Supporting Information

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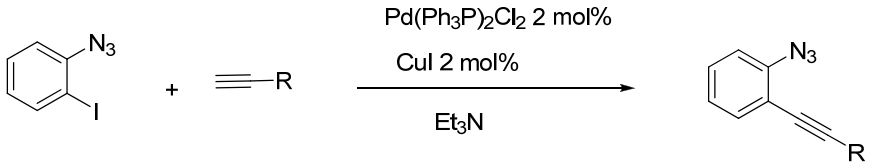
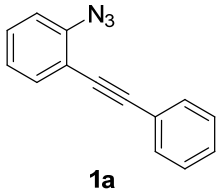
General Ethyl acetate (ACS grade), hexanes (ACS grade), diethyl ether (ACS grade) and anhydrous 1, 2-dichloroethane (HPLC grade) were purchased from Fisher Scientific and used without further purification. Methylene chloride and tetrahydrofuran were purified using MBraun Solvent Purifier. Commercially available reagents were used without further purification. 1-Azido-2-iodo-benzene and 1-Azido-2-ethynyl-benzene was prepared according to known procedure[1]. Reactions were monitored by thin layer chromatography (TLC) using Sorbent Technologies' pre-coated silica gel plates. Flash column chromatography was performed over Sorbent Technologies' 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 or Waters GCT Premier Time-of-Flight mass spectrometer with a field ionization (FI) ion source.

General procedure A: synthesis of *o*-azidoarylalkynes:



To a solution of 1-azido-2-iodobenzene (5 mmol), CuI (2 mol %), and $Pd(Ph_3P)_2Cl_2$ (2 mol %) in triethylamine (100mL) was added drop-wise an alkyne (6 mmol) under N_2. The reaction mixture was stirred for 5-10 h at room temperature. Upon completion, the mixture was diluted with diethyl ether and then washed with water and brine successively. The organic phase was dried with anhydrous $MgSO_4$, filtered, and concentrated under *vacuum*. The residue was purified through silica gel flash chromatography to give the desired product in mostly > 90% yield.

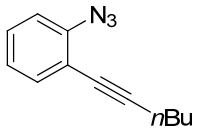
1-Azido-2-phenylethynylbenzene



1a

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 – 7.58 (m, 2H), 7.51 – 7.53 (m, 1H), 7.33 – 7.38 (m, 4H), 7.11 – 7.14 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 140.8, 133.6, 131.6, 129.5, 128.6, 128.3, 124.7, 122.9, 119.0, 115.6, 95.3, 84.9; IR (neat): 3063, 2917, 2127, 2092, 1599, 1569, 1495, 1481, 1442, 1302, 1293, 1262, 1088, 752, 711. MS (FI^+): Calculated for $[C_{14}H_9N_3]^+$: 219.08; Found: 219.08.

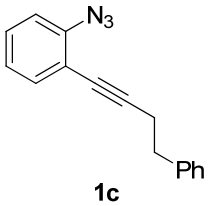
1-Azido-2-hex-1-ynylbenzene



1b

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38 (dd, *J* = 7.5 Hz, 1.5 Hz, 1H), 7.25 – 7.28 (m, 1H), 7.03 – 7.07 (m, 2H), 2.47 (t, *J* = 7.5 Hz, 2H), 1.59 – 1.63 (m, 2H), 1.47 – 1.52 (m, 2H), 0.96 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 140.6, 133.7, 128.7, 124.5, 118.7, 116.3, 96.9, 76.2, 30.7, 22.0, 19.4, 13.6; IR (neat): 2957, 2930, 2871, 2127, 2092, 1487, 1438, 1302, 748. MS (FI^+): Calculated for $[C_{12}H_{13}N_3]^+$: 199.11; Found: 199.11.

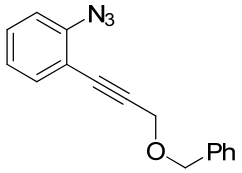
1-Azido-2-(4-phenyl-but-1-ynyl)benzene



1c

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.08 – 7.37(m, 7H), 7.04 – 7.09 (m, 2H), 2.96 (t, *J* = 7.6 Hz, 2H), 2.77 (t, *J* = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.6, 140.5, 133.7, 128.9, 128.5, 128.4, 126.3, 124.5, 118.6, 115.9, 95.8, 76.7, 35.0, 21.9; IR (neat): 3062, 3027, 2926, 2127, 2094, 1569, 1488, 1453, 1439, 1301, 750. MS (FI^+): Calculated for $[C_{16}H_{13}N_3]^+$: 247.11; Found: 247.11.

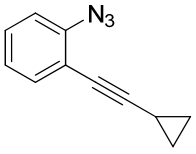
1-Azido-2-(3-benzyloxy-prop-1-ynyl)benzene



1d

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 – 7.46 (m, 7H), 7.08 – 7.14 (m, 2H), 4.71 (s, 2H), 4.45 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 141.2, 137.4, 133.8, 129.7, 128.4, 128.2, 127.9, 124.6, 118.6, 114.8, 91.1, 82.1, 71.6, 57.9; IR (neat): 3741, 2849, 2130, 2096, 1488, 1441, 1306, 1093, 1073, 752; MS (FI^+): Calculated for $[C_{16}H_{13}N_3]^+$: 263.11; Found: 263.10.

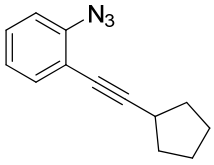
1-Azido-2-cyclopropylethynylbenzene



1e

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (d, *J* = 7.9 Hz, 1H), 7.24 – 7.28 (m, 2H), 7.02 – 7.06 (m, 2H), 1.47 – 1.54 (m, 1H), 0.83 – 0.93 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.6, 133.7, 128.6, 124.5, 118.7, 116.1, 99.8, 71.2, 8.8, 0.4. IR (neat): 3013, 2229, 2125, 2094, 1489, 1445, 1299, 954, 751; MS (FI^+): Calculated for $[C_{11}H_{19}N_3]^+$: 183.08; Found: 183.07.

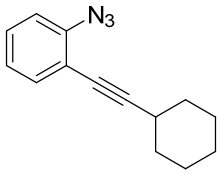
1-Azido-2-cyclopentylethynylbenzene



1f

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, *J* = 7.6 Hz, 1H), 7.25 (t, *J* = 7.6 Hz, 1H), 7.02 – 7.06 (m, 2H), 2.89 (quint, *J* = 7.4 Hz, 1H), 1.98 – 2.07 (m, 2H), 1.72 – 1.82 (m, 4H), 1.57 – 1.66 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.3, 133.6, 128.5, 124.4, 118.7, 116.3, 101.0, 75.5, 33.6, 30.9, 25.0. IR (neat): 2959, 2869, 2125, 2097, 1488, 1445, 1298, 749. MS (FI^+): Calculated for $[C_{13}H_{13}N_3]^+$: 211.11; Found: 211.11.

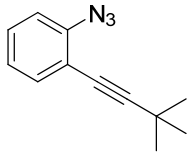
1-Azido-2-cyclohexylethynylbenzene



1g

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.38 (dd, 1H, *J* = 7.8 Hz, 1.8 Hz), 7.23 (td, 1H, *J* = 8.1 Hz, 1.2 Hz), 7.03 – 7.07 (m, 2H), 2.65 (quint, *J* = 4.6 Hz, 1H), 1.89 – 1.91(m, 2H), 1.75 – 1.80 (m, 2H), 1.56 – 1.60 (m, 2H), 1.33 – 1.40 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 140.6, 133.9, 128.7, 124.6, 118.9, 116.5, 101.1, 76.1, 32.6, 30.0, 26.0, 25.0. IR (neat): 2930, 2853, 2125, 2099, 1487, 1446, 1294, 748. MS (FI^+): Calculated for $[C_{14}H_{15}N_3]^+$: 225.13; Found: 225.12.

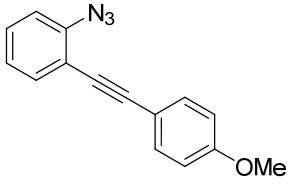
1-Azido-2-(3,3-dimethyl-but-1-ynyl)benzene



1h

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.37 (dd, *J* = 7.8 Hz, 1.8 Hz, 1H), 7.25 (td, *J* = 7.8 Hz, 1.2 Hz, 1H), 7.03 – 7.06 (m, 2H), 1.34 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 140.4, 133.8, 128.7, 124.6, 119.2, 116.6, 105.2, 74.6, 30.9, 28.4. IR (neat): 2969, 2128, 2104, 1571, 1489, 1474, 1446, 1362, 1297, 1264, 751. MS (FI^+): Calculated for $[C_{12}H_{13}N_3]^+$: 199.11; Found: 199.11.

1-azido-2-((4-methoxyphenyl)ethynyl)benzene

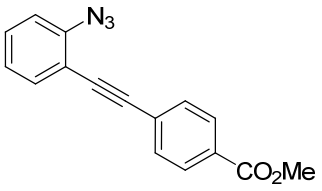


1j

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 – 7.52 (m, 3H), 7.29 – 7.34 (m, 1H), 7.09 – 7.13 (m, 2H), 6.87 – 6.90 (m, 2H), 3.83 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.9, 140.5, 133.5, 133.1, 129.2, 124.7, 118.9, 115.9, 114.9, 114.0, 95.5, 83.6, 55.3; IR (neat):2916, 2837, 2216, 2129,

2100, 1606, 1511, 1485, 1439, 1304, 1250, 1174, 1026, 834, 751; (ES^+) Calculated for $[C_{15}H_{12}N_3NaO]^+$: 272.08; Found: 272.08.

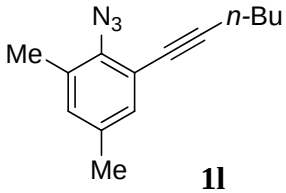
4-(2-Azido-phenylethynyl)benzoic acid methyl ester



1k

^1H NMR (500 MHz, $CDCl_3$) δ 8.02 – 8.04 (m, 2H), 7.61 – 7.63 (m, 2H), 7.51 – 7.53 (m, 1H), 7.36 – 7.39 (m, 1H), 7.12 – 7.16 (m, 2H), 3.93 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.5, 141.1, 133.7, 131.5, 130.0, 129.7, 129.5, 127.6, 124.7, 118.9, 114.9, 94.4, 87.8, 52.2; IR (neat):2951, 2342, 2127, 2088, 1724, 1484, 1434, 1277, 1192, 1175, 1104, 1095, 854, 765, 753; MS (ES^+) Calculated for $[C_{16}H_{11}KN_3O_2]^+$: 316.05; Found: 316.05.

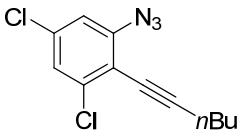
2-Azido-1-hex-1-ynyl-3, 5-dimethyl-benzene 1l



1l

^1H NMR (400 MHz, $CDCl_3$) δ 7.02 (s, 1H), 6.88 (s, 1H), 2.46 (t, *J* = 7.2 Hz, 2H), 2.23 (s, 3H), 2.21 (s, 3H), 1.58 – 1.85 (m, 2H), 1.46 – 1.53 (m, 2H), 0.95 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR 100 MHz, $CDCl_3$) δ 135.3, 134.3, 131.6, 131.2, 130.9, 118.0, 98.0,75.9, 30.4, 30.3, 22.1, 20.5, 19.4, 18.0, 13.6. IR (neat): 2958, 2932, 2121, 1469, 1428, 1230, 857, 728; MS: MS (FI^+): Calculated for $[C_{14}H_{17}N_3]^+$: 227.14; Found: 227.14.

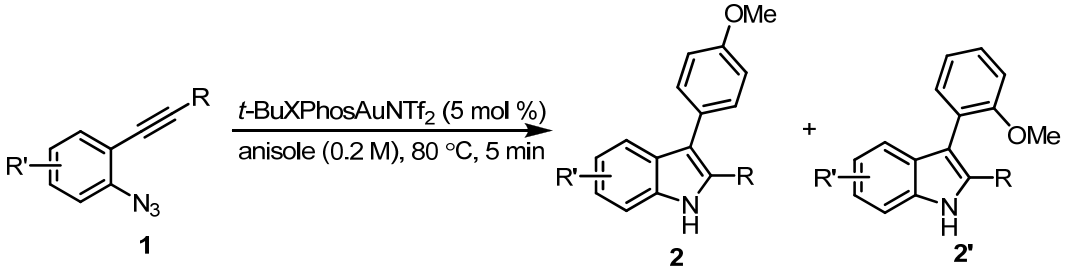
1-Azido-3, 5-dichloro-2-hex-1-ynylbenzene



1m

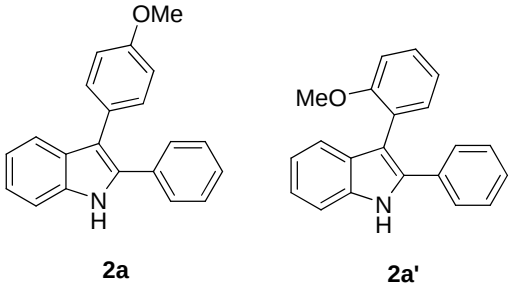
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.19(d, *J* = 2.0Hz, 1H), 6.97 (d, *J* = 2.0Hz, 1H), 2.53 (t, *J* = 7.2 Hz, 2H), 1.60 – 1.66 (m, 2H), 1.51 – 1.54 (m, 2H), 0.96 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 143.1, 138.1, 133.7, 125.4, 117.4, 116.3, 104.0, 72.5, 30.4, 21.9, 19.6, 13.6; IR (neat): 3441, 2112, 1642, 1461, 1400, 1295, 912, 715; MS: MS (FI^+): Calculated for $[C_{12}H_{11}Cl_2N_3]^+$: 267.03; Found: 267.03.

General procedure B: the reaction of *o*-azidoarylalkyne substrate 1 with anisole:



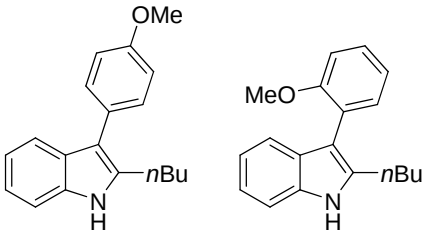
t-BuXPhosAuNTf$_2$ (13.8 mg, 0.015 mmol) was added to a solution of *o*-azidoarylalkyne **1** (0.30 mmol) in anisole (1.5 mL) at 80 °C, and the progress of the reaction was monitored by TLC. The reaction typically took 5 mins. Upon completion, the mixture was concentrated and the residue was purified by chromatography on silica gel to afford the desired products **2** and **2'**.

3-(4-Methoxy-phenyl)-2-phenyl-1*H*-indole



Yield of **2a**+**2a'**: 89% (**2a**/ **2a'** = 6.5/1). Major isomer **2a**: ^{1}H NMR (600 MHz, CD_3COCD_3) δ 10.6 (bs, 1H), 7.49 – 7.52 (m, 3H), 7.45 – 7.46 (m, 1H), 7.29 – 7.33 (m, 4H), 7.25 – 7.27 (m, 1H), 7.14 (t, *J* = 7.2 Hz, 1H), 7.04 (t, *J* = 7.2 Hz, 1H), 6.97 (d, *J* = 9.0 Hz, 2H), 3.82 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 158.3, 136.5, 133.8, 133.1, 131.1, 128.9, 128.4, 128.2, 128.1, 127.8, 127.3, 122.1, 119.6, 118.9, 114.0, 111.2, 54.6; IR (neat): 3054, 2934, 2834, 1602, 1554, 1513, 1484, 1456, 1329, 1284, 1245, 1175, 1029, 968, 907, 840, 744; MS (ES^+) Calculated for $[C_{21}H_{17}NNaO]^+$: 322.12; Found: 322.10.

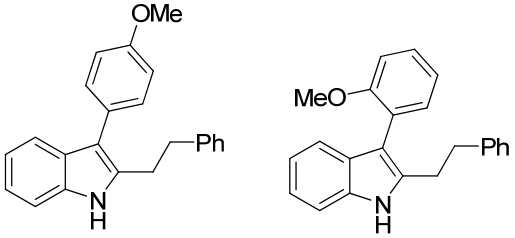
2-Butyl-3-(4-methoxy-phenyl)-1*H*-indole



2b **2b'**

Yield of **2b**+**2b'**: 74% (**2b**/ **2b'** = 7/1). Major isomer **2b**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.95 (bs, 1H), 7.64 (d, 1H, *J* = 8.0 Hz), 7.45 (d, 2H, *J* = 9.0 Hz), 7.35 (d, 1H, *J* = 8.0 Hz), 7.20 (t, 1H, *J* = 7.5 Hz), 7.14 (t, 1H, *J* = 7.5 Hz), 7.05 (d, 2H, *J* = 9.0 Hz), 3.90 (s, 3H), 2.85 (t, 2H, *J* = 7.8 Hz), 1.69 (quint, *J* = 7.8 Hz, 2H), 1.40 (sext, *J* = 7.5 Hz, 2H), 0.93 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.9, 135.8, 135.2, 130.7, 128.2, 127.9, 121.4, 119.8, 118.9, 114.0, 113.9, 110.4, 55.3, 32.1, 26.1, 22.6, 13.9; IR (neat):3404, 3056, 2955, 2930, 2870, 2834, 1611, 1561, 1510, 1448, 1330, 1282, 1174, 1036, 1019, 831, 744; MS (ES^+) Calculated for $[C_{19}H_{21}NNaO]^+$: 302.15; Found: 302.15

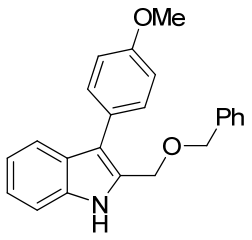
3-(4-Methoxy-phenyl)-2-phenethyl-1*H*-indole



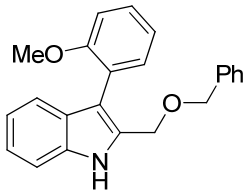
2c **2c'**

Yield of **2c**+**2c'**: 83% (**2c**/ **2c'** = 5/1). Major isomer **2c**: ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.76 (bs, 1H), 7.60 (d, *J* = 7.8 Hz, 1H), 7.34 – 7.36 (m, 2H), 7.29 – 7.31 (m, 3H), 7.23 – 7.25 (m, 1H), 7.16 – 7.19 (m, 3H), 7.10 – 7.13 (m, 1H), 7.00 – 7.02 (m, 2H), 3.89 (s, 3H), 3.16 (t, *J* = 7.8 Hz, 2H), 3.00 (t, *J* = 7.8 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 158.0, 141.0, 135.1, 134.6, 130.6, 128.6, 128.4, 128.0, 127.6, 126.3, 121.6, 119.8, 118.9, 114.5, 114.0, 110.4, 55.3, 36.1, 28.3; IR (neat):3403, 3026, 2930, 1611, 1562, 1510, 1459, 1331, 1284, 1244, 1174, 1021, 744; MS (ES^+) Calculated for $[C_{23}H_{21}NNaO]^+$: 350.15; Found: 350.14.

2-Benzyloxymethyl-3-(4-methoxy-phenyl)-1*H*-indole



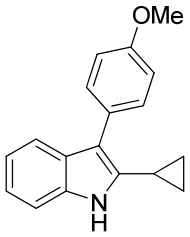
2d



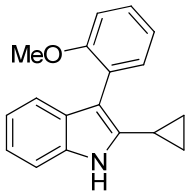
2d'

Yield of **2d**+**2d'**: 51% (**2d**/ **2d'** = 5/1). Major isomer **2d**: ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.40 (bs, 1H), 7.69 (d, *J* = 7.8 Hz, 1H), 7.41 – 7.37 (m, 3H), 7.36 – 7.28 (m, 5H), 7.23 (t, *J* = 7.8 Hz, 1H), 7.14 (t, *J* = 7.8 Hz, 1H), 7.00 (d, *J* = 9.0 Hz, 2H), 4.78 (s, 2H), 4.54 (s, 2H), 3.88 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 158.0, 137.7, 135.6, 131.1, 130.5, 128.5, 128.0, 127.9, 127.5, 126.9, 122.4, 120.0, 119.5, 116.0, 114.0, 110.9, 72.3, 63.8, 55.3; IR (neat): 3400, 3030, 2932, 2835, 2537, 1691, 1610, 1564, 1509, 1454, 1329, 1284, 1246, 1176, 1068, 1027, 837, 746; MS (ES^+) Calculated for $[C_{23}H_{21}NNaO_2]^+$: 366.15; Found: 366.14.

2-Cyclopropyl-3-(4-methoxy-phenyl)-1*H*-indole



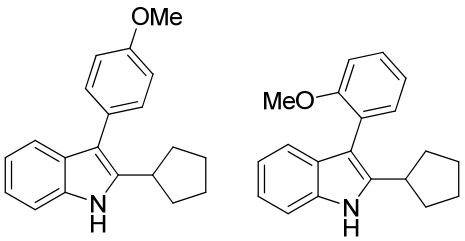
2e



2e'

Yield of **2e**+**2e'**: 76% (**2e**/ **2e'** = 8/1). Major isomer **2e**: ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.73 (bs, 1H), 7.64 (d, *J* = 7.8 Hz, 1H), 7.56 (d, *J* = 8.4 Hz, 2H), 7.30 (d, *J* = 7.8 Hz, 1H), 7.16 (t, *J* = 7.2 Hz, 1H), 7.11 (t, *J* = 7.5 Hz, 1H), 7.03 (d, *J* = 9.0 Hz, 2H), 3.89 (s, 3H), 2.18 – 2.23 (m, 1H), 0.97 – 1.00 (m, 2H), 0.71 – 0.76 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 157.8, 135.8, 134.7, 130.6, 128.2, 127.7, 121.5, 119.9, 118.7, 114.7, 113.8, 110.3, 55.4, 8.1, 7.5; IR (neat):3411, 3007, 2835, 1559, 1511, 1461, 1333, 1312, 1282, 1241, 1176, 1034, 987, 838, 744, 726; MS (ES^+) Calculated for $[C_{18}H_{17}NNaO]^+$: 286.12; Found: 286.10.

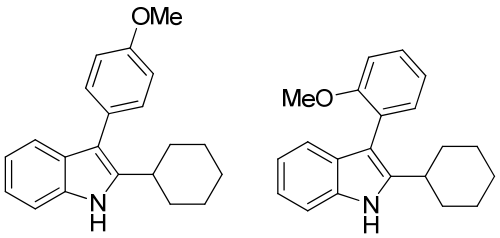
2-Cyclopentyl-3-(4-methoxy-phenyl)-1*H*-indole



2f **2f'**

Yield of **2f**+**2f'**: 75% (**2f**/ **2f'** = 15/1). Major isomer **2f**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.98 (bs, 1H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.45 (d, *J* = 8.5 Hz, 2H), 7.36 (d, *J* = 8.0 Hz, 1H), 7.19 (t, *J* = 7.5 Hz, 1H), 7.12 (t, *J* = 7.5 Hz, 1H), 7.05 (d, *J* = 9.0 Hz, 2H), 3.90 (s, 3H), 3.42 (quint, *J* = 8.8 Hz, 1H), 2.14 – 2.08 (m, 2H), 1.90 – 1.83 (m, 2H), 1.77 – 1.68 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.0, 138.8, 135.2, 130.9, 128.2, 127.9, 121.5, 119.8, 118.8, 114.0, 113.9, 110.4, 55.3, 36.9, 34.0, 26.0; IR (neat):3416, 3056, 2955, 2867, 2835, 1611, 1561, 1509, 1460, 1281, 1241, 1174, 1032, 1018, 908, 834, 745; MS (ES^+) Calculated for $[C_{20}H_{21}NNaO]^+$: 314.15; Found: 314.13.

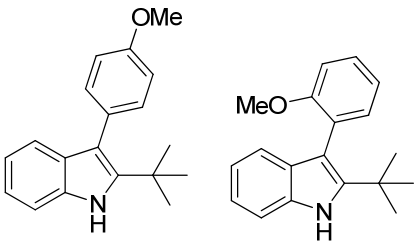
2-Cyclohexyl-3-(4-methoxy-phenyl)-1*H*-indole



2g **2g'**

Yield of **2g**+**2g'**: 82% (**2g**/ **2g'** = 16/1). Major isomer **2g**: ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.00 (bs, 1H), 7.59 (d, 1H, *J* = 7.8 Hz), 7.41 (d, 2H, *J* = 9.0 Hz), 7.35 (d, 1H, *J* = 7.8 Hz), 7.18 (t, 1H, *J* = 7.6 Hz), 7.11 (t, 1H, *J* = 7.5 Hz), 7.04 (d, 2H, *J* = 8.4 Hz), 3.90 (s, 3H), 2.99 (tt, 1H, *J* = 12.3 Hz, 3.6Hz), 1.96 – 1.99 (m, 2H), 1.84 – 1.87 (m, 2H), 1.71– 1.79 (m, 1H), 1.49 – 1.56 (m, 2H), 1.35 – 1.42 (m, 2H), 1.27 – 1.32 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 157.9, 140.4, 134.9, 130.8, 128.1, 127.9, 121.4, 119.7, 118.9, 114.0, 112.7, 110.4, 55.3, 35.5, 33.7, 26.5, 26.1; IR (neat): 3416, 3056, 2926, 2850, 1560, 1509, 1497, 1459, 1281, 1245, 1172, 1037, 1021, 831, 744; MS (ES^+) Calculated for $[C_{21}H_{23}NNaO]^+$: 328.17; Found: 328.16.

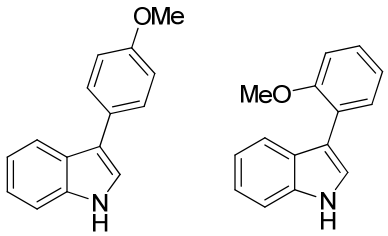
2-*tert*-Butyl-3-(4-methoxy-phenyl)-1*H*-indole



2h **2h'**

Yield of **2h**+**2h'**: 75% (**2h**/ **2h'** = 25/1). Major isomer **2h**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.02 (bs, 1H), 7.34 (d, 1H, *J* = 8.0 Hz), 7.29 (d, 2H, *J* = 4.5 Hz), 7.13 – 7.19 (m, 2H), 7.03 (t, 1H, *J* = 7.8 Hz), 6.96 (d, 2H, *J* = 8.5 Hz), 3.88 (s, 3H), 1.33 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.4, 142.6, 133.4, 132.5, 130.9, 129.0, 121.4, 119.5, 118.9, 113.3, 113.2, 110.0, 55.2, 33.2, 31.0; IR (neat): 3427, 2961, 1552, 1504, 1455, 1300, 1281, 1241, 1173, 1036, 829, 744; MS (ES^+) Calculated for $[C_{19}H_{21}NNaO]^+$: 302.15; Found: 302.12.

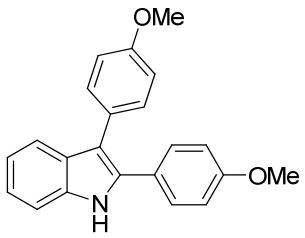
3-(4-Methoxy-phenyl)-1*H*-indole



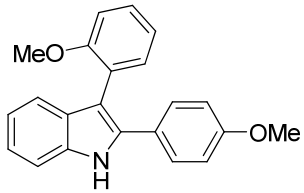
2i **2i'**

Yield of **2i**+**2i'**: 91% (**2i**/ **2i'** = 3/1). Major isomer **2i**: ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.13 (bs, 1H), 7.92 – 7.95 (m, 1H), 7.60 – 7.64 (m, 2H), 7.39 – 7.43 (m, 1H), 7.25 – 7.28 (m, 3H), 7.17 – 7.25 (m, 1H), 7.01 – 7.05 (m, 2H), 3.89 (s, 3H); **2i** and **2i'**: ^{13}C NMR (150 MHz, $CDCl_3$) δ 158.2 (major) 156.8 (minor), 136.7(major), 136.2 (minor), 128.7, 128.2, 130.6, 127.4 (major), 126.7, 126.0, 124.3, 124.2, 122.4 (major), 122.2, 121.3 (major), 120.8, 120.6, 120.2 (major), 120.0, 119.8 (major), 118.1 (major), 114.4, 113.6, 111.5 (major), 111.4, 111.3, 55.6 (major), 55.5 (minor); IR (neat):3410, 3055, 2956, 2834, 1550, 1502, 1456, 1331, 1280, 1246, 1179, 1196, 1030, 961, 836, 744; MS (ES^+) Calculated for $[C_{15}H_{13}NNaO]^+$: 246.09; Found: 246.08.

2,3-Bis-(4-methoxy-phenyl)-1*H*-indole



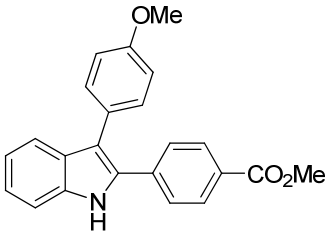
2j



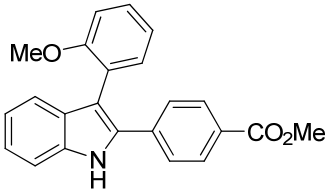
2j'

Yield of **2j**+**2j'**: 76% (**2j**/ **2j'** = 7/1). Major isomer **2j**: ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.15 (bs, 1H), 7.65 (d, *J* = 7.8 Hz, 1H), 7.39 – 7.41 (m, 1H), 7.33 – 7.38 (m, 4H), 7.21 – 7.24 (m, 1H), 7.13 – 7.17 (m, 1H), 6.95 (d, *J* = 8.4 Hz, 2H), 6.87 (d, *J* = 8.4 Hz, 2H), 3.86 (s, 3H), 3.82 (s, 3H); **2j** and **2j':** ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.1 (major), 158.9 (minor), 158.0 (major), 149.8 (minor), 135.7 (major), 133.7 (major), 132.6, 131.1 (major), 129.3 (major), 129.0, 128.4, 128.1, 127.5, 126.0, 125.3, 122.3, 122.1, 120.7, 120.2, 120.0, 119.4, 114.1 (major), 114.0 (major), 113.9 113.8, 111.3 (minor), 110.7 (major), 55.3, 55.2; IR (neat): 3403, 3001, 2936, 2836, 1610, 1576, 1556, 1519, 1497, 1456, 1289, 1246, 1178, 1030, 909, 832, 747, 730; MS (ES^+) Calculated for $[C_{22}H_{19}NNaO_2]^+$: 352.13; Found: 352.12.

4-[3-(4-Methoxy-phenyl)-1*H*-indol-2-yl]-benzoic acid methyl ester



2k

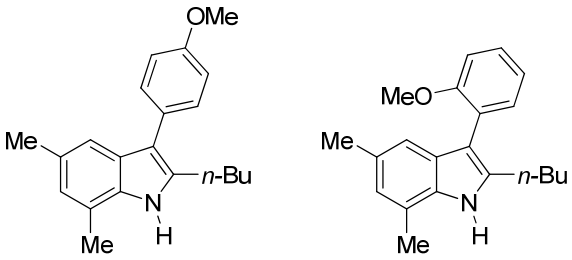


2k'

Yield of **2k**+**2k'**: 95%, (**2k**/ **2k'** = 7/1). Major isomer **2k**: ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.44 (bs, 1H), 7.93 – 8.00 (m, 2H), 7.62 – 7.68 (m, 1H), 7.39 – 7.51 (m, 3H), 7.32 – 7.37 (m, 2H), 7.24 – 7.28 (m, 1H), 7.14 – 7.19 (m, 1H), 6.93 – 6.98 (m, 2H), 3.92 (s, 3H), 3.87 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 166.9 (major), 158.5 (major), 157.3 (minor), 138.0, 137.3 (major), 136.3 (major), 133.3, 132.4, 131.2 (major), 129.9 (major), 129.8, 129.3, 129.0, 128.6, 128.4, 127.7 (major), 126.9, 126.7, 123.5, 123.3 (major), 123.1, 120.9, 120.5 (major), 120.4, 120.0

(major), 116.4, 114.2 (major), 112.8, 111.4, 110.1 (major), 55.3, 55.1, 52.2; IR (neat):3339, 2950, 1688, 1605, 1567, 1518, 1432, 1286, 1240, 1177, 1110, 741; MS (ES^+) Calculated for $[C_{23}H_{19}NNaO_3]^+$: 380.13; Found: 380.12.

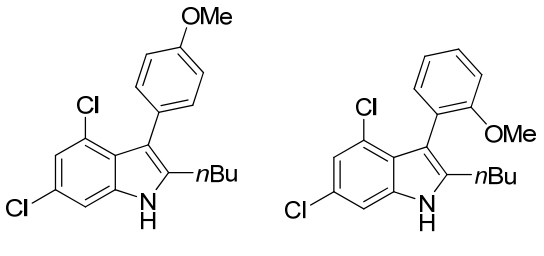
2-Butyl-3-(4-methoxy-phenyl)-5,7-dimethyl-1*H*-indole 2l



2l **2l'**

Yield of **2l**+**2l'**: 82 % (**2l**/ **2l'** = 8/1). Major isomer **2l**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (bs, 1H), 7.45 (dt, *J* = 9.6 Hz, 2.4 Hz, 2H), 7.28 (s, 1H), 7.06 (td, *J* = 9.6 Hz, 2.4 Hz, 2H), 6.87 (s, 1H), 3.92 (s, 3H), 2.87 (t, *J* = 7.6 Hz, 2H), 2.52 (s, 3H), 2.45 (s, 3H), 1.68 – 1.76 (m, 2H), 1.38 – 1.47 (m, 2H), 0.95 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.8 (major), 135.6 (major), 132.8, 132.4, 130.7 (major), 129.2, 128.9, 128.1, 127.9, 127.7, 123.7 (major), 123.4, 120.4, 119.1, 116.7, 116.2 (major), 114.0, 113.8, 111.0 (major), 55.3, 55.2, 32.2 (major), 31.6(minor), 26.7(minor), 26.1(major), 22.5, 21.4, 16.5, 13.8; IR (neat): 2956, 1645, 1597, 1509, 1458, 1314, 1248, 1170, 1030, 835; MS (ES^+) Calculated for $[C_{21}H_{26}NO]^+$: 308.20; Found: 308.18.

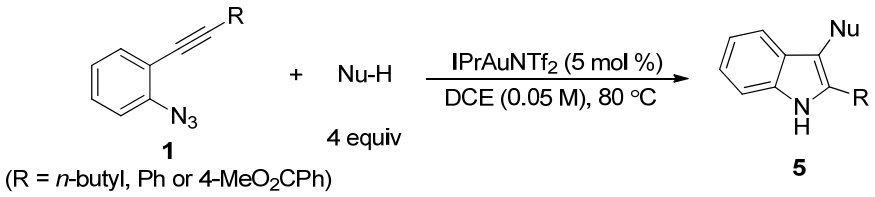
2-Butyl-4,6-dichloro-3-(4-methoxy-phenyl)-1*H*-indole



2m **2m'**

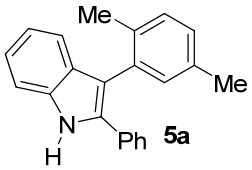
Yield of **2m**+**2m'**: 78% (**2m**/ **2m'** = 7/1). Major isomer **2m**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (bs, 1H), 7.25 – 7.31 (m, 3H), 7.08 (d, *J* = 1.6Hz, 1H), 6.96 – 6.98 (m, 2H), 4.09 (s, 3H), 2.66 (t, *J* = 7.6 Hz, 2H), 1.59 – 1.65 (m, 2H), 1.30 – 1.36 (m, 2H), 0.89 (t, *J* = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.5, 138.6, 136.1, 132.7, 126.7, 126.5, 126.0, 123.8, 121.0, 120.9, 112.8, 109.1, 55.2, 31.7, 25.7, 22.3, 13.8; IR (neat): 3428, 2956, 2930, 1614, 1553, 1509, 1444, 1243, 1175, 1036, 831; MS (ES^+) Calculated for $[C_{19}H_{20}Cl_2NO]^+$: 348.09; Found: 348.06.

General procedure B: the synthesis of indole derivatives 5 using different nucleophiles:



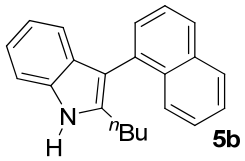
o-Alkynylarylazides **1** (0.30 mmol) and $IPrAuNTf_2$ (12.9 mg, 0.015 mmol) were added to a solution of the nucleophiles (1.2 mmol or 0.6 mmol) in DCE (3 mL) at room temperature. The reaction mixture was then stirred at 80 °C and the progress of the reaction was monitored by TLC. The reaction typically took 3 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 products **5**.

3-(2,5-Dimethyl-phenyl)-2-phenyl-1*H*-indole



Yield: 70%. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.28 (bs, 1H), 7.43 (d, *J* = 7.8 Hz, 1H), 7.35 (t, *J* = 9.3 Hz, 3H), 7.29 – 7.20 (m, 4H), 7.17 – 7.09 (m, 2H), 7.11 – 7.07 (m, 2H), 2.32 (s, 3H), 1.95(s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.8, 135.1, 134.5, 134.2, 133.0, 132.0, 130.1, 129.7, 128.7, 128.3, 127.9, 127.3, 126.6, 122.6, 120.1, 120.0, 114.9, 110.7, 21.0, 19.6; IR (neat):3407, 3055, 2917, 1603, 1505, 1484, 1456, 1446, 1327, 1252, 909, 811, 761, 745, 728; MS (ES^+) Calculated for $[C_{22}H_{19}KN]^+$: 336.12; Found: 336.11.

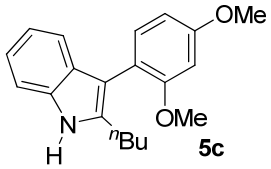
2-Butyl-3-naphthalen-1-yl-1*H*-indole



5b

Yield: 78%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.10 (bs, 1H),7.89 – 7.95 (m, 2 H), 7.78 (d, *J* = 8.5 Hz, 1H), 7.57 (dd, *J* = 7.5, 7.0 Hz, 1H), 7.48 – 7.51 (m, 2H), 7.41 – 7.42 (m, 1H), 7.35 – 7.38 (m, 1H), 7.18 – 7.21 (m, 2H), 7.03 – 7.06 (m, 1H), 2.62 – 2.76 (m, 2H), 1.56 –1.63 (m, 2H), 1.23 – 1.30 (m, 2H), 0.79 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.2, 135.1, 133.9, 133.8, 133.2, 133.0, 129.4, 128.7, 128.2, 127.2, 126.8, 125.6, 125.5, 121.4, 119.7, 119.5, 112.7, 110.3, 31.7, 30.9, 26.3, 22.3, 13.7; IR (neat):3407, 3051, 2955, 2927, 2870, 1591, 1506, 1457, 1438, 1316, 1244, 1011, 800, 778, 762, 743, 716; MS (ES^+) Calculated for $[C_{22}H_{21}NaN]^+$: 322.16; Found: 322.16.

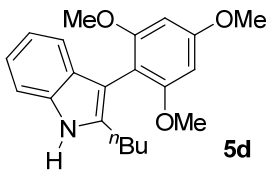
2-Butyl-3-(2,4-dimethoxy-phenyl)-1*H*-indole



5c

Yield: 84%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (bs, 1H), 7.38 (d, *J* = 8.0 Hz, 1H), 7.32 (dd, *J* = 8.4 Hz, 0.8 Hz, 1H), 7.26 (d, *J* = 8.0 Hz, 1H), 7.11 – 7.15 (m, 1H), 7.04 – 7.08 (m, 1H), 6.59 – 6.62 (m, 2H), 3.89 (s, 3H), 2.71(t, *J* = 8.0 Hz, 2H), 1.58 – 1.64 (m, 2H), 1.32 – 1.38 (m, 2H), 0.89 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.7, 158.4, 136.8, 135.2, 132.7, 128.7, 121.0, 119.4, 119.3, 116.5, 110.2, 109.9, 104.2, 98.9, 55.4, 55.3, 31.6, 26.5, 22.6, 13.9; IR (neat):3391, 2955, 2932, 2870, 2834, 1610, 1565, 1505, 1460, 1332, 1299, 1260, 1207, 1157, 1131, 1109, 1033, 743; MS (ES^+) Calculated for $[C_{20}H_{23}NNaO_2]^+$: 332.16; Found: 332.16.

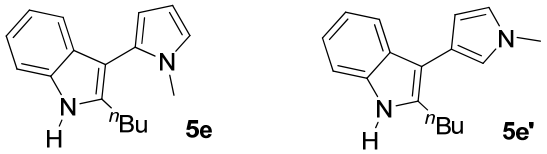
2-Butyl-3-(2,4,6-trimethoxy-phenyl)-1H-indole



5d

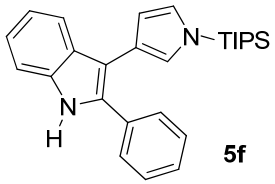
Yield: 84%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.96 (bs, 1H), 7.28 (dd, *J* = 8.0 Hz, 1.0 Hz, 1H), 7.21 (d, *J* = 7.5 Hz, 1H), 7.08 – 7.12 (m, 1H), 7.01 – 7.04 (m, 1H), 6.30 (s, 2H), 3.91 (s, 3H), 3.71 (s, 6H), 2.61(t, *J* = 7.5 Hz, 2H), 1.59 – 1.68 (m, 2H), 1.32 – 1.38 (m, 2H), 0.89 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.4, 159.6, 137.6, 135.4, 129.0, 120.6, 119.7, 119.1, 110.4, 105.3, 105.0, 90.9, 55.7, 55.4, 31.1, 26.9, 22.6, 13.9; IR (neat): 3390, 2955, 2934, 2870, 2837, 1607, 1585, 1499, 1458, 1411, 1334, 1224, 1203, 1154, 1125, 1063, 810, 742; MS (ES^+) Calculated for $[C_{21}H_{25}NNaO_3]^+$: 362.17; Found: 362.17.

2-Butyl-3-(1-methyl-1*H*-pyrrol-2-yl)-1*H*-indole and 2-Butyl-3-(2-methyl-1*H*-pyrrol-3-yl)-1*H*-indole



Yield: 91% (**5e** /**5e'** = 1:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.02 (bs, 0.5H), 7.86 (bs, 0.5H), 7.74 (d, *J* = 8.0 Hz, 0.5H), 7.30 – 7.37 (m, 1.5H), 7.10 – 7.18 (m, 1H), 6.79 (d, *J* = 9.0 Hz, 0.5H), 6.71 (s, 0.5H), 6.37 (s, 0.5H), 6.26 (s, 0.5H), 6.14 (s, 0.5H), 3.75 (s, 1.5H), 3.47 (s, 1.5H), 2.91(t, *J* = 7.2 Hz, 1H), 2.70 – 2.79 (m, 1H), 1.56 – 1.73 (m, 2H), 1.32 – 1.48 (m, 2H), 0.96 (t, *J* = 7.2 Hz, 1.5H), 0.90 (t, *J* = 7.2 Hz, 1.5H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 138.8, 135.2, 135.1, 135.0, 129.3, 128.3, 127.0, 121.9, 121.7, 121.4, 121.1, 119.9, 119.7, 119.4, 119.4, 119.3, 117.5, 110.4, 110.1, 109.6, 108.9, 108.5, 107.3, 105.7, 36.3, 34.3, 32.0, 31.8, 26.5, 26.2, 24.7, 22.7, 22.4, 14.0, 13.8; IR (neat):3396, 3055, 2956, 2927, 2871, 2859, 1504, 1488, 1458, 1440, 1417, 1326, 1286, 1241, 1171, 781, 743; MS (ES^+) Calculated for $[C_{17}H_{20}KN_2]^+$: 291.13; Found: 291.14.

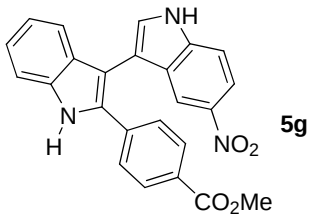
2-Phenyl-3-(1-triisopropylsilanyl-1*H*-pyrrol-3-yl)-1*H*-indole



Yield: 69%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.10 (bs, 1H), 7.77 (d, *J* = 7.5 Hz, 1H), 7.58 – 7.60 (m, 2H), 7.38 – 7.40 (m, 1H), 7.31– 7.35 (m, 2H), 7.23 – 7.29 (m, 1H), 7.20 – 7.23 (m, 1H), 7.13 – 7.16 (m, 1H), 6.83 (s, 1H), 6.79 (s, 1H), 6.41– 6.42 (m, 1H), 1.41–1.47 (m, 3H), 1.12 (d, *J* =

6.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 136.0, 133.6, 133.1, 129.4, 128.4, 127.9, 127.2, 124.1, 122.7, 122.3, 120.3, 119.9, 118.5, 111.7, 110.6, 110.0, 17.9, 11.7; IR (neat):3408, 2945, 2866, 1652, 749, 706; MS (ES^+) Calculated for $[C_{27}H_{34}N_2NaSi]^+$: 437.24; Found: 437.22.

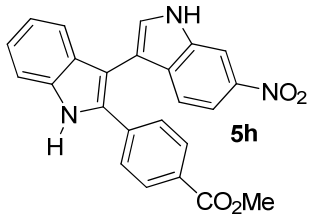
4-(5'-Nitro-1*H*,1'*H*-[3,3']biindolyl-2-yl)-benzoic acid methyl ester



5g

Yield: 83%. ^{1}H NMR (400 MHz, d_6-DMSO) δ 12.15 (bs, 1H), 11.90 (bs, 1H), 8.05 (dd, *J* = 8.5 Hz, 2.5 Hz, 1H), 7.92 (d, *J* = 10.5 Hz, 1H), 7.88 (s, 1H), 7.85 (s, 1H), 7.68 –7.72 (m, 3 H), 7.58 (d, *J* = 10.0 Hz, 1H), 7.49 (d, *J* = 10.5 Hz, 1H), 7.27–7.31 (m, 1H), 7.10–7.14 (m, 1H), 3.88 (s, 3H); ^{13}C NMR (100 MHz, d_6-DMSO) δ 166.5, 140.9, 140,2, 137.9, 137.3, 133.6, 129.9, 129.4, 128.8, 128.4, 128.0, 126.2, 123.4, 120.4, 119.9, 117.2, 117.0, 112.9, 112.3, 111.6, 107.1, 52.7, 31.3; IR (neat):3435, 2916, 2848, 1635, 1264, 740; MS (ES^+) Calculated for $[C_{23}H_{17}N_3NaO_4]^+$: 434.11; Found: 434.11

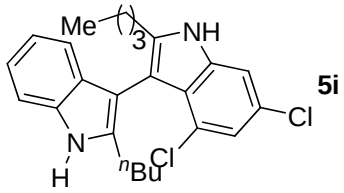
4-(6'-Nitro-1*H*,1'*H*-[3,3']biindolyl-2-yl)-benzoic acid methyl ester



5h

Yield: 81%. ^{1}H NMR (400 MHz, d_6-acetone) δ 11.26 (bs, 1H), 10.93 (bs, 1H), 8.53 (s, 1H), 7.87–7.90 (m, 2 H), 7.79 (dd, *J* = 7.2 Hz, 0.8 Hz, 1H), 7.69 (d, *J* = 8.4 Hz, 1H), 7.55 (d, *J* = 8.0 Hz, 1H), 7.49 (d, *J* = 8.0 Hz, 1H), 7.20 –7.25 (m, 2H), 7.06 – 7.10 (m, 1H), 3.84 (s, 3H); ^{13}C NMR (100 MHz, d_6-acteone) δ 166.8, 143.1, 137.8, 137.7, 137.2, 137.0, 135.5, 133.6, 131.6, 131.0, 130.9, 129.6, 128.7, 127.4, 123.1, 120.07, 120.05, 119.8, 114.2, 111.6, 111.5, 108.7, 108.6, 51.5; IR (neat):3376, 1700, 1607, 1504, 1435, 1329, 1106, 707; MS (ES^+) Calculated for $[C_{23}H_{17}N_3NaO_4]^+$: 434.11; Found: 434.11

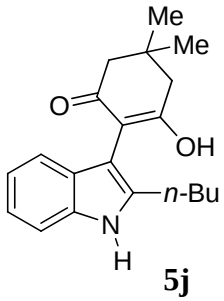
2,2'-dibutyl-4,6-dichloro-1*H*,1'*H*-3,3'-biindole



5i

Yield: 64%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (bs, 1H), 8.01 (bs, 1H), 7.36 (d, 1H, *J* = 8.0 Hz), 7.25 (d, 1H, *J* = 1.6 Hz), 7.19 – 7.12 (m, 2H), 7.00 – 7.05 (m, 2H), 2.53 – 2.67 (m, 4H), 1.50 – 1.64 (m, 4H), 1.22 – 1.32 (m, 4H), 0.79 – 0.84 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.2, 138.5, 136.6, 135.0, 130.9, 126.3, 125.2, 120.8, 119.3, 119.2, 110.0, 109.0, 105.7, 105.6, 31.4, 31.2, 26.5, 26.0, 22.4, 22.3, 22.2, 13.8; IR (neat): 3734, 2955, 2360, 2341, 1636, 1457, 1321, 745; MS (ES^+) Calculated for $[C_{24}H_{27}Cl_2N_2]^+$: 413.16; Found: 413.15.

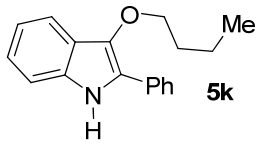
2-(2-butyl-1*H*-indol-3-yl)-3-hydroxy-5,5-dimethylcyclohex-2-enone 5j



5j

Yield: 49 %. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (bs, 1H), 7.22 (t, *J* = 9.2 Hz, , 2H), 7.10 (td, *J* = 8.0 Hz, 1.2 Hz, 1H), 7.04 (td, *J* = 7.2 Hz,1.2 Hz, 1H), 5.23 (s, 1H), 2.61(s, 2H), 2.54 (t, *J* = 7.6 Hz, 2H), 2.28 (s, 2H), 1.51 – 1.59 (m, 2H), 1.24 – 1.33 (m, 2H), 1.19 (s, 6H), 0.86 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.0, 177.2, 132.8, 128.2, 128.0, 121.8, 120.4, 119.9, 116.4, 111.0, 104.1, 50.8, 42.1, 32.9, 30. 6, 28.3, 24.3, 22.2, 12.7; IR (neat): 2957, 2871, 1637, 1609, 1459, 1373, 1349, 1319, 1198, 1162, 1144, 738; MS (ES^+) Calculated for $[C_{20}H_{25}NNaO_2]^+$: 334.18; Found: 334.14.

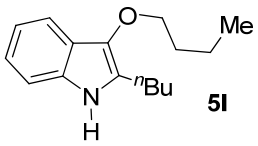
3-Butoxy-2-phenyl-1*H*-indole



5k

Compound **5k** was air sensitive. Its purification proceeded under N_2 protection. Yield: 66%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, 2H, *J* = 7.2 Hz), 7.80 (bs, 1H), 7.68 (d, 1H, *J* = 8.0 Hz), 7.46 (t, 2H, *J* = 7.8 Hz), 7.29 – 7.34 (m, 2H), 7.20 (t, 1H, *J* = 8.0 Hz), 7.13 (t, 1H, *J* = 7.4 Hz), 4.12 (t, 2H, *J* = 6.6 Hz), 1.80 (quint, 2H, *J* = 7.1 Hz), 1.54 (sext, 2H, *J* = 7.4 Hz), 0.97 (t, 3H, *J* = 7.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.7, 133.8, 131.6, 128.8, 126.9, 125.5, 124.4, 123.0, 122.7, 119.6, 118.2, 111.3, 73.9, 32.3, 19.3 13.9; IR (neat): 3410, 2957, 2932, 2871, 1665, 1604, 1457, 1338, 1316, 1238, 1073, 741, 692; MS (ES^+) Calculated for $[C_{18}H_{19}NNaO]^+$: 288.14; Found: 288.16.

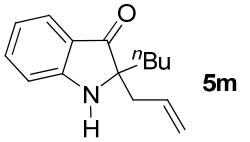
3-Butoxy-2-butyl-1*H*-indole



5l

Compound **5l** was air sensitive. Its purification proceeded under N_2 protection. Yield: 62%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, 1H, *J* = 8.0 Hz), 7.44 (bs, 1H), 7.22 – 7.25 (m, 1H), 7.06 – 7.14 (m, 2H), 4.06 (t, *J* = 6.6 Hz, 2H), 2.76 (t, *J* = 7.6 Hz, 2H), 1.74 – 1.81 (m, 2H), 1.51 – 1.70 (m, 4H), 1.37 – 1.46 (m, 2H), 1.00 (t, 3H, *J* = 7.4 Hz), 0.96 (t, 3H, *J* = 7.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.9, 132.8, 127.2, 122.1, 121.1, 119.0, 117.2, 110.7, 74.4, 32.3, 31.4, 24.4, 22.5, 19.3, 14.0, 13.9; IR (neat): 3406, 2957, 2932, 1638, 1620, 1459, 1241, 913, 742; MS (ES^+) Calculated for $[C_{16}H_{23}NNaO]^+$: 268.17; Found: 268.15.

2-Allyl-2-butyl-1,2-dihydroindol-3-one



5m

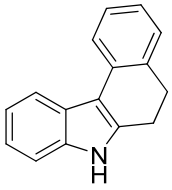
Yield: 65%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, 1H, *J* = 8.0 Hz), 7.42 (t, 1H, *J* = 7.6 Hz), 6.85 (d, 1H, *J* = 8.4 Hz), 6.79 (t, 1H, *J* = 7.4 Hz), 5.62 – 5.72 (m, 1H), 5.02 – 5.12 (m, 2H), 4.61 (bs, 1H), 2.34 – 2.45 (m, 2H), 1.75 – 1.83 (m, 1H), 1.60 – 1.69 (m, 1H), 1.18 – 1.29 (m, 3H), 1.00 – 1.09 (m, 1H), 0.81 (t, 3H, *J* = 7.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.5, 160.6,

137.1, 132.2, 124.5, 121.3, 119.2, 118.6, 112.2, 69.5, 41.8, 36.4, 25.3, 22.9, 13.9; IR (neat): 3340, 2957, 2933, 1680, 1621, 1492, 1469, 1326, 1142, 1100, 919, 752; MS (ES^+) Calculated for $[C_{15}H_{19}NNaO]^+$: 252.14; Found: 252.15.

General procedure for the synthesis of 6 and 7:

$IPrAuNTf_2$ (12.9 mg, 0.015 mmol) was added to the solution of **1c** or **1d** (0.30 mmol) in DCE (6.0 mL) at room temperature. The reaction mixture was then stirred at 80 °C and the progress of the reaction was monitored by TLC. The reaction typically took 3 hours. Upon completion, the mixture was concentrated and the residue was purified by chromatography on silica gel (eluent: hexanes/ethyl acetate) to afford the desired products **6** or **7**.

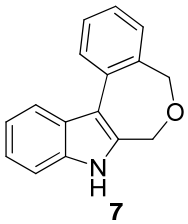
5,7-Dihydro-6*H*-benzo[c]carbazole



6

Yield: 73%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 8.4 Hz, 1H), 7.99 (bs, 1H), 7.87 (d, *J* = 7.6 Hz, 1H), 7.30 –7.37 (m, 2H), 7.18 – 7.27 (m, 3H), 7.08 – 7.12 (m, 1H), 3.07 (t, *J* = 8.0 Hz, 2H), 2.96(t, *J* = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.2, 136.1, 133.8, 133.3, 127.9, 126.9, 124.9, 124.3, 122.3, 121.4, 120.5, 119.5, 111.1, 29.5, 22.5; IR (neat):3397, 3054, 2924, 1599, 1548, 1496, 1456, 1356, 1326, 1276, 1254, 1183, 1027, 767, 749; MS (ES^+) Calculated for $[C_{16}H_{13}NK]^+$: 258.07; Found: 258.06.

5,8-Dihydro-7*H*-6-oxa-8-aza-dibenzo[a,h]azulene



7

Yield: 72%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (bs, 1H), 8.05 (dd, *J* = 7.6 Hz, 2.4 Hz, 2H), 7.47–7.52 (m, 1H), 7.35 – 7.40 (m, 2H), 7.21 – 7.29 (m, 3H), 5.08 (s, 2H), 4.64 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.4, 159.6, 137.6, 135.4, 129.0, 120.6, 119.7, 119.1, 110.4, 105.3, 105.0, 90.9, 55.7, 55.4, 31.1, 26.9, 22.6, 13.9; IR (neat):3391, 3275, 3059, 2855, 1603, 1552, 1494, 1459, 1392, 1328, 1259, 1231, 1185, 1124, 1101, 1051, 1020, 771, 741; MS (ES^+) Calculated for $[C_{16}H_{13}NNaO]^+$: 258.09; Found: 258.09.

Reference:

1. Tomiok, H.; Sawai, S. *Org. Biomol. Chem.* **2003**, *1*, 4441.

lb-IV-modelsubstrate

exp1 s2pul

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	lsubstrate.fid	dmf	200
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at	2.500	math	i
np	42518		
sw	8503.4	werr	
fb	not used	wexp	
bs	2	wbs	
pw	7.7	wnt	
pw	7.7	DISPLAY	
tpwr	57	sp	-280.0
d1	4.800	wp	5833.6
tof	0	vs	62
nt	32	sc	0
ct	22	wc	250
alock	n	hzmm	23.33
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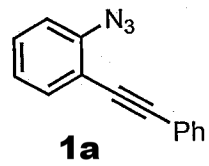
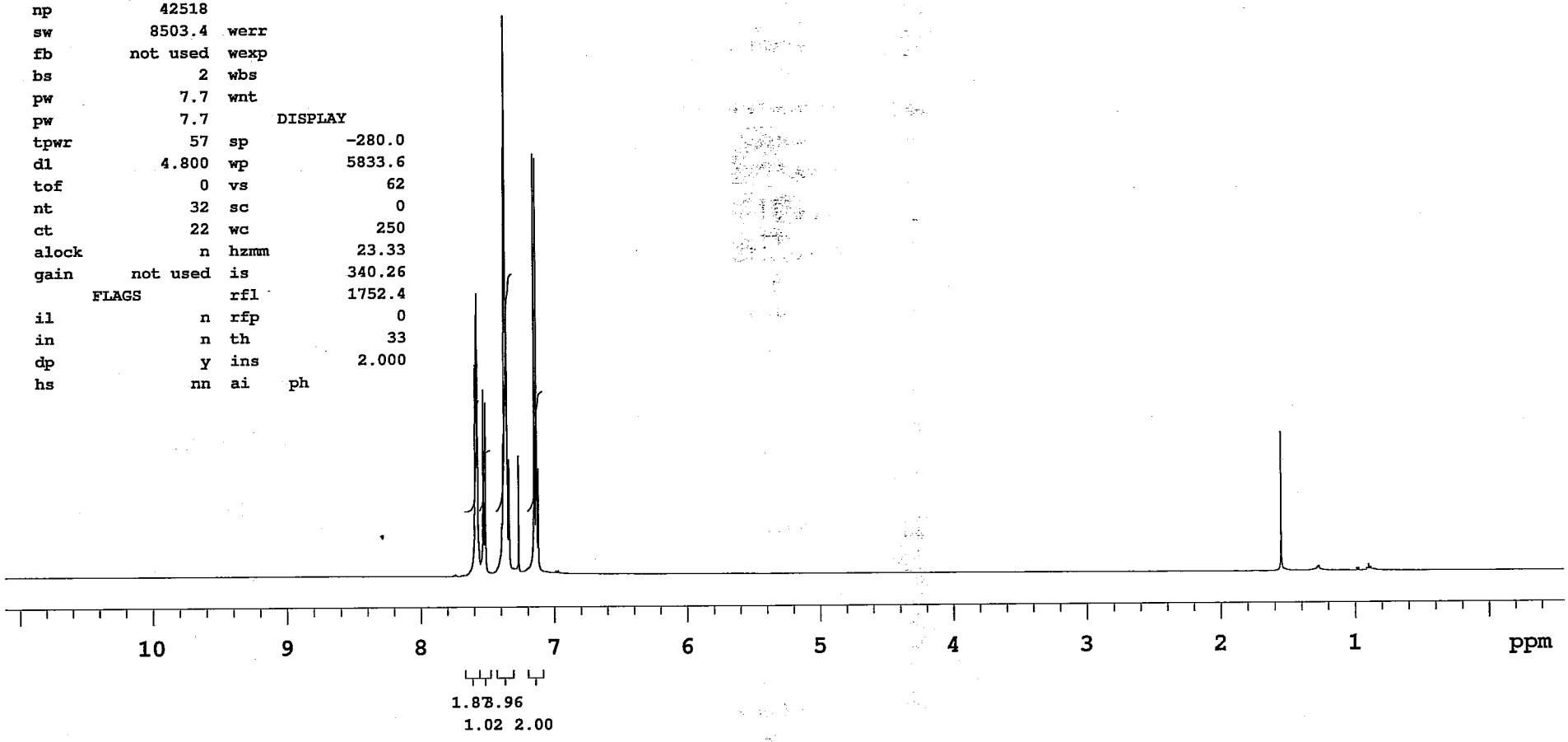
hs	nn	ai ph	



1a



Std carbon

exp1 Carbon

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sw	30165.9	FLAGS	
at	1.303	il	n
np	78590	in	n
fb	not used	dp	y
bs	4	hs	nn
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nt	10000	fn	not used
ct	116	DISPLAY	
TRANSMITTER		sp	-422.8
tn	C13	wp	24087.7
sfrq	125.702	rfl	1885.6
tof	1285.5	rfp	0
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pw	7.000	lp	-180.3
DECOUPLER		PLOT	
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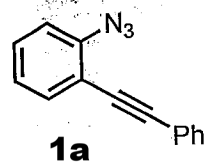
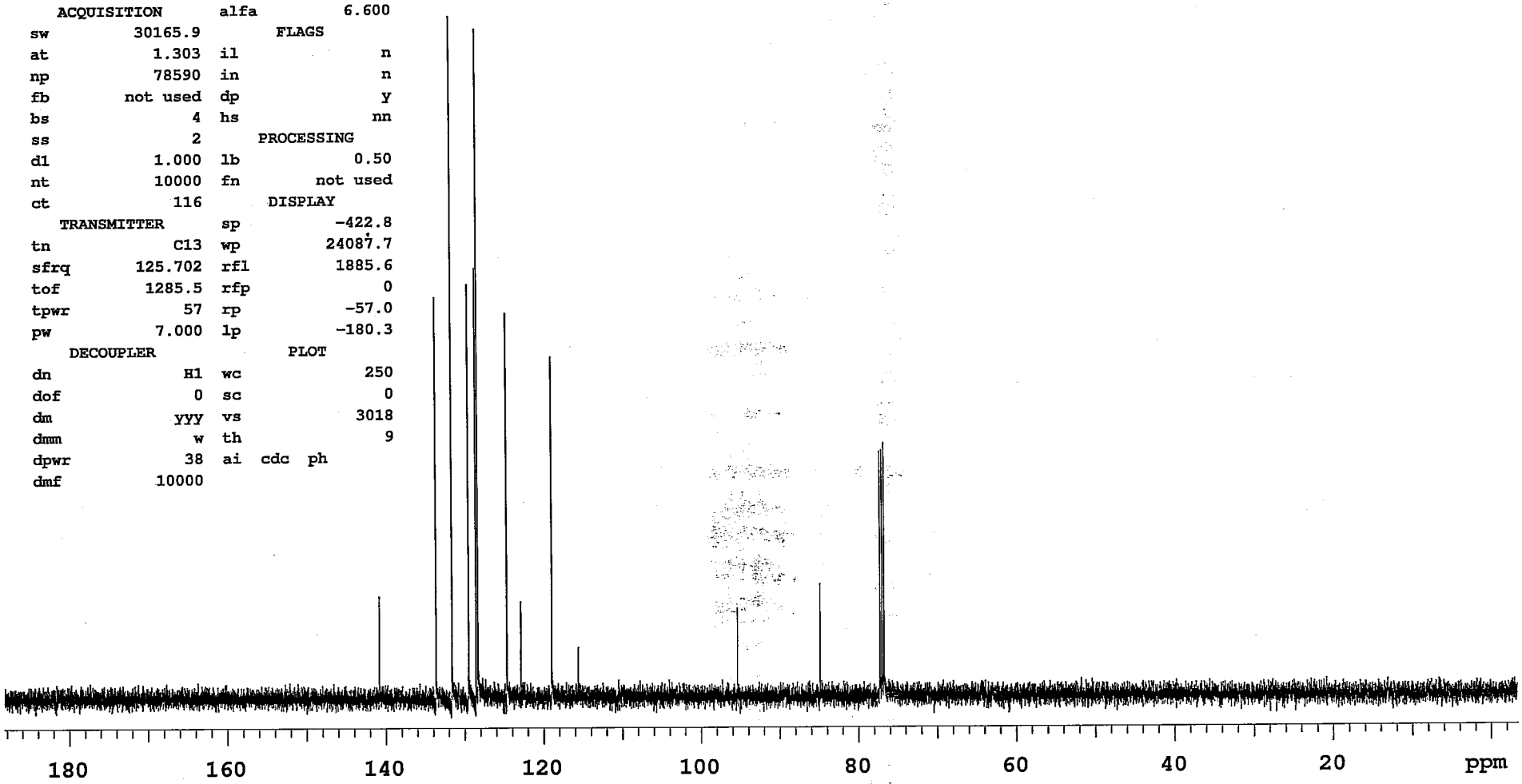
dof	0	sc	0
dm	yyy	vs	3018
dmm	w	th	9
dpwr	38	ai cdc ph	
dmf	10000		



1a



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Apr 22 2011
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AT1 = 2.50 sec
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LB1 = 0.00 Hz
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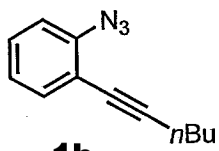
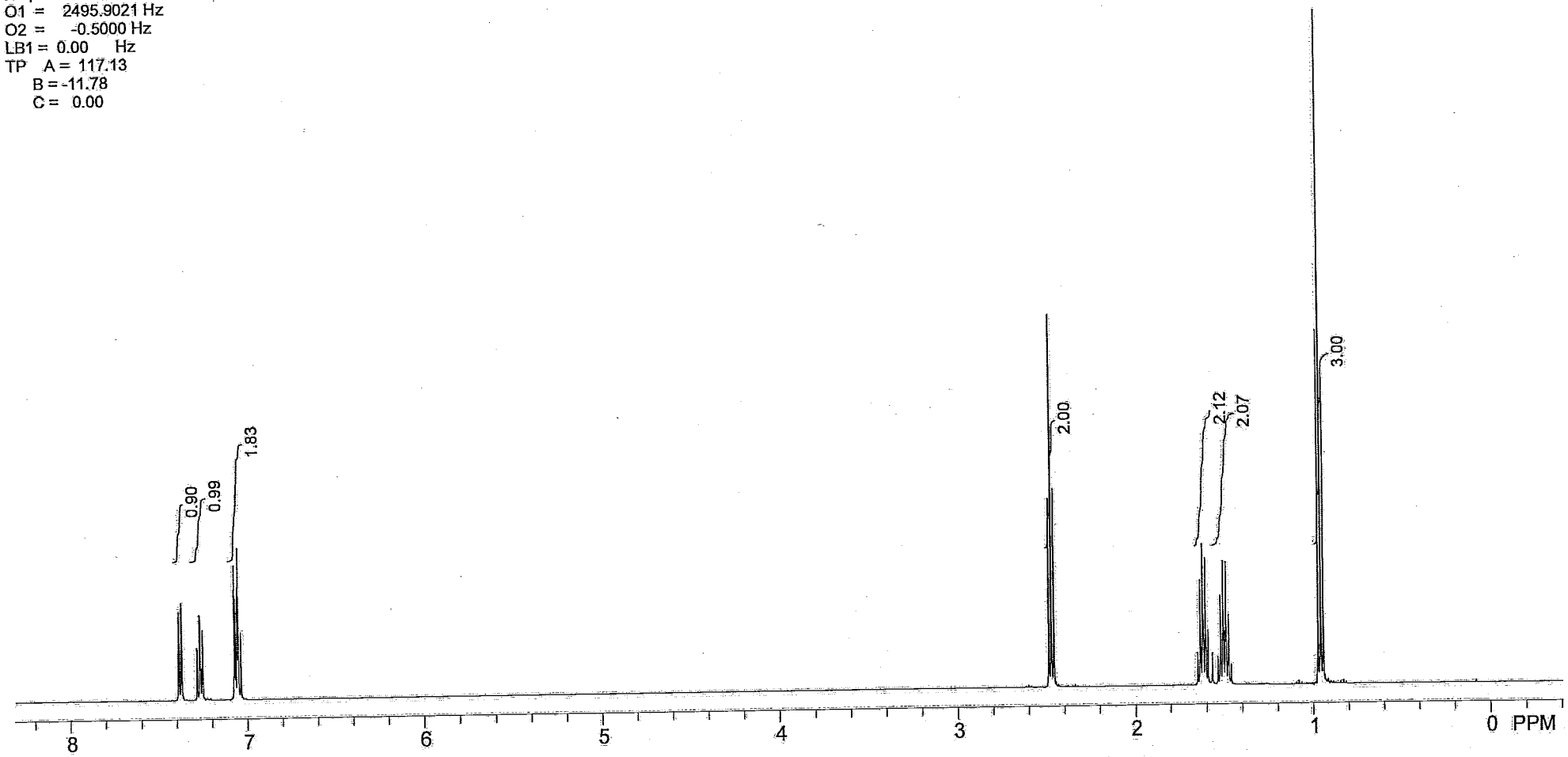
B = -11.78
C = 0.00

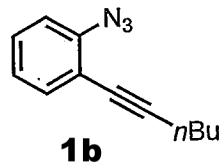


1b

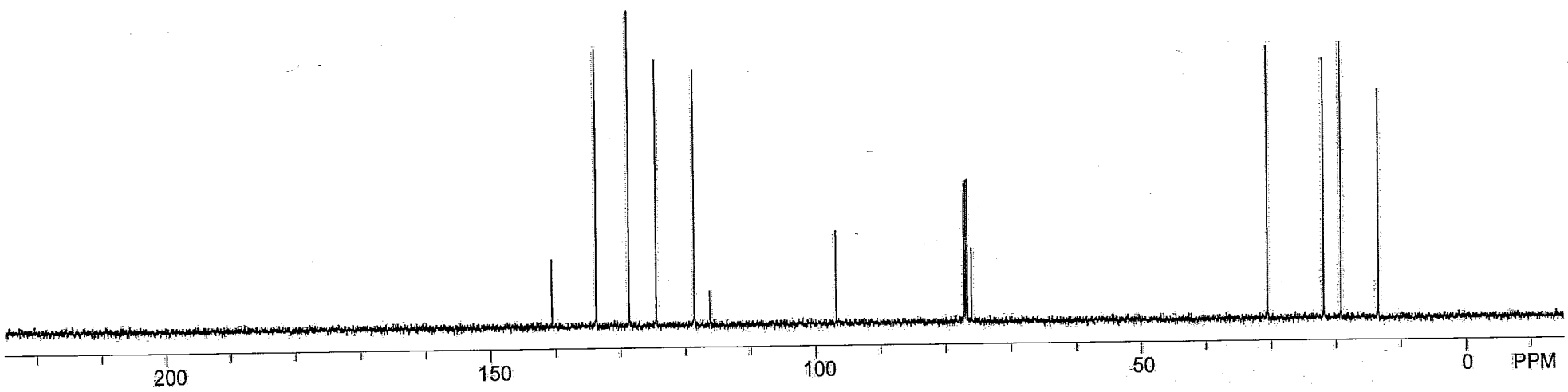


C:\Users\zhang laptop\Desktop\NMR\nuts\DATA\$llz-1-132-13c.fid
Std carbon;blank line7_t
May 1 2011
USER:
SOLVENT: CDCl3
Experiment = s2pul
Pulse length = 7.000 usec
Relaxation delay = 1.000 sec
NA = 136
Solvent = CDCl3
FID PTS1d = 39295
PTS1d = 65536
F1 = 125.702103 MHz
F2 = 499.858551 MHz
SW1 = 30165.91 Hz
AT1 = 1.30 sec
Hz per Pt 1stD = 0.46 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 13197.3711 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -185.16
B = 143.44
C = 0.00

140.577
133.736
128.715
124.544
118.703
116.307
96.931
77.283
77.026
76.774
76.151
30.688
22.042
19.368
13.633



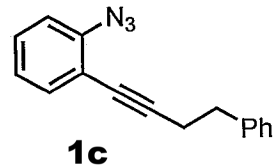
1b



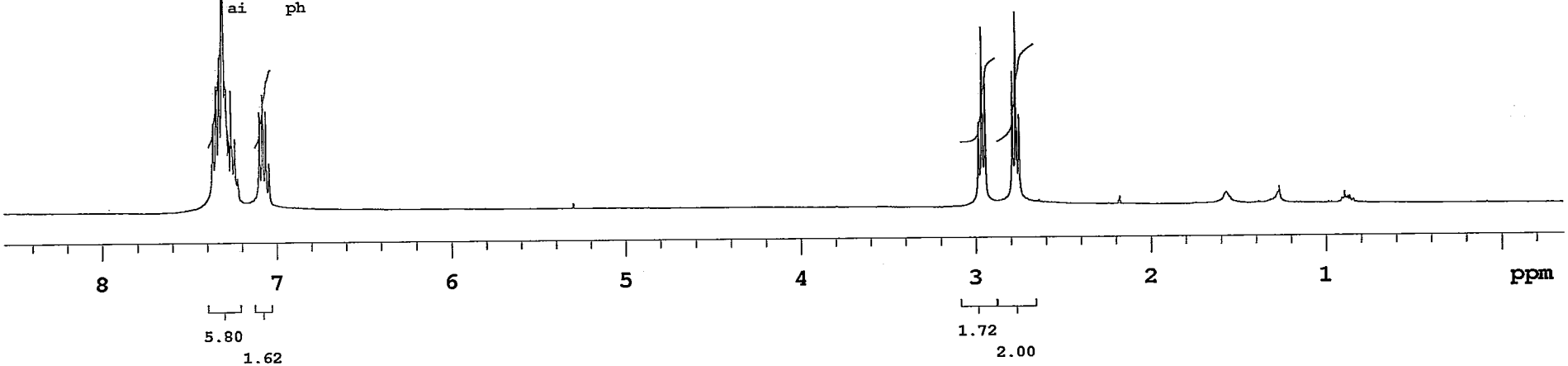
new experiment

expl s2pul

SAMPLE		DEC. & VT	
date	May 1 2011	dn	C13
solvent	cdcl3	dof	-1425.0
file	exp	dm	nnn
ACQUISITION		dmm	c
sfrq	399.951	dmf	200
tn	H1	PROCESSING	
at	2.500	lb	0.20
np	40012	fn	65536
sw	8002.4	math	i
fb	not used		
bs	2	werr	
pw	11.7	wexp	
pw	11.7	wbs	
tpwr	60	wnt	
d1	4.800	DISPLAY	
tof	0	sp	-142.1
nt	16	wp	3567.2
ct	10	vs	78
alock	n	sc	0
gain	not used	wc	250
FLAGS		hzmm	14.27
il	n	is	500.00
in	n	rfl	1994.5
dp	y	rfp	0
hs	nn	th	5
		ins	2.000
		ai ph	



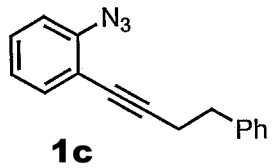
1c



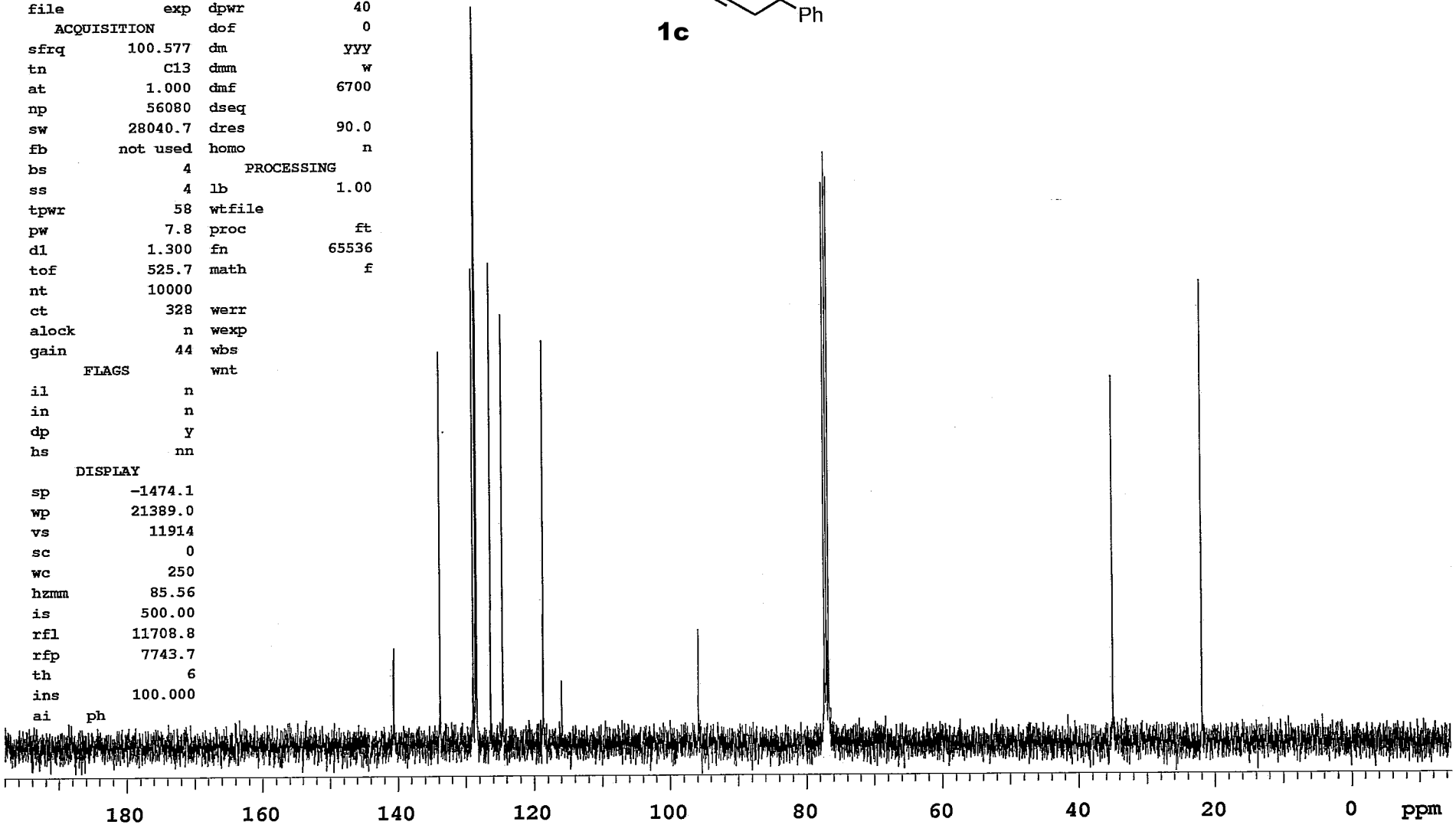
Standard c13 run using qnp probe

exp1 std13c

SAMPLE		DEC. & VT	
date	May 1 2011	dfrq	399.951
solvent	cdcl3	dn	H1
file	exp	dpwr	40
ACQUISITION		dof	0
sfrq	100.577	dm	yyy
tn	C13	dmm	w
at	1.000	dmf	6700
np	56080	dseq	
sw	28040.7	dres	90.0
fb	not used	homo	n
bs	4	PROCESSING	
ss	4	lb	1.00
tpwr	58	wtfile	
pw	7.8	proc	ft
d1	1.300	fn	65536
tof	525.7	math	f
nt	10000		
ct	328	werr	
alock	n	wexp	
gain	44	wbs	
FLAGS		wnt	
il	n		
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-1474.1		
wp	21389.0		
vs	11914		
sc	0		
wc	250		
hzmm	85.56		
is	500.00		
rfl	11708.8		
rfp	7743.7		
th	6		
ins	100.000		
ai	ph		



1c

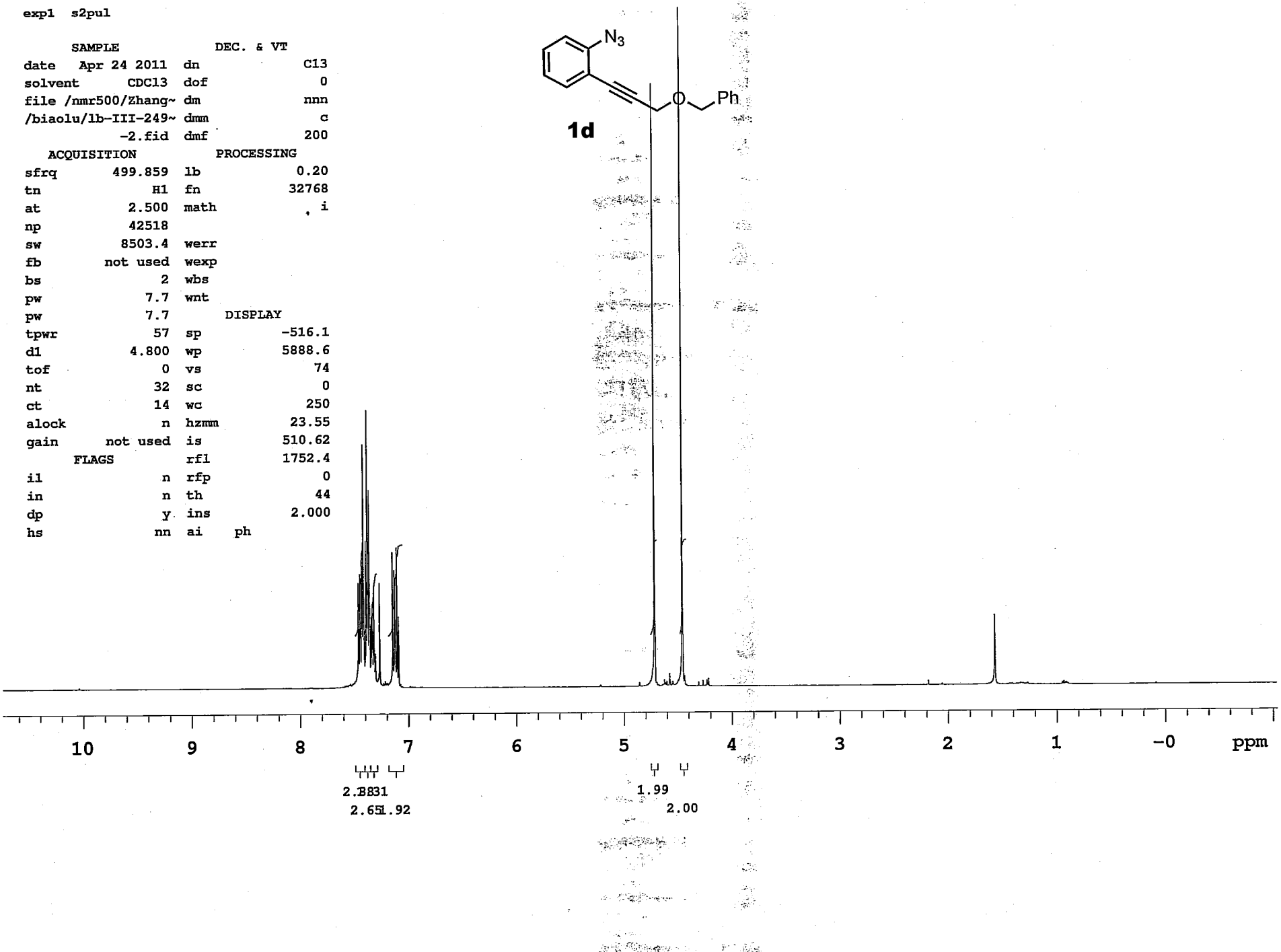


lb-III-249-2-C13

exp1 s2pul

SAMPLE		DEC. & VT	
date	Apr 24 2011	dn	C13
solvent	CDCl3	dof	0
file	/nmr500/Zhang~	dm	nnn
	/biaolu/lb-III-249~	dmm	c
	-2.fid	dmf	200
ACQUISITION		PROCESSING	
sfrq	499.859	lb	0.20
tn	H1	fn	32768
at	2.500	math	, i
np	42518		
sw	8503.4	werr	
fb	not used	wexp	
bs	2	wbs	
pw	7.7	wnt	
pw	7.7	DISPLAY	
tpwr	57	sp	-516.1
d1	4.800	wp	5888.6
tof	0	vs	74
nt	32	sc	0
ct	14	wc	250
alock	n	hzmm	23.55
gain	not used	is	510.62
FLAGS		rfl	1752.4
il	n	rfp	0
in	n	th	44
dp	y	ins	2.000
hs	nn	ai ph	

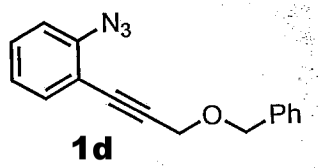
1d



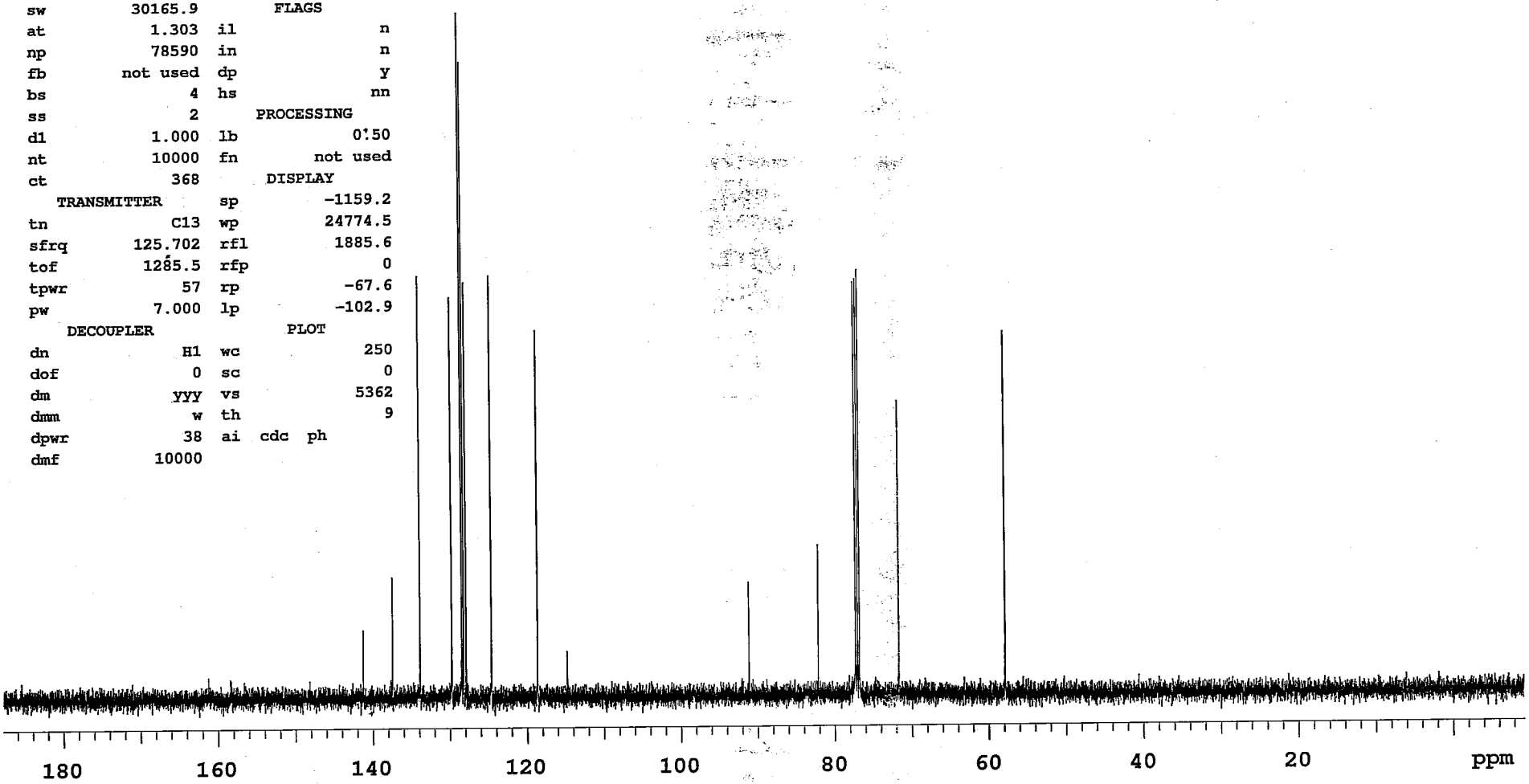
lb-III-249-2-C13

exp1 Carbon

SAMPLE		SPECIAL	
date	Apr 24 2011	temp	not used
solvent	CDCl3	gain	46
file	/nmr500/Zhang~	spin	not used
/biaolu/lb-III-249~		hst	0.008
	-2-C13.fid	pw90	14.600
ACQUISITION		alfa	6.600
sw	30165.9	FLAGS	
at	1.303	il	n
np	78590	in	n
fb	not used	dp	y
bs	4	hs	nn
ss	2	PROCESSING	
d1	1.000	lb	0.50
nt	10000	fn	not used
ct	368	DISPLAY	
TRANSMITTER		sp	-1159.2
tn	C13	wp	24774.5
sfrq	125.702	rfl	1885.6
tof	1285.5	rfp	0
tpwr	57	rp	-67.6
pw	7.000	lp	-102.9
DECOUPLER		PLOT	
dn	H1	wc	250
dof	0	sc	0
dm	yyy	vs	5362
dmm	w	th	9
dpwr	38	ai	cdc ph
dmf	10000		

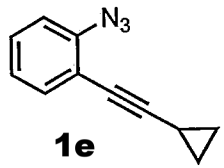


1d

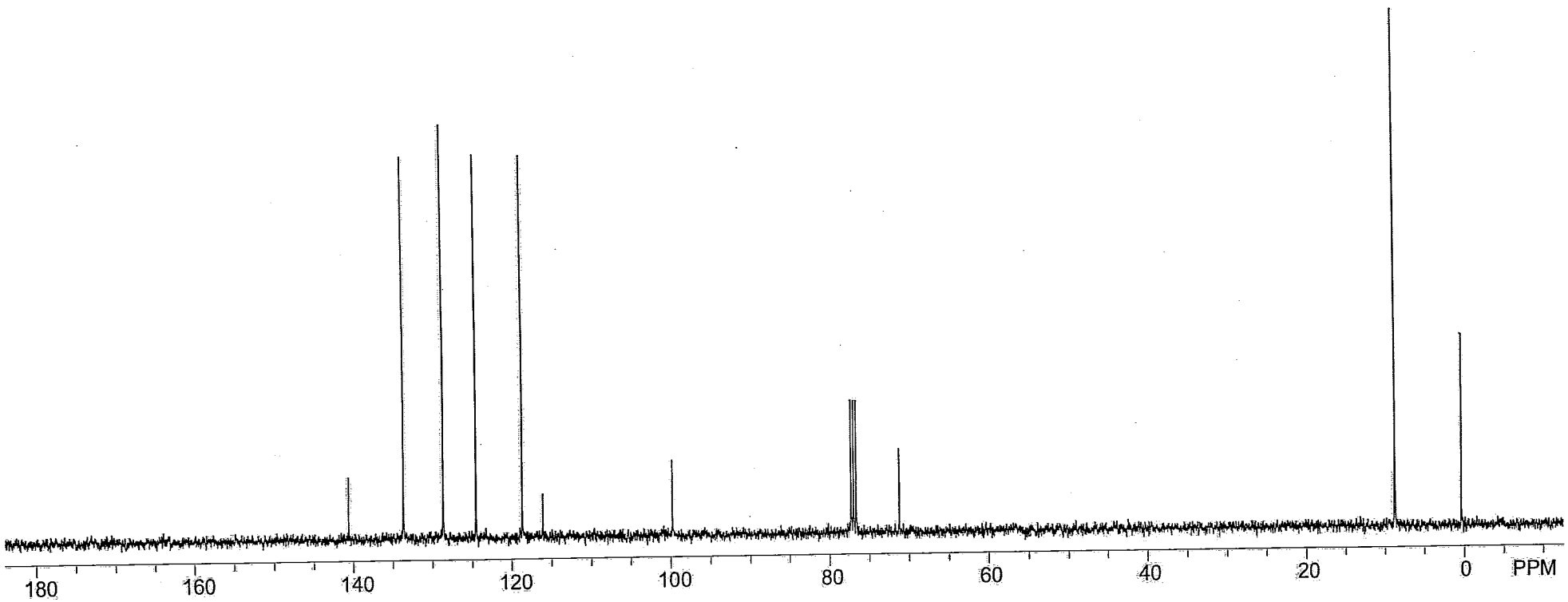


C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-169-3ring-c1.fid

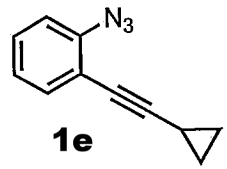
Apr 22 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 102
Solvent = cdcl3
FID PTS1d = 28040
PTS1d = 32768
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 28040.66 Hz
AT1 = 1.00 sec
Hz per Pt 1stD = 0.86 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 10052.9395 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -28.59
B = 4.22
C = 0.00



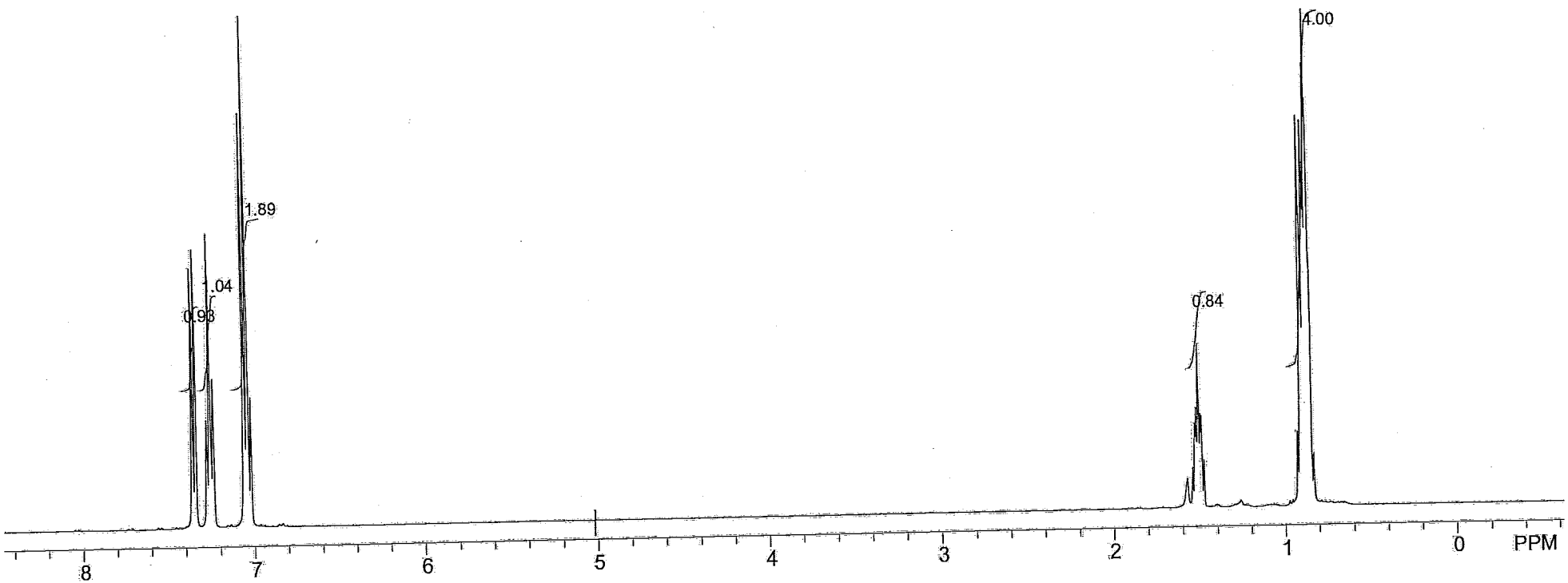
1e



C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-169-3ring.fid
new experiment
Apr 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 = -46.11
B = -36.81
C = 0.00

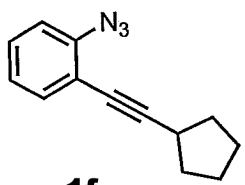


1e

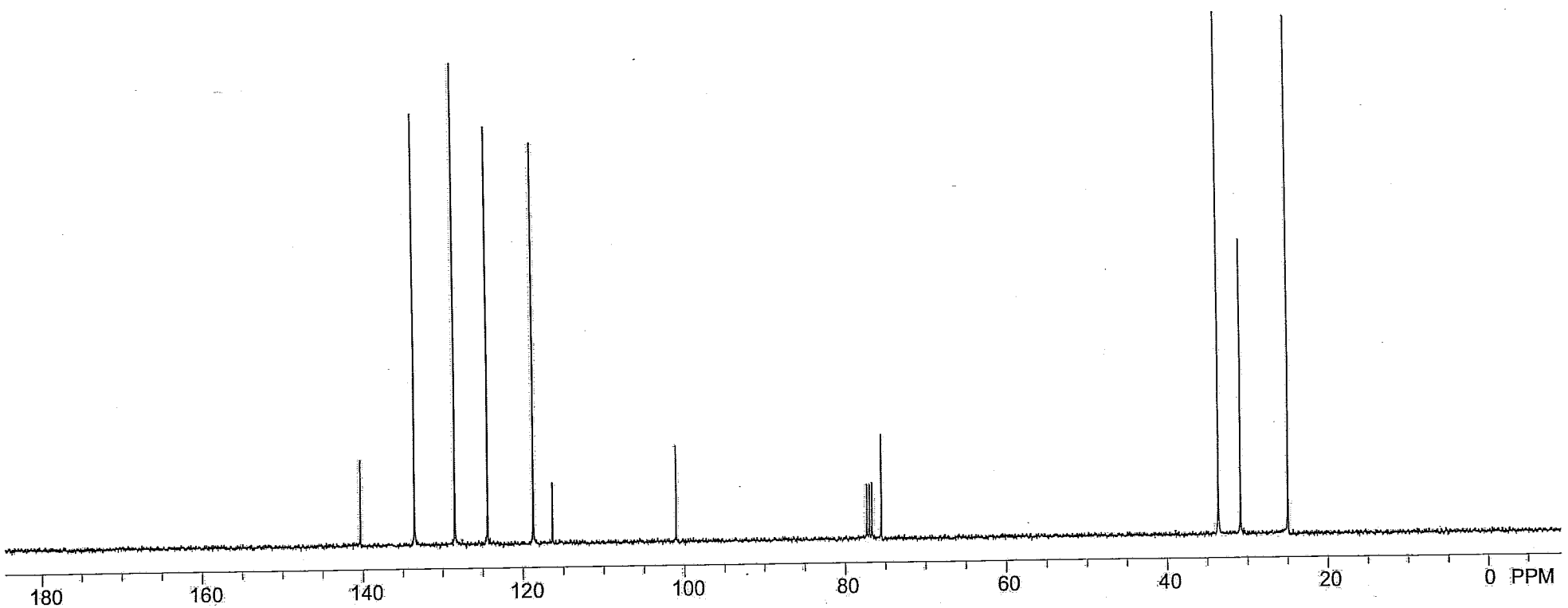


C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-169-5ring-c1.fid

Apr 22 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 74
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 = -37.97
B = 22.50
C = 0.00

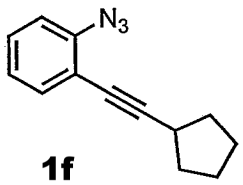


1f

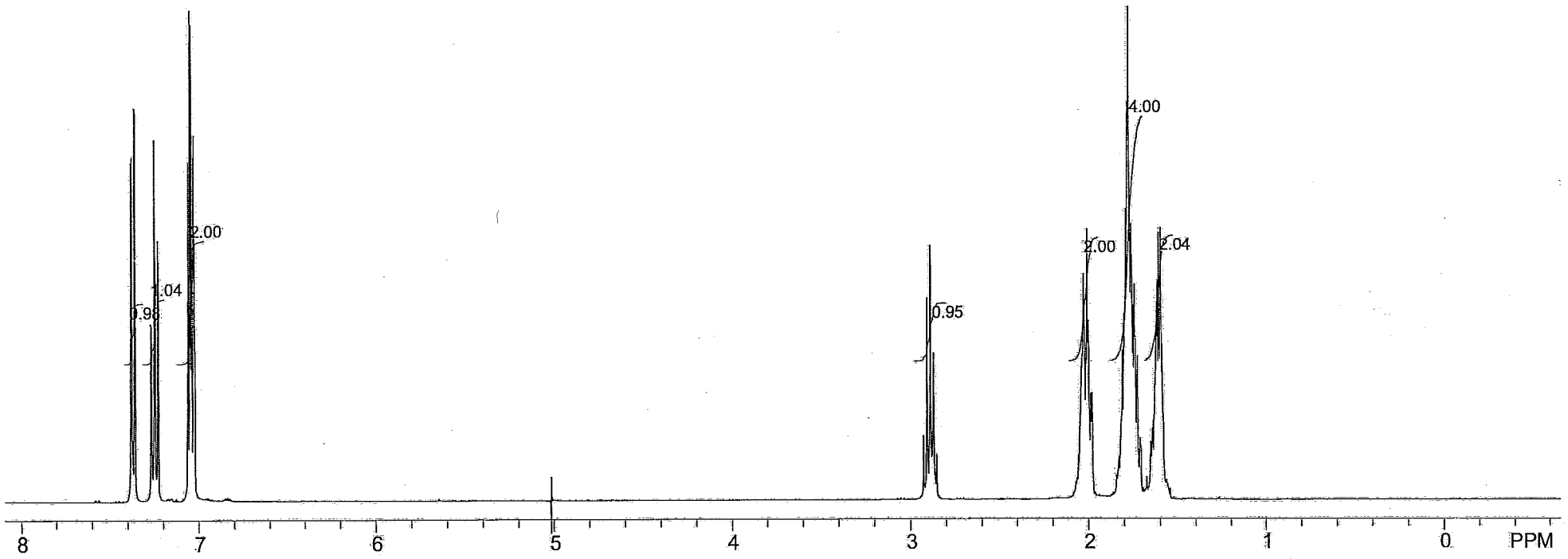


C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-169-5ring-h.fid

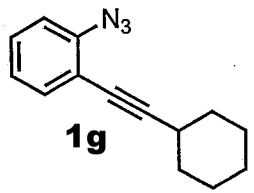
Apr 22 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 6
Solvent = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 0.24 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2006.7504 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -48.09
B = -26.16
C = 0.00



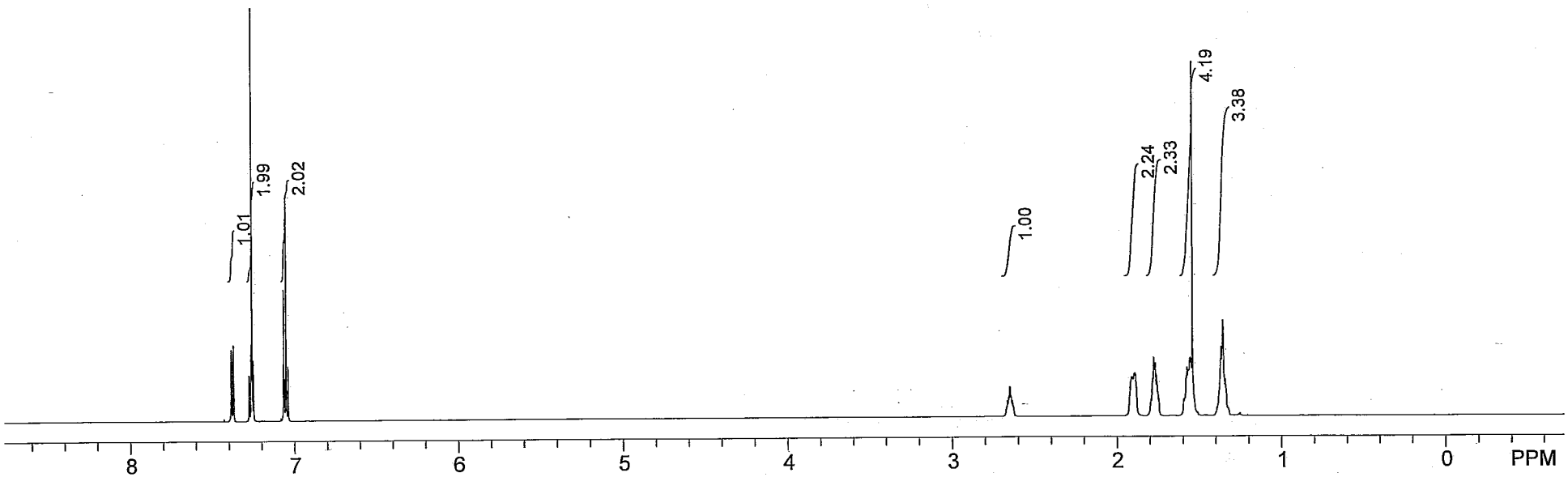
1f



C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$lyd-1-274-2.fid
lyd-1-274-2
Apr 23 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 5.825 usec
Relaxation delay = 4.800 sec
NA = 12
Solvent = cdcl3
FID PTS1d = 25000
PTS1d = 32768
F1 = 599.634705 MHz
F2 = 599.635132 MHz
SW1 = 10000.00 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 0.31 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2605.6868 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -134.06
B = 3.52
C = 0.00



1g



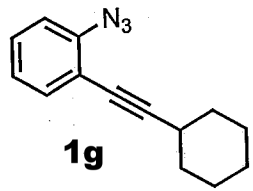
lyd-1-274-2-C

Sample: 1_Indanone
File: nmr600/Zhang/yluo/lyd-1-274-2-C.fid

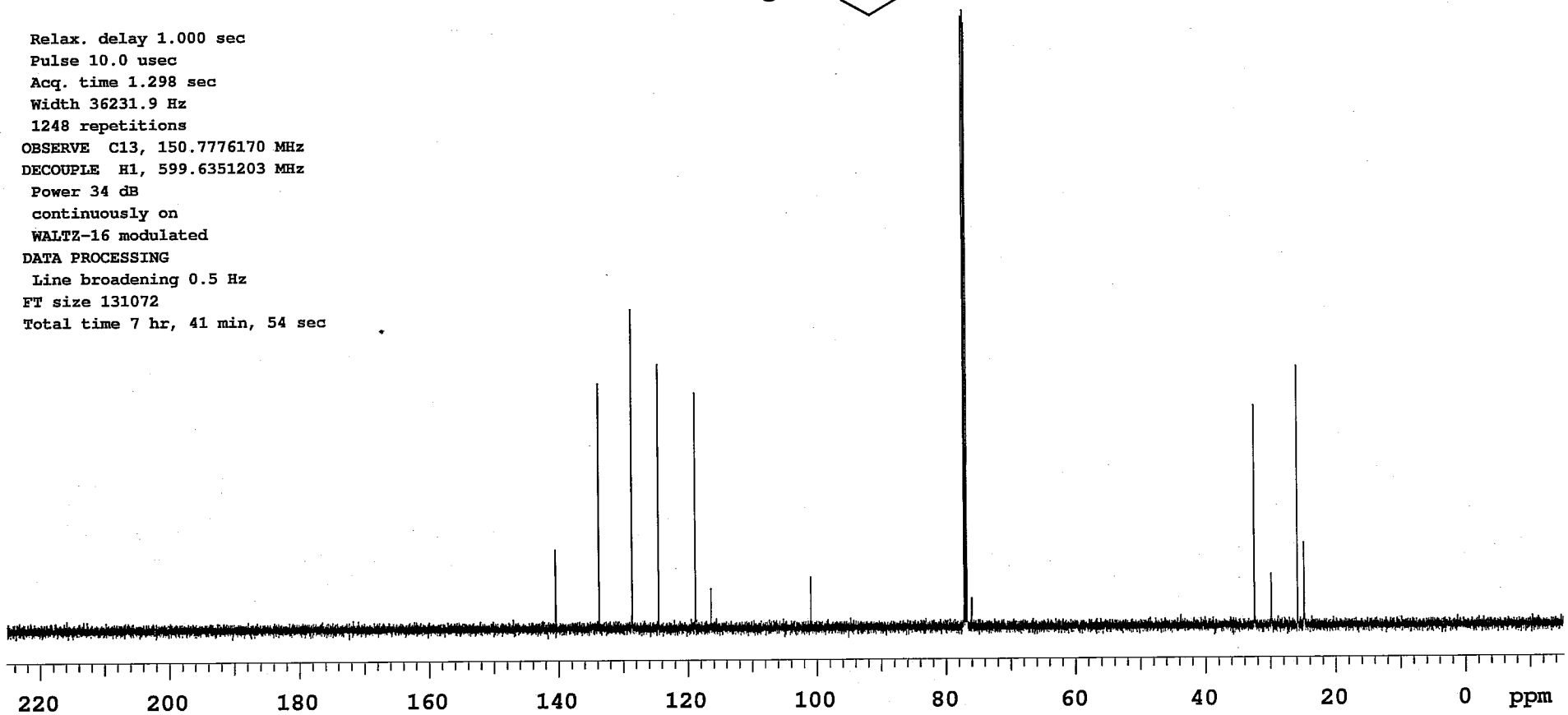
Pulse Sequence: s2pul

Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: yluo
File: lyd-1-274-2-C
INOVA-500 "nmrserver"

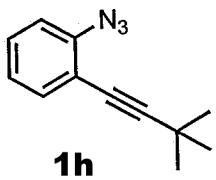
Relax. delay 1.000 sec
Pulse 10.0 usec
Acq. time 1.298 sec
Width 36231.9 Hz
1248 repetitions
OBSERVE C13, 150.7776170 MHz
DECOUPLE H1, 599.6351203 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 7 hr, 41 min, 54 sec



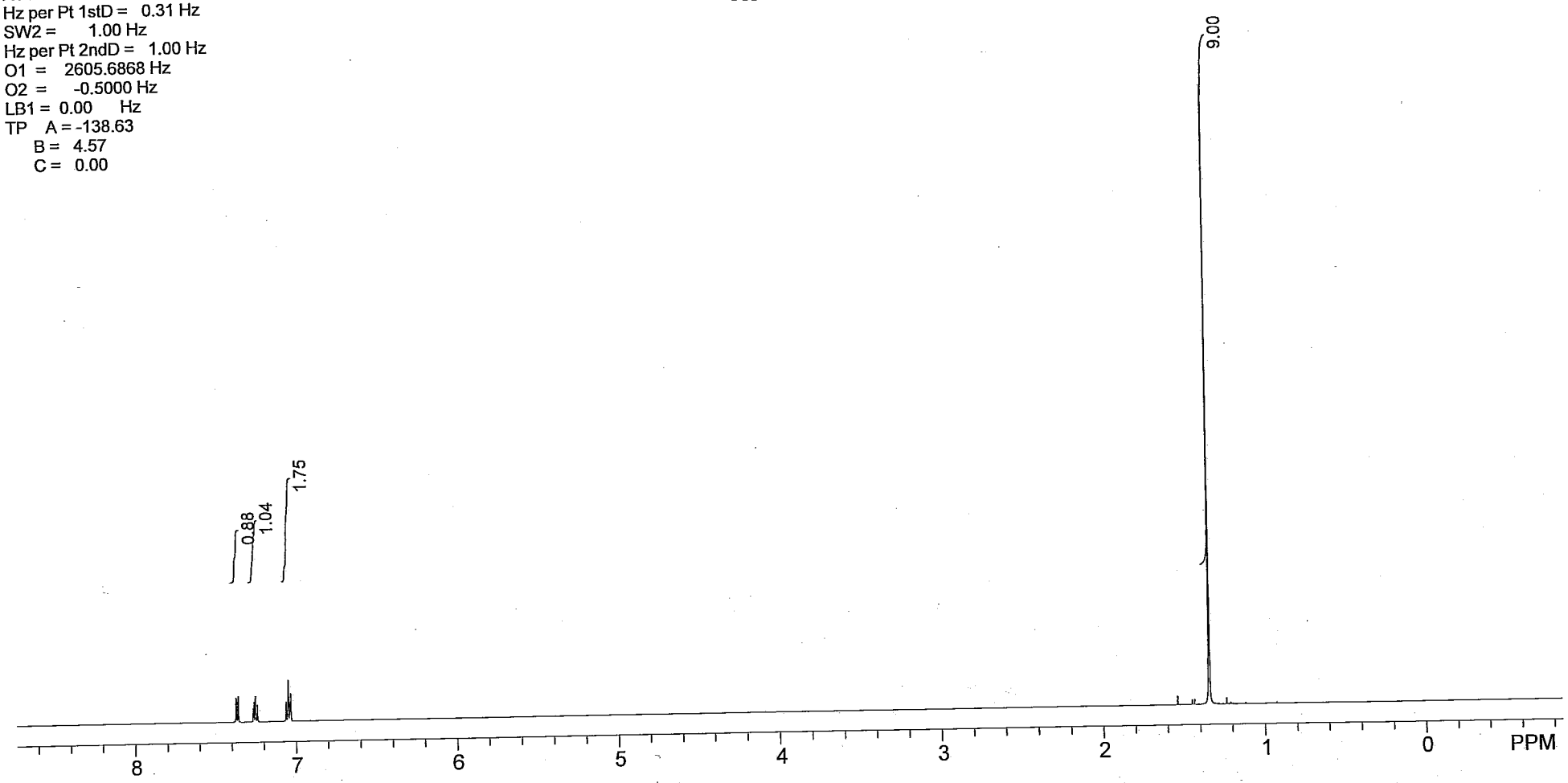
1g



C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$lyd-1-274-1.fid
lyd-1-274-1
Apr 23 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 5.825 usec
Relaxation delay = 4.800 sec
NA = 8
Solvent = cdcl3
FID PTS1d = 25000
PTS1d = 32768
F1 = 599.634705 MHz
F2 = 599.635132 MHz
SW1 = 10000.00 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 0.31 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2605.6868 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -138.63
B = 4.57
C = 0.00



1h



lyd-1-274-1-C

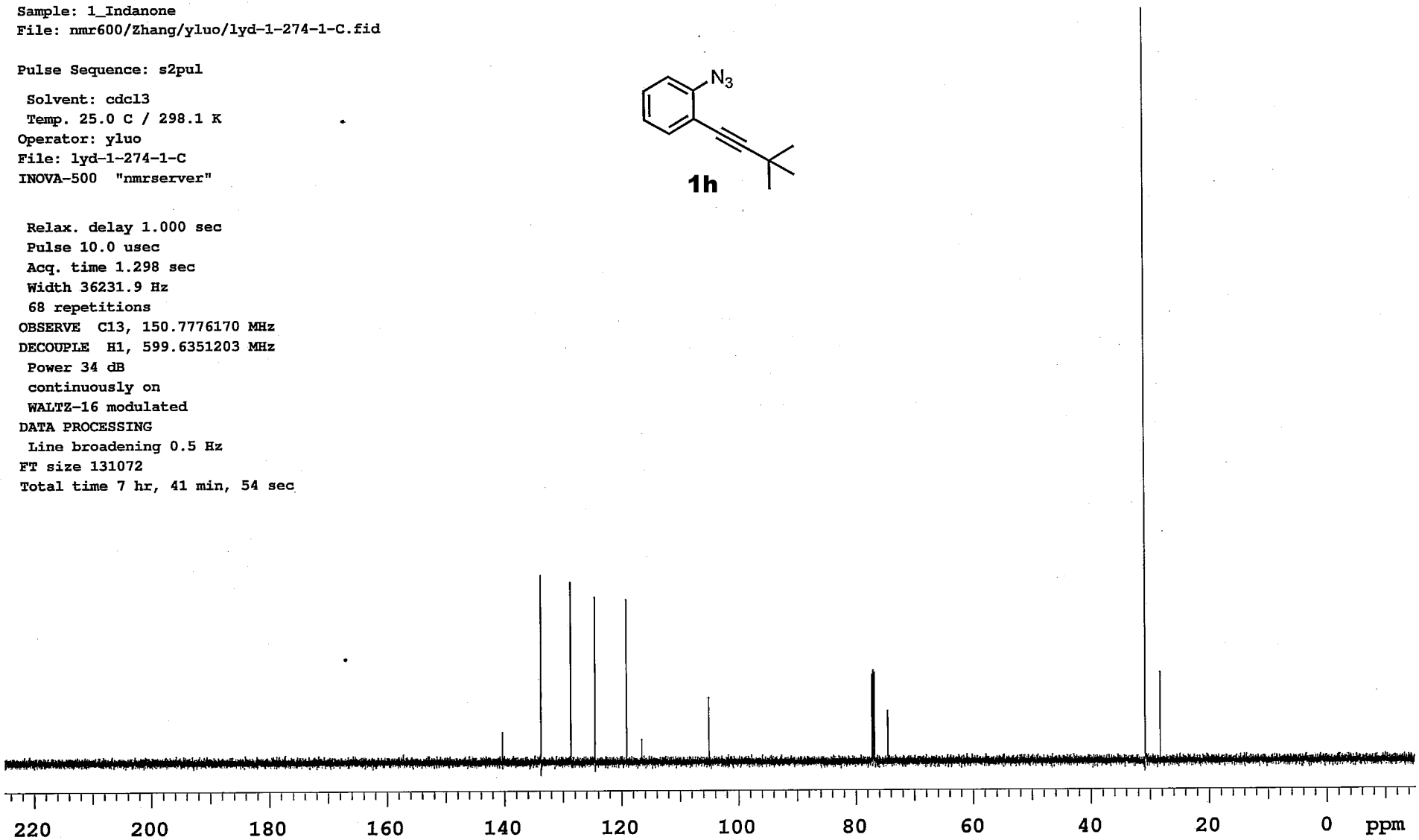
Sample: 1_Indanone
File: nmr600/Zhang/yluo/lyd-1-274-1-C.fid

Pulse Sequence: s2pul

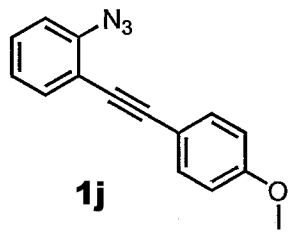
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: yluo
File: lyd-1-274-1-C
INOVA-500 "nmrserver"

Relax. delay 1.000 sec
Pulse 10.0 usec
Acq. time 1.298 sec
Width 36231.9 Hz
68 repetitions
OBSERVE C13, 150.7776170 MHz
DECOUPLE H1, 599.6351203 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 7 hr, 41 min, 54 sec

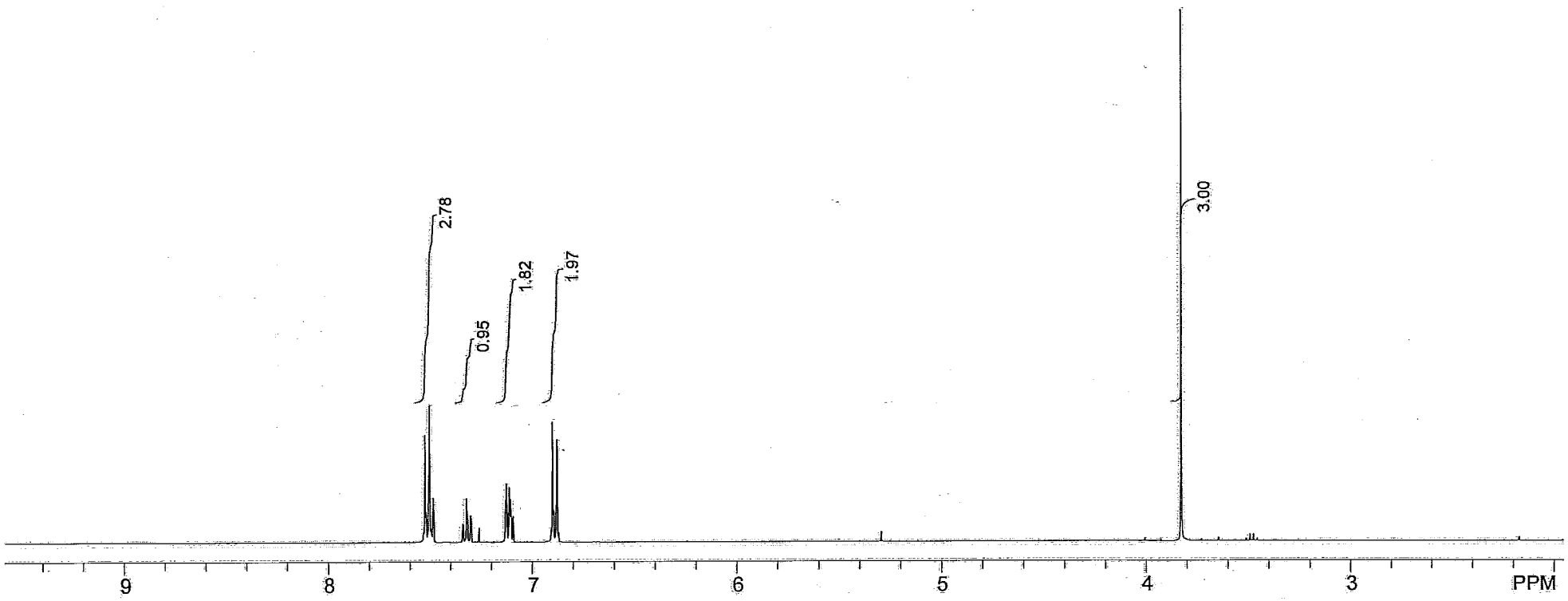
1h



C:\Users\zhang laptop\Desktop\NMR\nuts\DATA\$llz-1-139-1h.fid
new experimentU
Apr 24 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 = -33.20
B = -50.92
C = 0.00

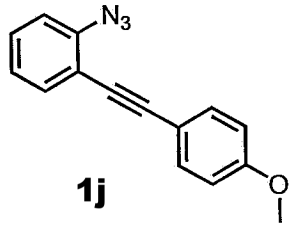


1j

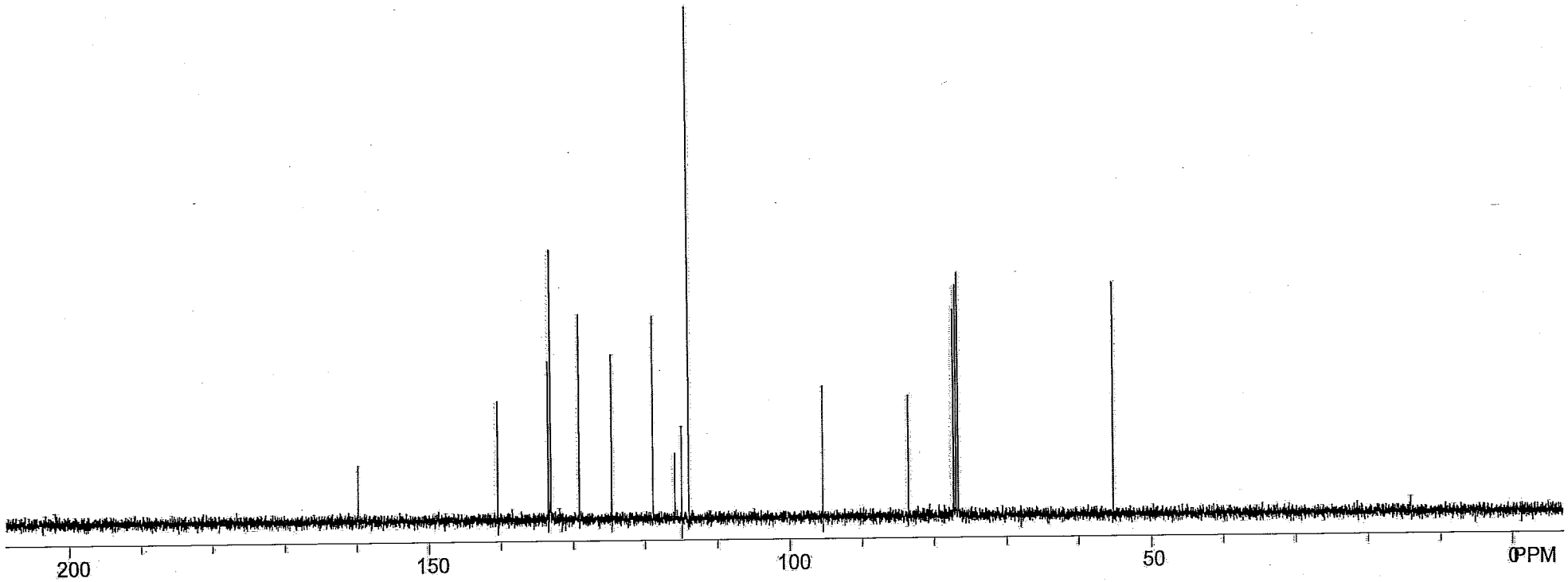


C:\Users\zhang laptop\Desktop\NMR\nuts\DATA\$llz-1-139-13c.fid
Standard c13 run using qnp probeU
Apr 24 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 9.500 usec
Relaxation delay = 5.000 sec
NA = 108
Solvent = cdcl3
FID PTS1d = 16000
PTS1d = 16384
F1 = 100.576706 MHz
F2 = 399.949585 MHz
SW1 = 25000.00 Hz
AT1 = 0.64 sec
Hz per Pt 1stD = 1.53 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 9531.0605 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -120.94
B = 189.84
C = 0.00

159.853
140.493
133.470
133.113
129.182
124.660
118.942
115.897
114.949
113.986
95.480
83.609
77.363
77.037
76.726
55.284



1j

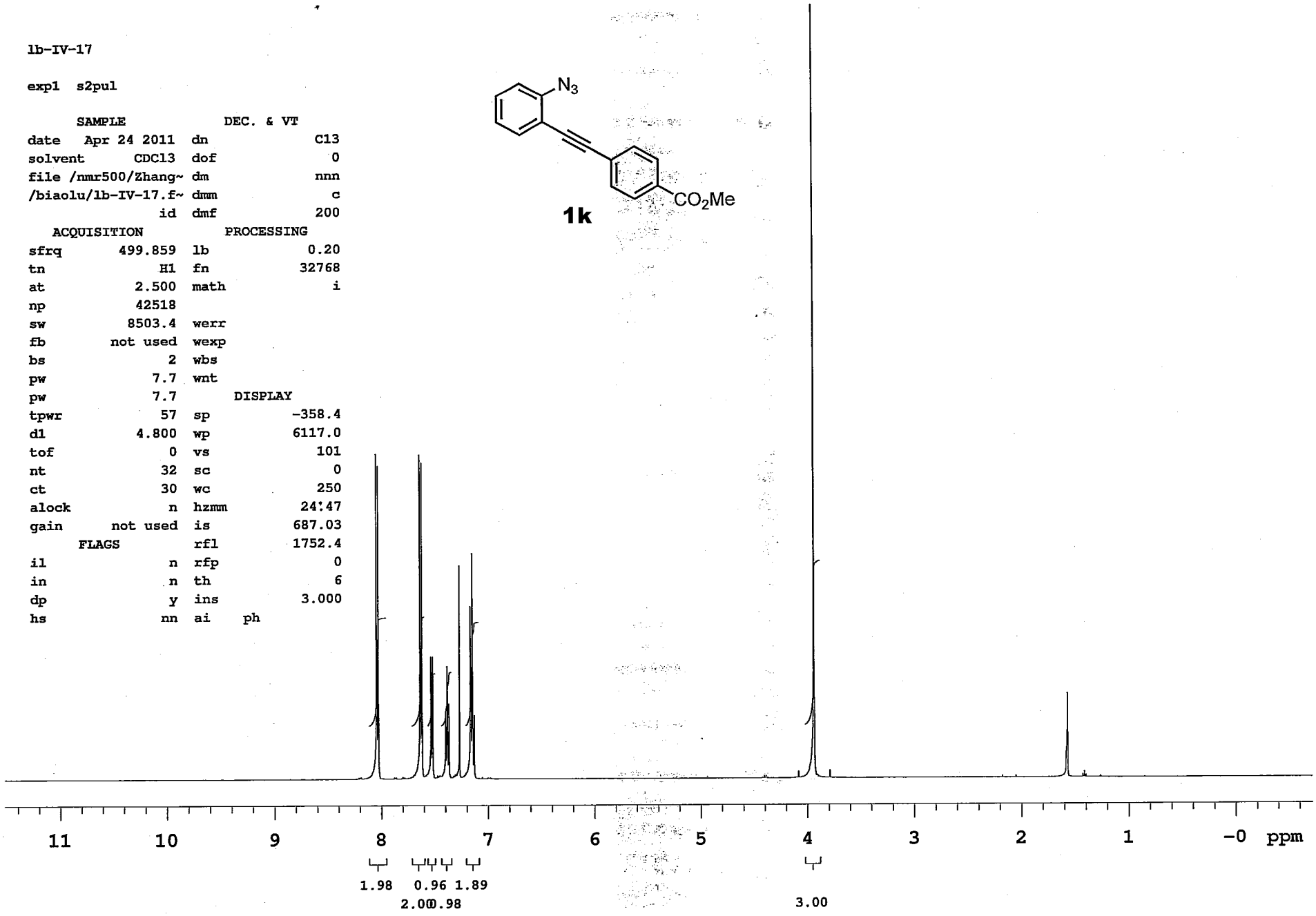


lb-IV-17

exp1 s2pul

SAMPLE		DEC. & VT	
date	Apr 24 2011	dn	C13
solvent	CDCl3	dof	0
file	/nmr500/Zhang~	dm	nnn
	/biaolu/lb-IV-17.f~	dmm	c
	id	dmf	200
ACQUISITION		PROCESSING	
sfrq	499.859	lb	0.20
tn	H1	fn	32768
at	2.500	math	i
np	42518		
sw	8503.4	werr	
fb	not used	wexp	
bs	2	wbs	
pw	7.7	wnt	
pw	7.7	DISPLAY	
tpwr	57	sp	-358.4
d1	4.800	wp	6117.0
tof	0	vs	101
nt	32	sc	0
ct	30	wc	250
alock	n	hzmm	24.47
gain	not used	is	687.03
FLAGS		rfl	1752.4
il	n	rfp	0
in	n	th	6
dp	y	ins	3.000
hs	nn	ai ph	

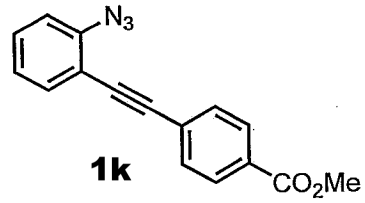
1k



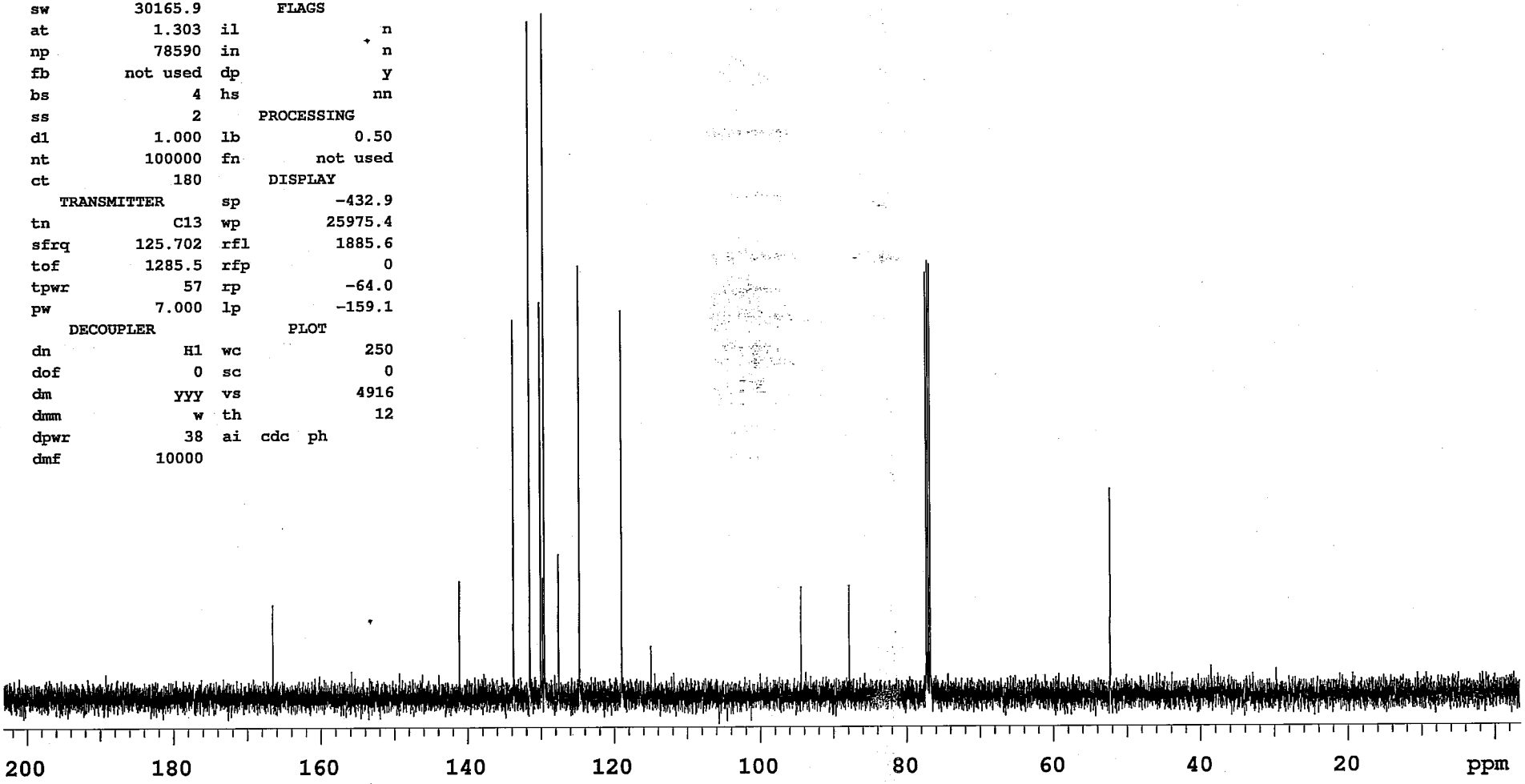
lb-IV-17-C13

exp1 Carbon

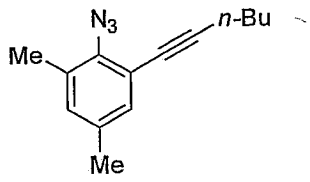
SAMPLE		SPECIAL	
date	Apr 24 2011	temp	not used
solvent	CDCl3	gain	46
file	/nmr500/Zhang~	spin	not used
	/biaolu/lb-IV-17-C~	hst	0.008
	13.fid	pw90	14.600
ACQUISITION		alfa	6.600
sw	30165.9	FLAGS	
at	1.303	il	n
np	78590	in	n
fb	not used	dp	y
bs	4	hs	nn
ss	2	PROCESSING	
d1	1.000	lb	0.50
nt	100000	fn	not used
ct	180	DISPLAY	
TRANSMITTER		sp	-432.9
tn	C13	wp	25975.4
sfrq	125.702	rfl	1885.6
tof	1285.5	rfp	0
tpwr	57	rp	-64.0
pw	7.000	lp	-159.1
DECOUPLER		PLOT	
dn	H1	wc	250
dof	0	sc	0
dm	yyy	vs	4916
dmm	w	th	12
dpwr	38	ai cdc ph	
dmf	10000		



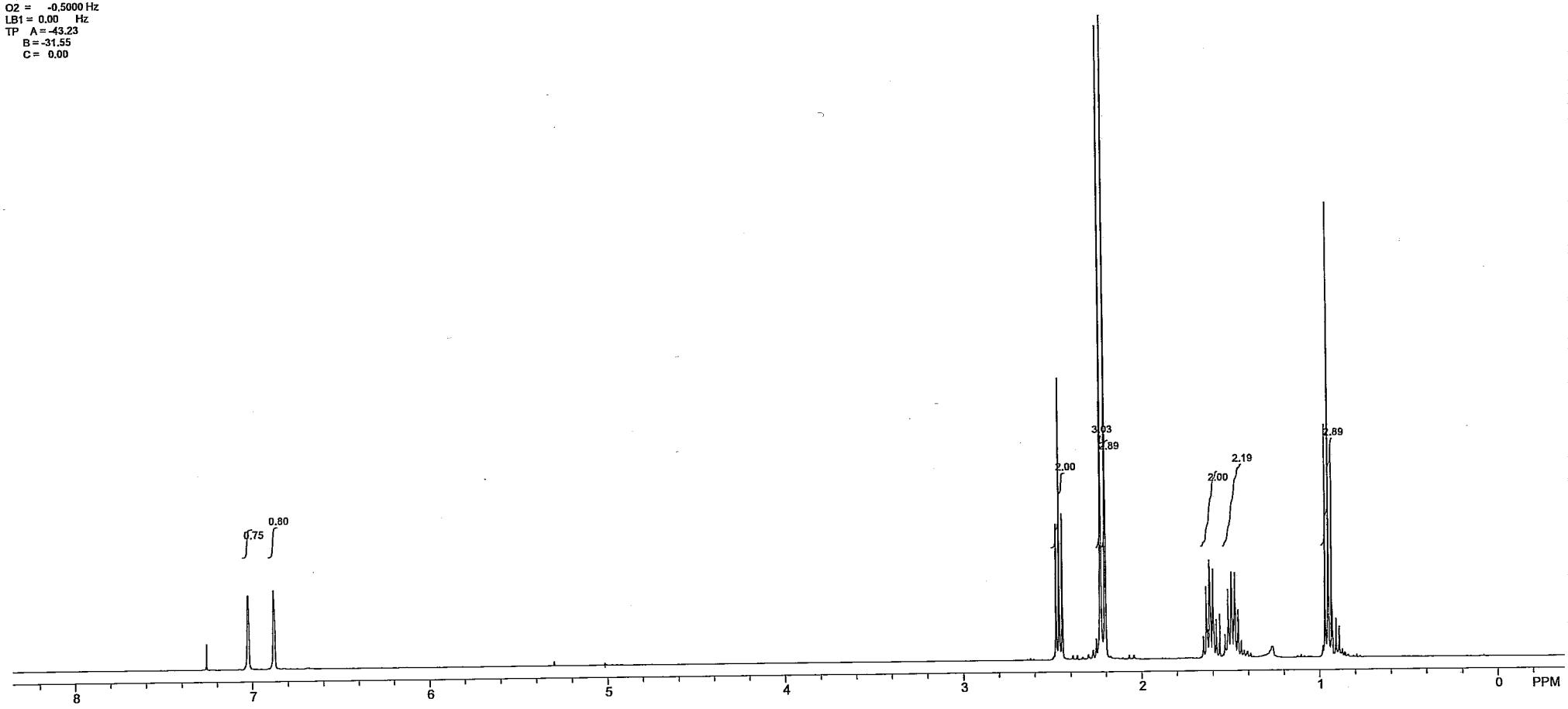
1k



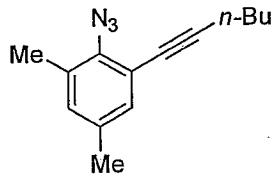
D:\Greenware\Ntus 20080731\DATA\$wyz3-253-pro.fid
new experiment
Apr 28 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 1.000 sec
NA = 20
Solvent = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 0.24 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2005.9918 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -43.23
B = -31.55
C = 0.00



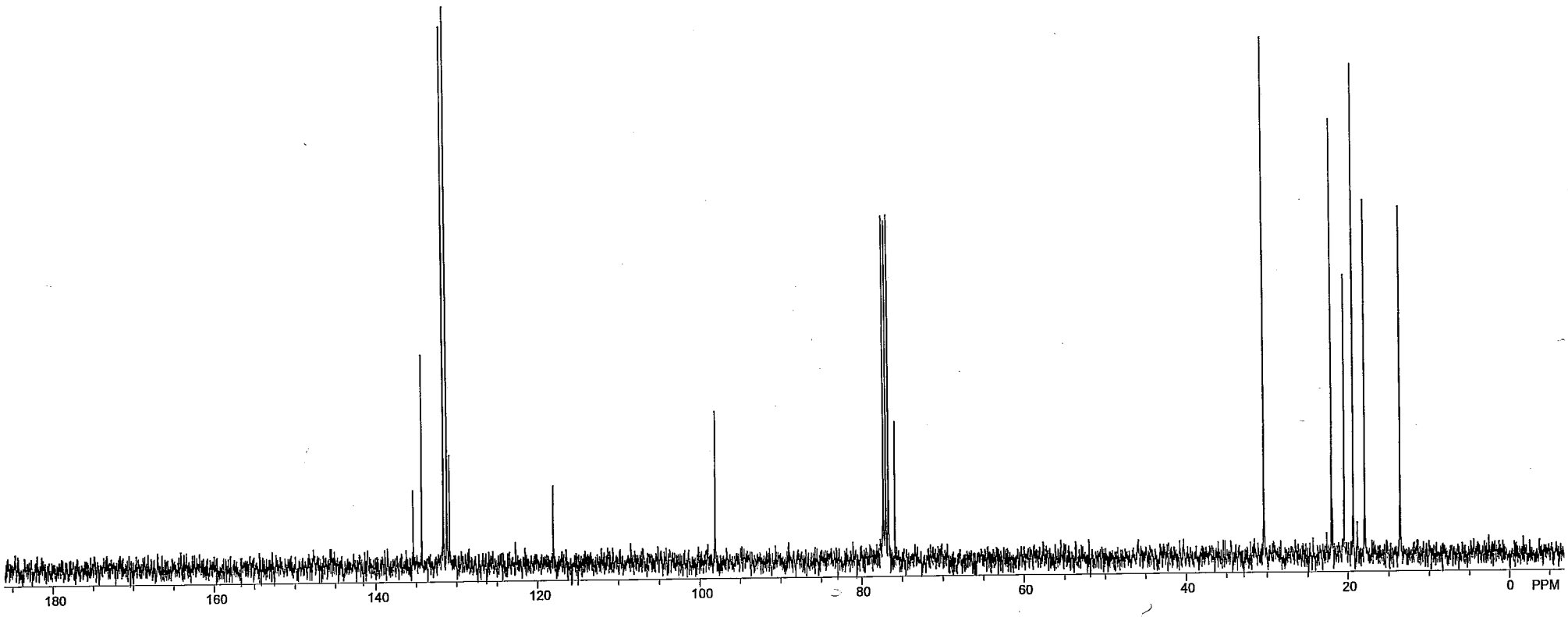
1l



D:\Greenware\Ntus 20080731\DATA\$wyz3-253-pro-c13.fid
Standard c13 run using qnp probe
Apr 28 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 100
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 = -30.47
B = 11.25
C = 0.00



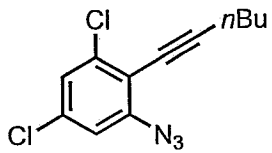
1l



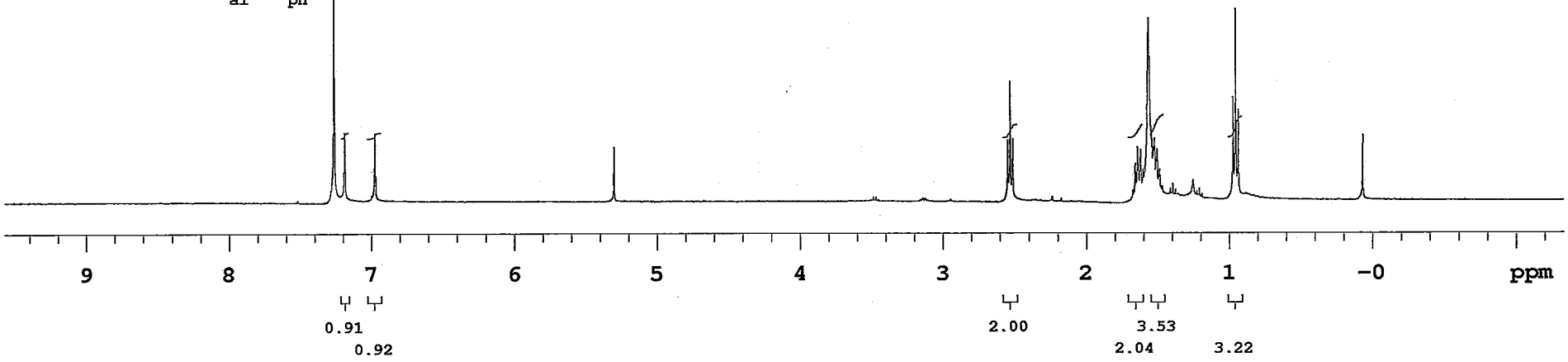
lb-IV-37

exp1 s2pul

SAMPLE		DEC. & VT	
date	May 1 2011	dn	C13
solvent	cdcl3	dof	-1425.0
file	exp	dm	nnn
ACQUISITION		dmm	c
sfrq	399.951	dmf	200
tn	H1	PROCESSING	
at	2.500	lb	0.20
np	40012	fn	65536
sw	8002.4	math	i
fb	not used		
bs	2	werr	
pw	11.7	wexp	
pw	11.7	wbs	
tpwr	60	wnt	
d1	4.800	DISPLAY	
tof	0	sp	-533.6
nt	16	wp	4362.9
ct	16	vs	219
alock	n	sc	0
gain	not used	wc	250
FLAGS		hzmm	17.45
il	n	is	500.00
in	n	rfl	1994.5
dp	y	rfp	0
hs	nn	th	5
		ins	2.000
		ai ph	



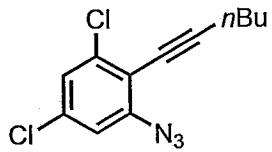
1m



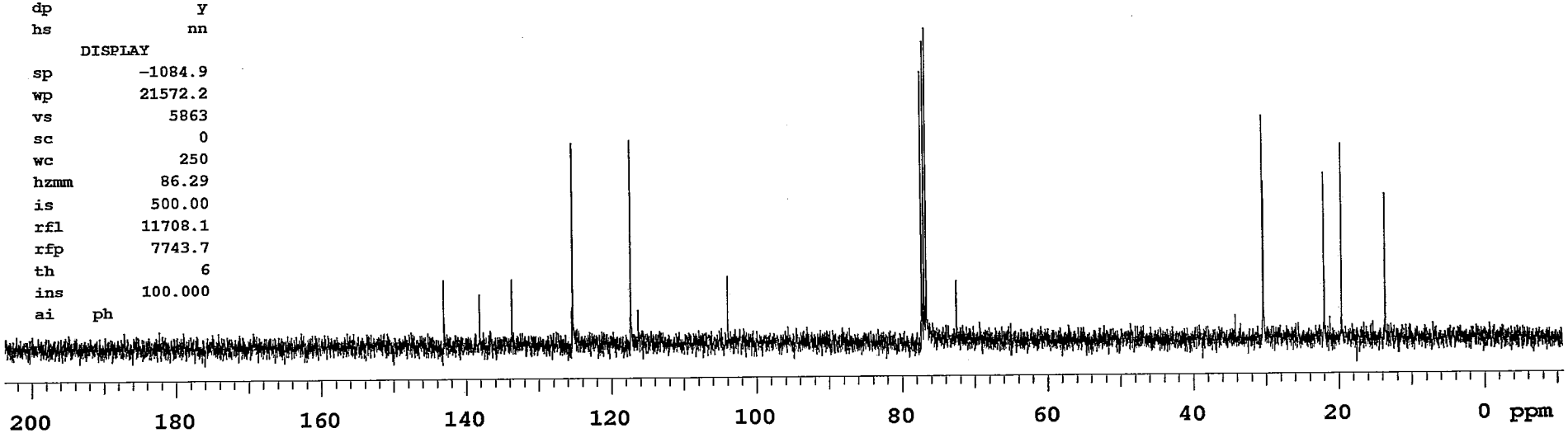
Standard c13 run using qnp probe

expl std13c

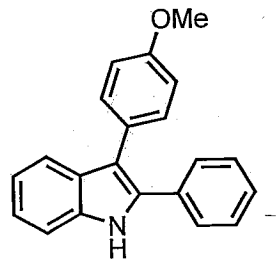
SAMPLE		DEC. & VT	
date	May 1 2011	dfrq	399.951
solvent	cdcl3	dn	H1
file	exp	dpwr	40
ACQUISITION		dof	0
sfrq	100.577	dm	yyy
tn	C13	dmm	w
at	1.000	dmf	6700
np	56080	dseq	
sw	28040.7	dres	90.0
fb	not used	homo	n
bs	4	PROCESSING	
ss	4	lb	1.00
tpwr	58	wtfile	
pw	7.8	proc	ft
d1	1.300	fn	65536
tof	525.7	math	f
nt	10000		
ct	248	werr	
alock	n	wexp	
gain	44	wbs	
FLAGS		wnt	
il	n		
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-1084.9		
wp	21572.2		
vs	5863		
sc	0		
wc	250		
hzmm	86.29		
is	500.00		
rfl	11708.1		
rfp	7743.7		
th	6		
ins	100.000		
ai ph			



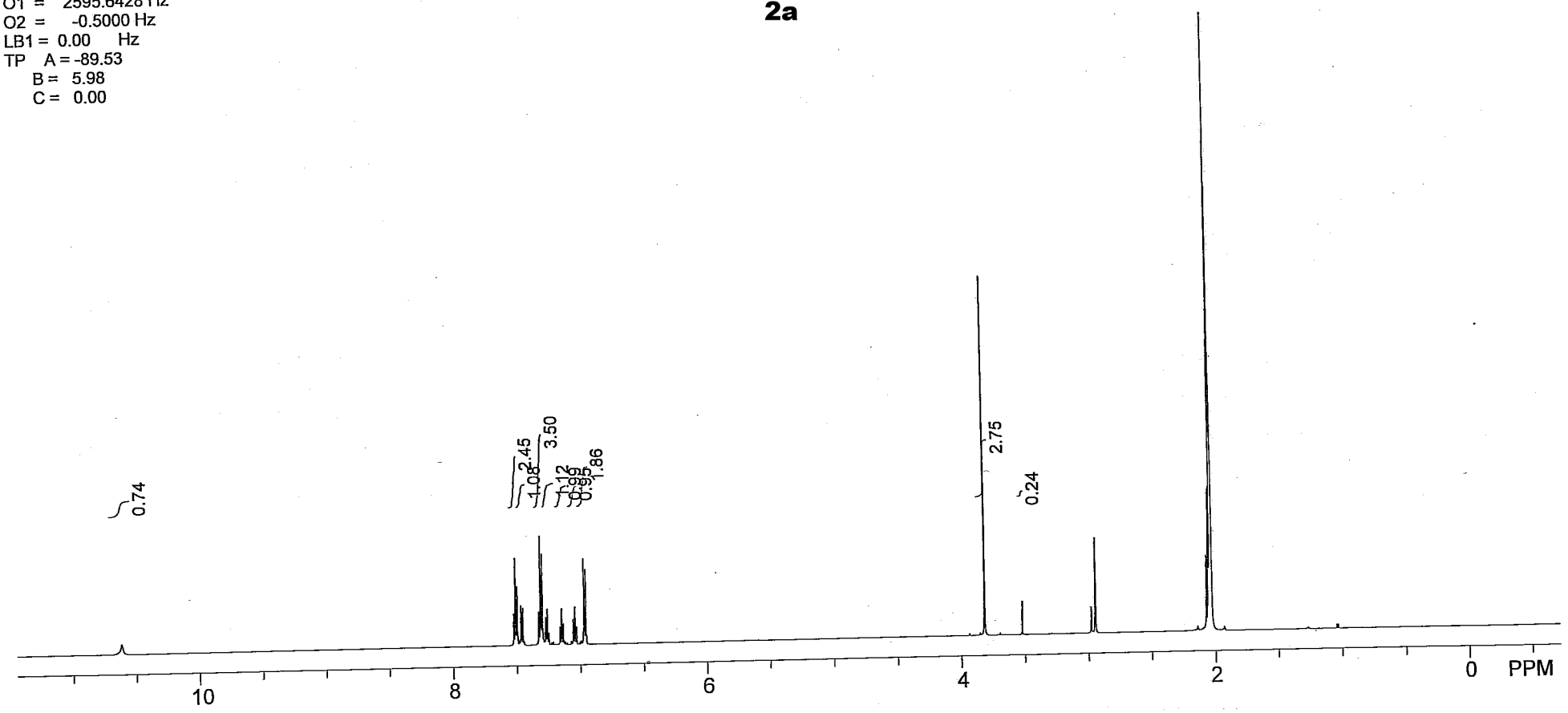
1m



C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$lyd-1-287-2-acetone.fid
lyd-1-287-2-acetone
Apr 26 2011
USER:
SOLVENT: acetone
Experiment = s2pul
Pulse length = 5.825 usec
Relaxation delay = 4.800 sec
NA = 28
Solvent = acetone
FID PTS1d = 25000
PTS1d = 32768
F1 = 599.637817 MHz
F2 = 599.638245 MHz
SW1 = 10000.00 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 0.31 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2595.6428 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -89.53
B = 5.98
C = 0.00



2a



lyd-1-287-2-C-acetone

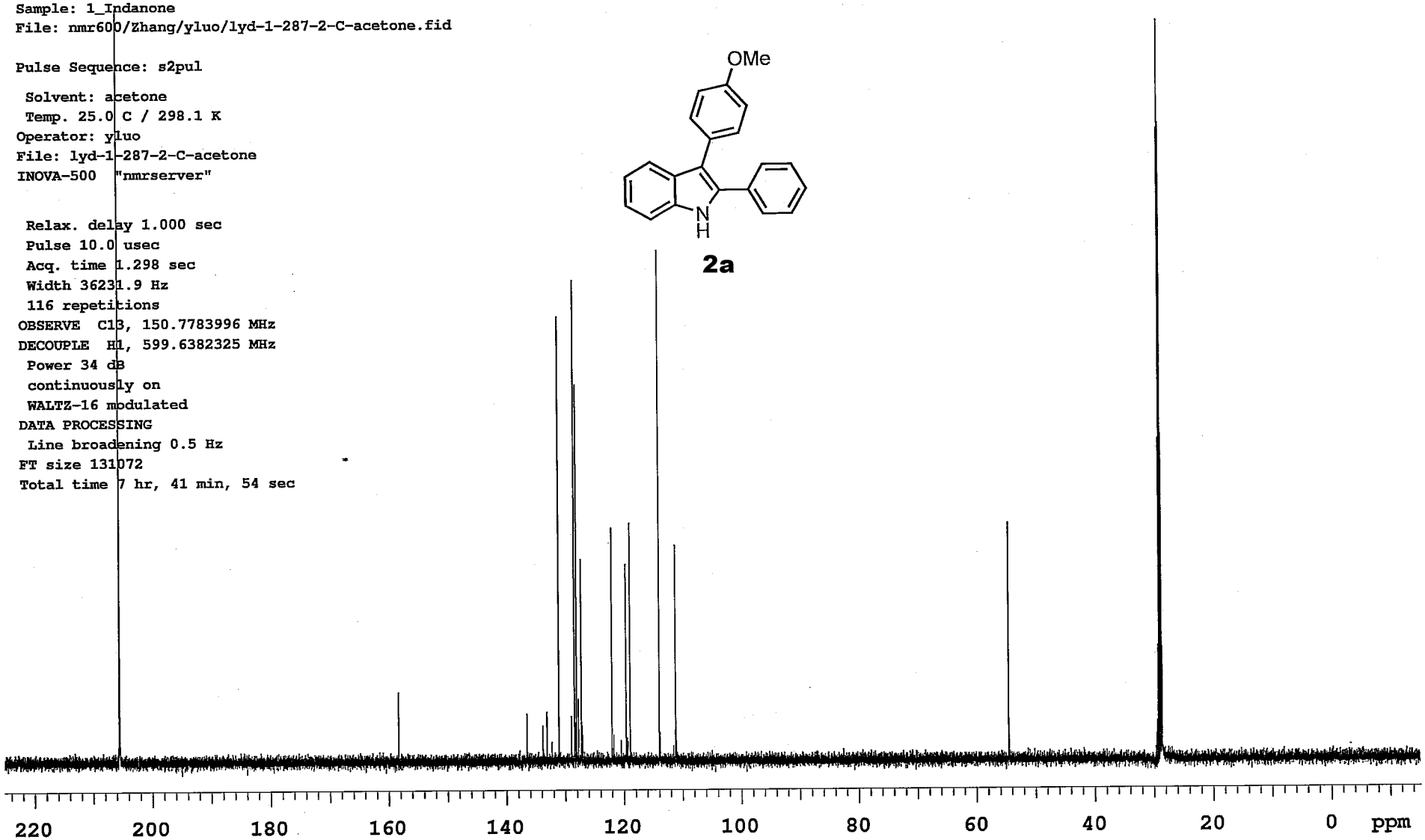
Sample: 1_Indanone
File: nmr600/Zhang/yluo/lyd-1-287-2-C-acetone.fid

Pulse Sequence: s2pul

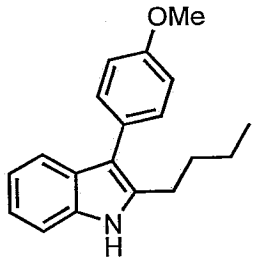
Solvent: acetone
Temp. 25.0 C / 298.1 K
Operator: yluo
File: lyd-1-287-2-C-acetone
INOVA-500 "nmrserver"

Relax. delay 1.000 sec
Pulse 10.0 usec
Acq. time 1.298 sec
Width 36231.9 Hz
116 repetitions
OBSERVE C13, 150.7783996 MHz
DECOUPLE H1, 599.6382325 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 7 hr, 41 min, 54 sec

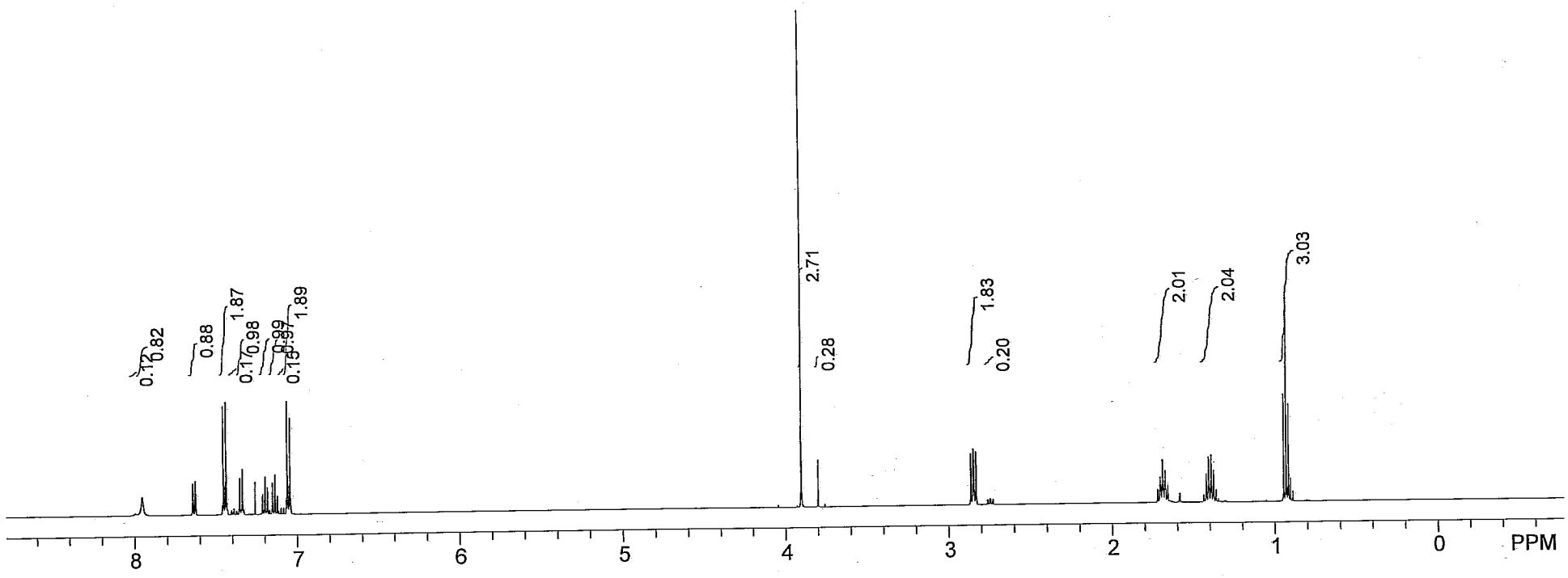
2a



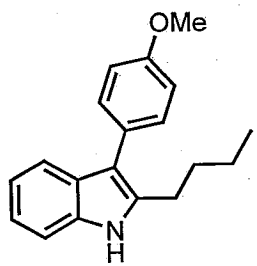
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$lyd-1-284-1.fid
lyd-1-284-1
Apr 25 2011
USER:
SOLVENT: CDCl3
Experiment = s2pul
Pulse length = 7.700 usec
Relaxation delay = 4.800 sec
NA = 12
Solvent = CDCl3
FID PTS1d = 21259
PTS1d = 32768
F1 = 499.858551 MHz
F2 = 125.700813 MHz
SW1 = 8503.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 0.26 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2495.9019 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = 32.84
B = 1.46
C = 0.00



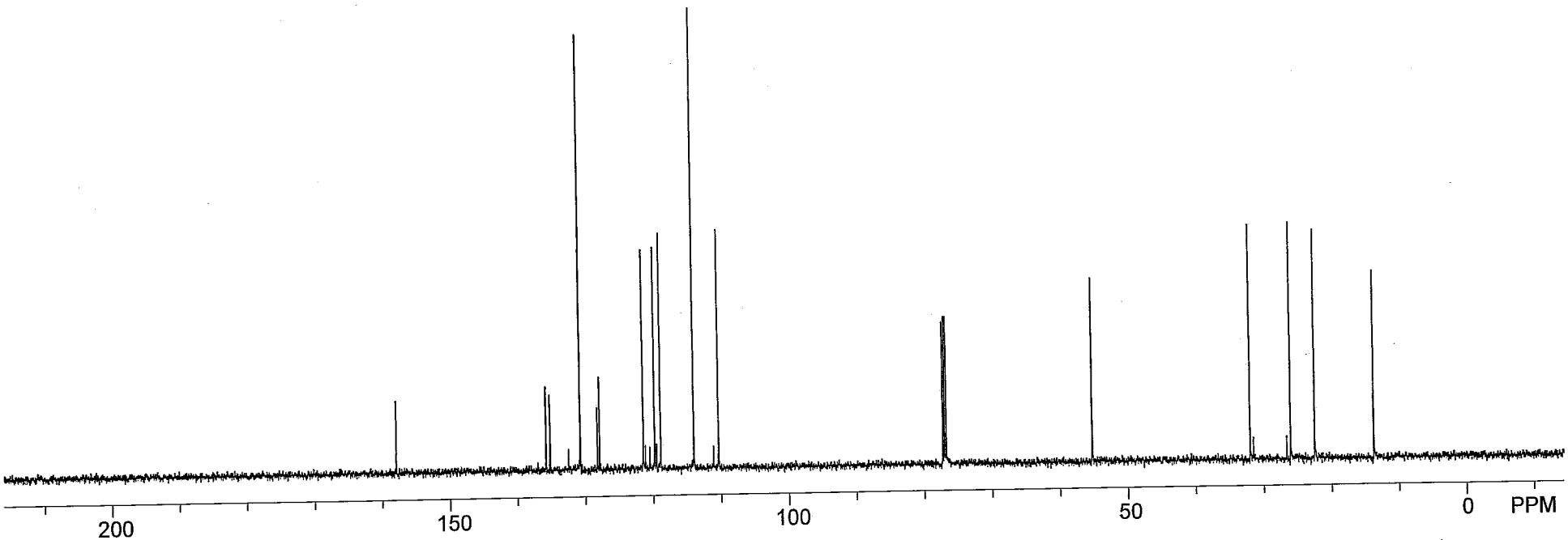
2b



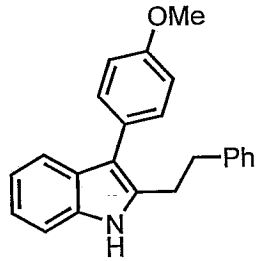
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$lyd-1-284-1.fid
lyd-1-284-1
Apr 25 2011
USER:
SOLVENT: CDCl3
Experiment = s2pul
Pulse length = 7.700 usec
Relaxation delay = 4.800 sec
NA = 12
Solvent = CDCl3
FID PTS1d = 21259
PTS1d = 32768
F1 = 499.858551 MHz
F2 = 125.700813 MHz
SW1 = 8503.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 0.26 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2495.9019 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = 32.84
B = 1.46
C = 0.00



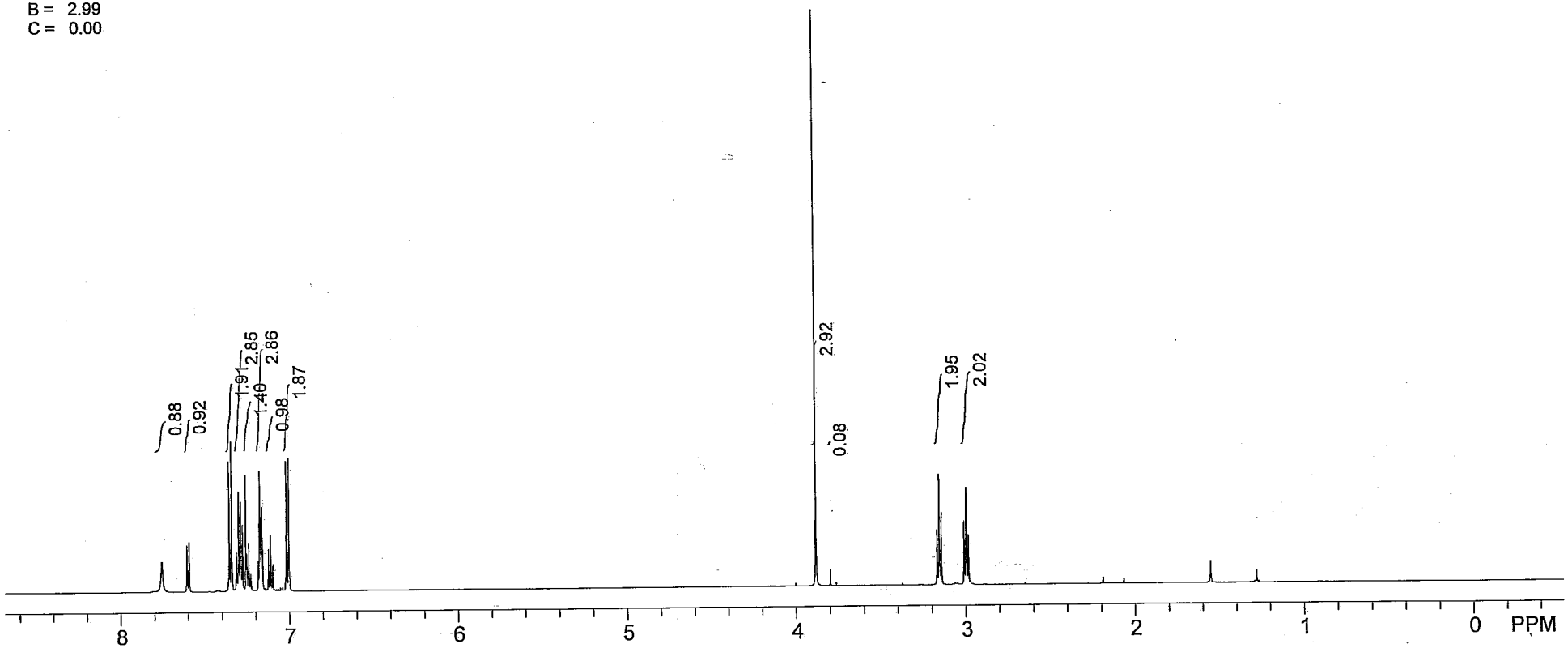
2b



C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$lyd-1-286-2.fid
lyd-1-286-2
Apr 26 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 5.825 usec
Relaxation delay = 4.800 sec
NA = 12
Solvent = cdcl3
FID PTS1d = 25000
PTS1d = 32768
F1 = 599.634705 MHz
F2 = 599.635132 MHz
SW1 = 10000.00 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 0.31 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2605.6868 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -137.58
B = 2.99
C = 0.00



2c



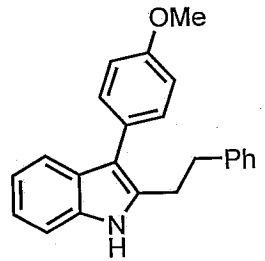
lyd-1-286-2-C

Sample: 1_Indanone
File: nmr600/Zhang/yluo/lyd-1-286-2-C.fid

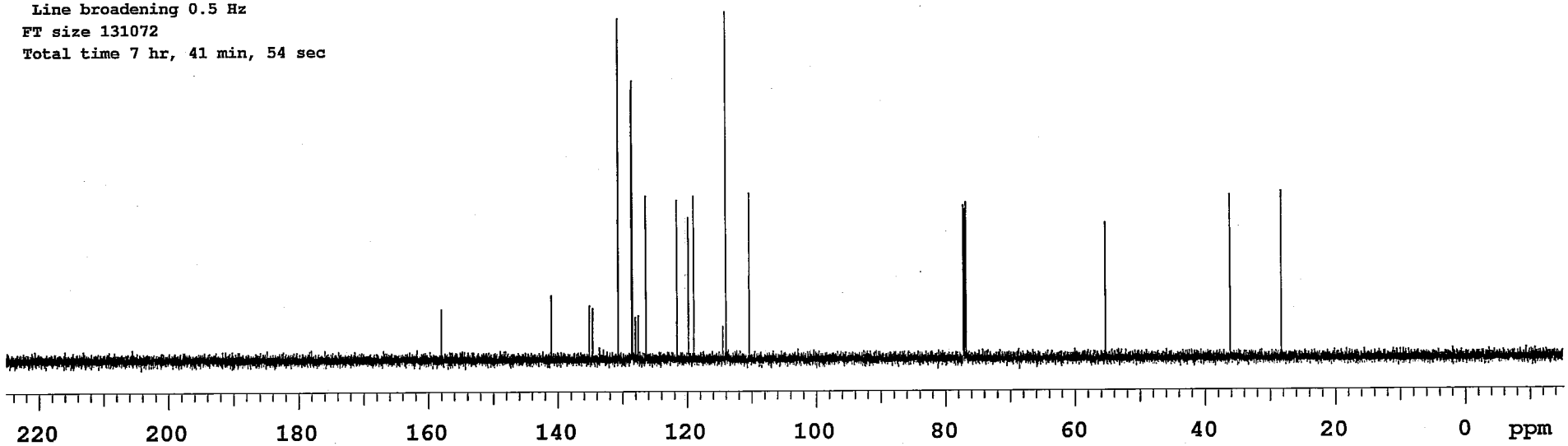
Pulse Sequence: s2pul

Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: yluo
File: lyd-1-286-2-C
INOVA-500 "nmrserver"

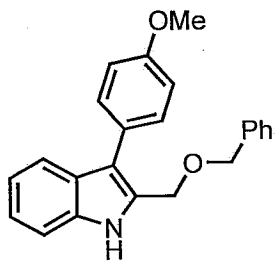
Relax. delay 1.000 sec
Pulse 10.0 usec
Acq. time 1.298 sec
Width 36231.9 Hz
68 repetitions
OBSERVE C13, 150.7776170 MHz
DECOUPLE H1, 599.6351203 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 7 hr, 41 min, 54 sec



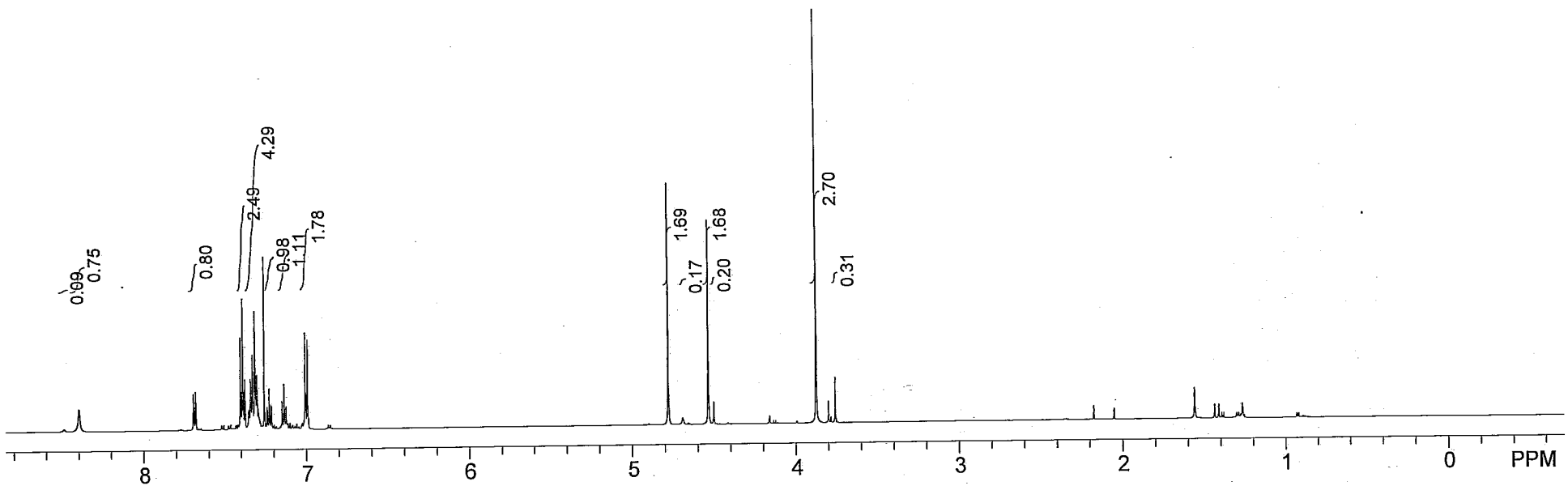
2c



C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$lyd-1-287-1-3rd.fid
lyd-1-287-1-3rd
Apr 26 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 5.825 usec
Relaxation delay = 4.800 sec
NA = 16
Solvent = cdcl3
FID PTS1d = 25000
PTS1d = 32768
F1 = 599.634705 MHz
F2 = 599.635132 MHz
SW1 = 10000.00 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 0.31 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2605.0764 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -134.59
B = 2.81
C = 0.00



2d



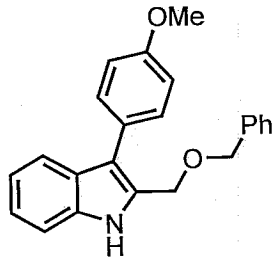
lyd-1-287-1-3rd-C

Sample: 1_Indanone
File: nmr600/Zhang/yluo/lyd-1-287-1-3rd-C.fid

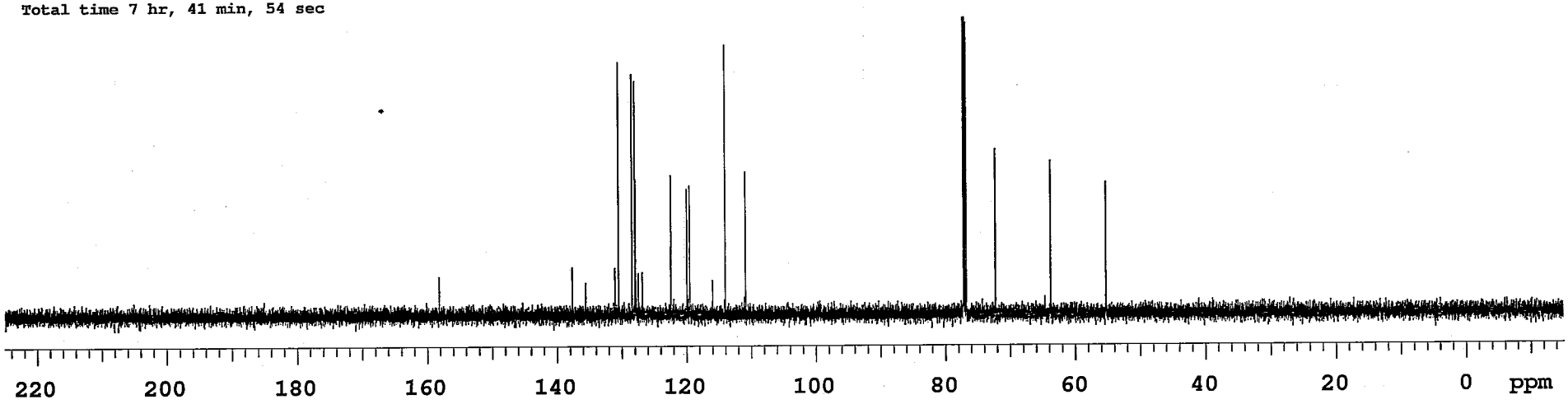
Pulse Sequence: s2pul

Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: yluo
File: lyd-1-287-1-3rd-C
INOVA-500 "nmrserver"

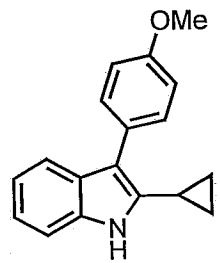
Relax. delay 1.000 sec
Pulse 10.0 usec
Acq. time 1.298 sec
Width 36231.9 Hz
120 repetitions
OBSERVE C13, 150.7776170 MHz
DECOUPLE H1, 599.6351203 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 7 hr, 41 min, 54 sec



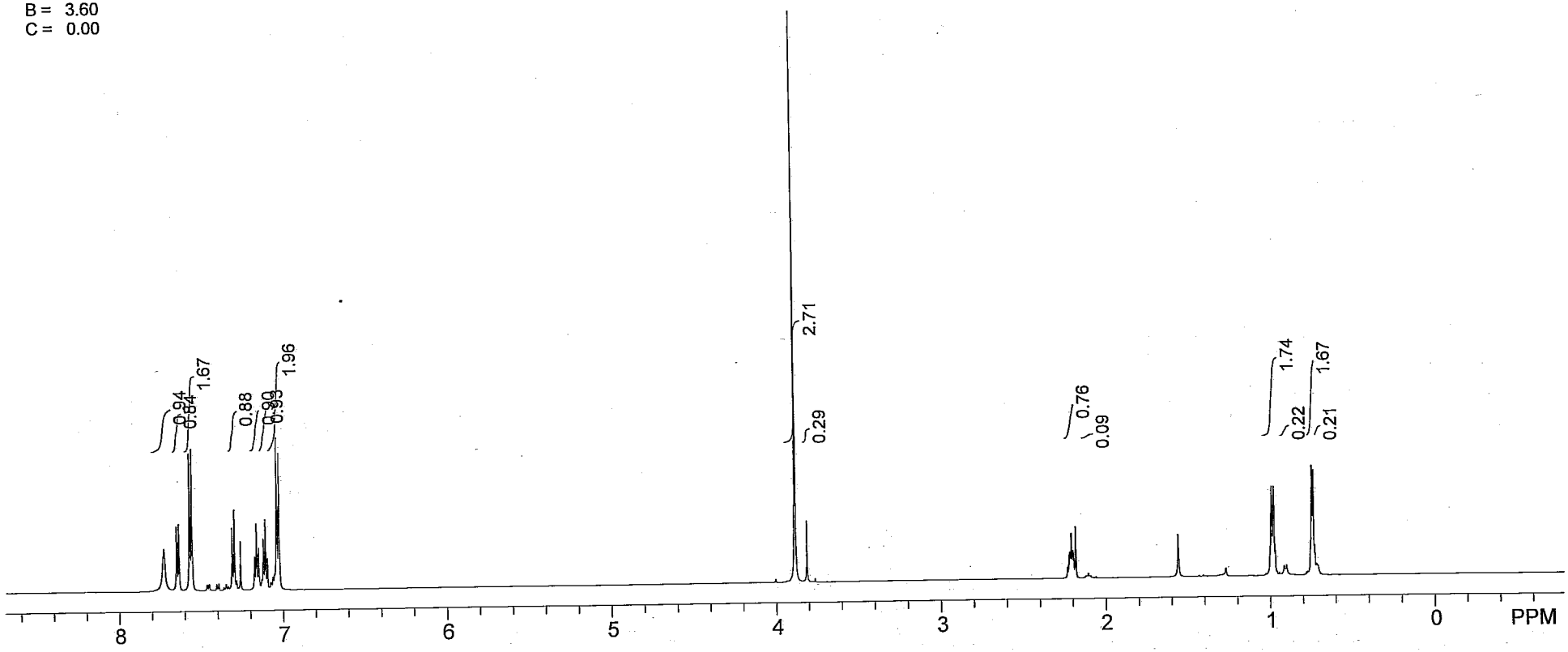
2d



C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$lyd-1-284-2.fid
lyd-1-284-2
Apr 25 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 5.825 usec
Relaxation delay = 4.800 sec
NA = 16
Solvent = cdcl3
FID PTS1d = 25000
PTS1d = 32768
F1 = 599.634705 MHz
F2 = 599.635132 MHz
SW1 = 10000.00 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 0.31 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2605.6877 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -133.24
B = 3.60
C = 0.00



2e



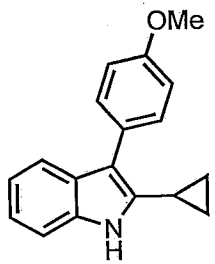
lyd-1-284-2-C

Sample: 1_Indanone
File: nmr600/Zhang/yluo/lyd-1-284-2-C.fid

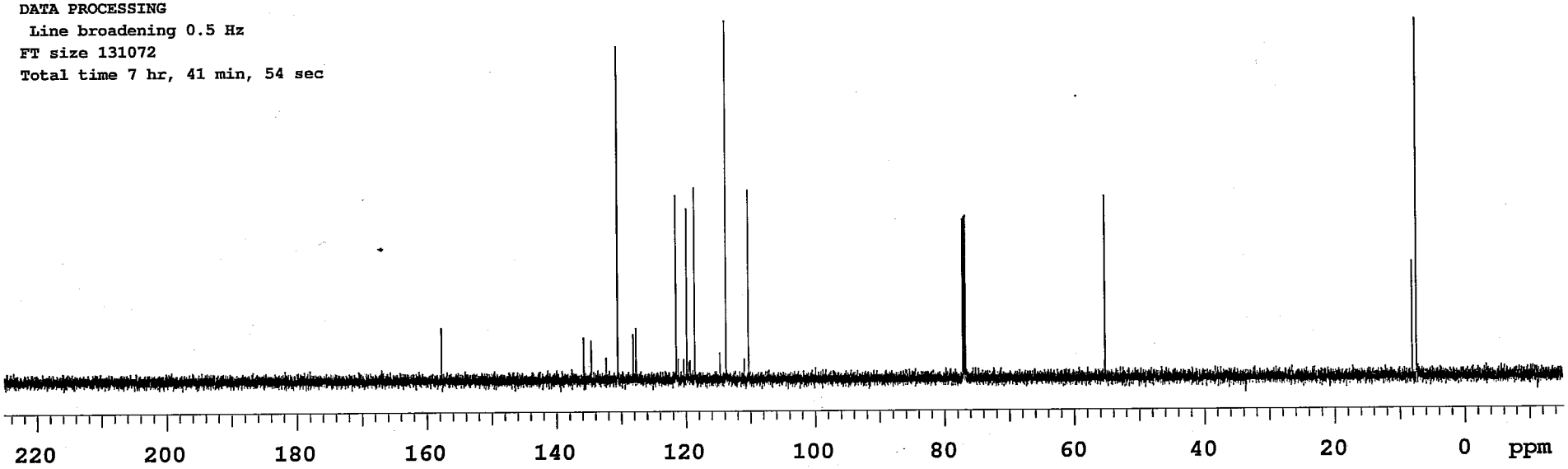
Pulse Sequence: s2pul

Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: yluo
File: lyd-1-284-2-C
INOVA-500 "nmrserver"

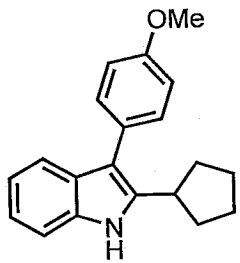
Relax. delay 1.000 sec
Pulse 10.0 usec
Acq. time 1.298 sec
Width 36231.9 Hz
136 repetitions
OBSERVE C13, 150.7776170 MHz
DECOUPLE H1, 599.6351203 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 7 hr, 41 min, 54 sec



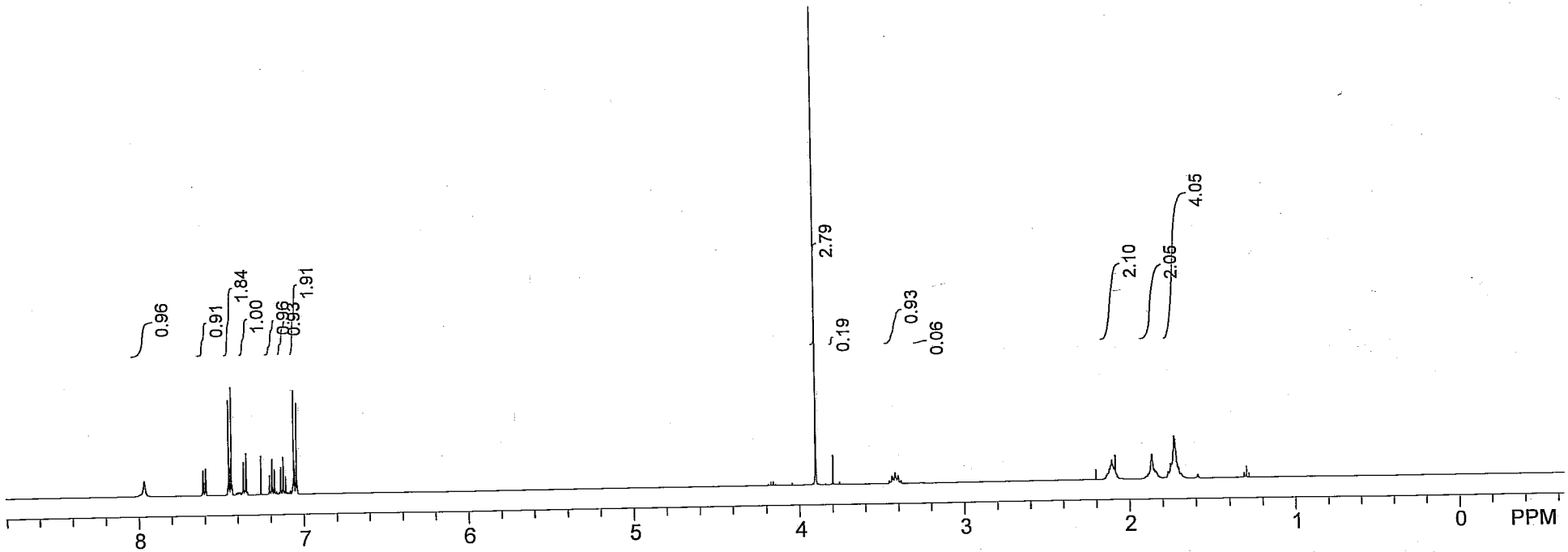
2e



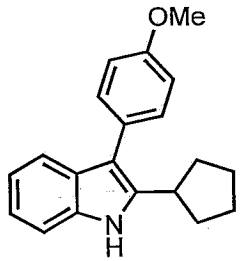
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$lyd-1-285-2-C.fid
lyd-1-285-2-C
Apr 25 2011
USER:
SOLVENT: CDCl3
Experiment = s2pul
Pulse length = 7.000 usec
Relaxation delay = 1.000 sec
NA = 132
Solvent = CDCl3
FID PTS1d = 39295
PTS1d = 65536
F1 = 125.702103 MHz
F2 = 499.858551 MHz
SW1 = 30165.91 Hz
AT1 = 1.30 sec
Hz per Pt 1stD = 0.46 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 13197.3711 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = 71.25
B = 106.88
C = 0.00



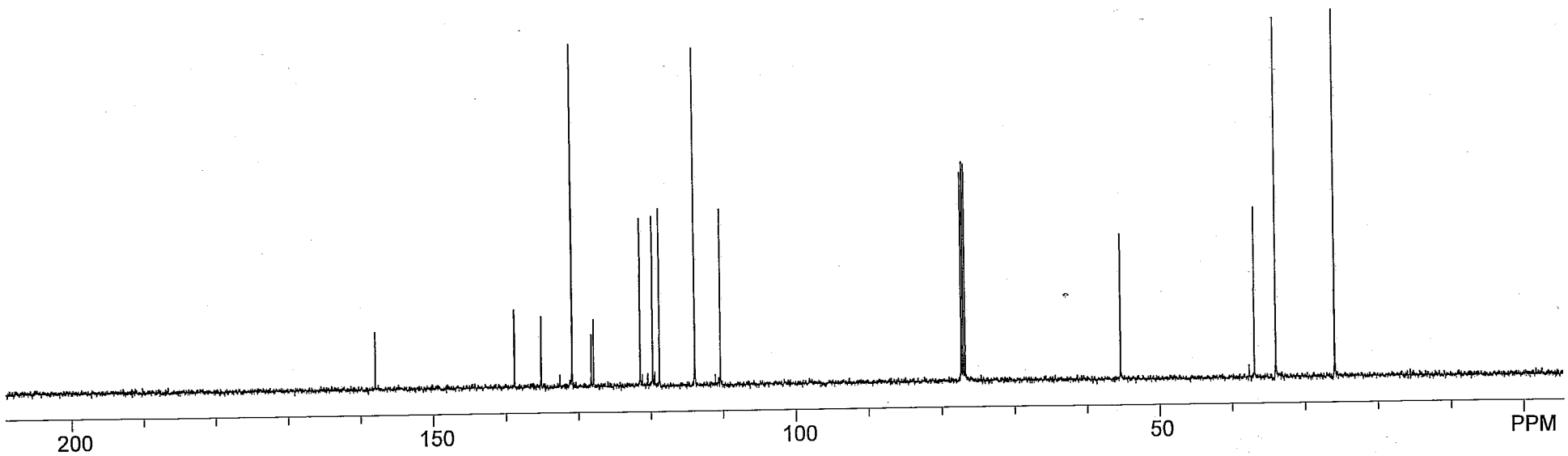
2f



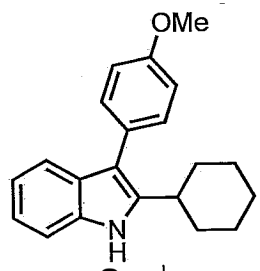
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$lyd-1-285-2-C.fid
lyd-1-285-2-C
Apr 25 2011
USER:
SOLVENT: CDCl3
Experiment = s2pul
Pulse length = 7.000 usec
Relaxation delay = 1.000 sec
NA = 132
Solvent = CDCl3
FID PTS1d = 39295
PTS1d = 65536
F1 = 125.702103 MHz
F2 = 499.858551 MHz
SW1 = 30165.91 Hz
AT1 = 1.30 sec
Hz per Pt 1stD = 0.46 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 13197.3711 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = 71.25
B = 106.88
C = 0.00



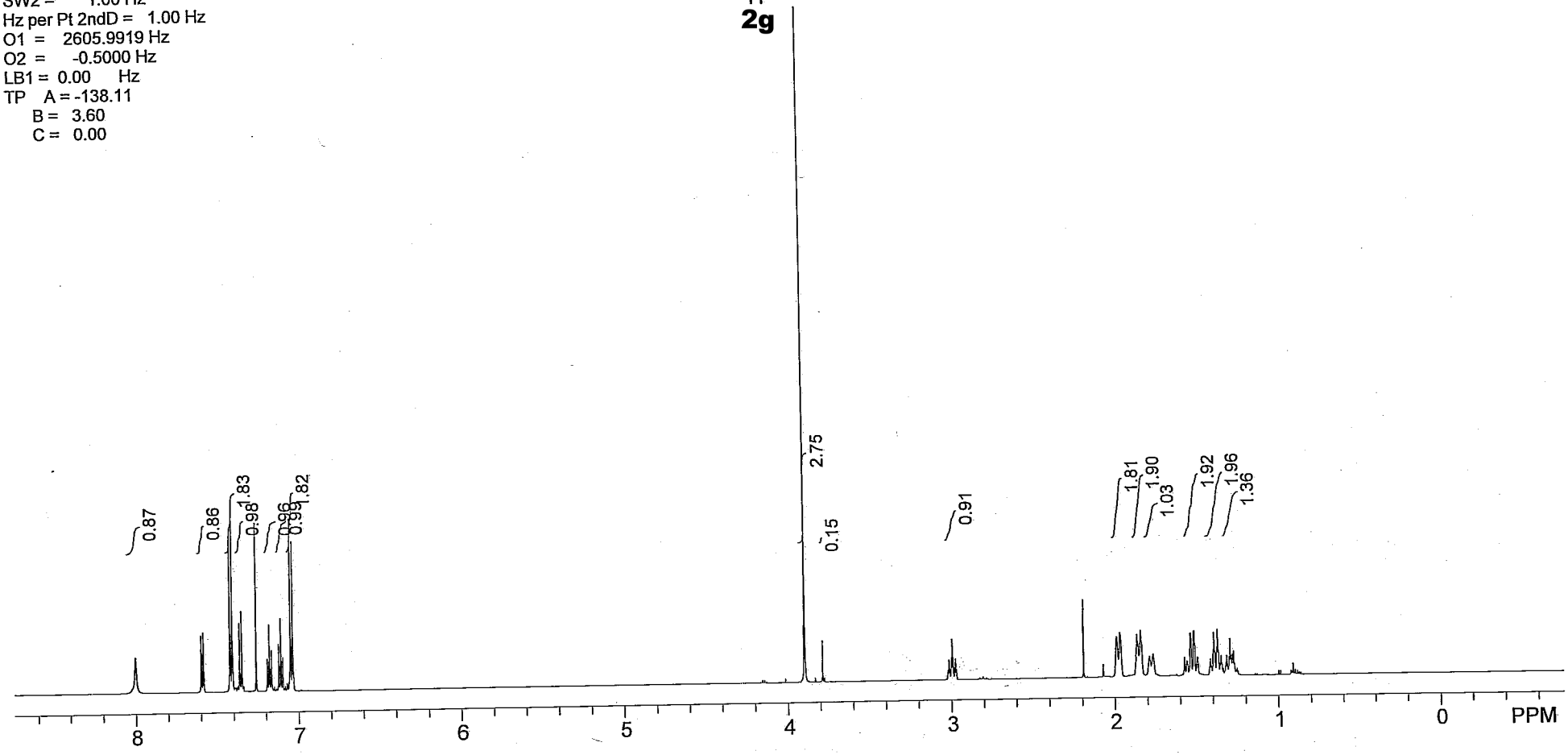
2f



C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$lyd-1-285-1-2nd.fid
lyd-1-285-1-2nd
Apr 26 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 5.825 usec
Relaxation delay = 4.800 sec
NA = 8
Solvent = cdcl3
FID PTS1d = 25000
PTS1d = 32768
F1 = 599.634705 MHz
F2 = 599.635132 MHz
SW1 = 10000.00 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 0.31 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2605.9919 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -138.11
B = 3.60
C = 0.00



2g



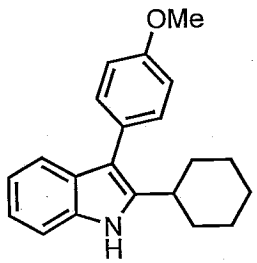
lyd-1-285-1-2nd-C

Sample: 1_Indanone
File: nmr600/Zhang/yluo/lyd-1-285-1-2nd-C.fid

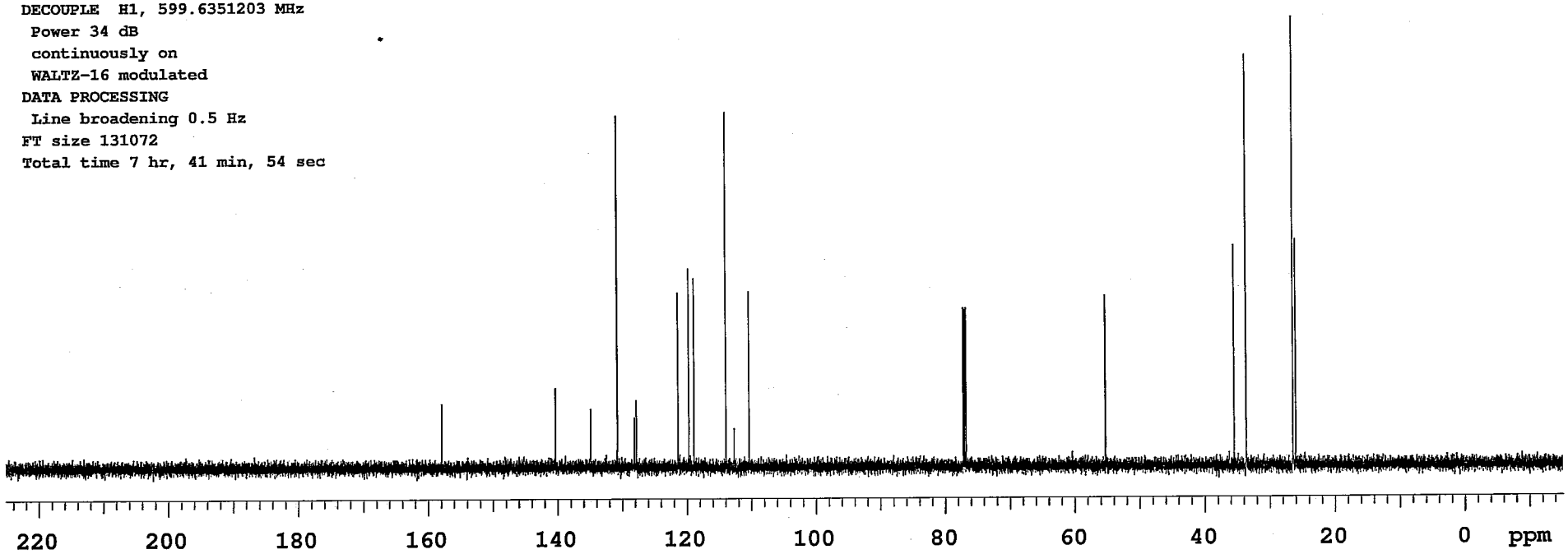
Pulse Sequence: s2pul

Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: yluo
File: lyd-1-285-1-2nd-C
INOVA-500 "nmrserver"

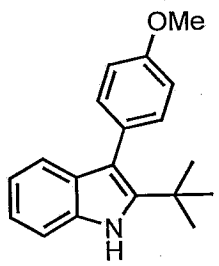
Relax. delay 1.000 sec
Pulse 10.0 usec
Acq. time 1.298 sec
Width 36231.9 Hz
44 repetitions
OBSERVE C13, 150.7776170 MHz
DECOUPLE H1, 599.6351203 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 7 hr, 41 min, 54 sec



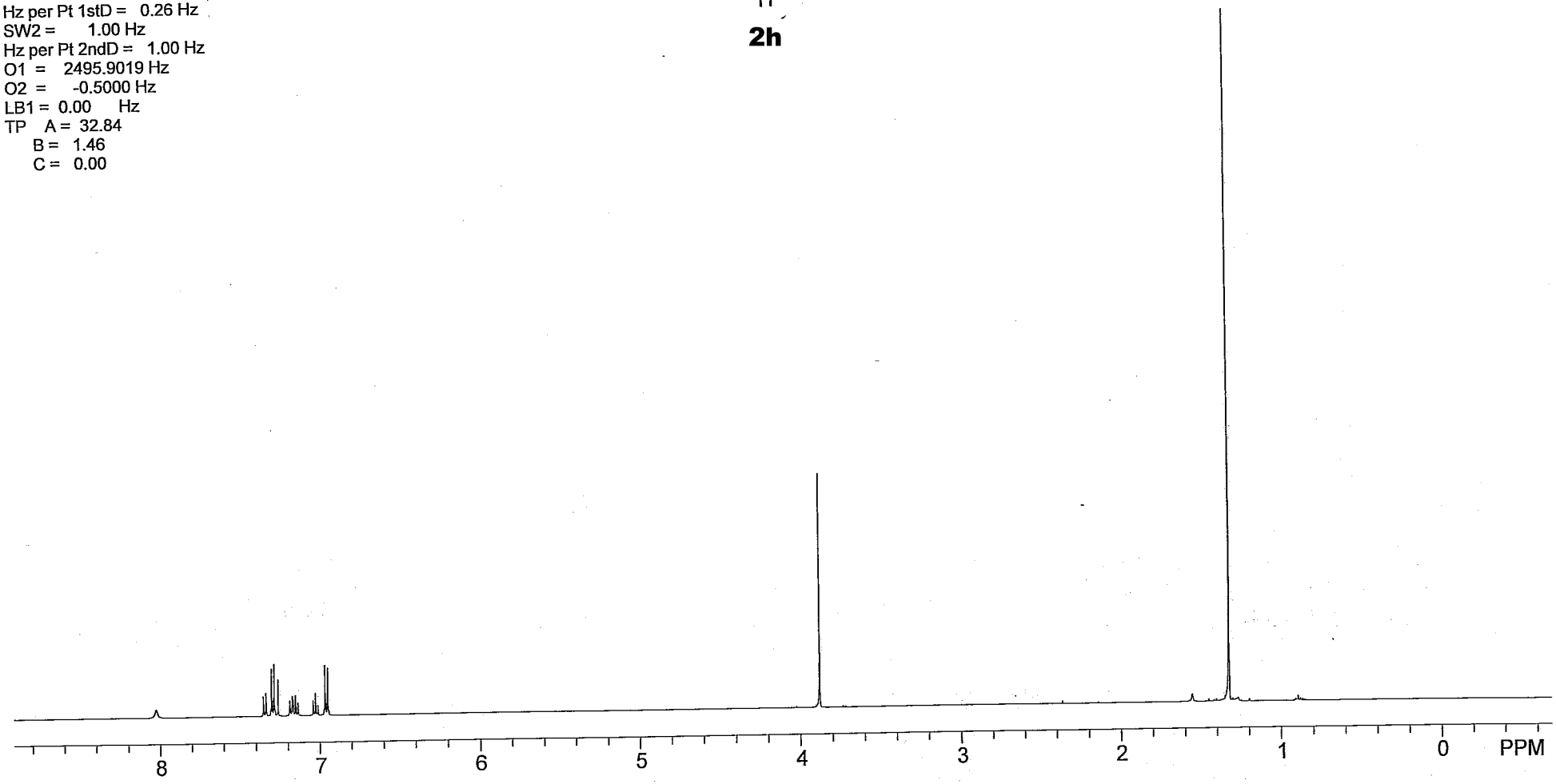
2g



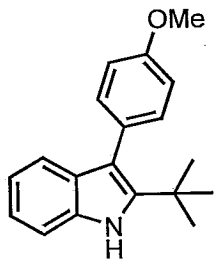
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$lyd-1-284-1.fid
lyd-1-284-1
Apr 25 2011
USER:
SOLVENT: CDCl3
Experiment = s2pul
Pulse length = 7.700 usec
Relaxation delay = 4.800 sec
NA = 12
Solvent = CDCl3
FID PTS1d = 21259
PTS1d = 32768
F1 = 499.858551 MHz
F2 = 125.700813 MHz
SW1 = 8503.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 0.26 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2495.9019 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = 32.84
B = 1.46
C = 0.00



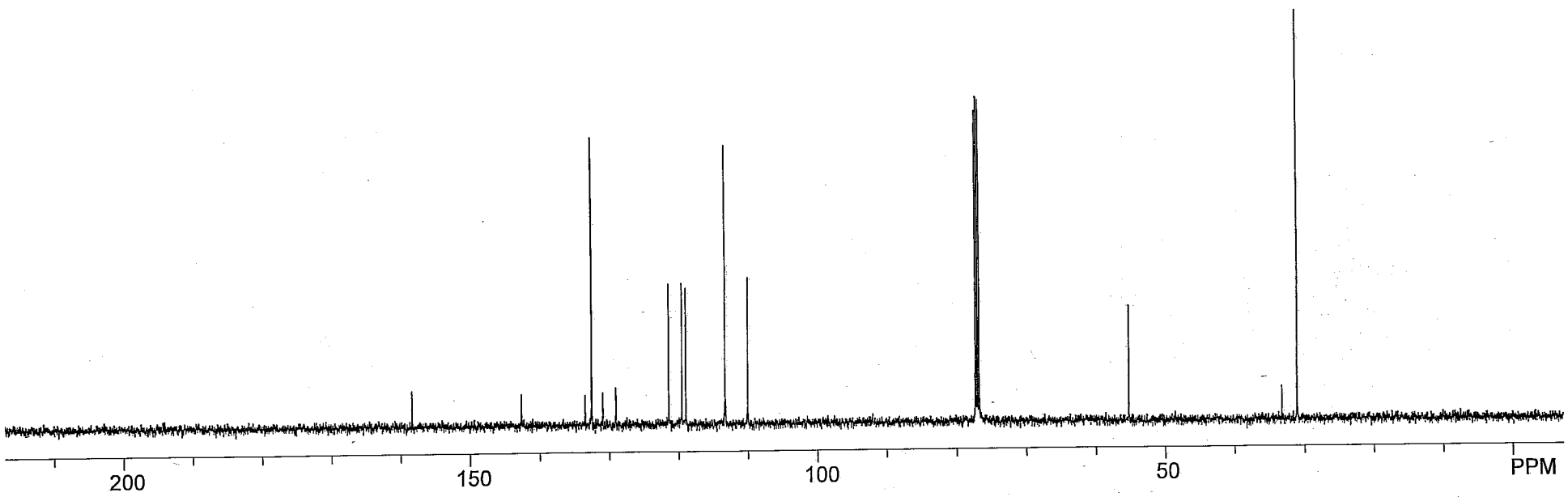
2h



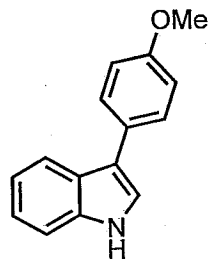
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$lyd-1-284-1.fid
lyd-1-284-1
Apr 25 2011
USER:
SOLVENT: CDCl3
Experiment = s2pul
Pulse length = 7.700 usec
Relaxation delay = 4.800 sec
NA = 12
Solvent = CDCl3
FID PTS1d = 21259
PTS1d = 32768
F1 = 499.858551 MHz
F2 = 125.700813 MHz
SW1 = 8503.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 0.26 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2495.9019 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = 32.84
B = 1.46
C = 0.00



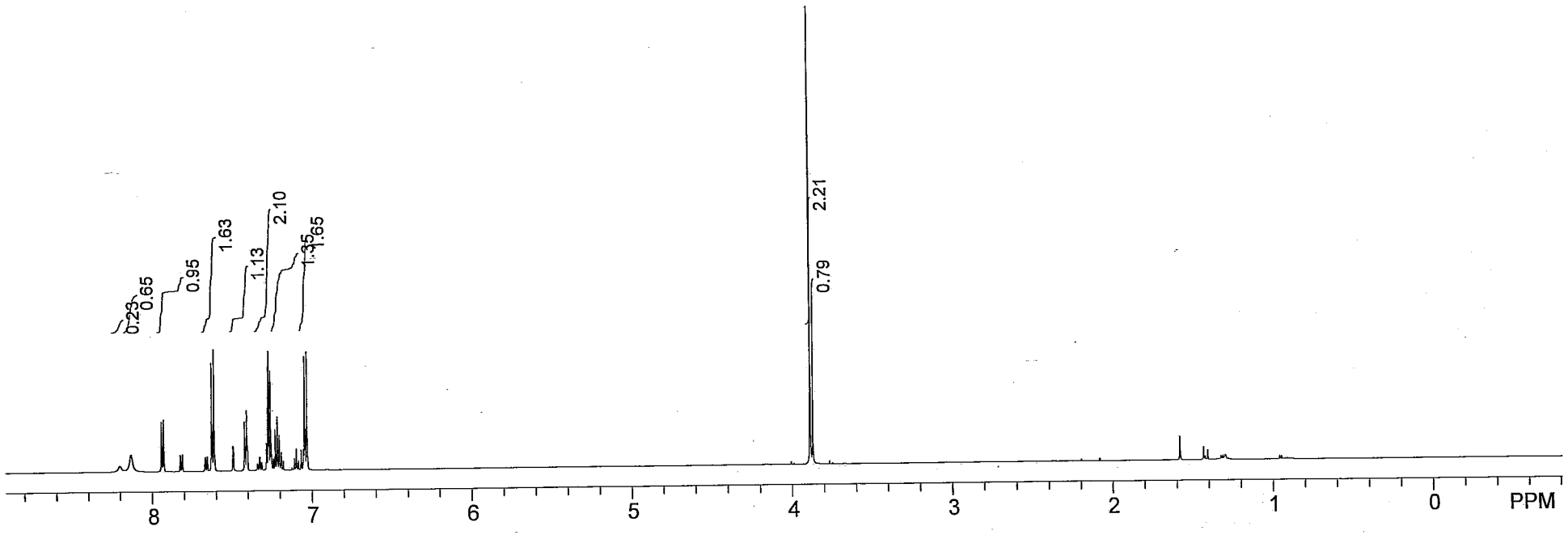
2h



C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$lyd-1-291-2.fid
lyd-1-291-2
Apr 29 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 5.825 usec
Relaxation delay = 4.800 sec
NA = 8
Solvent = cdcl3
FID PTS1d = 25000
PTS1d = 32768
F1 = 599.634705 MHz
F2 = 599.635132 MHz
SW1 = 10000.00 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 0.31 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2605.6868 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -143.91
B = 2.81
C = 0.00



2i



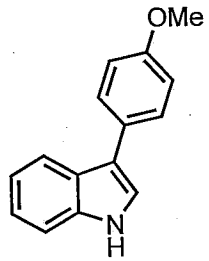
lyd-1-291-2-C

Sample: 1_Indanone
File: nmr600/Zhang/yluo/lyd-1-291-2-C.fid

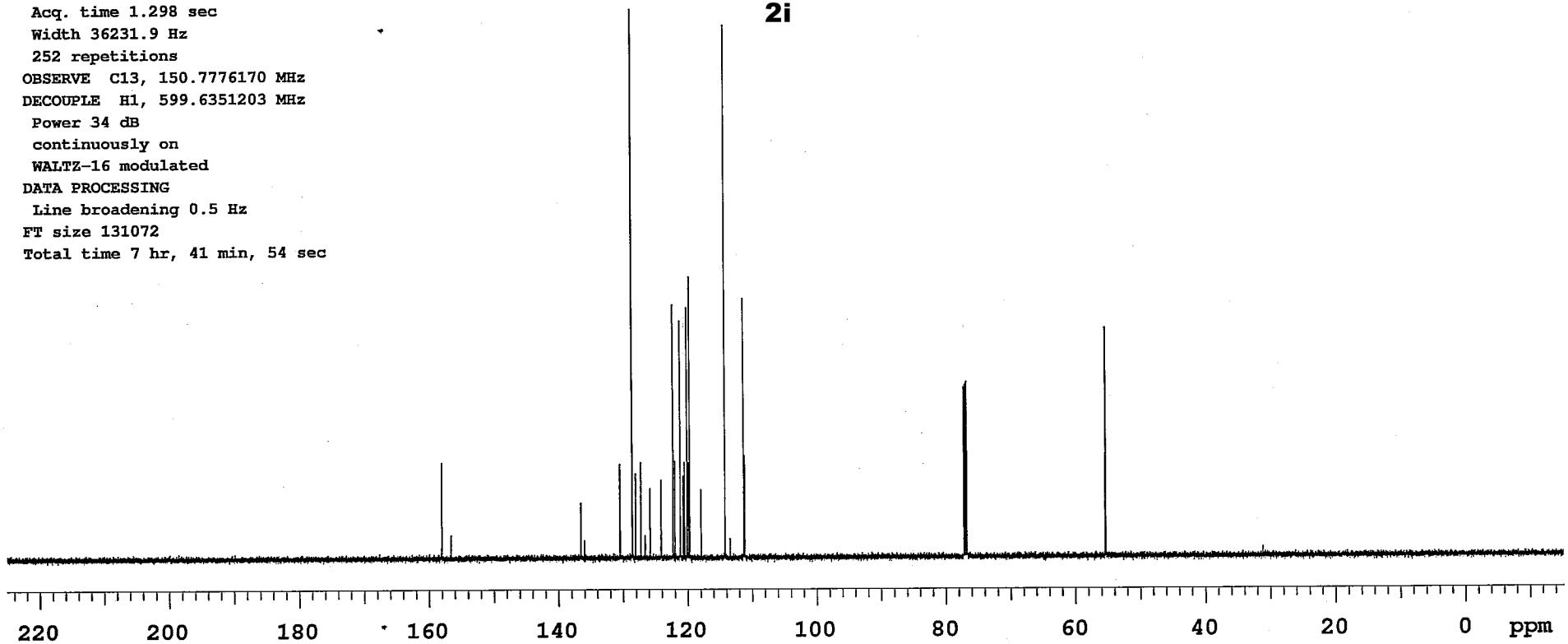
Pulse Sequence: s2pul

Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: yluo
File: lyd-1-291-2-C
INOVA-500 "nmrserver"

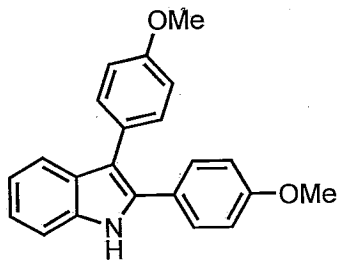
Relax. delay 1.000 sec
Pulse 10.0 usec
Acq. time 1.298 sec
Width 36231.9 Hz
252 repetitions
OBSERVE C13, 150.7776170 MHz
DECOUPLE H1, 599.6351203 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 7 hr, 41 min, 54 sec



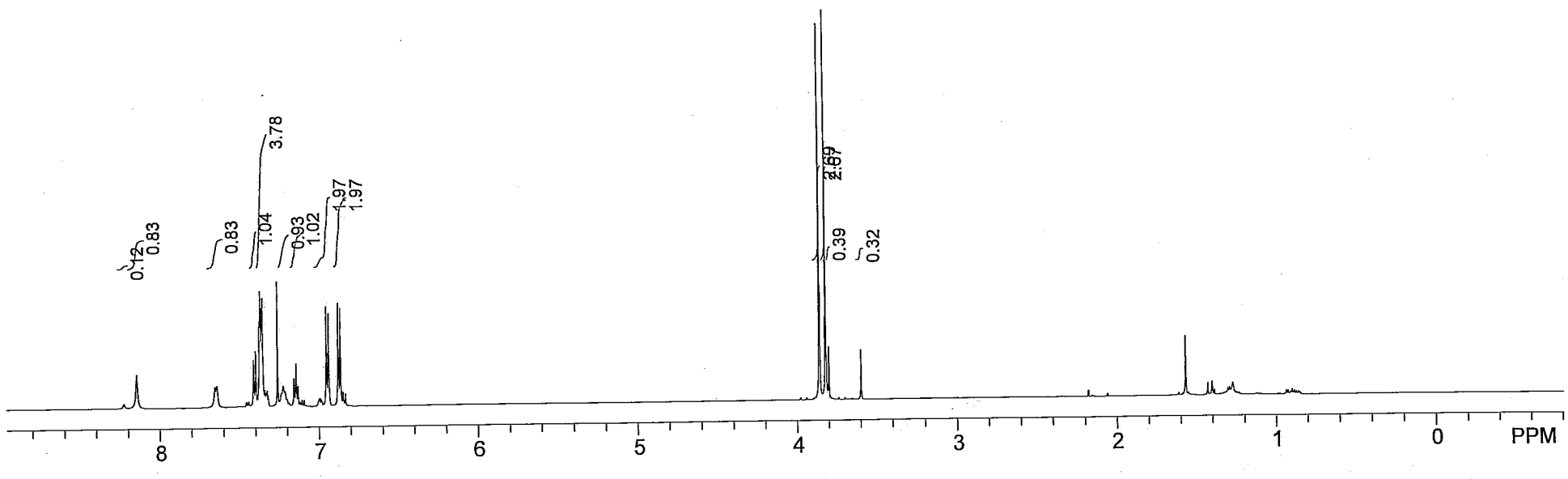
2i



C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$lyd-1-290-1.fid
lyd-1-290-1
Apr 28 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 5.825 usec
Relaxation delay = 4.800 sec
NA = 12
Solvent = cdcl3
FID PTS1d = 25000
PTS1d = 32768
F1 = 599.634705 MHz
F2 = 599.635132 MHz
SW1 = 10000.00 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 0.31 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2605.9919 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -136.88
B = 2.81
C = 0.00



2j



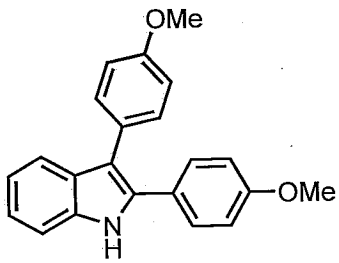
lyd-1-290-1-C

Sample: 1_Indanone
File: nmr600/Zhang/yluo/lyd-1-290-1-C.fid

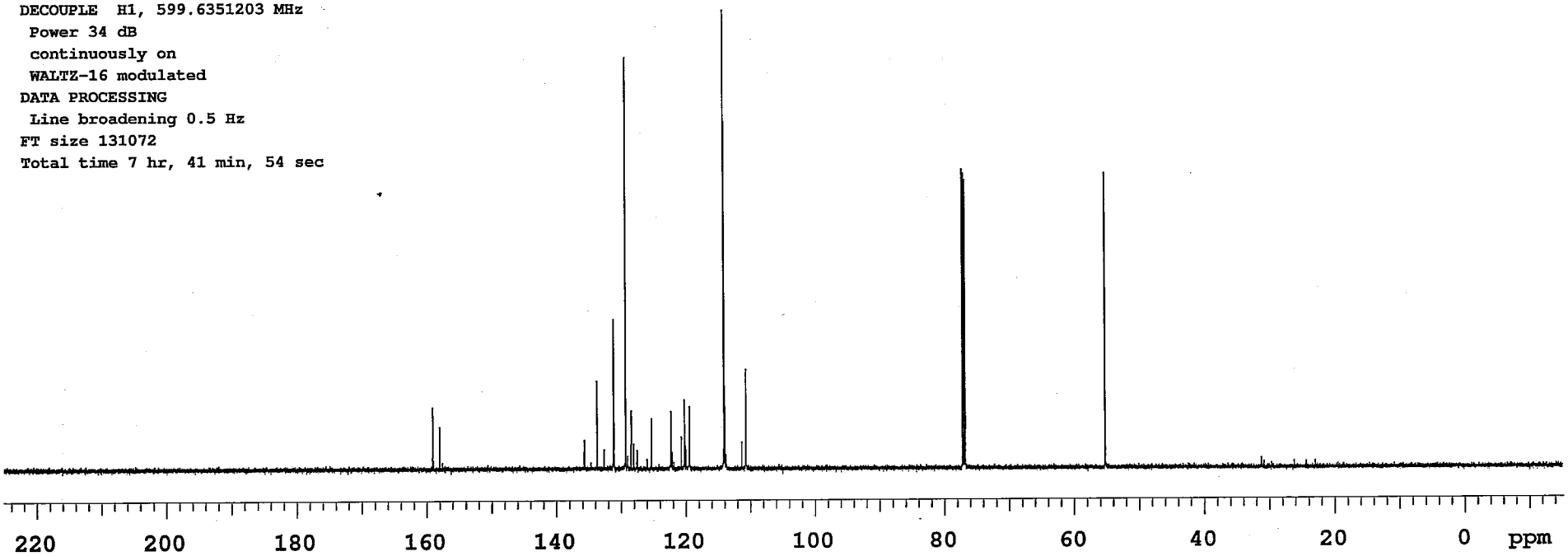
Pulse Sequence: s2pul

Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: yluo
File: lyd-1-290-1-C
INOVA-500 "nmrserver"

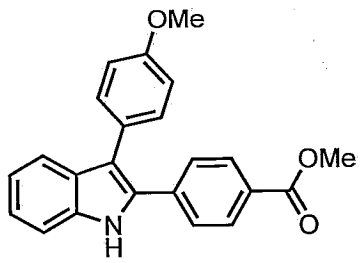
Relax. delay 1.000 sec
Pulse 10.0 usec
Acq. time 1.298 sec
Width 36231.9 Hz
1676 repetitions
OBSERVE C13, 150.7776170 MHz
DECOUPLE H1, 599.6351203 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 7 hr, 41 min, 54 sec



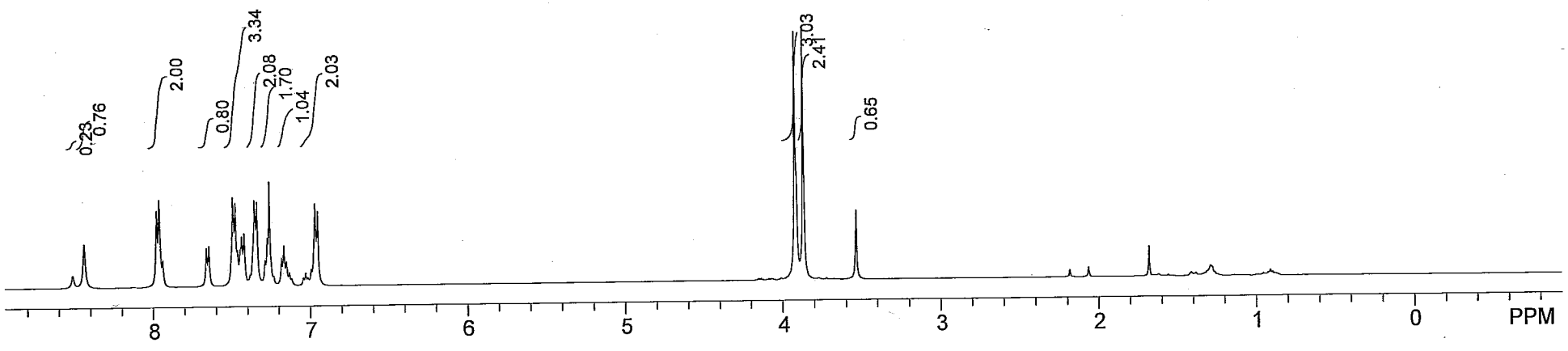
2j



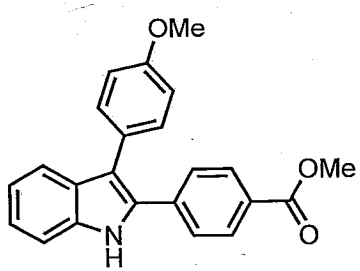
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$lyd-1-290-2.fid
lyd-1-290-2
Apr 28 2011
USER:
SOLVENT: CDCl3
Experiment = s2pul
Pulse length = 7.700 usec
Relaxation delay = 4.800 sec
NA = 12
Solvent = CDCl3
FID PTS1d = 21259
PTS1d = 32768
F1 = 499.858551 MHz
F2 = 125.700813 MHz
SW1 = 8503.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 0.26 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2495.9019 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = 49.69
B = -11.25
C = 0.00



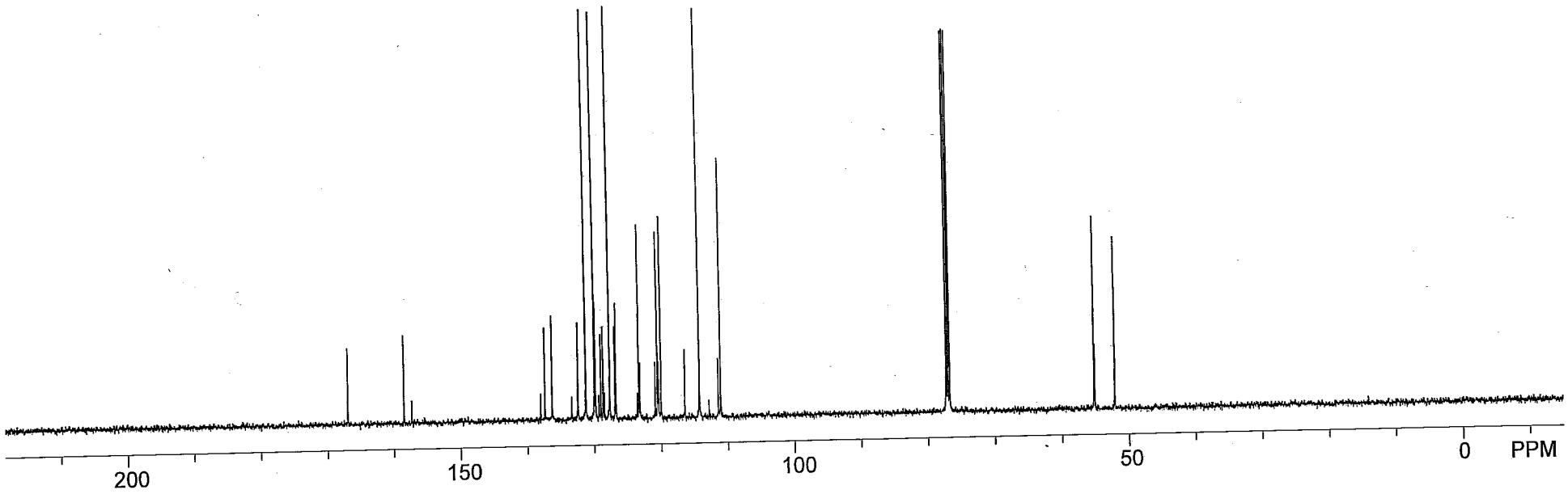
2k



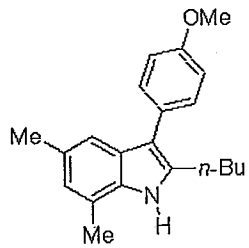
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$lyd-1-290-2-C.fid
lyd-1-290-2-C
Apr 28 2011
USER:
SOLVENT: CDCl3
Experiment = s2pul
Pulse length = 7.000 usec
Relaxation delay = 1.000 sec
NA = 512
Solvent = CDCl3
FID PTS1d = 39295
PTS1d = 65536
F1 = 125.702103 MHz
F2 = 499.858551 MHz
SW1 = 30165.91 Hz
AT1 = 1.30 sec
Hz per Pt 1stD = 0.46 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 13197.3711 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = 63.28
B = 127.97
C = 0.00



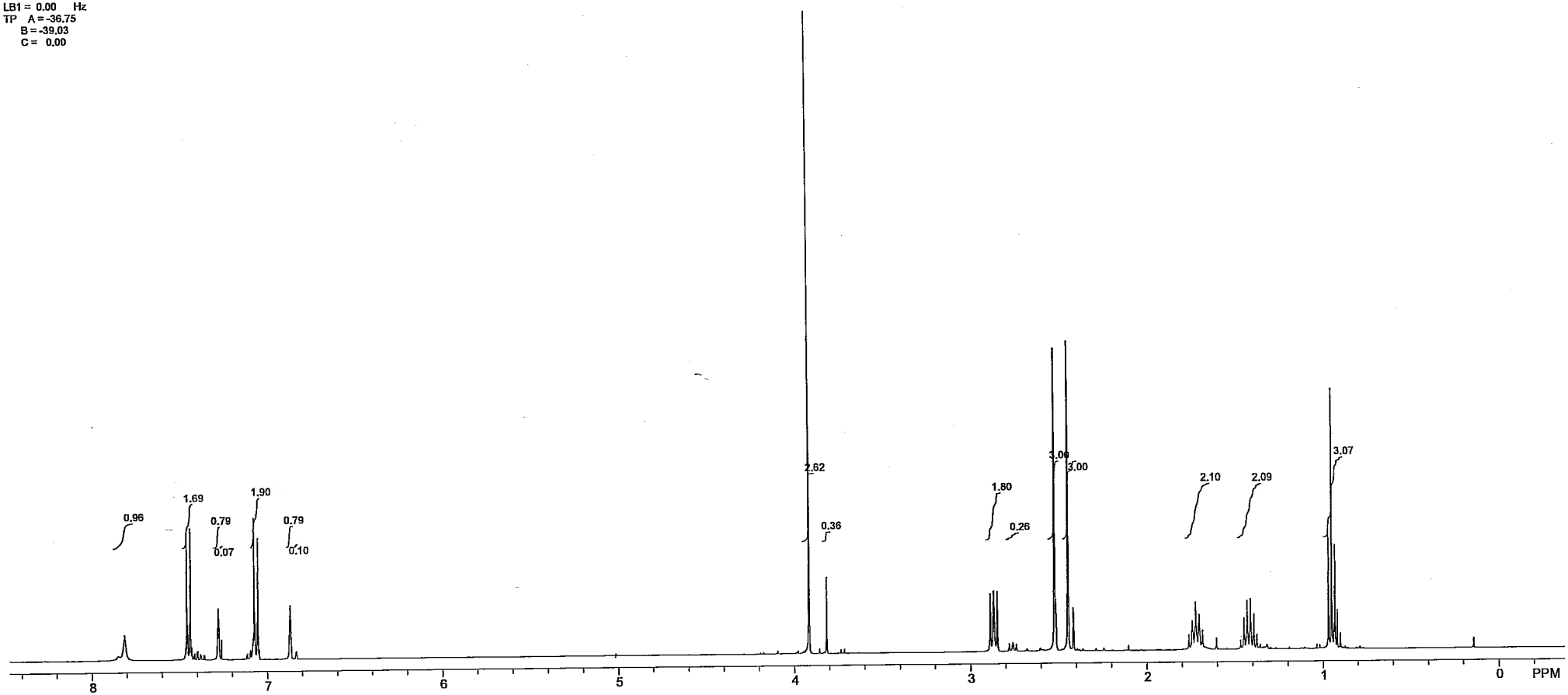
2k



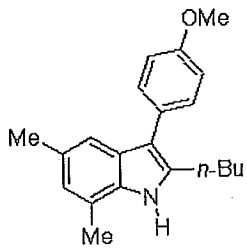
D:\Greenware\Ntus 20080731\DATA\$wyz3-256-pro-h1.fid
new experiment
Apr 29 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 2.000 sec
NA = 16
Solvent = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
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 = -36.75
B = -39.03
C = 0.00



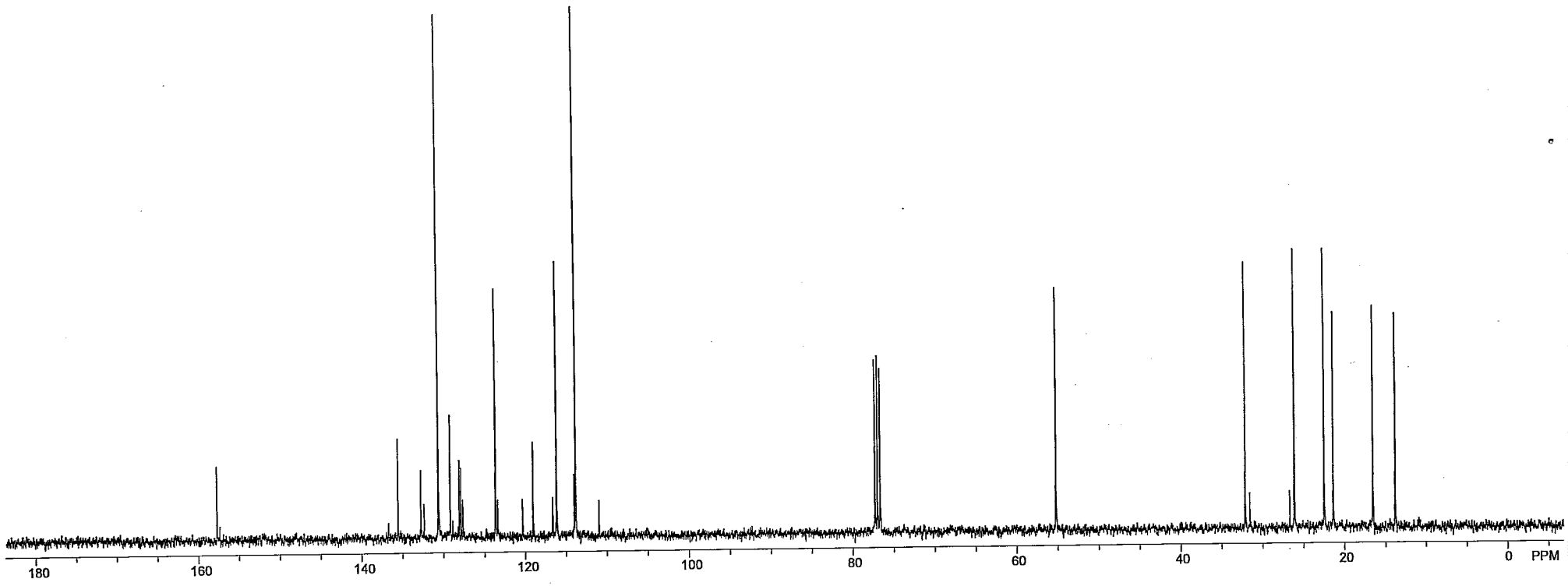
2l



D:\Greenware\Ntus 20080731\DATA\$wyz3-256-pro-c13.fid
Standard c13 run using qnp probe
Apr 29 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 132
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 = 10049.5137 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -37.97
B = 22.50
C = 0.00



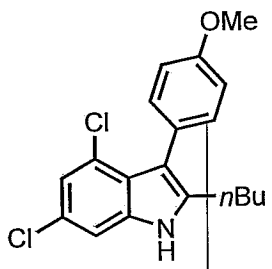
2l



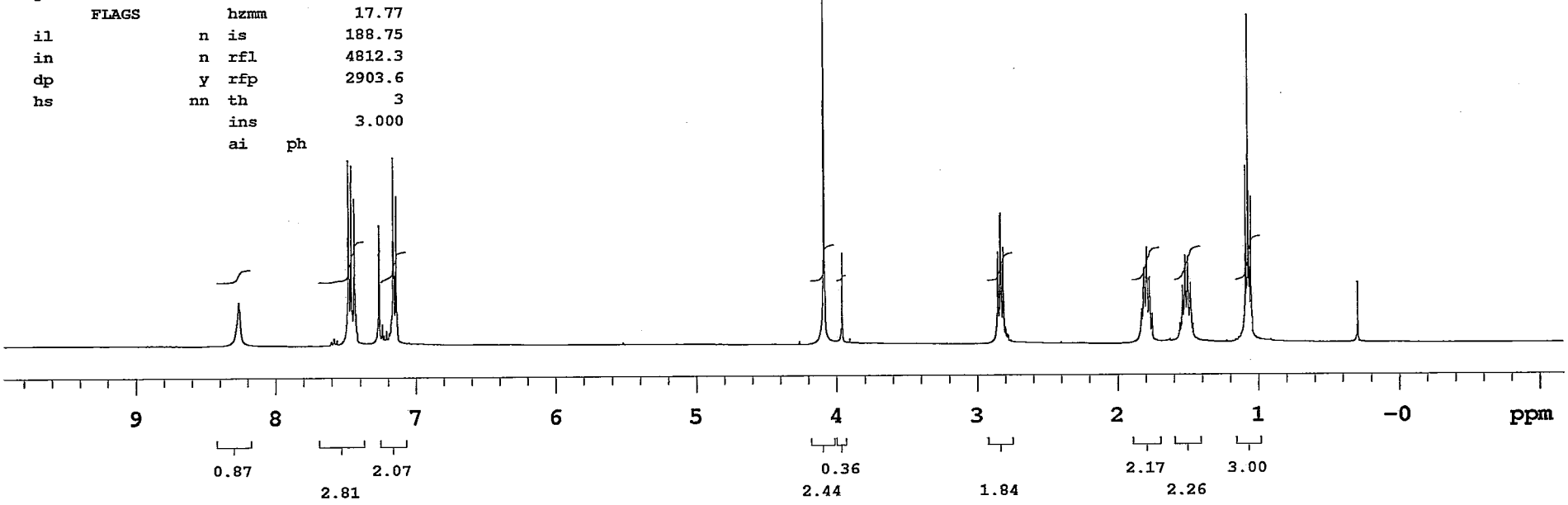
lb-IV-38

exp1 s2pul

SAMPLE		DEC. & VT	
date	May 1 2011	dn	C13
solvent	cdcl3	dof	-1425.0
file	exp	dm	nnn
ACQUISITION		dmm	c
sfrq	399.951	dmf	200
tn	H1	PROCESSING	
at	2.500	lb	0.20
np	40012	fn	65536
sw	8002.4	math	i
fb	not used		
bs	2	werr	
pw	11.7	wexp	
pw	11.7	wbs	
tpwr	60	wnt	
d1	4.800	DISPLAY	
tof	0	sp	-467.3
nt	16	wp	4441.3
ct	16	vs	75
alock	n	sc	0
gain	not used	wc	250
FLAGS		hzmm	17.77
il	n	is	188.75
in	n	rfl	4812.3
dp	y	rfp	2903.6
hs	nn	th	3
		ins	3.000
		ai ph	



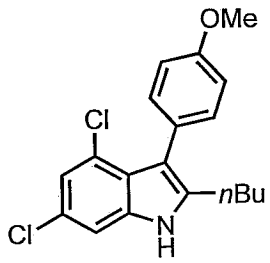
2m



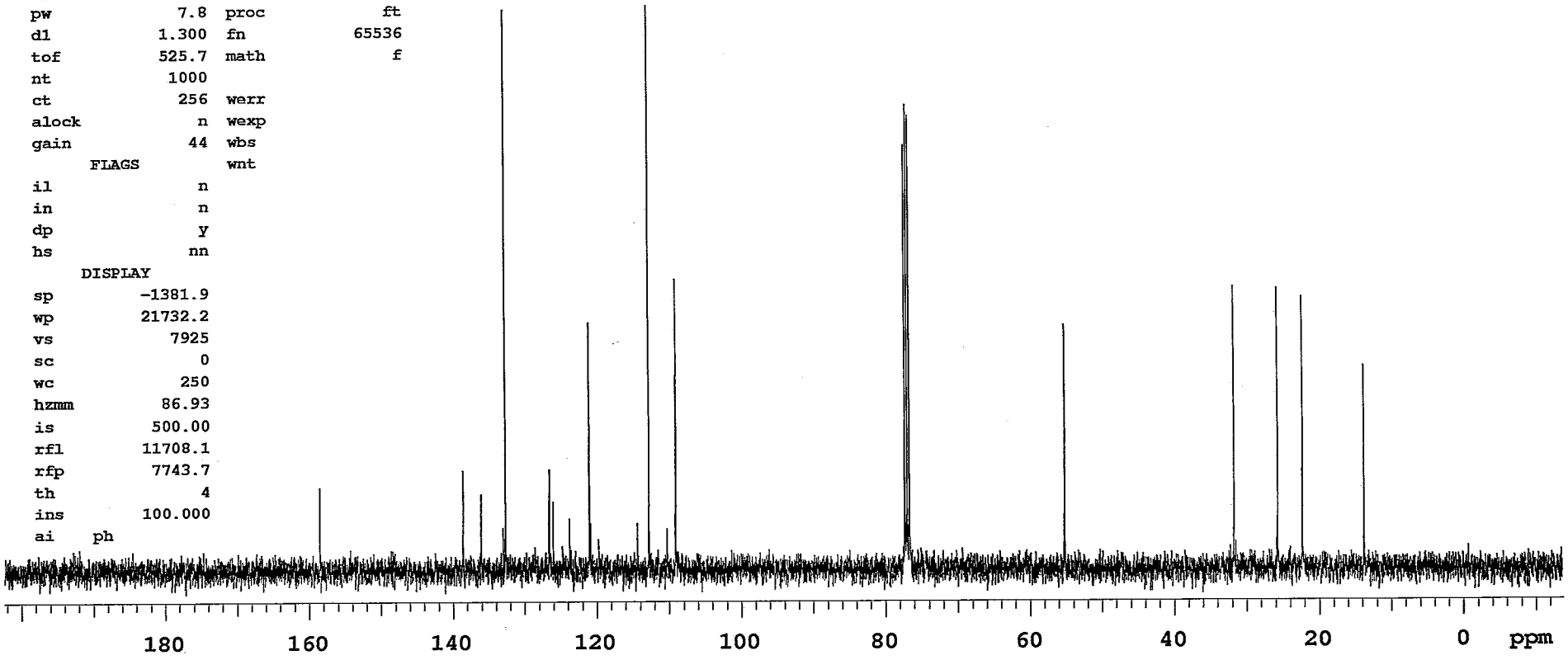
lb-IV-38-C13

expl std13c

SAMPLE		DEC. & VT	
date	May 1 2011	dfrq	399.951
solvent	cdcl3	dn	H1
file	exp	dpwr	40
ACQUISITION		dof	0
sfrq	100.577	dm	yyy
tn	C13	dmm	w
at	1.000	dmf	6700
np	56080	dseq	
sw	28040.7	dres	90.0
fb	not used	homo	n
bs	4	PROCESSING	
ss	4	lb	1.00
tpwr	58	wtfile	
pw	7.8	proc	ft
d1	1.300	fn	65536
tof	525.7	math	f
nt	1000		
ct	256	werr	
alock	n	wexp	
gain	44	wbs	
FLAGS		wnt	
il	n		
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-1381.9		
wp	21732.2		
vs	7925		
sc	0		
wc	250		
hzmm	86.93		
is	500.00		
rfl	11708.1		
rfp	7743.7		
th	4		
ins	100.000		
ai ph			



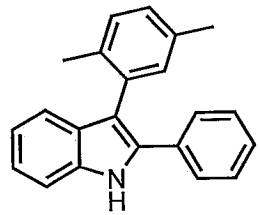
2m



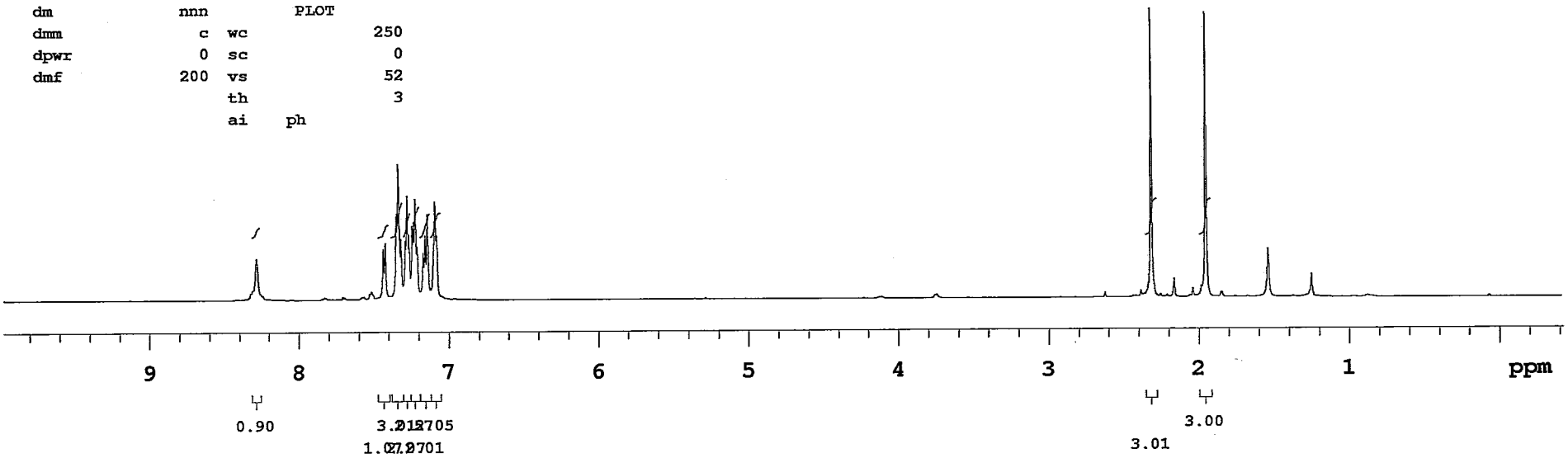
nt=8
pw=pw90

exp1 s2pul

SAMPLE		SPECIAL	
date	Apr 30 2011	temp	25.0
solvent	cdcl3	gain	not used
file	exp	spin	not used
ACQUISITION		hst	0.008
sw	10000.0	pw90	7.000
at	2.500	alfa	6.600
np	50000	FLAGS	
fb	not used	il	n
bs	2	in	n
d1	4.800	dp	y
nt	16	hs	nn
ct	14	PROCESSING	
TRANSMITTER		lb	0.20
tn	H1	fn	32768
sfrq	599.635	DISPLAY	
tof	-402.5	sp	-251.0
tpwr	53	wp	6231.7
pw	5.825	rfl	2404.4
DECOUPLER		rfp	0
dn	H1	rp	-113.5
dof	0	lp	-7.7
dm	nnn	PLOT	
dmm	c	wc	250
dpwr	0	sc	0
dmf	200	vs	52
		th	3
		ai	ph



5a

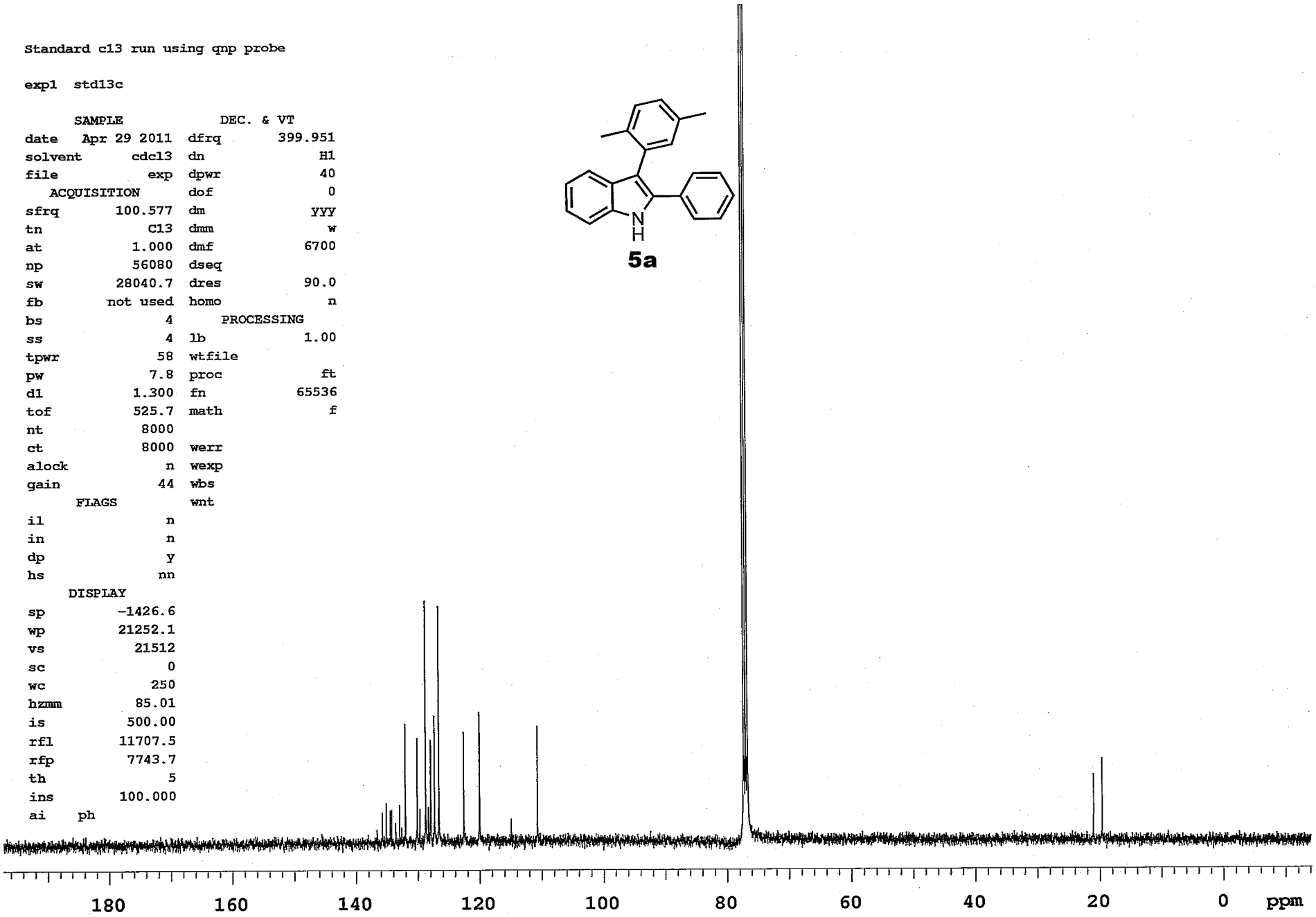


Standard c13 run using qnp probe

exp1 std13c

SAMPLE		DEC. & VT	
date	Apr 29 2011	dfrq	399.951
solvent	cdcl3	dn	H1
file	exp	dpwr	40
ACQUISITION		dof	0
sfrq	100.577	dm	yyy
tn	C13	dmm	w
at	1.000	dmf	6700
np	56080	dseq	
sw	28040.7	dres	90.0
fb	not used	homo	n
bs	4	PROCESSING	
ss	4	lb	1.00
tpwr	58	wtfile	
pw	7.8	proc	ft
d1	1.300	fn	65536
tof	525.7	math	f
nt	8000		
ct	8000	werr	
alock	n	wexp	
gain	44	wbs	
FLAGS		wnt	
il	n		
in	n		
dp	y		
hs	nn		
DISPLAY			
sp	-1426.6		
wp	21252.1		
vs	21512		
sc	0		
wc	250		
hzmm	85.01		
is	500.00		
rfl	11707.5		
rfp	7743.7		
th	5		
ins	100.000		
ai	ph		

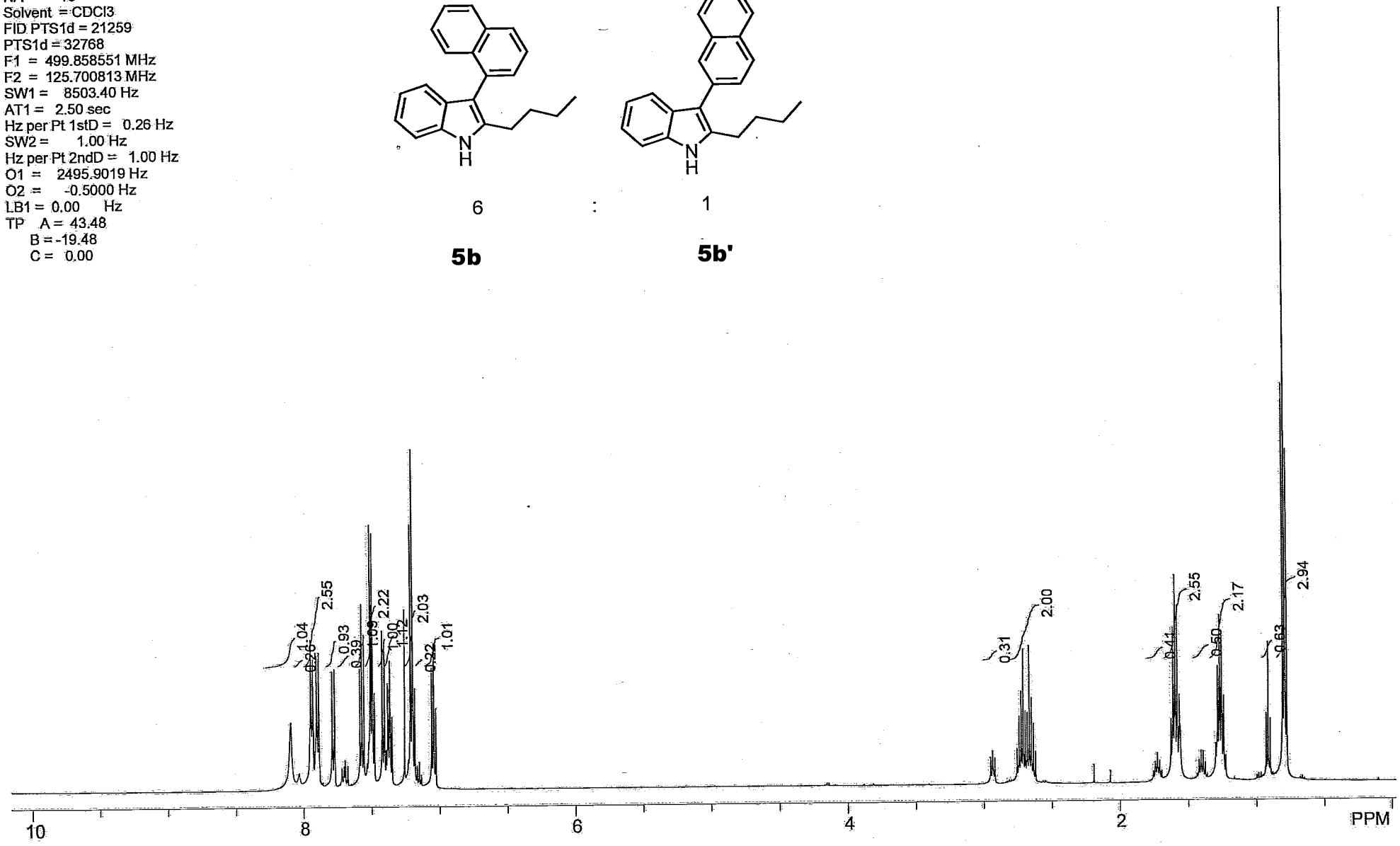
5a

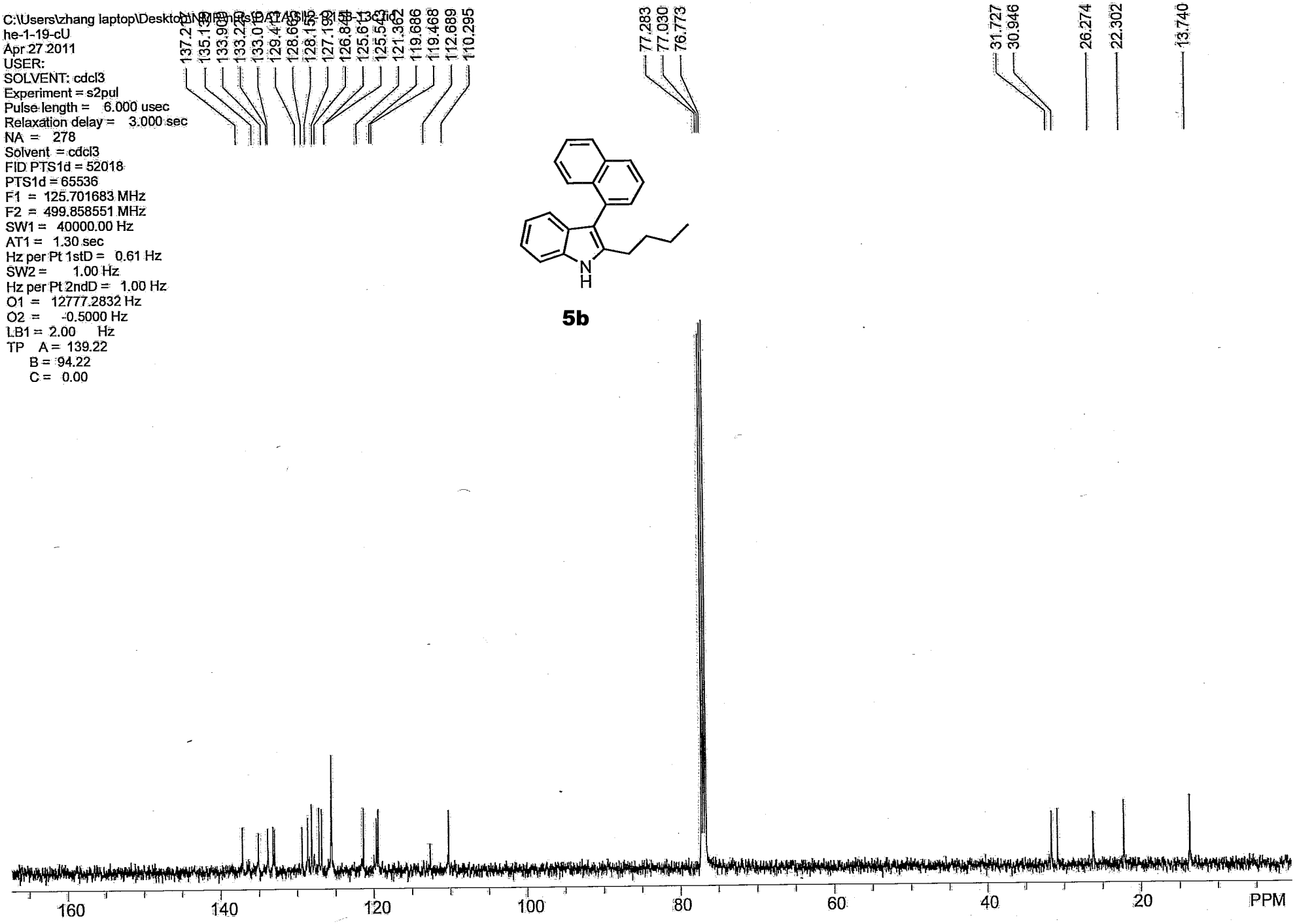


C:\Users\zhang laptop\Desktop\NMR\nuts\DATA\$llz-1-158-1h.fid
H1_CDCL3U
Apr 28 2011
USER:
SOLVENT: CDCl3
Experiment = s2pul
Pulse length = 7.700 usec
Relaxation delay = 4.800 sec
NA = 16
Solvent = CDCl3
FID PTS1d = 21259
PTS1d = 32768
F1 = 499.858551 MHz
F2 = 125.700813 MHz
SW1 = 8503.40 Hz
AT1 = 2.50 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 = 43.48
B = -19.48
C = 0.00

6 : 1

5b **5b'**




C:\Users\zhang laptop\Desktop\NMR\nmrs\DATA\5b2-9-15b-13c.fid
he-1-19-cU
Apr 27 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 6.000 usec
Relaxation delay = 3.000 sec
NA = 278
Solvent = cdcl3
FID PTS1d = 52018
PTS1d = 65536
F1 = 125.701683 MHz
F2 = 499.858551 MHz
SW1 = 40000.00 Hz
AT1 = 1.30 sec
Hz per Pt 1stD = 0.61 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 12777.2832 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = 139.22
B = 94.22
C = 0.00
137.217
135.139
133.908
133.220
133.016
129.413
128.665
128.155
127.199
126.845
125.613
125.543
121.362
119.686
119.468
112.689
110.295
77.283
77.030
76.773
31.727
30.946
26.274
22.302
13.740
N
H
5b
160
140
120
100
80
60
40
20
PPM

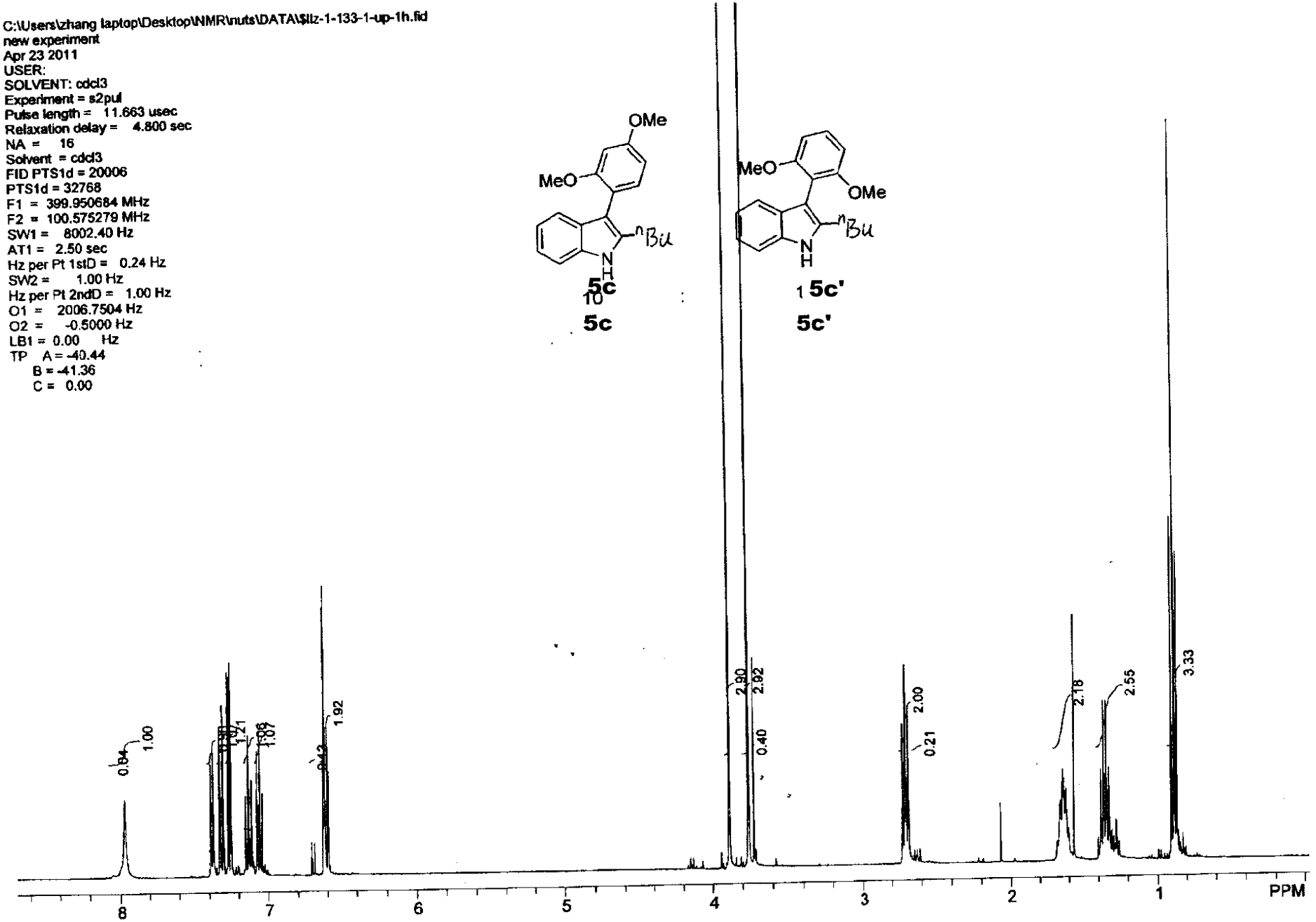
C:\Users\zhang laptop\Desktop\NMR\nuts\DATA\$llz-1-133-1-up-1h.fid
new experiment
Apr 23 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 16
Solvent = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
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 = -40.44
B = -41.36
C = 0.00

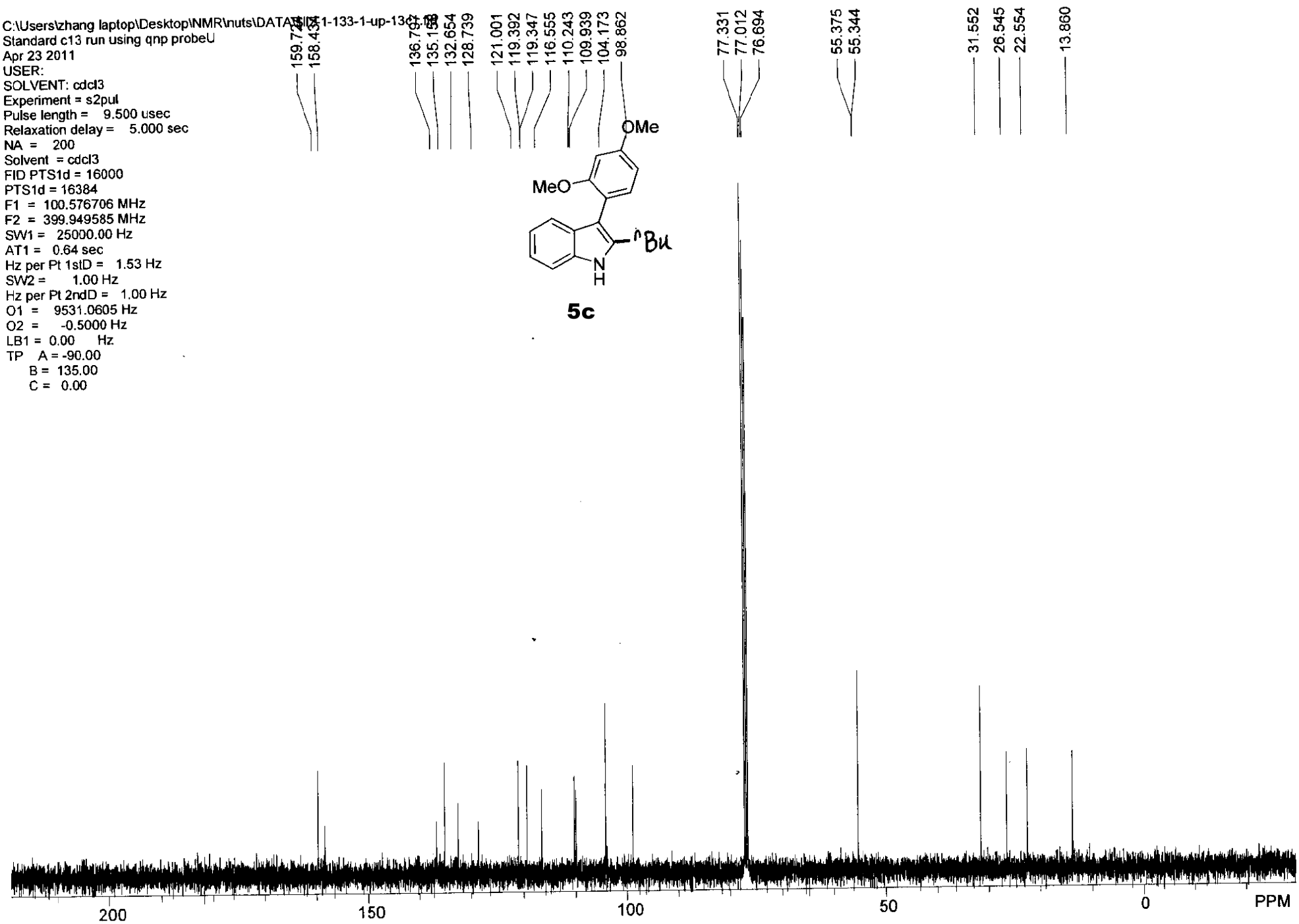
5c

5c'

5c

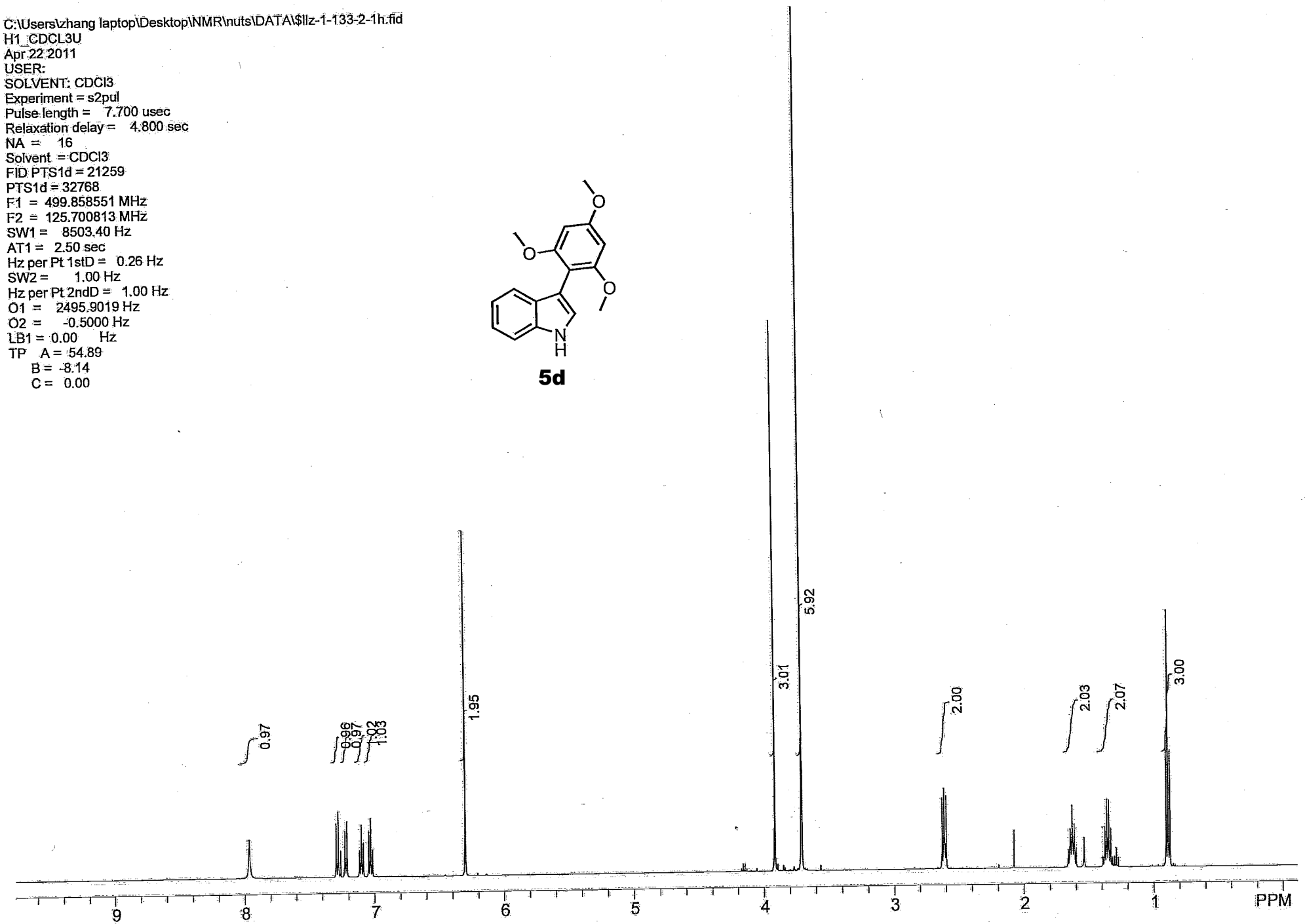
5c'




C:\Users\zhang laptop\Desktop\NMR\nuts\DATA\SIDZ-1-133-1-up-13c
Standard c13 run using qnp probeU
Apr 23 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 9.500 usec
Relaxation delay = 5.000 sec
NA = 200
Solvent = cdcl3
FID PTS1d = 16000
PTS1d = 16384
F1 = 100.576706 MHz
F2 = 399.949585 MHz
SW1 = 25000.00 Hz
AT1 = 0.64 sec
Hz per Pt 1stD = 1.53 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 9531.0605 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -90.00
B = 135.00
C = 0.00
159.744
158.437
136.797
135.158
132.654
128.739
121.001
119.392
119.347
116.555
110.243
109.939
104.173
98.862
77.331
77.012
76.694
55.375
55.344
31.552
26.545
22.554
13.860
OMe
MeO
nBu
N
H
5c
200
150
100
50
0
PPM

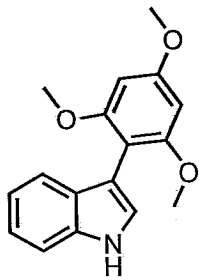
C:\Users\zhang laptop\Desktop\NMR\nuts\DATA\$llz-1-133-2-1h.fid
H1_CDCL3U
Apr 22 2011
USER:
SOLVENT: CDCl3
Experiment = s2pul
Pulse length = 7.700 usec
Relaxation delay = 4.800 sec
NA = 16
Solvent = CDCl3
FID PTS1d = 21259
PTS1d = 32768
F1 = 499.858551 MHz
F2 = 125.700813 MHz
SW1 = 8503.40 Hz
AT1 = 2.50 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 = 54.89
B = -8.14
C = 0.00

5d

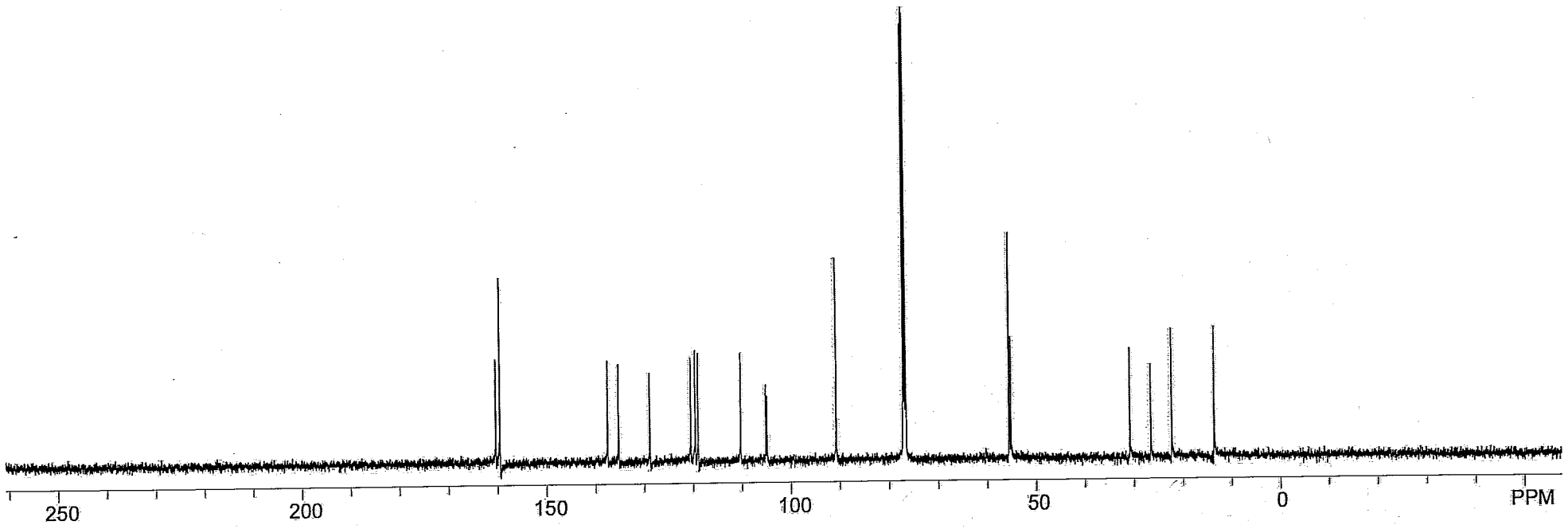


C:\Users\zhang laptop\Desktop\NMR\nuts\DATA\$llz-1-133-2-13c-d
he-1-19-cU
Apr 22 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 6.000 usec
Relaxation delay = 3.000 sec
NA = 724
Solvent = cdcl3
FID PTS1d = 52018
PTS1d = 65536
F1 = 125.701683 MHz
F2 = 499.858551 MHz
SW1 = 40000.00 Hz
AT1 = 1.30 sec
Hz per Pt 1stD = 0.61 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 12777.2832 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -138.75
B = 45.00
C = 0.00

160.428
159.599
137.620
135.376
129.000
120.609
119.715
119.118
110.382
105.273
105.006
90.909
77.341
77.084
76.831
55.741
55.377
31.111
26.857
22.617
13.930



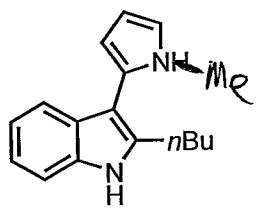
5d



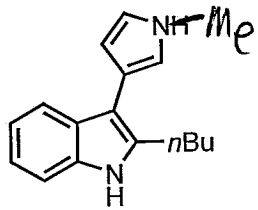
lb-IV-21-2

exp1 s2pul

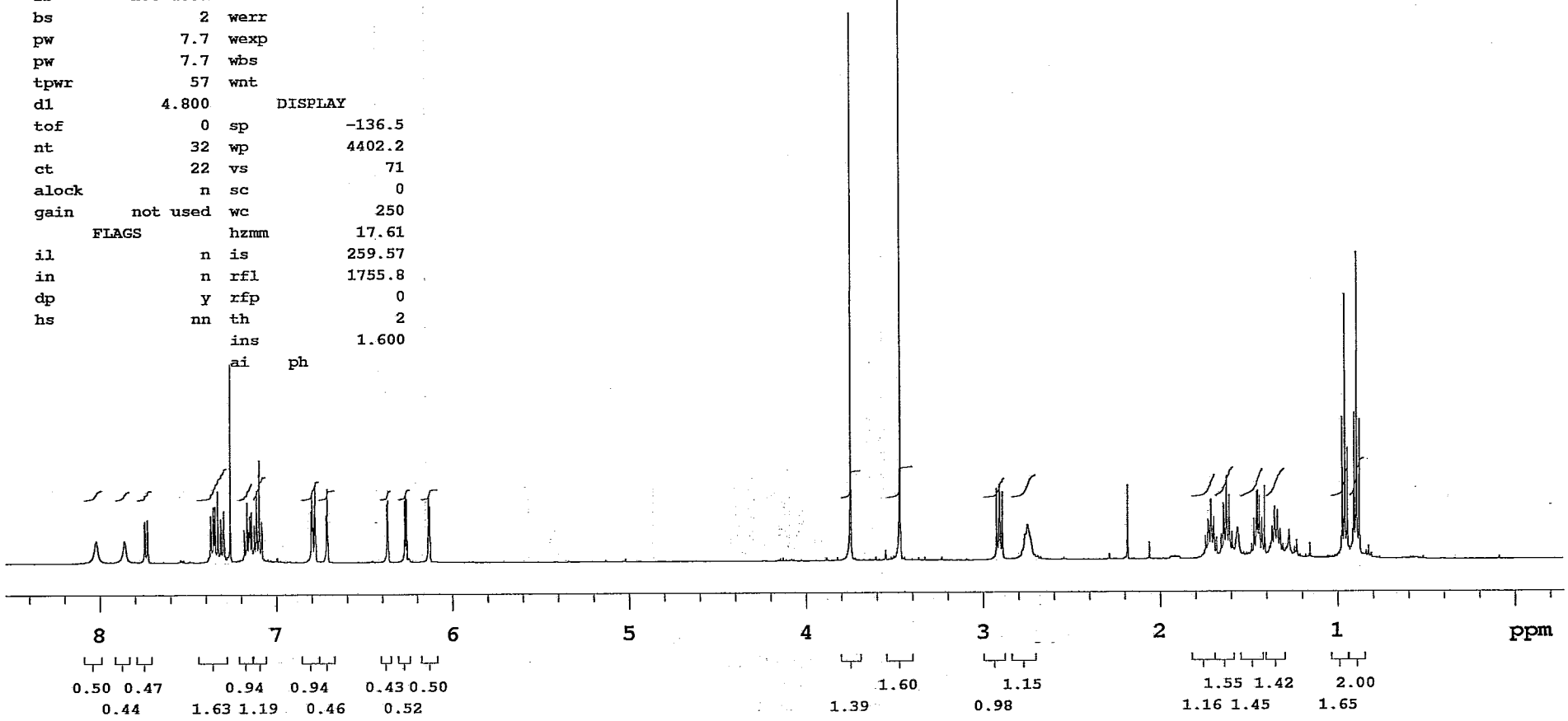
SAMPLE		DEC. & VT	
date	Apr 26 2011	dn	C13
solvent	CDCl3	dof	0
file	exp	dm	nnn
ACQUISITION		dmm	c
sfrq	499.859	dmf	200
tn	H1	PROCESSING	
at	2.500	lb	0.20
np	42518	fn	32768
sw	8503.4	math	i
fb	not used		
bs	2	werr	
pw	7.7	wexp	
pw	7.7	wbs	
tpwr	57	wnt	
d1	4.800	DISPLAY	
tof	0	sp	-136.5
nt	32	wp	4402.2
ct	22	vs	71
alock	n	sc	0
gain	not used	wc	250
FLAGS		hzmm	17.61
il	n	is	259.57
in	n	rfl	1755.8
dp	y	rfp	0
hs	nn	th	2
		ins	1.600
		ai ph	



5e



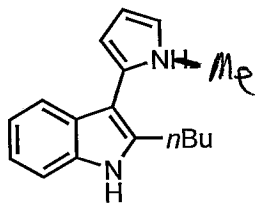
5e'



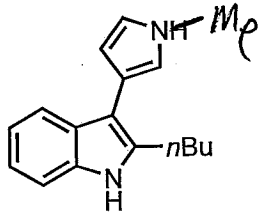
lb-IV-21-2-C13

exp1 Carbon

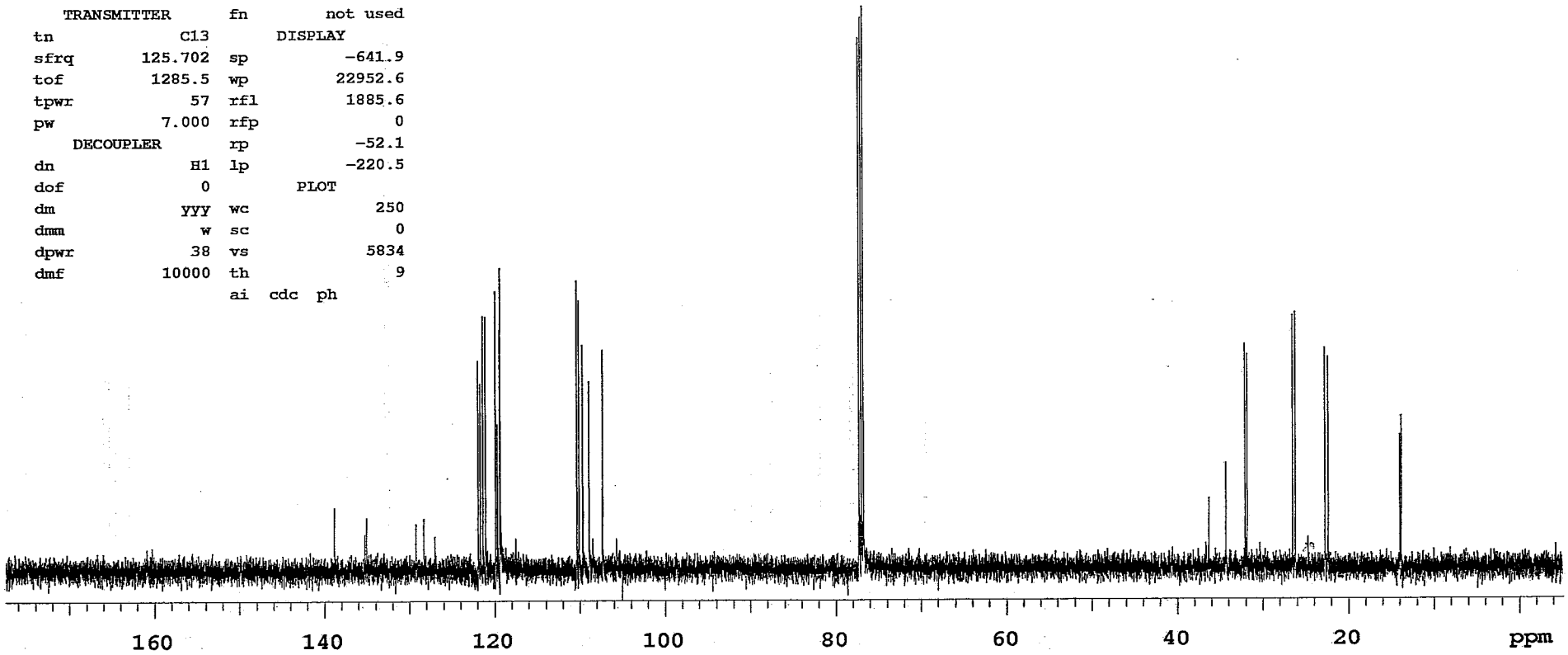
SAMPLE		SPECIAL	
date	Apr 26 2011	temp	not used
solvent	CDCl3	gain	46
file	exp	spin	not used
ACQUISITION		hst	0.008
sw	30165.9	pw90	14.600
at	1.303	alfa	6.600
np	78590	FLAGS	
fb	not used	il	n
bs	4	in	n
ss	2	dp	y
d1	1.000	hs	nn
nt	10000	PROCESSING	
ct	296	lb	0.50
TRANSMITTER		fn	not used
tn	C13	DISPLAY	
sfrq	125.702	sp	-641.9
tof	1285.5	wp	22952.6
tpwr	57	rfl	1885.6
pw	7.000	rfp	0
DECOUPLER		rp	-52.1
dn	H1	lp	-220.5
dof	0	PLOT	
dm	yyy	wc	250
dmm	w	sc	0
dpwr	38	vs	5834
dmf	10000	th	9
		ai	cdc ph



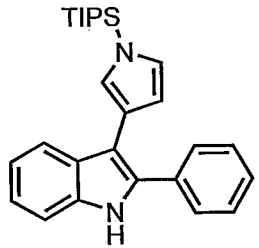
5e



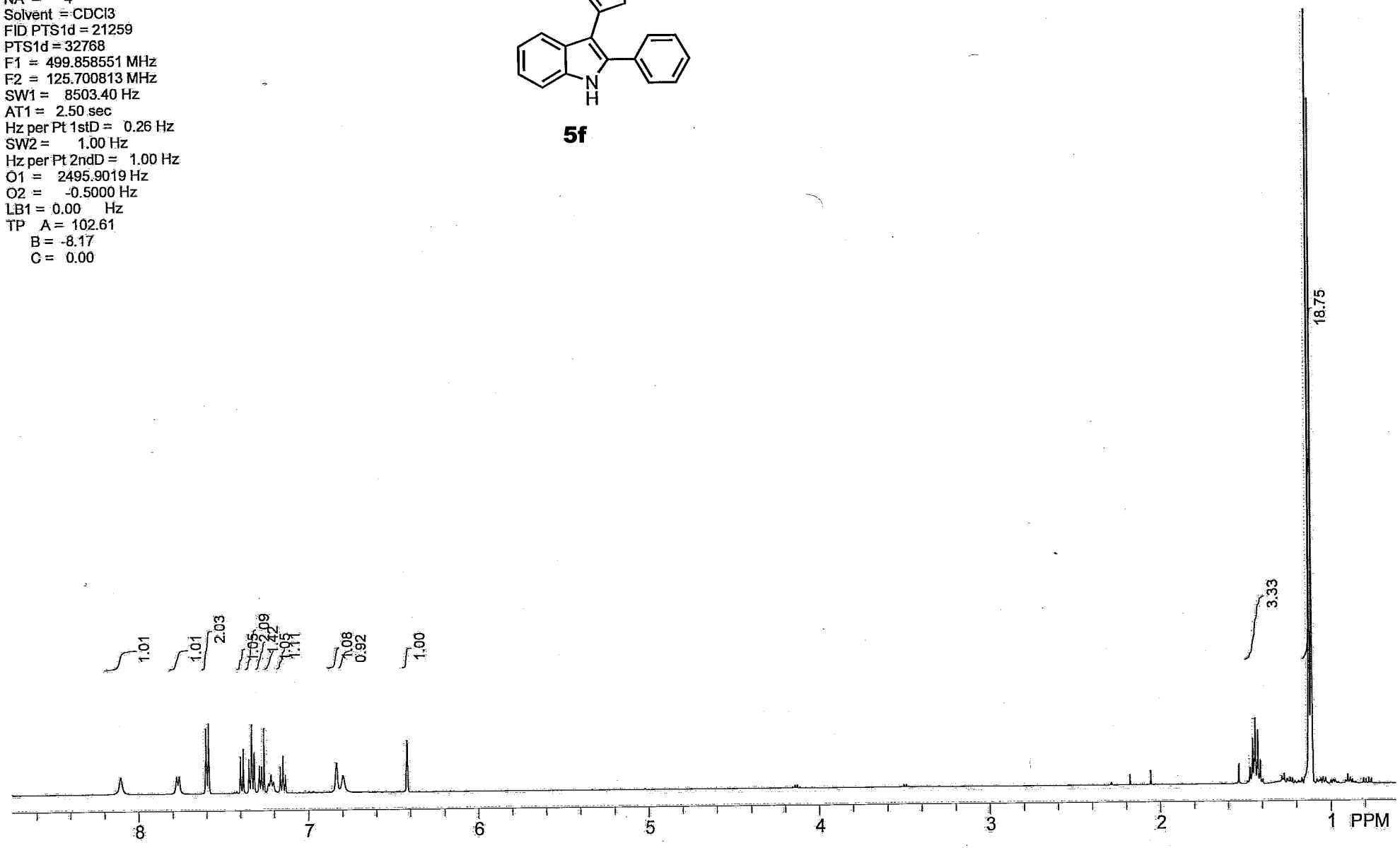
5e'

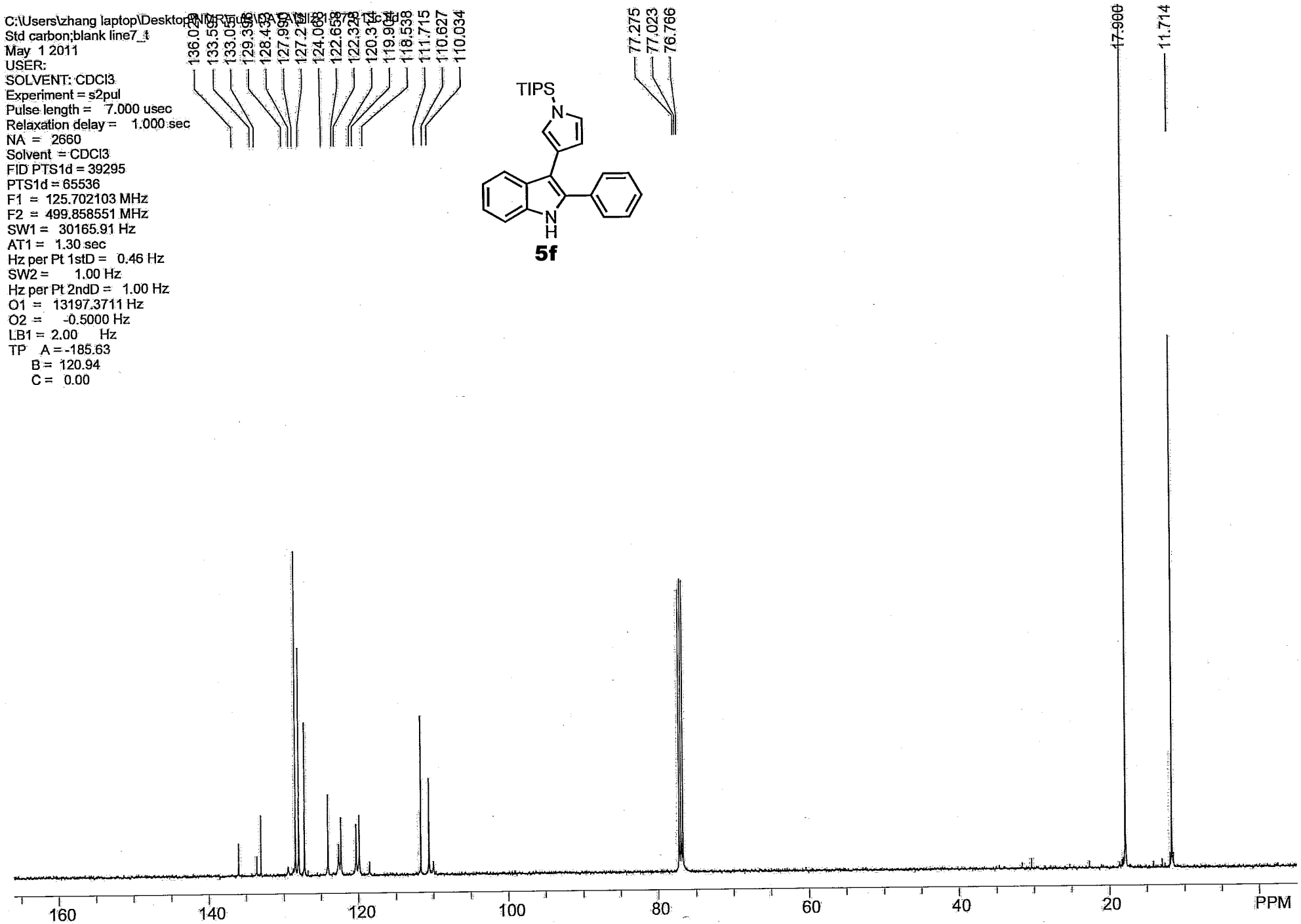


C:\Users\zhang laptop\Desktop\NMR\nuts\DATA\$llz-1-173-1h.fid
H1_CDCL3U
May 1 2011
USER:
SOLVENT: CDCl3
Experiment = s2pul
Pulse length = 7.700 usec
Relaxation delay = 4.800 sec
NA = 4
Solvent = CDCl3
FID PTS1d = 21259
PTS1d = 32768
F1 = 499.858551 MHz
F2 = 125.700813 MHz
SW1 = 8503.40 Hz
AT1 = 2.50 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 = 102.61
B = -8.17
C = 0.00



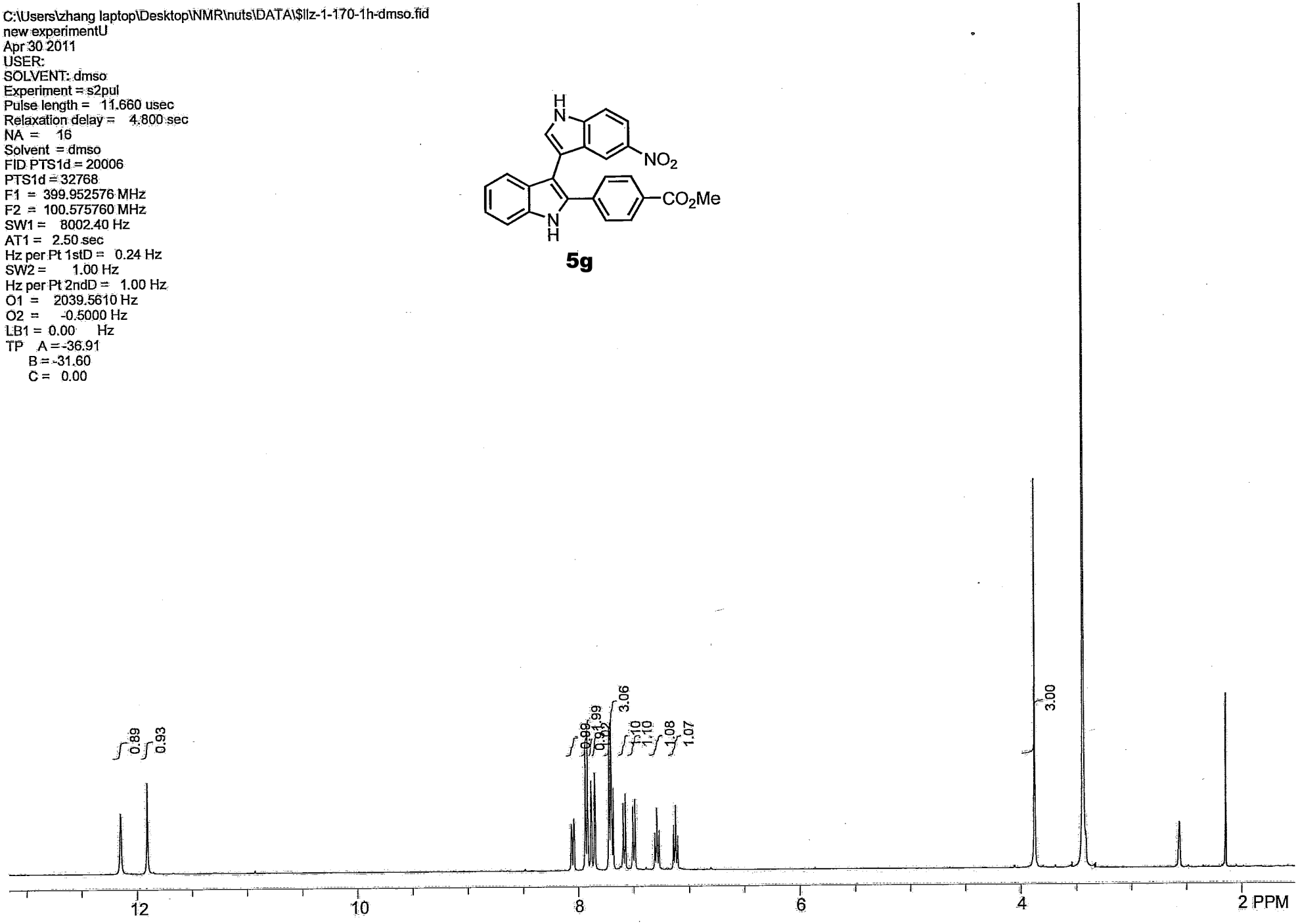
5f

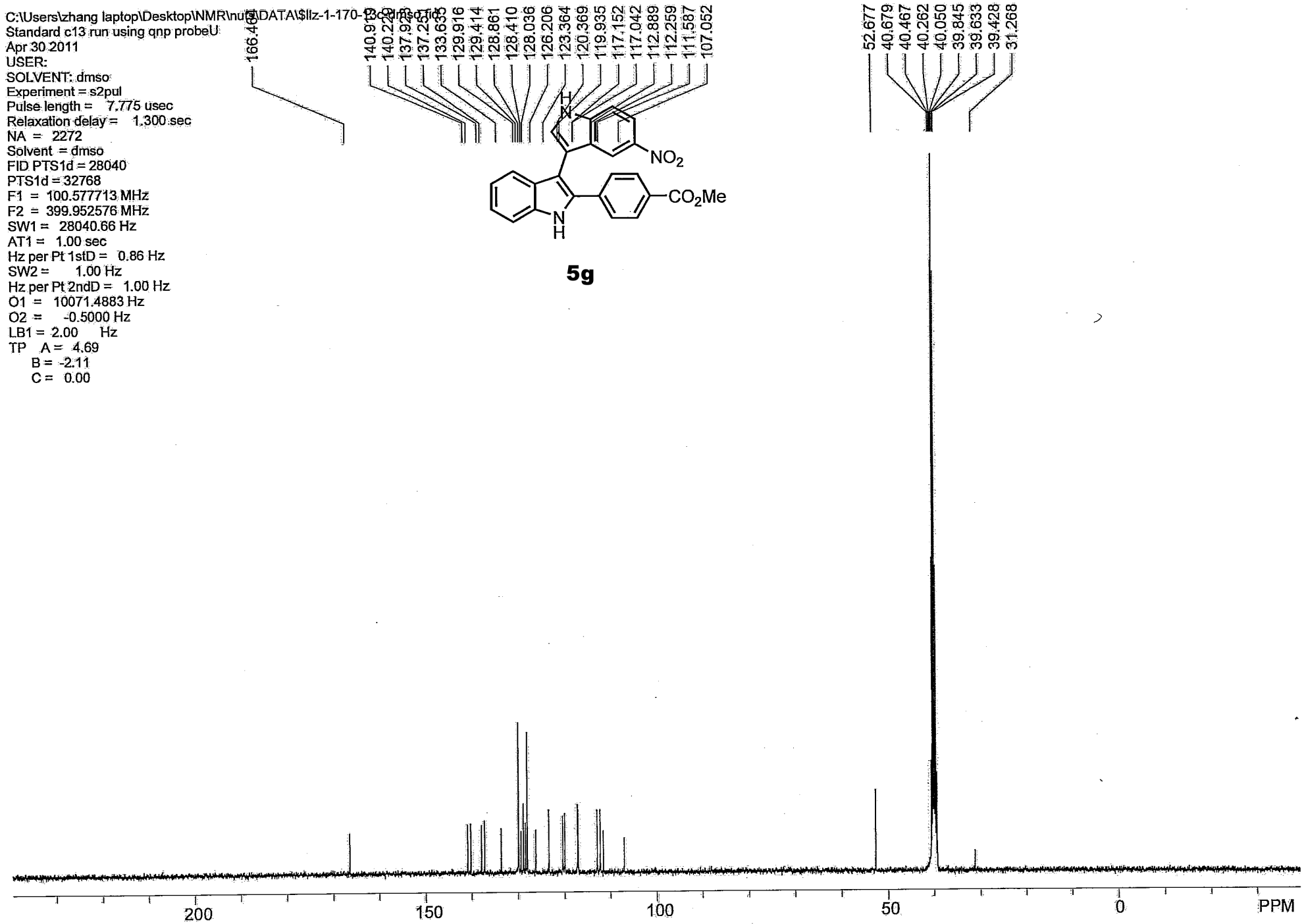



C:\Users\zhang laptop\Desktop\NMR\Tuo\DATA\Slize_9723_13c.fid
Std carbon;blank line7_t
May 1 2011
USER:
SOLVENT: CDCl3
Experiment = s2pul
Pulse length = 7.000 usec
Relaxation delay = 1.000 sec
NA = 2660
Solvent = CDCl3
FID PTS1d = 39295
PTS1d = 65536
F1 = 125.702103 MHz
F2 = 499.858551 MHz
SW1 = 30165.91 Hz
AT1 = 1.30 sec
Hz per Pt 1stD = 0.46 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 13197.3711 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -185.63
B = 120.94
C = 0.00
136.029
133.595
133.051
129.396
128.432
127.990
127.215
124.063
122.658
122.328
120.314
119.904
118.538
111.715
110.627
110.034
77.275
77.023
76.766
17.900
11.714
TIPS
N
N
H
5f
160
140
120
100
80
60
40
20
PPM

C:\Users\zhang laptop\Desktop\NMR\nuts\DATA\$llz-1-170-1h-dmso.fid
new experimentU
Apr 30 2011
USER:
SOLVENT: dmso
Experiment = s2pul
Pulse length = 11.660 usec
Relaxation delay = 4.800 sec
NA = 16
Solvent = dmso
FID PTS1d = 20006
PTS1d = 32768
F1 = 399.952576 MHz
F2 = 100.575760 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 = 2039.5610 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -36.91
B = -31.60
C = 0.00

5g

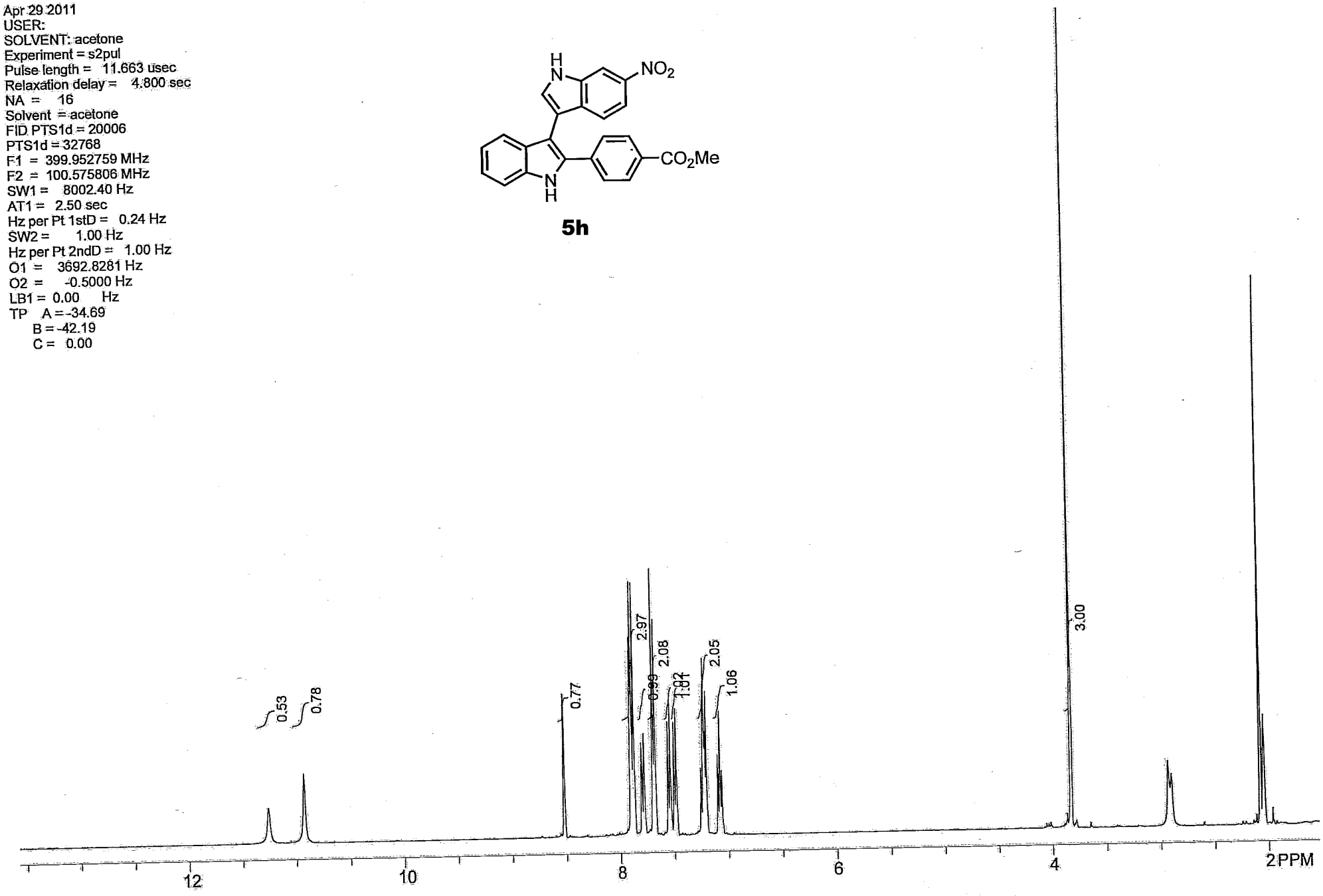


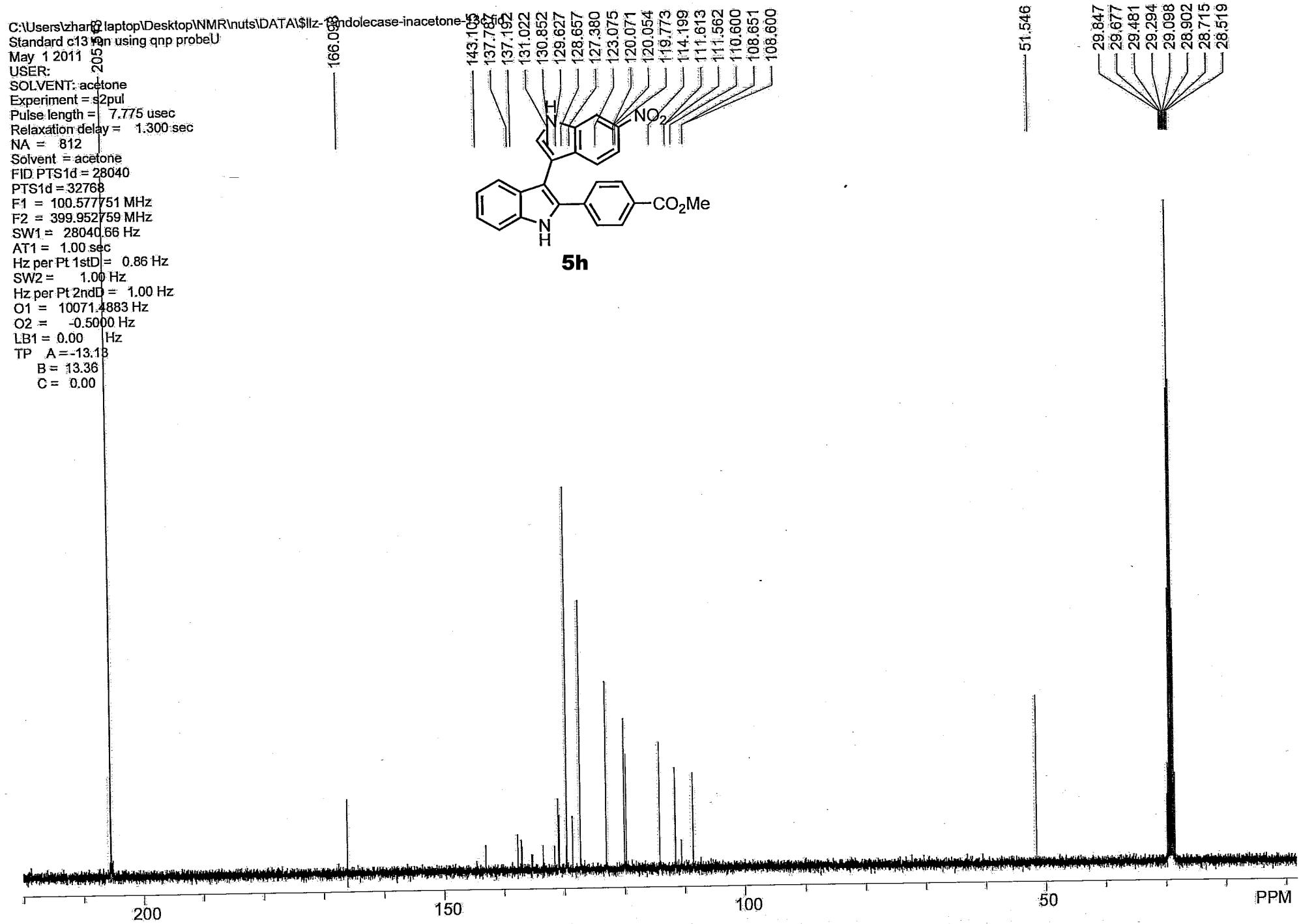

C:\Users\zhang laptop\Desktop\NMR\nuts\DATA\$llz-1-170-13c-dmso.fid
Standard c13 run using qnp probeU
Apr 30 2011
USER:
SOLVENT: dmso
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 2272
Solvent = dmso
FID PTS1d = 28040
PTS1d = 32768
F1 = 100.577713 MHz
F2 = 399.952576 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 = 4.69
B = -2.11
C = 0.00
166.464
140.913
140.220
137.923
137.251
133.635
129.916
129.414
128.861
128.410
128.036
126.206
123.364
120.369
119.935
117.152
117.042
112.889
112.259
111.587
107.052
52.677
40.679
40.467
40.262
40.050
39.845
39.633
39.428
31.268
H
N
NO2
CO2Me
N
H
5g
200
150
100
50
0
PPM

C:\Users\zhang laptop\Desktop\NMR\nuts\DATA\$llz-1-indolecase-inacetone-1h.fid

Apr 29 2011
USER:
SOLVENT: acetone
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 16
Solvent = acetone
FID PTS1d = 20006
PTS1d = 32768
F1 = 399.952759 MHz
F2 = 100.575806 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 = 3692.8281 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -34.69
B = -42.19
C = 0.00

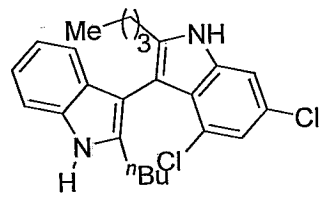
5h



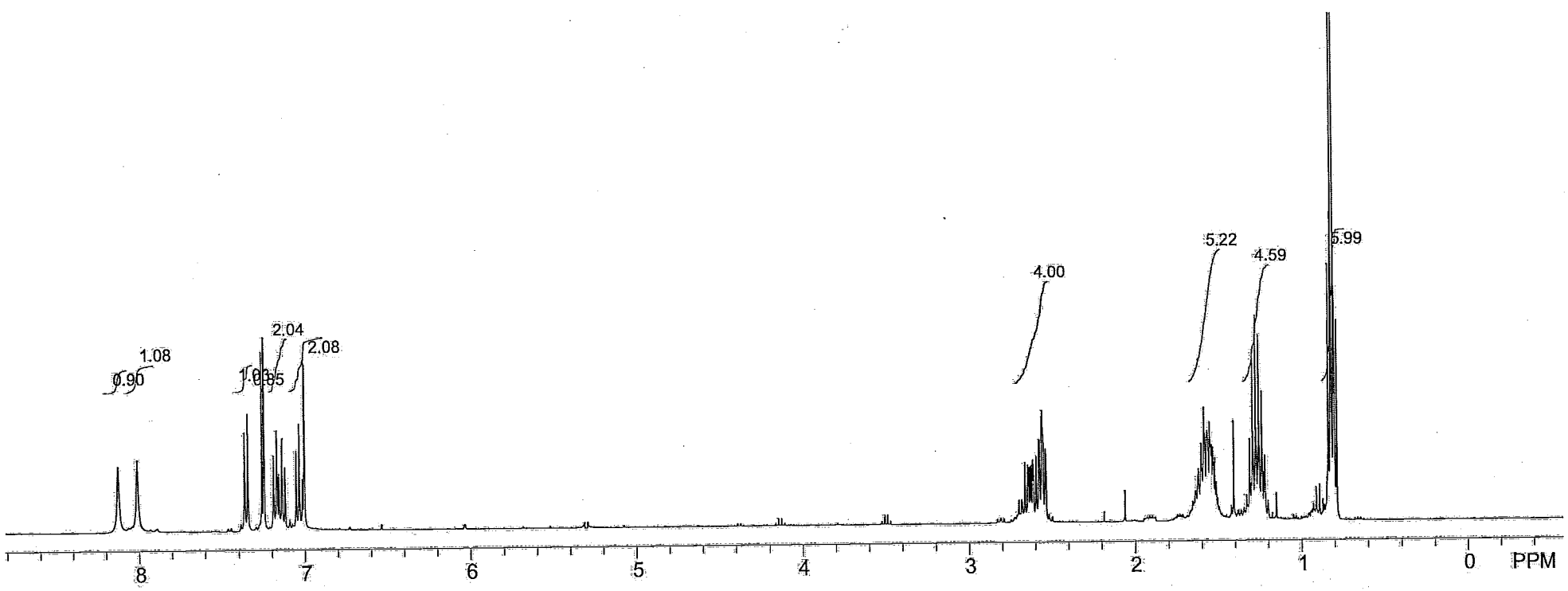

C:\Users\zhang laptop\Desktop\NMR\nuts\DATA\$llz-1indolecase-inacetone-13c.fid
Standard c13 run using qnp probeU
May 1 2011
USER:
SOLVENT: acetone
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 812
Solvent = acetone
FID PTS1d = 28040
PTS1d = 32768
F1 = 100.577751 MHz
F2 = 399.952759 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 = 0.00 Hz
TP A = -13.13
B = 13.36
C = 0.00
166.093
143.105
137.787
137.192
131.022
130.852
129.627
128.657
127.380
123.075
120.071
120.054
119.773
114.199
111.613
111.562
110.600
108.651
108.600
51.546
29.847
29.677
29.481
29.294
29.098
28.902
28.715
28.519
NO2
CO2Me
5h
200
150
100
50
PPM

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

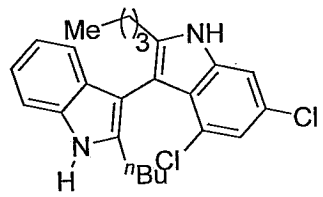
May 1 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 16
Solvent = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 0.24 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2006.7504 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -52.47
B = -19.74
C = 0.00



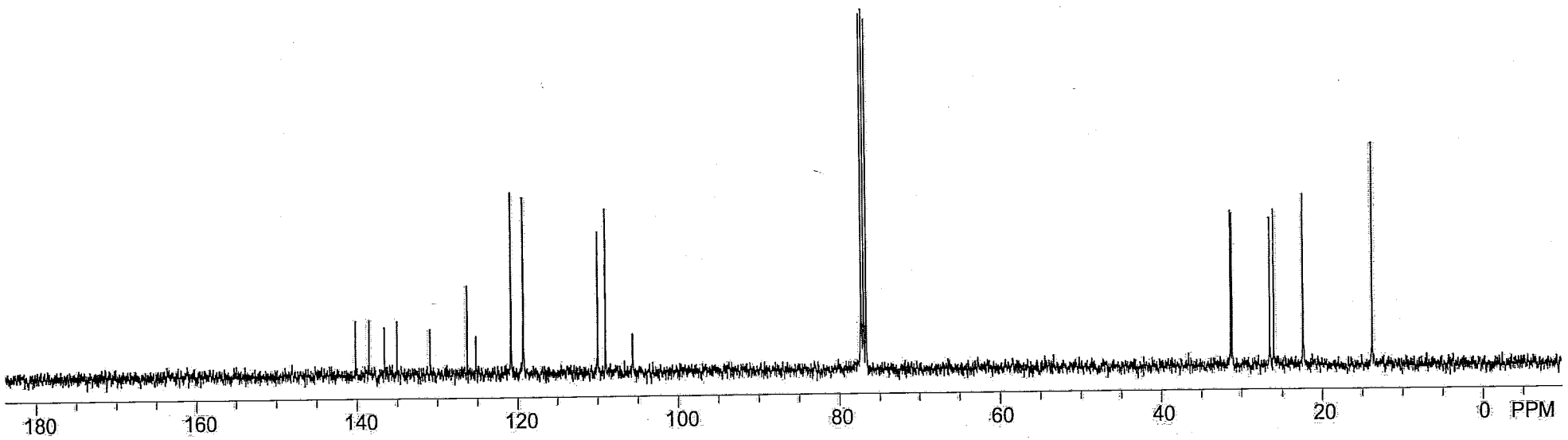
5i



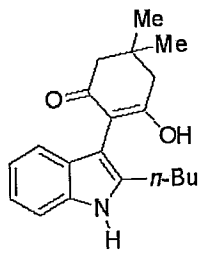
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-158-c1.fid
Standard c13 run using qnp probe
May 1 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 396
Solvent = cdcl3
FID PTS1d = 28040
PTS1d = 32768
F1 = 100.577232 MHz
F2 = 399.950684 MHz
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 = -30.00
B = 8.44
C = 0.00



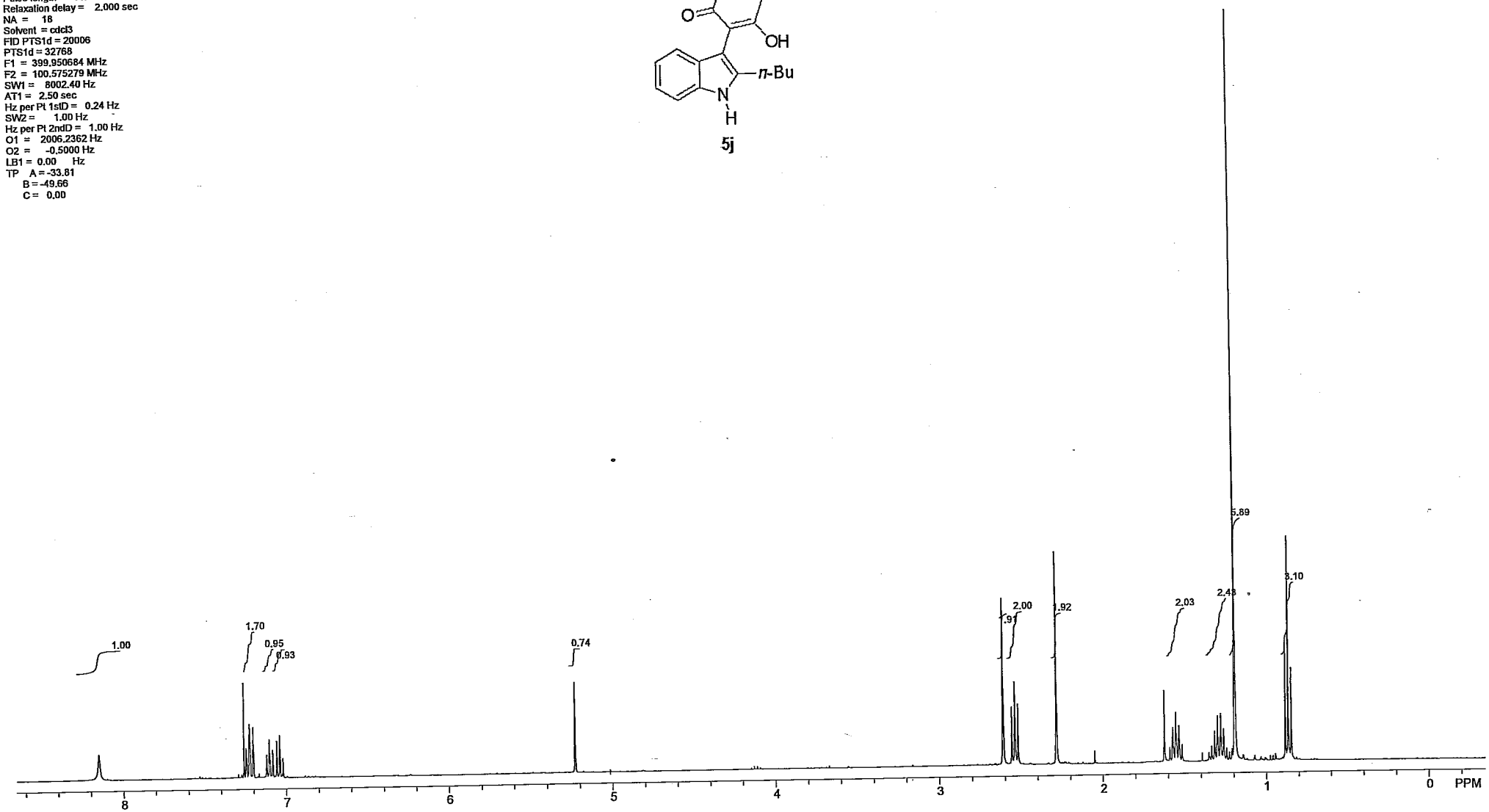
5i



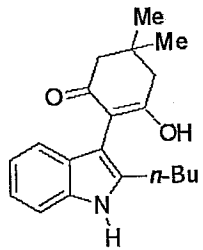
D:\Greenware\Ntus 20080731\DATA\$wyz3-267-pro-h1.fid
new experiment
May 1 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 2.000 sec
NA = 16
Solvent = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
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 = -33.81
B = -49.66
C = 0.00



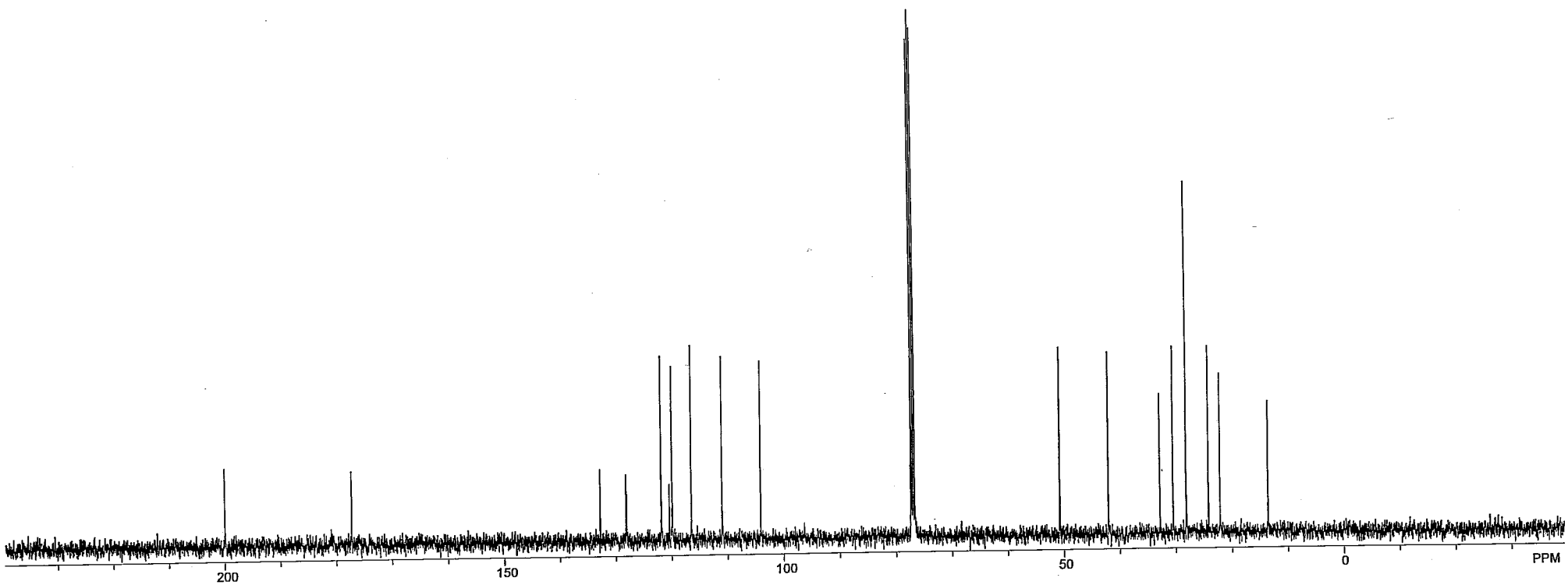
5j



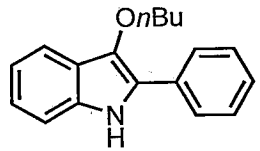
D:\Greenware\Ntus 20080731\DATA\$wyz3-267-pro-c13.fid
Standard c13 run using qnp probe
May 1 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 460
Solvent = cdcl3
FID PTS1d = 28040
PTS1d = 32768
F1 = 100.577232 MHz
F2 = 399.950684 MHz
SW1 = 28040.66 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 = -19.69
B = -15.47
C = 0.00



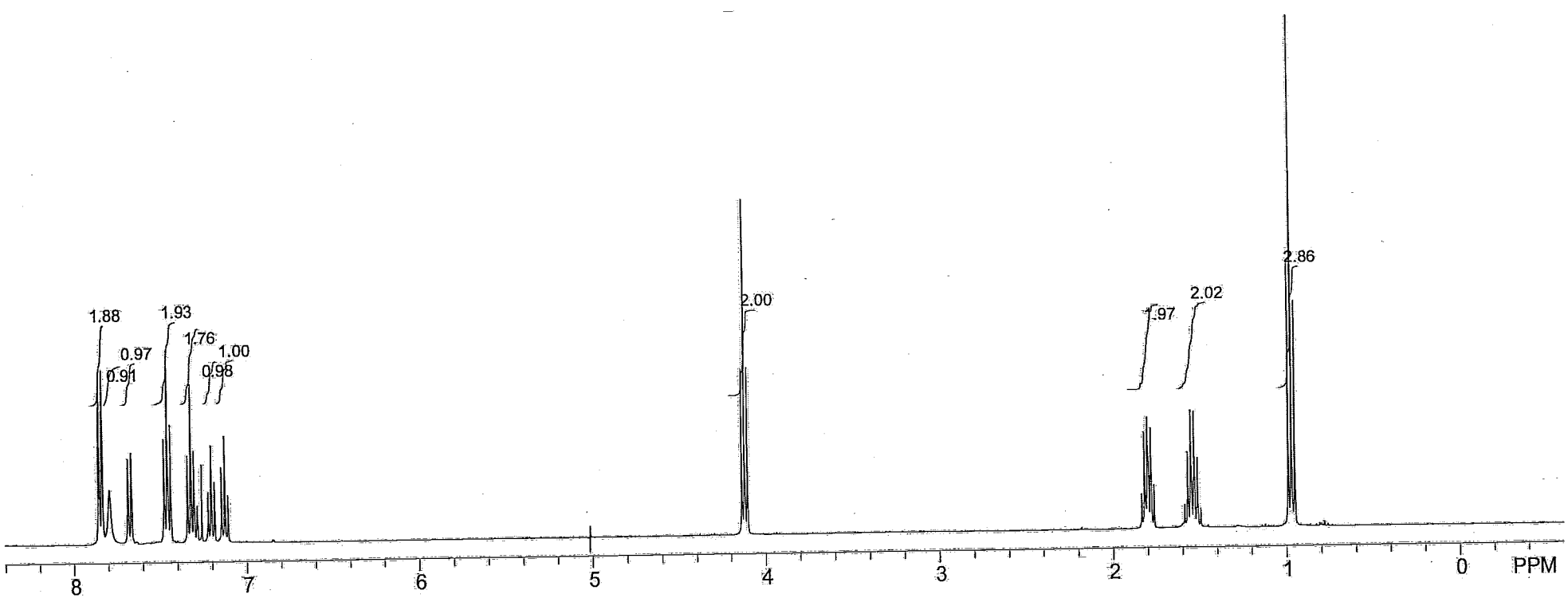
5j



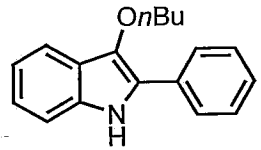
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-178-Ph-h.fid
new experiment
Apr 28 2011
USER:
SOLVENT; cdcl3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 6
Solvent = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 0.24 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2006.2362 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -44.62
B = -33.90
C = 0.00



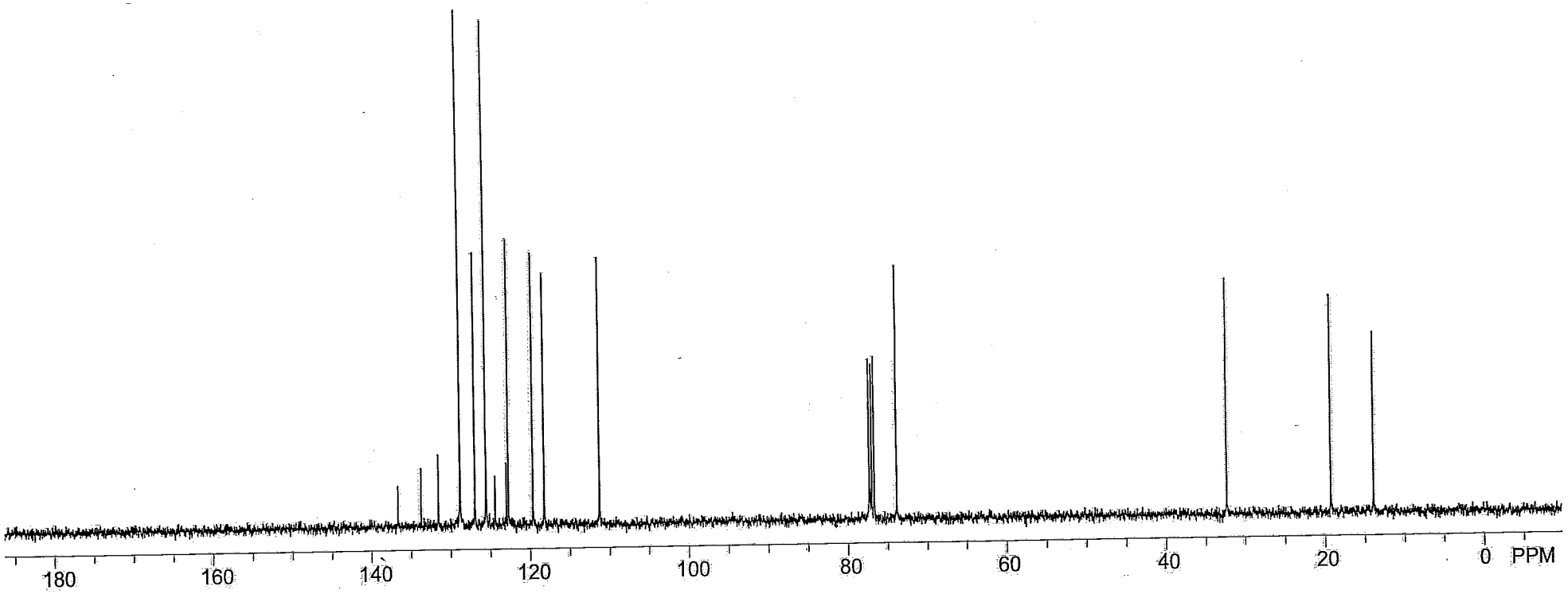
5k



C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-178-Ph-c3.fid
Standard c13 run using qnp probe
Apr 28 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 264
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 = -30.94
B = 4.22
C = 0.00

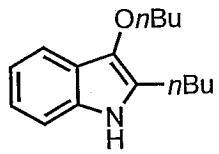


5k

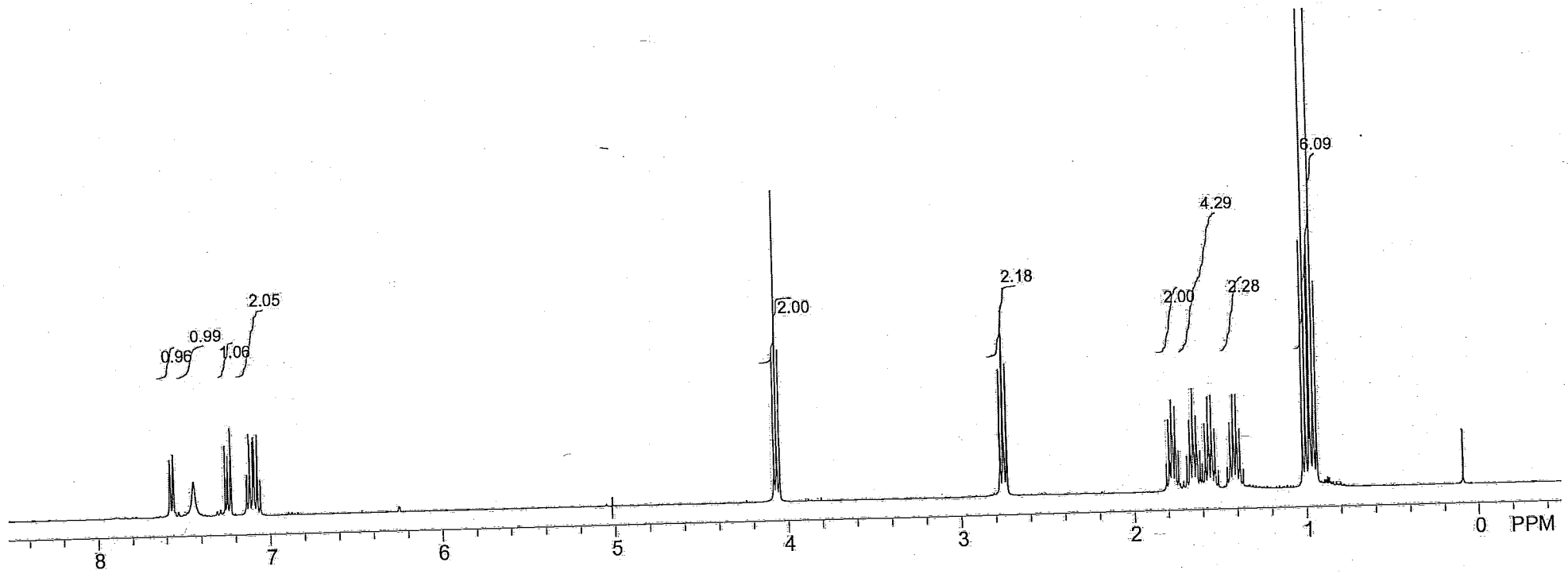


C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-176-hhhh.fid

Apr 27 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 = -37.03
B = -48.52
C = 0.00

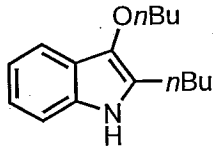


5l

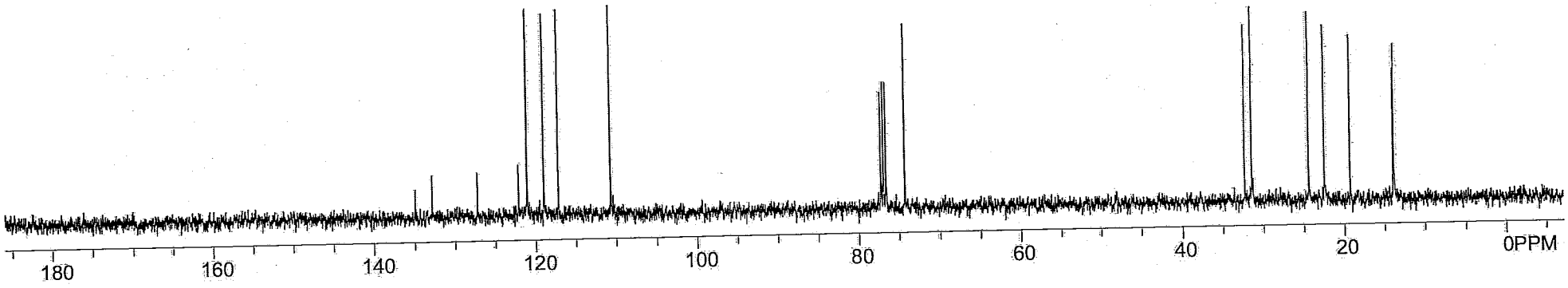


C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-176-c2.fid

Apr 27 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 = 10055.5059 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -30.47
B = -2.81
C = 0.00

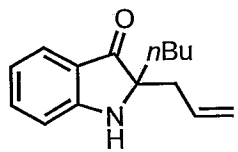


5l

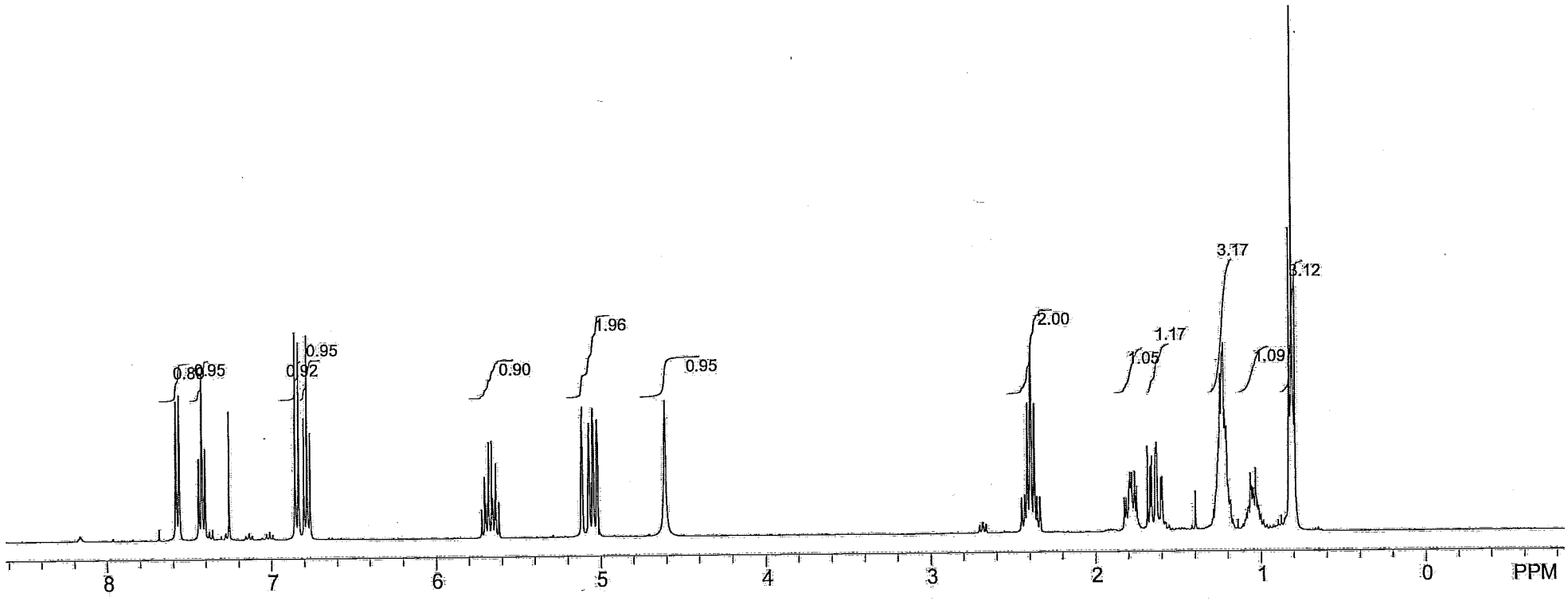


C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-184-h.fid

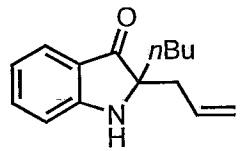
Apr 29 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 11.663 usec
Relaxation delay = 4.800 sec
NA = 14
Solvent = cdcl3
FID PTS1d = 20006
PTS1d = 32768
F1 = 399.950684 MHz
F2 = 100.575279 MHz
SW1 = 8002.40 Hz
AT1 = 2.50 sec
Hz per Pt 1stD = 0.24 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 2005.9918 Hz
O2 = -0.5000 Hz
LB1 = 0.00 Hz
TP A = -45.74
B = -34.27
C = 0.00



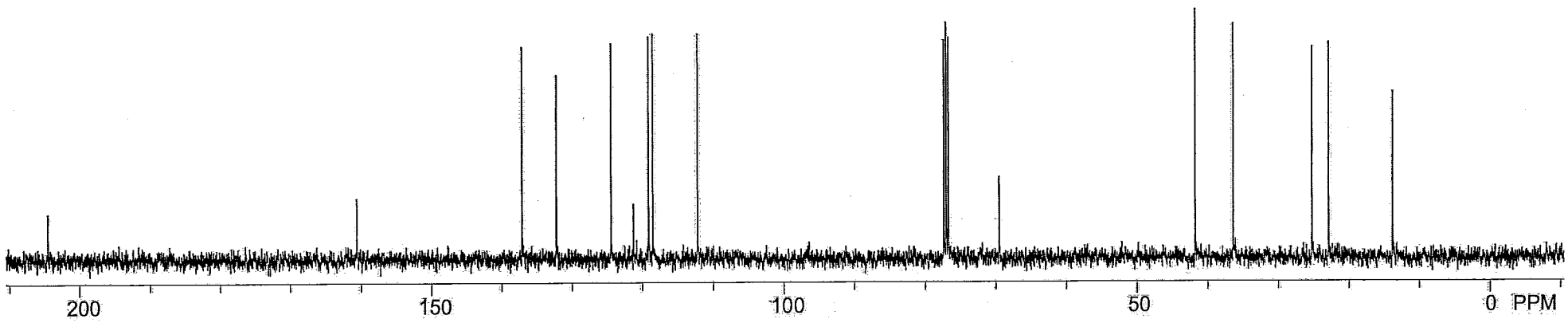
5m



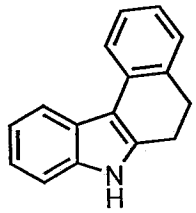
C:\Users\zhanglab1\Desktop\NMR\Ntus 20080731\DATA\$ylw-5-184-c.fid
Standard c13 run using qnp probe
Apr 29 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 7.775 usec
Relaxation delay = 1.300 sec
NA = 68
Solvent = cdcl3
FID PTS1d = 28040
PTS1d = 32768
F1 = 100.577232 MHz
F2 = 399.950684 MHz
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 = -40.78
B = 5.63
C = 0.00



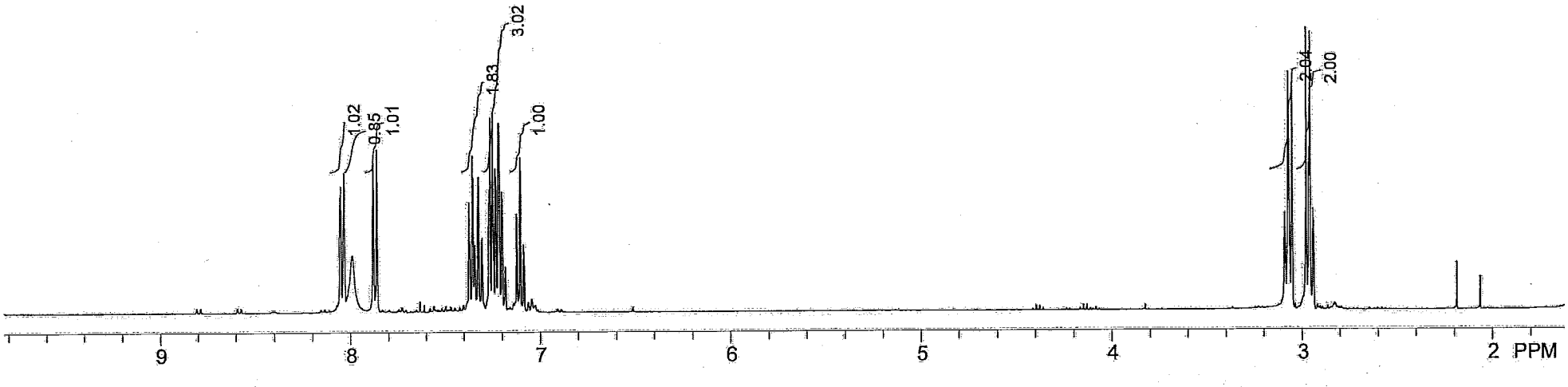
5m



C:\Users\zhang laptop\Desktop\NMR\nuts\DATA\$llz-1-150-1h.fid
new experimentU
Apr 26 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 = -55.78
B = -0.70
C = 0.00

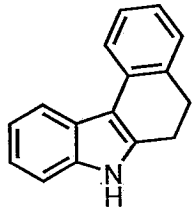


6

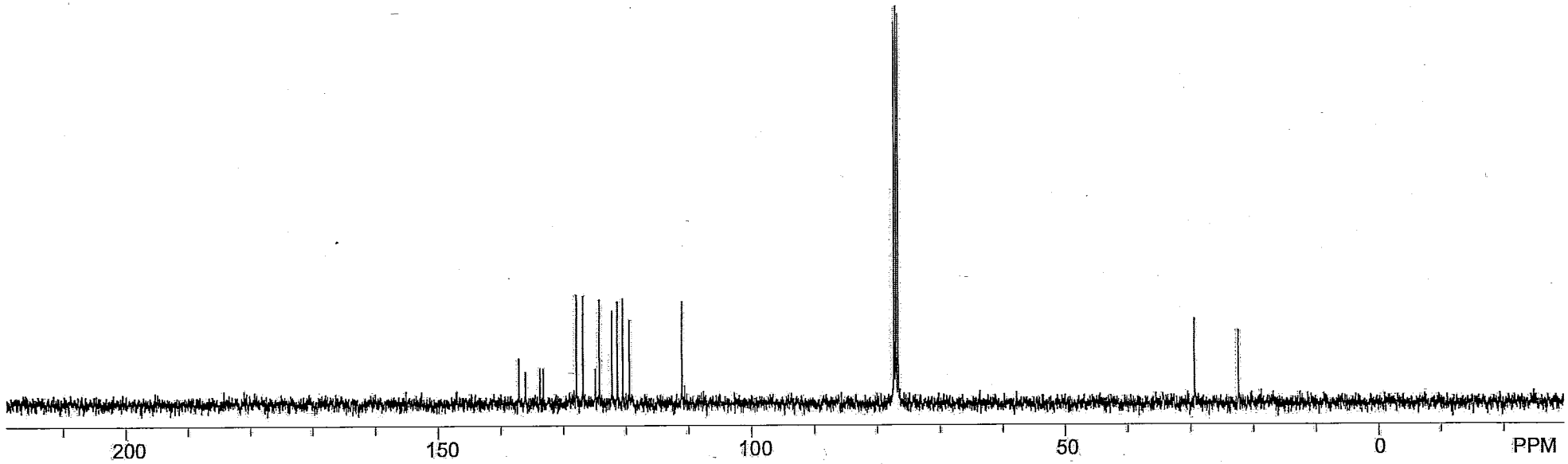


C:\Users\zhang laptop\Desktop\NMR\nuts\DATA\$llz-1-150-13C-1
Standard c13 run using qnp probeU
Apr 26 2011
USER:
SOLVENT: cdcl3
Experiment = s2pul
Pulse length = 9.500 usec
Relaxation delay = 5.000 sec
NA = 352
Solvent = cdcl3
FID PTS1d = 16000
PTS1d = 16384
F1 = 100.576706 MHz
F2 = 399.949585 MHz
SW1 = 25000.00 Hz
AT1 = 0.64 sec
Hz per Pt 1stD = 1.53 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 9531.0605 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -126.09
B = 174.38
C = 0.00

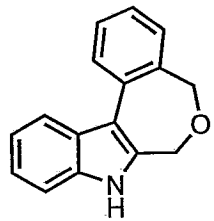
137.176
136.129
133.807
133.276
127.950
126.903
124.900
124.263
122.260
121.395
120.530
119.483
111.077
77.331
77.012
76.694
29.458
22.478



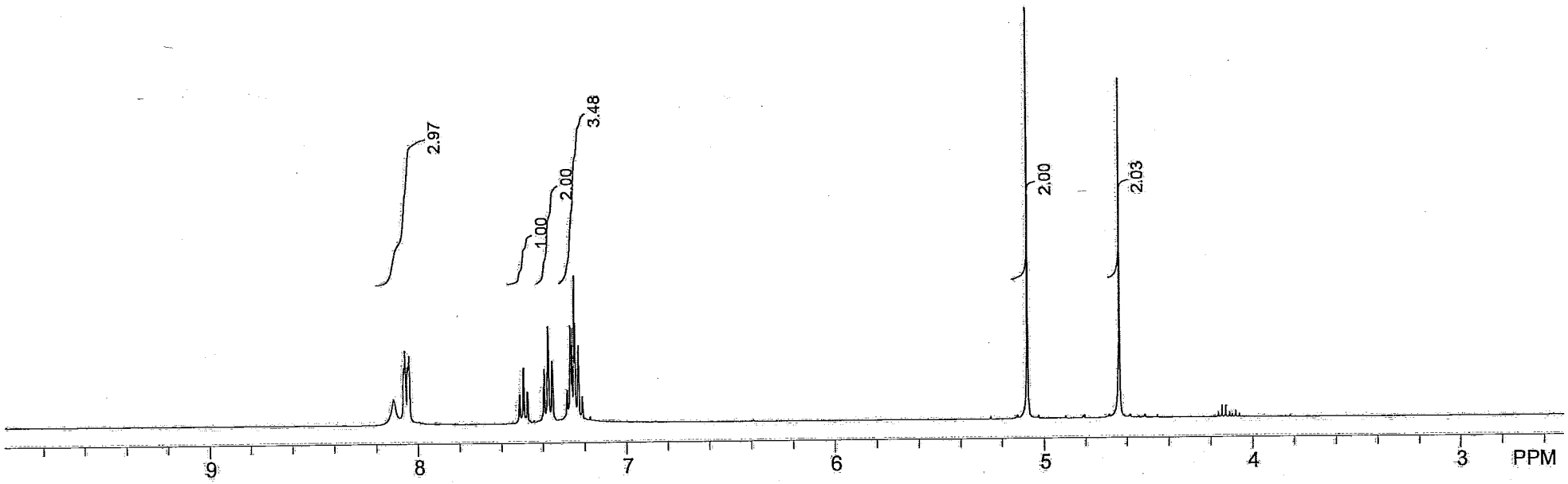
6



C:\Users\zhang laptop\Desktop\NMR\nuts\DATA\$llz-1-145-1h.fid
new experimentU
Apr 25 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 = -57.11
B = -16.77
C = 0.00



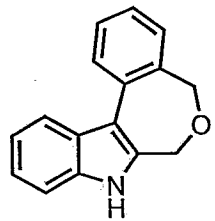
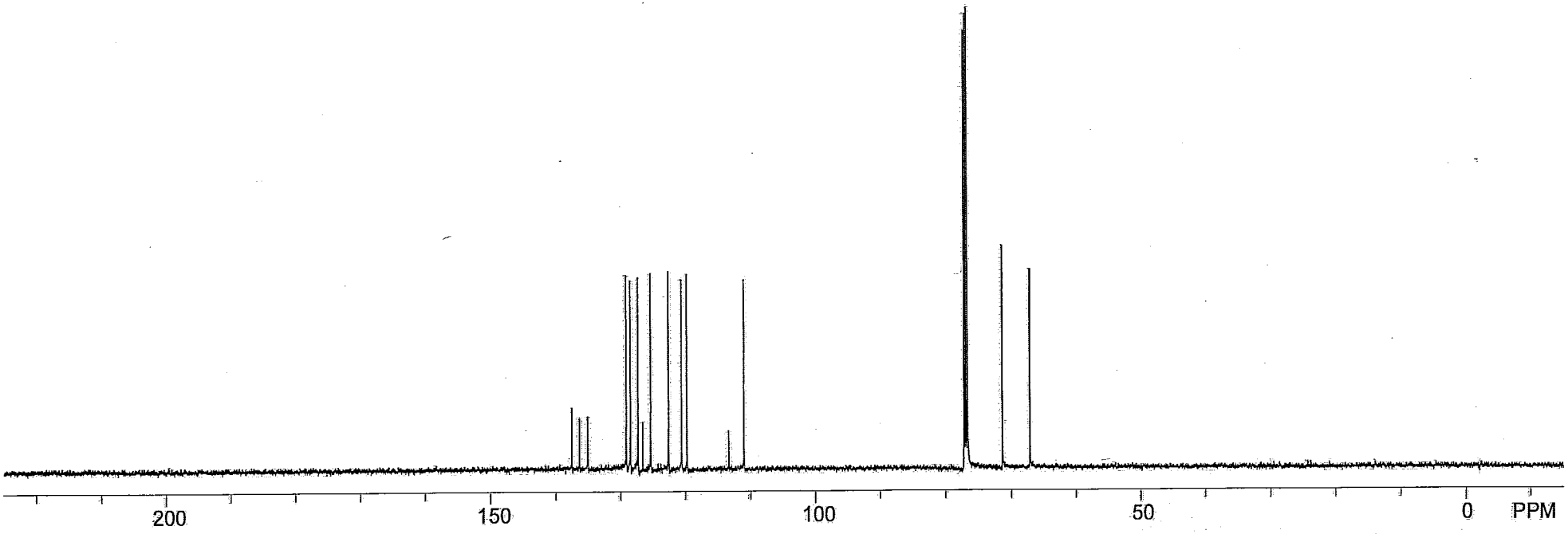
7



C:\Users\zhang laptop\Desktop\NMR\nuts\DATA\$llz-1-132-13c.fid
Std carbon;blank line7_t
May 1 2011
USER:
SOLVENT: CDCl3
Experiment = s2pul
Pulse length = 7.000 usec
Relaxation delay = 1.000 sec
NA = 136
Solvent = CDCl3
FID PTS1d = 39295
PTS1d = 65536
F1 = 125.702103 MHz
F2 = 499.858551 MHz
SW1 = 30165.91 Hz
AT1 = 1.30 sec
Hz per Pt 1stD = 0.46 Hz
SW2 = 1.00 Hz
Hz per Pt 2ndD = 1.00 Hz
O1 = 13197.3711 Hz
O2 = -0.5000 Hz
LB1 = 2.00 Hz
TP A = -185.16
B = 143.44
C = 0.00

137.501
136.322
135.084
135.014
129.114
128.484
127.305
126.609
125.371
122.621
120.625
119.805
113.385
111.026

77.275
77.019
76.766
71.423
67.212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