H); ^{13}C NMR (100 MHz, CDCl$_3$) δ 153.8, 150.9, 149.0, 137.6, 129.7, 127.8, 123.0, 122.0, 120.1, 1155.6, 98.9, 66.0, 62.2, 50.1, 35.4, 30.7, 30.3, 25.4, 19.5; IR (neat): 3065, 3044, 2938, 2869, 1602, 1323, 1352, 1136, 1075, 1034; MS (ES$^+$) Calculated for [$C_{19}H_{22}NaO_2$]$^+$: 305.2; Found: 305.2.

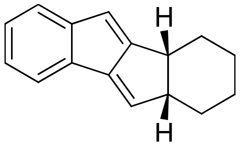
(3aR,9aR)-2,3,3a,9a-tetrahydro-1H-pentaleno[2,1-a]indene (2h)



2h

Compound **2h** was prepared in 86% yield using 2,6-dibromopyridine *N*-oxide (**5**) as the additive according to the general procedure B. The reaction time was 2 h. ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.57 (d, 1H, J = 7.2 Hz), 7.21 – 7.26 (m, 2H), 7.07 – 7.11 (m, 1H), 6.59 (dd, 1H, J_1 = 2.4 Hz, J_2 = 1.6 Hz), 6.25 (t, 1H, J = 1.6 Hz), 3.84 – 3.89 (m, 1H), 3.40 – 3.44 (m, 1H), 1.67 – 1.87 (m, 4H), 1.53 – 1.60 (m, 1H), 1.35 – 1.45 (m, 1H); ^{13}C NMR (100 MHz, CDCl$_3$) δ 159.8, 151.0, 149.7, 137.4, 129.8, 127.7, 123.1, 122.0, 120.3, 115.4, 58.1, 41.1, 33.3, 30.4, 24.9; IR (neat): 3065, 3010, 2947, 2861, 1602, 1443, 1294, 1192, 1011, 829; GCMS *m*/*z* 194 (M$^+$).

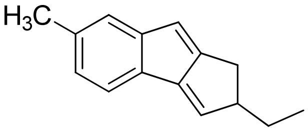
(4aR,10aS)-1,2,3,4,4a,10a-hexahydroindeno[2,1-a]indene (2i)



2i

Compound **2i** was prepared in 83% yield using 2,6-dibromopyridine *N*-oxide (**5**) as the additive according to the general procedure B. The reaction time was 2 h. ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.58 (d, 1H, J = 7.6 Hz), 7.19 – 7.25 (m, 2H), 7.05 – 7.12 (m, 1H), 6.68 (t, 1H, J = 2.4 Hz), 6.25 (s, 1H), 3.36 – 3.44 (m, 1H), 3.04 – 3.10 (m, 1H), 1.87 – 1.95 (m, 2H), 1.38 – 1.65 (m, 6H); ^{13}C NMR (100 MHz, CDCl$_3$) δ 159.1, 150.6, 148.4, 138.5, 129.9, 127.7, 123.0, 122.0, 120.2, 115.2, 51.8, 36.6, 26.9, 26.6, 20.8, 20.5; IR (neat): 3060, 2928, 2855, 1708, 1602, 1447, 1295, 1084, 909; GCMS *m*/*z* 208 (M$^+$).

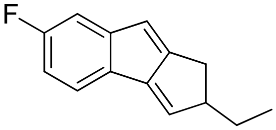
2-ethyl-6-methyl-1,2-dihydrocyclopenta[a]indene (2j)



2j

Compound **2j** was prepared in 93% yield using lutidine *N*-oxide (**6**) as the additive according to the general procedure B. The reaction time was 6 h. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (d, 1H, J = 7.6 Hz), 7.07 (s, 1H), 6.91 (d, 1H, J = 7.6 Hz), 6.67 (d, 1H, J = 2.0 Hz), 6.22 (s, 1H), 3.33 – 3.39 (m, 1H), 2.93 (ddd, 1H, J_1 = 18.4 Hz, J_2 = 6.4 Hz, J_3 = 2.0 Hz), 2.40 (s, 3H), 2.32 – 2.38 (m, 1H), 1.62 –1.71 (m, 1H), 1.53 – 1.60 (m, 1H), 1.04 (t, 3H, J = 7.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.5, 151.3, 148.8, 137.7, 136.8, 127.2, 123.7, 121.7, 121.0, 115.3, 54.5, 29.9, 28.4, 21.8, 12.3; IR (neat): 3060, 2959, 2923, 2871, 1706, 1606, 1454, 1292, 809; GCMS *m/z* 196 (M^+).

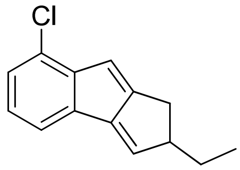
2-ethyl-6-fluoro-1,2-dihydrocyclopenta[a]indene (2k)



2k

Compound **2k** was prepared in 97% yield using lutidine *N*-oxide (**6**) as the additive according to the general procedure B. The reaction time was 6 h. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (dd, 1H, J_1 = 8.0 Hz, J_2 = 1.6 Hz), 6.92 (dd, 1H, J_1 = 9.6 Hz, J_2 = 2.4 Hz), 6.74 – 6.79 (m, 1H), 6.70 (t, 1H, J = 2.4 Hz), 6.22 (d, 1H, J = 1.6 Hz), 3.33 – 3.39 (m, 1H), 2.94 (ddd, 1H, J_1 = 18.4 Hz, J_2 = 6.4 Hz, J_3 = 2.0 Hz), 2.36 (dt, 1H, J_1 = 18.4 Hz, J_2= 2.0 Hz), 1.62 – 1.73 (m, 1H), 1.51 – 1.60 (m, 1H), 1.03 (t, 3H, J = 7.6 Hz); ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.1 (d, J = 243.4 Hz), 156.5, 153.0 (d, J = 9.4 Hz), 147.7, 138.1, 125.6, 122.7 (d, J = 9.3 Hz), 114.9 (d, J = 2.5 Hz), 109.3 (d, J = 23.0 Hz), 107.4 (d, J = 23.0 Hz), 54.6, 30.1, 28.3, 12.3; IR (neat): 3069, 2960, 2927, 2872, 1605, 1593, 1458, 1428, 1222, 1130, 861; GCMS *m/z* 200 (M^+).

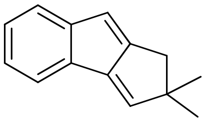
7-chloro-2-ethyl-1,2-dihydrocyclopenta[a]indene (2l)



2l

Compound **2l** was prepared in 78% yield using lutidine *N*-oxide (**6**) as the additive according to the general procedure B. The reaction time was 6 h. ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.46 (d, 1H, J = 7.2 Hz), 7.20 (d, 1H, J = 7.6 Hz), 7.01 (t, 1H, J = 7.6 Hz), 6.82 (s, 1H), 6.43 (s, 1H), 3.36 – 3.41 (m, 1H), 2.96 (ddd, 1H, J_1 = 18.4 Hz, J_2 = 6.4 Hz, J_3 = 2.0 Hz), 2.38 (d, 1H, J = 18.8 Hz), 1.51 – 1.71 (m, 2H), 1.03 (t, 3H, J = 7.6 Hz); ^{13}C NMR (100 MHz, CDCl$_3$) δ 155.1, 148.9, 148.3, 140.4, 131.3, 127.8, 125.0, 124.0, 120.3, 113.3, 54.8, 30.0, 28.2, 12.2; IR (neat): 3057, 2960, 2925, 2872, 1598, 1559, 1458, 1408, 1180, 1132, 829; GCMS *m*/*z* 216 (M$^+$).

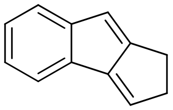
2,2-dimethyl-1,2-dihydrocyclopenta[a]indene (2m)



2m

Compound **2m** was prepared in 96% yield using lutidine *N*-oxide (**6**) as the additive according to the general procedure B. The reaction time was 6 h. ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.56 (d, 1H, J = 7.2 Hz), 7.22 (d, 2H, J = 4.0 Hz), 7.06 – 7.10 (m, 1H), 6.54 (d, 1H, J = 2.0 Hz), 6.25 (d, 1H, J = 2.0 Hz), 2.61 (d, 2H, J = 1.6 Hz), 1.32 (s, 6H); ^{13}C NMR (100 MHz, CDCl$_3$) δ 154.0 150.6, 146.3, 130.0, 127.8, 123.1, 122.1, 120.1, 116.1, 53.6, 39.6, 28.6; IR (neat): 3066, 3013, 2955, 2924, 2863, 1602, 1461, 1445, 1432, 816; GCMS *m*/*z* 182 (M$^+$).

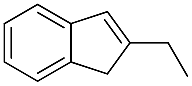
1,2-dihydrocyclopenta[a]indene (2n)



2n

Compound **2n** was prepared in 62% yield using 2,6-dibromopyridine *N*-oxide (**5**) as the additive according to the general procedure B. The reaction time was 4 h. ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.59 (d, 1H, J = 6.8 Hz *),* 7.20 – 7.25 (m, 2H), 7.06 – 7.10 (m, 1H), 6.79 (dd, 1H, J_1 = 4.8 Hz, J_2 = 2.8 Hz), 6.28 (s, 1H), 3.10 – 3.14 (m, 2H), 2.73 – 2.76 (m, 2H); ^{13}C NMR (100 MHz, CDCl$_3$) δ 154.9, 151.0, 150.0, 134.1, 129.8, 127.7, 122.9, 121.9, 120.1, 115.2, 39.3, 23.1; IR (neat): 3066, 3004, 2925, 2856, 1643, 1458, 1445, 1282; GCMS *m*/*z* 154 (M$^+$).

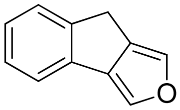
2-ethyl-1H-indene (7)



7

This compound was isolated as the minor component in the above reaction and its spectroscopic data match those reported.[5]

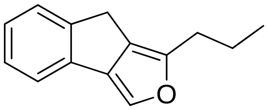
8H-indeno[1,2-c]furan (9)



9

Compound **9** was prepared in 93% yield using lutidine *N*-oxide (**6**) as the additive according to the general procedure B. The reaction time was 15 min. ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.60 (d, 1H, J = 0.8 Hz), 7.56 (d, 1H, J = 7.2 Hz), 7.43 (d, 1H, J = 7.2 Hz), 7.22 – 7.32 (m, 3H), 3.76 (s, 2H); ^{13}C NMR (100 MHz, CDCl$_3$) δ 147.6, 134.5, 134.1, 133.5, 131.3, 129.3, 126.9, 126.5, 125.8, 122.0, 29.0; IR (neat): 3119, 3057, 3026, 2913, 2822, 1634, 1462, 1265, 1198, 1094, 1011, 903; GCMS *m*/*z* 156 (M$^+$).

1-propyl-8H-indeno[1,2-c]furan (10)

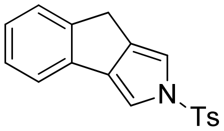


10

Compound **10** was prepared in 85% yield using lutidine *N*-oxide (**6**) as the additive according to the general procedure B. The reaction time was 12 h. ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.52 (d, 1H, J = 6.0

Hz), 7.47 (s, 1H), 7.40 (d, 1H, *J* = 6.4 Hz), 7.26 – 7.30 (m, 1H), 7.20 – 7.23 (m, 1H), 3.69 (s, 2H), 2.66 – 2.70 (m, 2H), 1.72 – 1.79 (m, 2H), 1.00 (t, 3H, *J* = 7.5 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.7, 147.1, 135.0, 133.8, 129.2, 126.8, 126.2, 125.7, 123.8, 121.8, 29.5, 29.0, 20.9, 13.9; IR (neat): 3060, 2961, 2931, 2872, 1764, 1631, 1565, 1462, 1174, 949; GCMS *m*/*z* 198 (M^+).

2-tosyl-2,8-dihydroindeno[1,2-c]pyrrole (11)



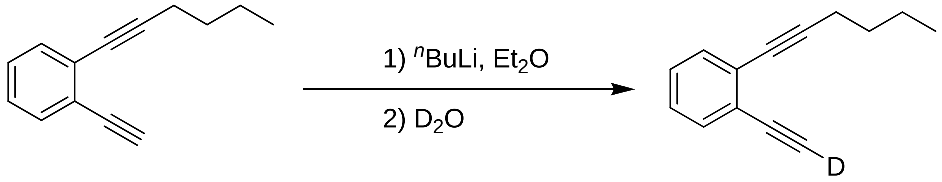
11

Compound **11** was prepared in 97% yield using lutidine *N*-oxide (**6**) as the additive according to the general procedure B. The reaction time was 18 h. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.78 (d, 2H, *J* = 8.5 Hz), 7.51 (d, 1H, *J* = 7.5 Hz), 7.39 (d, 1H, *J* = 7.5 Hz), 7.26 – 7.29 (m, 4H), 7.20 – 7.23 (m, 1H), 7.05 – 7.06 (m, 1H), 3.67 (s, 2H), 2.38 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 147.1, 144.6, 136.2, 136.0, 135.5, 133.1, 129.8, 126.9, 126.7, 126.5, 125.5, 121.4, 113.4, 109.7, 30.2, 21.6; IR (neat): 3119, 3060, 2916, 1593, 1366, 1317, 1270, 1092, 1050, 812; MS (ES^+) Calculated for $[C_{18}H_{15}NNaO_2S]^+$: 332.1; Found: 332.1.

Mechanistic studies:

A. Preparation of substrates:

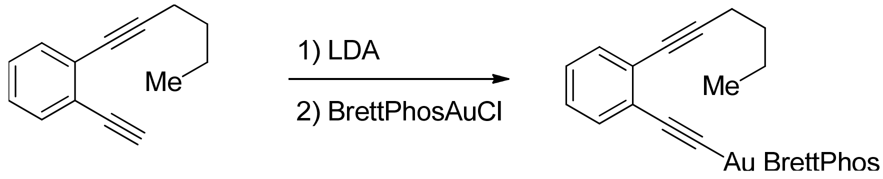
A1: Compound 1a-d$_1$



1a **1a**-d$_1$

In an oven-dried, 20 mL Schlenk flask, **1a** (128 mg, 0.70 mmol) was dissolved in 1.5 mL of anhydrous diethylether. The flask was cooled to 0 °C before the slow addition of 0.53 mL of ^{n}BuLi solution (1.6 M in hexanes, 0.84 mmol) and stirring for 15 min at 0 °C, followed by 30 min at room temperature. The flask was recooled to 0 °C, and D_2O (42 uL, 2.1 mmol) was slowly added. The reaction was stirred overnight at room temperature before the solvent was removed in vacuo. The crude product was purified with flash silica gel column chromatography (eluents: hexanes : ethyl acetate = 200:1) to give **1a'** (0.087 g) in 68% yield. The deuterium incorporation was determined to be >98% D by ^{1}H NMR. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (d, 1H, *J* = 8.0 Hz), 7.41 (d, 1H, *J* = 8.0 Hz), 7.19 – 7.28 (m, 2H), 2.48 (t, 2H, *J* = 7.2 Hz), 1.49 – 1.66 (m, 4H), 0.96 (t, 3H, *J* = 7.2 Hz); ^{13}C NMR (125 MHz, $CDCl_3$) δ 132.4, 131.8, 128.3, 127.1, 124.3, 95.0, 82.0 (t, *J* = 7.4 Hz), 80.1 (t, *J* = 152.5 Hz), 79.0, 30.8, 22.0, 19.3, 13.7; IR (neat): 3286, 3061, 3026, 2957, 2932, 2871, 2232, 1982, 1477, 1441, 1328, 1100, 950; GCMS *m*/*z* 183 (M^+).

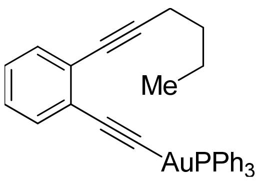
A2: Compound 1a-Au



1a-Au

1a (71.1 mg, 0.39 mmol) in THF (2 mL) was added dropwise to a solution of lithium diisopropylamine (0.5 mmol) in 2 mL THF at -78 °C for one hour. BrettPhosgold chloride (277 mg, 0.36 mmol) was added and the solution allowed to warm to 0 °C. After 5 hours at 0 °C, the solution was filtered, concentrated to dryness, and recrystallized from chloroform/pentane to afford **1a-Au** (228 mg, 64% yield) as a beige powder.[4] ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34 (dd, 1H, J_1 = 7.5 Hz, J_2 = 1.5 Hz), 7.29 (dd, 1H, J_1 = 7.5 Hz, J_2 = 1.5 Hz), 7.05 – 7.10 (m, 3H), 6.96 – 7.02 (m, 2H), 6.91 (dd, 1H, J_1 = 9.0 Hz, J_2 = 3.0 Hz), 3.88 (s, 3H), 3.56 (s, 3H), 2.92 – 2.97 (m, 1H), 2.59 – 2.66 (m, 2H), 2.46 (t, 2H, *J* = 7.5 Hz), 2.30 – 2.36 (m, 2H), 1.96 – 1.98 (m, 2H), 1.69 – 1.79 (m, 6H), 1.60 – 1.66 (m, 4H), 1.45 – 1.52 (m, 4H), 1.38 (d, 6H, *J* = 6.5 Hz), 1.15 – 1.35 (m, 14H), 0.87 – 0.94 (m, 10H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.5, 153.0 (d, *J* = 44.5 Hz), 148.9, 145.4, 143.0, 141.9, 138.6 (d, *J* = 63.5 Hz), 132.3, 131.3, 130.4 (d, *J* = 29.0 Hz), 129.2, 126.3 (d, *J* = 20.5 Hz), 124.7, 121.8, 119.1, 118.1, 113.0, 109.6, 99.7 (d, *J* = 96.0 Hz), 92.9, 80.8, 68.0, 55.5, 54.7, 39.0, 38.7, 33.8 (d, *J* = 31.0 Hz), 33.6, 31.6, 31.0, 30.7, 30.0, 27.5 (d, *J* = 48.0 Hz), 26.9 (d, *J* = 61.5 Hz), 25.9, 25.6, 25.1, 24.3, 23.8, 22.7, 22.1, 19.6, 14.1, 13.7; ^{31}P NMR (161.9 MHz, $CDCl_3$) δ 45.3; IR (neat): 3433, 3059, 2955, 2930, 2853, 2115, 1640, 1582, 1458, 1354, 1254, 1200, 1058; MS (ES^+) Calculated for $[AuC_{49}H_{67}O_2P]^+$: 915.5; Found: 915.5.

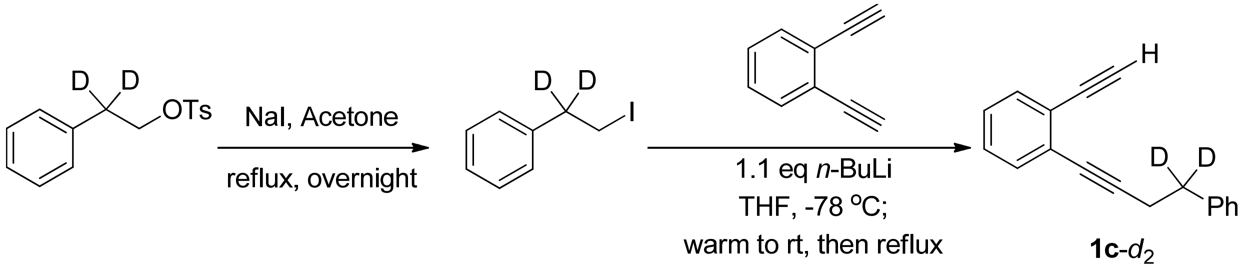
A3: Compound 1a'-Au



1a'-Au

The same procedure was applied to prepare **1a'-Au** (60% yield). ^{1}H NMR (500 MHz, CDCl$_3$) δ 7.57 (ddd, 5H, J_1 = 12.6 Hz, J_2 = 5.2 Hz, J_3 = 3.2 Hz,), 7.54 – 7.42 (m, 10H), 7.36 (dt, 1H, J_1 = 9.0 Hz, , J_2 = 4.2 Hz), 7.17 – 7.09 (m, 2H), 2.51 (t, 2H, J = 7.0 Hz), 1.70 – 1.60 (m, 2H), 1.59 – 1.50 (m, 2H), 0.91 – 0.83 (t, 3H, J = 7.5 Hz). ^{13}C NMR (125 MHz, CDCl$_3$) δ 155.5, 153.0 (d, J = 44.5 Hz), 148.9, 145.4, 143.0, 141.9, 138.6 (d, J = 63.5 Hz), 132.3, 131.3, 130.4 (d, J = 29.0 Hz), 129.2, 126.3 (d, J = 20.5 Hz), 124.7, 121.8, 119.1, 118.1, 113.0, 109.6, 99.7 (d, J = 96.0 Hz), 92.9, 80.8, 68.0, 55.5, 54.7, 39.0, 38.7, 33.8 (d, J = 31.0 Hz), 33.6, 31.6, 31.0, 30.7, 30.0, 27.5 (d, J = 48.0 Hz), 26.9 (d, J = 61.5 Hz), 25.9, 25.6, 25.1, 24.3, 23.8, 22.7, 22.1, 19.6, 14.1, 13.7; ^{31}P NMR (161.9 MHz, CDCl$_3$) δ 42.2.

A4: 1-ethynyl-2-(4-phenyl-4,4-*d*$_2$-but-1-yn-1-yl)benzene (1c-d$_2$)



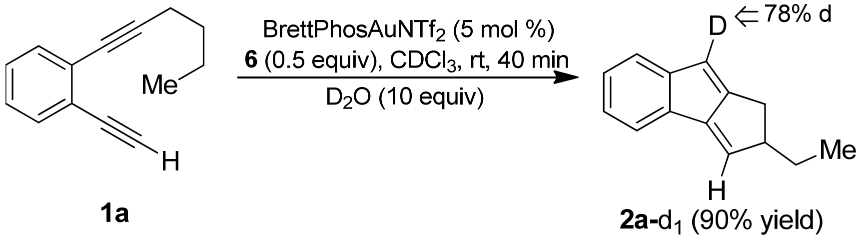
2-phenyl-2,2-*d*$_2$-ethyl 4-methylbenzenesulfonate (>98% deuterium) was prepared in 87% yield according to literature procedures[6].

(2-iodo-1,1-*d*$_2$-ethyl)benzene (>98% deuterium) was prepared from 2-phenyl-2,2-*d*$_2$-ethyl 4-methylbenzenesulfonate in 90 % yield according to literature procedures[7]. ^{1}H NMR (600 MHz, CDCl$_3$) δ 7.34 – 7.29 (m, 2H), 7.29 – 7.24 (m, 1H), 7.22 – 7.17 (m, 2H), 3.34 (d, J = 9.8 Hz, 2H; ^{13}C NMR (200 MHz, CDCl$_3$) δ 128.6, 128.3, 126.8, 5.33.

1,2-diethynylbenzene was prepared in 89% yield according to literature procedures[8].

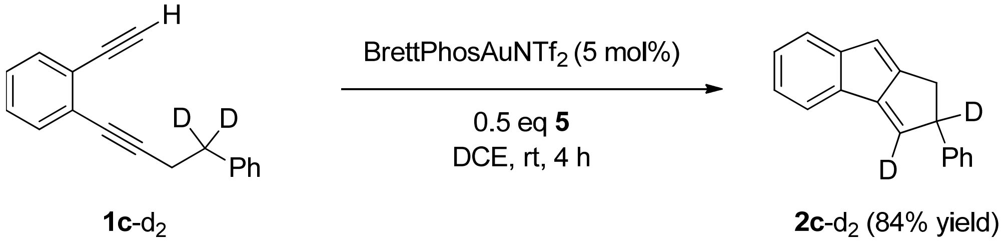
Compound **1c**-*d*$_2$ was prepared in 62% yield by the following procedure: to a THF solution (10 ml) of 1,2-diethynylbenzene (3 mmol) at -78 °C was slowly added n-butyllithium (2.5 M in hexanes, 3.3 mmol) under N_2. After stirring for 0.5 h, a THF solution (1ml) of 2-iodo-1,1-d_2-ethyl)benzene (3 mmol) was added dropwise and then the reaction was warmed to room temperature, followed by refluxing overnight. Upon completion, the mixture was concentrated and the residue was purified by chromatography on silica gel (eluent: hexanes) to afford the desired product. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.50 – 7.46 (m, 1H), 7.39 (dd, 1H, J_1 = 7.7 Hz, J_2 = 1.2 Hz), 7.34 – 7.30 (m, 4H), 7.28 (dd, 1H, J_1 = 7.2 Hz, J_2 = 1.2 Hz), 7.26 – 7.21 (m, 2H), 3.25 (s, 1H), 2.77 (d, 2H, J = 7.0 Hz); ^{13}C NMR (125 MHz, $CDCl_3$) δ 140.6, 132.5, 132.0, 128.6, 128.41, 128.37, 127.3, 126.9, 126.3, 124.3, 94.0, 82.4, 80.5, 79.7, 21.6; GCMS *m/z* 232 (M^+).

B. Deuterium-labeling studies



The reaction was run following the general procedure B except that 10 equivalents of D_2O was added to the reaction mixture. The reaction proceeded surprisingly faster than that in the absence of D_2O. **2a**-d$_1$: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, 1H, J = 7.6 Hz), 7.21 – 7.24 (m, 2H), 7.05 – 7.11 (m, 1H), 6.74 (d, 1H, J = 2.4 Hz), 3.33 – 3.40 (m, 1H), 2.93 (dd, 1H, J_1 = 18.4 Hz, J_2 = 6.4 Hz), 2.35 (dd, 1H, J_1 = 18.4 Hz, J_2 = 2.0 Hz), 1.61- 1.70 (m, 1H), 1.50 – 1.59 (m, 1H), 1.02 (t, 3H, J = 7.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.1 (d, J = 13.6 Hz), 150.9, 149.0, 138.0, 129.8, 128.8, 123.0, 122.0, 120.1, 115.4, 54.6, 29.9, 28.4, 12.3; IR (neat): 3066, 3044, 2960, 2928, 2873, 1711, 1603, 1460, 1443, 1325, 1185, 1087, 910; GCMS *m/z* 183 (M^+).

2-phenyl-2,3-*d*$_2$-1,2-dihydrocyclopenta[a]indene (2c-*d*$_2$)

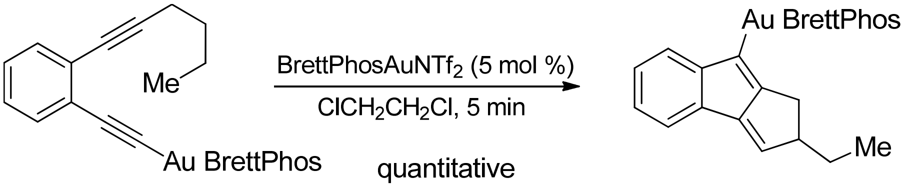


Compound **2c**-*d*$_2$ was prepared in 84% yield using 2,6-dibromopyridine *N*-oxide (**5**) as the additive according to the general procedure B. The reaction time was 4 h. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.62 (t,

J = 10.9 Hz, 1H), 7.38 – 7.18 (m, 7H), 7.17 – 7.09 (m, 1H), 6.73 (s, 1H), 6.35 (s, 1H), 4.62 (d, 1H, J = 7.8 Hz), 3.32 (d, 1H, J = 18.3 Hz), 2.67 (dd, 1H, J_1 = 18.4 Hz, J_2 = 1.4 Hz,). ^{13}C NMR (125 MHz, $CDCl_3$) δ 154.0, 151.0, 150.1, 143.8, 129.8, 128.7, 128.2, 127.3, 126.7, 123.3, 122.3, 120.3, 116.4, 33.9; GCMS *m/z* 232 (M^+).

C. Studies using alkynylgold intermediates as substrates

C1: the formation of 8-aurated 1,2-dihydrocyclopenta-[a]indene (2a-Au)



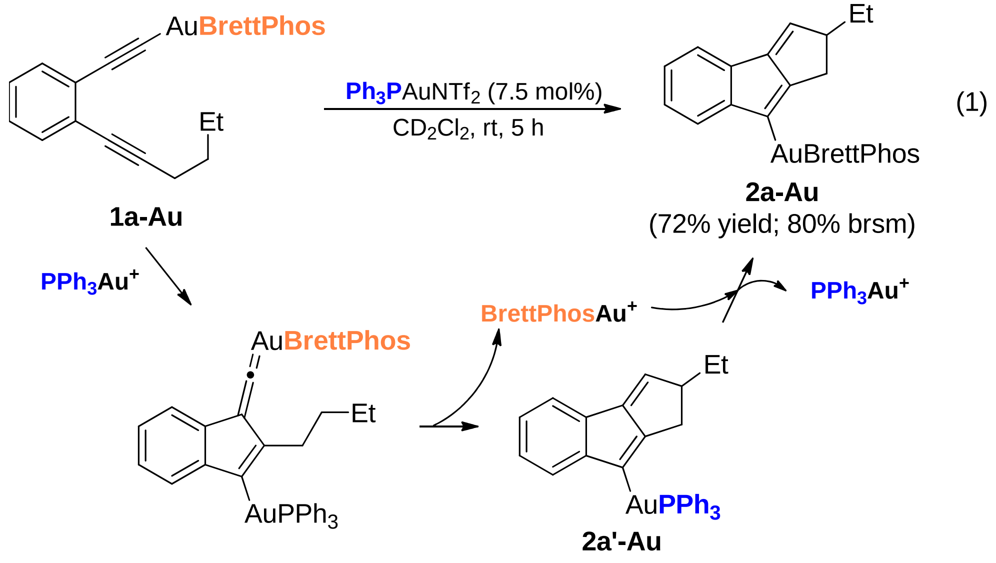
2a-Au

BrettPhosAuNTf$_2$ (5.1 mg, 0.005 mmol) was added to a solution of the compound **1a-Au** (0.10 mmol) in DCE (1.0 mL) at room temperature. The reaction mixture was stirred at rt and the progress of the reaction was monitored by TLC. Upon completion (5 min), the mixture was concentrated and the residue was purified by chromatography on silica gel (eluent: hexanes/ethyl acetate with 5% Et_3N) to afford the desired product **2a-Au** quantitatively. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (d, 1H, J = 7.6 Hz), 7.14 (d, 1H, J = 7.2 Hz), 7.06 (t, 1H, J = 7.6 Hz), 6.90 – 6.98 (m, 2H), 6.82 – 6.85 (m, 3H), 6.33 (d, 1H, J = 1.2 Hz), 3.90 (s, 3H), 3.54 (s, 3H), 3.19 – 3.21 (m, 1H), 2.70 – 2.80 (m, 3H), 2.39 – 2.43 (m, 2H), 2.18 – 2.22 (m, 2H), 2.02 – 2.06 (m, 2H), 1.11 – 1.90 (m, 3H), 1.00 – 1.04 (m, 3H), 0.89 (d, 6H, J = 6.4 Hz), 0.74 (dd, 6H, J_1 = 8.8 Hz, J_2 = 7.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.0, 162.4 (d, J = 25.5 Hz), 161.9, 159.5, 156.0, 153.1 (d, J = 55.0 Hz), 151.1 (d, J = 34.0 Hz), 148.0, 145.3 (d, J = 17.0 Hz), 139.1, 138.9, 132.1 (d, J = 17.0 Hz), 130.8 (d, J = 21.5 Hz), 55.5, 54.7, 53.4, 39.5, 39.3, 33.9 (t, J = 49.0 Hz), 32.8, 32.0, 30.7, 30.0, 29.0, 27.6 (d, J = 55.0 Hz), 27.1, 27.0, 26.2, 25.0, 24.3, 22.9, 22.7, 12.5; ^{31}P NMR (161.9 MHz, $CDCl_3$) δ 48.8; IR (neat): 3057, 2955, 2928, 2851, 1577, 1456, 1422, 1253, 1016, 909; MS (ES^+) Calculated for $[AuC_{49}H_{67}O_2P]^+$: 915.5; Found: 915.5.

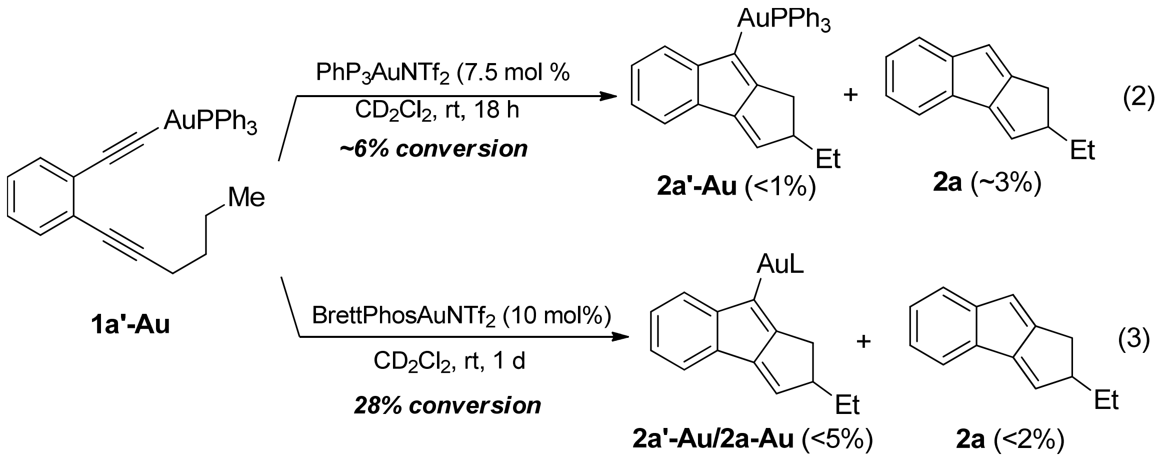
Discussion:

The rapid reaction above is expected as the concentration of BrettPhosAu was high in the system. When $Ph_3PauNTf_2$ (7.5 mol %) was used as the catalyst, the reaction was rather sluggish and did not proceed to completion in 5 h (90% conversion, Eq. 1). The reaction yield for **2a-Au** was lower but still good.

Due to the likely low quantity of **2a'-Au**, we were not able to identify its NMR signals, let alone purifying and characterizing it. Considering that BrettPhosAu$^+$ is generated during the reaction, the observed sluggishness was somewhat surprising. However, it can be explained if the gold exchange between **2a'-Au** and BrettPhosAu$^+$ is fast. Alternatively, Ph$_3$PAu$^+$ may somehow slow the reaction catalyzed by in-situ generated BrettPhosAu$^+$. In either event, it is clear that Ph$_3$PAu$^+$ is a catalyst much inferior to BrettPhosAu$^+$ for the cycloisomerization, consistent with the results shown in the condition studies (Table 1 in the manuscript).



The results using **1a'-Au** with Ph$_3$PAu attached at the ethynyl terminus as the substrate further confirmed the above conclusion. Hence, as shown in Eq. 2, when Ph$_3$PAuNTf$_2$ was used as the catalyst, little peak around 6.4 ppm, which might be attributed to **2a'-Au**, was observable; instead, the protonated product **2a** was formed in a ~3 % yield. The overall conversion was only 6% after 18 h reaction. This result further confirmed the ineffecitiveness of Ph$_3$P as the metal ligand for this reaction. The formation of **2a** is likely due to the strong acidity of Ph$_3$PAu$^+$, leading to higher concentration of H$^+$ in the reaction



medial in the presence of adventitious H_2O.

Eq. 3 was performed using BrettPhosAuNTf$_2$ as the catalyst. Again, the reaction was not productive at all. In fact, it is worse than Eq. 2 in terms of yielded based on conversion, suggesting that some side reactions occurred competitively. This is surprising to us.

These studies strongly support the notion that BrettPhos is much more efficient than Ph_3P in catalyzing this reaction. We attribute this difference partly to its steric bulk and partly to its more σ-donating nature.

Reference:

1 Taduri, B. P.; Ran, Y.-F.; Huang, C.-W.; Liu, R.-S. *Org. Lett.* **2006**, *8,* 883-886.

2. Hirano, K.; Inaba, Y.; Takahashi, N.; Shimano, M.; Oishi, S.; Fujii, N.; Ohno, H. *J. Org. Chem.* **2011**, *76,* 1212-1227.
3. Grissom, J. W.; Klingberg, D.; Huang, D.; Slattery, B. J. *J. Org. Chem.* **1997**, *62,* 603-626.
4. Cheong, P. H.-Y.; Morganelli, P.; Luzung, M. R.; Houk, K. N.; Toste, F. D. *J. Am. Chem. Soc.* **2008**, *130*, 4517–4526.
5. Adamczyk, M.; Watt, D. S.; Netzel, D. A. *J. Org. Chem.* **1984**, *49,* 4226-4237.
6. Ishii, Shingo; Zhao, Shikai; Helquist, Paul. *J. Am. Chem. Soc.*, **2000**, *122*, 5897 – 5898.
7. Toshiro Suenaga, Caroline Schutz, Tadashi Nakat. *Tetrahedron Lett.*, **2003**, *44*, 5799-5801;
8. Li, Jian-Rong; Yakovenko, Andrey A.; Lu, Weigang; Zhuang, Wenjuan; Yuan, Daqiang; Zhou, Hong-Cai; Timmons, Daren J. *J. Am. Chem. Soc.* **2010**, *132*, 17599 – 17610.

Computational studies:

Theoretical Methods. For hydrocarbons with no gold, complete geometry optimizations were carried out using density functional theory (DFT) methods using Becke's three-parameter exchange functional with the Lee, Yang, and Parr correlation functional at the B3LYP/6-311G(d,p),[1] M06-2X/6-31+G(d,p), and M06-2X/6-311+G(d,p) levels.[2] Frequency calculations were carried out in order to verify that the stationary points thus obtained were true minima and to determine thermodynamic parameters for the determination of reaction energetics. For the hydrocarbons, M06/6-31+G(d,p) geometries and thermochemistry were used for later calculations to be consistent with levels used for the gold complexes. For the pyridine N-oxide and conjugate acid calculations, M06-2X/6-311+G(d,p) geometries and thermochemistry was used in place of the M06/6-31+G(d,p) energies and theromochemistry, and for other single-point calculations. Geometries and thermochemical data are found in Supplemental Table S3 below. Diffuse functions sometimes result in linear dependencies that interfere with self-consistent field (SCF) convergence in DFT methods, however single-point B3LYP/6-31+G(d,p), B3LYP/6-311+G(2df,2pd), and aug-cc-pVTZ calculations at the M06-2X/6-31+G(d,p) geometries were carried out to account for the effect of diffuse functions on reaction energetics with no SCF convergence problems until aug-cc-pVXZ-PP basis sets were used for gold. In these cases, various methods, up to xqc, were used to achieve SCF convergence, and stability tests on the wave function were done when xqc methods were required. All of these DFT single-point calculations were carried out with the scf=tight option. All M06 and M06-2X calculations were done with the Gaussian 'int=ultrafine' option.

For organogold compounds, calculations were carried out using the M06 method, shown to be optimal for metals.[2] The basis sets used for gold species were the LANL2DZ, LANL2TZ(f),[3,4] and aug-cc-pVDZ-PP[4,5] effective core potentials. M06/LANL2DZ and M06/6-31+G(d,p)(C,H,P)/LANL2DZ(Cu) level geometry optimizations and frequency calculations were carried out in order to verify that the stationary points thus obtained were true minima and to determine thermodynamic parameters for the determination of reaction energetics. M06 single-point calculations were done with the 6-311+G(d,p)(C,H,P)/ LANL2TZ(f)(Au), aug-cc-pVDZ-PP, and aug-cc-pVTZ-PP basis sets using M06/LANL2DZ and M06/6-31+G(d,p)(C,H,P)/LANL2DZ(Au) geometries. All M06 calculations were done with the Gaussian 'int=ultrafine' option. For non-gold species, 6-31 basis sets were used with the 5d option when energies are compared with those from 6-311+G(d,p)(C,H,P) /LANL2TZ(f)(Au) and 6-31+G(d,p)(C,H,P)/LANL2DZ(Au) bases.

Thermochemical data were calculated with zero-point energy corrections from scaled M06 frequencies using a scaling factor of 0.99 for zero-point energies.[6] A scaling factor of 1.00 for M06 frequencies for the thermal and entropy terms was used.[6] Intrinsic reaction coordinate (IRC) calculations[7] were carried out on transition-state structures to assure that the calculated transition states lead to the expected products and starting materials.

To establish confidence in the computational methods employed here in the analysis of the energies of organogold compounds, we have calculated energies at a variety of theoretical levels to try to estimate the limits of accuracy of the methods used. We have chosen a polarized continuum model in ether solvent for our calculations using the SMD method of Truhlar and Cramer.[8] Solvent effects by similar methods have been treated successfully for cases where quantitative comparison with experiment is possible.[9] Preliminary atom-centered density matrix propagation molecular dynamics (ADMP) calculations[10] for a model reaction without the benzo ring fusion and with a methyl substituent were carried out at the B3LYP/6-31G(d)/LANL2DZ(Au) level to compute reaction trajectories. All calculations were performed using the Gaussian 03 and 09 program suites.[11]

Theoretical Results. Electronic reaction energies, reaction energies, transition-state energies, and solvation energies from quantum calculations are reported for the numerous reactions studied in Tables S1 and S2. Chemical structures and a reaction mechanism are depicted in Scheme S1. Thermochemical data and structures are reported for each compound in Table S3. Figures S1 and S2 show energy diagrams and structures of the transition states and intermediates.

Table S1 contains differences in energies at several M06 DFT levels with different basis sets. Comparisons of the electronic energies, $\Delta E^\circ_{g,e}$, at each level shows that the levels are consistent, usually within 1-2 kcal/mol. Effects of zero-point energy, thermal energy and entropy at 298K are shown for the geometry optimization level in the $\Delta E^\circ_{g,0K}$, $\Delta H^\circ_{g,298}$, and $\Delta G^\circ_{g,298}$ terms, respectively. The effect of chloroform solvation with the SMD model is contained in the $\Delta\Delta G^\circ_{solv,298}$ term, and the final free energy difference including all these effects in chloroform is in the ΔG°_{CHCl3} term at 298K. It can be seen that solvation is predicted to play a very large role for these ionic species, and generally favoring smaller ions with high charge density, as seen in Table S2. [12] Smaller zero-point energy and entropy differences are also seen. Final ΔG°_{CHCl3} energies with the largest basis set are shown in the far right column of Table S1.

The energy diagram in Figure S1 is based upon free energies in chloroform, while that showing the bifurcation region in Figure S2 has relative electronic energies with no zero-point energy corrections. The possibility that **E** and **J** might equilibrate through **TS1a** is relevant to the question of whether product ratios will be predictable from the dynamical factors affecting reaction trajectories as they traverse **TS1** and the ridge region or whether subsequent rapid equilbration could, in the end, make the bifurcation irrelevant to the product ratio prediction. The calculated free energy barrier in chloroform from **E** to **J** is 7.5 kcal/mole. This is compararable to the 8.6 kcal/mol barrier for C-H insertion into a methyl group for E via **TS2** and significantly higher than the 4.6 kcal barrier for a secondary CH bond in **L** via **TS3**. The barrier from the lower energy intermediate **J** to **E** via **TS1a** is 11.7 kcal/mole, while the gold migration product **K** is 6.5 kcal/mol lower in free energy than **J** with a gas-phase free energy barrier for formation of **K** from **J** of only 1.5 kcal/mol from B3LYP/6-31+G(d,p)/LANL2DZ(Au) calculations. The barrier for CH insertion into a methyl group in **M** to give **N** is then 9.8 kcal/mol. So the intermediate **J** would rapidly rearrange and undergo CH insertion before equilibrating with **E**, and **E** would undergo CH insertion faster than rearrangement to **J** for secondary CH bonds. The insertion product **N** would ultimately be predicted to lead to 2,3-cyclopentano-fused naphthalenes, rather than the 1,2-fusion seen in **4** from platinum.

Figure S3 shows some bond lengths for the vinylidene structure **E** along with the sigma-bound gold complex **G**. Comparisons of bond lengths shows that the vinylidene resonance structure for **E** is a very reasonable representation of its structure. A similar comparison of atomic charges by the natural population analysis method within Gaussian 09 in Figure S4 is also most consistent with the vinylidene representation of structure **E** with the positive charge mainly on the second gold, rather than on the carbons. The triplet vinylidene was calculated to be 9.2 kcal/mol less stable in electronic energy than the singet state at the geometry-optimized B3LYP/6-31+G(d,p)/LANL2DZ(Au) level. The CCAu angle at the charged gold decreases from 179.2º to 172.7º and some C-C bond distances increase.

Preliminary atom-centered density matrix propagation molecular dynamics (ADMP) calculations[10] for a model reaction without the benzo ring fusion and with a methyl substituent were carried out at the B3LYP/6-31G(d)/LANL2DZ(Au) level with step sizes of 0.07 fs for 112 to 224 fs time periods and settings of ElectronMass=-1000 (for a fictitious electron mass of 0.1 amu and uniform weighting of core and valence basis functions), geom=crowd, nosym, scf=NoVarAcc, and int=ultrafine. The trajectories were started at the simplified transition-state geometry analogous to **TS1** with random thermal energies. Of 140 trajectories, most went back to starting material, but the 29 that went to products favored the 5-membered over the 6-membered ring by 21/8, suggesting that, when statistically meaningful numbers of trajectories are collected, the 5-membered ring product will likely prevail, though not overwhelmingly. Assuming that these trajectory calculations give a reasonably accurate picture of the expected product ratio with simple phosphine ligands, the effect of the bulky BrettPhos ligand must be to steer the reaction toward the 5-membered ring product. This seems reasonable considering that one of the BrettPhos ligands is held further away from the main structure by the extra exocyclic carbon in the 5-membered ring product **E** than in the 6-membered ring product **J**. For the very large BrettPhos ligand, time-consuming trajectory calculations are entirely out of reach computationally to test this. To confirm that such steric factors could, indeed, favor the 5-membered ring formation, however, we carried out geometry optimizations at the B3LYP/LANL2DZ and B3LYP/6-31G(d)/LANL2DZ(Au) levels on the products **E** and **J** with a full BretPhos ligand attached in the critical position (next to the vinyidene carbon of **E** and corresponding position in **J**) and a trimethylphosphine in the other, less relevant, ligand position as shown in Figure S6. With simple phosphine ligands at this level of theory, the 6-membered ring is favored by 1.37 (3.13) kcal/mol in electronic energy and 0.96 (2.72) kcal/mol in free energy for the comparable pair of conformations chosen in Figure S6 at the B3LYP/LANL2DZ [and B3LYP/6-31G(d)/LANL2DZ(Au) (energies shown throughout in parentheses)] levels using thermochemistry from B3LYP/LANL2DZ frequencies scaled by 0.99 for ZPE and 0.96 for thermal and entropy terms.[6] The conformations within the BrettPhos group were chosen to correspond to that in the published X-ray structure.[13] Two other sets of conformations were tested as well to give similar results, but these were higher energy conformations. With the trimethylphosphino-BrettPhos ligands, these electronic and free energies now favor the five-membered ring by 1.31 (0.39) and 3.26 (2.34) kcal/mol, respectively, for a shift of 2.68 (3.52) kcal/mol in electronic energy and 4.22 (5.06) kcal/mol in free energy as a result of the steric interactions in the BrettPhos complex. We expect that this large steric effect will, in part, be felt along the energy surface on the reaction pathways and could reasonably be expected to steer the reaction course more toward the 5-membered ring product. For triethylphosphine ligands on **E** and **J**, B3LYP/LANL2DZ geometry optimizations showed a smaller steric effect of 1.21(1.65) kcal/mol in electronic energy, suggesting that reaction products derived from **J** would be more probable there than with BrettPhos ligands.

Further confirmation that the steric effect in the products **E** and **J** was sought at points along the energy surface was found in B3LYP/SDD level calculations. Geometry optimizations with these lower-level calculations show separate transition states for formation of the 5- and 6-membered ring products instead of the ridge-valley inflection and bifurcation surface for higher-level calculations. With larger basis sets and the M06 method, M06/6-31G(d)/LANL2DZ(Au) and M06/6-31+G(d,p)/LANL2DZ(Au), however, the bifurcated surface is seen. Using the two B3LYP/SDD transition-state geometries for the core structures, partial geometry optimizations with the trimethylphosphino and BrettPhos ligands were carried out. These calculations were very slow to converge, but after about 300 optimization steps and 1800 cpu-hours the energies largely leveled out. Full geometry optimization led to a slightly (0.3 kcal/mole) lower energy structure for the transition state leading to the **J** BrettPhos product, but did not converge for the **E** BrettPhos product. These electronic energies favored the 5-membered ring transition state by about 2 kcal/mol, similar to the 2.06 kcal/mole electronic energy difference (2.65 kcal/mol free energy difference) with PH_3 ligands, and consistent with experiment. This suggests that the steric effects in the **E** and **J** trimethylphosphino-BrettPhos products is likely diminished at these transition states, but might be felt in transitional structures along the energy surface leading to products and that this might lead to a steering of trajectories toward the 5-membered ring product. Within the traditional transition state model, as applied through B3LYP/SDD level calculations, there is still a significant approximate 2-3 kcal/mol free energy preference for the 5-membered ring product with the BrettPhos ligand as observed experimentally.

Acknowledgment. We are pleased to acknowledge support from the National Center for Supercomputing Applications, NSF (CHE100123) utilizing the NCSA Ember system and the use of software for 3-D drawings from CYLview, 1.0b; Legault, C. Y., Université de Sherbrooke, 2009 (http://www.cylview.org).

References:

1 A. D. Becke *J. Chem. Phys.* **1993**, *98*, 5648.
2 Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, **120** (2008) 215-41.
3 P. J. Hay and W. R. Wadt *J. Chem. Phys.* 82, 299 (1985).
4 From EMSL Library of Basis Set Exchange: Schuchardt, K.L., Didier, B.T., Elsethagen, T., Sun, L., Gurumoorthi, V., Chase, J., Li, J., and Windus, T.L. J. Chem. Inf. Model., 47(3), 1045-1052, 2007.
5 K.A. Peterson and C. Puzzarini, Theor. Chem. Acc., 114, 283 (2005).
6 (a) A. P. Scott, L. Radom *J. Phys. Chem.* **1996**, *100*, 16502. (b) D. H. Aue, J. Caras, M. Guidoni, to be published. We have evaluated optimum scale factors for numerous organic molecules and find that the DFT scale factors differ with basis set between 0.96 for the B3LYP/4-31G or 6-31G(d) levels to 0.97 for the B3LYP/ 6-311G(d,p) level. For thermal terms and entropies, such variation has little effect, and one may argue that a scaling factor close to 1.00 might be best for the dominant low frequencies (ref. 6a). For zero point energies (ZPE), the 0.99 scale factor fits experimental zero-point energies for organic molecules reasonably well for B3LYP methods and 0.98 for M06-2X/6-311+G(d,p). Here we chose a 0.99 scale factor for ZPE with the M06 frequency calculations.
7 C. Gonzalez, H. B. Schlegel *J. Phys. Chem.* **1990**, *94*, 5523.
8 A. V. Marenich, C. J. Cramer, and D. G. Truhlar, J. Phys. Chem. B, 113 (2009) 6378-96.
9 (a) K. S. Raymond, A. K. Grafton, R. A. Wheeler, *J. Phys. Chem. B* **1997**, *101*, 623 (and references therein); (b) M. Namazian, P. Norouzi, *J. Electroanal. Chem.* **2004**, *573*, 49.
10 H. B. Schlegel, S. S. Iyengar, X. Li, J. M. Millam, G. A. Voth, G. E. Scuseria, and M. J. Frisch, *J. Chem. Phys.*, **117** (2002) 8694-704.
11 Gaussian 09, Revision **A.1**, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J.

Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

12 (a) D. H. Aue, H. M. Webb, and M. T. Bowers, *J. Am. Chem. Soc.* **1976**, *98*, 318. (b) H. P. Hopkins Jr., D. V. Jahagirdar, S. P. Moulik, D. H. Aue, H. M. Webb, W. R. Davidson, and M. D. Pedley, *J. Am. Chem. Soc.*, **1984**, *106*, 4341. (c) D. H. Aue, H. M. Webb, W. R. Davidson, P. Toure, H. P. Hopkins, Jr., S. P. Moulik, and D. V. Jahagirdar, *J. Am. Chem. Soc.* **1991**, *113*, 1770(1991).

13 Ye, L.; He, W.; Zhang, L. *Angew. Chem., Int. Ed.* **2011**, *50*, 3236-3239.

Scheme S1.

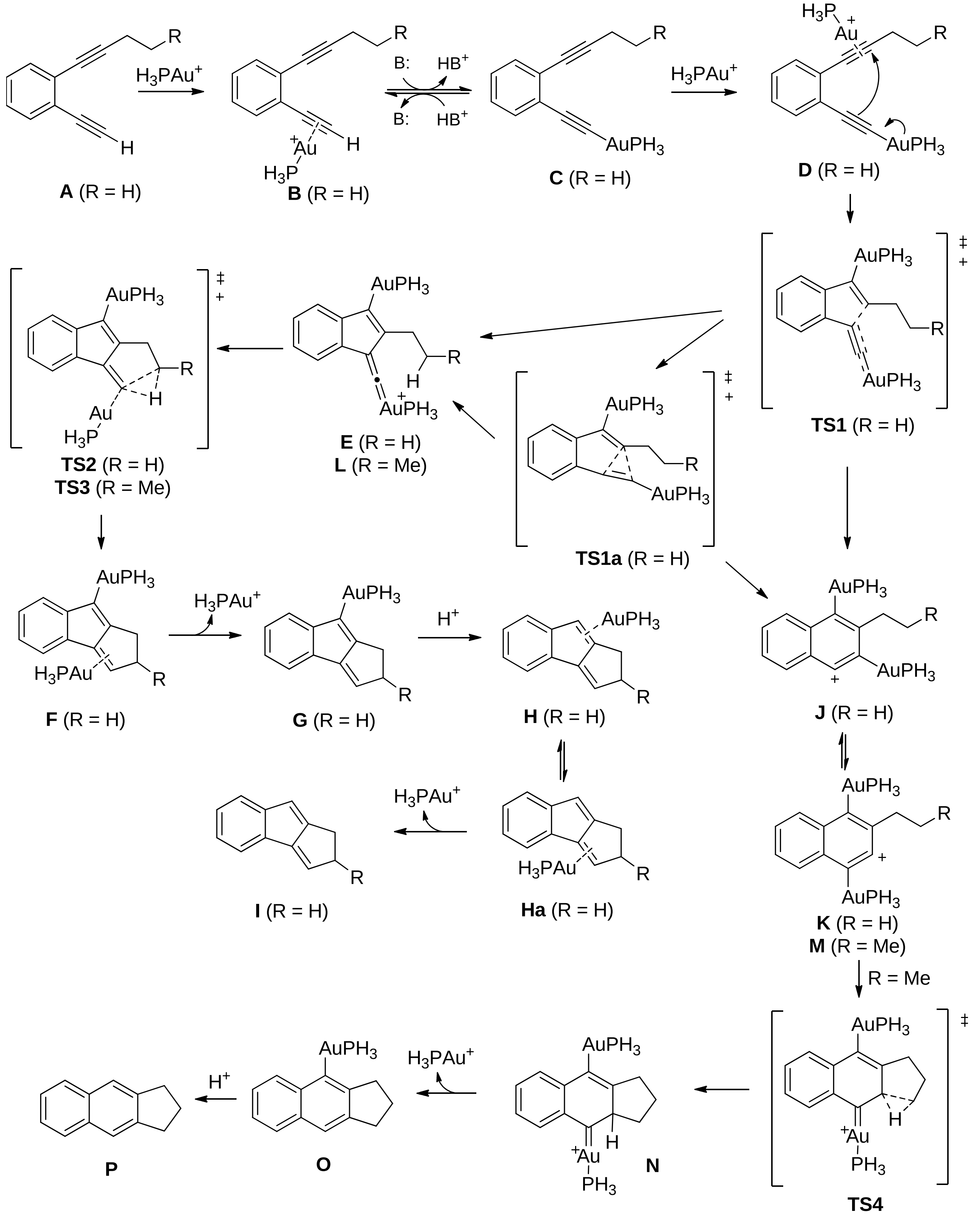

H3PAu+
B:
HB+
B:
HB+
H3PAu+
A (R = H)
B (R = H)
C (R = H)
D (R = H)
TS1 (R = H)
TS1a (R = H)
E (R = H)
L (R = Me)
TS2 (R = H)
TS3 (R = Me)
F (R = H)
H3PAu+
G (R = H)
H+
H (R = H)
J (R = H)
Ha (R = H)
H3PAu+
I (R = H)
K (R = H)
M (R = Me)
R = Me
TS4
N
H3PAu+
O
H+
P
AuPH3
R
‡
+

Figure S1. Free energy diagram calculated in chloroform at the M06/aug-cc-pVTZ-PP(SMD)//M06/6-31+G(d,p)/LANL2DZ(Cu) level. For proton-transfer and ligand-transfer reactions, energy barriers were not computed and small barriers are shown in the diagram simply for clarity. All relative free energies in kcal/mol at 298K.

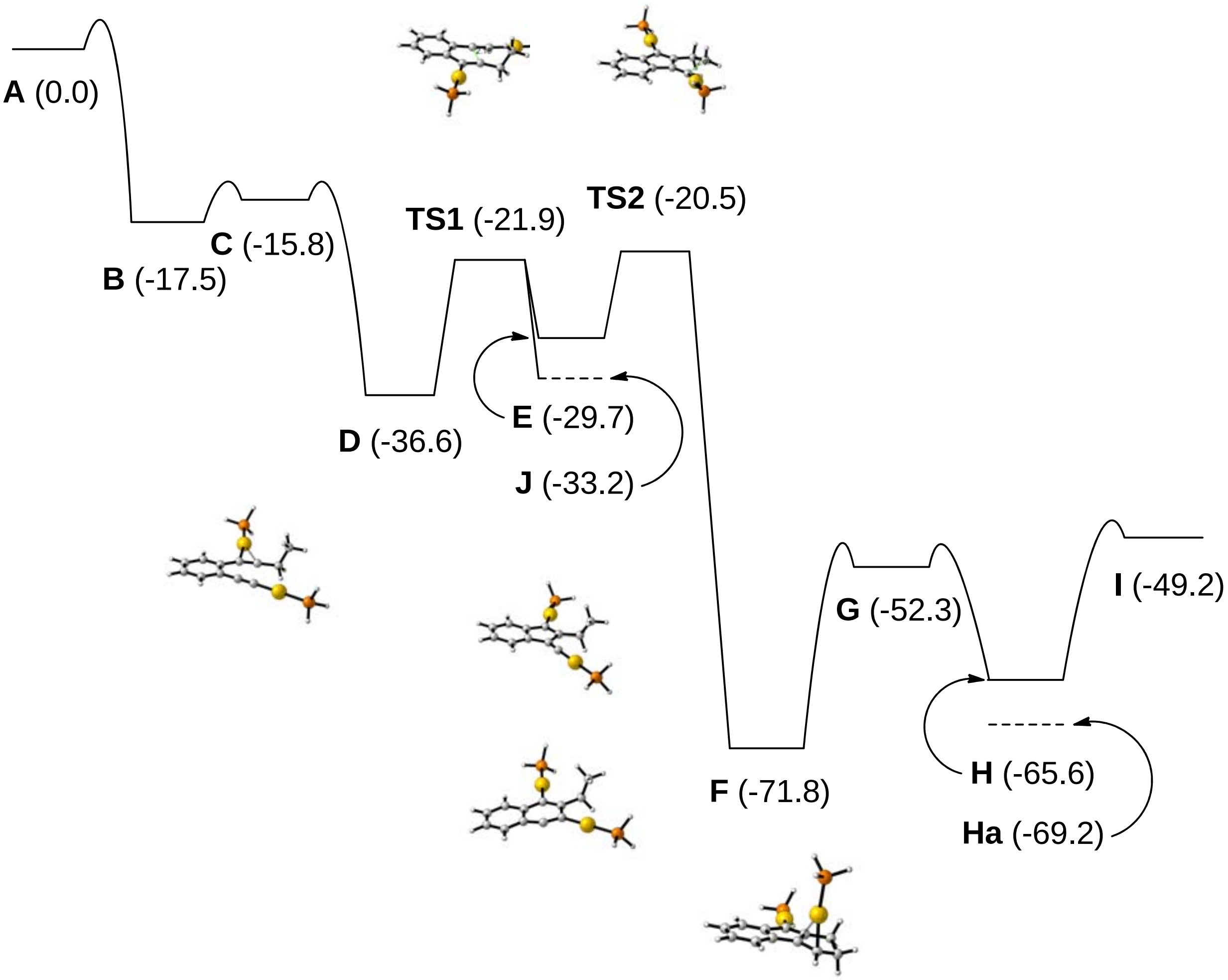


Figure S2. Energy diagram showing a bifurcation at a ridge-valley inflection, calculated at the M06/aug-cc-pVTZ-PP(SMD)//M06/6-31+G(d,p)/LANL2DZ(Cu) level. Relative electronic energies in parentheses, relative free energies in chloroform in brackets, all in kcal/mol at 298K. For pictures of typical 3D surfaces see Ess, D. H.; Wheeler, S. E.; Iafe, R. G.; Xu, L.; Çelebi-Ölçüm, N.; Houk, K. N. *Angew. Chem., Int. Ed.* **2008**, *47*, 7592-7601.

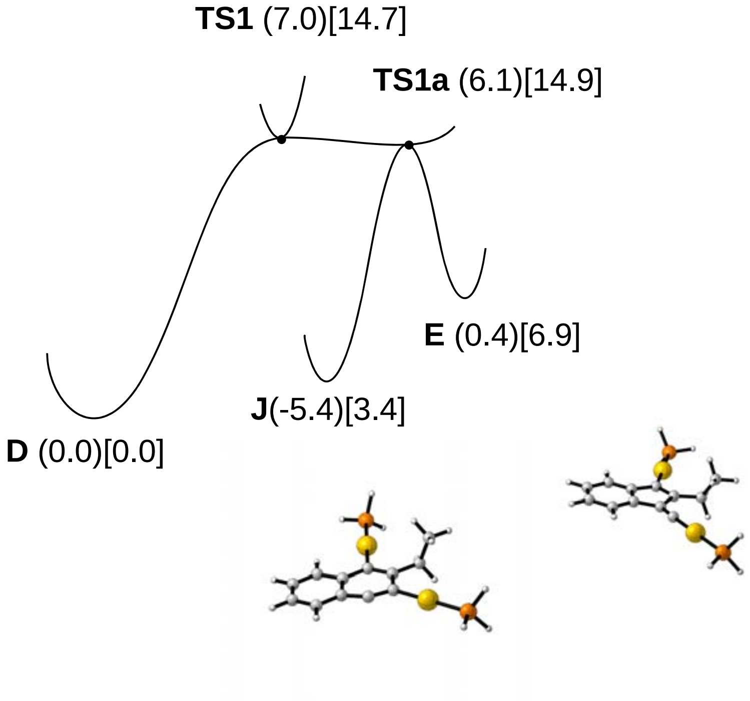


Figure S3. Bond lengths in Angstroms for intermediates **E** and **G** at the geometry-optimized M06/6-31+G(d,p)/LANL2DZ(Cu) level.

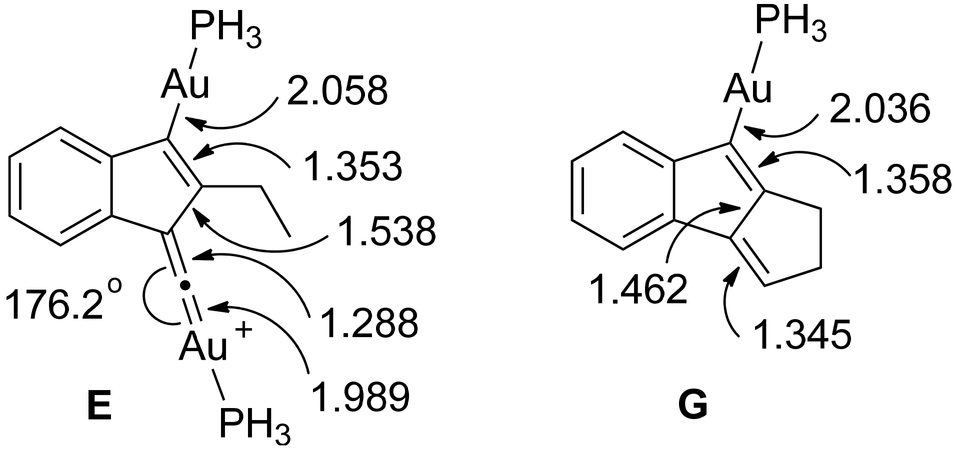


Figure S4. Natural population analysis charges for intermediates **E** and **G** at the geometry-optimized M06/6-31+G(d,p)/LANL2DZ(Cu) level.

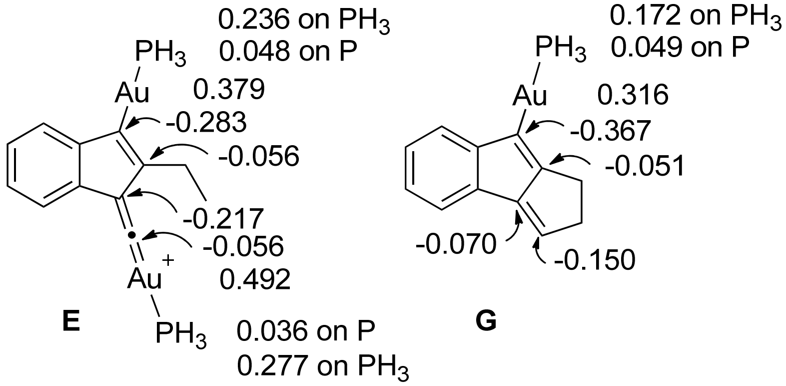
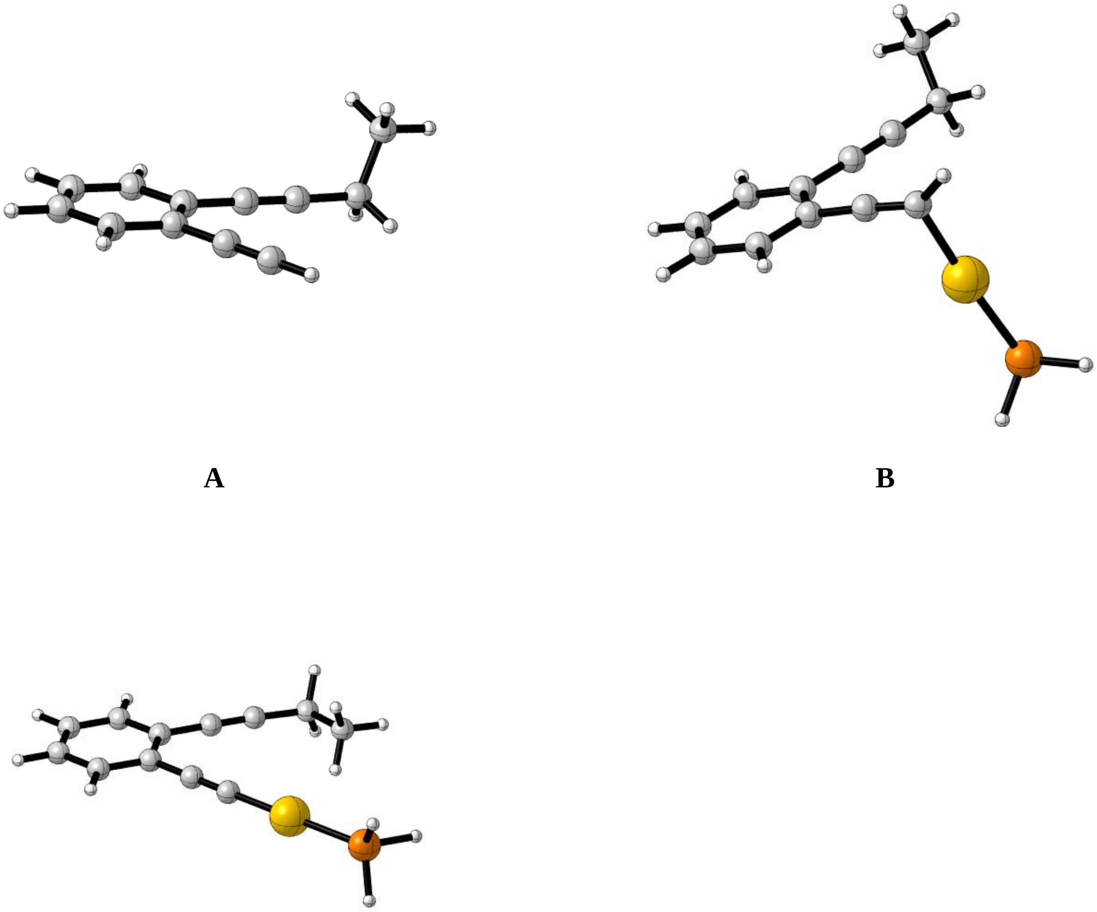


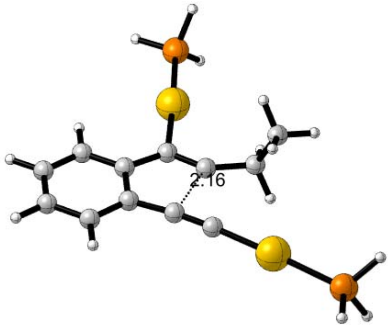
Figure S5. Structures of the intermediates and transition states from geometries optimized at the M06/6-31+G(d,p)/LANL2DZ(Cu) level.



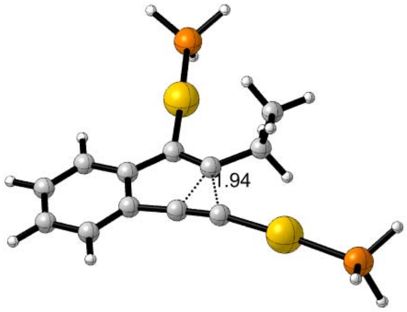
A

B

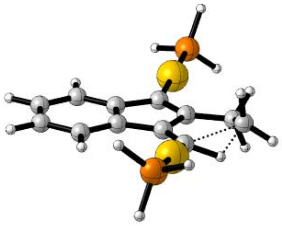
C



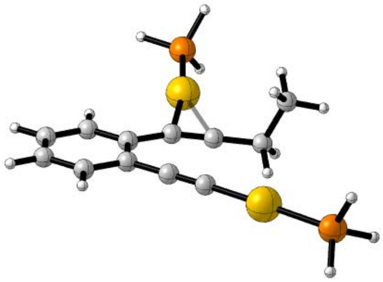
TS1



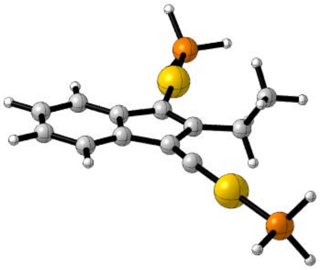
TS1a



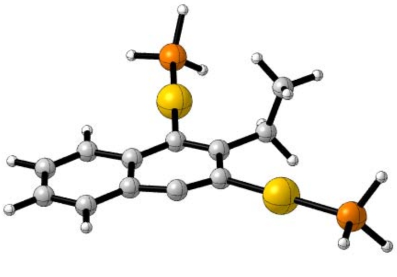
TS2



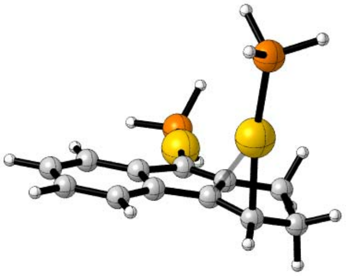
D



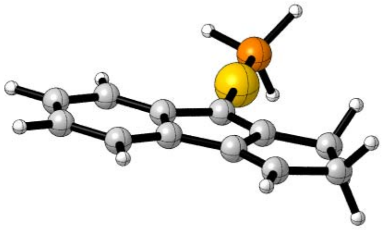
E



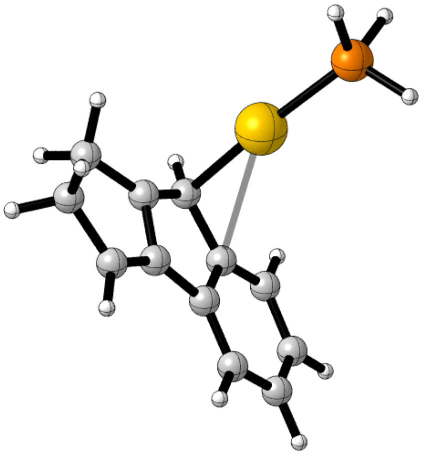
J



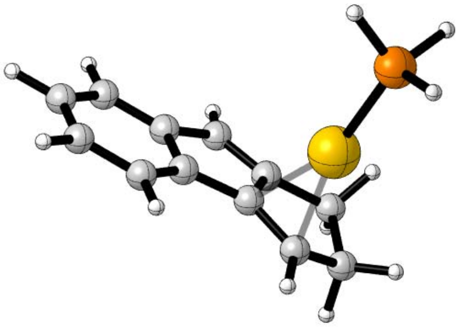
F



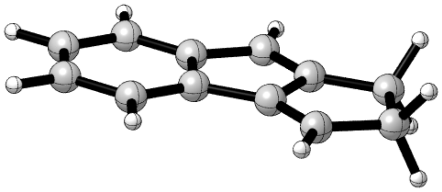
G



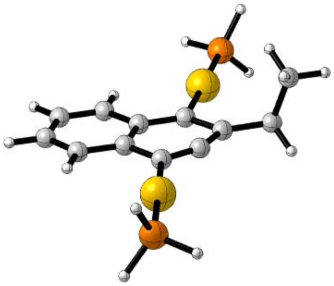
H



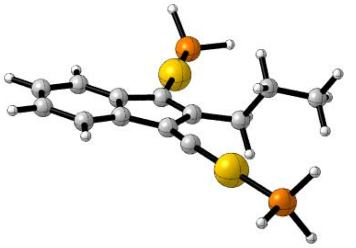
Ha



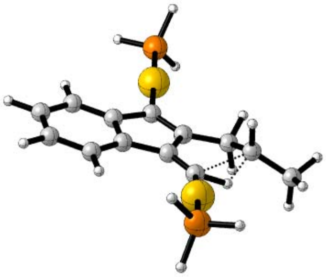
I



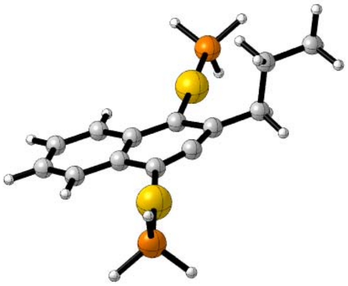
K



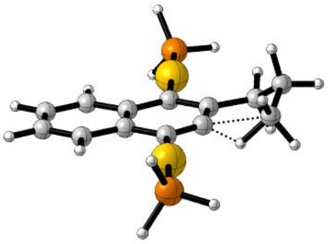
L



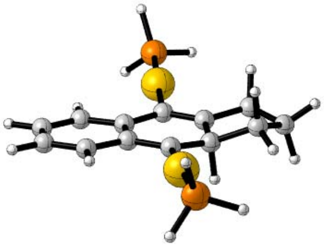
TS3



M

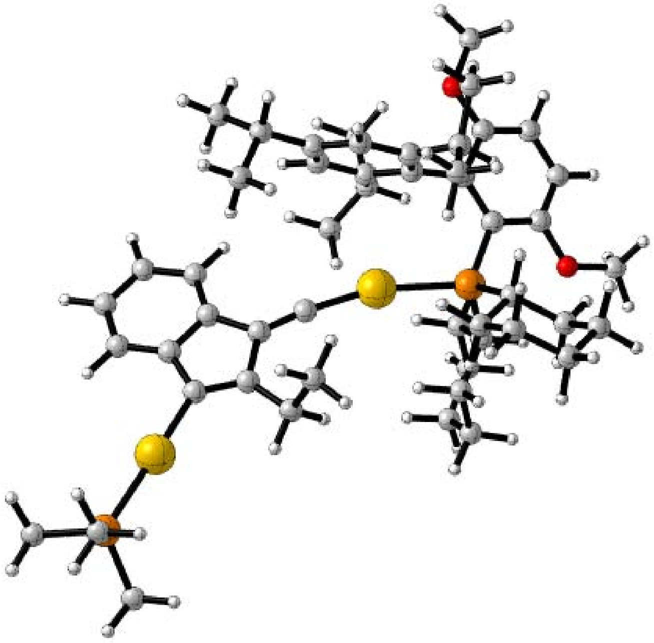


TS4



N

Figure S6. Structures of the trimethylphosphino-BrettPhos complexes of the 5- and 6-membered ring intermediates **E** and **J**, respectively, optimized at the B3LYP/LANL2DZ level.



X

Y

Table S1. Reaction energies of 3,4-benzoocta-3-ene-1,5diyne with PH_3Au^+ from quantum calculations at 298K at M06/6-31+G(d,p)/LANL2DZ(Au) level. (All values in kcal/mol).

Reaction Step:	M06/6-31+G(d,p)/LANL2DZ(Au)[a]					SMD[a,b]	M06/6-311+G(d,p) /LANL2TZ(f)(Au)[a]	M06/aug-cc-pVDZ/ aug-cc-pVDZ-PP(Au)[a]	M06/aug-cc-pVTZ/ aug-cc-pVTZ-PP(Au)[a]	
	$\Delta E^{o}_{g,e}$	$\Delta E^{o}_{g,0K}$	$\Delta H^{o}_{g,298}$	$\Delta G^{o}_{g,298}$	ΔG^{o}_{CHCl3}	$\Delta\Delta G^{o}_{solv,298}$	$\Delta E^{o}_{g,e}$	$\Delta E^{o}_{g,e}$	$\Delta E^{o}_{g,e}$	ΔG^{o}_{CHCl3}
A to **B**	-51.70	-51.20	-50.69	-41.76	-15.03	26.73	-52.81	-56.34	-54.14	-17.46
B to **C**	13.85	15.73	15.60	16.54	2.23	-14.31	11.50	12.26	13.31	1.70
C to **D**	-57.78	-57.75	-57.01	-48.28	-17.84	30.44	-59.49	-62.91	-60.72	-20.79
D to **E**	-4.26	-3.67	-4.43	-1.43	2.22	3.65	-1.65	-4.37	0.41	6.90
E to **F**	-46.24	-44.13	-45.00	-42.64	-43.61	-0.96	-45.56	-46.43	-44.74	-42.12
F to **G**	58.67	57.83	57.38	47.14	17.01	-30.12	61.30	62.05	61.13	19.47
G to **H**	-21.66	-21.86	-22.17	-21.24	-13.51	7.72	-19.88	-19.20	-21.44	-13.29
H to **I**	47.88	47.16	46.65	36.83	13.22	-23.61	50.78	51.59	51.03	16.38
Overall Rxn **A** to **I**	-61.24	-57.88	-59.66	-54.84	-55.30	-0.46	-55.82	-63.35	-55.15	-49.21
E to **J**	-5.99	-6.07	-6.13	-5.38	-3.75	1.63	-5.81	-5.18	-5.78	-3.54
H to **Ha**	-5.30	-5.30	-5.29	-5.62	-4.32	1.29	-4.80	-4.92	-4.58	-3.59
$\Delta G^{\ddagger}$ for **TS1** (**D** to **E**)[c]	4.39	4.38	3.62	6.98	12.04	5.06	5.98	4.99	7.04	14.68
$\Delta\Delta G^{\ddagger}$ **TS1** to **TS1a**[c]	-1.33	-1.01	-1.30	-0.08	-0.21	-0.13	-0.94	-1.69	-0.89	0.23
$\Delta G^{\ddagger}$ for **TS1a** (**J** to **E**)[c]	13.32	13.12	12.88	13.72	13.36	-0.36	12.50	12.86	11.51	11.55
$\Delta G^{\ddagger}$ for **TS2** (**E** to **F**)[c]	7.36	6.42	5.51	8.32	8.35	0.03	7.97	7.68	8.12	9.11
J to **K**	-6.74	-6.36	-6.35	-6.57	-6.89	-0.32	-6.33	-6.77	-6.43	-6.58
$\Delta G^{\ddagger}$ for **TS3** (from **L**)[c]	2.38	1.29	0.46	3.32	3.90	0.58	3.09	1.54	3.34	4.86
M to **N**	-30.85	-28.89	-30.01	-26.46	-24.08	2.38	-30.56	-31.75		
$\Delta G^{\ddagger}$ for **TS4** (**M** to **N**)[c]	7.97	7.52	6.55	9.43	8.70	-0.73	8.24	6.42	8.96	9.70

---

a) Geometry optimized at the M06/6-31+G(d,p)/LANL2DZ(Au) level.

b) Solvation energy term from the difference in free energies of solvation from SMD model M06/6-31+G(d,p)/LANL2DZ//M06/6-31+G(d,p)/LANL2DZ in chloroform. (Ref. 8)

c) Activation energies, enthalpies, and free energies in appropriate columns.

Table S2. Free energies of solvation in chloroform calculated by SMD model at 298K. (All values in kcal/mol)[a]

	$\Delta\Delta G^{o}_{CHCl3,298}$
A	-10.00
B	-45.21
C	-17.20
D	-48.70
E	-45.05
F	-46.01
G	-14.19
H	-48.79
Ha	-47.50
I	-10.46
J	-43.42
K	-43.73
L	-45.64
M	-44.27
N	-41.89
TS1	-43.64
TS1a	-43.77
TS2	-45.02
TS3	-45.06
TS4	-45.00
pyridine N-oxide	-9.67
prot. pyridine N-oxide	-52.00
PH3Au+	-61.94

---

a) Solvation free energy in chloroform from the SMD model at the M06/6-31+G(d,p)/LANL2DZ(Cu)//M06/6-31+G(d,p)/LANL2DZ(Cu) level. (Ref. 8)

Table S3. Calculated geometries, thermochemical data, and vibrational frequencies for hydrocarbons and gold complexes. Compound numbering from Supporting Information schemes.

1-ethynyl-2-but-1’-yn-1’-yl-benzene (3,4-benzoocta-3-ene-1,5diyne) (**A**):

```
Processing: etbendiyn6plam6.log
PG=C01

Method        BasisSet      Imaginary Freqs
RM06          6-31+G(d,p)    0

HF Energy
-462.8225160

       ZPE        E298       S298      Strans       Srot
   109.88371     117.140     107.885      41.007      31.174

Processing: etbendiyn6plam6.log
22
C     1.305667   0.723803   0.016160
C     0.525853  -0.449288  -0.119484
C     2.695061   0.613066   0.161077
C     1.167830  -1.695399  -0.104959
C     3.312626  -0.630374   0.173061
C     2.545704  -1.787614   0.039754
H     3.280984   1.523497   0.264016
H     0.561179  -2.591891  -0.209878
H     4.391856  -0.697731   0.286366
H     3.023577  -2.764382   0.048401
C     0.697407   2.013140   0.006614
C    -0.889152  -0.375615  -0.269615
C     0.202385   3.118315   0.001044
C    -2.093266  -0.318445  -0.407245
C    -3.542626  -0.245411  -0.533670
C    -4.260518  -0.548166   0.781872
H    -3.820301   0.756086  -0.890382
H    -3.874691  -0.947063  -1.311630
H    -5.346305  -0.482237   0.654104
H    -3.961222   0.161469   1.560213
H    -4.016431  -1.555149   1.136435
H    -0.240473   4.089331  -0.005301

Population analysis using the SCF density.
Label   Frequencies    IR Inten      Dipole
A        3467.7222     69.6164      0.7336
A        3202.0500     19.0132
```

A	3194.5447	15.7866
A	3186.2744	3.9882
A	3178.0338	0.2903
A	3134.0568	22.5376
A	3131.6101	30.5790
A	3069.5057	5.0348
A	3038.8892	42.4049
A	3025.6387	32.3638
A	2349.0838	18.1182
A	2219.9570	5.7002
A	1660.6853	4.7641
A	1619.8972	1.8078
A	1517.5382	29.0721
A	1473.9763	4.6307
A	1468.7250	9.5904
A	1464.3924	10.9126
A	1446.9714	6.1814
A	1387.7551	3.4984
A	1357.8434	1.3932
A	1342.0535	16.6686
A	1289.0787	0.9142
A	1264.9152	0.0886
A	1263.0146	0.0476
A	1218.8304	0.6356
A	1161.5648	0.0632
A	1117.4981	3.9930
A	1084.3383	0.4271
A	1077.4421	7.6095
A	1065.8065	3.6461
A	1030.0339	2.4982
A	989.8512	0.0007
A	959.7214	1.9668
A	911.5478	1.0023
A	884.4558	0.0111
A	786.6047	4.4475
A	769.0352	4.2466
A	768.2290	55.3468
A	752.0603	4.3118
A	690.1058	35.1635
A	682.8158	15.6287
A	656.4661	58.3632
A	594.9441	1.2242
A	590.1458	1.2856
A	566.9101	2.2371
A	545.0975	1.5089
A	498.0077	0.3974
A	457.1183	0.6634
A	389.5059	2.7329
A	377.0974	1.4523

```
A          329.3471       1.0943
A          318.0621       1.0997
A          214.5498       0.0808
A          178.1480       1.7135
A          154.7616       2.5501
A          126.0051       1.4184
A           72.0628      1.0144
A           68.3705      1.3173
A           24.0166      0.0302

Processing: etbendiynm6x.log
PG=C01

Method        BasisSet      Imaginary Freqs
RM062X        6-311+G(d,p)   0

HF Energy
-463.0908299

       ZPE        E298        S298      Strans        Srot
   111.04856     118.301     110.298      41.007      31.156

Processing: etbendiynm6x.log
22
C     1.291471   0.726293   0.012124
C     0.537867  -0.458282  -0.122098
C     2.679701   0.647705   0.163472
C     1.200650  -1.690544  -0.099870
C     3.320166  -0.582300   0.183032
C     2.578010  -1.753550   0.050986
H     3.244197   1.566249   0.265055
H     0.615299  -2.595652  -0.203300
H     4.395852  -0.627926   0.300976
H     3.073594  -2.716697   0.065725
C     0.652210   2.006939  -0.005433
C    -0.882832  -0.409147  -0.277931
C     0.133176   3.090602  -0.018221
C    -2.078802  -0.366394  -0.413187
C    -3.533481  -0.303445  -0.541206
C    -4.243653  -0.508079   0.803271
H    -3.805430   0.667454  -0.964256
H    -3.860591  -1.062534  -1.257123
H    -5.325601  -0.450970   0.673135
H    -3.937574   0.257256   1.517280
H    -3.995171  -1.483341   1.223544
H    -0.331467   4.047375  -0.030670
```

```
Processing etbendiyn6be.log
PG=C01

Method        BasisSet      Imaginary Freqs
RB3LYP        6-311G(d,p)    0

HF Energy
-463.2962070

Thermochemistry will use frequencies scaled by 0.9600
        ZPE        E298        S298      Strans        Srot
   105.39932     112.912     109.093      41.007      31.088

22
C    -1.174893   0.768743  -0.000022
C    -0.604568  -0.531347  -0.000006
C    -2.572078   0.905051   0.000000
C    -1.461266  -1.644536   0.000041
C    -3.399139  -0.209992   0.000038
C    -2.840809  -1.488386   0.000060
H    -2.995088   1.902125  -0.000013
H    -1.022020  -2.634533   0.000054
H    -4.475484  -0.083228   0.000052
H    -3.481051  -2.363105   0.000091
C    -0.354973   1.934998  -0.000046
C     0.806897  -0.721391  -0.000045
C     0.312538   2.937110  -0.000055
C     1.999362  -0.907832  -0.000094
C     3.446805  -1.095123  -0.000175
C     4.229925   0.229884   0.000239
H     3.730079  -1.691697   0.875118
H     3.730042  -1.691115  -0.875877
H     5.305332   0.035087   0.000125
H     3.986208   0.823488   0.883571
H     3.986125   0.824076  -0.882674
H     0.909057   3.815834  -0.000059

Population analysis using the SCF density.
Label   Frequencies    IR Inten      Dipole
A         3477.1178     78.5344      0.6307
A         3198.5485     13.0230
A         3193.3281     14.7822
A         3181.7185      9.5114
A         3169.0278      0.6186
A         3112.1139     27.2548
A         3104.5940     36.7354
A         3036.8360     33.9843
A         3035.0158      9.7353
A         3012.1984     28.7878
```

A	2330.6449	23.5839
A	2206.4971	1.8649
A	1633.6204	3.6917
A	1592.6101	0.7741
A	1509.9941	13.3851
A	1505.8122	25.9828
A	1496.8180	7.4556
A	1476.3141	2.5286
A	1471.2600	10.7193
A	1414.4622	2.2776
A	1357.4108	37.7382
A	1311.9126	1.1379
A	1299.2078	0.3545
A	1288.2805	0.0786
A	1267.9259	0.0687
A	1217.7353	0.4494
A	1185.2698	0.1717
A	1124.9620	3.8707
A	1104.6392	0.3088
A	1087.4494	0.8764
A	1062.7045	2.5767
A	1022.0764	4.6399
A	995.4118	0.0016
A	965.7256	1.7279
A	908.1701	0.2728
A	888.4863	0.0177
A	788.9132	4.9079
A	788.2670	1.8108
A	771.8547	65.0769
A	746.9279	0.7322
A	690.1413	19.6781
A	679.4388	24.4739
A	630.0920	37.6272
A	607.8310	0.6992
A	567.6123	0.1456
A	549.2496	1.4270
A	529.2327	2.3447
A	525.0435	5.7809
A	433.2921	1.2631
A	400.9323	0.0037
A	366.6713	2.5844
A	360.7560	0.9204
A	281.1141	0.3372
A	205.0124	0.0412
A	188.7520	0.2248
A	140.0510	1.5412
A	133.6713	3.7774
A	79.5480	1.2802
A	55.8372	0.7316

```
A          33.8343      0.0240
```

3,4-benzobicyclo[3.3.0]octa-1,3,5-triene (**I**):

```
Processing: bbc33dien6plam6.log
PG=CS

Method        BasisSet      Imaginary Freqs
RM06          6-31+G(d,p)    0

HF Energy
-462.9201070

       ZPE        E298        S298      Strans       Srot
   113.31488     118.786      91.703      41.007      30.159

Processing: bbc33dien6plam6.log
22
C     0.000000   0.753074   0.000000
C     1.262272   0.100382   0.000000
C    -0.089261   2.136863   0.000000
C     2.429694   0.856781   0.000000
C     1.089456   2.887237   0.000000
C     2.331664   2.250509   0.000000
H    -1.059507   2.631789   0.000000
H     3.405234   0.373245   0.000000
H     1.039702   3.973689   0.000000
H     3.239509   2.850510   0.000000
C    -0.995982  -0.308916   0.000000
C     1.056130  -1.353753   0.000000
C    -2.324978  -0.513396   0.000000
C    -0.277546  -1.582774   0.000000
C    -1.266969  -2.704958   0.000000
C    -2.644141  -1.984362   0.000000
H    -1.154149  -3.352750   0.878307
H    -1.154149  -3.352750  -0.878307
H    -3.250726  -2.256433  -0.875601
H    -3.250726  -2.256433   0.875601
H    -3.096910   0.253291   0.000000
H     1.859705  -2.084280   0.000000



Processing: bbc33dienm6x.log
PG=CS

Method        BasisSet      Imaginary Freqs
RM062X          6-311+G(d,p)   0
```

```
HF Energy
-463.1820392

       ZPE        E298        S298      Strans        Srot
   114.42531    119.887      91.970     41.007      30.161

Processing: bbc33dienm6x.log
22
C     0.000000   0.758311   0.000000
C     1.260170   0.107624   0.000000
C    -0.088985   2.140139   0.000000
C     2.427145   0.860459   0.000000
C     1.089615   2.888069   0.000000
C     2.329860   2.252770   0.000000
H    -1.053819   2.634851   0.000000
H     3.398516   0.378974   0.000000
H     1.040713   3.970179   0.000000
H     3.233859   2.850645   0.000000
C    -1.000924  -0.308677   0.000000
C     1.054073  -1.353992   0.000000
C    -2.323747  -0.515202   0.000000
C    -0.273310  -1.584002   0.000000
C    -1.262037  -2.714473   0.000000
C    -2.645186  -1.993642   0.000000
H    -1.145980  -3.351546   0.878972
H    -1.145980  -3.351546  -0.878972
H    -3.243478  -2.260407  -0.876186
H    -3.243478  -2.260407   0.876186
H    -3.094949   0.246223   0.000000
H     1.854547  -2.081271   0.000000


Processing bbc33dien6be.log
PG=C01

Method        BasisSet      Imaginary Freqs
RB3LYP        6-311G(d,p)    0

HF Energy
-463.3826571

Thermochemistry will use frequencies scaled by 0.9600
       ZPE        E298        S298      Strans        Srot
   108.75273    114.412      92.724     41.007      30.171

22
C    -0.567143  -0.502168  -0.000103
C    -0.915160   0.879598   0.000040
```

C	-1.549207	-1.482490	-0.000142
C	-2.255228	1.254307	0.000137
C	-2.892545	-1.093774	-0.000049
C	-3.237033	0.258668	0.000091
H	-1.284822	-2.534771	-0.000243
H	-2.539177	2.301439	0.000245
H	-3.671715	-1.847526	-0.000082
H	-4.284076	0.542096	0.000166
C	0.894224	-0.546602	-0.000115
C	0.317230	1.688028	0.000046
C	1.927058	-1.406166	0.000057
C	1.371125	0.841790	-0.000077
C	2.874872	0.849471	-0.000290
C	3.249958	-0.670294	0.000336
H	3.282535	1.360049	0.877031
H	3.282110	1.359123	-0.878349
H	3.852429	-0.942335	-0.874370
H	3.851615	-0.941790	0.875773
H	1.866715	-2.488567	0.000126
H	0.335474	2.770078	0.000109

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Dipole
A	3201.4504	13.2338	1.6520
A	3185.7927	32.6254	
A	3184.8488	7.8692	
A	3172.3740	32.4783	
A	3162.4919	1.8219	
A	3155.6962	3.3375	
A	3067.8366	24.3457	
A	3039.3426	39.9026	
A	3032.8313	10.8392	
A	3014.5050	39.7123	
A	1694.6044	10.5321	
A	1647.7175	3.1855	
A	1640.7116	52.1757	
A	1610.5550	3.6596	
A	1495.5611	3.9991	
A	1489.3340	7.4859	
A	1473.3707	44.6000	
A	1468.2014	3.5381	
A	1381.0926	2.5277	
A	1355.5008	1.2790	
A	1328.4108	9.4422	
A	1318.2981	5.8102	
A	1279.0336	0.4868	
A	1246.8715	9.2555	
A	1229.8318	0.4442	
A	1207.8652	10.8216	

```
A       1190.7920      2.2989
A       1172.5795      5.8064
A       1163.4516      0.1065
A       1134.5519      2.1039
A       1111.7568      0.1584
A       1041.6686      3.1393
A       1020.3510      3.5078
A        992.7850     11.7374
A        983.3724      0.0517
A        960.2604      2.5995
A        944.3651      1.3121
A        901.4457      6.7868
A        889.7021      6.3091
A        886.5726      0.6078
A        845.3191      0.6391
A        840.0251     17.8098
A        825.8227      2.2287
A        786.2899      0.6286
A        766.1910     58.9140
A        757.7711      0.0122
A        726.5894      2.6237
A        683.3477      1.0544
A        676.3415     11.7566
A        590.5507      0.7815
A        568.0792      5.4897
A        518.9956      0.5547
A        453.8494      0.3445
A        436.7983      1.6897
A        326.1966      4.2708
A        311.5448      0.2094
A        243.1667      0.9230
A        198.0794      0.0132
A        122.3723      3.1756
A         88.3445     0.5480
```

Pyridine N-oxide:

```
Processing: pyro61pbe.log
PG=C02V

Method      BasisSet      Imaginary Freqs
RB3LYP        6-311+G(d,p)   0

HF Energy
-323.5400821

Thermochemistry will use frequencies scaled by 0.9600
       ZPE       E298       S298      Strans       Srot
```

55.66165 58.976 72.390 39.566 25.353

12

C	0.000000	1.192886	-1.097905
C	0.000000	0.000000	-1.818744
C	0.000000	-1.192886	-1.097905
C	0.000000	-1.178914	0.283063
N	0.000000	0.000000	0.984084
C	0.000000	1.178914	0.283063
H	0.000000	-2.058797	0.909205
H	0.000000	2.058797	0.909205
H	0.000000	-2.151987	-1.601225
H	0.000000	2.151987	-1.601225
H	0.000000	0.000000	-2.900661
O	0.000000	0.000000	2.260837

Population analysis using the SCF density.

Label	Frequencies	IR Inten	Dipole
A1	3239.6672	0.1870	4.4175
A1	3210.1275	3.0242	
A1	3187.1790	0.2051	
A1	1655.1333	43.5325	
A1	1491.6973	116.1350	
A1	1322.5110	206.2756	
A1	1193.9764	32.3934	
A1	1058.2901	0.0388	
A1	1025.9566	43.3188	
A1	857.1152	14.4299	
A1	553.7679	6.6849	
A2	965.0951	0.0000	
A2	828.2027	0.0000	
A2	421.9917	0.0000	
B1	978.6391	0.1293	
B1	886.4334	4.2720	
B1	764.6996	67.4166	
B1	677.8863	26.7691	
B1	515.0461	9.2082	
B1	209.1553	3.8839	
B2	3238.1464	0.4007	
B2	3193.3032	6.4030	
B2	1578.9243	4.1288	
B2	1506.0798	4.4558	
B2	1355.0104	0.1281	
B2	1250.9342	2.8214	
B2	1171.2891	0.5615	
B2	1091.0303	3.9437	
B2	649.5834	0.5832	
B2	481.3907	5.3571	

Pyridine N-oxide, protonated:

```
Processing: pyroh61pbe.log
PG=CS

Method        BasisSet       Imaginary Freqs
RB3LYP        6-311+G(d,p)   0

HF Energy
-323.8997106

Thermochemistry will use frequencies scaled by 0.9600
      ZPE        E298       S298      Strans      Srot
   63.17266     66.902     76.510     39.598     26.830

13
C    -0.004075   0.231793   1.190248
C    -0.004075  -1.150136   1.207160
C    -0.001786  -1.849823   0.000000
C    -0.004075  -1.150136  -1.207160
C    -0.004075   0.231793  -1.190248
N     0.018783   0.867360   0.000000
O    -0.092430   2.246369   0.000000
H    -0.027869   0.865282  -2.066586
H    -0.027869   0.865282   2.066586
H    -0.016150  -1.662643  -2.160076
H    -0.016150  -1.662643   2.160076
H    -0.007741  -2.933093   0.000000
H     0.812247   2.604391   0.000000

Population analysis using the SCF density.
Label   Frequencies    IR Inten      Dipole
A'       3703.9378    158.2550      1.6864
A'       3235.2690      4.9850
A'       3220.2003     16.0761
A'       3204.1604      0.1416
A'       1648.5041     17.7162
A'       1514.2928     14.2219
A'       1396.6266     78.6832
A'       1215.3963     10.2599
A'       1187.4181     14.8931
A'       1071.0190      2.5652
A'       1040.2712      0.0530
A'       1038.8728      0.2844
A'        962.2152      1.4770
A'        822.8124     11.4306
A'        780.3414     64.7064
A'        667.6220     33.9253
```

```
A'       542.8110      0.8681
A'       461.2652     13.6981
A'       221.1914      4.3495
A"      3233.1071     38.9916
A"      3217.6670      1.8618
A"      1613.1195      0.6358
A"      1510.1242     41.2161
A"      1366.9282      1.1734
A"      1313.4309     19.5552
A"      1194.3692      2.4896
A"      1112.2727      3.5782
A"      1000.8305      0.0342
A"       858.2024      0.3555
A"       651.6922      0.0426
A"       436.4789      0.2474
A"       413.4771      2.3776
A"       175.2873    123.9327
```

B:

```
Processing: pauetbendiyn6plam6.log
PG=C01

Method       BasisSet                        Imaginary Freqs
RM06         6-31+G(d,p)/LANL2DZ(Au)           0

HF Energy
-941.2018467

      ZPE       E298      S298     Strans     Srot
  127.74562   138.460   144.097    43.737    34.099

27
C    -0.289911  -0.397913  -1.841439
Au   -1.667422  -0.080912  -0.237369
P    -3.310619   0.324811   1.403286
C     0.694897  -0.865601  -1.225851
C     1.749014  -1.369597  -0.461265
C     2.619212  -0.473406   0.229368
C     2.411608   0.927774   0.188434
C     2.249524   2.131675   0.157004
C     2.118021   3.579927   0.110253
H    -4.521902   0.858610   0.934419
H    -3.758480  -0.784511   2.139029
H    -2.982174   1.228816   2.426797
H    -0.585022  -0.103716  -2.838975
C     1.960654  -2.765137  -0.400440
C     3.681395  -1.020941   0.957683
```

C	3.445970	4.273067	-0.201818
H	1.361680	3.849281	-0.639359
H	1.729229	3.930256	1.076747
H	3.309503	5.358083	-0.226733
H	4.197548	4.039769	0.558611
H	3.835797	3.954583	-1.173442
C	3.023343	-3.273626	0.319676
H	1.281584	-3.422721	-0.937658
H	3.194526	-4.345222	0.360483
C	3.878914	-2.395766	0.996551
H	4.351811	-0.351308	1.489299
H	4.715709	-2.794804	1.564691

C:

Processing: sauetbendiyn6plam6.log
PG=C01

Method	BasisSet	Imaginary Freqs
RM06	6-31+G(d,p)/LANL2DZ(Au)	0

HF Energy
-940.8176680

ZPE	E298	S298	Strans	Srot
121.76584	131.972	137.231	43.729	34.316

26

C	-0.094121	-0.659876	-0.000994
C	-1.311430	-0.792221	0.000256
C	-2.725999	-0.947083	0.001668
C	-3.581010	0.183949	-0.005854
C	-3.026356	1.495544	-0.015971
C	-2.524872	2.600047	-0.024645
C	-1.821242	3.874876	-0.037631
Au	1.887697	-0.409902	-0.001844
P	4.223653	-0.102139	-0.002614
C	-3.301075	-2.226778	0.010670
C	-4.969714	-0.003263	-0.004062
C	-0.308807	3.677996	0.067510
H	-2.179191	4.504825	0.789287
H	-2.067102	4.421393	-0.959493
H	4.977687	-0.684538	-1.040873
H	4.965609	-0.566522	1.101718
H	4.724498	1.213153	-0.072155
C	-4.679393	-2.394038	0.012388
H	-2.638700	-3.089479	0.016344
H	-5.101990	-3.396301	0.019463
C	-5.517855	-1.279066	0.005049

```
H    -5.611721   0.874960  -0.010018
H    -6.598126  -1.404959   0.006321
H     0.214110   4.640742   0.039162
H    -0.051645   3.166316   1.001531
H     0.054954   3.054199  -0.756740

WARNING: Geometry optimization converged in opt job, but not in freq job
```

AuPH$_3$:

```
Processing: aup6plam6.log
PG=C03V

Method        BasisSet                              Imaginary Freqs
RM06          6-31+G(d,p)/LANL2DZ(Au)                  0

HF Energy
-478.2969361

      ZPE        E298        S298      Strans       Srot
   17.34994      19.705      66.176      42.213      21.152

5
P     0.000000   0.000000  -1.864018
Au     0.000000   0.000000   0.446233
H     0.000000   1.281584  -2.430711
H     1.109884  -0.640792  -2.430711
H    -1.109884  -0.640792  -2.430711
```

D:

```
Processing: etbendiynau2p2-sp6plam6.log
PG=C01

Method        BasisSet      Imaginary Freqs
RM06          6-31+G(d,p)/LANL2DZ(Au)        0

HF Energy
-1419.2066756

      ZPE        E298        S298      Strans       Srot
  139.14482     153.038     174.136      45.133      36.693

31
C     2.365787   4.140449   0.070798
C     2.494766   2.766237  -0.066921
```

C	1.361565	1.948692	-0.085802
C	0.064258	2.511002	0.037873
C	-0.038637	3.902299	0.178297
C	1.094814	4.703904	0.194391
C	-1.087658	1.681778	0.018854
C	-2.081018	0.963360	0.000888
Au	-3.775961	-0.112285	-0.007068
P	-5.813358	-1.313389	-0.014163
C	1.425989	0.519635	-0.224073
C	0.860116	-0.584452	-0.356193
C	0.154200	-1.847456	-0.483362
C	-0.022632	-2.584181	0.842214
Au	3.280295	-0.647736	-0.060664
P	5.440197	-1.567945	0.156035
H	-5.839803	-2.585175	-0.615692
H	-6.906341	-0.711262	-0.663441
H	-6.398730	-1.616472	1.228673
H	0.638900	-2.476489	-1.242378
H	-0.825425	-1.568415	-0.904041
H	5.916525	-2.331121	-0.922319
H	6.479762	-0.639157	0.325513
H	5.657574	-2.435464	1.238799
H	-0.604494	-3.498352	0.692640
H	0.945535	-2.864152	1.273408
H	-0.548694	-1.950791	1.563724
H	-1.028554	4.340694	0.273103
H	0.988019	5.780213	0.302784
H	3.482028	2.317659	-0.170712
H	3.249477	4.772341	0.080897

WARNING: Geometry optimization converged in opt job, but not in freq job

TS1:

Processing: etbcpau2p2-sprcts6plam6.log
PG=C01

Method	BasisSet	Imaginary Freqs
RM06	6-31+G(d,p)/LANL2DZ(Au)	1

HF Energy
-1419.1996758

ZPE	E298	S298	Strans	Srot
139.13454	152.264	162.863	45.133	36.578

31

C	-2.463905	4.151631	0.099391

```
C    -2.618766   2.770261   0.035913
C    -1.492446   1.951961   0.013147
C    -0.204571   2.532200   0.054175
C    -0.054758   3.918436   0.116091
C    -1.190272   4.721350   0.138887
C    -1.467600   0.502872  -0.049264
Au   -3.201583  -0.679829  -0.070076
P    -5.214579  -1.928555  -0.081472
C     0.858285   1.592152   0.022971
C     1.878833   0.890926  -0.005154
Au    3.614582  -0.131158  -0.059911
P     5.697371  -1.248920  -0.128944
C    -0.363194  -0.186473  -0.071646
C     0.246107  -1.524194  -0.051601
C     0.678365  -1.992087   1.334351
H     6.051410  -1.883466  -1.332176
H     5.908217  -2.290860   0.790625
H     6.838335  -0.460754   0.099680
H    -0.536707  -2.191592  -0.444725
H     1.068690  -1.580596  -0.774223
H    -6.406924  -1.200283  -0.237132
H    -5.517206  -2.682977   1.065692
H    -5.370818  -2.901866  -1.084047
H     1.084688  -3.007666   1.286319
H     1.445971  -1.330645   1.752124
H    -0.172512  -1.992390   2.024938
H     0.938635   4.357618   0.146214
H    -1.082705   5.801657   0.187552
H    -3.612570   2.327558   0.003128
H    -3.341796   4.792105   0.117673
```

TS1a:

```
Processing: etbcpau2p2-sprcts-a6plam6.log
PG=C01

Method       BasisSet                          Imaginary Freqs
RM06         6-31+G(d,p)/LANL2DZ(Au)              1

HF Energy
-1419.2017914

       ZPE        E298       S298      Strans       Srot
   139.46338     152.295     158.746      45.133      36.453

ccl00:~/aue/ark/pj/au> gtg etbcpau2p2-sprcts-a6plam6.log
Processing: etbcpau2p2-sprcts-a6plam6.log
31
```

C	-2.606902	4.134698	0.049880
C	-2.696242	2.749203	-0.006896
C	-1.526009	1.989308	0.008242
C	-0.286867	2.657641	0.084778
C	-0.186752	4.049540	0.136470
C	-1.365525	4.781132	0.120240
C	-1.366154	0.548326	-0.041680
Au	-3.007134	-0.725904	-0.074377
P	-4.931227	-2.131288	-0.110822
C	0.742638	1.695433	0.070885
C	1.666290	0.859912	0.014744
Au	3.436497	-0.141834	-0.067774
P	5.554359	-1.172987	-0.168538
C	-0.102084	0.072207	-0.026118
C	0.318901	-1.369854	0.051449
C	0.676592	-1.834822	1.458620
H	6.122247	-1.334995	-1.443145
H	5.659824	-2.476077	0.345726
H	6.596198	-0.524554	0.515008
H	-0.557632	-1.931653	-0.301286
H	1.124075	-1.595556	-0.659424
H	-6.057825	-1.708984	0.618367
H	-4.797850	-3.443106	0.380380
H	-5.527758	-2.394547	-1.357657
H	0.915044	-2.903866	1.462790
H	1.540616	-1.293143	1.864541
H	-0.165206	-1.667625	2.140739
H	0.780536	4.540802	0.190928
H	-1.325685	5.866013	0.163568
H	-3.664709	2.255365	-0.063132
H	-3.515818	4.731000	0.039253

E:

Processing: etmebcpau2p2-sp6plam6.log
PG=C01

Method	BasisSet	Imaginary Freqs
RM06	6-31+G(d,p)/LANL2DZ(Au)	0

HF Energy
-1419.2134688

ZPE	E298	S298	Strans	Srot
139.74491	152.882	164.159	45.133	36.601

31

C	-1.774851	4.207109	0.157690

C	-2.280476	2.904052	0.097103
C	-1.393909	1.839975	0.033873
C	-0.007990	2.103724	0.032643
C	0.505352	3.386630	0.093291
C	-0.403515	4.448486	0.155078
C	0.666195	0.791668	-0.034648
C	-0.449418	-0.265163	-0.086081
C	-1.628705	0.396302	-0.040157
Au	-3.481335	-0.500247	-0.060868
P	-5.651971	-1.498288	-0.079808
C	-0.142446	-1.723045	-0.139326
C	0.418276	-2.273807	1.169059
C	1.906334	0.445543	-0.033740
Au	3.783349	-0.213368	-0.055636
P	6.028143	-1.010935	-0.084284
H	6.468058	-1.718042	1.046538
H	6.369671	-1.896050	-1.119810
H	7.028730	-0.033222	-0.210577
H	-1.076686	-2.243903	-0.387065
H	0.553813	-1.929865	-0.967185
H	-5.735223	-2.901417	-0.014069
H	-6.539685	-1.152231	0.955616
H	-6.472663	-1.256924	-1.197158
H	1.576247	3.575958	0.091394
H	-0.033363	5.469151	0.200387
H	-3.353963	2.725001	0.100454
H	-2.464055	5.046445	0.206972
H	0.618029	-3.347759	1.092128
H	1.359636	-1.779300	1.448125
H	-0.289294	-2.112793	1.990682

J:

Processing: etbchau2p2-sprcprod6plam6.log
PG=C01

Method	BasisSet	Imaginary Freqs
RM06	6-31+G(d,p)/LANL2DZ(Au)	0

HF Energy
-1419.2230174

ZPE	E298	S298	Strans	Srot
139.66987	152.741	161.571	45.133	36.293

31

C	0.199163	-1.717764	-0.166918
C	0.055057	-0.217842	-0.119816

C	-1.149754	0.457542	-0.064537
Au	-2.928569	-0.632558	-0.065487
P	-4.962924	-1.878572	-0.057972
C	-1.194133	1.885811	0.017690
C	0.025105	2.714819	0.052295
C	1.019460	1.792912	-0.002170
C	1.323900	0.549942	-0.074288
Au	3.271194	-0.180451	-0.060792
P	5.490568	-0.995346	-0.047872
H	5.917325	-1.703654	-1.184024
H	5.836135	-1.894526	0.975146
H	6.514819	-0.041217	0.075056
C	-0.016218	4.118998	0.123485
C	-2.396384	2.635635	0.067282
H	-0.735205	-2.146818	-0.552635
H	0.985895	-1.982243	-0.887960
C	0.514509	-2.311384	1.200875
H	-6.167672	-1.166402	-0.205205
H	-5.266148	-2.636586	1.088298
H	-5.136105	-2.858922	-1.052671
H	0.627601	-3.399266	1.144867
H	1.447423	-1.897431	1.609696
H	-0.285090	-2.083875	1.916382
C	-1.231797	4.755753	0.167477
H	0.915719	4.675231	0.143280
H	-1.270786	5.839974	0.223362
C	-2.424769	4.007998	0.140336
H	-3.329431	2.075458	0.044118
H	-3.381311	4.522170	0.175756
H	-0.285090	-2.083875	1.916382
C	-1.231797	4.755753	0.167477
H	0.915719	4.675231	0.143280
H	-1.270786	5.839974	0.223362
C	-2.424769	4.007998	0.140336
H	-3.329431	2.075458	0.044118
H	-3.381311	4.522170	0.175756

K:

Processing: etbchau2p2-sprcprod6plam6.log

31

C	0.199163	-1.717764	-0.166918
C	0.055057	-0.217842	-0.119816
C	-1.149754	0.457542	-0.064537
Au	-2.928569	-0.632558	-0.065487
P	-4.962924	-1.878572	-0.057972
C	-1.194133	1.885811	0.017690
C	0.025105	2.714819	0.052295

C	1.019460	1.792912	-0.002170
C	1.323900	0.549942	-0.074288
Au	3.271194	-0.180451	-0.060792
P	5.490568	-0.995346	-0.047872
H	5.917325	-1.703654	-1.184024
H	5.836135	-1.894526	0.975146
H	6.514819	-0.041217	0.075056
C	-0.016218	4.118998	0.123485
C	-2.396384	2.635635	0.067282
H	-0.735205	-2.146818	-0.552635
H	0.985895	-1.982243	-0.887960
C	0.514509	-2.311384	1.200875
H	-6.167672	-1.166402	-0.205205
H	-5.266148	-2.636586	1.088298
H	-5.136105	-2.858922	-1.052671
H	0.627601	-3.399266	1.144867
H	1.447423	-1.897431	1.609696
H	-0.285090	-2.083875	1.916382
C	-1.231797	4.755753	0.167477
H	0.915719	4.675231	0.143280
H	-1.270786	5.839974	0.223362
C	-2.424769	4.007998	0.140336
H	-3.329431	2.075458	0.044118
H	-3.381311	4.522170	0.175756

Processing: etbchau2p2-sprcprod-a6plam6.log
PG=C01

Method	BasisSet	Imaginary Freqs
RM06	6-31+G(d,p)/LANL2DZ(Au)	0

HF Energy
-1419.2337626

ZPE	E298	S298	Strans	Srot
140.05902	153.137	162.310	45.133	36.212

31

C	-0.729443	3.681368	0.248644
C	-1.358860	2.466758	0.123655
C	-0.622715	1.255559	0.038740
C	0.812427	1.356301	0.087831
C	1.438768	2.614533	0.214323
C	0.677753	3.756606	0.294624
C	1.543373	0.110446	-0.012688
C	0.668295	-0.842389	-0.106678
C	-0.618706	-1.250714	-0.193196
C	-1.283153	-0.008114	-0.089501
C	-1.214216	-2.619984	-0.265074

C	-1.385701	-3.239603	1.119125
Au	-3.381395	-0.123958	-0.081996
P	-5.758801	-0.204971	-0.071683
Au	3.591066	-0.223094	-0.042670
P	5.928391	-0.591148	-0.077251
H	6.628954	-0.393036	1.124976
H	6.686814	0.196974	-0.959798
H	6.365534	-1.879502	-0.429954
H	-2.184637	-2.536472	-0.772741
H	-0.580969	-3.257284	-0.894341
H	-6.440592	1.025050	-0.074626
H	-6.387635	-0.841091	1.013857
H	-6.394624	-0.850121	-1.147733
H	-1.827861	-4.238006	1.044576
H	-0.423205	-3.333415	1.634609
H	-2.039476	-2.620285	1.745065
H	2.525173	2.662535	0.248127
H	1.162873	4.724412	0.393886
H	-2.446400	2.422218	0.086545
H	-1.318752	4.592360	0.311350

WARNING: Geometry optimization converged in opt job, but not in freq job

TS2:

Processing: etmebcpau2p2-spts6plam6.log
PG=C01

Method	BasisSet	Imaginary Freqs
RM06	6-31+G(d,p)/LANL2DZ(Au)	1

HF Energy
-1419.2017431

ZPE	E298	S298	Strans	Srot
138.79445	151.022	154.664	45.133	36.371

31

C	-0.842834	3.882211	0.014892
C	-1.666557	2.746691	0.021967
C	-1.081861	1.497232	-0.077826
C	0.325334	1.391090	-0.184390
C	1.140615	2.508100	-0.191771
C	0.539862	3.769401	-0.090408
C	-1.697285	0.146644	-0.099113
C	-0.672692	-0.732146	-0.233359
C	0.617638	-0.038913	-0.277469
Au	-3.701882	-0.242733	0.035799

P	-6.053986	-0.673176	0.185892
C	-0.540107	-2.219845	-0.327337
C	0.880918	-2.545485	0.047218
C	1.777458	-0.720418	-0.332805
Au	3.773543	-0.383288	-0.017330
P	6.070013	0.092826	0.354536
H	6.368674	1.113123	1.273892
H	6.868616	-0.951532	0.852512
H	6.833136	0.503448	-0.752287
H	-6.607517	-1.639806	-0.674536
H	-6.568911	-1.123630	1.416025
H	-6.929887	0.399993	-0.063229
H	1.334845	-3.442132	-0.389967
H	1.142118	-2.453106	1.100795
H	1.622473	-1.825670	-0.793942
H	-0.761741	-2.589341	-1.338457
H	-1.225091	-2.733245	0.361440
H	2.222714	2.415056	-0.279168
H	1.156262	4.664427	-0.094841
H	-2.747456	2.846970	0.105273
H	-1.292789	4.869024	0.093432

F:

Processing: etmebcpau2p2-spprod6plam6.log
PG=C01

Method	BasisSet	Imaginary Freqs
RM06	6-31+G(d,p)/LANL2DZ(Au)	0

HF Energy
-1419.2871509

ZPE	E298	S298	Strans	Srot
141.90342	154.163	156.180	45.133	36.017

31

C	-1.947508	-0.228098	1.943812
C	-0.993535	0.452031	1.188175
C	0.153689	-0.401200	0.908967
C	-0.119006	-1.774692	1.444534
C	-1.344377	-1.563001	2.370945
C	-0.696207	1.789200	0.680525
C	0.618919	1.699816	0.157546
C	1.154200	0.317975	0.332956
C	-1.411566	2.972546	0.670048
C	-0.804797	4.108416	0.115495
C	0.483170	4.030173	-0.401950

C	1.209512	2.826849	-0.380889
Au	3.048158	-0.296587	-0.131304
P	5.276270	-1.016375	-0.644854
Au	-2.937265	-0.446779	-0.060470
P	-4.239484	-0.832048	-1.996597
H	-4.831096	-2.100416	-2.116062
H	-5.348133	0.009188	-2.187013
H	-3.585178	-0.713854	-3.234334
H	6.199463	-0.044037	-1.072879
H	6.021841	-1.620328	0.384844
H	5.448231	-1.975545	-1.660655
H	-1.022561	-1.460323	3.417773
H	-2.056206	-2.394993	2.348244
H	-2.723321	0.266556	2.531012
H	0.735208	-2.210464	1.974115
H	-0.370801	-2.470820	0.629155
H	-2.418437	3.027117	1.083400
H	-1.340380	5.053597	0.095727
H	2.222861	2.785629	-0.776712
H	0.941185	4.920840	-0.825647

G:

Processing: saupetmeb33dien6plam6.log
PG=C01

Method	BasisSet	Imaginary Freqs
RM06	6-31+G(d,p)/LANL2DZ(Au)	0

HF Energy
-940.8967129

ZPE	E298	S298	Strans	Srot
123.69203	132.558	124.372	43.729	33.509

26

C	-1.356354	-2.304627	0.000420
C	-1.539236	-0.925620	0.000255
C	-2.861590	-0.401126	-0.000385
C	-3.967643	-1.236940	-0.000870
C	-3.768066	-2.620425	-0.000717
C	-2.473981	-3.143380	-0.000072
C	-0.550918	0.173687	0.000613
C	-1.273711	1.323641	0.000317
C	-2.709352	1.046711	-0.000378
C	-1.063851	2.805916	0.000291
C	-2.505366	3.387728	-0.000616
C	-3.419045	2.188646	-0.000919

Au	1.475022	-0.029153	0.000787
P	3.862667	-0.265904	-0.002133
H	4.408849	-1.561458	-0.116480
H	4.616034	0.367864	-1.012953
H	4.603514	0.174301	1.115171
H	-2.691310	4.026250	-0.876619
H	-2.692288	4.026594	0.874926
H	-4.503660	2.278580	-0.001578
H	-0.494429	3.137928	-0.878285
H	-0.495483	3.138093	0.879485
H	-4.975884	-0.823781	-0.001374
H	-4.623609	-3.292339	-0.001099
H	-0.349663	-2.722645	0.000930
H	-2.334128	-4.222973	0.000055

H:

Processing: paupetmeb33dien6plam6.log
PG=C01

Method	BasisSet	Imaginary Freqs
RM06	6-31+G(d,p)/LANL2DZ(Au)	0

HF Energy
-941.2933387

ZPE	E298	S298	Strans	Srot
131.39304	140.324	124.956	43.737	33.007

27

C	-3.791946	-0.588578	-1.027315
C	-2.699302	0.200662	-0.713572
C	-1.926132	-0.091439	0.438141
C	-2.232384	-1.158455	1.267546
C	-3.336543	-1.953699	0.941249
C	-4.099031	-1.670283	-0.189112
C	-2.156966	1.404992	-1.373955
C	-1.079213	1.825929	-0.679967
C	-0.891179	0.940825	0.481732
C	-0.066707	2.928013	-0.629655
C	0.519453	2.816869	0.802468
C	0.088931	1.455937	1.316843
Au	1.193337	-0.180592	0.120081
P	2.753033	-1.700306	-0.788450
H	-2.597518	1.865495	-2.252765
H	3.438304	-1.280534	-1.939561
H	3.809028	-2.072500	0.058405
H	2.246920	-2.947471	-1.188044

H	0.073398	3.573289	1.464862
H	1.601889	2.978723	0.845043
H	0.261966	1.137142	2.344996
H	-0.493754	3.916287	-0.826240
H	0.720613	2.775187	-1.382202
H	-1.636941	-1.372689	2.154440
H	-3.604408	-2.793027	1.576927
H	-4.407207	-0.375413	-1.898364
H	-4.955309	-2.297763	-0.423571

Ha:

Processing: paupetmeb33dien-a6plam6.log
PG=C01

Method	BasisSet	Imaginary Freqs
RM06	6-31+G(d,p)/LANL2DZ(Au)	0

HF Energy
-941.3017909

ZPE	E298	S298	Strans	Srot
131.39754	140.338	126.048	43.737	33.080

27

C	1.957195	-2.029961	-1.028908
C	1.642244	-0.713278	-0.714158
C	2.279910	-0.059925	0.369669
C	3.222039	-0.726739	1.144597
C	3.532811	-2.046925	0.823172
C	2.912074	-2.686977	-0.252576
C	0.668906	0.217957	-1.349890
C	0.804570	1.443769	-0.680458
C	1.762789	1.299642	0.398971
C	0.395920	2.870465	-0.814936
C	1.046455	3.544851	0.415387
C	1.924463	2.493952	1.016545
Au	-1.173140	-0.174142	-0.166368
P	-3.125881	-0.871522	0.951864
H	0.308959	0.105951	-2.373247
H	-2.947009	-1.678376	2.087503
H	-3.969612	0.134614	1.450516
H	-4.024809	-1.641650	0.196069
H	0.298633	3.888555	1.144856
H	1.623765	4.439196	0.147744
H	2.612531	2.702348	1.832777
H	-0.687762	3.018044	-0.871012
H	0.807031	3.282666	-1.746958

H	3.716555	-0.228935	1.976171
H	4.272922	-2.583480	1.410816
H	1.479112	-2.536293	-1.865251
H	3.179712	-3.713593	-0.489365

L:

Processing: prmebcpau2p2-sp6plam6.log
PG=C01

Method	BasisSet	Imaginary Freqs
RM06	6-31+G(d,p)/LANL2DZ(Au)	0

HF Energy
-1458.4971445

ZPE	E298	S298	Strans	Srot
157.48131	171.457	170.580	45.200	36.782

34

C	-1.652703	0.513833	-0.043376
C	-1.467931	1.960942	0.088249
C	-0.091736	2.271695	0.088304
C	0.627497	0.991711	-0.033698
C	-0.453034	-0.105365	-0.122424
C	0.378893	3.568046	0.195825
C	-0.564320	4.595195	0.304564
C	-1.926778	4.307299	0.306448
C	-2.389331	2.991166	0.198331
C	1.868612	0.652218	-0.048582
Au	3.731109	-0.047403	-0.094702
P	5.952324	-0.904507	-0.153848
C	-0.089424	-1.544877	-0.237707
C	0.476087	-2.148478	1.049052
Au	-3.469181	-0.452578	-0.096832
P	-5.599912	-1.531568	-0.153424
H	6.383898	-1.639278	0.962457
H	6.260808	-1.782974	-1.205358
H	6.977482	0.048023	-0.275725
H	-0.993273	-2.098818	-0.529440
H	0.634458	-1.686446	-1.058493
H	-5.633340	-2.936251	-0.075917
H	-6.521390	-1.208931	0.859905
H	-6.404598	-1.330227	-1.290125
H	1.442874	3.792664	0.193959
H	-0.228636	5.625428	0.386632
H	-3.456267	2.776550	0.201457
H	-2.643440	5.120303	0.392384

C	0.947151	-3.578768	0.848957
H	1.310860	-1.527367	1.414036
H	-0.294891	-2.096464	1.831139
H	1.327741	-4.015808	1.777802
H	0.131364	-4.219412	0.491712
H	1.749979	-3.629005	0.100181

TS3:

Processing: prmebcpau2p2-spts6plam6.log
PG=C01

Method	BasisSet	Imaginary Freqs
RM06	6-31+G(d,p)/LANL2DZ(Au)	1

HF Energy
-1458.4933569

ZPE	E298	S298	Strans	Srot
156.37109	169.518	160.984	45.200	36.625

34

C	0.582041	0.079267	-0.243598
C	0.258499	1.505644	-0.183565
C	-1.149930	1.589374	-0.084882
C	-1.740598	0.229718	-0.083532
C	-0.702183	-0.635445	-0.194584
C	1.053778	2.637368	-0.208161
C	0.431042	3.888831	-0.132854
C	-0.954650	3.980089	-0.035090
C	-1.757116	2.831249	-0.009873
Au	-3.741974	-0.182040	0.038767
P	-6.092136	-0.629070	0.174435
C	-0.573127	-2.122560	-0.272026
C	0.797130	-2.499935	0.208089
C	1.752541	-0.575696	-0.280541
Au	3.744506	-0.208866	-0.001993
P	6.042267	0.309514	0.322180
H	6.339950	1.342822	1.227553
H	6.873840	-0.712860	0.812334
H	6.777312	0.726977	-0.801207
H	-6.636255	-1.599467	-0.688022
H	-6.614100	-1.081121	1.401189
H	-6.973211	0.438423	-0.081384
C	1.433470	-3.777246	-0.244102
H	0.992380	-2.250082	1.253496
H	1.593211	-1.710333	-0.597090
H	-0.726588	-2.503708	-1.293987

H	-1.315304	-2.618285	0.371862
H	2.137743	2.561455	-0.289291
H	1.031807	4.794356	-0.151872
H	-2.840077	2.913425	0.068016
H	-1.421936	4.960275	0.022954
H	2.493744	-3.826570	0.024991
H	0.930541	-4.604682	0.275439
H	1.319614	-3.939673	-1.321004

M:

Processing: prbchau2p2-sprcprod-a6plam6.log
PG=C01

Method	BasisSet	Imaginary Freqs
RM06	6-31+G(d,p)/LANL2DZ(Au)	0

HF Energy
-1458.5172158

ZPE	E298	S298	Strans	Srot
157.62215	171.610	170.939	45.200	36.543

34

C	-1.195546	2.640322	0.224413
C	-0.502103	1.409852	0.077618
C	0.935563	1.455531	0.141048
C	1.605201	2.681711	0.340521
C	0.884656	3.844122	0.479052
C	-0.524130	3.822534	0.420085
C	1.621732	0.191513	-0.022637
C	0.714136	-0.723369	-0.173883
C	-0.585100	-1.079091	-0.291166
C	-1.205096	0.180345	-0.123709
Au	-3.306256	0.125982	-0.123603
P	-5.684495	0.102558	-0.118846
Au	3.656060	-0.213960	-0.058311
P	5.978645	-0.664959	-0.098169
C	-1.241680	-2.411741	-0.440395
C	-1.575704	-3.054075	0.907227
C	-2.334993	-4.357825	0.731239
H	6.834409	0.415691	-0.372454
H	6.430504	-1.606124	-1.039192
H	6.556592	-1.168665	1.079865
H	-2.163103	-2.272071	-1.025160
H	-0.595561	-3.080464	-1.024570
H	-6.338161	0.344041	-1.340588
H	-6.336536	1.035243	0.707606

H	-6.325331	-1.083601	0.282554
H	-0.646792	-3.220029	1.471101
H	-2.169017	-2.342822	1.501688
H	2.692335	2.688741	0.383629
H	1.403130	4.786898	0.634618
H	-2.283629	2.636589	0.177531
H	-1.080829	4.749533	0.529202
H	-2.565929	-4.822042	1.695057
H	-3.284242	-4.192106	0.204871
H	-1.756229	-5.081527	0.144227

TS4:

Processing: prbchau2p2-insts6plam6.log
PG=C01

Method	BasisSet	Imaginary Freqs
RM06	6-31+G(d,p)/LANL2DZ(Au)	1

HF Energy
-1458.5045211

ZPE	E298	S298	Strans	Srot
157.16237	170.180	161.261	45.200	36.364

34

C	-0.727864	3.656187	0.198027
C	-1.398408	2.458897	0.125225
C	-0.717562	1.218993	0.033824
C	0.720561	1.253492	0.024771
C	1.382642	2.503436	0.104893
C	0.680244	3.680785	0.188021
C	1.479354	0.029797	-0.049669
C	0.644047	-1.019717	-0.138875
C	-0.741761	-1.193405	-0.106280
C	-1.457405	-0.013324	-0.028591
C	-1.223334	-2.610344	-0.143057
C	-0.176007	-3.435926	0.614199
Au	-3.532461	-0.059890	-0.033259
P	-5.924045	-0.106976	-0.051922
Au	3.548710	-0.052057	-0.042181
P	5.927997	-0.122000	-0.040385
H	6.586892	0.235258	1.149813
H	6.594870	0.706923	-0.960244
H	6.549302	-1.353897	-0.313720
H	-2.211674	-2.707395	0.318533
H	-1.320081	-2.957050	-1.183821
H	-6.584916	0.684946	-1.009674

H	-6.602507	0.304740	1.110656
H	-6.563194	-1.340498	-0.278660
H	-0.275192	-3.234896	1.686633
C	1.214783	-3.043361	0.163312
H	-0.325109	-4.510697	0.460457
H	2.472236	2.512361	0.097152
H	1.208922	4.628872	0.244884
H	-2.487728	2.444630	0.136811
H	-1.284954	4.587383	0.263928
H	1.960596	-2.866568	0.938364
H	1.632956	-3.673634	-0.635399
H	1.230893	-2.095091	-0.596162

N:

Processing: prbchau2p2-insprod6plam6.log
PG=C01

Method	BasisSet	Imaginary Freqs
RM06	6-31+G(d,p)/LANL2DZ(Au)	0

HF Energy
-1458.5663707

ZPE	E298	S298	Strans	Srot
159.61252	172.486	159.044	45.200	36.320

34

C	-1.474186	-0.015323	-0.127658
C	-0.717097	1.212476	-0.126435
C	0.734620	1.234771	-0.075776
C	1.477146	0.048428	-0.100756
C	0.723889	-1.188168	-0.320068
C	-0.756707	-1.170673	-0.178570
C	1.406346	2.494144	0.005427
C	0.721386	3.677501	0.011281
C	-0.688852	3.650491	-0.064412
C	-1.378233	2.459612	-0.125287
Au	3.536659	-0.057129	0.007665
P	5.925073	-0.218771	0.149134
C	-1.238084	-2.585556	-0.043048
C	0.018137	-3.456168	-0.197889
C	1.164959	-2.544203	0.242892
Au	-3.543284	-0.064000	0.012830
P	-5.930504	-0.171626	0.170002
H	6.521671	0.081143	1.387140
H	6.682564	0.605144	-0.702732
H	6.513148	-1.467932	-0.119293

H	-1.670193	-2.702318	0.963499
H	-2.039580	-2.831798	-0.751083
H	-6.686685	0.678210	-0.659136
H	-6.525635	0.115121	1.413036
H	-6.553534	-1.401059	-0.115979
H	-0.035188	-4.387759	0.372277
H	0.157819	-3.728537	-1.253382
H	2.494878	2.483691	0.051041
H	1.247860	4.625896	0.066908
H	-2.466093	2.461884	-0.169905
H	-1.241162	4.587675	-0.068735
H	1.221479	-2.477469	1.338460
H	2.147969	-2.859072	-0.125934
H	0.875574	-1.261650	-1.430554

E with trimethylphosphine and BrettPhos ligands:

Processing: ebrettpme36labe.log
PG=C01

Method	BasisSet	Imaginary Freqs
RB3LYP	LANL2DZ	0

HF Energy
-2381.9592659

Thermochemistry will use frequencies scaled by 0.9600

ZPE	E298	S298	Strans	Srot
665.31317	707.699	378.929	47.023	41.050

127

C	-4.371742	3.866563	-2.090585
C	-4.931519	2.716390	-1.488876
C	-4.079950	1.741147	-0.952480
C	-2.668563	1.936078	-1.024581
C	-2.103575	3.067050	-1.619746
C	-2.975998	4.041176	-2.158147
C	-2.039797	0.734799	-0.388878
C	-3.200959	-0.166107	0.058337
C	-4.379520	0.449189	-0.286990
Au	-6.265306	-0.275853	0.032664
P	-8.552081	-1.103591	0.377340
C	-2.966331	-1.478448	0.764343
C	-2.422031	-1.326178	2.208196
C	-0.766198	0.459572	-0.245507
Au	1.083740	-0.176364	-0.159171
P	3.138545	-1.519486	-0.158725
C	3.288635	-2.537490	1.481282

C	2.981491	-2.719235	-1.647442
C	4.755117	-0.543747	-0.325395
H	-3.922380	-2.014614	0.797308
H	-2.270556	-2.102526	0.181635
C	-9.885106	-0.045333	-0.424058
C	-9.093550	-1.219001	2.175764
C	-8.875672	-2.827352	-0.303769
H	-1.027642	3.203152	-1.676193
H	-2.565385	4.930544	-2.628711
H	-6.009371	2.586071	-1.443932
H	-5.026438	4.626586	-2.509378
H	-2.290281	-2.311434	2.674069
H	-1.450636	-0.814244	2.220804
H	-3.117957	-0.742919	2.823098
C	4.013178	-3.898828	1.331089
H	3.903559	-1.886508	2.119578
C	4.161127	-4.590844	2.709116
H	3.432800	-4.556093	0.666381
H	4.993833	-3.756073	0.868991
C	2.796184	-4.769203	3.409058
H	4.650294	-5.565490	2.575036
H	4.823758	-3.988351	3.349914
C	2.057802	-3.418369	3.534735
H	2.177620	-5.471997	2.828911
H	2.935732	-5.215206	4.402870
C	1.906306	-2.718724	2.162187
H	1.064493	-3.565956	3.980315
H	2.617269	-2.759982	4.216974
H	1.250735	-3.325154	1.519508
H	1.413390	-1.746013	2.291517
C	3.143125	-1.954874	-2.984315
H	3.806662	-3.429163	-1.549415
C	3.024775	-2.924887	-4.185358
H	2.361267	-1.183406	-3.067310
H	4.112481	-1.441714	-3.016682
C	1.696103	-3.712505	-4.153249
H	3.108675	-2.358285	-5.122734
H	3.868838	-3.631851	-4.163984
C	1.518417	-4.450951	-2.808179
H	0.855618	-3.016162	-4.300647
H	1.662909	-4.429892	-4.984112
C	1.632005	-3.480574	-1.605846
H	0.543627	-4.956567	-2.777014
H	2.286449	-5.234765	-2.716979
H	0.799082	-2.761889	-1.642228
H	1.528544	-4.046156	-0.669918
C	4.802776	0.845762	-0.036668
C	6.054956	1.523317	-0.143627
C	7.217805	0.847361	-0.536206

C	7.164671	-0.523691	-0.824277
C	5.951223	-1.215616	-0.714003
C	3.627629	1.692620	0.393660
O	6.034285	2.884014	0.169532
H	8.165563	1.367499	-0.620018
H	8.071451	-1.035599	-1.125769
O	5.852222	-2.587981	-0.973608
C	7.041858	-3.325087	-1.393236
H	6.707663	-4.355368	-1.529489
H	7.433403	-2.935160	-2.341445
H	7.821936	-3.289499	-0.621881
C	7.276701	3.647269	0.093212
H	7.003349	4.663268	0.382266
H	8.028413	3.253696	0.790728
H	7.680824	3.648751	-0.928170
C	3.371903	1.892270	1.782810
C	2.389156	2.823069	2.165850
C	1.658312	3.583666	1.231556
C	1.928534	3.375910	-0.132196
C	2.904323	2.452837	-0.574226
C	4.194620	1.196085	2.875500
H	2.204684	2.988847	3.225496
C	0.624799	4.591912	1.743870
H	1.407309	3.974640	-0.873525
C	3.233395	2.382951	-2.072911
C	3.990665	3.664219	-2.521191
H	3.906806	1.532943	-2.237904
C	1.989800	2.164586	-2.970465
H	2.296479	2.062063	-4.019615
H	1.437599	1.258387	-2.688206
H	1.295521	3.013415	-2.916597
H	4.298274	3.579126	-3.571861
H	3.348912	4.550209	-2.428779
H	4.880203	3.827134	-1.904461
H	4.787944	0.399560	2.408544
C	5.199140	2.191198	3.519794
C	3.313328	0.543535	3.970253
H	5.828818	1.677681	4.258574
H	5.844623	2.642398	2.758855
H	4.667942	3.002486	4.034336
H	3.939154	-0.024725	4.671103
H	2.773691	1.298229	4.555486
H	2.568554	-0.136758	3.539408
C	-0.686662	3.872709	2.167898
H	1.050110	5.045170	2.652812
C	0.316057	5.740348	0.758469
H	-1.385635	4.588649	2.619461
H	-1.181503	3.418989	1.300106
H	-0.490000	3.079815	2.900309

```
H    -0.335347   6.481079   1.238833
H     1.230554   6.252870   0.433954
H    -0.211005   5.377311  -0.134053
H   -10.123590  -1.586300   2.245550
H    -8.428718  -1.899889   2.715843
H    -9.029808  -0.230358   2.640273
H    -9.918792  -3.119175  -0.137893
H    -8.662098  -2.841634  -1.376814
H    -8.215864  -3.546401   0.191254
H   -10.878132  -0.468701  -0.235703
H    -9.841368   0.968778  -0.015344
H    -9.712672   0.006348  -1.503349

Method        BasisSet
RB3LYP        6-31G(d)/LANL2DZ(Au)

HF Energy
-3051.99518920

Processing: ebrettpme3-b6dlabe.log
Frequency job incomplete: ebrettpme3-b6dlabe.log
127
C    -4.025700  -2.648114  -2.305105
C    -3.333501  -2.937500  -0.957305
C    -1.907541  -3.480103  -1.210985
C    -1.946088  -4.753439  -2.072600
C    -2.669415  -4.508918  -3.403777
C    -4.068205  -3.919551  -3.173680
P    -3.298728  -1.490973   0.260763
Au   -1.132290  -0.455242   0.334446
C     0.743993   0.112232   0.503406
C     1.995519   0.399147   0.662146
C     2.590515   1.542052   1.411102
C     3.994702   1.416910   1.271623
C     4.321037   0.231506   0.461651
C     3.170968  -0.391422   0.090431
C     4.814651   2.362232   1.883336
C     4.233538   3.404964   2.617919
C     2.846801   3.508759   2.745989
C     2.003087   2.568551   2.136770
Au    6.224794  -0.363297  -0.027129
P     8.457260  -1.003481  -0.582905
C     8.808010  -1.049128  -2.390726
C     2.958156  -1.624106  -0.739843
C     2.341808  -1.355841  -2.124424
C    -4.721154  -0.364213  -0.090973
C    -4.562530   1.009857  -0.396176
C    -5.725900   1.785208  -0.650035
C    -6.995660   1.217037  -0.580617
```

C	-7.147543	-0.135221	-0.281612
C	-6.026921	-0.925097	-0.049422
C	-3.252272	1.754649	-0.509688
C	-2.749386	2.491870	0.594488
C	-1.627860	3.312583	0.404861
C	-0.997046	3.455323	-0.832639
C	-1.512039	2.721611	-1.904201
C	-2.624273	1.881874	-1.775790
C	-3.436003	2.500194	1.960382
C	-4.246681	3.799385	2.159088
C	-3.154799	1.188340	-3.030118
C	-3.814706	2.204226	-3.986188
C	0.160477	4.430969	-1.005323
C	1.359609	3.826706	-1.756422
O	-6.106834	-2.268158	0.208165
C	-7.388980	-2.888840	0.239222
O	-5.511688	3.097038	-0.964894
C	-6.635661	3.925743	-1.239746
C	-3.629618	-2.273419	1.941448
C	-3.763930	-1.206933	3.045289
C	-4.053873	-1.847356	4.413859
C	-2.987148	-2.885130	4.788539
C	-2.845106	-3.945528	3.689597
C	-2.551865	-3.314329	2.315826
C	-2.065828	0.383464	-3.764857
C	-0.320875	5.726382	-1.691386
C	-2.456410	2.311692	3.134520
C	8.953541	-2.674180	0.014122
C	9.747131	0.120871	0.098954
H	3.932691	-2.108715	-0.865677
H	2.322697	-2.335430	-0.191927
H	0.925076	2.649953	2.234198
H	2.414891	4.321016	3.323081
H	5.894595	2.288554	1.791232
H	4.871996	4.141990	3.096791
H	2.219065	-2.293563	-2.678091
H	1.355239	-0.883973	-2.042261
H	2.982059	-0.689804	-2.712775
H	-3.919374	-3.707858	-0.438993
H	-1.322955	-2.708044	-1.731099
H	-1.385079	-3.680200	-0.269645
H	-0.922469	-5.105104	-2.250674
H	-2.457732	-5.552274	-1.516236
H	-2.077628	-3.811043	-4.013692
H	-2.740095	-5.441662	-3.975923
H	-4.547844	-3.688129	-4.132560
H	-4.703410	-4.669626	-2.680069
H	-3.475448	-1.864315	-2.840106
H	-5.041674	-2.277456	-2.147641

H	-4.589102	-2.788513	1.833380
H	-2.829178	-0.633518	3.108024
H	-4.558263	-0.495616	2.792485
H	-4.112681	-1.062553	5.177741
H	-5.041070	-2.331093	4.386017
H	-2.021574	-2.378735	4.932997
H	-3.237269	-3.360521	5.744402
H	-2.046238	-4.654152	3.939385
H	-3.773526	-4.531382	3.625776
H	-1.564751	-2.829715	2.340209
H	-2.498874	-4.107628	1.562224
H	-7.881205	1.812884	-0.765607
H	-8.144507	-0.556413	-0.242698
H	-7.202332	-3.943189	0.447613
H	-8.017313	-2.466611	1.032494
H	-7.900740	-2.792871	-0.725750
H	-6.225529	4.910372	-1.467460
H	-7.202730	3.558844	-2.104532
H	-7.301272	4.001261	-0.370609
H	-1.049982	2.822166	-2.881898
H	-1.256462	3.893771	1.245396
H	-4.144243	1.665819	1.986973
H	-3.010385	2.198175	4.073438
H	-1.826082	1.425106	3.002509
H	-1.795464	3.177552	3.255046
H	-4.793676	3.768804	3.108900
H	-3.583125	4.671968	2.182038
H	-4.963358	3.946799	1.347409
H	-3.933021	0.481897	-2.724328
H	-4.259381	1.690089	-4.846519
H	-4.599384	2.770480	-3.475983
H	-3.079612	2.922016	-4.369025
H	-2.502461	-0.168405	-4.605731
H	-1.284695	1.033636	-4.174520
H	-1.579051	-0.337069	-3.096861
H	0.507402	4.699872	0.001715
H	2.184751	4.546976	-1.791129
H	1.723435	2.918801	-1.264302
H	1.104456	3.573178	-2.792079
H	0.496362	6.453803	-1.759516
H	-0.675536	5.522527	-2.708871
H	-1.144494	6.188846	-1.136604
H	9.846298	-1.341099	-2.582339
H	8.137677	-1.764384	-2.876480
H	8.625563	-0.061342	-2.823983
H	9.986078	-2.901694	-0.272284
H	8.864132	-2.716146	1.103585
H	8.287379	-3.429641	-0.412883
H	10.750612	-0.211446	-0.188029

H	9.583896	1.135714	-0.275724
H	9.674124	0.142592	1.190367

J with trimethylphosphine and BrettPhos ligands:

Processing: jbrettpme36labe.log
PG=C01

Method	BasisSet	Imaginary Freqs
RB3LYP	LANL2DZ	0

HF Energy
-2381.9445231

Thermochemistry will use frequencies scaled by 0.9600

ZPE	E298	S298	Strans	Srot
665.59352	707.811	373.613	47.023	40.794

127

C	-4.724710	3.251829	2.666503
C	-4.789040	2.145247	1.825742
C	-3.626117	1.447648	1.367477
C	-2.340446	2.012577	1.864282
C	-2.292011	3.141783	2.720459
C	-3.473677	3.754796	3.119306
C	-1.359900	1.210490	1.314867
C	-1.227866	0.172881	0.563515
C	-2.516434	-0.376651	0.077508
C	-3.681811	0.288404	0.493903
C	-2.477382	-1.628724	-0.781569
C	-2.267334	-2.914060	0.057137
Au	-5.530449	-0.409600	-0.147933
P	-7.718578	-1.215845	-0.905682
Au	0.774456	-0.418573	0.371624
P	2.992135	-1.394533	0.164910
C	4.420016	-0.208031	-0.239564
C	2.820657	-2.661334	-1.296924
C	3.424851	-2.316606	1.808349
H	-3.416981	-1.712878	-1.340201
H	-1.665977	-1.536408	-1.516183
C	-9.185709	-0.392874	-0.063632
C	-8.019755	-3.053486	-0.638347
C	-8.050584	-0.961929	-2.739872
H	-2.203623	-3.795662	-0.594047
H	-1.340697	-2.852247	0.642957
H	-3.099592	-3.059098	0.757145
H	-1.327673	3.505837	3.060479
H	-3.443964	4.617868	3.778196

H	-5.755351	1.777571	1.493463
H	-5.642676	3.738566	2.983843
C	1.891770	-3.840351	-0.908909
H	2.282657	-2.057445	-2.041498
C	1.557367	-4.699319	-2.153279
H	2.391671	-4.475720	-0.163493
H	0.961955	-3.468515	-0.457442
C	2.837345	-5.208288	-2.852032
H	0.924105	-5.545313	-1.852441
H	0.969107	-4.096203	-2.862665
C	3.781095	-4.036802	-3.200652
H	3.360209	-5.911947	-2.185339
H	2.574847	-5.767190	-3.760324
C	4.119811	-3.181224	-1.953804
H	4.711959	-4.417545	-3.643148
H	3.305956	-3.399667	-3.963033
H	4.682205	-3.787816	-1.233437
H	4.766124	-2.345939	-2.246619
C	2.162125	-2.937697	2.461608
H	4.123292	-3.110057	1.519857
C	2.537893	-3.717712	3.746242
H	1.455883	-2.134945	2.722979
H	1.641588	-3.607367	1.769290
C	3.279402	-2.820426	4.760111
H	1.625636	-4.130295	4.198703
H	3.175421	-4.575473	3.480138
C	4.509157	-2.150880	4.109009
H	2.592603	-2.041614	5.126921
H	3.587108	-3.410057	5.634174
C	4.130369	-1.379522	2.820775
H	4.987971	-1.462152	4.818811
H	5.255901	-2.921670	3.861169
H	3.456322	-0.550265	3.081690
H	5.032076	-0.942677	2.381127
C	4.226174	1.154766	-0.596261
C	5.378806	1.961166	-0.842774
C	6.673493	1.428637	-0.784544
C	6.858210	0.079692	-0.451147
C	5.747247	-0.725935	-0.170788
C	2.893255	1.864276	-0.692530
O	5.125359	3.302821	-1.138947
H	7.541556	2.045854	-0.988034
H	7.864064	-0.321747	-0.403029
O	5.875951	-2.065385	0.212742
C	2.379313	2.503442	0.478003
C	1.203257	3.276147	0.387817
C	0.506330	3.443834	-0.822152
C	1.035269	2.816536	-1.960721
C	2.227766	2.056656	-1.942538

C	3.114249	2.454412	1.825835
H	0.835634	3.784661	1.277168
C	-0.729464	4.341956	-0.894852
H	0.528856	2.940919	-2.915816
C	2.711081	1.639582	-3.350868
C	3.561862	0.362907	-3.516997
H	1.790164	1.463076	-3.927256
C	3.432473	2.839657	-4.032929
H	3.653273	0.137813	-4.588103
H	4.574080	0.474626	-3.117503
H	3.095170	-0.501547	-3.036202
H	3.686329	2.588118	-5.071427
H	2.796390	3.732575	-4.042622
H	4.353083	3.091848	-3.496754
C	2.185259	2.112931	3.018123
H	3.880669	1.672742	1.777218
C	3.849241	3.798519	2.088628
H	4.433488	3.743044	3.016961
H	4.523933	4.041046	1.260942
H	3.131348	4.623163	2.189802
H	2.776682	1.991491	3.935255
H	1.457631	2.913494	3.206721
H	1.626795	1.183917	2.842632
C	7.200843	-2.676067	0.241521
C	6.250615	4.199441	-1.383775
H	5.799287	5.174257	-1.575292
H	6.908076	4.261441	-0.505970
H	6.830777	3.882569	-2.261186
H	7.034080	-3.714019	0.535763
H	7.672422	-2.643954	-0.749355
H	7.847165	-2.184262	0.979994
C	-0.351328	5.736074	-1.467416
C	-1.892845	3.719869	-1.704727
H	-1.087632	4.496563	0.133796
H	-2.775153	4.371389	-1.659265
H	-1.627212	3.601314	-2.763465
H	-2.174564	2.734690	-1.313826
H	-1.223346	6.403377	-1.465150
H	0.443776	6.207551	-0.876346
H	0.005742	5.648764	-2.502208
H	-9.046407	-1.332716	-3.007281
H	-7.984986	0.104013	-2.977804
H	-7.296063	-1.495292	-3.325980
H	-9.015535	-3.337038	-0.997020
H	-7.262992	-3.631469	-1.177340
H	-7.939865	-3.284806	0.428091
H	-10.127757	-0.797237	-0.450431
H	-9.133846	-0.567282	1.015377
H	-9.154692	0.685772	-0.245168

Method	BasisSet
RB3LYP	6-31G(d)/LANL2DZ(Au)

HF Energy
-3051.99456170

127

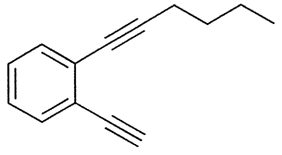
C	1.734671	-3.633700	-0.958532
C	3.121947	-2.964687	-0.822256
C	3.709855	-2.705086	-2.224504
C	3.810609	-4.016978	-3.024149
C	2.455245	-4.728157	-3.135975
C	1.831083	-4.948879	-1.751419
P	3.042644	-1.440281	0.295564
Au	0.858011	-0.507743	0.352382
C	-1.120881	0.162778	0.533575
C	-1.261567	1.225751	1.228865
C	-2.198061	2.056152	1.774506
C	-3.490667	1.482280	1.331268
C	-3.572323	0.301530	0.510481
C	-2.426003	-0.375158	0.105100
C	-4.625414	2.209230	1.788215
C	-4.532452	3.338049	2.575898
C	-3.277215	3.844673	2.974923
C	-2.119793	3.212401	2.577034
Au	-5.439969	-0.409950	-0.080047
P	-7.579121	-1.201351	-0.775812
C	-7.854683	-3.005110	-0.521836
C	-2.415105	-1.660733	-0.696602
C	-2.284737	-2.912030	0.187962
C	4.394494	-0.274204	-0.203428
C	4.168925	1.069864	-0.591971
C	5.286644	1.860822	-0.974682
C	6.578797	1.343291	-0.941830
C	6.798290	0.024666	-0.550230
C	5.723211	-0.782000	-0.194322
C	2.834241	1.778297	-0.665296
C	2.110925	1.796307	-1.886185
C	0.973602	2.605596	-1.996209
C	0.525954	3.414399	-0.950762
C	1.252543	3.380085	0.243491
C	2.400774	2.593762	0.410149
C	2.565318	1.021000	-3.121442
C	1.450099	0.130120	-3.701922
C	3.174415	2.701448	1.724086
C	2.275956	2.549104	2.966576
C	-0.656395	4.362910	-1.106877
C	-0.210448	5.665860	-1.803601
O	5.872670	-2.096024	0.164014

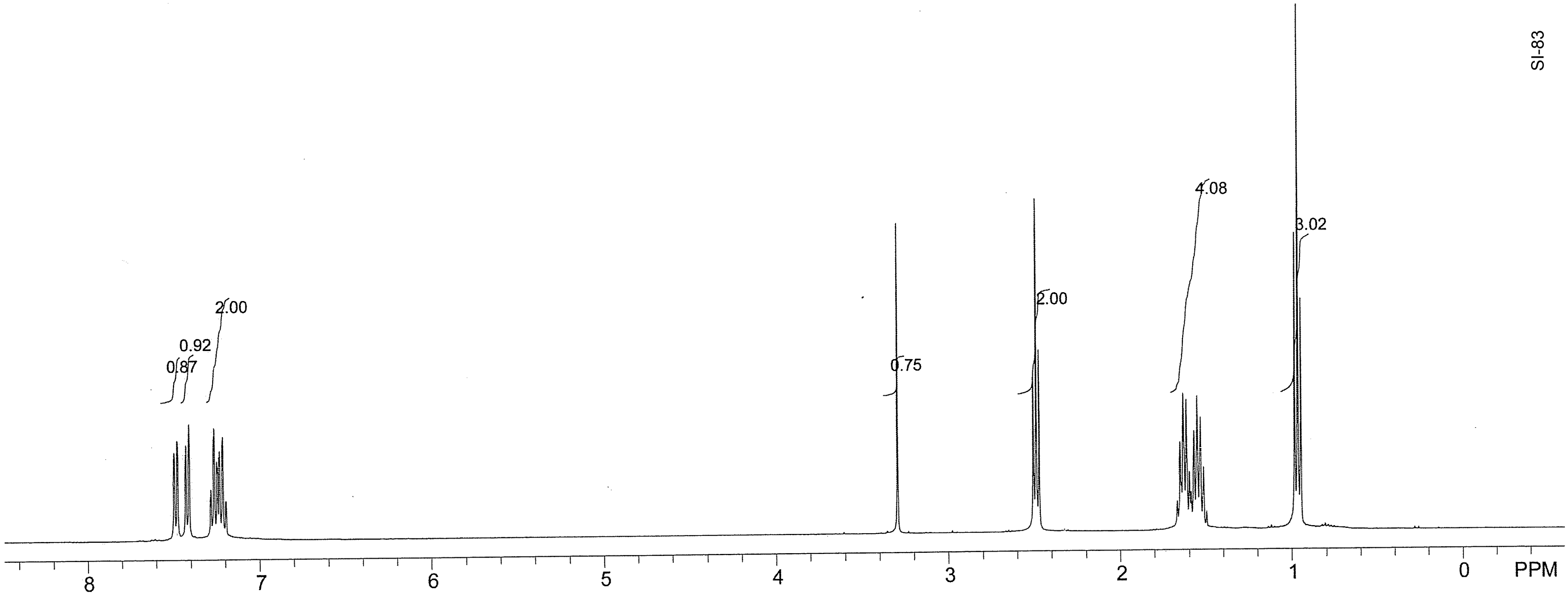
C	7.178428	-2.664820	0.168410
O	5.005434	3.137794	-1.371677
C	6.077606	3.974998	-1.788646
C	3.490828	-2.072241	2.012588
C	2.429282	-3.048845	2.562472
C	2.810840	-3.555511	3.965993
C	3.056757	-2.399954	4.944963
C	4.112405	-1.432292	4.395106
C	3.731244	-0.912261	2.998207
C	3.956496	4.029853	1.801097
C	-1.857231	3.738133	-1.837602
C	3.111695	1.977182	-4.202520
C	-7.933336	-0.936629	-2.563993
C	-8.998729	-0.405003	0.086641
H	-3.338467	-1.724669	-1.282660
H	-1.582286	-1.628934	-1.409860
H	-2.256765	-3.819046	-0.427031
H	-1.365557	-2.877988	0.784962
H	-3.131998	-2.988988	0.878373
H	-1.143580	3.577882	2.876167
H	-3.221919	4.732370	3.597439
H	-5.602991	1.839534	1.495629
H	-5.439329	3.843246	2.894299
H	3.795148	-3.652950	-0.295119
H	3.063875	-2.002443	-2.765846
H	4.697202	-2.242363	-2.153051
H	4.214325	-3.804637	-4.021726
H	4.533162	-4.683479	-2.530782
H	1.774691	-4.116641	-3.746107
H	2.569859	-5.685040	-3.659147
H	0.831989	-5.391660	-1.846593
H	2.438863	-5.669159	-1.184614
H	1.057182	-2.943209	-1.480742
H	1.286101	-3.821472	0.022339
H	4.431478	-2.615996	1.880241
H	1.453810	-2.542832	2.608025
H	2.310847	-3.907227	1.892108
H	2.018577	-4.215507	4.339751
H	3.719957	-4.169889	3.892369
H	2.115235	-1.855967	5.110263
H	3.368616	-2.790021	5.921164
H	4.246724	-0.582651	5.075663
H	5.084018	-1.944313	4.339142
H	2.817254	-0.308529	3.076254
H	4.519016	-0.250509	2.621216
H	7.428870	1.952521	-1.223855
H	7.811102	-0.358590	-0.537523
H	0.936422	4.025288	1.060101
H	0.439159	2.619509	-2.941136

H	3.388647	0.363013	-2.826650
H	1.837658	-0.473685	-4.531077
H	1.043964	-0.547481	-2.941589
H	0.616763	0.723857	-4.093983
H	3.501861	1.409656	-5.055736
H	2.324192	2.642733	-4.575130
H	3.916265	2.601964	-3.803701
H	3.905444	1.887399	1.749346
H	4.562129	4.066954	2.714436
H	4.617119	4.150394	0.938894
H	3.270902	4.885464	1.818694
H	2.888898	2.502800	3.874098
H	1.597040	3.402254	3.082343
H	1.668441	1.638560	2.919209
H	5.617994	4.924487	-2.066045
H	6.796337	4.143362	-0.976557
H	6.599512	3.555546	-2.658026
H	7.047482	-3.704563	0.471393
H	7.631371	-2.630324	-0.829691
H	7.832603	-2.155968	0.886516
H	-0.990245	4.629036	-0.094591
H	-2.703901	4.433889	-1.831309
H	-1.625665	3.520567	-2.886876
H	-2.179392	2.805409	-1.362460
H	-1.042859	6.376696	-1.864703
H	0.610669	6.147144	-1.261224
H	0.136185	5.463077	-2.824002
H	-8.930196	-1.306560	-2.827131
H	-7.873284	0.131145	-2.794353
H	-7.184965	-1.458657	-3.167553
H	-8.852699	-3.301617	-0.862159
H	-7.102461	-3.573533	-1.076699
H	-7.750800	-3.245665	0.540303
H	-9.952179	-0.801327	-0.278993
H	-8.923419	-0.586891	1.162870
H	-8.971803	0.675698	-0.081916

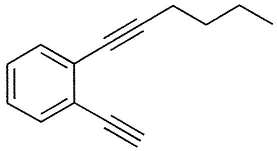
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-146-h.fid

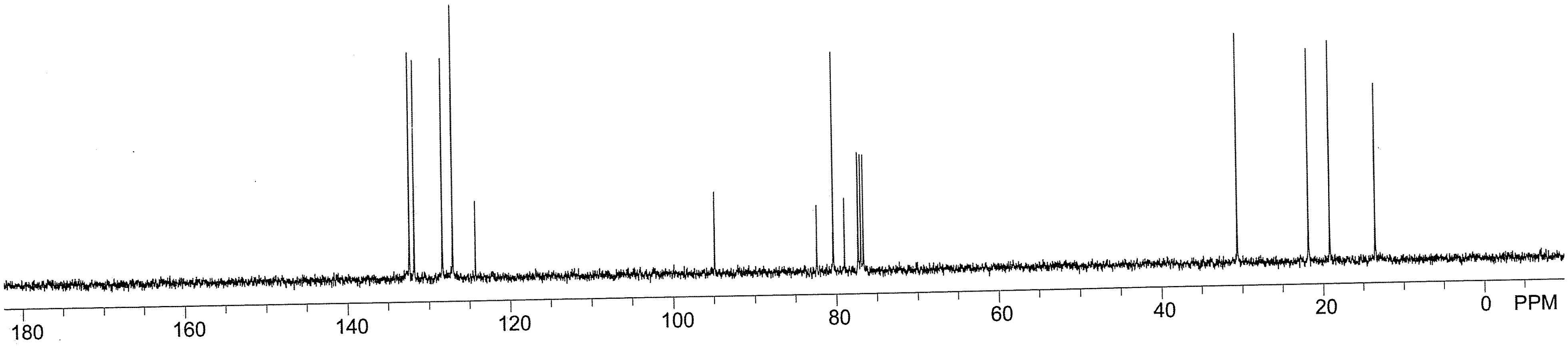
Apr 6 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 8
Solvent = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 0.24 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2006.7504 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -46.54
B = -28.31
C = 0.00

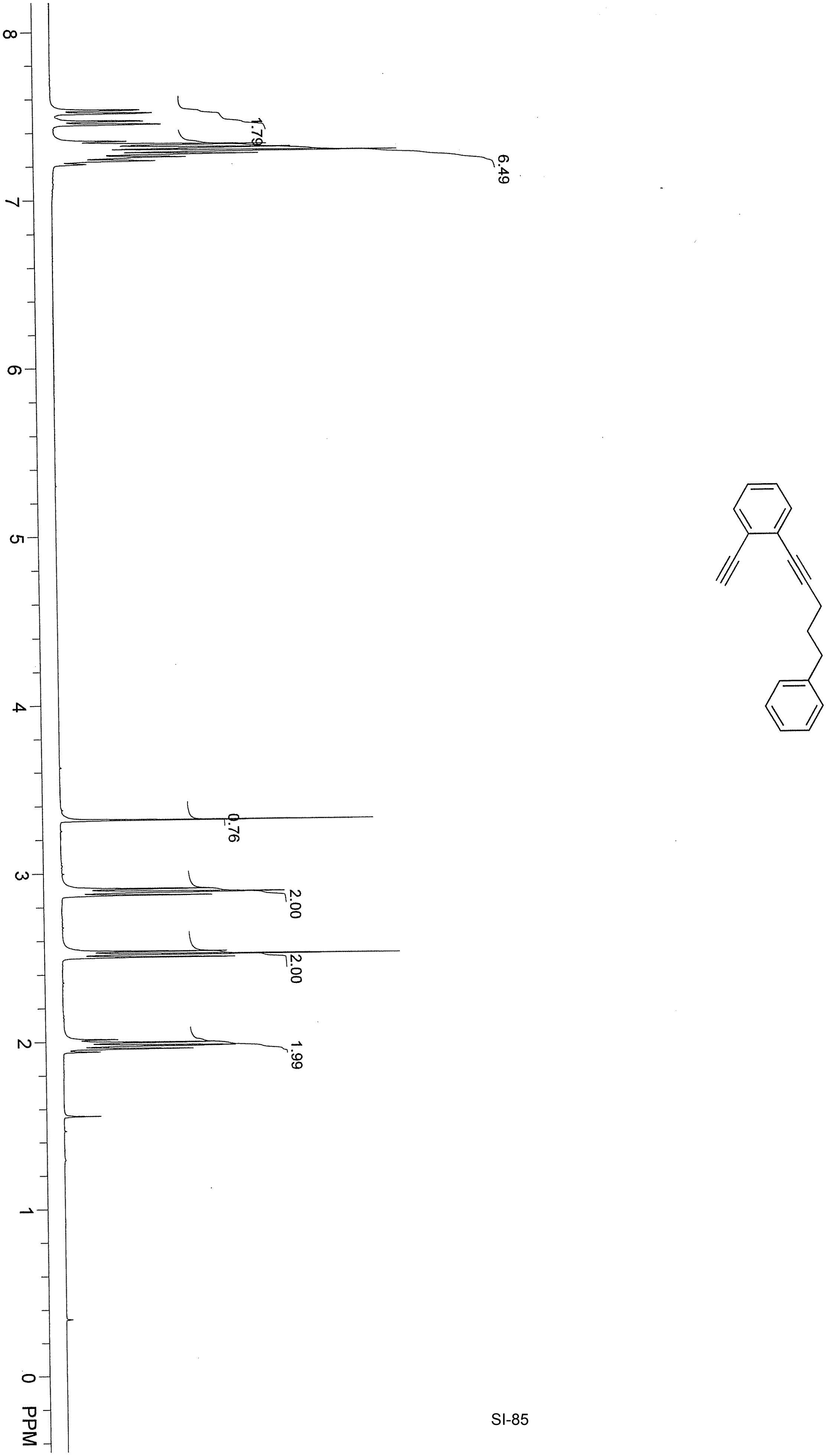




```
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-146-c1.fid
ylw-5-146-c
Apr  6 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length =    7.775 usec
Relaxation delay =    1.300 sec
NA  =    138
Solvent  = cdcl3
FID PTS1d = 28040
PTS1d = 32768
F1  =  100.577232 MHz
F2  =  399.950684 MHz
SW1 =   28040.66 Hz
AT1 =   1.00 sec
Hz per Pt 1stD =   0.86 Hz
SW2 =       1.00 Hz
Hz per Pt 2ndD =   1.00 Hz
O1  =   10049.5156 Hz
O2  =      -0.5000 Hz
LB1 = 2.00       Hz
TP    A = 99.84
     B = -5.63
     C =   0.00
```

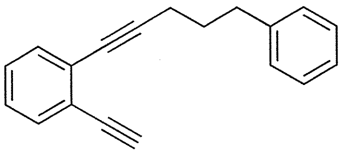


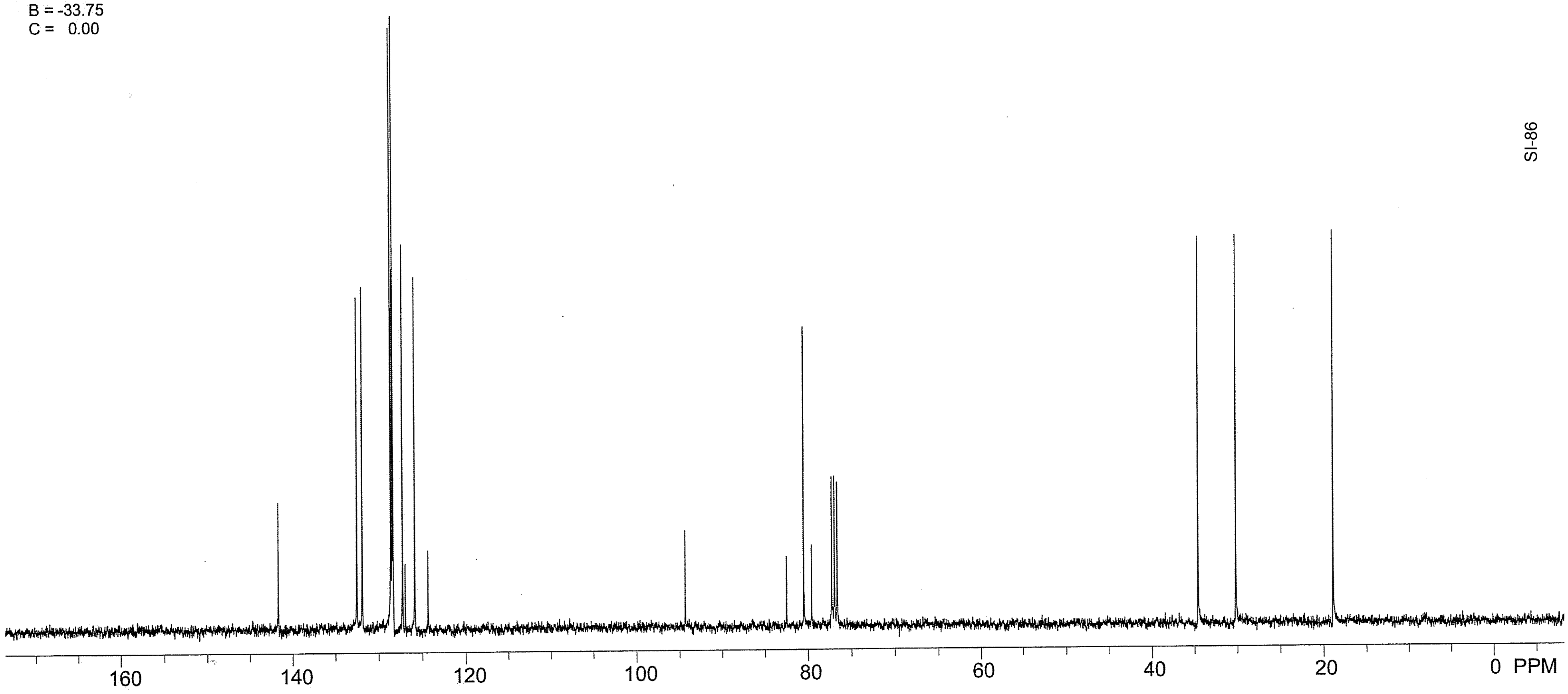



8
7
6
5
4
3
2
1
0
PPM
1.79
6.49
0.76
2.00
2.00
1.99

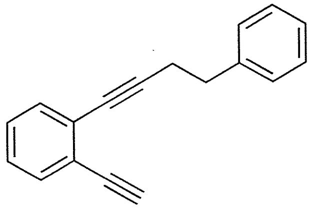
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-158-2-s-c1.fid

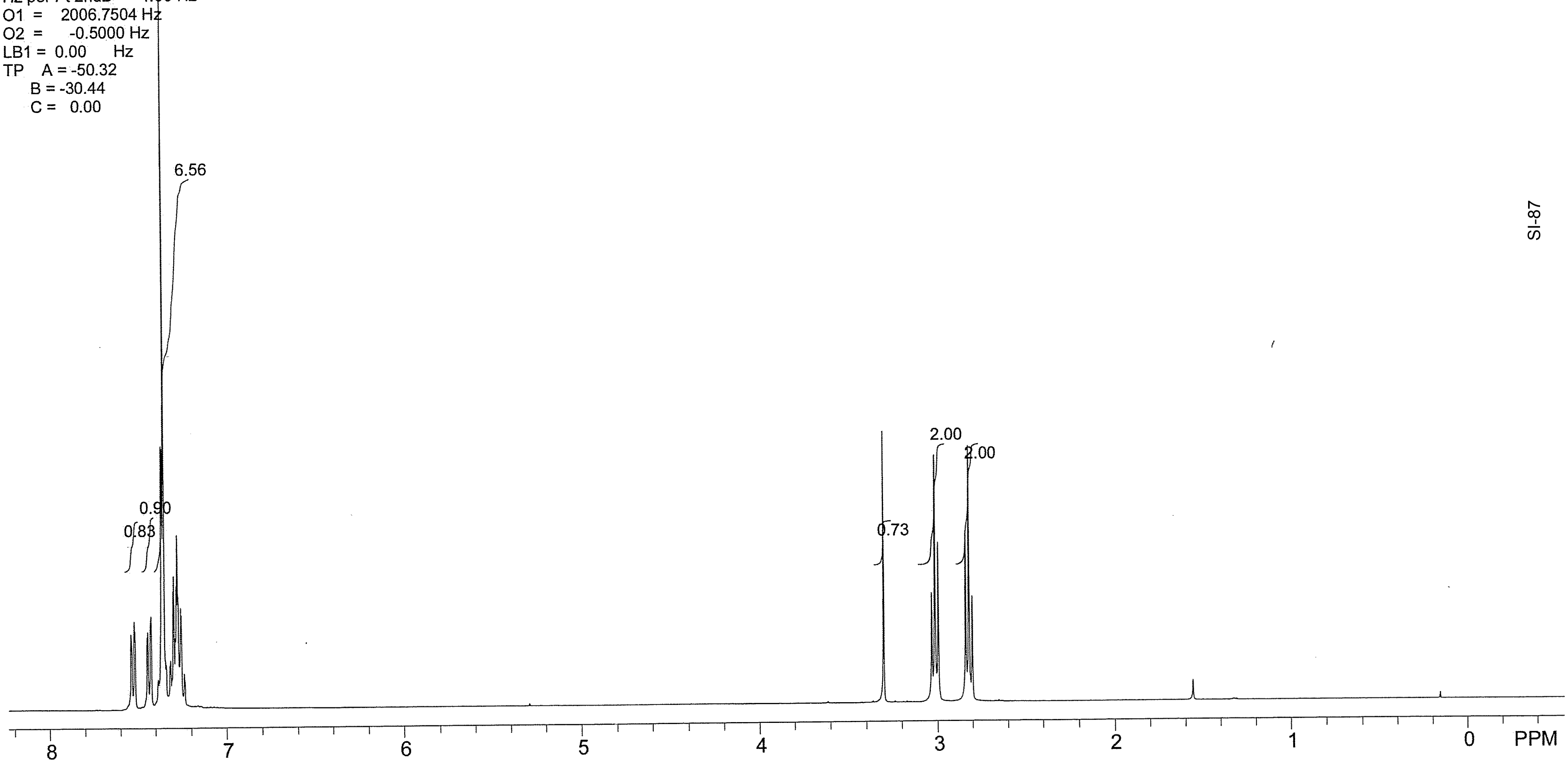
Apr 12 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 106
Solvent = cdcl3
FID PTS1d = 28040
PTS1d = 32768
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 28040.66 Hz
AT1 = 1.00 sec
Hz per Pt 1stD = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 10050.3711 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -7.50
B = -33.75
C = 0.00



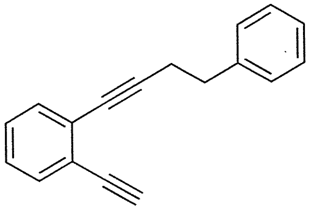


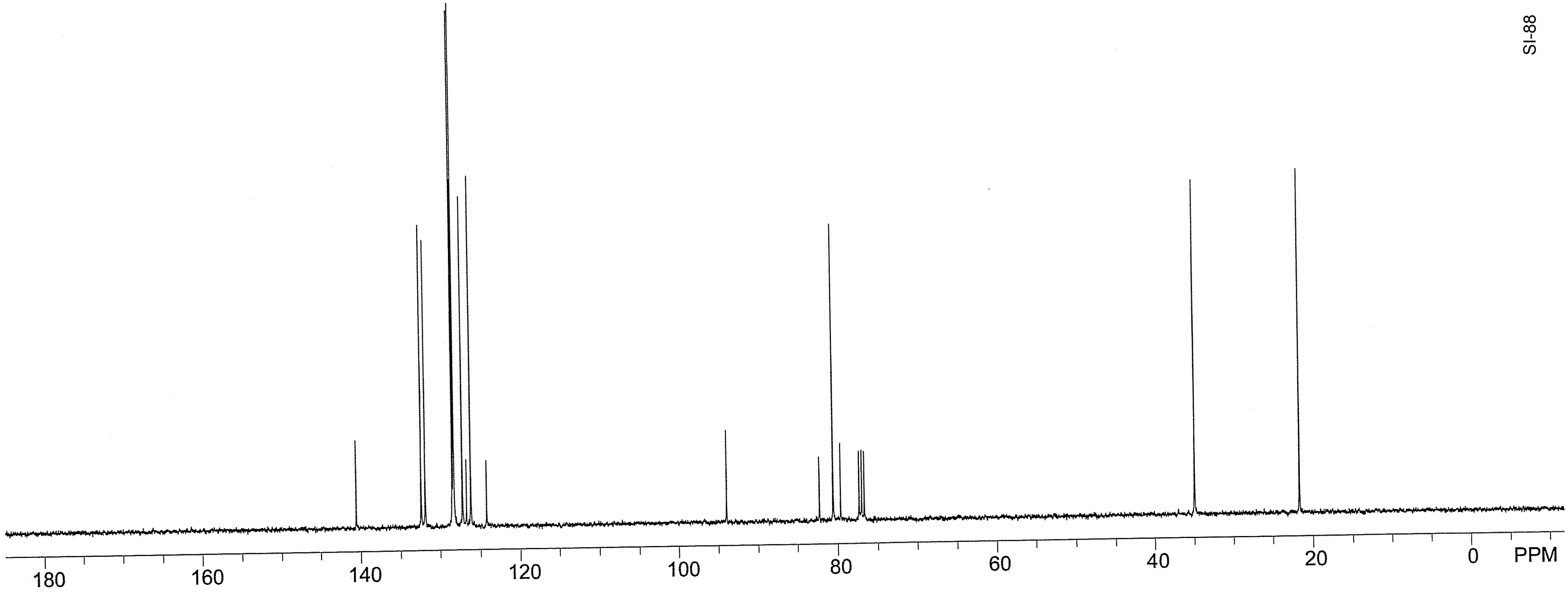
```
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-163-s-h.fid
new experiment
Apr 18 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length =   11.663 usec
Relaxation delay =    4.800 sec
NA =      8
Solvent  = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1  =  399.950684 MHz
F2  =  100.575279 MHz
SW1 =    8002.40 Hz
AT1 =   2.50 sec
Hz per Pt 1stD =   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 = -50.32
      B = -30.44
      C =   0.00
```





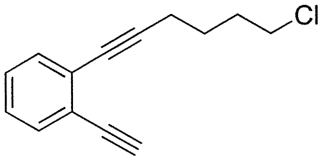
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-163-s-c.fid
ylw-5-163-s-c
Apr 18 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 106
Solvent = cdcl3
FID PTS1d = 28040
PTS1d = 32768
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 28040.66 Hz
AT1 = 1.00 sec
Hz per Pt 1stD = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 10044.3818 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -36.56
B = 15.47
C = 0.00

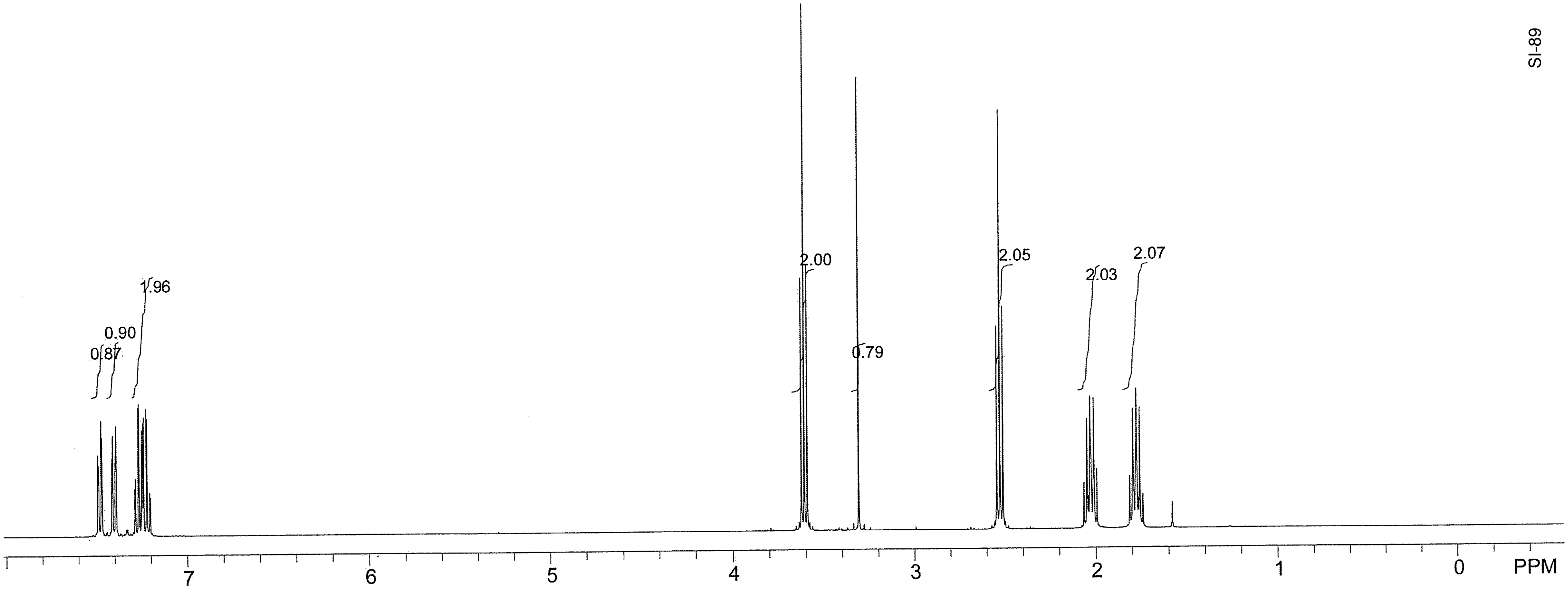




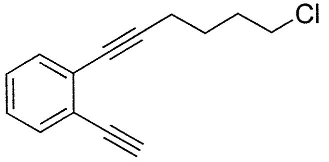
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-152-Cl-h.fid

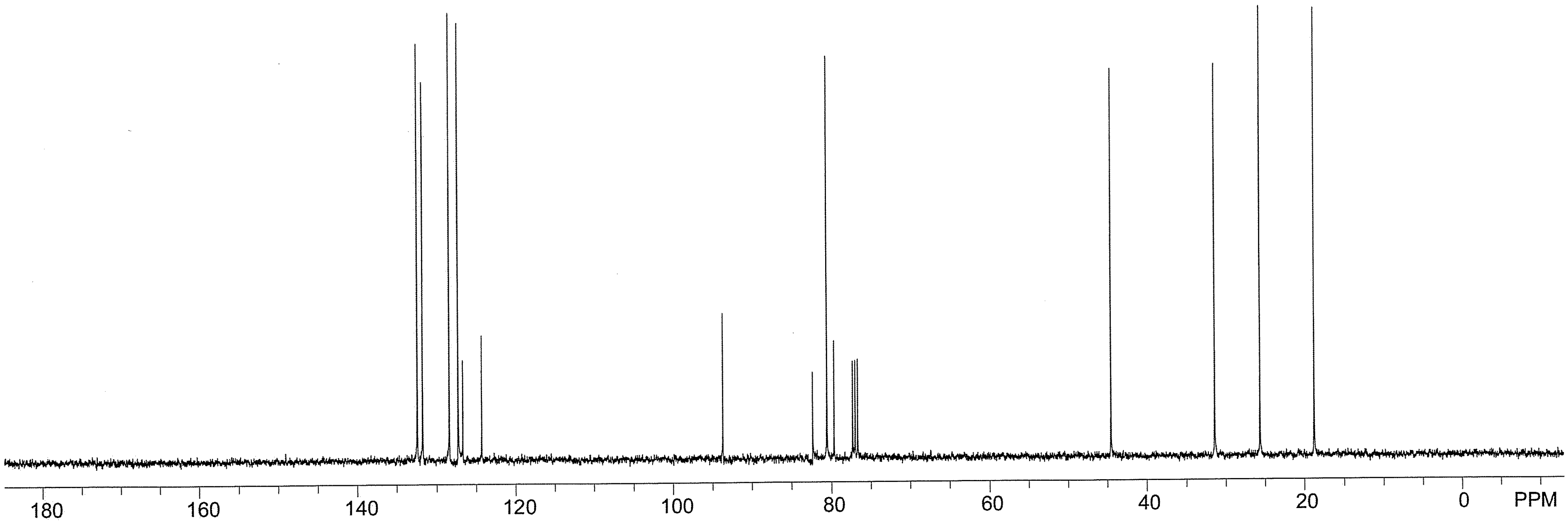
Apr 14 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 8
Solvent = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 0.24 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2006.2362 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -45.74
B = -36.00
C = 0.00



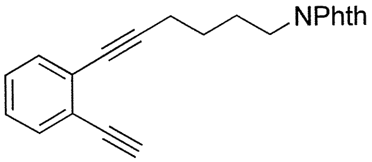


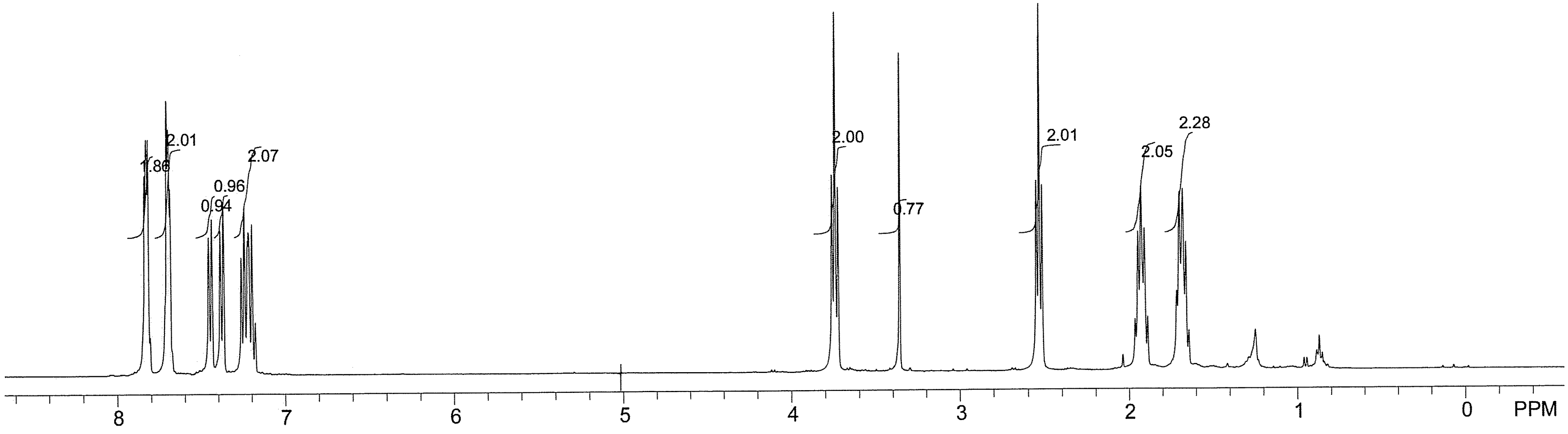
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-152-Cl-c1.fid
ylw-5-152-Cl-c
Apr 14 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 78
Solvent = cdcl3
FID PTS1d = 28040
PTS1d = 32768
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 28040.66 Hz
AT1 = 1.00 sec
Hz per Pt 1stD = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 10049.5156 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -36.09
B = 18.28
C = 0.00



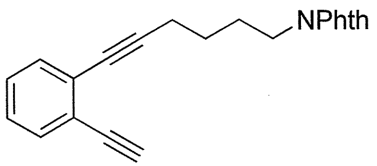


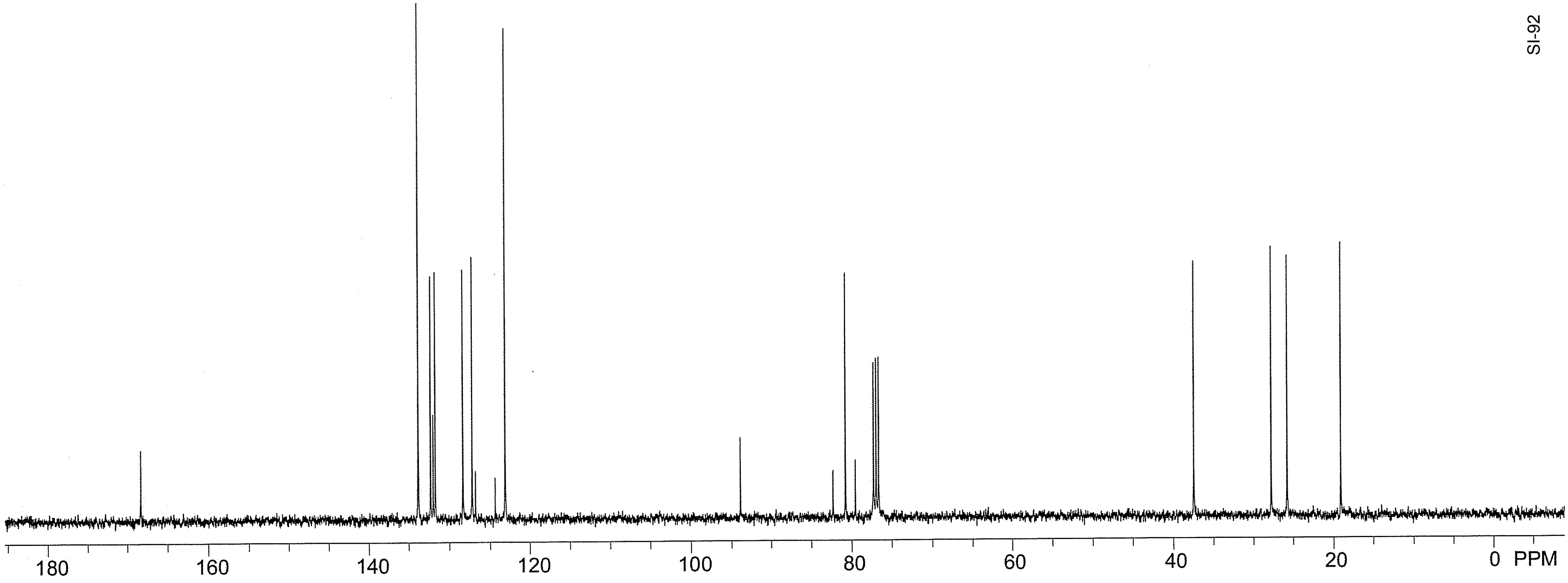
```
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-150-h.fid
new experiment
Apr  8 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length =   11.663 usec
Relaxation delay =    4.800 sec
NA =     14
Solvent  = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1  =  399.950684 MHz
F2  =  100.575279 MHz
SW1 =    8002.40 Hz
AT1 =   2.50 sec
Hz per Pt 1stD =   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 = -49.99
      B = -36.87
      C =   0.00
```



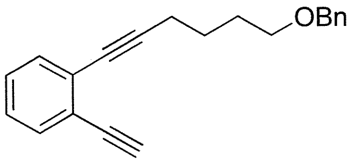


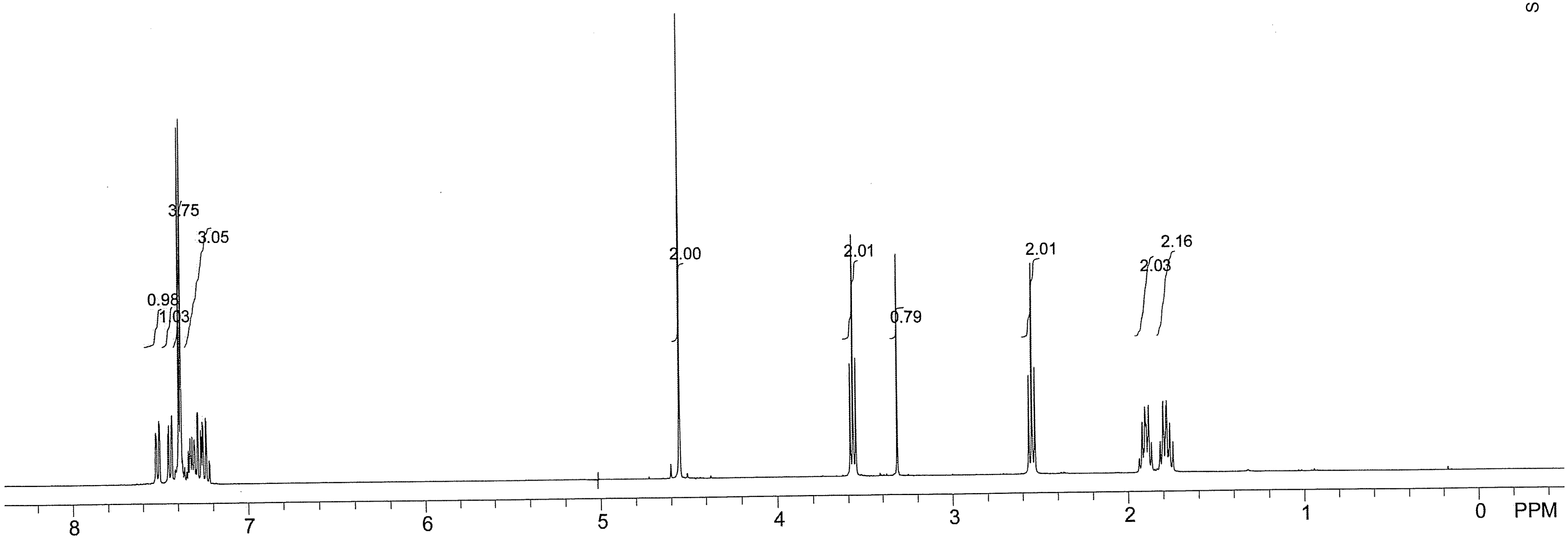
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-150-c1.fid
ylw-5-150-c
Apr 8 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 160
Solvent = cdcl3
FID PTS1d = 28040
PTS1d = 32768
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 28040.66 Hz
AT1 = 1.00 sec
Hz per Pt 1stD = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 10052.0830 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -22.03
B = -1.41
C = 0.00



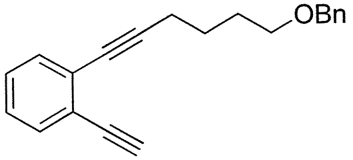


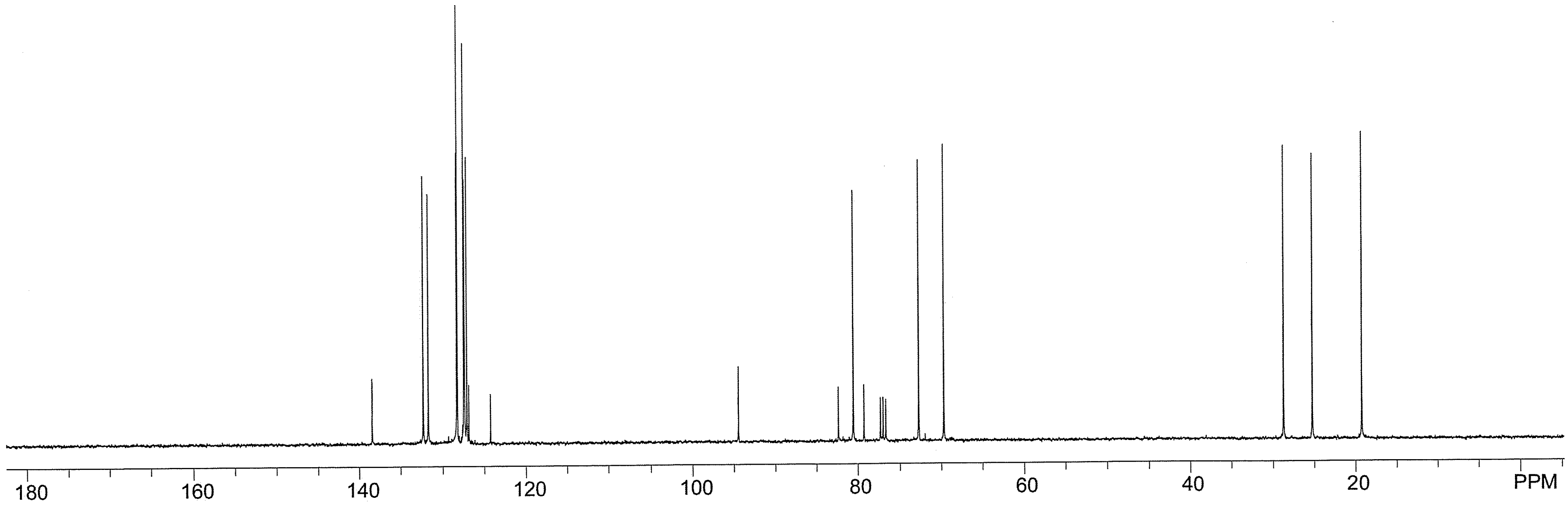
```
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-191-OBn.fid

May  6 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length =   11.663 usec
Relaxation delay =    4.800 sec
NA =      6
Solvent  = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1  =  399.950684 MHz
F2  =  100.575279 MHz
SW1 =    8002.40 Hz
AT1 =   2.50 sec
Hz per Pt 1stD =   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 = -37.27
      B = -44.73
      C =   0.00
```



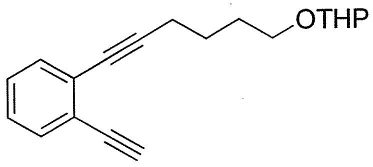


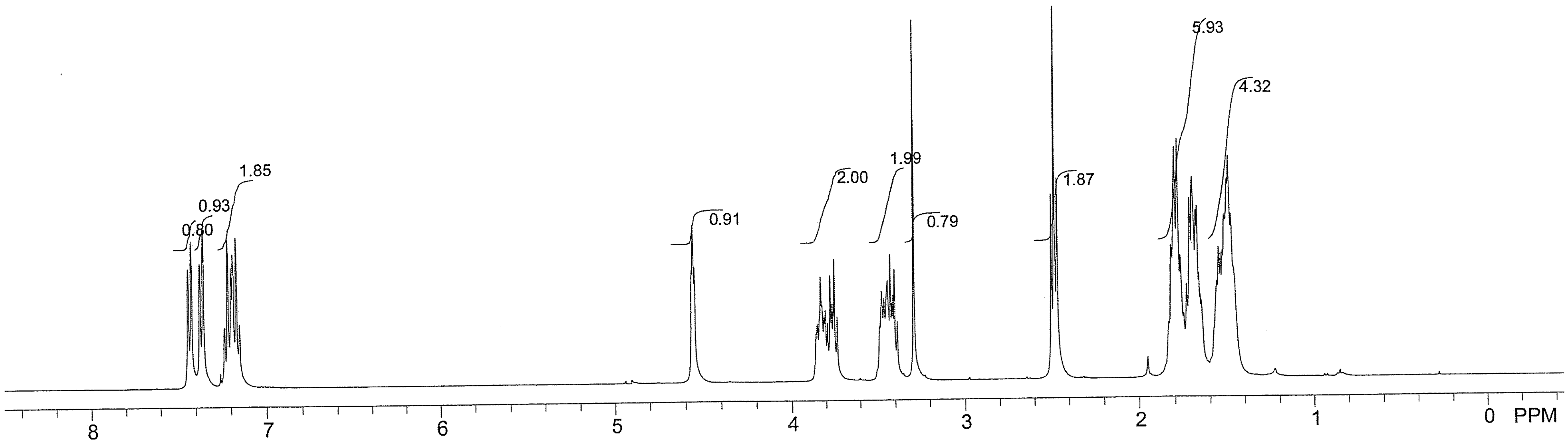
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-191-OBn-c1.fid
Standard c13 run using qnp probe
May 6 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 128
Solvent = cdcl3
FID PTS1d = 28040
PTS1d = 32768
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 28040.66 Hz
AT1 = 1.00 sec
Hz per Pt 1stD = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 10039.2451 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -37.50
B = 4.22
C = 0.00



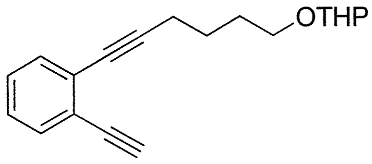


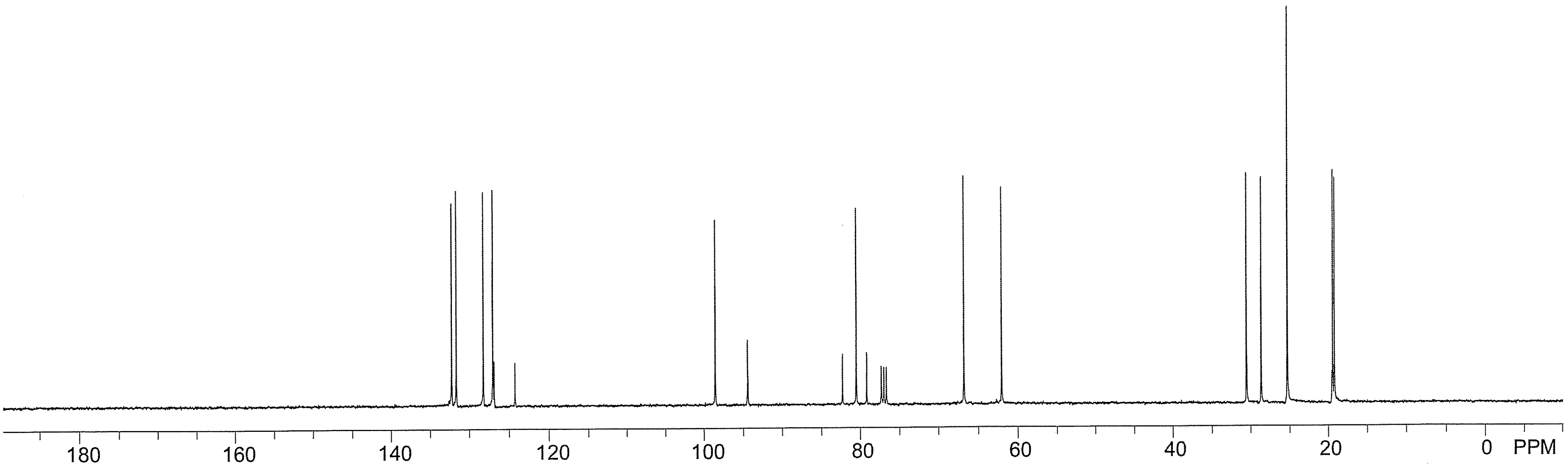
```
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-298-THP-s-h.fid
new experiment
Jun  1 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length =   11.663 usec
Relaxation delay =    4.800 sec
NA  =     8
Solvent  = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1  =  399.950684 MHz
F2  =  100.575279 MHz
SW1 =    8002.40 Hz
AT1 =   2.50 sec
Hz per Pt 1stD =   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 = -44.83
      B = -33.79
      C =   0.00
```



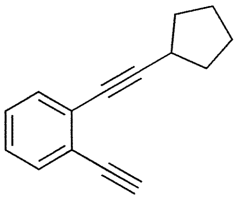


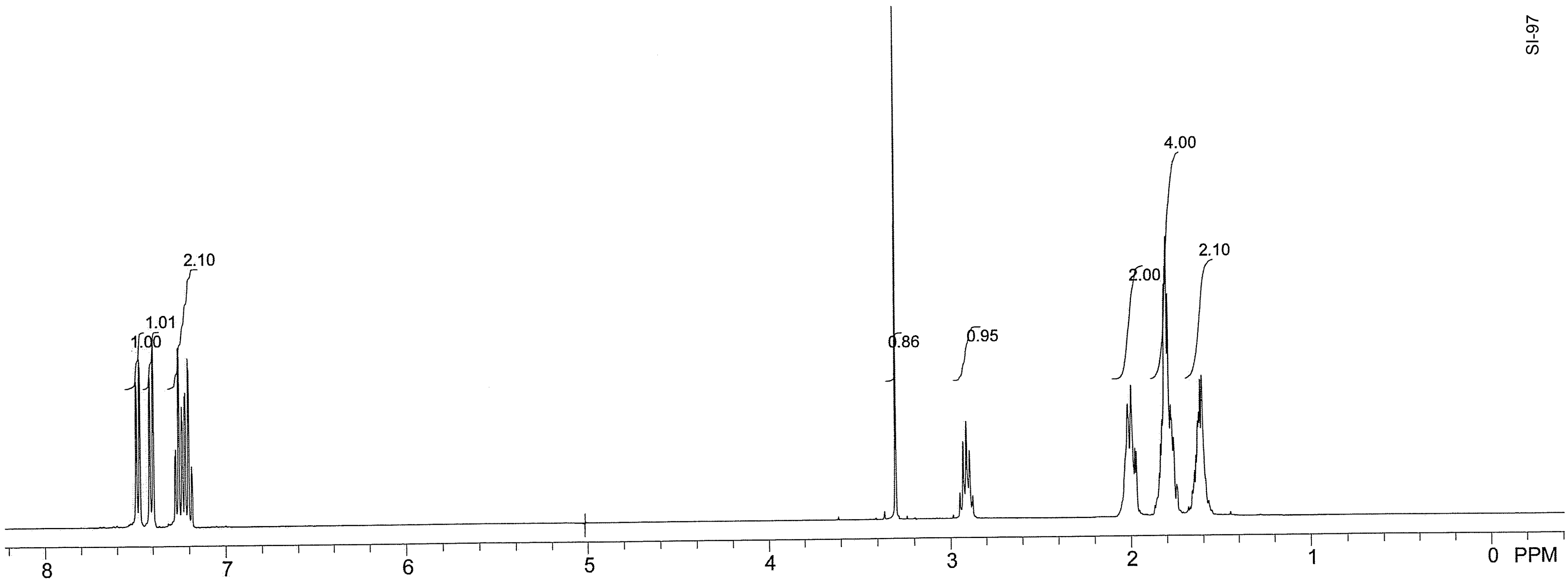
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-298-THP-s-c2.fid
Standard c13 run using qnp probe
Jun 1 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 112
Solvent = cdcl3
FID PTS1d = 28040
PTS1d = 32768
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 28040.66 Hz
AT1 = 1.00 sec
Hz per Pt 1stD = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 10043.5234 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -13.13
B = -16.88
C = 0.00



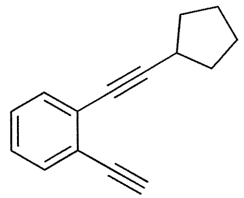


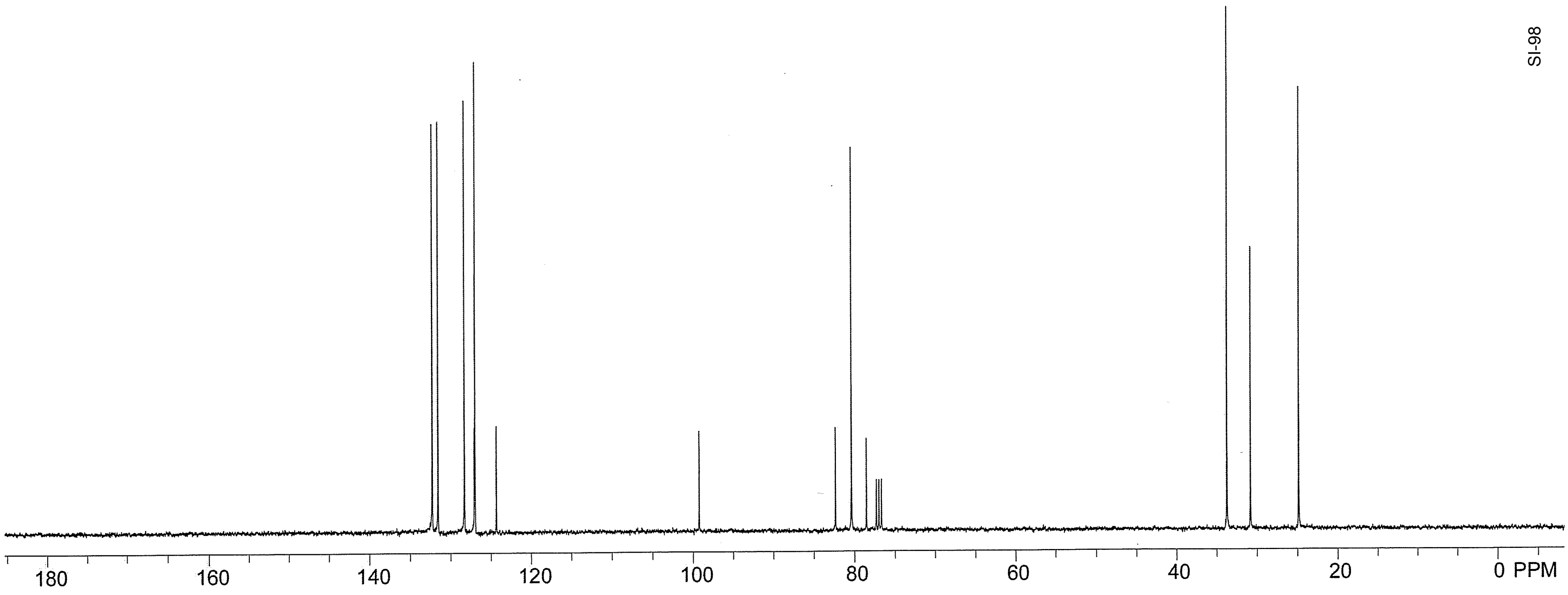
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-216-h1.fid
new experiment
May 21 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 6
Solvent = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 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 = -38.53
B = -45.16
C = 0.00



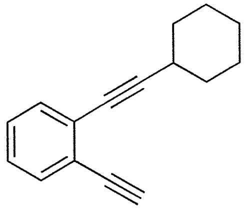


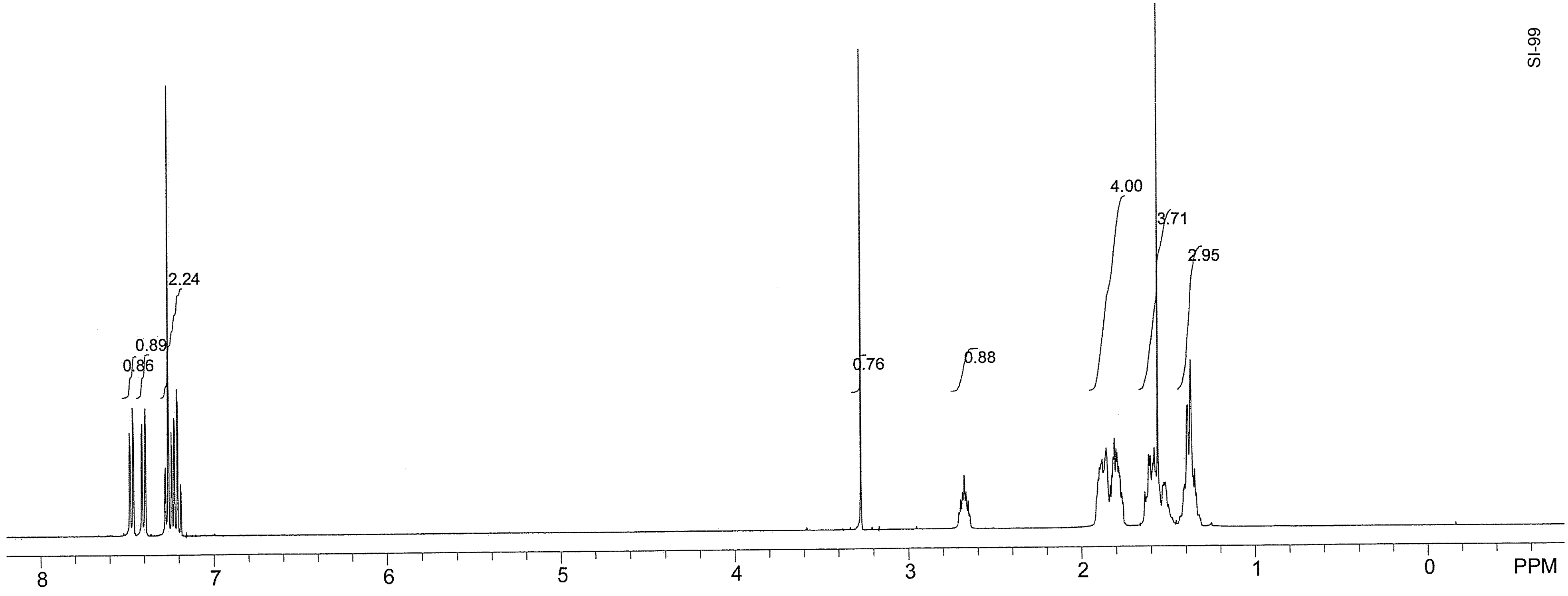
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-216-c1.fid
Standard c13 run using qnp probe
May 21 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 76
Solvent = cdcl3
FID PTS1d = 28040
PTS1d = 32768
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 28040.66 Hz
AT1 = 1.00 sec
Hz per Pt 1stD = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 10046.9473 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -20.63
B = -11.25
C = 0.00



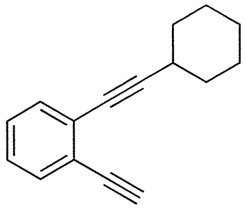


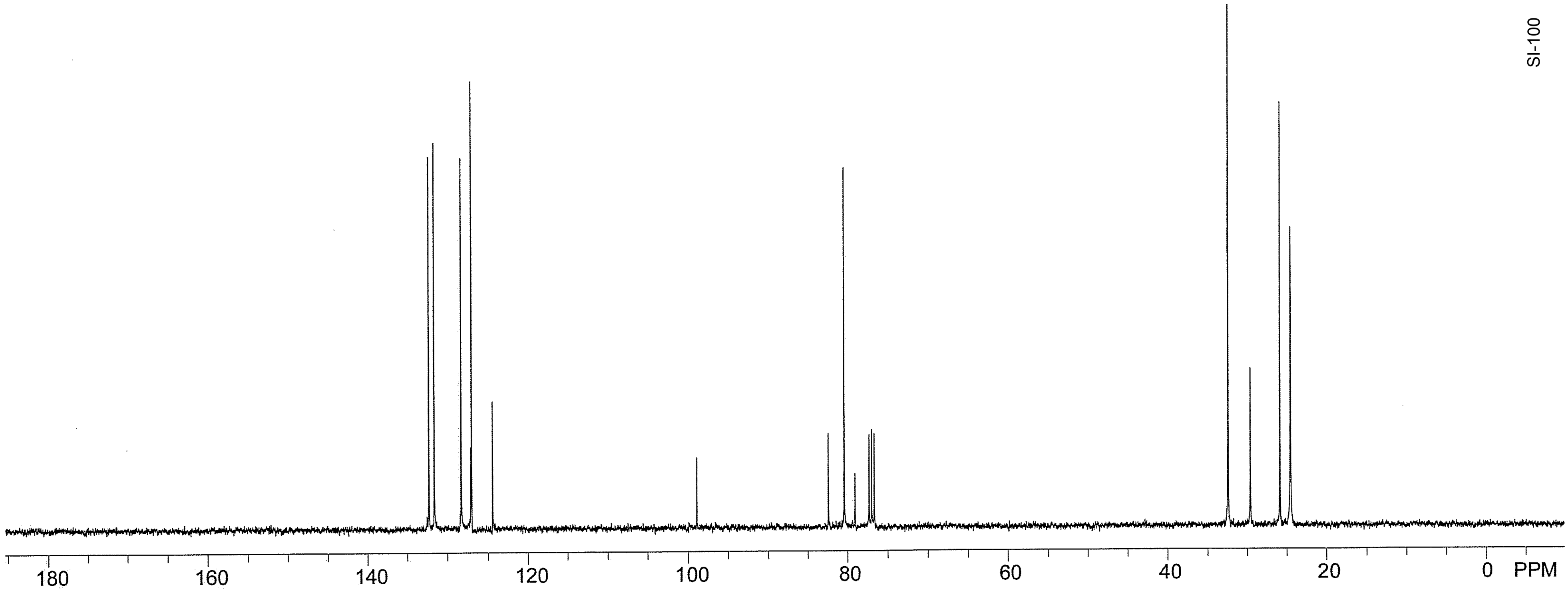
```
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-217-hh.fid
new experiment
May 20 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length =   11.663 usec
Relaxation delay =    4.800 sec
NA  =     16
Solvent  = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1  =  399.950684 MHz
F2  =  100.575279 MHz
SW1 =    8002.40 Hz
AT1 =   2.50 sec
Hz per Pt 1stD =   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 = -43.93
      B = -37.63
      C =   0.00
```



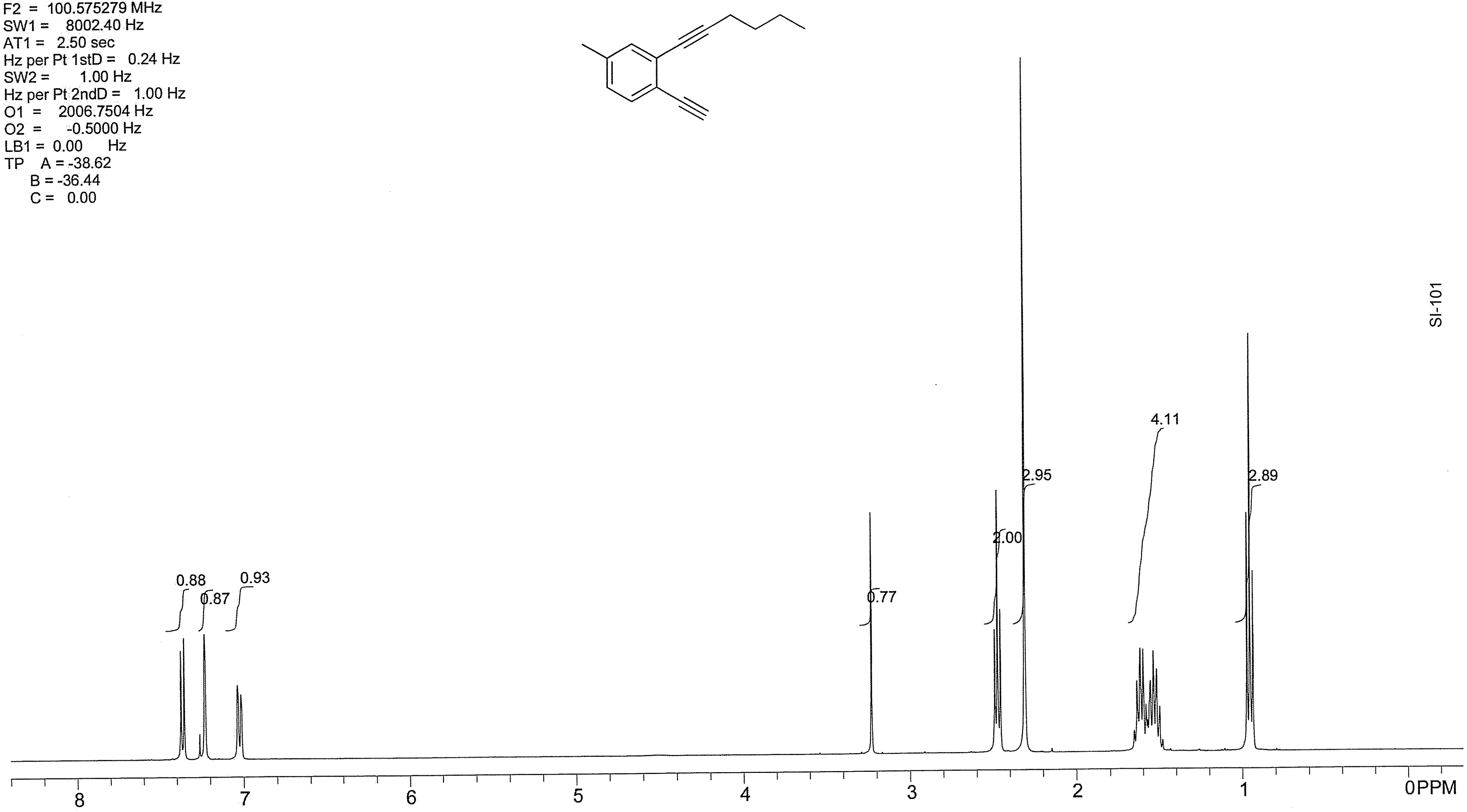


C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-217-s-c1.fid
Standard c13 run using qnp probe
May 20 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 102
Solvent = cdcl3
FID PTS1d = 28040
PTS1d = 32768
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 28040.66 Hz
AT1 = 1.00 sec
Hz per Pt 1stD = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 10052.0820 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -26.72
B = 5.63
C = 0.00

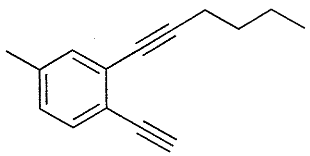


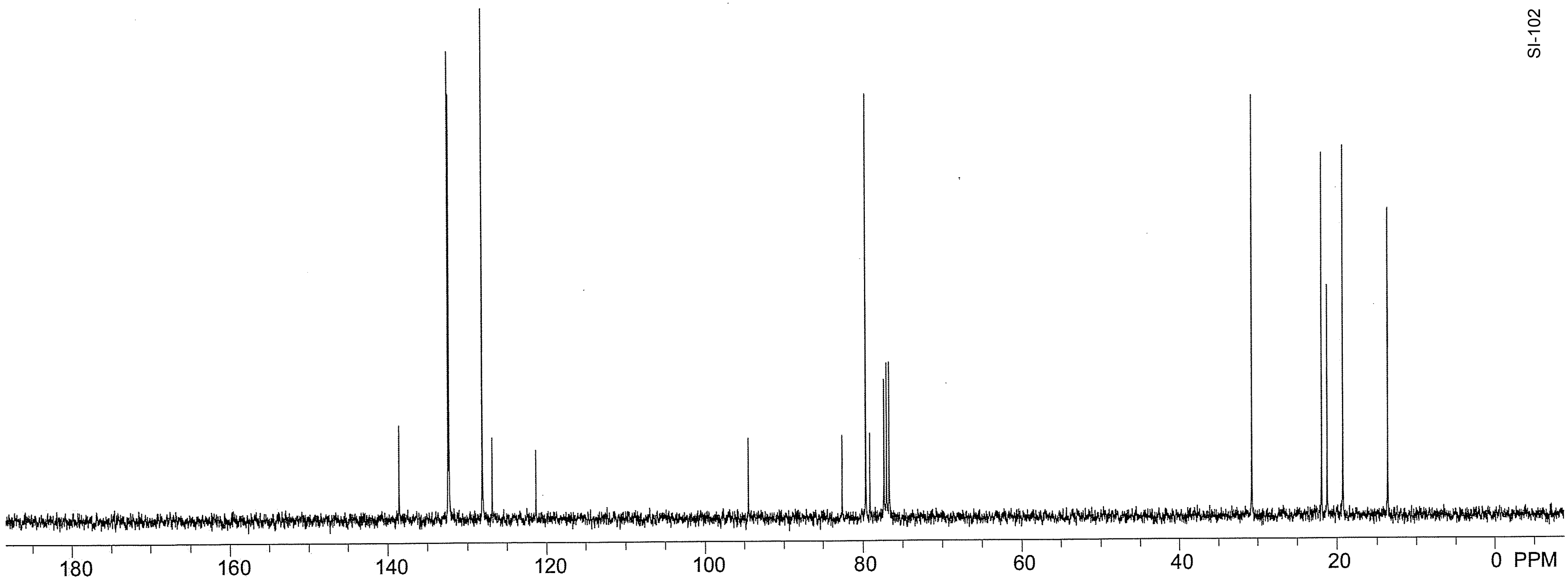


C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-220-h-1.fid
new experiment
May 27 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 8
Solvent = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 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 = -38.62
B = -36.44
C = 0.00

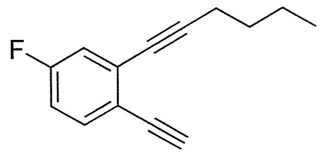


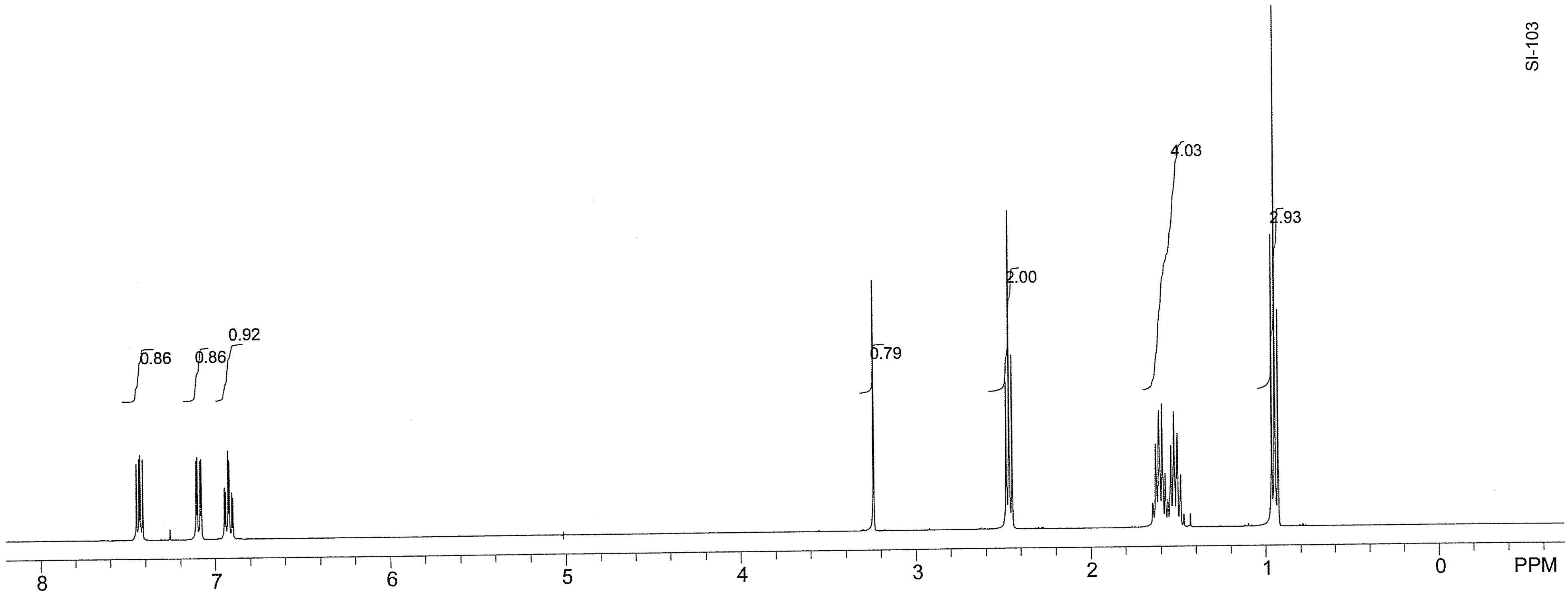
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-220-c2.fid
Standard c13 run using qnp probe
May 27 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 116
Solvent = cdcl3
FID PTS1d = 28040
PTS1d = 32768
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 28040.66 Hz
AT1 = 1.00 sec
Hz per Pt 1stD = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 10055.5039 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -63.75
B = 39.38
C = 0.00



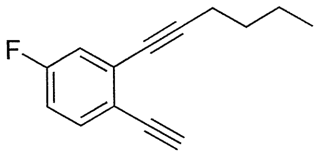


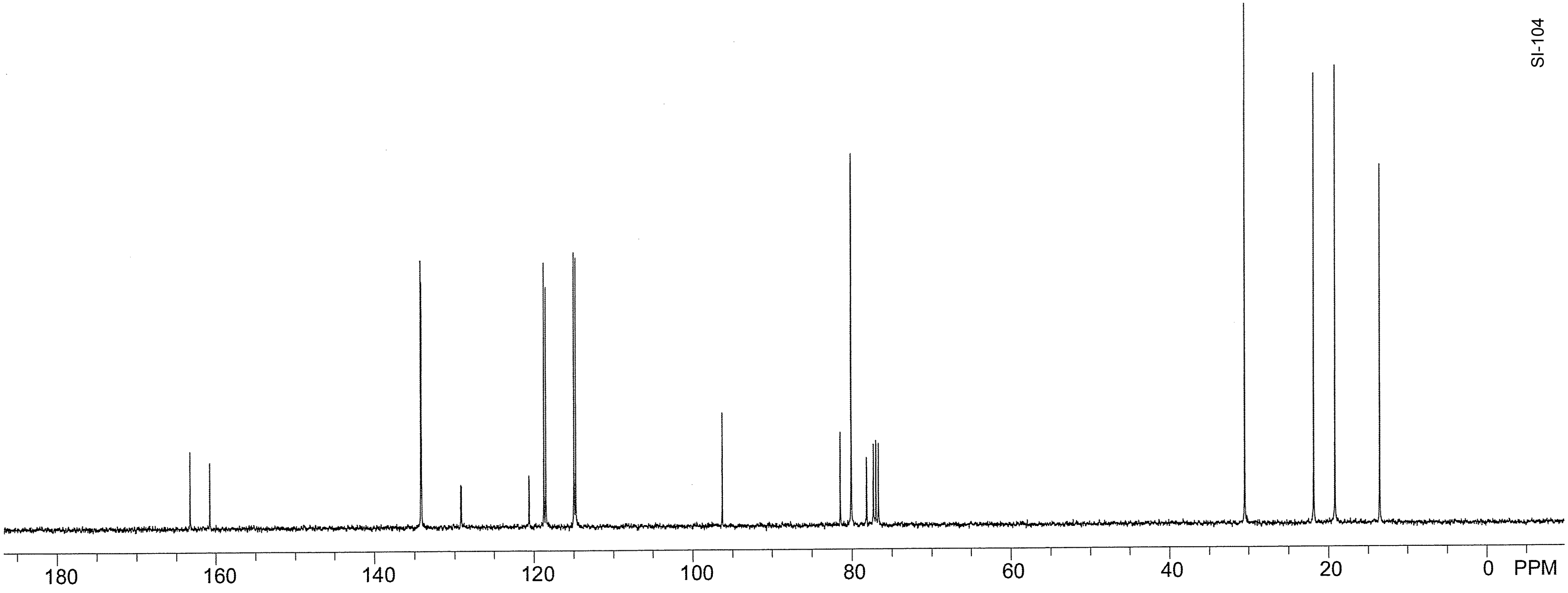
```
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-208-h.fid
new experiment
May 16 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length =   11.663 usec
Relaxation delay =    4.800 sec
NA =     12
Solvent  = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1  =  399.950684 MHz
F2  =  100.575279 MHz
SW1 =    8002.40 Hz
AT1 =   2.50 sec
Hz per Pt 1stD =   0.24 Hz
SW2 =        1.00 Hz
Hz per Pt 2ndD =   1.00 Hz
O1  =    2006.2362 Hz
O2  =      -0.5000 Hz
LB1 =  0.00      Hz
TP    A = -45.44
      B = -28.81
      C =   0.00
```



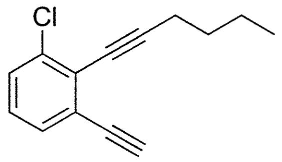


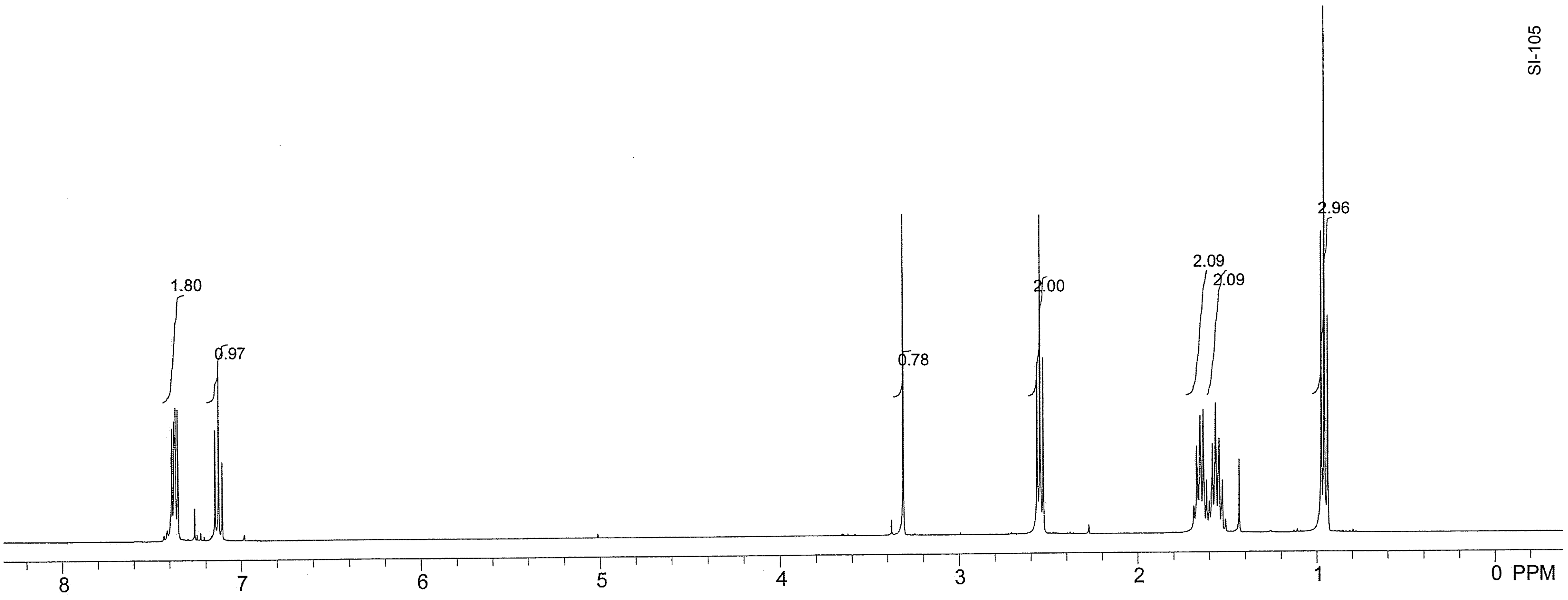
```
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-208-c1.fid
Standard c13 run using qnp probe
May 16 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length =    7.775 usec
Relaxation delay =    1.300 sec
NA  =    146
Solvent  = cdcl3
FID PTS1d = 28040
PTS1d = 32768
F1  =  100.577232 MHz
F2  =  399.950684 MHz
SW1 =   28040.66 Hz
AT1 =   1.00 sec
Hz per Pt 1stD =   0.86 Hz
SW2 =        1.00 Hz
Hz per Pt 2ndD =   1.00 Hz
O1  =    10053.7930 Hz
O2  =       -0.5000 Hz
LB1 =  2.00      Hz
TP    A = -37.97
      B =  18.28
      C =   0.00
```



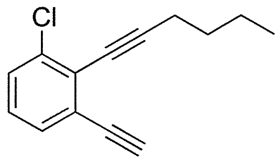


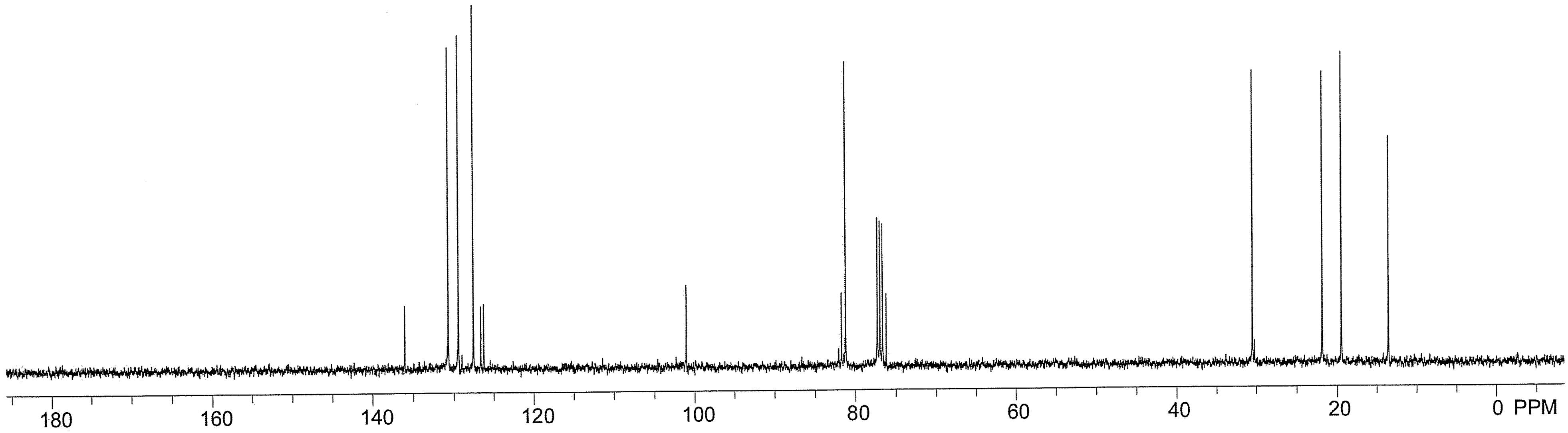
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-211-Cl-s-h.fid
new experiment
May 23 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 12
Solvent = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 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 = -50.77
B = -27.39
C = 0.00



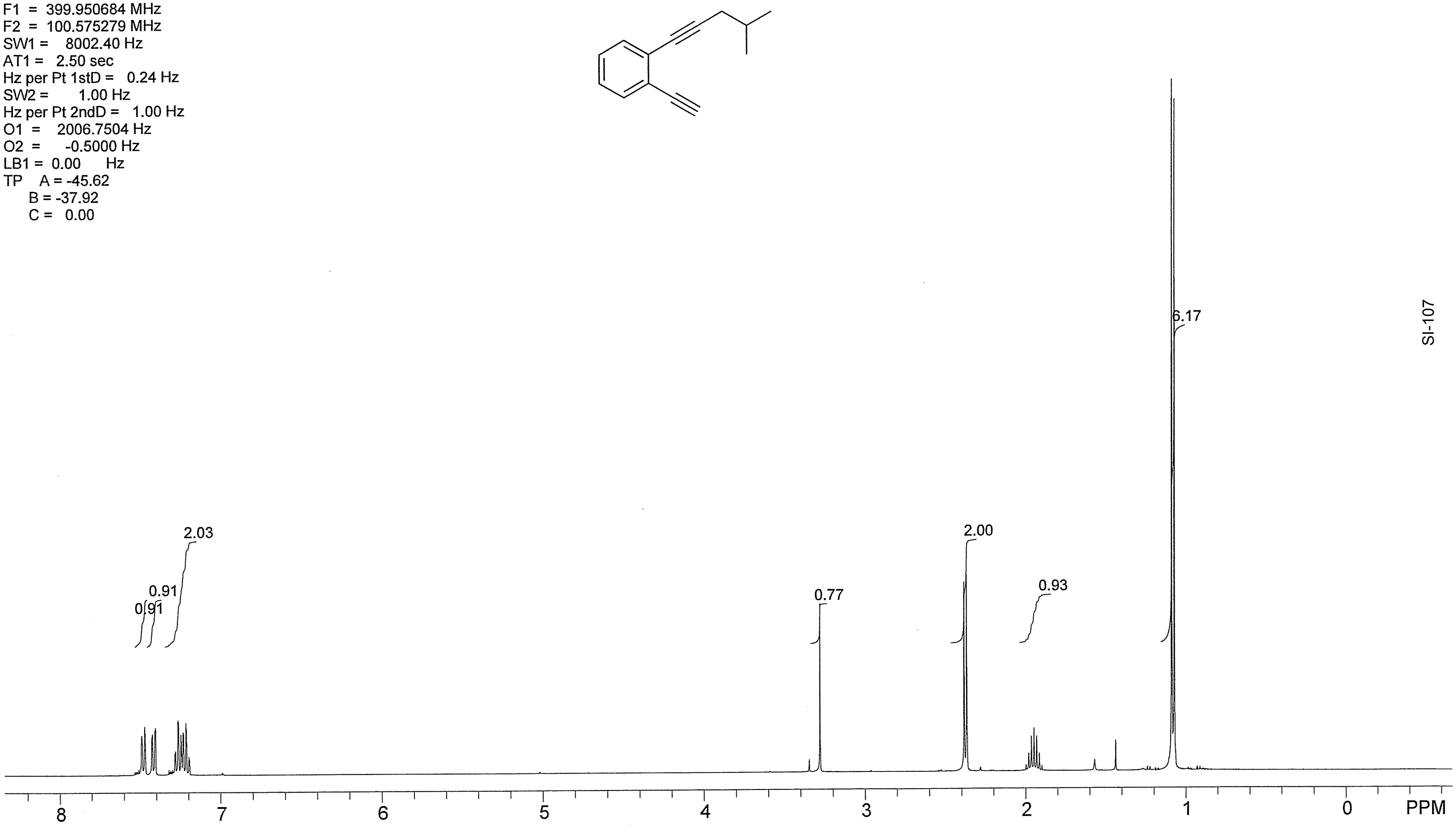


```
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-211-Cl-s-c1.fid
Standard c13 run using qnp probe
May 23 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length =   7.775 usec
Relaxation delay =   1.300 sec
NA =   154
Solvent = cdcl3
FID PTS1d = 28040
PTS1d = 32768
F1 =  100.577232 MHz
F2 =  399.950684 MHz
SW1 =  28040.66 Hz
AT1 =  1.00 sec
Hz per Pt 1stD =  0.86 Hz
SW2 =      1.00 Hz
Hz per Pt 2ndD =  1.00 Hz
O1 =  10054.6484 Hz
O2 =     -0.5000 Hz
LB1 = 2.00     Hz
TP   A = -31.41
     B =  12.66
     C =   0.00
```

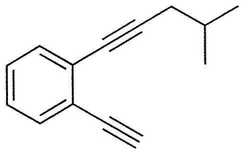


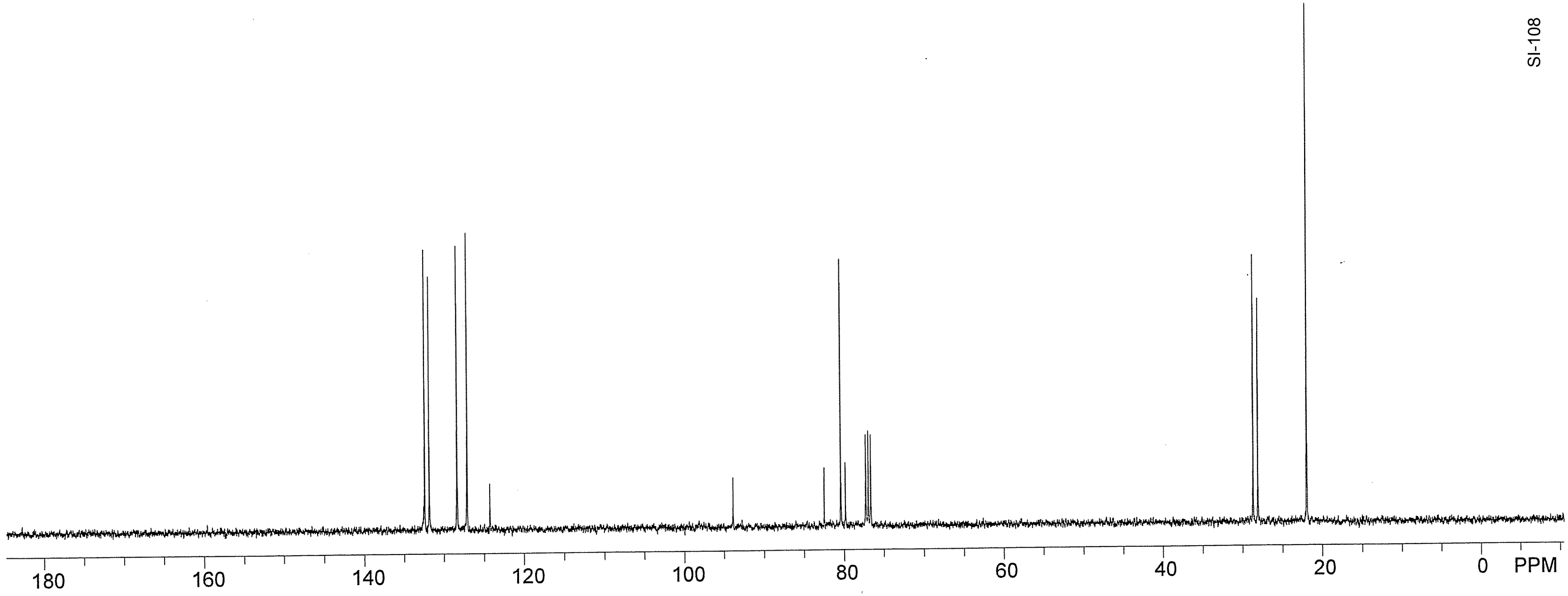


C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-295-s-h.fid
new experiment
Jun 11 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 12
Solvent = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 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 = -45.62
B = -37.92
C = 0.00

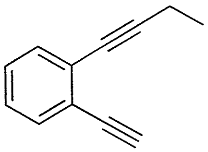


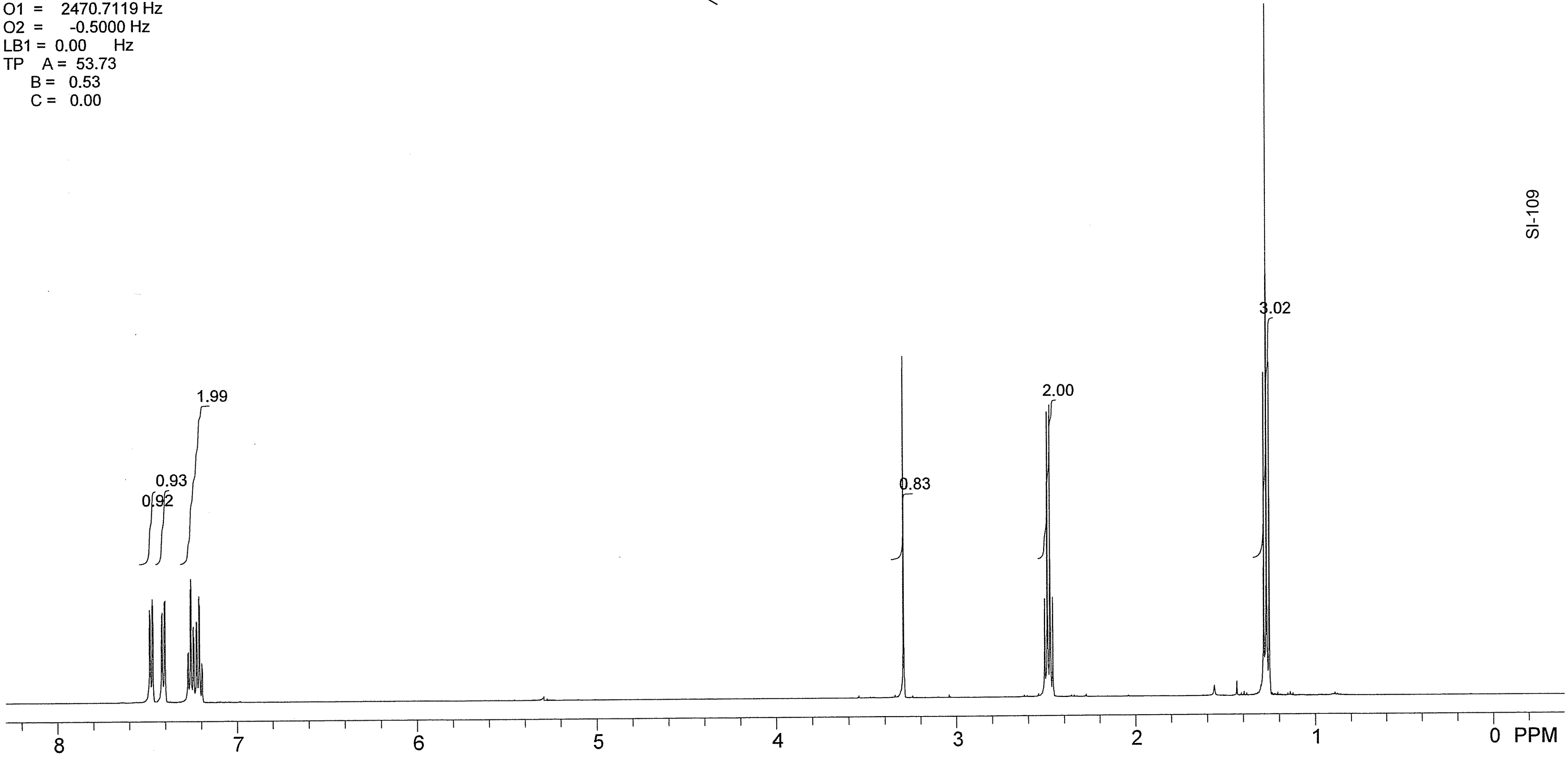
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-295-s-c2.fid
Standard c13 run using qnp probe
Jun 11 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 102
Solvent = cdcl3
FID PTS1d = 28040
PTS1d = 32768
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 28040.66 Hz
AT1 = 1.00 sec
Hz per Pt 1stD = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 10053.7930 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -31.88
B = 11.25
C = 0.00



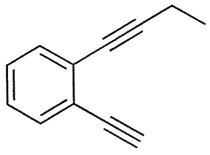


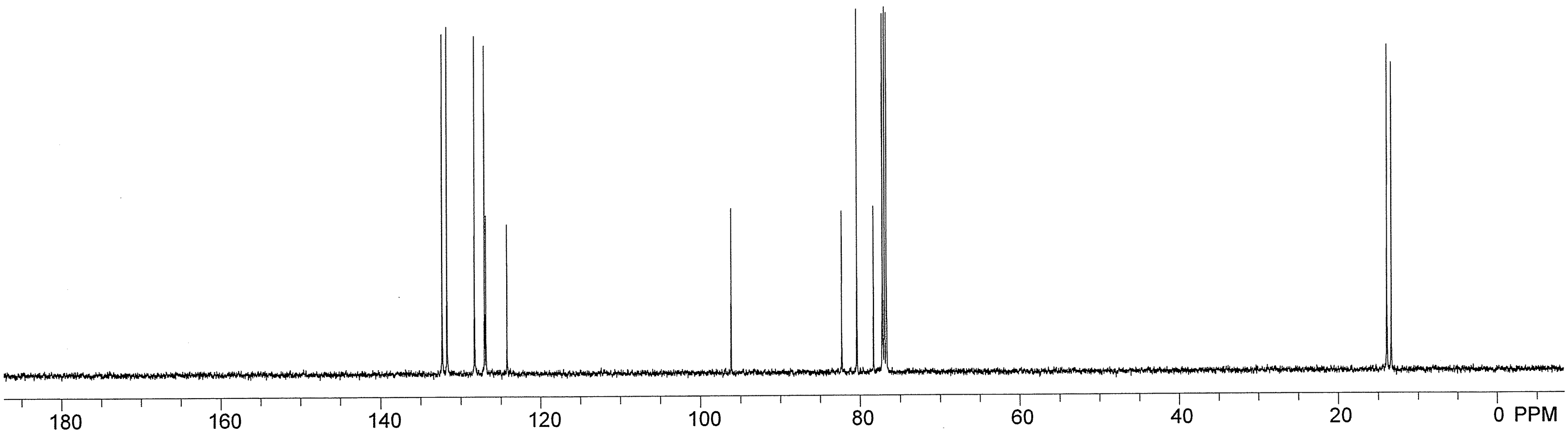
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-238-s.fid
STANDARD PROTON PARAMETERS
Jun 9 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.912 usec
Relaxation delay = 4.800 sec
NA = 16
Solvent = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1 = 499.858521 MHz
F2 = 125.700813 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 0.24 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2470.7119 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = 53.73
B = 0.53
C = 0.00





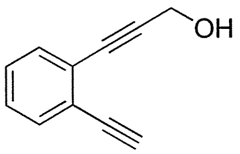
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-238-s-c1.fid
STANDARD CARBON PARAMETERS
Jun 9 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 6.000 usec
Relaxation delay = 3.000 sec
NA = 90
Solvent = cdcl3
FID PTS1d = 36749
PTS1d = 65536
F1 = 125.701683 MHz
F2 = 499.858551 MHz
SW1 = 28258.57 Hz
AT1 = 1.30 sec
Hz per Pt 1stD = 0.43 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 12766.0713 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = 61.88
B = 167.34
C = 0.00

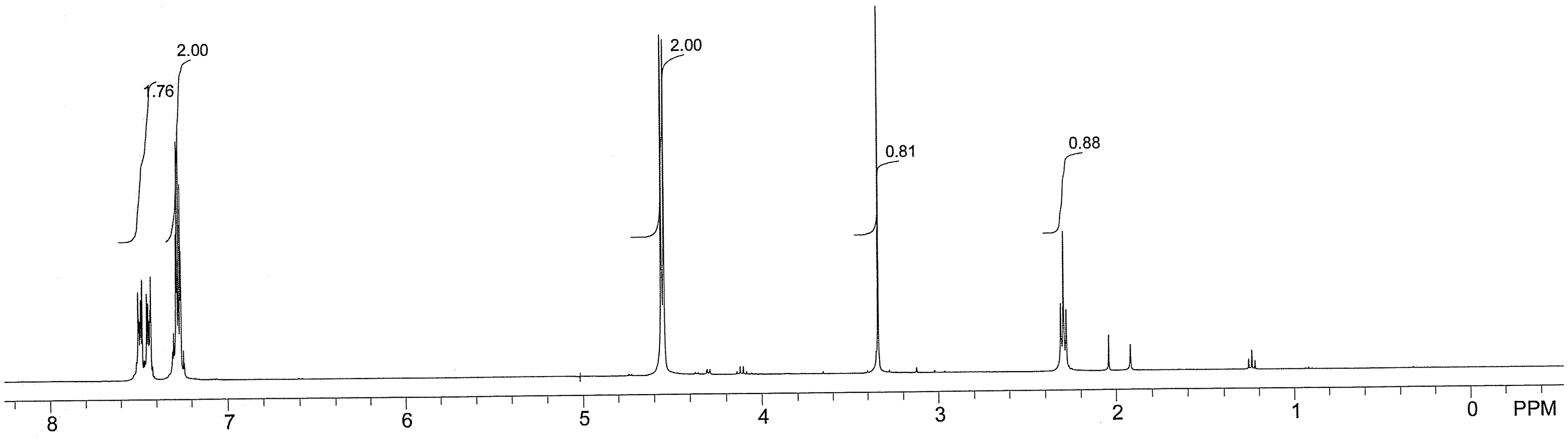




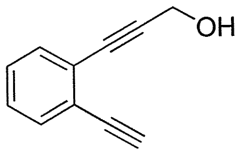
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-189-s-h.fid

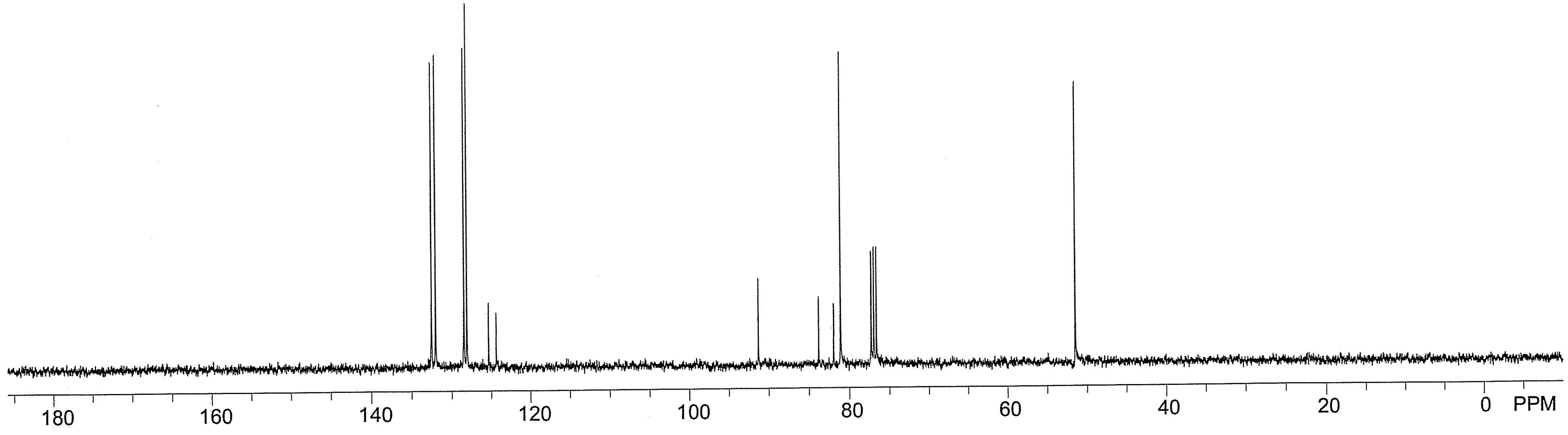
May 4 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 8
Solvent = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 0.24 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2006.7504 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -39.22
B = -45.70
C = 0.00





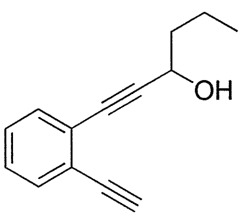
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-189-s-c1.fid
Standard c13 run using qnp probe
May 4 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 108
Solvent = cdcl3
FID PTS1d = 28040
PTS1d = 32768
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 28040.66 Hz
AT1 = 1.00 sec
Hz per Pt 1stD = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 10051.2256 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -17.34
B = -36.56
C = 0.00

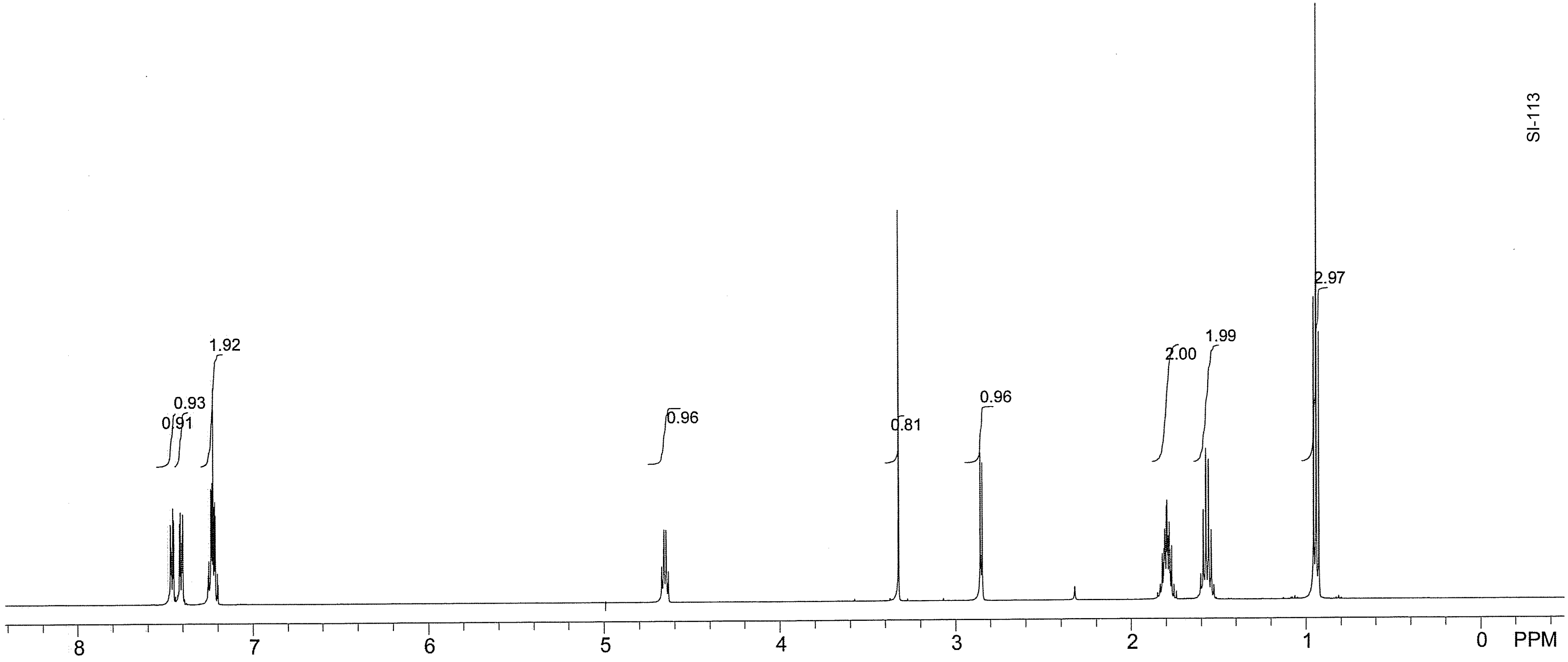




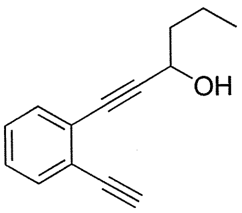
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-198-s-h.fid

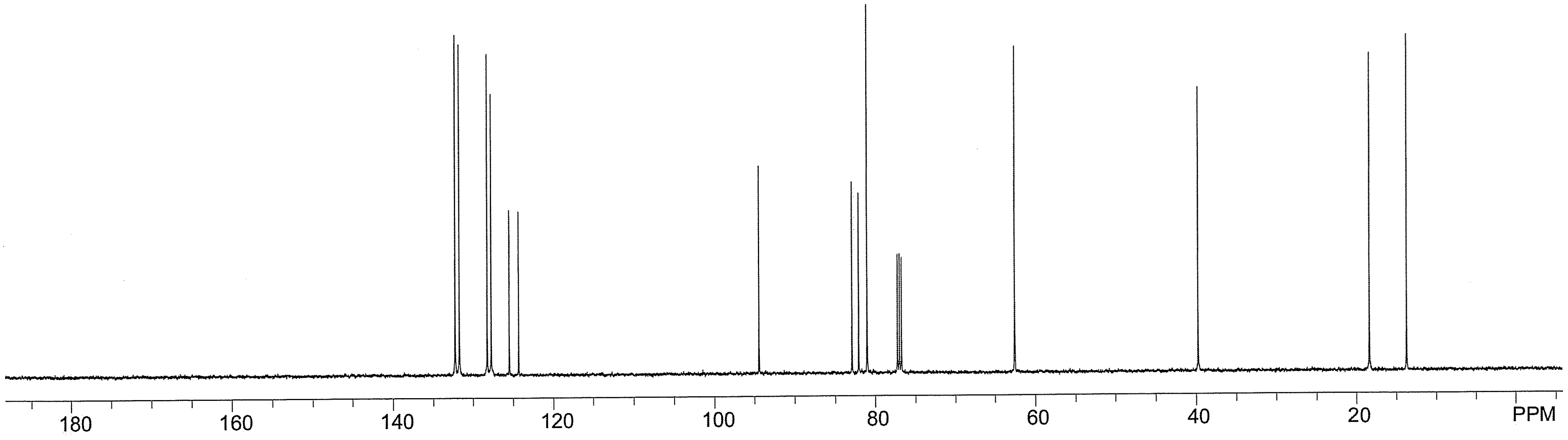
May 10 2011
USER:
SOLVENT: CDCl3
Experiment = s2pul
Pulse length = 7.700 usec
Relaxation delay = 4.800 sec
Solvent = CDCl3
FID PTS1d = 21259
PTS1d = 32768
F1 = 499.858551 MHz
F2 = 125.700813 MHz
SW1 = 8503.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 0.26 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2495.9019 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = 75.31
B = -11.07
C = 0.00



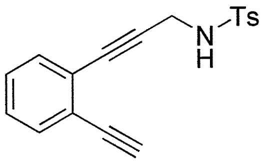


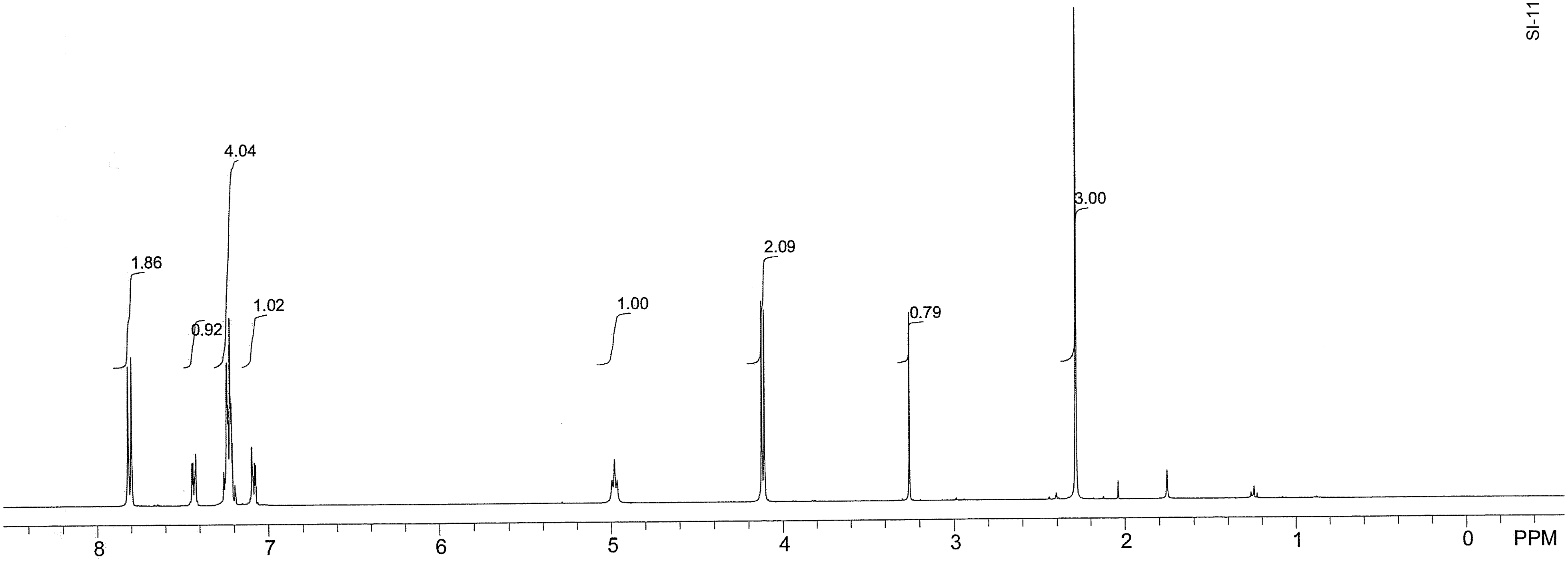
```
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-198-s-c1.fid
ylw-5-198-s-c
May 10 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length =    6.000 usec
Relaxation delay =    3.000 sec
NA =    54
Solvent  = cdcl3
FID PTS1d = 36749
PTS1d = 65536
F1  =  125.701683 MHz
F2  =  499.858551 MHz
SW1 =   28258.57 Hz
AT1 =   1.30 sec
Hz per Pt 1stD =   0.43 Hz
SW2 =       1.00 Hz
Hz per Pt 2ndD =   1.00 Hz
O1  =   12753.5664 Hz
O2  =      -0.5000 Hz
LB1 =  2.00      Hz
TP    A = -234.38
      B =  154.69
      C =   0.00
```



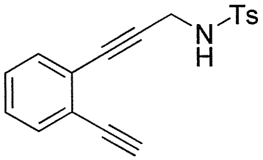


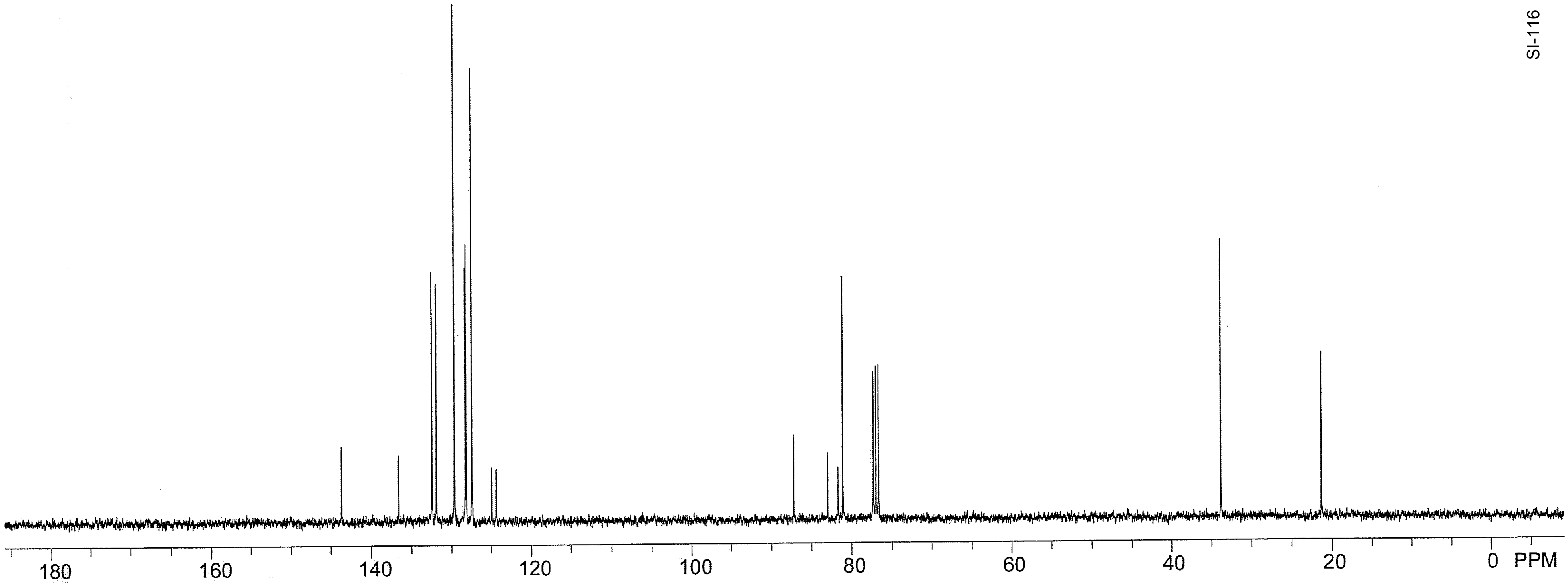
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-197-s-h.fid
new experiment
May 11 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 12
Solvent = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 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 = -45.92
B = -36.04
C = 0.00



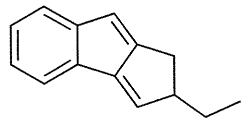


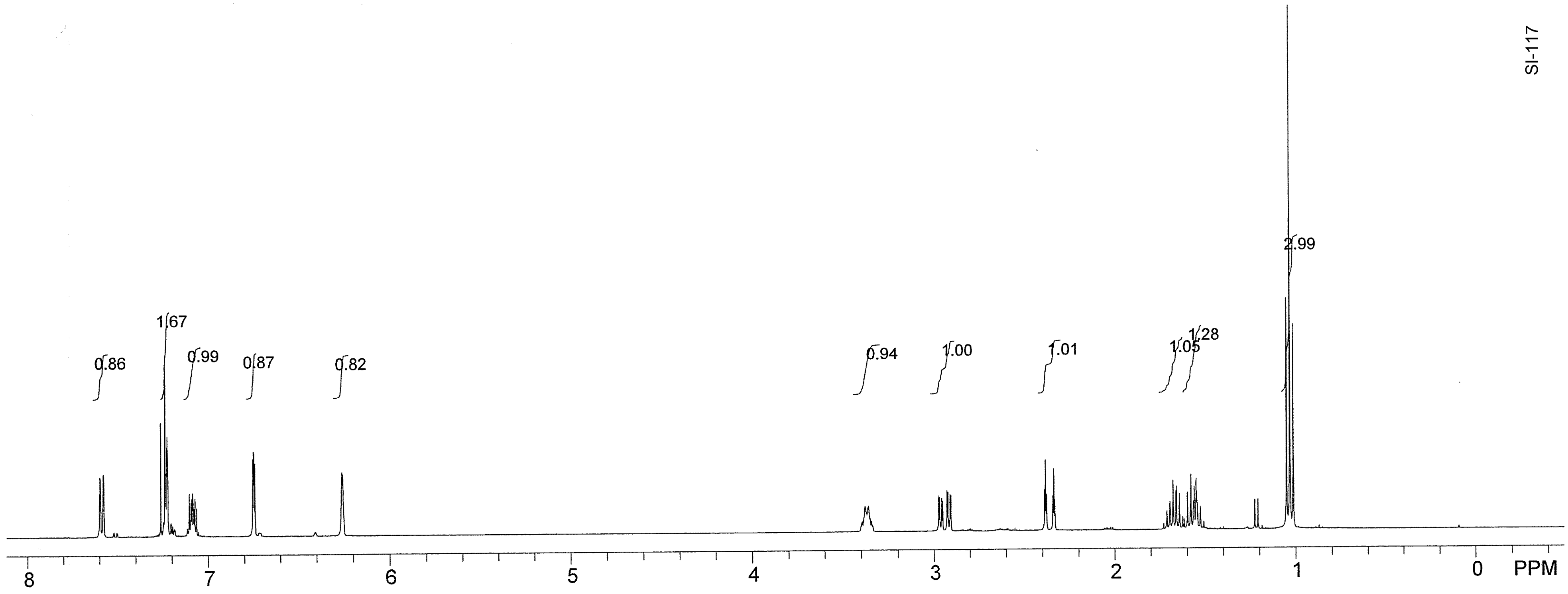
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-197-s-c2.fid
Standard c13 run using qnp probe
May 11 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 128
Solvent = cdcl3
FID PTS1d = 28040
PTS1d = 32768
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 28040.66 Hz
AT1 = 1.00 sec
Hz per Pt 1stD = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 10052.0820 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -18.28
B = -11.25
C = 0.00



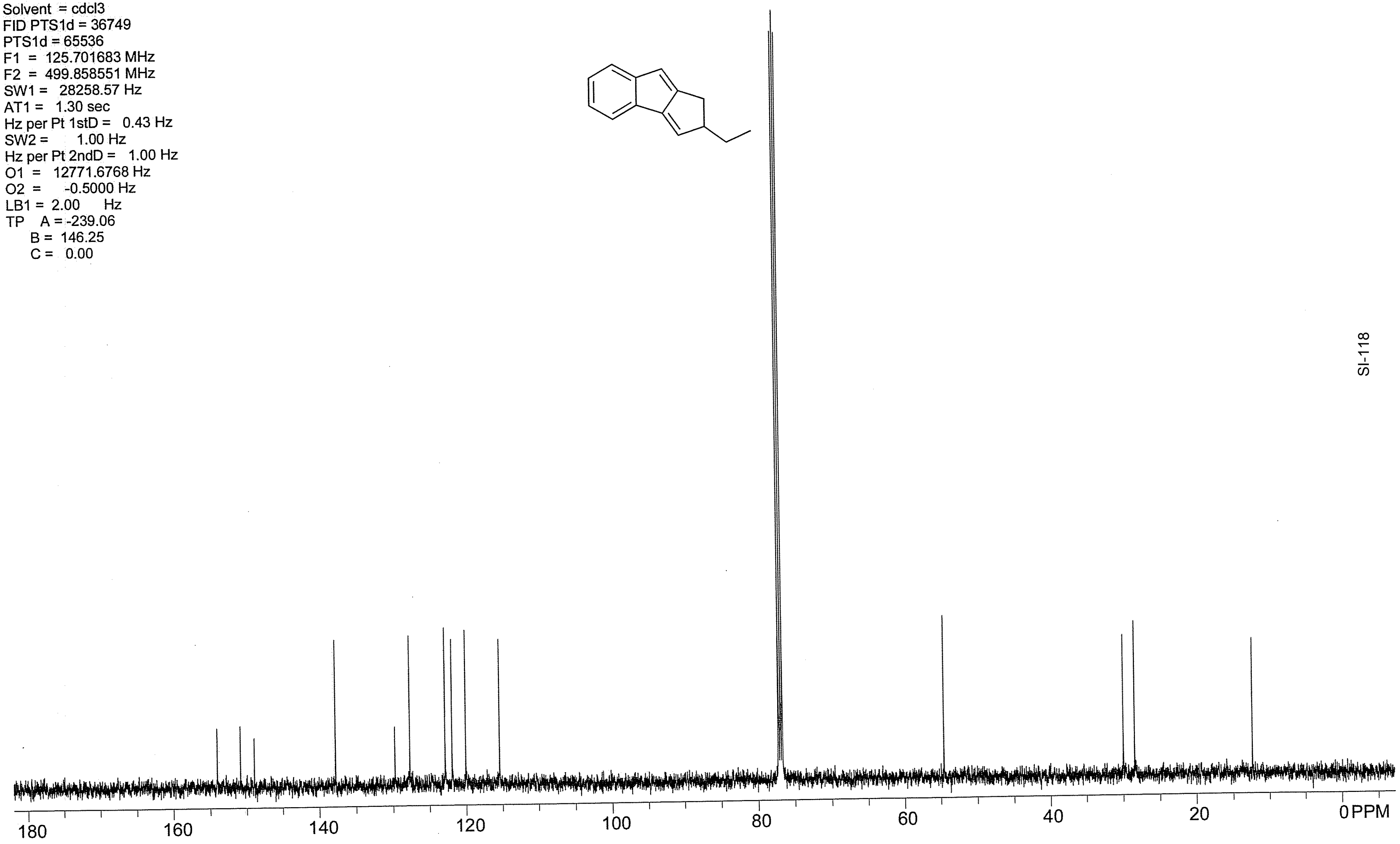


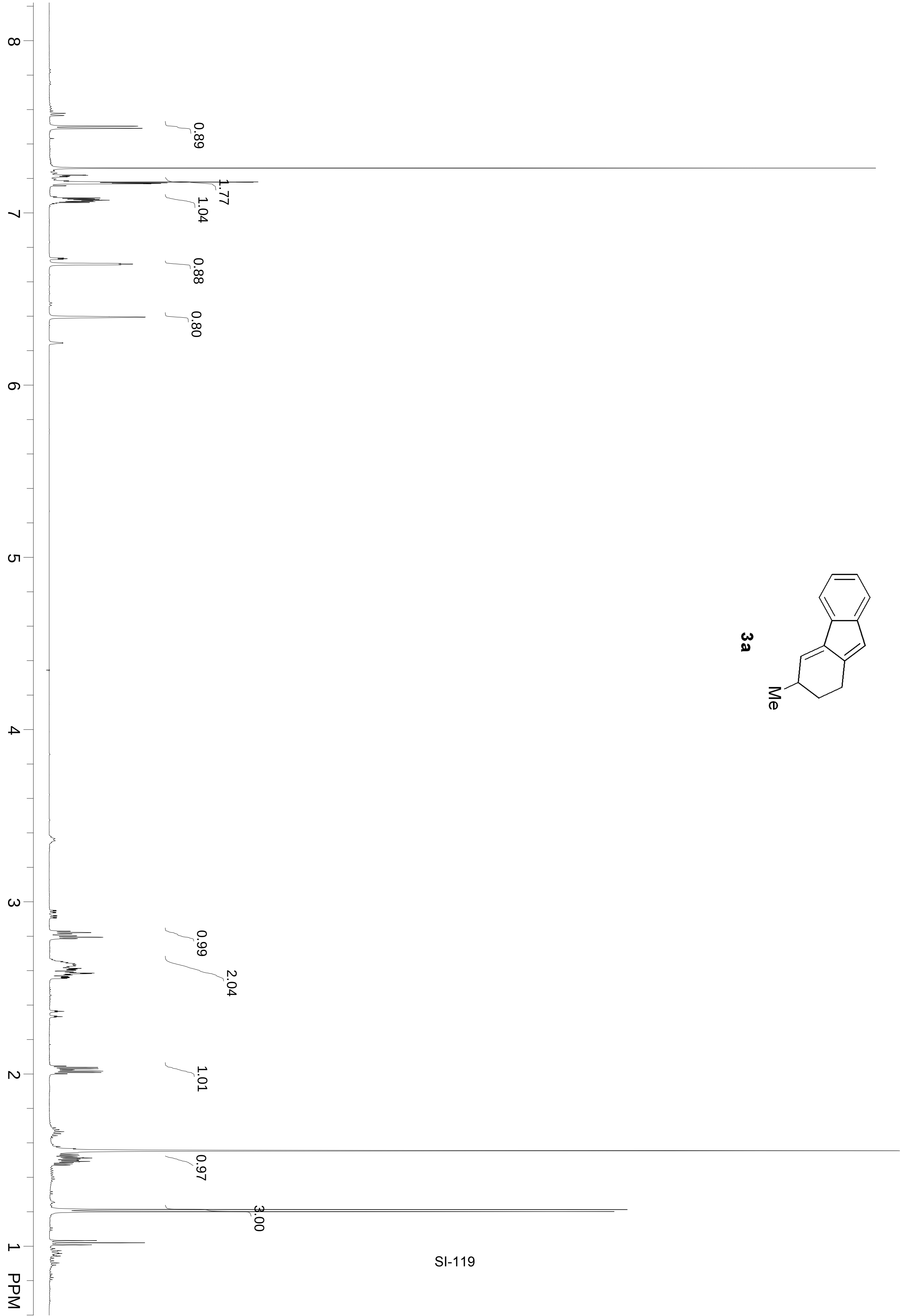
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-149-2.fid
new experiment
Apr 8 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 16
Solvent = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 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 = -49.28
B = -33.09
C = 0.00



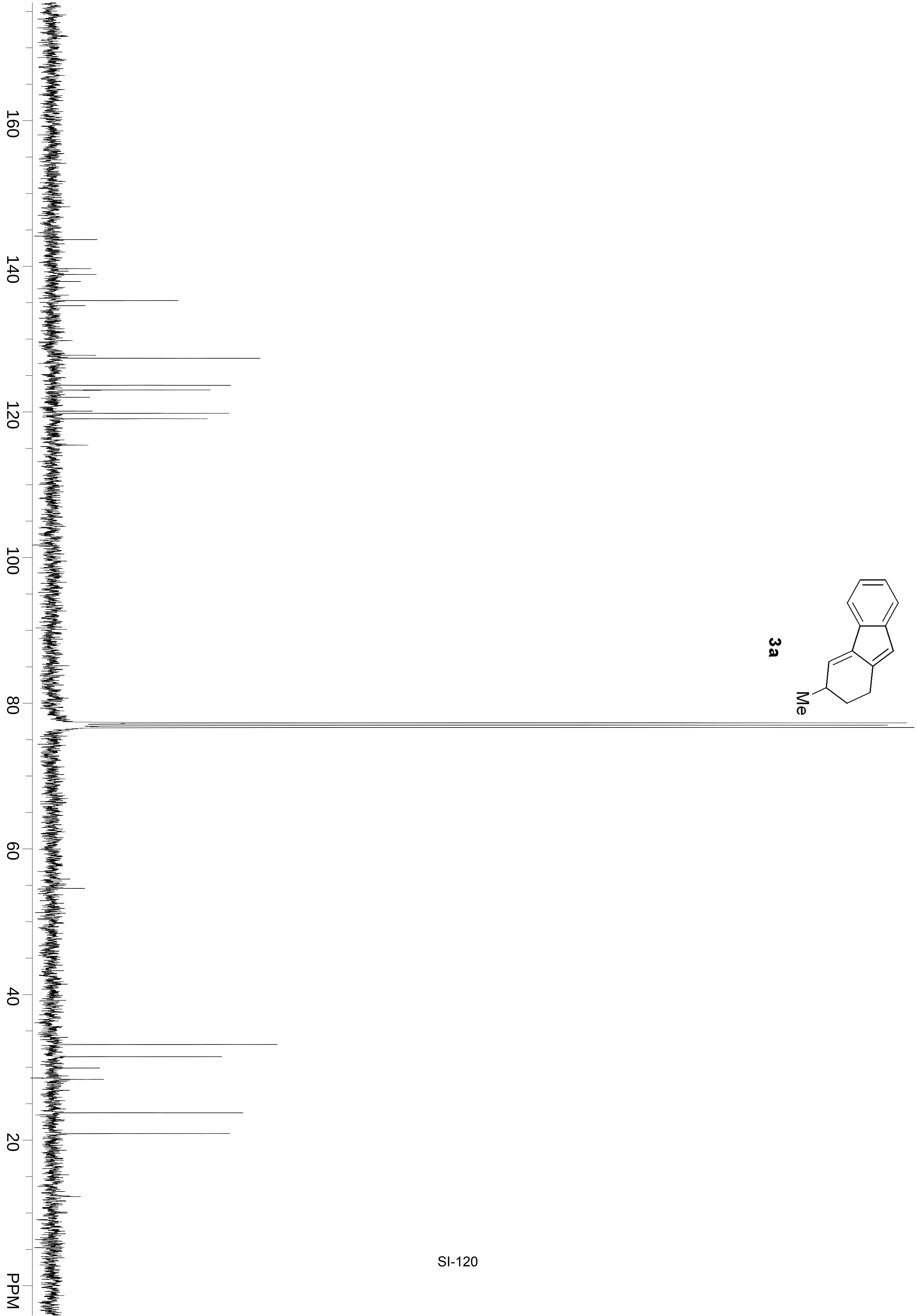


C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-139-c.fid
STANDARD CARBON PARAMETERSvU
Mar 31 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 6.000 usec
Relaxation delay = 3.000 sec
NA = 76
Solvent = cdcl3
FID PTS1d = 36749
PTS1d = 65536
F1 = 125.701683 MHz
F2 = 499.858551 MHz
SW1 = 28258.57 Hz
AT1 = 1.30 sec
Hz per Pt 1stD = 0.43 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 12771.6768 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -239.06
B = 146.25
C = 0.00

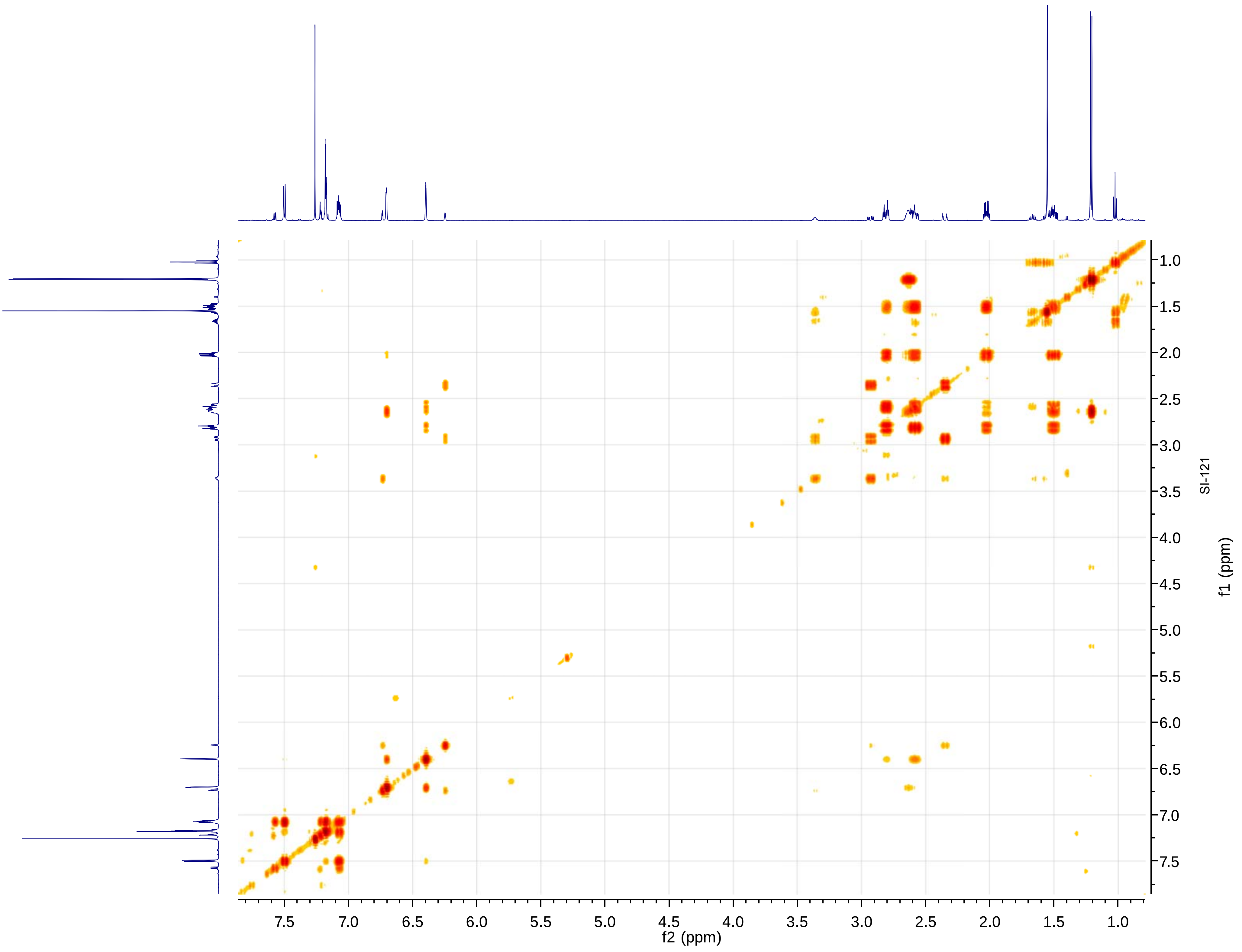




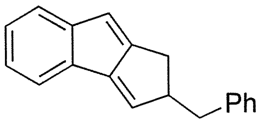
3a

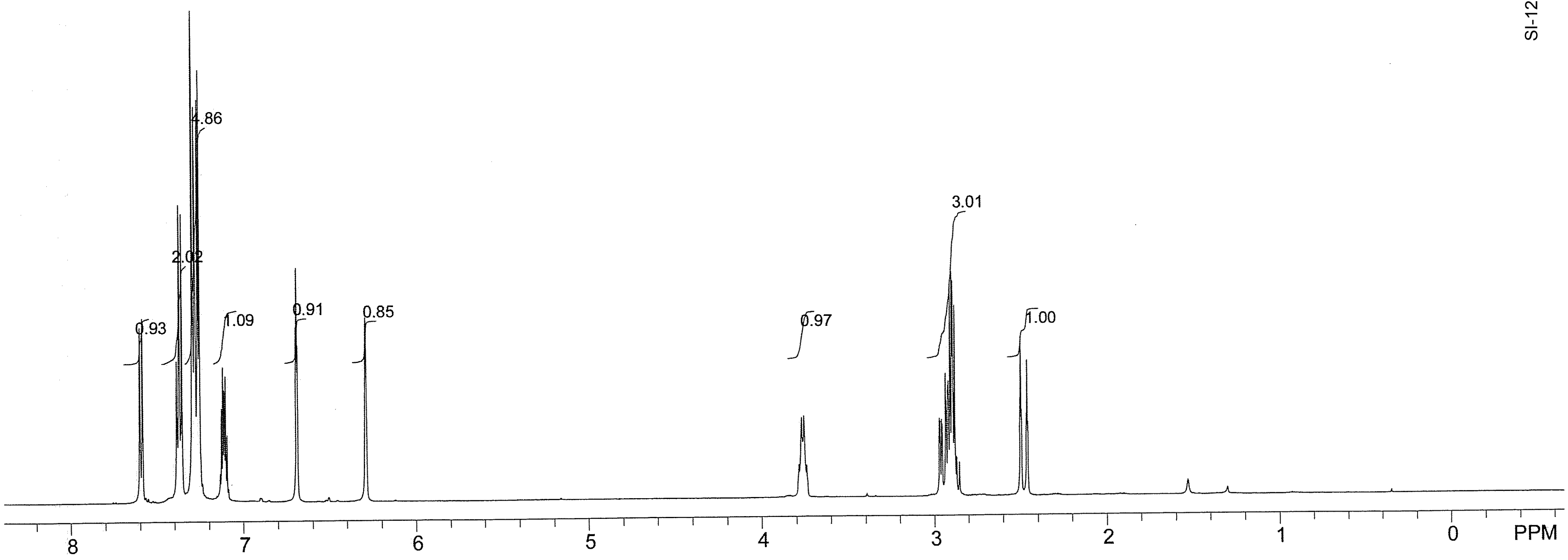


3a

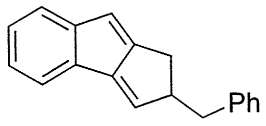

f2 (ppm)
f1 (ppm)
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0

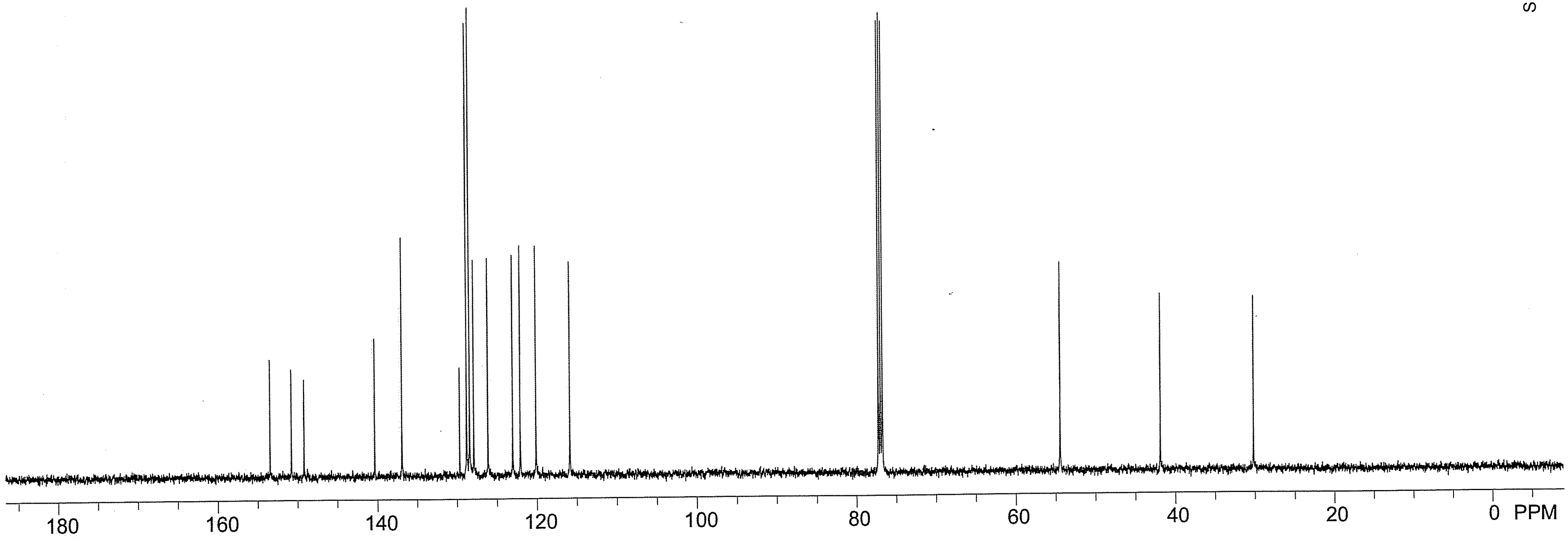
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-160-hh.fid
H1_CDCL3
Apr 14 2011
USER:
SOLVENT: CDCl3
Experiment = s2pul
Pulse length = 7.700 usec
Relaxation delay = 4.800 sec
NA = 8
Solvent = CDCl3
FID PTS1d = 21259
PTS1d = 32768
F1 = 499.858551 MHz
F2 = 1.000000 MHz
SW1 = 8503.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 0.26 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2499.2932 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = 70.55
B = -13.01
C = 0.00





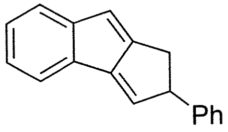
```
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-160-p-c1.fid

Apr 14 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length =    6.000 usec
Relaxation delay =    3.000 sec
NA  =    164
Solvent  = cdcl3
FID PTS1d = 36749
PTS1d = 65536
F1  =  125.701683 MHz
F2  =  499.858551 MHz
SW1 =   28258.57 Hz
AT1 =   1.30 sec
Hz per Pt 1stD =   0.43 Hz
SW2 =       1.00 Hz
Hz per Pt 2ndD =   1.00 Hz
O1  =   12766.5029 Hz
O2  =      -0.5000 Hz
LB1 =  2.00      Hz
TP    A =  104.53
      B =  160.31
      C =   0.00
```

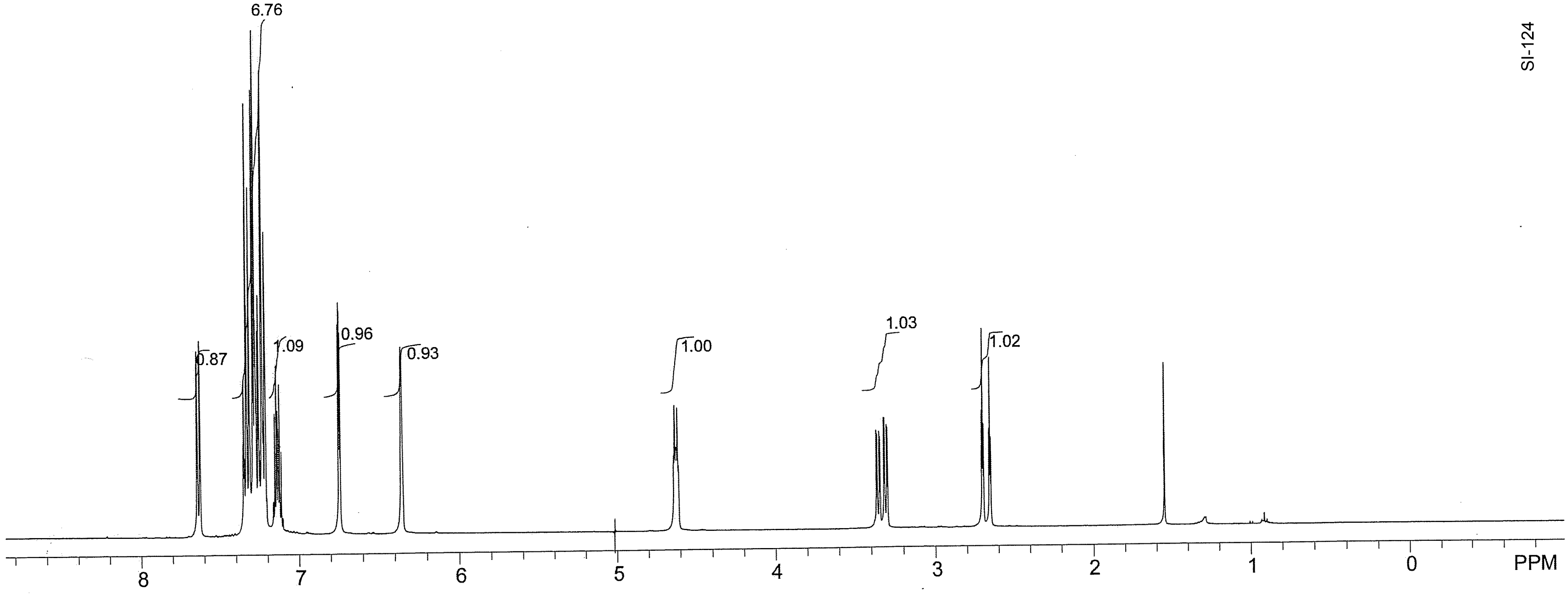




C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-301-h.fid

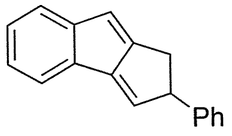
May 3 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 10
Solvent = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 0.24 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2006.7504 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -50.63
B = -29.06
C = 0.00

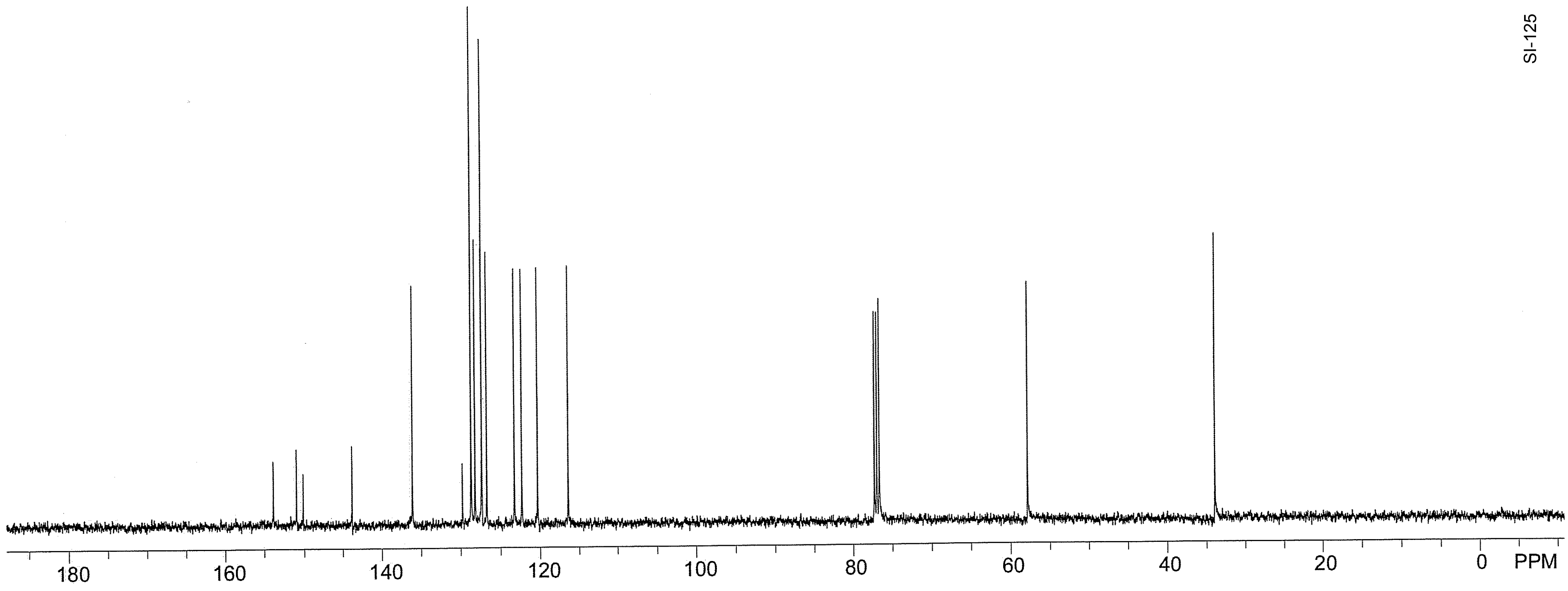




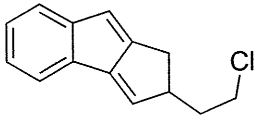
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-301-c2.fid

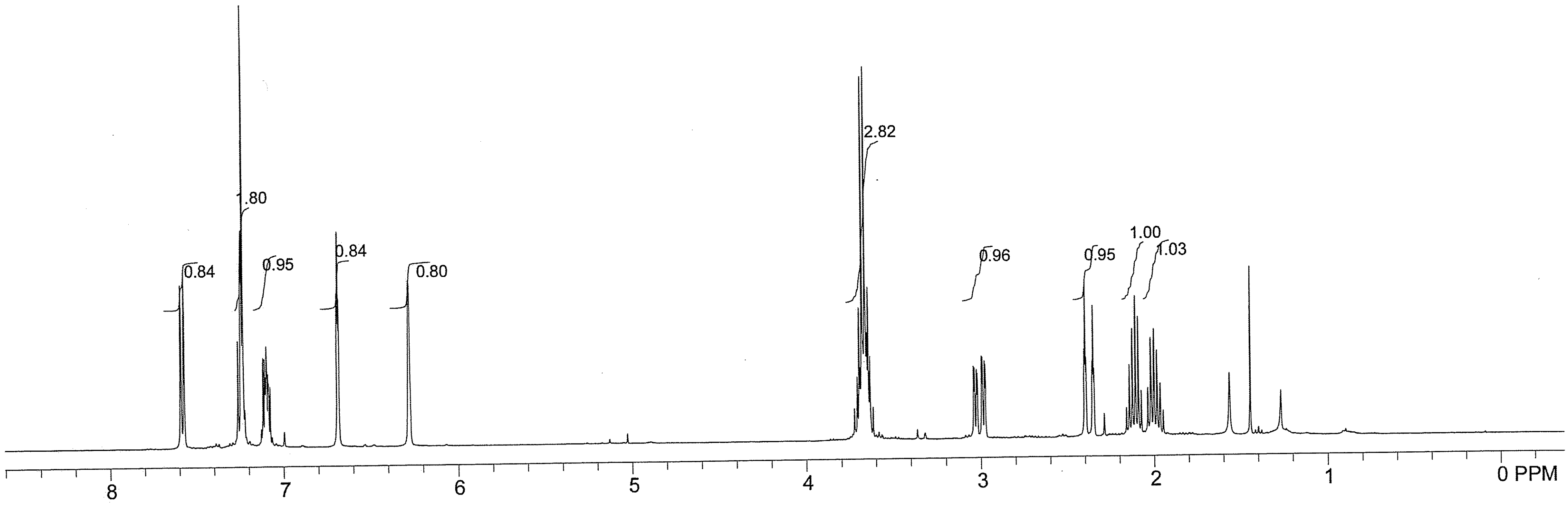
May 3 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 300
Solvent = cdcl3
FID PTS1d = 28040
PTS1d = 32768
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 28040.66 Hz
AT1 = 1.00 sec
Hz per Pt 1stD = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 10053.7930 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -11.25
B = -45.00
C = 0.00



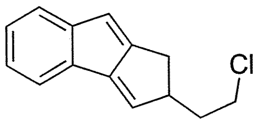


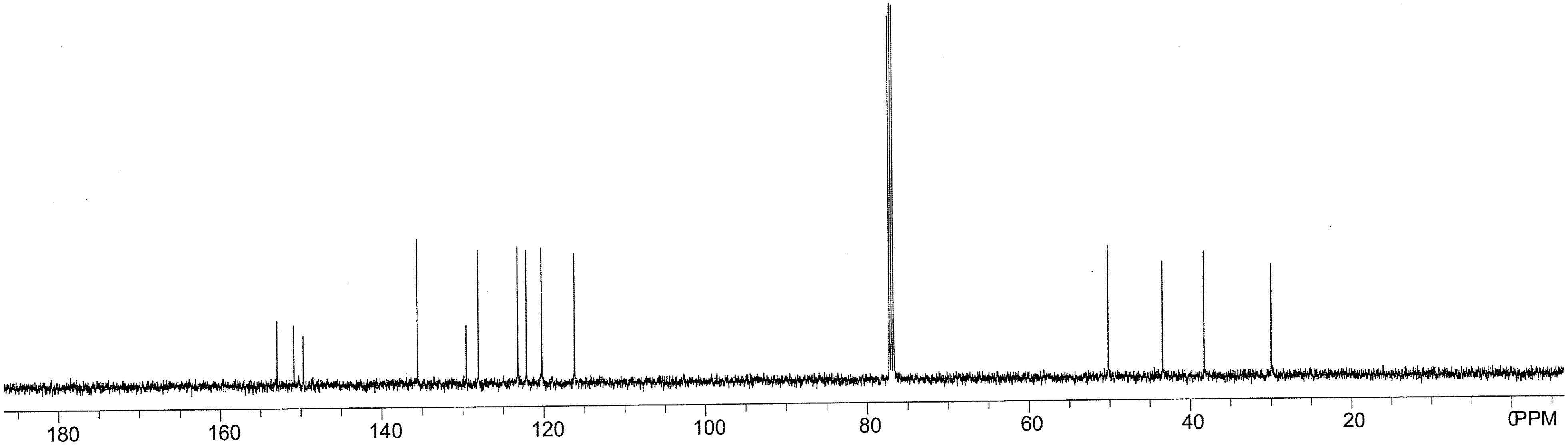
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-162-Cl-04242011.fid
new experiment
Apr 24 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 8
Solvent = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 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 = -46.60
B = -28.25
C = 0.00



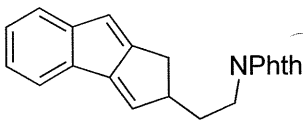


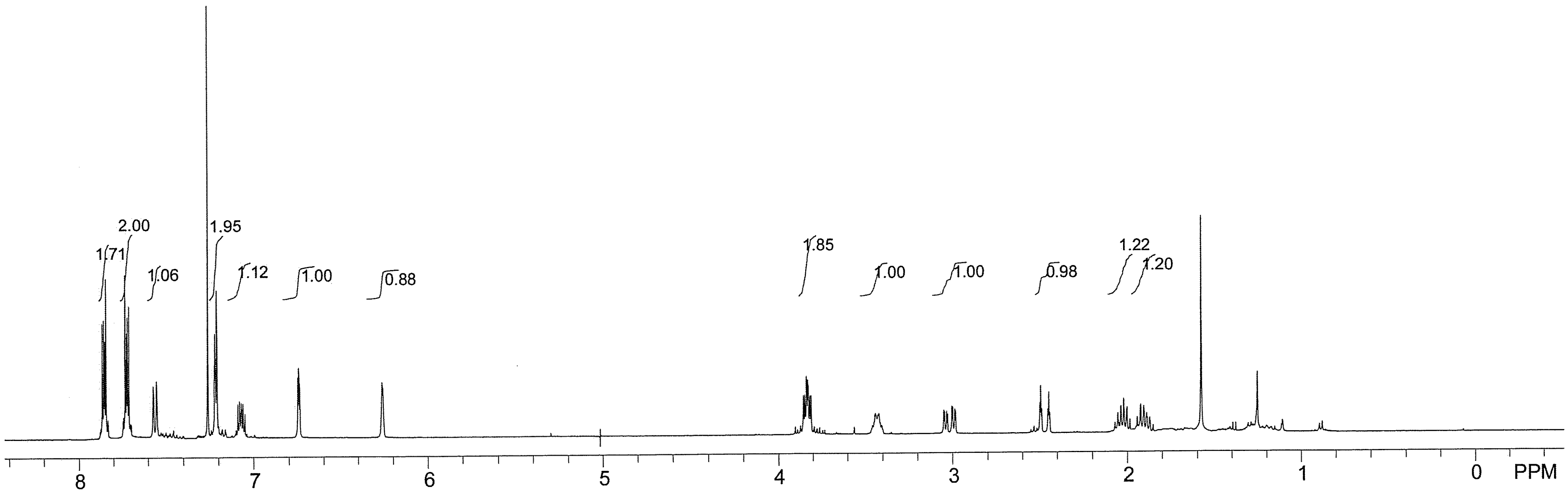
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-162-04252011-Cl-c5.fid
STANDARD CARBON PARAMETERS
Apr 25 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 6.000 usec
Relaxation delay = 3.000 sec
NA = 84
Solvent = cdcl3
FID PTS1d = 36749
PTS1d = 65536
F1 = 125.701683 MHz
F2 = 499.858551 MHz
SW1 = 28258.57 Hz
AT1 = 1.30 sec
Hz per Pt 1stD = 0.43 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 12768.6582 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -170.16
B = 132.19
C = 0.00

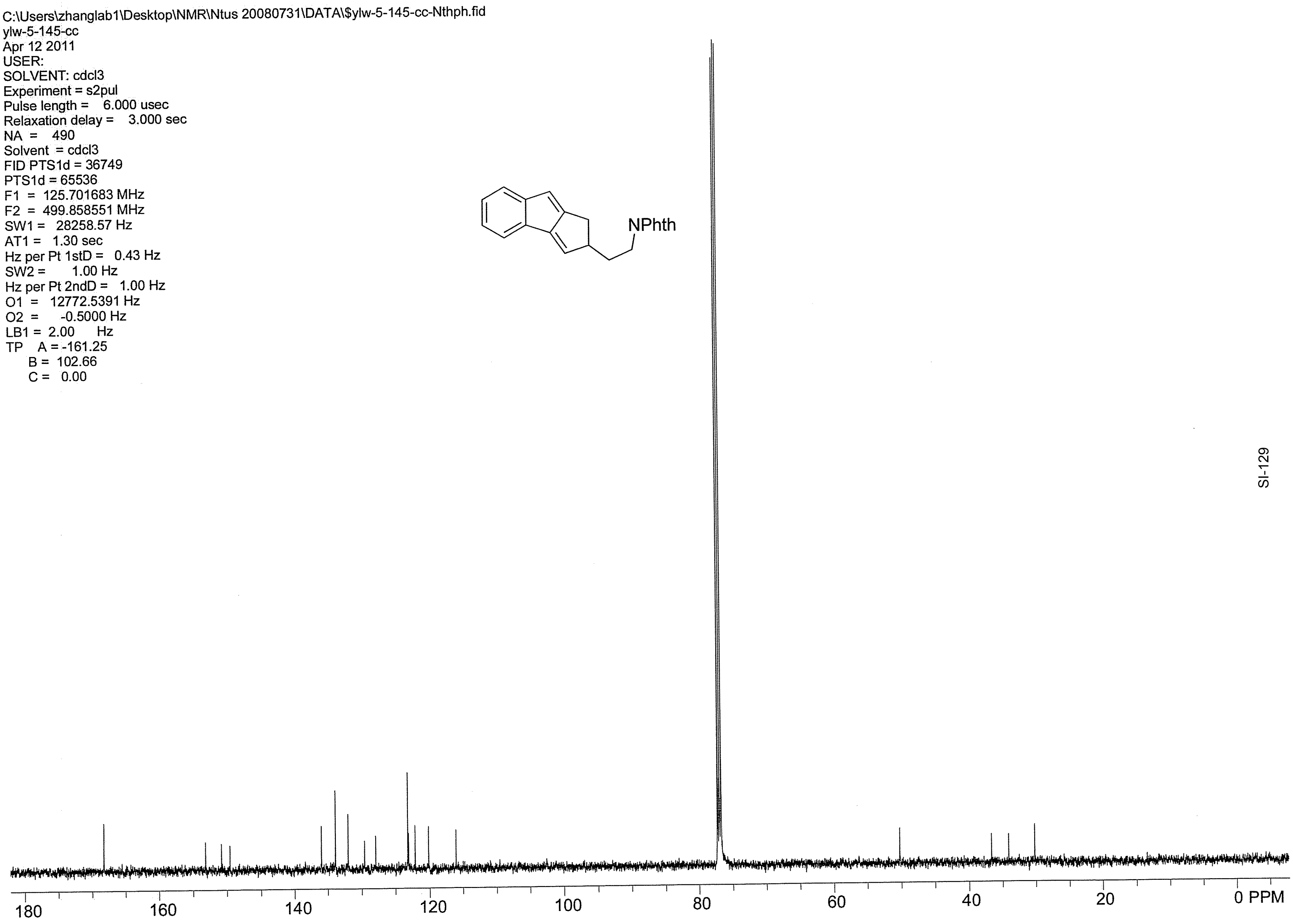




C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-145-p-hh.fid
new experiment
Apr 11 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 14
Solvent = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 0.24 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2006.2362 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -47.04
B = -27.06
C = 0.00

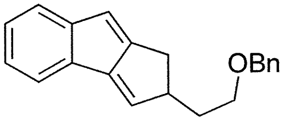


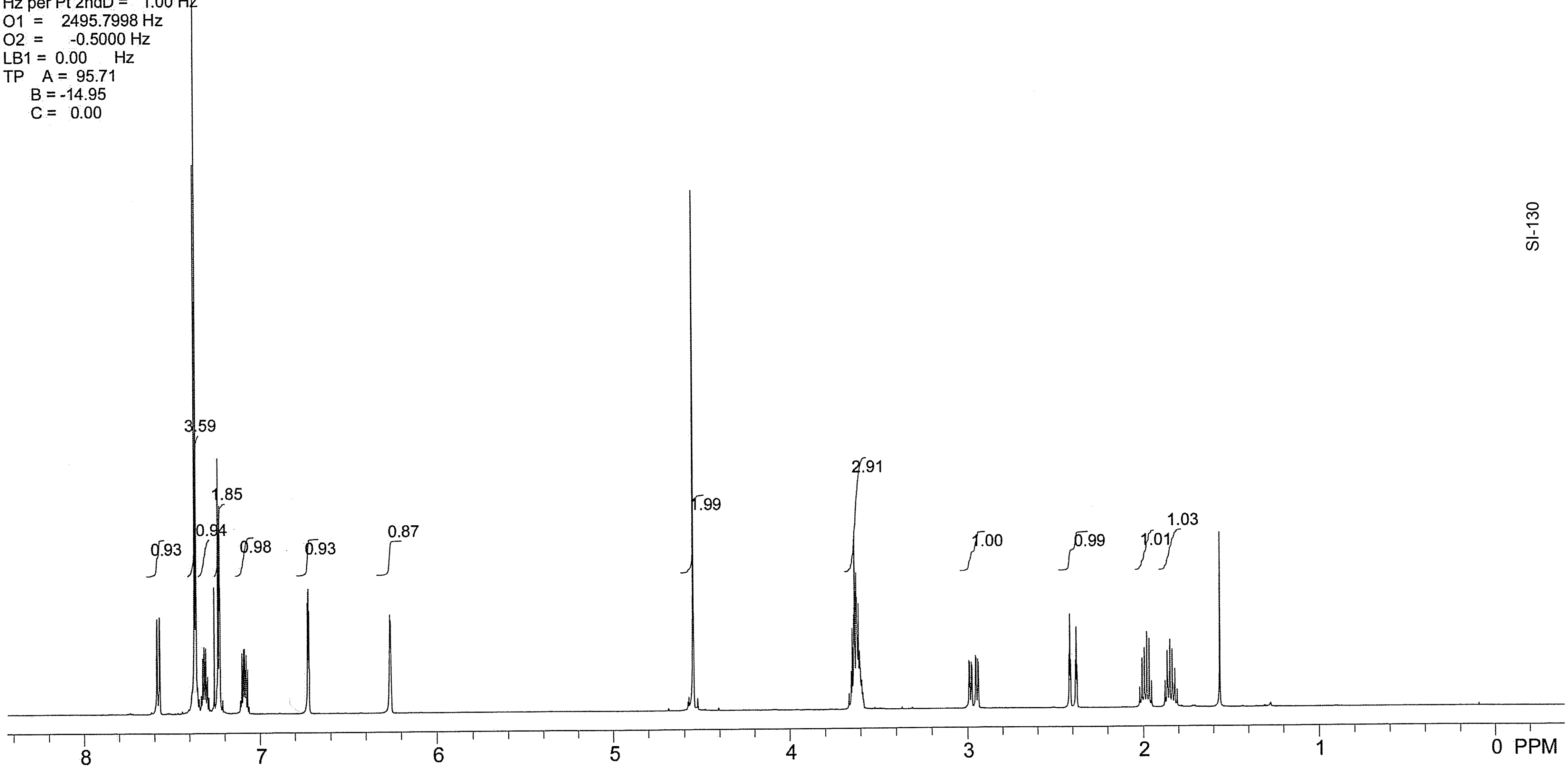




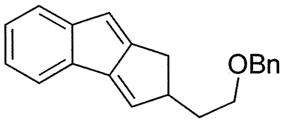
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-145-cc-Nthph.fid
ylw-5-145-cc
Apr 12 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 6.000 usec
Relaxation delay = 3.000 sec
NA = 490
Solvent = cdcl3
FID PTS1d = 36749
PTS1d = 65536
F1 = 125.701683 MHz
F2 = 499.858551 MHz
SW1 = 28258.57 Hz
AT1 = 1.30 sec
Hz per Pt 1stD = 0.43 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 12772.5391 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -161.25
B = 102.66
C = 0.00

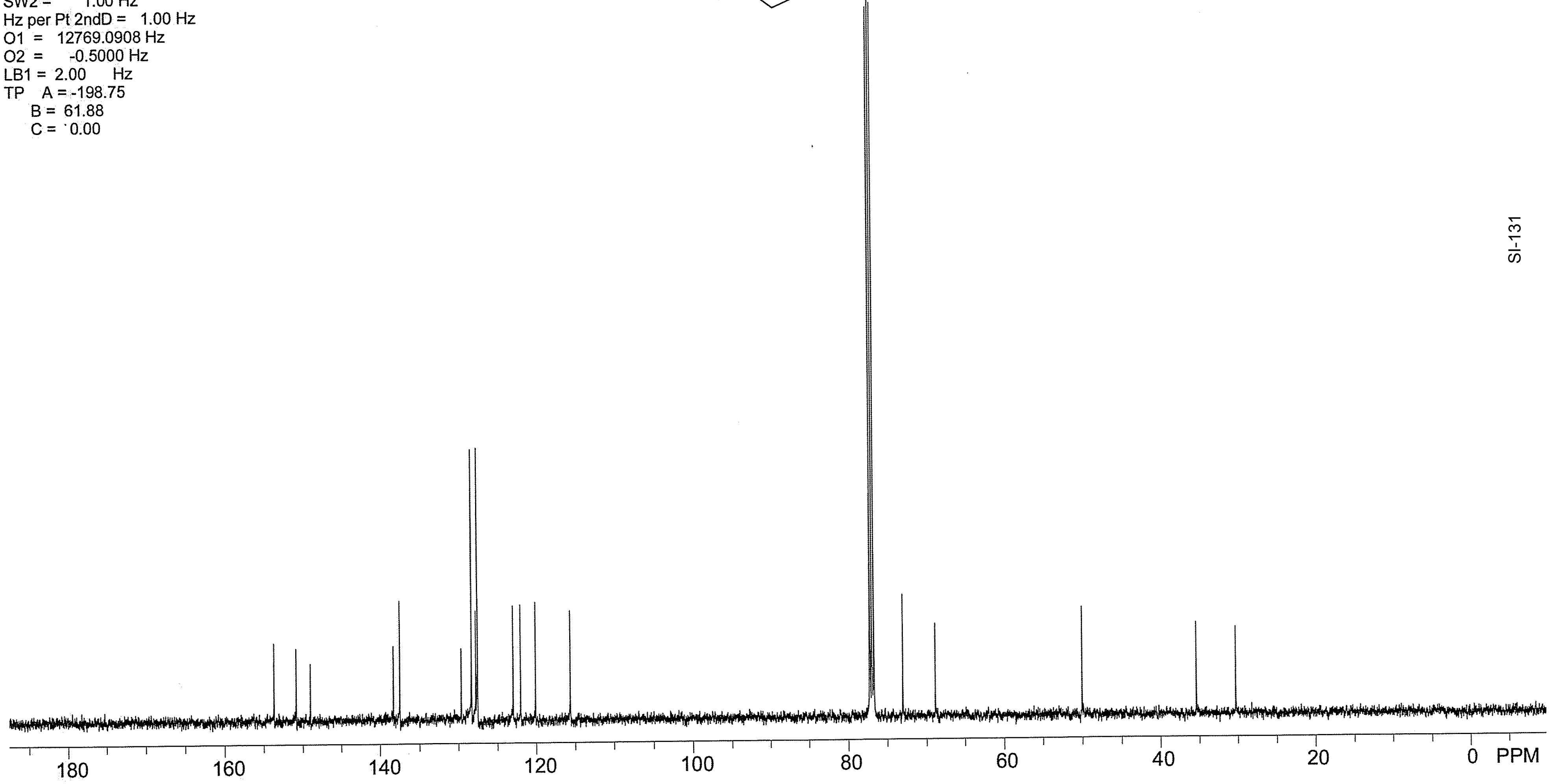
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-196-OBn-p.fid
H1_CDCL3
May 7 2011
USER:
SOLVENT: CDCl3
Experiment = s2pul
Pulse length = 7.700 usec
Relaxation delay = 4.800 sec
NA = 12
Solvent = CDCl3
FID PTS1d = 21259
PTS1d = 32768
F1 = 499.858551 MHz
F2 = 125.700813 MHz
SW1 = 8503.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 0.26 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2495.7998 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = 95.71
B = -14.95
C = 0.00





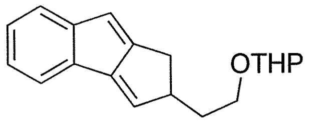
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-196-OBn-p-c1.fid
ylw-5-196-OBn-p-c
May 7 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 6.000 usec
Relaxation delay = 3.000 sec
NA = 176
Solvent = cdcl3
FID PTS1d = 36749
PTS1d = 65536
F1 = 125.701683 MHz
F2 = 499.858551 MHz
SW1 = 28258.57 Hz
AT1 = 1.30 sec
Hz per Pt 1stD = 0.43 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 12769.0908 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -198.75
B = 61.88
C = 0.00

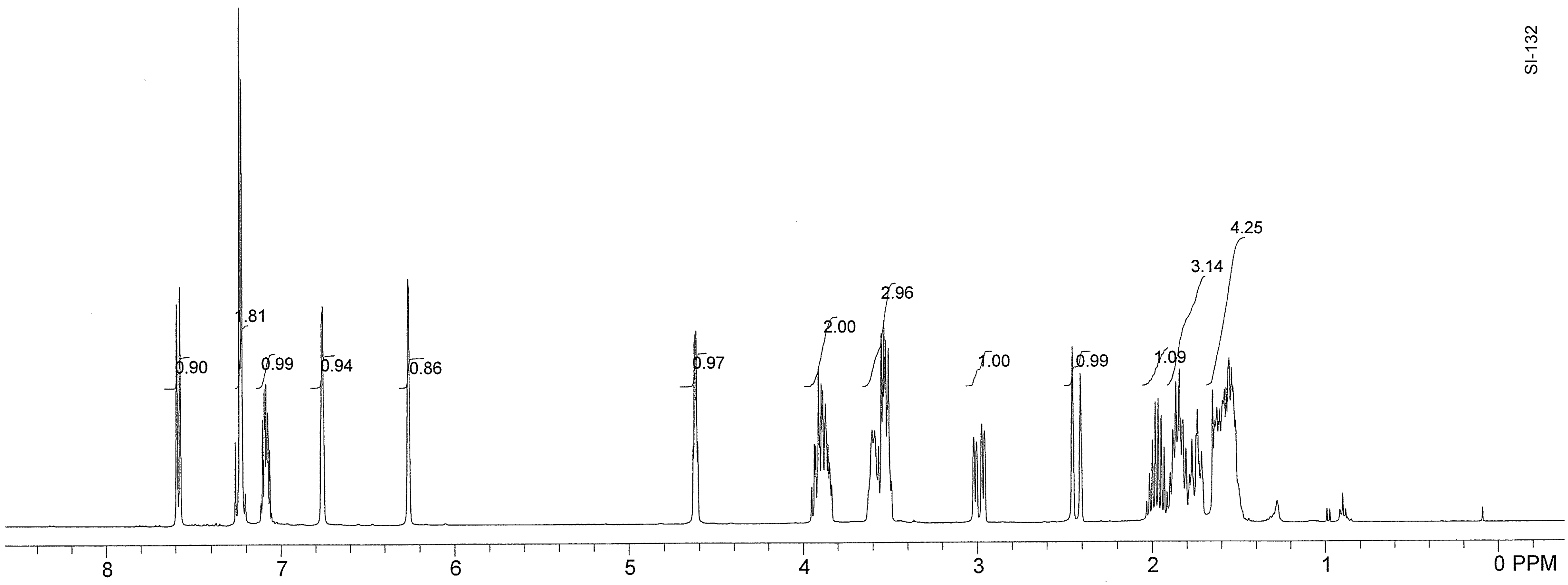




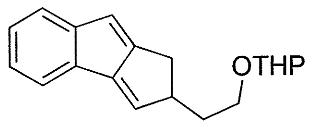
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-297-h.fid

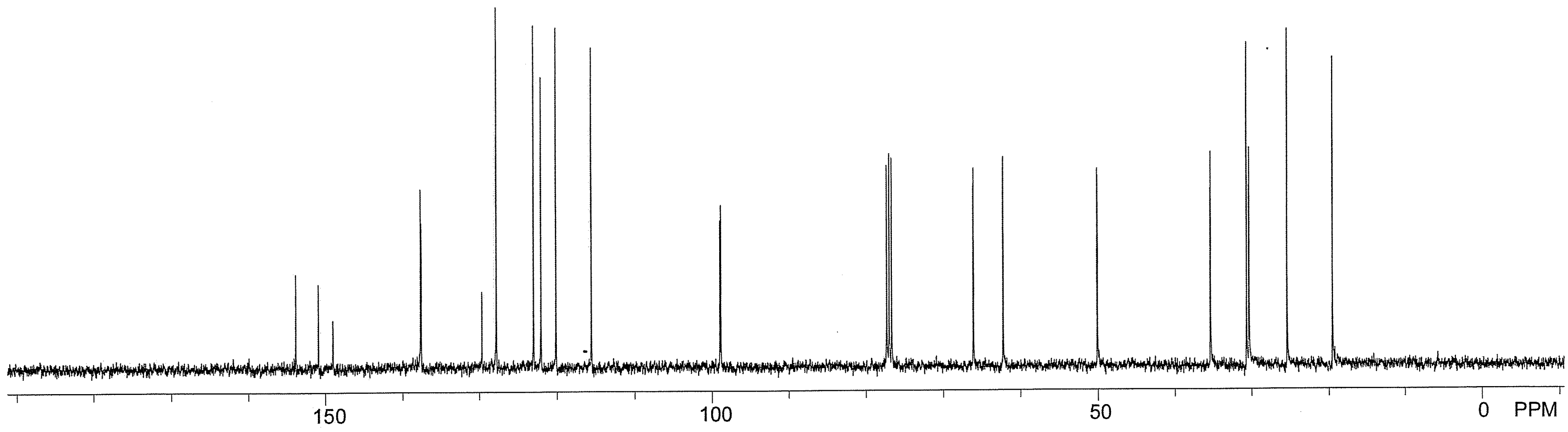
Jun 2 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 16
Solvent = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 0.24 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2006.7504 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -54.85
B = -24.46
C = 0.00





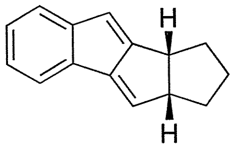
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-297-c2.fid
Standard c13 run using qnp probe
Jun 2 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 166
Solvent = cdcl3
FID PTS1d = 28040
PTS1d = 32768
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 28040.66 Hz
AT1 = 1.00 sec
Hz per Pt 1stD = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 10052.9375 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = 0.00
B = -50.63
C = 0.00

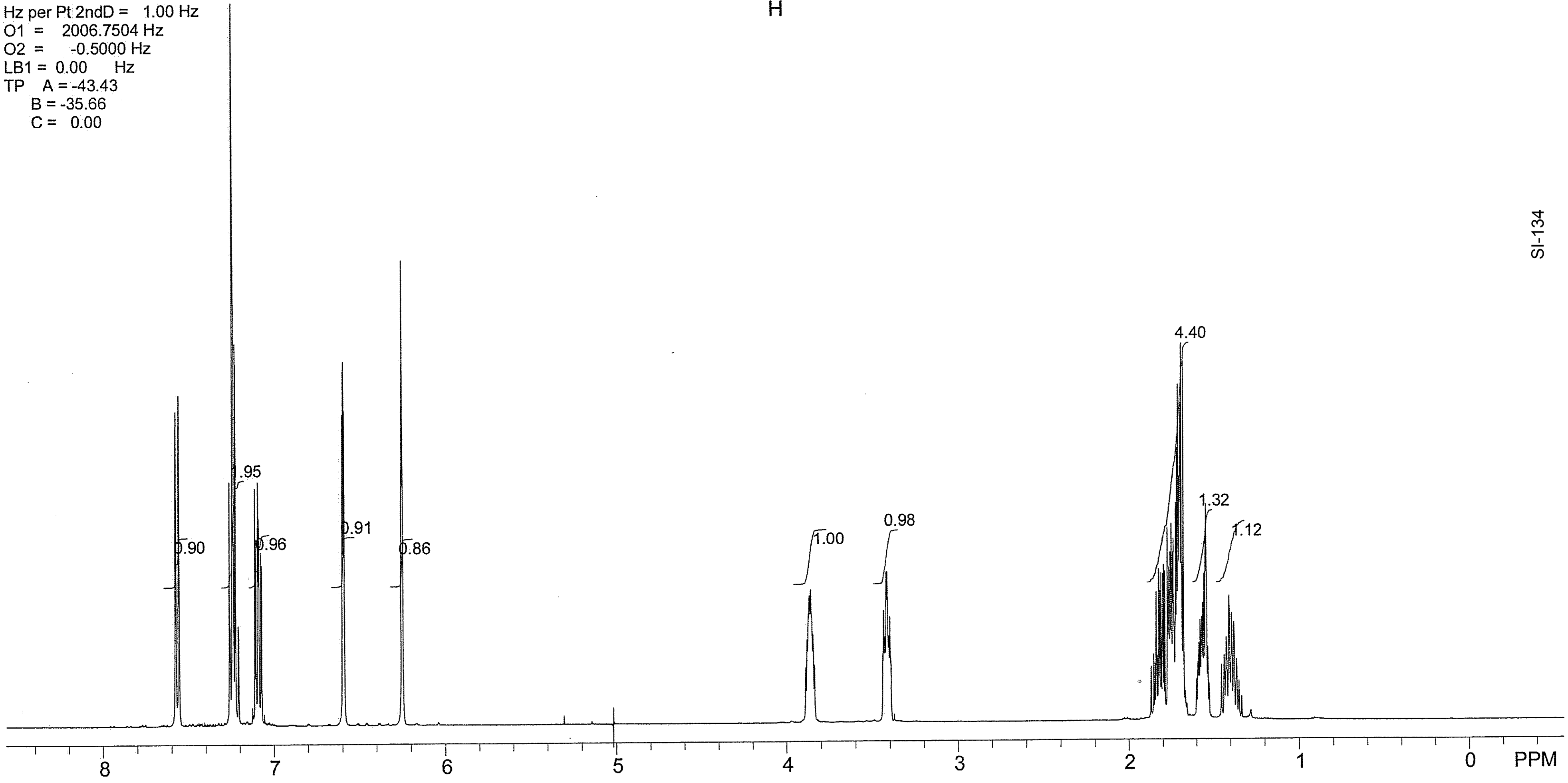




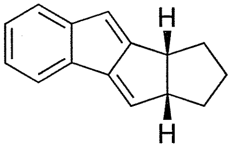
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-215-5ring-h.fid

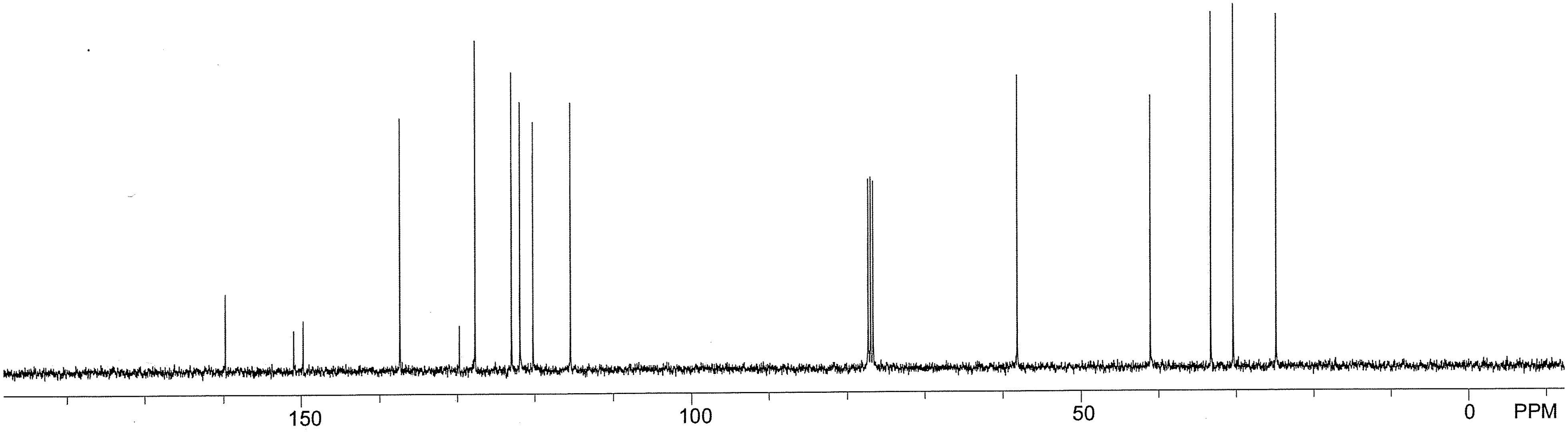
May 22 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 10
Solvent = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 0.24 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2006.7504 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -43.43
B = -35.66
C = 0.00



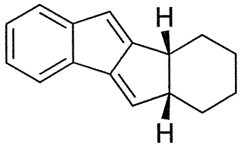


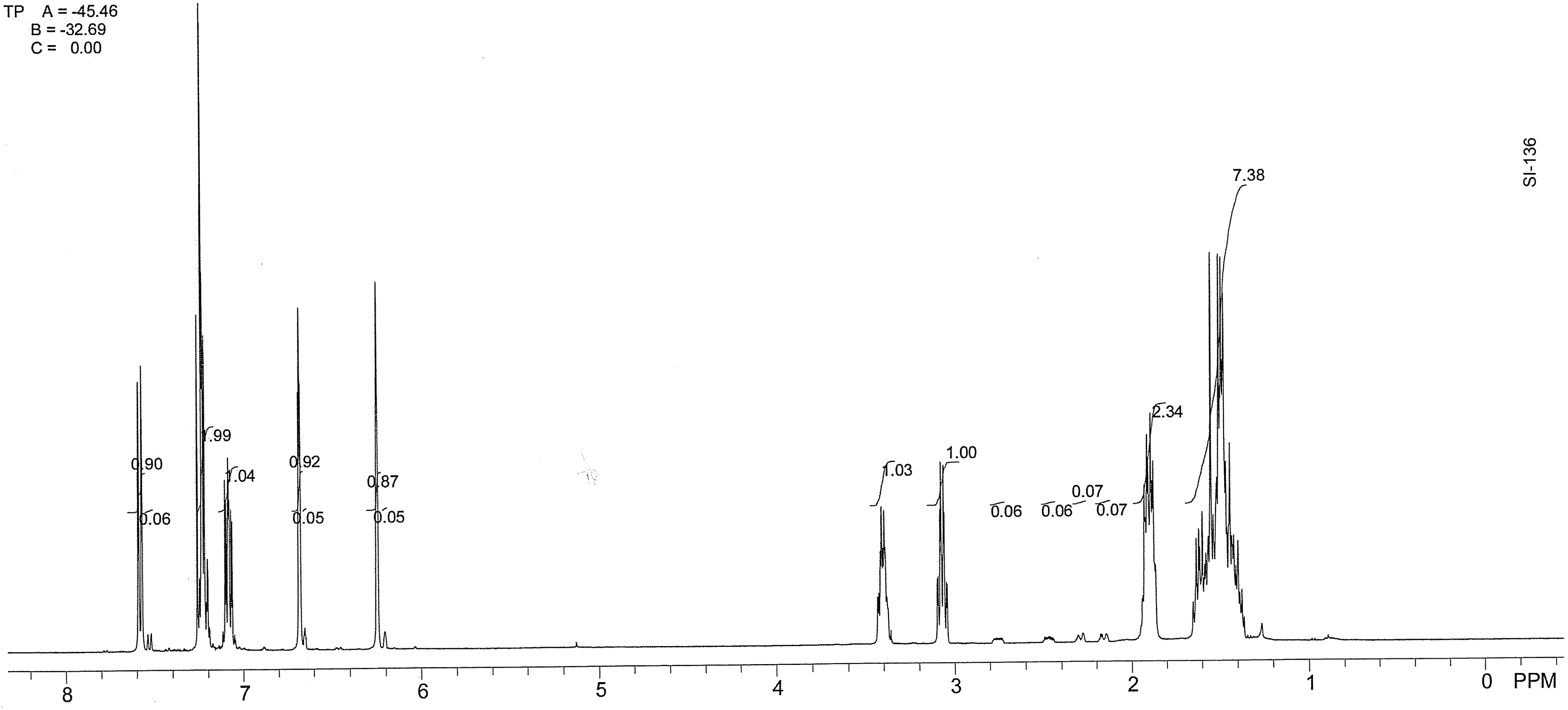
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-215-5ring-c1.fid
Standard c13 run using qnp probe
May 22 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 218
Solvent = cdcl3
FID PTS1d = 28040
PTS1d = 32768
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 28040.66 Hz
AT1 = 1.00 sec
Hz per Pt 1stD = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 10053.7930 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -31.88
B = 7.03
C = 0.00



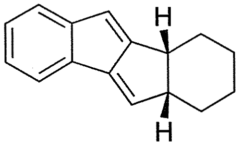


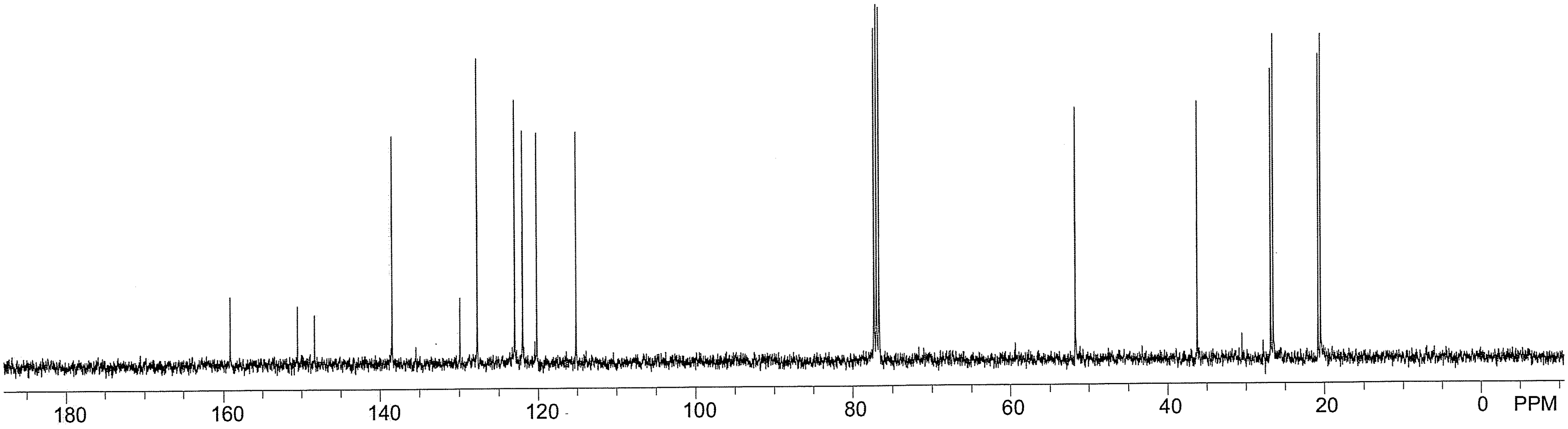
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-218-h.fid
new experiment
May 20 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 16
Solvent = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 0.24 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2006.2362 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -45.46
B = -32.69
C = 0.00



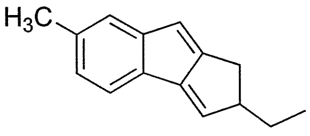


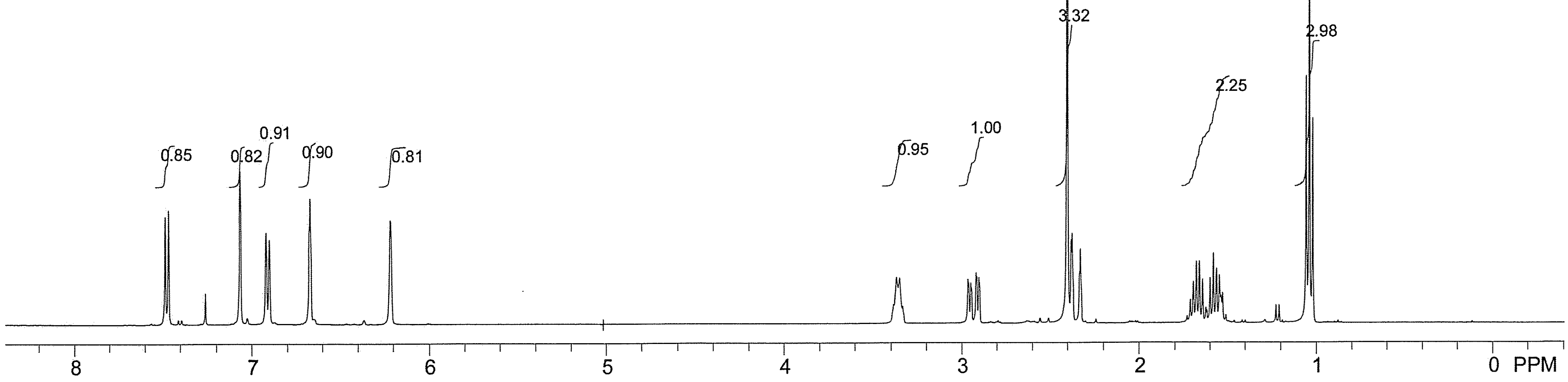
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-218-c3.fid
Standard c13 run using qnp probe
May 20 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 442
Solvent = cdcl3
FID PTS1d = 28040
PTS1d = 32768
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 28040.66 Hz
AT1 = 1.00 sec
Hz per Pt 1stD = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 10056.3604 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -15.47
B = -22.50
C = 0.00



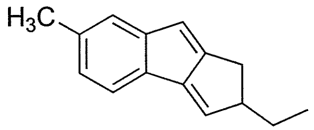


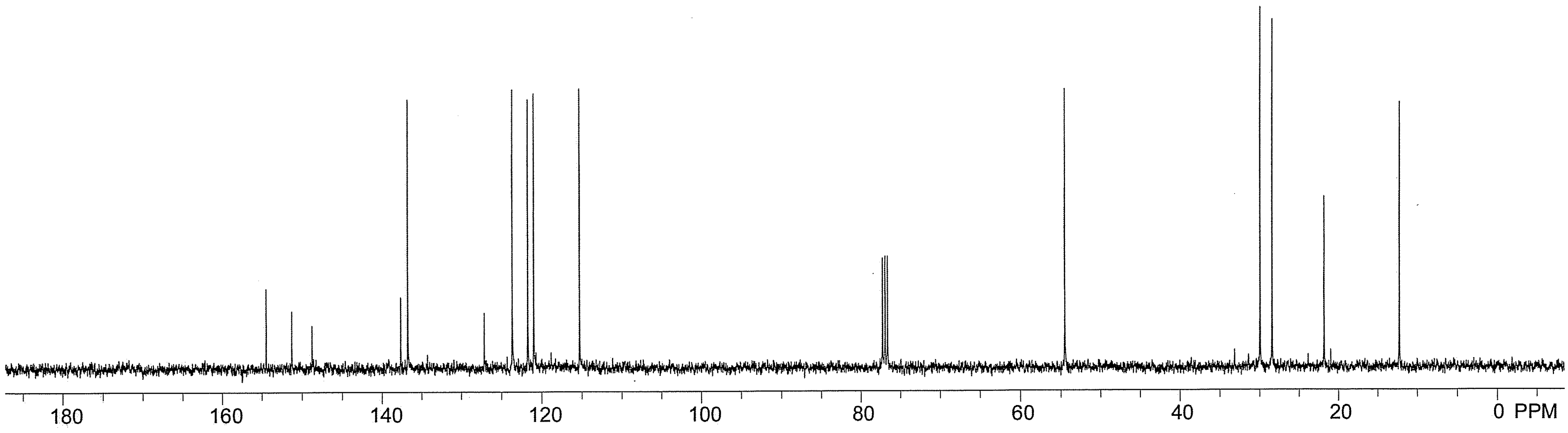
```
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-230-h.fid
new experiment
May 29 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length =  11.663 usec
Relaxation delay =   4.800 sec
NA =    12
Solvent  = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1  =  399.950684 MHz
F2  =  100.575279 MHz
SW1 =    8002.40 Hz
AT1 =  2.50 sec
Hz per Pt 1stD =  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 = -25.77
      C =  0.00
```



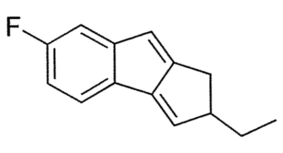


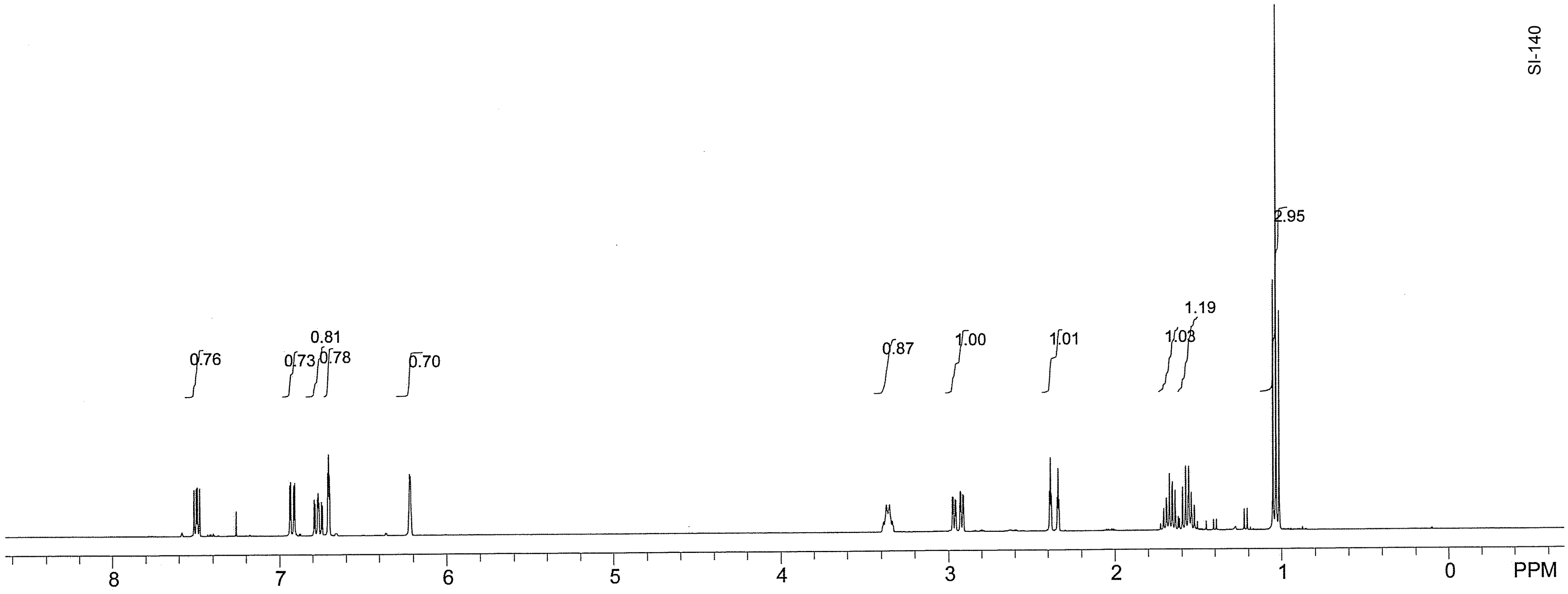
```
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-230-c2.fid
Standard c13 run using qnp probe
May 29 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length =    7.775 usec
Relaxation delay =    1.300 sec
NA =    128
Solvent  = cdcl3
FID PTS1d = 28040
PTS1d = 32768
F1  =  100.577232 MHz
F2  =  399.950684 MHz
SW1 =   28040.66 Hz
AT1 =   1.00 sec
Hz per Pt 1stD =   0.86 Hz
SW2 =       1.00 Hz
Hz per Pt 2ndD =   1.00 Hz
O1  =   10054.6484 Hz
O2  =      -0.5000 Hz
LB1 =  2.00      Hz
TP    A = -75.47
      B =  47.81
      C =   0.00
```



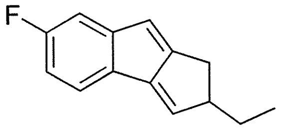


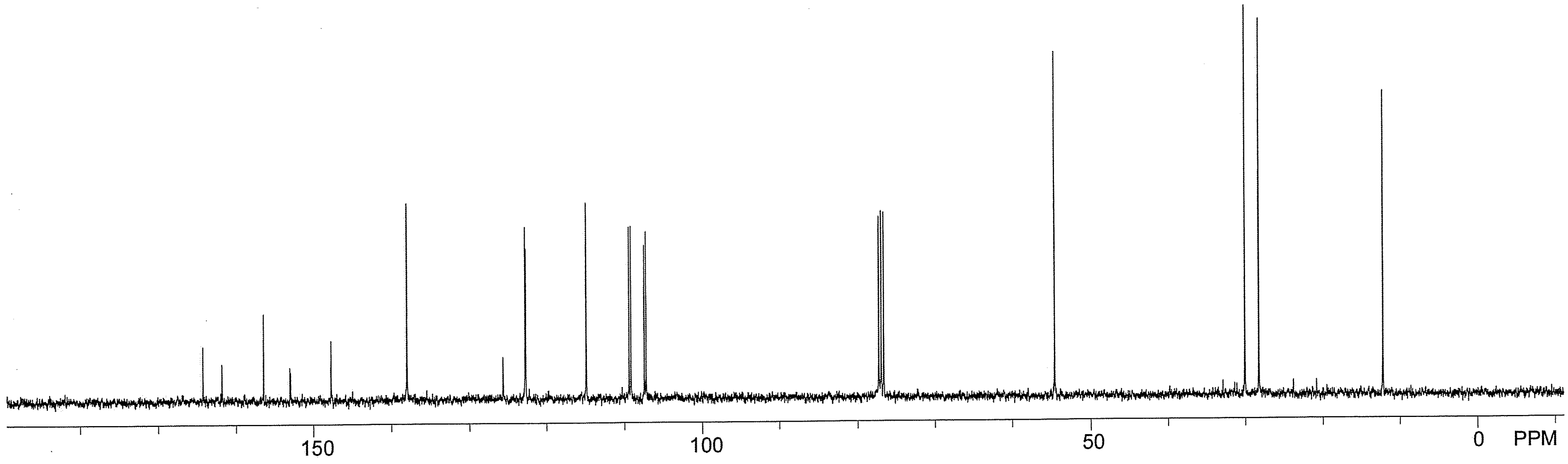
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-209-F-h.fid
new experiment
May 18 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 2.000 sec
NA = 12
Solvent = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 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 = -44.20
B = -35.16
C = 0.00





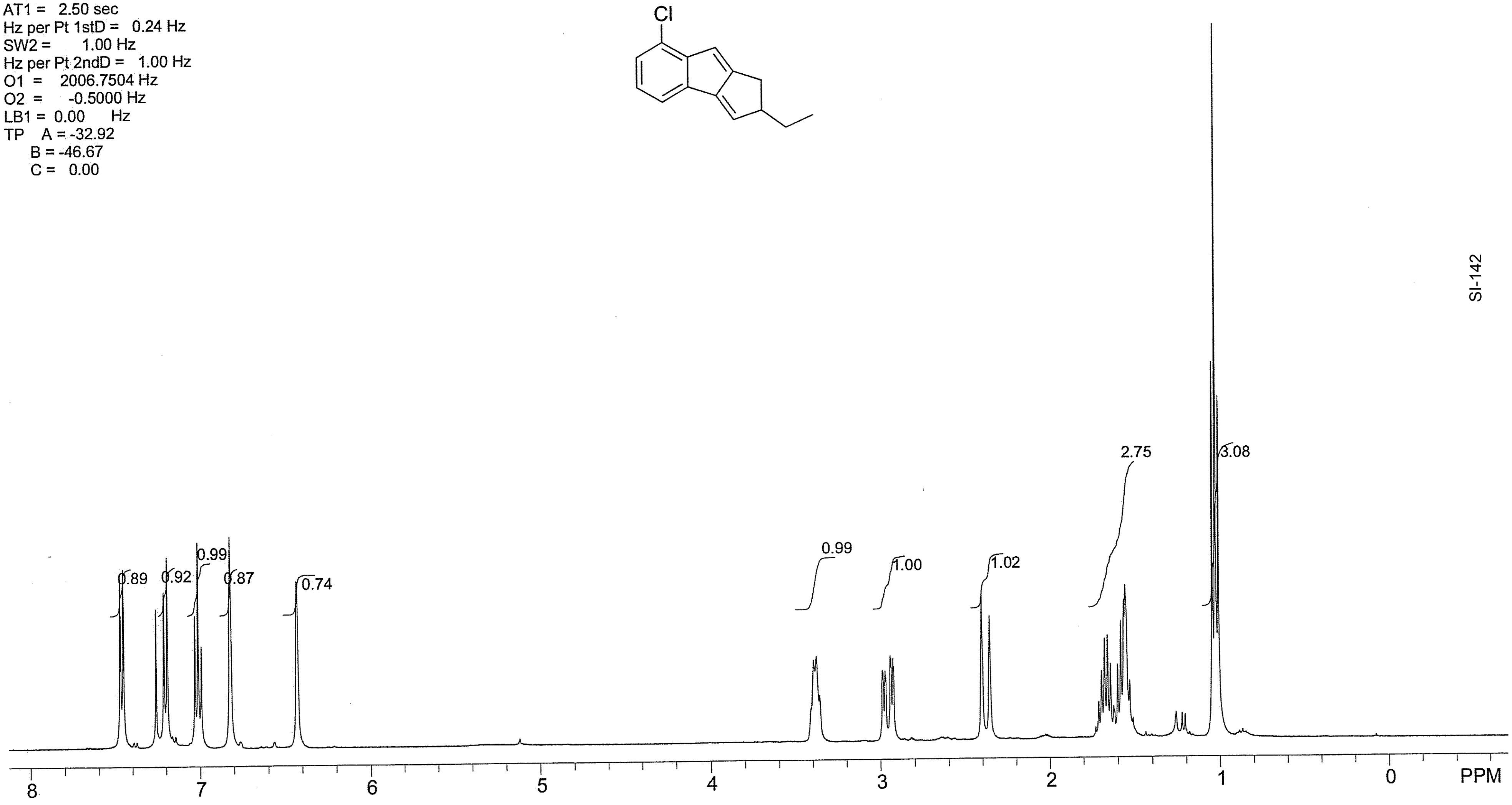
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-209-F-c2.fid
Standard c13 run using qnp probe
May 18 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 176
Solvent = cdcl3
FID PTS1d = 28040
PTS1d = 32768
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 28040.66 Hz
AT1 = 1.00 sec
Hz per Pt 1stD = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 10053.7930 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -25.78
B = 8.44
C = 0.00



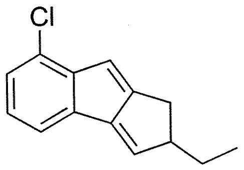


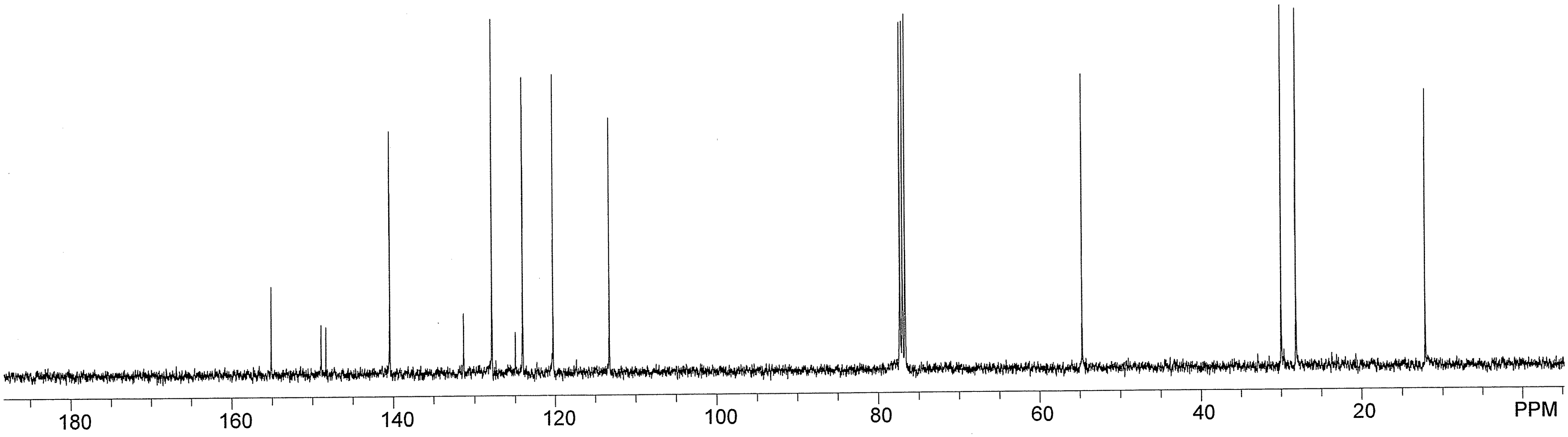
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-224-Cl-h.fid

May 26 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 12
Solvent = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 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 = -32.92
B = -46.67
C = 0.00

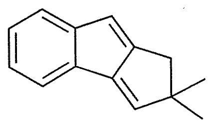


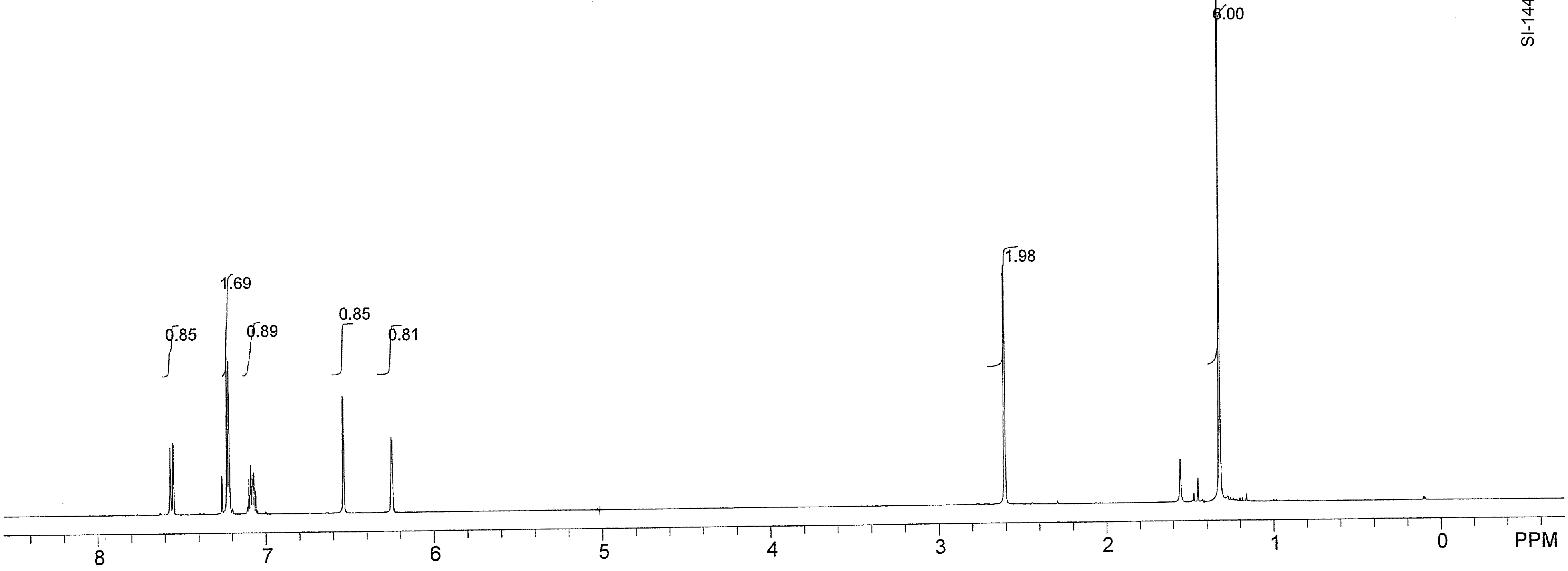
```
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-224-c2.fid
Standard c13 run using qnp probe
May 26 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length =    7.775 usec
Relaxation delay =    1.300 sec
NA  =   1212
Solvent  = cdcl3
FID PTS1d = 28040
PTS1d = 32768
F1  =  100.577232 MHz
F2  =  399.950684 MHz
SW1 =   28040.66 Hz
AT1 =   1.00 sec
Hz per Pt 1stD =   0.86 Hz
SW2 =       1.00 Hz
Hz per Pt 2ndD =   1.00 Hz
O1  =   10057.2168 Hz
O2  =      -0.5000 Hz
LB1 =  2.00      Hz
TP    A = -17.34
      B = -36.56
      C =   0.00
```





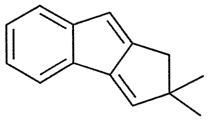
```
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-294-hh.fid

Jun 13 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length =   11.663 usec
Relaxation delay =    4.800 sec
NA =     10
Solvent  = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1  =  399.950684 MHz
F2  =  100.575279 MHz
SW1 =    8002.40 Hz
AT1 =   2.50 sec
Hz per Pt 1stD =   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 = -43.64
      B = -39.89
      C =   0.00
```

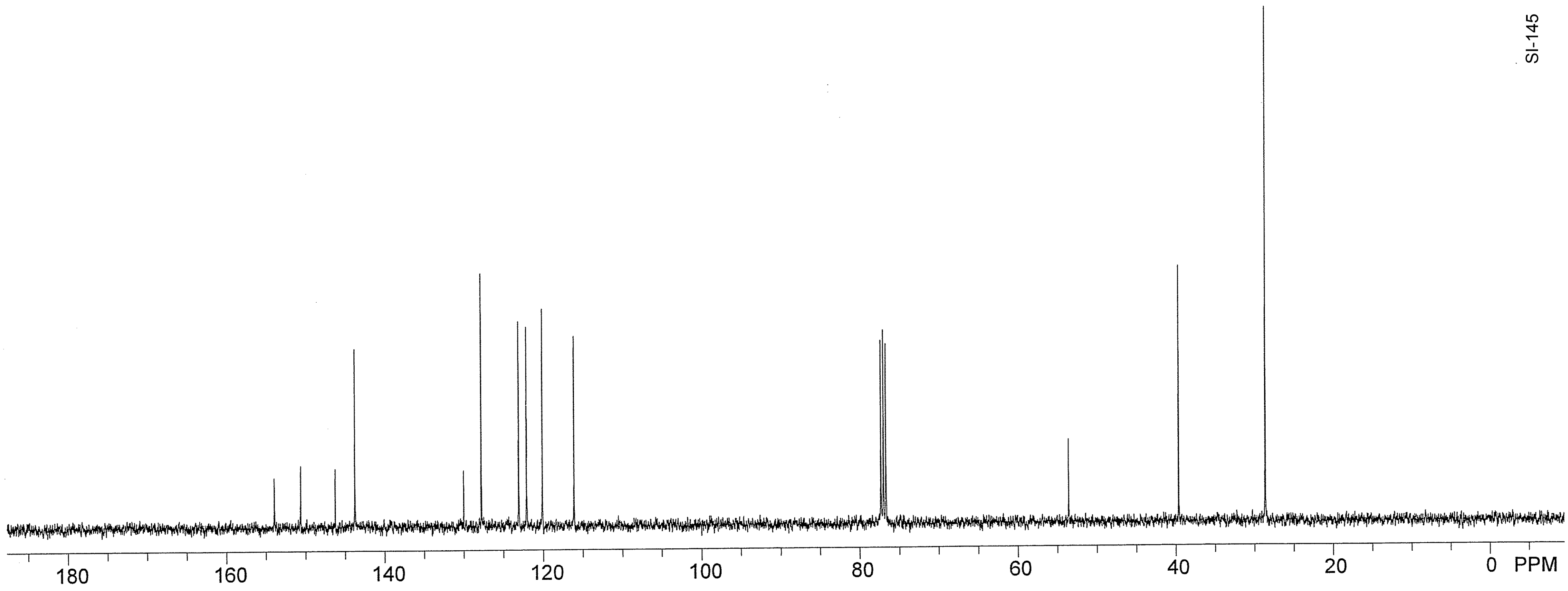




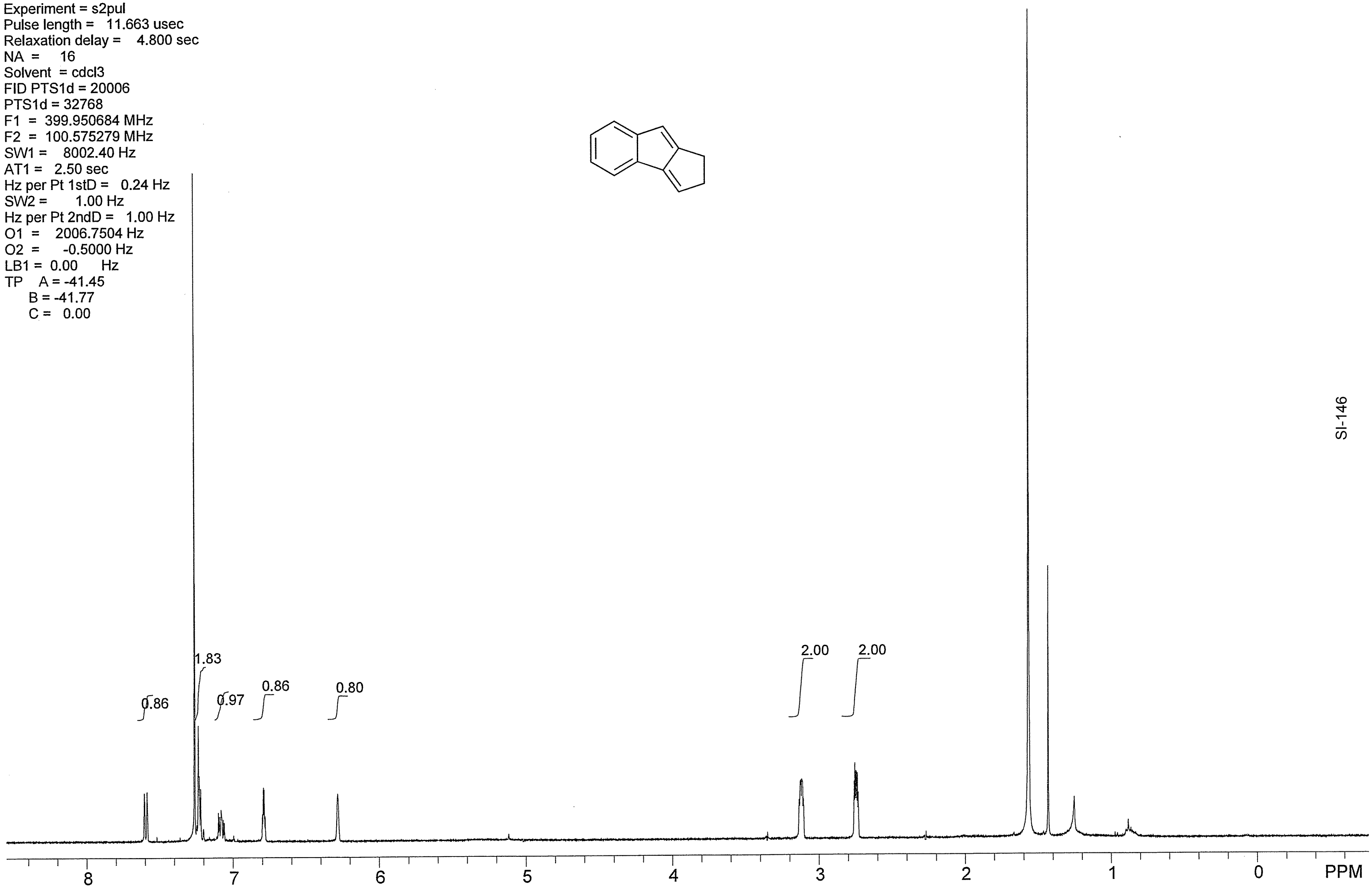
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-294-c1.fid

Jun 13 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 150
Solvent = cdcl3
FID PTS1d = 28040
PTS1d = 32768
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 28040.66 Hz
AT1 = 1.00 sec
Hz per Pt 1stD = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 10054.6484 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -33.05
B = 18.98
C = 0.00

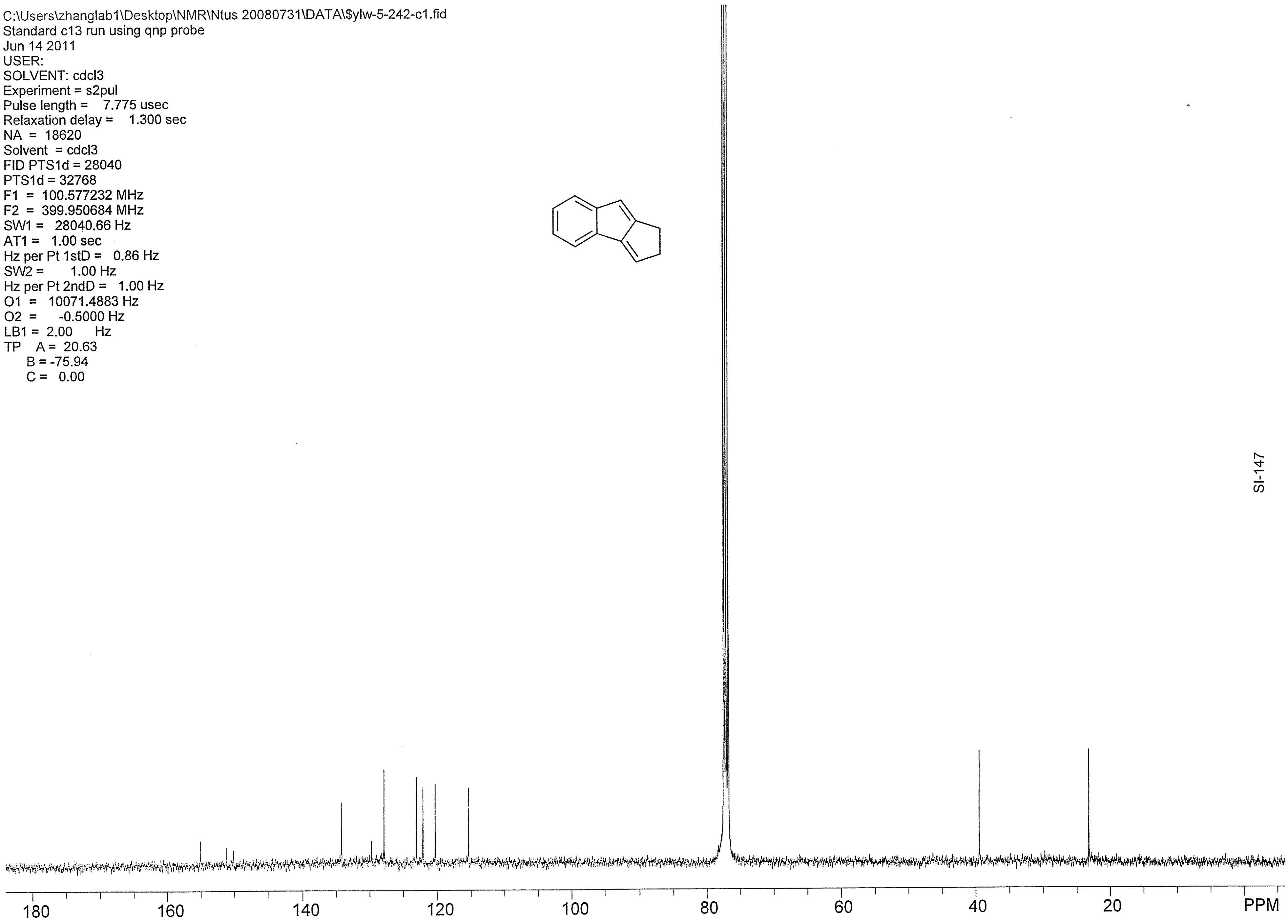




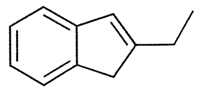
```
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-242-h.fid
new experiment
Jun 14 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length =   11.663 usec
Relaxation delay =    4.800 sec
NA =    16
Solvent  = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1  =  399.950684 MHz
F2  =  100.575279 MHz
SW1 =    8002.40 Hz
AT1 =   2.50 sec
Hz per Pt 1stD =   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 = -41.45
      B = -41.77
      C =   0.00
```

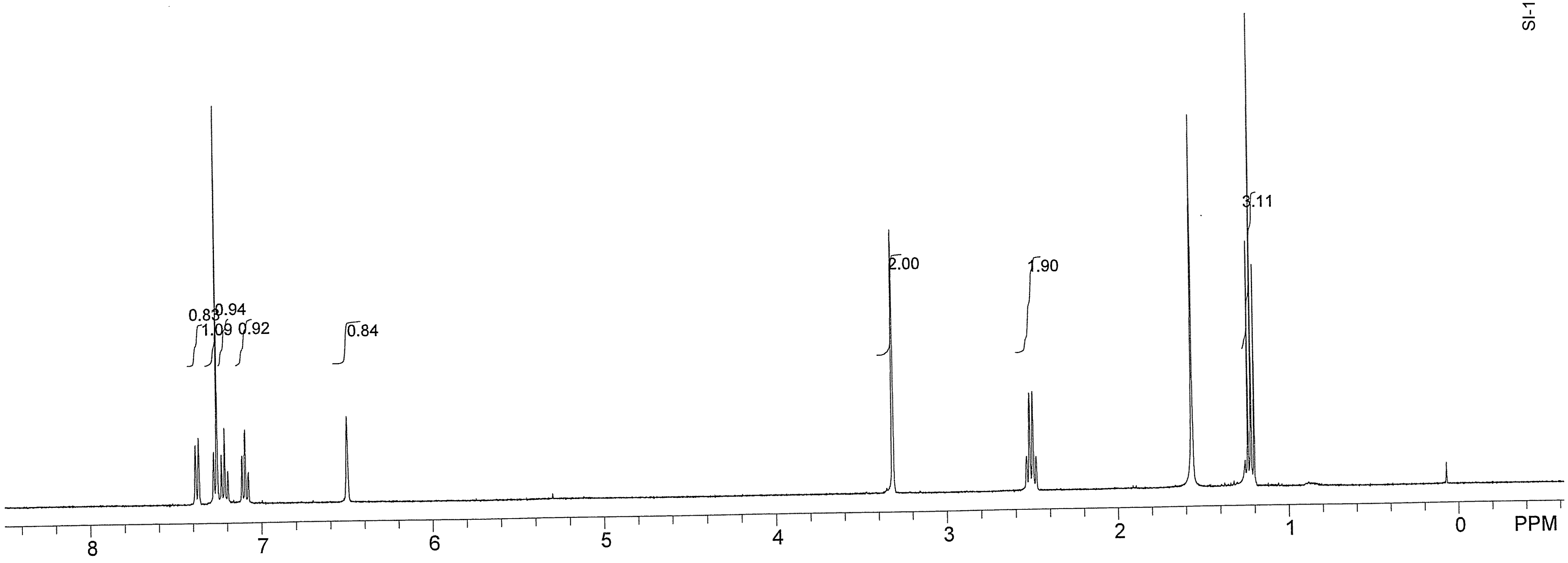


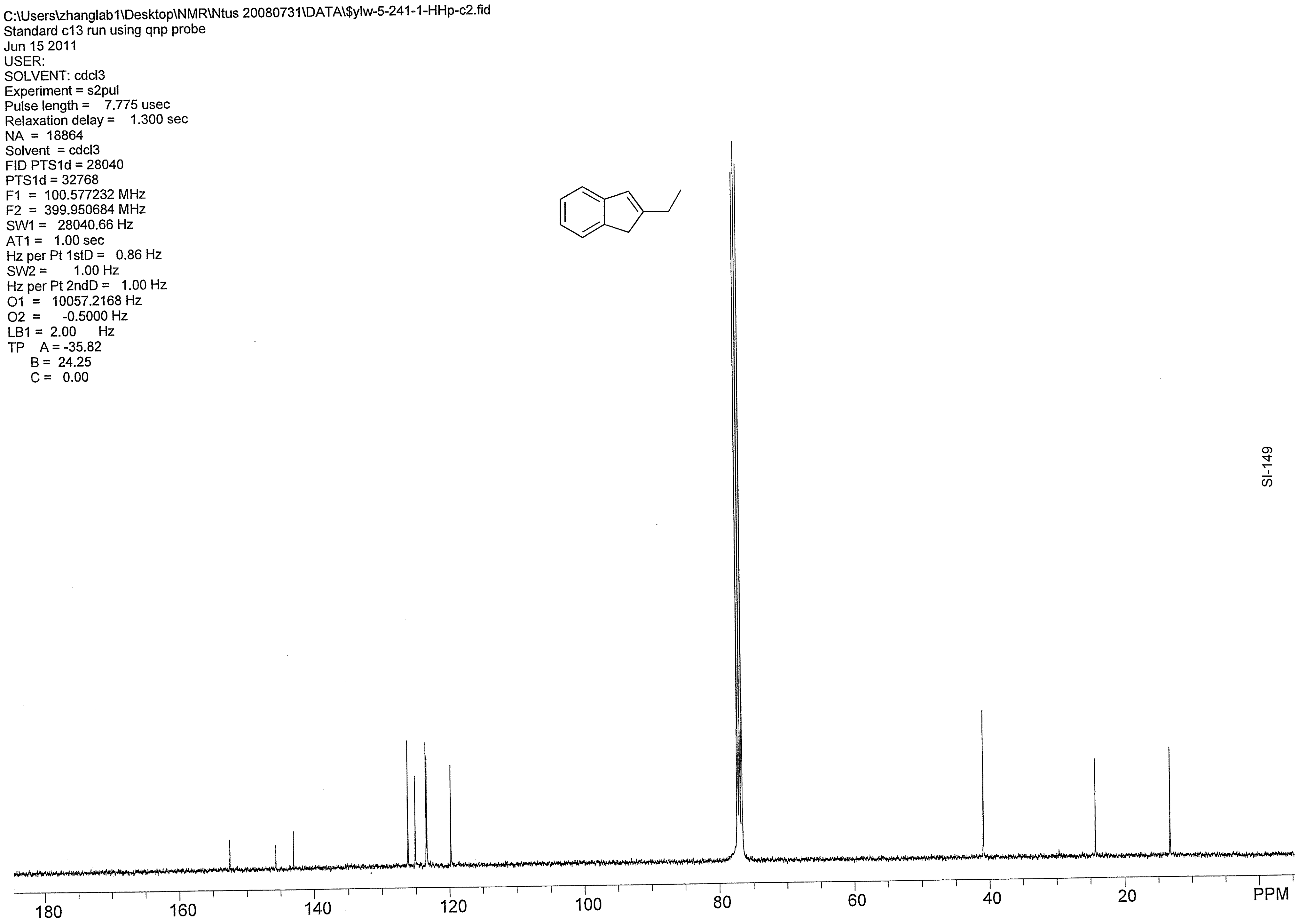
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-242-c1.fid
Standard c13 run using qnp probe
Jun 14 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 18620
Solvent = cdcl3
FID PTS1d = 28040
PTS1d = 32768
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 28040.66 Hz
AT1 = 1.00 sec
Hz per Pt 1stD = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 10071.4883 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = 20.63
B = -75.94
C = 0.00



C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-241-1.fid
new experiment
Jun 15 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 16
Solvent = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 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 = -52.09
B = -26.55
C = 0.00



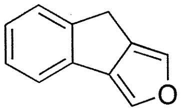


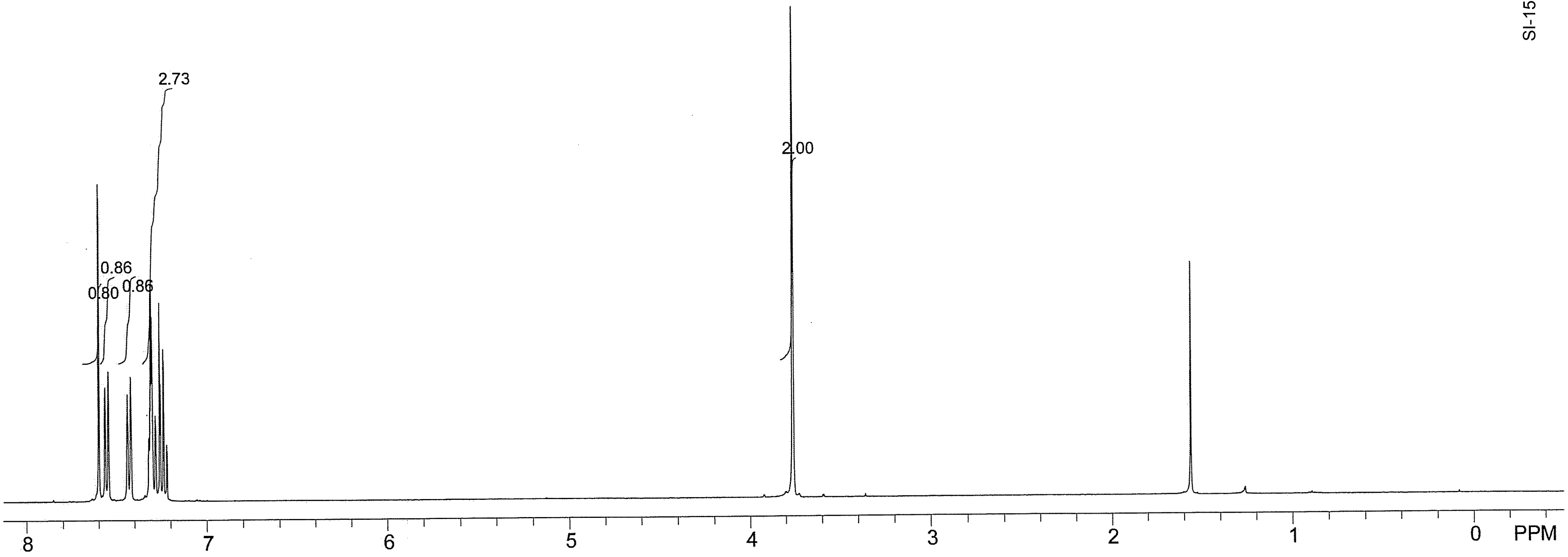


C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-241-1-HHp-c2.fid
Standard c13 run using qnp probe
Jun 15 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 18864
Solvent = cdcl3
FID PTS1d = 28040
PTS1d = 32768
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 28040.66 Hz
AT1 = 1.00 sec
Hz per Pt 1stD = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 10057.2168 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -35.82
B = 24.25
C = 0.00

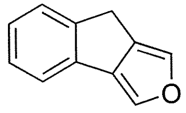
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-192-h.fid

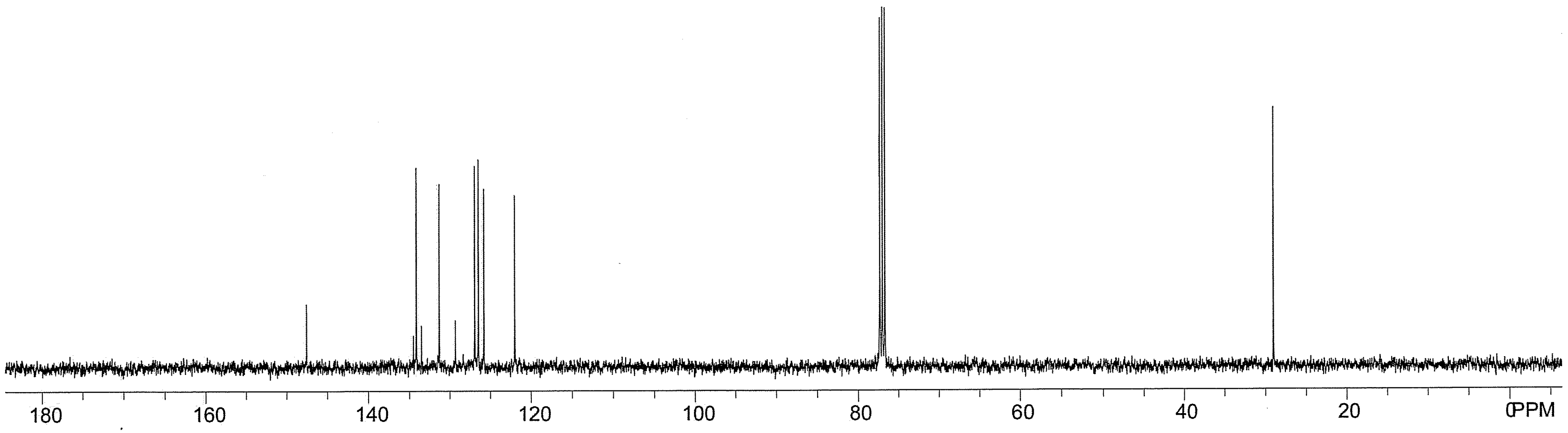
May 4 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 10
Solvent = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 0.24 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2006.7504 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -42.31
B = -28.55
C = 0.00



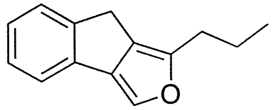


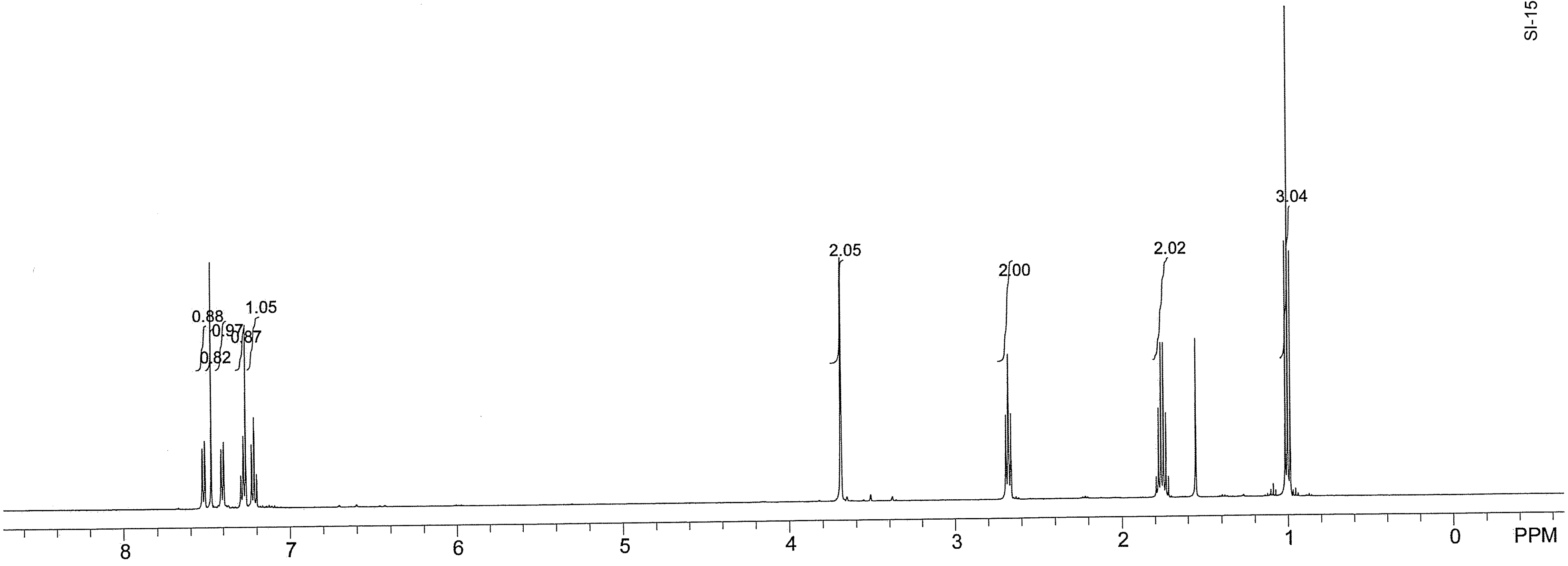
```
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-192-c.fid
Standard c13 run using qnp probe
May  4 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length =    7.775 usec
Relaxation delay =    1.300 sec
NA  =    306
Solvent  = cdcl3
FID PTS1d = 28040
PTS1d = 32768
F1  =  100.577232 MHz
F2  =  399.950684 MHz
SW1 =   28040.66 Hz
AT1 =   1.00 sec
Hz per Pt 1stD =   0.86 Hz
SW2 =        1.00 Hz
Hz per Pt 2ndD =   1.00 Hz
O1  =    10056.3604 Hz
O2  =       -0.5000 Hz
LB1 = 2.00      Hz
TP    A = -12.19
      B = -25.31
      C =   0.00
```



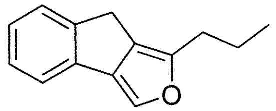


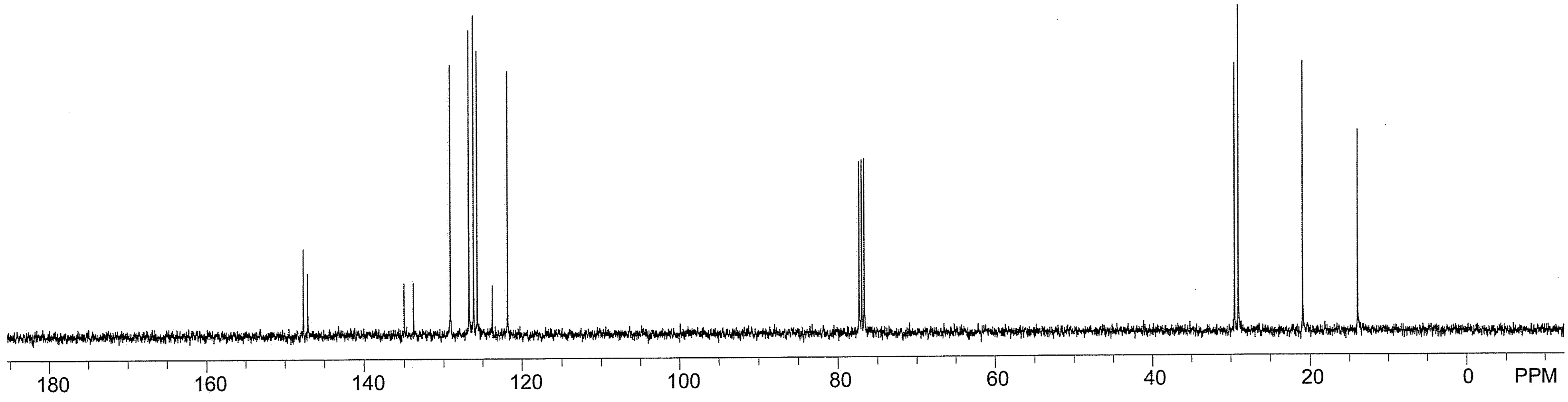
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-202-1.fid
STANDARD PROTON PARAMETERS
May 11 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.700 usec
Relaxation delay = 4.800 sec
NA = 8
Solvent = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1 = 499.858521 MHz
F2 = 125.700813 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 0.24 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2474.4551 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = 49.11
B = 8.65
C = 0.00





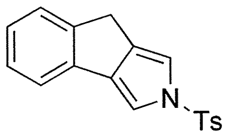
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-202-c1.fid
Standard c13 run using qnp probe
May 11 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 146
Solvent = cdcl3
FID PTS1d = 28040
PTS1d = 32768
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 28040.66 Hz
AT1 = 1.00 sec
Hz per Pt 1stD = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 10053.7930 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -27.66
B = -1.41
C = 0.00

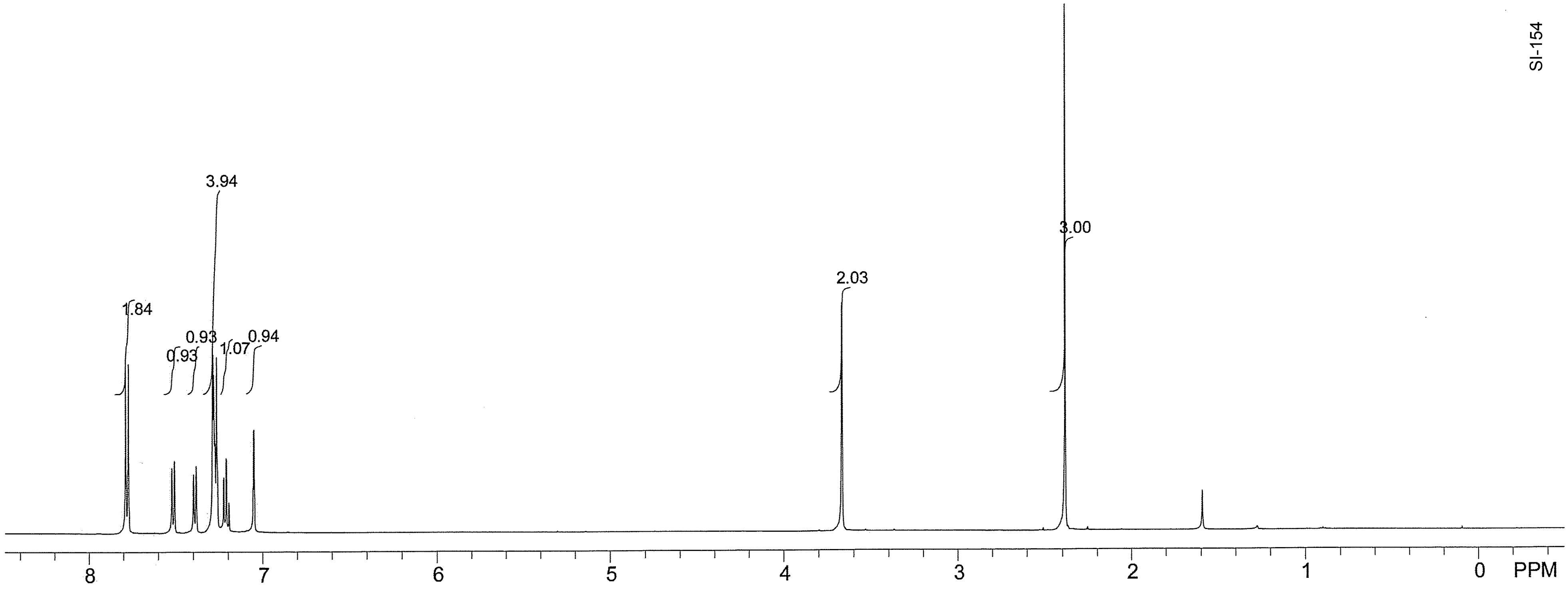




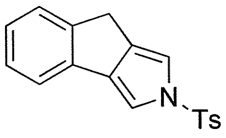
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-203-NTs-p.fid

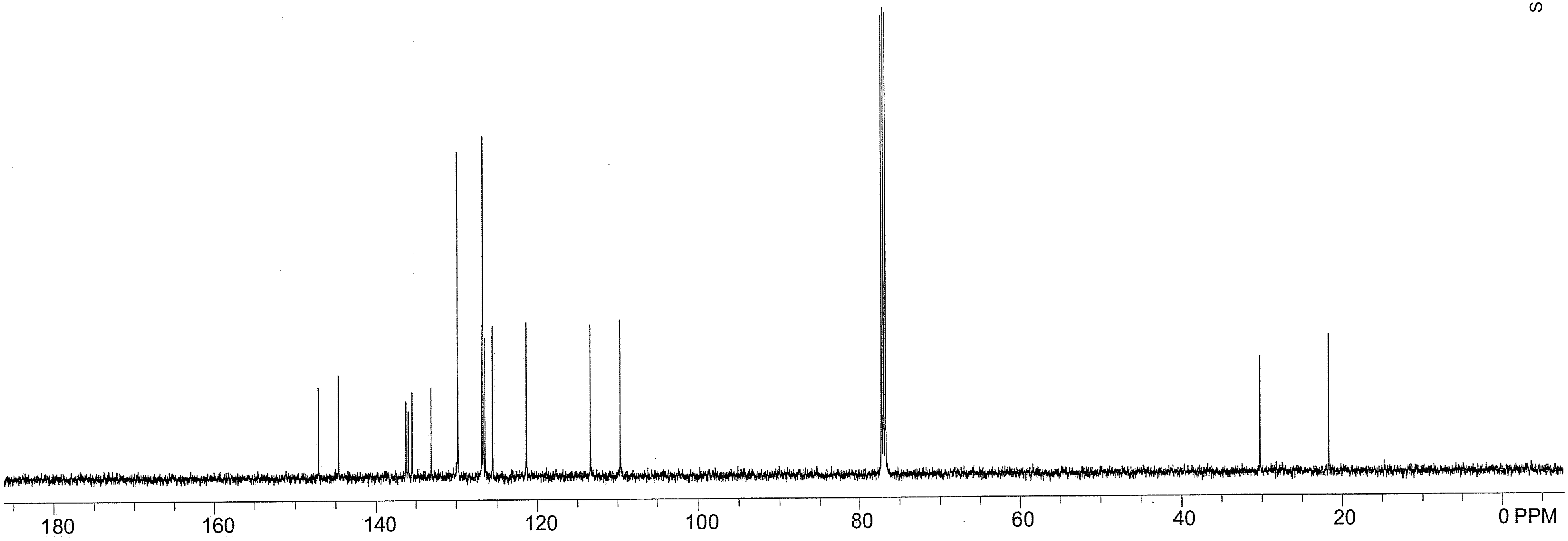
May 12 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.700 usec
Relaxation delay = 4.800 sec
NA = 8
Solvent = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1 = 499.858521 MHz
F2 = 125.700813 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 0.24 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2474.4551 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = 32.08
B = 6.59
C = 0.00



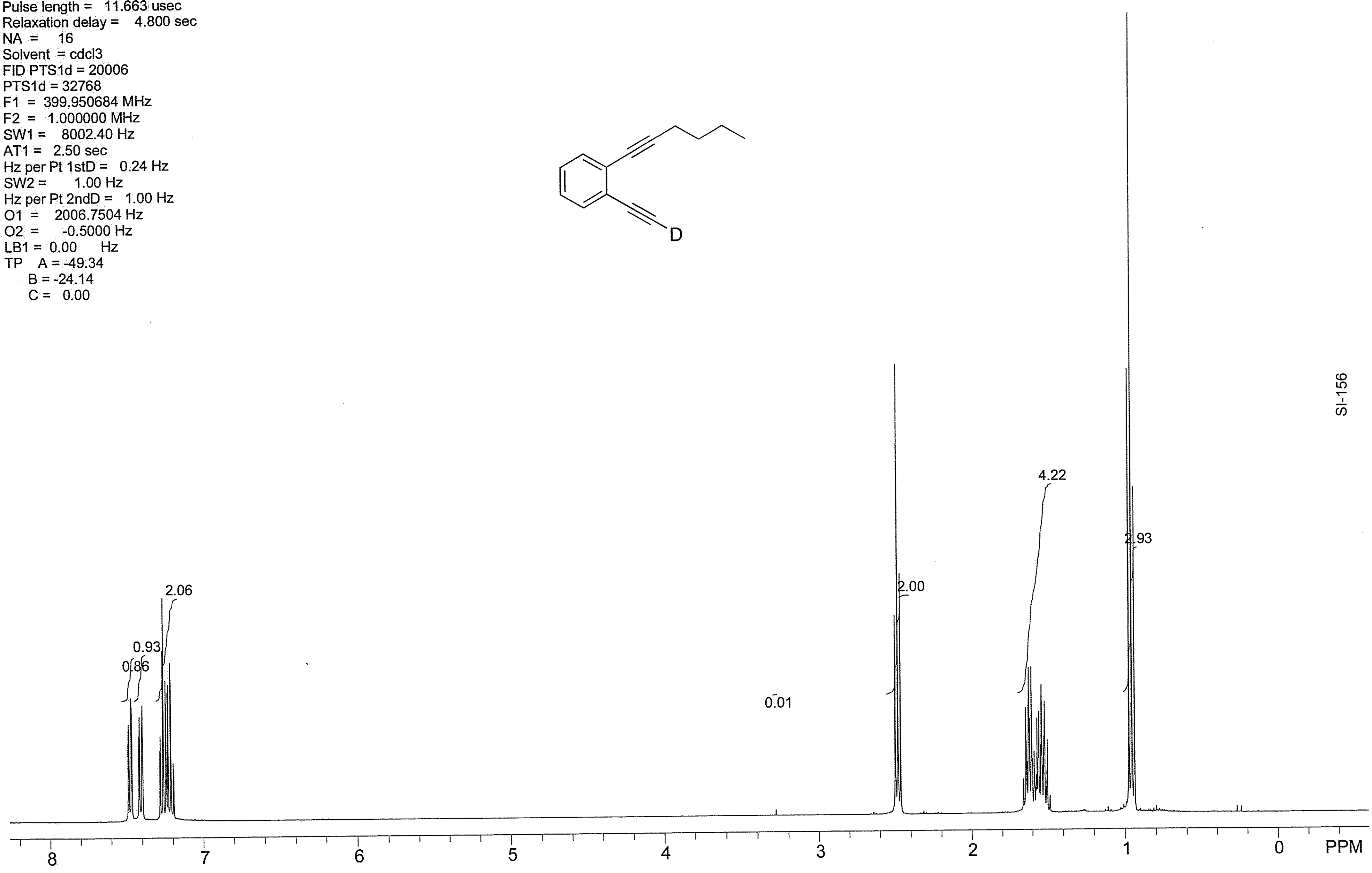


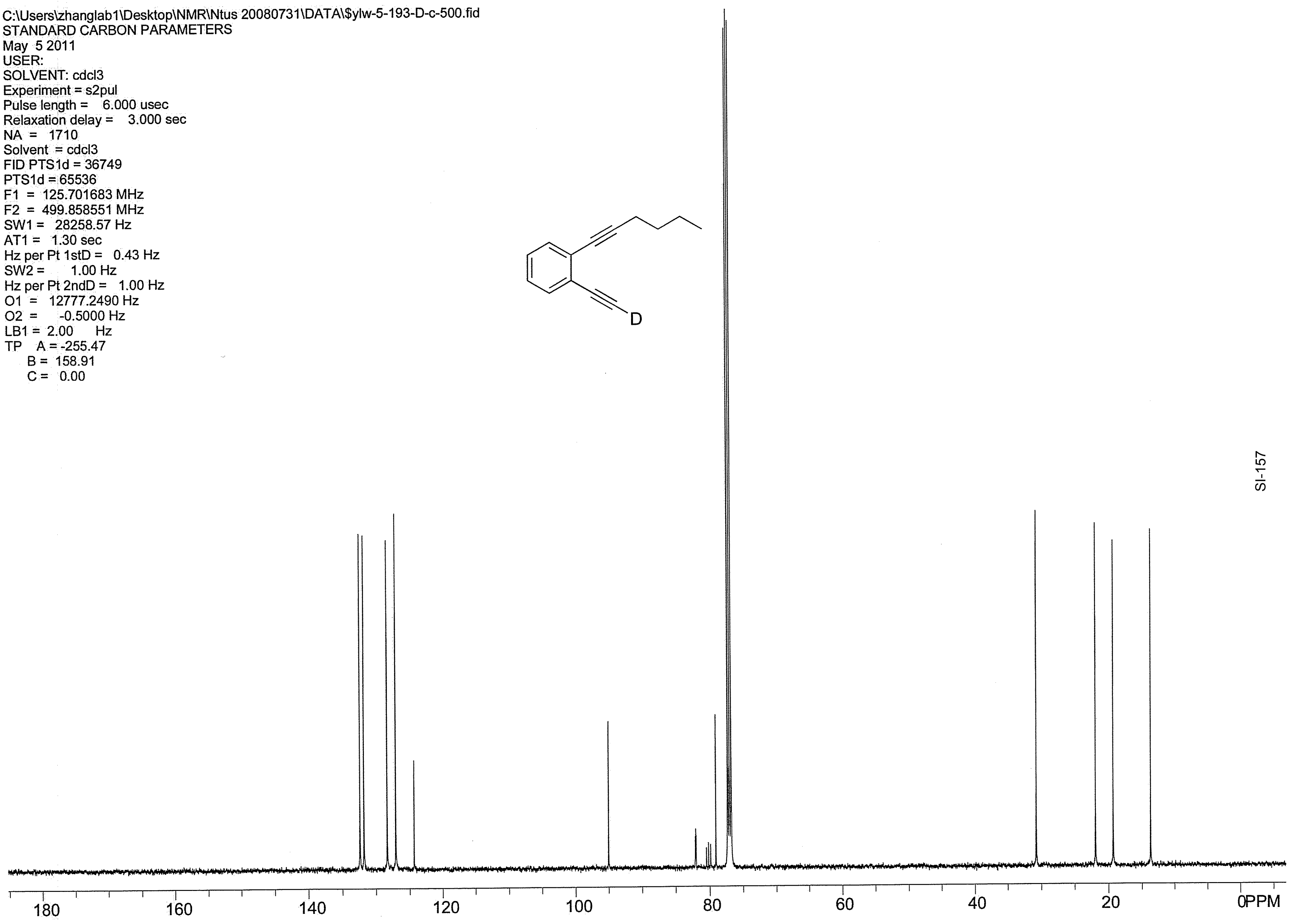
```
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-203-NTs-p-c1.fid
STANDARD CARBON PARAMETERS
May 12 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length =    6.000 usec
Relaxation delay =    3.000 sec
NA =    108
Solvent  = cdcl3
FID PTS1d = 36749
PTS1d = 65536
F1  =  125.701683 MHz
F2  =  499.858551 MHz
SW1 =   28258.57 Hz
AT1 =   1.30 sec
Hz per Pt 1stD =   0.43 Hz
SW2 =       1.00 Hz
Hz per Pt 2ndD =   1.00 Hz
O1  =   12767.7959 Hz
O2  =      -0.5000 Hz
LB1 = 2.00      Hz
TP    A = -231.56
      B =  142.03
      C =   0.00
```



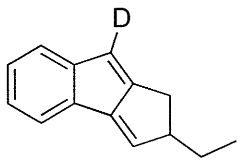


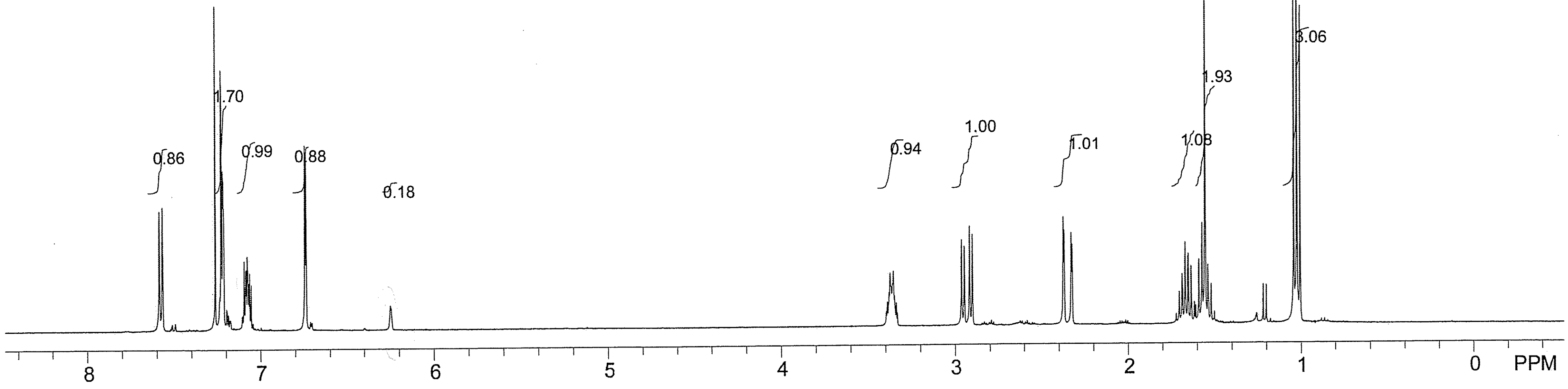
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-193-D.fid
new experiment
May 5 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 16
Solvent = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1 = 399.950684 MHz
F2 = 1.000000 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 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 = -49.34
B = -24.14
C = 0.00



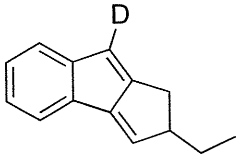

C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-193-D-c-500.fid
STANDARD CARBON PARAMETERS
May 5 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 6.000 usec
Relaxation delay = 3.000 sec
NA = 1710
Solvent = cdcl3
FID PTS1d = 36749
PTS1d = 65536
F1 = 125.701683 MHz
F2 = 499.858551 MHz
SW1 = 28258.57 Hz
AT1 = 1.30 sec
Hz per Pt 1stD = 0.43 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 12777.2490 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -255.47
B = 158.91
C = 0.00

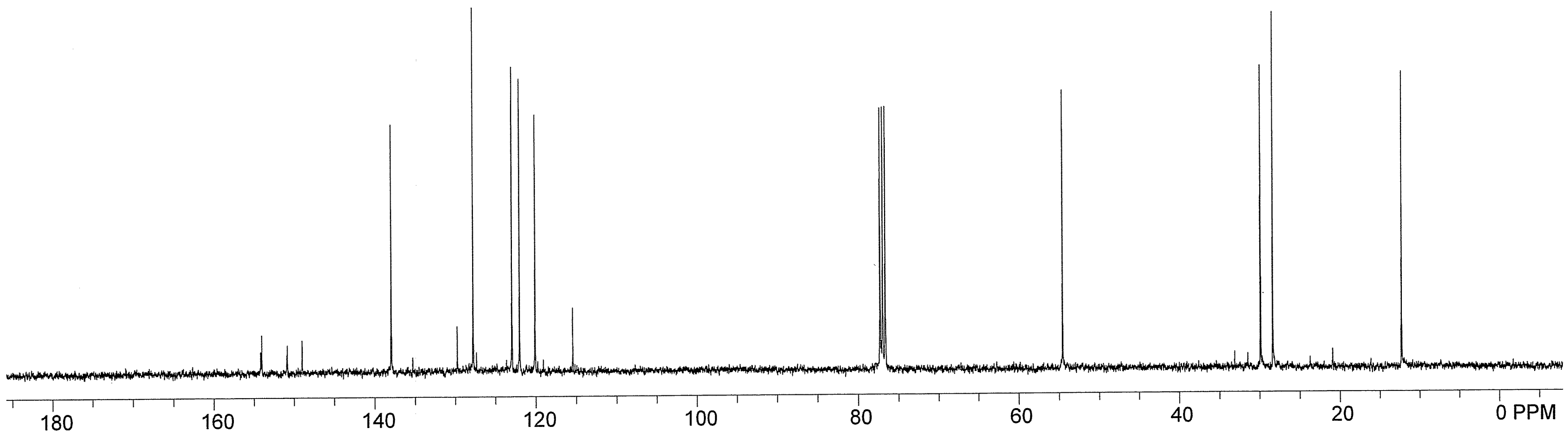
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-194-D2O-2.fid
new experiment
May 8 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 16
Solvent = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 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 = -46.40
B = -31.34
C = 0.00



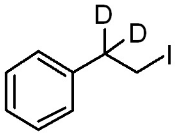


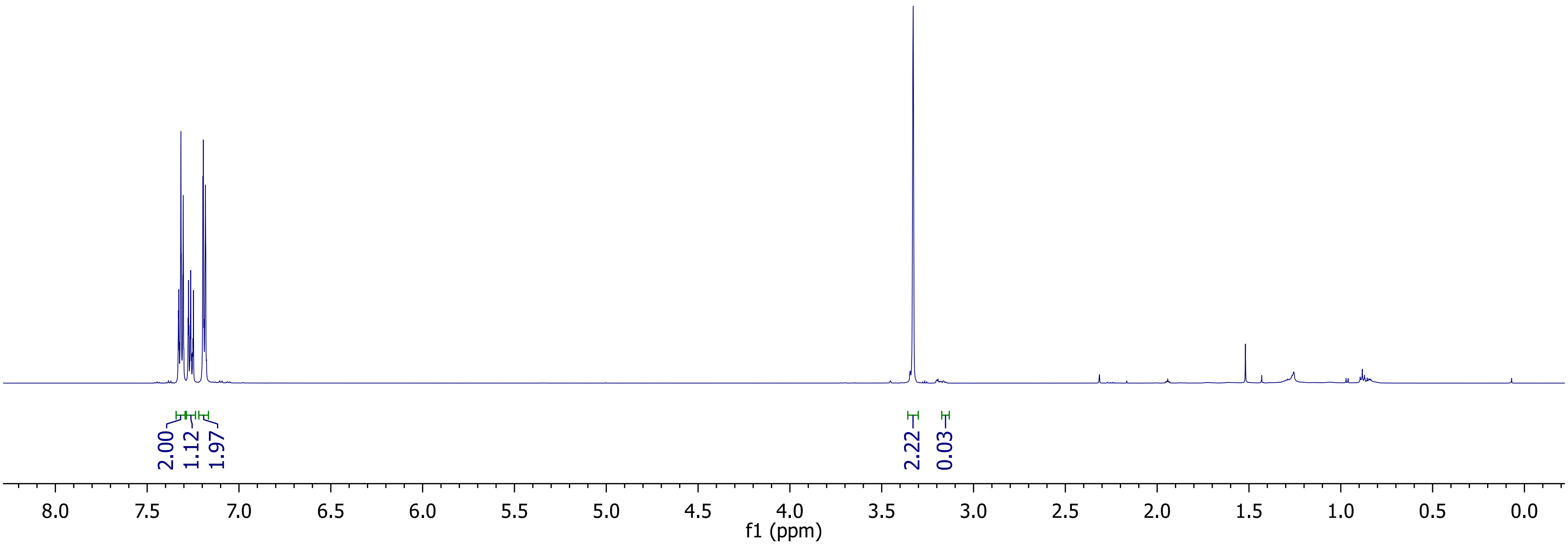
```
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-194-D2O-c1.fid
Standard c13 run using qnp probe
May  9 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length =    7.775 usec
Relaxation delay =    1.300 sec
NA  =  2144
Solvent  = cdcl3
FID PTS1d = 28040
PTS1d = 32768
F1  =  100.577232 MHz
F2  =  399.950684 MHz
SW1 =   28040.66 Hz
AT1 =   1.00 sec
Hz per Pt 1stD =   0.86 Hz
SW2 =       1.00 Hz
Hz per Pt 2ndD =   1.00 Hz
O1  =   10056.3613 Hz
O2  =      -0.5000 Hz
LB1 =  2.00      Hz
TP    A = -18.75
      B = -12.66
      C =   0.00
```

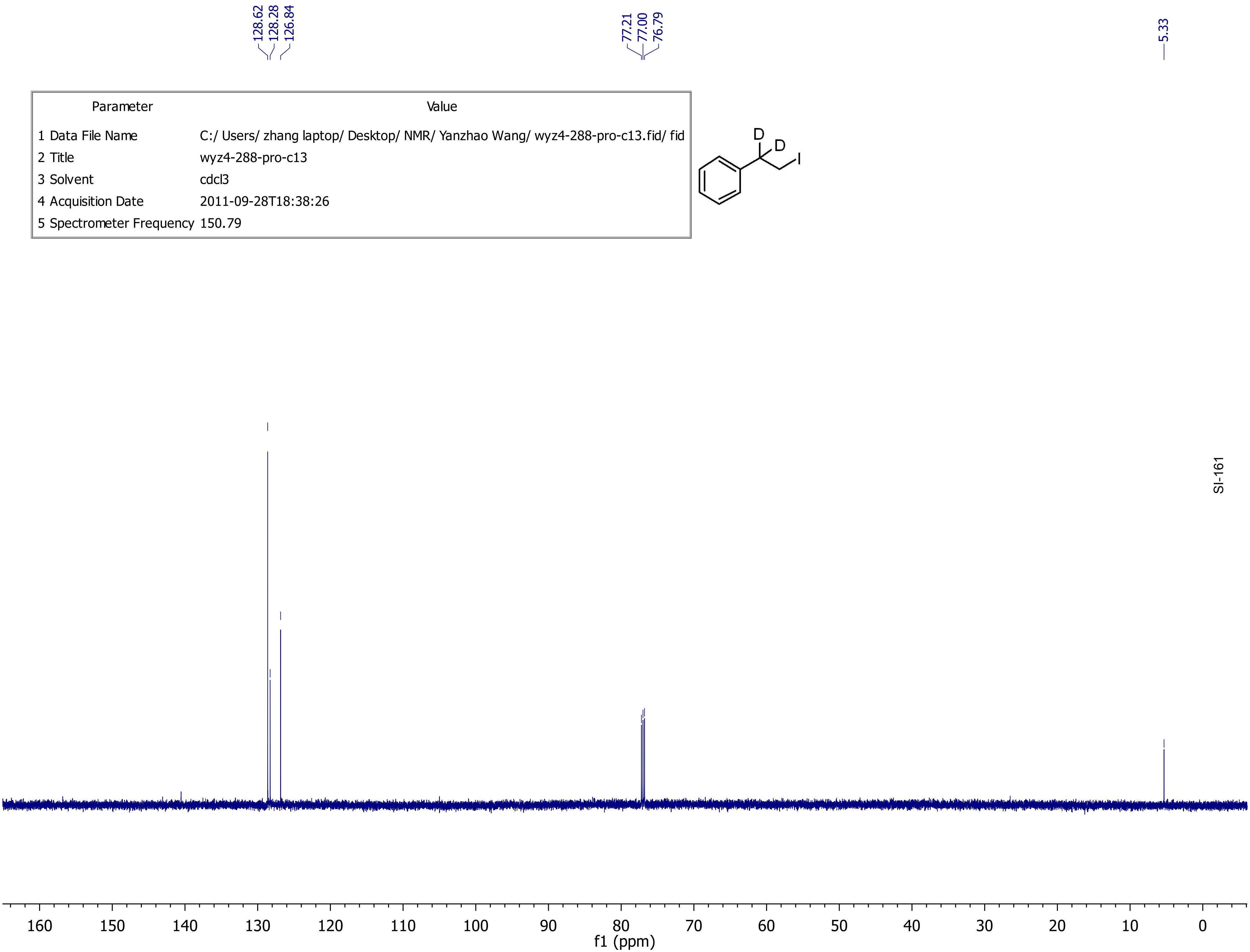




Parameter	Value
1 Data File Name	C:/ Users/ zhang laptop/ Desktop/ NMR/ Yanzhao Wang/ wyz4-288-pro-c13.fid/ fid
2 Title	wyz4-288-pro-c13
3 Solvent	cdcl3
4 Acquisition Date	2011-09-28T18:38:26
5 Spectrometer Frequency	150.79

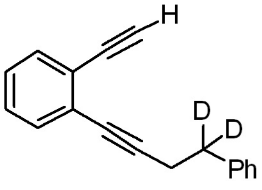


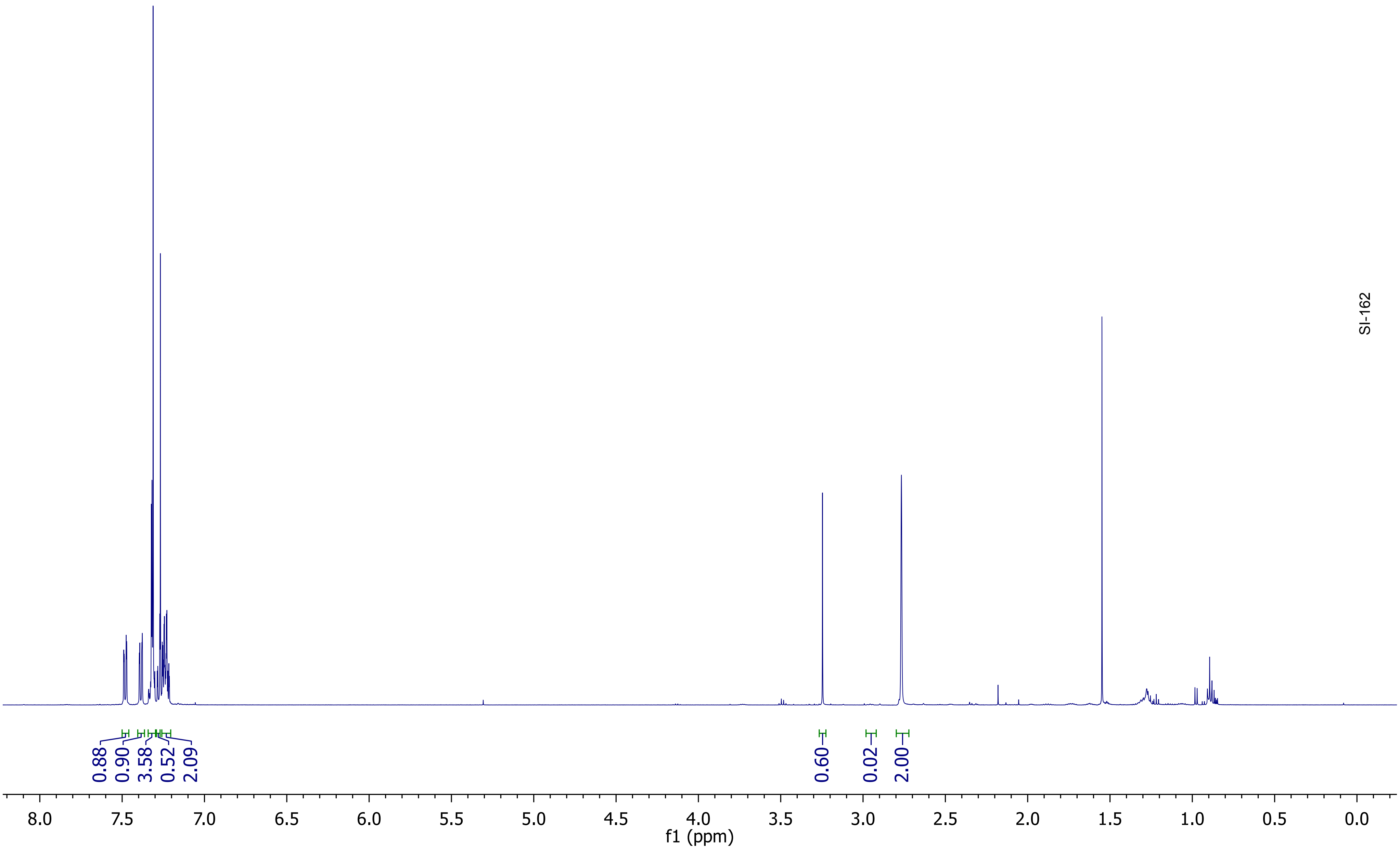


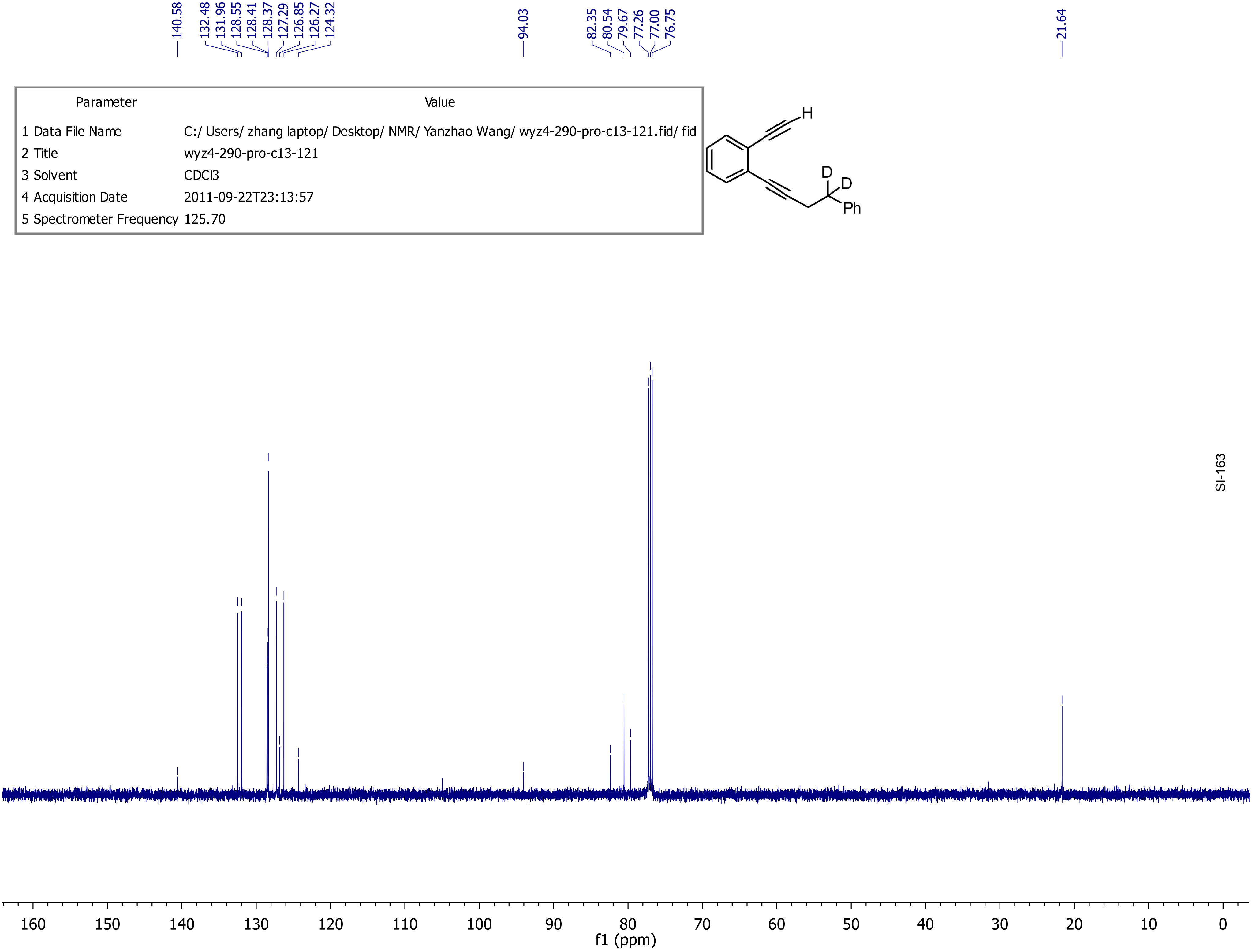


Parameter	Value
1 Data File Name	C:/ Users/ zhang laptop/ Desktop/ NMR/ Yanzhao Wang/ wyz4-288-pro-c13.fid/ fid
2 Title	wyz4-288-pro-c13
3 Solvent	cdcl3
4 Acquisition Date	2011-09-28T18:38:26
5 Spectrometer Frequency	150.79

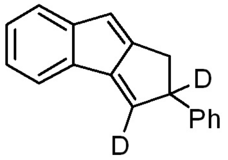
Parameter	Value
1 Data File Name	C:/ Users/ zhang laptop/ Desktop/ NMR/ Yanzhao Wang/ wyz4-290-por-h1.fid/ fid
2 Title	wyz4-290-por-h1
3 Solvent	CDCl3
4 Acquisition Date	2011-09-22T23:10:53
5 Spectrometer Frequency	499.86

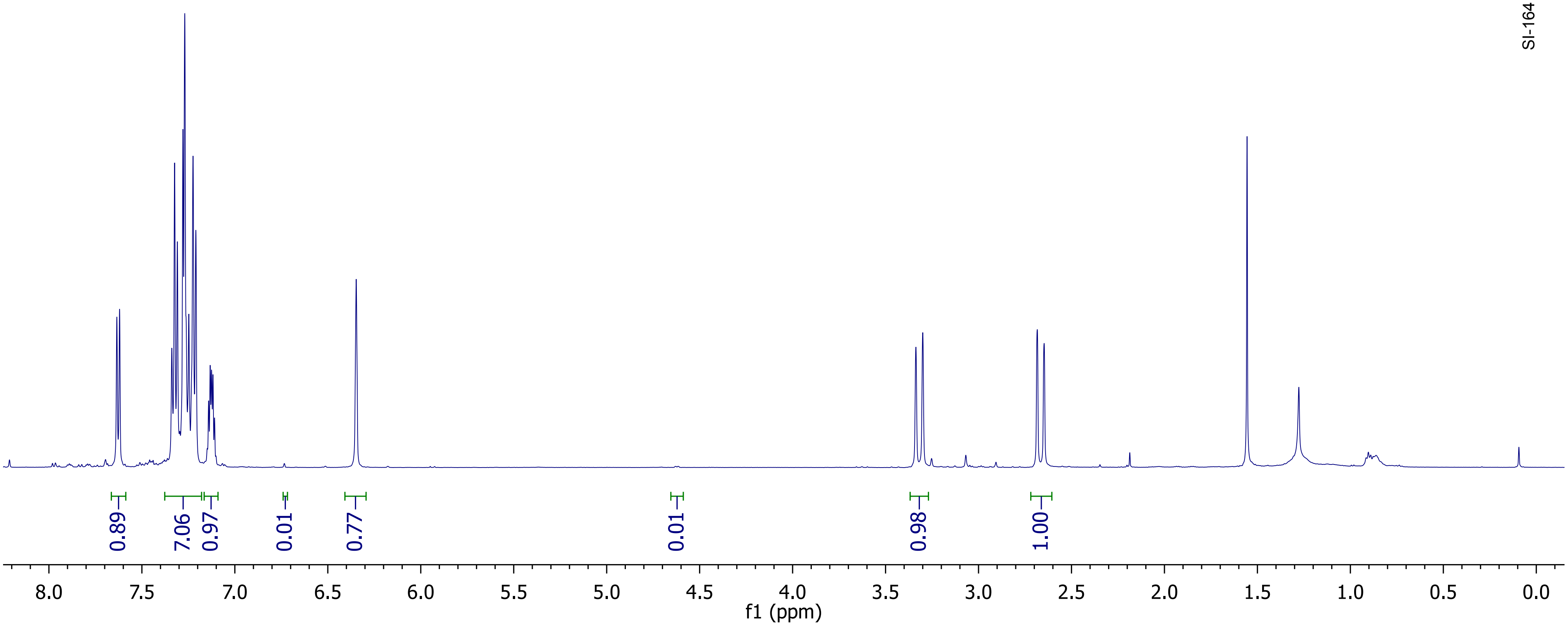




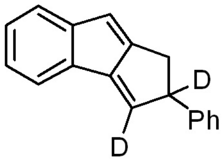


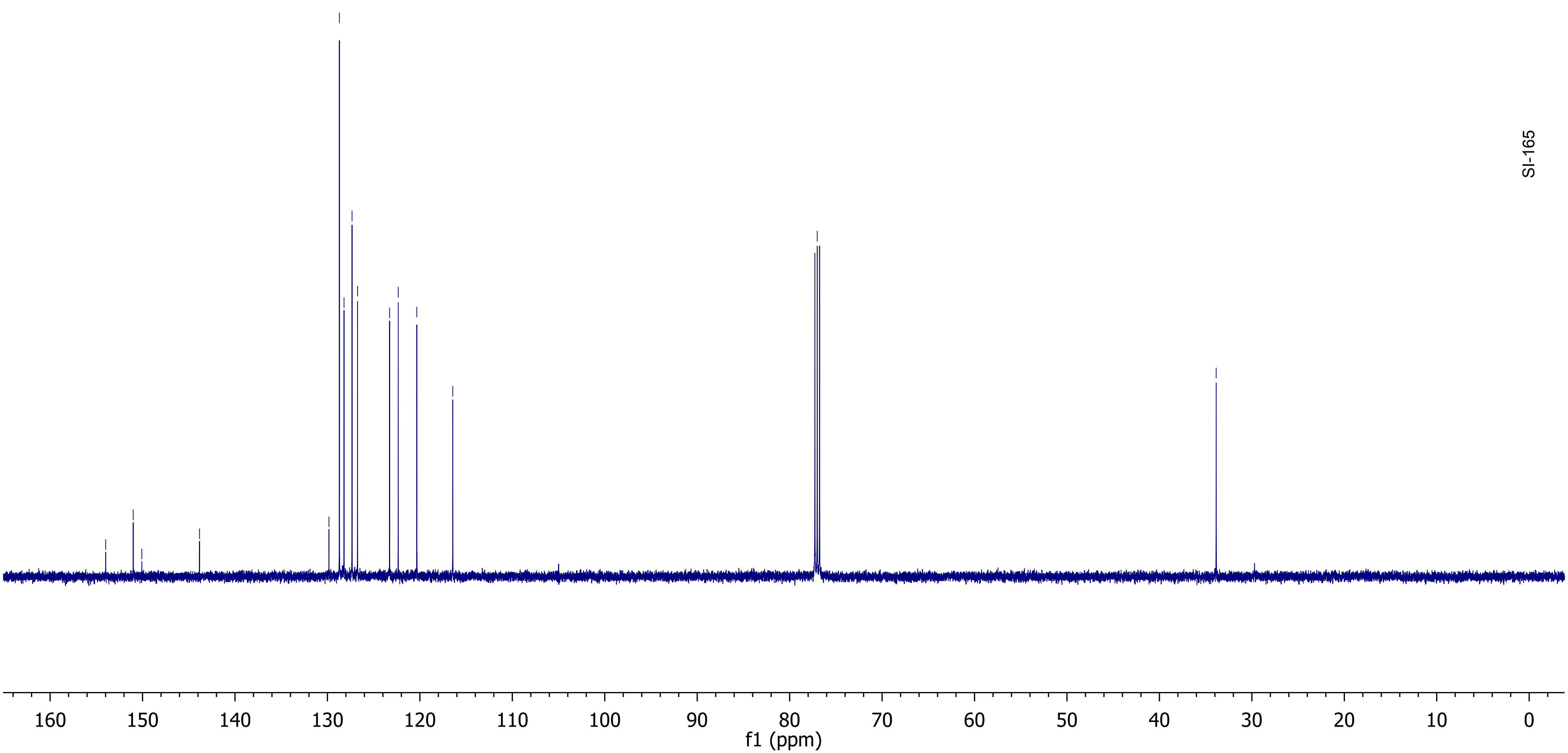
Parameter	Value
1 Data File Name	C:/ Users/ zhang laptop/ Desktop/ NMR/ Yanzhao Wang/ wyz4-292-pro-h1.fid/ fid
2 Title	wyz4-292-pro-h1
3 Solvent	CDCl3
4 Acquisition Date	2011-09-22T22:47:00
5 Spectrometer Frequency	499.86



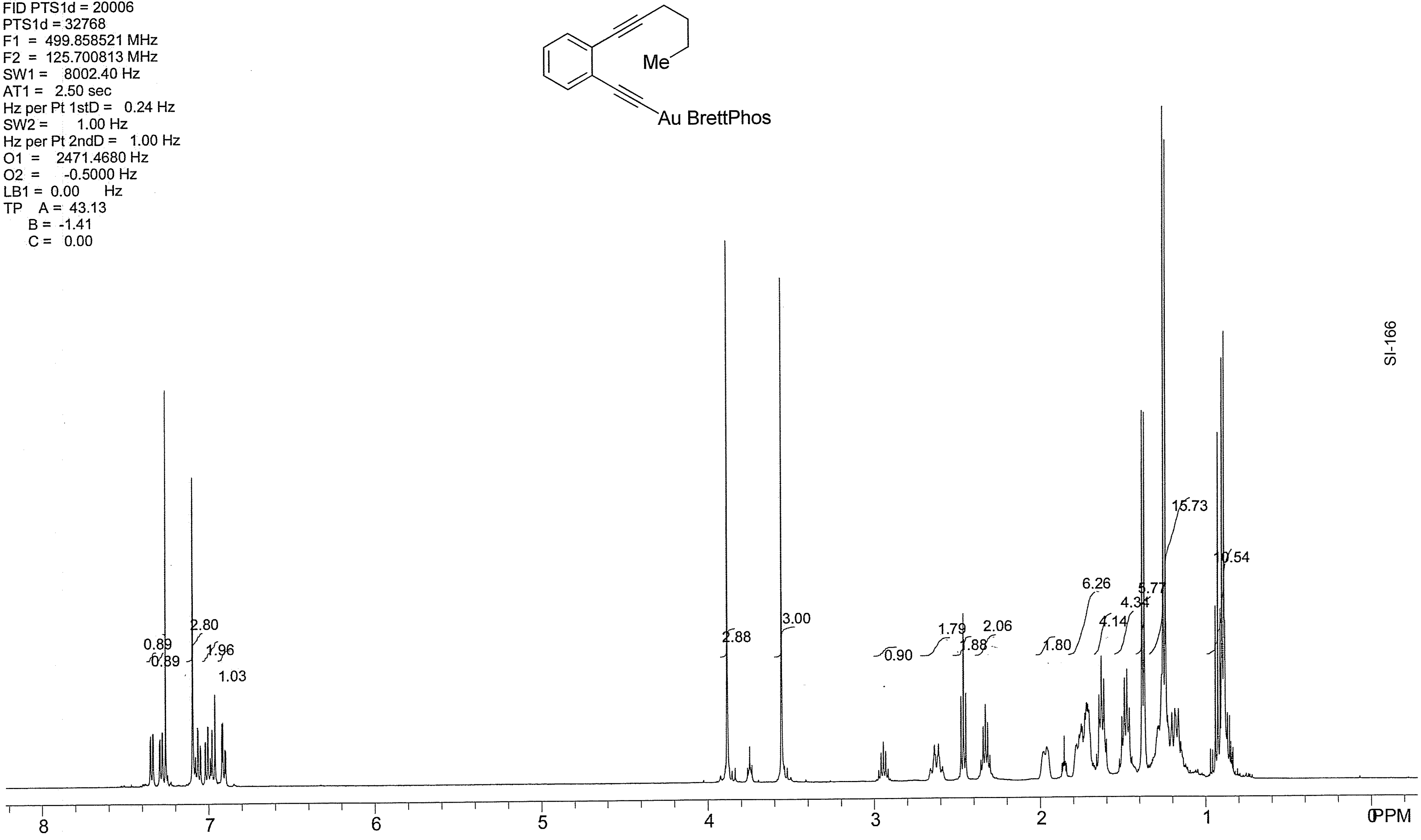


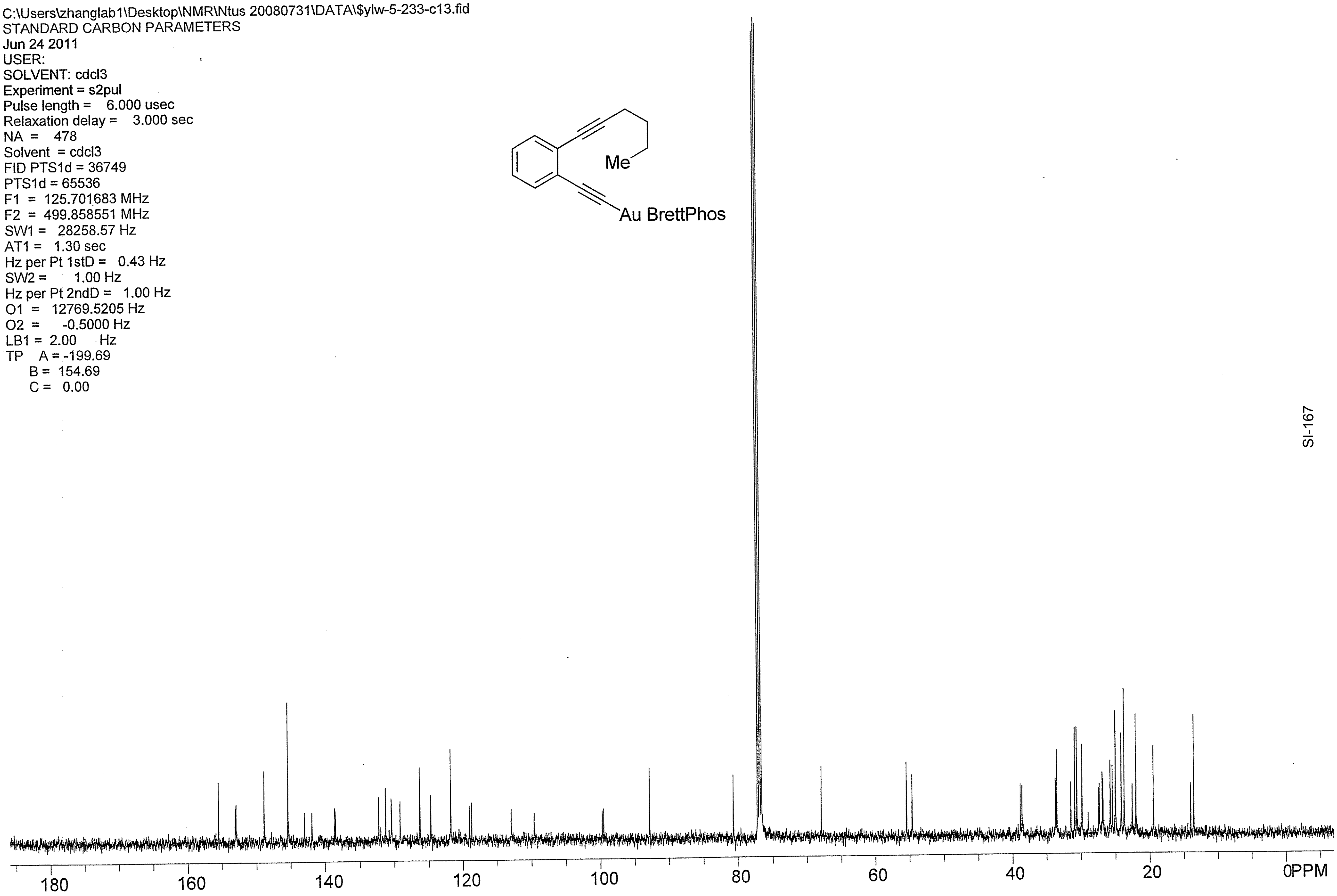
Parameter	Value
1 Data File Name	C:/ Users/ zhang laptop/ Desktop/ NMR/ Yanzhao Wang/ wyz4-292-pro-c13.fid/ fid
2 Title	wyz4-292-pro-c13
3 Solvent	CDCl3
4 Acquisition Date	2011-09-22T22:49:16
5 Spectrometer Frequency	125.70





C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-235-Aualkyne-h2.fid
STANDARD PROTON PARAMETERS
Jun 8 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.912 usec
Relaxation delay = 4.800 sec
NA = 32
Solvent = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1 = 499.858521 MHz
F2 = 125.700813 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 0.24 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2471.4680 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = 43.13
B = -1.41
C = 0.00

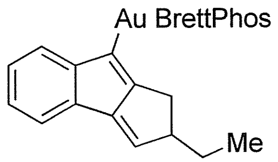


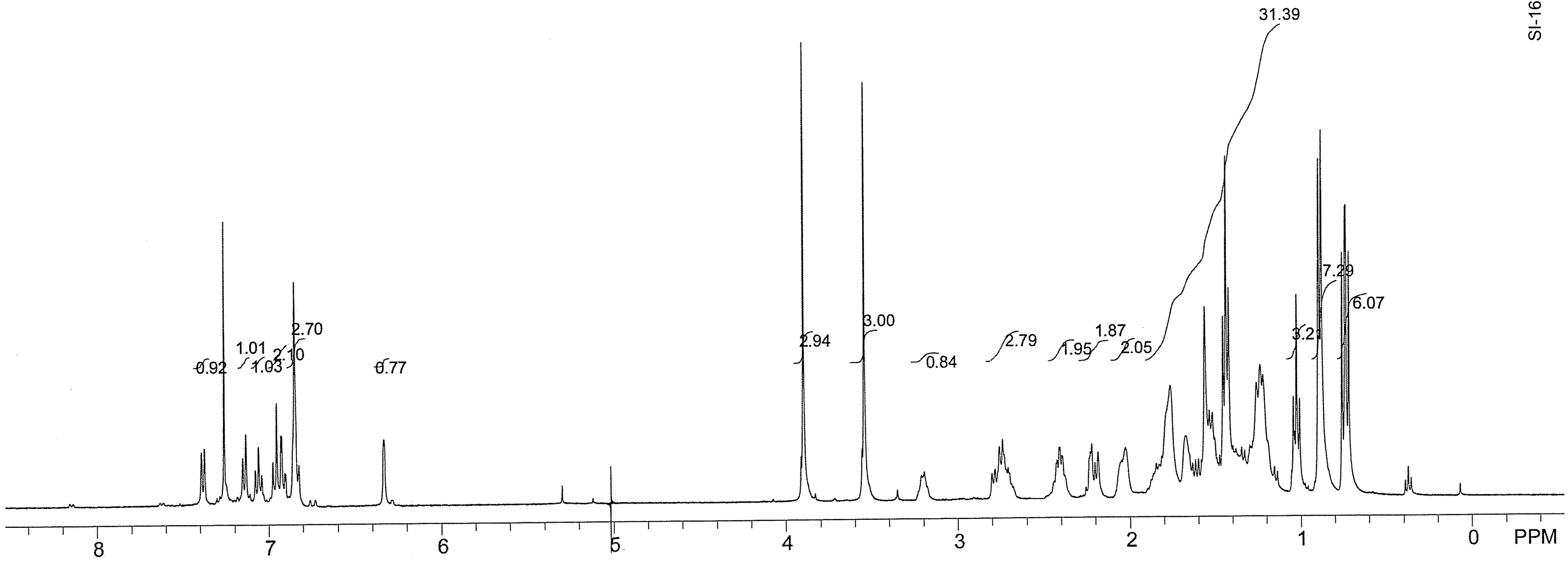


C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-233-c13.fid
STANDARD CARBON PARAMETERS
Jun 24 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 6.000 usec
Relaxation delay = 3.000 sec
NA = 478
Solvent = cdcl3
FID PTS1d = 36749
PTS1d = 65536
F1 = 125.701683 MHz
F2 = 499.858551 MHz
SW1 = 28258.57 Hz
AT1 = 1.30 sec
Hz per Pt 1stD = 0.43 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 12769.5205 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -199.69
B = 154.69
C = 0.00

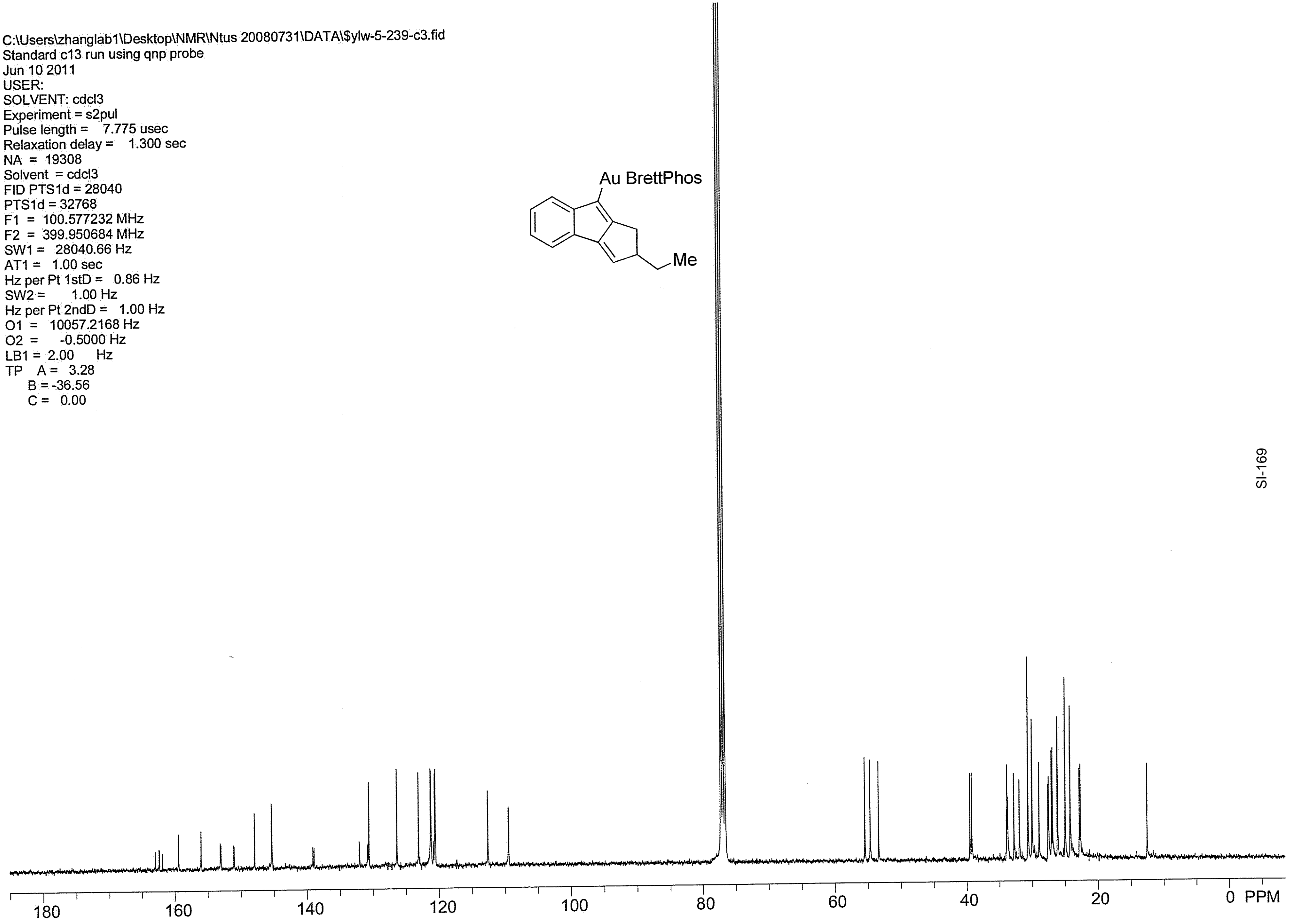
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-239-h2.fid

Jun 10 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 10
Solvent = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 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 = -27.41
B = -64.86
C = 0.00

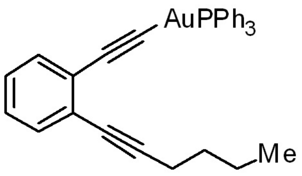


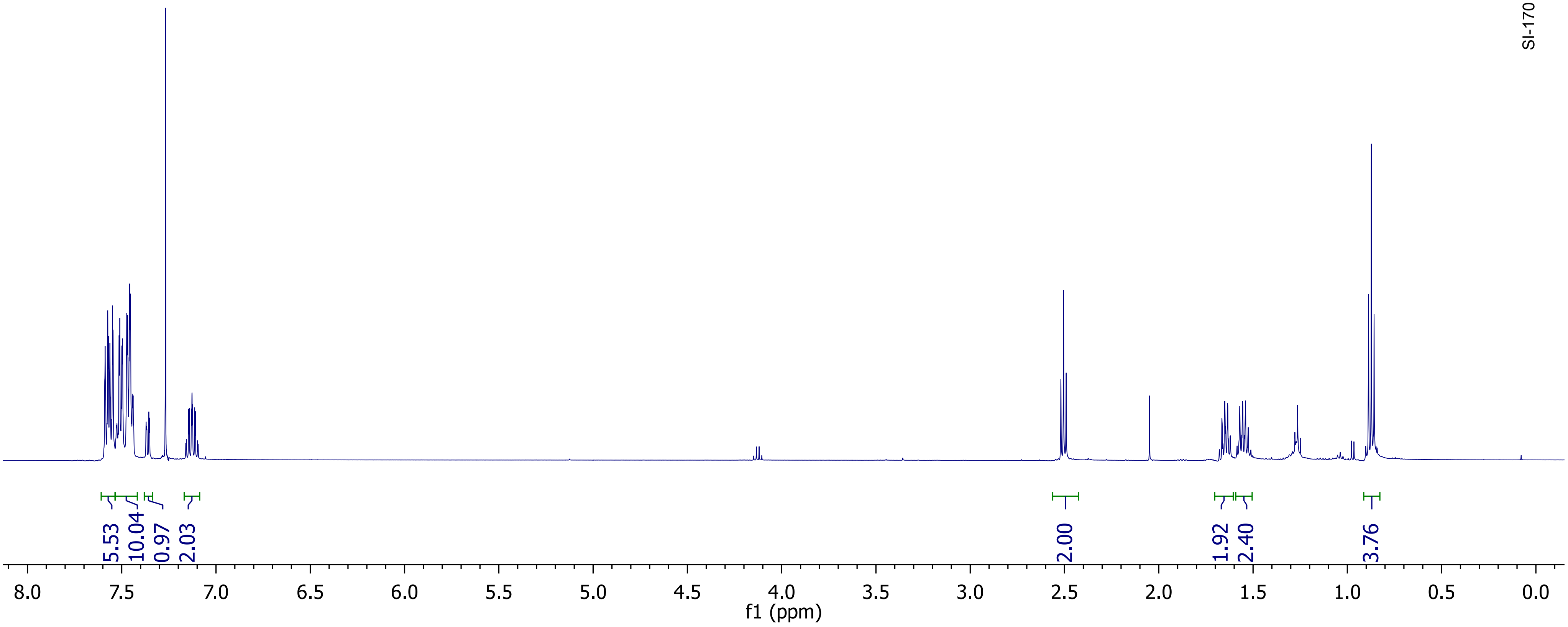


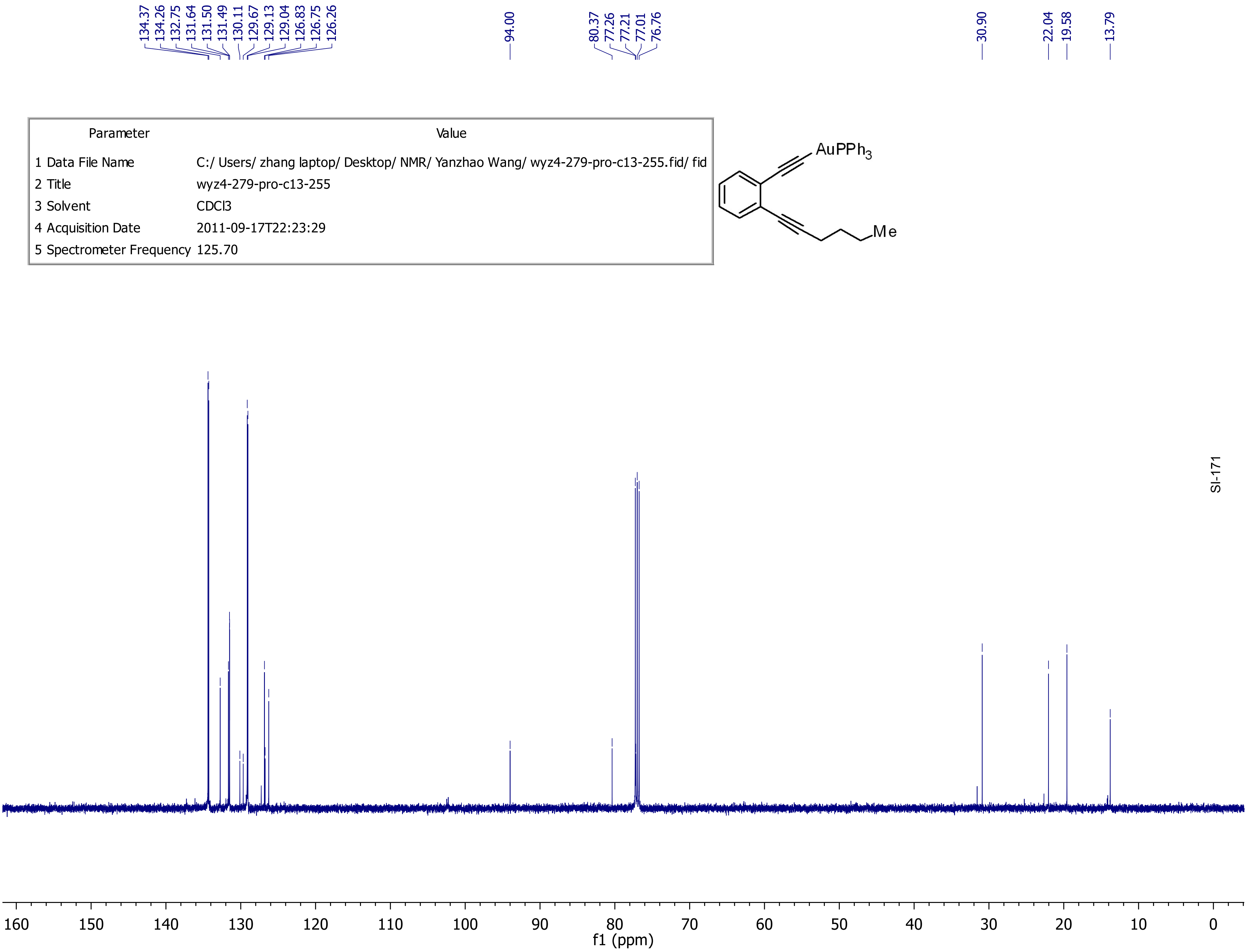
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-239-c3.fid
Standard c13 run using qnp probe
Jun 10 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 19308
Solvent = cdcl3
FID PTS1d = 28040
PTS1d = 32768
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 28040.66 Hz
AT1 = 1.00 sec
Hz per Pt 1stD = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 10057.2168 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = 3.28
B = -36.56
C = 0.00



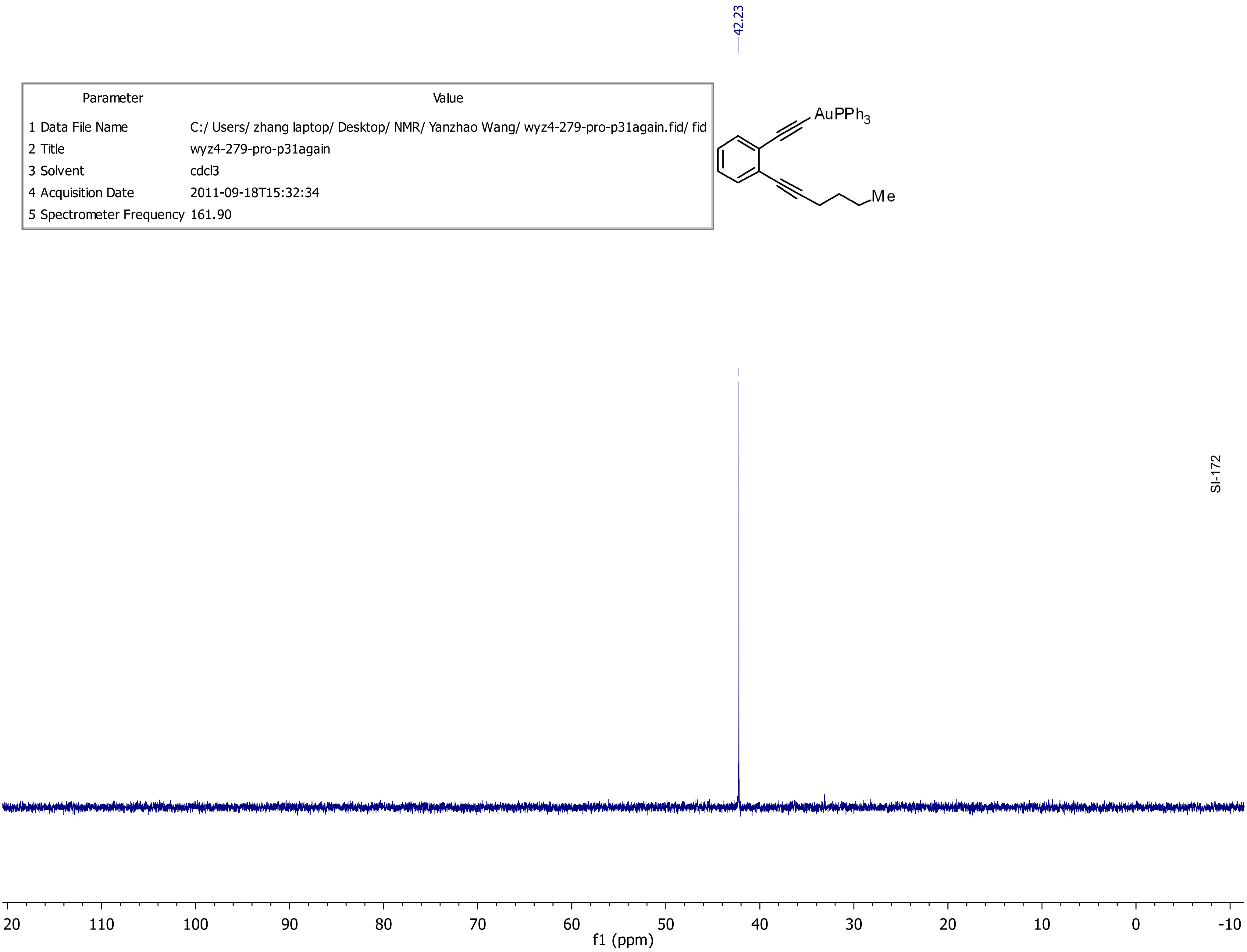
Parameter	Value
1 Data File Name	C:/ Users/ zhang laptop/ Desktop/ NMR/ Yanzhao Wang/ wyz4-279-pro-h1.fid/ fid
2 Title	wyz4-279-pro-h1
3 Solvent	CDCl3
4 Acquisition Date	2011-09-17T22:20:50
5 Spectrometer Frequency	499.86







Parameter	Value
1 Data File Name	C:/ Users/ zhang laptop/ Desktop/ NMR/ Yanzhao Wang/ wyz4-279-pro-c13-255.fid/ fid
2 Title	wyz4-279-pro-c13-255
3 Solvent	CDCl3
4 Acquisition Date	2011-09-17T22:23:29
5 Spectrometer Frequency	125.70



Parameter	Value
1 Data File Name	C:/ Users/ zhang laptop/ Desktop/ NMR/ Yanzhao Wang/ wyz4-279-pro-p31again.fid/ fid
2 Title	wyz4-279-pro-p31again
3 Solvent	cdcl3
4 Acquisition Date	2011-09-18T15:32:34
5 Spectrometer Frequency	161.90