Synthesis of Heterocycles via Pd-Ligand Controlled Cyclization of 2-Chloro-*N*-(2-vinyl)aniline: Preparation of Carbazoles, Indoles, Dibenzazepines and Acridines

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Supporting Information

General Reagent Information

All reagents were used as received unless otherwise noted. 1,4-Dioxane was purchased from Aldrich Chemical Company in Sure-Seal bottle. Anhydrous toluene was purchased from J. T. Baker in CYCLE-TAINER® solvent delivery kegs. The solvent was further purified by passing it through two packed columns of neutral alumina under argon. Flash column chromatography was performed using a Biotage SP4 Flash Purification System using KP-Sil flash cartridges. $Pd_2(dba)_3$, $Pd(OAc)_2$ and $Cu(OAc)_2$ were purchased from Sigma-Aldrich and used as received. 2-Bromostyrene 97.0% (Alfa Aesar, used as received). Derivates of 2-bromostyrene (1-bromo-4-methoxy-2-vinylbenzene and 4-bromo-2-methoxy-5-vinylphenol) that not commercially available, were prepared based on literature procedure.[1] Ligands **L2-3, L8** and **L10-11** were purchased from Strem Chemicals, Inc., Ligands **L1, L7** and **L9** were synthesized according to the methods described in literature.[2] Ligands **L4-6** were purchased from Sigma-Aldrich and used as received. All amines were purchased from Alfa Aesar and Sigma-Aldrich and used as reseived, sodium *tert*-butoxide was purchased from Sigma-Aldrich and stored in an inert atmosphere glovebox.

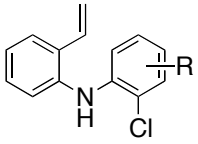
S1. General Experimental Details.

All reactions requiring a dry and inert atmosphere were performed in glassware flame-dried or dried overnight in a 110 °C oven, sealed with septa and flushed with Argon. 1,4-Dioxane was purged with argon before use. Infrared spectra were recorded on a Perkin-Elmer Model 2000 FT-IR. ^1H, ^{19}F and ^{13}C NMR spectra were obtained in $CDCl_3$ at 25 °C on a Bruker AVANCE spectrometer at the following frequencies: 400 MHz (^1H), 100

MHz (^{13}C) and 282 MHz (^{19}F). All ^{1}H NMR experiments are reported in ppm downfield of TMS and were measured relative to the signals for chloroform (7.27 ppm). All ^{13}C NMR spectra were reported in ppm relative to residual chloroform (77 ppm). Gas chromatographic analyses were preformed on Hewlett-Packard 6890 gas chromatography instrument with a FID detector using HP 10m x 0.10 mm capillary column.

General Procedure 1:

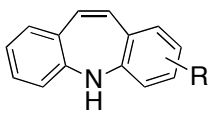
Synthesis of diarylamine intermediates (Table 2)



Generally, 0.025 mmol (13.5 mg) of BrettPhos[2], 0.0075 mmol (6.9 mg) of $Pd_2(dba)_3$, 3.0 mmol (288 mg) of NaO*t*Bu and 1.2 mmol of the appropriate substituted 2-chloroaniline (if solid) were mixed in oven-dried schlenk tube and degassed. Flask was refilled with argon (repeated 3-5 times) and 1.0 mmol (182 mg, 130 μL) of 2-Bromostyrene in degassed dioxane (1 mL) was added under an argon atmosphere (liquid amines were added with 2-bromostyrene in the same manner). The tube was then placed in a preheated oil bath at 110°C, and mixture was stirred until completion of the reaction (followed by GC analysis). After cooled down to room temperature, the solution was quenched with water (5 mL) and diluted with ethyl acetate (10 mL). Organic layer was dried on Na_2SO_4 and filtered. After concentration under reduced pressure, the crude mixture was purified, either by silica gel chromatography, or by Biotage SP4 technique, eluting with hexanes/ethyl acetate mixtures to afford desired intermediate. Products were characterized by analysis of their characteristic IR, MS, and NMR spectra.

General Procedure 2:

A. Synthesis of dibenzazepines from diarylamine intermediates*:*

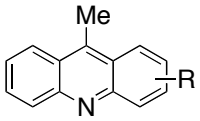


Typically, unless otherwise noted, 0.0225 mmol (8.8 mg) of DavePhos, 0.0075 mmol (6.9 mg) of $Pd_2(dba)_3$, 1.5 mmol (144 mg) of NaO*t*Bu and 1.0 mmol of the appropriate diarylamine intermediate (if solid) were mixed in oven-dried schlenk tube and degassed. Flask was refilled with argon (repeated 3-5 times) and degassed dioxane (1 mL) was added under an argon atmosphere (liquid intermediates were added with dioxane in same manner). The tube was then

placed in a preheated oil bath at 110°C, and mixture was stirred until completion of the reaction (followed by GC analysis). After cooled down to room temperature, the solution was quenched with water (5 mL) and diluted with ethyl acetate (10 mL). Organic layer was separated and dried on Na_2SO_4, then filtered. After concentration under reduced pressure, the crude mixture was purified, either by silica gel chromatography, or by Biotage SP4 technique, eluting with hexanes/ethyl acetate mixtures to afford pure dibenzazepines, as yellow/orange solids. Products were characterized either by direct comparison with authentic samples, obtained by synthetic routes described in the literature,[3] or by analysis of their characteristic IR, MS, and NMR spectra.

General Procedure 3:

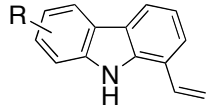
Synthesis of 9-methylacridines (Table 3)



Generally, 0.075 mmol (21.8 mg) of tri-*tert*-butylphosphonium tetrafluoroborate, 0.025 mmol (22.9 mg) of $Pd_2(dba)_3$, 1.5 mmol (144 mg) of NaO*t*Bu and 1.0 mmol of the appropriate diarylamine intermediate (if solid) were mixed in oven-dried schlenk tube and degassed. Flask was refilled with argon (repeated 3-5 times) and degassed toluene (1 mL) was added under an argon atmosphere (liquid intermediates were added with toluene in same manner). Reaction mixture was then placed in a preheated oil bath at 110°C, and mixture was stirred until completion of the reaction (followed by GC analysis). After cooled down to room temperature, the solution was quenched with water (5 mL) and diluted with ethyl acetate (15 mL). Organic layer was separated and dried on Na_2SO_4, then filtered. After concentration under reduced pressure, the crude mixture was purified, either by silica gel chromatography, or by Biotage SP4 technique, eluting with hexanes/ethyl acetate mixtures to afford desired light yellow acridines. Products were characterized by analysis of their characteristic IR, MS, and NMR spectra.

General Procedure 4:

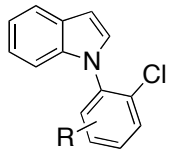
Synthesis of vinyl-9H-carbazoles (Table 3)



Generally, 0.06 mmol (23.9 mg) of racemic-2-di-*t*-butylphosphino-1,1'-binaphthyl, 0.02 mmol (18.3 mg) of $Pd_2(dba)_3$, 1.5 mmol (144 mg) of NaO*t*Bu and 1.0 mmol of the appropriate diarylamine intermediate were mixed in oven-dried schlenk tube and degassed. Tube was refilled with argon (repeated 3-5 times) and degassed dioxane (1 mL) was added under an argon atmosphere. Reaction mixture was then placed in a preheated oil bath at 110°C, and mixture was stirred until completion of the reaction (followed by GC analysis). After cooled down to room temperature, the solution was quenched with water (5 mL) and diluted with ethyl acetate (15 mL). Organic layer was dried on Na_2SO_4 and filtered. After concentration under reduced pressure, the crude mixture was purified, either by silica gel chromatography, or by Biotage SP4 technique, eluting with hexanes/ethyl acetate or hexanes/diethyl ether mixtures to afford desired white carbazole. Products were characterized by analysis of their characteristic IR, MS, and NMR spectra.

General Procedure 5:

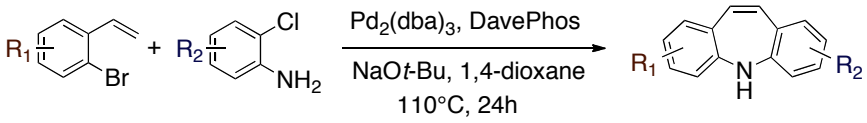
Synthesis of 2-chlorophenyl-1H-indoles (Table 4)



Generally, 0.10 mmol (22.4 mg) of $Pd(OAc)_2$, 1.5 mmol (272.5 mg) of $Cu(OAc)_2$ and 1.0 mmol of the appropriate diarylamine intermediate were mixed in schlenk tube. DMF (3 mL) and acetic acid (1 mL) were added. Reaction mixture was then placed in a preheated oil bath at 110°C, and mixture was stirred until completion of the reaction (followed by GC analysis). After cooled down to room temperature, the solution was quenched with saturated $NaHCO_3$ (5 mL), water (10 mL) and diluted with ethyl acetate (15 mL). Organic layer was dried on Na_2SO_4 and filtered. After concentration under reduced pressure, the crude mixture was purified, either by silica gel chromatography, or by Biotage SP4 technique, eluting with hexanes/ethyl acetate mixtures to afford desired *N*-arylindole. Products were characterized by analysis of their characteristic IR, MS, and NMR spectra.

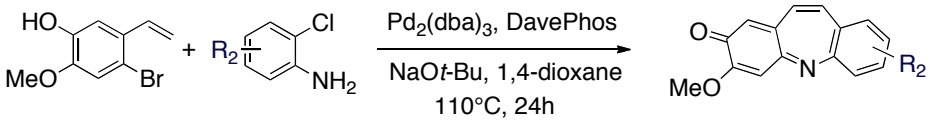
General Procedure 6:

***A. One-pot synthesis of dibenzazepines (Table 1)**:*



Typically, unless otherwise noted, 0.0225 mmol (8.8 mg) of DavePhos, 0.0075 mmol (6.9 mg) of $Pd_2(dba)_3$, 3.0 mmol (288 mg) of NaO*t*Bu and 1.2 mmol of the appropriate substituted 2-chloroaniline (if solid) were mixed in oven-dried schlenk tube and degassed. Flask was refilled with argon (repeated 3-5 times) and 1.0 mmol (182 mg, 130 μL) of 2-Bromostyrene in degassed dioxane (1 mL) was added under an argon atmosphere (liquid amines were added with 2-bromostyrene in same manner). The tube was then placed in a preheated oil bath at 110°C, and mixture was stirred until completion of the reaction (followed by GC analysis).

***B. One-pot synthesis of dibenzazepinones (Table 1)**:*



0.08 mmol (31.4 mg) of DavePhos, 0.025 mmol (22.9 mg) of $Pd_2(dba)_3$, 3.0 mmol (288 mg) of NaO*t*Bu, 1.2 mmol of the appropriate substituted 2-chloroaniline and 1.0 mmol (229 mg) of 4-bromo-2-methoxy-5-vinylphenol were mixed in oven-dried schlenk tube and degassed. Tube was refilled with argon (repeated 3-5 times) and 1 mL of dry 1,4-dioxane was added under an argon atmosphere. The flask was then placed in a preheated oil bath at 120°C, and mixture was stirred until completion of the reaction (followed by GC analysis).

<u>*Continue for A. and B*</u>. After cooled down to room temperature, the solution was quenched with water (5 mL) and diluted with ethyl acetate (10 mL). Organic layer was dried on Na_2SO_4 and filtered. After concentration under reduced pressure, the crude mixture was purified, either by silica gel chromatography, or by Biotage SP4 technique,

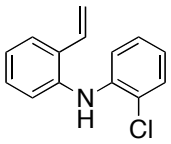
eluting with hexanes/ethyl acetate mixtures to afford pure dibenzazepines or dibenzazepinones, as yellow/orange or red solids respectively. Products were characterized either by direct comparison with authentic samples, obtained by synthetic routes described in the literature,[3] or by analysis of their characteristic IR, MS, and NMR spectra.

General Procedure 7:

Preparation of substituted 2-bromostyrenes:

To a suspension of 13.2g (37 mmol) CH_3PPh_3Br in 50 mL THF (oven-dried and degassed flask) was added a solution of 4.14g (37 mmol) KO*t*-Bu in 50 ml THF in 0°C. The mixture was stirred for 1 hour at 0 °C and to yellow suspension was added an aldehyde (23 mmol) in 20 ml of dry THF under an argon atmosphere. The ice bath was removed and mixture stirred for 20 hours. Saturated ammonium chloride (60 mL) was added and mixture was stirred for additional 10 minutes. Resultant mixture was extracted with Et_2O (100 mL × 3). The combined organic layer was dried (Na_2SO_4) and concentrated. The residue was purified by flash column chromatography (EtOAc/hexanes mixtures) to afford **8** and **9**.

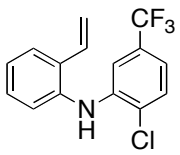
Experimental data for compounds described in Table 2



2-Chloro-N-(2-vinylphenyl)aniline (7)

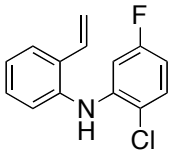
According to *General Procedure 1*, a solution of 1.2 mmol (153.6 mg) 2-chloroaniline, 1.0 mmol (182 mg) of 2-bromostyrene, 1.0 mmol (182 mg) of 2-bromostyrene, 0.025 mol (13.5 mg) of BrettPhos, 0.0075 mol% (6.9 mg) of $Pd_2(dba)_3$ and 3.0 mmol (288 mg) of NaO*t*Bu in 1 mL of 1,4-dioxane was heated at 110°C for 1 hour. The crude was purified using Biotage SP4 (100% hexanes) to provide a pure adduct as colorless oil (203 mg, 91%). **^{1}H NMR (400 MHz, $CDCl_3$)** δ: 7.56-7.58 (d, J = 8.4 Hz, 1H), 7.33-7.36 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.23-7.27 (m, 2H), 7.13-7.17 (m, 1H), 7.05-7.09 (t, J = 8.4 Hz, 1H), 6.85-6.92(dd, J_1 = 17.6 Hz, J_2 = 10.8 Hz, 1H), 6.88-6.90 (d, J = 8.4 Hz, 1H), 6.74-6.78 (t, J = 8.0 Hz, 1H), 5.98 (s, 1H), 5.71-5.76 (d, J = 17.6 Hz, 1H), 5.31-5.34 (d, J = 11.2 Hz, 1H) ppm. **^{13}C NMR (100 MHz, $CDCl_3$)**

δ: 141.35, 138.42, 132.51, 132.31, 129.56, 128.72, 127.49, 126.97, 124.44, 123.21, 120.72, 119.74, 116.40, 115.10 ppm. **IR (KBr disc, cm^{-1})**: 3401, 3064, 1591, 1501, 1455, 1315, 1034, 743. Anal. Calc. for $C_{14}H_{12}ClN$: C, 73.20; H, 5.27. Found: C, 73.47; H, 5.52.



2-chloro-5-(trifluoromethyl)-*N*-(2-vinylphenyl)aniline

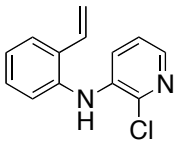
According to *General Procedure 1*, a solution of 1.2 mmol (234 mg) of 2-chloro-5-(trifluoromethyl)aniline, 1.0 mmol (182 mg) of 2-bromostyrene, , 0.025 mol (13.5 mg) of BrettPhos, 0.0075 mol% (6.9 mg) of $Pd_2(dba)_3$ and 3.0 mmol (288 mg) of NaO*t*Bu in 1 mL of 1,4-dioxane was heated at 110°C for 4 hours. The crude was purified using Biotage SP4 (15/85% EtOAc/hexanes mixture) to provide a pure adduct as a light yellow oil (193 mg, 65%). **^{1}H NMR (400 MHz, $CDCl_3$)** δ: 7.58-7.60 (d, J = 7.6 Hz, 1H), 7.281-7.323 (t, J = 7.6.0 Hz, 1H), 7.19-7.25 (m 2H), 7.00 (s, 2H), 6.95-6.97 (dd, J_1 = 8.0 J_2 = 1.6 Hz, 1H), 6.77-6.84 (dd, J_1 = 17.6, J_2 = 11.2, 1H), 6.10 (s, 1H), 5.71-5.76 (d, J = 18.8, 1H), 5.30-5.33 (d, J = 12, 1H) ppm. **^{13}C NMR (100 MHz, $CDCl_3$)** Due to the complexity of the spectra all the peaks are listing without take into consideration C-F couplings, δ: 142.04, 137.05, 133.18, 132.22, 130.21, 129.84, 129.00, 127.21, 125.67, 125.14, 124.23, 123.30, 122.43, 116.86, 115.67, 115.63, 110.82, 110.79 ppm. **^{19}F NMR (282 MHz, $CDCl_3$)** δ: -113.654. **IR (KBr disc, cm^{-1})**: 3410, 1587, 1511, 1436, 1334, 1274, 1170, 1127, 1080, 767. Anal. Calc. for $C_{14}H_{14}ClN_3$: C, 60.52; H, 3.72; N, 4.70. Found: C, 60.76; H, 3.62; N, 4.64.



2-Chloro-5-fluoro-N-(2-vinylphenyl)aniline

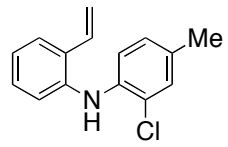
Following *General Procedure 1*, a solution of 1.2 mmol (175.2 mg) of 2-chloro-5-fluoroaniline, 1.0 mmol (182 mg, 130 μL) of 2-bromostyrene, 0.025 mol (13.5 mg) of BrettPhos, 0.0075 mol% (6.9 mg) of $Pd_2(dba)_3$ and 3.0 mmol (288 mg) of NaO*t*Bu in 1 mL of 1,4-dioxane was heated at 110°C for 4 hours. The crude was purified using Biotage SP4 (5/95% EtOAc/hexanes mixture) to provide a pure adduct as light yellow oil (166 mg, 67%). **^{1}H NMR (400 MHz, $CDCl_3$)** δ: 7.56-7.58 (d, J = 7.6 Hz, 1H), 7.17-7.30 (m, 4H), 6.79-6.86 (dd, J_1 = 17.6 Hz, J_2 = 11.2 Hz, 1H), 6.40-6.45 (m, 2H), 6.02 (s, 1H), 5.66-5.75 (d, J = 18.8 Hz, 1H) ppm. **^{13}C NMR (100 MHz, $CDCl_3$) δ**: 162.43 (d, J = 243 Hz, 1C), 143.01 (d, J = 11 Hz, 1C), 137.32, 131.17, 132.21, 130.12 (d,

J = 10 Hz, 1C), 128.90, 127.00, 125.54, 124.54, 116.69, 114.88, 105.96 (d, *J* = 23 Hz, 1C), 101.45 (d, *J* = 28 Hz, 1C) ppm. **^{19}F NMR (282 MHz)** δ: -63.218. **IR (KBr disc, cm^{-1})**: 3404, 1611, 1507, 1438, 1303, 1164, 768. Anal. Calc. for $C_{14}H_{11}ClFN$: C, 67.89; H, 4.48; N. Found: C, 68.00; H, 4.46.



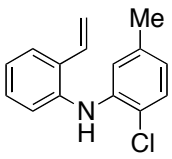
2-chloro-*N*-(2-vinylphenyl)pyridin-3-amine

According to *General Procedure 1*, a solution of 1.2 mmol (194.4 mg) of 2-amino-3-chloropyridine, 1.0 mmol (182 mg) of 2-bromostyrene, 0.025 mol (13.5 mg) of BrettPhos, 0.0075 mol% (6.9 mg) of $Pd_2(dba)_3$ and 3.0 mmol (288 mg) of NaO*t*Bu in 1 mL of 1,4-dioxane was heated at 110°C for 4 hours. The crude was purified using Biotage SP4 (100% hexanes) to provide a pure adduct as light yellow oil (209 mg, 91%). **^{1}H NMR (400 MHz, $CDCl_3$)** δ: 7.79 (m, 1H), 7.56-7.58 (d, *J* = 8.0, 1H), 7.23-7.28 (m, 1H), 7.16-7.20 (m, 2H), 6.97-7.03 (m, 2H), 6.75-6.83 (dd, J_1 = 17.6, J_2 = 11.2 Hz, 2H), 5.98 (s, 1H), 5.70-5.74 (d, *J* = 17.2 Hz, 1H), 5.26-5.29 (d, *J* = 10.4 Hz, 1H) ppm. **^{13}C NMR (100 MHz, $CDCl_3$)** δ: 138.74, 138.68, 137.86, 136.89, 133.21, 132.14, 128.93, 127.07, 125.67, 124.27, 123.16, 120.90, 116.86 ppm. **IR (KBr disc, cm^{-1})**: 3393, 1581, 153, 1479, 1451, 1318, 1056, 767. Anal. Calc. for $C_{13}H_{11}ClN$: C, 67.68; H, 4.81; N, 12.14. Found: C, 67.62; H, 4.75.



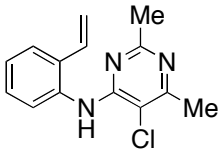
2-Chloro-4-methyl-*N*-(2-vinylphenyl)aniline

Following *General Procedure 1*, a solution of 1.2 mmol (169.2 mg) of 2-chloro-4-methylaniline, 1.0 mmol (182 mg) of 2-bromostyrene, 0.025 mol (13.5 mg) of BrettPhos, 0.0075 mmol (6.9 mg) of $Pd_2(dba)_3$ and 3.0 mmol (288 mg) of NaO*t*Bu in 1 mL of 1,4-dioxane was heated at 110°C for 4 hours. The crude was purified using Biotage SP4 (100% hexanes) to provide a pure adduct as colorless oil (240 mg, 99%). **^{1}H NMR (400 MHz, $CDCl_3$)** δ: 7.52-7.54 (d, *J* = 7.6 Hz, 1H), 7.18-7.26 (m, 3H), 7.05-7.11 (m, 1H), 6.84-6.92 (m, 3H), 5.83 (s, 1H), 5.70-5.75 (dd, J_1 = 17.6, J_2 = 1.6 Hz, 1H), 5.31-5.33 (dd, J_1 = 11.2, J_2 = 1.2 Hz, 1H), 2.26 (s, 3H) ppm. **^{13}C NMR (100 MHz, $CDCl_3$)** δ: 139.15, 138.59, 132.61, 131.46, 129.95, 128.68, 128.09, 127.05, 123.68, 121.93, 121.18, 116.34, 115.98, 20.38 ppm. **IR (KBr disc, cm^{-1})**: 3406, 1612, 1600, 1513, 1457, 1312, 1049, 995, 914, 810, 761. Anal. Calc. for $C_{15}H_{14}ClN$: C, 73.92; H, 5.79. Found: C, 73.99; H, 5.77.



2-Chloro-5-methyl-*N*-(2-vinylphenyl)aniline (Table 2)

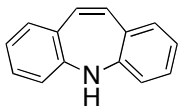
Following *General Procedure 1*, a solution of 1.2 mmol (169.2 mg) of 2-chloro-5-methylaniline, 1.0 mmol (182 mg) of 2-bromostyrene, 0.025 mol (13.5 mg) of BrettPhos, 0.0075 mol% (6.9 mg) of $Pd_2(dba)_3$ and 3.0 mmol (288 mg) of NaO*t*Bu in 1 mL of 1,4-dioxane was heated at 110°C for 4 hours. The crude was purified using Biotage SP4 (2/98% EtOAc/hexanes mixture) to provide a pure adduct as white powder (177 mg, 73%), mp. 35-36 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ: 7.55-7.57 (d, J = 8.0 Hz, 1H), 7.26-7.27 (d, J = 3.6 Hz, 2H), 7.20-7.22 (d, J = 8.0 Hz, 1H), 7.10-7.16 (m, 1H), 6.84-6.91 (dd, J_1 = 17.6, J_2 = 11.2 Hz, 1H), 6.71 (s, 1H), 6.56-6.58 (d, J = 8.0 Hz, 1H), 5.91 (s, 1H), 5.70-5.75 (d, J = 17.6 Hz, 1H), 5.30-5.33 (d, J = 12, 1H), 2.18 (s, 3H) ppm. **^{13}C NMR (100 MHz, $CDCl_3$)** δ: 140.87, 138.57, 137.54, 132.56, 132.19, 129.18, 128.70, 126.97, 124.26, 123.13, 120.70, 117.87, 116.34, 115.71, 21.35 ppm. **IR (KBr disc, cm^{-1})**: 3341, 1420, 1384, 818, 748. Anal. Calc. for $C_{15}H_{14}ClN$: C, 73.92; H, 5.79; N, 5.75. Found: C, 74.09; H, 5.73; N, 5.79.



4-Amino-5-chloro-2,6-dimethyl-*N*-(2-vinylphenyl)pyrimidine

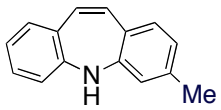
According to *General Procedure 1*, a solution of 1.2 mmol (188.8 mg) of 4-amino-5-chloro-2,6-dimethylpyrimidine, 1.0 mmol (182 mg) of 2-bromostyrene, , 0.025 mol (13.5 mg) of BrettPhos, 0.0075 mol% (6.9 mg) of $Pd_2(dba)_3$ and 3.0 mmol (288 mg) of NaO*t*Bu in 1 mL of 1,4-dioxane was heated at 110°C for 4 hours. The crude was purified using Biotage SP4 (15/85% EtOAc/hexanes mixture) to provide a pure adduct as white solid (142 mg, 55%), mp. 69-70 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ: 7.98-8.00 (d, J = 10.0 Hz, 1H), 7.43-7.45 (d, J = 10.0 Hz, 1H), 7.30-7.31 (t, J = 5.0 Hz, 1H), 7.11-7.15 (m, 2H), 6.80-6.85 (dd, J_1 = 19.0 Hz, J_2 = 12.0 Hz, 1H), 5.68-5.72 (d, J = 16.0 Hz, 1H), 5.39-5.41 (d, J = 8.0 Hz, 1H), 2.49 (s, 6H) ppm**. ^{13}C NMR (100 MHz, $CDCl_3$)** δ: 164.46, 161.47, 155.51, 135.12, 132.28, 130.94, 128.30, 127.08, 124.86, 123.43, 118.20, 111.20, 25.66, 22.13 ppm. **IR (KBr disc, cm^{-1})**: 3191, 1564, 1490, 1416, 1057, 769. Anal. Calc. for $C_{14}H_{14}ClN_3$: C, 64.74; H, 5.43. Found: C, 64.96; H, 5.59.

Experimental data for compounds described in Table 1



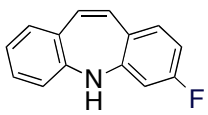
5*H*-Dibenz[*b,f*]azepine (1)

According to *General Procedure 1A*, a solution of 1.2 mmol (153.6 mg) 2-chloroaniline, 1.0 mmol (182 mg) of 2-bromostyrene, 2.25 mmol (9.8 mg) of DavePhos, 0.0075 mmol (6.9 mg) of $Pd_2(dba)_3$ and 3.0 mmol (288 mg) of NaO*t*Bu in 1 mL of 1,4-dioxane was heated at 110°C for 6 hours. The crude was purified using Biotage SP4 (100% hexanes) to provide a pure adduct as yellow powder (193 mg, 99%), mp. 197-199 °C (lit.[3b] m.p. 195-196 °C). **^{1}H NMR (400 MHz, $CDCl_3$)** δ: 6.85-7.7.01 (dd, J_1 = 9.2 Hz, J_2 = 2.0 Hz, 1H), 7.005-7.028 (dd, J_1 = 9.2 Hz, J_2 = 2.4 Hz, 1H), 6.79-6.85 (m, 4H), 6.46-6.48 (d, J = 8 Hz, 2H), 6.30 (s, 2H), 4.82 (s, 1H), ppm. ^{13}C NMR (100 MHz, $CDCl_3$) δ: 148.39, 132.16, 130.53, 129.77, 129.49, 123.06, 119.36 ppm. **IR (KBr disc, cm^{-1})**: 3361, 1580, 1434, 933, 756.



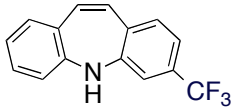
3-Methyl-*5H*-dibenz[*b,f*]azepine

According to *General Procedure 2A*, a solution of 1.2 mmol (169.2 mg) of 2-chloro-5-methylaniline, 1.0 mmol (182 mg) of 2-bromostyrene, 2.25 mmol (9.8 mg) of DavePhos, 0.0075 mmol (6.9 mg) of $Pd_2(dba)_3$ and 3.0 mmol (288 mg) of NaO*t*Bu in 1 mL of 1,4-dioxane was heated at 110°C for 6 hours. The crude was purified using Biotage SP4 (2/98% EtOAc/hexanes mixture) to provide a pure adduct as orange crystal needles (188 mg, 91%), mp. 219-221 °C (***lit.***[3b] m.p. 213-215 °C). **^{1}H NMR (400 MHz, $CDCl_3$)** δ: 6.96-7.01 (dt, J_1 = 8.6 Hz, J_2 = 2.0 Hz, 1H), 6.77-6.83 (m, 2H), 6.71-6.73 (d, J = 7.6 Hz, 1H), 6.60-6.62 (d, J = 8.4 Hz, 1H), 6.44-6.46 (d, J = 8.0 Hz, 1H), 6.30 (s, 1H), 6.21-6.24(d, J = 11.6 Hz, 1H), 6.25-6.28(d, J = 11.6 Hz, 1H), 4.85 (s, 1H), 2.17 (s, 3H) ppm. **^{13}C NMR (100 MHz, $CDCl_3$)** δ: 148.24, 139.71, 132.03, 131.15, 130.49, 130.44, 129.85, 129.30, 126.88, 123.70, 122.96, 120.12, 119.25, 20.89 ppm. **IR (KBr disc, cm^{-1})**: 3345, 1384, 819, 748.



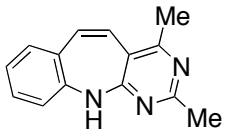
3-Fluoro-*5H*-dibenz[*b,f*]azepine

According to *General Procedure 2A*, a solution of 1.2 mmol (175.2 mg) of 2-chloro-5-fluoroaniline, 1.0 mmol (182 mg) of 2-bromostyrene, 2.25 mmol (9.8 mg) of DavePhos, 0.0075 mmol (6.9 mg) of $Pd_2(dba)_3$ and 3.0 mmol (288 mg) of NaO*t*Bu in 1 mL of 1,4-dioxane was heated at 110°C for 24 hours. The crude was purified using Biotage SP4 (5/95% EtOAc/hexanes mixture) to provide a pure adduct as yellow crystal plates (193 mg, 92%), mp. 186-188 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ: 6.99-7.02 (m, 1H), 6.81-6.82 (d, *J* = 4.0 Hz, 2H), 6.74-6.77 (t, *J* = 8.0 Hz, 1H), 6.43-6.50 (m, 2H), 6.02-6.21 (m, 3H), 4.89 (s 1H) ppm. **^{13}C NMR (100 MHz, $CDCl_3$)** δ: 165.21, 162.74, 150.00-150.09 (*J* = 9 Hz, 1C), 147.36, 131.77-131.86 (*J* = 9), 131.18, 130.56, 129.64, 129.53, 125.78-125.82 (*J* = 4 Hz, 1C), 123.44, 119.40, 109.28-109.49 (*J* = 21, 1C), 106.45-106.69 (J = 24, 1C) ppm. **^{19}F NMR (282 MHz, $CDCl_3$)** δ: -114.249. **IR (KBr disc, cm^{-1})**: 3365, 1590, 1524, 1423, 1271, 851, 750.



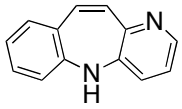
3-(Trifluoromethyl)-5*H*-dibenz[*b,f*]azepine

According to *General Procedure 1*, a solution of 1.2 mmol (243.4 mg) of 2-chloro-5-(trifluoromethyl)aniline, 1.0 mmol (182 mg) of 2-bromostyrene, 2.25 mmol (9.8 mg) of DavePhos, 0.0075 mmol (6.9 mg) of $Pd_2(dba)_3$ and 3.0 mmol (288 mg) of NaO*t*Bu in 1 mL of 1,4-dioxane was heated at 110°C for 24 hours. The crude was purified using Biotage SP4 (5/95% EtOAc/hexanes mixture) to provide a pure adduct as orange plates (232 mg, 89%), mp. 177-179 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ: 7.02, 7.07 (m, 2H), 6.88-6.90 (d, *J* = 7.6 Hz, 1H), 6.81-6.86 (m, 2H), 6.69 (s, 1H), 6.47-6.49 (d, *J* = 8.0 Hz, 1H), 6.33-6.36 (d, *J* = 12.0 Hz, 1H), 6.24-6.27 (d, *J* = 12.0 Hz, 1H), 4.99 (s, 1H) ppm. **^{13}C NMR (100 MHz, $CDCl_3$)** Due to the complexity of the spectra all the peaks are listing without take into consideration C-F couplings, δ: 148.67, 147.74, 134.26, 133.29, 131.72, 131.39, 131.07, 130.89, 130.82, 130.75, 130.06, 129.33, 125.22, 123.55, 122.52, 119.81, 119.81, 119.77, 119.73, 119.54, 115.93, 115.89, 115.85 ppm. **^{19}F NMR (282 MHz, $CDCl_3$)** δ: -63.461. **IR (KBr disc, cm^{-1})**: 3333, 1583, 1424, 1335, 1169, 1122, 1078, 844, 757. Anal. Calc. for $C_{15}H_{10}F_3N$: C, 68.96; H, 3.86. Found: C, 68.69; H, 3.81.



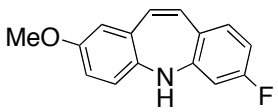
2,4-Dimethyl-11*H*-benzo[*b*]pyrimido[5,4-*f*]azepine

According to *General Procedure 2B*, a solution of 1.2 mmol (188.8 mg) of 4-amino-5-chloro-2,6-dimethylpyrimidine, 1.0 mmol (182 mg) of 2-bromostyrene, 8 mol% (31.4 mg) of DavePhos, 2.5 mol% (22.9 mg) of $Pd_2(dba)_3$ and 3.0 mmol (288 mg) of NaO*t*Bu in 2 mL of dioxane was heated at 120°C for 24 hours. The crude was purified using Biotage SP4 (25/75% EtOAc/hexanes mixture) to provide a pure adduct as orange crystals (162 mg, 73%), mp. 138-140 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ: 6.93-6.97 (t, *J* = 9.2 Hz, 1H), 6.75-6.78 (t, *J* = 7.6 Hz, 1H), 6.71-6.75 (t, *J* = 6.4 Hz, 1H), 6.33-6.35 (d, *J* = 8.0 Hz, 1H), 6.06-6.09 (d, *J* = 12.0 Hz, 1H), 6.95-6.98 (d, *J* = 12.0 Hz, 1H), 5.85 (s, 1H), 2.35 (s, 3H), 2.21 (s, 3H) ppm. **^{13}C NMR (100 MHz, $CDCl_3$)** δ: 166.36, 166.28, 164.14, 144.10, 133.01, 131.31, 130.20, 128.14, 125.31, 123.85, 119.65, 115.00, 25.17, 21.90 ppm. **IR (KBr disc, cm^{-1})**: 3254, 1580, 1543, 1485, 1422, 1397, 1256, 804, 752.



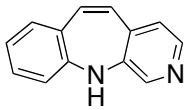
11*H*-Benzo[*b*]pyrido[3,2-*f*]azepine

Following *General Procedure 2A*, a solution of 1.2 mmol (194.4 mg) of 3-amino-2-chloropyridine, 1.0 mmol (182 mg) of 2-bromostyrene, 2.25 mmol (9.8 mg) of DavePhos, 0.0075 mmol (6.9 mg) of $Pd_2(dba)_3$ and 3.0 mmol (288 mg) of NaO*t*Bu in 1 mL of 1,4-dioxane was heated at 110°C for 24 hours. The crude was purified using Biotage SP4 (100% hexanes) to provide a pure adduct as orange solid (172 mg, 89%), mp. 182-185 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ: 8.02-8.04 (dd, J_1= 4.8 Hz, J_2= 1.6 Hz, 1H), 7.00-7.04 (dt, J_1= 8.6 Hz, J_2= 2.0 Hz, 1H), 6.81-6.92 (m, 3H), 6.71-6.74 (d, *J* = 8.0 Hz, 1H), 6.41-6.48 (m, 3H), 4.75 (s, 1H) ppm. **^{13}C NMR (100 MHz, $CDCl_3$)** δ: 149.26, 147.88, 144.61, 143.66, 135.03, 133.31, 131.19, 130.04, 129.19, 125.88, 123.58, 123.52, 119.28 ppm. **IR (KBr disc, cm^{-1})**: 3266, 1611, 1448, 1437, 1390, 1284, 1110, 802, 762, 749. Anal. Calc. for $C_{13}H_{10}N_2$: C, 80.39; H, 5.19. Found: C, 80.01; H, 5.29.



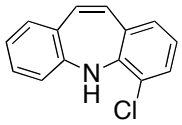
7-Fluoro-2-methoxy-5*H*-dibenzo[*b*,*f*]azepine

According to *General Procedure 2A*, a solution of 1.2 mmol (175.2 mg) of 2-chloro-5-fluoroaniline, 1.0 mmol (212 mg) of 2-bromo-4-methoxy-1-vinylbenzene, 2.25 mmol (9.8 mg) of DavePhos, 0.0075 mmol (6.9 mg) of $Pd_2(dba)_3$ and 3.0 mmol (288 mg) of NaO*t*Bu in 1 mL of 1,4-dioxane was heated at 110°C for 24 hours. The crude was purified using Biotage SP4 (10/90% EtOAc/hexanes mixture) to provide a pure adduct as orange solid (197 mg, 82%), mp. 145-147 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ: 6.77-6.81 (dd, J_1 = 14.8, J_2 = 6.4 Hz, 1H), 6.57-6.60 (dd, J_1 = 8.4, J_2 = 2.8, 1H), 6.45-6.52 (dt, J_1 = 8.4 Hz, J_2 = 2.4, 1H), 6.42-6.43 (d, J = 4.8 Hz, 1H), 6.41-6.42 (d, J = 5.6 Hz, 1H), 6.22-6.32 (m, 3H), 4.81 (s, 1H), 3.69 (s, 3H), ppm. **^{13}C NMR (100 MHz, $CDCl_3$)** Due to the complexity of the spectra all the peaks are listing without take into consideration C-F couplings, δ: 165.21, 162.75, 156.04, 150.81, 150.72, 140.44, 131.91, 131.87, 131.81, 130.91, 130.83, 130.81, 125.72, 125.69, 120.36, 115.55, 114.36, 109.38, 109.17, 106.57, 106.33, 55.54. ppm. **^{19}F NMR (282 MHz, $CDCl_3$)** δ: -114.053. **IR (KBr disc, cm^{-1})**: 3361, 1613, 1519, 1396, 1270, 1220, 1145, 1037, 811. Anal. Calc. for $C_{15}H_{12}FNO$: C, 74.67; H, 5.01.Found: C, 74.45; H, 5.04.



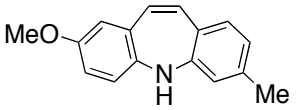
11*H*-Benzo[*b*]pyrido[4,3-*f*]azepine

According to *General Procedure 2A*, a solution of 1.2 mmol (194.4 mg) of 3-amino-4-chloropyridine, 1.0 mmol (182 mg) of 2-bromostyrene, 2.25 mmol (9.8 mg) of DavePhos, 0.0075 mmol (6.9 mg) of $Pd_2(dba)_3$ and 3.0 mmol (288 mg) of NaO*t*Bu in 1 mL of 1,4-dioxane was heated at 110°C for 24 hours. The crude was purified using Biotage SP4 (100% hexanes) to provide a pure adduct as orange solid (187 mg, 97%), mp. 126-127 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ: 7.97-7.99 (d, J = 4.8 Hz, 1H), 7.75 (s, 1H), 6.99-7.06 (m, 1H), 6.78-6.82 (m, 2H), 6.64-6.66 (d, J = 4.8 Hz, 1H), 6.46-6.48(d, J = 8.0 Hz, 1H), 6.36-6.39 (d, J = 11.6, 1H), 6.09-6.12 (d, J = 12, 1H), 5.07 (s, 1H) ppm. **^{13}C NMR (100 MHz, $CDCl_3$)** δ: 148.38, 144.75, 144.01, 140.02, 137.00, 136.88, 131.43, 129.57, 128.90, 123.52, 123.38, 123.43, 119.60 ppm. **IR (KBr disc, cm^{-1})**: 3281, 3217, 3029, 1593, 1474, 1307, 1282, 839, 760. Anal. Calc. for $C_{14}H_{10}ClN$: C, 73.85; H, 4.43; N, 6.15. Found: C, 73.57; H, 4.56; N, 5.95.



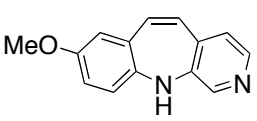
4-Chloro-5*H*-dibenzo[*b*,*f*]azepine

According to *General Procedure 2A*, a solution of 1.2 mmol (194.4 mg) of 2,6-dichloroaniline, 1.0 mmol (182 mg) of 2-bromostyrene, 2.25 mmol (9.8 mg) of DavePhos, 0.0075 mmol (6.9 mg) of $Pd_2(dba)_3$ and 3.0 mmol (288 mg) of NaO*t*Bu in 1 mL of 1,4-dioxane was heated at 110°C for 24 hours. The crude was purified using Biotage SP4 (100% hexanes) to provide a pure adduct as orange solid (181 mg, 80%), mp. 56-57 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ: 7.14-7.16 (dd, J_1 = 7.2 Hz, J_2= 2.0 Hz 1H), 7.07-7.12 (m, 1H), 6.86-6.91 (m, 2H), 6.73-6.78 (m, 2H), 6.65-6.67 (d, J = 8.0 Hz, 1H), 6.38-6.41(d, J = 11.6 Hz, 1H), 6.31-6.34(d, J = 11.6 Hz, 1H), 5.82 (s, 1H), ppm. **^{13}C NMR (100 MHz, $CDCl_3$)** δ: 147.50, 144.24, 132.97, 131.60, 131.52, 130.41, 129.81, 129.76, 129.13, 129.05, 123.58, 123.41, 123.16, 120.61 ppm. **IR (KBr disc, cm^{-1})**: 3353, 3049, 3025, 1610, 1457, 1432, 1263, 1138, 924, 801, 702. Anal. Calc. for $C_{14}H_{10}ClN$: C, 73.85; H, 4.43; N, 6.15. Found: C, 73.57; H, 4.56; N, 5.95.



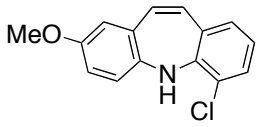
2-Methoxy-7-methyl-5*H*-dibenzo[*b*,*f*]azepine

According to *General Procedure 2A*, a solution of 1.2 mmol (169.2 mg) of 2-chloro-5-methylaniline, 1.0 mmol (212 mg) of 2-bromo-4-methoxy-1-vinylbenzene, 2.25 mmol (9.8 mg) of DavePhos, 0.0075 mmol (6.9 mg) of $Pd_2(dba)_3$ and 3.0 mmol (288 mg) of NaO*t*Bu in 1 mL of 1,4-dioxane was heated at 110°C for 24 hours. The crude was purified using Biotage SP4 (35/65% EtOAc/hexanes mixture) to provide a pure adduct as yellow crystalline powder (218 mg, 92%), mp. 187-189 °C**. ^{1}H NMR (400 MHz, $CDCl_3$)** δ: 6.75-6.77 (d, J = 8.0 Hz, 1H), 6.62-6.64 (d, J = 7.6 Hz, 1H), 6.56-6.59 (dd, J_1 = 8.4 Hz, J_2 = 2.4 Hz, 1H), 6.42-6.44 (m, 2H), 6.34 (s, 2H), 4.79 (s, 1H), 3.69 (s, 3H), 2.19 (s, 3H) ppm. **^{13}C NMR (100 MHz, $CDCl_3$)** δ: 155.76, 148.91, 141.31, 139.75, 132.70, 131.09, 130.73, 130.47, 126.79, 123.59, 120.14, 120.02, 115.36, 114.26, 55.55, 20.93 ppm. **IR (KBr disc, cm^{-1})**: 3357, 1502, 1271, 1037, 860, 839, 807. Anal. Calc. for $C_{16}H_{15}NO$: C, 80.98; H, 6.37. Found: C, 80.64; H, 6.43.



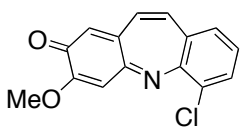
8-Methoxy-11*H*-benzo[*b*]pyrido[4,3-*f*]azepine

According to *General Procedure 2A*, a solution of 1.2 mmol (194.4 mg) of 3-amino-4-chloropyridine, 1.0 mmol (212 mg) of 2-bromo-4-methoxy-1-vinylbenzene, 2.25 mmol (9.8 mg) of DavePhos, 0.0075 mmol (6.9 mg) of $Pd_2(dba)_3$ and 3.0 mmol (288 mg) of NaO*t*Bu in 1 mL of 1,4-dioxane was heated at 110°C for 24 hours. The crude was purified using Biotage SP4 (60/40% EtOAc/hexanes mixture) to provide a pure adduct as orange viscose oil (175 mg, 94%). **^{1}H NMR (400 MHz, $CDCl_3$)** δ: 8.02-8.03 (d, J = 4.8 Hz, 1H), 7.82 (s, 1H), 6.71-6.72 (d, J = 4.8, 2H), 6.62-6.65 (dd, J_1 = 11.2, J_2 = 2.8, 1H), 6.43-6.49 (m, 3H), 6.23-6.26 (d, J = 11.6 Hz, 1H), 4.91 (s, 1H), 3.71 (s, 3H) ppm. **^{13}C NMR (100 MHz, $CDCl_3$)** δ: 155.98, 144.58, 141.27, 140.08, 136.68, 136.47, 130.27, 130.12, 123.51, 120.54, 116.43, 115.21, 55.58 ppm. **IR (KBr disc, cm^{-1})**: 3278, 3208, 1584, 1504, 1477, 1400, 1271, 1241, 1041, 840.



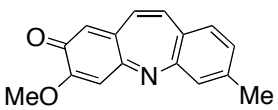
6-Chloro-2-methoxy-5*H*-dibenzo[*b*,*f*]azepine

According to *General Procedure 2A*, a solution of 1.2 mmol (194.4 mg) of 2,6-dichloroaniline, 1.0 mmol (212 mg) of 2-bromo-4-methoxy-1-vinylbenzene, 2.25 mmol (9.8 mg) of DavePhos, 0.0075 mmol (6.9 mg) of $Pd_2(dba)_3$ and 3.0 mmol (288 mg) of NaO*t*Bu in 1 mL of 1,4-dioxane was heated at 110°C for 24 hours. The crude was purified using Biotage SP4 (10/90% EtOAc/hexanes mixture) to provide a pure adduct as yellow twinkle powder (226 mg, 88%), mp. 98-100 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ: 7.13-7.16 (d, J = 12.0 Hz, 1H), 6.72-6.80 (m, 2H), 6.60-6.66 (m, 2H), 6.46-6.48 (d, J = 2.4 Hz, 1H), 6.39 (s, 2H), 5.70 (s, 1H) ppm. **^{13}C NMR (100 MHz, $CDCl_3$)** δ: 156.12, 144.86, 140.46, 132.54, 132.18, 131.36, 130.98, 129.09, 129.02, 123.38, 122.97, 121.49, 115.32, 114.67 ppm. **IR (KBr disc, cm^{-1})**: 3359, 1455, 1418, 1384, 1255, 1038, 796, 711. Anal. Calc. for $C_{15}H_{12}ClNO$: C, 69.91; H, 4.69; Cl, 13.76. Found: C, 69.78; H, 4.59.



6-chloro-3-methoxy-2*H*-dibenzo[*b*,*f*]azepin-2-one

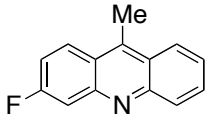
According to *General Procedure 2B*, a solution of 1.2 mmol (194.4 mg) of 2,6-dichloroaniline, 1.0 mmol (228 mg) of 4-bromo-2-methoxy-5-vinylphenol, 2.25 mmol (9.8 mg) of DavePhos, 0.0075 mmol (6.9 mg) of $Pd_2(dba)_3$ and 3.0 mmol (288 mg) of NaO*t*Bu in 1 mL of 1,4-dioxane was heated at 120°C for 24 hours. The crude was purified using Biotage SP4 (60/40% EtOAc/hexanes mixture) to provide a pure adduct as red powder (177 mg, 65%), mp. 157-159 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ: 7.74-7.79 (dd, J_1 = 6.4 Hz, J_2 = 2.8 Hz, 1H), 7.40-7.7.45 (m, 2H), 7.05-7.08 (d, J = 12 Hz, 1H), 7.00 (s, 1H), 6.92-6.95 (d, J = 12 Hz, 1H), 6.72(s, 1H), 4.00 (s, 3H), ppm**. ^{13}C NMR (100 MHz, $CDCl_3$)** δ: 180.01, 157.91, 154.54, 142.05, 140.01, 138.11, 135.96, 133.38, 132.16, 131.70, 131.16, 130.76, 126.46, 115.16, 56.34. **IR (KBr disc, cm^{-1})**: 2964, 2920, 2848, 1629, 1609, 1589, 1468, 1237, 1209, 1162, 882. Anal. Calc. for $C_{15}H_{10}ClNO_2$: C, 66.31; H, 3.71. Found: C, 65.96; H, 3.82.



6-chloro-3-methoxy-2*H*-dibenzo[*b*,*f*]azepin-2-one

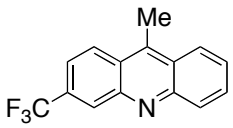
According to *General Procedure 2B*, a solution of 1.2 mmol (169.2 mg) of 2-chloro-5-methylaniline, 1.0 mmol (228 mg) of 4-bromo-2-methoxy-5-vinylphenol, 2.25 mmol (9.8 mg) of DavePhos, 0.0075 mmol (6.9 mg) of $Pd_2(dba)_3$ and 3.0 mmol (288 mg) of NaO*t*Bu in 1 mL of 1,4-dioxane was heated at 120°C for 24 hours. The crude was purified using Biotage SP4 (30/70% EtOAc/hexanes mixture) to provide a pure adduct as red powder (210 mg, 83%), mp. 141-143 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ: 7.79 (s, 1H), 7.45-7.47 (d, J = 8 Hz, 1H), 7.34-7.36 (dd, J_1 = 9.6 Hz, J_2 = 1.6 Hz, 1H), 7.08-7.11 (d, J = 12 Hz, 1H), 6.91 (s, 1H), 6.89-6.91 (d, J = 10.4 Hz, 1H), 6.70 (s, 1H), 3.96 (s, 3H), 2.2.49 (s, 3H) ppm. **^{13}C NMR (100 MHz, $CDCl_3$)** δ: 179.83, 157.60, 154.48, 146.26, 141.42, 138.91, 136.59, 136.36, 132.22, 131.98, 130.77, 129.45, 125.69, 115.81, 56.13, 21.24 ppm. **IR (KBr disc, cm^{-1})**: 3402, 2361, 2338, 1591, 1496, 1457, 1315, 1049, 1034, 743.

Experimental data for acridines described in Table 3



3-Fluoro-9-methylacridine

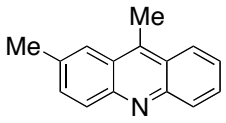
According to *General Procedure 5*, a solution of 0.10 mmol (29 mg) of tri-*tert*-butylphosphonium tetrafluoroborate, 0.025 mmol (22.9 mg) of $Pd_2(dba)_3$, 1.5 mmol (144 mg) of NaO*t*Bu and 1.0 mmol (247 mg) of 2-chloro-5-fluoro-*N*-(2-vinylphenyl)aniline (Table 1) in 1 mL of dry toluene was heated at 100°C for 24 hours. The crude was purified using Biotage SP4 (15/85% diethyl ether/hexanes mixture) to provide a pure adduct as yellow solid (165 mg, 78%), m.p 132-133 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ: 8.16-8.19 (m, 2H), 8.12-8.14 (d, J = 8.4 Hz, 1H), 7.17-7.76 (m, 2H), 7.48-7.52 (t, J = 6.4 Hz, 1H), 7.30-7.33 (dt, J_1 = 8.0 Hz, J_2 = 2.8 Hz, 1H), 3.05 (s, 3H) ppm. **^{13}C NMR (100 MHz, $CDCl_3$)** Due to the complexity of the spectra all the peaks are listing without take into consideration C-F couplings, δ: 164.46, 161.95, 149.30, 149.17, 149.08, 142.87, 130.32, 129.88, 127.21, 125.37, 125.05, 124.62, 122.91, 117.35, 117.08, 112.26, 112.07, 13.89 ppm. **^{19}F NMR (282 MHz)** δ: -109.15. **IR (KBr disc, cm^{-1})**: 1618, 1569, 1528, 1459, 1439, 1274, 1154, 977, 850, 746. Anal. Calc. for $C_{14}H_{10}FN$: C, 79.60; H, 4.77. Found: C, 79.44; H, 5.01.



9-Methy-3-(trifluoromethyl)lacridine

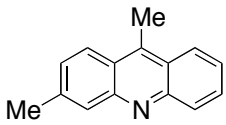
According to *General Procedure 5*, a solution of 0.10 mmol (29 mg) of tri-*tert*-butylphosphonium tetrafluoroborate, 0.025 mmol (22.9 mg) of $Pd_2(dba)_3$, 1.5 mmol (144 mg) of NaO*t*Bu and 1.0 mmol (261 mg) of 2-chloro-5-(trifluoromethyl)-*N*-(2-vinylphenyl)aniline (Table 1) in 1 mL of dry toluene was heated at 100°C for 24 hours. The crude was purified using Biotage SP4 (15/85% diethyl ether/hexanes mixture) to provide a pure adduct as light yellow needles (208 mg, 80%), m.p 117-119 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ: 8.44 (s, 1H), 8.18-8.20 (d, J = 9.2 Hz, 1H), 8.11-8.13 (d, J = 8.8 Hz, 1H), 8.10-8.13 (d, J = 8.8 Hz, 1H), 7.71-7.75 (t, J = 6.4 Hz, 1H), 7.54-7.57 (d, J = 9.2 Hz, 1H), 7.50-7.57 (t, J = 6.4 Hz, 1H), 2.98 (s, 3H) ppm. **^{13}C NMR (100 MHz, $CDCl_3$)** Due to the complexity of the spectra all the peaks are listing without take into consideration C-F couplings, δ: 149.04, 146.76, 142.59, 131.53, 131.20, 130.88, 130.48, 130.33, 128.36, 128.31, 128.27, 128.22, 128.06, 126.46, 126.10, 126.06,

126.02, 125.35, 124.48, 122.64, 120.34, 120.31, 119.93, 13.64 ppm. **^{19}F NMR (282 MHz)** δ: -63.65. **IR (KBr disc, cm^{-1})**: 1557, 1521, 1421, 1349, 1319, 1270, 1238, 1157, 1114, 943, 898, 811, 755, 665. Anal. Calc. for $C_{15}H_{10}F_3N$: C, 68.96; H, 3.86. Found: C, 68.80; H, 3.76.



2,9-Dimethylacridine (Table 3)

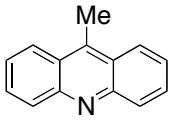
According to *General Procedure 5*, a solution of 0.10 mmol (29 mg) of tri-*tert*-butylphosphonium tetrafluoroborate, 0.025 mmol (22.9 mg) of $Pd_2(dba)_3$, 1.5 mmol (144 mg) of NaO*t*Bu and 1.0 mmol (243 mg) of 2-chloro-4-methyl-*N*-(2-vinylphenyl)aniline (Table 1) in 1 mL of dry toluene was heated at 100°C for 24 hours. The crude was purified using Biotage SP4 (40/60% diethyl diethylether/hexanes mixture) to provide a pure adduct as light yellow solid (203 mg, 98%), m.p 89-90 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ: 8.14-8.16 (d, *J* = 8.8 Hz, 1H), 8.11-8.13 (d, *J* = 8.8 Hz, 1H), 8.05-8.08 (d, *J* = 8.8 Hz, 1H), 7.86 (s, 1H), 7.66-7.69 (t, *J* = 8.2 Hz, 1H), 7.52-7.55 (d, *J* = 9.2 Hz, 1H), 7.44-7.48 (t, *J* = 7.8 Hz 1H), 2.96 (s, 3H), 2.53 (s, 3H) ppm. **^{13}C NMR (100 MHz, $CDCl_3$)** δ: 147.88, 147.29, 140.91, 135.02, 13016, 129.86, 29.22, 125.58, 122.46, 125.22, 124.44, 122.75, 22.22, 13.48 ppm. **IR (KBr disc, cm^{-1})**: 1718, 1635, 1560, 1516, 1447, 1416, 1148, 819, 752. Anal. Calc. for $C_{15}H_{13}N$: C, 86.92; H, 6.32. Found: C, 86.54; H, 6.27.



3,9-Dimethylacridine

According to *General Procedure 5*, a solution of 0.10 mmol (29 mg) of tri-*tert*-butylphosphonium tetrafluoroborate, 0.025 mmol (22.9 mg) of $Pd_2(dba)_3$, 1.5 mmol (144 mg) of NaO*t*Bu and 1.0 mmol (243 mg) of 2-chloro-5-methyl-*N*-(2-vinylphenyl)aniline (Table 1) in 1 mL of dry toluene was heated at 100°C for 24 hours. The crude was purified using Biotage SP4 (25/75% diethyl ether/hexanes mixture) to provide a pure adduct as light yellow solid (186 mg, 90%), m.p 81-83°C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ: 8.12-8.14 (d, *J* = 8.8 Hz, 1H), 8.04-8.06 (d, *J* = 8.4 Hz, 1H), 7.93-7.95 (d, *J* = 9.2 Hz, 1H), 7.90 (s, 1H), 7.64-7.67 (t, *J* = 8.0 Hz, 1H), 7.38-7.42 (t, *J* = 6.4 Hz, 1H), 7.21-7.24 (d, *J* = 9.2 Hz 1H), 2.90 (s, 3H), 2.51 (s, 3H) ppm. **^{13}C NMR (100 MHz, $CDCl_3$)** δ: 148.51, 148.23, 141.89, 139.95, 129.86, 129.51, 128.25, 128.03,

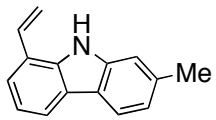
125.07, 124.81, 124.45, 124.09, 123.73, 21.89, 13.42 ppm. **IR (KBr disc, cm^{-1})**: 1636, 1616, 1561, 1515, 1442, 1384, 1017, 878, 805, 752, 647, 602. Anal. Calc. for $C_{15}H_{13}N$: C, 86.92; H, 6.32. Found: C, 86.87; H6.38.



9-Methylacridine

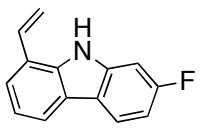
According to *General Procedure 5*, a solution of 0.10 mmol (29 mg) of $Pd_2(dba)_3$, 1.5 mmol (144 mg) of NaO*t*Bu and 1.0 mmol (229 mg) of 2-chloro-*N*-(2-vinylphenyl)aniline (Table 1) in 1 mL of dry toluene was heated at 100°C for 24 hours. The crude was purified using Biotage SP4 (25/75% diethyl ether/hexanes mixture) to provide a pure adduct as yellow solid (168 mg, 77%), m.p 114-116 °C (lit.[5] m.p. 117-119 °C) **^{1}H NMR (400 MHz, $CDCl_3$)** δ: 8.14-8.18 (t, *J* = 8.0 Hz, 4H), 7.68-7.72 (t, *J* = 8.0 Hz, 2H), 7.74-7.50 (t, *J* = 6.8 Hz, 2H), 3.2 (s, 3H) ppm. **^{13}C NMR (100 MHz, $CDCl_3$)** δ: 148.39, 142.26, 130.19, 129.75, 125.50, 125.37, 124.54, 13.61 ppm.

Experimental data for vinylcarbazoles described in Table 3



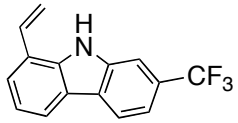
7-Methyl-1-vinyl-9*H*-carbazole

According to *General Procedure 3*, a solution of 1.0 mmol (243 mg) of 2-chloro-5-methyl-*N*-(2-vinylphenyl)aniline (Table 1), 0.06 mmol (23.9 mg) of racemic-2-di-*t*-butylphosphino-1,1'-binaphthyl, 0.03 mmol (6.7 mg) of $Pd(OAc)_2$, 1.5 mmol (144 mg) of NaO*t*Bu in 1 mL of 1,4-dioxane was heated at 110°C for 24 hours. The crude was purified using Biotage SP4 (5/95% diethyl ether/hexanes mixture) to provide a pure adduct as white solid (178 mg, 86%), mp. 182-184 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ: 8.14 (s, 1H), 7.93-7.95 (d, *J* = 7.6 Hz, 1H), 7.91-7.93 (d, *J* = 8.0 Hz, 1H), 7.41-7.43 (d, *J* = 7.2 Hz, 1H), 7.17-7.21 (t, *J* = 7.6 Hz, 1H), 7.00-7.07- (m, 2H), 5.83-5.87 (d, *J* = 17.6 Hz, 1H), 5.46-5.49 (d, *J* = 11.2 Hz, 1H) ppm. **^{13}C NMR (100 MHz, $CDCl_3$)** δ: 140.02, 137.25, 136.22, 133.27, 124.08, 123.33, 121.31, 121.16, 121.01, 120.07, 119.59, 119.57, 115.38, 110.96, 22.11 ppm. **IR (KBr disc, cm^{-1})**: 3412, 1412, 1334, 990, 905, 821, 794, 742, 561. Anal. Calc. for $C_{15}H_{13}N$: C, 86.92; H, 6.32. Found: C, 86.65; H, 6.30.



7-Fluoro-1-vinyl-9*H*-carbazole

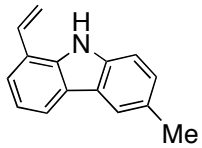
According to *General Procedure 3*, a solution of 1.0 mmol (247 mg) of 2-chloro-5-fluoro-*N*-(2-vinylphenyl)aniline (Table 1), 0.06 mmol (23.9 mg) of racemic-2-di-*t*-butylphosphino-1,1'-binaphthyl, 0.03 mmol (6.7 mg) of $Pd(OAc)_2$, 1.5 mmol (144 mg) of NaO*t*Bu in 1 mL of 1,4-dioxane was heated at 110°C for 24 hours. The crude was purified using Biotage SP4 (5/95% EtOAc/hexanes mixture) to provide a pure adduct as white powder (162 mg, 78%), mp. 98-100 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ: 8.26 (s, 1H), 7.94-7.98 (dd, J_1= 8.8 Hz, J_2 = 5.6, 1H), 7.91-7.93 (d, J = 7.6 Hz, 1H), 7.43-7.45 (d, J = 7.2 Hz, 1H), 7.20-7.24 (t, J = 7.6 Hz, 1H), 7.11-7.14 (d, J = 9.6 Hz, 1H), 6.99-7.06 (dd, J_1= 17.6 Hz, J_2 = 11.2 Hz, 1H), 6.93-6.98 (dt, J_1 = 10.8 Hz, J_2 = 2.0 Hz, 1H), 5.83-5.88 (d, J = 17.6 Hz, 1H), 5.49-5.51 (d, J = 11.2 Hz, 1H) ppm. **^{13}C NMR (100 MHz, $CDCl_3$)** Due to the complexity of the spectra all the peaks are listing without take into consideration C-F couplings, δ: 163.25, 160.85, 140.09, 139.96, 137.63, 133.21, 132.95, 126.02, 123.89, 123.53, 123.49, 121.38, 121.28, 121.19, 120.42, 120.15, 119.89, 119.76, 119.69, 119.45, 115.86, 115.57, 110.81, 108.11, 107.87, 97.75, 97.49 ppm. **^{19}F NMR (282 MHz, $CDCl_3$)** δ: -115.66. **IR (KBr disc, cm^{-1})**: 3437, 1625, 1599, 1497, 1413, 1339, 1139, 1116, 848, 797. Anal. Calc. for $C_{14}H_{10}FN$: C, 80.60; H, 4.77. Found: C, 80.33; H, 4.87.



7-(Trifluoromethyl)-1-vinyl-9*H*-carbazole

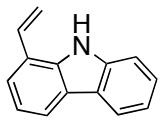
According to *General Procedure 3*, a solution of 1.0 mmol (247 mg) of 2-chloro-5-fluoro-*N*-(2-vinylphenyl)aniline (Table 1), 0.06 mmol (23.9 mg) of racemic-2-di-*t*-butylphosphino-1,1'-binaphthyl, 0.03 mmol (6.7 mg) of $Pd(OAc)_2$, 1.5 mmol (144 mg) of NaO*t*Bu in 1 mL of 1,4-dioxane was heated at 110°C for 24 hours. The crude was purified using Biotage SP4 (5/95% EtOAc/hexanes mixture) to provide a pure adduct as white powder (232 mg, 89%), mp. 93-94 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ: 8.42 (s, 1H), 8.11-8.13 (d, J= 8.4 Hz, 1H), 8.00-8.02 (d, J = 7.6 Hz, 1H), 7.72 (s, 1H), 7.51-7.52 (d, J = 7.2 Hz, 1H), 7.46-7.48 (d, J = 8.4 Hz, 1H), 7.24-7.28 (m, 1H), 7.00-7.07 (dd, J_1= 17.6 Hz, J_2 = 11.2 Hz, 1H), 5.85-5.89 (d, J = 17.6 Hz, 1H), 5.51-5.54 (d, J = 11.2 Hz, 1H) ppm. **^{13}C NMR (100 MHz, $CDCl_3$)** Due to the complexity of the spectra all the peaks are listing without take into consideration C-F couplings, δ:

138.56, 138.14, 132.80, 127.96, 127.64, 126.03, 125.06, 122.98, 121.58, 120.70, 120.39, 120.36, 116.51, 116.48, 116.22, 108.16, 118.11, 29.73 ppm. **^{19}F NMR (282 MHz, $CDCl_3$)** δ: -61.41. **IR (KBr disc, cm^{-1})**: 3415, 2919, 2854, 2355, 2330, 1503, 1331, 1244, 1164, 1108, 1054, 801, 755.



6-Methyl-1-vinyl-9*H*-carbazole

According to *General Procedure 3*, a solution of 1.0 mmol (243 mg) of 2-chloro-4-methyl-*N*-(2-vinylphenyl)aniline (Table 1), 0.06 mmol (23.9 mg) of racemic-2-di-*t*-butylphosphino-1,1'-binaphthyl, 0.03 mmol (6.7 mg) of $Pd(OAc)_2$, 1.5 mmol (144 mg) of NaO*t*Bu in 1 mL of 1,4-dioxane was heated at 110°C for 24 hours. The crude was purified using Biotage SP4 (5/95% diethyl ether/hexanes mixture) to provide a pure adduct as white solid (188 mg, 91%), mp. 129-130 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ: 8.13 (s, 1H), 7.97-7.99 (d, J = 8.0 Hz, 1H), 7.88 (s, 1H), 7.46-7.48 (d, J = 8.4 Hz, 1H), 7.34-7.36 (d, J = 8.0 Hz, 1H), 7.21-7.27 (m, 1H), 7.00-7.07 (dd, J_1= 17.6 Hz, J_2 = 11.2 Hz, 1H), 5.85-5.90 (d, J = 17.6 Hz, 1H), 5.48-5.51 (d, J = 10.8 Hz, 1H), 2.55 (s, 3H) ppm. **^{13}C NMR (100 MHz, $CDCl_3$)** δ: 137.79, 137.62, 133.30, 129.09, 127.39, 123.89, 123.74, 123.64, 121.08, 120.36, 119.83, 119.49, 115.39, 110.50, 21.52 ppm. **IR (KBr disc, cm^{-1})**: 3420, 1455, 1410, 1334, 985, 895, 801, 752. Anal. Calc. for $C_{15}H_{13}N$: C, 86.92; H, 6.32. Found: C, 86.66; H, 6.50.

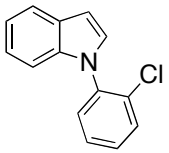


1-Vinyl-9*H*-carbazole

According to *General Procedure 3*, a solution of 1.0 mmol (229 mg) of 2-chloro-*N*-(2-vinylphenyl)aniline (**7**), 0.06 mmol (23.9 mg) of racemic-2-di-*t*-butylphosphino-1,1'-binaphthyl, 0.03 mmol (6.7 mg) of $Pd(OAc)_2$, 1.5 mmol (144 mg) of NaO*t*Bu in 1 mL of 1,4-dioxane was heated at 110°C for 24 hours. The crude was purified using Biotage SP4 (2/98% EtOAc/hexanes mixture) to provide a pure adduct as white solid (181 mg, 94%), mp. 82-83 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ: 8.23 (s, 1H), 8.06-8.08 (d, J = 7.6 Hz, 1H), 7.99-8.01 (d, J = 7.6 Hz, 1H), 7.40-7.48 (m, 3H), 7.18-7.27 (m, 2H), 6.99-7.08 (dd, J_1= 18.00 Hz, J_2 = 11.2 Hz, 1H), 5.85-5.89 (d, J = 17.6 Hz, 1H), 5.48-5.51 (d, J = 10.8 Hz, 1H) ppm. **^{13}C NMR (100 MHz, $CDCl_3$)** δ: 139.53, 137.26, 133.22, 126.03, 123.97, 123.89, 123.46, 121.13, 120.44, 119.90, 199.77, 119.71, 115.57,

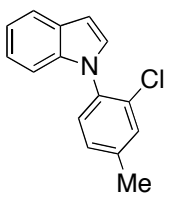
110.82 ppm. **IR (KBr disc, cm^{-1})**: 3415, 1619, 1596, 1457, 1414, 1339, 1324, 1228, 984, 908, 753. Anal. Calc. for $C_{14}H_{11}N$: C, 87.01; H, 5.74. Found: C, 86.61; H, 5.70.

Experimental data for compounds described in Table 4



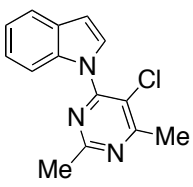
1-(2-Chlorophenyl)-1*H*-indole (Table 4)

According to *General Procedure 4*, a solution of 1.0 mmol (229 mg) of 2-chloro-*N*-(2-vinylphenyl)aniline (Table 1), 0.10 mmol (22.4 mg) of $Pd(OAc)_2$, 1.5 mmol (272.5 mg) of $Cu(OAc)_2$ in 1 mL of acetic acid and 3 mL of DMF was heated at 110°C for 12 hours. The crude was purified using Biotage SP4 (5/95% EtOAc/hexanes mixture) to provide a pure adduct as light yellow oil (222 mg, 98%). **^{1}H NMR (400 MHz, $CDCl_3$)** δ: 7.67-7.69 (dd, J_1= 6.4 Hz, J_2 = 1.6 Hz, 1H), 7.56-7.59 (m, 1H), 7.35-7.46 (m, 3H), 7.24-7.25 (d, J = 3.2 Hz, 1H), 7.12-7.21 (m, 3H), 6.69-6.70 (d, J = 3.2 Hz, 1H) ppm. **^{13}C NMR (100 MHz, $CDCl_3$)** δ: 136.92, 136.77, 131.85, 130.85, 129.45, 129.09, 128.79, 128.49, 127.69, 122.32, 121.00, 120.35, 110.62, 103.28 ppm. **IR (KBr disc, cm^{-1})**: 3072, 1588, 1514, 1489, 1455, 1331, 1308, 1232, 1212, 739. Anal. Calc. for $C_{14}H_{10}ClN$: C, 73.85; H, 4.43. Found: C, 74.06; H, 4.50.



1-(5-Chloro-4-methylphenyl)-1*H*-indole

According to *General Procedure 4*, a solution of 1.0 mmol (259 mg) of 2-chloro-4-methyl-*N*-(2-vinylphenyl)aniline (Table 1), 0.10 mmol (22.4 mg) of $Pd(OAc)_2$, 1.5 mmol (272.5 mg) of $Cu(OAc)_2$ in 1 mL of acetic acid and 3 mL of DMF was heated at 110°C for 12 hours. The crude was purified using Biotage SP4 (15/85% dichloromethane/hexanes mixture) to provide a pure adduct as yellow oil (210 mg, 87%). **^{1}H NMR (400 MHz, $CDCl_3$)** δ: 7.65-7.68 (dd, J_1= 6.8 Hz, J_2 = 1.6 Hz, 1H), 7.38-7.39 (d, J = 1.2 Hz, 1H), 7.27-7.30 (d, J = 13.2 Hz, 1H), 7.09-7.20 (m, 5H), 7.66-7.67 (d, J = 3.2 Hz, 1H), 2.42 (s, 3H) ppm. **^{13}C NMR (100 MHz, $CDCl_3$)** δ: 139.54, 136.88, 134.22, 131.47, 131.12, 129.08, 128.89, 128.39, 122.19, 120.93, 120.20, 110.60, 103.00, 21.00 ppm. **IR (KBr disc, cm^{-1})**: 3052, 2922, 1515, 1504, 1457, 1332, 1235, 1212, 1135, 1052, 740. Anal. Calc. for $C_{15}H_{12}ClN$: C, 74.53; H, 5.00. Found: C, 74.93; H, 5.40.

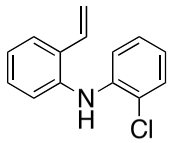


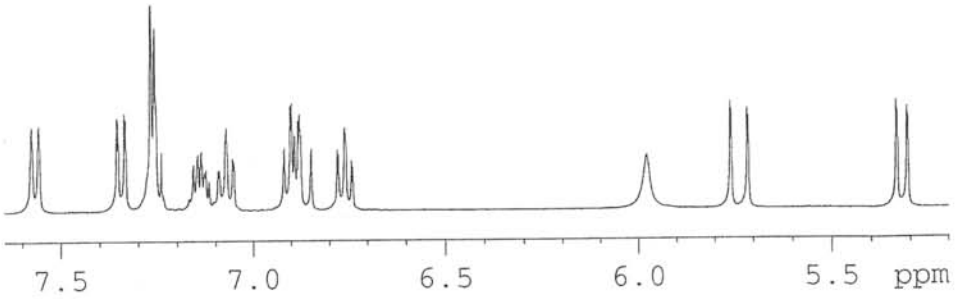
1-(5-Chloro-2,6-dimethylpyrimidine-4-yl)-1*H*-indole (Table 4)

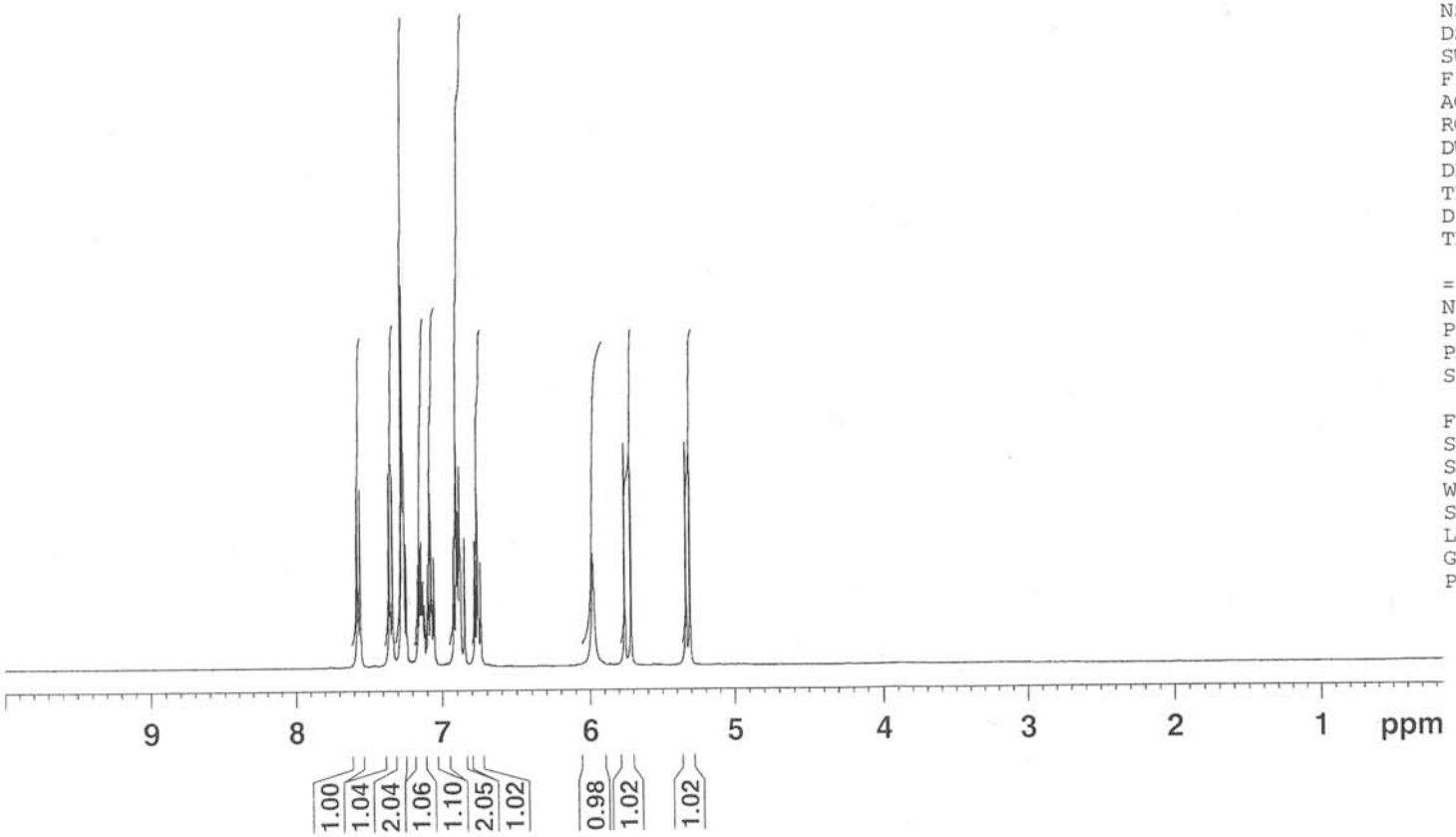
According to *General Procedure 4*, a solution of 1.0 mmol (259 mg) of 2-chloro-2,6-dimethyl-*N*-(2-vinylphenyl)pyrimidin-4-amine (Table 1), 0.10 mmol (22.4 mg) of $Pd(OAc)_2$, 1.5 mmol (272.5 mg) of $Cu(OAc)_2$ in 1 mL of acetic acid and 3 mL of DMF was heated at 110°C for 12 hours. The crude was purified using Biotage SP4 (50/50% dichloromethane/hexanes mixture) to provide a pure adduct as yellow oil (234 mg, 91%). **^{1}H NMR (400 MHz, $CDCl_3$)** δ: 7.74-7.76 (d, *J* = 8.4 Hz, 1H), 7.63-7.64 (d, *J* = 3.6 Hz, 1H), 7.61-7.63 (d, *J* = 8.4 Hz, 1H), 7.18-7.28 (m, 2H), 7.69-7.70 (d, *J* = 3.6 Hz, 1H), 2.70 (s, 1H), 2.68 (s, 1H) ppm. **^{13}C NMR (100 MHz, $CDCl_3$)** δ: 167.94, 165.18, 154.45, 135.66, 129.67, 127.21, 123.30, 121.97, 121.07, 118.86, 113.50, 25.34, 23.26 ppm. **IR (KBr disc, cm^{-1})**: 2918, 2850, 1550, 1523, 1454, 1399, 1366, 1123, 1063, 741.

References:

1. Inoue, M.; Nakada, M. *J. Am. Chem. Soc.*, **2007**, *129*, 4164
2. Fors, B. P.; Watson, D. A.; Biscoe, M. R.; Buchwald. S. L. *J. Am. Chem. Soc.* **2008**, *130*, 13552.
3. (a) Kricka, L. J.; Ledwith, A. *Chem. Rev*. **1974**, *74*, 101; and references therein. (b) Tokmakov, G. P.; Grandberg, I. I. *Tetrahedron*, **1995**, *51*, 2091.
4. Morrow, G. W.; Marks, T. M.; Sear D. L. *Tetrahedron*, **1995**, *51*, 10115.
5. Rogness, D. C.; Larock, R. C. *J. Org. Chem.* **2010**, *75*, 2289.







BRUKER

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PROCNO                      1

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FIDRES            0.126314 Hz
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RG                   228.1
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DE                   6.00 usec
TE                  300.0 K
D1              1.00000000 sec
TD0                      1

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PL1                  0.00 dB
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F2 - Processing parameters
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PC                    1.00
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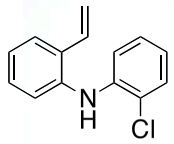

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77.39
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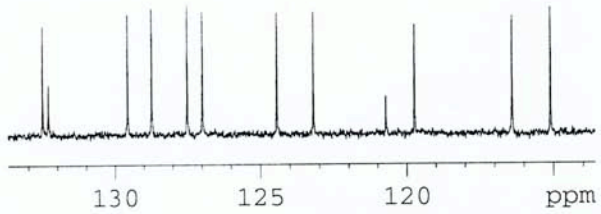
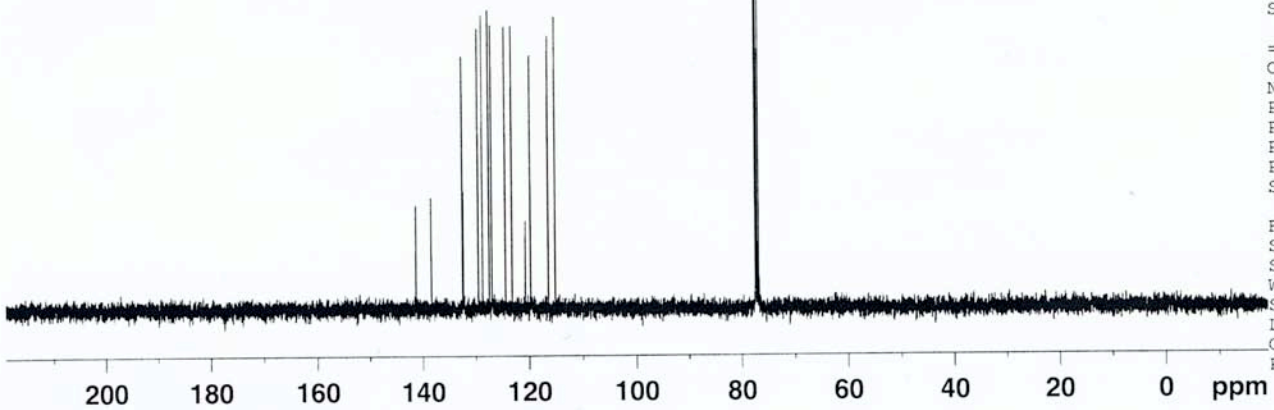
76.75





BRUKER

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PROCNO                     1

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TD                   65536
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NS                     106
DS                       4
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FIDRES           0.365918 Hz
AQ               1.3664756 sec
RG                  1824.6
DW                  20.850 usec
DE                   6.00 usec
TE                  294.2 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
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P1                    9.38 usec
PL1                   0.00 dB
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2                90.00 usec
PL2                   0.00 dB
PL12                 16.10 dB
PL13                 19.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
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WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
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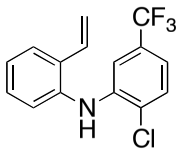

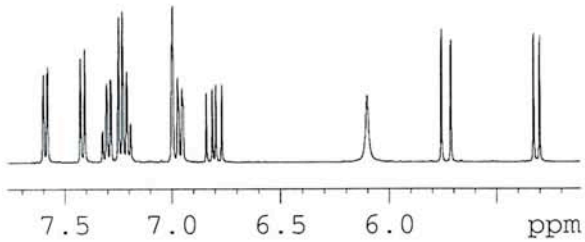

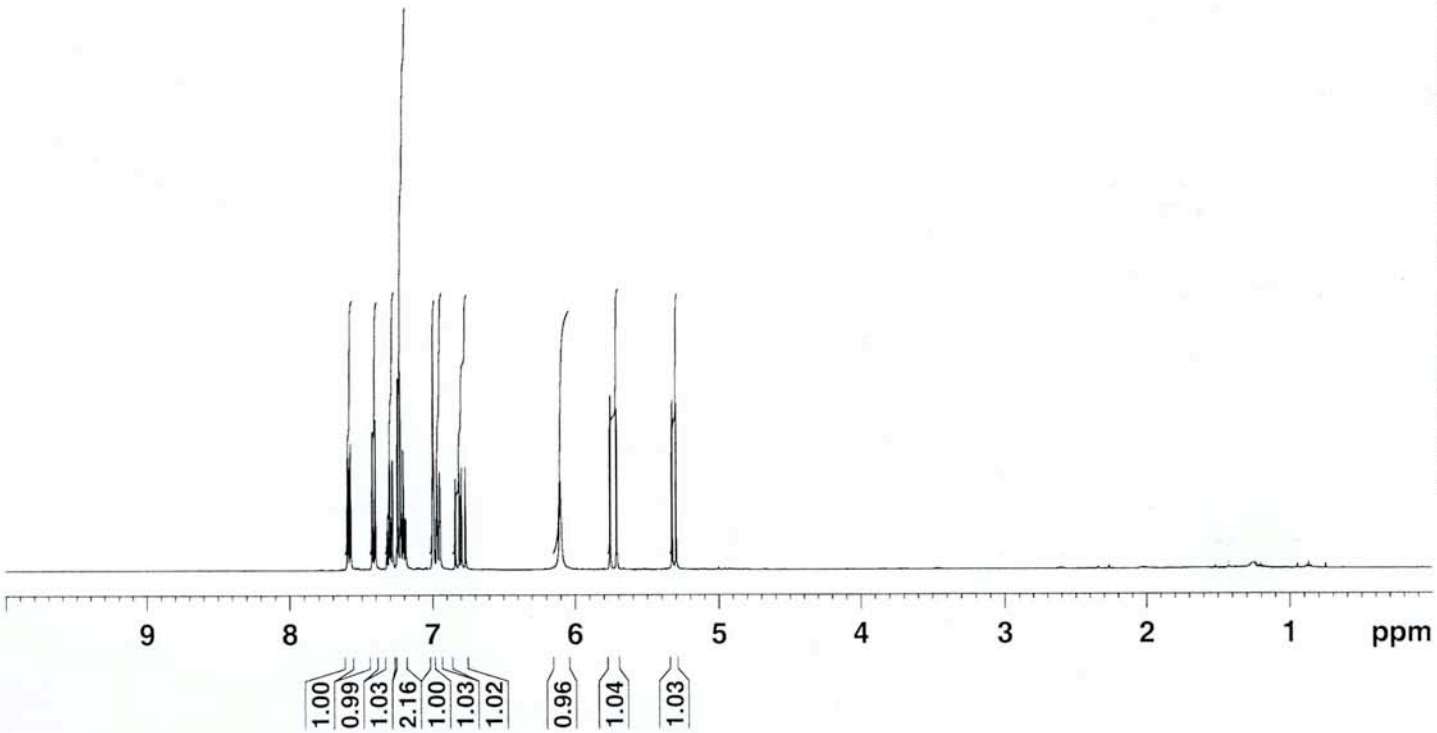


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DS                          2
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FIDRES               0.126314
AQ                   3.9584243
RG                        128
DW                     60.400
DE                       6.00
TE                      294.2
D1                1.00000000
TD0                         1

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PL1                      0.00
SFO1           400.1324710

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WDW                       EM
SSB                        0
LB                      0.30
GB                         0
PC                      1.00
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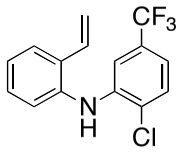

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130.37
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127.38
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123.46
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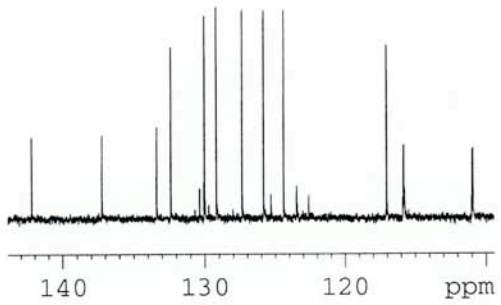
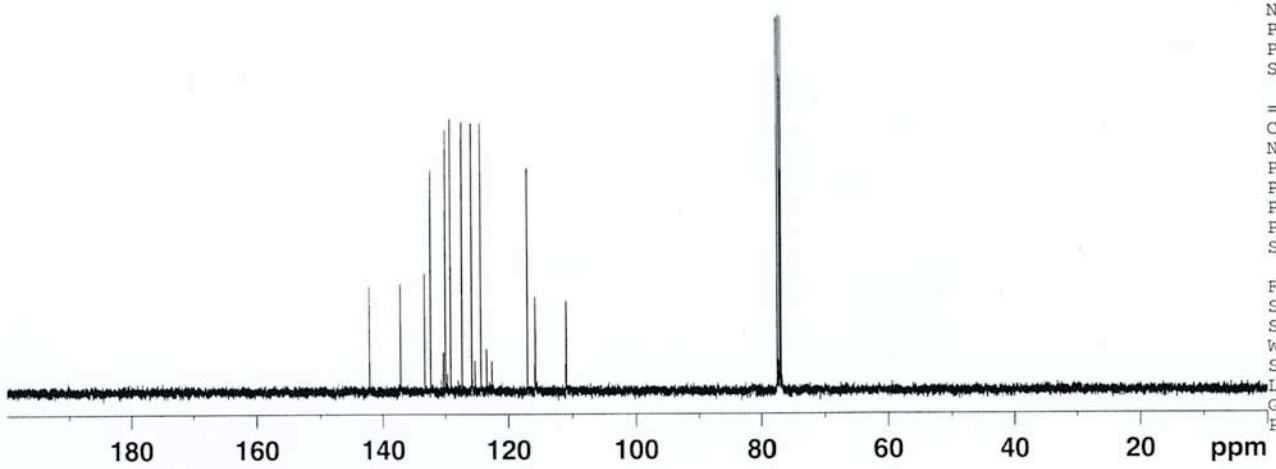
115.81
110.98
110.94

77.54
77.22
76.90





BRUKER

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EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
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PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 128
DS 2
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FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 8192
DW 20.850 usec
DE 6.00 usec
TE 294.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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PL1 -3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
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NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 14.52 dB
PL13 18.00 dB
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F2 - Processing parameters
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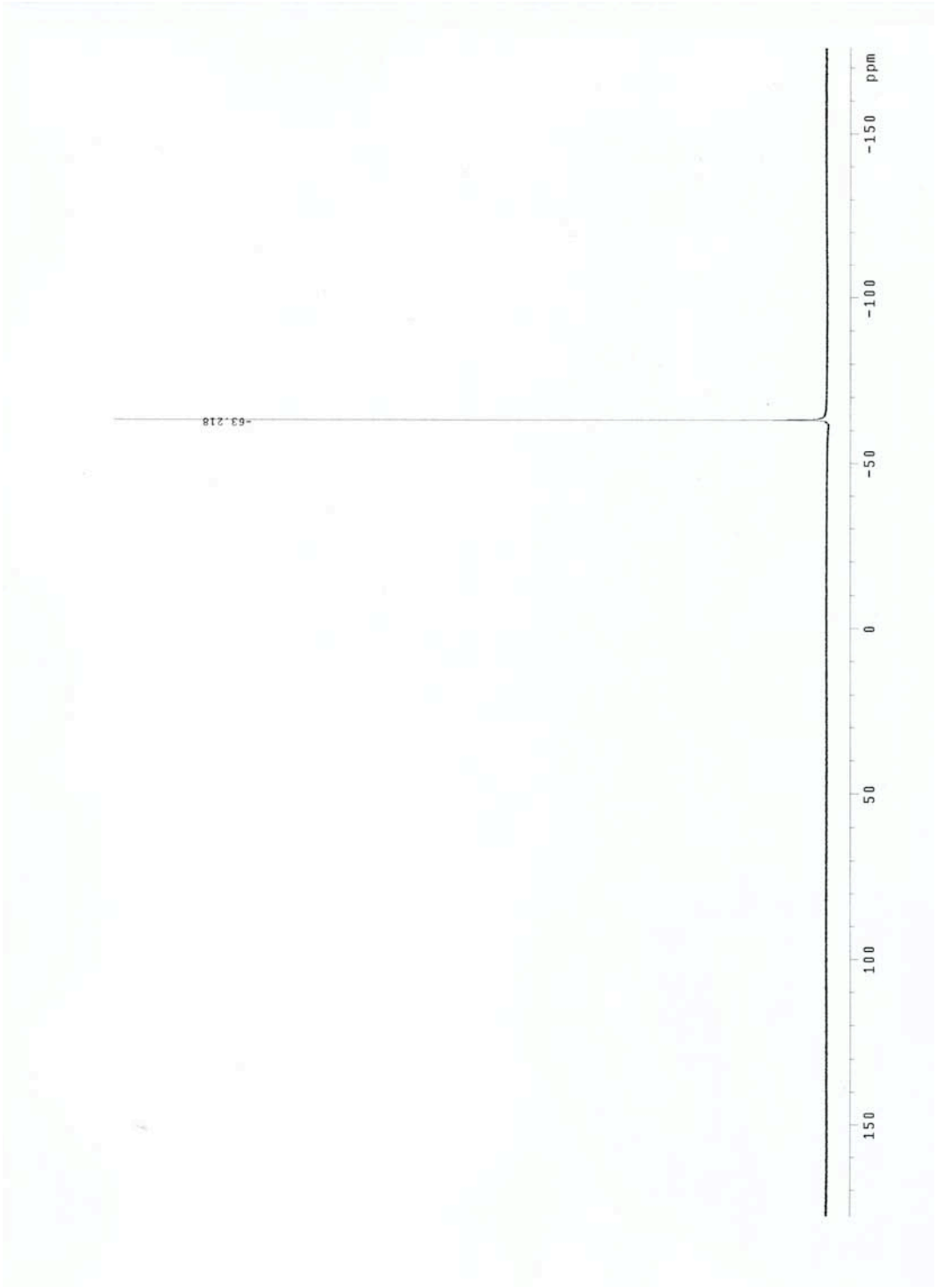
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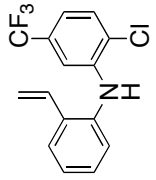
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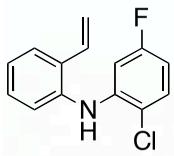

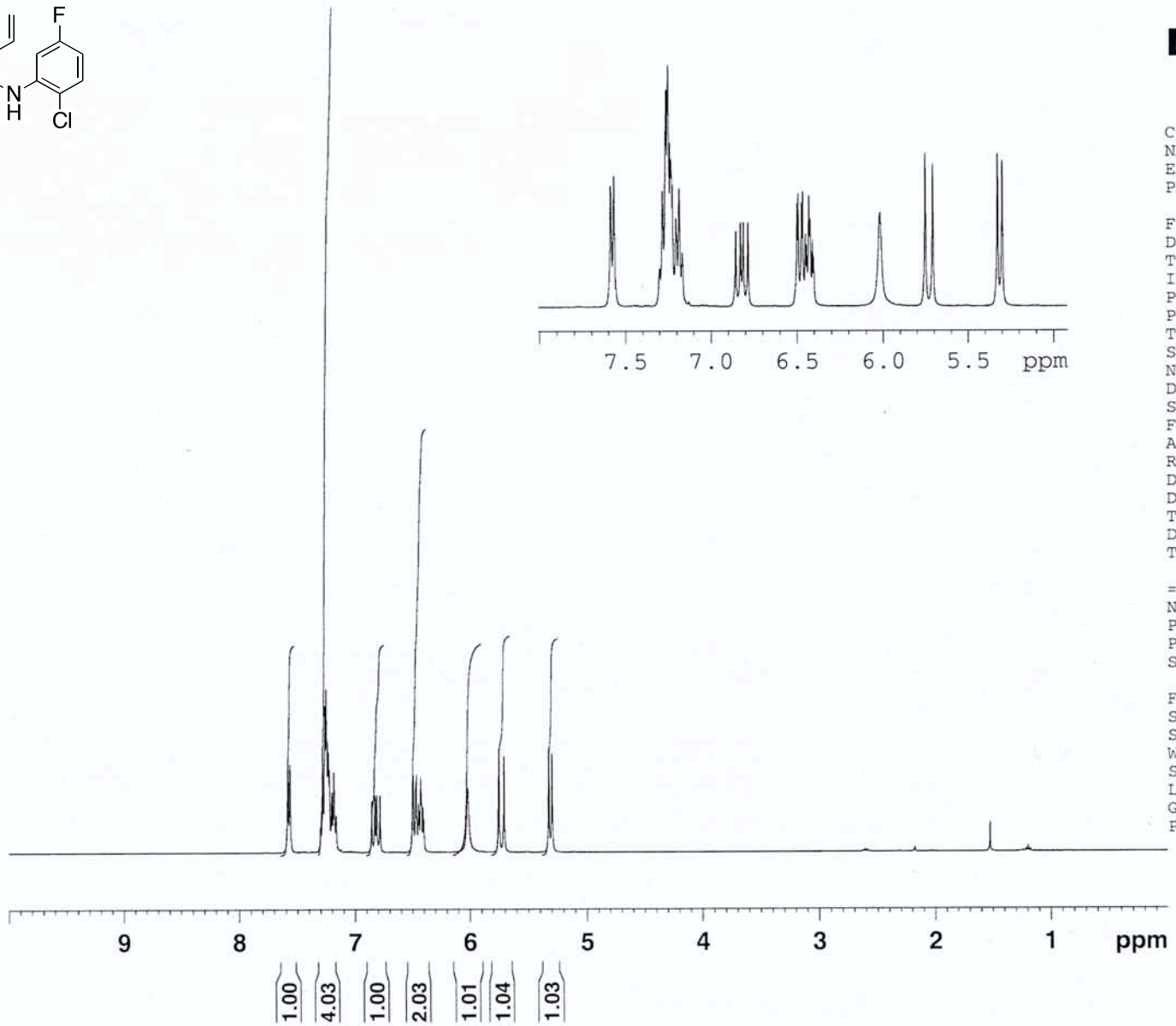

BRUKER

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PROCNO                  1

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DS                      2
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FIDRES           0.126314 Hz
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RG                     57
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TE                292.2 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
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PL1                 0.00 dB
SFO1         400.1324710 MHz

F2 - Processing parameters
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WDW                    EM
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LB                 0.30 Hz
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PC                   1.00
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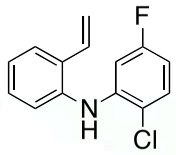

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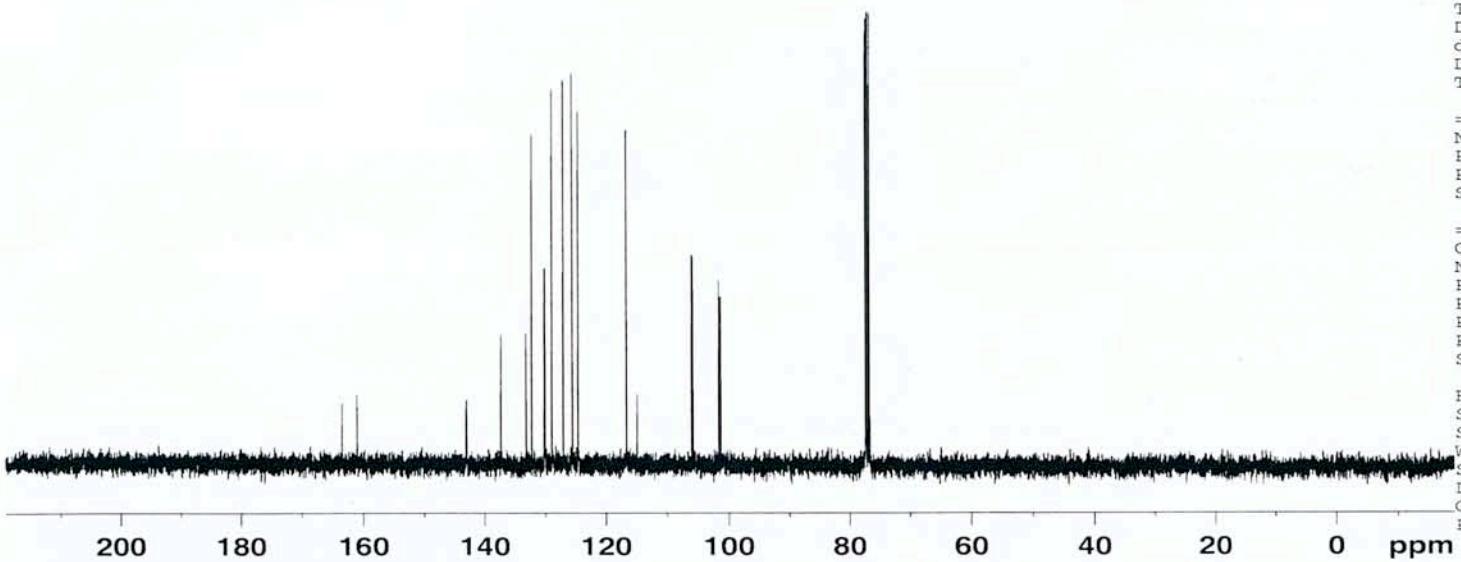

BRUKER

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PROCNO 1

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SOLVENT CDC13
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FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 4597.6
DW 20.850 usec
DE 6.00 usec
TE 296.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.10 dB
PL13 19.00 dB
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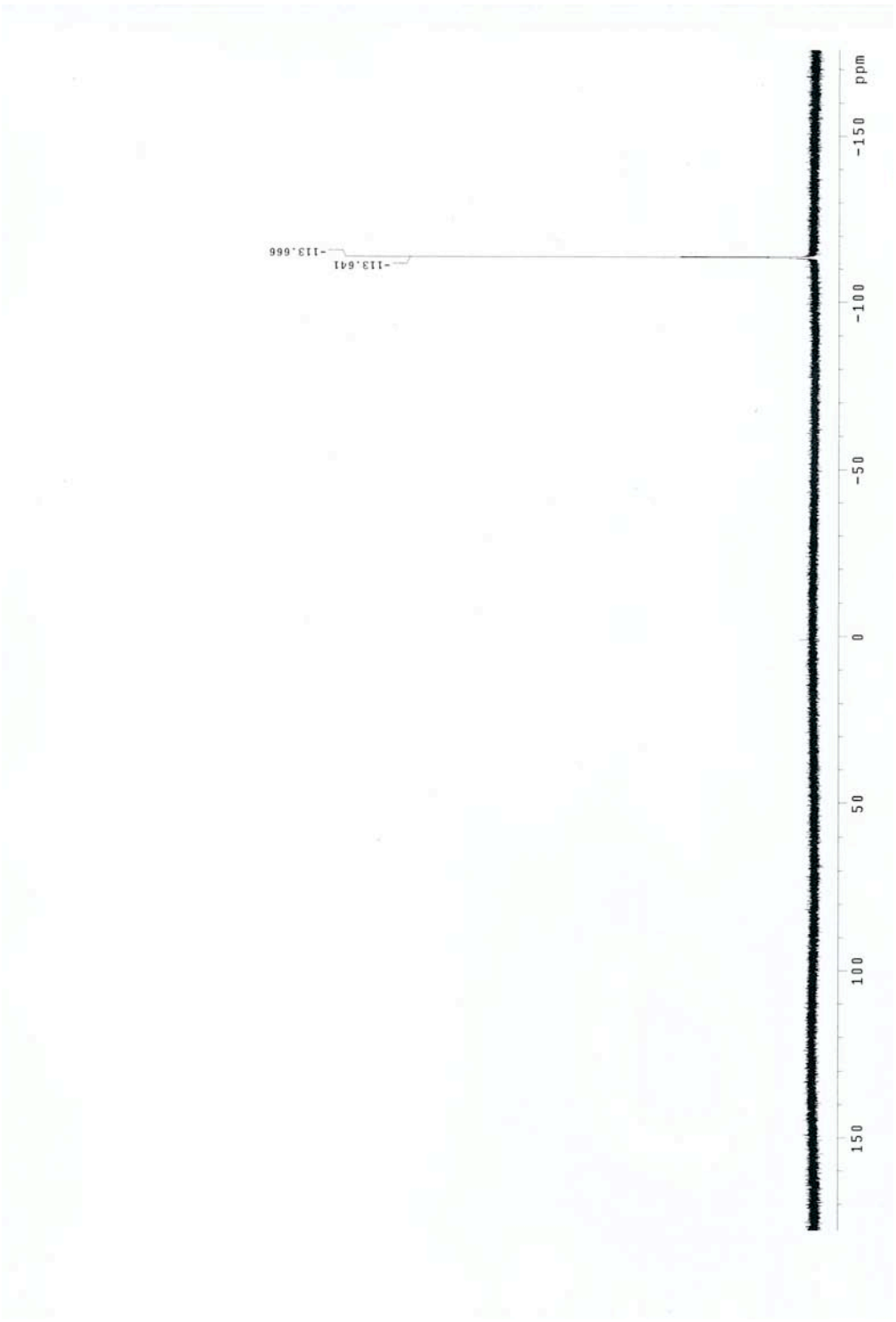
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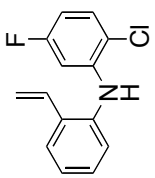
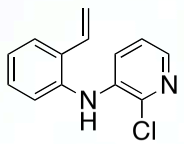
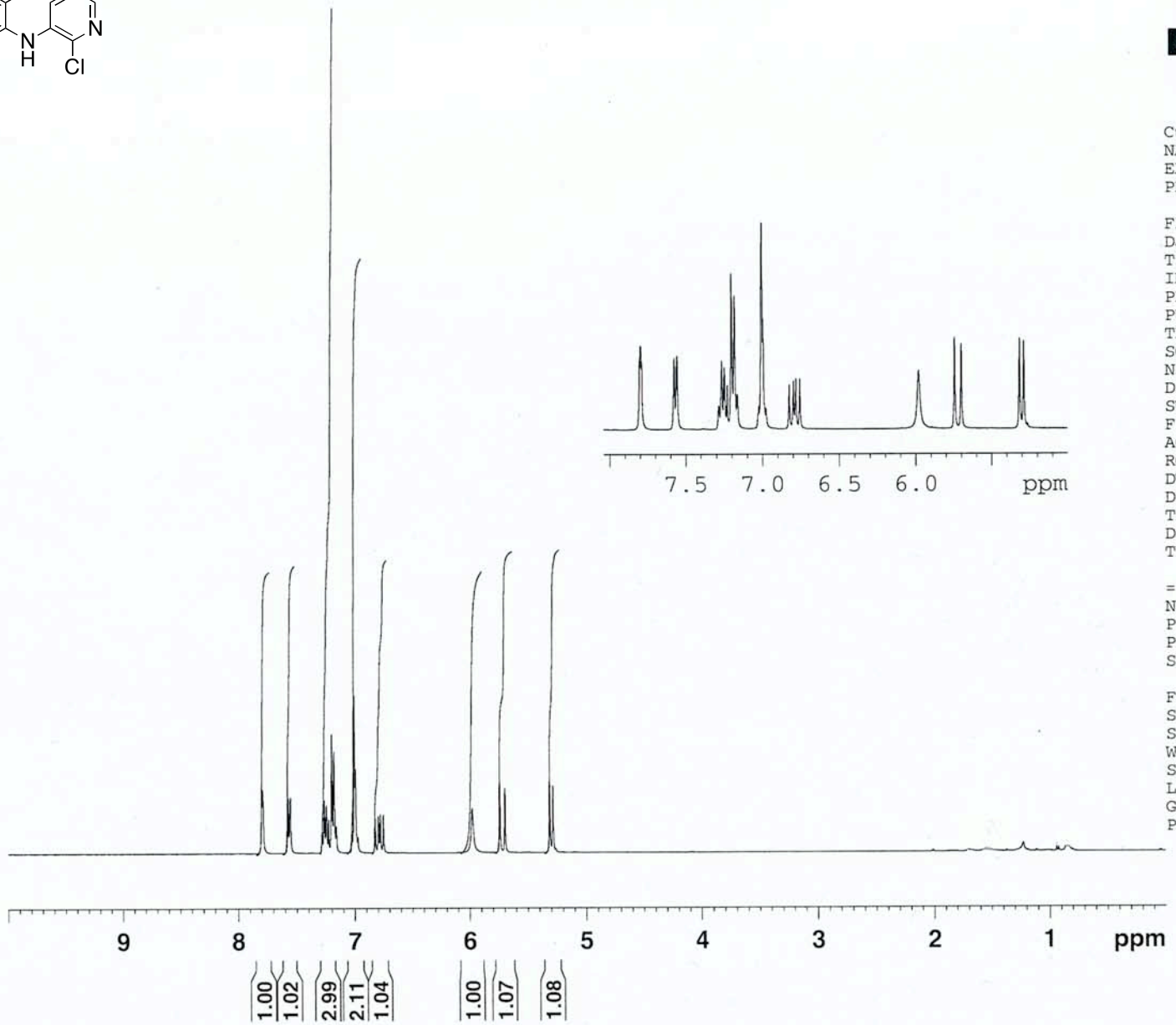

F
Cl
NH





BRUKER

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RG                  322.5
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TE                291.2 K
D1           1.00000000 sec
TD0                     1

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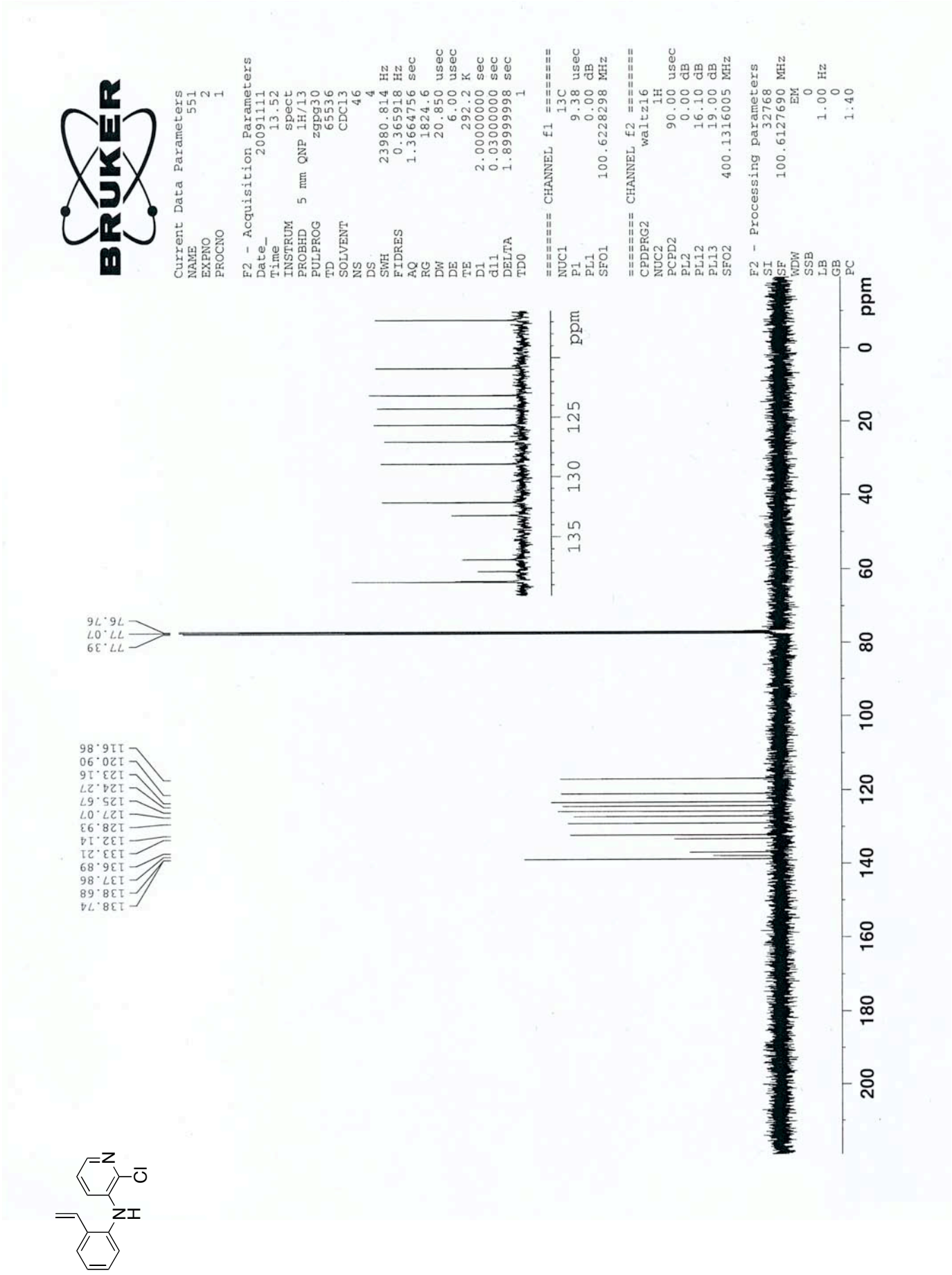
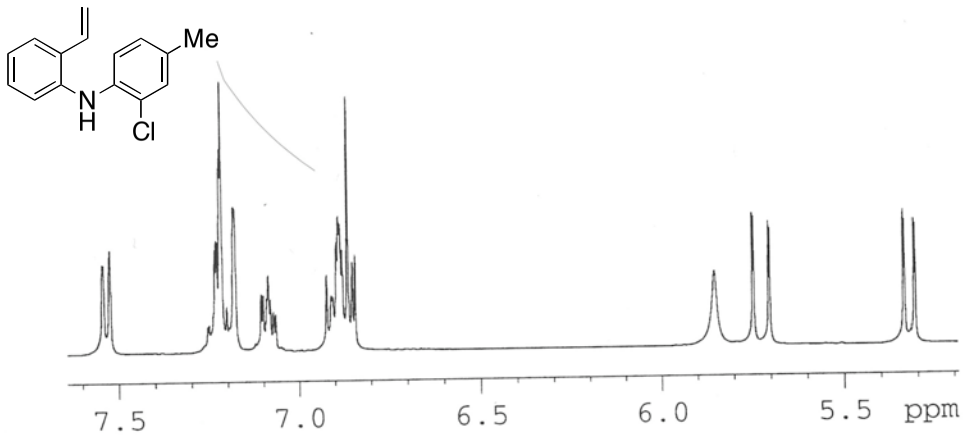
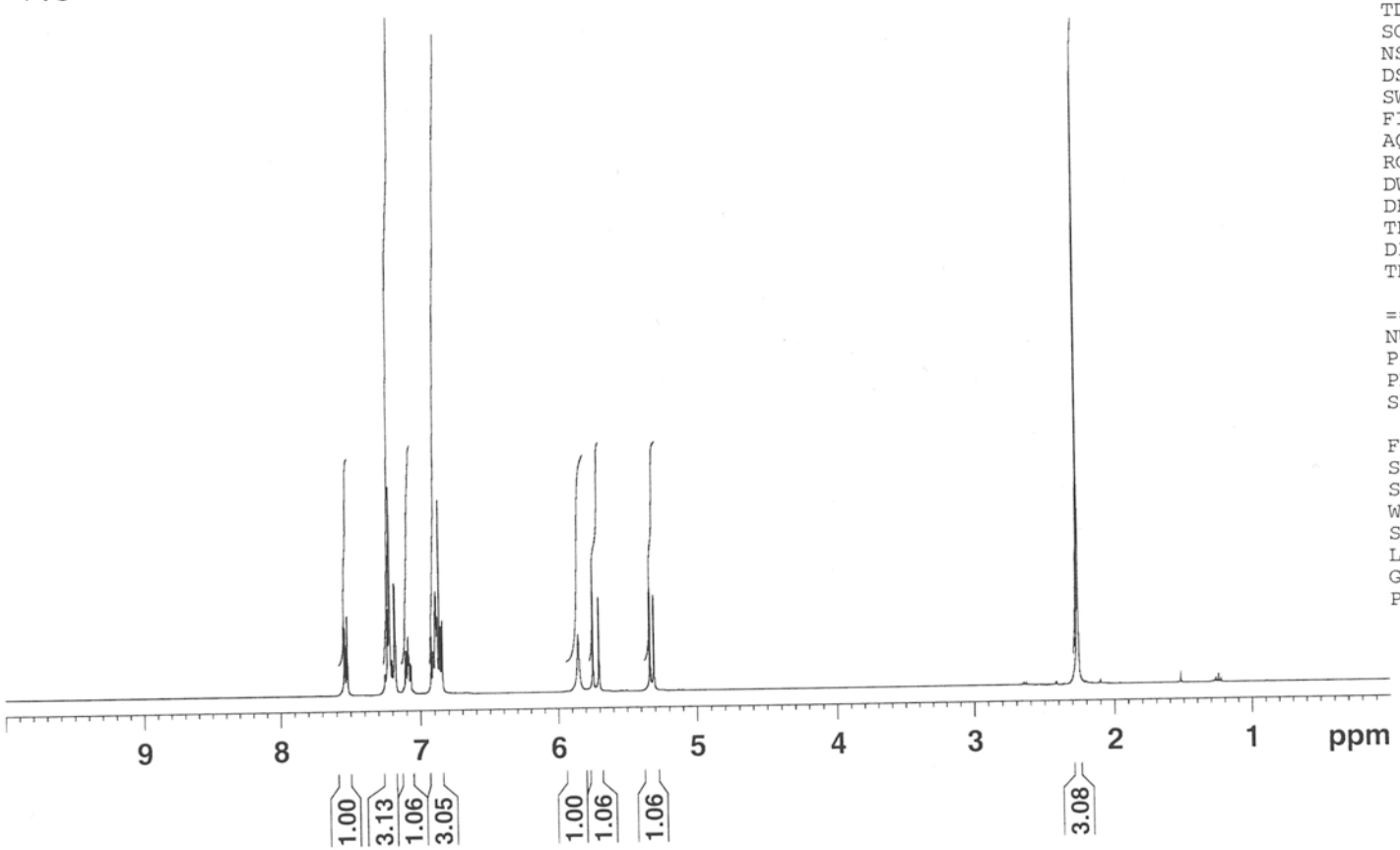
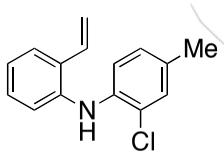

BRUKER
Current Data Parameters
NAME 551
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20091111
Time 13.52
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 46
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 1824.6
DW 20.850 usec
DE 6.00 usec
TE 292.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.38 usec
PL1 0.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.10 dB
PL13 19.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
77.39
77.07
76.76
138.74
138.68
137.86
136.89
133.21
132.14
128.93
127.07
125.67
124.27
123.16
120.90
116.86
135 130 125 ppm
200 180 160 140 120 100 80 60 40 20 0 ppm
N
Cl
H
N





BRUKER

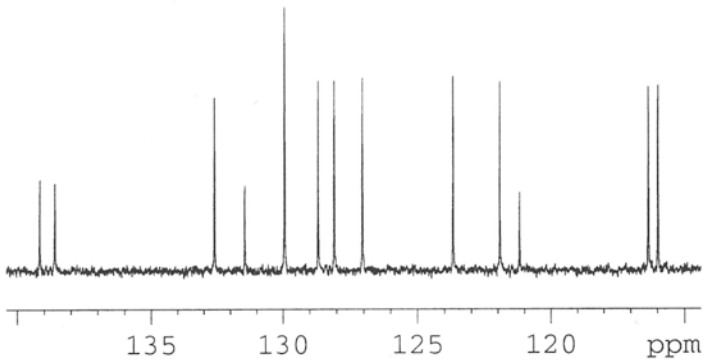
```
Current Data Parameters
NAME                  690
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20100610
Time                7.10
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                      7
DS                      2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 sec
RG                    114
DW               60.400 usec
DE                6.00 usec
TE                294.2 K
D1           1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  1H
P1               14.00 usec
PL1               0.00 dB
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF          400.1300220 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```

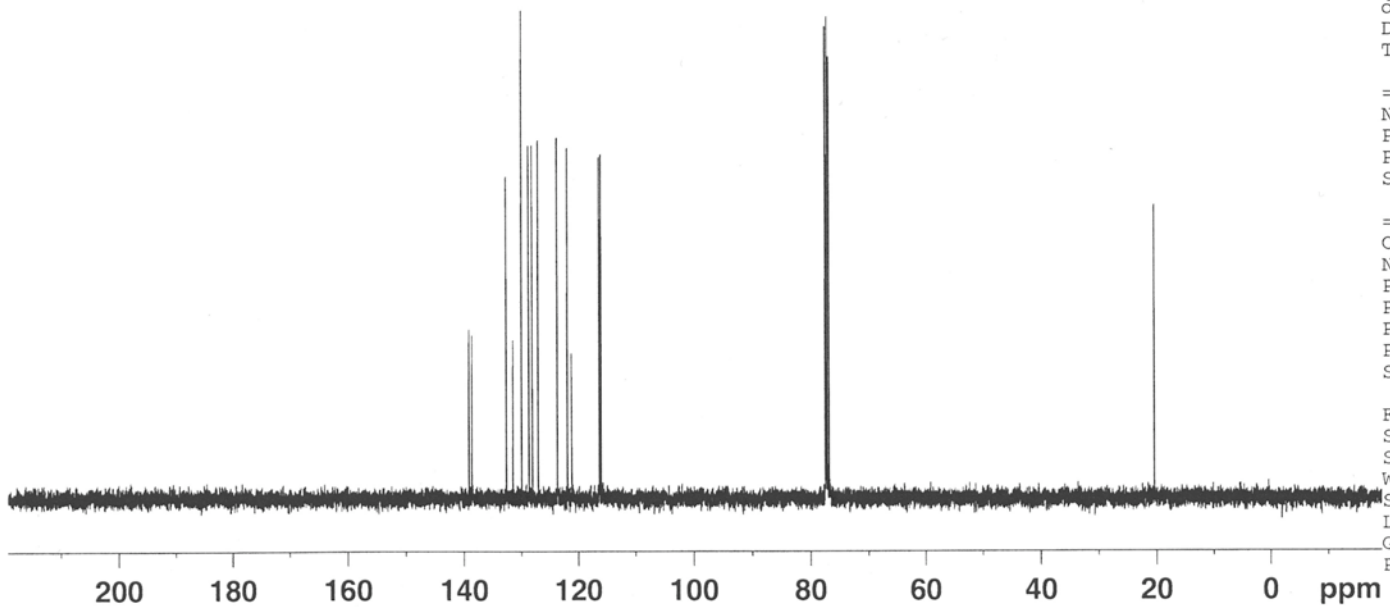


139.15
138.59
132.61
131.46
129.95
128.68
128.09
127.05
123.68
121.93
121.18
116.34
115.98

77.41
77.09
76.77

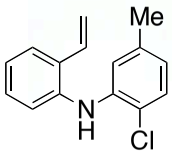
20.38

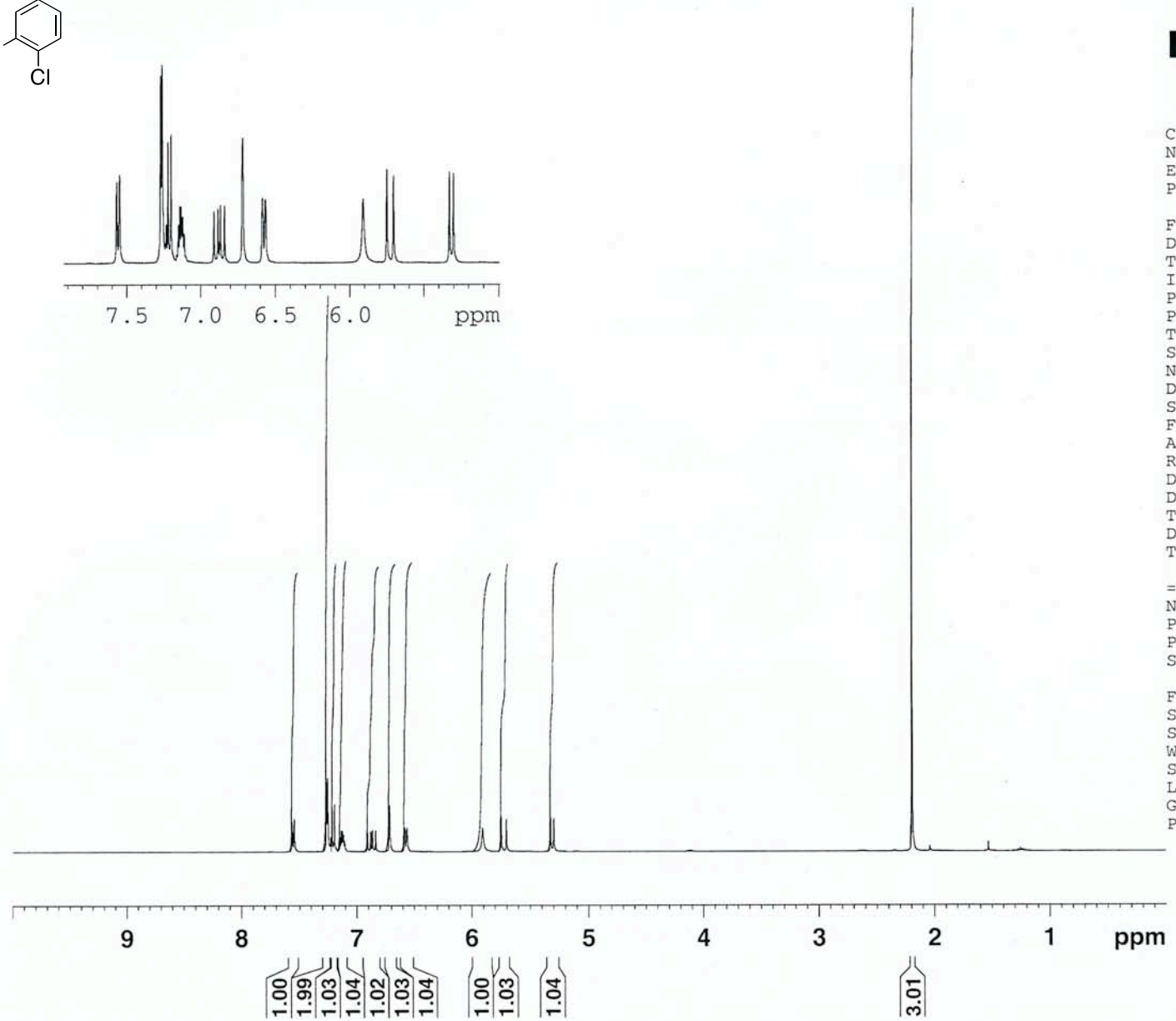




BRUKER

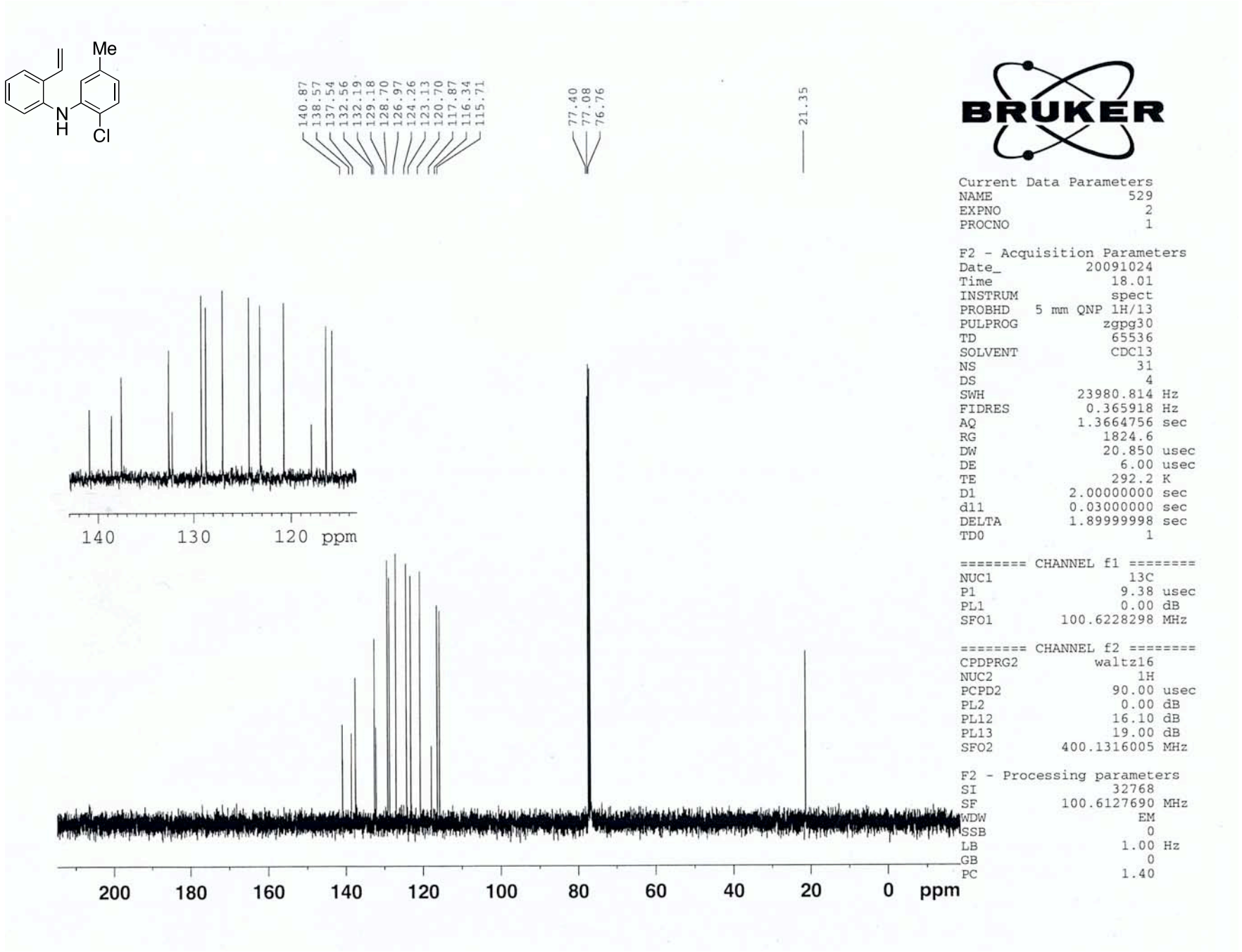
```
Current Data Parameters
NAME                  690
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20100610
Time                7.19
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    70
DS                     4
SWH            23980.814 Hz
FIDRES             0.365918 Hz
AQ                 1.3664756 sec
RG                 1824.6
DW                 20.850 usec
DE                 6.00 usec
TE                 294.2 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 9.38 usec
PL1                0.00 dB
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2                0.00 dB
PL12               16.10 dB
PL13               19.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF            100.6127690 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```

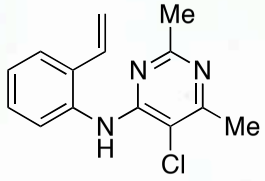


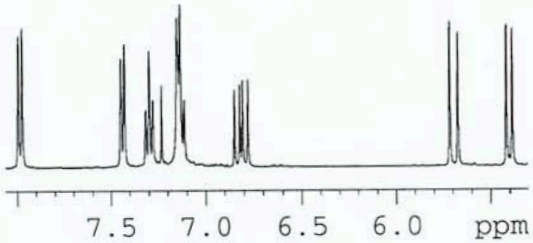


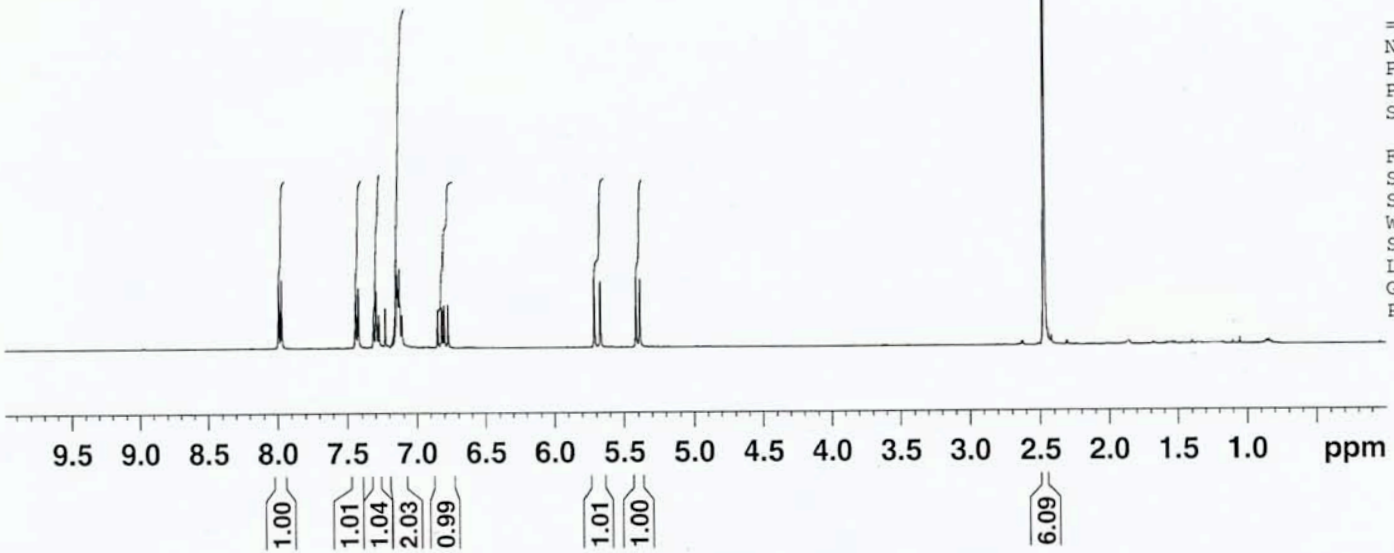
BRUKER

```
Current Data Parameters
NAME                  529
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20091024
Time                17.52
INSTRUM             spect
PROBHD   5 mm QNP 1H/13
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      8
DS                      2
SWH              8278.146 Hz
FIDRES           0.126314 Hz
AQ               3.9584243 sec
RG                    181
DW                 60.400 usec
DE                  6.00 usec
TE                 292.2 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 14.00 usec
PL1                 0.00 dB
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                  65536
SF           400.1300220 MHz
WDW                    EM
SSB                     0
LB                  0.30 Hz
GB                      0
PC                  1.00
```


Me
N
H
Cl
140.87
138.57
137.54
132.56
132.19
129.18
128.70
126.97
124.26
123.13
120.70
117.87
116.34
115.71
77.40
77.08
76.76
21.35
140
130
120 ppm
200
180
160
140
120
100
80
60
40
20
0 ppm
BRUKER
Current Data Parameters
NAME 529
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20091024
Time 18.01
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 31
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 1824.6
DW 20.850 usec
DE 6.00 usec
TE 292.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.38 usec
PL1 0.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.10 dB
PL13 19.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

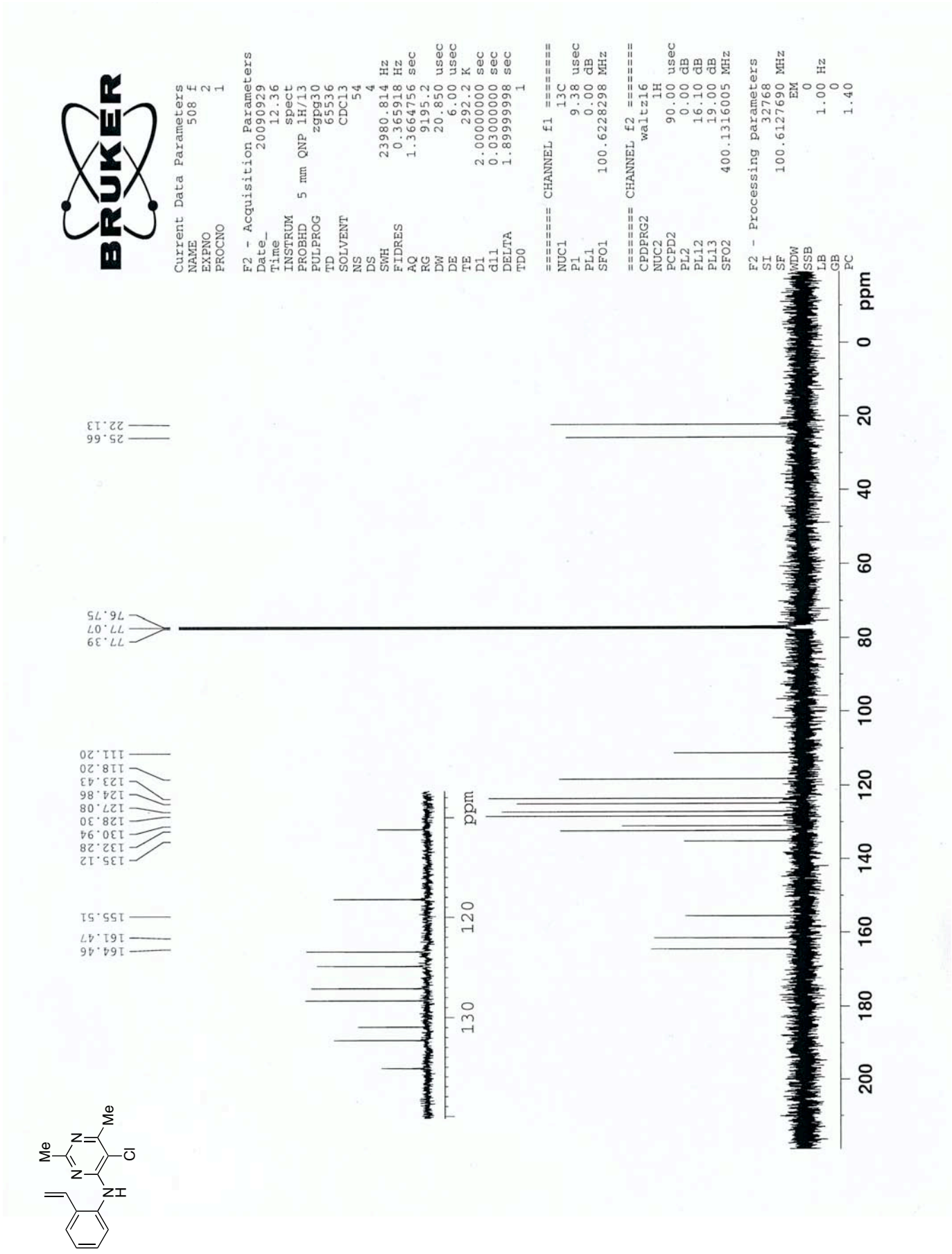


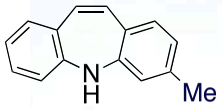


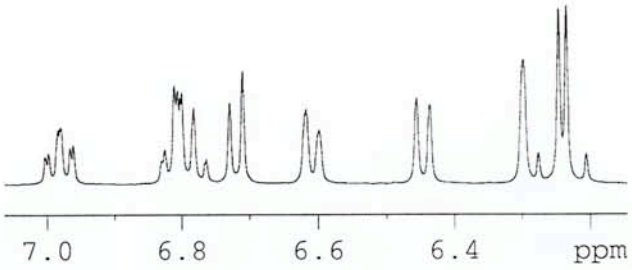


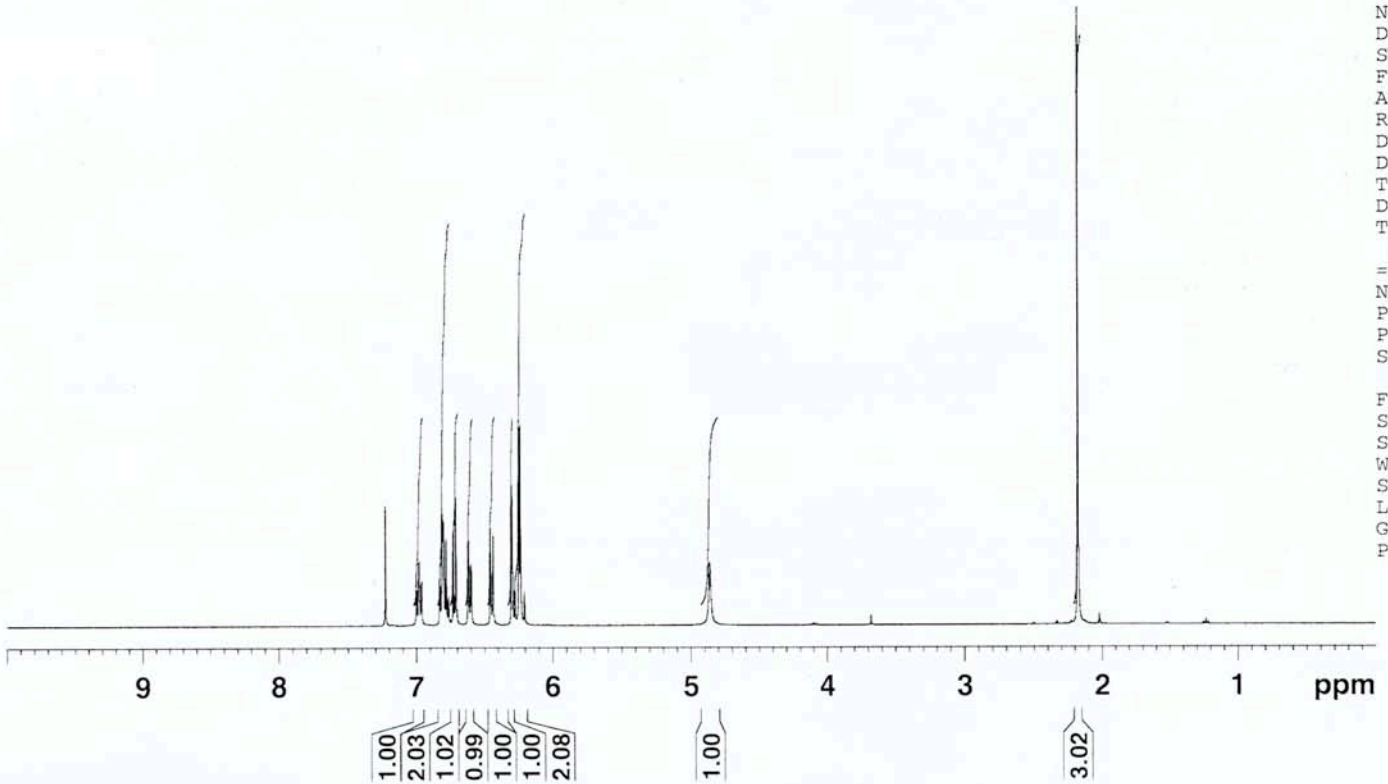
BRUKER

```
Current Data Parameters
NAME                  508 f
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20090929
Time                  12.25
INSTRUM               spect
PROBHD   5 mm QNP 1H/13
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8278.146 Hz
FIDRES            0.126314 Hz
AQ                3.9584243 sec
RG                    203.2
DW                   60.400 usec
DE                    6.00 usec
TE                   292.2 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                   14.00 usec
PL1                   0.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                    65536
SF            400.1300220 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                     1.00
```

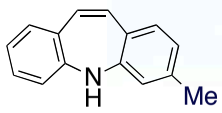

Me
Me
Cl
N
N
H
BRUKER
Current Data Parameters
NAME 508 f
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090929
Time 12.36
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 54
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 9195.2
DW 20.850 usec
DE 6.00 usec
TE 292.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.38 usec
PL1 0.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.10 dB
PL13 19.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
164.46
161.47
155.51
135.12
132.28
130.94
128.30
127.08
124.86
123.43
118.20
111.20
77.39
77.07
76.75
25.66
22.13
ppm
130
120
200
180
160
140
120
100
80
60
40
20
0
ppm

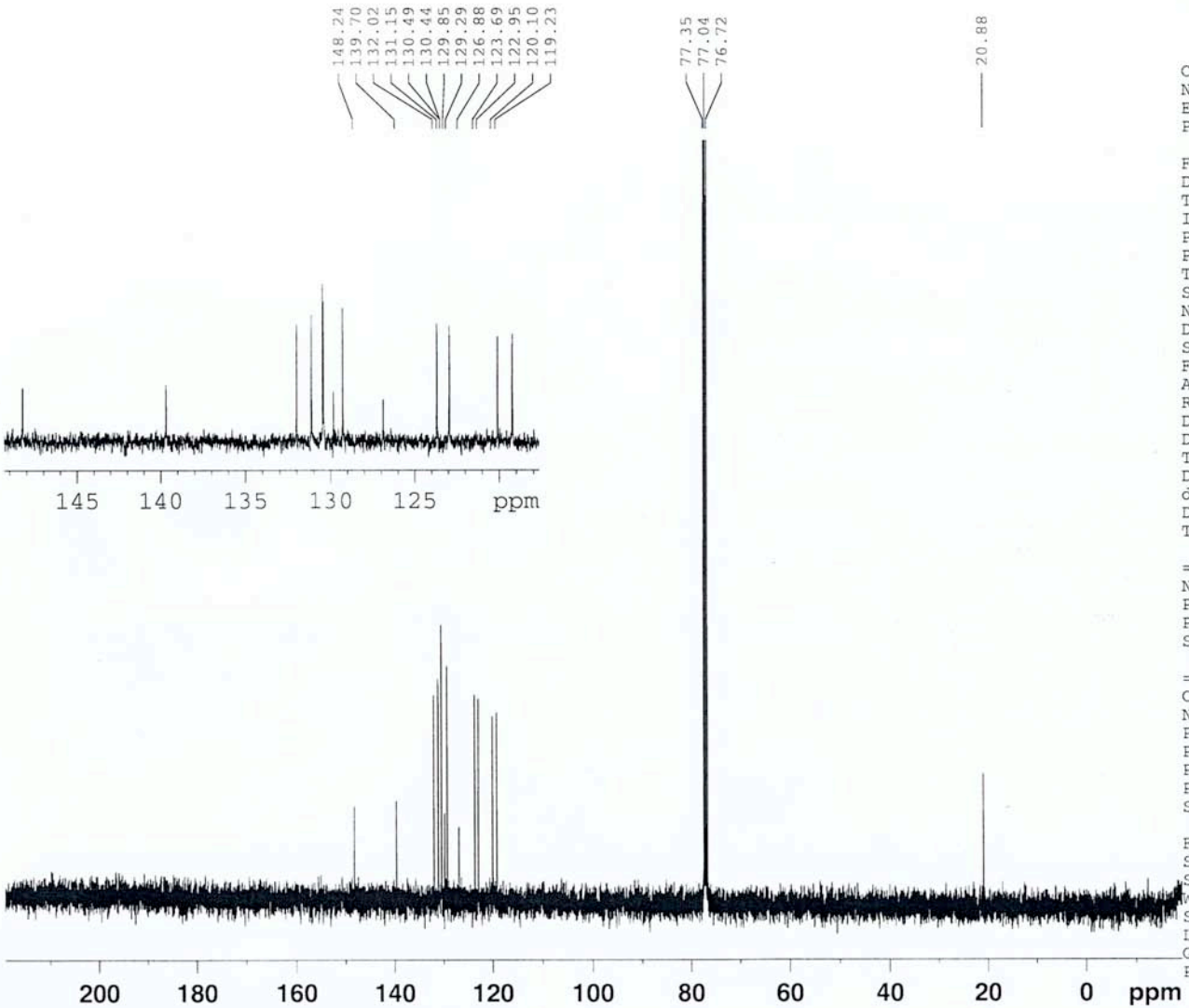







```
Current Data Parameters
NAME                  583-2
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20100327
Time                  9.23
INSTRUM              spect
PROBHD   5 mm QNP 1H/13
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      18
DS                       2
SWH               8278.146 Hz
FIDRES            0.126314 Hz
AQ                3.9584243 sec
RG                      57
DW                  60.400 usec
DE                   6.00 usec
TE                  294.2 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                  14.00 usec
PL1                  0.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                   65536
SF            400.1300220 MHz
WDW                     EM
SSB                      0
LB                   0.30 Hz
GB                       0
PC                    1.00
```





BRUKER

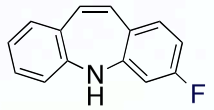
Current Data Parameters
NAME 583-2
EXPNO 1
PROCNO 1

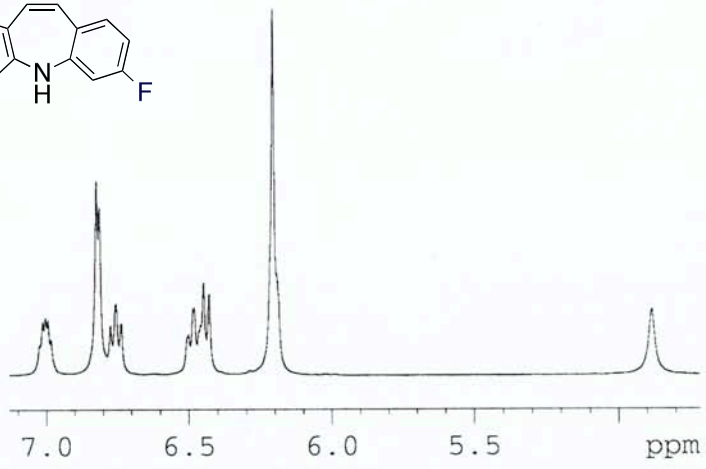
F2 - Acquisition Parameters
Date_ 20100327
Time 9.20
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 1625.5
DW 20.850 usec
DE 6.00 usec
TE 294.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

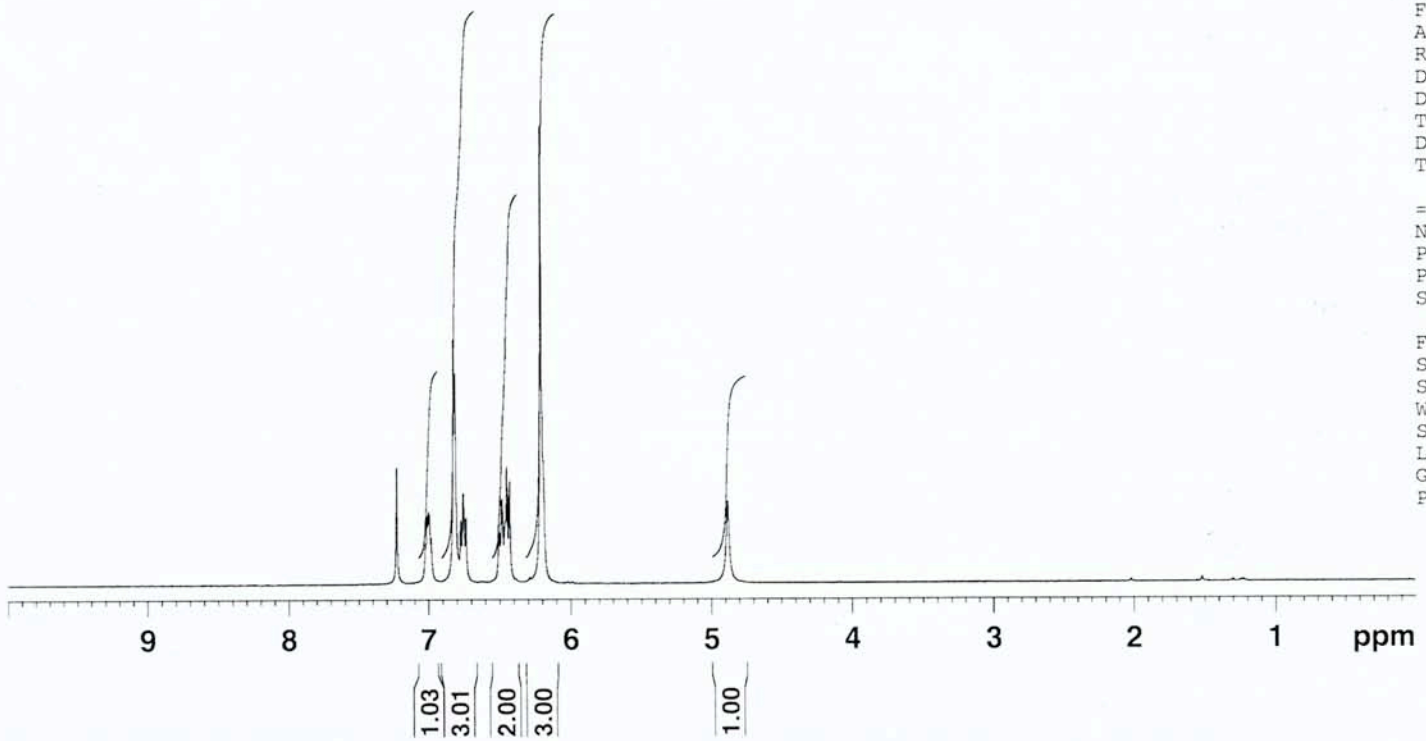
======== CHANNEL f1 ========
NUC1 13C
P1 9.38 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.10 dB
PL13 19.00 dB
SFO2 400.1316005 MHz

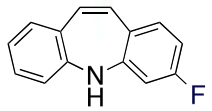
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

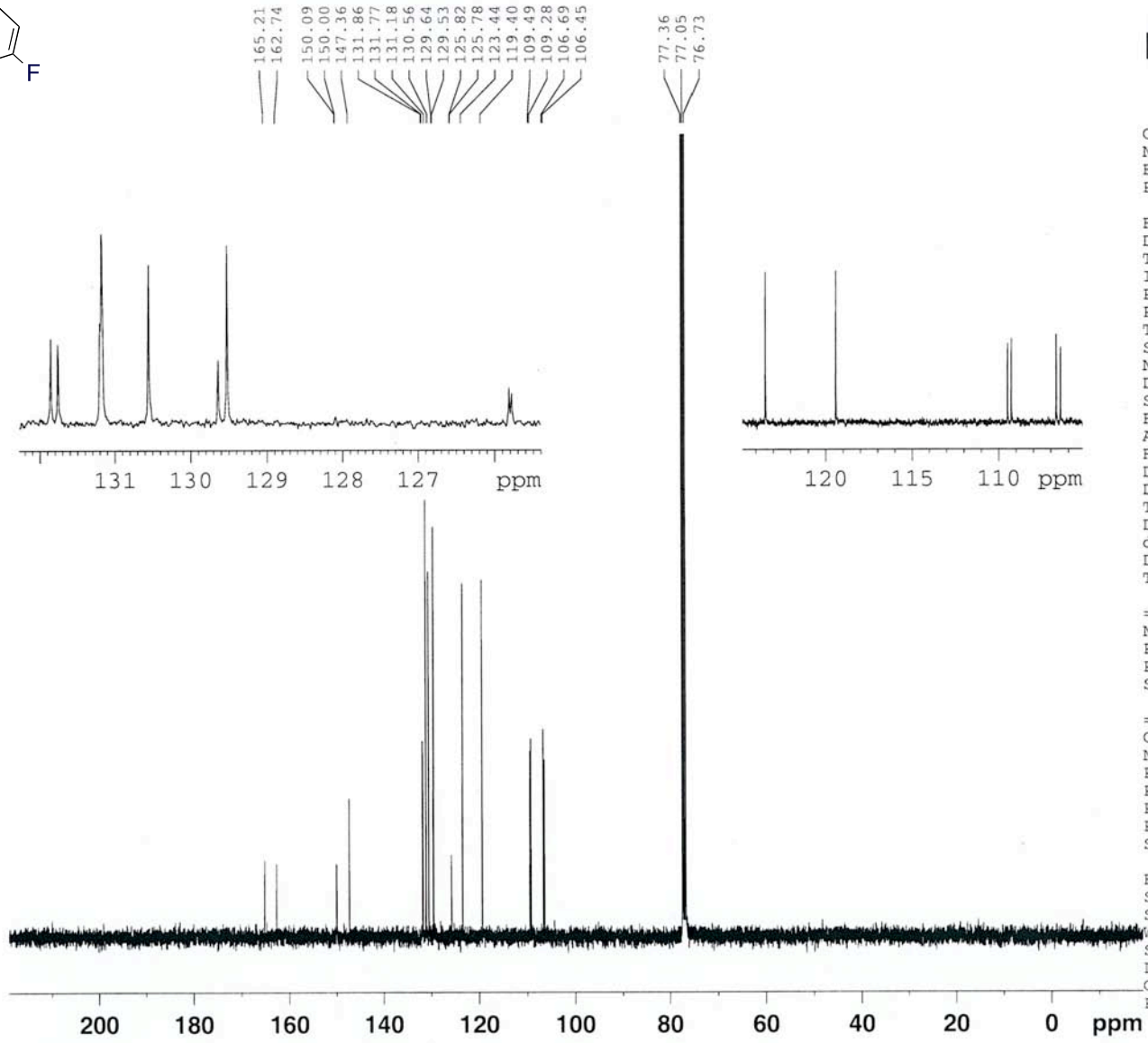






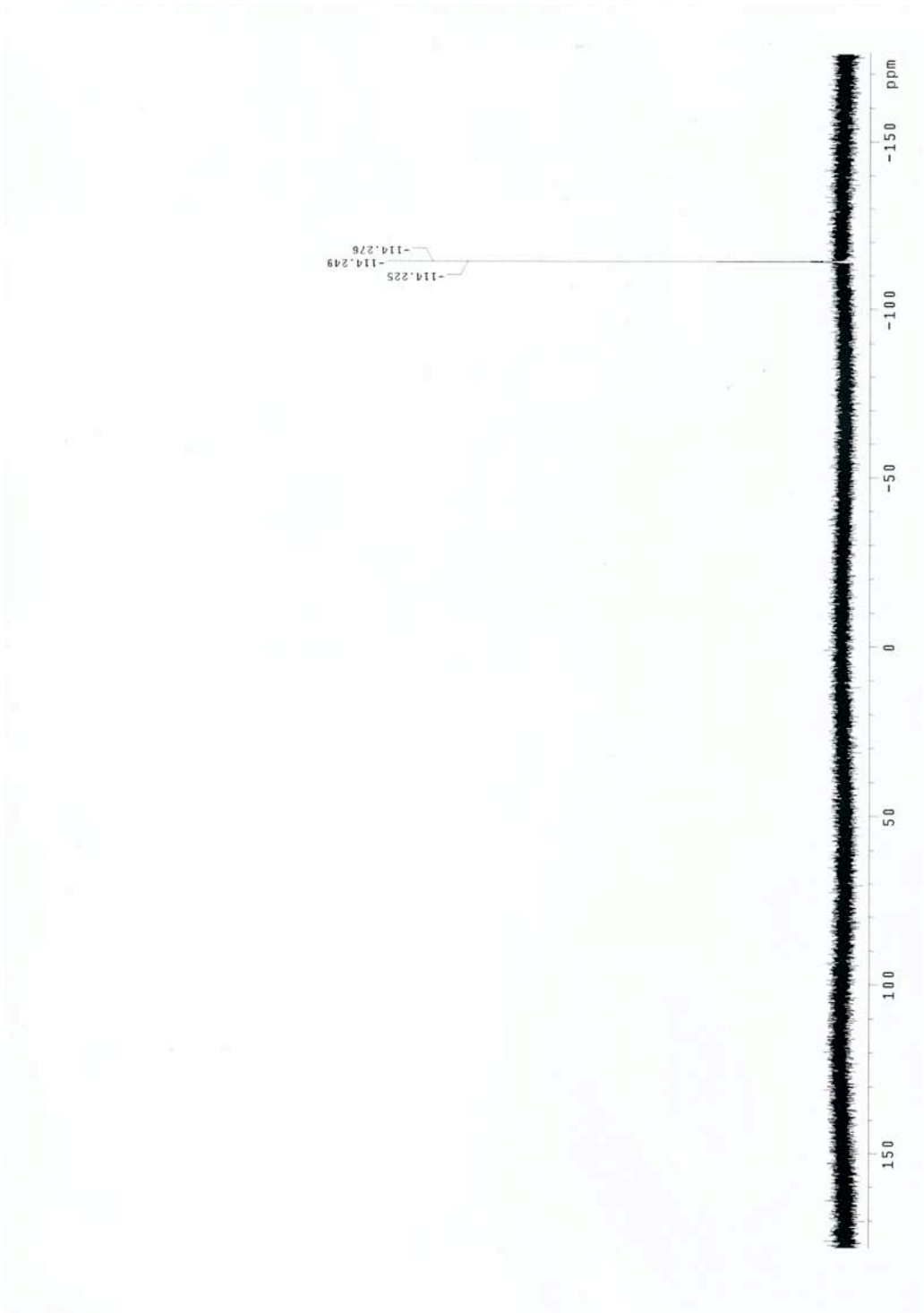

```
Current Data Parameters
NAME                  533-2
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20100327
Time                   9.31
INSTRUM               spect
PROBHD   5 mm QNP 1H/13
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       17
DS                        2
SWH                8278.146 Hz
FIDRES             0.126314 Hz
AQ                 3.9584243 sec
RG                     322.5
DW                    60.400 usec
DE                     6.00 usec
TE                     294.2 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                    14.00 usec
PL1                    0.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                        65536
SF            400.1300220 MHz
WDW                       EM
SSB                        0
LB                     0.30 Hz
GB                         0
PC                      1.00
```

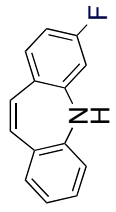


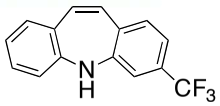


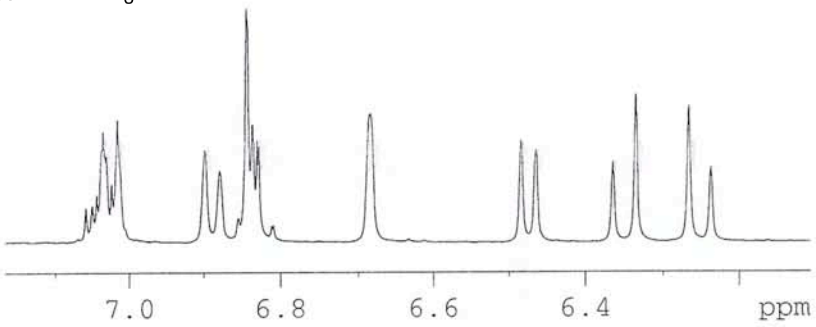
BRUKER

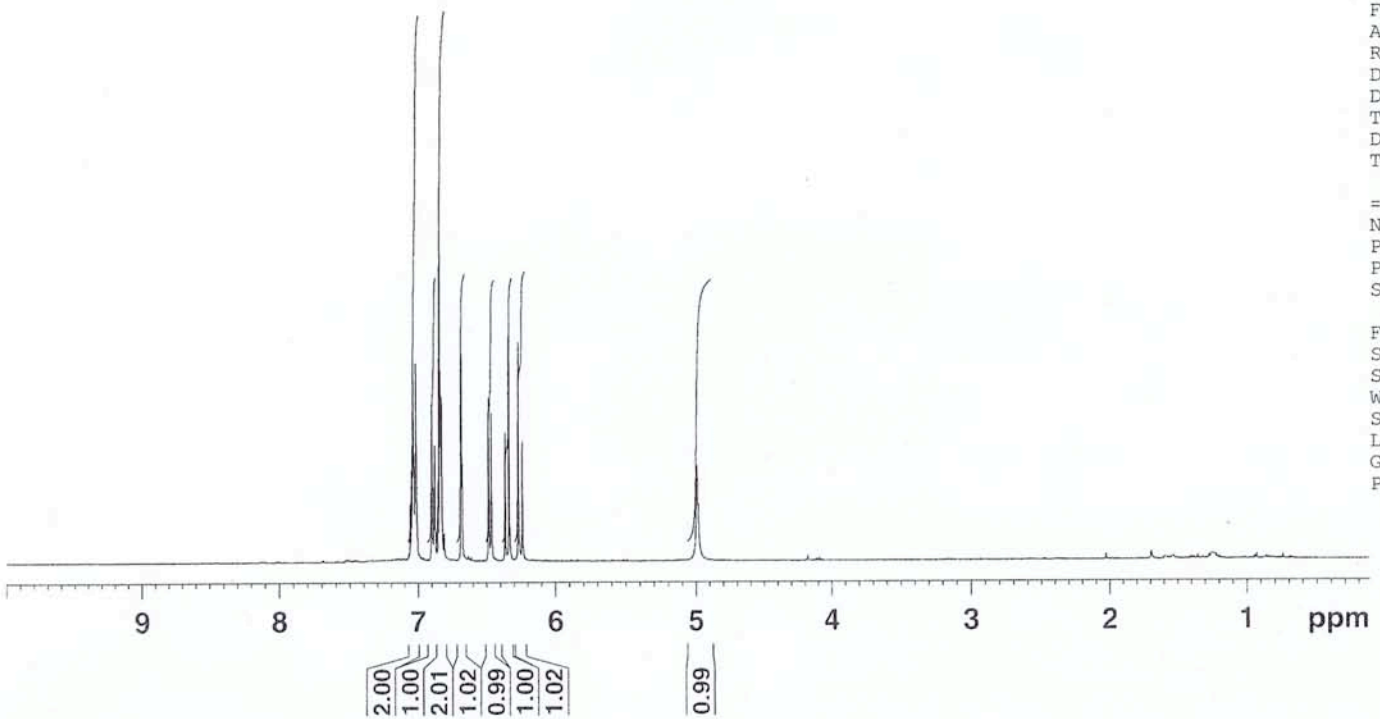
```
Current Data Parameters
NAME                  533 4
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20100331
Time                   8.30
INSTRUM               spect
PROBHD    5 mm QNP 1H/13
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      839
DS                        4
SWH               23980.814 Hz
FIDRES             0.365918 Hz
AQ                1.3664756 sec
RG                   1824.6
DW                   20.850 usec
DE                    6.00 usec
TE                   295.2 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                    9.38 usec
PL1                   0.00 dB
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                   0.00 dB
PL12                 16.10 dB
PL13                 19.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF            100.6127690 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```


-114.225
-114.249
-114.276
150
100
50
0
-50
-100
-150
ppm

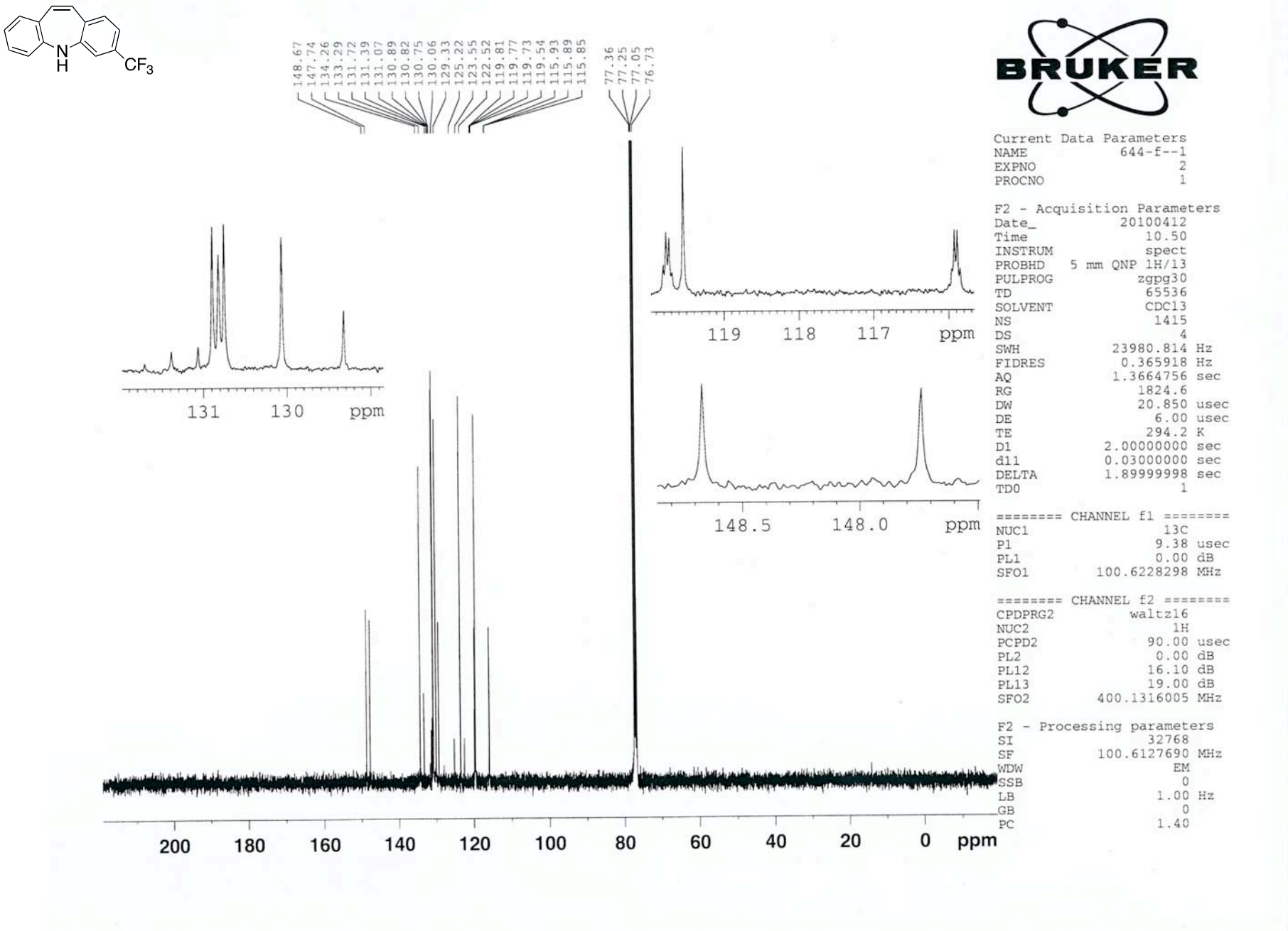

F
NH

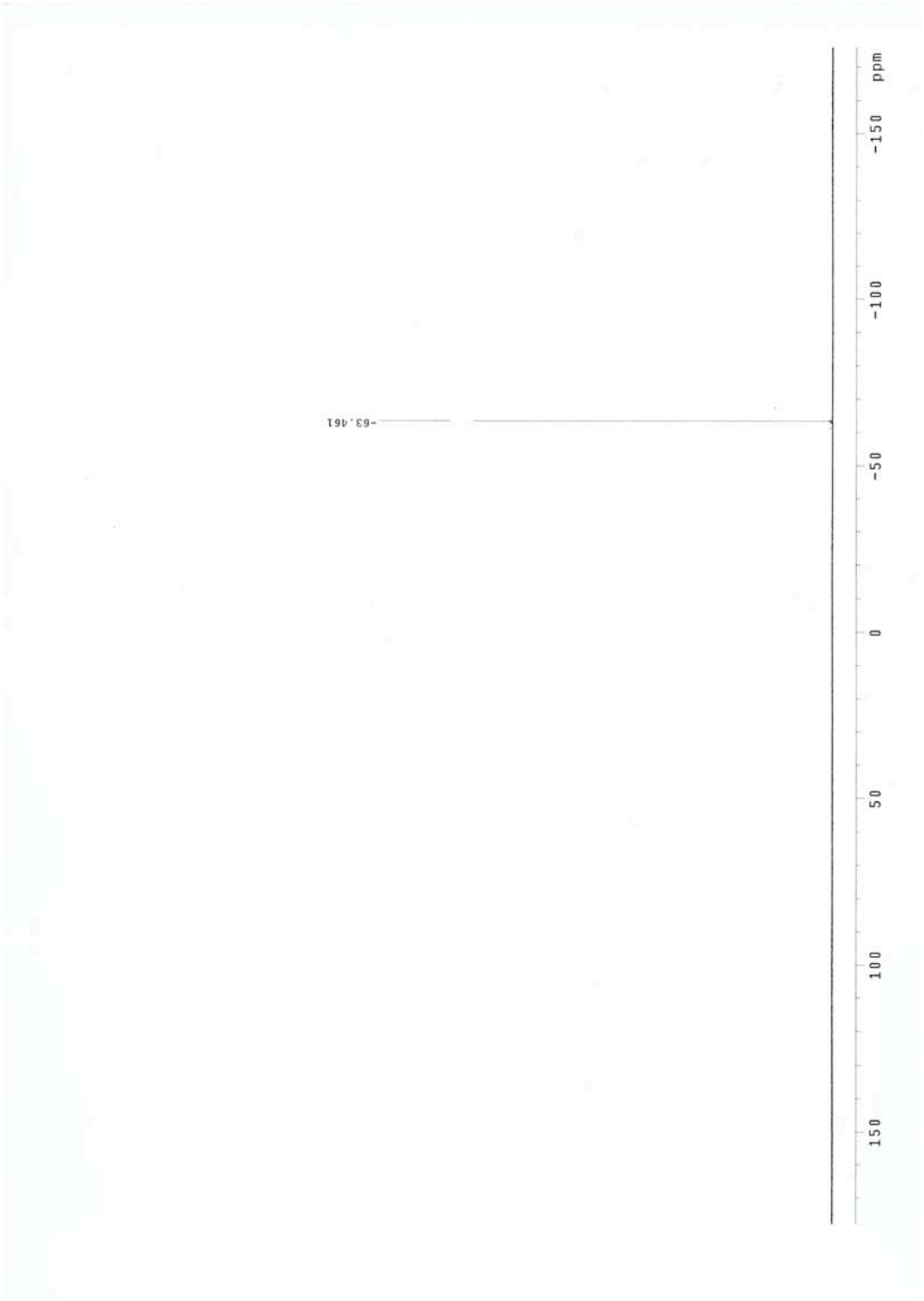


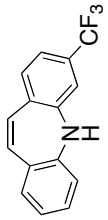


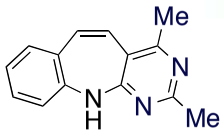


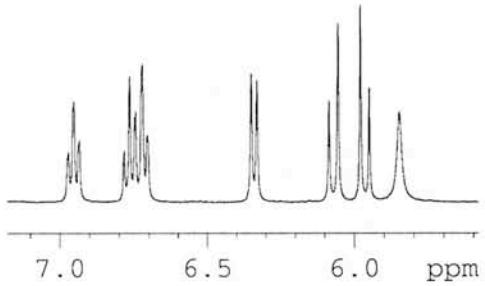

```
Current Data Parameters
NAME                  644-f
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20100408
Time                 11.56
INSTRUM              spect
PROBHD   5 mm QNP 1H/13
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       6
DS                       2
SWH               8278.146 Hz
FIDRES               0.126314 Hz
AQ                3.9584243 sec
RG                      57
DW                   60.400 usec
DE                    6.00 usec
TE                   294.2 K
D1             1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   14.00 usec
PL1                   0.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                   65536
SF            400.1300220 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

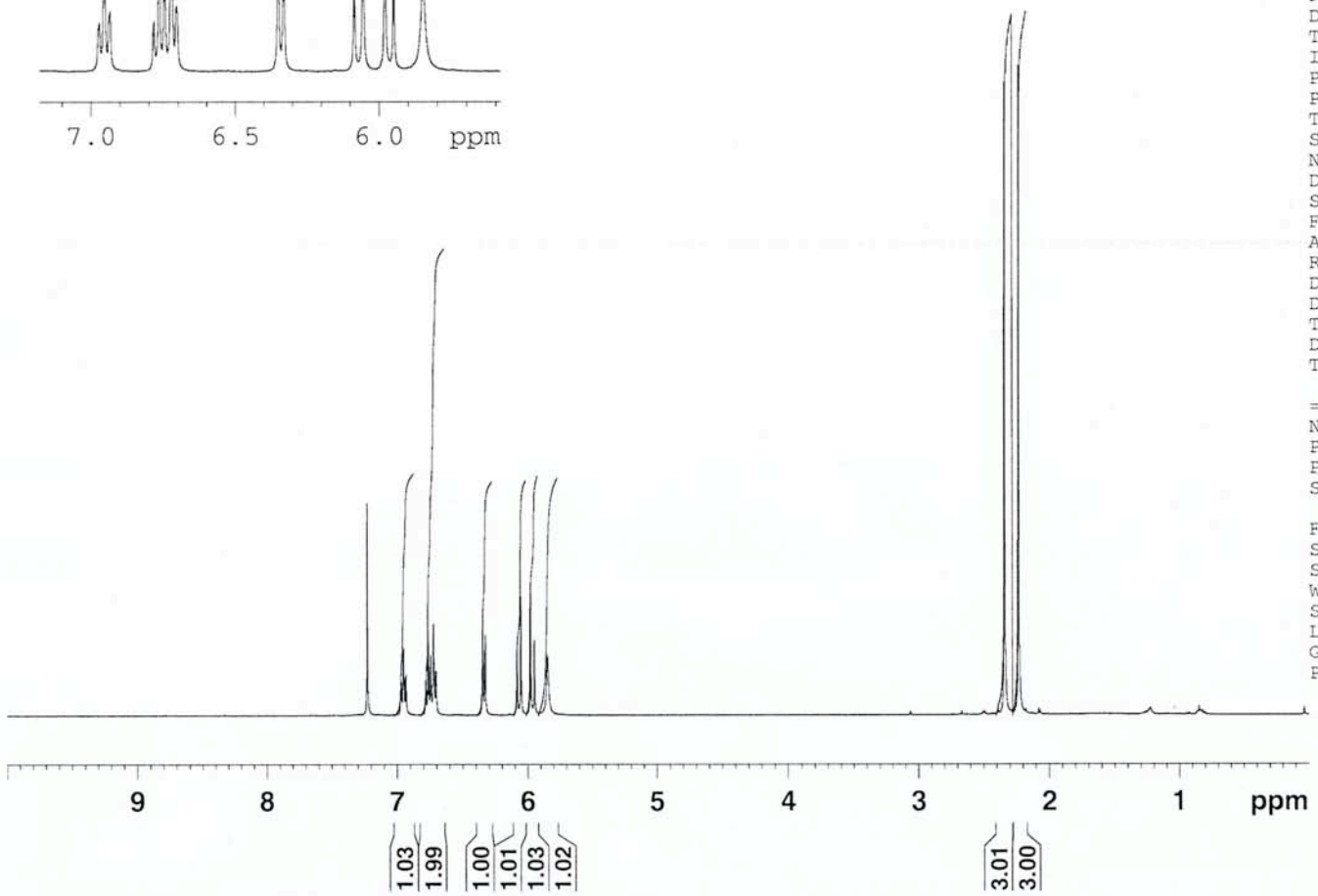

148.67
147.74
134.26
133.29
131.72
131.39
131.07
130.89
130.82
130.75
130.06
129.33
125.22
123.55
122.52
119.81
119.77
119.73
119.54
115.93
115.89
115.85
77.36
77.25
77.05
76.73
131
130
ppm
119
118
117
ppm
148.5
148.0
ppm
200
180
160
140
120
100
80
60
40
20
0
ppm
BRUKER
Current Data Parameters
NAME 644-f--1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100412
Time 10.50
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1415
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 1824.6
DW 20.850 usec
DE 6.00 usec
TE 294.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.38 usec
PL1 0.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.10 dB
PL13 19.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


-63.461
150
100
50
0
-50
-100
-150
ppm

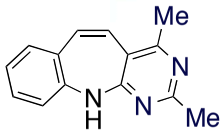

CF3
N
H

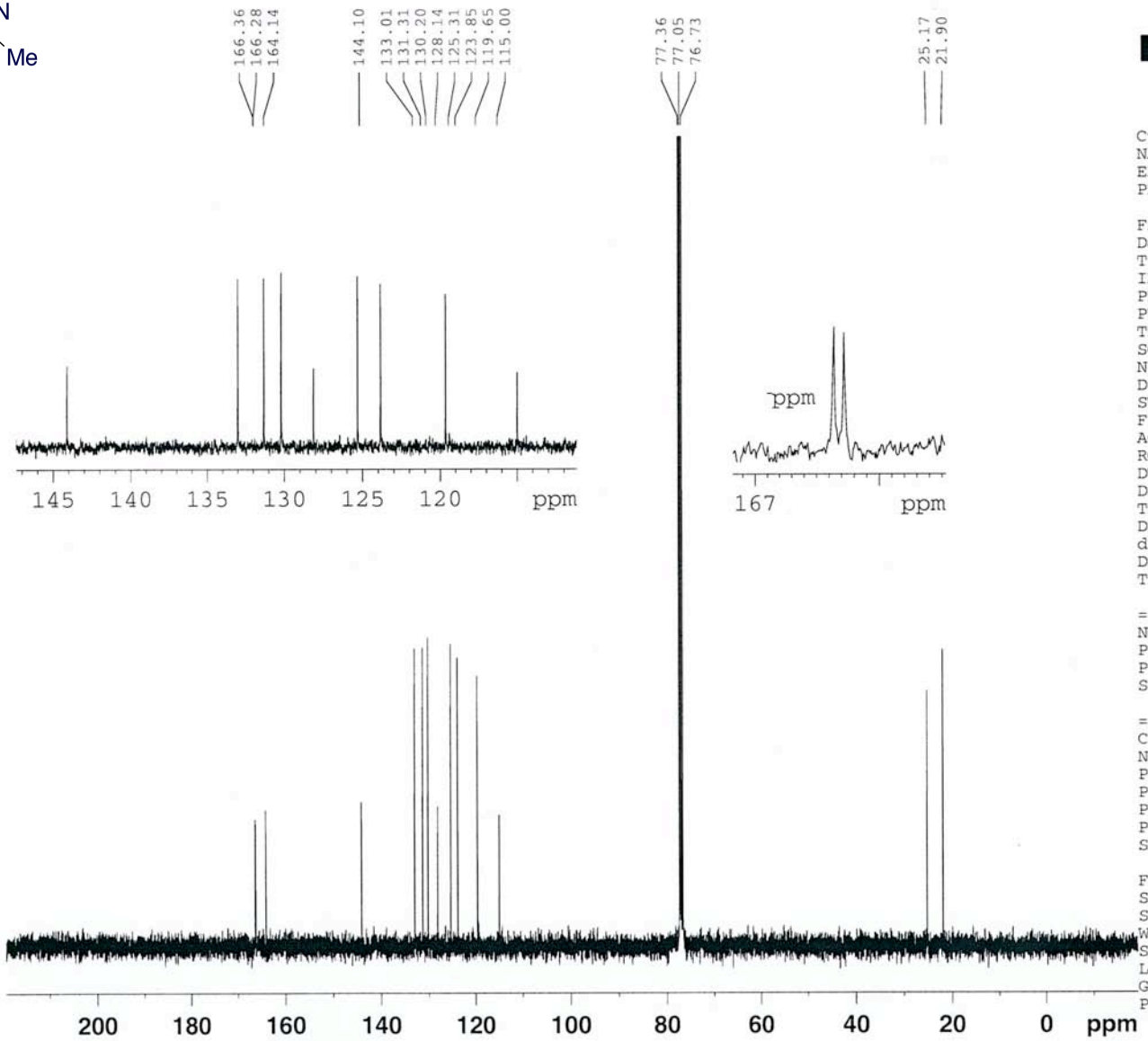







```
Current Data Parameters
NAME                  559 1
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20091217
Time                 17.20
INSTRUM              spect
PROBHD    5 mm QNP 1H/13
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               8278.146 Hz
FIDRES            0.126314 Hz
AQ                3.9584243 sec
RG                     512
DW                  60.400 usec
DE                   6.00 usec
TE                  292.2 K
D1             1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                  14.00 usec
PL1                  0.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                   65536
SF            400.1300220 MHz
WDW                     EM
SSB                      0
LB                   0.30 Hz
GB                       0
PC                    1.00
```

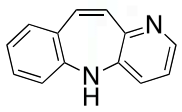


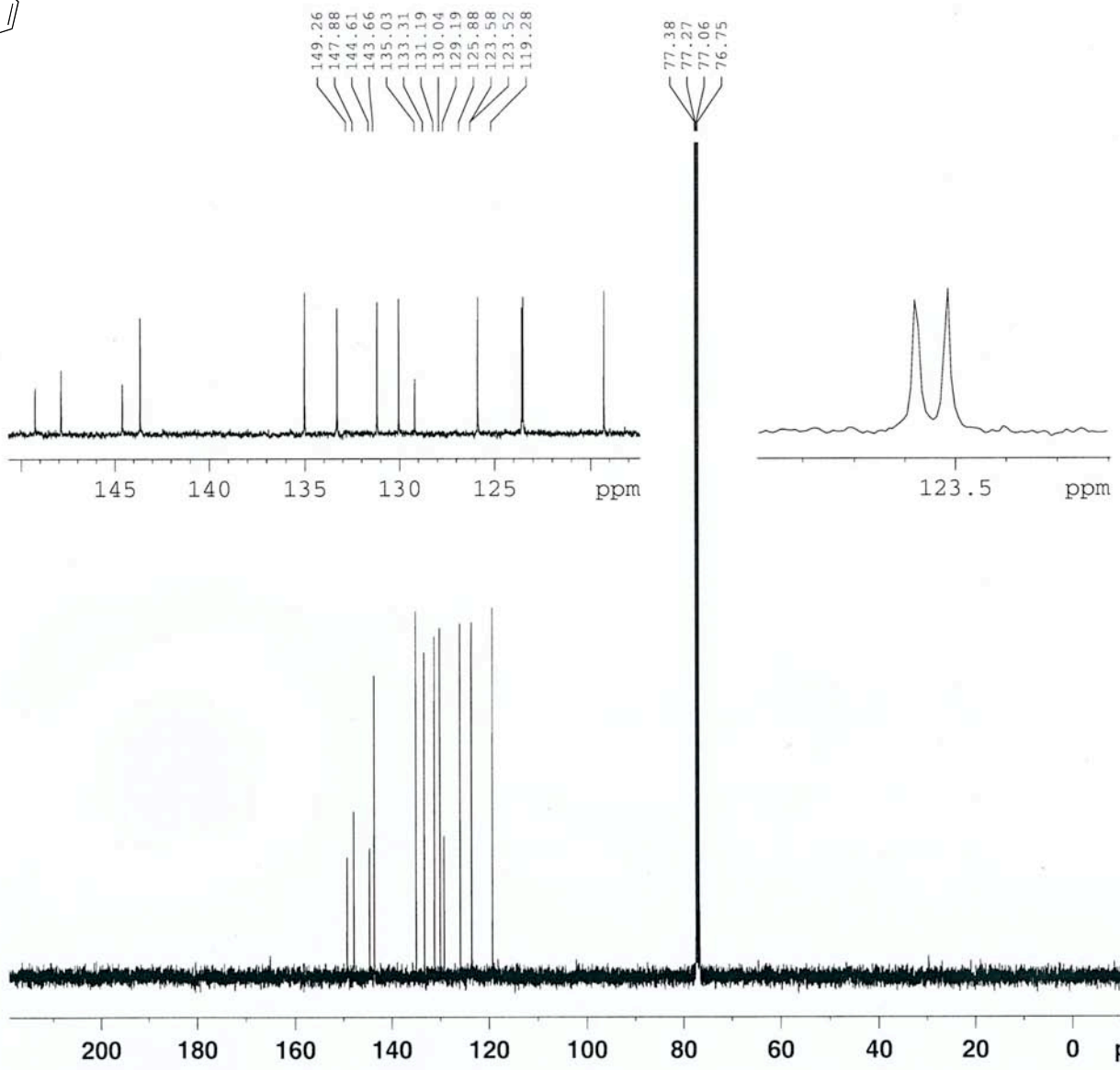


BRUKER

```
Current Data Parameters
NAME                   3N
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20100406
Time                9.58
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  576
DS                    4
SWH           23980.814 Hz
FIDRES        0.365918 Hz
AQ            1.3664756 sec
RG              11585.2
DW               20.850 usec
DE                6.00 usec
TE               294.2 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                  9.38 usec
PL1                 0.00 dB
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              90.00 usec
PL2                 0.00 dB
PL12               16.10 dB
PL13               19.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                  32768
SF          100.6127690 MHz
WDW                    EM
SSB                     0
LB                 1.00 Hz
GB                      0
PC                   1.40
```

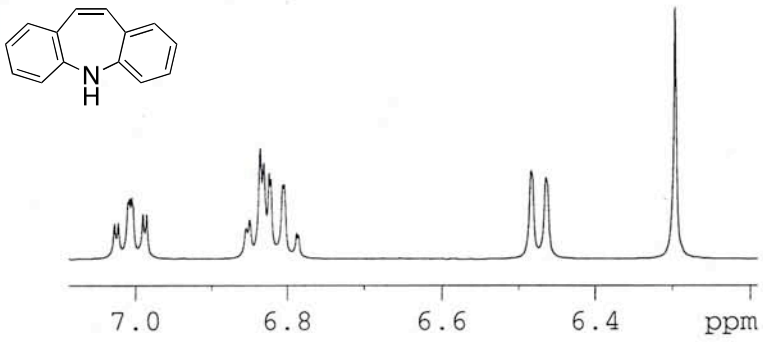
BRUKER
Current Data Parameters
NAME 644-c--1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100412
Time 9.12
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 77
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 362
DW 60.400 usec
DE 6.00 usec
TE 294.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 65536
SF 400.1300220 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.0
7.5
7.0
6.5 ppm
9
8
7
6
5
4
3
2
1 ppm
1.00
1.08
3.07
1.07
3.07
1.07

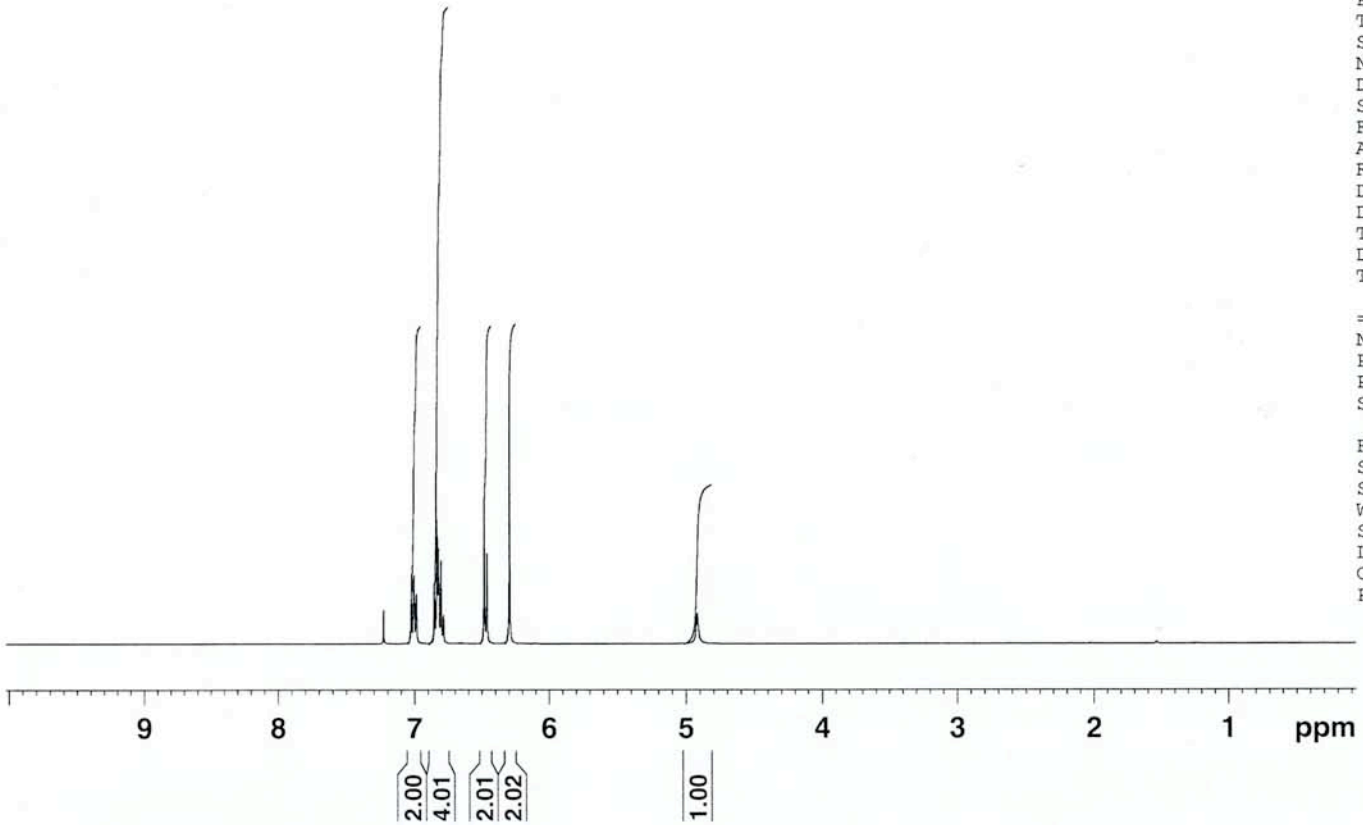




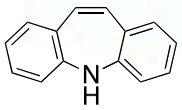
BRUKER

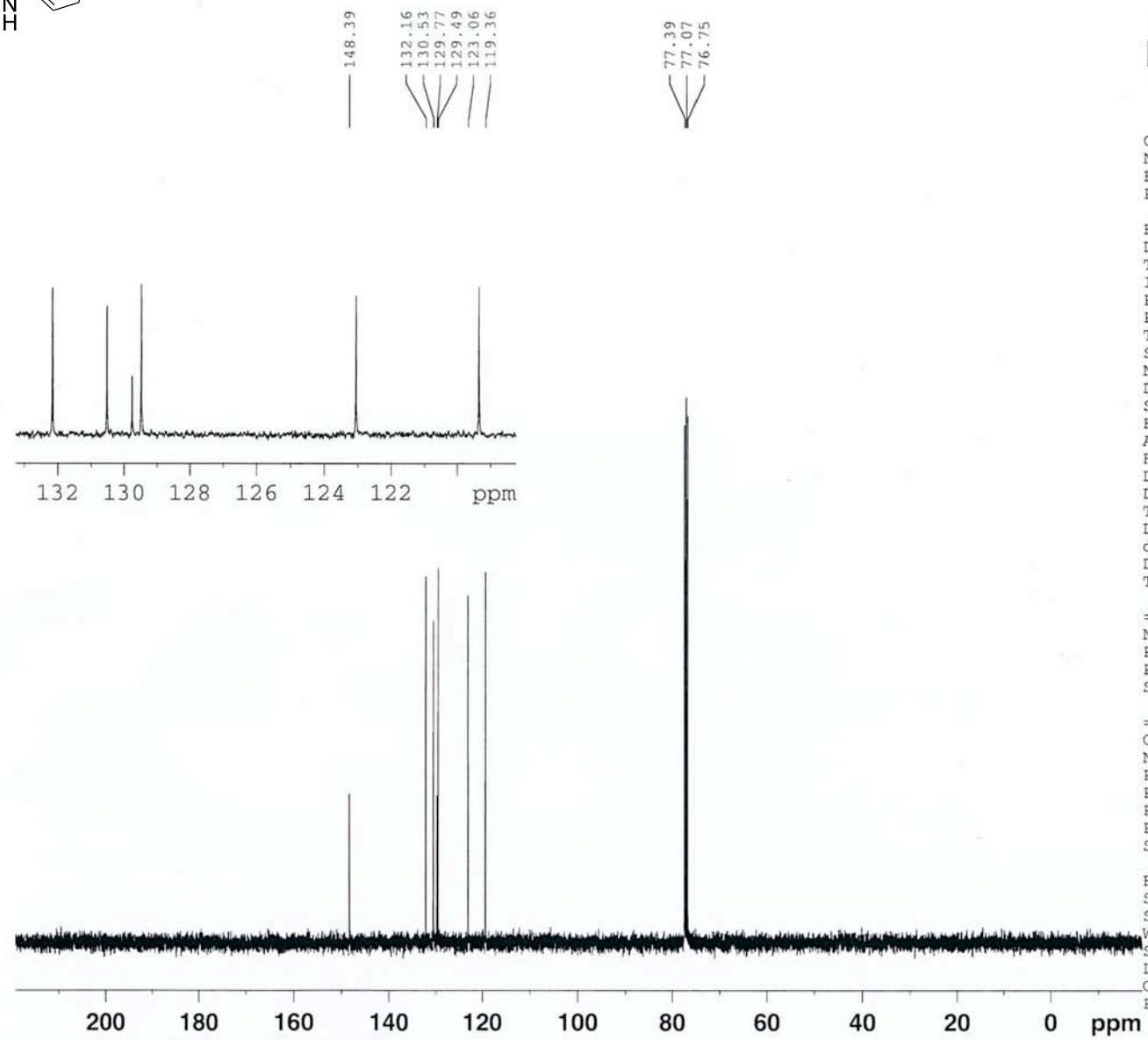
```
Current Data Parameters
NAME                  644-c
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20100408
Time                 11.37
INSTRUM              spect
PROBHD    5 mm QNP 1H/13
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     345
DS                       4
SWH             23980.814 Hz
FIDRES              0.365918 Hz
AQ                1.3664756 sec
RG                   1824.6
DW                  20.850 usec
DE                   6.00 usec
TE                  294.2 K
D1               2.00000000 sec
d11              0.03000000 sec
DELTA            1.89999998 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                   9.38 usec
PL1                  0.00 dB
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2               90.00 usec
PL2                  0.00 dB
PL12                16.10 dB
PL13                19.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF            100.6127690 MHz
WDW                     EM
SSB                      0
LB                   1.00 Hz
GB                       0
PC                    1.40
```





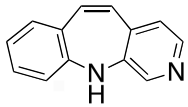

```
Current Data Parameters
NAME      Dibenzazepine-1
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20100330
Time                  8.16
INSTRUM              spect
PROBHD   5 mm QNP 1H/13
PULPROG               zg30
TD                   65536
SOLVENT              CDC13
NS                      11
DS                       2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 sec
RG                   322.5
DW                60.400 usec
DE                 6.00 usec
TE                294.2 K
D1             1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                  14.00 usec
PL1                  0.00 dB
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                   65536
SF           400.1300220 MHz
WDW                     EM
SSB                      0
LB                  0.30 Hz
GB                       0
PC                    1.00
```

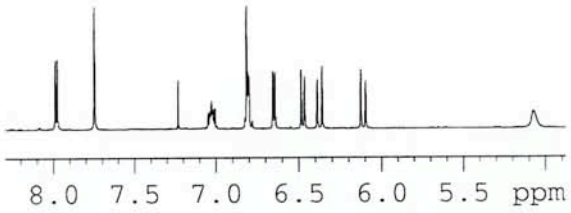


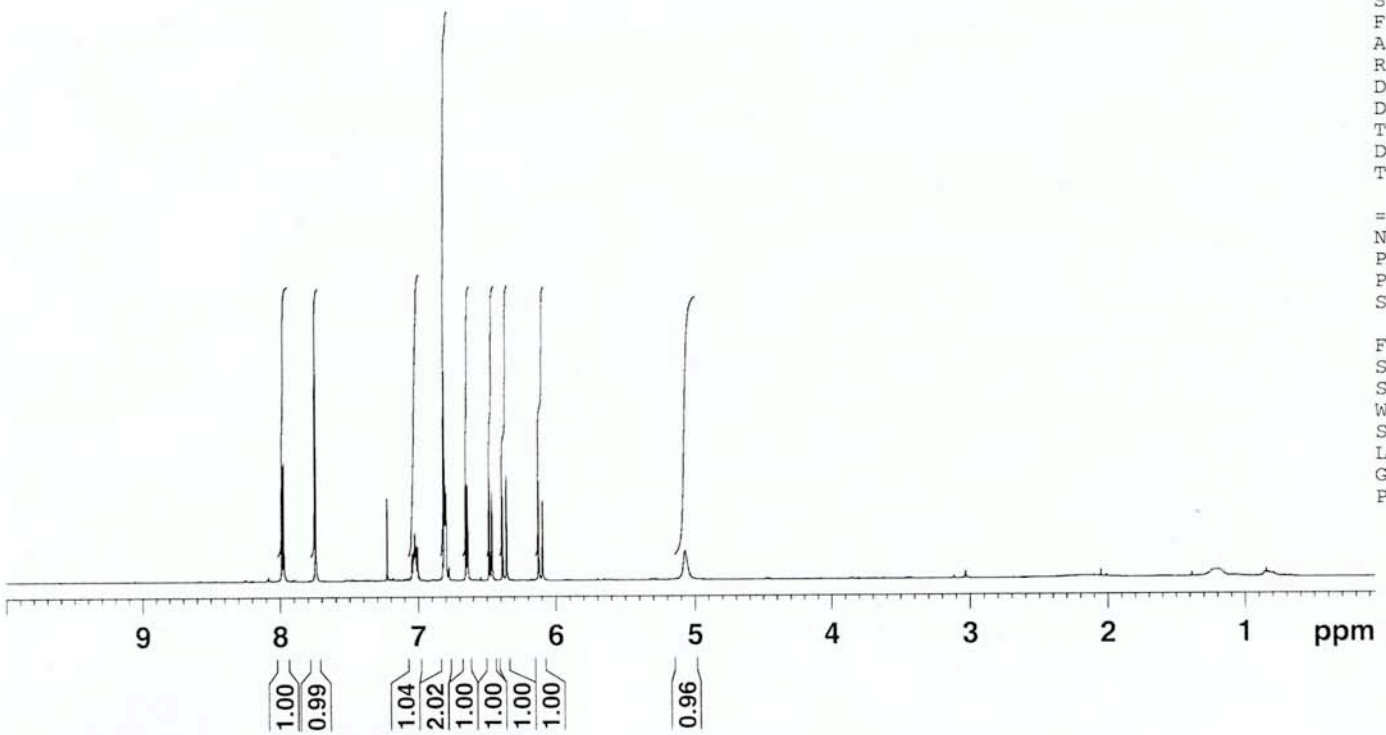


BRUKER

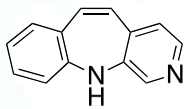
```
Current Data Parameters
NAME      Dibenzazepine-1
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20100330
Time                8.27
INSTRUM             spect
PROBHD   5 mm QNP 1H/13
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                     85
DS                      4
SWH             23980.814 Hz
FIDRES           0.365918 Hz
AQ               1.3664756 sec
RG                  1824.6
DW                  20.850 usec
DE                   6.00 usec
TE                  294.2 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.38 usec
PL1                   0.00 dB
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2                90.00 usec
PL2                   0.00 dB
PL12                 16.10 dB
PL13                 19.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF            100.6127690 MHz
WDW                      EM
SSB                       0
LB                    1.00 Hz
GB                        0
PC                    1.40
```





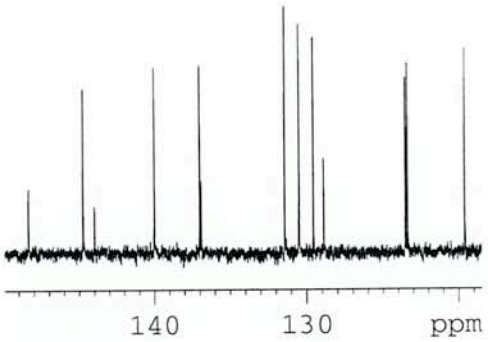


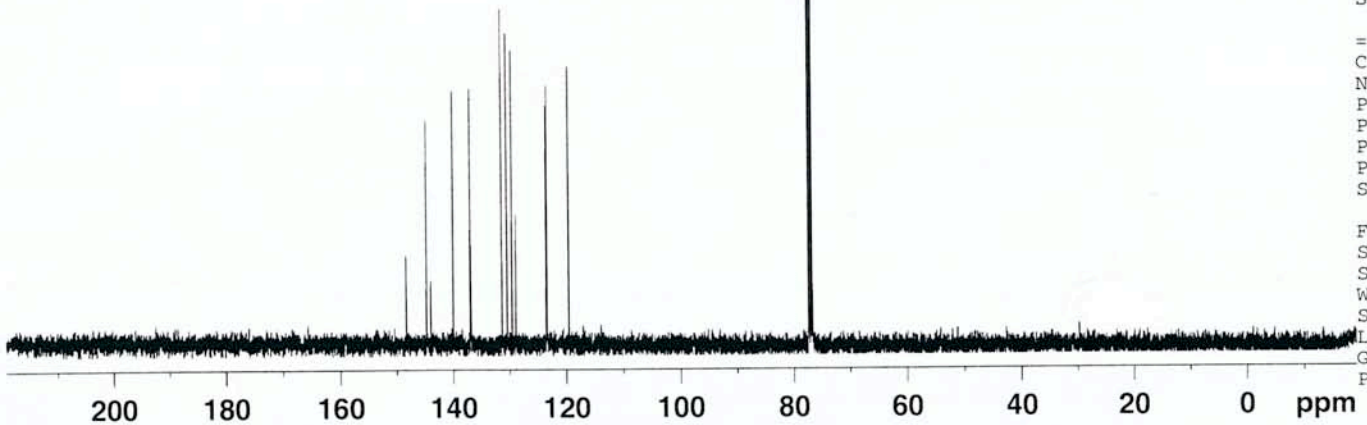

```
Current Data Parameters
NAME                  517-2
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20100320
Time                   9.54
INSTRUM               spect
PROBHD    5 mm QNP 1H/13
PULPROG                zg30
TD                    65536
SOLVENT               CDC13
NS                       16
DS                        2
SWH                8278.146 Hz
FIDRES            0.126314 Hz
AQ                3.9584243 sec
RG                       57
DW                  60.400 usec
DE                   6.00 usec
TE                   293.2 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                  14.00 usec
PL1                  0.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                    65536
SF            400.1300220 MHz
WDW                      EM
SSB                       0
LB                   0.30 Hz
GB                        0
PC                     1.00
```



148.38
144.75
144.01
140.02
137.00
136.88
131.43
130.50
129.57
128.90
123.52
123.38
119.60

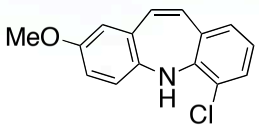
77.37
77.06
76.74

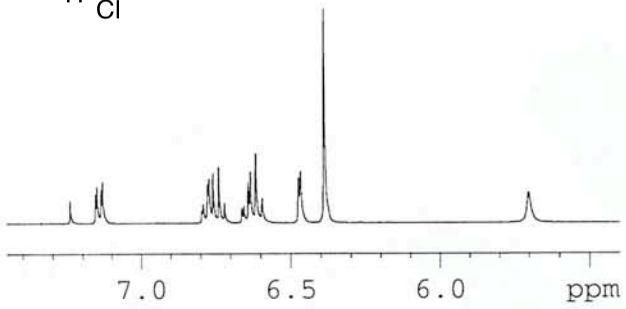


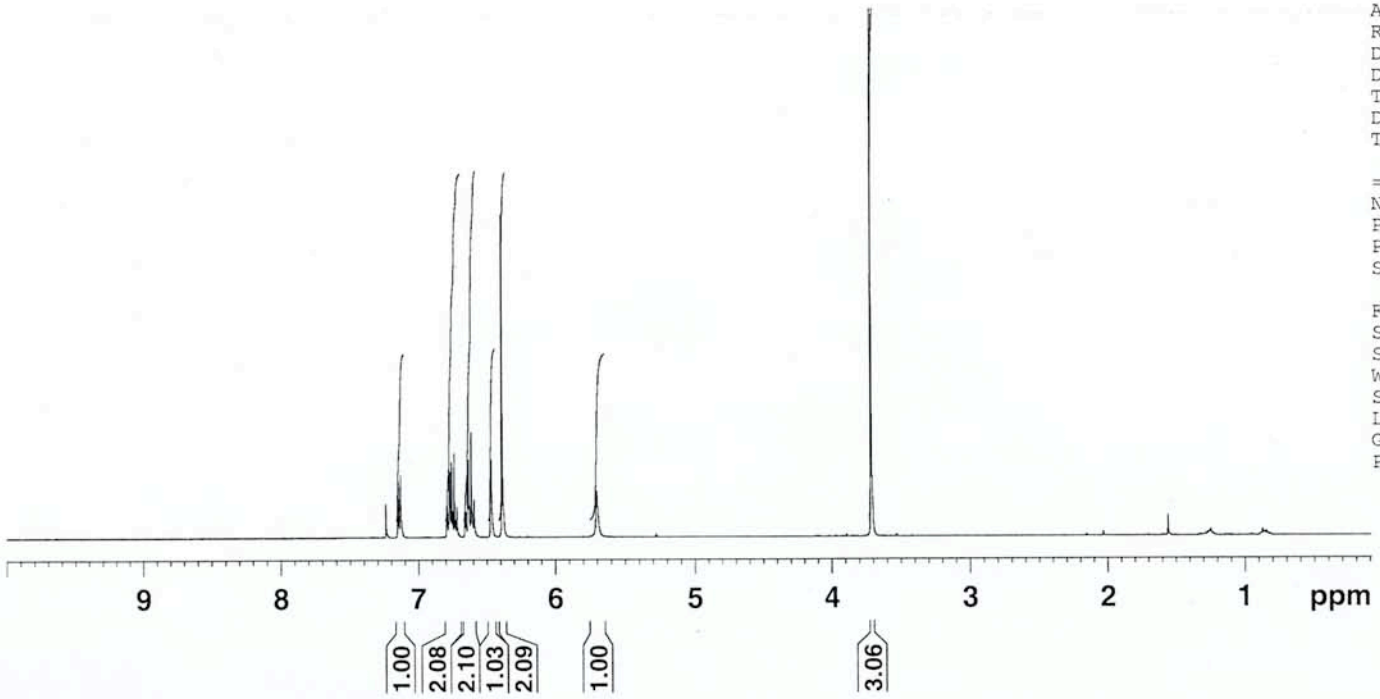


BRUKER

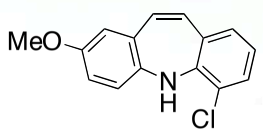
```
Current Data Parameters
NAME                  517-1
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20100320
Time                   9.50
INSTRUM               spect
PROBHD   5 mm QNP 1H/13
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     119
DS                       4
SWH              23980.814 Hz
FIDRES           0.365918 Hz
AQ               1.3664756 sec
RG                  2580.3
DW                  20.850 usec
DE                   6.00 usec
TE                  294.2 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                  9.38 usec
PL1                 0.00 dB
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                   1H
PCPD2              90.00 usec
PL2                 0.00 dB
PL12               16.10 dB
PL13               19.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF           100.6127690 MHz
WDW                     EM
SSB                      0
LB                  1.00 Hz
GB                       0
PC                   3.00
```







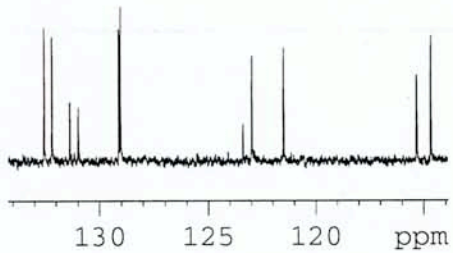

```
Current Data Parameters
NAME                  635
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20100302
Time                8.52
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 sec
RG                 228.1
DW                60.400 usec
DE                 6.00 usec
TE                294.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.00 usec
PL1                0.00 dB
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF          400.1300175 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                  1.00
```

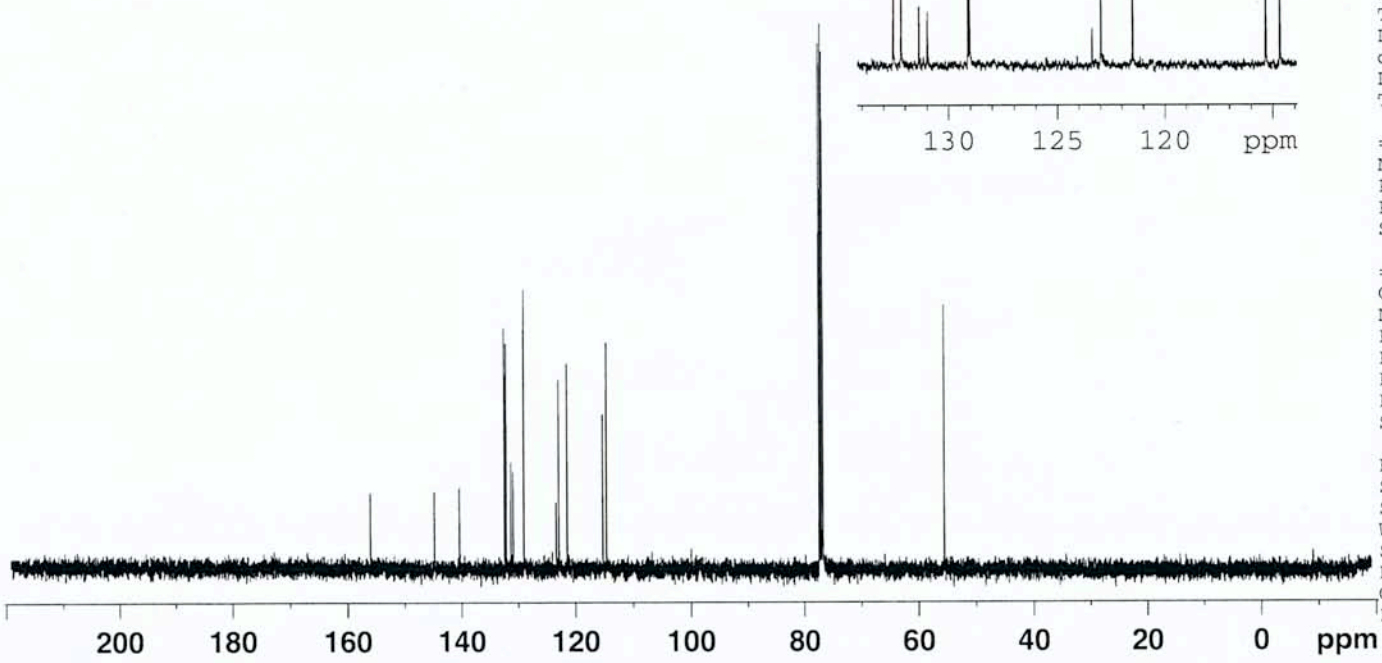


156.12
144.86
140.46
132.54
132.18
131.36
130.98
129.09
129.02
123.38
122.97
121.49
115.32
114.67

77.37
77.05
76.73

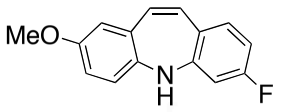
55.57

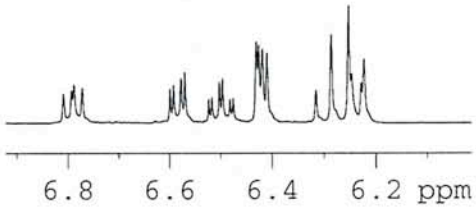


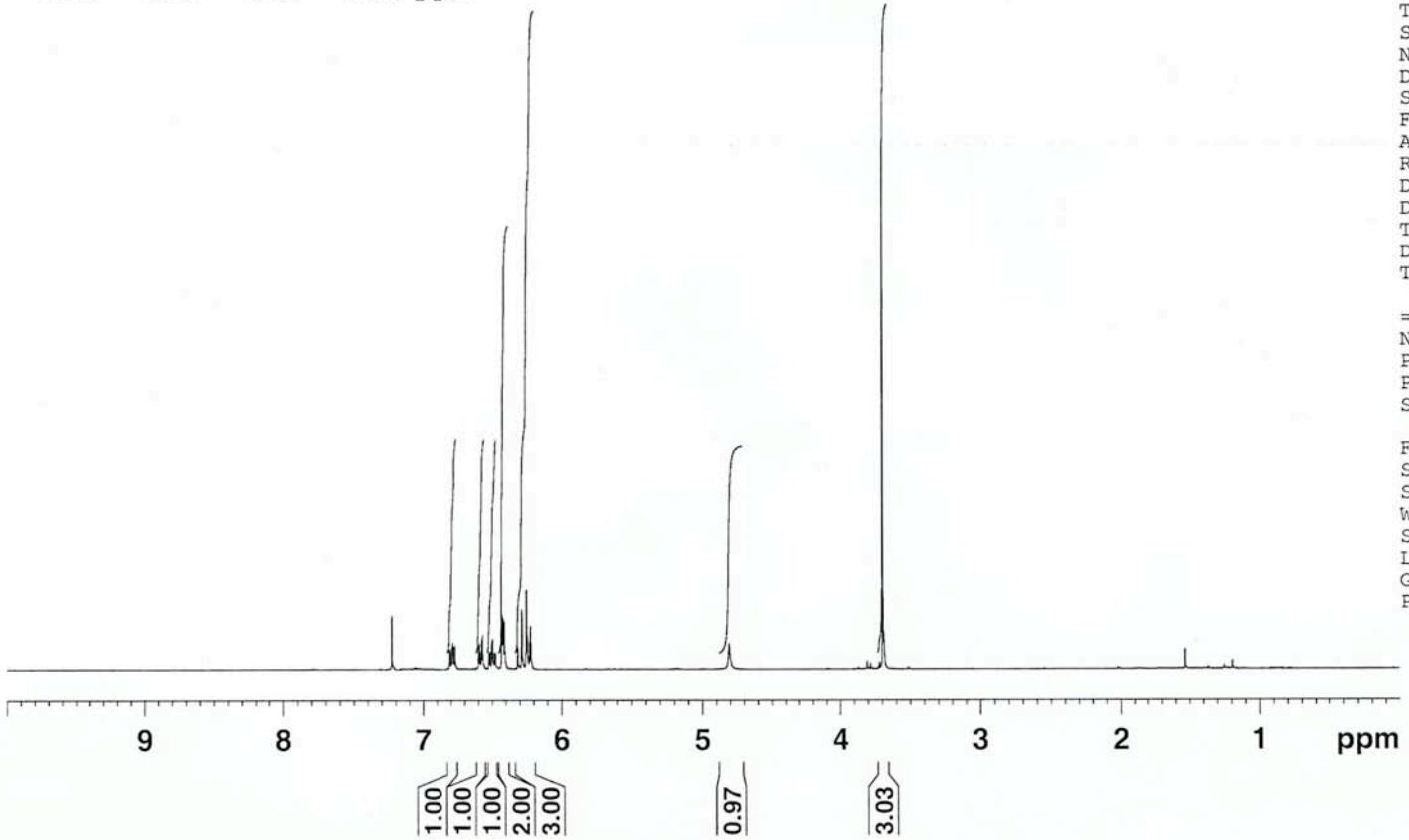


BRUKER

```
Current Data Parameters
NAME                  635
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20100302
Time                9.06
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  118
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                1824.6
DW                20.850 usec
DE                 6.00 usec
TE                295.2 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.38 usec
PL1                0.00 dB
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2           90.00 usec
PL2                0.00 dB
PL12              16.10 dB
PL13              19.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                  1.40
```

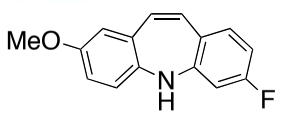






BRUKER

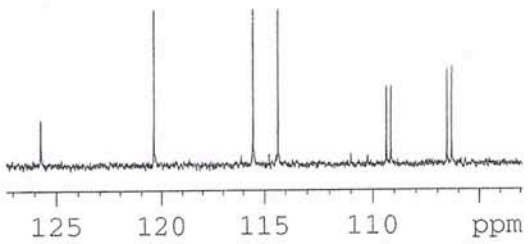
```
Current Data Parameters
NAME                  617
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20100224
Time                9.04
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 sec
RG                 322.5
DW                60.400 usec
DE                 6.00 usec
TE                294.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.00 usec
PL1                0.00 dB
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF          400.1300220 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```

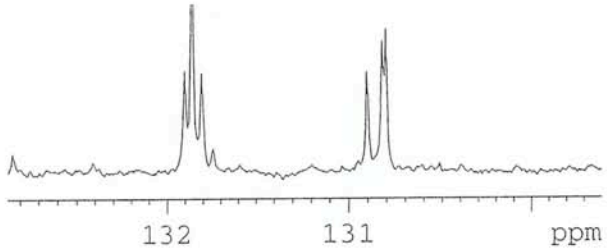


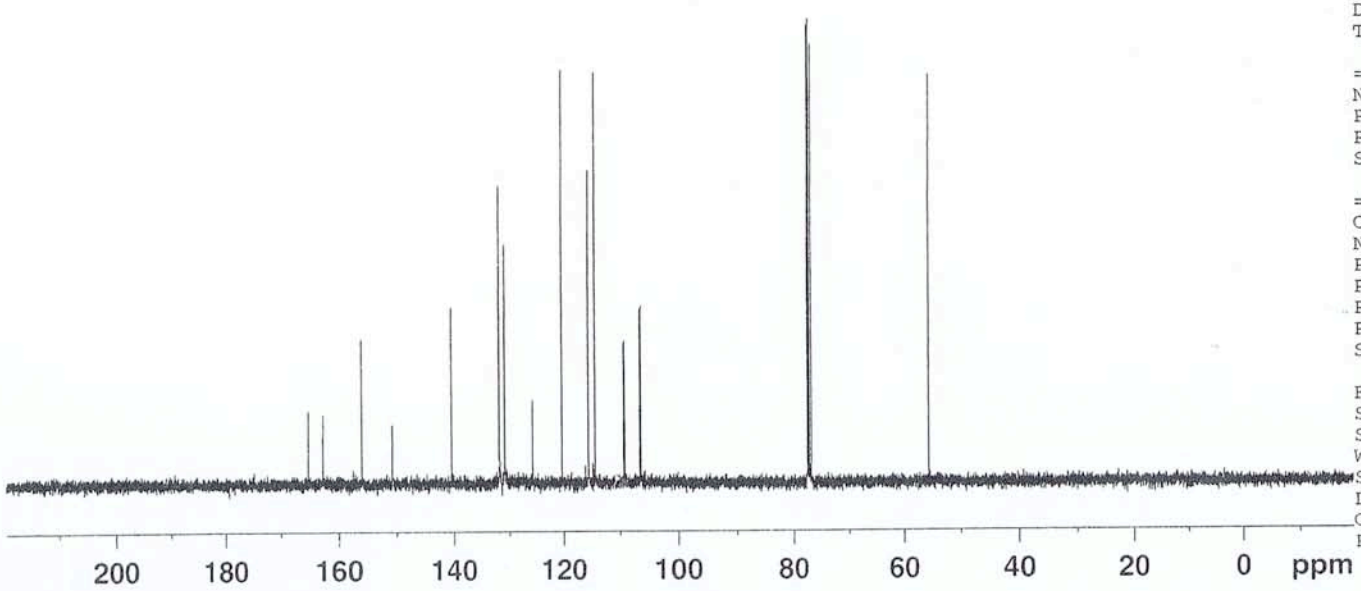
165.21
162.75
156.04
150.81
150.72
140.44
131.91
131.87
131.81
130.91
130.83
130.81
125.72
125.69
120.36
115.55
114.36
109.38
109.17
106.57
106.33

77.44
77.12
76.80

55.54







BRUKER

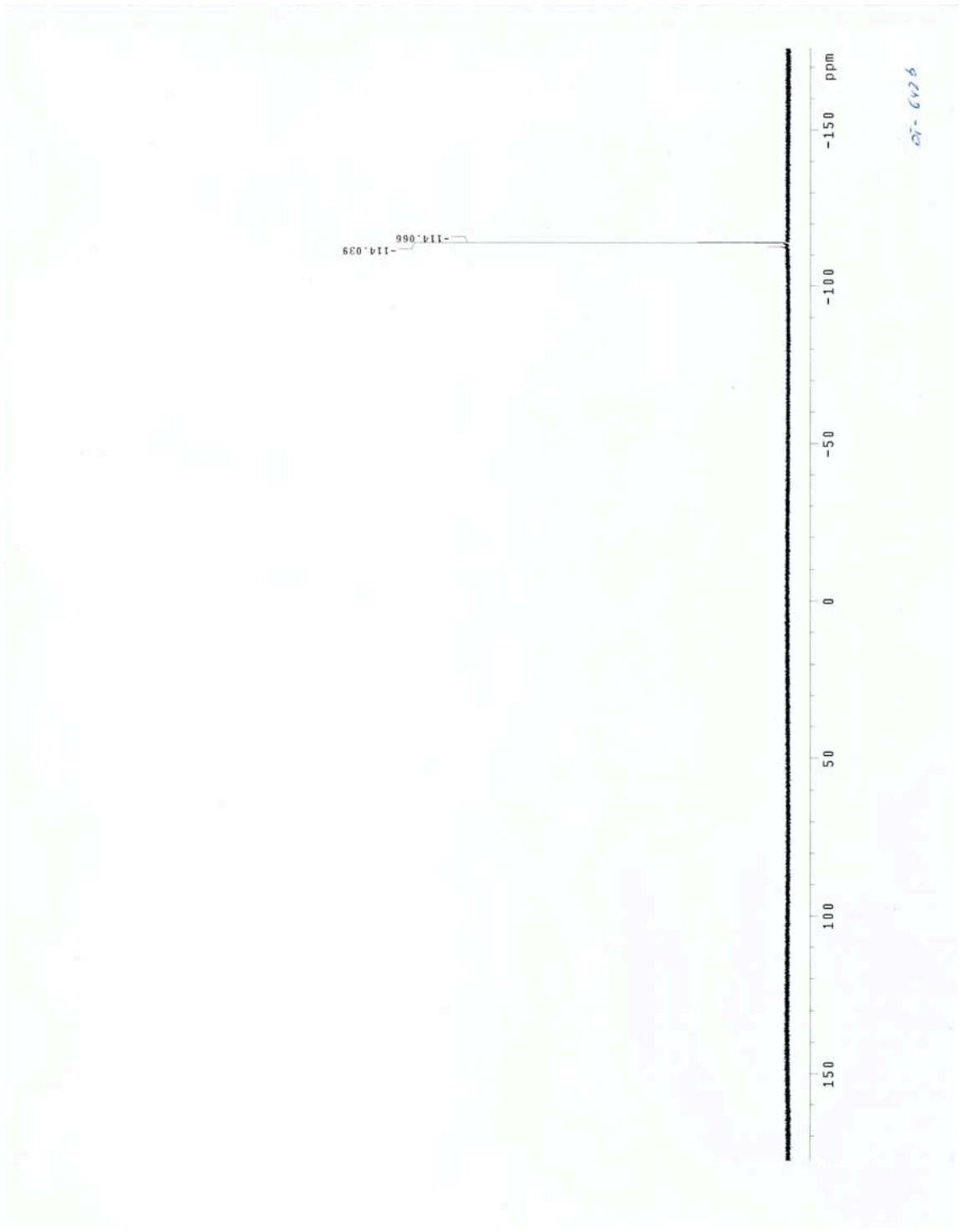
Current Data Parameters
NAME 642-b 5
EXPNO 1
PROCNO 1

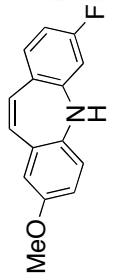
F2 - Acquisition Parameters
Date_ 20100406
Time 19.32
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 113
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 1824.6
DW 20.850 usec
DE 6.00 usec
TE 294.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

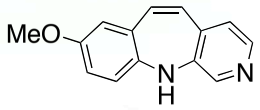
======== CHANNEL f1 ========
NUC1 13C
P1 9.38 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

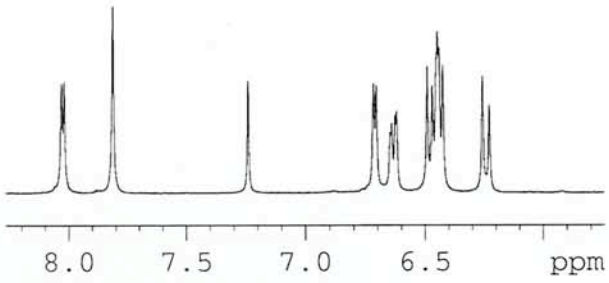
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.10 dB
PL13 19.00 dB
SFO2 400.1316005 MHz

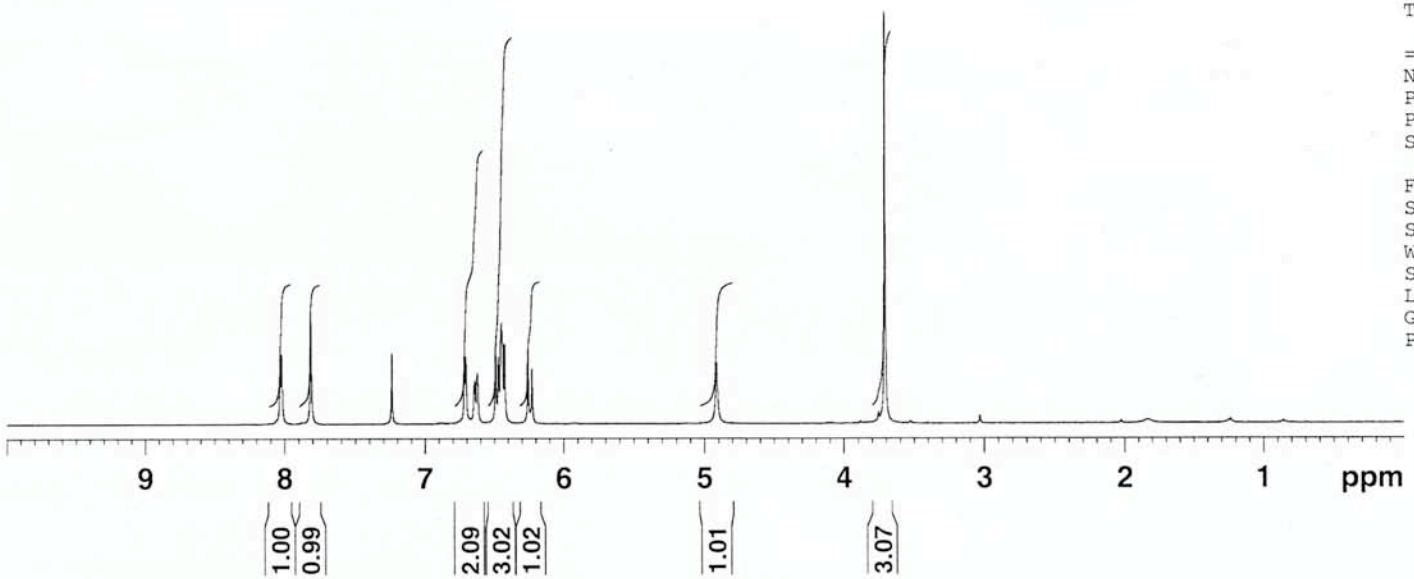
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 3.00


-114.039
-114.066
150
100
50
0
-50
-100
-150
ppm

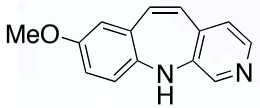

F
H
N
MeO



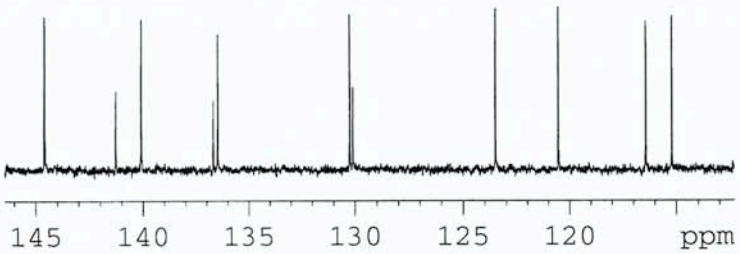


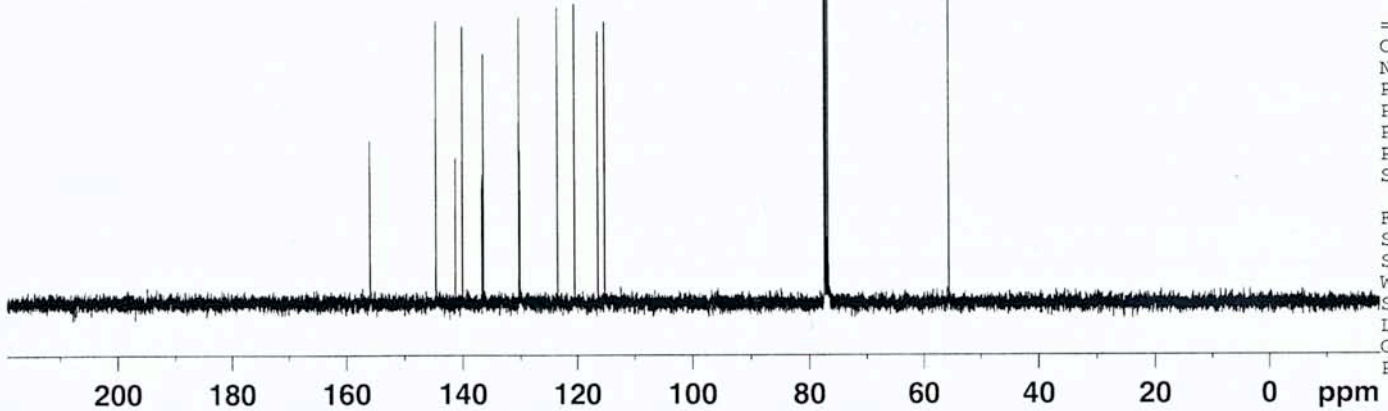



```
Current Data Parameters
NAME                  618
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20100208
Time                14.17
INSTRUM             spect
PROBHD   5 mm QNP 1H/13
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      8
DS                      2
SWH              8278.146 Hz
FIDRES           0.126314 Hz
AQ               3.9584243 sec
RG                    362
DW                60.400 usec
DE                 6.00 usec
TE                292.2 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 14.00 usec
PL1                 0.00 dB
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                  65536
SF           400.1300174 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                   1.00
```



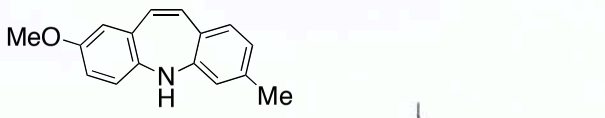
155.98
144.58
141.27
140.08
136.68
136.47
130.27
130.12
123.51
120.54
116.43
115.21
77.40
77.08
76.76
55.58

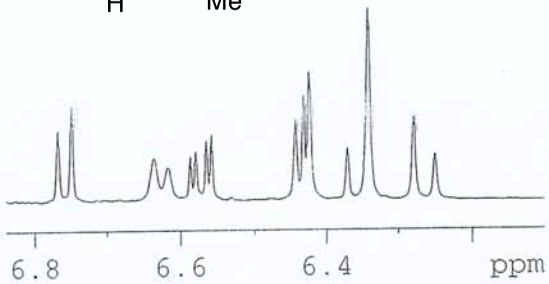


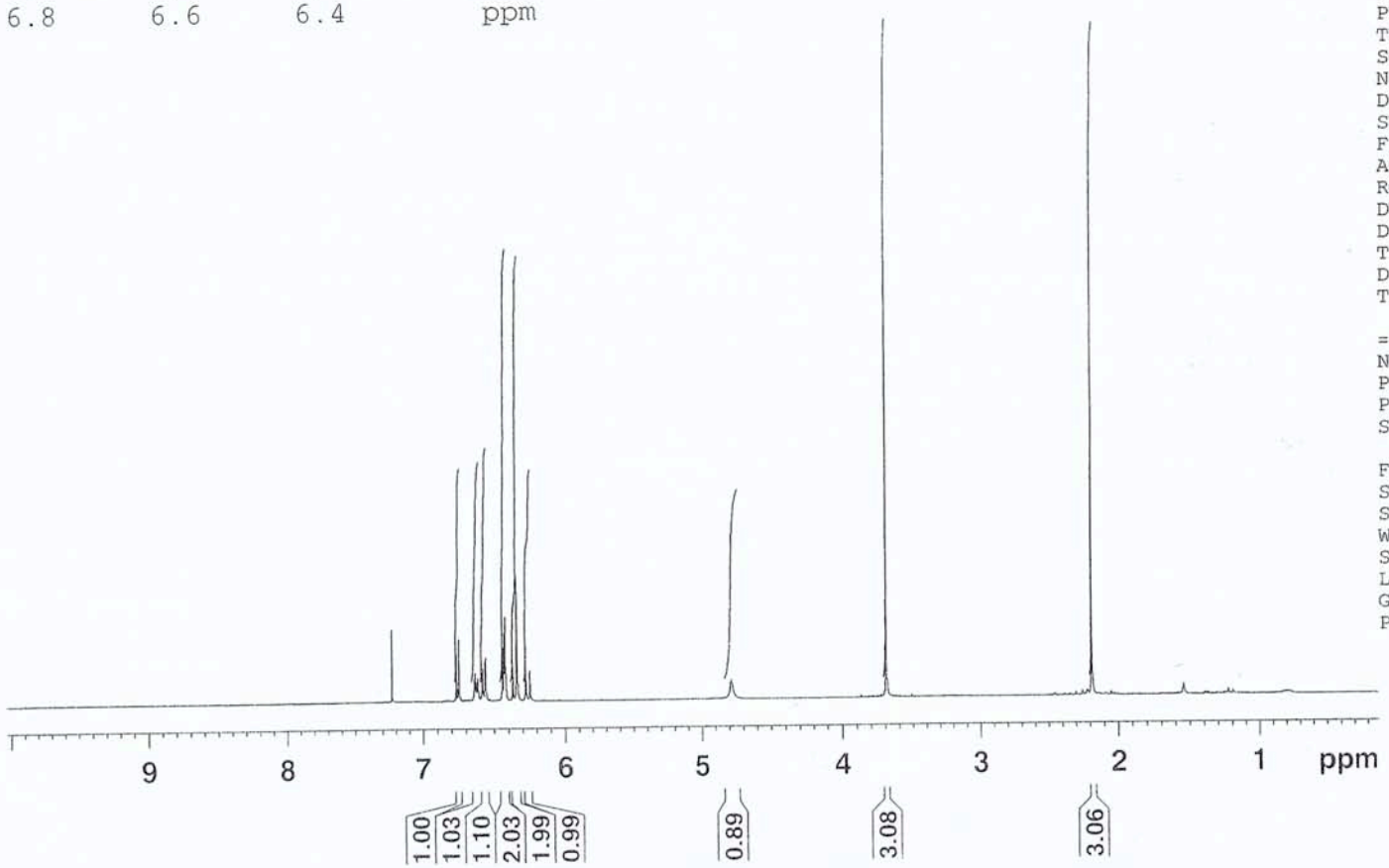


BRUKER

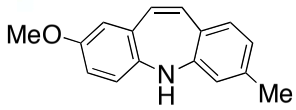
```
Current Data Parameters
NAME                  642 d
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20100405
Time                  16.12
INSTRUM               spect
PROBHD    5 mm QNP 1H/13
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      188
DS                        4
SWH               23980.814 Hz
FIDRES             0.365918 Hz
AQ                 1.3664756 sec
RG                    1824.6
DW                   20.850 usec
DE                    6.00 usec
TE                   294.2 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                   9.38 usec
PL1                  0.00 dB
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                    1H
PCPD2               90.00 usec
PL2                  0.00 dB
PL12                16.10 dB
PL13                19.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF            100.6127690 MHz
WDW                      EM
SSB                       0
LB                   1.00 Hz
GB                        0
PC                    1.40
```



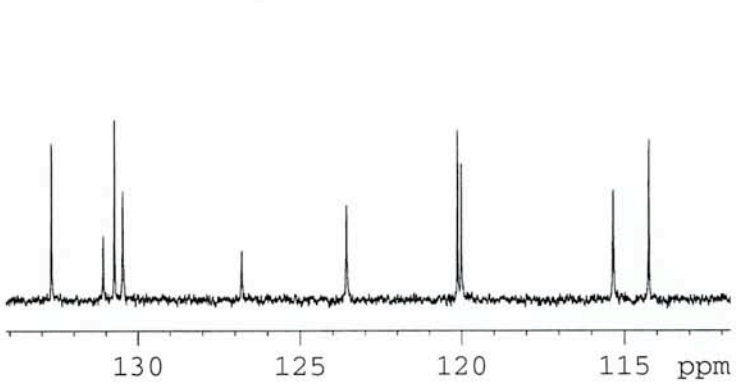


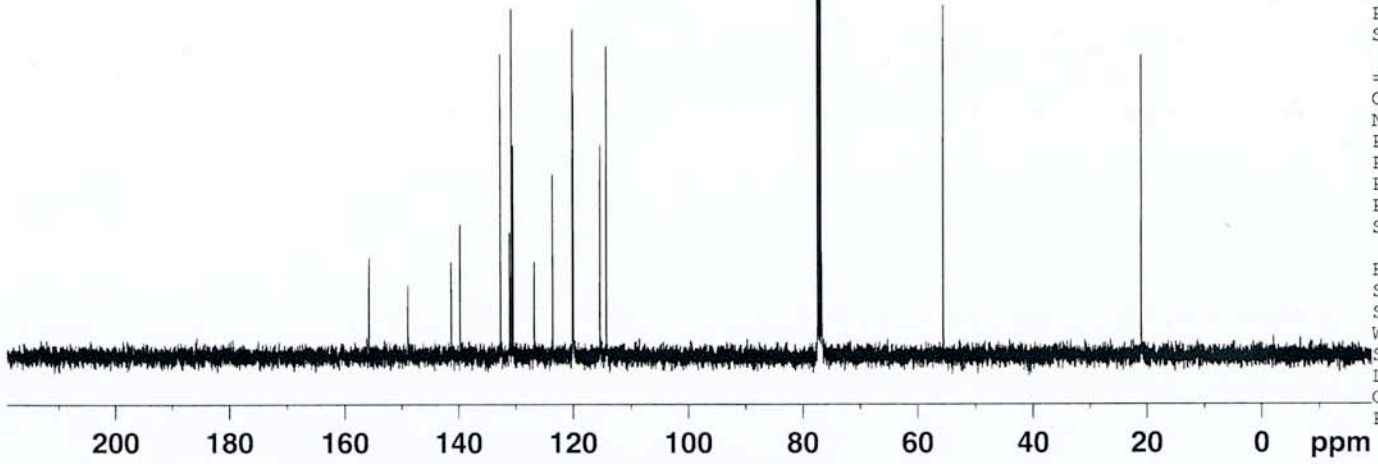



```
Current Data Parameters
NAME                  616-1
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20100320
Time                 10.30
INSTRUM              spect
PROBHD    5 mm QNP 1H/13
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH              8278.146 Hz
FIDRES           0.126314 Hz
AQ               3.9584243 sec
RG                   287.4
DW                60.400 usec
DE                 6.00 usec
TE                 293.2 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                 14.00 usec
PL1                 0.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                   65536
SF            400.1300220 MHz
WDW                     EM
SSB                      0
LB                  0.30 Hz
GB                       0
PC                    1.00
```

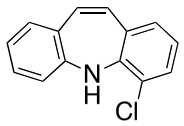


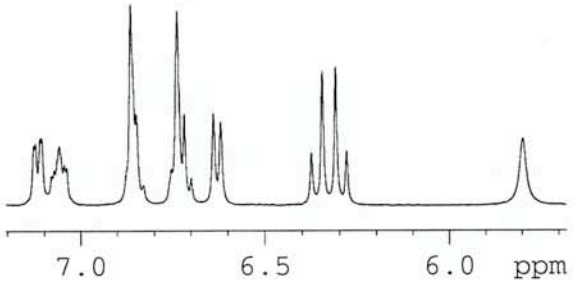
155.76
148.91
141.31
139.75
132.70
131.09
130.73
130.47
126.79
123.59
120.14
120.02
115.35
114.26
77.37
77.06
76.74
55.55
20.93

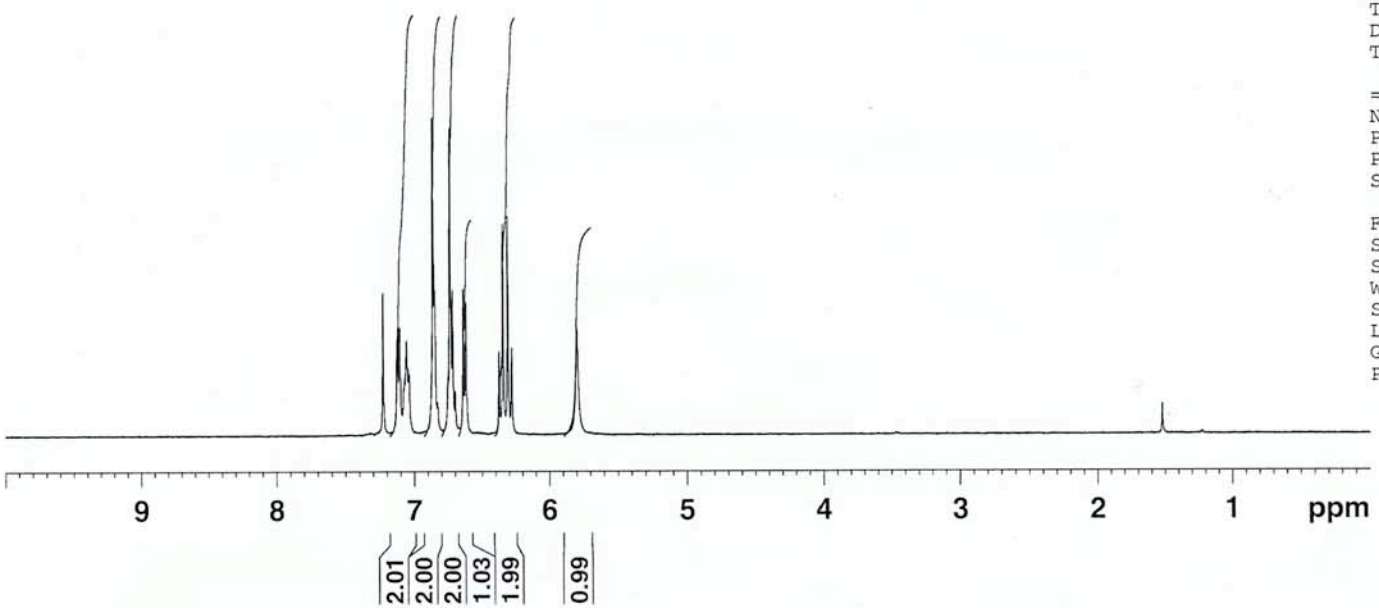




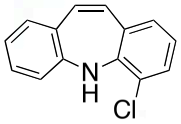

```
Current Data Parameters
NAME                  642 c
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20100402
Time                   8.30
INSTRUM               spect
PROBHD   5 mm QNP 1H/13
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      400
DS                        4
SWH              23980.814 Hz
FIDRES           0.365918 Hz
AQ               1.3664756 sec
RG                   1625.5
DW                  20.850 usec
DE                   6.00 usec
TE                  295.2 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                   9.38 usec
PL1                  0.00 dB
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2               90.00 usec
PL2                  0.00 dB
PL12                16.10 dB
PL13                19.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF            100.6127690 MHz
WDW                      EM
SSB                       0
LB                   1.00 Hz
GB                        0
PC                    1.40
```





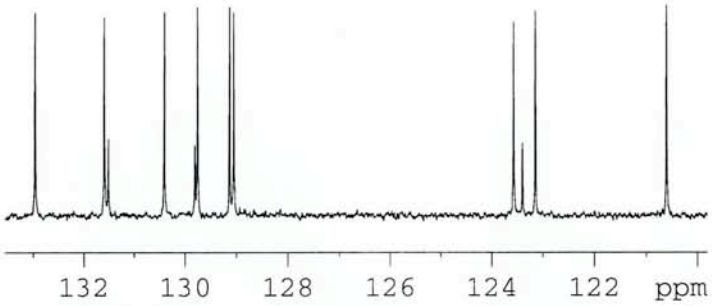


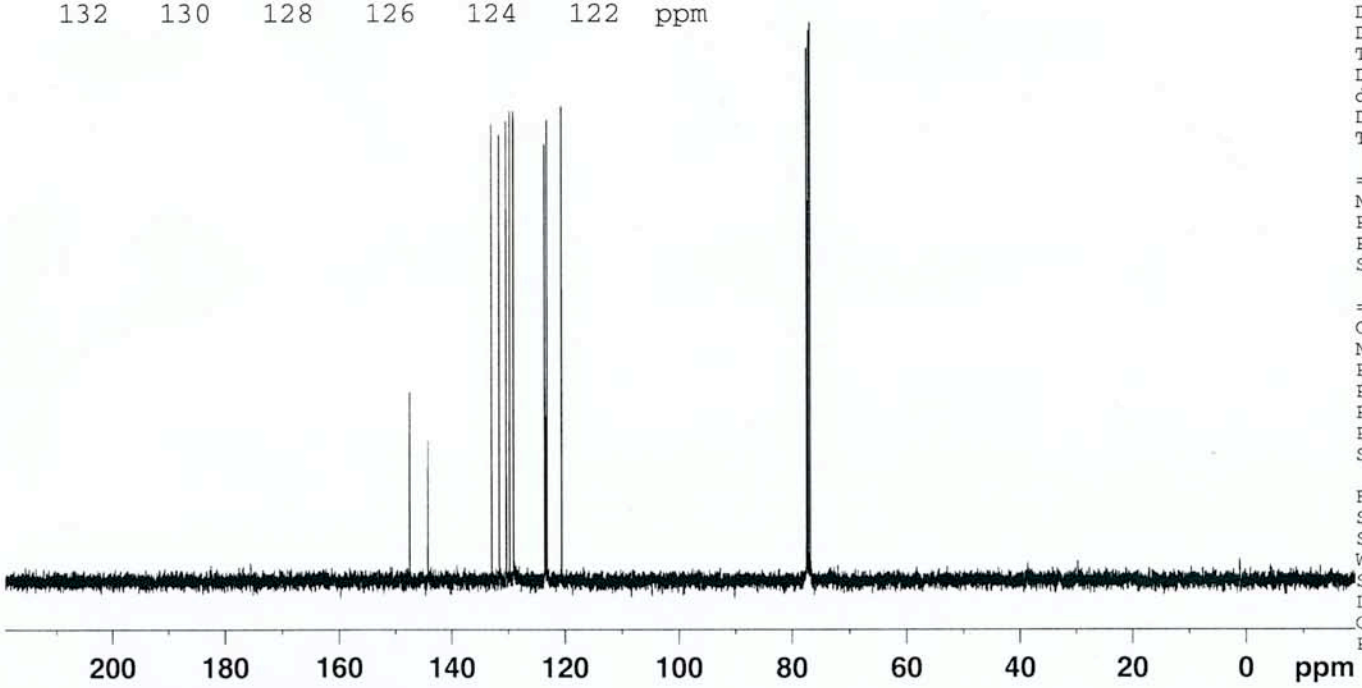

```
Current Data Parameters
NAME                  553-2-2
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20091115
Time                   8.16
INSTRUM               spect
PROBHD   5 mm QNP 1H/13
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        7
DS                        2
SWH                8278.146 Hz
FIDRES            0.126314 Hz
AQ                3.9584243 sec
RG                    724.1
DW                 60.400 usec
DE                  6.00 usec
TE                  292.2 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                 14.00 usec
PL1                 0.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                    65536
SF            400.1300220 MHz
WDW                      EM
SSB                       0
LB                  0.30 Hz
GB                        0
PC                     1.00
```



147.50
144.24
132.97
131.60
131.52
130.41
129.81
129.76
129.13
129.05
123.58
123.41
123.16
120.61

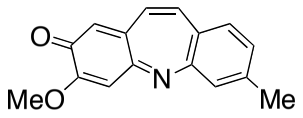
77.41
77.10
76.78

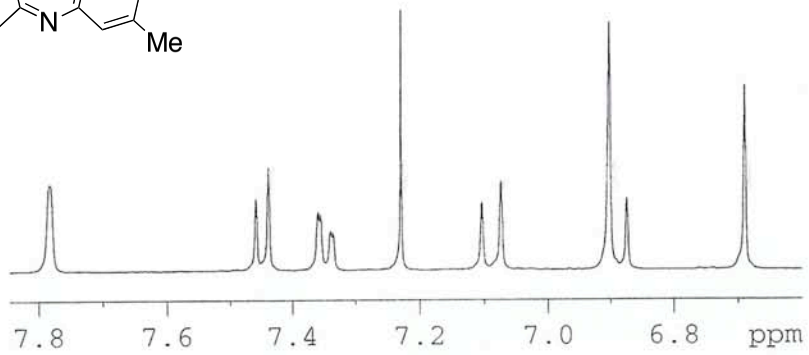


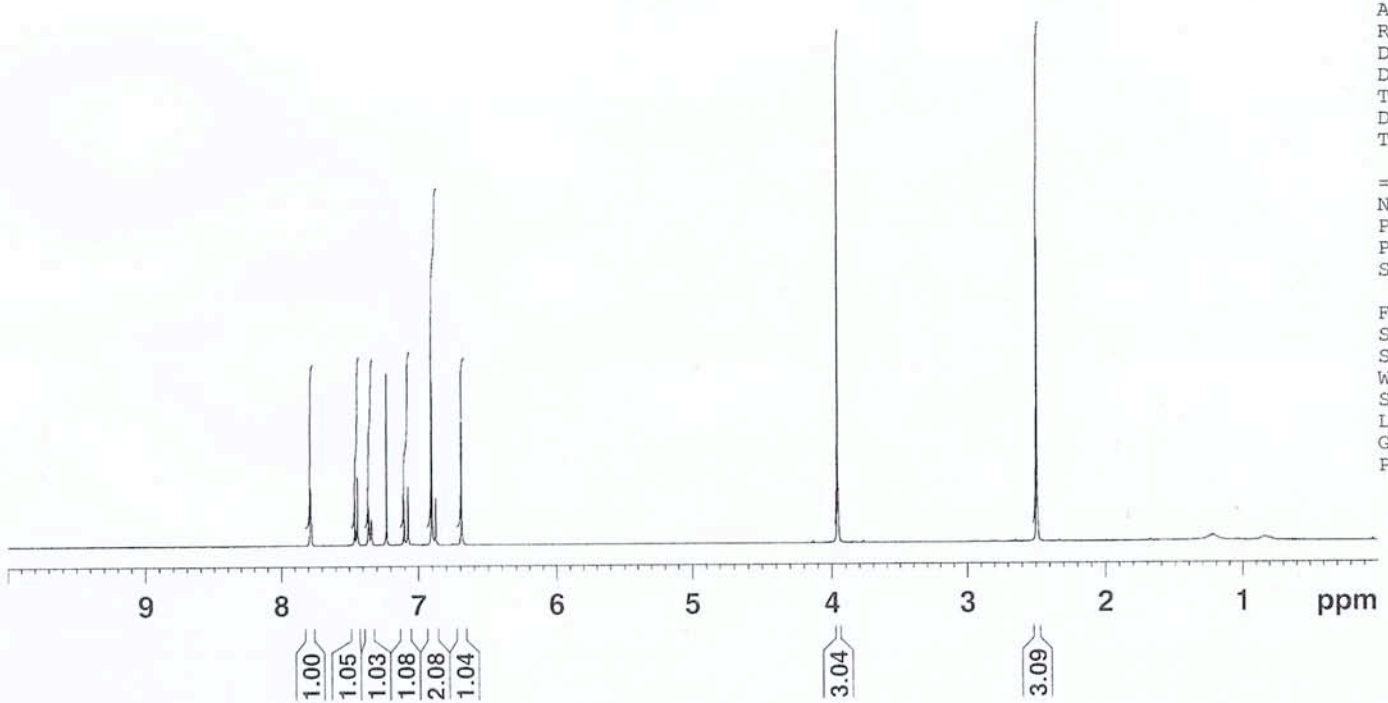


BRUKER

```
Current Data Parameters
NAME                  519-2
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20100331
Time                   8.44
INSTRUM               spect
PROBHD   5 mm QNP 1H/13
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     101
DS                       4
SWH             23980.814 Hz
FIDRES          0.365918 Hz
AQ              1.3664756 sec
RG                  1625.5
DW                20.850 usec
DE                 6.00 usec
TE                294.2 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                  9.38 usec
PL1                 0.00 dB
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2              90.00 usec
PL2                 0.00 dB
PL12               16.10 dB
PL13               19.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF           100.6127690 MHz
WDW                     EM
SSB                      0
LB                1.00 Hz
GB                       0
PC                   1.60
```

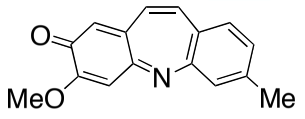




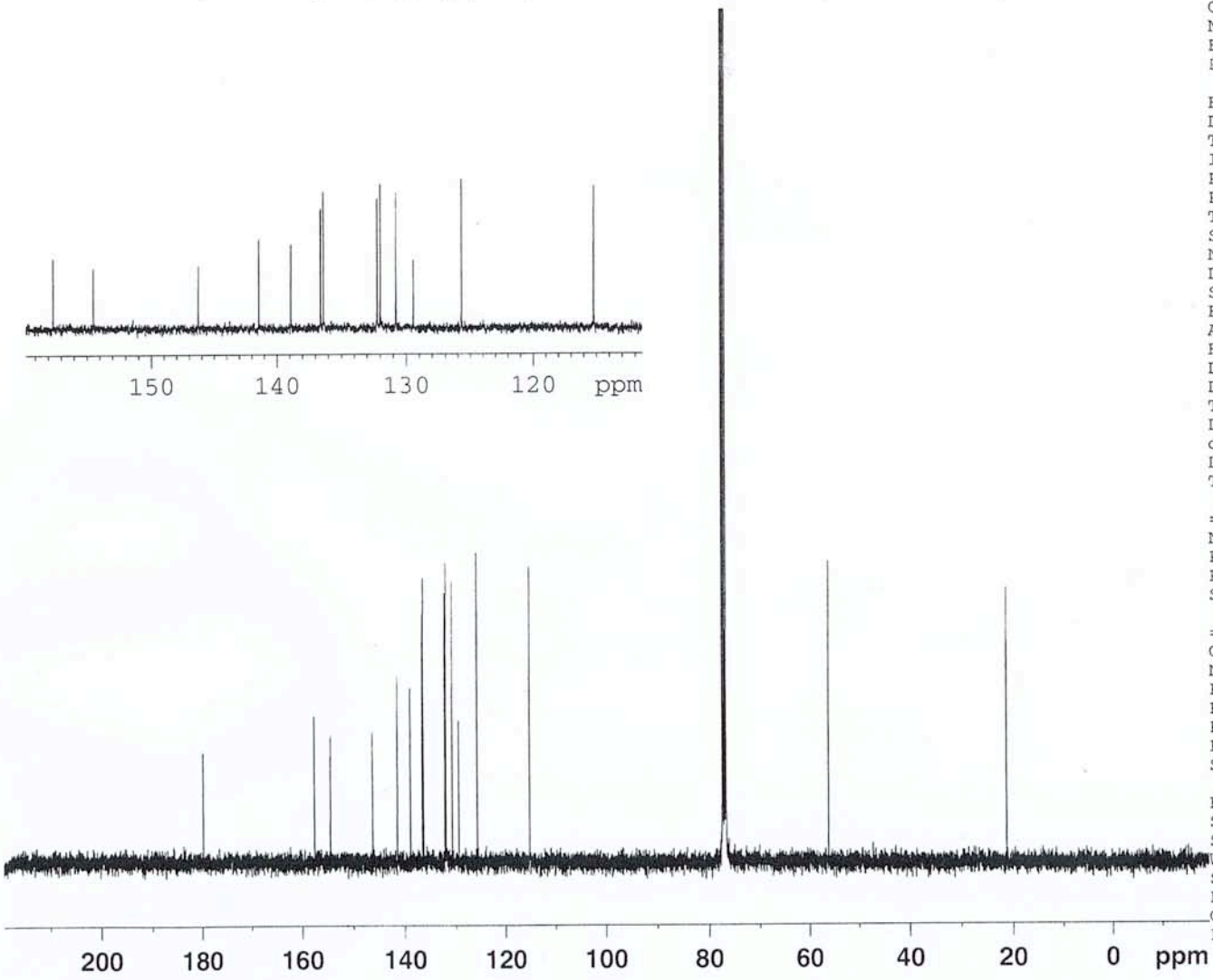


BRUKER

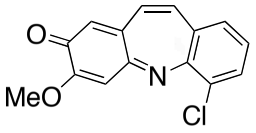
```
Current Data Parameters
NAME                  631--1
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20100413
Time                  15.08
INSTRUM               spect
PROBHD    5 mm QNP 1H/13
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       27
DS                        2
SWH                8278.146 Hz
FIDRES            0.126314 Hz
AQ                3.9584243 sec
RG                      362
DW                 60.400 usec
DE                  6.00 usec
TE                  294.2 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                 14.00 usec
PL1                 0.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                    65536
SF            400.1300220 MHz
WDW                      EM
SSB                       0
LB                  0.30 Hz
GB                        0
PC                     1.00
```

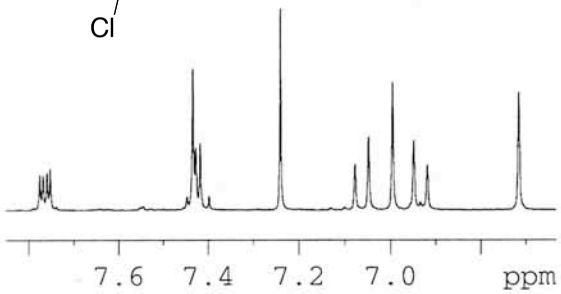


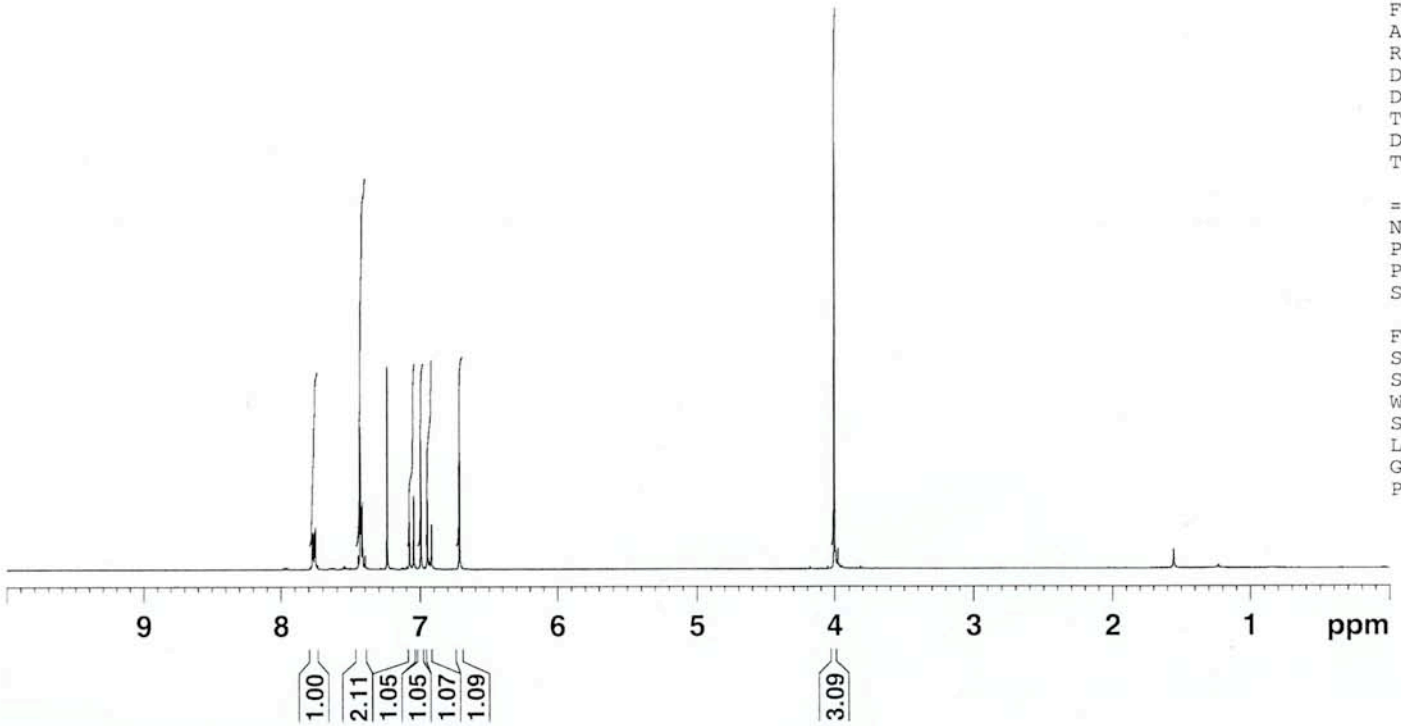
179.83
157.60
154.48
146.26
141.42
138.91
136.59
136.36
132.22
131.98
130.77
129.45
125.69
115.18
77.36
77.04
76.73
56.13
21.24



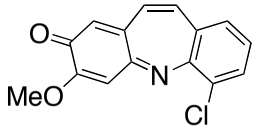

```
Current Data Parameters
NAME                  631-C
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20100413
Time                  20.29
INSTRUM               spect
PROBHD    5 mm QNP 1H/13
PULPROG             zgpg30
TD                    65536
SOLVENT               CDC13
NS                     2431
DS                        4
SWH             23980.814 Hz
FIDRES          0.365918 Hz
AQ              1.3664756 sec
RG                     3251
DW                20.850 usec
DE                 6.00 usec
TE                 294.2 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                   13C
P1                  9.38 usec
PL1                 0.00 dB
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                   1H
PCPD2              90.00 usec
PL2                 0.00 dB
PL12               16.10 dB
PL13               19.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF           100.6127690 MHz
WDW                      EM
SSB                       0
LB                  1.00 Hz
GB                        0
PC                     2.00
```

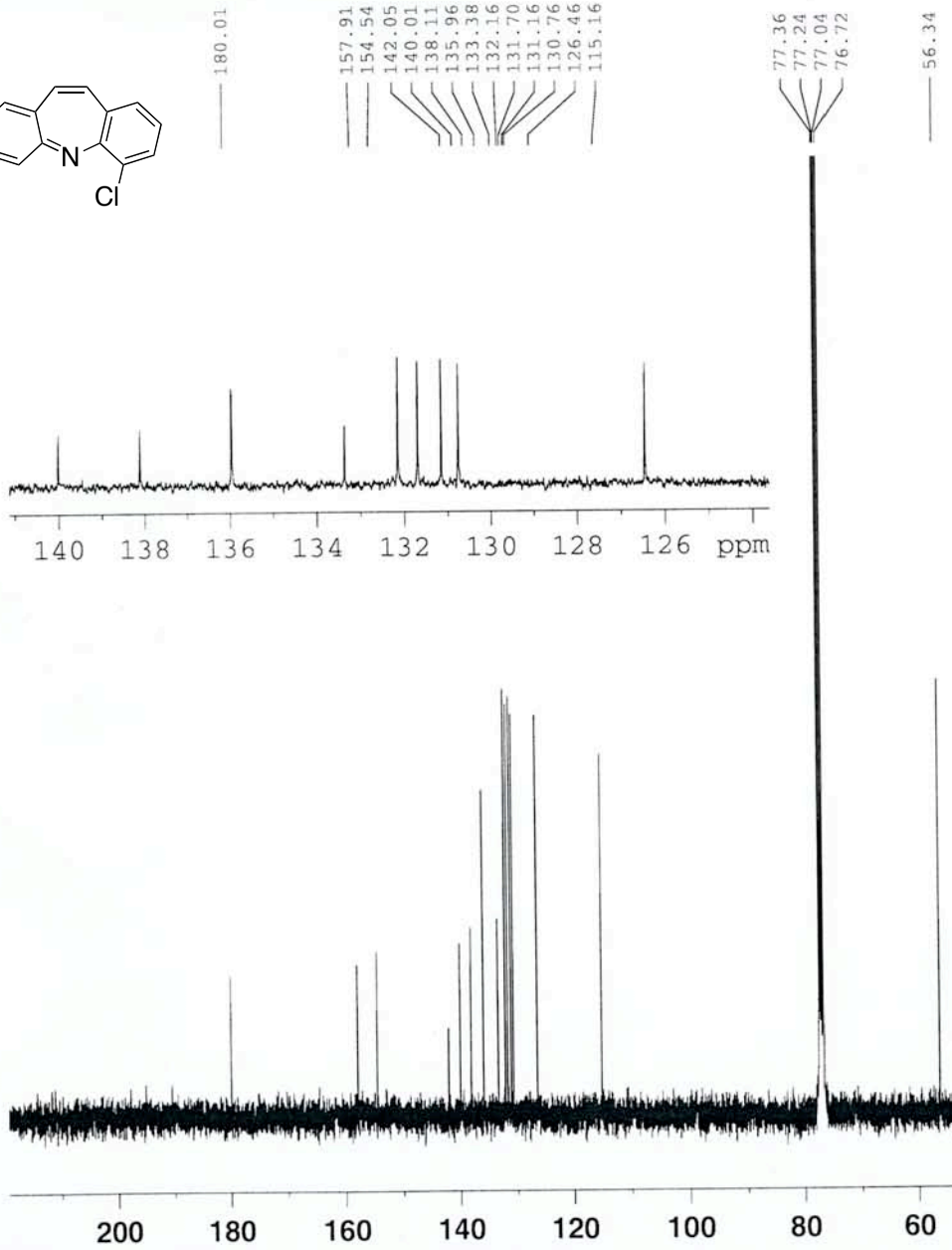






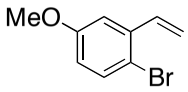

```
Current Data Parameters
NAME                  632-3
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20100326
Time                 18.11
INSTRUM              spect
PROBHD    5 mm QNP 1H/13
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               8278.146 Hz
FIDRES            0.126314 Hz
AQ                3.9584243 sec
RG                     362
DW                  60.400 usec
DE                   6.00 usec
TE                  295.2 K
D1               1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    1H
P1                  14.00 usec
PL1                  0.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                   65536
SF            400.1300175 MHz
WDW                     EM
SSB                      0
LB                  0.30 Hz
GB                       0
PC                    1.00
```

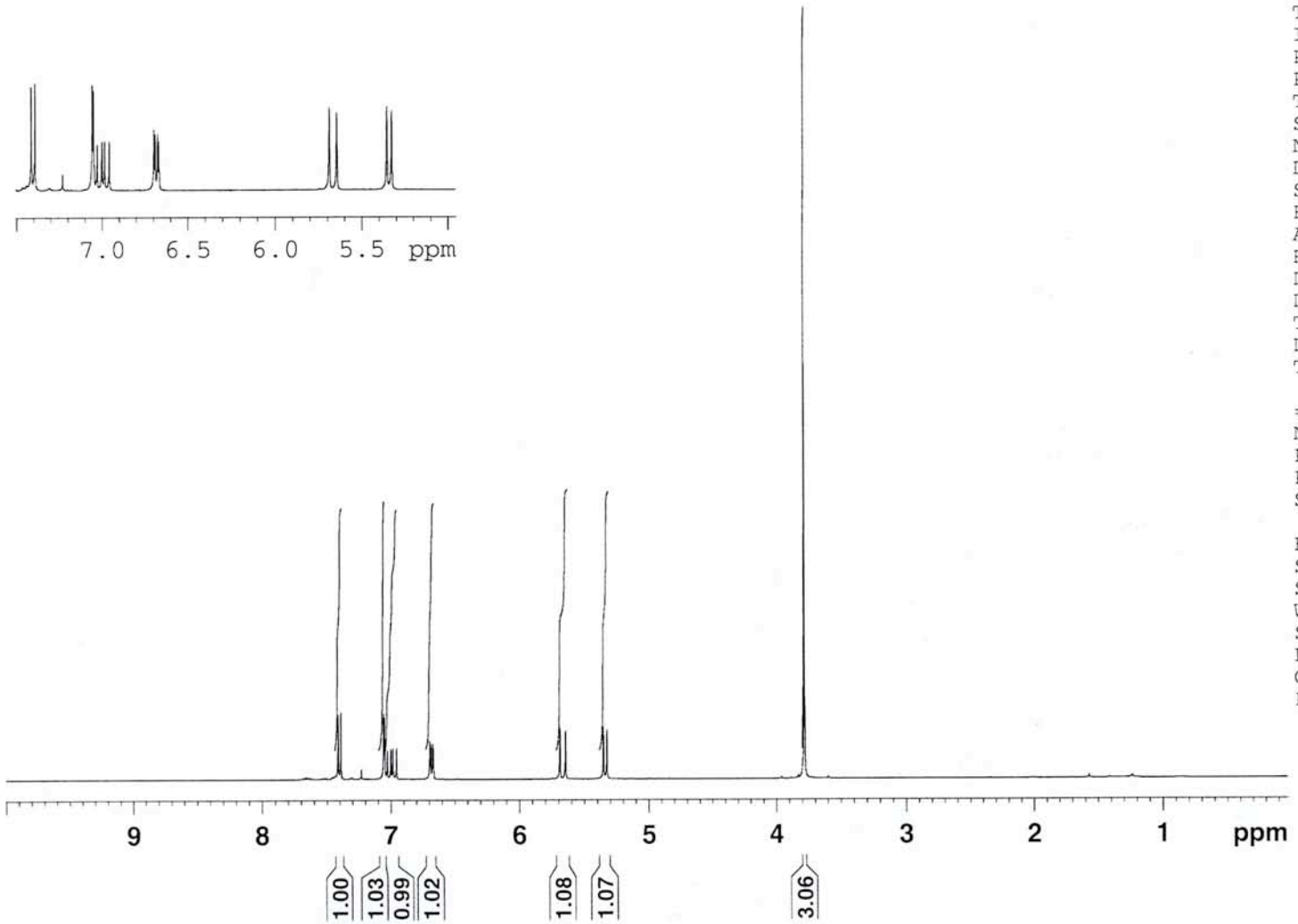




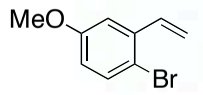
BRUKER

```
Current Data Parameters
NAME                  632---C
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20100414
Time                  20.54
INSTRUM               spect
PROBHD    5 mm QNP 1H/13
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    2752
DS                       4
SWH             23980.814 Hz
FIDRES           0.365918 Hz
AQ               1.3664756 sec
RG                  5160.6
DW                  20.850 usec
DE                   6.00 usec
TE                  294.2 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                   9.38 usec
PL1                  0.00 dB
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                   1H
PCPD2               90.00 usec
PL2                  0.00 dB
PL12                16.10 dB
PL13                19.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF           100.6127690 MHz
WDW                      EM
SSB                       0
LB                   1.00 Hz
GB                        0
PC                     1.40
```

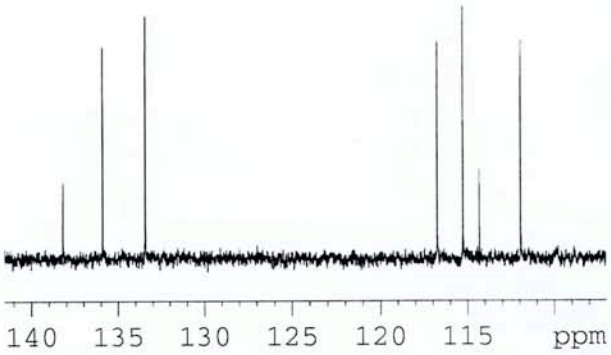


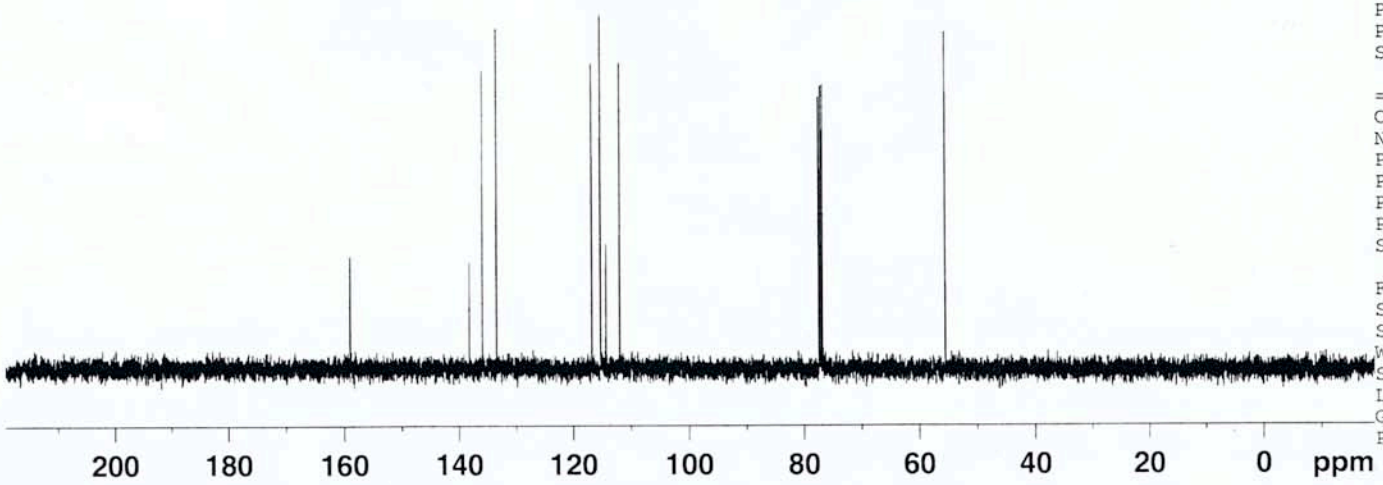



```
Current Data Parameters
NAME                      610
EXPNO                       1
PROCNO                      1

F2 - Acquisition Paramet
Date_                20100114
Time                    16.51
INSTRUM                 spect
PROBHD    5 mm BBO BB-1H
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                          8
DS                          2
SWH                  8278.146
FIDRES               0.126314
AQ                  3.9584243
RG                       80.6
DW                     60.400
DE                       6.00
TE                      293.2
D1                1.00000000
TD0                         1

======== CHANNEL f1 ====
NUC1                       1H
P1                      15.07
PL1                      0.00
SFO1           400.1324710

F2 - Processing paramete
SI                     65536
SF                400.1300212
WDW                       EM
SSB                        0
LB                      0.30
GB                         0
PC                      1.00
```



159.01
138.18
135.89
133.43
116.75
115.28
114.34
111.95
77.39
77.07
76.75
55.49





BRUKER

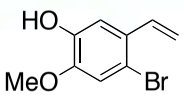
Current Data Parameters
NAME 610-1
EXPNO 2
PROCNO 1

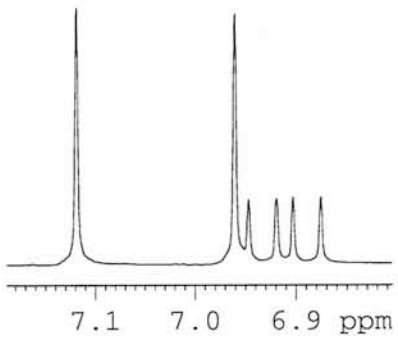
F2 - Acquisition Parameters
Date_ 20100326
Time 18.53
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 15
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 1625.5
DW 20.850 usec
DE 6.00 usec
TE 295.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

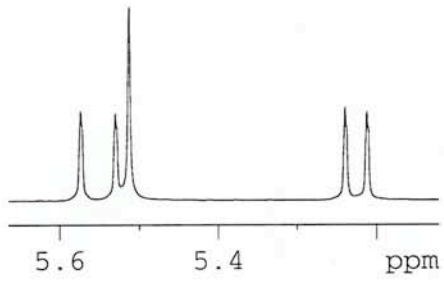
======== CHANNEL f1 ========
NUC1 13C
P1 9.38 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

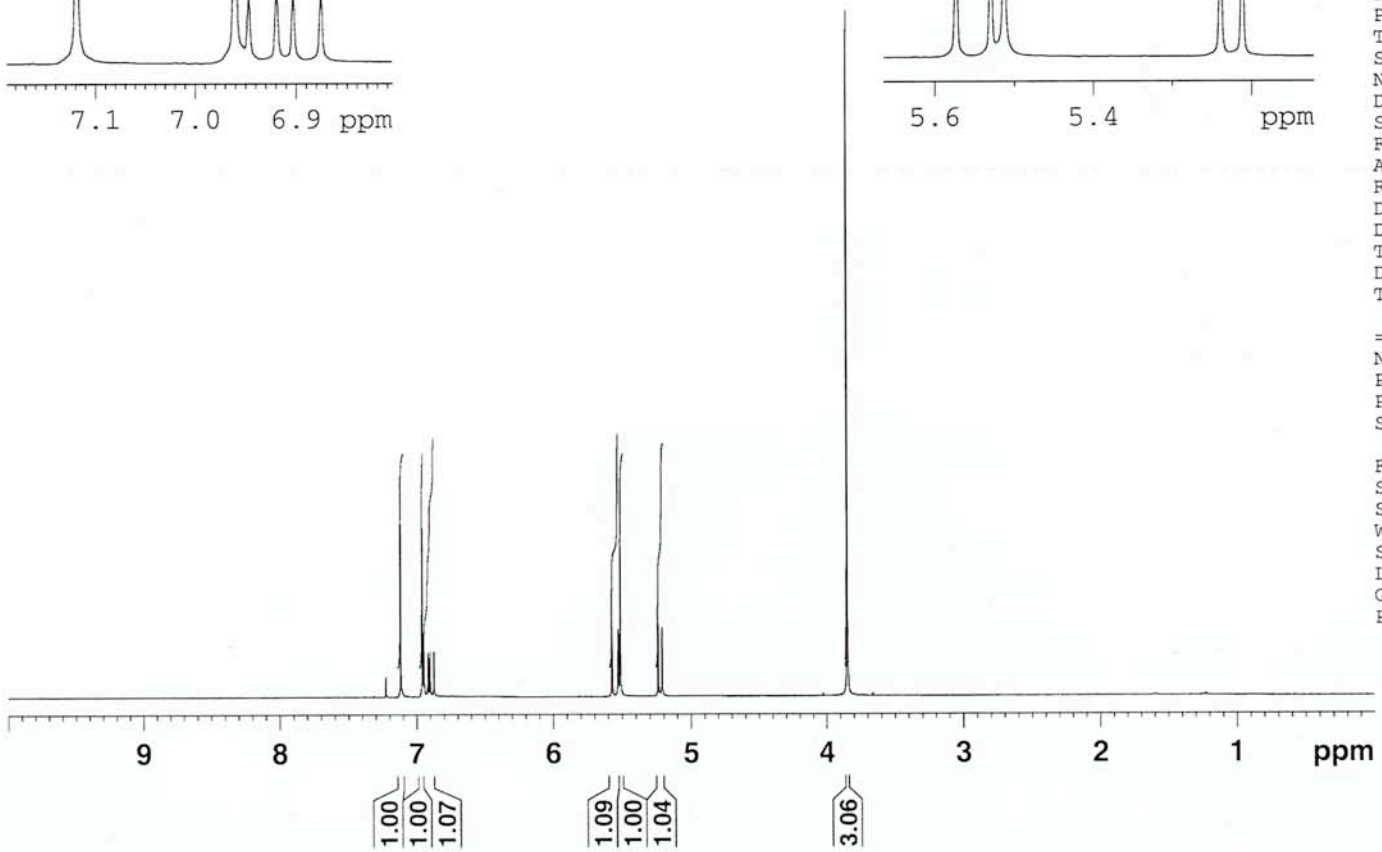
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.10 dB
PL13 19.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

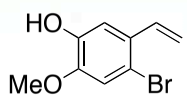


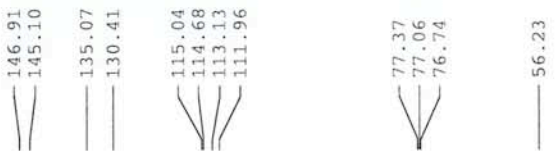


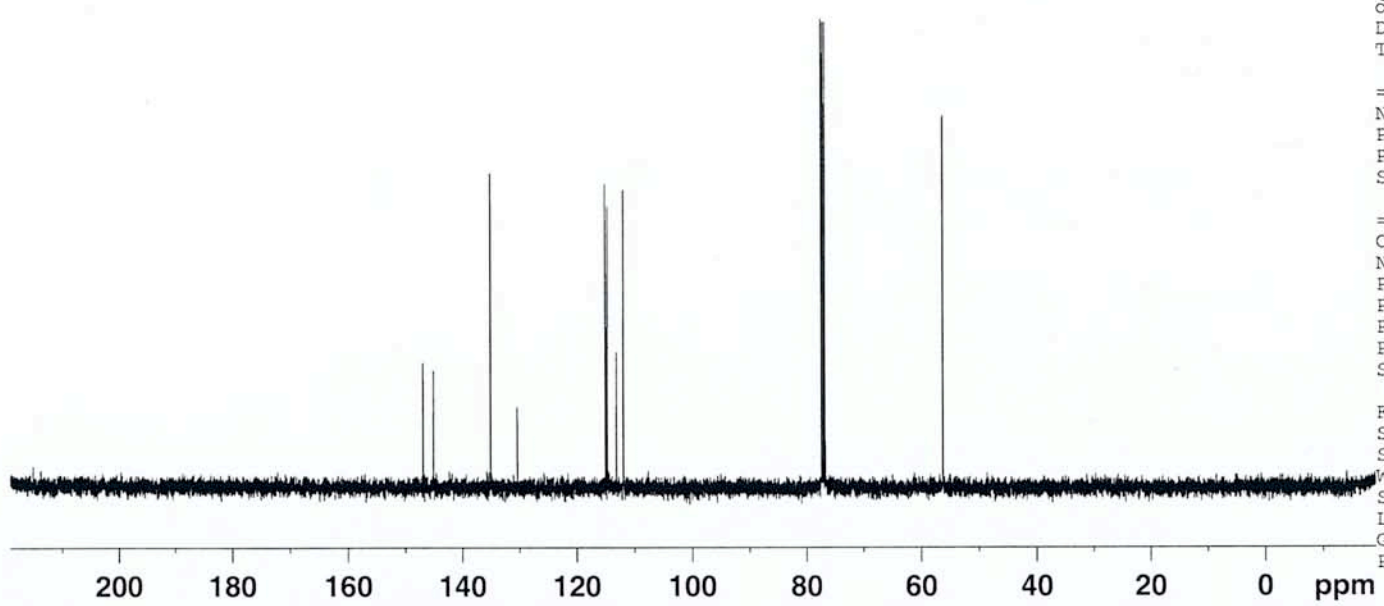




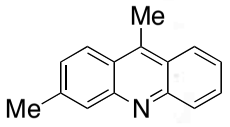

```
Current Data Parameters
NAME                  620
EXPNO                   3
PROCNO                  1

F2 - Acquisition Parameters
Date_            20100223
Time                 8.04
INSTRUM             spect
PROBHD   5 mm QNP 1H/13
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      8
DS                      2
SWH              8278.146 Hz
FIDRES           0.126314 Hz
AQ               3.9584243 sec
RG                    181
DW                 60.400 usec
DE                  6.00 usec
TE                 294.2 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 14.00 usec
PL1                 0.00 dB
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                  65536
SF           400.1300220 MHz
WDW                    EM
SSB                     0
LB                  0.30 Hz
GB                      0
PC                   1.00
```

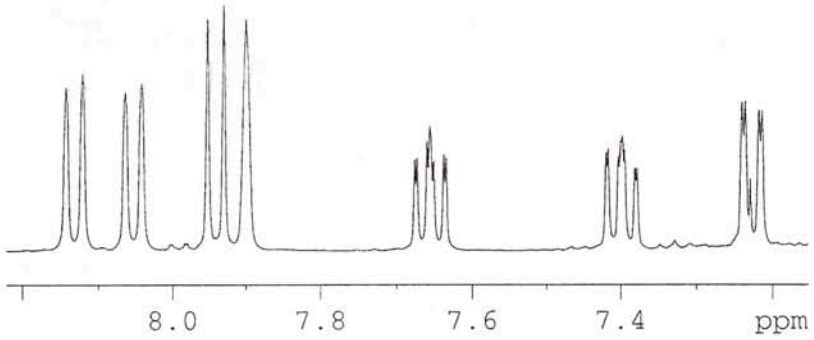


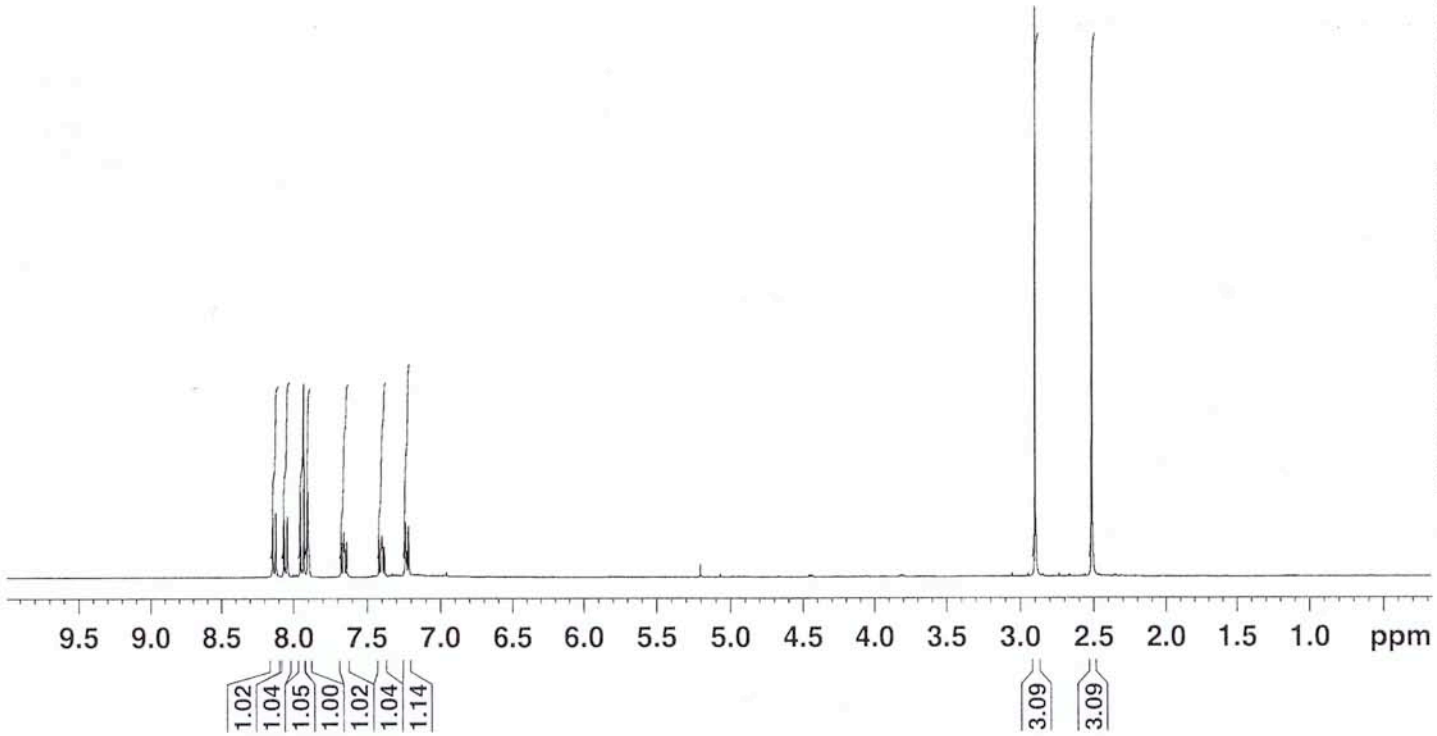




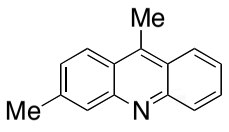

```
Current Data Parameters
NAME                  620
EXPNO                   4
PROCNO                  1

F2 - Acquisition Parameters
Date_            20100223
Time                 8.16
INSTRUM             spect
PROBHD   5 mm QNP 1H/13
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    87
DS                     4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                1824.6
DW                20.850 usec
DE                 6.00 usec
TE                295.2 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 9.38 usec
PL1                0.00 dB
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             90.00 usec
PL2                0.00 dB
PL12              16.10 dB
PL13              19.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF           100.6127690 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                 1.40
```








```
Current Data Parameters
NAME          685(2,1)-r
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parame
Date_           20100606
Time                8.12
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8278.146
FIDRES          0.126314
AQ              3.9584243
RG                  40.3
DW                60.400
DE                 6.00
TE                296.2
D1           1.00000000
TD0                    1

======== CHANNEL f1 ===
NUC1                  1H
P1                 15.07
PL1                 0.00
SFO1        400.1324710

F2 - Processing paramet
SI                 65536
SF          400.1300212
WDW                   EM
SSB                    0
LB                  0.30
GB                     0
PC                  1.00
```

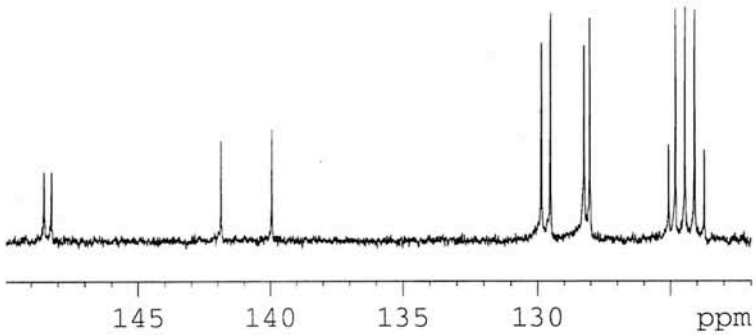


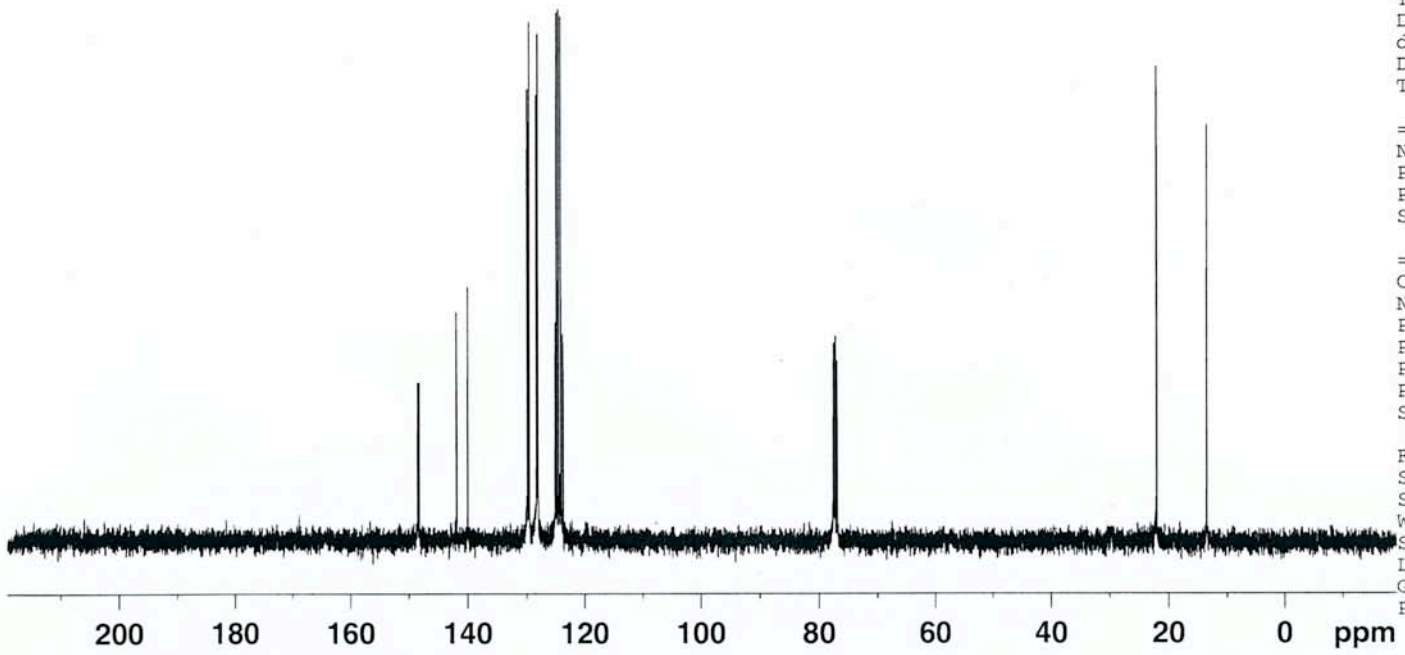
148.51
148.23
141.89
139.95
129.86
129.51
128.25
128.03
125.07
124.81
124.45
124.09
123.73

77.52
77.20
76.88

21.98

13.42





BRUKER

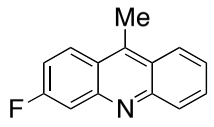
Current Data Parameters
NAME 685
EXPNO 3
PROCNO 1

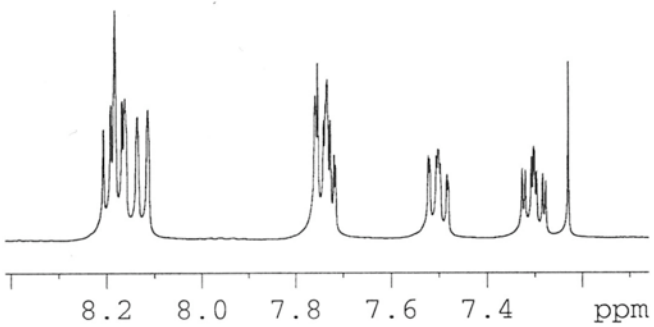
F2 - Acquisition Parameters
Date_ 20100612
Time 11.28
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 43
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 1625.5
DW 20.850 usec
DE 6.00 usec
TE 295.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

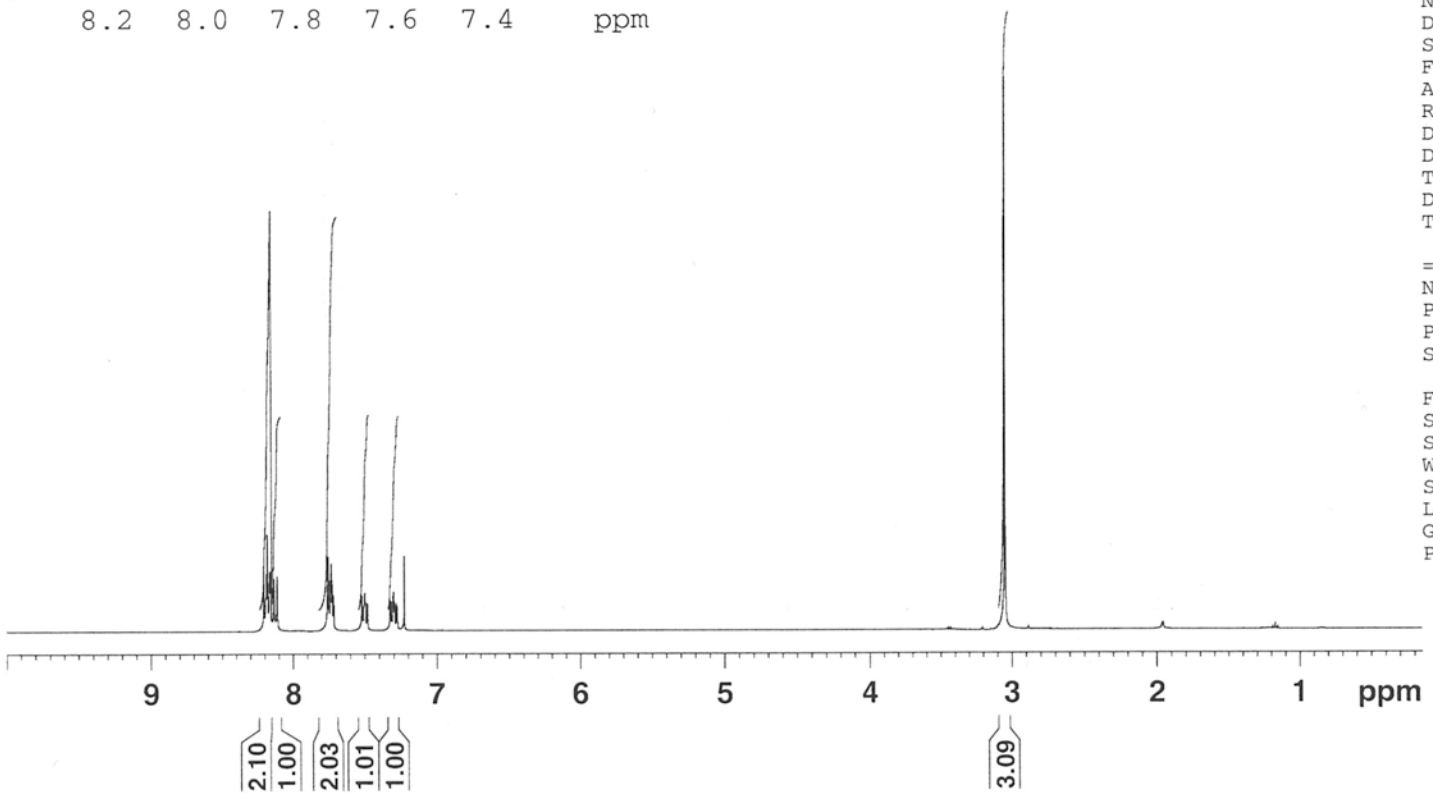
======== CHANNEL f1 ========
NUC1 13C
P1 9.38 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.10 dB
PL13 19.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 3.00

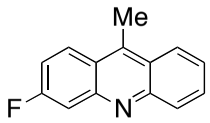


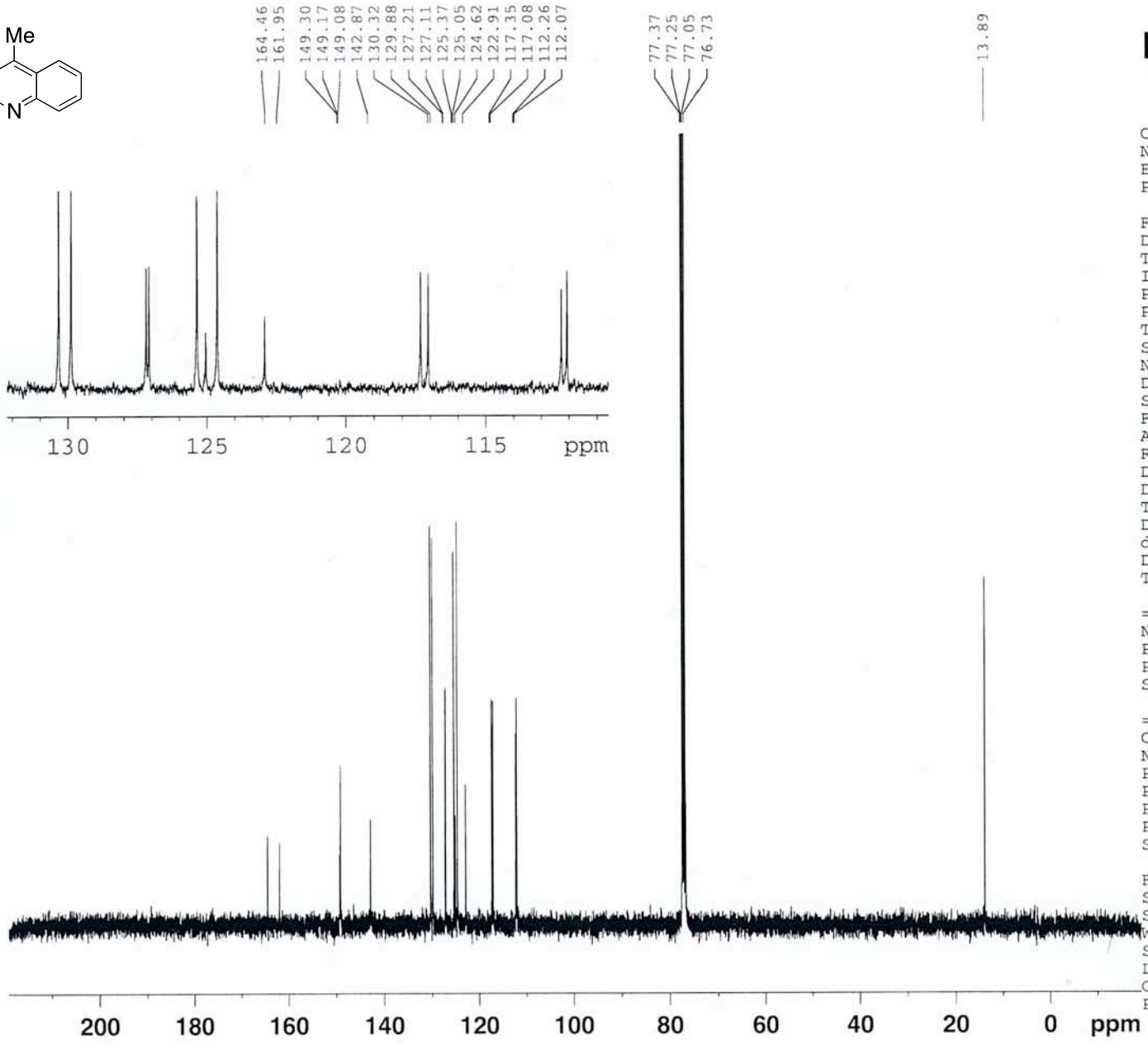




BRUKER

```
Current Data Parameters
NAME                  687
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20100610
Time                6.48
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    14
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 sec
RG                   256
DW                60.400 usec
DE                 6.00 usec
TE                300.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.00 usec
PL1                0.00 dB
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF           400.1300220 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```





BRUKER

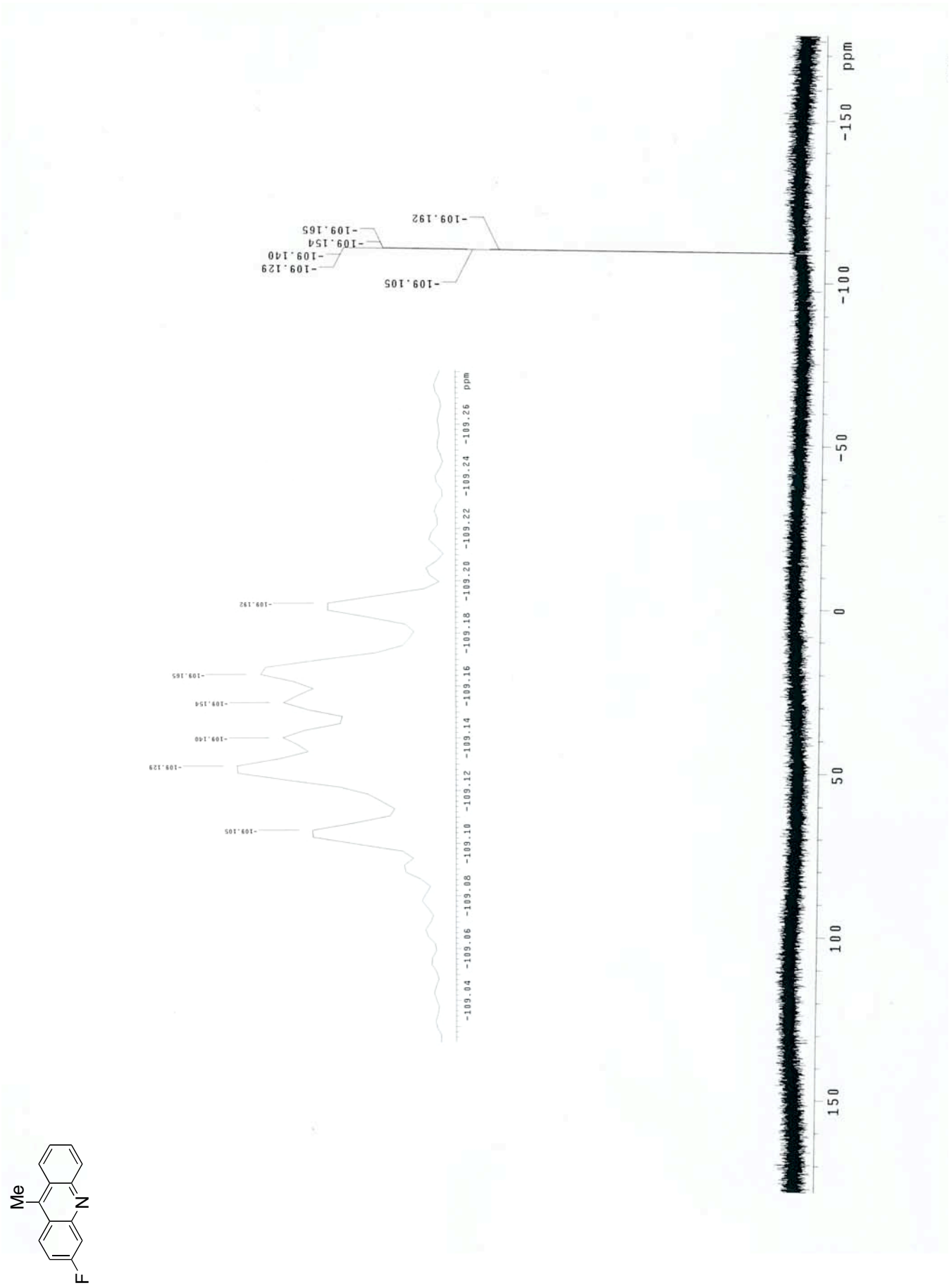
Current Data Parameters
NAME 687
EXPNO 2
PROCNO 1

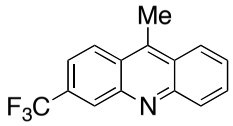
F2 - Acquisition Parameters
Date_ 20100610
Time 19.39
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 600
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 2896.3
DW 20.850 usec
DE 6.00 usec
TE 295.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

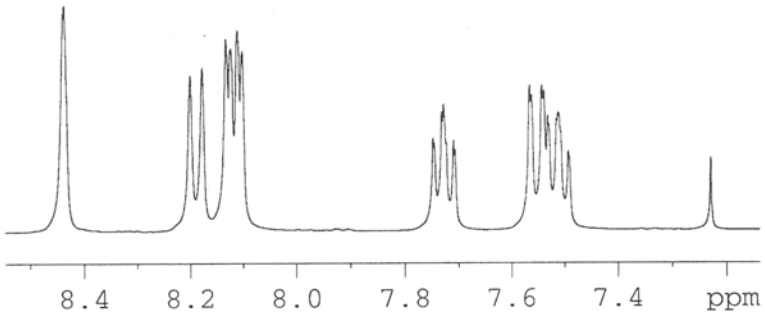
======== CHANNEL f1 ========
NUC1 13C
P1 9.38 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

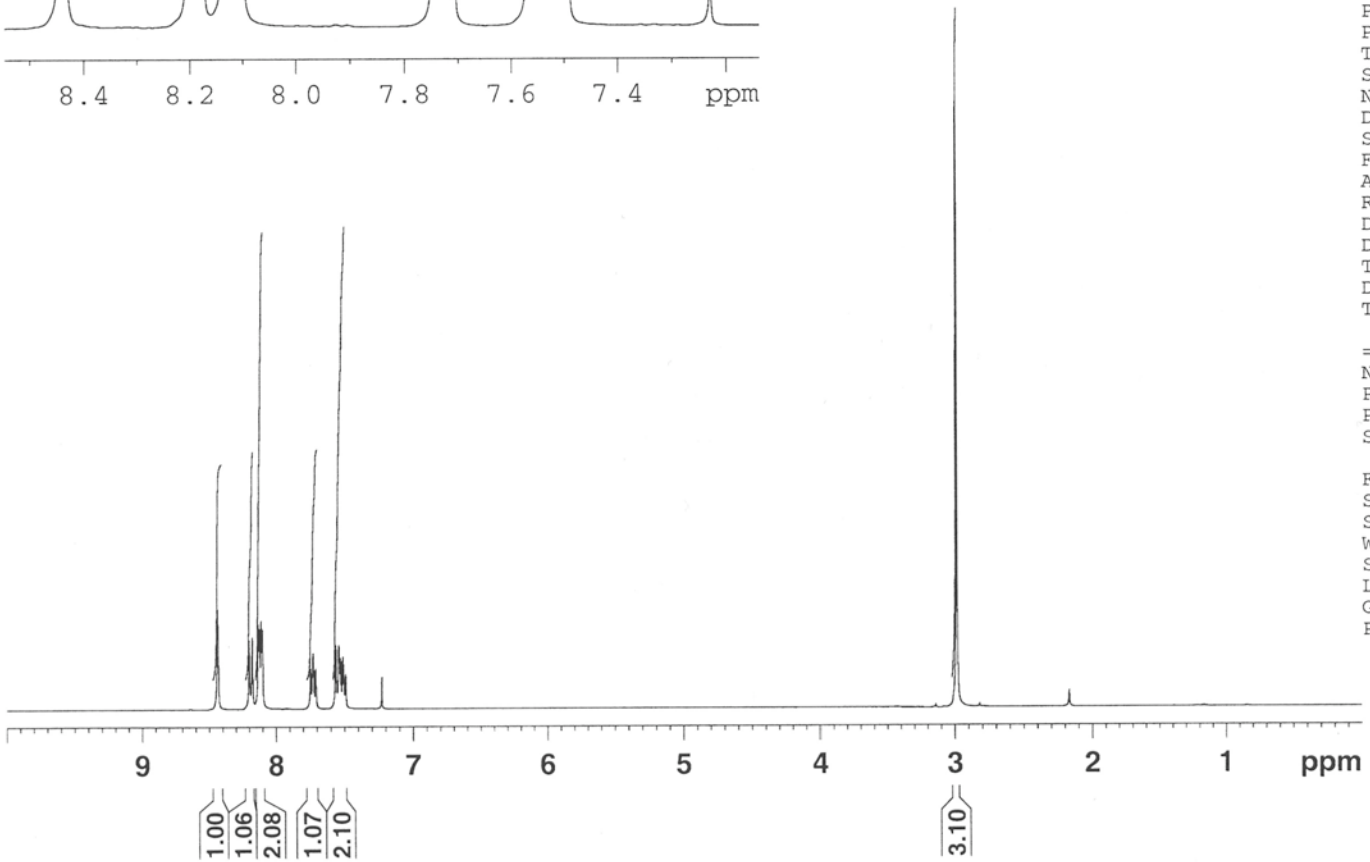
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.10 dB
PL13 19.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.60


-109.192
-109.165
-109.154
-109.140
-109.129
-109.105
ppm
150
100
50
0
-50
-100
-150
-109.04
-109.06
-109.08
-109.10
-109.12
-109.14
-109.16
-109.18
-109.20
-109.22
-109.24
-109.26
Me
N
F

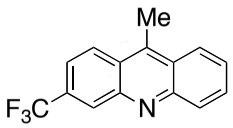






BRUKER

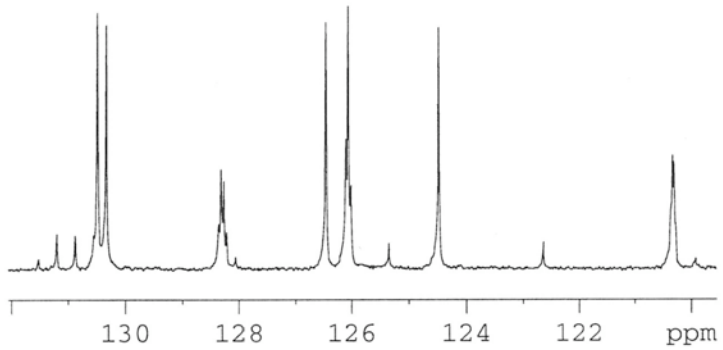
```
Current Data Parameters
NAME                  688
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20100610
Time                7.01
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    12
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 sec
RG                 161.3
DW                60.400 usec
DE                 6.00 usec
TE                294.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.00 usec
PL1                0.00 dB
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF          400.1300220 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                 1.00
```

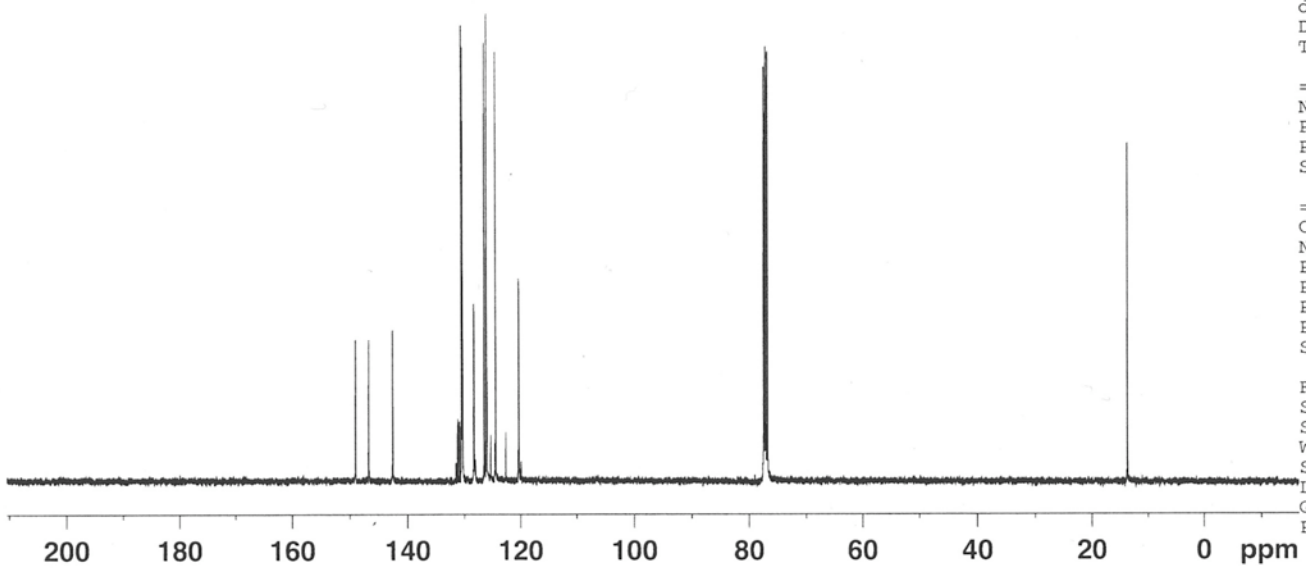


149.04
146.76
142.59
131.53
131.20
130.88
130.48
130.33
128.36
128.31
128.27
128.22
128.06
126.46
126.10
126.06
126.02
125.35
124.48
122.64
120.34
120.31
119.93

77.38
77.06
76.74

13.64





BRUKER

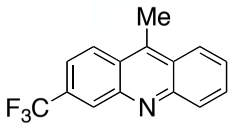
Current Data Parameters
NAME 688
EXPNO 3
PROCNO 1

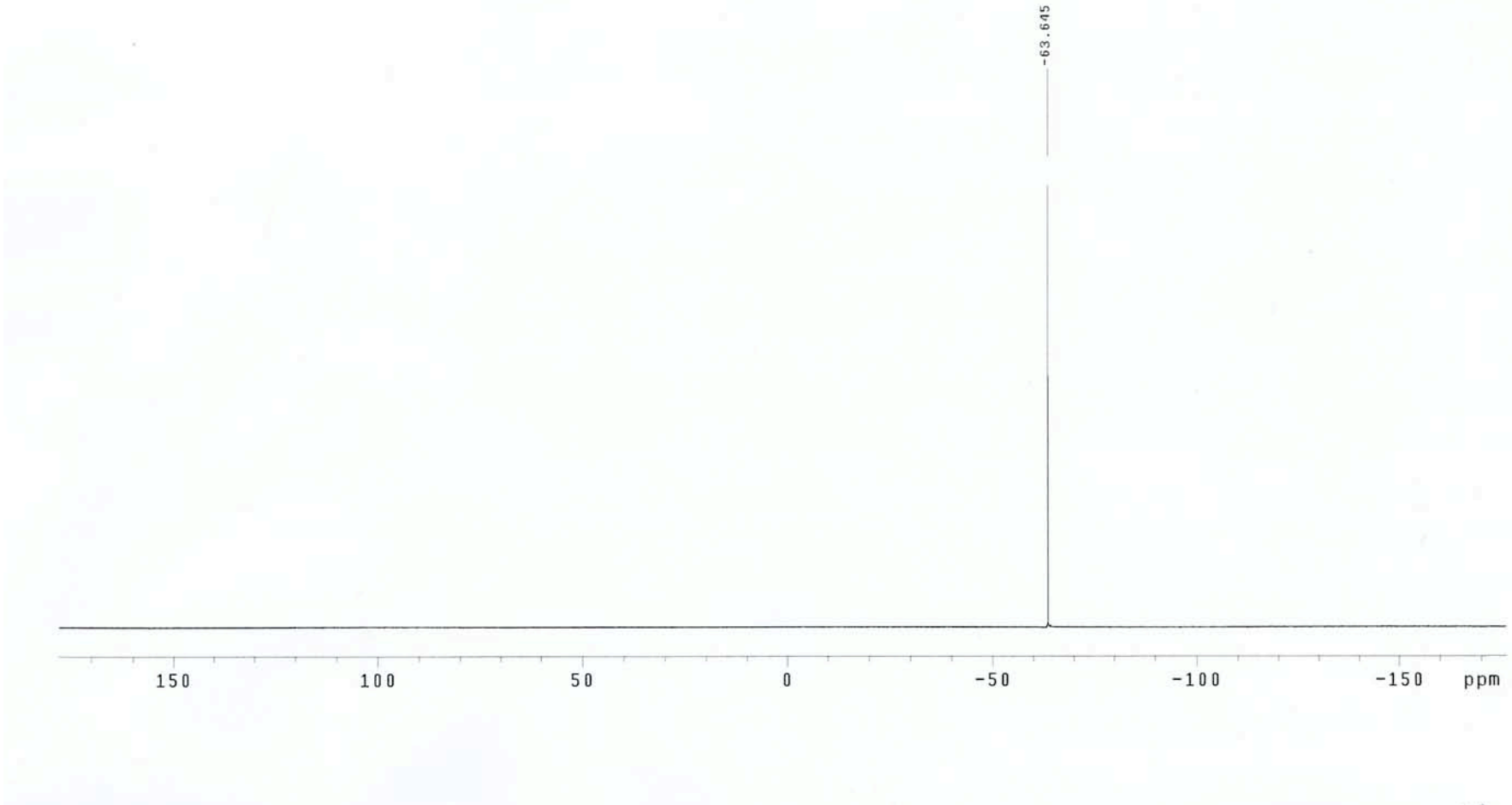
F2 - Acquisition Parameters
Date_ 20100612
Time 11.14
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1089
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 1625.5
DW 20.850 usec
DE 6.00 usec
TE 295.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

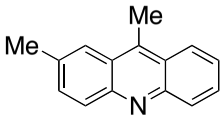
======== CHANNEL f1 ========
NUC1 13C
P1 9.38 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

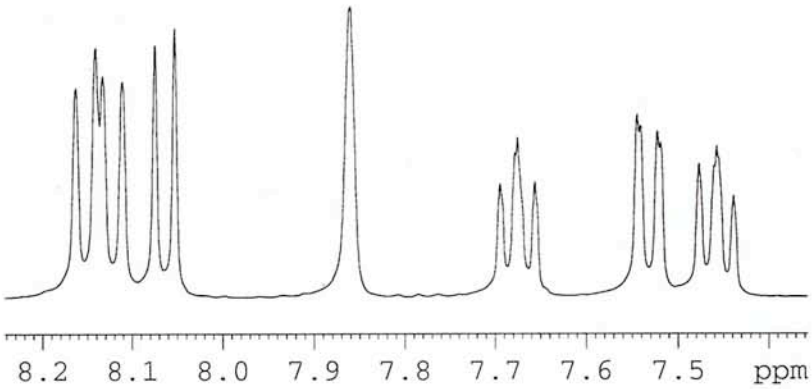
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.10 dB
PL13 19.00 dB
SFO2 400.1316005 MHz

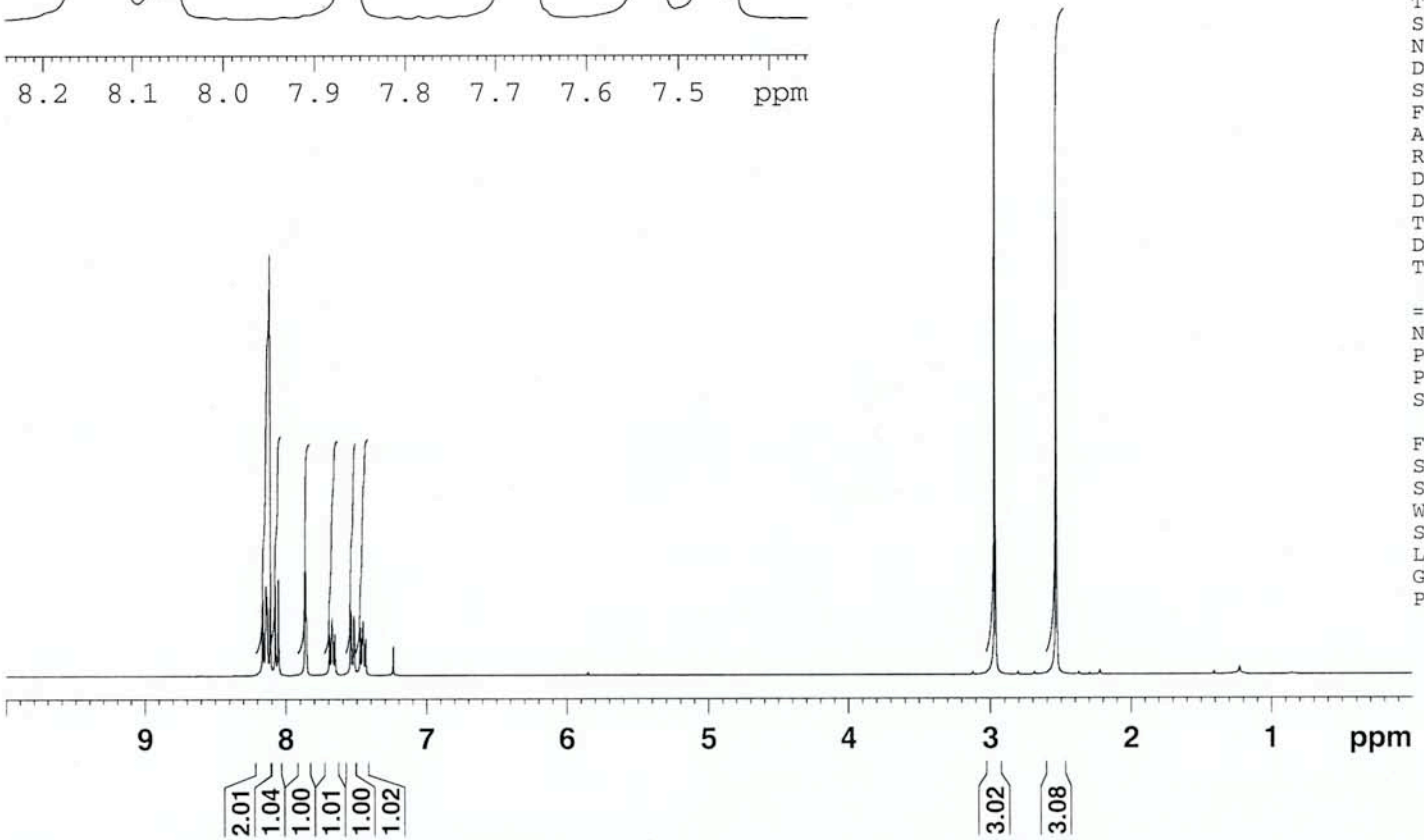
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.80


Me
F3C
N

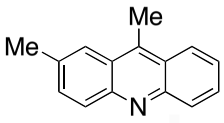

-63.645
150
100
50
0
-50
-100
-150
ppm








```
Current Data Parameters
NAME                  692
EXPNO                   4
PROCNO                  1

F2 - Acquisition Parameters
Date_            20100619
Time                11.06
INSTRUM             spect
PROBHD   5 mm QNP 1H/13
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      6
DS                      2
SWH              8278.146 Hz
FIDRES           0.126314 Hz
AQ               3.9584243 sec
RG                    128
DW                60.400 usec
DE                 6.00 usec
TE                 294.2 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 14.00 usec
PL1                 0.00 dB
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                  65536
SF           400.1300174 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                 1.00
```

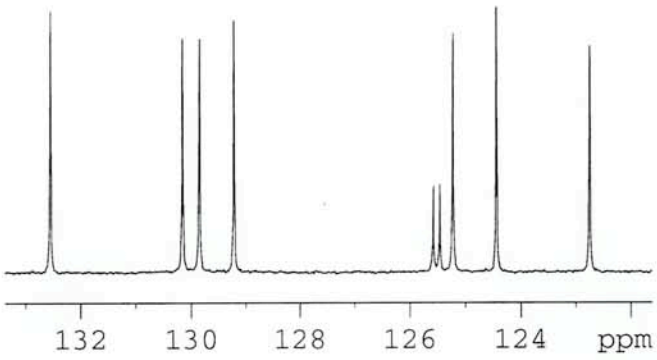


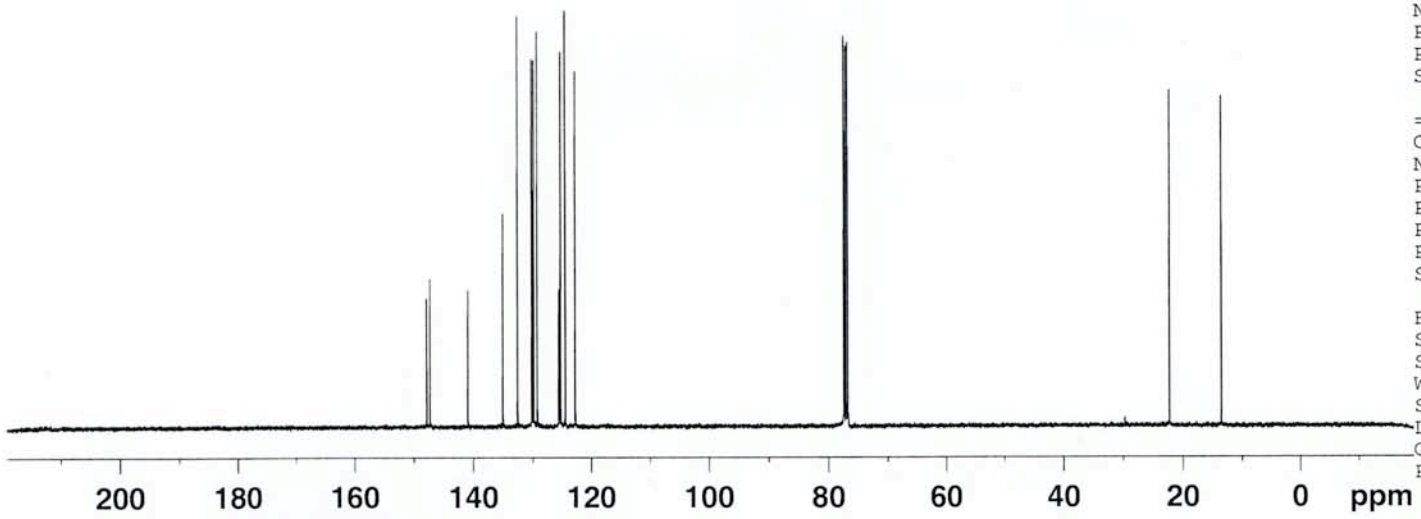
147.88
147.29
140.91
135.02
132.55
130.16
129.86
129.22
125.58
125.46
125.22
124.44
122.75

77.42
77.10
76.78

22.22

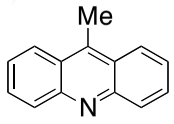
13.48

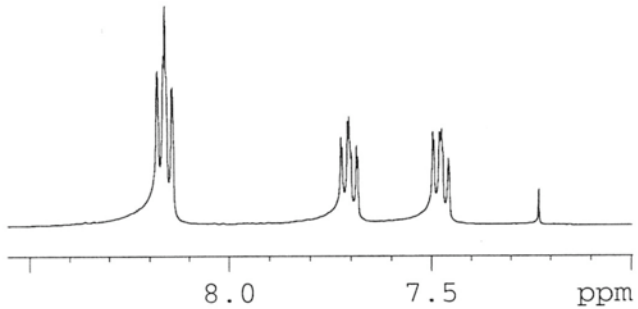


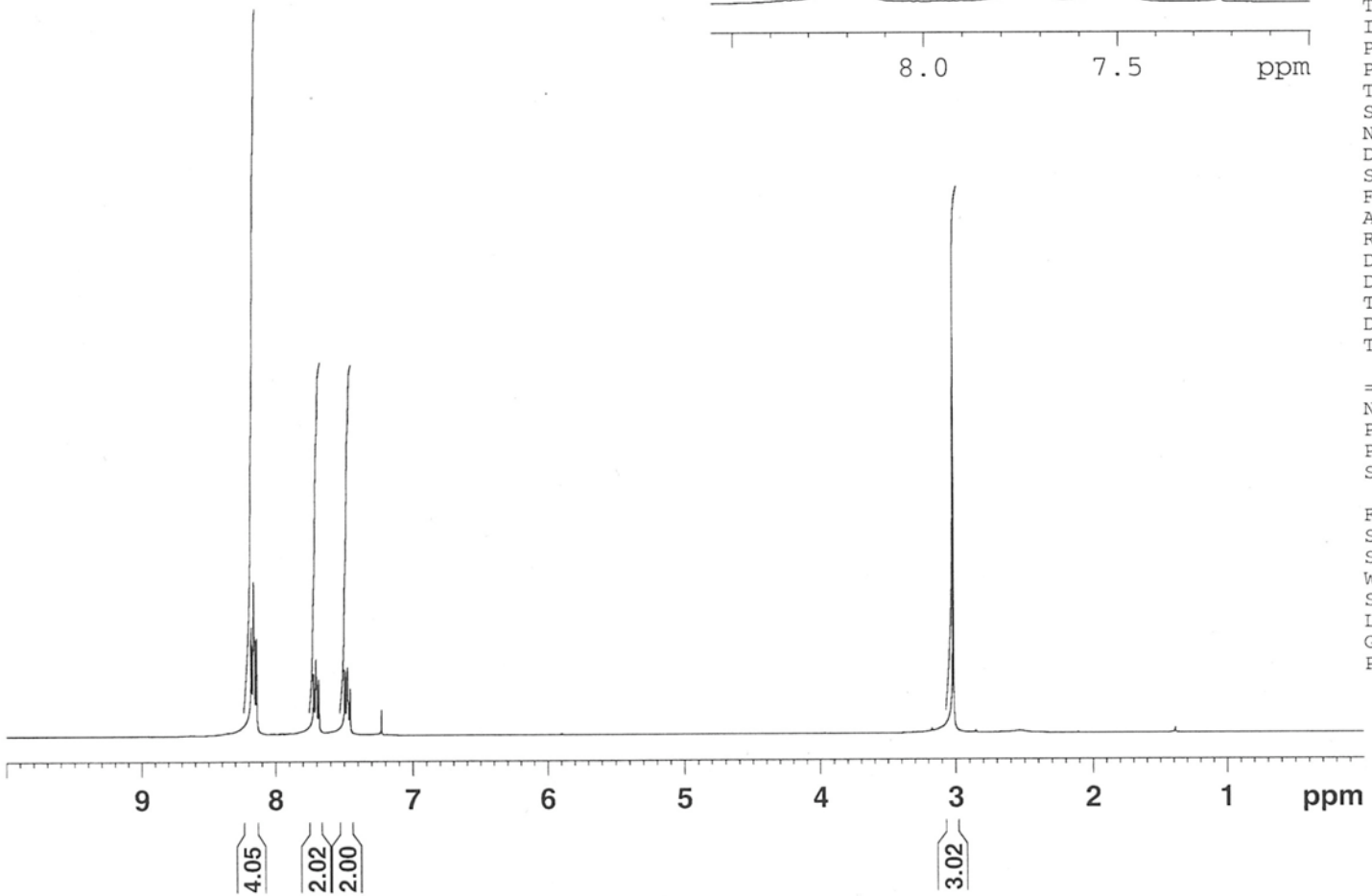


BRUKER

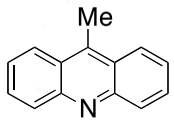
```
Current Data Parameters
NAME                  692
EXPNO                   5
PROCNO                  1

F2 - Acquisition Parameters
Date_            20100619
Time                12.37
INSTRUM             spect
PROBHD   5 mm QNP 1H/13
PULPROG           zgpg30
TD                 65536
SOLVENT             CDCl3
NS                   1491
DS                      4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                1824.6
DW                20.850 usec
DE                 6.00 usec
TE                295.2 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                 9.38 usec
PL1                0.00 dB
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             90.00 usec
PL2                0.00 dB
PL12              16.10 dB
PL13              19.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                 6.00
```

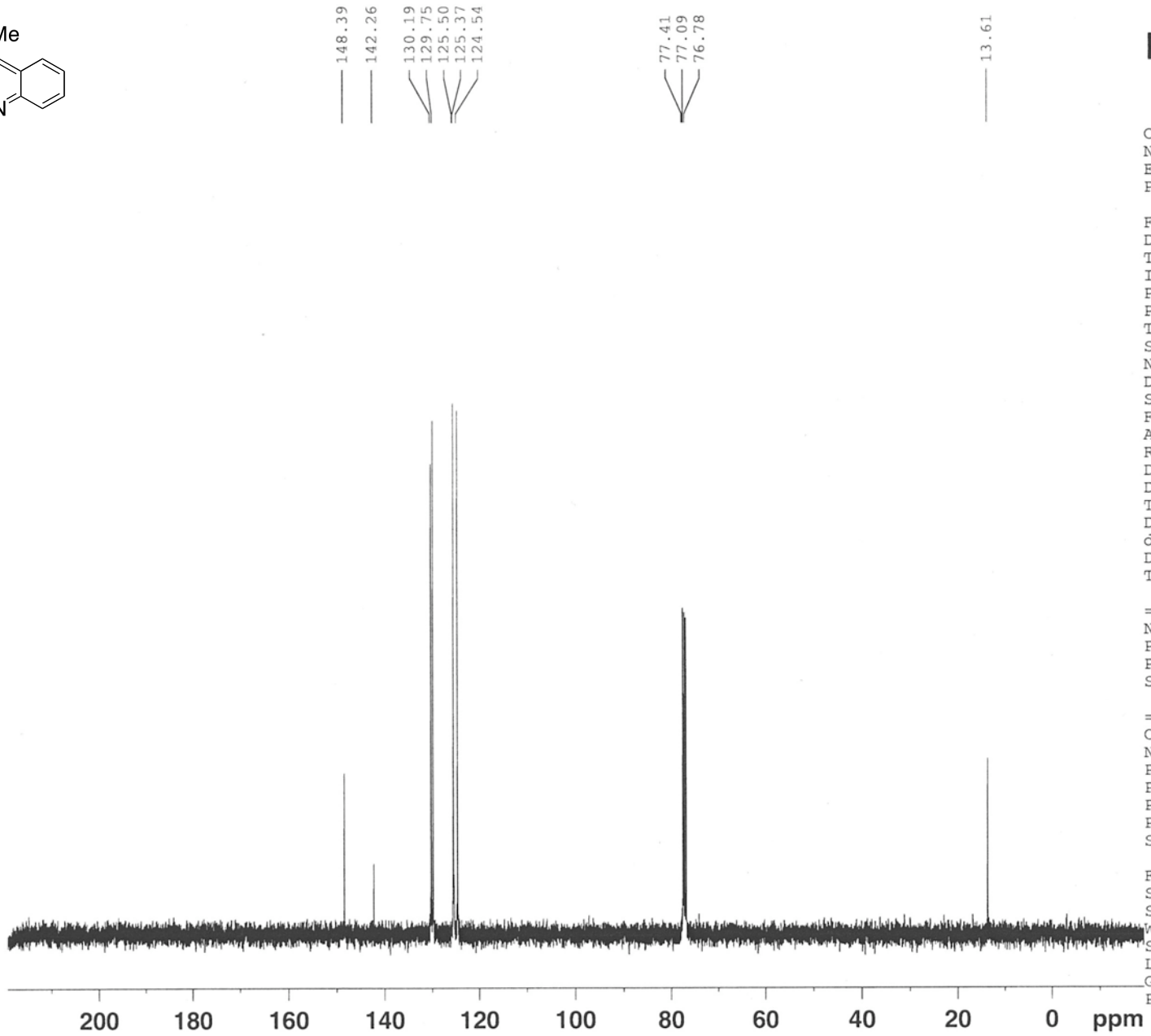






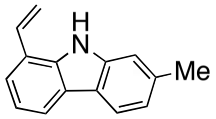

```
Current Data Parameters
NAME      9-methylacridine
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20100612
Time                 10.00
INSTRUM              spect
PROBHD   5 mm QNP 1H/13
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       6
DS                       2
SWH               8278.146 Hz
FIDRES             0.126314 Hz
AQ                3.9584243 sec
RG                    143.7
DW                   60.400 usec
DE                    6.00 usec
TE                   294.2 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   14.00 usec
PL1                   0.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                   65536
SF            400.1300220 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

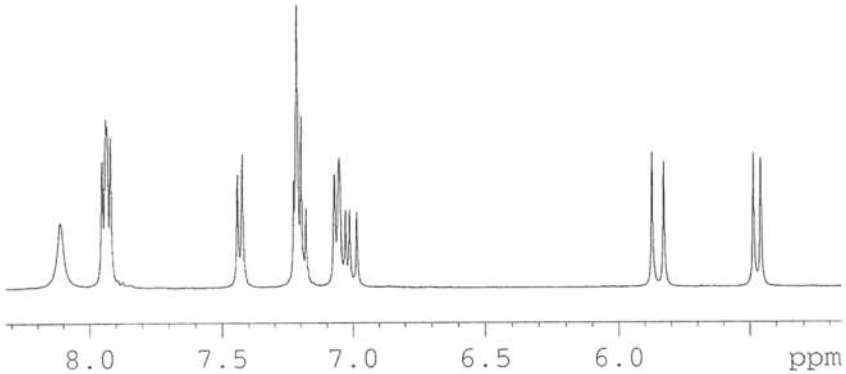


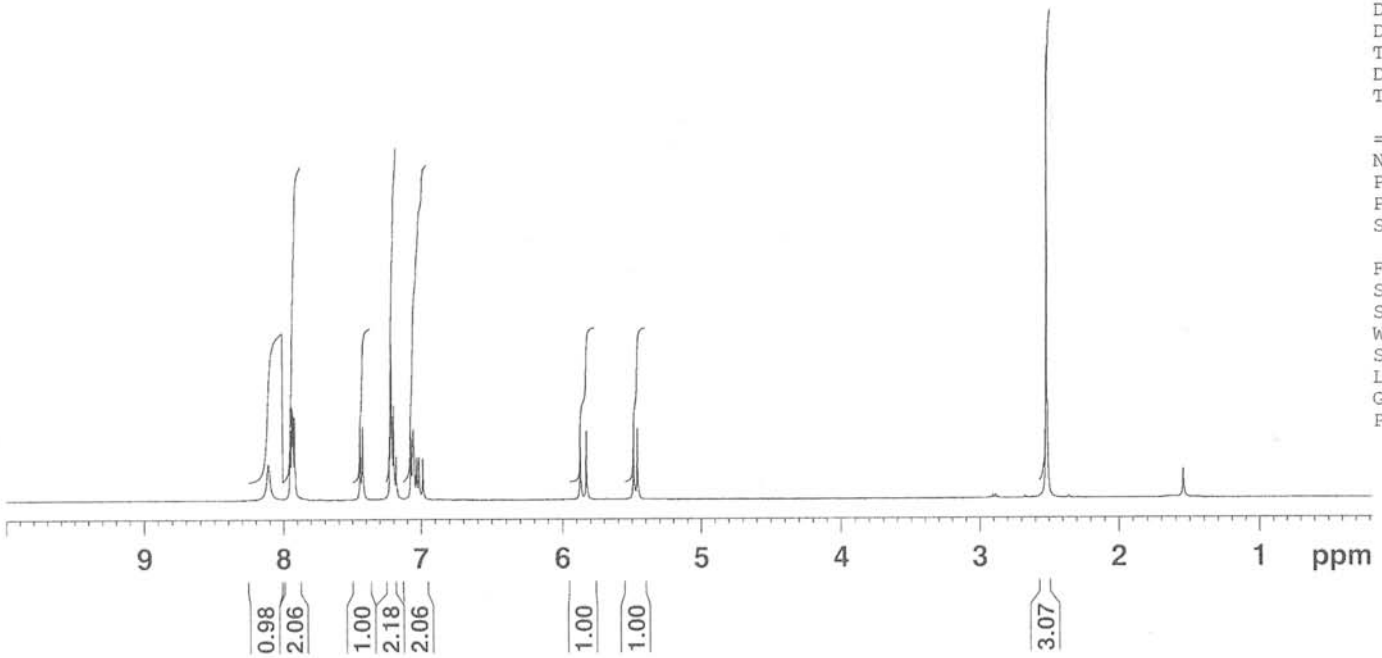


BRUKER

```
Current Data Parameters
NAME      9-methylacridine
EXPNO                    3
PROCNO                   1

F2 - Acquisition Parameters
Date_             20100612
Time                 10.07
INSTRUM              spect
PROBHD   5 mm QNP 1H/13
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                      57
DS                       4
SWH             23980.814 Hz
FIDRES          0.365918 Hz
AQ              1.3664756 sec
RG                 1824.6
DW                20.850 usec
DE                 6.00 usec
TE                295.2 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                  9.38 usec
PL1                 0.00 dB
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                   1H
PCPD2              90.00 usec
PL2                 0.00 dB
PL12               16.10 dB
PL13               19.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF           100.6127690 MHz
WDW                     EM
SSB                      0
LB                  1.00 Hz
GB                       0
PC                    1.40
```

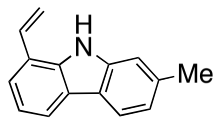


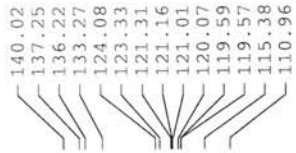


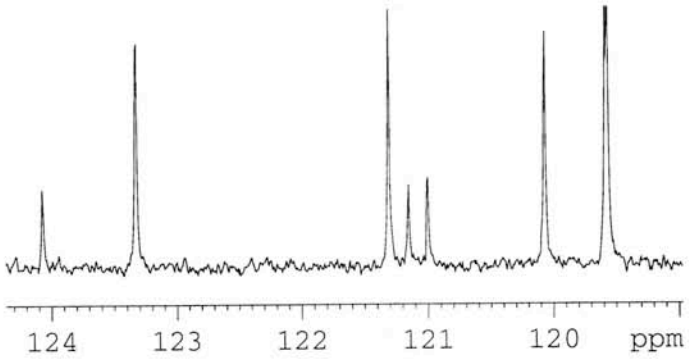


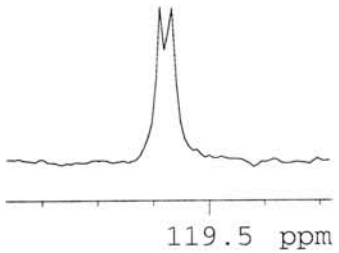
BRUKER

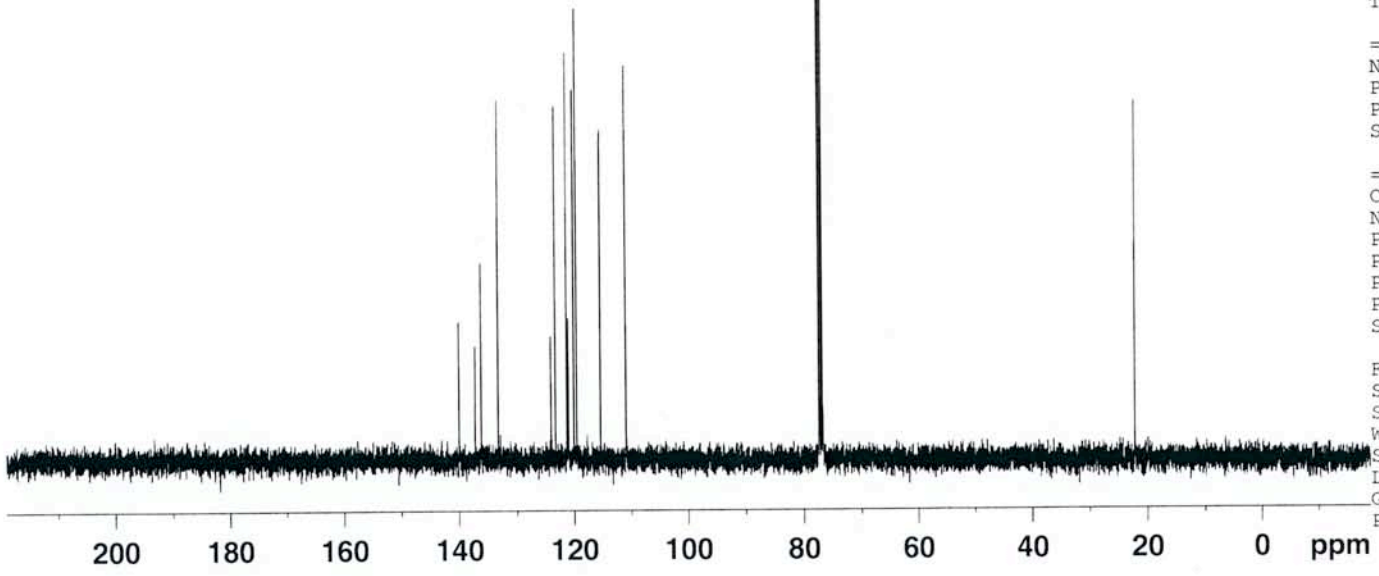
```
Current Data Parameters
NAME                  696
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20100630
Time                6.19
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    12
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 sec
RG                   256
DW                60.400 usec
DE                 6.00 usec
TE                294.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.00 usec
PL1                0.00 dB
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF           400.1300220 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                 1.00
```



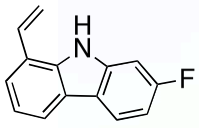


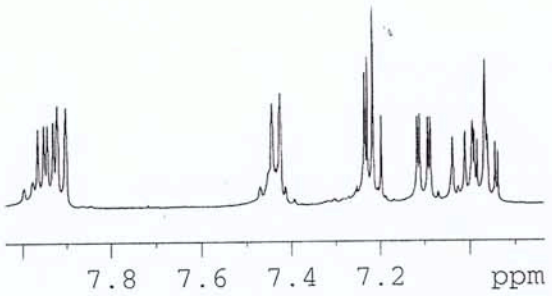


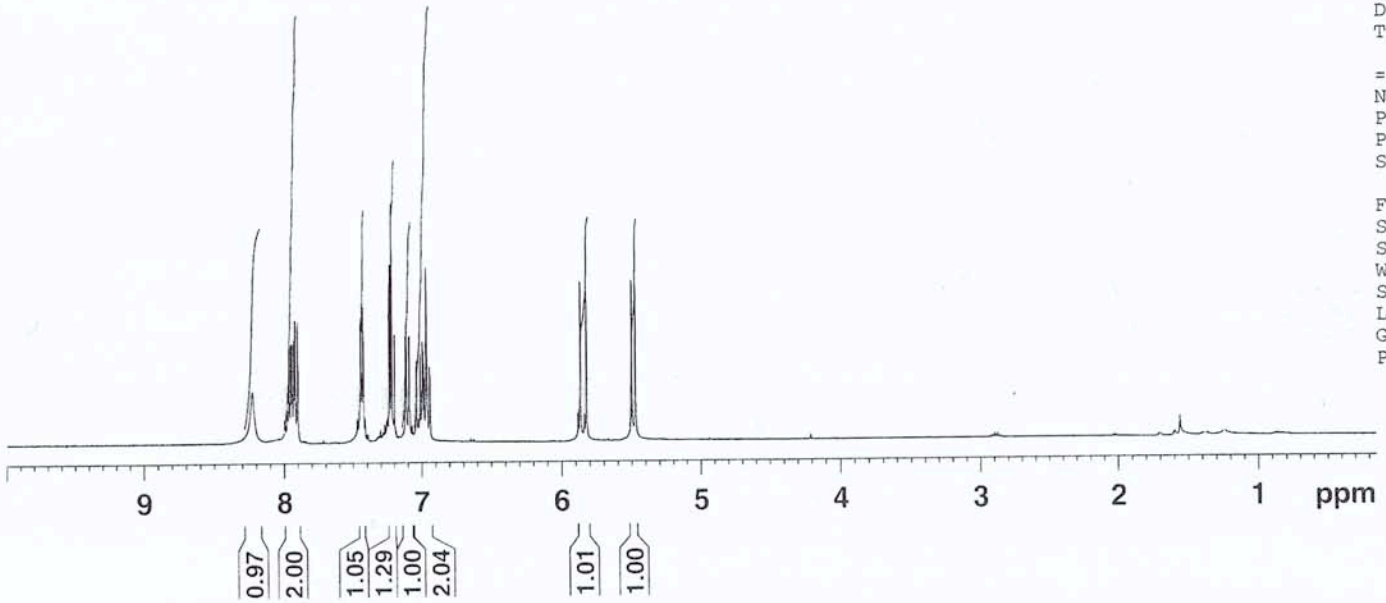





```
Current Data Parameters
NAME                  696
EXPNO                   6
PROCNO                  1

F2 - Acquisition Parameters
Date_            20100630
Time                18.14
INSTRUM             spect
PROBHD    5 mm QNP 1H/13
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   110
DS                     4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                4597.6
DW                20.850 usec
DE                 6.00 usec
TE                296.2 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                  9.38 usec
PL1                 0.00 dB
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2                 0.00 dB
PL12               16.10 dB
PL13               19.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF           100.6127690 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                 1.40
```







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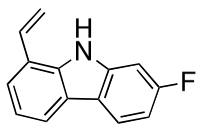
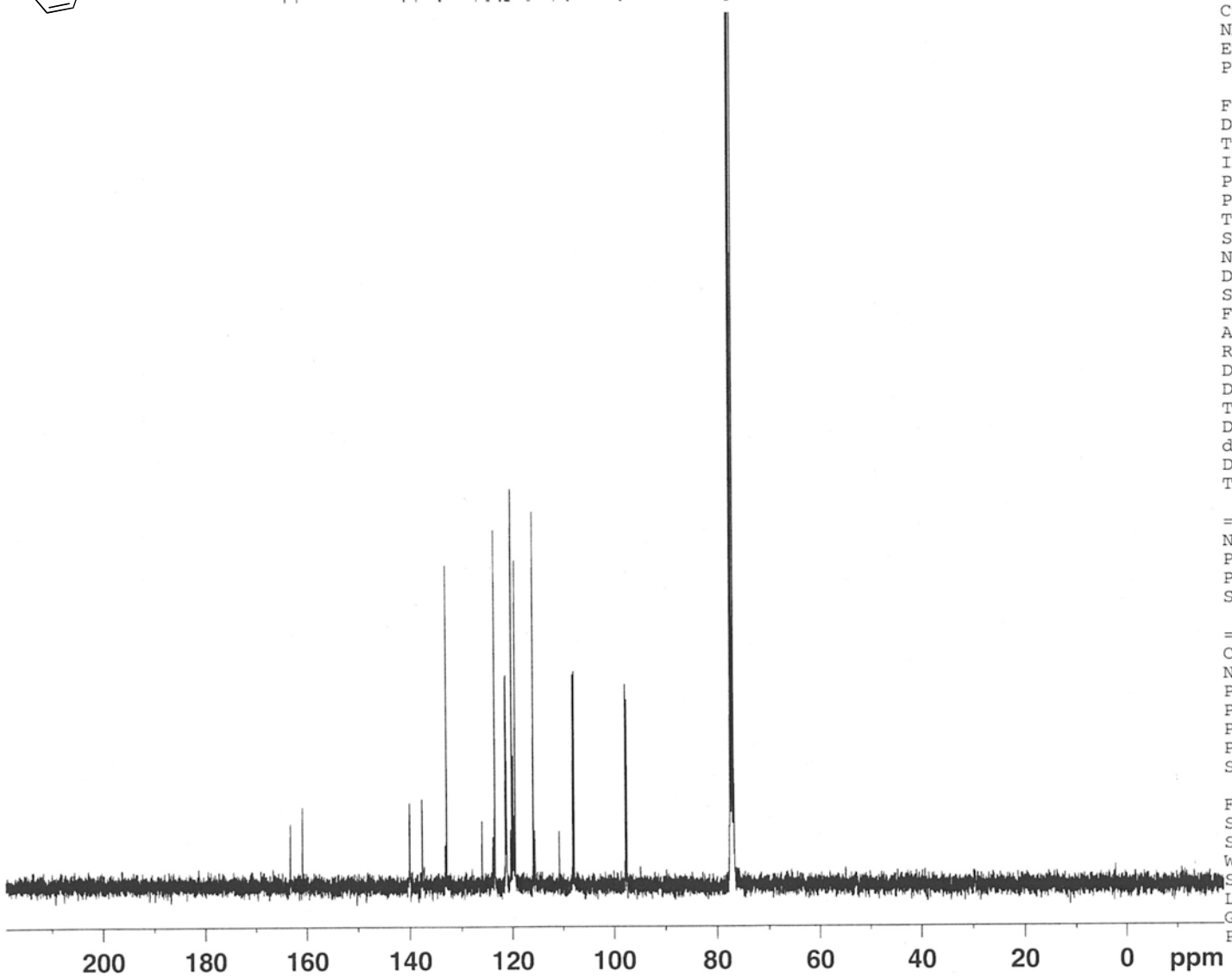
BRUKER

```
Current Data Parameters
NAME                  656
EXPNO                   4
PROCNO                  1

F2 - Acquisition Parameters
Date_            20100514
Time                14.12
INSTRUM             spect
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    17
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 sec
RG                 161.3
DW                60.400 usec
DE                 6.00 usec
TE                294.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.00 usec
PL1                0.00 dB
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF           400.1300220 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                  1.00
```



163.25
160.85
140.09
139.96
137.63
133.21
132.95
126.02
123.89
123.53
123.49
121.38
121.28
121.19
120.42
120.15
119.89
119.76
119.69
119.45
115.86
115.57
110.81
108.11
107.87
97.75
97.49
77.38
77.07
76.75



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BRUKER

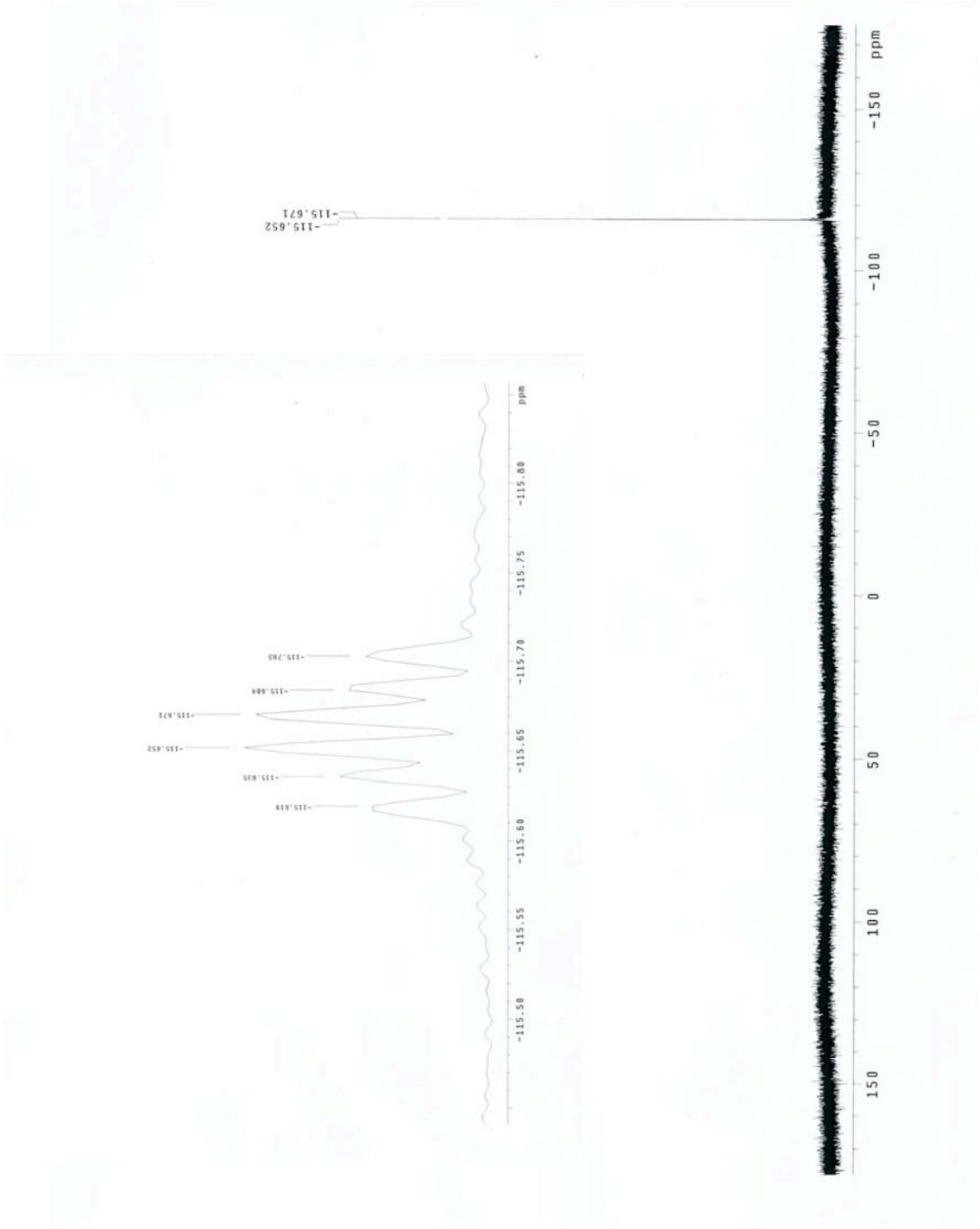
Current Data Parameters
NAME 656-1
EXPNO 2
PROCNO 1

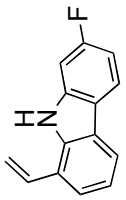
F2 - Acquisition Parameters
Date_ 20100515
Time 9.22
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1167
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 1824.6
DW 20.850 usec
DE 6.00 usec
TE 295.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

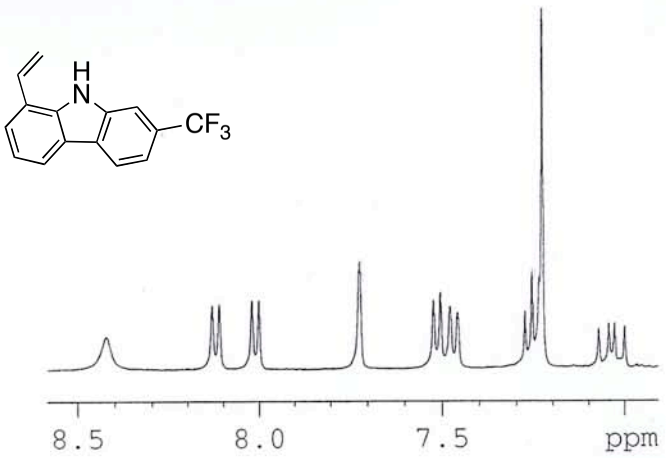
======== CHANNEL f1 ========
NUC1 13C
P1 9.38 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

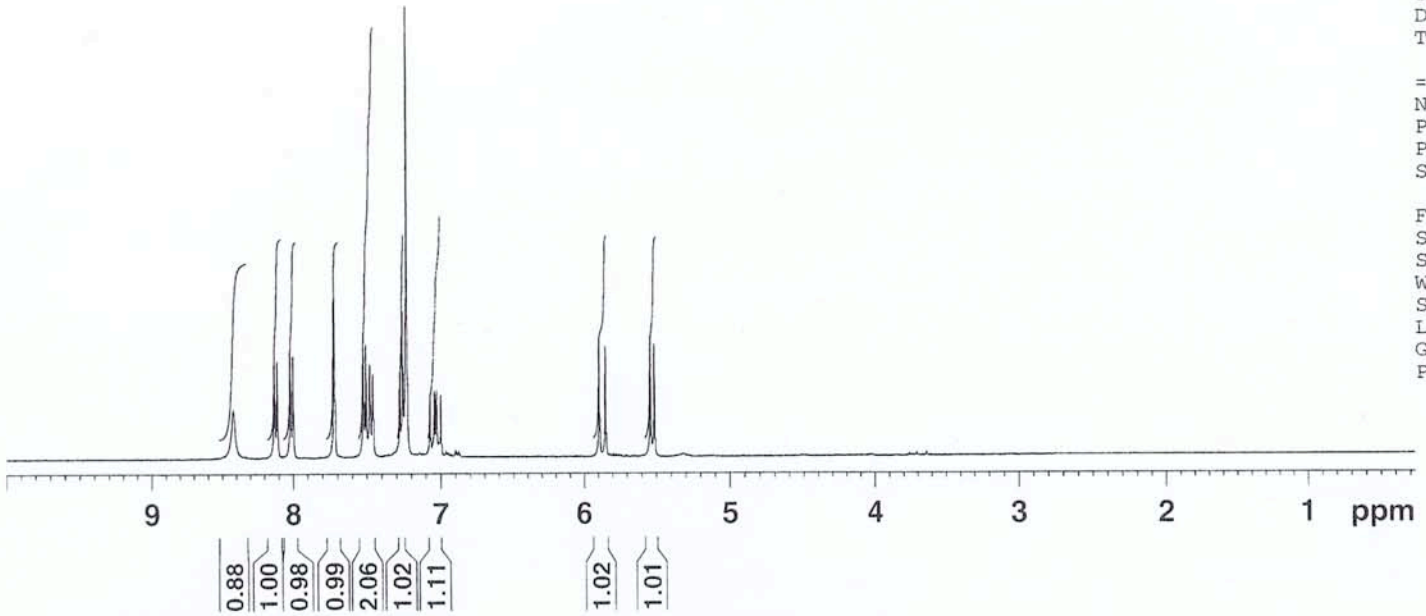
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.10 dB
PL13 19.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


-115.652
-115.671
150
100
50
0
-50
-100
-150
ppm
-115.50
-115.55
-115.60
-115.65
-115.70
-115.75
-115.80
ppm
-115.619
-115.635
-115.652
-115.671
-115.686
-115.703

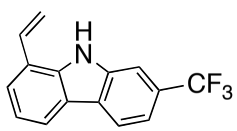

F
H
N

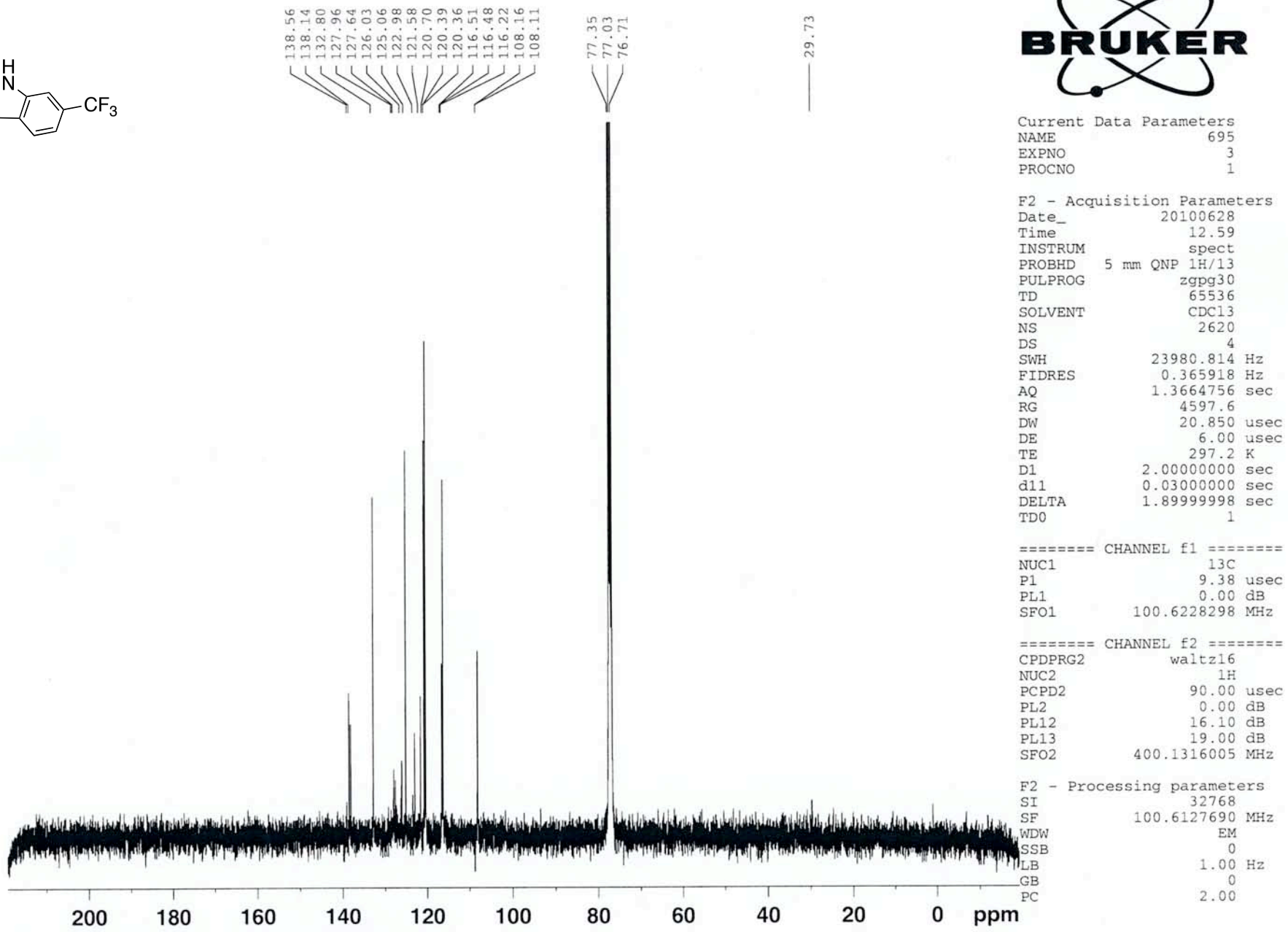




BRUKER

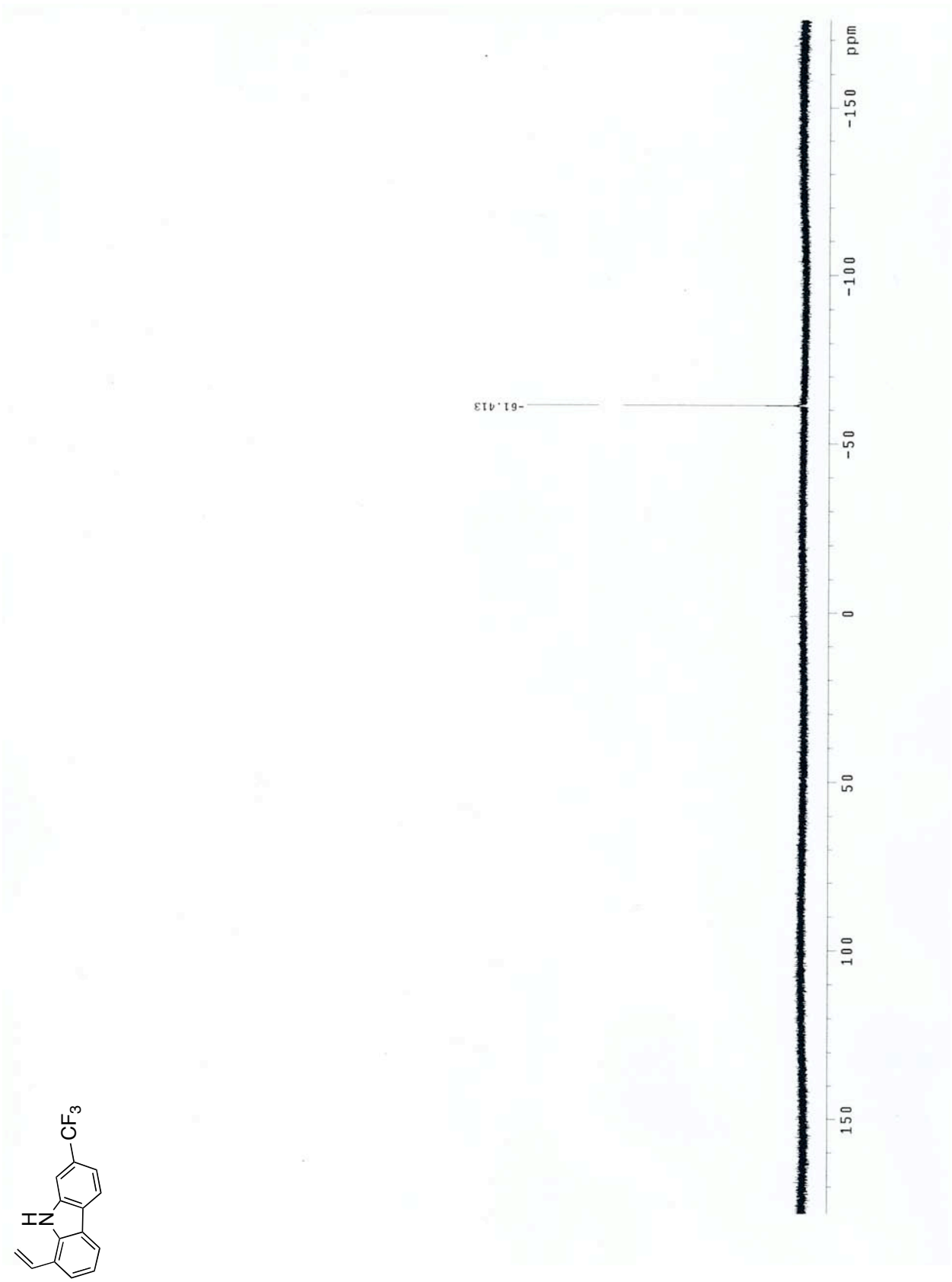
```
Current Data Parameters
NAME                  676-1
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20100527
Time                  7.07
INSTRUM              spect
PROBHD   5 mm QNP 1H/13
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       59
DS                        2
SWH               8278.146 Hz
FIDRES             0.126314 Hz
AQ                3.9584243 sec
RG                    322.5
DW                   60.400 usec
DE                    6.00 usec
TE                   294.2 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                   14.00 usec
PL1                   0.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                    65536
SF            400.1300220 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                     1.00
```



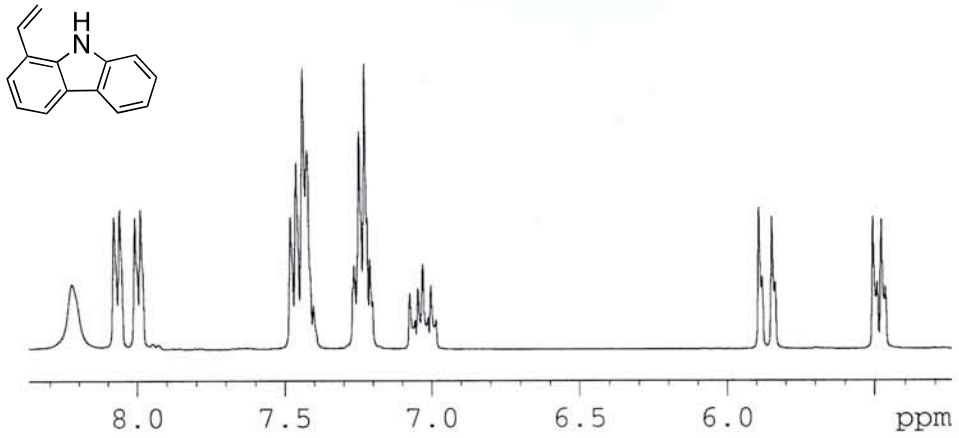


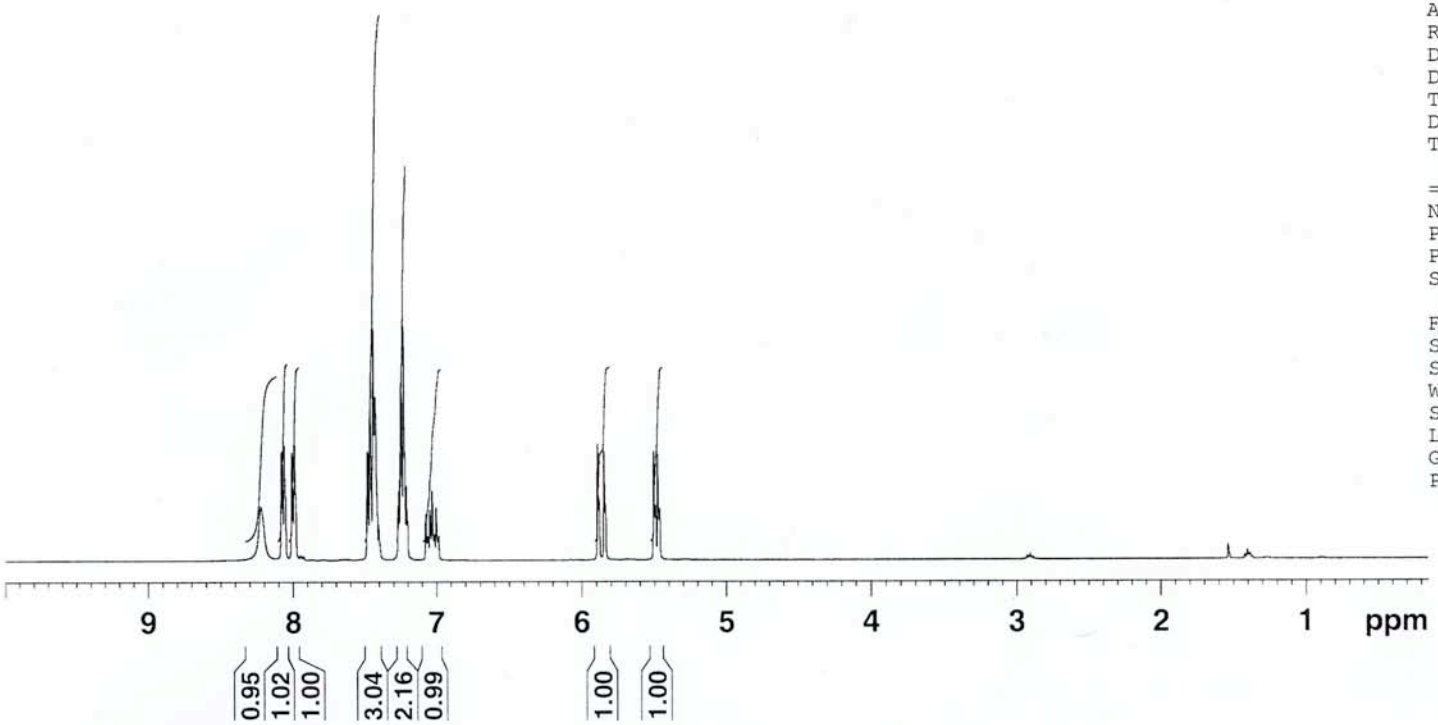
BRUKER

```
Current Data Parameters
NAME                  695
EXPNO                   3
PROCNO                  1

F2 - Acquisition Parameters
Date_            20100628
Time                12.59
INSTRUM             spect
PROBHD   5 mm QNP 1H/13
PULPROG           zgpg30
TD                 65536
SOLVENT             CDCl3
NS                   2620
DS                      4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                4597.6
DW                20.850 usec
DE                 6.00 usec
TE                297.2 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                 9.38 usec
PL1                0.00 dB
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                   1H
PCPD2             90.00 usec
PL2                0.00 dB
PL12              16.10 dB
PL13              19.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                2.00
```


-61.413
150
100
50
0
-50
-100
-150
ppm

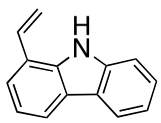
CF3
H
N

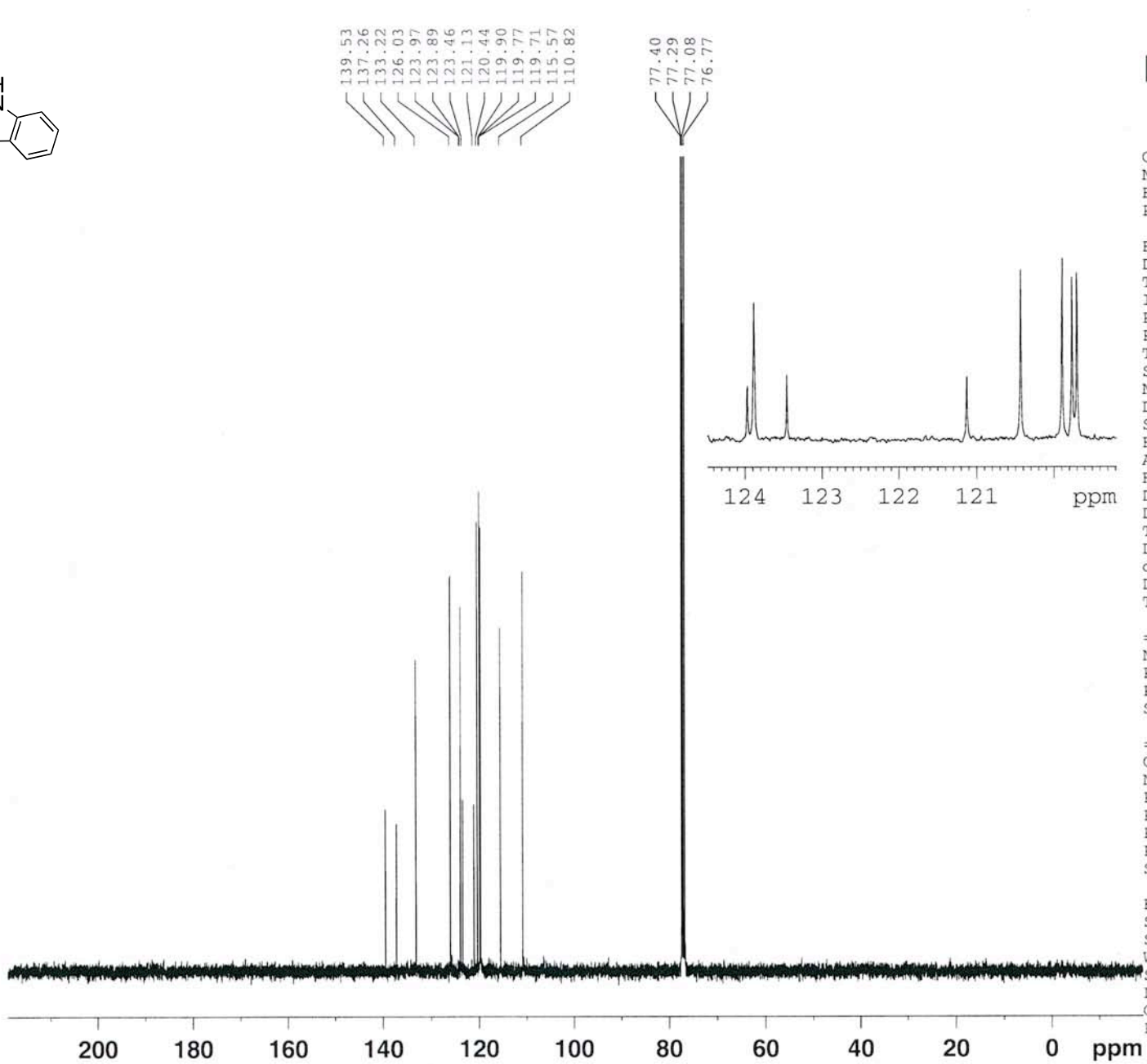




BRUKER

```
Current Data Parameters
NAME                  677-3
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20100603
Time                   7.13
INSTRUM               spect
PROBHD    5 mm QNP 1H/13
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       15
DS                        2
SWH                8278.146 Hz
FIDRES             0.126314 Hz
AQ                 3.9584243 sec
RG                      256
DW                   60.400 usec
DE                    6.00 usec
TE                   294.2 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                   14.00 usec
PL1                   0.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                    65536
SF            400.1300220 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                     1.00
```

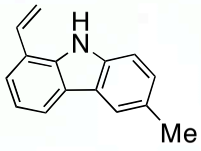


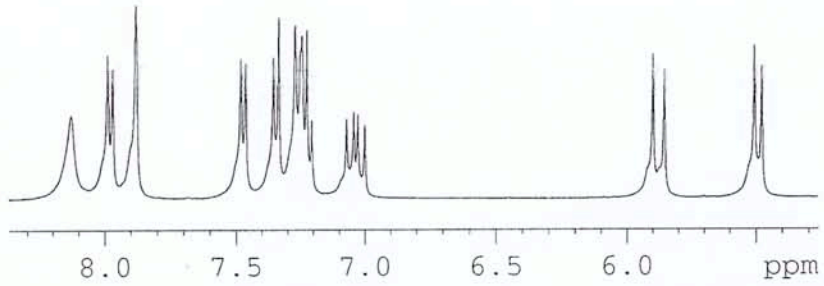


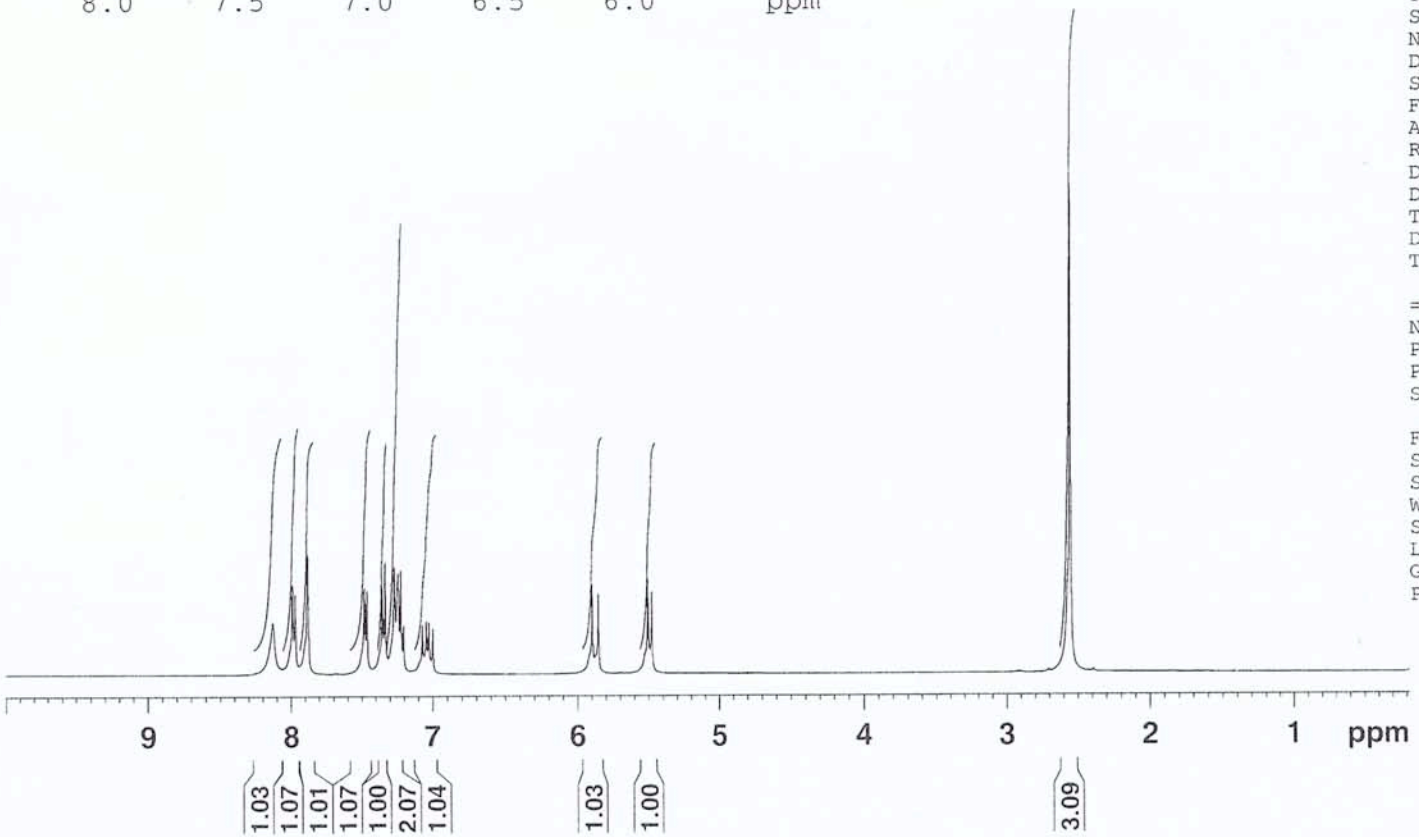
BRUKER

```
Current Data Parameters
NAME                  677-3
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20100603
Time                   7.51
INSTRUM               spect
PROBHD    5 mm QNP 1H/13
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     534
DS                       4
SWH            23980.814 Hz
FIDRES          0.365918 Hz
AQ             1.3664756 sec
RG                  1824.6
DW                 20.850 usec
DE                  6.00 usec
TE                 295.2 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                  9.38 usec
PL1                 0.00 dB
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                   1H
PCPD2              90.00 usec
PL2                 0.00 dB
PL12               16.10 dB
PL13               19.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF           100.6127690 MHz
WDW                     EM
SSB                      0
LB                  1.00 Hz
GB                       0
PC                   1.40
```

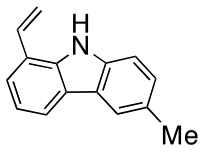
96-IS







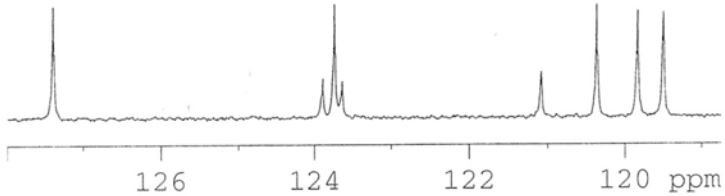

```
Current Data Parameters
NAME                  658
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20100507
Time                10.00
INSTRUM             spect
PROBHD   5 mm QNP 1H/13
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8278.146 Hz
FIDRES           0.126314 Hz
AQ               3.9584243 sec
RG                  228.1
DW                 60.400 usec
DE                  6.00 usec
TE                 295.2 K
D1            1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 14.00 usec
PL1                 0.00 dB
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                  65536
SF           400.1300175 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                   1.00
```

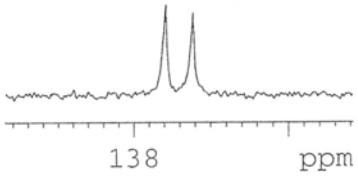


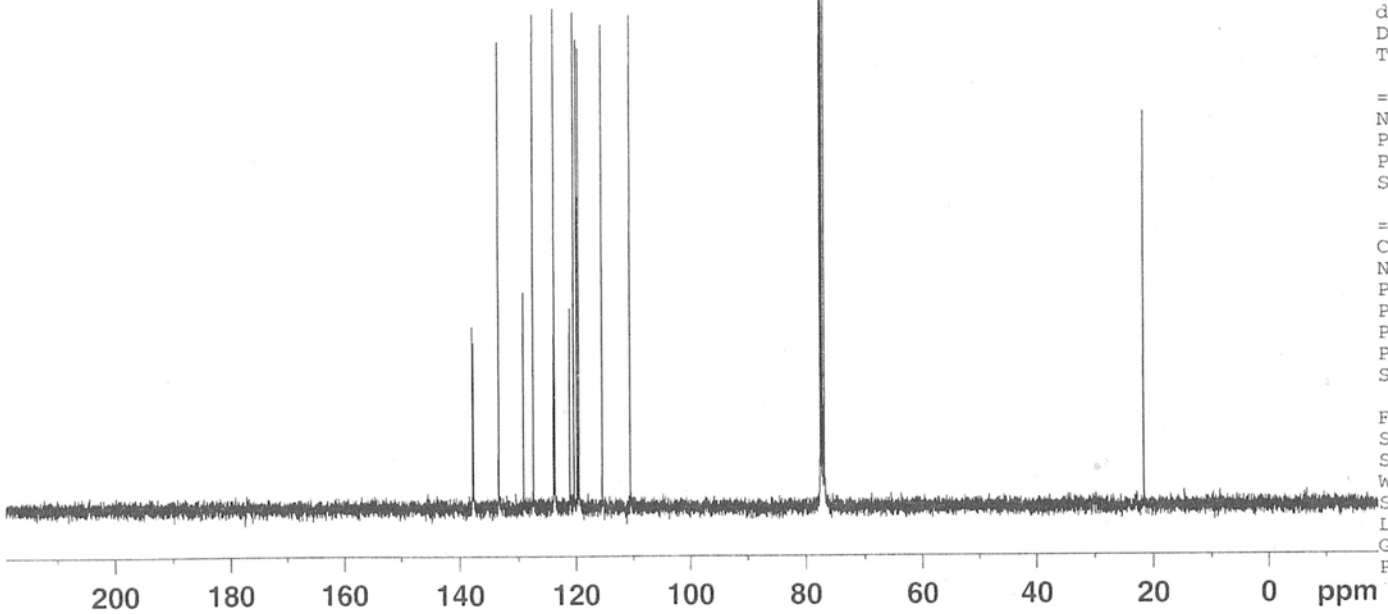
137.79
137.62
133.30
129.09
127.39
123.89
123.74
123.64
121.08
120.36
119.83
119.49
115.39
110.50

77.42
77.10
76.78

21.52







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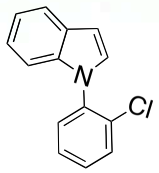
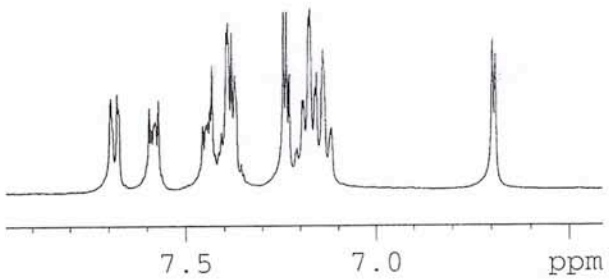
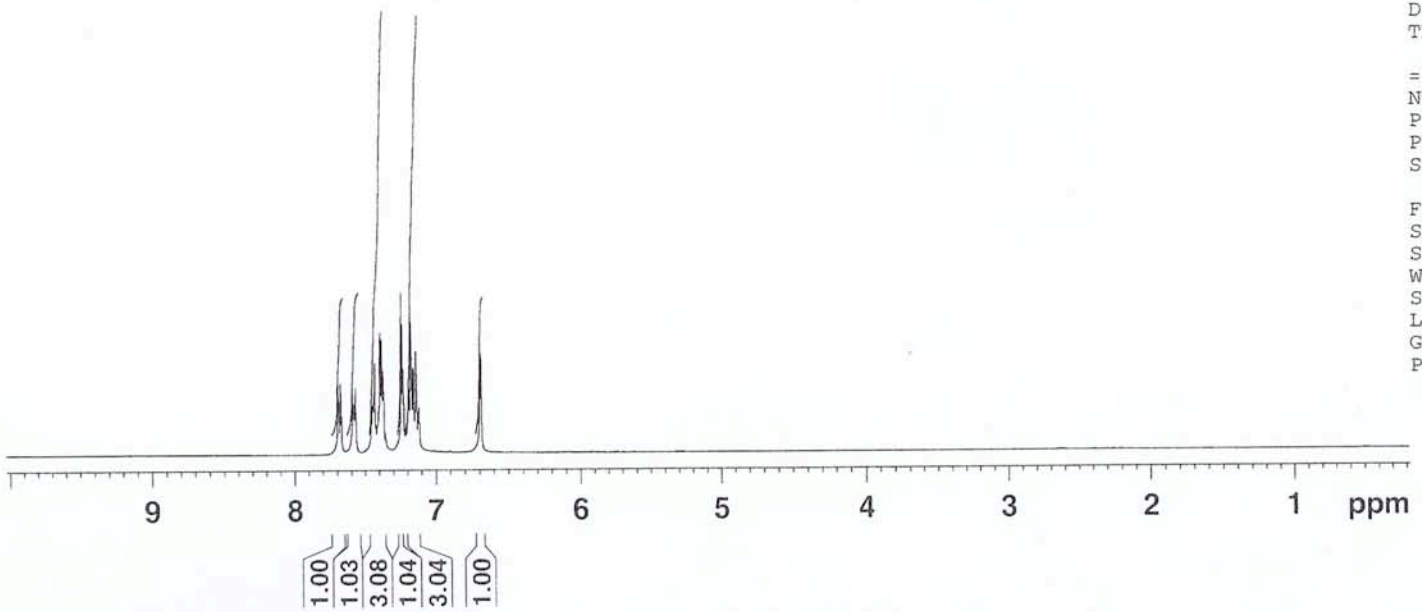
```
Current Data Parameters
NAME                  658
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20100507
Time                10.50
INSTRUM             spect
PROBHD   5 mm QNP 1H/13
PULPROG           zgpg30
TD                 65536
SOLVENT             CDCl3
NS                    749
DS                      4
SWH             23980.814 Hz
FIDRES          0.365918 Hz
AQ              1.3664756 sec
RG                 1824.6
DW                20.850 usec
DE                 6.00 usec
TE                295.2 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                 9.38 usec
PL1                0.00 dB
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             90.00 usec
PL2                0.00 dB
PL12              16.10 dB
PL13              19.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF           100.6127690 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                 5.00
```

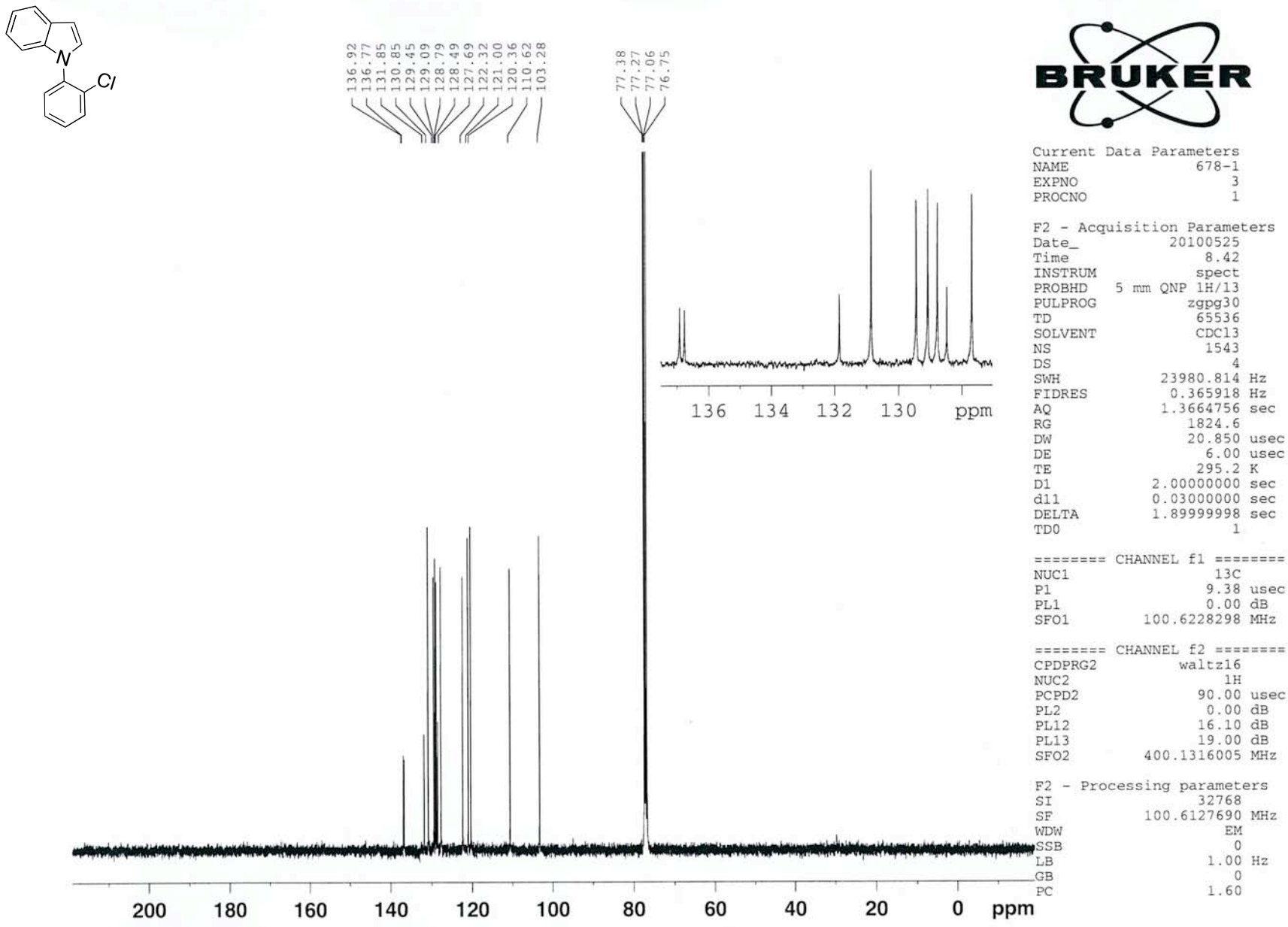


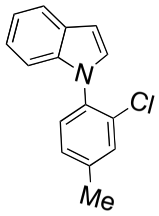


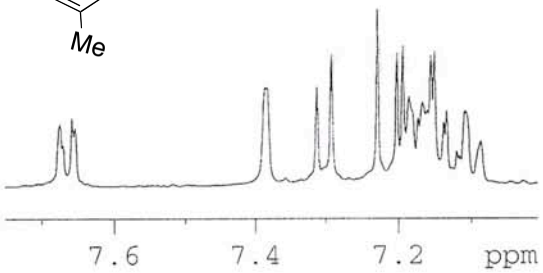


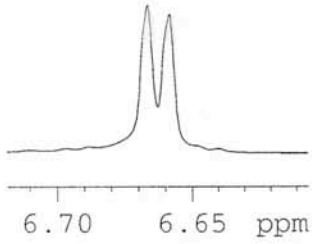
BRUKER

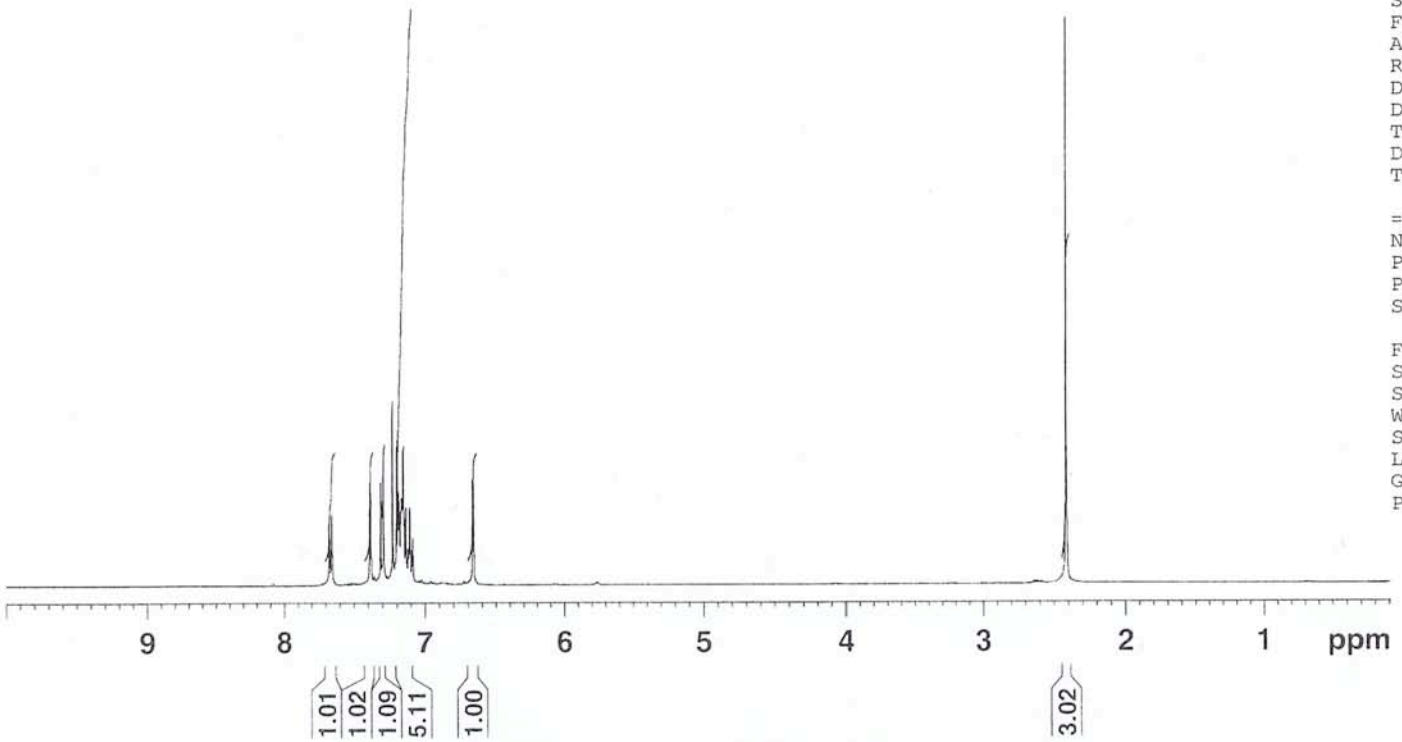
```
Current Data Parameters
NAME                  678-1
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20100524
Time                 13.38
INSTRUM              spect
PROBHD    5 mm QNP 1H/13
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      13
DS                       2
SWH               8278.146 Hz
FIDRES               0.126314 Hz
AQ                3.9584243 sec
RG                     256
DW                  60.400 usec
DE                   6.00 usec
TE                  294.2 K
D1               1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                  14.00 usec
PL1                  0.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                   65536
SF            400.1300220 MHz
WDW                     EM
SSB                      0
LB                   0.30 Hz
GB                       0
PC                    1.00
```

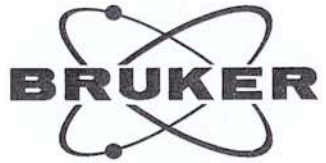

136.92
136.77
131.85
130.85
129.45
129.09
128.79
128.49
127.69
122.32
121.00
120.36
110.62
103.28
77.38
77.27
77.06
76.75
136
134
132
130
ppm
200
180
160
140
120
100
80
60
40
20
0
ppm
BRUKER
Current Data Parameters
NAME 678-1
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100525
Time 8.42
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1543
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 1824.6
DW 20.850 usec
DE 6.00 usec
TE 295.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.38 usec
PL1 0.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.10 dB
PL13 19.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.60



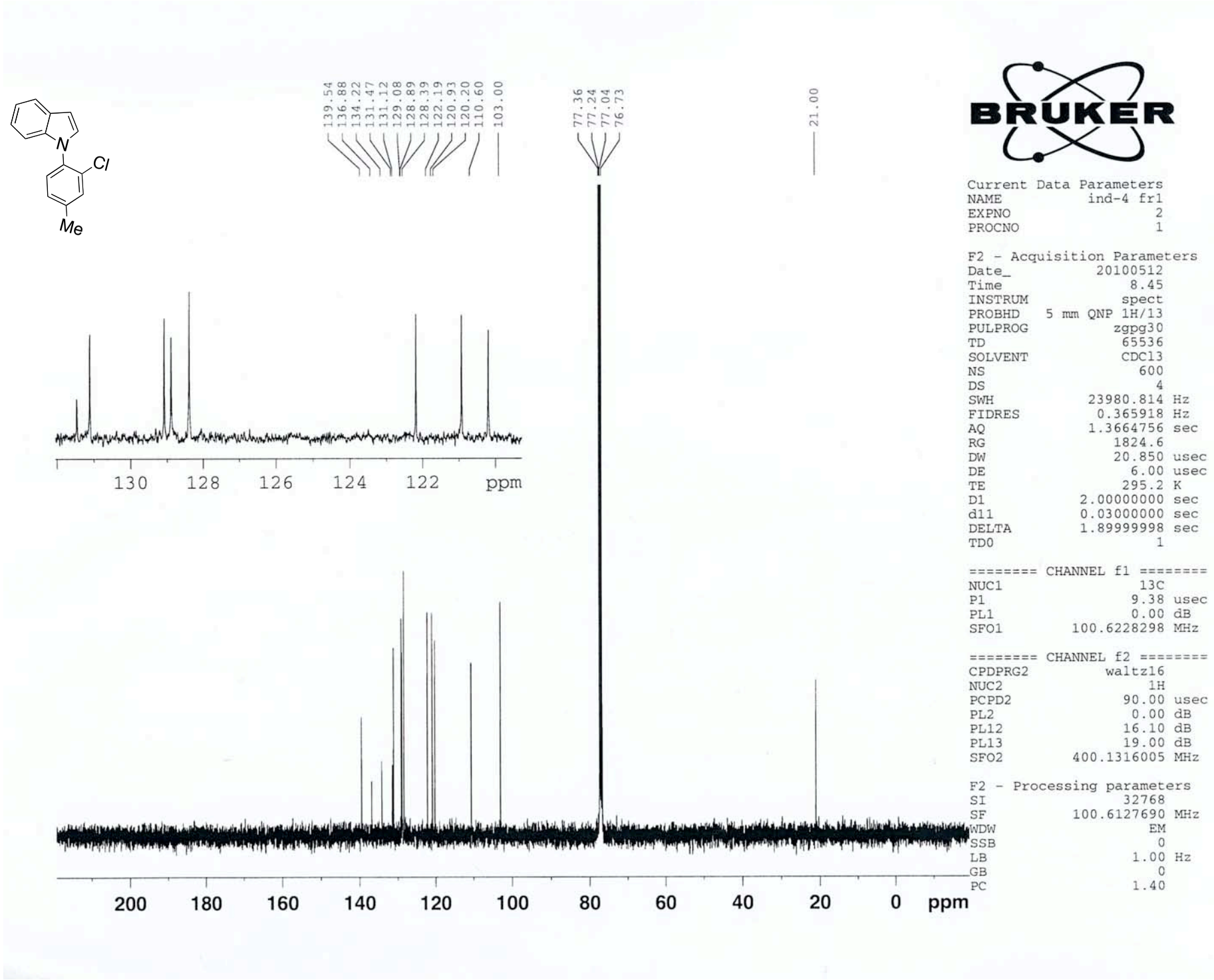


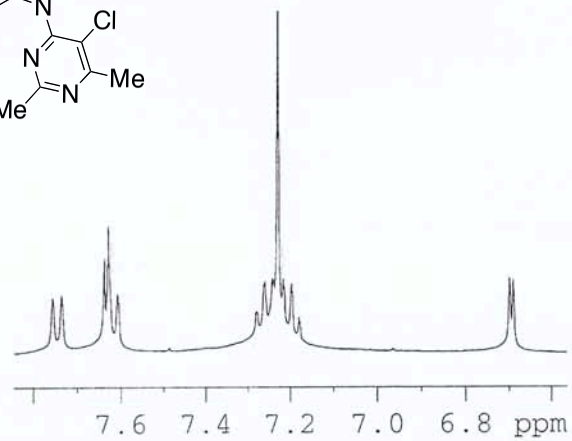


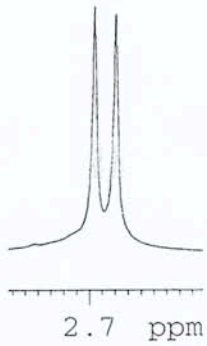


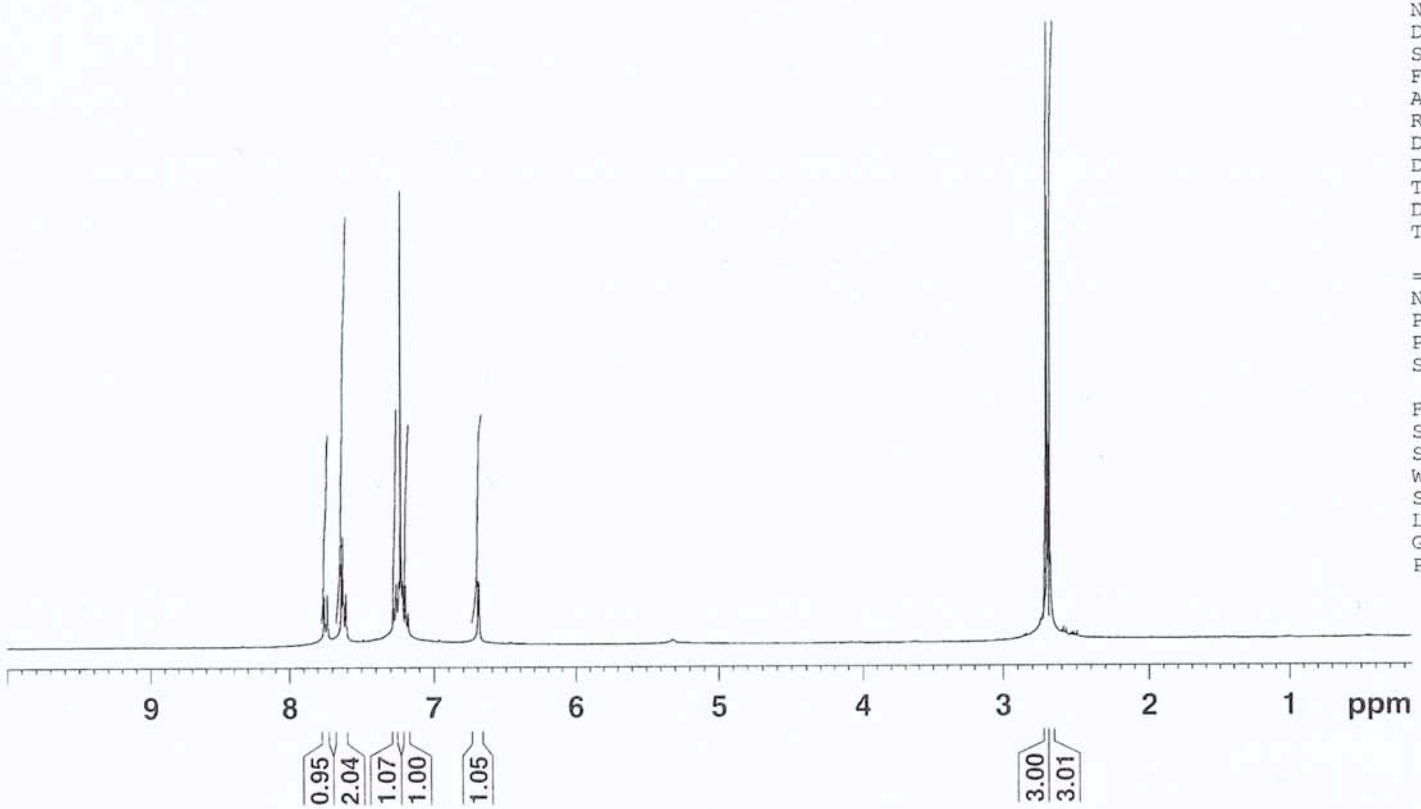



```
Current Data Parameters
NAME                  ind-4 fr1
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20100512
Time                       7.57
INSTRUM                   spect
PROBHD    5 mm QNP 1H/13
PULPROG                    zg30
TD                        65536
SOLVENT                   CDCl3
NS                           43
DS                            2
SWH                    8278.146 Hz
FIDRES                 0.126314 Hz
AQ                     3.9584243 sec
RG                          256
DW                       60.400 usec
DE                        6.00 usec
TE                       294.2 K
D1                    1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         1H
P1                       14.00 usec
PL1                       0.00 dB
SFO1             400.1324710 MHz

F2 - Processing parameters
SI                        65536
SF               400.1300220 MHz
WDW                          EM
SSB                           0
LB                        0.30 Hz
GB                            0
PC                         1.00
```


139.54
136.88
134.22
131.47
131.12
129.08
128.89
128.39
122.19
120.93
120.20
110.60
103.00
77.36
77.24
77.04
76.73
21.00
N
Cl
Me
130
128
126
124
122
ppm
200
180
160
140
120
100
80
60
40
20
0
ppm
BRUKER
Current Data Parameters
NAME ind-4 fr1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100512
Time 8.45
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 600
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 1824.6
DW 20.850 usec
DE 6.00 usec
TE 295.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.38 usec
PL1 0.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.10 dB
PL13 19.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

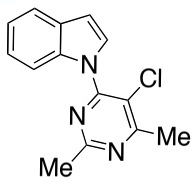


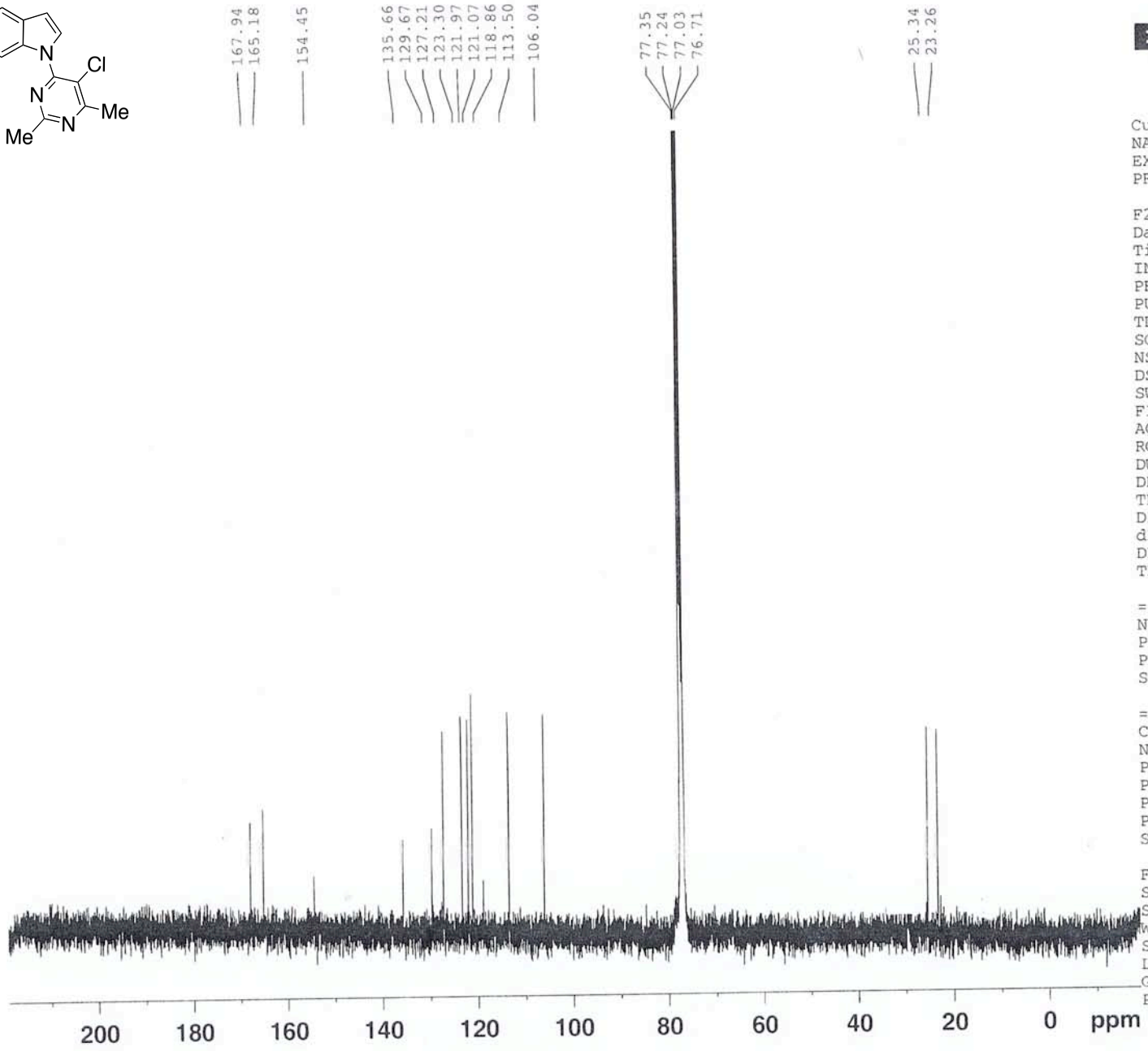




BRUKER

```
Current Data Parameters
NAME                  ind2-1
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20100513
Time                   7.52
INSTRUM               spect
PROBHD   5 mm QNP 1H/13
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                      578
DS                        2
SWH                8278.146 Hz
FIDRES             0.126314 Hz
AQ                 3.9584243 sec
RG                      362
DW                   60.400 usec
DE                    6.00 usec
TE                   294.2 K
D1              1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                   14.00 usec
PL1                   0.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                    65536
SF              400.1300220 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                     1.00
```





BRUKER

```
Current Data Parameters
NAME                  ind2
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_              20100519
Time                  7.37
INSTRUM              spect
PROBHD    5 mm QNP 1H/13
PULPROG             zgpg30
TD                   65536
SOLVENT              CDC13
NS                   12838
DS                       4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                1824.6
DW               20.850 usec
DE                6.00 usec
TE                294.2 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                  13C
P1                 9.38 usec
PL1                0.00 dB
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             90.00 usec
PL2                0.00 dB
PL12              16.10 dB
PL13              19.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF          100.6127690 MHz
WDW                    EM
SSB                     0
LB                1.00 Hz
GB                      0
PC                   1.40
```