

Supporting Information for

Allenylazide Cycloaddition Chemistry. Synthesis of Annelated Indoles from 2-(Allenyl)phenylazide Substrates.

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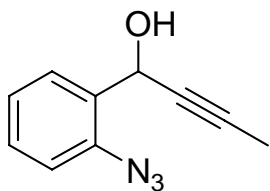
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General Experimental

Moisture and oxygen sensitive reactions were carried out in flame-dried glassware under a nitrogen atmosphere. Solvents were dried by passage through an activated alumina column under nitrogen. All organic reagents were used as purchased. Flash chromatography was performed using 32 – 63 μm silica gel with the indicated solvent systems. Melting points are uncorrected. Low and high resolution mass spectra were obtained according to the specified technique and were performed at the Proteomics and Mass Spectrometry Core Facility at the Pennsylvania State University. Copies of ^1H and ^{13}C NMR spectra are supplied in the Supporting Information as criteria of purity.

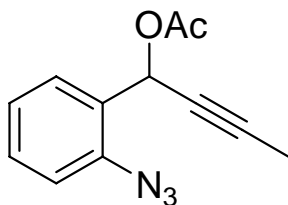
1-(2-Azidophenyl)but-2-yn-1-ol.



To a solution of 2-azidobenzaldehyde (**8**) (2.0 g, 14 mmol) in 20 mL of THF at $-20\text{ }^\circ\text{C}$ was added 1-propynylmagnesium bromide (0.50 M, 30 mL, 15 mmol) and the mixture was stirred for 2 h. The reaction mixture was warmed to room temperature over an additional hour and poured into 20 mL of saturated NH_4Cl solution. The organic layer was extracted with 3x30 mL of Et_2O and the combined organic extracts were washed with water and brine, dried over Na_2SO_4 and the solvent was evaporated to yield a brown oil. The crude material was carried over to the next step. A small batch was purified by column chromatography (40% Et_2O in hexanes) to give a white solid: mp $49 - 50\text{ }^\circ\text{C}$; IR (neat): $3400, 2125\text{ cm}^{-1}$; ^1H NMR (300 MHz, C_6D_6) δ 7.69 (m, 1H), 6.86 (m, 2H), 6.61 (m, 1H), 5.67 (d, $J = 2.1\text{ Hz}$, 1H), 3.07 (br s, 1H), 1.47 (d, $J = 2.2\text{ Hz}$, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 137.0, 131.9, 129.4, 128.1, 124.9, 118.0, 82.9, 78.2, 60.3, 3.6; TOFESMS m/z relative intensity 210.1 (MNa^+ 100%); HRMS (+ES) Calcd for $\text{C}_{10}\text{H}_9\text{N}_3\text{ONa}$: 210.0643, Found: 210.0639.

Representative Procedure 1. Azidophenyl Alkynyl Acetate Synthesis.

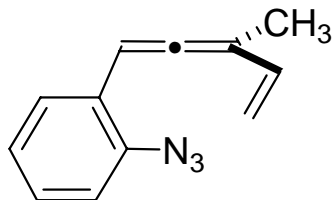
1-Acetoxy-1(2-azidophenyl)but-2-yne (**9a**).



Acetic anhydride (1.2 mL, 13 mmol) and DMAP (1.6 g, 13 mmol) were added to an ice-cold solution of 1-(2-azidophenyl)but-2-yn-1-ol (2.0 g, 11 mmol) in 40 mL of CH₂Cl₂, and the mixture was stirred for 24 h with warming to room temperature. The reaction mixture was poured into 30 mL of saturated NaHCO₃ solution. The mixture was then extracted with 3x30 mL of CH₂Cl₂ and the combined organic layers were washed with water and brine, dried over Na₂SO₄ and concentrated *in vacuo*. The crude material was purified by column chromatography (25% Et₂O in hexanes) to give the acetate **9a** as a pale yellow solid (1.5 g, 61%): mp 49 – 50 °C; IR (neat): 2140, 1736 cm⁻¹; ¹H NMR (360 MHz, C₆D₆) δ 7.75 (dd, *J* = 7.5, 1.8 Hz, 1H), 6.91 (m, 3H), 6.64 (dd, *J* = 7.6, 1.4 Hz, 1H), 1.66 (s, 3H), 1.45 (d, *J* = 2.3 Hz, 3H); ¹³C NMR (90 MHz, C₆D₆) δ 168.9, 138.1, 130.2, 129.5, 129.3, 124.9, 118.4, 83.6, 76.4, 61.3, 20.4, 3.3; TOFESMS *m/z* (relative intensity) 252.0 (MNa⁺, 100%), 284.0 (MMeOH⁺, 70%); HRMS Calcd for C₁₂H₁₁N₃O₂Na : 252.0749, Found: 252.0762.

Representative Procedure 2. Allenylazide Synthesis.

1-(2-Azidophenyl)3-methylpent-1,2,4-triene (**6a**).

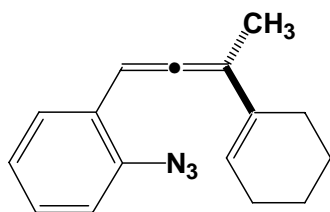


To a solution of ZnCl₂ (0.34 g, 2.5 mmol) in 10 mL of THF was added vinylMgBr (1.0 M in THF, 2.5 mL, 2.5 mmol) and the mixture was stirred at room temperature for 1 h. Pd(PPh₃)₄ (58 mg, 5.0 mol%) in 2 mL of THF and the propargylic acetate **9a** (0.23 g, 1.0 mmol) in 5 mL of THF were added sequentially. The reaction mixture was stirred at

room temperature for 20 min. After addition of 10 mL of saturated NH₄Cl solution, the reaction mixture was extracted with 2x20 mL of Et₂O and the combined organic layers were washed with water and brine. Drying over Na₂SO₄ and removal of solvent under reduced pressure resulted in a brown oil. The crude product was purified by flash chromatography using pure hexanes as the eluent to give **6a** as a pale yellow oil (114 mg, 58%). IR (neat): 2120, 1930 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.36 (d, *J* = 7.4 Hz, 1H), 7.27 (d, *J* = 7.4, 1H), 7.16 (d, *J* = 7.3 Hz, 1H), 7.10 (t, *J* = 7.3 Hz, 1H), 6.54 (m, 1H), 6.42 (dd, *J* = 17.4, 10.5 Hz, 1H), 5.25 (d, *J* = 17.4 Hz, 1H), 5.15 (d, *J* = 10.5 Hz, 1H), 1.97 (d, *J* = 2.8 Hz, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 210.3, 136.8, 135.0, 128.9, 128.4, 126.3, 125.3, 118.9, 114.0, 104.6, 89.1, 14.9; TOFESMS *m/z* relative intensity 170 (MH⁺-N₂ 100); HRMS (+ES) Calcd for C₁₂H₁₂N: 170.0970, Found: 170.0977.

Representative Procedure 3. Allenylazide Synthesis.

1-(2-Azidophenyl)3-cyclohex-1-enylbut-1,2-diene (**6h**).



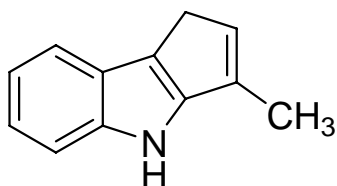
To a solution of CuBr•Me₂S (2.5 g, 12 mmol) in 20 mL of THF at -40 °C was added MeMgBr (3.0 M in THF, 4.0 mL, 12 mmol) and the mixture was stirred for 1 h, after which acetate **9h** (0.30 g, 1.3 mmol) in 5 mL of THF was cannulated into the reaction mixture at -40 °C. The reaction mixture was warmed to room temperature over a period of 8 h to allow complete consumption of starting material. The excess cuprate was then quenched with drop-wise addition of saturated NH₄Cl solution. The organic layer was extracted with 3x50 mL of Et₂O and washed with water and brine. Drying the combined extracts over Na₂SO₄ and removal of solvent under reduced pressure resulted in a brown oil. The crude product was purified by column chromatography using pure hexanes as the eluent to give **6h** as a pale yellow oil (120 mg, 37%). IR (neat): 2123, 1928 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.38 (d, *J* = 7.5 Hz, 1H), 7.24 (d, *J* = 7.3 Hz, 1H), 7.16 (d, *J* = 7.0, 1H), 7.09 (t, *J* = 7.5 Hz, 1H), 6.57 (m, 1H), 5.81 (m, 1H), 2.2 (m, 3H), 2.07 (m, 1H), 1.97 (d, *J* = 2.7 Hz, 3H), 1.63-1.68 (m, 4H); ¹³C NMR (75 MHz, CDCl₃) δ 207.6, 136.5,

133.4, 128.4, 128.2, 127.2, 125.2, 123.9, 118.8, 107.1, 90.5, 27.4, 26.4, 23.2, 22.7, 16.3 ; TOFESMS m/z relative intensity 224 ($MH^+ - N_2$ 100); HRMS (+ES) Calcd for $C_{16}H_{18}N$: 224.1439, Found: 224.1459

Representative Procedure 4. Cyclization.

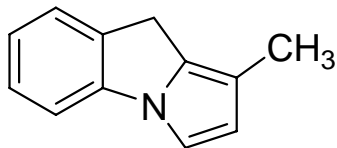
A deoxygenated solution of allenylazide **6a** (35 mg, 0.18 mmol) in toluene- d_8 , (1.8 mL) was heated at 110 °C in a clean, sealed tube for 15 min, after which the reaction mixture was cooled to room temperature. Evaporation of the solvent *in vacuo* gave a brown oil. The ratio of the products was determined at this stage by 1H NMR analysis. Purification of this crude oil using an alumina column resulted in two products; **7a** (80% Et₂O in hexanes, 12 mg, 40%) and **11a** (10% Et₂O in hexanes 17 mg, 56%).

3-Methyl-1,4-dihydrocyclopenta[b]indole (**7a**).



IR (neat): 3406 cm^{-1} ; 1H NMR (300 MHz, $CDCl_3$) δ 8.03 (bs, 1H), 7.58 (d, $J = 7.43$ Hz, 1H), 7.41 (d, $J = 7.8$ Hz, 1H), 7.09-7.24 (m, 2H), 6.22 (m, 1H), 3.25 (s, 2H), 2.22 (d, $J = 1.6$ Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 148.7, 140.5, 132.7, 131.6, 125.2, 121.0, 120.6, 120.3, 118.5, 112.3, 31.9, 13.5; TOFESMS m/z relative intensity 170 ($MH^+ 35$); HRMS (+ES) Calcd for $C_{12}H_{12}N$:170.0970, Found: 170.0967.

1-Methyl-9H-pyrrolo[1,2-a]indole (**11a**).

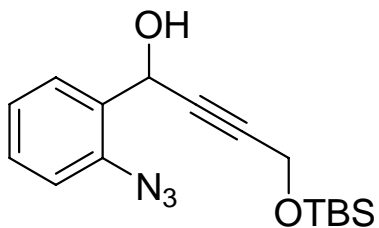


Crystals suitable for X-ray crystallographic analysis were obtained by slow evaporation of an Et₂O solution of **11a** over a period of 48 h at 25 °C. 1H NMR (300 MHz, $CDCl_3$) δ 7.42 (d, $J = 7.4$ Hz, 1H), 7.24-7.33 (m, 2H), 7.10 (t, $J = 7.3$ Hz, 1H), 7.05 (d, $J = 2.6$ Hz, 1H), 6.25 (d, $J = 2.6$ Hz, 1H), 3.77 (s, 2H), 2.18 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 141.8, 135.3, 132.7, 127.7, 126.3, 123.0, 114.8, 111.9, 109.8, 109.6, 28.4, 11.7;

TOFESMS m/z relative intensity 170 (MH^+ 35); HRMS (+ES) Calcd for $C_{12}H_{12}N$:170.0970, Found: 170.0967.

Representative Procedure 5. Azidophenyl Alkynyl Alcohol Synthesis.

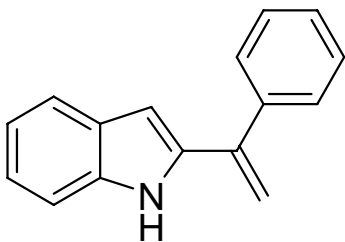
1-*t*-Butyldimethylsilyloxy-4-(2-azidophenyl)but-2-yn-4-ol.



A solution of 1-*t*-butyldimethylsilyloxybut-2-yne (0.68 g, 4.0 mmol) in THF (20 mL) was cooled to -78 °C and *n*-butyllithium (2.3 M in hexanes, 1.8 mL, 4.0 mmol) was added. The reaction mixture was stirred at -78 °C for 30 min. 2-Azidobenzaldehyde (**8**) (0.59 g, 4.0 mmol) in 5 mL of THF was cannulated into the reaction mixture and the reaction was warmed to room temperature over a period of 2 h. The reaction mixture was poured into 10 mL of saturated NH_4Cl solution and extracted with 3x30 mL of Et_2O . The combined organic layers were washed with water and brine, dried over Na_2SO_4 and the solvent was evaporated. The crude alcohol was purified by flash chromatography using 40% Et_2O in hexanes to give 1.2 g (96%) of the alcohol as yellow oil. IR (neat): 3404, 2127 cm^{-1} ; 1H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, $J = 7.8$ Hz, 1H), 7.39 (t, $J = 7.6$ Hz, 1H), 7.19 (d, $J = 7.3$ Hz, 2H), 5.68 (m, 1H), 4.44 (s, 2H), 0.91 (s, 9H), 0.12 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 137.7, 131.5, 130.1, 128.8, 125.5, 118.7, 85.7, 84.0, 61.1, 52.2, 26.2, 18.7, -4.8; TOFESMS m/z relative intensity 318 (MH^+ 30); HRMS (+ES) Calcd for $C_{16}H_{24}N_3O_2Si$: 318.1638, Found: 318.1636.

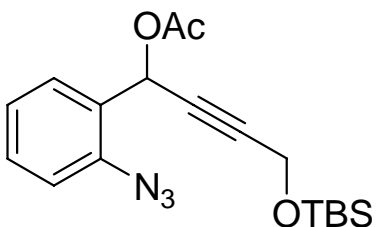
Representitive Procedure 6. Thermolysis of Crude Phenyl-substituted Allenylazides.

2-(1-Phenyl-vinyl)-1H-indole (14j)



To a solution of propargyl acetate **9a** (77 mg, 0.34 mmol) and Pd(PPh₃)₄ (35 mg, 0.03 mmol) in 3.4 mL of THF was added drop-wise phenylzinc bromide (0.50 M in THF, 1.0 mL, 0.50 mmol) and the reaction mixture was stirred at room temperature for 1 h, and then brought to reflux and held there for 14 h. The reaction mixture was allowed to cool to room temperature and added to 30 mL of ice-cold saturated NH₄Cl solution. The mixture was extracted with Et₂O (3x30 mL), and the combined organic layers were washed with water and brine, then dried over MgSO₄ and concentrated *in vacuo*. This crude material was purified by column chromatography (5% EtOAc in hexanes) to give the product **14j** as a yellow oil (25 mg, 34%). IR (neat): 3416 cm⁻¹; ¹H NMR (400 MHz, (CD₃)₂CO) δ 10.30 (br s, 1H), 7.51-7.48 (m, 3H), 7.42-7.36 (m, 4H), 7.10 (m, 1H), 6.99 (m, 1H), 6.30 (dd, *J* = 2.2, 0.8 Hz, 1H), 5.76 (s, 1H), 5.33 (d, *J* = 0.6 Hz, 1H); ¹³C NMR (100 MHz, (CD₃)₂CO) δ 143.0, 141.5, 138.8, 138.3, 129.5, 129.3, 129.1, 128.9, 123.1, 121.3, 120.3, 112.7, 111.9, 104.0; APCI *m/z* (relative intensity) 220.1 (MH⁺, 100%); HRMS Calcd for C₁₆H₁₄N: 220.1126, Found: 220.1121.

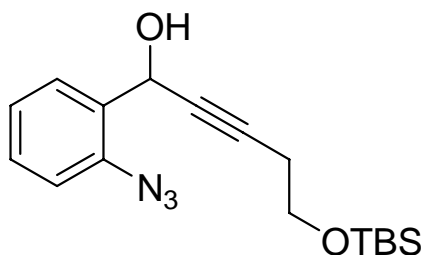
1-*t*-Butyldimethylsilyloxy-4-acetoxy-4-(2-azidophenyl)but-2-yne (9b).



Following representative procedure (1) for acetate synthesis, 1-*t*-butyldimethylsilyloxy-4-(2-azidophenyl)but-2-yn-4-ol (1.3 g, 3.9 mmol) was converted to acetate **9b** (1.3 g, 92%). IR (neat): 2127, 1745 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.69 (d, *J* = 7.6 Hz, 1H), 7.40 (t, *J* = 7.6 Hz, 1H), 7.18 (d, *J* = 7.8 Hz, 2H), 6.68 (m, 1H), 4.44 (d, *J* = 1.8 Hz, 2H), 2.11 (s, 3H), 0.91 (s, 9H), 0.11 (s, 3H), 0.10 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 169.8,

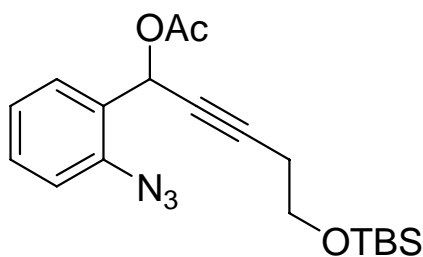
138.2, 130.7, 129.7, 128.3, 125.3, 118.6, 86.3, 81.2, 61.2, 52.2, 26.1, 21.3, 18.6, -4.8; TOFESMS m/z relative intensity 360 (MH^+ 80); HRMS (+ES) Calcd for $C_{18}H_{26}N_3O_3Si$: 360.1743, Found: 360.1731.

1-*t*-butyldimethylsilyloxy-5-(2-azidophenyl)pent-3-yn-5-ol.



Following the representative procedure (5) for alcohol synthesis, 2-azidobenzaldehyde (8) (0.66 g, 4.4 mmol) was treated with 1-*t*-butyldimethylsilyloxypent-3-ynyllithium (1.0 equiv, 4.4 mmol) to give 1-*t*-butyldimethylsilyloxy-5-(2-azidophenyl)pent-3-yn-5-ol as a yellow oil (1.3 g, 96%). IR (neat): 3423, 2110 cm^{-1} ; 1H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, $J = 7.5$ Hz, 1H), 7.37 (t, $J = 7.2$ Hz, 1H), 7.18 (t, $J = 7.3$ Hz, 2H), 5.64 (m, 1H), 3.76 (t, $J = 7.1$ Hz, 2H), 2.50 (dt, $J = 7.0, 1.8$ Hz, 2H), 0.91 (s, 9H), 0.08 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 137.8, 132.3, 130.1, 128.9, 125.5, 118.7, 85.0, 80.4, 62.1, 61.2, 26.3, 23.7, 18.7, -4.9 (2C); TOFESMS m/z relative intensity 332 (MH^+ 40); HRMS (+ES) Calcd for $C_{17}H_{26}N_3O_2Si$: 332.1794, Found: 332.1780.

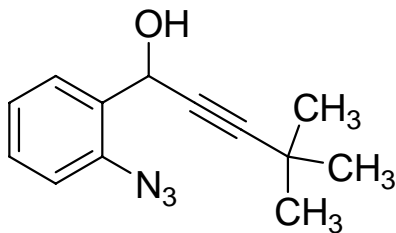
1-*t*-Butyldimethylsilyloxy-5-acetoxy-5-(2-azidophenyl)pent-3-yne (9c).



Following representative procedure (1) for acetate synthesis, 1-*t*-butyldimethylsilyloxy-5-(2-azidophenyl)pent-3-yn-5-ol (1.3g, 3.9 mmol) was converted to acetate 9c (1.2 g, 82%). IR (neat): 2129, 1747 cm^{-1} ; 1H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, $J = 7.7$ Hz, 1H), 7.41 (dt, $J = 7.7, 1.5$ Hz, 1H), 7.19 (t, $J = 7.7$ Hz, 2H), 6.64 (t, $J = 2.0$ Hz, 1H), 3.75 (t, $J = 6.9$ Hz, 2H), 2.49 (dt, $J = 6.9, 2.1$ Hz, 1H), 2.11 (s, 3H), 0.89 (s, 9H), 0.07 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 169.9, 138.2, 130.6, 129.9, 128.9, 125.4, 118.7, 85.7.3, 82.2,

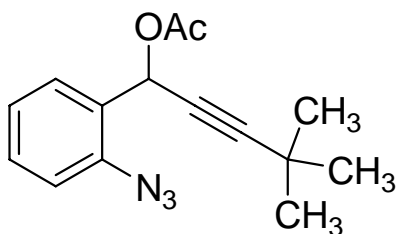
61.9 61.5, 26.3, 23.7, 21.4, 18.7, -4.9 (2C); TOFESMS m/z relative intensity 396 (MNa^+ 65); HRMS (+ES) Calcd for $C_{19}H_{27}N_3O_3SiNa$: 396.1719, Found: 396.1716.

1-(2-Azidophenyl)4,4-dimethylpent-2-yn-1-ol.



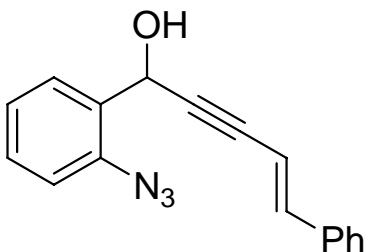
Following the representative procedure (5) for alcohol synthesis, 2-azidobenzaldehyde (8) (0.60 g, 4.0 mmol) was treated with 3,3-dimethylbutynyllithium (1.0 equiv, 4.0 mmol) to give 1-(2-azidophenyl)4,4-dimethylpent-2-yn-1-ol as a yellow oil (800 mg, 87%). IR (neat): 3375, 2128 cm^{-1} ; 1H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, $J = 7.6$ Hz, 1H), 7.37 (t, $J = 7.5$ Hz, 1H), 7.17-7.28 (m, 2H), 5.67 (s, 1H), 2.53 (bs, 1H) 1.28 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 137.9, 132.6, 130.0, 128.9, 125.4, 118.7, 96.4, 77.7, 60.1, 31.3 27.9; TOFESMS m/z relative intensity 230 (MH^+ 80); HRMS (+ES) Calcd for $C_{12}H_{16}N_3O$: 230.1293, Found: 230.1280.

1-Acetoxy-1-(2-azidophenyl)4,4-dimethylpent-2-yne (9d).



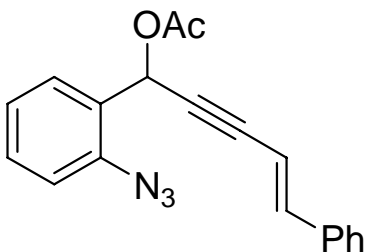
Following representative procedure (1) for acetate synthesis, 1-(2-azidophenyl)4,4-dimethylpent-2-yn-1-ol (0.80 g, 3.5 mmol) was converted to acetate 9d (850 mg, 90%). IR (neat): 2127, 1745 cm^{-1} ; 1H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, $J = 7.8$ Hz, 1H), 7.39 (t, $J = 7.7$ Hz, 1H), 7.20 (t, $J = 8.3$ Hz, 2H), 6.64 (s, 1H), 2.10 (s, 3H), 1.26 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 169.9, 138.4, 130.5, 130.0, 129.1, 125.3, 118.7, 96.7, 74.9 61.6, 31.2, 27.9, 21.5; TOFESMS m/z relative intensity 272 (MH^+ 32); HRMS (+MSES) Calcd for $C_{15}H_{18}N_3O_2$: 272.1399, Found: 272.1392.

1-(2-Azidophenyl)5-phenylpent-4-en-2-yn-ol.



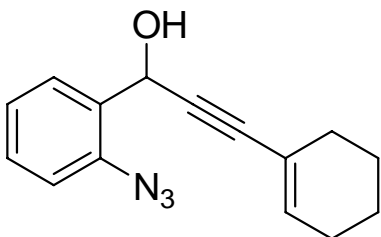
Following the representative procedure (**5**) for alcohol synthesis, 2-azidobenzaldehyde (**8**) (0.46 g, 3.1 mmol) was treated with 4-phenylbut-3-en-1-ynyllithium (1.0 equiv, 3.1 mmol) to give 1-(2-azidophenyl)5-phenylpent-4-en-2-yn-ol as a bright yellow oil (460 mg, 54%). IR (neat): 3396, 2126 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.71 (dd, $J = 8.1$, 1.3 Hz, 1H), 7.44-7.23 (m, 8H), 7.02 (d, $J = 16.3$ Hz, 1H), 6.24 (dd, $J = 16.3$, 1.9 Hz, 1H), 5.84 (m, 1H), 2.75 (bs, 1H); ^{13}C NMR (75 MHz, CDCl_3) δ 142.6, 137.8, 136.5, 132.2, 130.2, 129.3, 129.2, 128.9, 126.8, 125.6, 118.8, 107.8, 90.7, 86.1, 61.5; TOFESMS m/z relative intensity 276 (MH^+ 30); HRMS (+ES) Calcd for $\text{C}_{13}\text{H}_{15}\text{N}_3\text{O}$: 276.1137, Found: 276.1123.

1-Acetoxy-1-(2-azidophenyl) 5-phenylpent-4-en-2-yn-ol (**9g**).



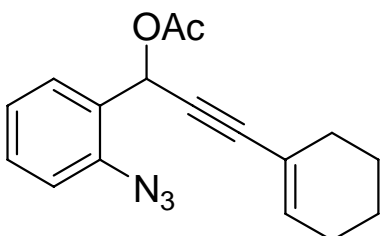
Following representative procedure (**1**) for acetate synthesis, 1-(2-azidophenyl)5-phenylpent-4-en-2-yn-ol (0.40 g, 1.6 mmol) was converted to acetate **9g** (460 mg, 91%). IR (neat): 2127, 1742 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.78 (dd, $J = 7.8$, 1.3 Hz, 1H), 7.44-7.20 (m, 8H), 7.04 (d, $J = 16.3$ Hz, 1H), 6.87 (d, $J = 1.8$ Hz, 1H) 6.22 (dd, $J = 16.3$, 2.0 Hz, 1H), 2.16 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 170.0, 143.2, 138.3, 136.3, 130.8, 129.8, 129.4, 129.2, 128.6, 126.8, 125.5, 118.8, 107.5, 87.5, 86.7, 61.9, 21.4; TOFESMS m/z relative intensity 318 (MH^+ 68); HRMS (+ES) Calcd for $\text{C}_{19}\text{H}_{16}\text{N}_3\text{O}_2$: 318.1243, Found: 318.1261.

1-(2-Azidophenyl)3-cyclohex-1-enylprop-2-yn-1-ol.



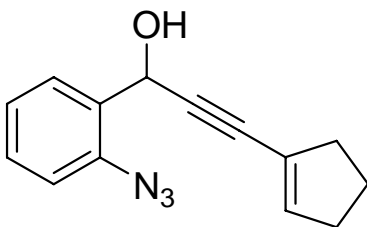
Following the representative procedure (5) for alcohol synthesis, 2-azidobenzaldehyde (8) (0.50 g, 3.4 mmol) was treated with 1-cyclohexenylethynyllithium (0.85 equiv, 2.9 mmol) to give 1-(2-azidophenyl)3-cyclohex-1-enylprop-2-yn-1-ol as a yellow oil (280 mg, 38%). IR (neat): 3390, 2126 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) δ 7.67 (d, $J = 7.7$ Hz, 1H), 7.36 (m, 1H), 7.19-7.11 (m, 2H), 6.16 (m, 1H), 5.76 (d, $J = 4.6$ Hz, 1H), 3.23 (d, $J = 5.3$ Hz, 1H), 2.15-2.09 (m, 4H), 1.64-1.58 (m, 4H); ^{13}C NMR (75 MHz, CDCl_3) δ 137.7, 136.1, 132.5, 130.0, 128.9, 125.5, 120.5, 118.7, 88.7, 85.9, 61.1, 29.5, 26.1, 22.7, 21.9; TOFESMS m/z relative intensity 254 (MH^+ 75); HRMS (+ES) Calcd for $\text{C}_{15}\text{H}_{16}\text{N}_3\text{O}$: 254.1293, Found: 254.1302.

1-Acetoxy-1-(2-azidophenyl) 3-cyclohex-1-enylprop-2-yne (9h).



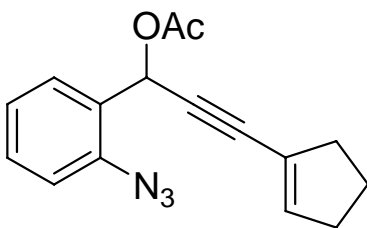
Following representative procedure (1) for acetate synthesis, 1-(2-azidophenyl)3-cyclohex-1-enylprop-2-yn-1-ol (0.28 g, 1.1 mmol) was converted to acetate 9h (260 mg, 80%). IR (neat): 2127, 1742 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.72 (dd, $J = 7.5, 1.3$ Hz, 1H), 7.42 (dd, $J = 7.2, 1.5$ Hz, 1H), 7.18-7.22 (m, 2H), 6.76 (m, 1H), 6.20 (m, 1H), 2.11 (s, 3H), 2.16-2.10 (m, 4H), 1.67-1.55 (m, 4H); ^{13}C NMR (75 MHz, CDCl_3) δ 169.9, 138.2, 137.0, 130.6, 129.8, 128.9, 125.4, 120.2, 118.7, 89.3, 82.7, 61.7, 29.3, 26.0, 22.6, 21.8, 21.5; TOFESMS m/z relative intensity 318 (MNa^+ 100); HRMS (+ES) Calcd for $\text{C}_{17}\text{H}_{17}\text{N}_3\text{O}_2\text{Na}$: 318.1203, Found: 318.1218.

1-(2-Azidophenyl)3-cyclopent-1-enylprop-2-yn-1-ol.



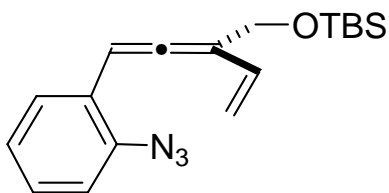
Following the representative procedure (**5**) for alcohol synthesis, 2-azidobenzaldehyde (**8**) (0.35 g, 2.4 mmol) was treated with 1-cyclopentynylethynyllithium (1.3 equiv, 3.2 mmol) to give 1-(2-Azidophenyl)3-cyclopent-1-enylprop-2-yn-1-ol as a yellow oil (330 mg, 54%). IR (neat): 3354, 2126 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.67 (dd, $J = 8.2$, 1.6 Hz, 1H), 7.43 (m, 1H), 7.22-7.15 (m, 2H), 6.12 (t, $J = 2.4$ Hz, 1H), 5.80 (d, $J = 6.2$ Hz, 1H), 2.61 (d, $J = 6.1$ Hz, 1H), 2.51-2.42 (m, 4H), 1.96-1.89 (m, 2H); ^{13}C NMR (75 MHz, CDCl_3) δ 139.0, 137.4, 131.7, 129.8, 128.5, 125.1, 123.8, 118.3, 88.9, 84.1, 61.2, 36.3, 33.3, 23.3; TOFESMS m/z relative intensity 240 ($\text{MH}^+ 30$); HRMS (+ES) Calcd for $\text{C}_{14}\text{H}_{14}\text{N}_3\text{O}$: 240.1127, Found: 240.1137.

1-Acetoxy-1(2-azidophenyl) 3-cyclopent-1-enylprop-2-yne (9i).



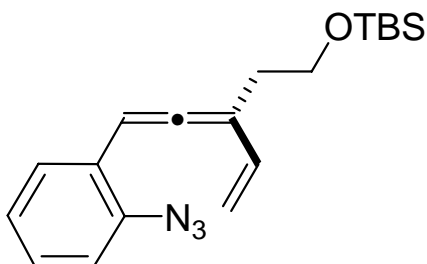
Following representative procedure (**1**) for acetate synthesis, 1-(2-azidophenyl)3-cyclopent-1-enylprop-2-yn-1-ol (0.33 g, 1.3 mmol) was converted to acetate **9i** (330 mg, 88%). IR (neat): 2126, 1746 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.71 (d, $J = 8.6$ Hz, 1H), 7.42 (d, $J = 7.7$ Hz, 1H), 7.25-7.18 (m, 2H), 6.79 (m, 1H), 6.22 (m, 1H), 2.62-2.45 (m, 4H), 2.12 (s, 3H), 1.96-1.88 (m, 2H); ^{13}C NMR (75 MHz, CDCl_3) δ 169.9, 140.1, 138.3, 130.6, 129.8, 128.7, 125.4, 124.0, 118.7, 86.4, 84.8, 61.9, 36.6, 33.7, 23.7, 21.5; TOFESMS m/z relative intensity 282 ($\text{MH}^+ 30$); HRMS (+ES) Calcd for $\text{C}_{16}\text{H}_{16}\text{N}_3\text{O}_2$: 282.1243, Found: 282.1229.

1-*t*-Butyldimethylsilyloxy-2-vinyl-4-(2-azidophenyl)but-2,3-diene (6b).



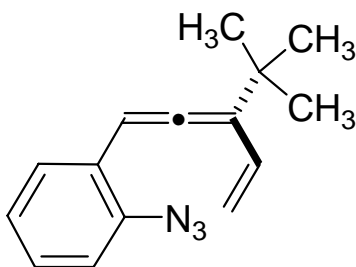
Following representative procedure (2) for allenylazide synthesis, acetate **9b** (0.50 g, 1.4 mmol) was converted to **6b** (250 mg, 55%). IR (neat): 2122, 1934 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.39 (dd, $J = 7.7, 1.5$ Hz, 1H), 7.29 (m, 1H), 7.18-7.09 (m, 2H), 6.10 (m, 1H), 6.38 (dd, $J = 17.7, 10.1$ Hz, 1H), 5.38 (dd, $J = 17.4, 1.1$ Hz, 1H), 5.16 (d, $J = 10.5, 1.2$ Hz, 1H), 4.48 (d, $J = 2.5$ Hz, 2H), 0.9 (s, 9H), 0.09 (s, 3H), 0.08 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 209.0, 136.8, 132.0, 129.0, 128.7, 125.9, 125.2, 118.8, 115.1, 109.8, 91.9, 61.9, 26.2, 18.7, -4.8, -4.9; TOFESMS m/z relative intensity 300 ($\text{MH}^+ - \text{N}_2$ 100); HRMS (+ES) Calcd for $\text{C}_{18}\text{H}_{26}\text{NOSi}$: 300.1784, Found: 300.1812.

1-*t*-Butyldimethylsilyloxy-3-vinyl-5-(2-azidophenyl)but-3,4-diene (6c).



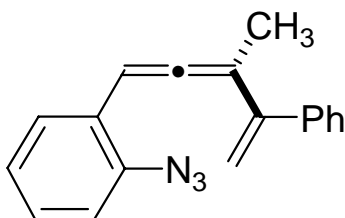
Following representative procedure (2) for allenylazide synthesis, acetate **9c** (0.50 g, 1.3 mmol) was converted to **6c** (259 mg, 57%). IR (neat): 2122, 1930 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.36 (d, $J = 7.9$ Hz, 1H), 7.25 (d, $J = 7.3$ Hz, 1H), 7.15 (d, $J = 8.0$ Hz, 1H), 7.08 (t, $J = 7.5$ Hz, 1H), 6.59 (m, 1H), 6.32 (dd, $J = 17.5, 10.7$ Hz, 1H), 5.29 (d, $J = 17.6$ Hz, 1H), 5.13 (d, $J = 10.7$ Hz, 1H), 3.81 (t, $J = 5.8$ Hz, 2H), 2.54-2.49 (m, 2H), 0.89 (s, 9H), 0.06 (s, 3H), 0.04 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 209.8, 136.7, 134.3, 128.8, 128.6, 126.1, 125.2, 118.9, 114.0, 106.2, 90.6, 62.1, 32.1, 26.3, 18.8, -4.8 (2C); TOFESMS m/z relative intensity 314 ($\text{MH}^+ - \text{N}_2$ 100); HRMS (+ES) Calcd for $\text{C}_{19}\text{H}_{28}\text{NOSi}$: 314.1940, Found: 314.1919.

1-(2-Azidophenyl)3-*t*-butylpent-1,2,4-triene (6d).



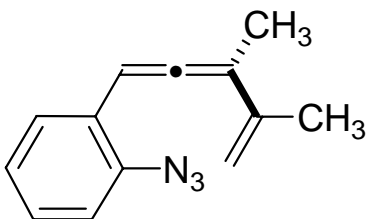
Following representative procedure (2) for allenylazide synthesis, acetate **9d** (0.27 g, 1.0 mmol) was converted to **6d** (150 mg, 63%). IR (neat): 2124, 1930 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.43 (dd, $J = 7.7, 1.4$ Hz, 1H), 7.27 (dt, $J = 8.1, 1.5$ Hz, 1H), 7.19 (d, $J = 7.0$ Hz, 1H), 7.12 (t, $J = 7.6$ Hz, 1H), 6.73 (m, 1H), 6.28 (ddd, $J = 17.0, 10.4, 1.3$ Hz, 1H), 5.51 (dd, $J = 17.1, 0.9$ Hz, 1H), 5.26 (dd, $J = 10.4, 0.9$ Hz, 1H), 1.24 (s, 9H); ^{13}C NMR (75 MHz, CDCl_3) δ 204.7, 136.6, 130.9, 128.3, 128.0, 126.9, 125.3, 119.0, 118.6, 117.2, 92.3, 34.3, 29.9; TOFESMS m/z relative intensity 210 ($\text{MH}^+ - \text{N}_2$ 100); HRMS (-ES) Calcd for $\text{C}_{15}\text{H}_{16}\text{N}$: 210.1283, Found: 210.1277.

1-(2-Azidophenyl)3-methyl-5-phenylpent-1,2,4-triene (6e).



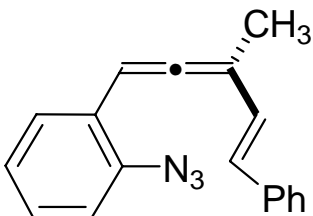
Following representative procedure (2) for allenylazide synthesis, acetate **9a** (0.20 g, 0.88 mmol) was converted to **6e** (160 mg, 67%). IR (neat): 2124, 1932 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) δ 7.25-7.55 (m, 7H), 7.16 (d, $J = 7.6$ Hz, 2H), 6.48 (m, 1H), 5.41 (s, 1H), 5.32 (s, 1H), 2.19 (d, $J = 2.7$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 209.8, 147.2, 141.7, 136.7, 128.6, 128.5, 128.4, 128.1, 128.0, 127.9, 126.4, 118.9, 114.4, 106.1, 90.4, 18.0; TOFESMS m/z relative intensity 246 ($\text{MH}^+ - \text{N}_2$ 100); HRMS (+ES) Calcd for $\text{C}_{18}\text{H}_{16}\text{N}$: 246.1283, Found: 246.1275.

1-(2-Azidophenyl)3-methyl-4-phenylpent-1,2,4-triene (6f).



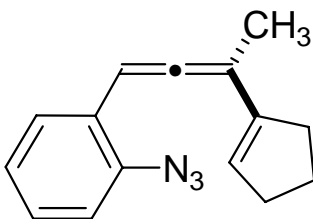
Following representative procedure (2) for allenylazide synthesis, acetate **9a** (0.23 g, 1.0 mmol) was converted to **6e** (125 mg, 59%). IR (neat): 2124, 1930 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) δ 7.41 (d, $J = 7.7$ Hz, 1H) 7.28 (t, $J = 7.9$ Hz, 1H), 7.16-7.10 (m, 2H), 6.6 (m, 1H), 5.08 (s, 1H), 5.04 (s, 1H), 2.05 (s, 3H), 2.04 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 208.7, 140.8, 136.7, 128.5, 128.4, 126.7, 125.3, 118.9, 112.0, 107.1, 90.3, 22.0, 16.7; TOFESMS m/z relative intensity 184 ($\text{MH}^+ - \text{N}_2$ 100); HRMS (+ES) Calcd for $\text{C}_{13}\text{H}_{14}\text{N}$: 184.1121, Found: 184.1126.

1-(2-Azidophenyl)3-methyl-4-phenylpent-1,2,4-triene (6g).



Following representative procedure (3) for allenylazide synthesis, acetate **9g** (0.21 g, 0.65 mmol) was converted to **6e** (60 mg, 34%). IR (neat): 2122, 1927 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) δ 7.55-7.10 (m, 9H), 6.82 (d, $J = 16.1$ Hz, 1H), 6.63 (m, 1H), 6.56 (d, $J = 16.2$ Hz, 1H), 2.09 (d, $J = 2.8$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 211.6, 137.7, 136.7, 130.5, 129.0, 128.9, 128.8, 128.6, 127.8, 126.9, 126.7, 125.3, 118.9, 104.8, 89.3, 15.7; TOFESMS m/z relative intensity 246 ($\text{MH}^+ - \text{N}_2$ 100); HRMS (+ES) Calcd for $\text{C}_{18}\text{H}_{16}\text{N}$: 246.1283, Found: 246.1289.

1-(2-Azidophenyl)3-cyclopent-1-enylbut-1,2-diene (6i).

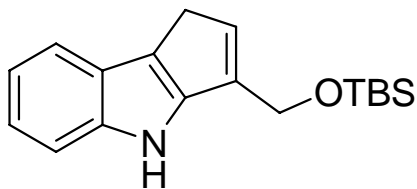


Following representative procedure (3) for allenylazide synthesis, acetate **9i** (0.30 g, 1.1 mmol) was converted to **6e** (75 mg, 30%). IR (neat): 2112, 1930 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.38 (dd, $J = 7.7, 1.5$ Hz, 1H), 7.25 (dt, $J = 7.0, 1.6$ Hz, 1H), 7.16 (dd, $J = 7.9, 1.1$ Hz, 1H), 7.09 (dt, $J = 7.3, 1.8$ Hz, 1H), 6.55 (m, 1H), 5.75 (d, $J = 1.4$ Hz, 1H), 2.50-2.35 (m, 4H), 2.02 (d, $J = 2.7$ Hz, 3H), 1.93 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 208.8, 140.6, 136.6, 128.6, 128.2, 127.1, 127.0, 125.2, 118.8, 103.0, 89.5, 34.1, 33.8, 23.7, 17.0; APCIMS m/z relative intensity 210 ($\text{MH}^+ - \text{N}_2$ 100); HRMS (+APMS) Calcd for $\text{C}_{15}\text{H}_{16}\text{N}$: 210.1283, Found: 210.1302.

Cyclization Studies

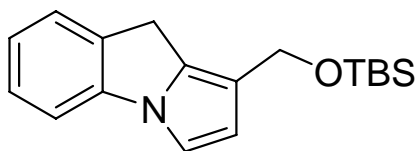
Following the representative procedure (4) for cyclization, allenylazide **6b** (49 mg, 0.15 mmol) was converted to compounds **7b** (10 mg, 40%) and **11b** (13 mg, 56%).

3-(*t*-Butyldimethylsilyloxymethyl)-1,4-dihydrocyclopenta[b]indole (**7b**).



IR (neat): 3395 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) δ 8.23 (bs, 1H), 7.58 (m, 1H), 7.41 (m, 1H), 7.14-7.06 (m, 2H), 6.29 (m, 1H), 4.76 (d, $J = 1.7$ Hz, 2H), 3.29 (d, $J = 1.6$ Hz, 2H), 0.97 (s, 1H), 0.14 (s, 6H); ^{13}C NMR (75 MHz, CDCl_3) δ 147.1, 140.4, 137.8, 129.7, 124.8, 121.2, 120.7, 120.2, 118.5, 112.4, 61.1, 32.0, 29.4, 18.8, -4.8 (2C); TOFESMS m/z relative intensity 300 (MH^+ 10); HRMS (+ES) Calcd for $\text{C}_{36}\text{H}_{51}\text{N}_2\text{O}_2\text{Si}_2$: 599.3489, Found: 599.3466.

1-(*t*-Butyldimethylsilyloxymethyl)-9H-pyrrolo[1,2-a]indole (**11b**).

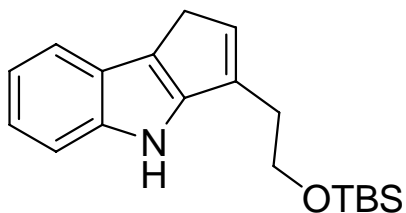


^1H NMR (300 MHz, CDCl_3) δ 7.41 (d, $J = 7.5$ Hz, 1H), 7.30-7.24 (m, 2H), 7.09 (t, $J = 7.3$ Hz, 1H), 7.06 (d, $J = 2.1$ Hz, 1H), 6.33 (d, $J = 2.6$ Hz, 1H), 4.73 (s, 2H), 3.85 (s, 2H), 0.96 (s, 9H) 0.13 (s, 6H); ^{13}C NMR (75 MHz, CDCl_3) δ 141.5, 135.2, 133.0, 127.7, 126.3, 123.3, 117.1, 112.8, 109.94, 109.92, 59.6, 29.1, 26.5, 18.9, -4.7 (2C); TOFESMS

m/z relative intensity 300 (MH^+ 10); HRMS (+ES) Calcd for $C_{36}H_{51}N_2O_2Si_2$: 599.3489, Found: 599.3466.

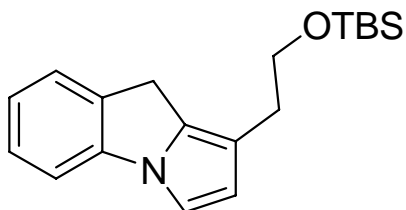
Following the representative procedure (4) for cyclization, allenylazide **6c** (25 mg, 0.07 mmol) was converted to compounds **7c** (12 mg, 52%) and **11c** (10 mg, 43%).

3-(*t*-Butyldimethylsilyloxyethyl)-1,4-dihydrocyclopenta[b]indole (7c).



IR (neat): 3372 cm^{-1} ; $^1\text{H NMR}$ (300 MHz, CDCl_3) δ 8.8 (bs, 1H), 7.57 (m, 1H), 7.38 (m, 1H), 7.13-7.07 (m, 2H), 6.22 (m, 1H), 3.95 (t, $J = 5.7\text{ Hz}$, 2H), 3.25 (s, 2H), 2.82 (t, $J = 5.6\text{ Hz}$, 1H), 0.99 (s, 9H), 0.14 (s, 6H); $^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ 148.5, 140.1, 136.1, 131.9, 125.2, 120.6, 120.4, 120.0, 118.4, 112.2, 63.9, 32.7, 31.8, 26.5, 18.9, -4.9; TOFMSSES m/z relative intensity 314 (MH^+ 25); HRMS (+MSES) Calcd for $C_{19}H_{28}NOSi$: 314.1940, Found: 314.1929.

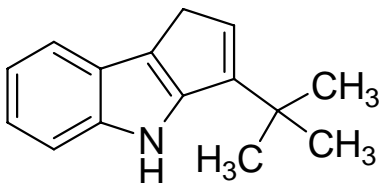
1-(*t*-Butyldimethylsilyloxyethyl)-9H-pyrrolo[1,2-*a*]indole (11c).



$^1\text{H NMR}$ (300 MHz, CDCl_3) δ 7.40 (d, $J = 7.6\text{ Hz}$, 1H), 7.30 (d, $J = 7.8\text{ Hz}$, 1H), 7.24 (d, $J = 7.7\text{ Hz}$, 1H), 7.07 (t, $J = 7.4\text{ Hz}$, 1H), 7.04 (d, $J = 2.4\text{ Hz}$, 1H), 6.25 (d, $J = 2.6\text{ Hz}$, 1H), 3.84 (t, $J = 7.7\text{ Hz}$, 2H), 3.79 (s, 2H), 2.78 (t, $J = 7.5\text{ Hz}$, 2H), 0.93 (s, 9H), 0.07 (s, 6H); $^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ 141.7, 135.1, 133.0, 127.8, 126.3, 123.3, 114.2, 113.6, 109.9, 109.7, 64.5, 31.0, 28.7, 26.4, 18.9, -4.8; TOFESMS m/z relative intensity 314 (MH^+ 25); HRMS (+ES) Calcd for $C_{19}H_{28}NOSi$: 314.1940, Found: 314.1929.

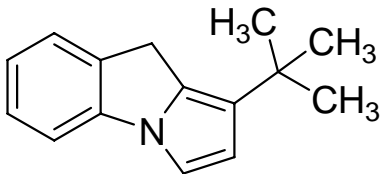
Following the representative procedure (4) for cyclization, allenylazide **6d** (60 mg, 0.25 mmol) was converted to compounds **7d** (30 mg, 57%) and **11d** (11 mg, 20%).

3-*t*-Butyl-1,4-dihydrocyclopenta[b]indole (7d).



IR (neat): 3414 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 8.09 (bs, 1H), 7.60 (m, 1H), 7.43 (m, 1H), 7.29-7.13 (m, 2H), 6.19 (t, $J = 1.6$ Hz, 1H), 3.24 (d, $J = 1.6$ Hz, 2H), 1.4 (s, 9H); ^{13}C NMR (75 MHz, CDCl_3) δ 147.5, 147.0, 140.5, 127.6, 124.8, 122.1, 120.7, 120.3, 118.5, 112.2, 32.8, 31.2, 30.2; TOFESMS m/z relative intensity 212 (MH^+ 100); HRMS (+ES) Calcd for $\text{C}_{15}\text{H}_{18}\text{N}$: 212.1439, Found: 212.1436.

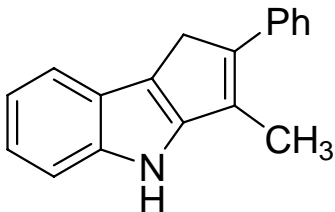
1-*t*-Butyl-9H-pyrrolo[1,2-*a*]indole (11d).



^1H NMR (400 MHz, CDCl_3) δ 7.38 (d, $J = 7.4$ Hz, 1H), 7.28-7.22 (m, 2H), 7.07 (dd, $J = 7.4, 1.2$ Hz, 1H), 7.04 (d, $J = 2.9$ Hz, 1H), 6.32 (d, $J = 2.8$ Hz, 1H), 3.92 (s, 2H), 1.36 (s, 9H); ^{13}C NMR (75 MHz, CDCl_3) δ 141.8, 135.2, 130.1, 127.8, 127.7, 126.0, 123.0, 111.7, 109.7, 109.2, 31.7, 31.3, 30.8; TOFESMS m/z relative intensity 212 (MH^+ 100); HRMS (+ES) Calcd for $\text{C}_{15}\text{H}_{18}\text{N}$: 212.1439, Found: 212.1436.

Following the representative procedure (4) for cyclization allenylazide **6e** (45 mg, 0.16 mmol) was converted to compounds **7e** (16 mg, 40%) and **11e** (12 mg, 30%).

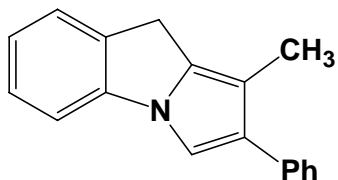
3-Methyl-2-phenyl-1,4-dihydrocyclopenta[b]indole (7e).



IR (neat): 3414 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 8.07 (bs, 1H), 7.60 (d, $J = 7.4$ Hz, 1H), 7.52 (m, 2H), 7.45-7.41 (m, 3H), 7.25 (m, 1H), 7.18-7.11 (m, 2H), 3.69 (q, $J = 1.8$ Hz, 2H), 2.39 (t, $J = 1.7$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 150.0, 143.5, 140.2,

138.3, 128.9, 128.1, 127.6, 126.6, 125.1, 120.8, 120.6, 118.7, 118.6, 112.3 34.7, 12.9;
TOFESMS m/z relative intensity 246 (MH^+ 100); HRMS (+ES) Calcd for $C_{18}H_{16}N$:
246.1283, Found: 246.1262.

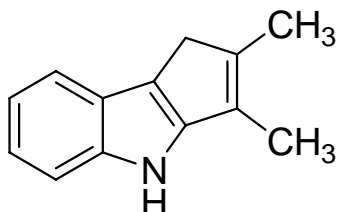
1-Methyl-2-phenyl-9H-pyrrolo[1,2-a]indole (11e).



1H NMR (300 MHz, $CDCl_3$) δ 7.54-7.52 (m, 2H), 7.45-7.40 (m, 3H), 7.34-7.28 (m, 3H),
7.24 (m, 1H), 7.11 (dt, $J = 7.2, 1.5$ Hz, 1H), 3.85 (s, 2H), 2.3 (s, 3H); ^{13}C NMR (75
MHz, $CDCl_3$) δ 141.6, 137.0, 134.8, 134.0, 130.0, 128.8, 128.2, 127.9, 126.3, 126.1,
123.2, 110.3, 109.9, 107.7, 28.6, 11.4; TOFESMS m/z relative intensity 246 (MH^+ 100);
HRMS (+ES) Calcd for $C_{18}H_{16}N$: 246.1283, Found: 246.1262.

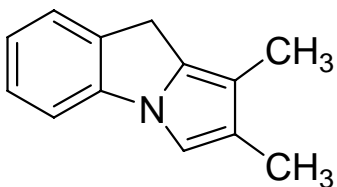
Following the representative procedure (4) for cyclization, allenylazide **6f** (35 mg, 0.17
mmol) was converted to compounds **7f** (11 mg, 36%) and **11f** (11 mg, 36%).

2,3-Dimethyl-1,4-dihydrocyclopenta[b]indole (7f).



IR (neat): 3406 cm^{-1} ; 1H NMR (400 MHz, $CDCl_3$) δ 7.94 (bs, 1H), 7.51 (d, $J = 7.7$ Hz,
1H), 7.38 (d, $J = 7.8$ Hz, 1H), 7.13-7.04 (m, 2H), 3.19 (s, 2H), 2.13 (s, 3H), 2.08 (s, 3H);
 ^{13}C NMR (75 MHz, $CDCl_3$) δ 149.9, 141.6, 139.7, 125.4, 125.3, 120.3, 119.7, 117.9,
116.9, 112.1, 36.5, 15.0, 10.8; TOFESMS m/z relative intensity 183 (MH^+ 100); HRMS
(+ES) Calcd for $C_{13}H_{14}N$: 184.1126, Found: 184.1095.

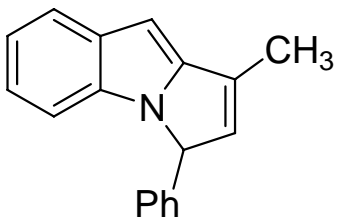
1,1-Dimethyl-9H-pyrrolo[1,2-a]indole (11f).



^1H NMR (300 MHz, CDCl_3) δ 7.37 (d, $J = 7.3$ Hz, 1H), 7.27 (t, $J = 7.6$ Hz, 1H), 7.16 (d, $J = 7.7$ Hz, 1H), 7.02 (t, $J = 7.2$ Hz, 1H), 6.88 (s, 1H), 3.75 (s, 2H), 2.14 (s, 3H), 2.08 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 141.9, 134.7, 132.8, 127.7, 126.1, 124.0, 122.4, 111.6, 109.3, 107.6, 28.5, 11.3, 9.8; TOFESMS m/z relative intensity 183 (MH^+ 100); HRMS (+ES) Calcd for $\text{C}_{13}\text{H}_{14}\text{N}$: 184.1126, Found: 184.1095.

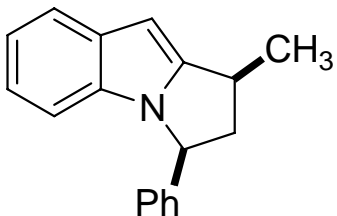
Following the representative procedure (**4**) for cyclization, allenylazide **6g** (35 mg, 0.13 mmol) was converted to compound **10g** (9 mg, 36%).

1-Methyl-3-phenyl-3H-pyrrolo[1,2-a]indole (10g).



^1H NMR (400 MHz, CDCl_3) δ 7.66 (dd, $J = 6.6, 1.7$ Hz, 1H), 7.36-7.30 (m, 3H), 7.21-7.11 (m, 2H), 7.05-7.01 (m, 2H), 6.94 (dd, $J = 7.7, 1.5$ Hz, 1H), 6.34 (s, 1H), 6.17 (m, 1H), 5.70 (s, 1H), 2.21 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 149.0, 138.2, 134.5, 133.9, 133.3, 132.1, 129.3, 128.4, 127.3, 122.0, 121.5, 119.5, 109.8, 90.6, 65.7, 12.9; TOFESMS m/z relative intensity 246 (MH^+ 20); HRMS (+ES) Calcd for $\text{C}_{18}\text{H}_{16}\text{N}$: 246.1283, Found: 246.1259.

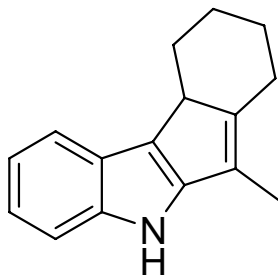
1-Methyl-3-phenyl-2,3-dihydro-1H-pyrrolo[1,2-a]indole (12g).



A deoxygenated solution of compound **10g** (9.0 mg, 0.04 mmol) and 5 mg of 10% Pd on carbon in 5 mL of THF was stirred at room temperature under H₂ at 1 atm for 2 h. The solution was then filtered through Celite and concentrated *in vacuo* to afford a yellow oil. The crude compound was purified over an alumina column using 20% Et₂O in hexanes to give **12g** as a yellow film (6 mg, 54%). Crystals suitable for X-ray crystallographic analysis were obtained by slow evaporation of an Et₂O solution of **12g** over a period of 48 h at 25 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.57 (d, *J* = 7.9 Hz, 1H), 7.38-7.35 (m, 3H), 7.28-7.24 (m, 2H), 7.03 (dt, *J* = 7.1, 0.8 Hz, 1H), 6.90 (dt, *J* = 7.1, 1.0 Hz, 1H), 6.59 (d, *J* = 8.1 Hz, 1H), 6.24 (s, 1H), 5.35 (t, *J* = 8.2 Hz, 1H), 3.45 (m, 1H), 3.18 (m, 1H), 2.13 (m, 1H), 1.49 (d, *J* = 6.8 Hz, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 150.6, 141.4, 133.8, 132.6, 129.2, 128.3, 127.1, 120.8, 120.4, 119.6, 110.8, 92.1, 61.9, 49.1, 32.7, 20.1; TOFESMS *m/z* relative intensity 248 (MH⁺ 45); HRMS (+ES) Calcd for C₁₈H₁₈N: 248.1439, Found: 248.1445.

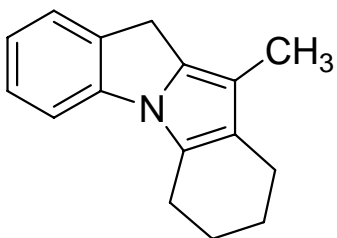
Following the representative procedure (**4**) for cyclization, allenylazide **6h** (31 mg, 0.12 mmol) was converted to compounds **7h** (10 mg, 36%) and **11h** (14 mg, 51%).

6-Methyl -5,7,8,9-hexahydroindeno[2,1-b]indole (7h).



IR (neat): 3406 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.95 (bs, 1H), 7.52 (d, *J* = 7.8 Hz, 1H), 7.39 (d, *J* = 8.0 Hz, 1H), 7.10 (t, *J* = 7.1 Hz, 1H), 7.03 (t, *J* = 7.2 Hz, 1H) 3.05 (dd, *J* = 12.5, 5.5 Hz, 1H), 2.8 (m, 1H), 2.68 (m, 1H), 2.27 (m, 1H), 2.08 (s, 3H), 2.6 (m, 1H), 1.85 (m, 1H), 1.28-1.21 (m, 2H), 1.00 (m, 1H); ¹³C NMR (75 MHz, CDCl₃) δ 149.7, 148.8, 136.0, 139.7, 122.3, 121.2, 120.2, 119.6, 117.9, 112.2, 45.2, 33.6, 28.9, 27.3, 26.0, 10.4; TOFESMS *m/z* relative intensity 224 (MH⁺ 10); HRMS (+ES) Calcd for C₁₆H₁₈N: 214.1422, Found: 224.1439.

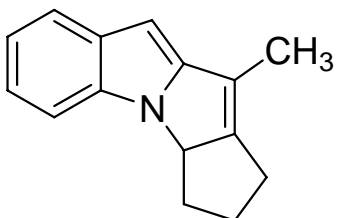
11-Methyl-2,3,4,10-tetrahydro-1H-indolo[1,2-a]indole (11h).



¹H NMR (400 MHz, CDCl₃) δ 7.37 (d, *J* = 7.4 Hz, 1H), 7.28-7.24 (m, 2H), 7.05 (m, 1H), 3.74 (s, 2H), 2.96(t, *J* = 5.6 Hz, 2H), 2.51(t, *J* = 6.0 Hz, 2H), 2.04 (s, 3H), 1.95-1.85 (m, 2H), 1.85-1.80 (m, 2H); ¹³C NMR (75 MHz, CDCl₃) δ 142.5, 135.2, 130.6, 127.6, 126.2, 122.5, 122.0, 121.6, 110.2, 109.5, 28.1, 23.8, 23.7, 23.2, 22.4, 9.6; TOFESMS *m/z* relative intensity 224 (MH⁺ 10); HRMS (+ES) Calcd for C₁₆H₁₈N: 214.1422, Found: 224.1439.

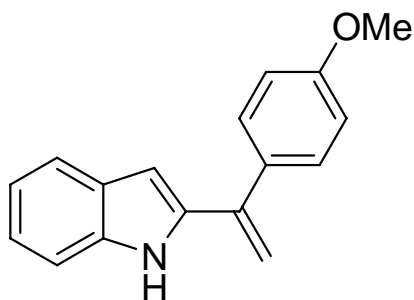
Following the representative procedure (**4**) for cyclization, allenylazide **6i** (40 mg, 0.17 mmol) was converted to compound **10i** (14 mg, 40%),

Pyrrolo-indole (10i)



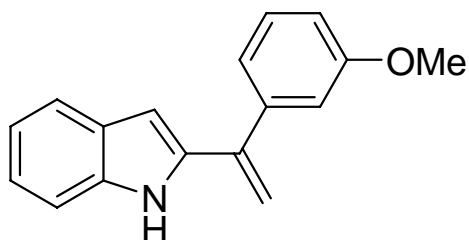
¹H NMR (400 MHz, CDCl₃) δ 7.59 (d, *J* = 8.2 Hz, 1H), 7.25 (s, 1H), 7.12 (t, *J* = 7.3 Hz, 1H), 7.03 (t, *J* = 7.1 Hz, 1H), 6.11 (s, 1H), 4.8 (t, *J* = 8.5 Hz, 1H), 2.46-2.27 (m, 6H), 2.04 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 154.1, 152.2, 135.2, 132.8, 123.4, 121.7, 121.0, 119.1, 108.9, 89.1, 66.3, 29.7, 27.8, 21.2, 11.2; TOFMSES *m/z* relative intensity 210 (MH⁺ 10); HRMS (+MSES) Calcd for C₁₅H₁₆N: 210.1283, Found: 210.1274.

2-[1-(4-Methoxy-phenyl)-vinyl]-1H-indole (14k)



Following representative procedure (6) for crude thermolysis, propargyl acetate **9a** (78 mg, 0.34 mmol) was treated with 4-methoxyphenylzinc iodide (0.50M in THF, 1.0 mL, 0.51 mmol) to give compound **14k** (30 mg, 35%) as a yellow solid: mp 145 - 146 °C; IR (neat): 3429 cm^{-1} ; ^1H NMR (300 MHz, $(\text{CD}_3)_2\text{CO}$) δ 10.35 (br s, 1H), 7.49 (dd, J = 6.8, 1.0 Hz, 1H), 7.42 (dd, J = 6.7, 2.2 Hz, 2H), 7.37 (dq, J = 8.1, 0.9 Hz, 1H), 7.10 (td, J = 7.1, 1.2 Hz, 1H), 7.01-6.94 (m, 3H), 6.32 (dd, J = 2.2, 0.8 Hz, 1H), 5.66 (d, J = 0.7, 1H), 5.27 (d, J = 0.8 Hz, 1H), 3.84 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 159.7, 141.0, 138.1, 136.3, 132.4, 129.6, 128.6, 122.6, 120.7, 120.0, 113.7, 111.7, 110.7, 103.1, 55.3; APCI m/z (relative intensity) 250.1 (MH^+ : 100%); HRMS Calcd for $\text{C}_{17}\text{H}_{16}\text{NO}$: 250.1232, Found: 250.1226.

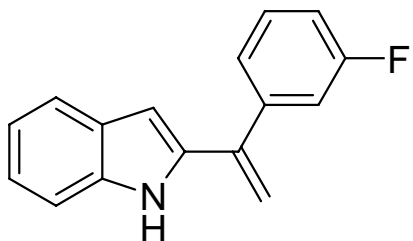
2-[1-(3-Methoxy-phenyl)-vinyl]-1H-indole (14l)



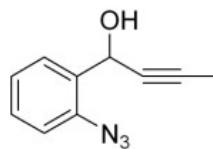
Following representative procedure (6) for crude thermolysis using a reflux time of 4 h and 6% Et_2O in hexanes as chromatography eleuent, propargyl acetate **9a** (81 mg, 0.35 mmol) was treated with 3-methoxyphenylzinc iodide (0.50 M in THF, 1.8 mL, 0.88 mmol) to give the product **14l** as a yellow oil (20 mg, 23%). IR (neat): 3413 cm^{-1} ; ^1H NMR (400 MHz, $(\text{CD}_3)_2\text{CO}$) δ 10.40 (br s, 1H), 7.49 (dd, J = 7.9, 0.8 Hz, 1H), 7.37 (dq, J = 8.2, 0.8 Hz, 1H), 7.32 (t, J = 7.9 Hz, 1H), 7.10 (m, 1H), 7.07-7.03 (m, 2H), 7.00-6.96 (m, 2H), 6.35 (dd, J = 5.1, 0.8 Hz, 1H), 5.76 (s, 1H), 5.34 (s, 1H), 3.82 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 159.5, 141.5, 141.4, 137.6, 136.4, 129.4, 128.6, 122.7, 121.0, 120.8,

120.1, 114.0, 113.9, 112.8, 110.8, 103.2, 55.3; ESI m/z (relative intensity) 250.1 (MH^+ , 100%); HRMS Calcd for $C_{17}H_{16}NO$: 250.1232, Found: 250.1230.

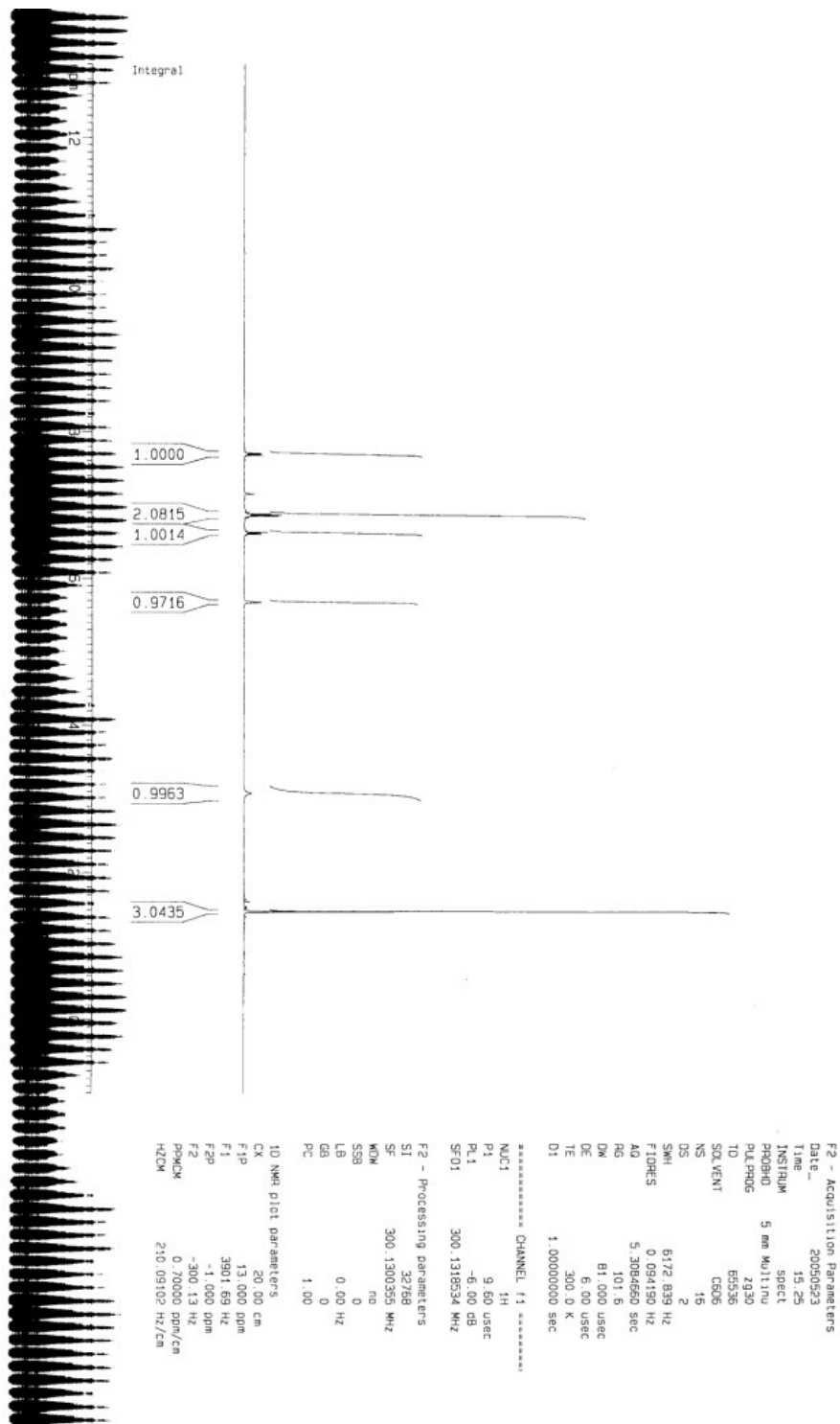
2-[1-(3-Fluoro-phenyl)-vinyl]-1H-indole (14m)

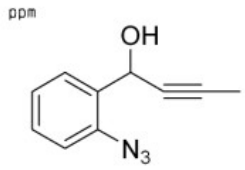


Following representative procedure (**6**) for crude thermolysis, propargyl acetate **9a** (82 mg, 0.36 mmol) was treated with 3-fluorophenylzinc iodide (0.50 M in THF, 1.1 mL, 0.54 mmol) to give compound **14m** (45 mg, 53%) as an orange solid: mp 74 - 75 °C; IR (neat): 3415 cm^{-1} ; 1H NMR (300 MHz, $(CD_3)_2CO$) δ 10.48 (br s, 1H), 7.52 (d, $J = 7.9$ Hz, 1H), 7.48-7.33 (m, 3H), 7.26 (d, $J = 10.2$ Hz, 1H), 7.21-7.11 (m, 2H), 7.01 (t, $J = 7.5$ Hz, 1H), 6.35 (s, 1H), 5.82 (s, 1H), 5.41 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.7 (d, $J_{CF} = 244.7$ Hz), 142.2 (d, $J_{CF} = 7.6$ Hz), 140.6 (d, $J_{CF} = 2.2$ Hz), 137.1, 136.5, 129.8 (d, $J_{CF} = 8.2$ Hz), 128.5, 124.2 (d, $J_{CF} = 2.9$ Hz), 122.9, 120.9, 120.2, 115.4 (d, $J_{CF} = 25.6$ Hz), 115.1 (d, $J_{CF} = 24.7$ Hz), 113.2, 110.8, 103.7; CI m/z (relative intensity) 238.0 (MH^+ , 100%); HRMS Calcd for $C_{16}H_{13}NF$: 238.1032, Found: 238.1027.



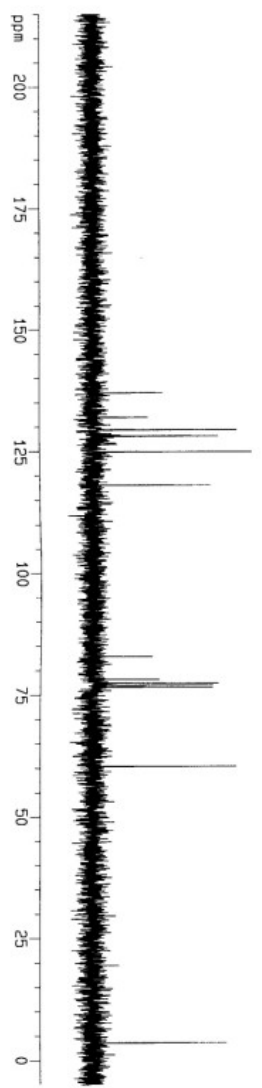
DKHI-43 Grignard Product (lower Rf than S.M., yellow oil)





DKM2-43 Yellow 011

- 136.987
- 131.948
- 129.375
- 128.105
- 124.885
- 118.043
- 82.874
- 78.151
- 77.432
- 77.008
- 76.584
- 60.346
- 3.617



Current Data Parameters
 NAME DKM2-43Carbon
 EXPNO 2
 PROCNO 1

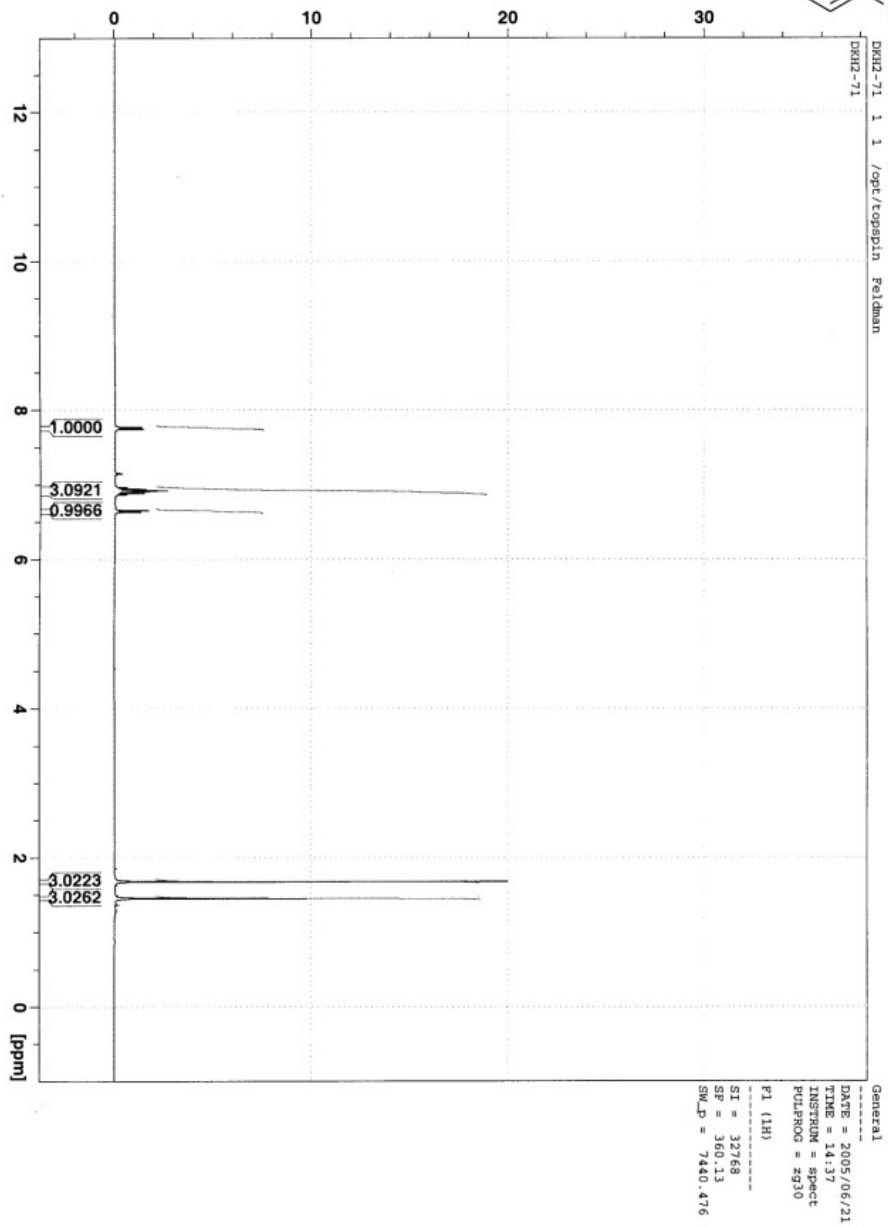
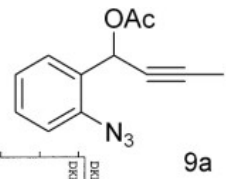
F2 - Acquisition Parameters
 Date_ 20050627
 Time 10:21
 INSTRUM spect
 PROBHD 5 mm WJ11nu
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 14
 DS 4
 SMI 18832.393 Hz
 FIDRES 0.287360 Hz
 AQ 1.7600368 sec
 RG 8192
 DW 26.556 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 d12 0.00002000 sec

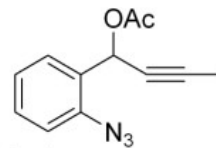
***** CHANNEL f1 *****
 NUC1 13C
 P1 11.80 usec
 PL1 0.00 dB
 SF01 75.4760200 MHz

***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 P2 110.00 usec
 PC202 0.00 dB
 PL2 0.00 dB
 PL12 17.30 dB
 PL13 17.30 dB
 SF02 300.1312000 MHz

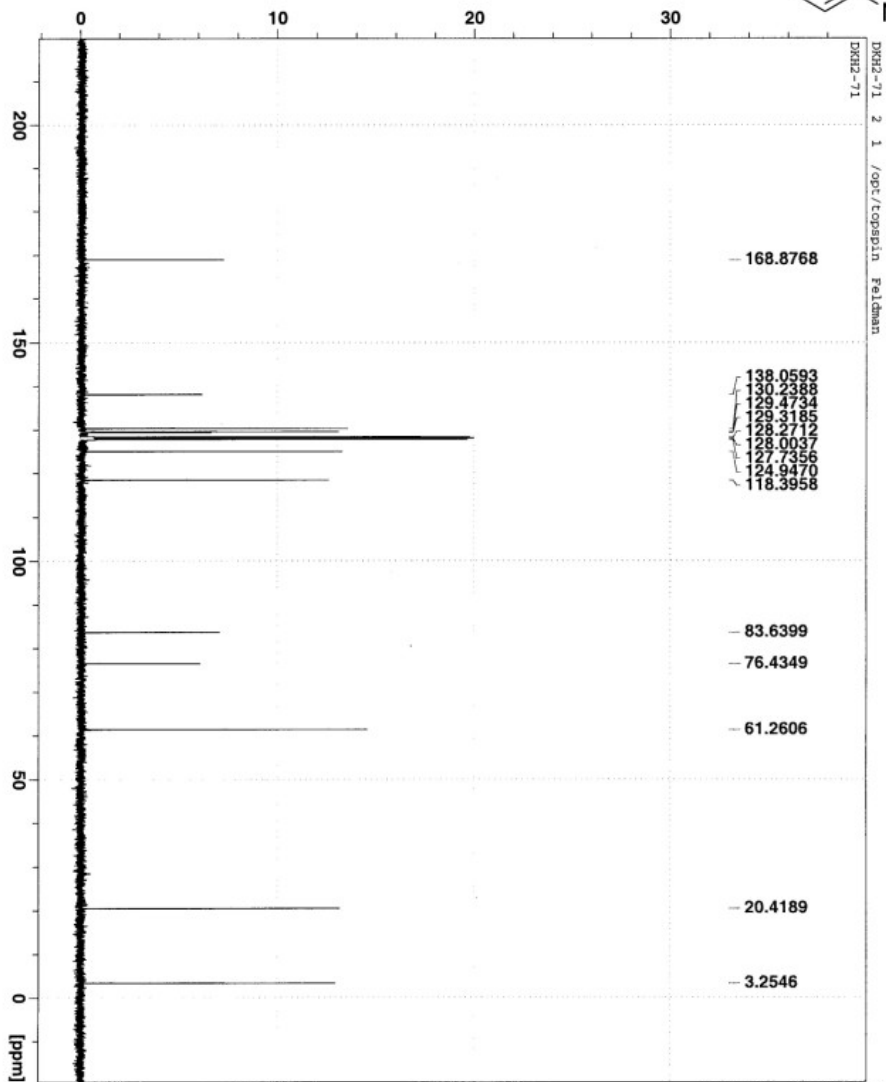
F2 - Processing parameters
 SI 32768
 SF 75.4677619 MHz
 KW 0
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 F1p 215.000 ppm
 F1 16229.57 Hz
 F2p -5.000 ppm
 F2 -377.34 Hz
 PPM/CX 11.00000 ppm/cm
 HZ/CX 830.14532 Hz/cm





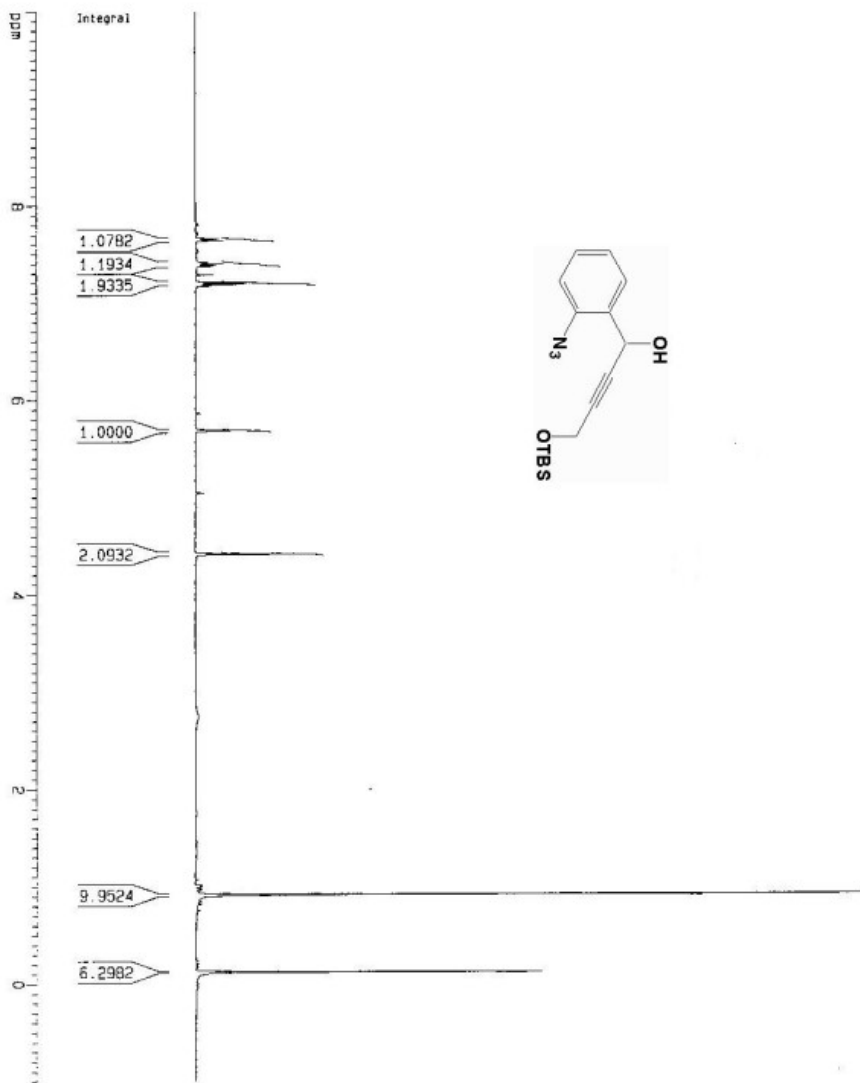
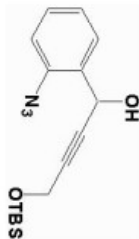
9a



General

 DATE = 2005/06/21
 TIME = 14:41
 INSTRUM = spect
 PULPROG = zgpg30
 FI (13C)

 SI = 32768
 SF = 90.555
 SWH = 21645.022



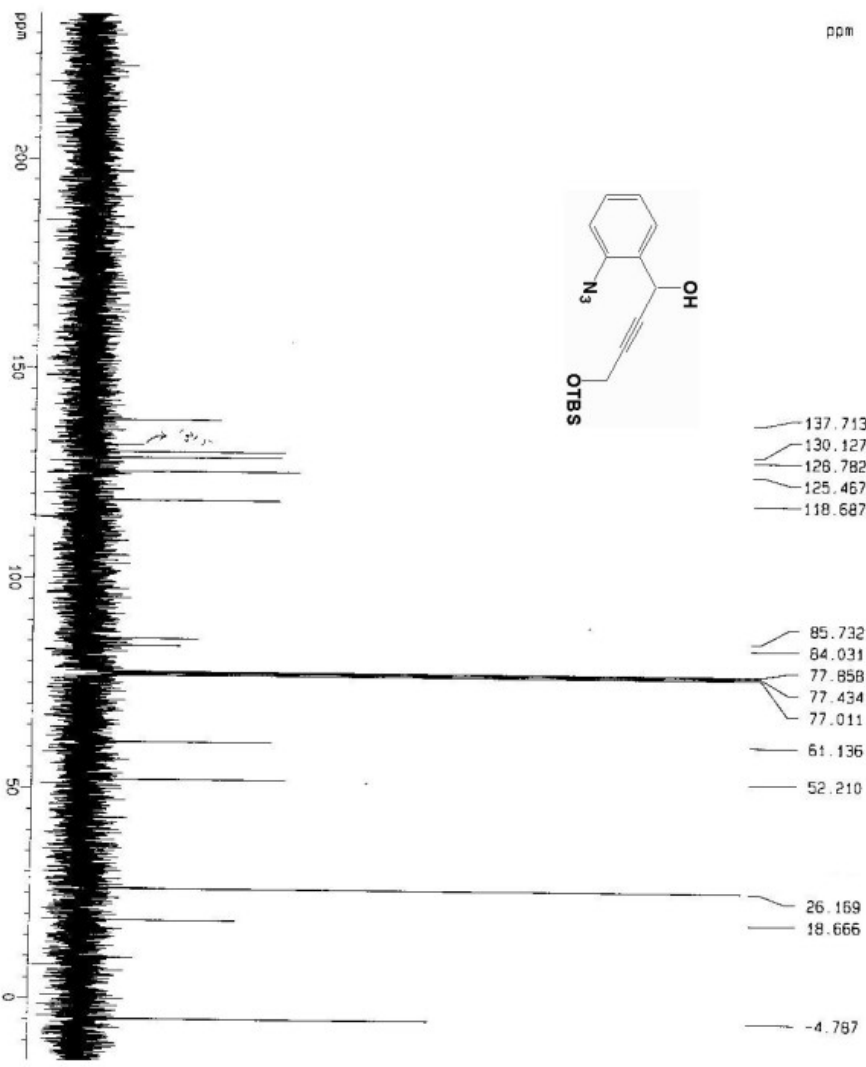
Current Data Parameters
 NAME: n01-dec-03-05
 EXPNO: 1
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20051203
 Time: 16.45
 INSTRUM: spect
 PROBRD: 5 mm BBI 1H-B
 PULPROG: zg30
 TO: 65536
 SOLVENT: CDCl3
 NS: 16
 DS: 2
 SWH: 8278.148 Hz
 FIDRES: 0.126314 Hz
 AQ: 3.9584243 sec
 RG: 512
 DM: 50.400 usec
 DE: 6.00 usec
 TE: 300.0 K
 D1: 1.00000000 sec

***** CHANNEL f1 *****
 NUC1: 1H
 P1: 6.43 usec
 PL1: 0.00 dB
 SF01: 400.1324710 MHz

F2 - Processing parameters
 SI: 32768
 SF: 400.1300000 MHz
 KW: no
 SSB: 0
 LB: 0.00 Hz
 GB: 0
 PC: 1.00

10 MHz plot parameters
 CX: 20.00 cm
 FIP: 10.000 ppm
 F1: 4001.30 Hz
 F2P: -1.040 ppm
 F2: -400.13 Hz
 FWHM: 0.55000 ppm/cm
 HZCM: 200.07150 Hz/cm



```

Current Data Parameters
NAME      M1-02013-03
EXPNO     3
PROCNO    1

F2 - Acquisition Parameters
Date_     20051203
Time      17:20
INSTRUM   spect
PROBHD    5 mm WALTZ16
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         203
DS         4
SMB       16832.393 Hz
FIDRES    0.267260 Hz
AQ         1.740038 sec
RG         16384
DM         28.580 usec
DE         6.00 usec
TE         300.0 K
D1         2.00000000 sec
d11        0.03000000 sec
d12        0.00002000 sec

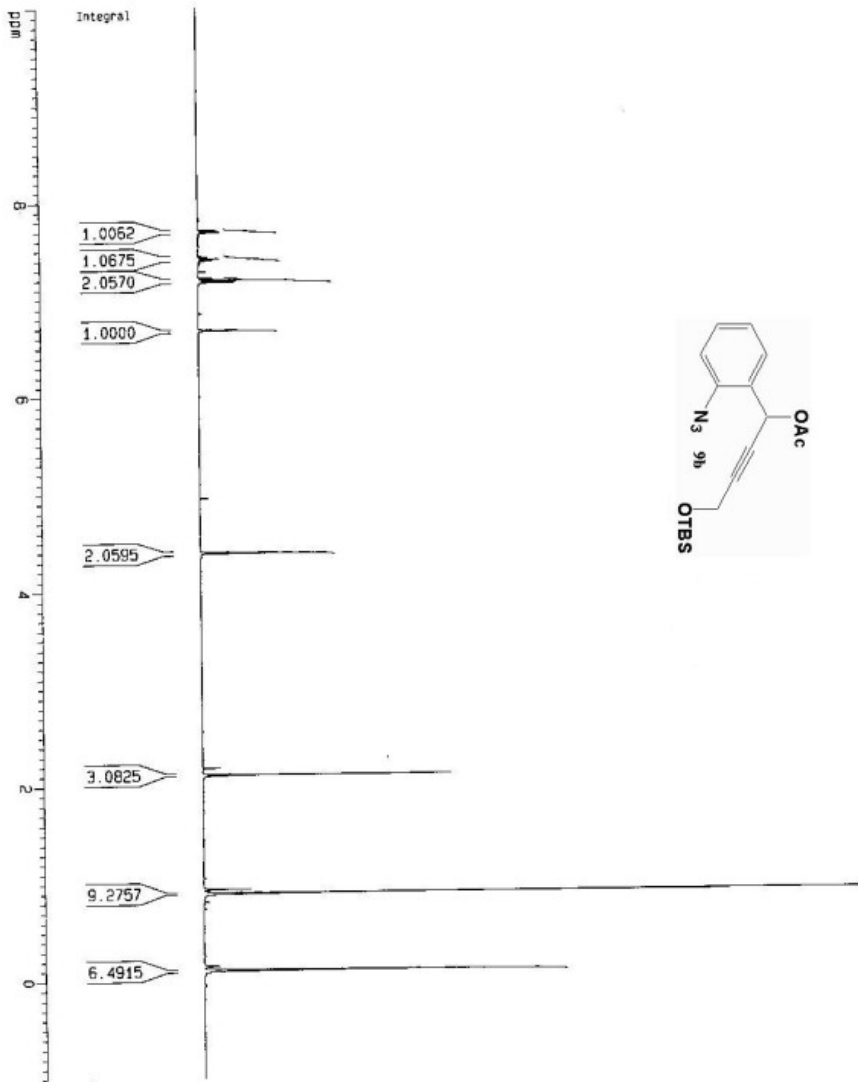
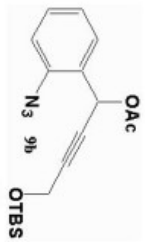
***** CHANNEL f1 *****
NUC1       13C
P1         11.80 usec
PL1        0.00 dB
SFO1       75.4763000 MHz

***** CHANNEL f2 *****
DPRGR2    waltz16
NUC2       1H
P2         110.00 usec
PL2        0.00 dB
PC2        0.00 dB
P12        17.50 dB
P13        17.50 dB
SFO2       300.1350000 MHz

F2 - Processing parameters
SI         32768
SF         75.4671990 MHz
WDW        EM
SSB         0
LB         1.00 Hz
GB         0
PC         1.40

1D NMR Plot Parameters
CX         20.00 cm
F1P        234.789 dB
F1         13717.15 Hz
F2P        -20.000 dB
F2         -1509.35 Hz
PRINCM    12.7383 dB/cm
HYDN       S61.30550 Hz/cm

```



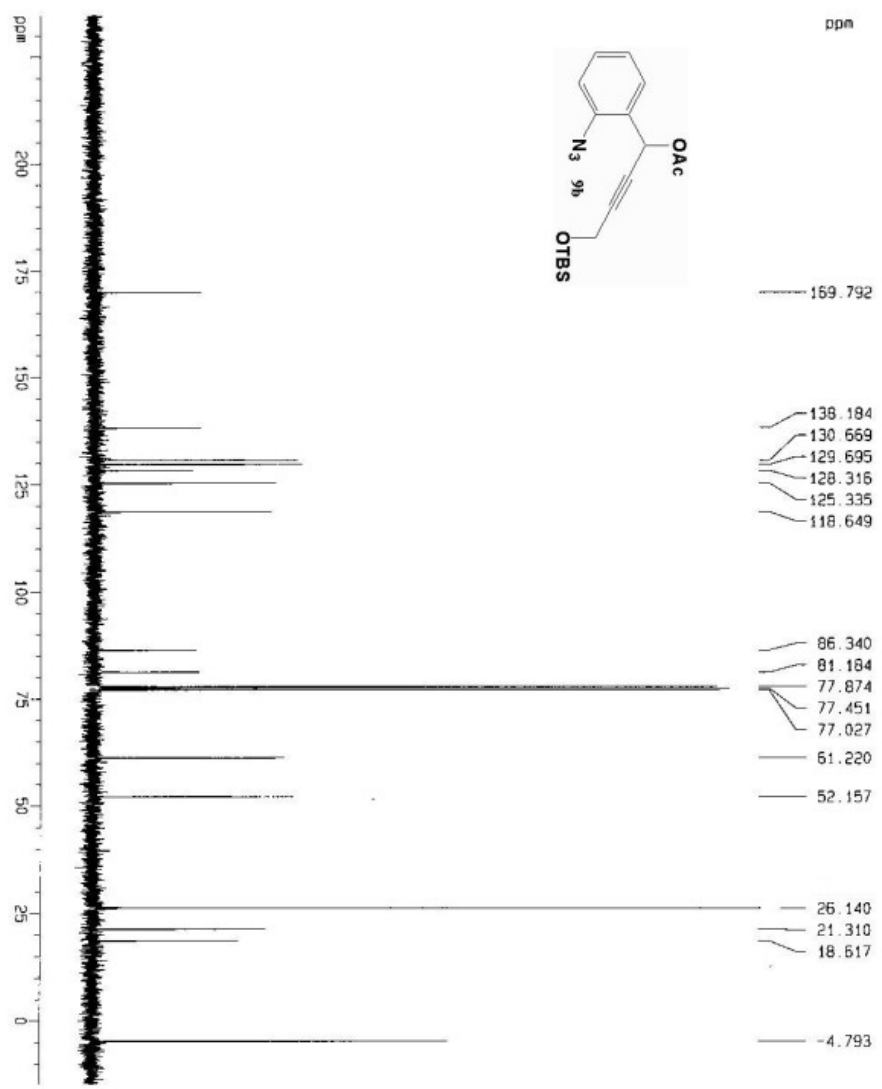
Current Data Parameters
 NAME HRI-DEC05-05
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051205
 Time 11:46
 INSTRUM spect
 PROBR0 5 mm BBI 1H-B
 PULPROG zg30
 TD 65536
 SOLVENT DMS-D3
 NS 16
 DS 2
 SFO1 8270.148 Hz
 FIDRES 0.18014 Hz
 AQ 3.598423 sec
 RG 256
 DM 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

----- CHANNEL f1 -----
 NUC1 31P
 P1 6.45 usec
 PL1 0.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 KW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

10 NMR plot parameters
 CX 20.00 cm
 FIP 10.000 DPM
 F1 4001.30 Hz
 F2P -1.000 ppm
 F2 -400.13 MHz
 PPM0H 0.55000 ppm/cm
 HZCM 220.07150 Hz/cm



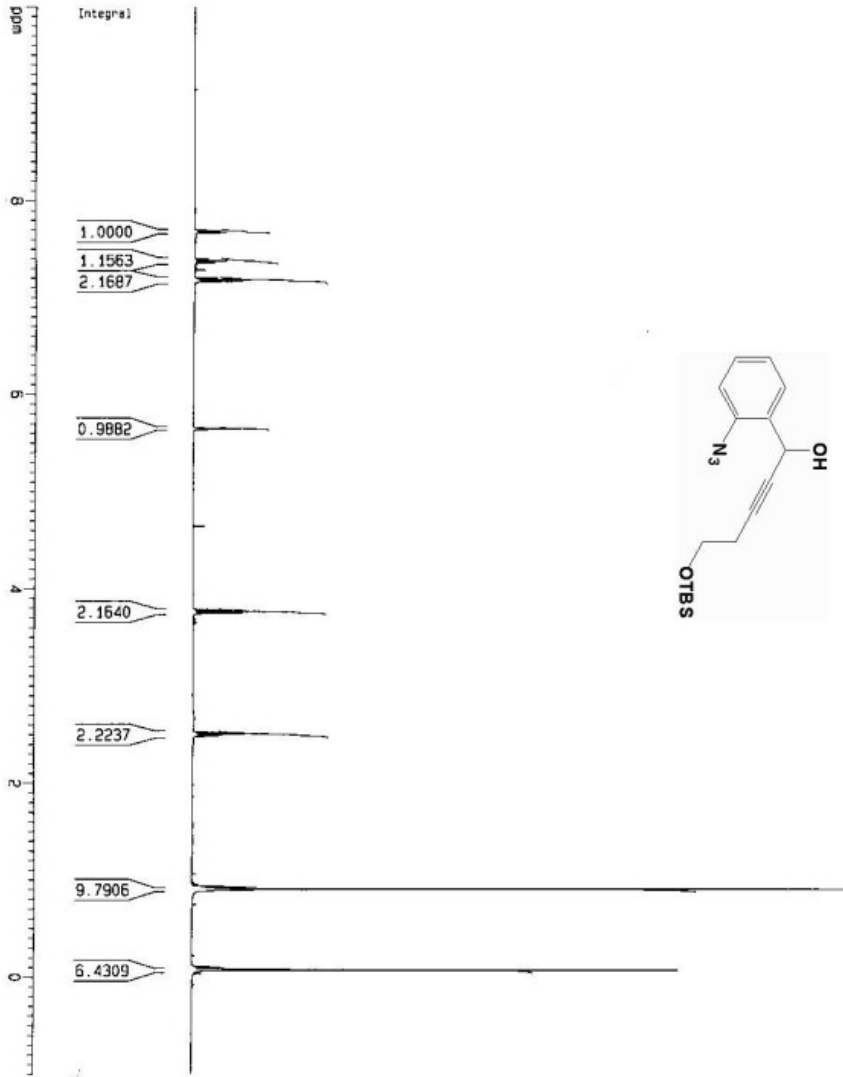
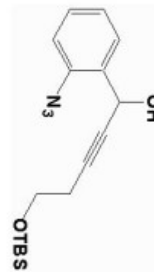
ppm

169.792
138.184
130.669
129.695
128.316
125.335
118.649
86.340
81.184
77.874
77.451
77.027
61.220
52.157
26.140
21.310
18.617
-4.793

```

Current Data Parameters
NAME      MR1-DEC03-05
EXPNO    2
PROCNO   1
-----
F2 - Acquisition Parameters
Date_    20051203
Time     18.46
INSTRUM  spect
PROBHD   5 mm Nu1190
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        417
DS        4
SFO1     100.62 303.36 Hz
FIDRES   0.287360 Hz
AQ        1.7400308 sec
RG         11596.2
DM        28.550 usec
DE         6.00 usec
TE        300.0 K
D1         2.00000000 sec
d12        0.03000000 sec
d122       0.00020000 sec
-----
***** CHANNEL f1 *****
NUC1      13C
P1         11.90 usec
PL1        0.00 dB
SFO1      75.4702000 MHz
-----
***** CHANNEL f2 *****
OPPRG2    waltz16
NUC2       1H
PCPD2     110.00 usec
RG2        0.00 dB
PL2        17.50 dB
PL12       17.50 dB
SFO2      300.1312005 MHz
-----
F2 - Processing parameters
SI         32768
SF         75.4677190 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
-----
10 NMR p101 parameters
CX         20.00 cm
F1P        234.765 ppm
F1         17217.15 Hz
F2P        -14.778 ppm
F2         -1115.24 Hz
PUNCH     12.47732 DDP/CA
HZCM      941.61951 HZ/CA

```



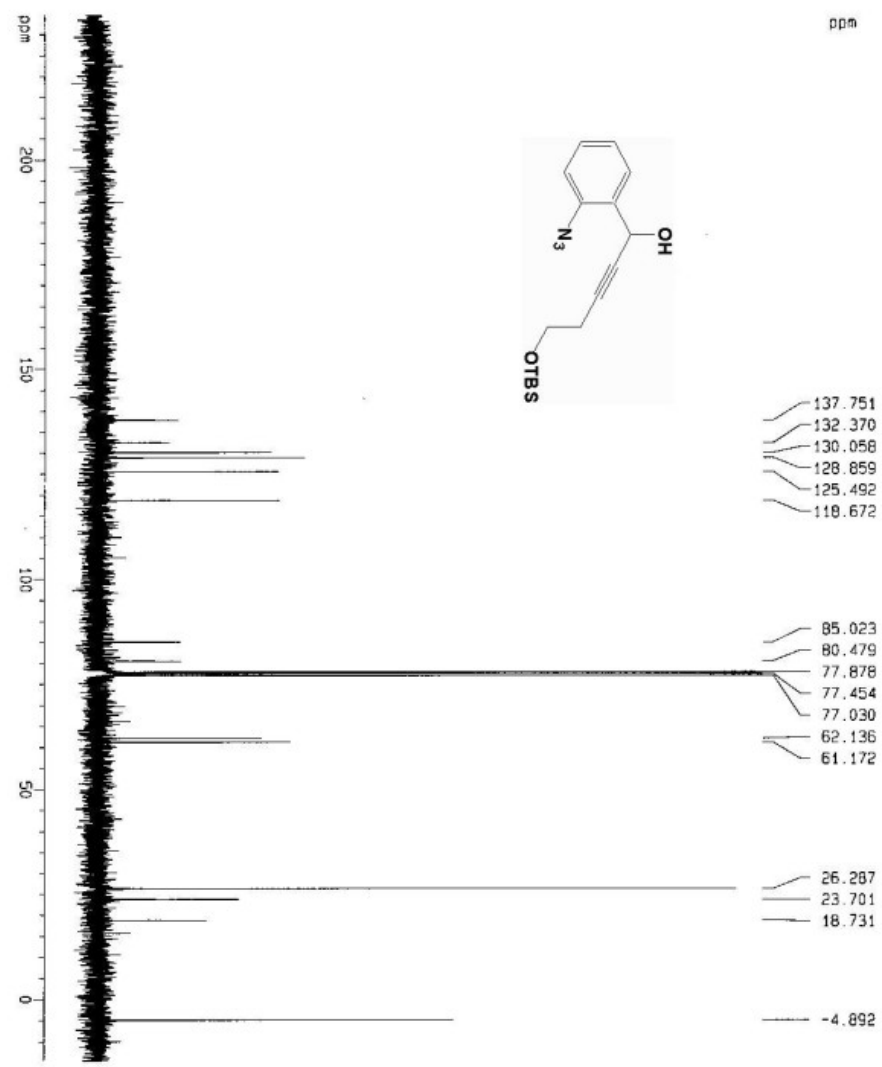
Current Data Parameters
 NAME MRI-Aug05-06
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050905
 Time 9:48
 INSTRUM spect
 PULPROG 5 ms 891 Tr-B
 PROBHD 2830
 PULPROG 2830
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SFO 82718.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 35.9
 DW 50.400 usec
 DE 5.00 usec
 TE 300.0 K
 D1 1.00000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 14
 PL1 6.43 usec
 PL1 0.00 dB
 SF 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 MDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR p1d1 parameters:
 CX 50.00 cm
 F1P 10.000 ppm
 F1 4001.30 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PRPCH 0.55000 ppm/cm
 HZCH 250.07150 Hz/cm



```

Current Data Parameters
NAME      MFL-06c03-05
EXPNO    1
PROCNO   1

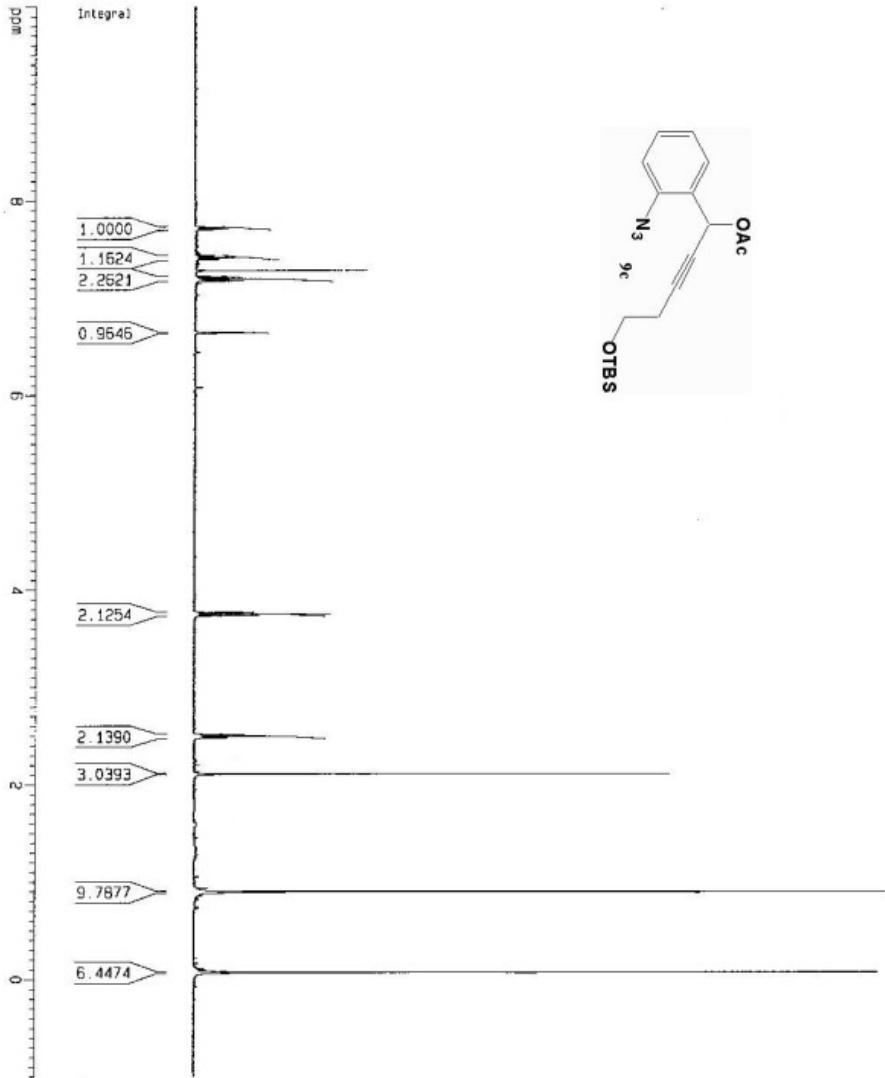
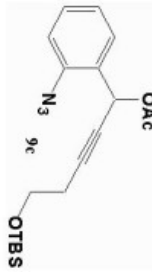
F2 - Acquisition Parameters
Date_     20051203
Time      17.44
INSTRUM   spect
PROBHD    5 mm QNP 1H/1
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         147
DS         4
SWH        18796.982 MHz
FIDRES     0.298619 Hz
AQ         1.7443076 sec
RG         325
DE         20.600 usec
TE         300.0 K
D1         2.00000000 sec
D11        0.03000000 sec
D12        0.00000000 sec

***** CHANNEL f1 *****
NUC1       13C
P1         5.40 usec
PL1        -9.00 dB
SFO1       75.470327 MHz

***** CHANNEL f2 *****
CPDPRG2    MZL145
NUC2       1H
P2         115.00 usec
PL2        0.00 dB
SFO2       299.871595 MHz

F2 - Processing parameters
SI         32768
SF         75.4023410 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

1D NMR Plot Parameters
CX         20.00 cm
F1P        234.551 ppm
F1         17693.24 Hz
F2P        -20.000 ppm
F2         -1508.05 Hz
AQ         12.73255 sec/cm
HZCM       560.06451 Hz/cm
  
```



Current Data Parameters
 NAME: M01-06c03-05
 EXPNO: 2
 PROCNO: 1

F2 - Acquisition Parameters

Date_: 20051203
 Time: 16.51
 INSTRUM: spect
 PROBRD: 5 mm BBT 1H-5
 PULPROG: zgpg30
 TD: 65536
 SOLVENT: CDCl3
 NS: 2
 DS: 2
 SWH: 8278.146 Hz
 FIDRES: 0.128314 Hz
 AQ: 3.5984243 sec
 RG: 1624.6
 DM: 50.400 USEC
 DE: 5.00 USEC
 TE: 300.0 K
 D1: 1.00000000 sec

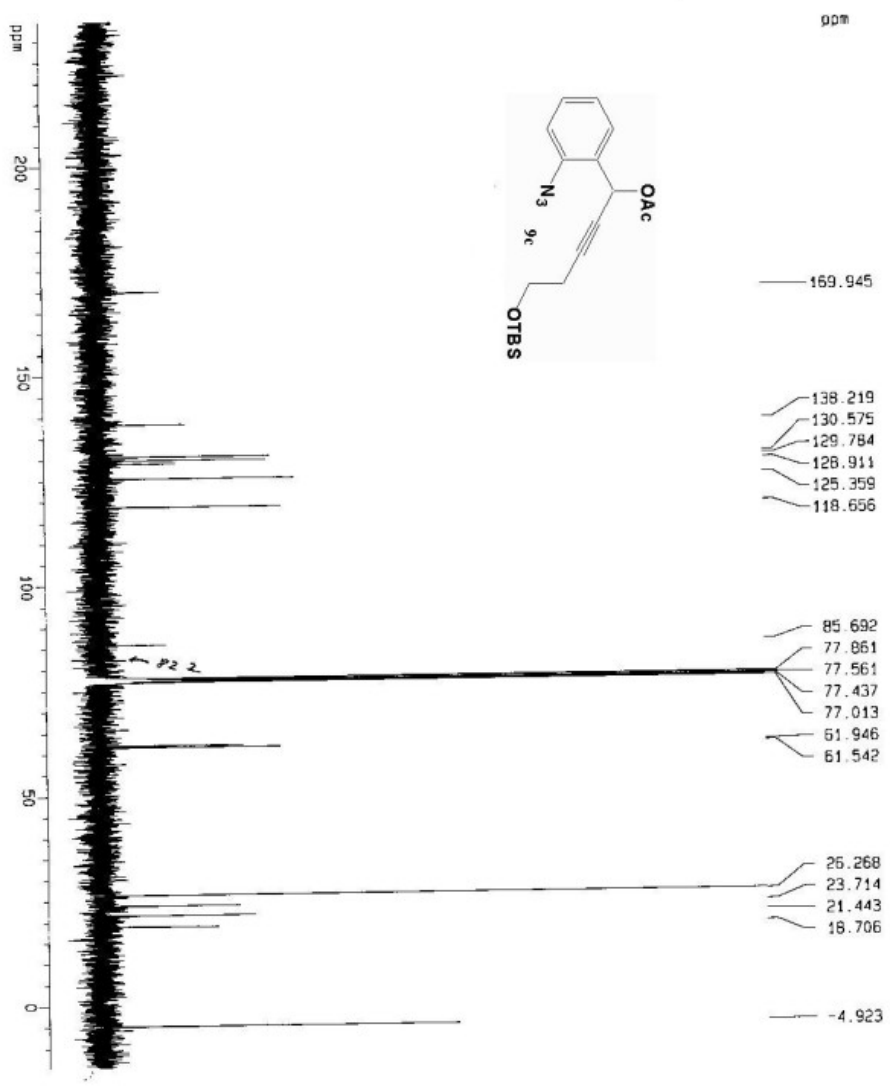
----- CHANNEL f1 -----
 NUC1: 1H
 P1: 6.45 USEC
 PL1: 0.00 DB
 SFO1: 400.1326710 MHz

F2 - Processing parameters

SF: 400.1300000 MHz
 SW: 32768
 MW: 0
 SSB: 0
 LB: 0.00 Hz
 GB: 0
 PC: 1.00

1D NMR plot parameters

CX: 20.00 cm
 F1P: 10.000 ppm
 F1: 4001.30 Hz
 F2P: -1.000 ppm
 F2: -400.13 Hz
 SFOCK: 0.55000 ppm/cm
 HZCK: 220.07150 Hz/cm



```

Current Data Parameters
NAME      N11-Dec03-05
EXPNO    3
PROCNO   1

F2 - Acquisition Parameters
Date_    20051203
Time     19.28
INSTRUM spect
PROBHD   5 mm QNP 1H/1
PULPROG zgpg30
TD        65535
SOLVENT  CDCl3
NS        1329
DS         4
SWH       18796.982 Hz
FIDRES    0.288819 Hz
AQ         1.743076 sec
RG         1024
DM         26.800 uvert
DE         6.00 uvert
TE         300.0 K
D1         2.00000000 sec
D11        0.07000000 sec
D12        0.00000000 sec

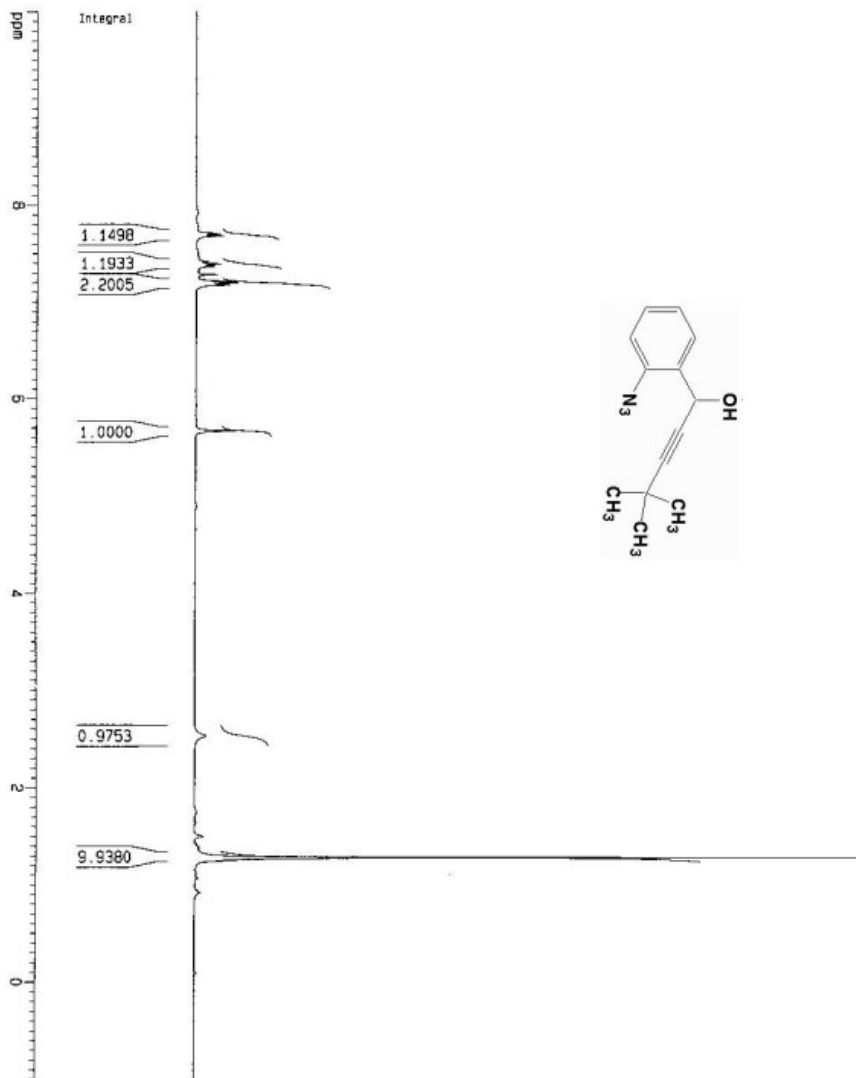
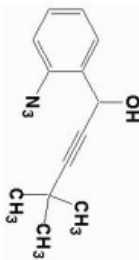
***** CHANNEL f1 *****
NUC1       13C
P1         5.40 uvert
PL1        -6.00 dB
SFO1       75.410927 MHz

***** CHANNEL f2 *****
CPDPRG2   waltz16
NUC2       1H
P2         115.00 uvert
PL2        0.00 dB
PL12       20.00 dB
PL13       20.00 dB
SFO2       259.8711995 MHz

F2 - Processing parameters
SI         32768
SF         75.4073410 MHz
WDW        EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40

1D NMR plot parameters
CX         20.08 cm
F1p        234.651 Dppm
F1         17693.24 Hz
F2p        -20.000 Dppm
F2         -1569.05 Hz
PCMCN     12.73266 Dppm/cm
HZCM      980.08451 Hz/cm

```



Current Data Parameters
 NAME M1-AP19-06
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060419
 Time 14:57

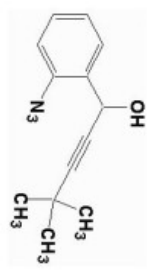
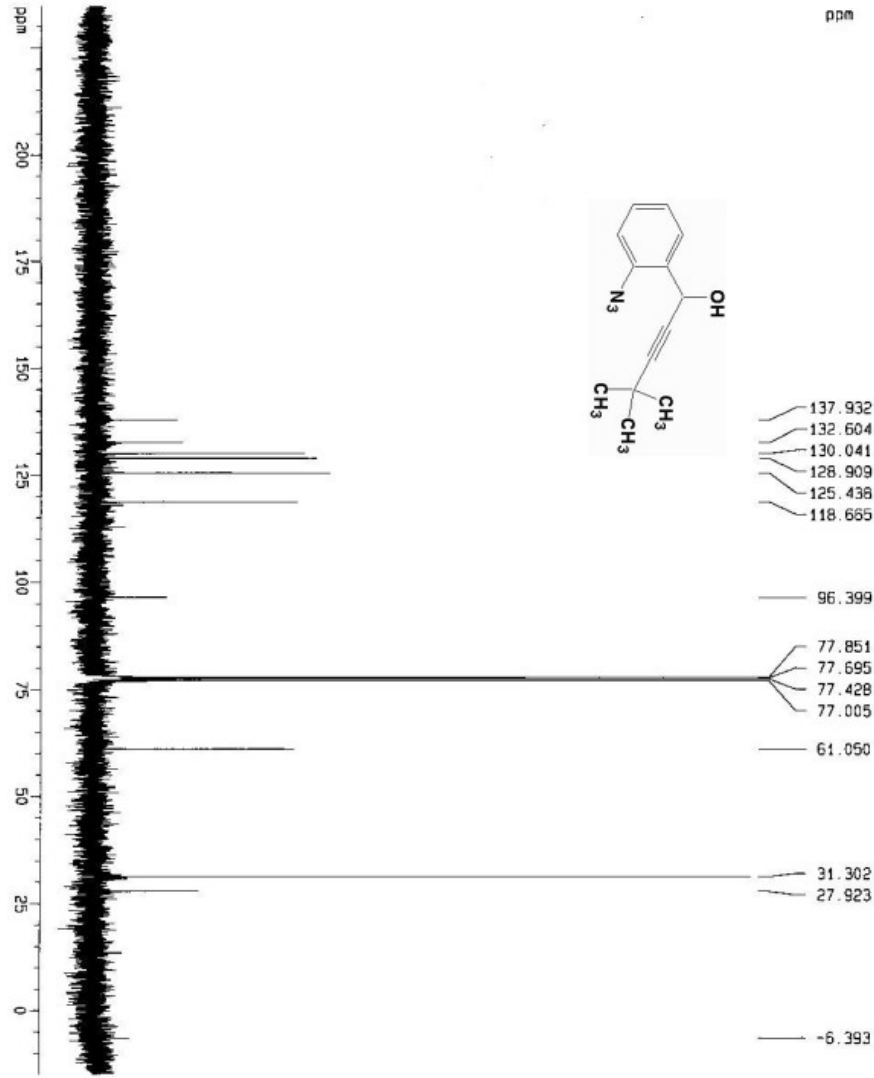
INSTRUM spect
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2

SI 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3994660 sec
 RG 362
 DM 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 9.80 usec
 PL1 -6.00 dB
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300000 MHz
 MM 0
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

3D NMR plot parameters
 CX 20.00 cm
 F1P 10.000 ppm
 F1 3001.30 Hz
 F2P -1.000 ppm
 F2 -300.13 Hz
 PRGCM 0.55000 ppm/cm
 HZCM 165.07150 Hz/cm

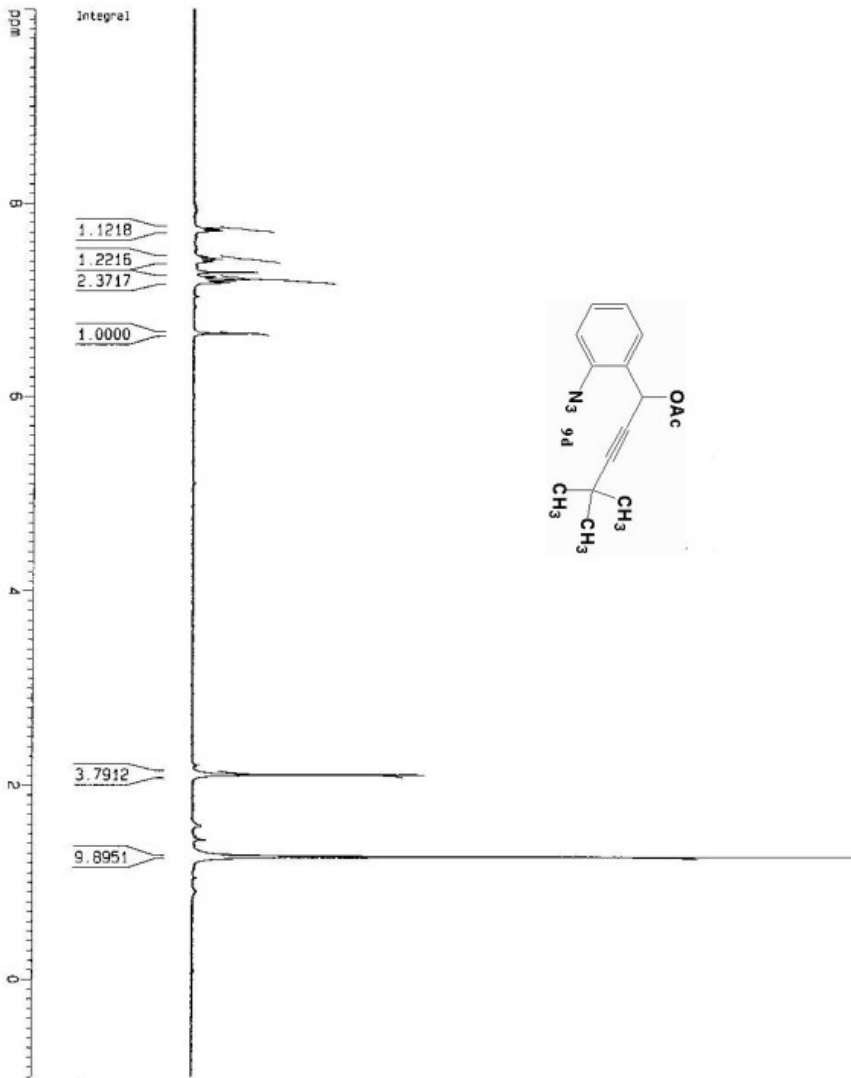
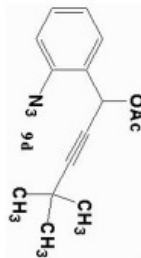


- 137.932
- 132.604
- 130.041
- 128.909
- 125.438
- 118.665
- 96.399
- 77.851
- 77.695
- 77.428
- 77.005
- 61.050
- 31.302
- 27.923
- 9.393

```

Current Data Parameters
NAME      M1-APR19-08
EXPNO     5
PROCNO    1
-----
F2 - Acquisition Parameters
Date_     20080418
Time      15:04
INSTRUM   spect
PROBHD    5 mm W111nu
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         311
DS         4
SWH        18682.393 Hz
FIDRES     0.287350 Hz
AQ         1.7400308 sec
RG         11585.2
CW         26.500 usec
DE         6.00 usec
TE         300.0 K
D1         2.00000000 sec
d11        0.03000000 sec
d12        0.00020000 sec
-----
***** CHANNEL f1 *****
NUC1       13C
P1         11.60 usec
PL1        0.00 dB
SFO1       75.4760000 MHz
-----
***** CHANNEL f2 *****
CPDPRG2    waltz16
NUC2       1H
P2         110.00 usec
PL2        0.00 dB
PL12       17.50 dB
PL13       17.50 dB
SFO2       300.1312005 MHz
-----
F2 - Processing parameters
SI         32768
SF         75.4677190 MHz
AQ         1.7400308 sec
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
-----
1D NMR plot parameters
CX         20.00 cm
F1P        234.705 ppm
F1         12717.16 Hz
F2P        -14.778 ppm
F2         -1119.23 Hz
FIDRES     12.47715 ppm/cm
HZCM       941.61951 Hz/cm

```



Current Data Parameters
 NAME M1-Apr20-06
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20050420
 Time 16.09
 INSTRUM spect
 PROBRD 5 mm MUltinu
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SMH 6172.833 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 512
 DM 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

***** CHANNEL f1 *****

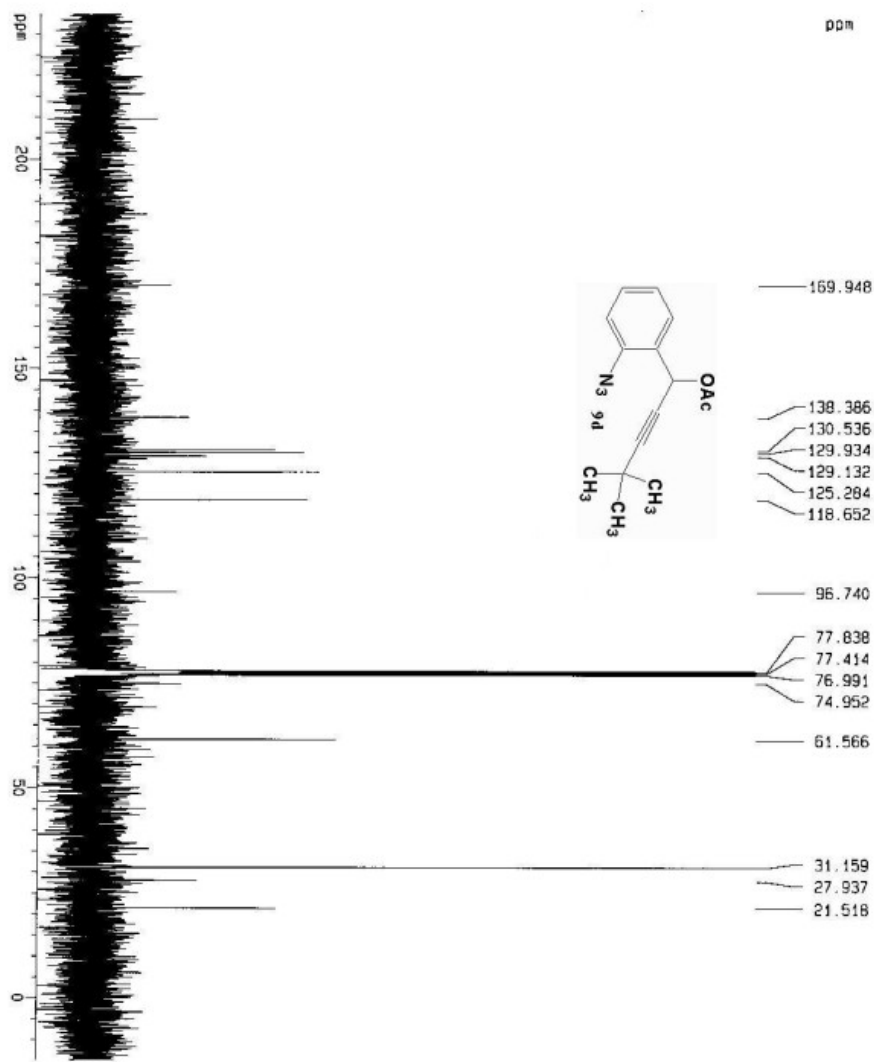
NUC1 1H
 P1 9.60 usec
 PL1 -8.00 dB
 SFO1 300.1318534 MHz

F2 - Processing parameters

SF 32768
 SF 300.1300000 MHz
 MDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters

CX 20.00 cm
 F1P 10.000 ppm
 F1 3001.30 Hz
 F2P -1.000 ppm
 F2 -300.13 Hz
 PPM/CM 0.550000 ppm/cm
 HZ/CM 165.07150 Hz/cm



Current Data Parameters
 NAME W1-Apr20-06
 EXPNO 3
 PROCNO 1

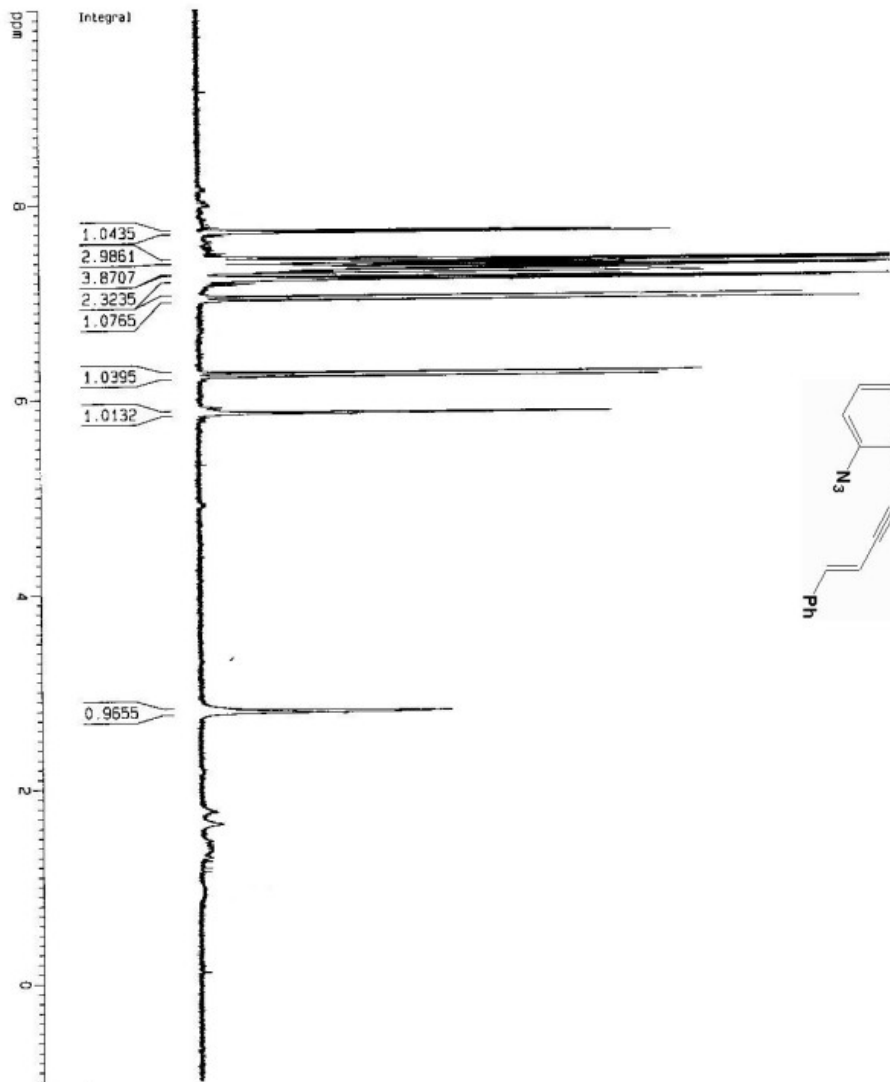
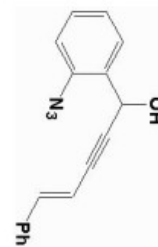
F2 - Acquisition Parameters
 Date_ 20060420
 Time 16:24
 INSTRUM spect
 PULPROG 5 pm Multivp
 FIDRES 2.99430
 T0 65536
 SOLVENT CDCl3
 NS 769
 DS 4
 SWH 18832.309 Hz
 FIDRES 0.282706 Hz
 AQ 1.7460008 sec
 RG 13004
 DN 26.350 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 d12 0.00012000 sec

***** CHANNEL f1 *****
 NUC1 13C
 P1 11.80 usec
 PL1 0.00 dB
 SFO1 75.4750200 MHz

***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 110.00 usec
 PL2 0.00 dB
 PL12 17.50 dB
 PL13 17.50 dB
 SFO2 300.1312000 MHz

F2 - Processing parameters
 S1 32768
 SF 75.4677150 MHz
 KW EM
 SSB 0
 LB 1.00 Hz
 DB 0
 PC 1.40

ID NMR plot parameters
 CS 20.00 cm
 CP 234.769 ppm
 F1 17.173 Hz
 F2 -150.000 ppm
 PPMCH 12.73893 Hz/cm
 HZCH 961.32544 Hz/cm

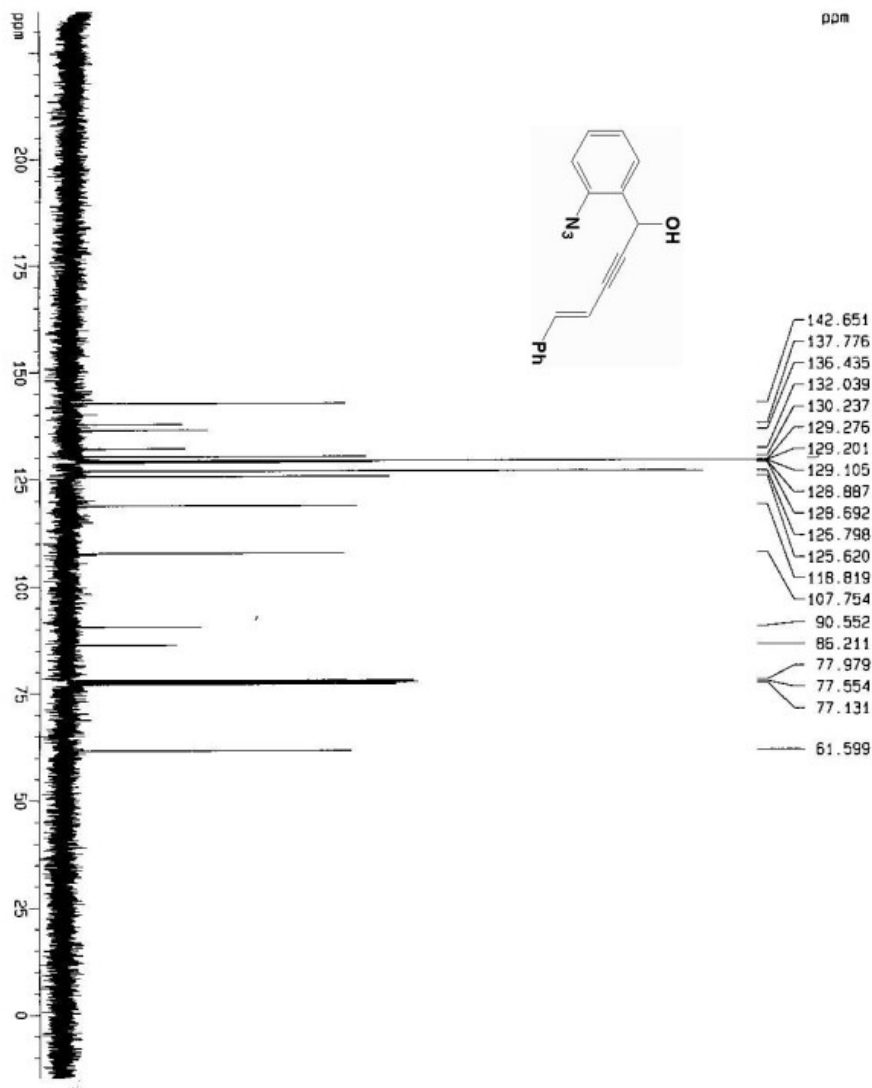


Current Data Parameters
 NAME M01-08C03-05
 EXPNO 3
 PRGNAME 1
 F2 - Acquisition Parameters
 Date_ 20051205
 Time 12.01
 INSTRUM spect
 PROCNO 5
 PULPROG zgpg30
 TD 4930
 FIDRES 0.5556
 SOLVENT CDCl3
 NS 12
 DS 2
 SWH 8278.145 Hz
 FIDRES 0.18514 Hz
 AQ 3.595443 sec
 RG 812.7
 DM 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 6.45 usec
 PL1 0.00 dB
 SF01 400.1364710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 KW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

10 NMR list parameters
 CX 20.00 cm
 F1P 10.000 ppm
 F1 4001.30 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 GPMCH 0.55000 ppm/cm
 KZCH 220.07150 Hz/cm



```

Current Data Parameters
NAME          N01-Sept13-05
EXPNO         4
PROCNO       1
PROCNAME     1

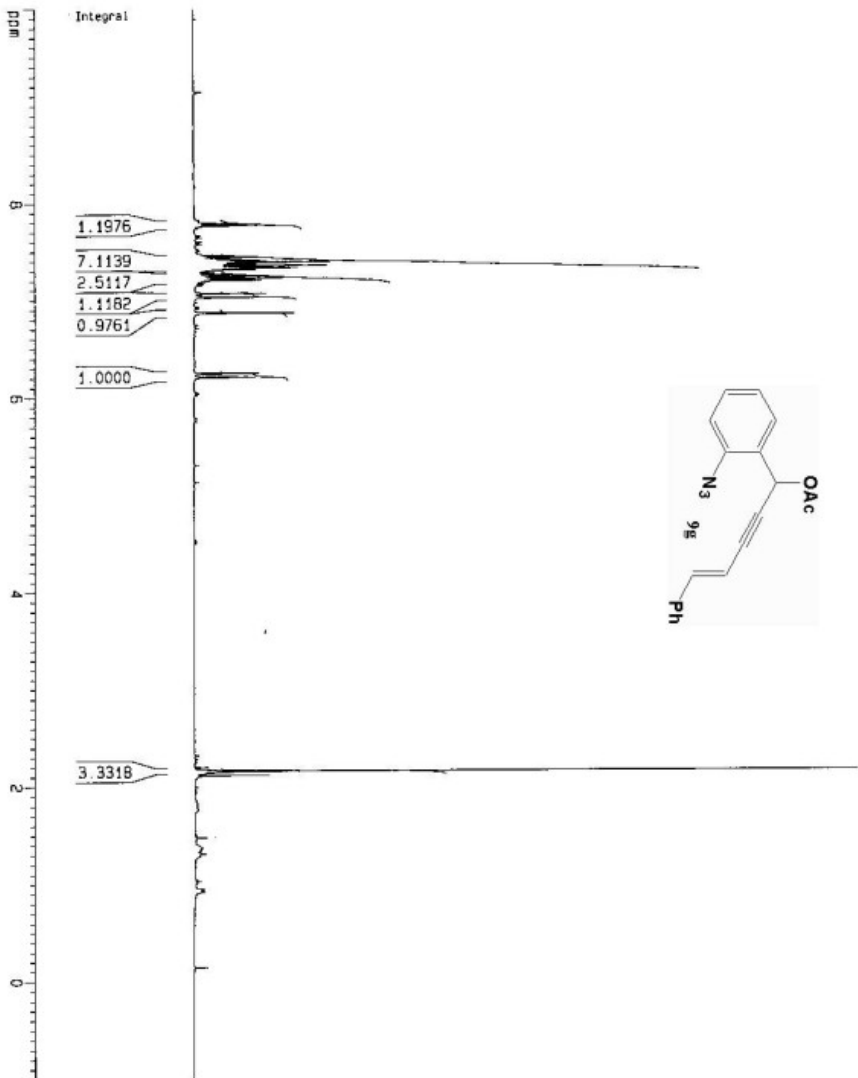
F2 - Acquisition Parameters
Date_        20050919
Time         17.13
INSTRUM     spect
PROBHD      5 mm DNP 1H/1
PULPROG     zgpg30
TD           65536
SOLVENT     CDCl3
NS           37
DS           4
SWH          18798.992 Hz
FIDRES      0.286819 Hz
AQ           1.7433076 sec
RG           1024
DE           28.800 umic
TE           300.0 K
D0           2.00000000 sec
O1           0.03000000 sec
O12          0.00000000 sec

***** CHANNEL f1 *****
NUC1         13C
P1           5.00 umic
PL1          -8.00 dB
SFO1         75.4108307 MHz

***** CHANNEL f2 *****
COPROG2     waltz16
NUC2         1H
P2           115.00 umic
PL2          0.00 dB
PL12         20.00 dB
PL13         20.00 dB
SFO2         299.8711995 MHz

F2 - Processing parameters
SI           32768
SF           75.4023410 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40

10 NMR plot parameters
CK           20.00 cm
F1P          234.651 ppm
F1           17593.24 Hz
F2P          -14.038 ppm
F2           -1103.75 Hz
PROCKM      12.40446 Deg/Ce
HZCKM       939.84987 Hz/Ce
  
```



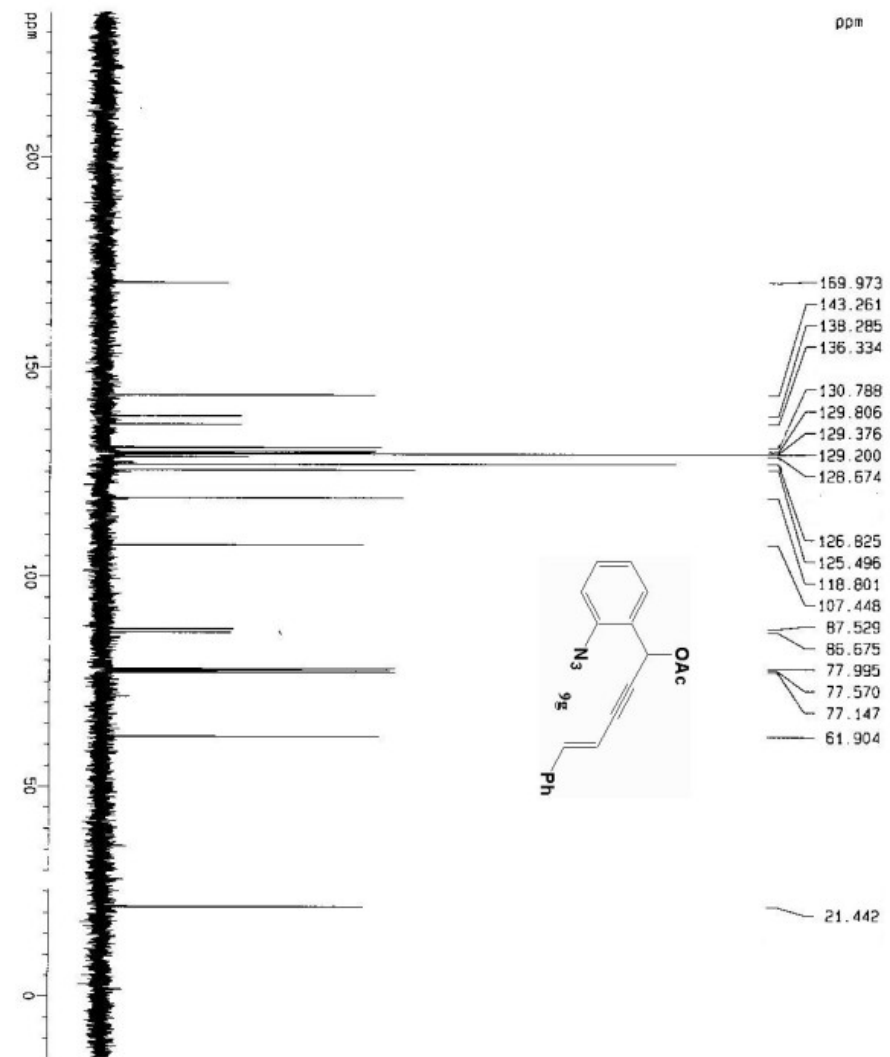
Current Data Parameters
 NAME W1-Nov10-05
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051110
 Time 10.10
 INSTRUM spect
 PROBR0 5 mm BBI 1H-6
 PULPROG zgpg30
 TO 85336
 SOLVENT CDCl3
 NS 7
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.5944243 sec
 RG 181
 DM 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

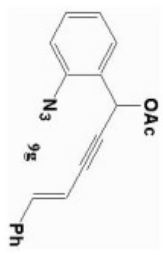
----- CHANNEL f1 -----
 NUC1 1H
 P1 6.45 usec
 PL1 0.00 dB
 SF01 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 KCM no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

10 MHz plot parameters
 CX 20.00 cm
 F1 10.000 GHz
 F2 4001.30 Hz
 F3 -1.000 GHz
 F4 -400.13 Hz
 PPMCM 0.55000 ppm/cm
 HZCM 250.07150 Hz/cm



- 169.973
- 143.261
- 138.285
- 136.334
- 130.788
- 129.806
- 129.376
- 129.200
- 128.674
- 126.825
- 125.496
- 118.801
- 107.448
- 87.529
- 86.675
- 77.995
- 77.570
- 77.147
- 61.904
- 21.442



```

Current Data Parameters
NAME      W1-MW1F-05
EXPNO    2
PROCNO   1

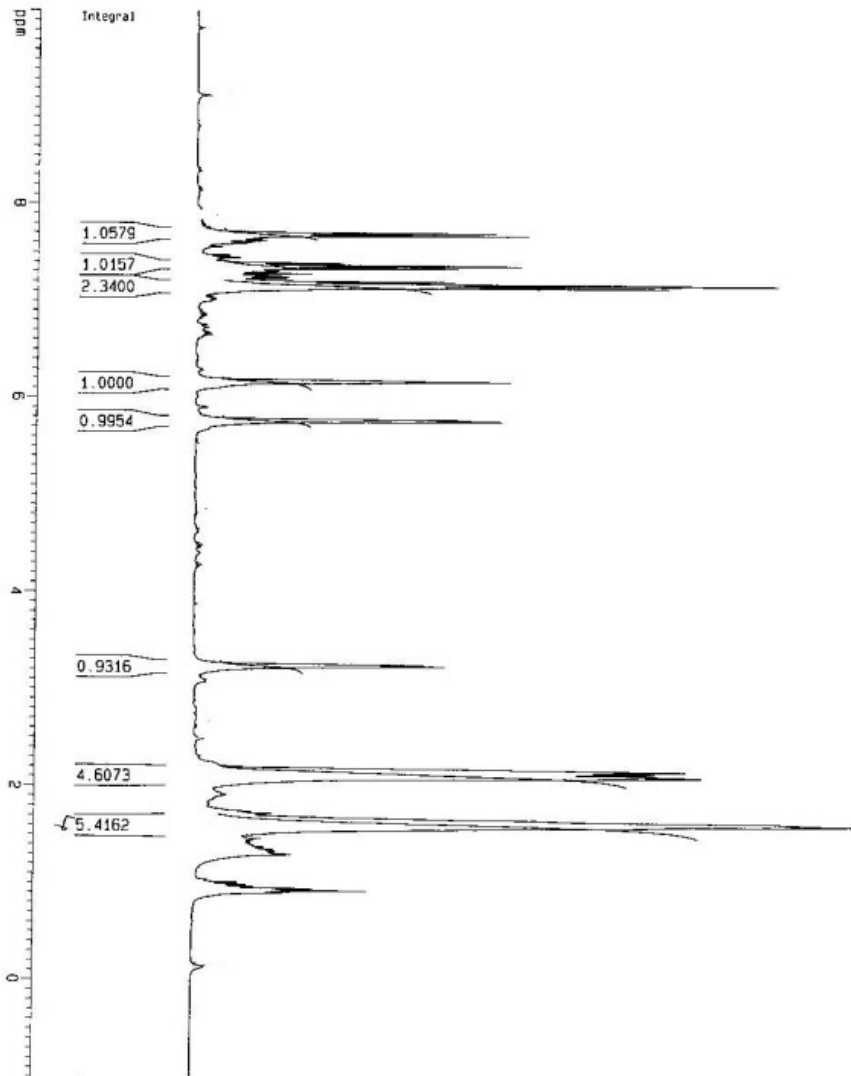
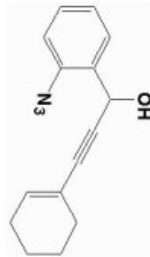
F2 - Acquisition Parameters
Date_    20051110
Time     10:22
INSTRUM  spect
PROBHD   5 mm QNP 1H/1
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        31
DS        4
SWH       18736.899 Hz
FIDRES    0.286813 Hz
AQ         1.7233075 sec
RG         512
AQ         26.600 usec
DE         6.00 usec
TE         300.0 K
D1         2.00000000 sec
D11        0.03000000 sec
D12        0.00020000 sec

----- CHANNEL f1 -----
NUC1      13C
P1         5.40 usec
PL1       -6.00 dB
SFO1      75.476327 MHz

----- CHANNEL f2 -----
CPDPRG2   waltz16
NUC2      1H
P2         115.00 usec
PL2        0.00 dB
PL12       20.00 dB
PL13       20.00 dB
SFO2      299.8711095 MHz

F2 - Processing parameters
SI         32768
SF         75.4623410 MHz
SOLVENT    CDCl3
NS         0
DS         0
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

1D NMR plot parameters
CX         30.00 cm
F1P        234.651 ppm
F1         11563.24 Hz
F2P        -20.000 ppm
F2         -1506.05 Hz
NUC1CH    13C
NUC2CH    1H
PCNCH     96.451 Hz/cm
  
```



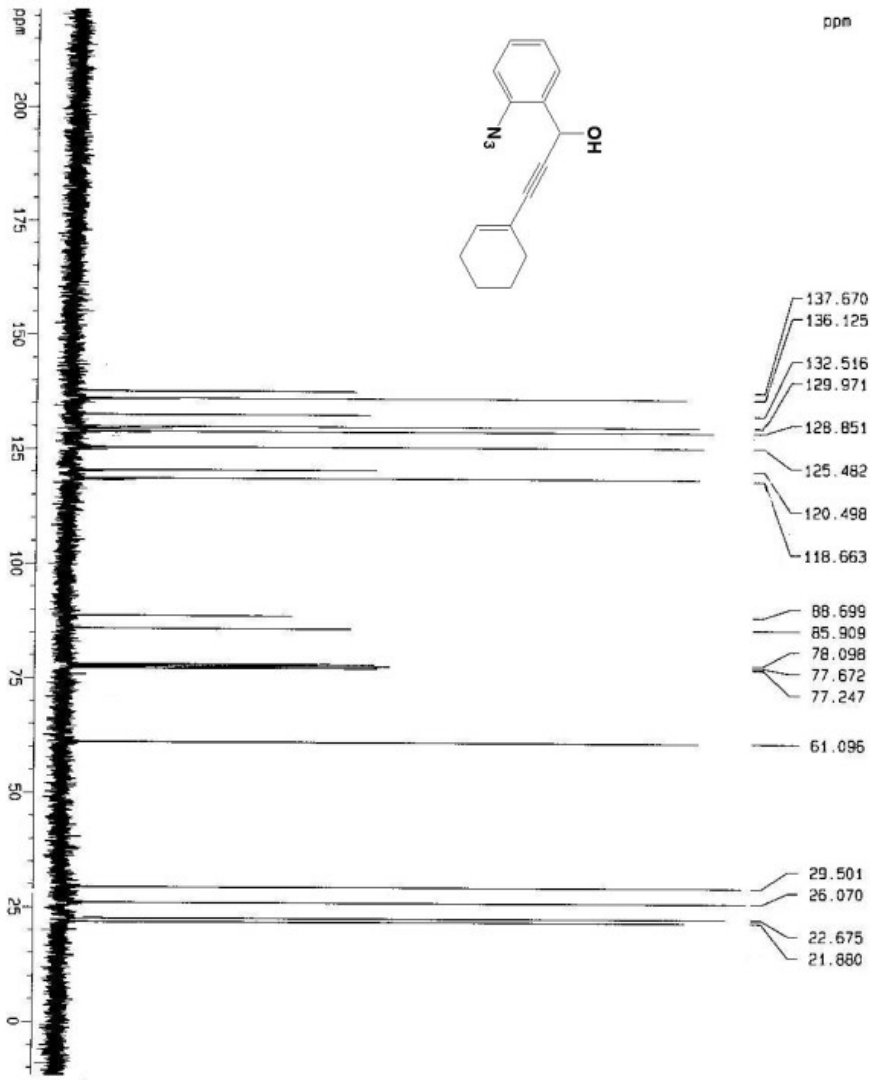
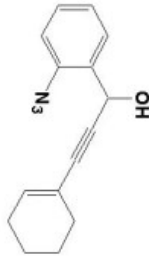
Current Data Parameters
 NAME M1-59019-05
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050919
 Time 16:51
 INSTRUM spect
 PROBRID 5 pr Omp 14/1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.034190 Hz
 AQ 5.3094660 sec
 RG 35.9
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 11.70 usec
 PL1 0.00 dB
 SF01 259.0716518 MHz

F2 - Processing parameters
 SI 32768
 SF 299.8700000 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

ID NMR plot parameters
 CX 20.00 cm
 F1P 10.000 ppm
 F1 2998.70 Hz
 F2P -1.000 ppm
 F2 -299.87 Hz
 PRCM 0.55000 ppm/cm
 HZCM 164.52950 Hz/cm

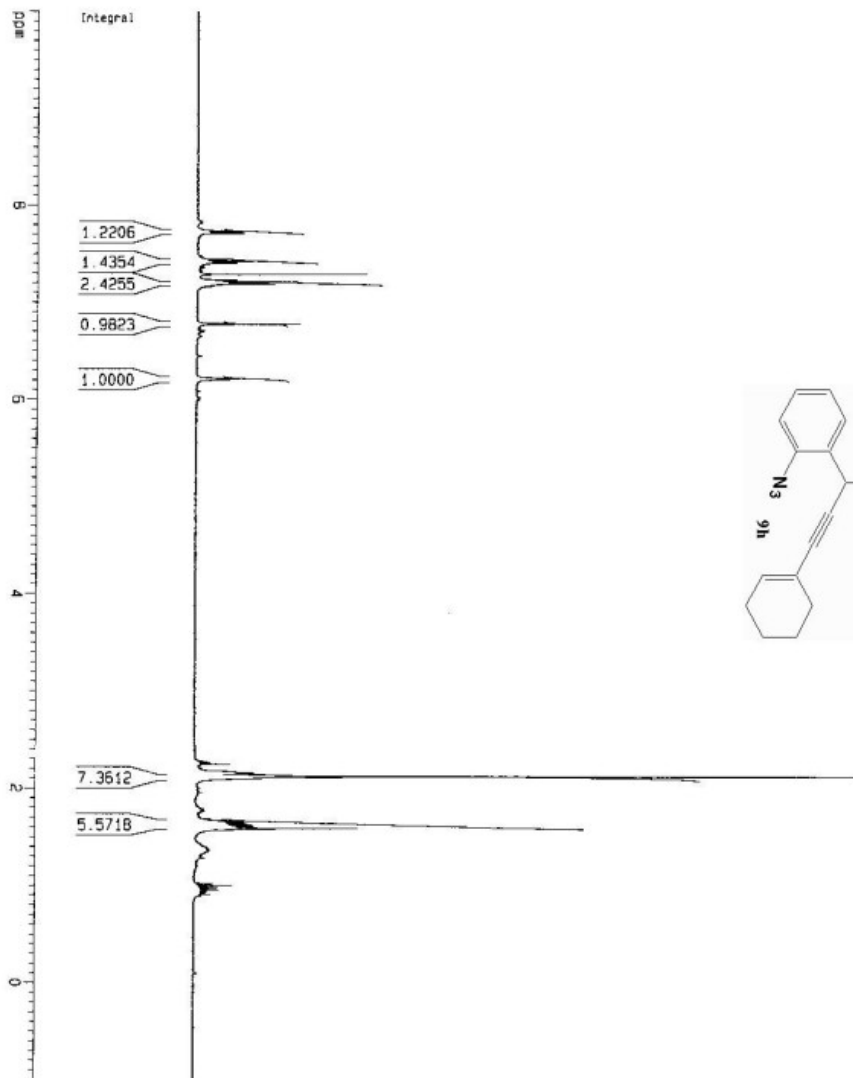
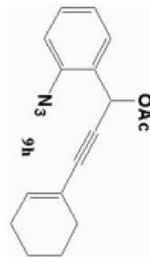


ppm

137.670
136.125
132.516
129.971
128.851
125.482
120.498
118.663
88.699
85.909
78.098
77.672
77.247
61.096
29.501
26.070
22.675
21.880

```

Current Data Parameters
NAME      M1-Sm19-05
EXPNO     2
PROCNO    1
-----
F2 - Acquisition Parameters
Date_     20050915
Time      16.39
INSTRUM   spect
PROBHD    5 mm QNP 1H/1
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         43
DS         4
SMH       18796.592 Hz
FIDRES    0.268819 Hz
AQ         1.7433076 sec
RG         1024
OR         25.600 usec
DE         300.0 K
TE         2.90000000 sec
D11        0.05000000 sec
D12        0.00000000 sec
-----
***** CHANNEL f1 *****
NUC1       13C
P1         5.40 usec
PL1        -6.00 dB
SFO1       75.410637 MHz
-----
***** CHANNEL f2 *****
CPDPRG2   waltz16
NUC2       1H
P2         115.00 usec
PL2         0.00 dB
PC12       20.00 dB
PL13       20.00 dB
SFO2       200.8711956 MHz
-----
F2 - Processing parameters
SI         32768
SF         75.4023410 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
-----
10 NMR 13C parameters
CX         20.00 cm
F1P        231.464 GHz
F1         15689.38 MHz
F2         -11.011 GHz
F3PCMK     11.85276 GHz/cm
HZCM       878.64528 Hz/cm
  
```



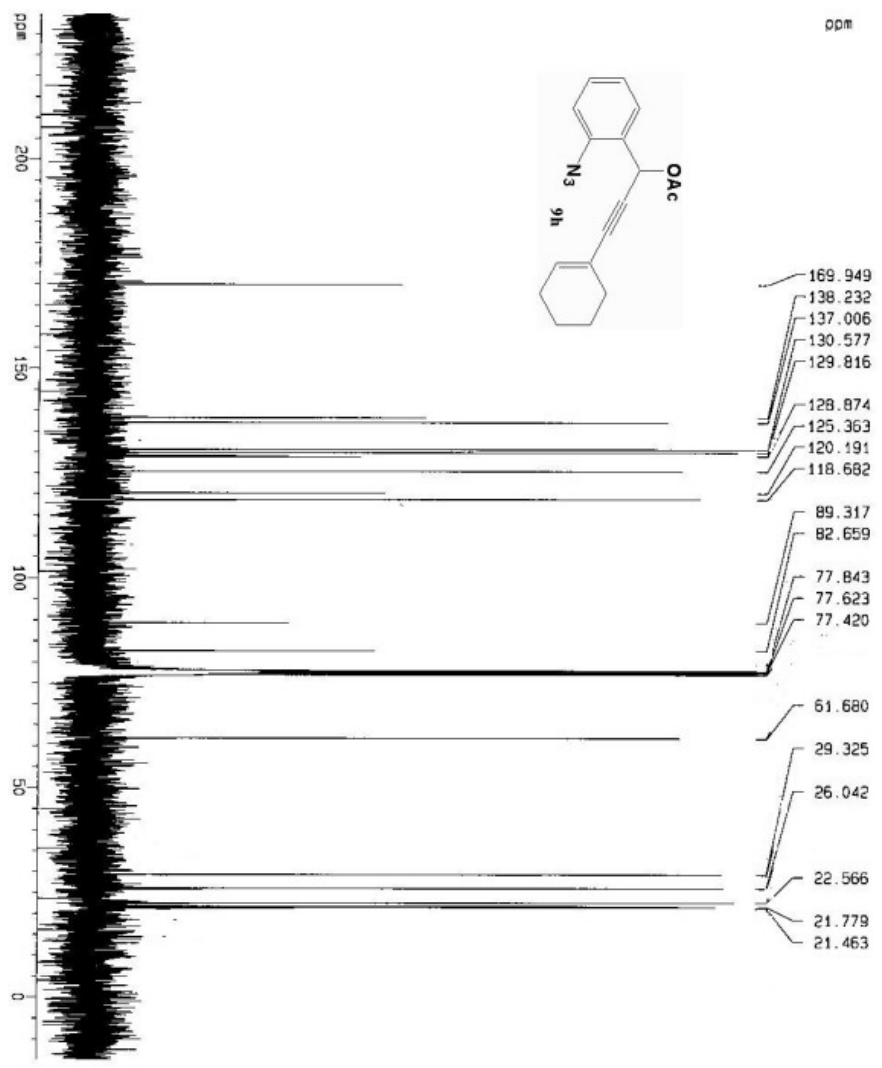
Current Data Parameters
 NAME: M01-Apr-21-06
 EXPNO: 4
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20060421
 Time: 10.30
 INSTRUM: spect
 PROBRW: 5 MHz
 PULPROG: zg30
 TD: 65536
 SOLVENT: CDCl3
 NS: 16
 DS: 2
 SWH: 8279.146 Hz
 FIDRES: 0.126314 Hz
 AQ: 3.9584243 sec
 RG: 1149.4
 DM: 60.400 usec
 DE: 6.00 usec
 TE: 300.0 K
 D1: 1.00000000 sec

===== CHANNEL f1 =====
 NUC1: 1H
 P1: 6.45 usec
 PL1: 0.00 dB
 SFO1: 400.1324710 MHz

F2 - Processing parameters
 SI: 32768
 SF: 400.1300000 MHz
 NDM: no
 SSB: 0
 LB: 0.00 Hz
 GB: 0
 PC: 1.00

1D NMR plot parameters
 CX: 20.00 cm
 F1P: 10.000 ppm
 F1: 4007.30 Hz
 F2P: -1.000 ppm
 F2: -400.13 Hz
 PRNCH: 0.55000 ppm/cm
 HZCH: 220.07149 Hz/cm



- 169.949
- 138.232
- 137.006
- 130.577
- 129.816
- 128.874
- 125.363
- 120.191
- 118.682
- 89.317
- 82.659
- 77.843
- 77.623
- 77.420
- 61.680
- 29.325
- 26.042
- 22.566
- 21.779
- 21.463

```

Current Data Parameters
NAME      MRI-Apr-22-06
EXPNO    1
PROCNO   1

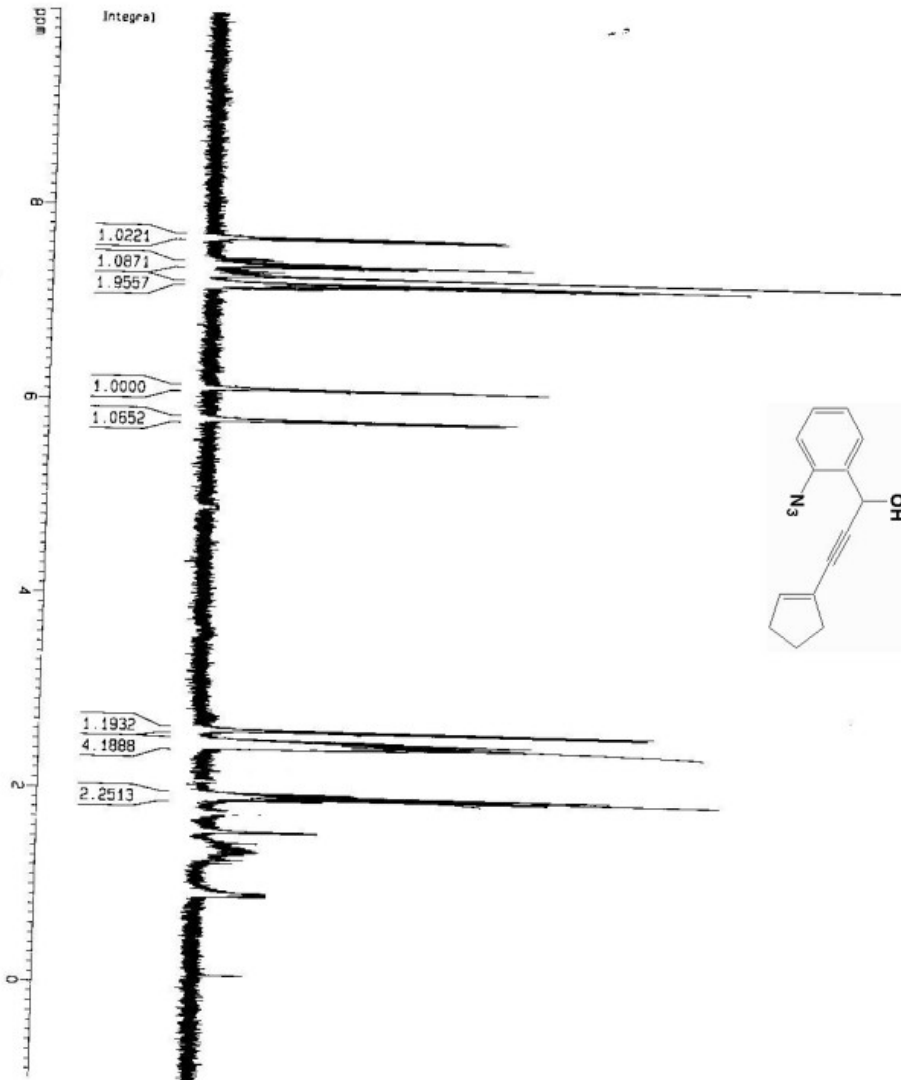
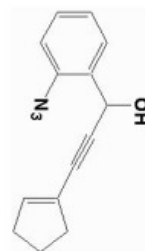
F2 - Acquisition Parameters
Date_    20060422
Time     19.18
INSTRUM  spect
PROBHD   5 mm Multinu
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        500
DS        4
SFO1     100.625383 Hz
FIDRES   0.287360 Hz
AQ        1.7460326 sec
RG        17004
OR        26.500 usec
DE        6.00 usec
TE        300.0 K
D1        2.00000000 sec
d12       0.03000000 sec
d12       0.00000000 sec

***** CHANNEL f1 *****
NUC1      13C
P1        11.80 usec
PL1       0.00 dB
SFO1      75.4763200 MHz

***** CHANNEL f2 *****
CPDPRG2  waltz16
NUC2      1H
P2        110.00 usec
PL2       0.00 dB
PL12      17.50 dB
PL13      17.50 dB
SFO2      300.1312005 MHz

F2 - Processing parameters
SI        32768
SF        75.4677190 MHz
WDW        EM
SSB        0
LB         3.00 Hz
GB         0
PC         1.40

10 NMR list parameters
C1         20.00 cm
F1P        234.30 ppm
F1         37317.46 Hz
F2P        300.000 MHz
F2         300131200.5 Hz
P1PICK     12 21824 um/cg
HZCM       951.32566 Hz/7%
  
```



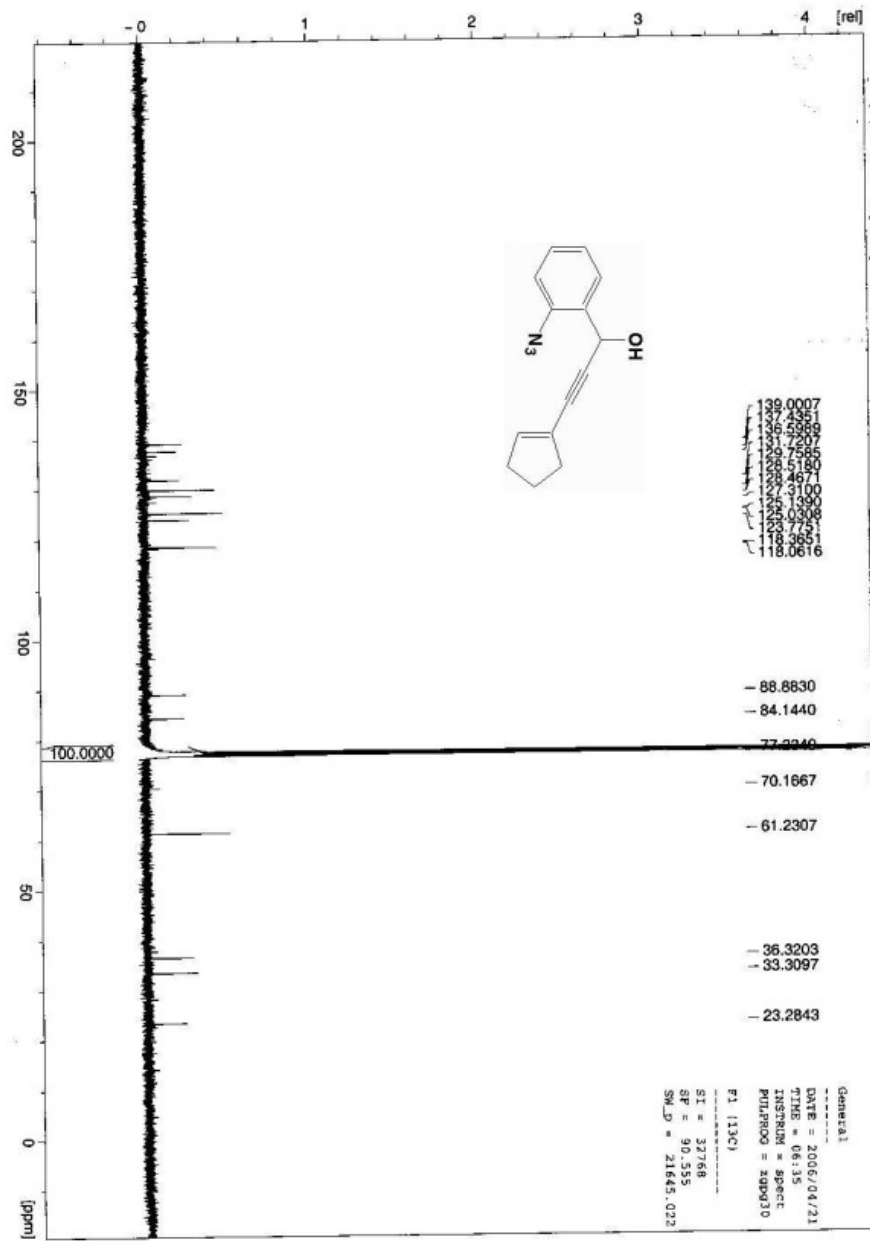
Current Data Parameters
 NAME NMR-Apr20-05
 EXPNO 6
 PROCNO 1

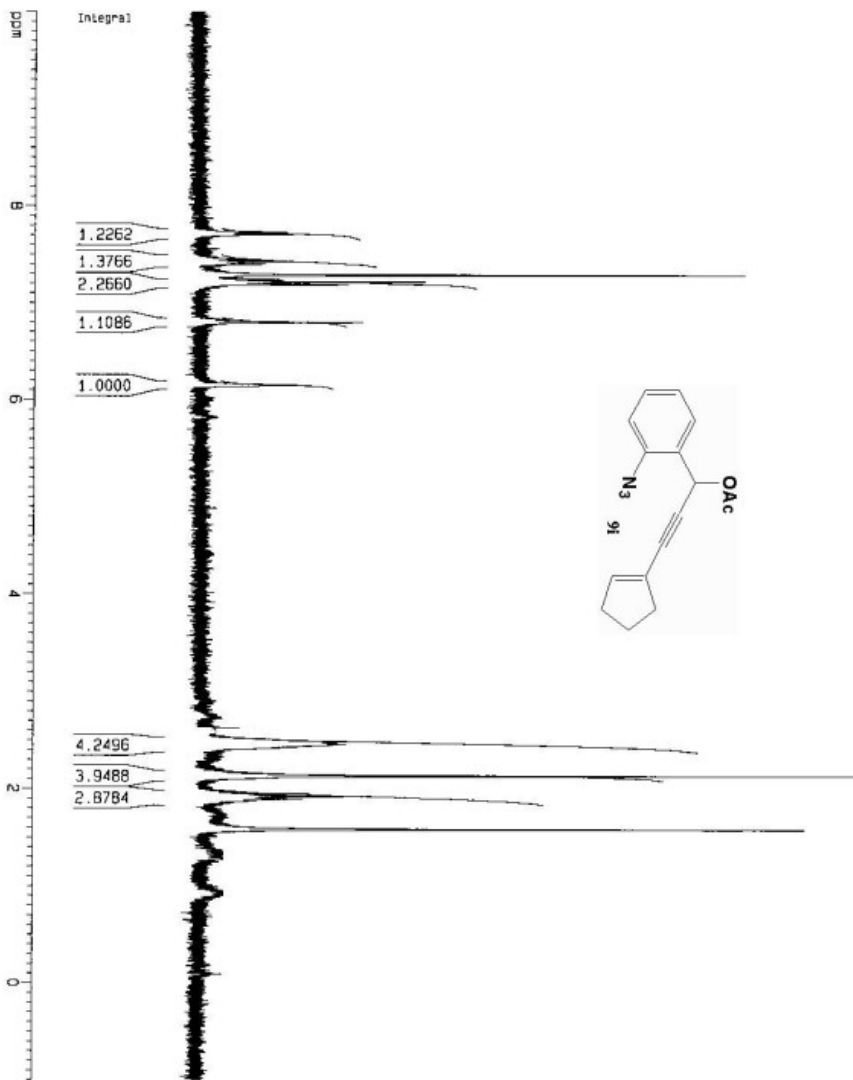
F2 - Acquisition Parameters
 Date_ 20050420
 Time 20:40
 INSTRUM spect
 PROBRD 5 mm BBI 1H-B
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9594243 sec
 RG 3281
 DM 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

***** CHANNEL f1 *****
 NUCL1 1H
 P1 6.45 usec
 PL1 0.00 dB
 SF01 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDM no
 SSB no
 LB 0.00 Hz
 GB 0
 PC 1.00

3D NMR plot parameters
 CX 20.00 cm
 F1P 10.000 ppm
 F1 4001.30 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPMCK 0.55000 ppm/cm
 HZCM 280.07150 Hz/cm





Current Data Parameters
 NAME M1-Apr21-06
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20060421
 Time 15.00
 INSTRUM spect
 PROGRAM 5 mm Multisnu
 PULPROG zg30
 TD 65536
 ID SOLVENT CDC13
 NS 16
 DS 2
 OS 6172.835 Hz
 SMH 0.094190 Hz
 FTDEFS 5.3084660 sec
 AQ 645.1
 RG 81.000 usec
 DW 5.00 usec
 DE 300.0 K
 TE 1.00000000 sec
 D1

***** CHANNEL f1 *****

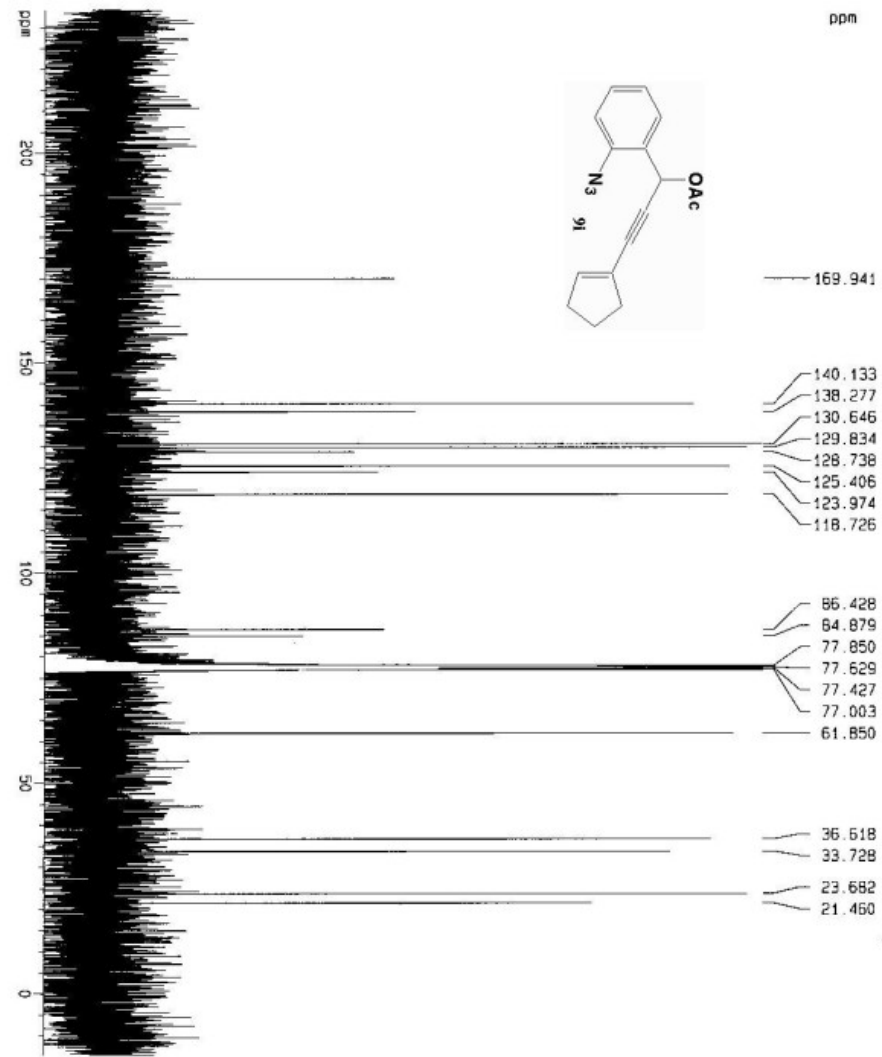
MUCL 1H
 P1 9.80 usec
 PL1 -6.00 dB
 SF01 300.1318534 MHz

F2 - Processing parameters

SF 32768
 SF 300.1300000 MHz
 NDM no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters

CX 80.00 cm
 F1P 10.000 ppm
 F1 3001.30 Hz
 F2P -1.000 ppm
 F2 -300.13 Hz
 PPMCM 0.55000 ppm/cm
 HQCM 165.07150 Hz/cm



```

Current Data Parameters
NAME      M1-4p-21-05
EXPNO    1
PROCNO   1

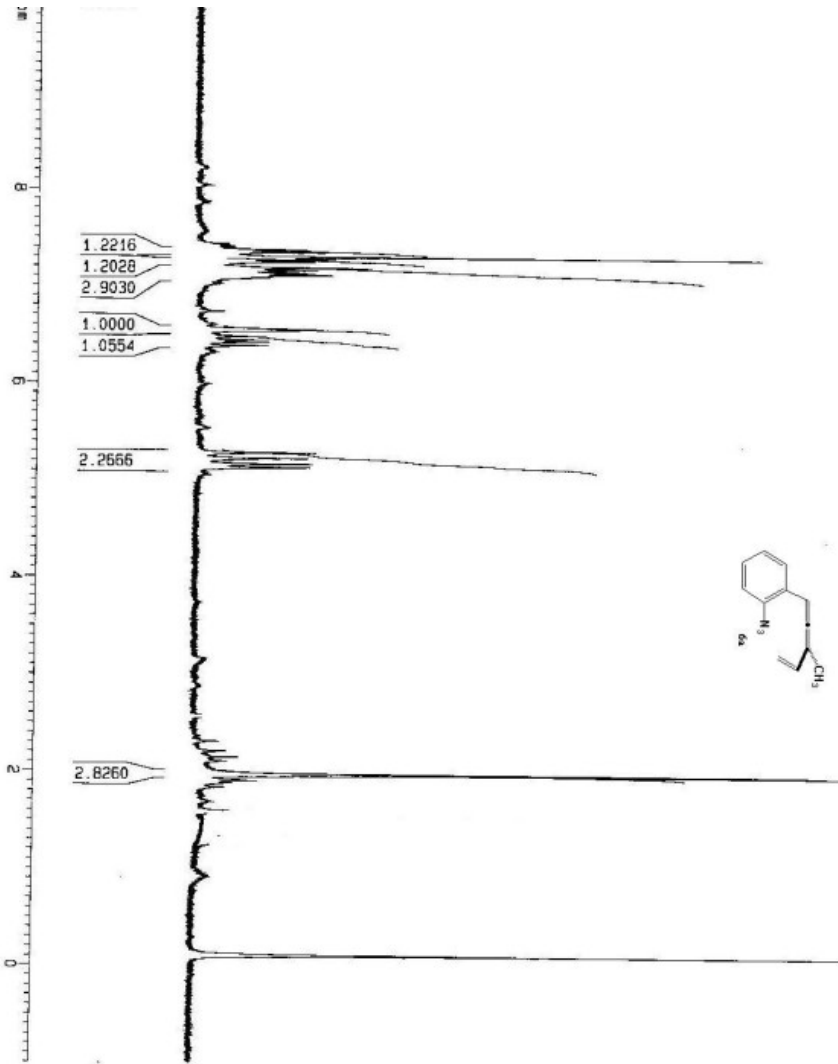
F2 - Acquisition Parameters
Date_    20080422
Time     9.28
INSTRUM  spect
PROBHD   5 mm QNP 1H/1
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        12000
DS        4
SMH       18798.882 Hz
FIDRES    0.288818 Hz
AQ         1.7433076 sec
RG         256
AQ         2.56
DE         28.500 uS/ac
TE         300.0 K
D1         2.00000000 sec
D12        0.03000000 sec
D12        0.00020000 sec

***** CHANNEL f1 *****
NUC1      13C
P1        13C
PC1       5.00 uS/ac
SFO1      75.4100517 MHz

***** CHANNEL f2 *****
CPDPRG2  MULLIS
NUC2      1H
P2        115.00 uS/ac
PC2       0.00 uS
R12       20.00 uS
R13       20.00 uS
SFO2      200.871995 MHz

F2 - Processing parameters
SI         32768
SF         75.4023410 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

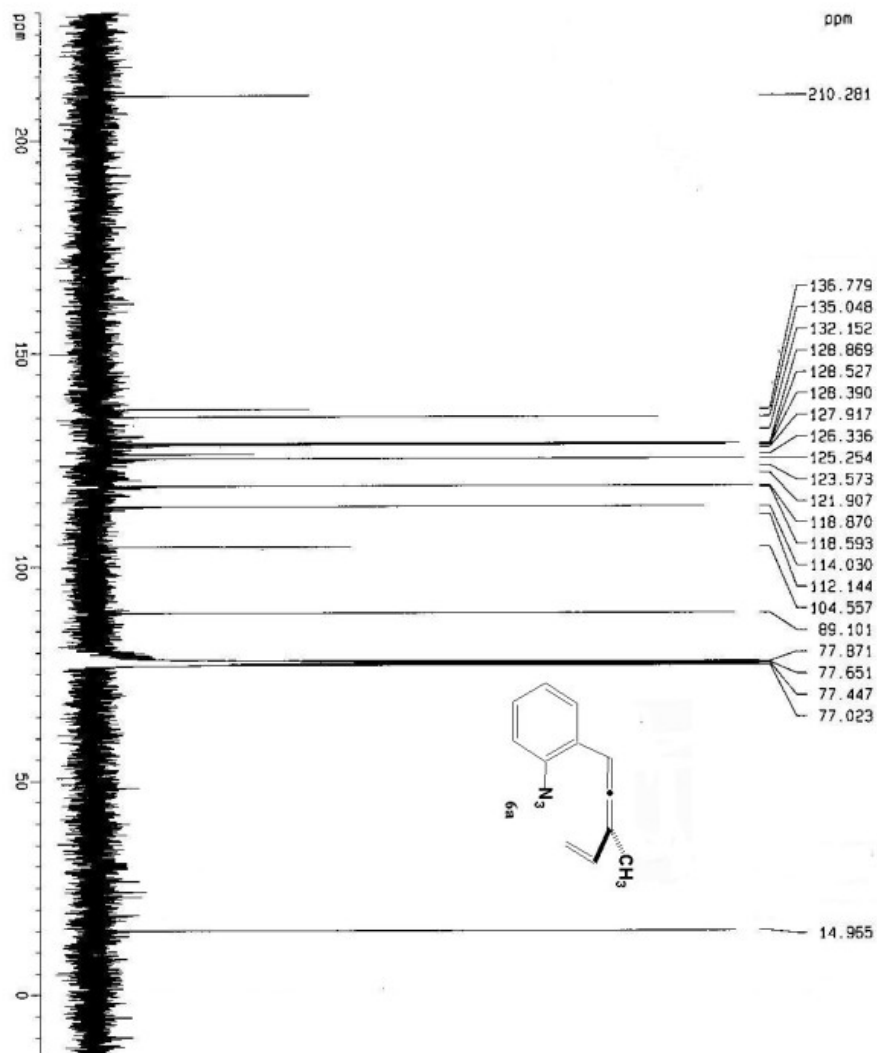
10 NMR data parameters
CX         20.00 cm
F1P        234.206 uS/n
F1         17693.55 Hz
F2P        -20.000 uS/n
F2         -1508.05 Hz
PWCW       12.71028 ppm/cm
HZCW       598.38477 Hz/cm
  
```



```

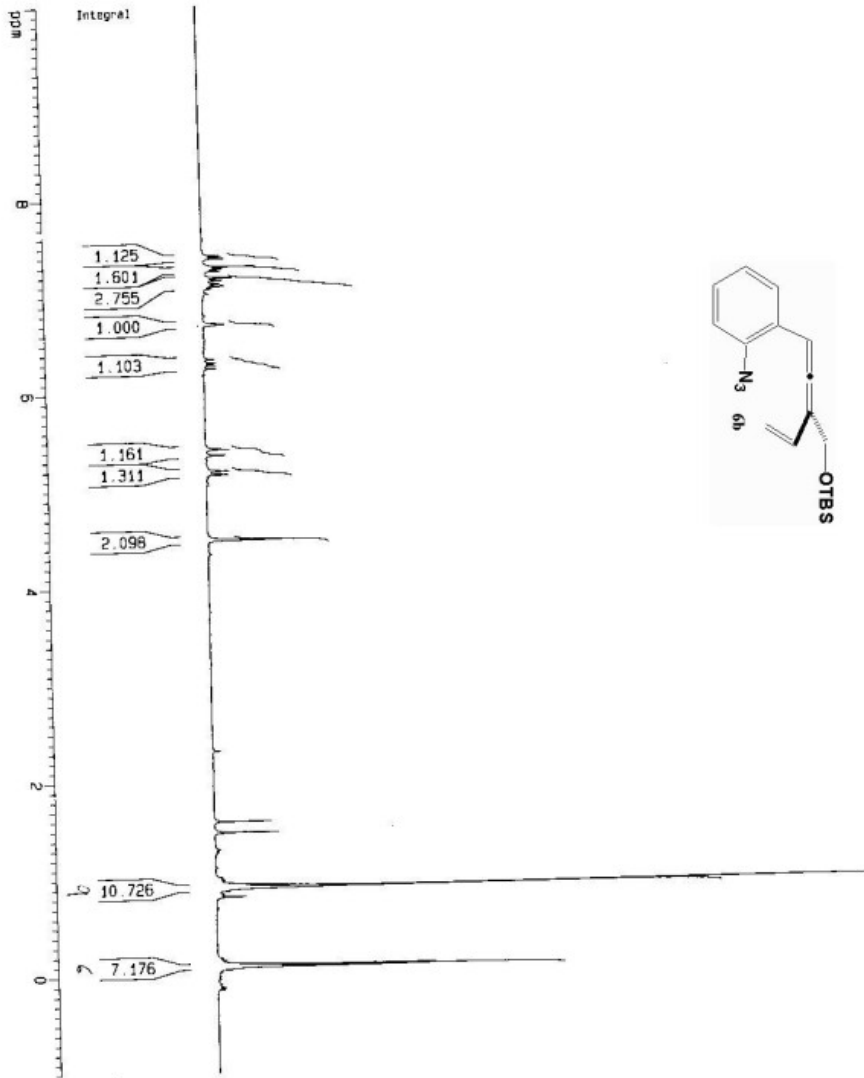
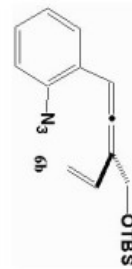
PROBHD 1
F2 - Acquisition Parameters
Date_ 20050308
Time 20.04
INSTNAM spect
PROBHD 5 mm DNP 1H/1
PULPROG zg30
TD 65536
SOLVENT DMS-D6
NS 11
DS 2
SWH 5172.899 Hz
FIDRES 0.054190 Hz
AQ 5.305459 sec
RG 812.7
DE 81.000 usec
TE 300.0 K
D1 1.00000000 sec
***** CHANNEL f1 *****
NUC1 1H
P1 11.70 usec
PL1 0.00 dB
SFO1 299.8716518 MHz
F2 - Processing parameters
SI 32768
SF 299.8700000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
FIP 10.000 ppm
F1 2998.70 Hz
F2 -1.000 ppm
PNUCH 0.55000 ppm/cm
HZCH 164.97650 MHz/cm

```

```

Current Data Parameters
NAME      MRI-MAR-06
EXPNO    7
PROCNO   1
-----
F2 - Acquisition Parameters
Date_    20050309
Time     6.07
INSTRUM  spect
PROBHD   5 mm QNP 1H/1
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        11500
DS        4
SWH       18396.992 Hz
FIDRES    0.166619 Hz
AQ         1.7453276 sec
RG         26
WDW        EM
SSB        0
GB         0
PC         300.0 K
TE         300.2 K
DE         5.00 usec
IE         2.00000000 sec
D11        0.03000000 sec
D12        0.00002000 sec
-----
***** CHANNEL f1 *****
NUC1      13C
P1         5.40 usec
PL1        -6.00 dB
SFO1      75.410657 MHz
-----
***** CHANNEL f2 *****
PROBHD2   MALT115
NUC2       1H
P2         115.00 usec
PL2         0.00 dB
SFO2      200.000000 MHz
-----
F2 - Processing parameters
SI         32768
SF         75.4023410 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
-----
1D NMR plot parameters
CK         20.00 cm
F1P        230.000 ppm
F1         173.94254 MHz
F2P        -260.000 ppm
F2         -1598.03 Hz
PFGMCH    12.50000 DPM/CM
SFC       32530 N/CM
  
```



Current Data Parameters
 NAME M01-02131-05
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20051031
 Time 14.05
 INSTRUM spect
 PROBRD 5 mm QNP 1H/1
 PULPROG zgpg
 TD 65535
 TO SOLVENT CDCl3
 NS 16
 DS 2
 SMH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 256
 DM 81.000 usec
 DE 5.00 usec
 TE 300.0 K
 TC 1.00000000 sec
 D1

***** CHANNEL f1 *****

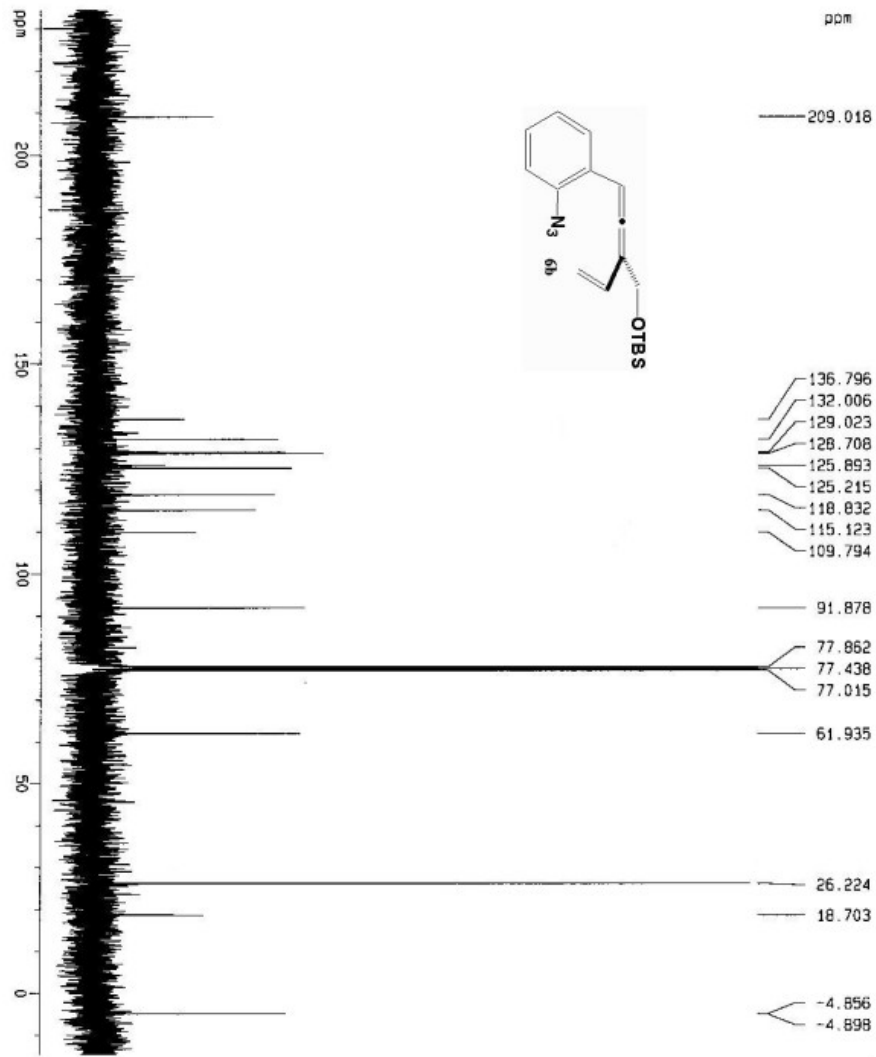
NUC1 1H
 P1 11.70 usec
 PL1 0.00 dB
 SFO1 299.9716918 MHz

F2 - Processing parameters

SI 32768
 SF 299.9700000 MHz
 WDM no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters:

CX 20.00 cm
 F1e 10.000 ppm
 F1 2998.70 Hz
 F2p -1.000 ppm
 F2 -299.87 Hz
 PPMCM 0.35000 ppm/cm
 NZCM 164.92850 Hz/cm



```

Current Data Parameters
NAME      MW1-DC131-05
EXPNO    2
PROCNO   1

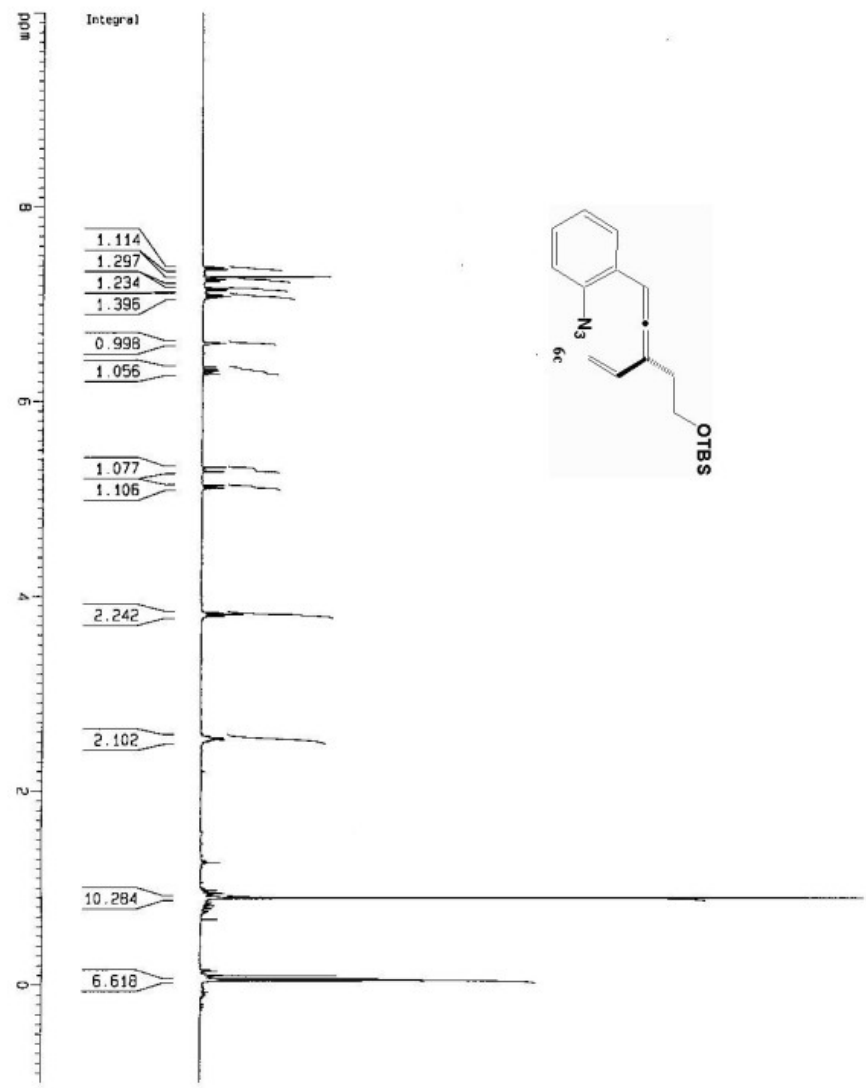
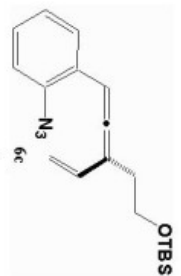
F2 - Acquisition Parameters
Date_    20051031
Time     14.20
INSTRUM  spect
PROBHD   5 mm DNP HV/1
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        209
DS        4
SWH       18796.952 Hz
FIDRES   0.768819 Hz
AQ        1.743076 sec
RG         256
DM         28.600 uS/ac
DE         6.00 uS/ac
TE        300.0 K
O1        2.00000000 sec
O2        0.03000000 sec
O3        0.00000000 sec
O4        0.00000000 sec

***** CHANNEL f1 *****
NUC1      13C
P1        5.00 uS/ac
PC1       8.00 dB
SFO1      75.410657 MHz

***** CHANNEL f2 *****
CPROG2    waltz16
NUC2       1H
P2        115.00 uS/ac
PC2       0.00 dB
R12       20.00 dB
R13       20.00 dB
SFO2      283.871985 MHz

F2 - Processing parameters
SI         32768
SF         75.4023410 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

10 NMR 01ct parameters
CX         20.00 cm
FLP        234.661 ppm
F1         17683.24 Hz
F2P        -20.000 ppm
F2         -1508.05 Hz
P1RCM     12.73255 ppm/cm
HZCM      960.08461 Hz/cm
  
```



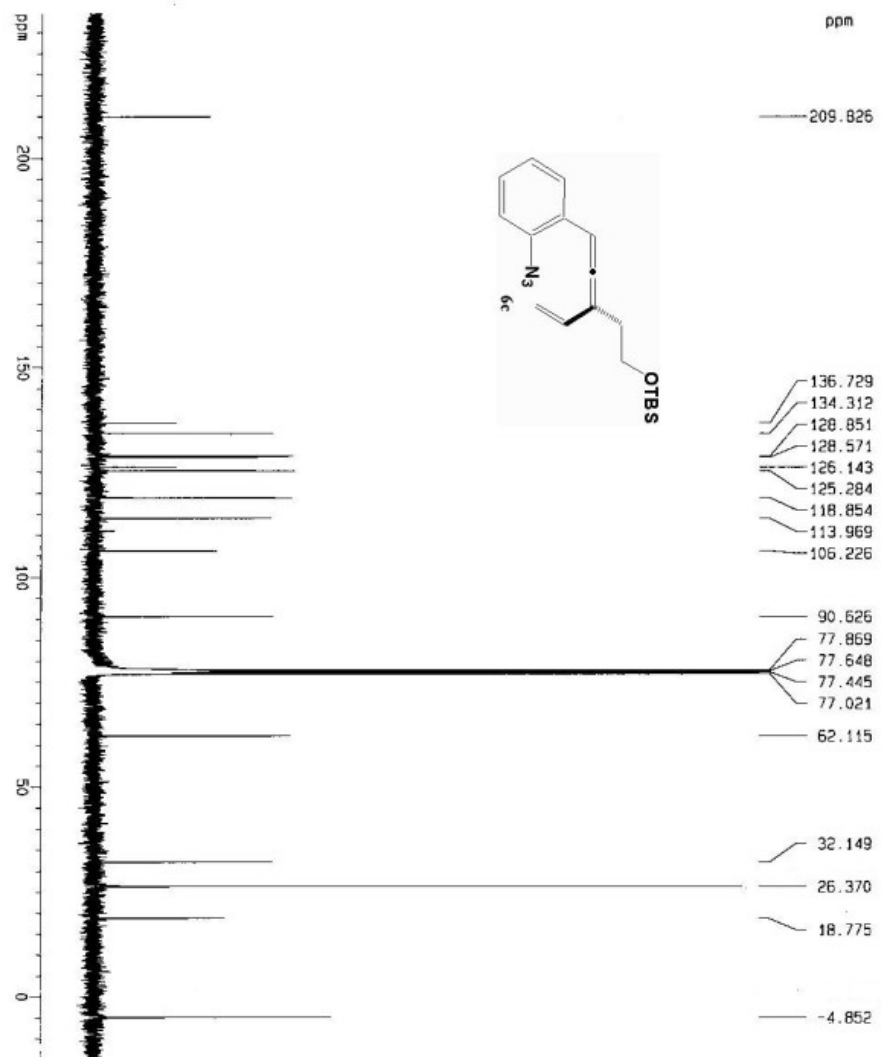
Current Data Parameters
 NAME N1-0127-05
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051027
 Time 9.43
 INSTRUM spect
 PULPROG 5 mm BBI 1H-B
 TD 4330
 FIDRES 0.5536
 SOLVENT DMS-D6
 NS 16
 DS 2
 SWH 8275.145 Hz
 F1RES 0.126314 Hz
 AQ 3.9584243 sec
 RG 574.7
 DW 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 6.45 usec
 PL1 0.00 dB
 SFO1 400.1264710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1000000 MHz
 KW 0
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

10 MHz plot parameters
 CX 20.00 cm
 FIP 10.000 ppm
 F1 4001.30 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 FREQM 0.55000 ppm/cm
 FZDM 220.07150 Hz/cm



Current Data Parameters

NAME	MT-NOV02-05
EXPNO	4
PROCNO	1

F2 - Acquisition Parameters

Date_	20051103
Time	8.12
INSTRUM	spect
PROBHD	5 mm QNP 1H/1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	11000
DS	4
SWH	18796.982 Hz
FIDRES	0.268819 Hz
AQ	1.7433276 sec
RG	1024
DM	26.600 usec
DE	18.000 usec
TE	300.2 K
D1	3.0000000 sec
D11	0.0300000 sec
D12	0.0000000 sec

***** CHANNEL f1 *****

NUC1	13C
P1	5.40 usec
PL1	-6.00 dB
SFO1	75.418337 MHz

***** CHANNEL f2 *****

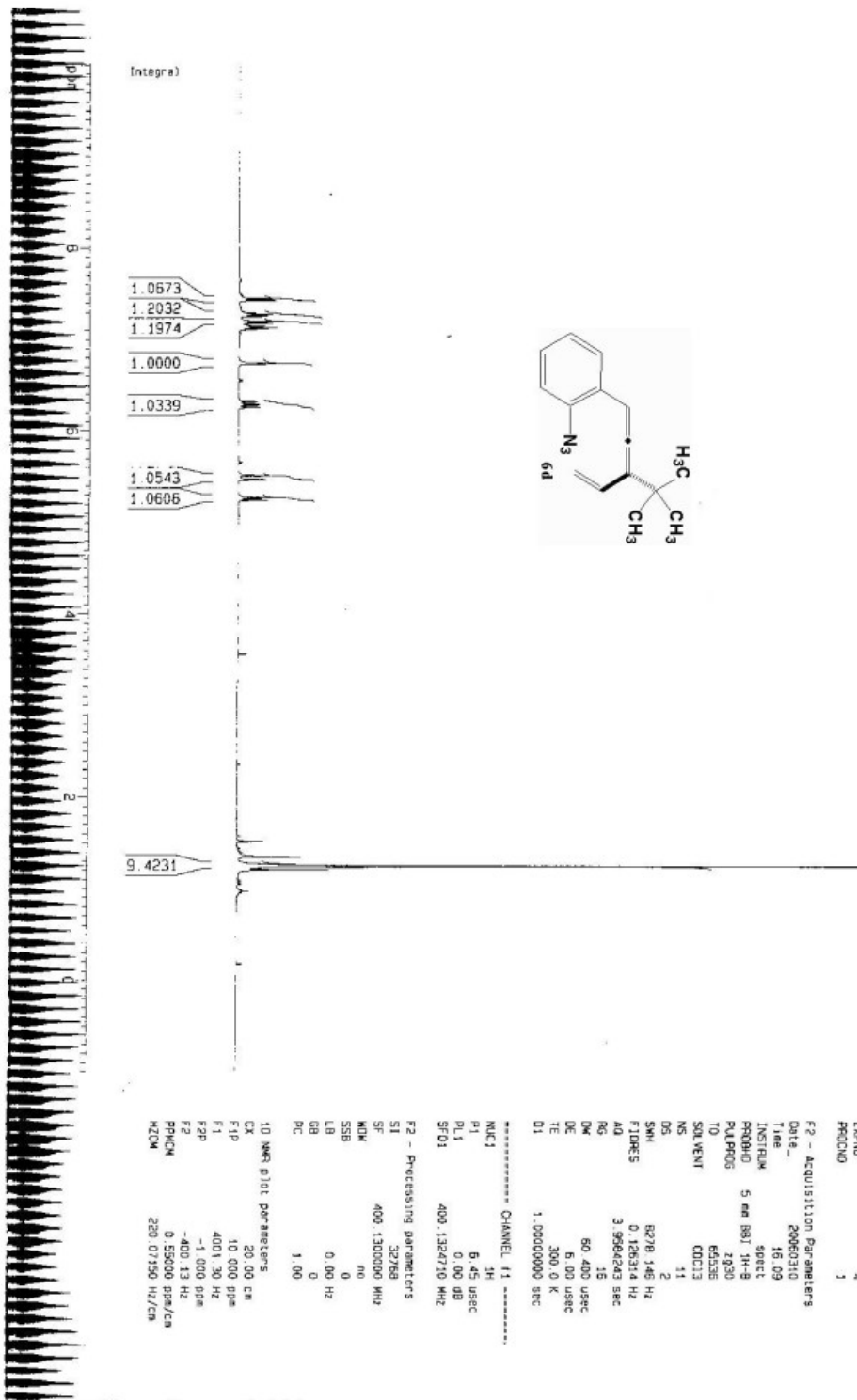
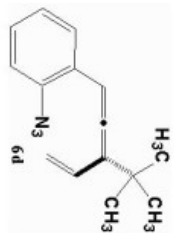
CROSSP2	WALTZ16
NUC2	1H
PCPD2	115.00 usec
PL2	0.00 dB
PL12	20.00 dB
PL13	20.00 dB
SFO2	298.871795 MHz

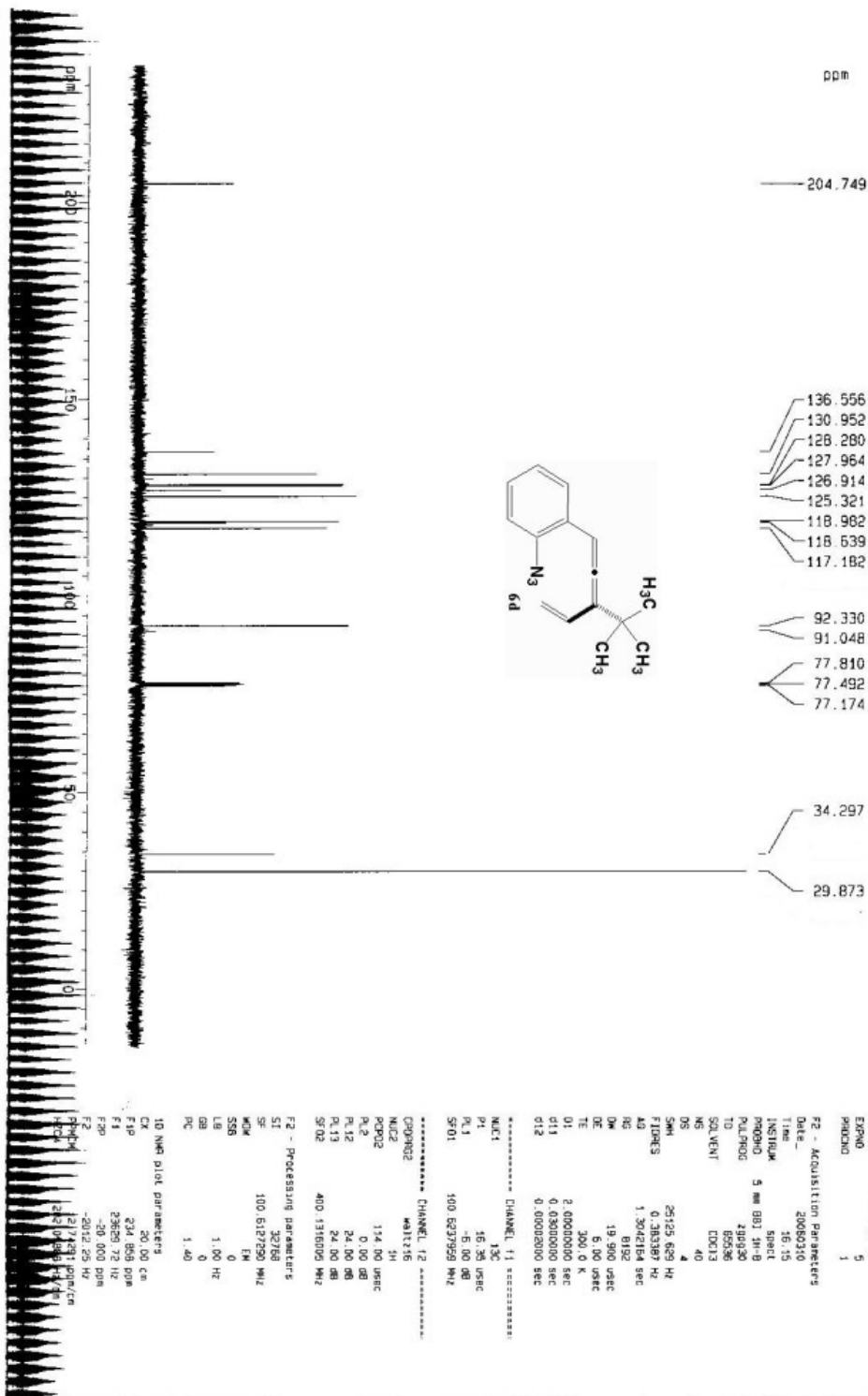
F2 - Processing parameters

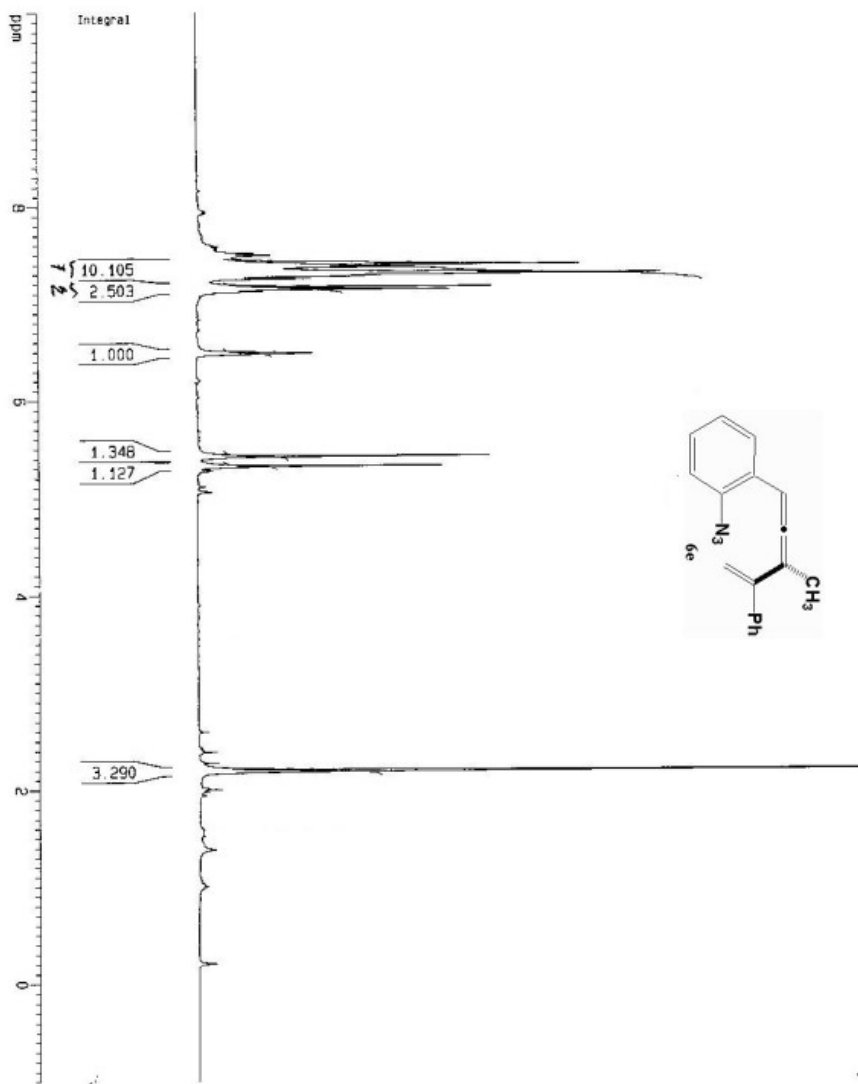
SF	327766
WF	75.4023410 MHz
MEM	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

10 MHz plot parameters

CX	20.00 cm
FIP	234.631 ppm
F1	17933.24 Hz
F2	-50.000 ppm
PRINCM	-1508.05 Hz
PRINCM	12.74250 ppm/cm
HZCM	950.08440 Hz/cm







Current Data Parameters
 Name: M81-DEC30-05
 ExpNO: 2
 PROCNO: 1

F2 - Acquisition Parameters

Date_: 20051230
 Time: 17.46
 INSTRUM: spect
 PROBDW: 5 mm QNP 1H/1
 PULPROG: zgpg30
 TD: 65536
 SOLVENT: CDCl3
 NS: 9
 DS: 2
 SWH: 8172.839 Hz
 FIDRES: 0.094190 Hz
 AQ: 5.208460 sec
 RG: 50.5
 DM: 81.000 usec
 DE: 6.00 usec
 TE: 300.2 K
 D1: 1.00000000 sec

CHANNEL f1

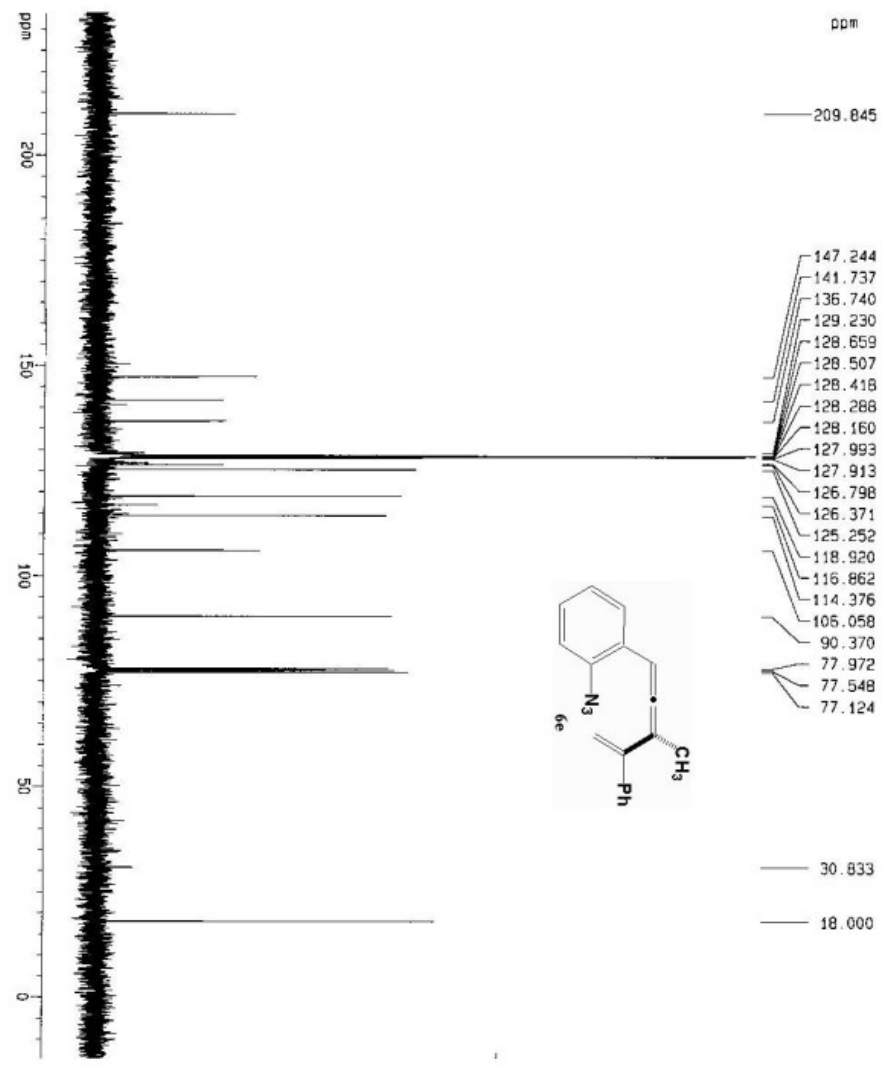
NUC1: 1H
 P1: 11.70 usec
 PL1: 0.00 dB
 SF01: 299.8718018 MHz

F2 - Processing parameters

SF: 32766
 FIDRES: 0.094190 Hz
 KOP: 0
 SSB: 0
 LB: 0.00 Hz
 GB: 0
 PC: 1.00

1D NMR F101 parameters

CX: 20.00 cm
 F1P: 10.000 ppm
 F1: 299.870 Hz
 F2P: -1.000 ppm
 F2: -299.87 Hz
 PPM/CM: 0.35000 ppm/cm
 HZ/CM: 164.32850 Hz/cm



```

Current Data Parameters
NAME      H4176230-05
EXPNO    2
PROCNO   1

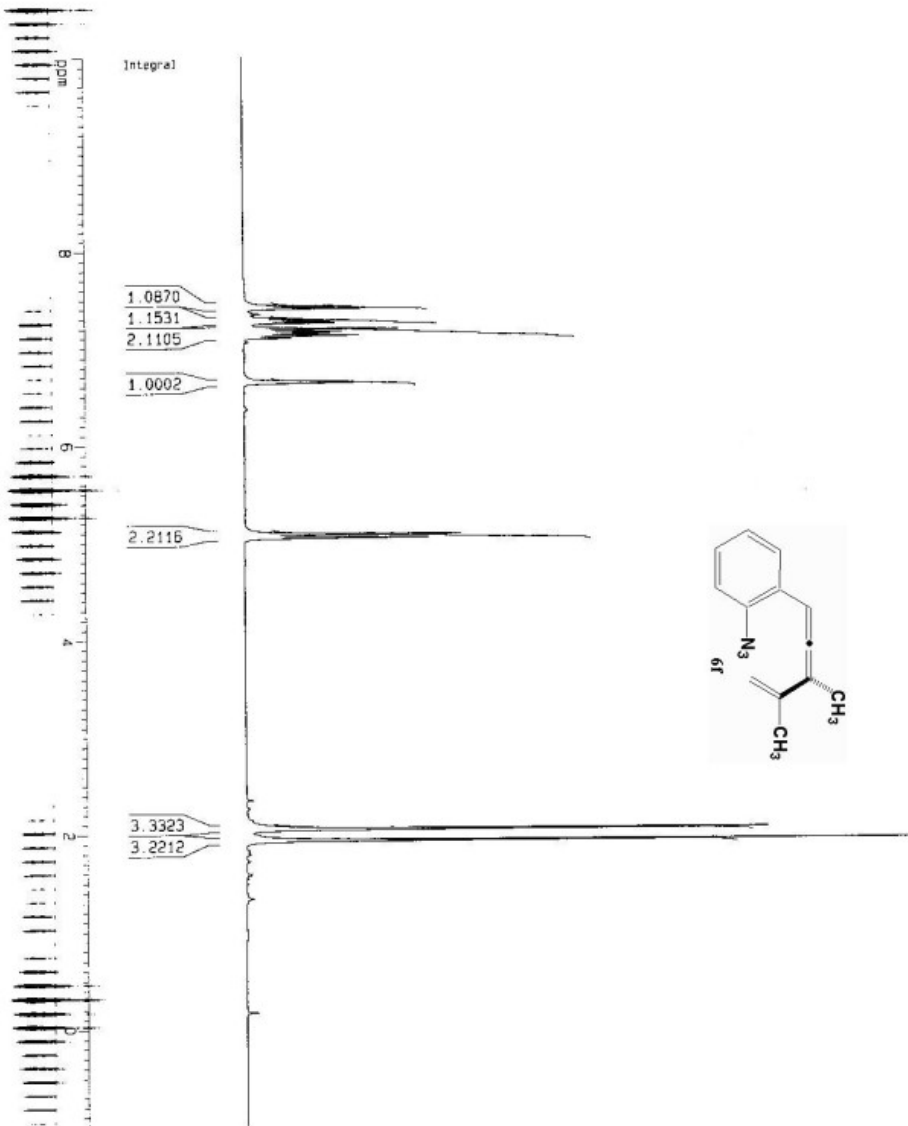
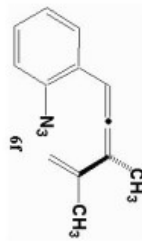
F2 - Acquisition Parameters
Date_    20051230
Time     17.52
INSTRUM  spect
PROBHD   5 mm QNP 1H/1
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        28
DS        4
SWH       16795.992 Hz
FIDRES    0.286819 Hz
AQ         1.7433075 sec
RG         1024
DE         26.800 usec
TE         300.0 K
D1         2.00000000 sec
D11        0.03600000 sec
D12        0.00020000 sec

***** CHANNEL f1 *****
NUC1       13C
P1         5.40 usec
PL1        -6.00 dB
SFO1       75.4706377 MHz

***** CHANNEL f2 *****
CPDPRG2   waltz16
NUC2       1H
PCPD2     115.00 usec
PL2        0.00 dB
PL12       20.00 dB
PL13       20.00 dB
SFO2       299.871592 MHz

F2 - Processing parameters
SI         32768
SF         75.4632410 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

1D NMR plot parameters
CX         20.00 cm
F1P        234.000 ppm
F1         17644.55 Hz
F2P        -20.000 ppm
F2         -1508.05 Hz
PULPROG    12.70000 usec/cm
NUC1       957.60874 Hz/cm
NUC2
  
```



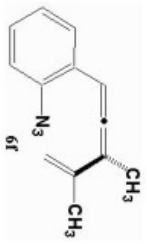
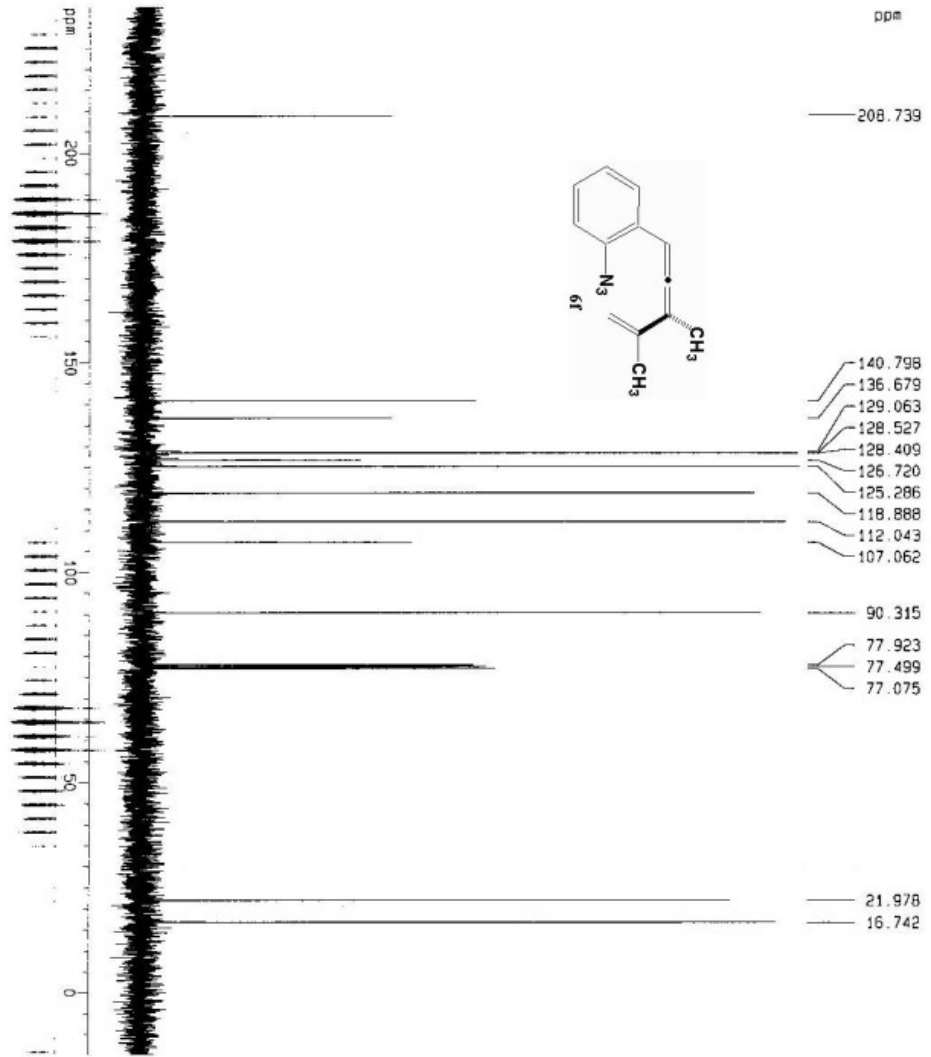
Current Data Parameters
 NAME MFL-JAN10-05
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060110
 Time 17:25
 INSTRUM spect
 PROBNM 5 mm WJ11nu
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 2
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084650 sec
 RG 90.5
 DM 91.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 9.60 usec
 PL1 -6.00 dB
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300000 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 10.000 ppm
 F1 3001.30 Hz
 F2P -1.000 ppm
 F2 -300.13 Hz
 PPGCM 0.95000 ppm/cm
 HZCM 165.07150 Hz/cm



- 140.798
- 136.679
- 129.063
- 128.527
- 128.409
- 126.720
- 125.286
- 118.888
- 112.043
- 107.062

- 90.315
- 77.923
- 77.499
- 77.075

- 21.978
- 16.742

```

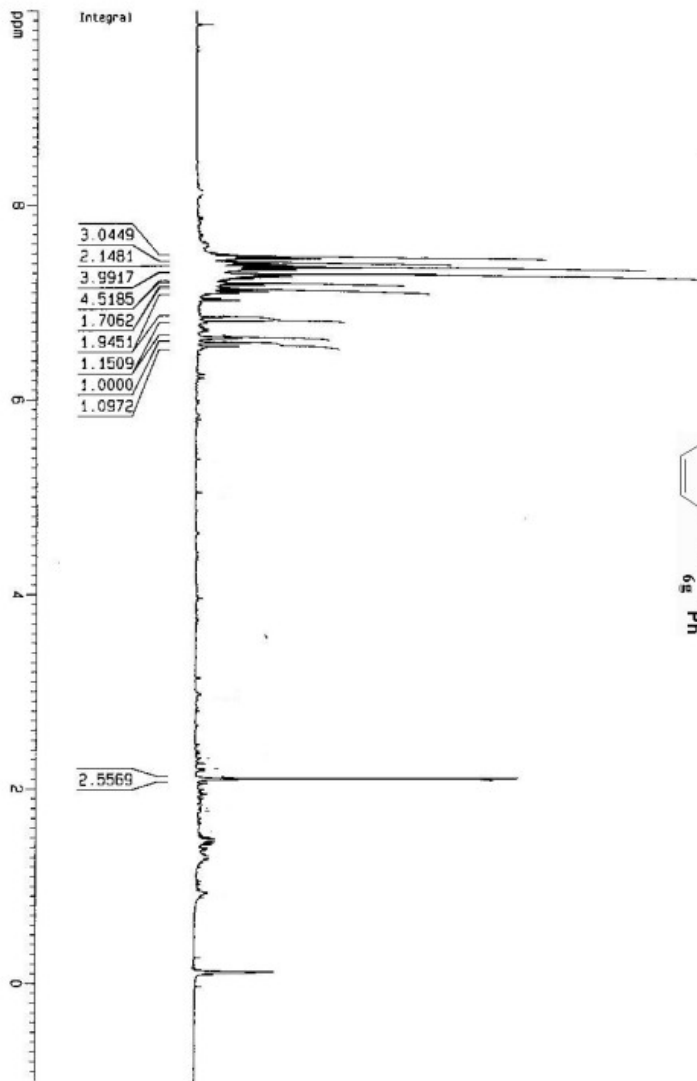
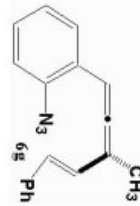
Current Data Parameters
NAME          M01-Jan10-05
EXPNO        2
PROCNO       1
Date_         20060110
Time         17.32
INSTRUM      spect
PROBHD       5 mm H-130
PULPROG      zgpg30
TD            65536
SOLVENT      CDCl3
NS            36
DS            4
SWH           18632.303 Hz
FIDRES        0.287360 Hz
AQ            1.7400308 sec
RG            16384
DE            26.550 usec
TE            300.0 K
D1            2.00000000 sec
d11           0.03000000 sec
d12           0.00020000 sec

***** CHANNEL f1 *****
NAC1          13C
P1            11.80 usec
PA.1          0.00 dB
SFO1          75.4760200 MHz

***** CHANNEL f2 *****
CPDPRG2      waltz16
NUC2          1H
PCPD2        110.00 usec
PL2           0.00 dB
PL12         17.50 dB
PL13         17.50 dB
SFO2         300.1312000 MHz

F2 - Processing parameters
SI            32768
SF            75.4671950 MHz
SM            EM
SOLVENT       CDCl3
GB            1.00 Hz
GB            0
PC            1.40

1D NMR plot 6f-deriv13
CX            20.00 cm
F1P           234.760 ppm
F1            17717.18 Hz
F2P           -20.000 ppm
F2            11808.35 Hz
PRINXM       127.8834 ppm/cm
          581.2555 MHz/cm
  
```



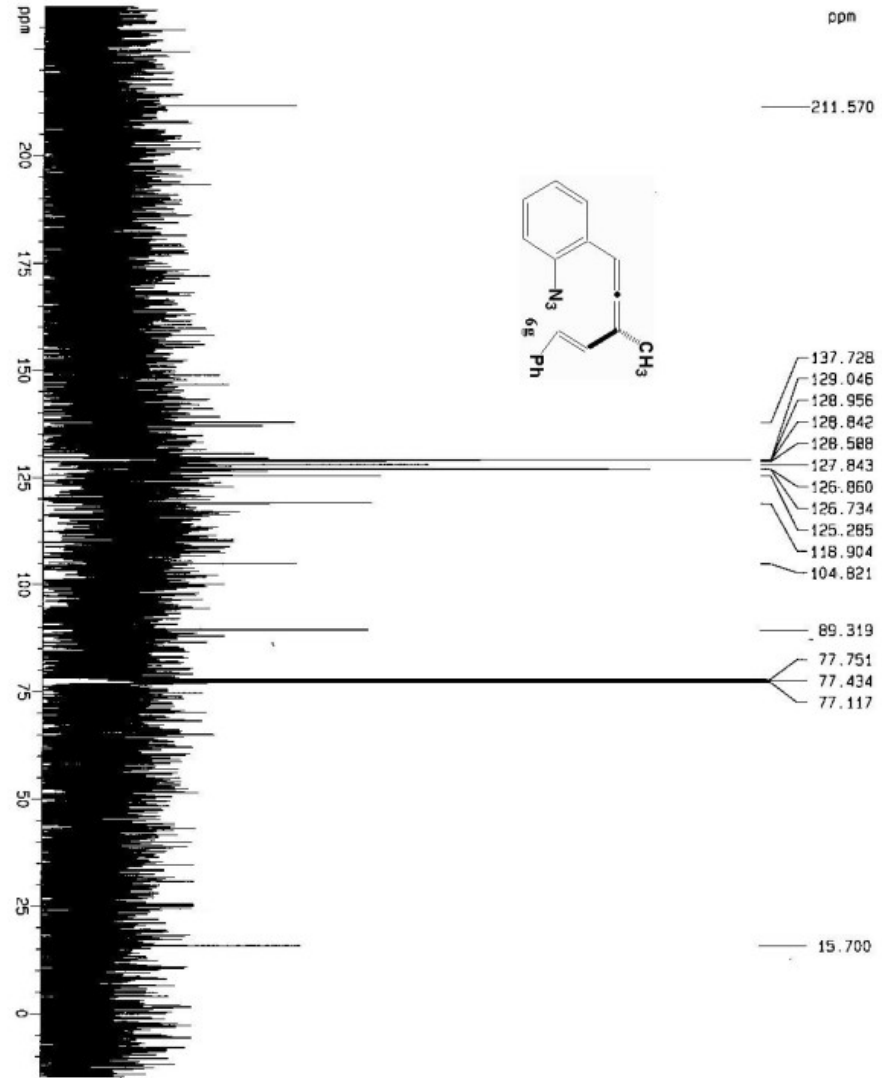
Current Data Parameters
 NAME H61-0127-05
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051027
 Time 9:12
 INSTRUM spect
 PROBHD 5 mm BBI 1H-5
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 9
 DS 2
 SWH 8278.145 Hz
 FIDRES 0.126314 Hz
 AQ 3.984243 sec
 RG 228.1
 DW 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 6.45 usec
 PL1 0.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 KHz
 WDW nc
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

10 MHz plot parameters
 CX 20.00 cm
 F1P 10.000 ppm
 F1 4001.30 Hz
 F2P -1.000 ppm
 F2 -40.13 Hz
 PRICK 0.55000 ppm/cm
 RFLW 220.07150 Hz/cm



```

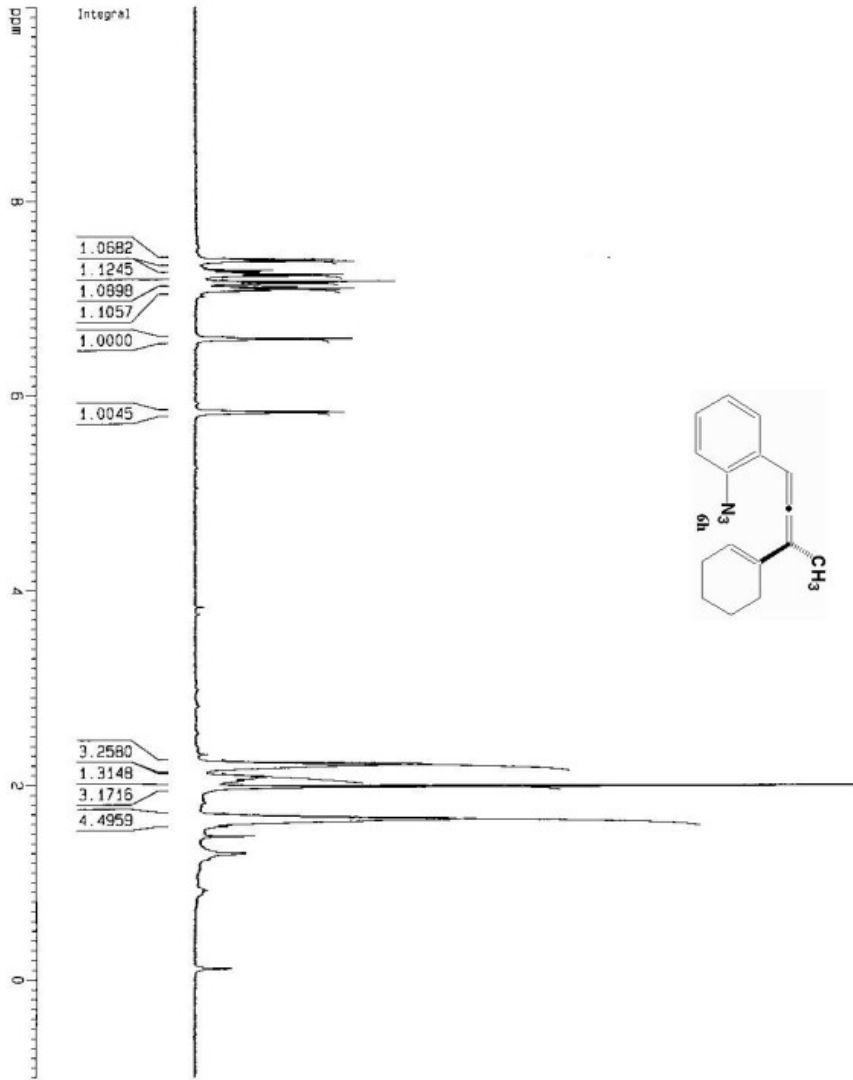
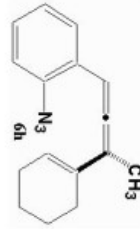
Current Data Parameters
NAME          M41-001271-05
EXPNO        2
PROCNO       1
F2 - Acquisition Parameters
Date_         20051027
Time          9.30
INSTRUM      spect
PROBHD       5 mm BBI 1H-8
PULPROG      zgpg30
TD           65536
SOLVENT      CDCl3
NS           311
DS           4
SWH          25125.629 Hz
FIDRES       0.36337 Hz
AQ           1.3042154 sec
RG           15384
DM           19.900 usec
DE           5.00 usec
TE           300.0 K
D1           2.00000000 sec
d12          0.03000000 sec
d122         0.00000000 sec

***** CHANNEL f1 *****
NUC1         13C
P1           15.35 usec
PL1         -5.00 dB
SFO1        100.6237959 MHz

***** CHANNEL f2 *****
CPDPRG2     MSL212B
NUC2         13C
PCPD2       114.00 usec
PL2         0.00 dB
PL12        24.00 dB
PL13        24.00 dB
SFO2        400.1315002 MHz

F2 - Processing parameters
SI           32768
SF           100.6127290 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40

ID NAME PLOT parameters.
CX          20.00 cm
F1p         234.685 ppm
F1          20629.72 Hz
F2p         -14.969 ppm
F2          -1495.51 Hz
PROMCHK     12.48531 muA/cm
HZDM        1265.28137 Hz/cm
  
```



Current Data Parameters
 NAME: M01-DEC05-05
 EXPNO: 1
 PROCNO: 1

F2 - Acquisition Parameters

Date_: 20051206
 Time: 9.27
 INSTRUM: spect
 PROBR0: 5 mm BBI 1H-8
 PULPROG: zgpg30
 TD: 65536
 SOLVENT: DMS-D6
 NS: 16
 DS: 2
 SWH: 8270.146 Hz
 FIDRES: 0.126314 Hz
 AQ: 3.3984243 sec
 RG: 645.1
 DE: 60.400 usec
 DM: 6.00 usec
 TE: 300.0 K
 D1: 1.00000000 sec

***** CHANNEL f1 *****

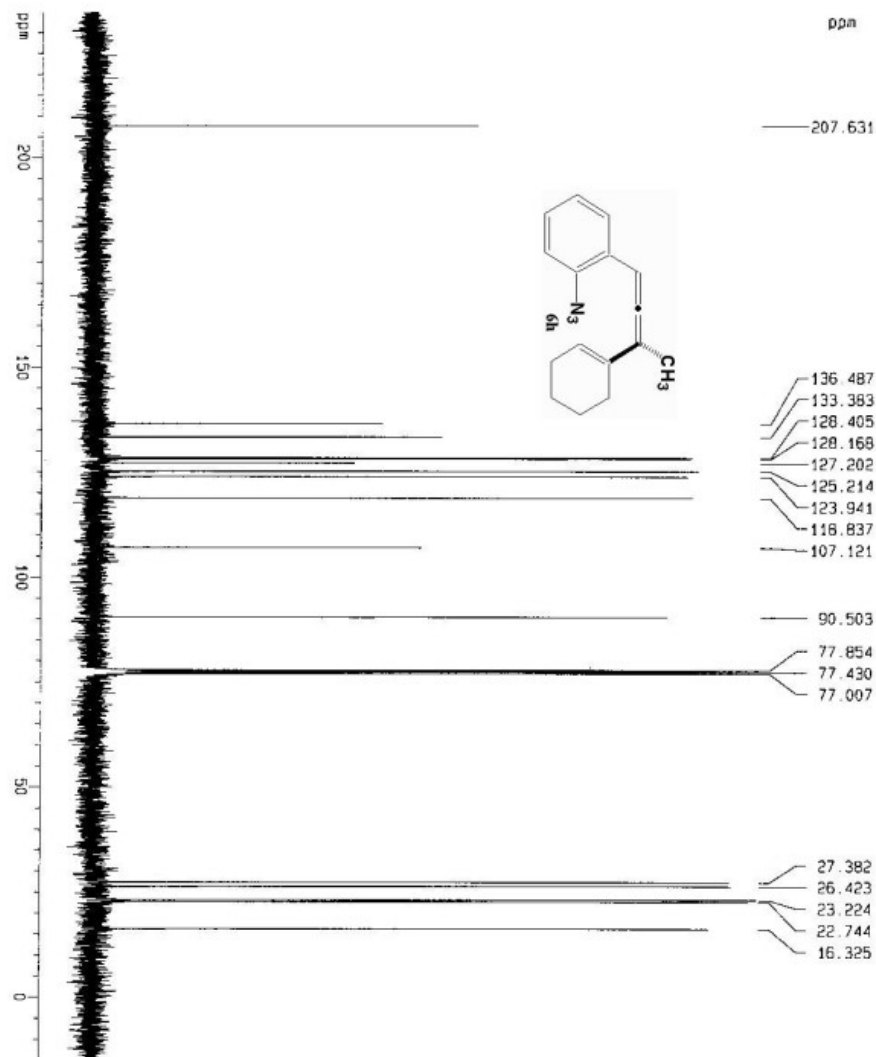
NUC1: 1H
 P1: 5.45 usec
 PA: 0.00 dB
 SF01: 400.1324710 MHz

F2 - Processing Parameters

SI: 32768
 SF: 400.1300000 MHz
 MDW: no
 SSB: 0
 LB: 0.00 Hz
 GB: 0
 PC: 1.00

1D NMR plot parameters

CX: 20.00 cm
 F1P: 10.000 dB
 F1: 4001.30 Hz
 F2P: -1.000 dBm
 F2: -400.13 Hz
 FREQH: 0.550000 ppm/cw
 HZDK: 220.07150 Hz/cm



```

Current Data Parameters
Name      M1-09c04-05
EXPNO    2
PROCNO   1

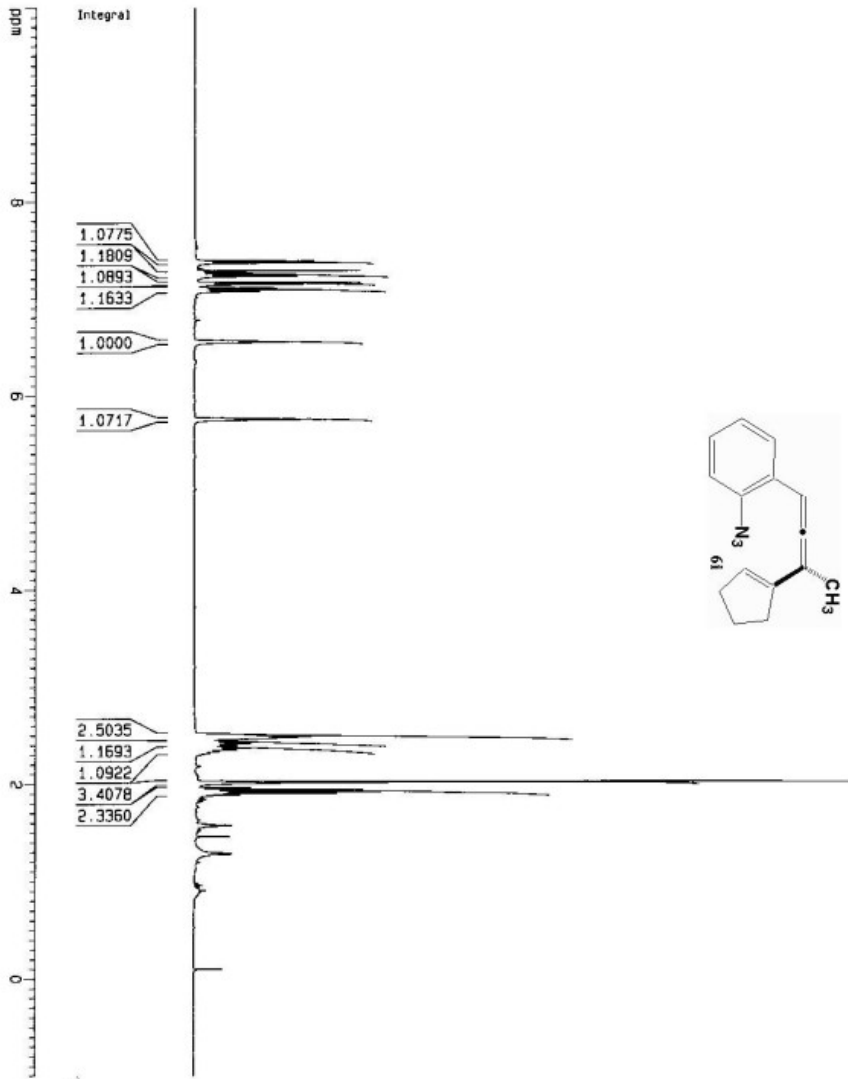
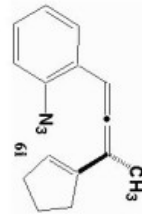
F2 - Acquisition Parameters
Date_    20071208
Time     19:10
INSTRUM  spect
PROBHD   5 mm WALTZ
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       2000
DS       4
SWH      16833.363 Hz
FIDRES   0.297360 Hz
AQ       1.7400368 sec
RG       8192
DM       25.550 usec
DE       5.00 usec
TE       300.0 K
D1       2.00000000 sec
d12      0.03000000 sec
D12      0.00020000 sec

***** CHANNEL f1 *****
NUC1      13C
P1       11.80 usec
PL1      0.00 dB
SFO1     75.4762000 MHz

***** CHANNEL f2 *****
CPDPRG2  waltz16
NUC2      1H
PCPDPR2  110.00 usec
PL2       0.00 dB
PL12     17.50 dB
PL13     17.50 dB
SFO2     300.1312005 MHz

F2 - Processing parameters
SI       32768
SF       75.4677150 MHz
RG       65536
AQ       1.00 Hz
AS       0
PC       1.40

ID - NMR plot parameters
CX       30.00 cm
C1P      234.755 ppm
F1       12717.56 Hz
F2P      -20.000 ppm
PCMKCH  12.73823 ppm/c
HZCM     561.32550 Hz/cm
  
```



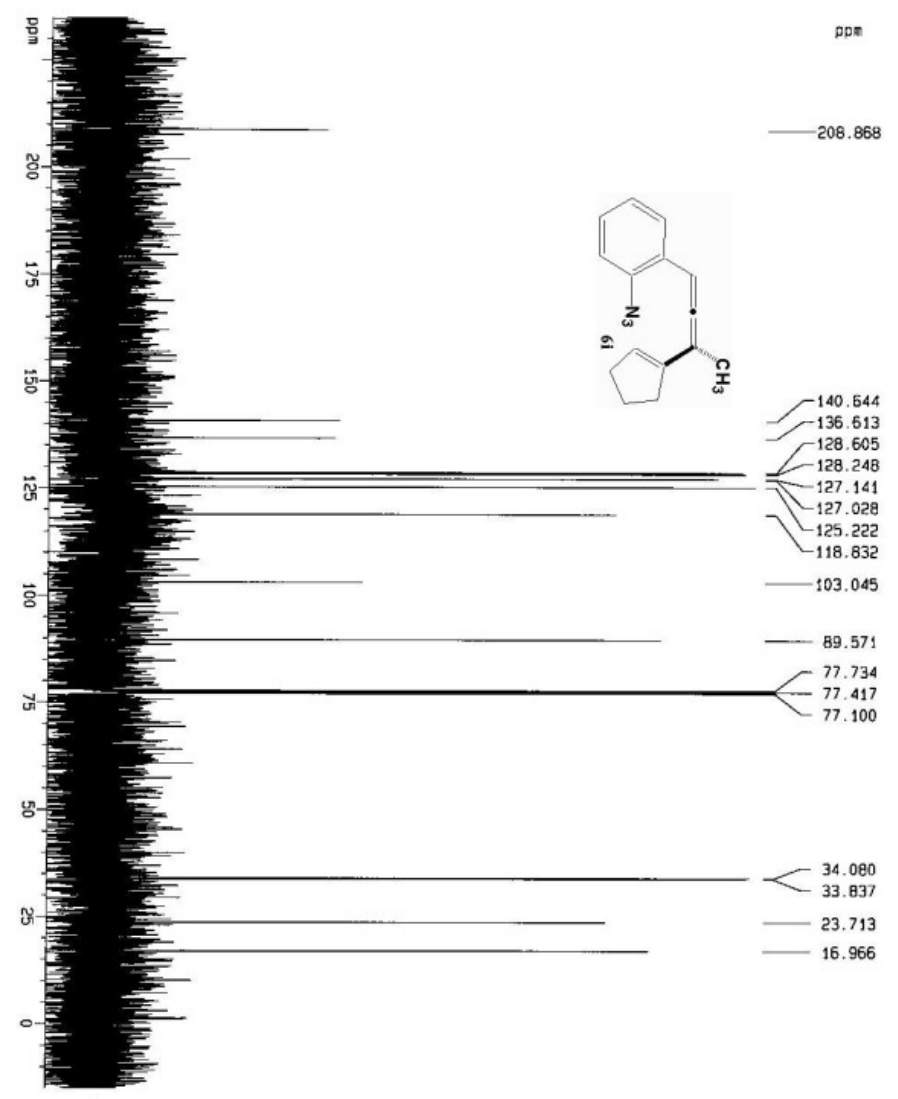
Current Data Parameters
 NAME nfi-jun25-05
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050528
 Time 13.31
 INSTRUM spect
 PROBRD 5 mm BBI 1H-B
 PULPROG zg30
 TD 65536
 TO SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.5084243 sec
 RG 143.7
 DM 80.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.000000000 sec

----- CHANNEL f1 -----
 NUC1 1H
 P1 6.45 usec
 PL1 0.00 dB
 SFO1 400.1324710 MHz

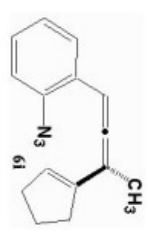
F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

10 NMR plot parameters
 CX 20.00 cm
 FIP 10.000 gpm
 F1 4001.30 Hz
 F2 -1.000 gpm
 -ADD 13 Hz
 PRPCK 0.55000 ppm/cm
 HZCM 220.07150 Hz/cm



ppm

- 208.868
- 140.544
- 136.613
- 128.605
- 128.248
- 127.141
- 127.028
- 125.222
- 118.832
- 103.045
- 89.571
- 77.734
- 77.417
- 77.100
- 34.080
- 33.837
- 23.713
- 16.966



```

Current Data Parameters
NAME      W1-jun28-05
EXPNO    2
PROCNO   1

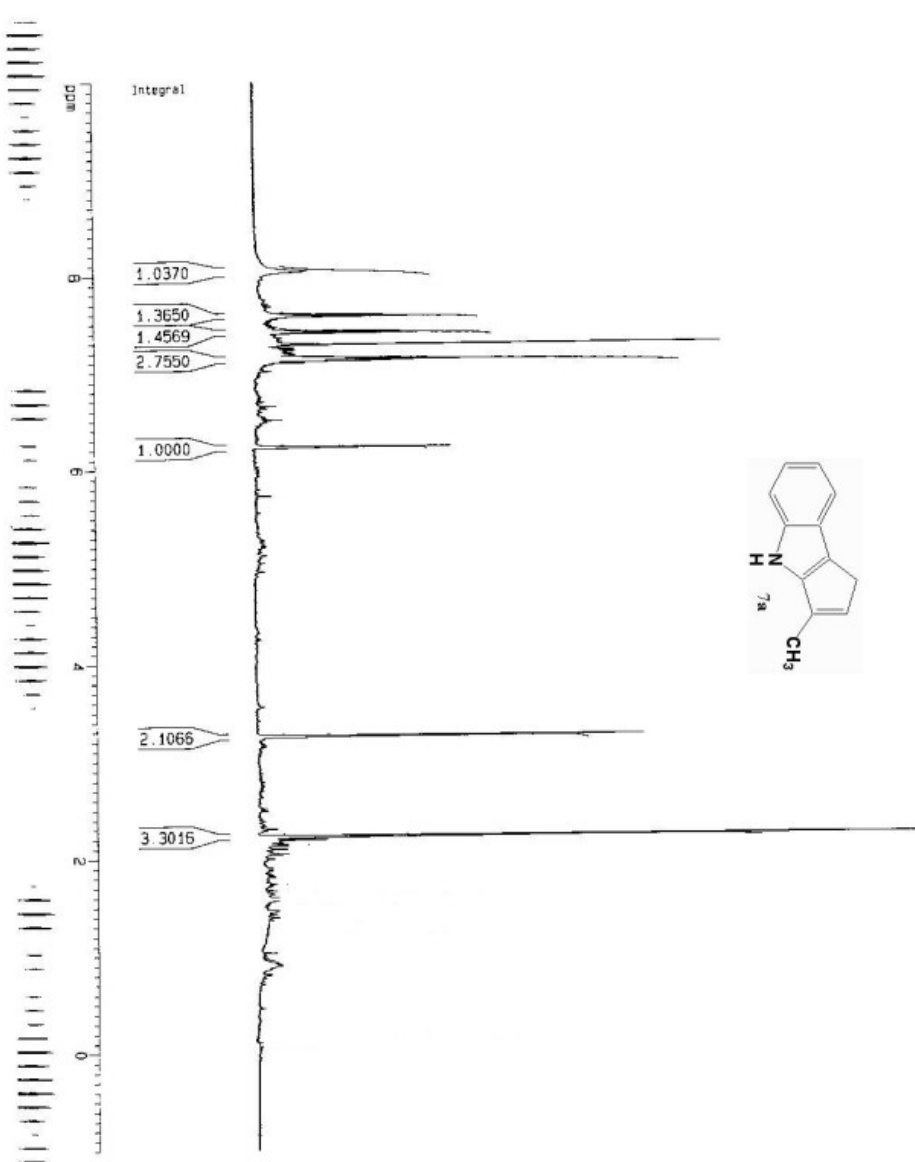
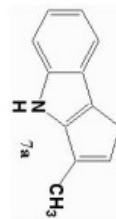
F2 - Acquisition Parameters
Date_     20050528
Time      13.45
INSTRUM   spect
PROBHD    5 mm BBI 1H-1
PULPROG   zgpg30
TD         65536
SOLVENT   DMS-d6
NS         513
DS         4
SWH        26126.629 Hz
FIDRES    0.58297 Hz
AQ         1.3045164 sec
RG         16384
DE         19.900 umsc
TE         300.2 K
D1         2.00000000 sec
d11        0.03000000 sec
d12        0.00002000 sec

***** CHANNEL f1 *****
NUC1       13C
P1         16.35 usec
PL1        -6.00 dB
SFO1       100.6277558 MHz

***** CHANNEL f2 *****
CPDPRG2   waltz16
NUC2       1H
PCPD2     114.00 usec
PL2        0.00 dB
P12       24.00 dB
P13       24.00 dB
SFO2       400.1418009 MHz

F2 - Processing parameters
SI         32768
SF         100.6172780 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

1D NMR plot parameters
CU         50.00 cm
F1P        234.4530 ppm
F1         238.9721 MHz
F2P        -14.046 ppm
F2         -1495.90 Hz
PRMCHN    12.46531 ppm/Hz
HZCM      1256.28137 Hz/cm
  
```



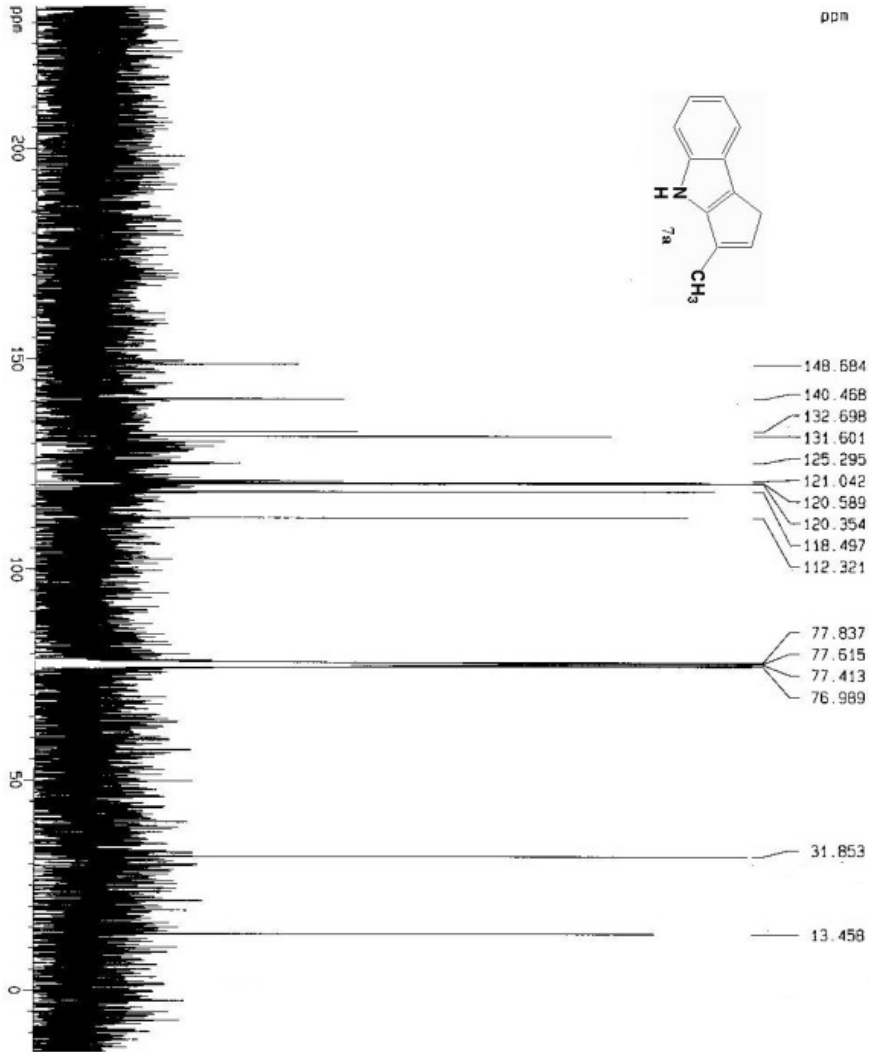
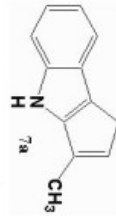
Current Data Parameters
 NAME MRI-0820-05
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060120
 Time 9:06
 INSTRUM spect
 PROBHD 5 mm BBI 1H-9
 PULPROG zg30
 TD 65536
 SCA VENT CDD13
 NS 16
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.18314 Hz
 AQ 3.988243 sec
 RG 322.5
 W2 50.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 6.45 usec
 PL1 0.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 NQW 0
 SSB 0
 LB 0.00 Hz
 GB 0

10 NMR plot parameters
 CX 20.00 cm
 FIP 10.000 ppm
 F1 4001.30 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PUNCH 0.55000 ppm/cm
 HZCM 220.07150 Hz/cm



```

Current Data Parameters
NAME      MR1-Jan22-06
EXPNO    1
PROCNO   1

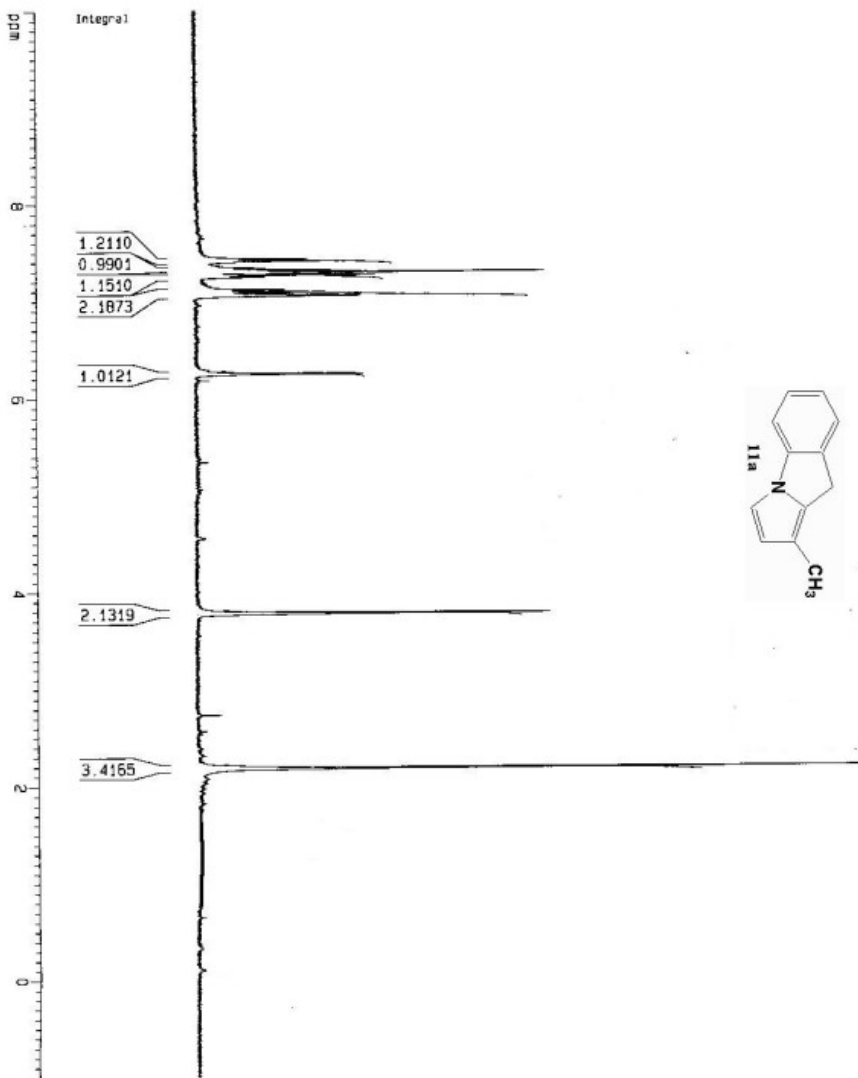
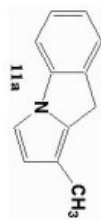
F2 - Acquisition Parameters
Date_    20060122
Time     17.32
INSTRUM  spect
PROBHD   5 mm QNP 1H/1
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS       6737
DS       4
SWH      18796.992 Hz
FIDRES   0.286619 Hz
AQ       1.7432076 sec
RG       512
OR       76.500 uSAC
DE       6.00 uSAC
TE       300.0 K
D1       2.00000000 sec
D11      0.03000000 sec
D12      0.00020000 sec

***** CHANNEL f1 *****
NUC1      13C
P1       5.40 uSAC
PL1      -6.00 dB
SFO1     75.4106357 MHz

***** CHANNEL f2 *****
CHARGE2   MALT235
NUC2      1H
P2       115.00 uSAC
PL2      0.00 dB
SFO2     200.0000000 MHz
SFO2     299.8719995 MHz

F2 - Processing parameters
SI       32768
SF       75.4023410 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40

1D NMR 0101 parameters
CX       30.00 cm
F1P      234.000 cm
F1       17664.75 Hz
F2P      -20.000 cm
F2       -1508.05 Hz
PNUC1M  12 70000 cm/cr
HZCM     957.60969 Hz/cm
  
```



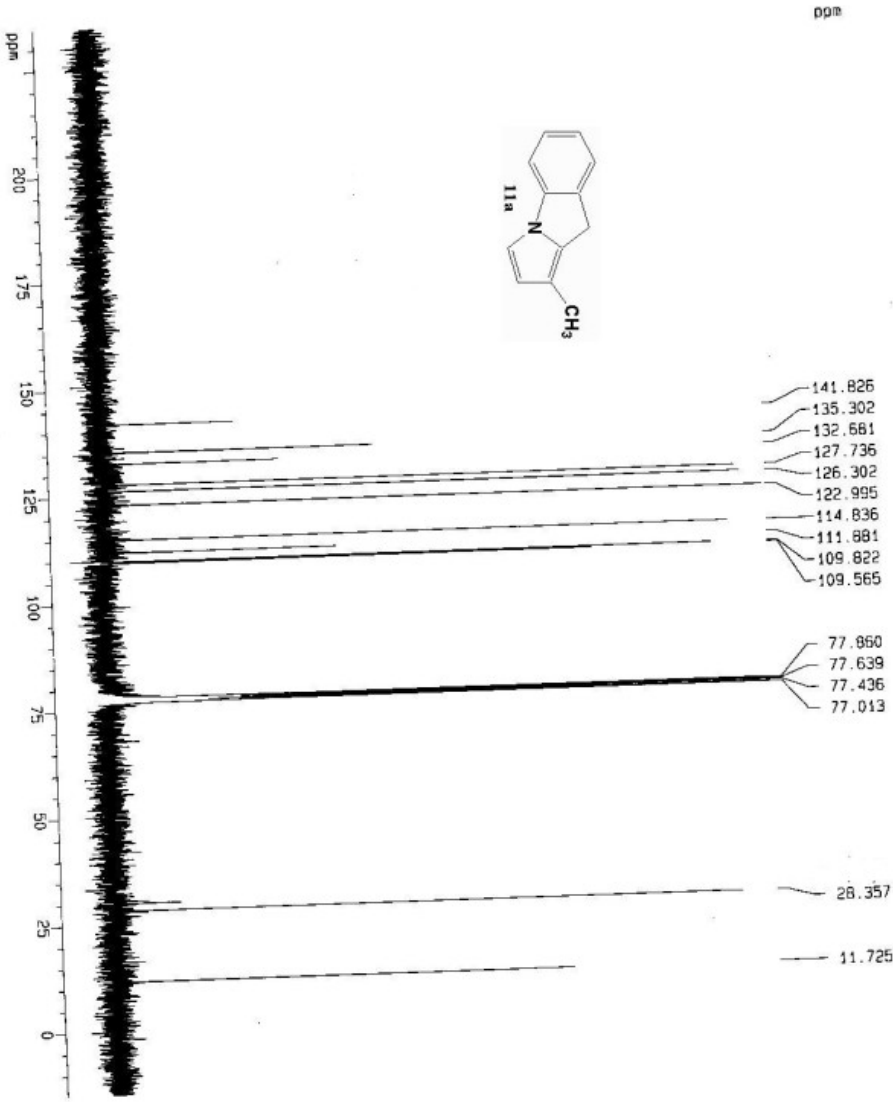
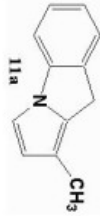
Current Data Parameters
 NAME M1-JUN03-05
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050603
 Time 20 01
 INSTRUM spect
 PROBS= 5 mm QNP 1H/1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SFO1 5172.839 Hz
 FIDRES 0.094150 Hz
 AQ 5.3694680 sec
 RG 724.1
 DM 81.000 uS/cic
 DE 6.00 uS/c
 TE 300.0 K
 O1 1.00000000 sec

***** CHANNEL f1 *****
 MUX1 H1
 P1 11.70 uS/c
 PL1 0.00 dB
 SFO1 299.870518 MHz

F2 - Processing parameters
 SI 32768
 SF 299.8705000 MHz
 KHZ
 MWM no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

10 NMR plot parameters
 CX 20.00 cm
 FIP 10.000 ppm
 F1 2398.70 Hz
 F2 -1.000 ppm
 F3 -259.87 Hz
 PUNCH 0.55000 gms/cm
 HZCM 164.82850 Hz/cm



```

Current Data Parameters
NAME          M1-14a13-05
EXPNO        4
PROCNO       1

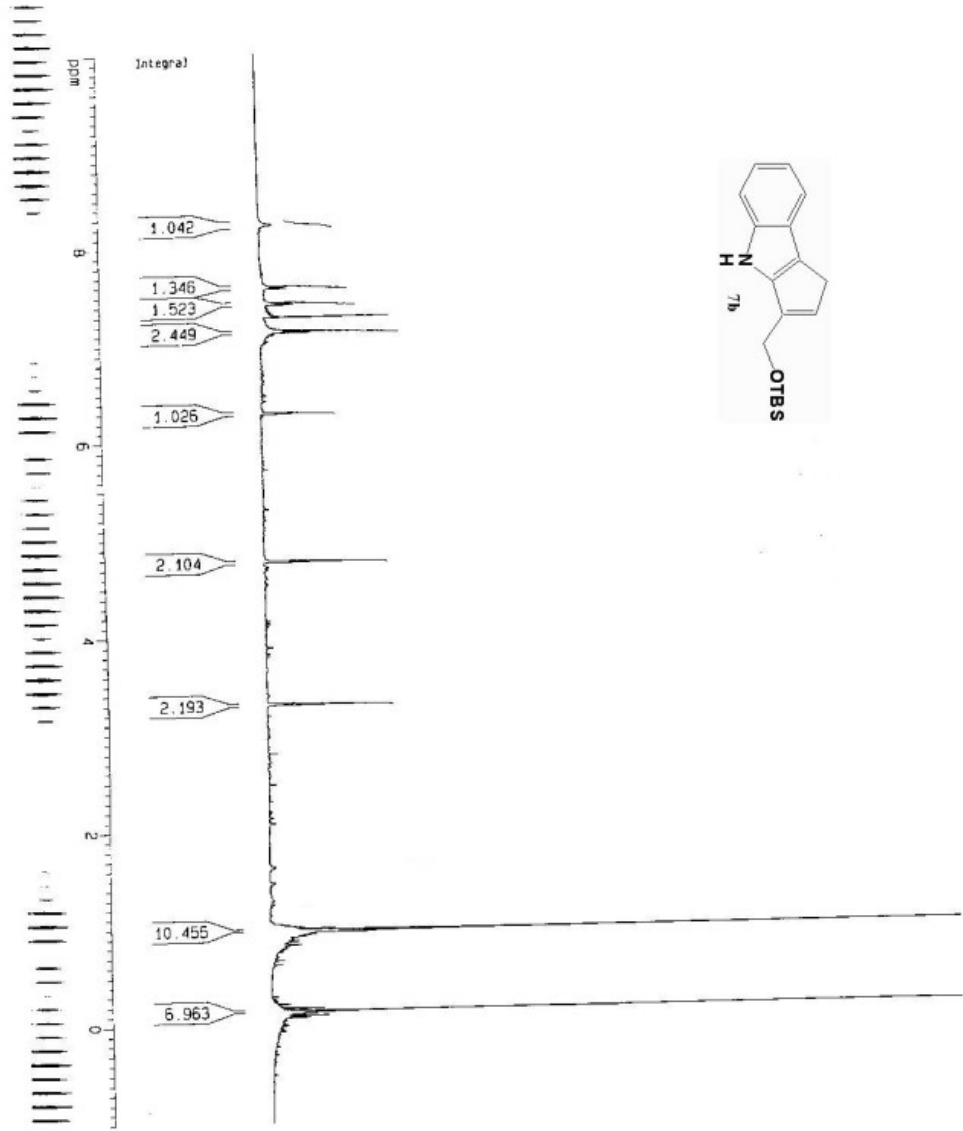
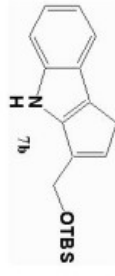
F2 - Acquisition Parameters
Date_         20030604
Time         5.36
INSTRUM      spect
PROBHD       5 mm QNP 1H/1
PULPROG      zgpg30
TD            65536
SOLVENT      CDCl3
NS           5000
DS           4
SWH           13796.592 Hz
FIDRES       0.286919 Hz
AQ           1.7453076 sec
RG           512
WB           26.600 usec
DE           300.0 K
TE           0.0000000 sec
D1           0.0000000 sec
D12          0.0000000 sec

***** CHANNEL f1 *****
NUC1          13C
P1           5.40 usec
PL           -5.00 dB
SFO1         75.410697 MHz

***** CHANNEL f2 *****
CPROG2       waltz16
NUC2          1H
P2           145.00 usec
PL2          0.00 dB
PC2         20.00 dB
PC12        20.00 dB
SFO2         298.871985 MHz

F2 - Processing parameters
SI           32768
SF           75.4023410 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40

1D NMR plot parameters
CX           20.00 cm
F1P          234.637 ppm
F1           17982.21 Hz
F2P          -14.629 ppm
F2           -1104.78 Hz
PC1M        939.94953 Hz/cm
  
```



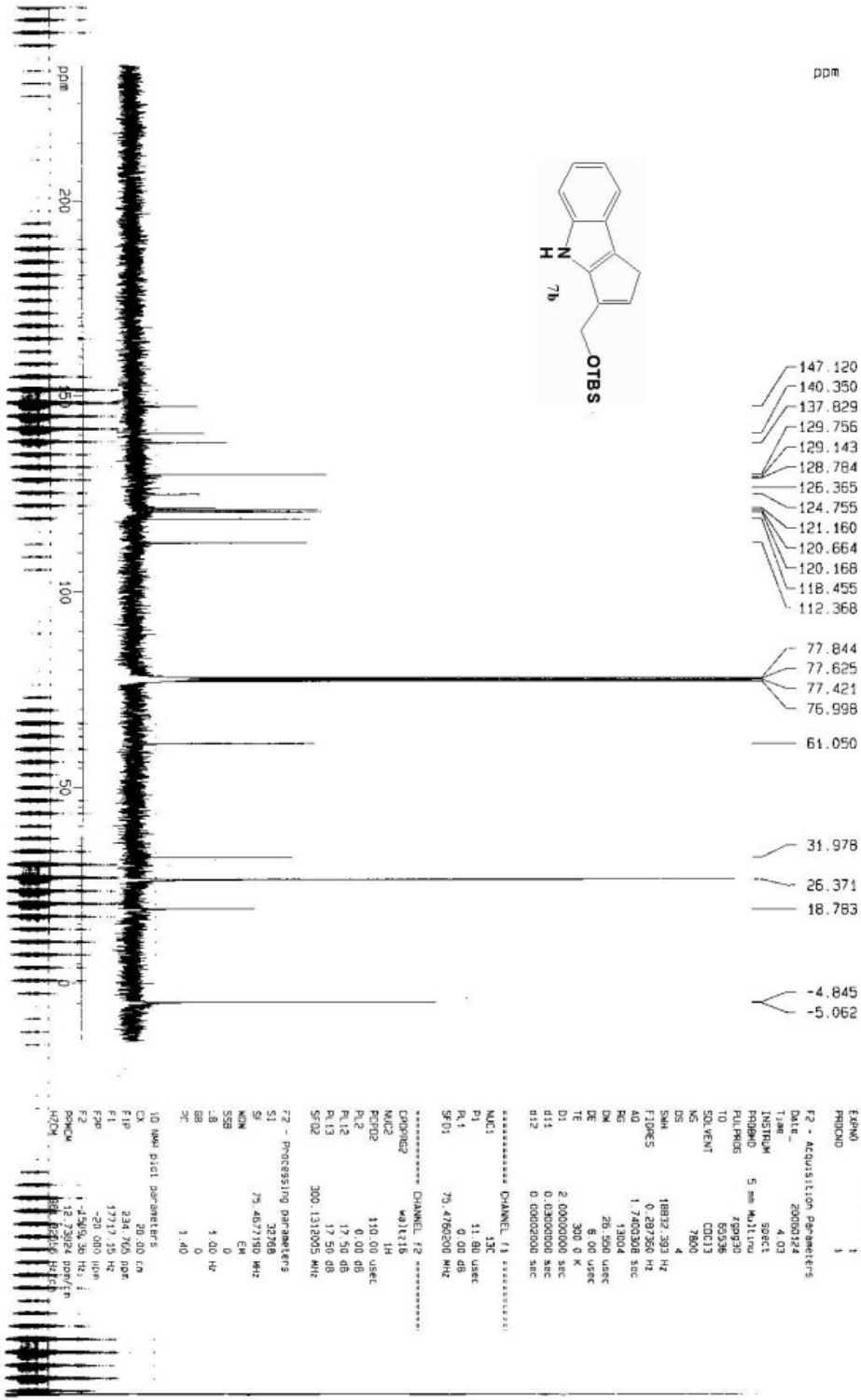
Current Data Parameters
 NAME MRI-Jan23-05
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060123
 Time 19.37
 INSTRUM spect
 PROBM 5 mm BBI 1H-8
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 128
 DM 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 5.45 usec
 PL1 0.00 dB
 SFO1 400.132470 MHz

F2 - Processing parameters
 SI 32768
 SF 400.130000 MHz
 MDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters.
 CX 20.00 cm
 F1P 10.000 ppm
 F1 4001.30 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 FPCWID 0.55000 ppm/cw
 HZCW 220.07150 Hz/cw



Experiment Parameters

NAME: M1-5873-08
 EXPNO: 1
 PROCNO: 1

F2 - Acquisition Parameters

DATE_: 20080324
 TIME: 14.02
 INSTRUM: spect
 PULPROG: zgpg30
 FIDRES: 5.00 Hz
 SFO1: 125.762 MHz
 SOLVENT: CDCl3
 NS: 7800
 DS: 4
 SWH: 18832.393 Hz
 FIDRES: 0.287560 Hz
 AQ: 1.7400308 sec
 RG: 13004
 DM: 28.500 usec
 DE: 6.00 usec
 TE: 300.0 K
 D1: 2.00000000 sec
 D11: 0.03000000 sec
 D12: 0.00000000 sec

CHANNEL f1

MUCL: 13C
 P1: 11.80 usec
 PL1: 0.00 dB
 SF01: 75.4760200 MHz

CHANNEL f2

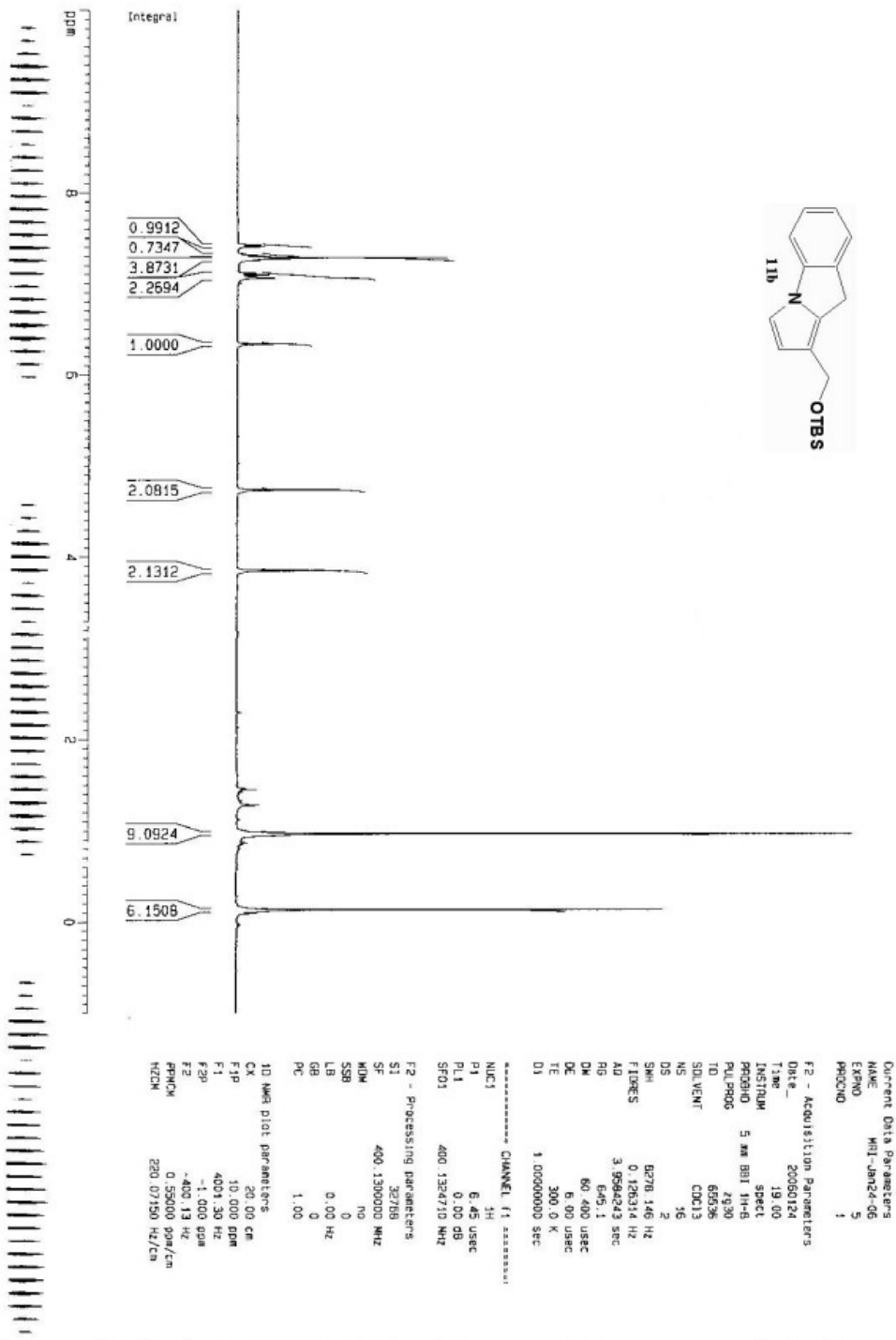
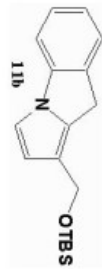
CPDPRG2: waltz16
 NUCL2: 1H
 PULPROG2: zgpg30
 PC2: 0.00 usec
 PL2: 0.00 dB
 PL12: 17.50 dB
 PL13: 17.50 dB
 SFO2: 300.1310005 MHz

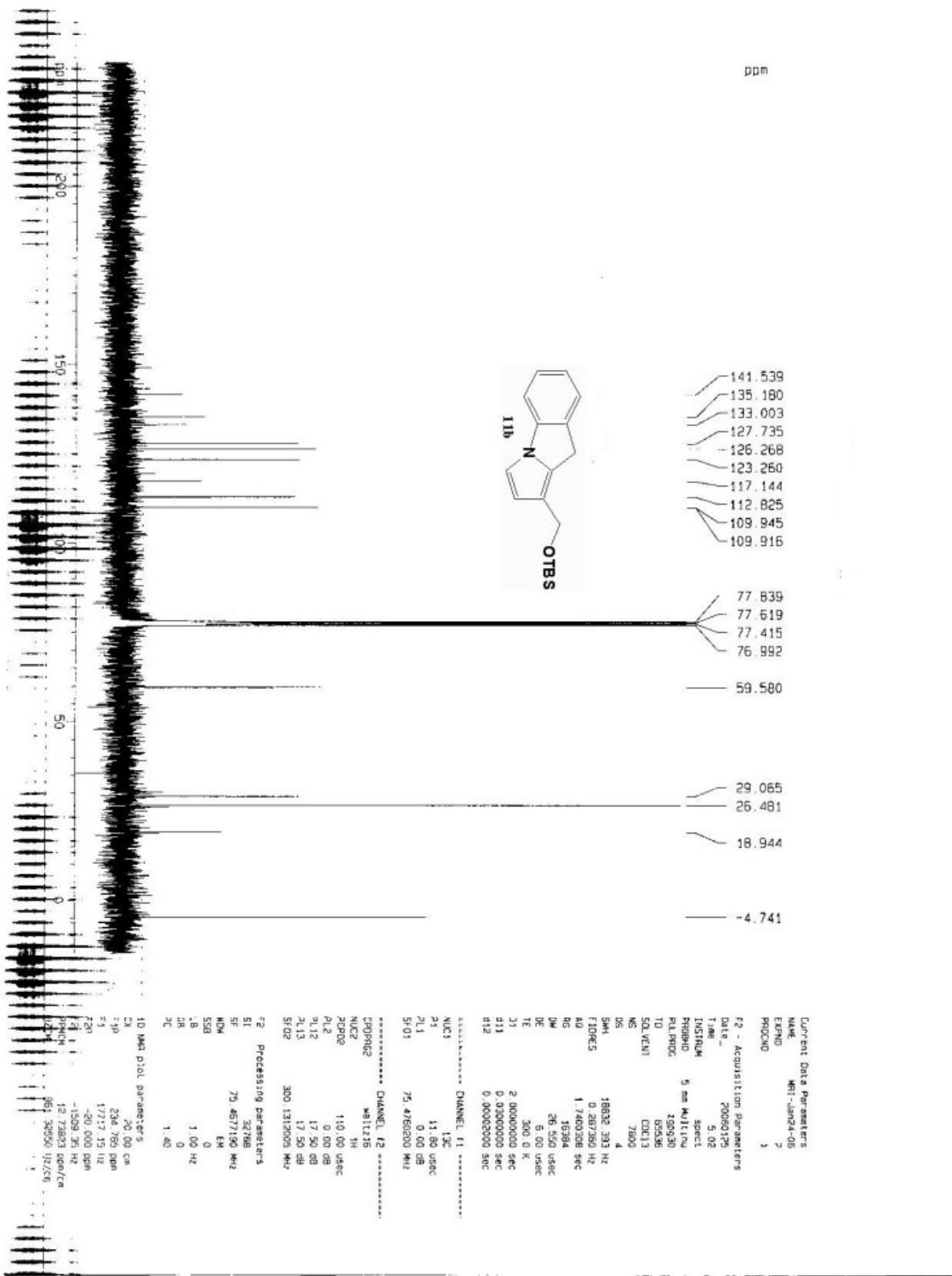
F2 - Processing parameters

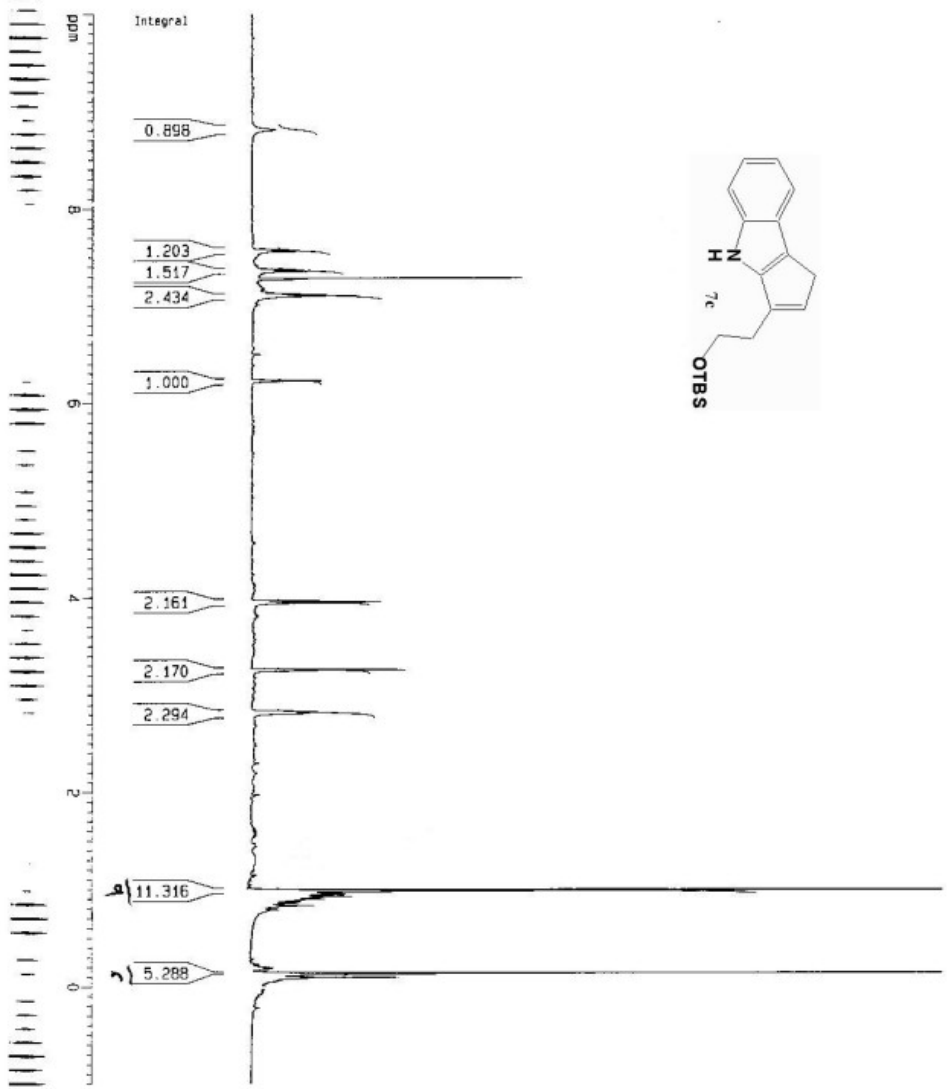
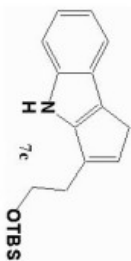
SF: 300.1310005 MHz
 WHW: 75.4677150 MHz
 EQ: 0
 SSB: 0
 GB: 1.00 Hz
 SC: 1.40

10 user def parameters

CX: 20.00 Hz
 F1P: 234.765 ppm
 F1: 17117.15 Hz
 FAP: -20.000 ppm
 F2: -12500.36 Hz
 POSPCW: -18.23000 ppm/Hz
 HZCW: 18.23000 Hz







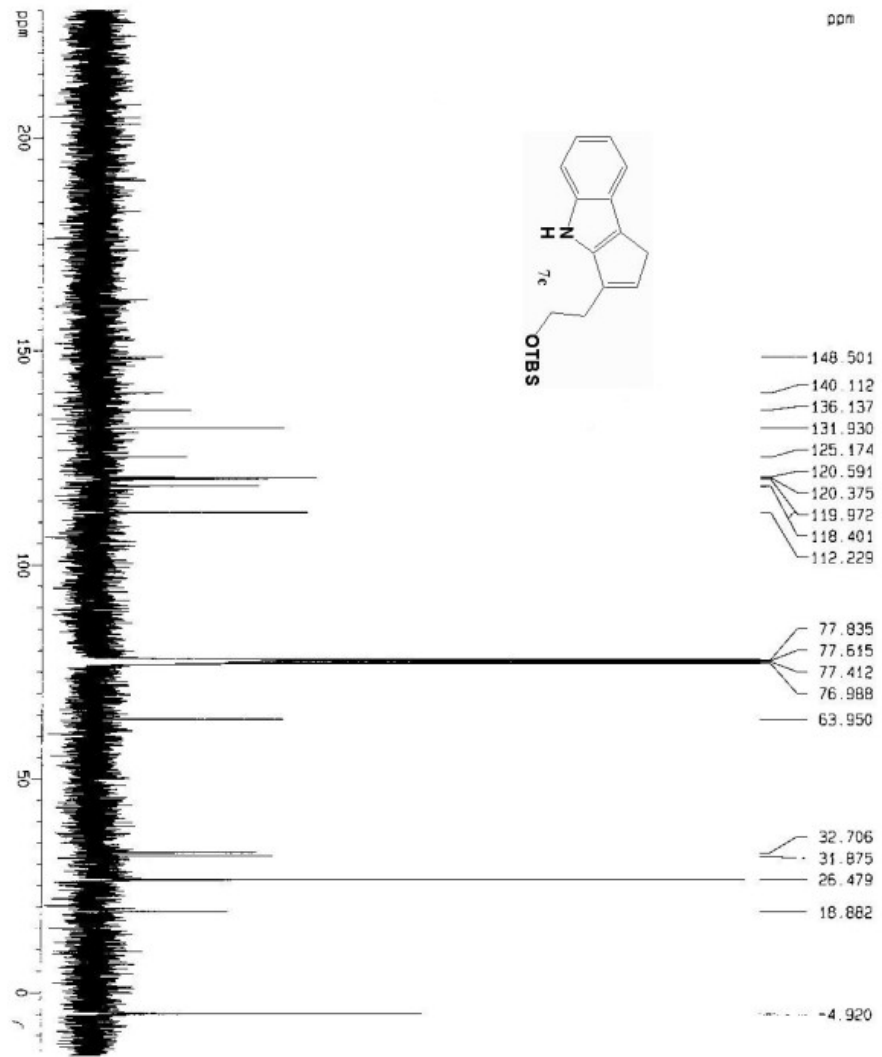
Current Data Parameters
 NAME: NRI-Jan21-06
 EXPNO: 3
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20060121
 Time: 11:19
 INSTRUM: spect
 PROBHD: 5 mm BBI 1H-8
 PULPROG: zg30
 TO: 65536
 SOLVENT: DMS-D3
 NS: 16
 DS: 2
 SWH: 8278.140 Hz
 FIDRES: 0.128314 Hz
 AQ: 3.9596243 sec
 RG: 228.1
 DW: 80.400 usec
 DE: 5.00 usec
 TE: 300.0 K
 D1: 1.00000000 sec

***** CHANNEL f1 *****
 NUC1: 1H
 P1: 6.45 usec
 PL1: 0.00 dB
 SFO1: 400.1326710 MHz

F2 - Processing parameters
 SI: 32768
 SF: 400.1300000 MHz
 KW: no
 SSB: 0
 LB: 0.00 Hz
 GB: 0
 PC: 1.00

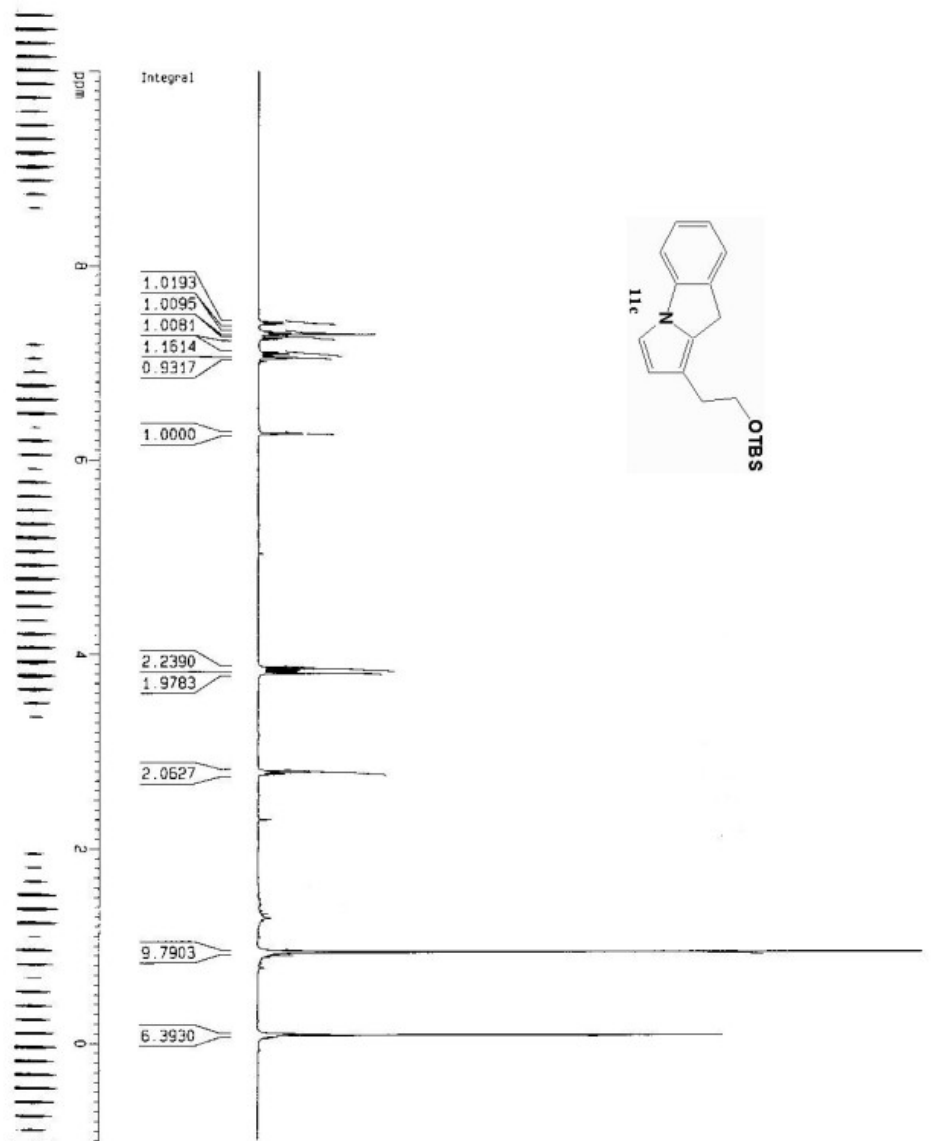
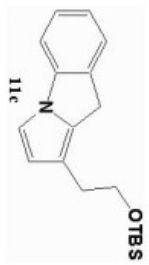
1D NMR plot parameters.
 CX: 20.00 cm
 FJP: 10.000 DPM
 F1: 4001.30 Hz
 F2: -400.13 Hz
 PPMCK: 0.58000 ppm/cm
 NZCM: 220.07150 Hz/cm



- 148.501
- 140.112
- 136.137
- 131.930
- 125.174
- 120.591
- 120.375
- 119.972
- 118.401
- 112.229
- 77.835
- 77.615
- 77.412
- 76.988
- 63.950
- 32.706
- 31.875
- 26.479
- 18.882
- 4.920

```

Current Data Parameters
NAME      MFL-3621-00
EXPNO     1
PROCNO    1
----- F2 - Acquisition Parameters -----
Date_     20060123
Time      16.42
INSTRUM   spect
PROBHD    5 mm DNP-HU/1
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         4000
DS         4
SWH        18796.992 Hz
FIDRES     0.268119 Hz
AQ         1.7433776 sec
RG         256
OR         26.600 usec
DE         6.00 usec
TE         300.0 K
D1         2.00000000 sec
D11        0.03000000 sec
D12        0.00002000 sec
----- CHANNEL f1 -----
NUC1       13C
P1         5.40 usec
PL1        -6.00 dB
SFO1       75.410657 MHz
----- CHANNEL f2 -----
CPDPRG2   waltz16
NUC2       1H
P2         115.00 usec
PL2        0.00 dB
PL12       20.00 dB
PL13       20.00 dB
SFO2       298.871995 MHz
----- F3 - Processing Parameters -----
SI         32768
SF         75.402340 MHz
WDW         EM
SSB         0
LB         1.00 Hz
GB         0
PC         1.40
----- 1D NMR plot parameters -----
CX         20.00 cm
FLP        230.000 gpm
FL         17342.54 Hz
FAP        -20.000 gpm
F2         -1506.05 Hz
PPMACH     12.50000 ppm/cm
HZCM       942.58320 Hz/cm
  
```



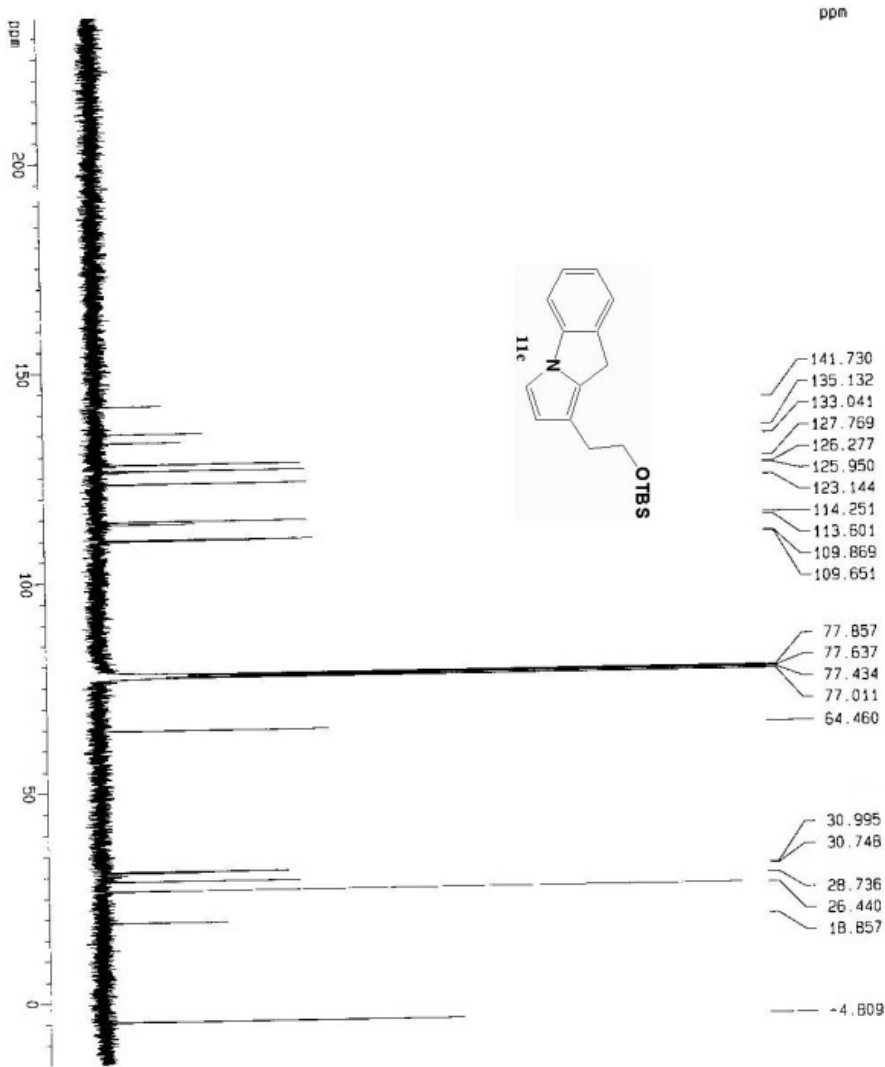
Current Data Parameters
 Name MRI-JAN24-05
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050124
 Time 16.52
 INSTRUM spect
 PNOBHD 5 mm BBI JH-9
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 11
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.186314 Hz
 AQ 3.9594243 sec
 RG 256
 DM 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 6.45 usec
 PL1 0.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 KW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

10 MHz plot parameters
 CX 20.00 cm
 FIP 10.000 ppm
 F1 4001.30 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPHZ 0.55000 ppm/cm
 MZCM 220.0/150 Hz/cm



```

Current Data Parameters
NAME      MRI-Jan24-06
EXPNO    2
PROCNO   1

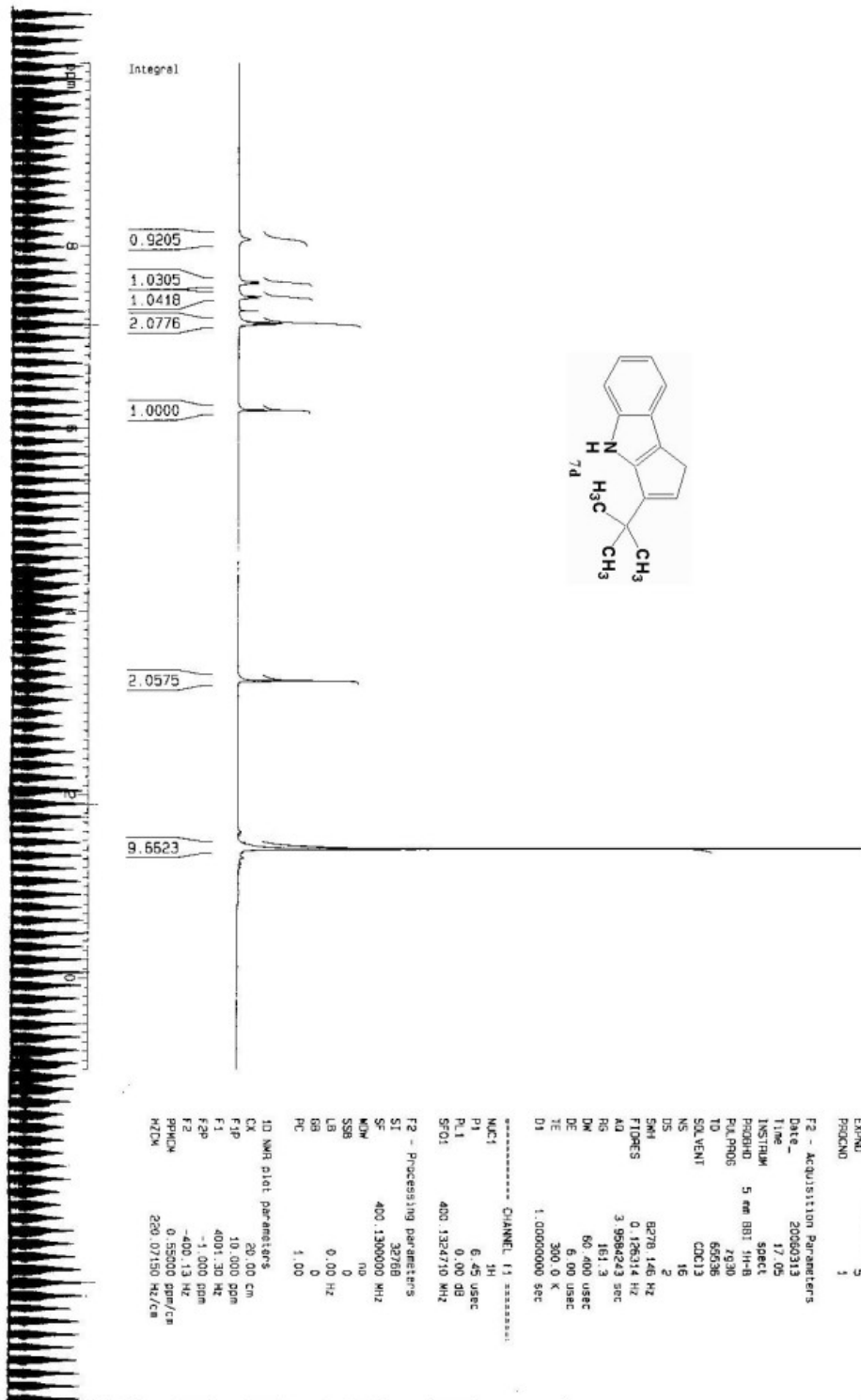
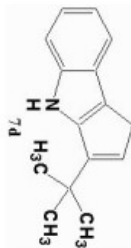
F2 - Acquisition Parameters
Date_    20080125
Time     5.05
INSTRUM  spect
PROBHD   5 mm QNP 1H/1
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        7500
DS        4
SMH       18750.592 Hz
FIDRES    0.288819 Hz
AQ         1.7432076 sec
RG         512
DE         28.800 uVsec
TE         300.0 K
D1         2.00000000 sec
D12        0.03000000 sec
D122       0.00002000 sec

***** CHANNEL f1 *****
NUC1       13C
P1         5.00 uVsec
PL1        -8.00 dB
SFO1       75.4109397 MHz

***** CHANNEL f2 *****
CPROG2    waltz16
NUC2       1H
P2         115.00 uVsec
PL2        0.00 dB
R12        20.00 dB
R122       20.00 dB
SFO2       299.8711995 MHz

F2 - Processing parameters
SI         32768
SF         75.4023410 MHz
KOH        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

10 MHz plot parameters
CX         20.00 cm
F1P        234.863 ppm
F1         17693.24 Hz
F2P        -20.000 ppm
F2         -1508.00 Hz
FREQH0     12.73255 ppm/cM
HZ0M       950.08433 Hz/cM
  
```



Current Data Parameters
 NAME MRI-MR13-06
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060313
 Time 17.05

INSTRUM spect
 PULPROG 5 mm BBI 1H-B
 PULPROG 7d30

SOLVENT CDCl3
 NS 16
 US 2

SMH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9564243 sec

RG 161.3
 DM 60.400 usec
 DE 6.00 usec

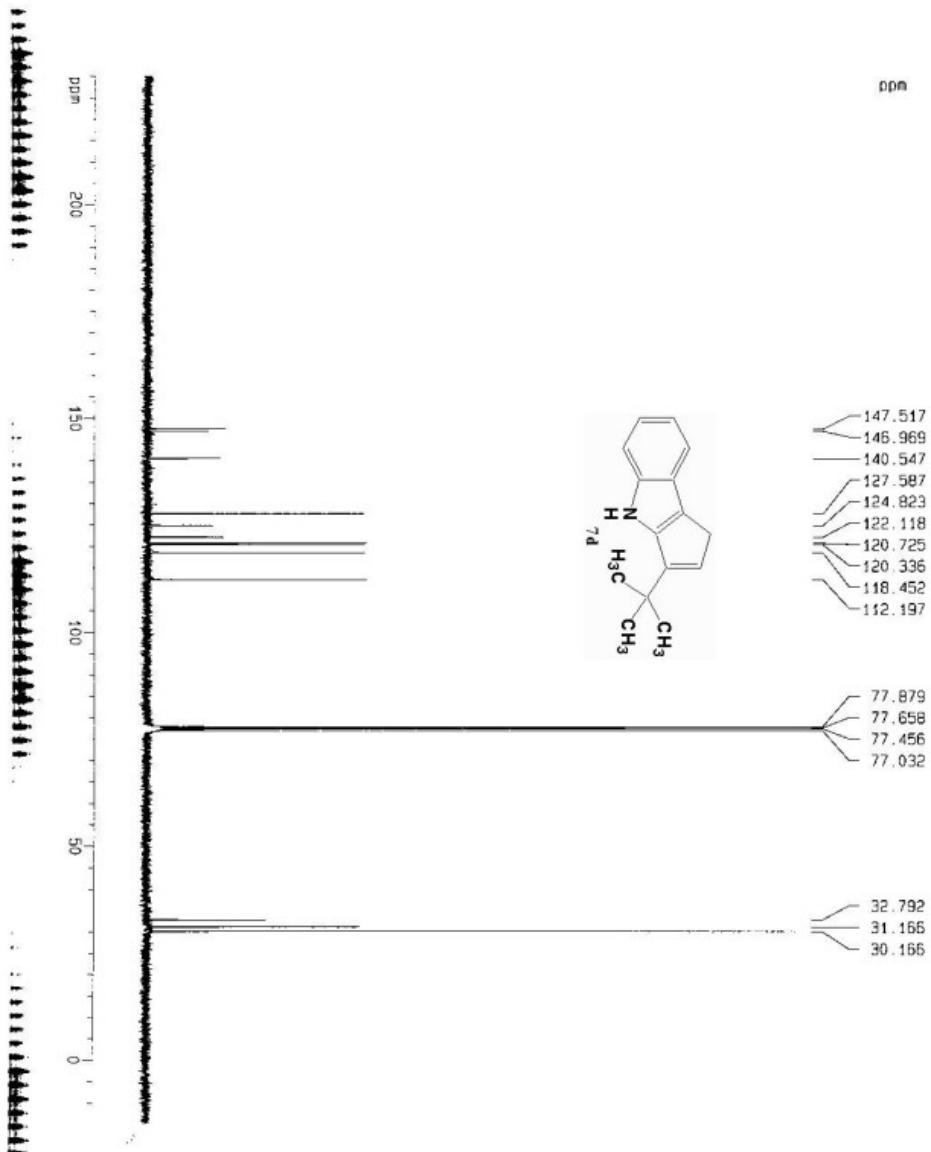
TE 300.0 K
 D1 1.00000000 sec

----- CHANNEL f1 -----
 NUC1 1H
 P1 6.45 usec
 PL1 0.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW no
 SSB 0

LB 0.00 Hz
 GB 0
 PC 1.00

ID NMR plot parameters
 CX 20.00 cm
 FXP 10.000 gpm
 F1 4001.30 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPM1CM 0.55000 ppm/cm
 MTCM 220.07150 Hz/cm



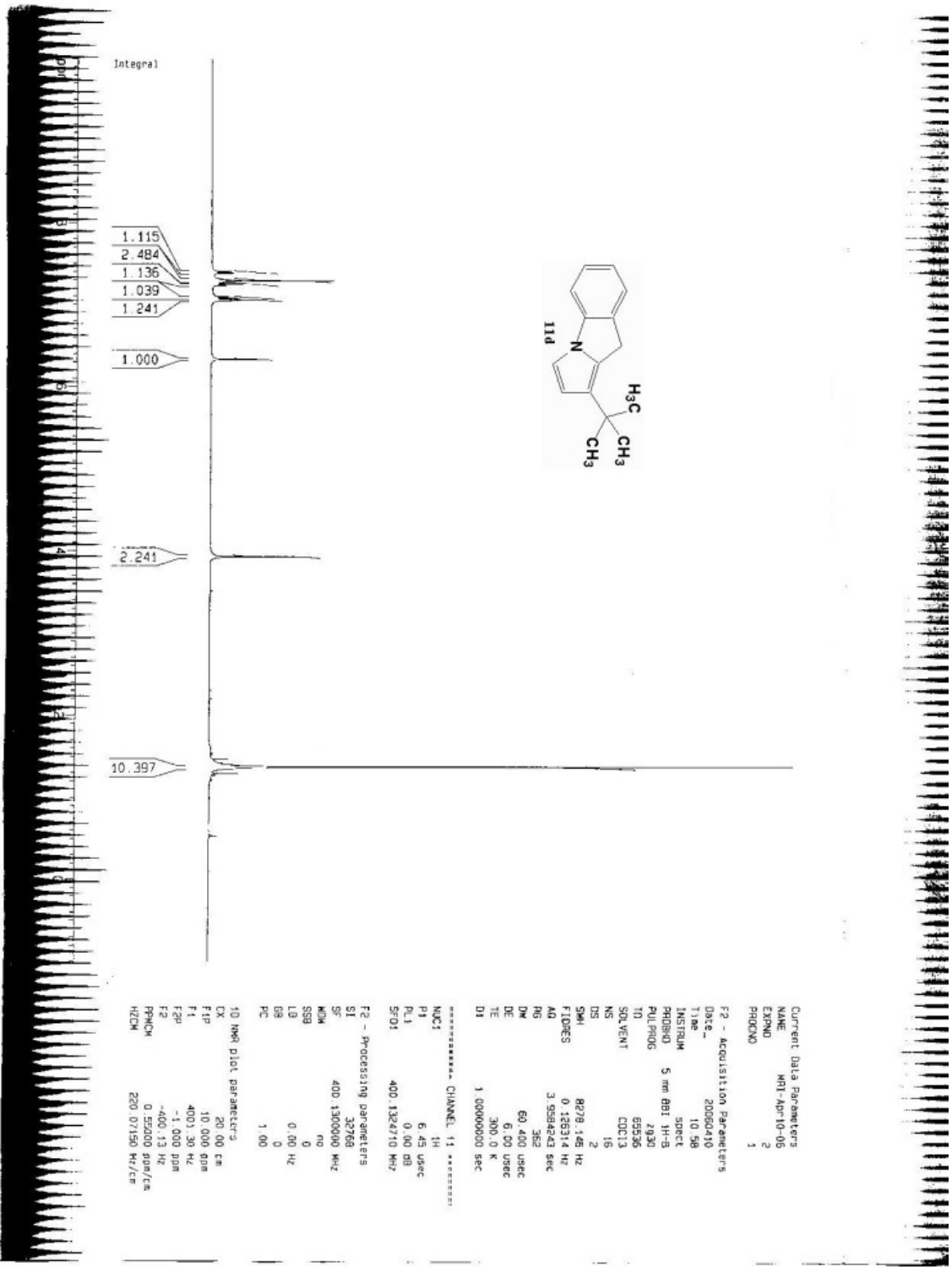
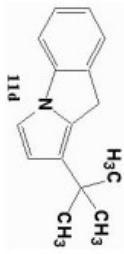
Current Data Parameters
 NAME: M07-MR-14-06
 EXPNO: 2
 F2ID: 1
 F2 - Acquisition Parameters
 Date_: 20080314
 Time: 17:00
 INSTRUM: spect
 PROBHD: 5 mm DNP HX/1
 PULPROG: zgpg30
 TO: E5536
 SOLVENT: CDCl3
 NS: 1637
 DS: 4
 SMH: 18796.592 Hz
 FIDRES: 0.266819 Hz
 AQ: 1.7433076 sec
 RG: 512
 DM: 28.600 usec
 DE: 6.00 usec
 TE: 300.0 K
 D1: 2.00000000 sec
 D12: 0.05000000 sec
 D12: 0.00002000 sec

***** CHANNEL f1 *****
 NUC1: 13C
 P1: 5.40 usec
 PL1: -6.00 dB
 SFO1: 75.410657 MHz

***** CHANNEL f2 *****
 CPDPRG2: waltz16
 NUC2: 1H
 P2: 115.00 usec
 PL2: 0.00 dB
 PL12: 20.00 dB
 PL13: 20.00 dB
 SFO2: 299.8711999 MHz

F2 - Processing parameters
 SI: 32768
 SF: 75.4023410 MHz
 WHW: EM
 SSB: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.40

10 NMR plot parameters
 EX: 20.00 cm
 F1P: 230.000 ppm
 F1: 17342.54 Hz
 F2P: -20.000 ppm
 F2: -1508.09 Hz
 PPMCH: 12.50000 ppm/cm
 SCA2: 52930 Hz/cm



Current Data Parameters
 NAME MRI-APR10-06
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060410
 Time 10.58

INSTRUM spect
 PROBHD 5 mm BBI 1H-3
 PULPROG zgpg30

TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2

SWH 8278.145 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec

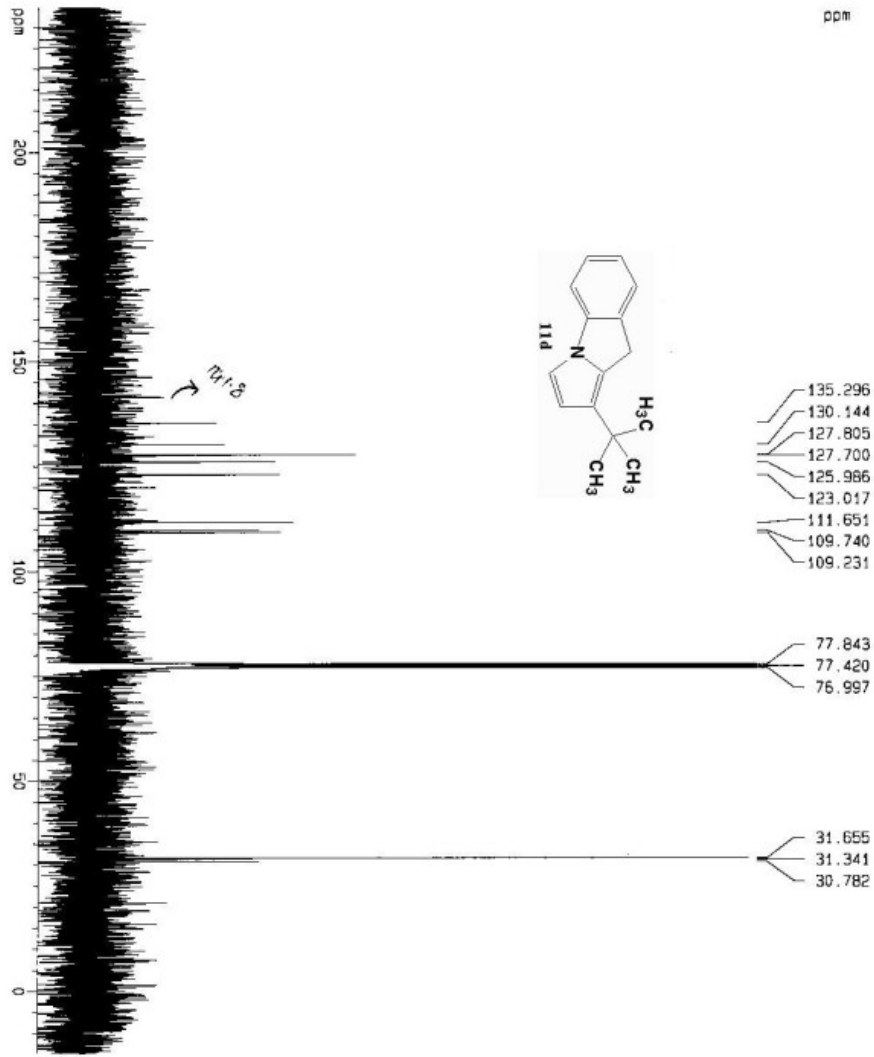
RG 382
 DW 60.400 usec
 DE 6.00 usec
 TE 300.0 K

D1 1.00000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 6.43 usec
 PL1 0.00 dB
 SFO1 400.1364710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 KW 64
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 FIP 10.000 GHz
 F1 4003.30 Hz
 F2 -1.000 ppm
 F2 -400.13 Hz
 PRNCK 0.55200 ppm/cm
 HZCM 220.07150 Hz/cm



```

Current Data Parameters
NAME      W11-30r10-06
EXPNO    1
PROCNO   1

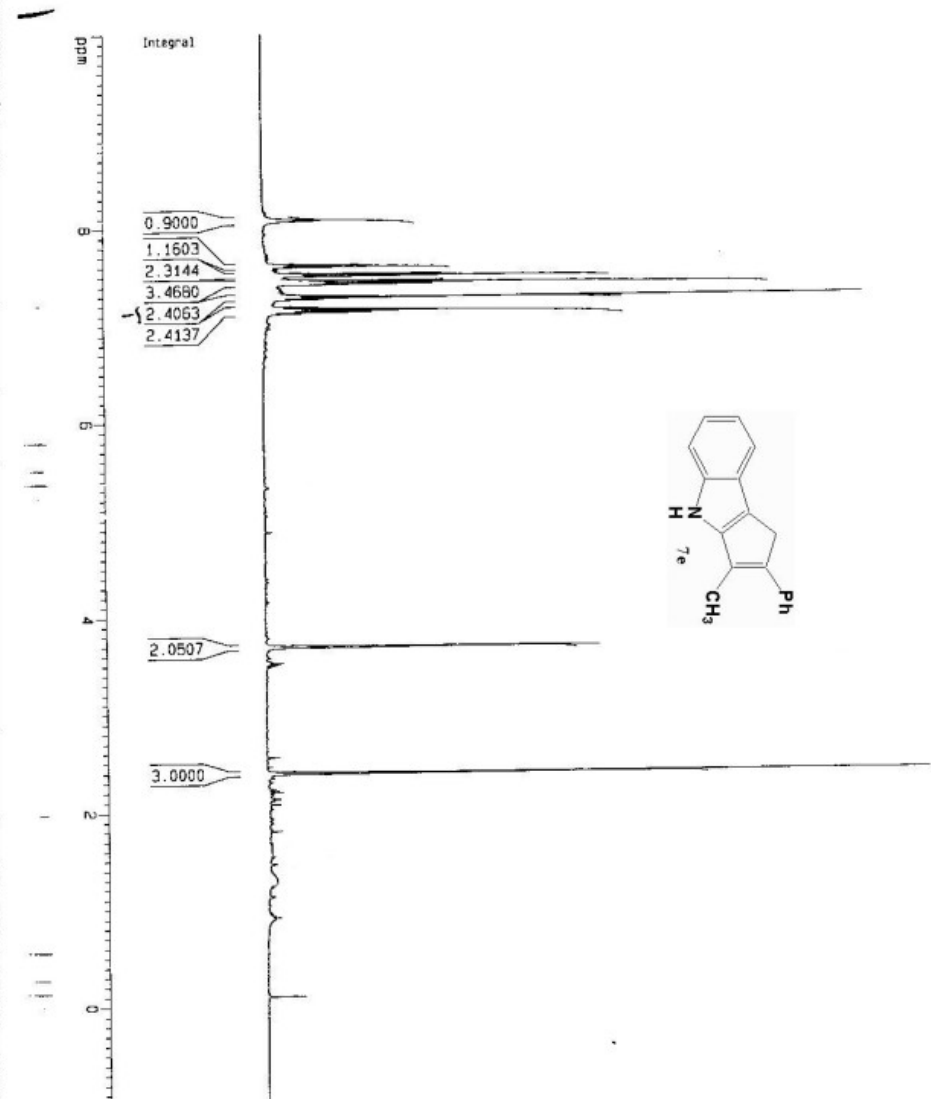
F2 - Acquisition Parameters
Date_    20050410
Time     23:45
INSTRUM  spect
PROBHD   5 mm WALTZ
PULPROG  zgpg30
TD       65536
SFO1     125.760 MHz
SOLVENT  CDCl3
NS       3754
DS       4
SWH      19832.393 Hz
FIDRES   0.2807360 Hz
AQ       1.7400000 sec
RG       16384
DE       26.7500 usec
TE       300.0 K
D1       2.00000000 sec
d11      0.03000000 sec
d12      0.00000000 sec

----- CHANNEL f1 -----
NUC1     13C
P1       11.80 usec
PL1      0.00 dB
SFO1     75.4760200 MHz

----- CHANNEL f2 -----
CPDPRG2  waltz16
NUC2     1H
P2       110.00 usec
PL2      0.00 dB
PL12     17.50 dB
PL13     17.50 dB
SFO2     300.1312005 MHz

F2 - Processing parameters
SI       32768
SF       75.4677190 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40

10 NMR P102 parameters:
CV       20.00 cm
F1P      234.785 ppm
F1       127.1716 Hz
F2P      -20.000 ppm
F2       -1519.98 Hz
P0MCHM  12.73124 ppm/cm
HZCM     951.26756 Hz/cm
  
```



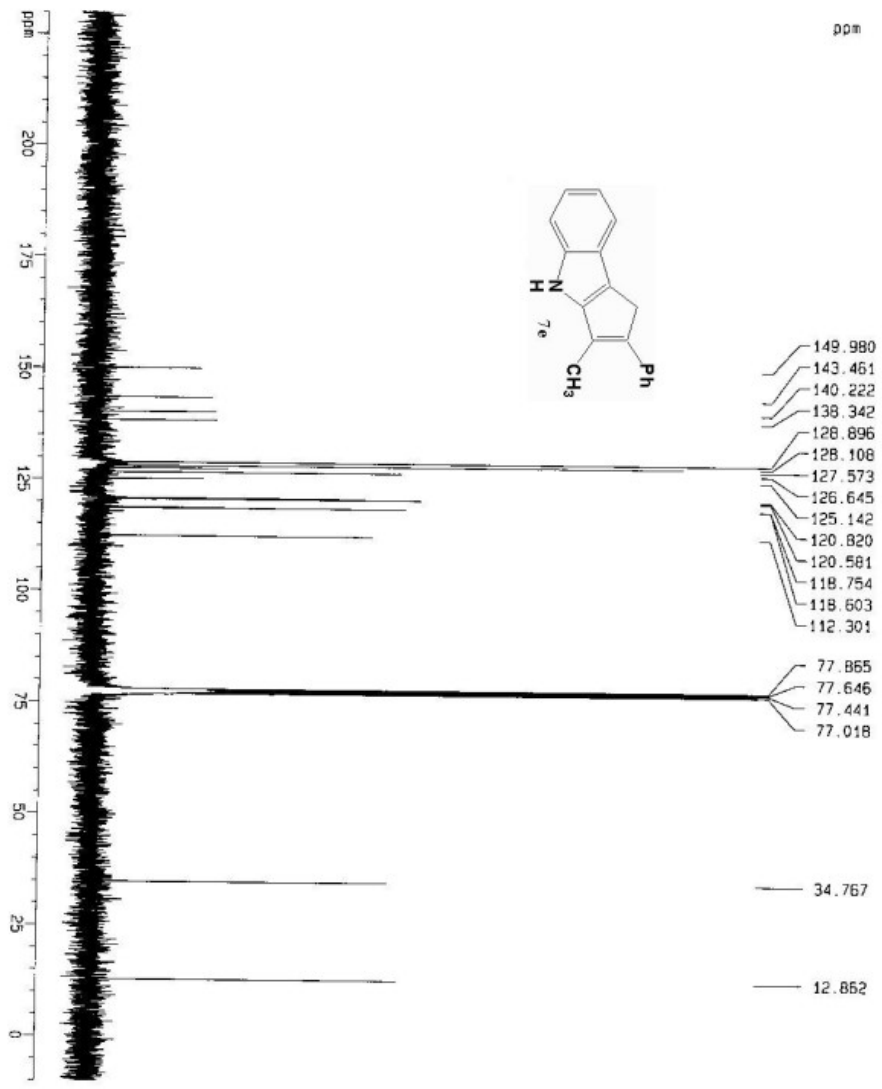
Current Data Parameters
 NAME: M01-Jan09-06
 EXPNO: 1
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20060108
 Time: 11:46
 INSTRUM: spect
 PROBR4: 5 mm BBI 1H-B
 PULPROG: zg30
 TD: 65536
 SOLVENT: CDCl3
 NS: 16
 DS: 2
 SWH: 6278.146 Hz
 FIDRES: 0.126314 Hz
 AQ: 3.5984243 sec
 RG: 287.4
 DW: 60.400 usec
 DE: 6.00 usec
 TE: 300.0 K
 D1: 1.00000000 sec

***** CHANNEL f1 *****
 NUCL1: 1H
 P1: 6.45 usec
 PL1: 0.00 dB
 SF01: 400.1324710 MHz

F2 - Processing Parameters
 SI: 32768
 SF: 400.1300000 MHz
 KW: no
 SSB: 0
 LB: 0.00 Hz
 GB: 0
 PC: 1.00

1D NMR plot parameters
 CX: 20.00 cm
 F1P: 10.000 ppm
 F1: 4001.30 Hz
 F2P: -1.000 ppm
 F2: -400.13 Hz
 PPM2H: 0.59300 ppm/cm
 HZCM: 220.07150 Hz/cm



- 149.980
- 143.461
- 140.222
- 138.342
- 128.896
- 128.108
- 127.573
- 126.645
- 125.142
- 120.820
- 120.581
- 118.754
- 118.603
- 112.301
- 77.865
- 77.646
- 77.441
- 77.018

- 34.767
- 12.852

```

Current Data Parameters
NAME      M01-JAN07-06
EXPNO    9
PROCNO   1

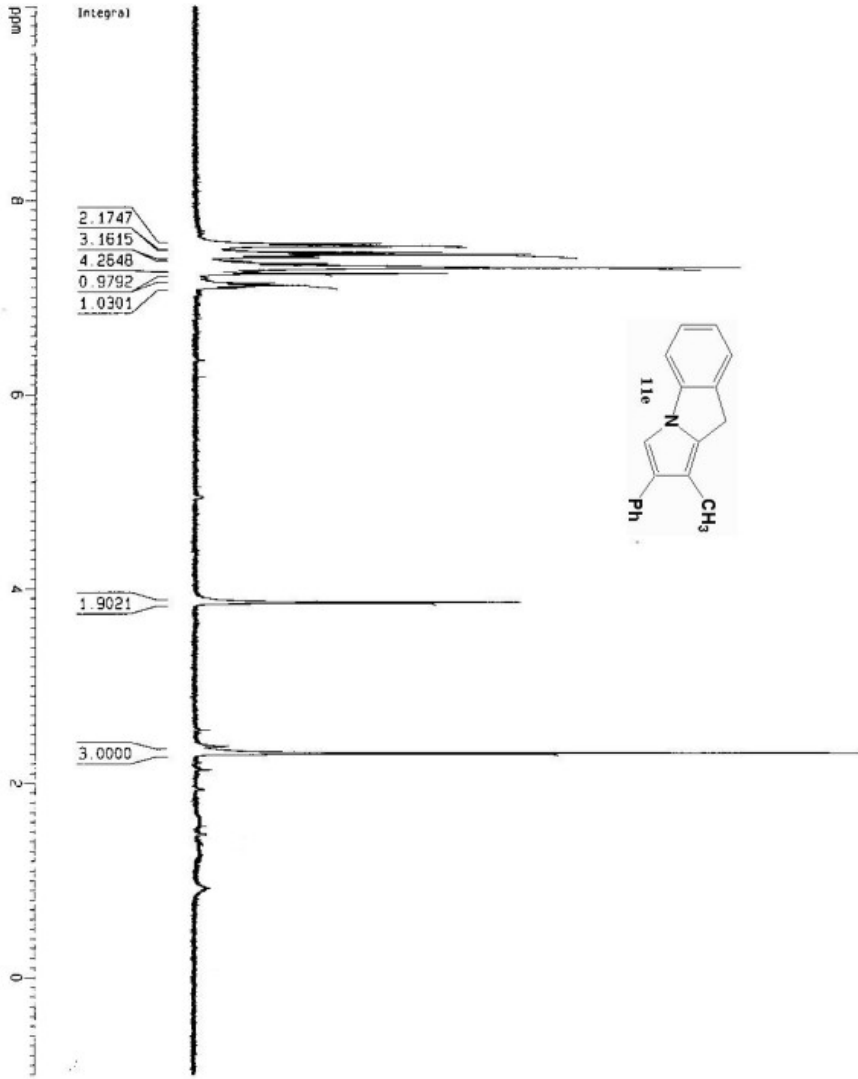
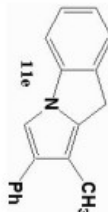
F2 - Acquisition Parameters
Date_    20060108
Time     1.47
INSTRUM  spect
PROBHD   5 mm QNP 1H/1
PULPROG  zgpg30
TD        65536
SOLVENT  DMS-D6
NS        4096
DS        4
SWH       18795.992 Hz
FIDRES   0.298819 Hz
AQ        1.7432976 sec
RG         2048
AQ        0.6000000 sec
TE        300.0 K
DE        6.00 uS/cm
D1         2.0000000 sec
D11        0.0200000 sec
D12        0.0000000 sec

***** CHANNEL f1 *****
NUC1      13C
P1         5.40 uS/cm
PL1       -6.00 dB
SFO1      75.418357 MHz

***** CHANNEL f2 *****
CPDPRG2  waltz16
NUC2      1H
PCPD2     115.00 uS/cm
PL2        0.00 dB
PL12       20.00 dB
PL13       20.00 dB
SFO2      285.871995 MHz

F2 - Processing Parameters
SI         32768
SF         75.4023410 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

10 NMR tick parameters
CX         20.00 cm
F1P        230.000 GHz
F2P        17342.54 Hz
F3P        -1754.02 Hz
P1P        12.00000 GHz/cm
P2P        504.82612 Hz/cm
  
```



Current Data Parameters
 NAME: 11e-14017-06
 EXPNO: 4
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20060107
 Time: 14.25

INSTRUM: spect
 PROCNO: 5
 PULPROG: zgpg30

TD: 65536
 SOLVENT: CDCl3
 NS: 16
 DS: 2

SWH: 6172.826 Hz
 FIDRES: 0.094190 Hz
 AQ: 5.3084660 sec

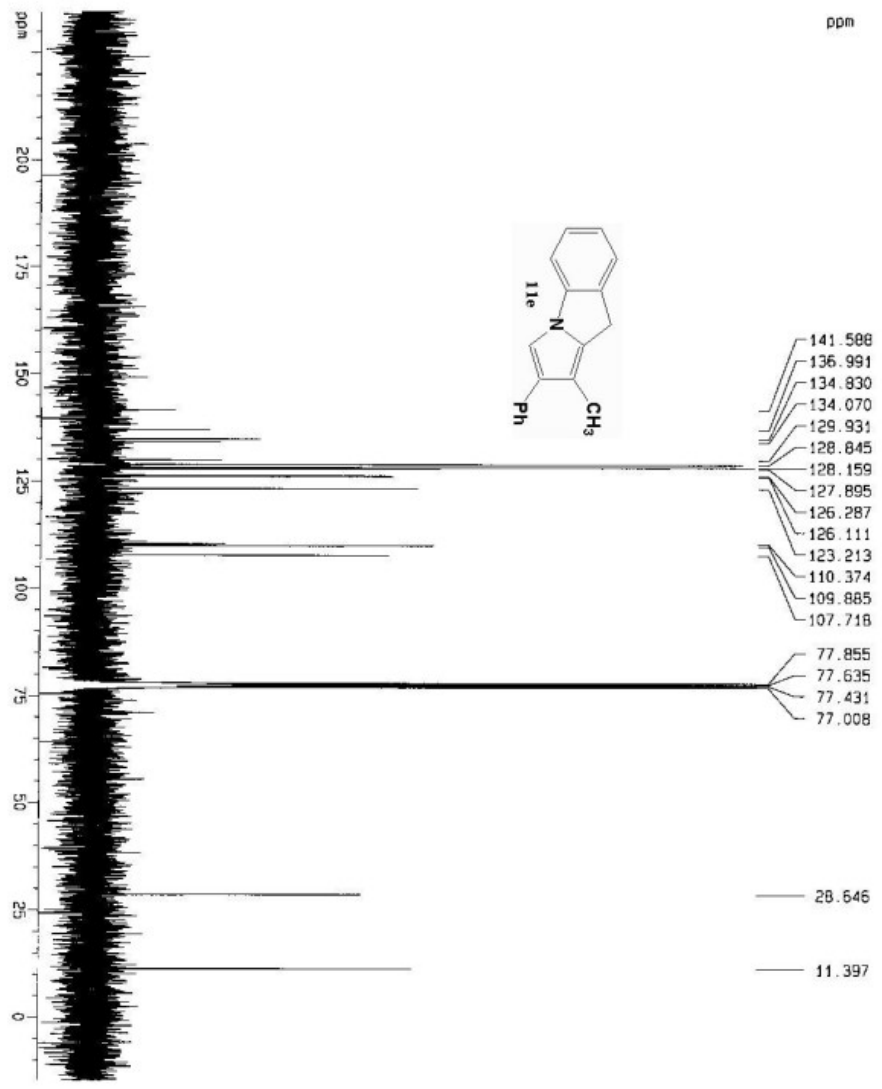
RG: 1024
 DW: 91.000 usec
 DE: 5.00 usec
 TE: 300.0 K

D1: 1.00000000 sec

***** CHANNEL f1 *****
 NUC1: 1H
 P1: 11.70 usec
 PL1: 0.00 dB
 SF01: 299.8718518 MHz

F2 - Processing parameters
 SI: 32768
 SF: 299.8700000 MHz
 WDM: no
 SSB: 0
 LB: 0.00 Hz
 GB: 0
 PC: 1.00

10 NMR plot parameters
 CX: 20.00 cm
 FIP: 10.000 ppm
 F1: 2998.70 Hz
 F2: -299.87 Hz
 PPMCN: 0.55000 ppm/cr
 HZCN: 184.96850 Hz/cm



```

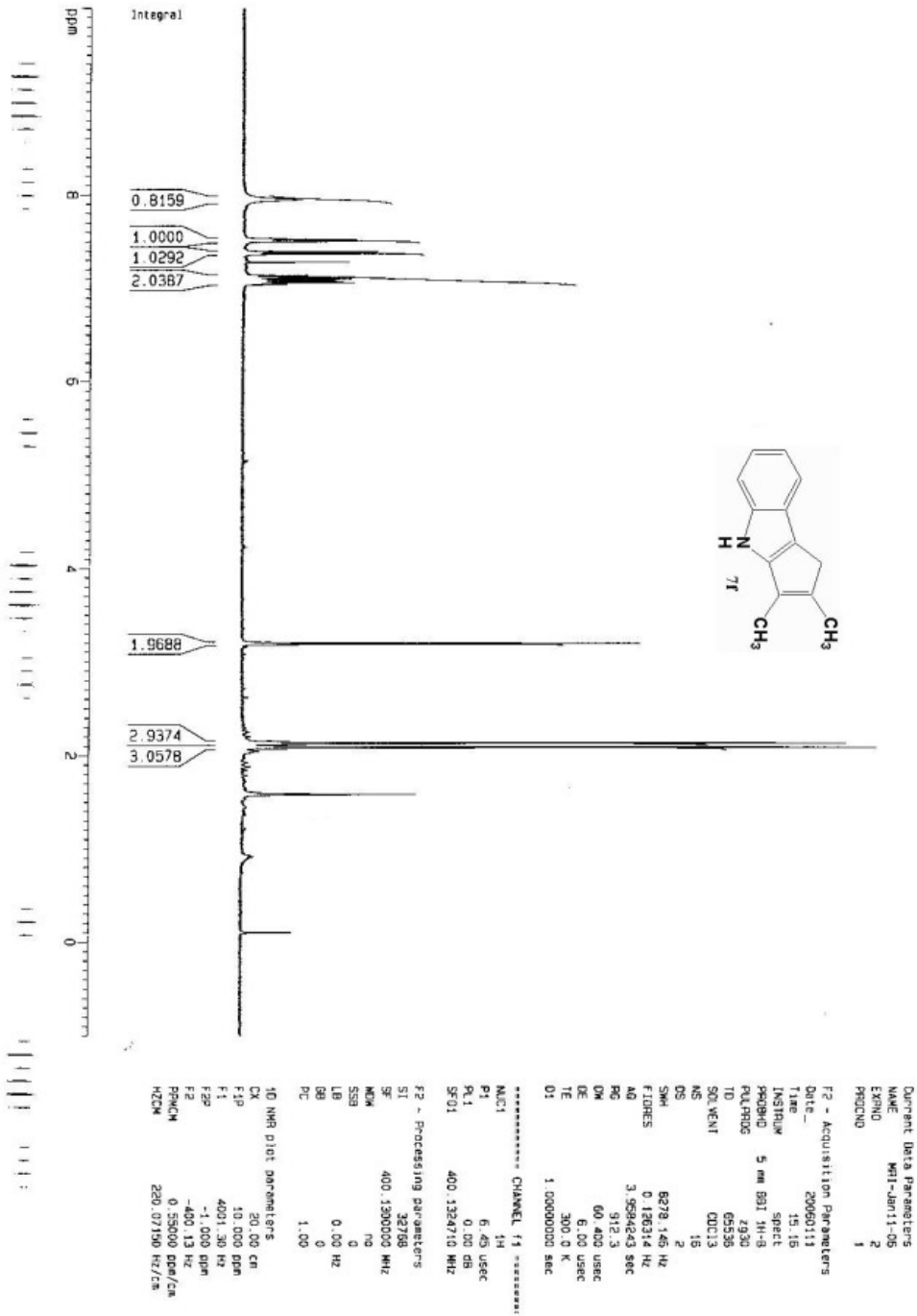
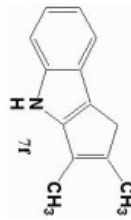
Current Data Parameters
NAME      MRI-IND7-08
EXPNO     5
PROCNO    1
F2 - Acquisition Parameters
Date_     20080107
Time      18.41
INSTRUM   spect
PROBHD    5 mm QNP 1H/1
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         2048
DS         4
SWH        18736.982 Hz
FIDRES     0.288919 Hz
AQ         1.7432075 sec
RG         512
DM         26.600 usec
DE         6.00 usec
TE         300.0 K
D1         2.00000000 sec
D11        0.03000000 sec
D12        0.00002000 sec

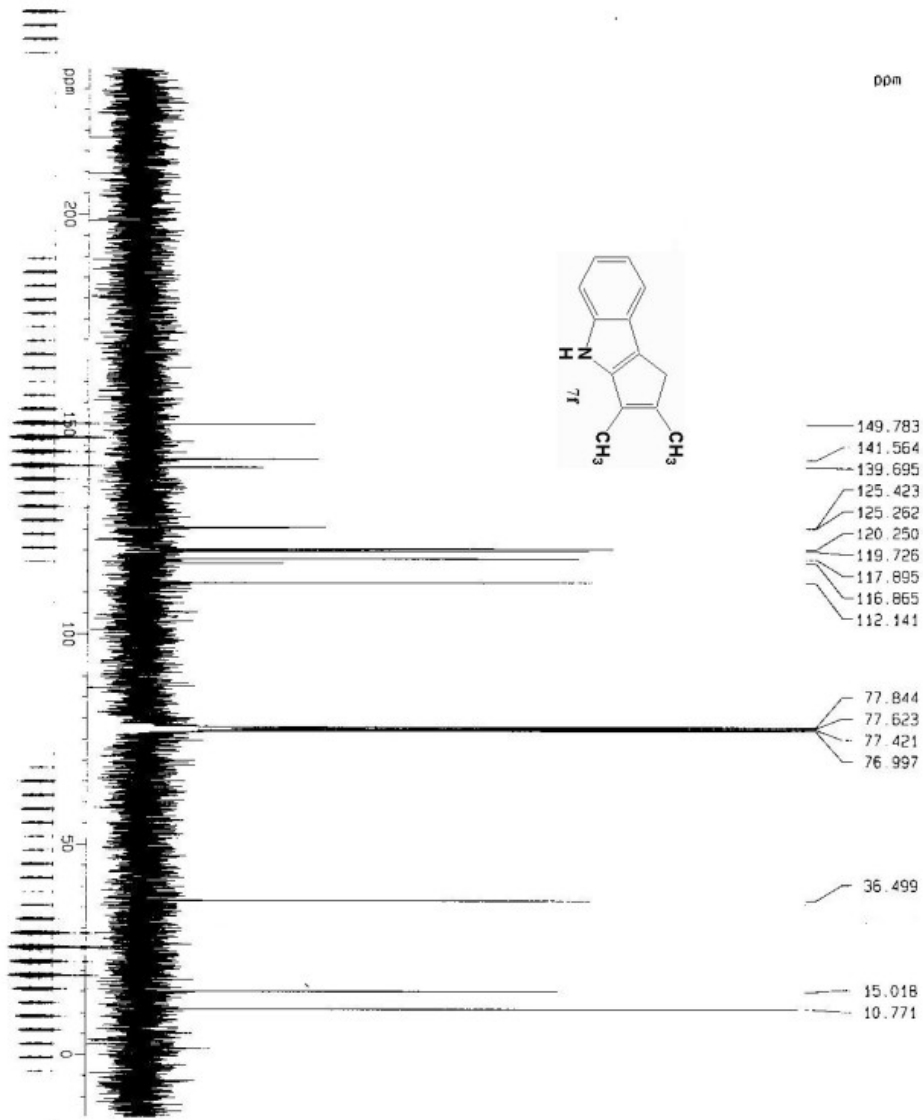
***** CHANNEL f1 *****
NUC1       13C
P1         5.40 usec
PL1        -5.00 dB
SFO1       75.4108357 MHz

***** CHANNEL f2 *****
CPDPRG2    waltz16
NUC2       1H
P2         115.00 usec
PL2         0.00 dB
PL12       20.00 dB
PL13       20.00 dB
SFO2       299.8711955 MHz

F2 - Processing parameters
SI         32768
SF         75.4023410 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

1D NMR plot parameters
CX         50.00 cm
F1P        23.651 ppm
F1         1.7503.21 Hz
F2P        -141.638 cm
F2         -1103.25 Hz
PPMCK      12.46445 pos/cm
HZCK       995.84967 Hz/cm
  
```





- 149.783
- 141.564
- 139.695
- 125.423
- 125.262
- 120.250
- 119.726
- 117.895
- 116.865
- 112.141

- 77.844
- 77.623
- 77.421
- 76.997

- 36.499

- 15.018
- 10.771

```

Current Data Parameters
NAME      WSI-JMS11-06
EXPNO    2
PROCNO   1

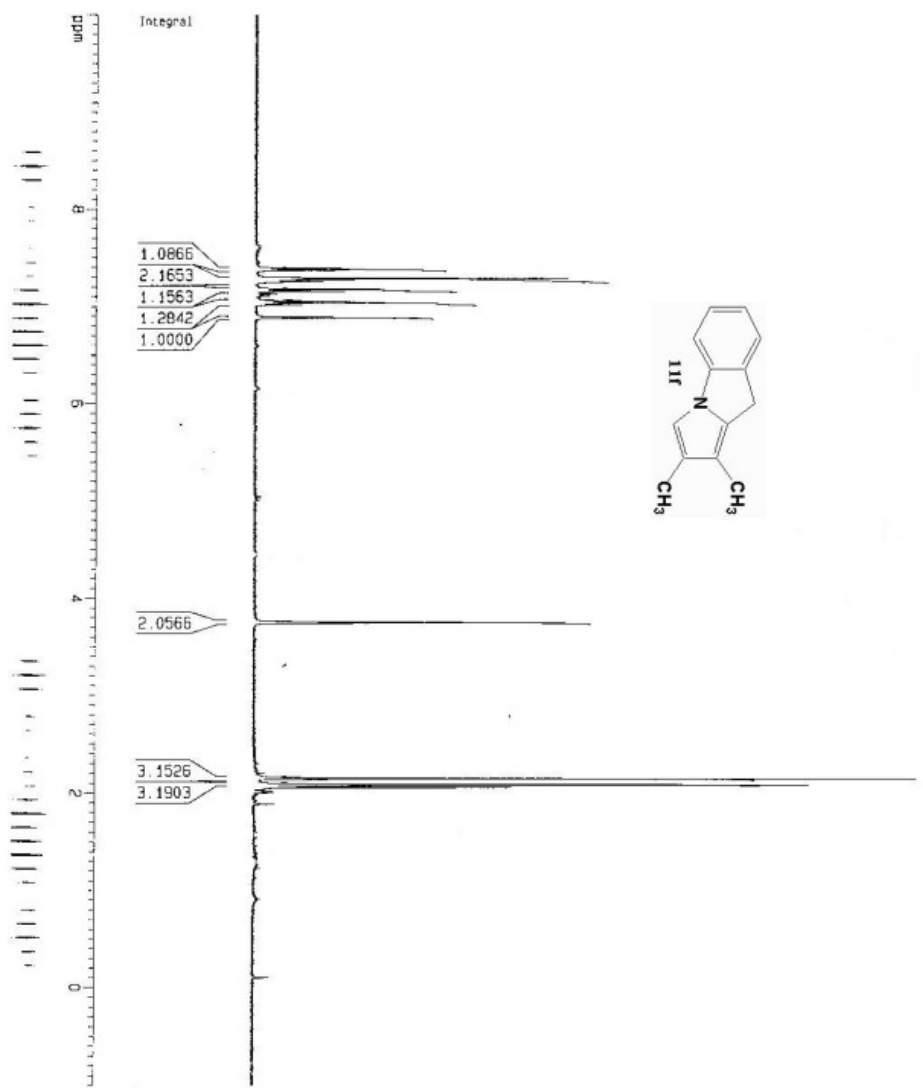
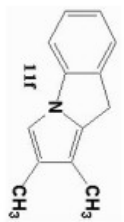
F2 - Acquisition Parameters
Date_    20060112
Time     0.35
INSTRUM  spect
PROBHD   5 mm WULS1nu
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        3500
DS        4
SWH       19832.363 Hz
FIDRES   0.297350 Hz
AQ        1.7400300 sec
RG         65804
DM        25.550 usec
DE        6.00 usec
TE        300.0 K
C1        2.00000000 sec
d11       0.03000000 sec
d12       0.00002000 sec

***** CHANNEL f1 *****
NUC1      13C
P1        11.80 usec
PL1       0.00 dB
SFO1      75.475000 MHz

***** CHANNEL f2 *****
COPROG2   waltz16
NUC2       1H
PCPD2     110.00 usec
PL2       0.00 dB
PL12      17.50 dB
PL13      17.50 dB
SFO2      300.1312000 MHz

F2 - Processing parameters
SI         32768
SF         75.4577190 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

10 NMR data parameters
D1         20.00 sec
F1         229.700 MHz
F2         127.700 MHz
SFO         20.000 MHz
-1500.00 Hz
PRNDM      12.23824 usec/cycle
SOL         CDCl3
HZTM
  
```



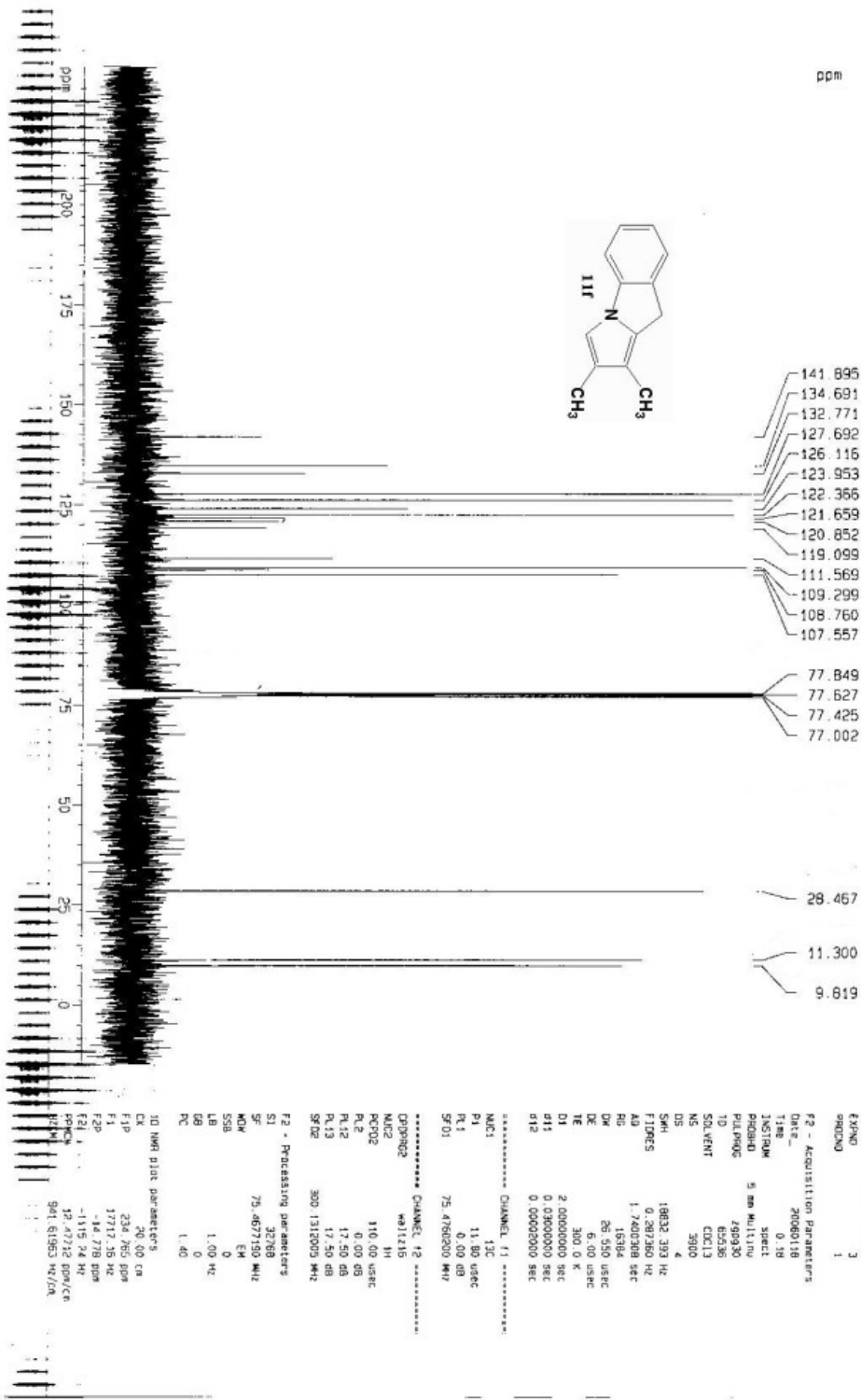
Current Data Parameters
 NAME: 11F-vent-09
 EXPNO: 2
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20050116
 Time: 13.51
 INSTRUM: spect
 PULPROG: zgpg30
 PU: 5.00
 PR: 14.8
 TD: 2930
 SOLVENT: CDCl₃
 NS: 15
 DS: 2
 SWH: 8228.146 Hz
 FIDRES: 0.126314 Hz
 AQ: 3.9594243 sec
 RG: 1448.2
 DW: 60.400 usec
 DE: 6.00 usec
 TE: 300.0 K
 D1: 1.00000000 sec

CHANNEL f1
 NUCl: 1H
 P1: 6.45 usec
 PL1: 0.00 dB
 SFO1: 400.1326710 MHz

F2 - Processing parameters
 SI: 32768
 SF: 400.1300000 MHz
 KW: no
 LB: 0
 GB: 0.00 Hz
 PC: 1.00

ID NMR plot parameters
 CX: 20.00 cm
 F1P: 10.000 gpm
 F1: 4001.30 Hz
 F2P: -1.000 gpm
 F2: -400.13 Hz
 PPM/CM: 0.56000 gpm/cm
 MZCK: 220.07150 Hz/cm



```

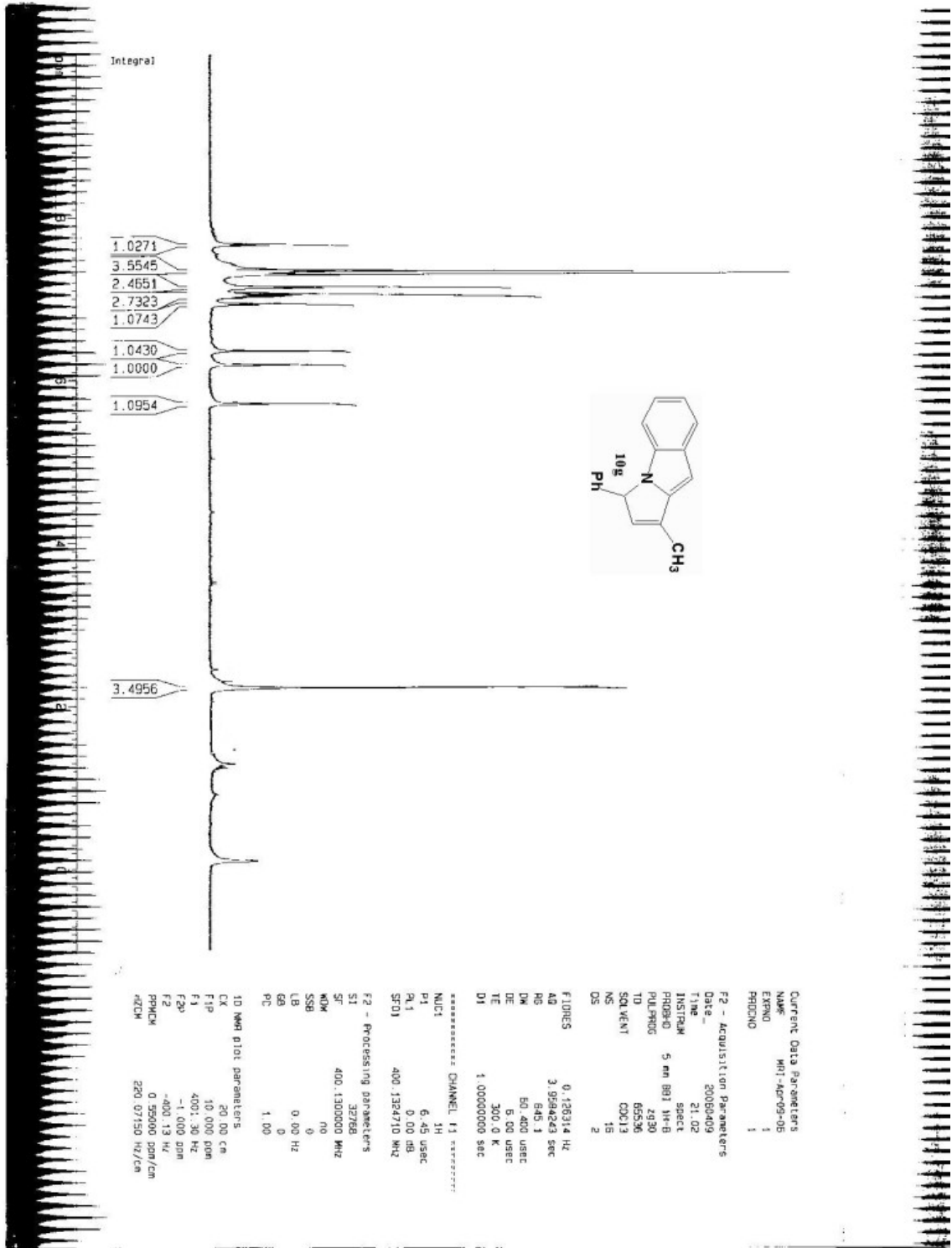
Current Data Parameters
NAME      MNI-1017-06
EXPNO    3
PROCNO   1
Date_     2006110
Time      08:19
INSTRUM  spect
PROBHD   5 mm MUX150
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        3990
DS        4
SWH       18632.393 Hz
FIDRES    0.287260 Hz
AQ        1.7240208 sec
RG         18784
DM        26.550 usec
DE        6.00 usec
TE        300.0 K
D1        2.00000000 sec
d11       0.03000000 sec
d12       0.00020000 sec

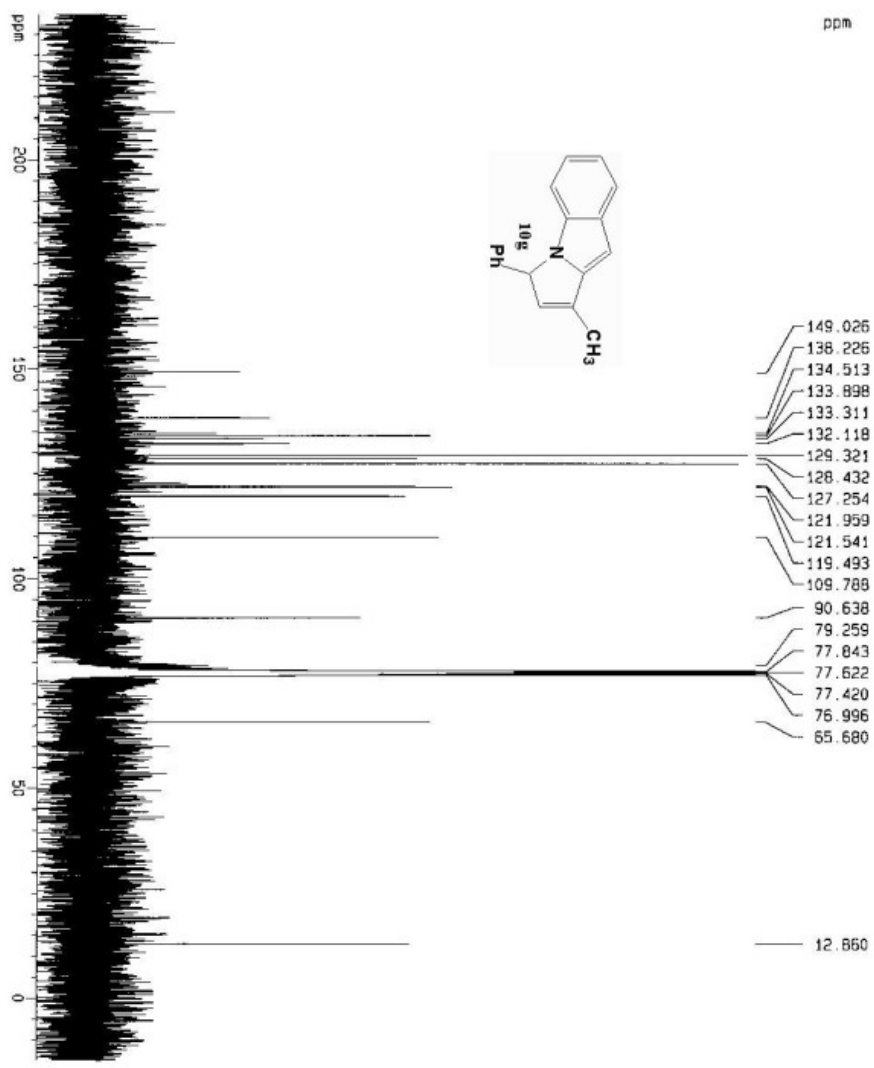
----- CHANNEL f1 -----
NUC1      13C
P1        11.80 usec
PL1       0.00 dB
SFO1      75.476200 MHz

----- CHANNEL f2 -----
OPPRG2   wa1z1b
NUC2      1H
PCPD2    110.00 usec
PL2       0.00 dB
PL12     17.50 dB
PL13     17.50 dB
SFO2     300.1312000 MHz

F2 - Processing parameters
SI        32768
SF        75.467150 MHz
WDW       EM
SSB       0
GB        1.00 Hz
DB        0
PC        1.40

3D NMR plot parameters
CX        20.00 cm
F1P       234.265 ppm
F1        17717.35 Hz
F2P       -14.778 ppm
F2        -1115.24 Hz
PPCK     32.47712 ppm/cm
RZNM     941.61963 Hz/cm
  
```



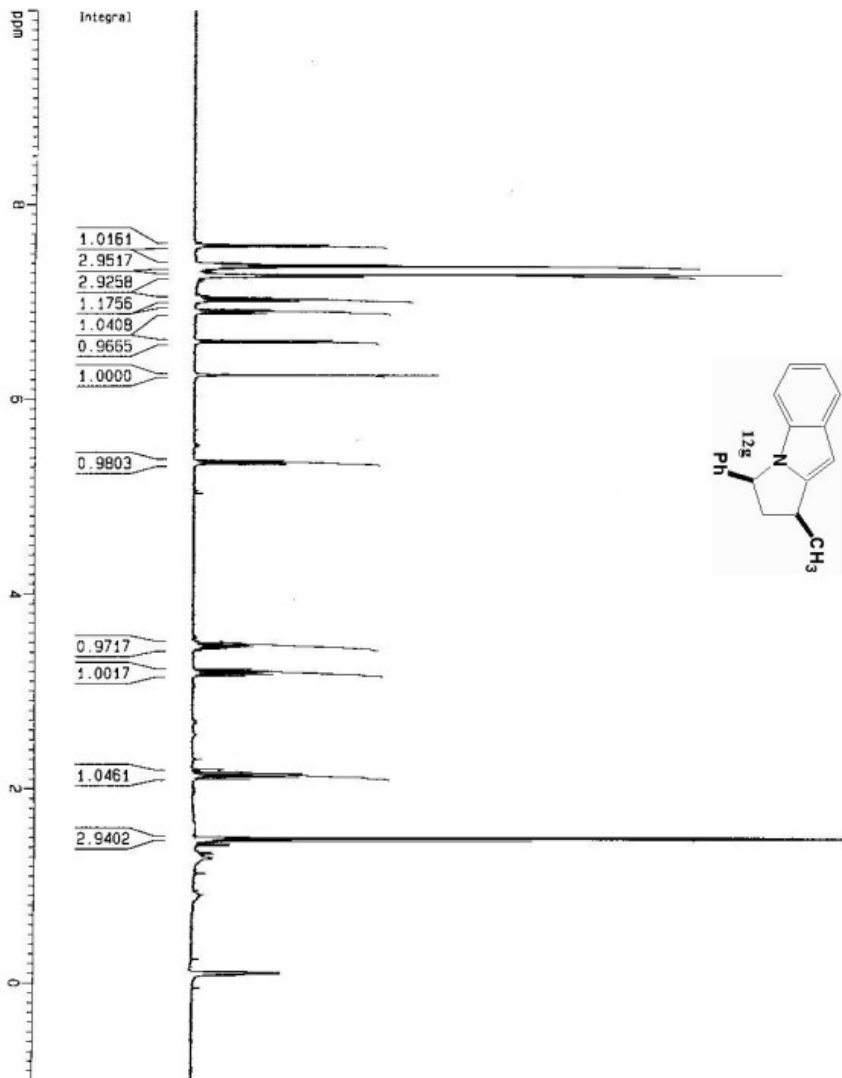
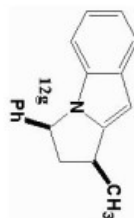


- 149.026
- 138.226
- 134.513
- 133.898
- 133.311
- 132.118
- 129.321
- 128.432
- 127.254
- 121.959
- 121.541
- 119.493
- 109.788
- 90.638
- 79.259
- 77.843
- 77.622
- 77.420
- 76.996
- 65.680

12.650

```

Current Data Parameters
NAME      MRI-AP09-06
EXPNO     3
PROCNO    1
-----
F2 - Acquisition Parameters
Date_     20060410
Time      8.13
INSTRUM   spect
PROBHD    5 mm Multicou
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         10448
DS         4
SWH        18932.393 Hz
FIDRES     0.267360 Hz
AQ          1.7460208 sec
RG          1119.6
DE         0E 500 usec
TE          300.0 K
D1          2.00000000 sec
d11         0.03000000 sec
d12         0.00000000 sec
-----
***** CHANNEL f1 *****
NUC1       13C
P1         14.90 usec
PL1        0.00 dB
SFO1       75.4763200 MHz
-----
***** CHANNEL f2 *****
CPDPRG2   mbl1215
NUC2       1H
PCPD2     110.00 usec
PL2        0.00 dB
PL12       17.50 dB
PL13       17.50 dB
SFO2       300.1318005 MHz
-----
F2 - Processing parameters
SI         32768
SF         75.467190 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
-----
1D NMR plot parameters
CX         50.00 cm
F1P        234.780 DPM
F1         17717.48 Hz
F2         -1009.36 Hz
PASCAL    13 73834 opa/cm
NTCPC     951 32956 Hz/cm
  
```



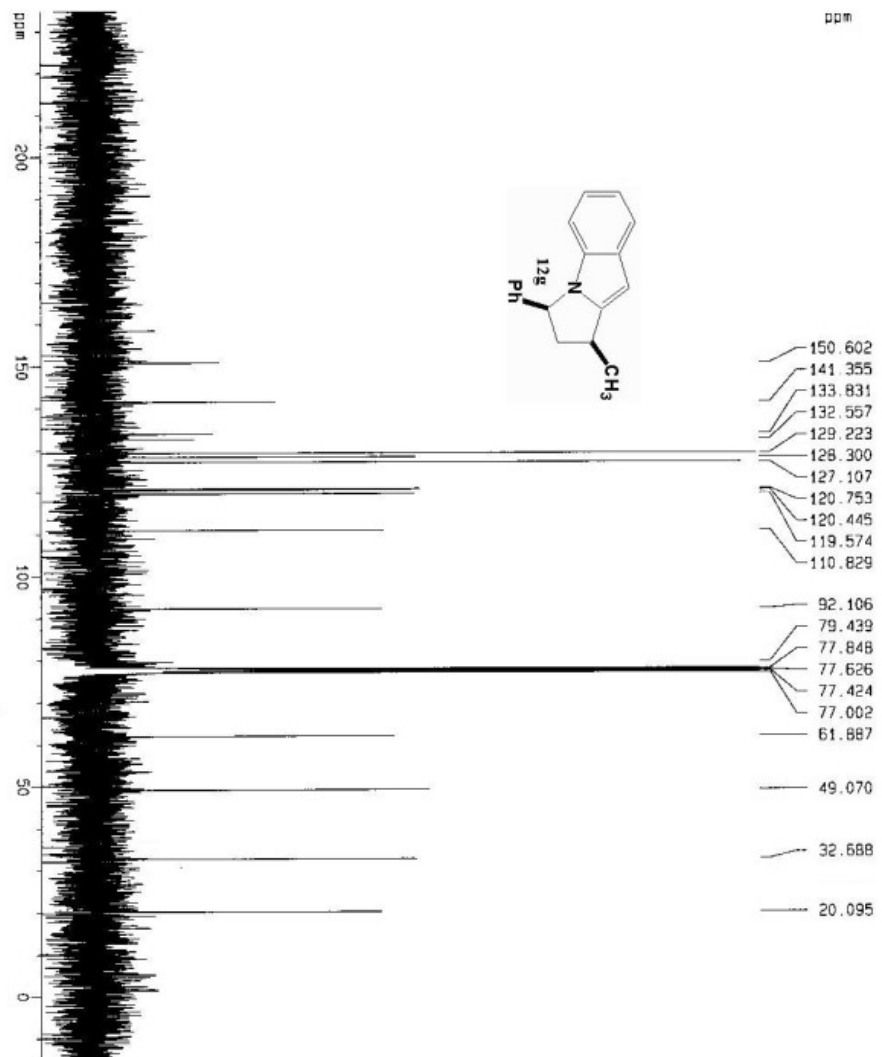
Current Data Parameters
 NAME M01-Nov12-05
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051112
 Time 10.58
 INSTRUM spect
 PROBHD 5 mm BBI 1H-3
 PULPROG zgpg30
 TD 65535
 SOLVENT DMS-D3
 NS 15
 DS 2
 SMH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.5984243 sec
 RG 724.1
 DE 50.400 usec
 DM 5.00 usec
 TE 300.0 K
 D1 1.00000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 8.45 usec
 PL1 0.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 27756
 SF 400.1300000 MHz
 MDW no
 SSB 0
 LB 0.00 Hz
 BR 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 FIP 10.000 ppm
 F1 4001.30 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPM0H 0.35000 ppm/cm
 NCHW 220.07150 Hz/cm



- 150.602
- 141.355
- 133.831
- 132.557
- 129.223
- 128.300
- 127.107
- 120.753
- 120.445
- 119.574
- 110.829
- 92.106
- 79.439
- 77.848
- 77.626
- 77.424
- 77.002
- 61.887
- 49.070
- 32.688
- 20.095

```

Current Data Parameters
NAME          M01-04/12-05
EXPNO         1
PROCNO        1

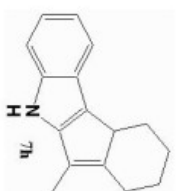
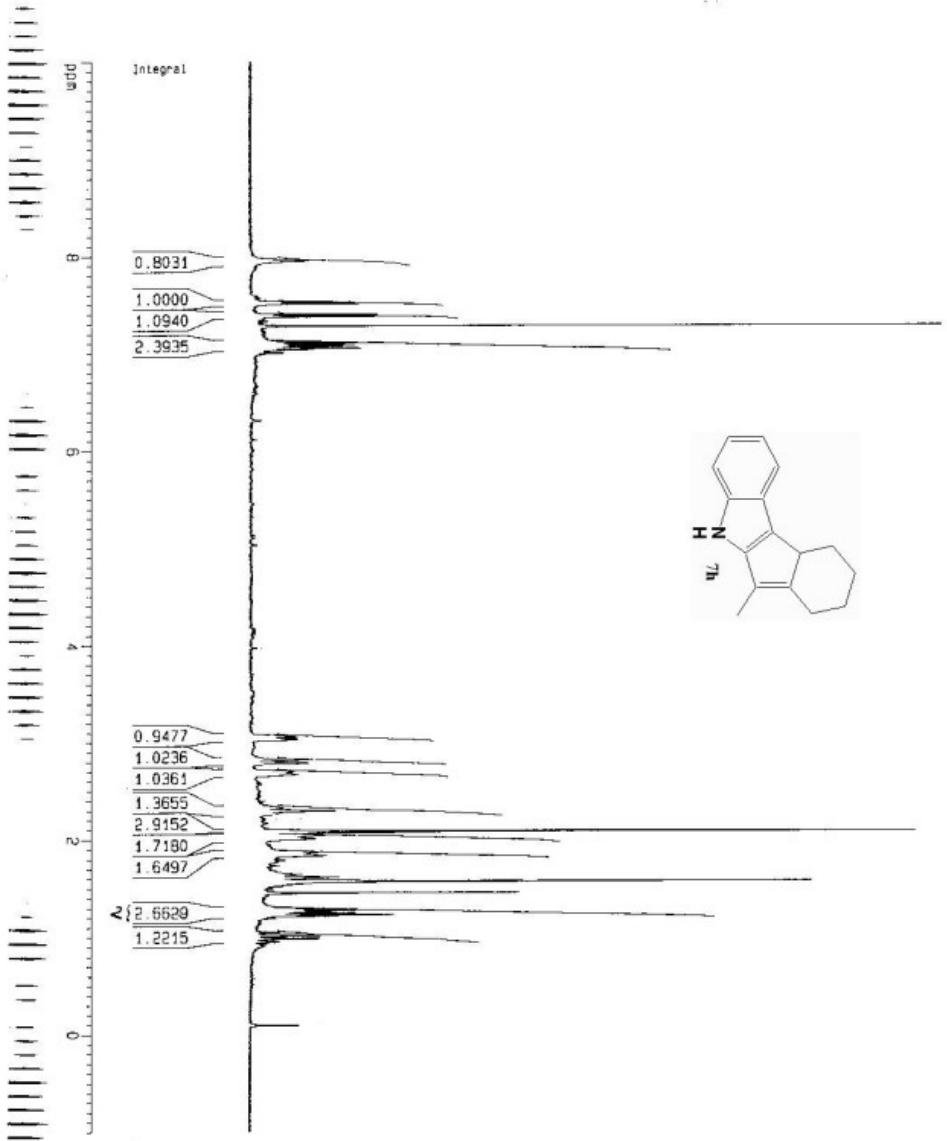
F2 - Acquisition Parameters
Date_         20051112
Time          13.38
INSTRUM      spect
PROBHD      5 mm HLL1nu
PULPROG      zgpg30
TD           65536
SOLVENT      CDCl3
NS           2233
DS           4
SFO1         100.625 MHz
FIDRES       0.2407860 Hz
AQ           1.7400308 sec
RG           11588.2
DM           26.550 usec
DE           5.00 usec
TE           300.0 K
O1           2.0000000 sec
O2           0.0300000 sec
O3           0.0002000 sec
O4           0.0002000 sec

***** CHANNEL f1 *****
NUC1          13C
P1           11.80 usec
PC1          0.00 dB
SFO1         75.4762000 MHz

***** CHANNEL f2 *****
CPDPRG2      waltz16
NUC2          1H
P2           110.00 usec
PC2          0.00 dB
SFO2         500.1320000 MHz

F2 - Processing parameters
SI           32768
SF           75.4671500 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40

1D NMR plot parameters
CK           20.00 cm
F1P          234.765 ppm
F2P          17171.15 Hz
F2           -20.000 ppm
DPRCHM      12.73854 ppm/cm
SFO1         75.4671500 MHz
SFO2         500.1320000 MHz
  
```



Current Data Parameters
 NAME KR1-JAN21-05
 EXPNO 7
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20080121
 Time 17.36
 INSTRUM spect
 PROBRD 5 mm BBI 1H-B
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8078.146 Hz
 FIDRES 0.189314 Hz
 AQ 3.9584243 sec
 RG 322.5
 DM 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

***** CHANNEL f1 *****

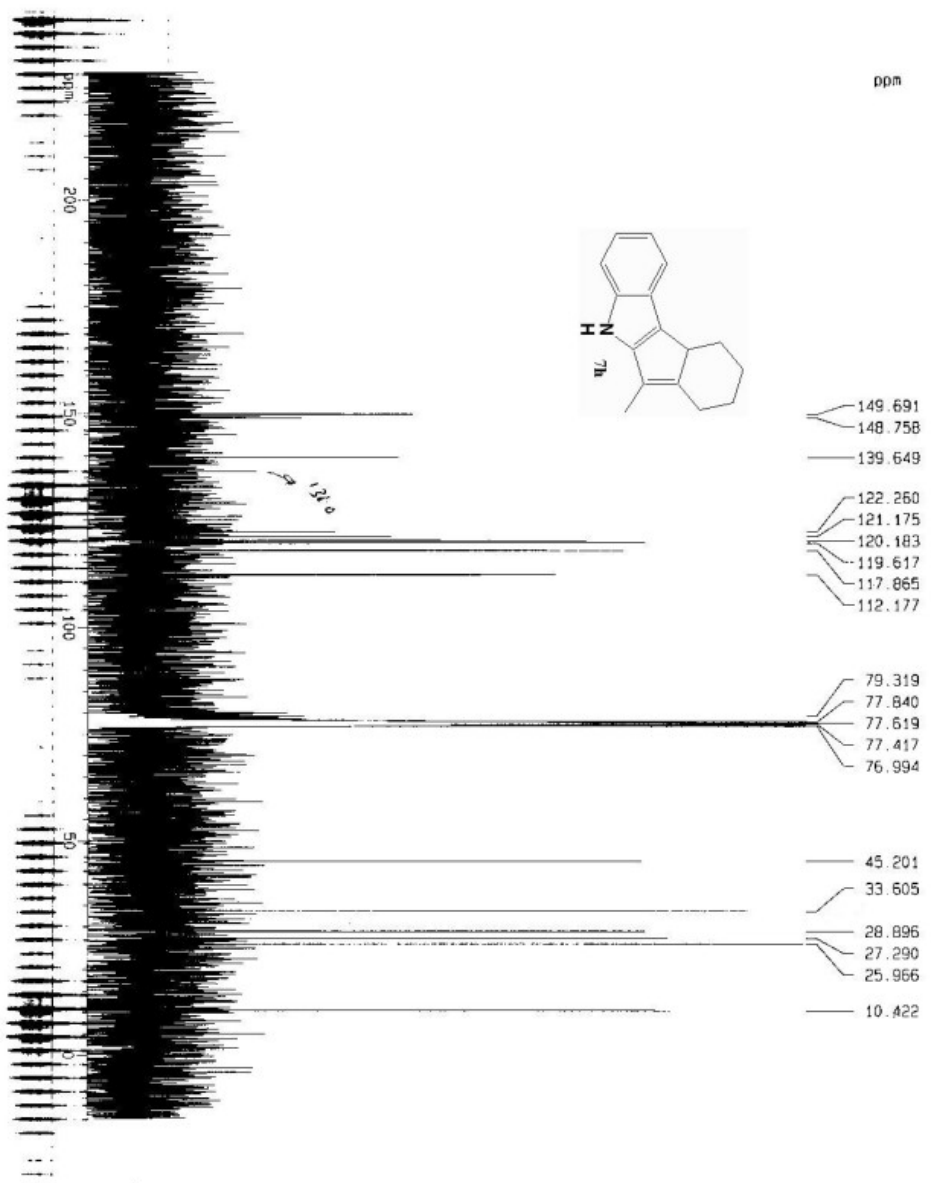
NUC1 1H
 P1 6.45 usec
 PL1 0.00 dB
 SF01 400.1326710 MHz

F2 - Processing parameters

SI 32768
 SF 400.1300000 MHz
 MDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR pilot parameters

CX 20.00 ca
 F1P 10.000 ppm
 F1 4001.30 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPM/CM 0.55000 ppm/cm
 HZ/CM 280.07150 Hz/cm



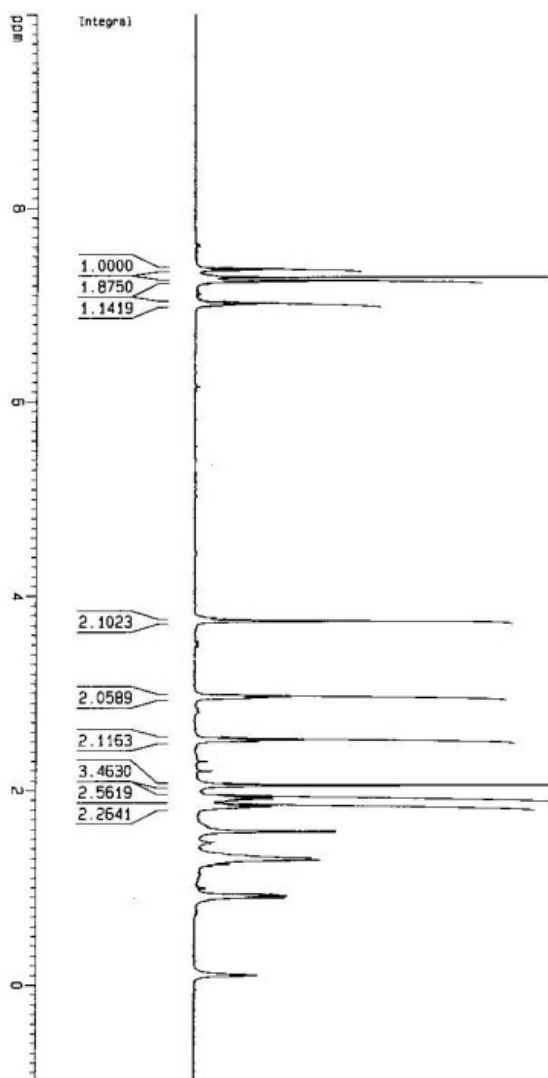
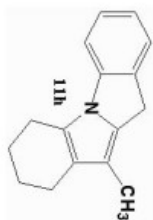
- 149.691
- 148.758
- 139.649
- 122.260
- 121.175
- 120.183
- 119.617
- 117.865
- 112.177

- 79.319
- 77.840
- 77.619
- 77.417
- 76.994

- 45.201
- 33.605
- 28.896
- 27.290
- 25.966
- 10.422

```

Current Data Parameters
NAME      M01-0007-05
EXPNO    4
PROCNO   1
-----
F2 - Acquisition Parameters
Date_    20080122
Time     08:31
INSTRUM  spect
PROBHD   5 mm WALTZ
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       7000
DS       4
SWH      19832.353 Hz
FIDRES   0.292760 Hz
AQ       1.72400108 sec
RG       115601.2
DM       25.540 usec
DE       6.00 usec
TE       300.0 K
SFO1     2.00000000 sec
SFO2     0.03000000 sec
SFO3     0.00020000 sec
-----
CHANNEL F1
NUC1      13C
P1       11.80 usec
PL1      0.00 dB
SFO1     75.4762000 MHz
-----
CHANNEL F2
PROBHD   WALTZ16
NUC2      1H
P2       110.00 usec
PL2      0.00 dB
PL12     47.50 dB
PL13     47.50 dB
SFO2     300.1312000 MHz
-----
F2 - Processing parameters
SI       32768
SF       75.4677150 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
-----
1D NMR plot parameters
CX       20.00 cm
F1P      230.000 MHz
F1       47257.57 Hz
F2P      20.000 MHz
F2       -15691.36 MHz
NUC1     12.50000000 MHz
PCWHICH 12.50000000 MHz
H2C1M   943.246500000 Hz
  
```



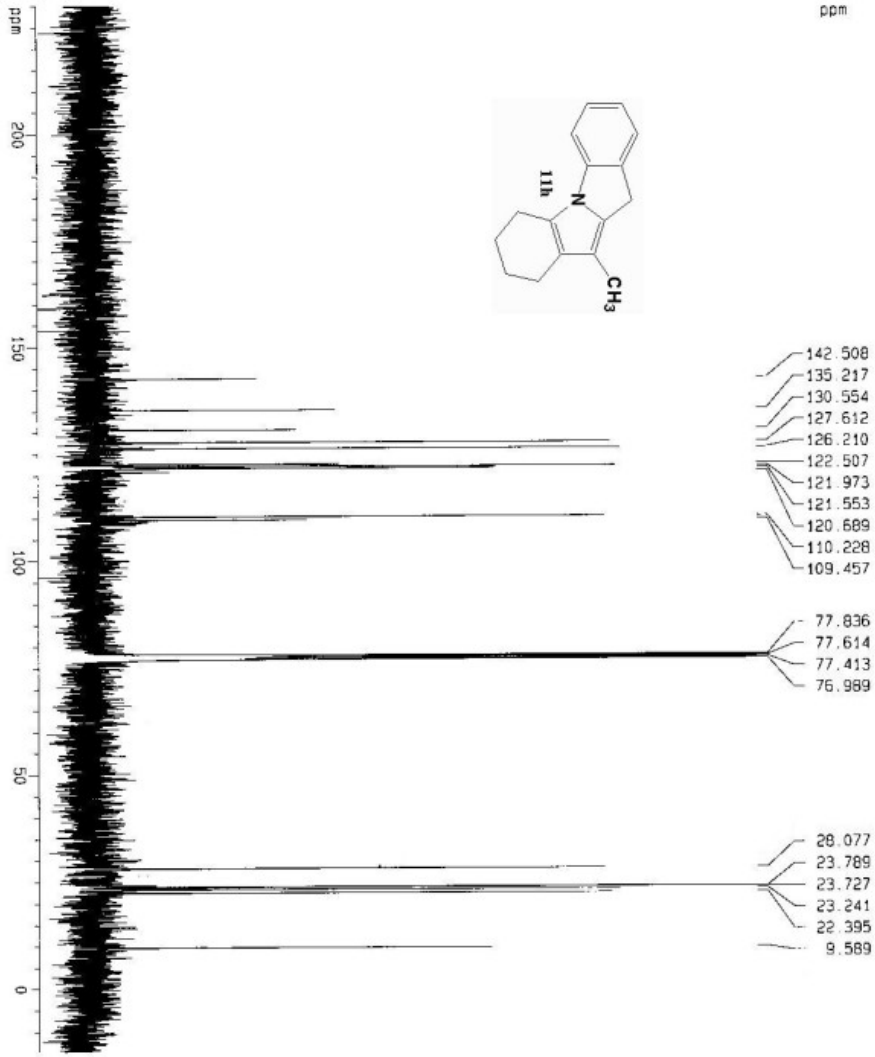
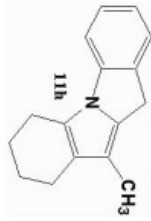
Current Data Parameters
 NAME NRI-JUNE1-05
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050621
 Time 19.00
 INSTRUM spect
 PROBRG 5 mm BBI 1H-9
 PULPROG zg30
 TO 65536
 SOLVENT CDCl₃
 NS 32
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.183314 Hz
 AQ 3.5584243 sec
 RG 512
 DM 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 6.45 usec
 PL1 0.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 10.000 ppm
 F1 -4001.30 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PRNOM 0.55000 ppm/cm
 NTCOM 220.07150 Hz/cm



```

Current Data Parameters
NAME      M01-0h21-05
EXPNO    4
PROCNO   1

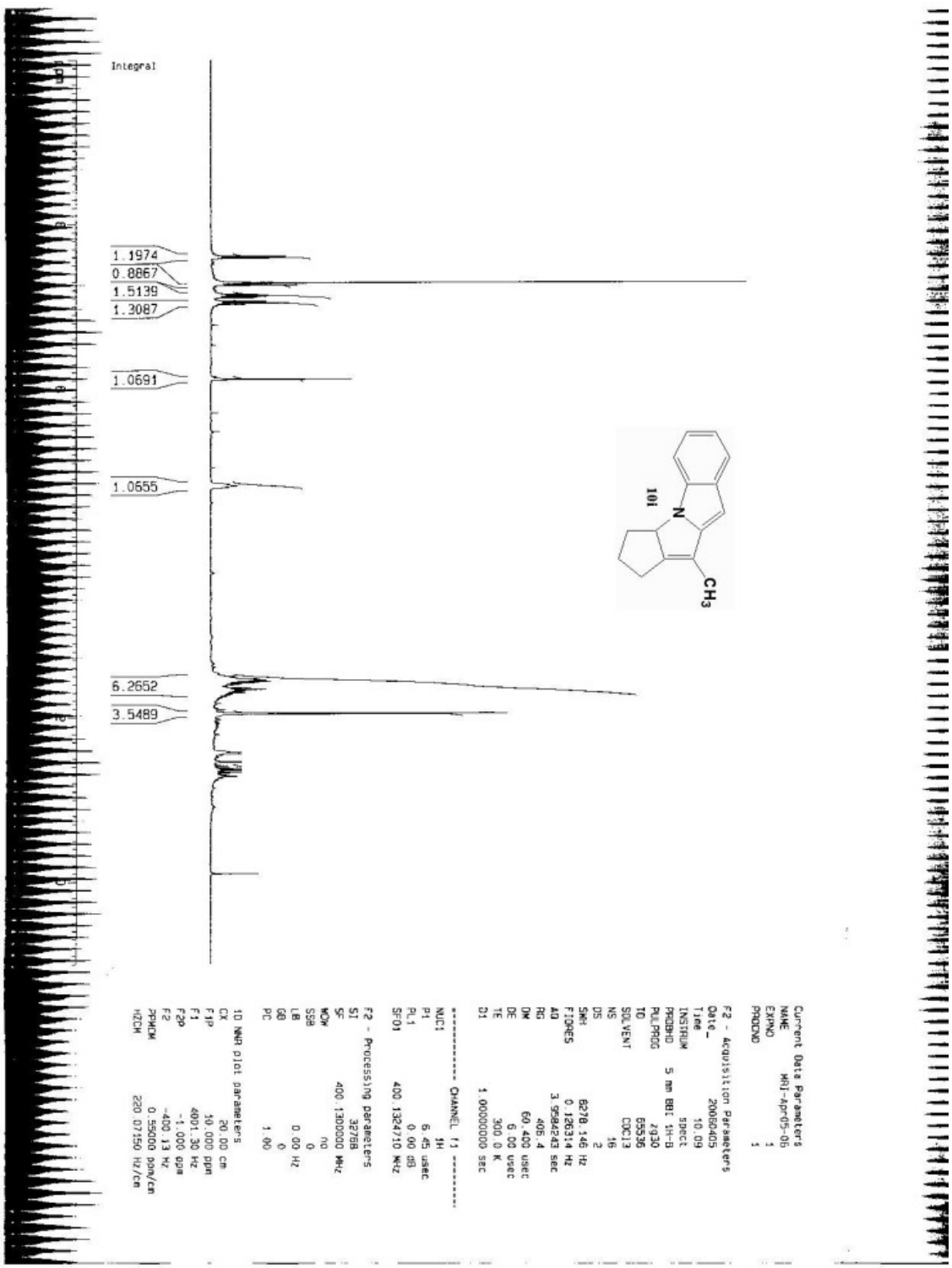
F2 - Acquisition Parameters
Date_    20080122
Time     5.40
INSTRUM  spect
PROBHD   5 mm QNP 1H/1
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        8000
DS        4
SWH       18795.992 Hz
FIDRES    0.286819 Hz
AQ         1.7423076 sec
RG         514.7
DE         26.600 usec
TE         300.0 K
D1         2.80000000 sec
D11        0.03000000 sec
D12        0.00020000 sec

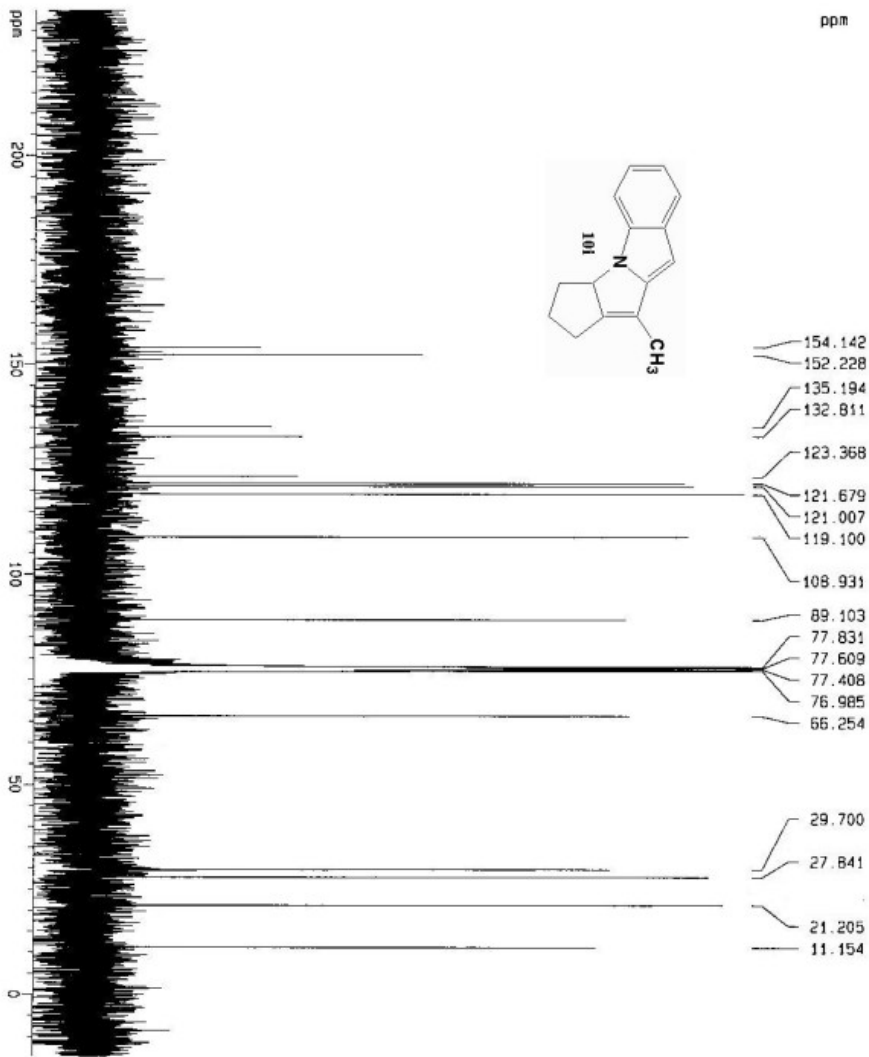
----- CHANNEL f1 -----
NUC1      13C
P1         5.40 usec
PL1       -6.00 dB
SFO1      75.410637 MHz

----- CHANNEL f2 -----
COPROG2   waltz16
NUC2       1H
P2         115.00 usec
PL2        0.00 dB
PL12       20.00 dB
PL13       20.00 dB
SFO2      299.8711995 MHz

F2 - Processing parameters
SI         32768
SF         75.4023410 MHz
WDW        EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40

10 NMR plot parameters
CX          20.00 cm
F1         230.000 ppm
F2         17342.54 Hz
F2a        -20.000 ppm
F2b        -1508.05 Hz
F2c        32.50000 ppm/cm
HZCM       542.58330 Hz/cm
  
```





- 154.142
- 152.228
- 135.194
- 132.811
- 123.368
- 121.679
- 121.007
- 119.100
- 108.931
- 89.103
- 77.831
- 77.609
- 77.408
- 76.985
- 66.254
- 29.700
- 27.841
- 21.205
- 11.154

```

Current Data Parameters
NAME      M1-467-06
EXPNO    2
PROCNO   1

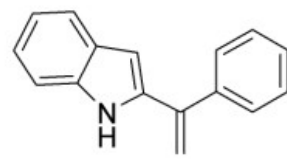
F2 - Acquisition Parameters
Date_    20040717
Time     09:49
INSTRUM  spect
PROBHD   5 mm M111pro
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        17000
DS        4
SFO1     100.625000 MHz
FIDRES   0.267360 Hz
AQ       1.7400308 sec
RG       11595.2
DM       28.550 usec
DE       6.00 usec
TE       300.0 K
D1       2.00000000 sec
d11      0.23000000 sec
d12      0.10000000 sec

***** CHANNEL f1 *****
NUC1      13C
P1       11.80 usec
PL1      0.00 dB
SFO1     75.4750200 MHz

***** CHANNEL f2 *****
CPDPRG2  waltz16
NUC2      1H
P2       150.00 usec
PL2      0.00 dB
PL12     17.50 dB
PL13     17.50 dB
SFO2     300.1352605 MHz

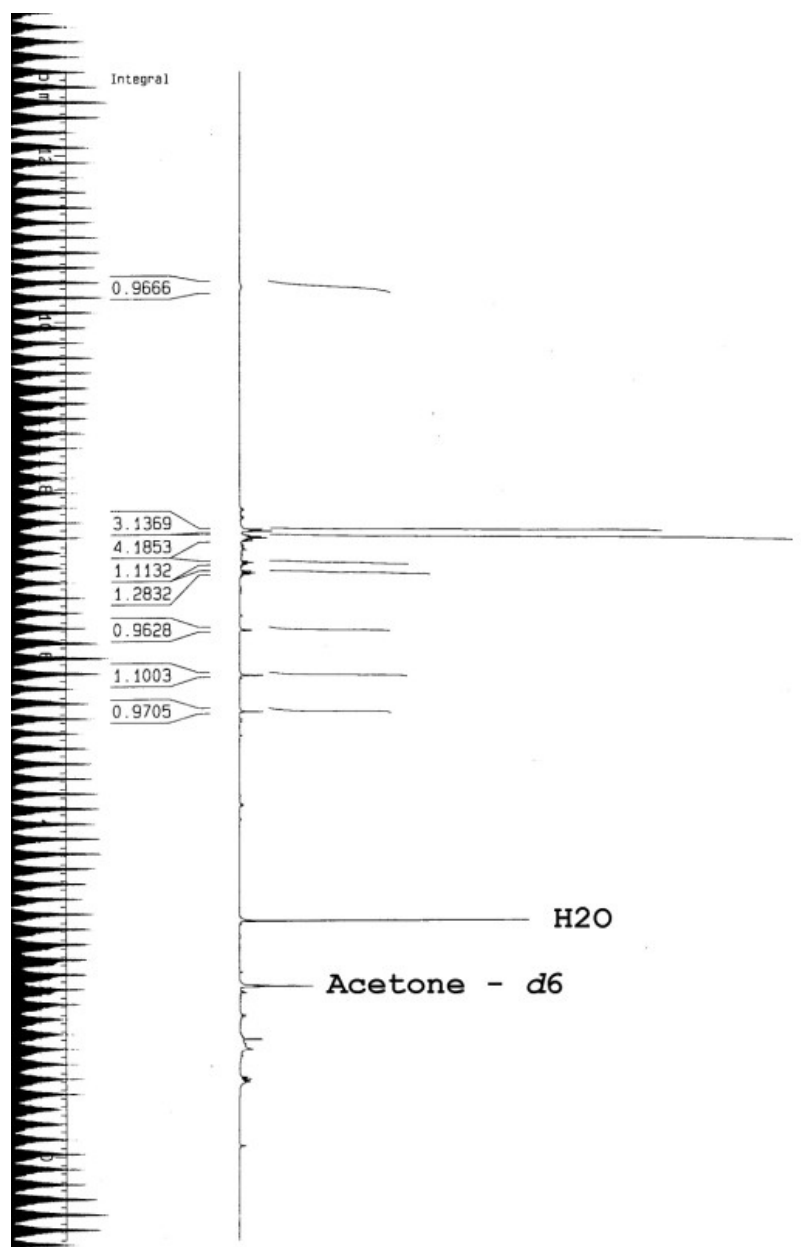
F2 - Processing parameters
SI       32768
SF       75.4677190 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40

1D NMR Data Parameters
CX       20.00 cm
F1P      234.765 ppm
F1       117.1715 Hz
F2P      -30.000 ppm
F2       -1501.35 Hz
PEPICK   12.73623 conv/cm
HZCW     581.32950 Hz/cm
  
```



14j

DKH2-297P



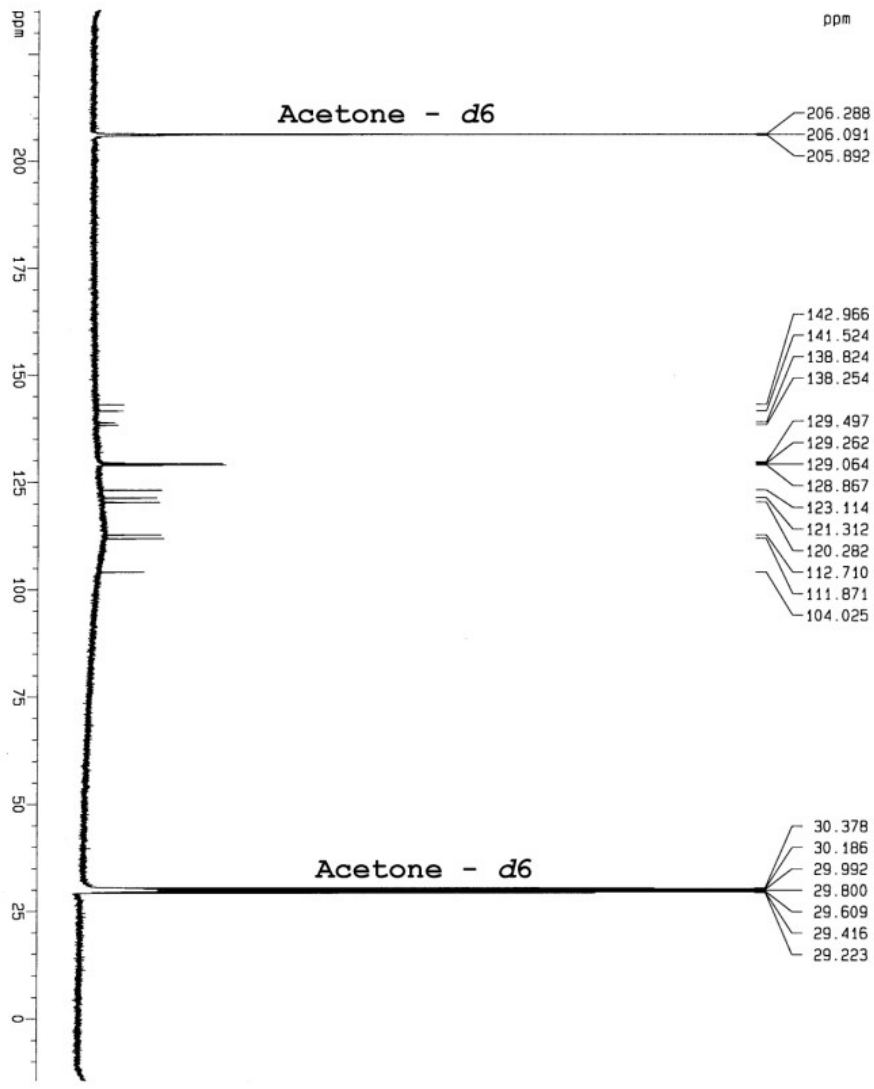
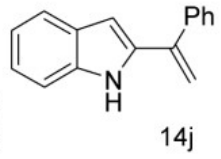
Current Data Parameters
 NAME DKH2-297P
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060407
 Time 13.44
 INSTRUM spect
 PROBRHD 5 mm BBI 1H-B
 PULPROG zg30
 TD 65536
 SOLVENT Acetone
 NS 16
 DS 2
 SMH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9598243 sec
 RG 228.1
 DM 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 6.45 usec
 PL1 0.00 dB
 SF01 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300106 MHz
 KDM no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

10 NMR plot parameters
 CX 20.00 cm
 FIP 13.000 ppm
 F1 5201.69 Hz
 F2p -1.000 ppm
 F2 -400.13 Hz
 PPM/CM 0.70000 ppm/cm
 HZCM 280.09100 Hz/cm



DKH2-110 Product

```

Current Data Parameters
NAME          DKH2-110
EXPNO         666
PROCNO        1

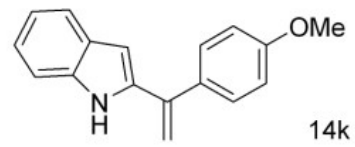
F2 - Acquisition Parameters
Date_         20060422
Time          17.36
INSTRUM       spect
PROBHD        5 mm BBO 1H-13
PULPROG       zgpg30
TD            65536
SOLVENT       Acetone
NS            2000
DS            4
SWH            25126.629 Hz
FIDRES        0.383397 Hz
AQ            1.3042164 sec
RG            4066
DE            13.900 usec
TE            300.0 K
D1            2.00000000 sec
d12           0.03000000 sec
d13           0.00002000 sec

***** CHANNEL f1 *****
NUC1           13C
P1            16.35 usec
PL1           -6.00 dB
SFO1          100.6237959 MHz

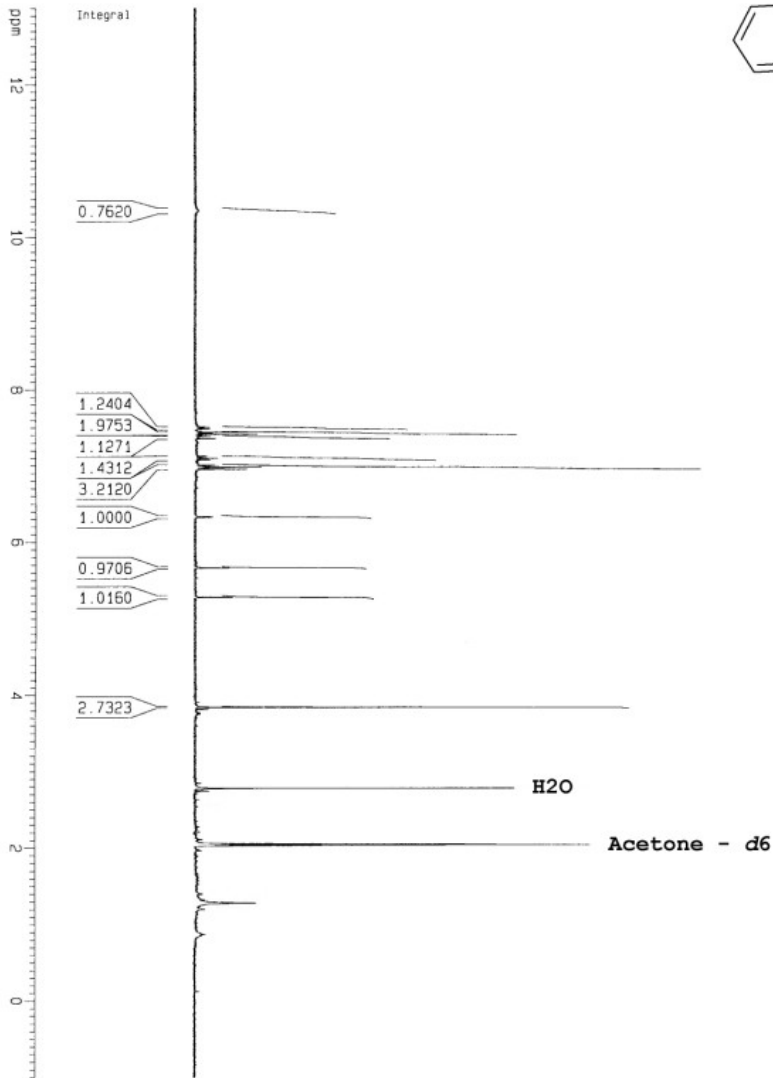
***** CHANNEL f2 *****
CPDPRG2       waltz16
NUC2           1H
PCPD2         114.00 usec
PL2           0.00 dB
PL12          24.00 dB
PL13          24.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI            32768
SF            100.6126821 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

1D NMR plot parameters
CX            20.00 cm
F1P           235.340 ppm
F1            2352.561 Hz
F2P           -149.03 Hz
F2            -12.48531 ppm/cm
H2C1M         1256.28137 Hz/cm
  
```



DKH2-172 Flush product purified



```

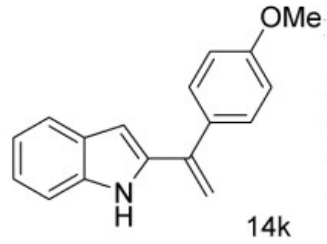
Current Data Parameters
NAME      DKH2-172FP
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20051123
Time     16.37
INSTRUM  spect
PROBHD   5 mm NUC1Hn
PULPROG  zg30
TD        65536
SOLVENT  Acetone
NS        16
DS        2
SH1       6172.839 Hz
FIDRES    0.094190 Hz
AQ         5.308660 sec
RG         724.1
DM         81.000 usec
DE         6.00 usec
TE         300.0 K
D1         1.00000000 sec

***** CHANNEL f1 *****
NUC1      1H
P1         9.60 usec
PL1       -6.00 dB
SFO1      300.1318934 MHz

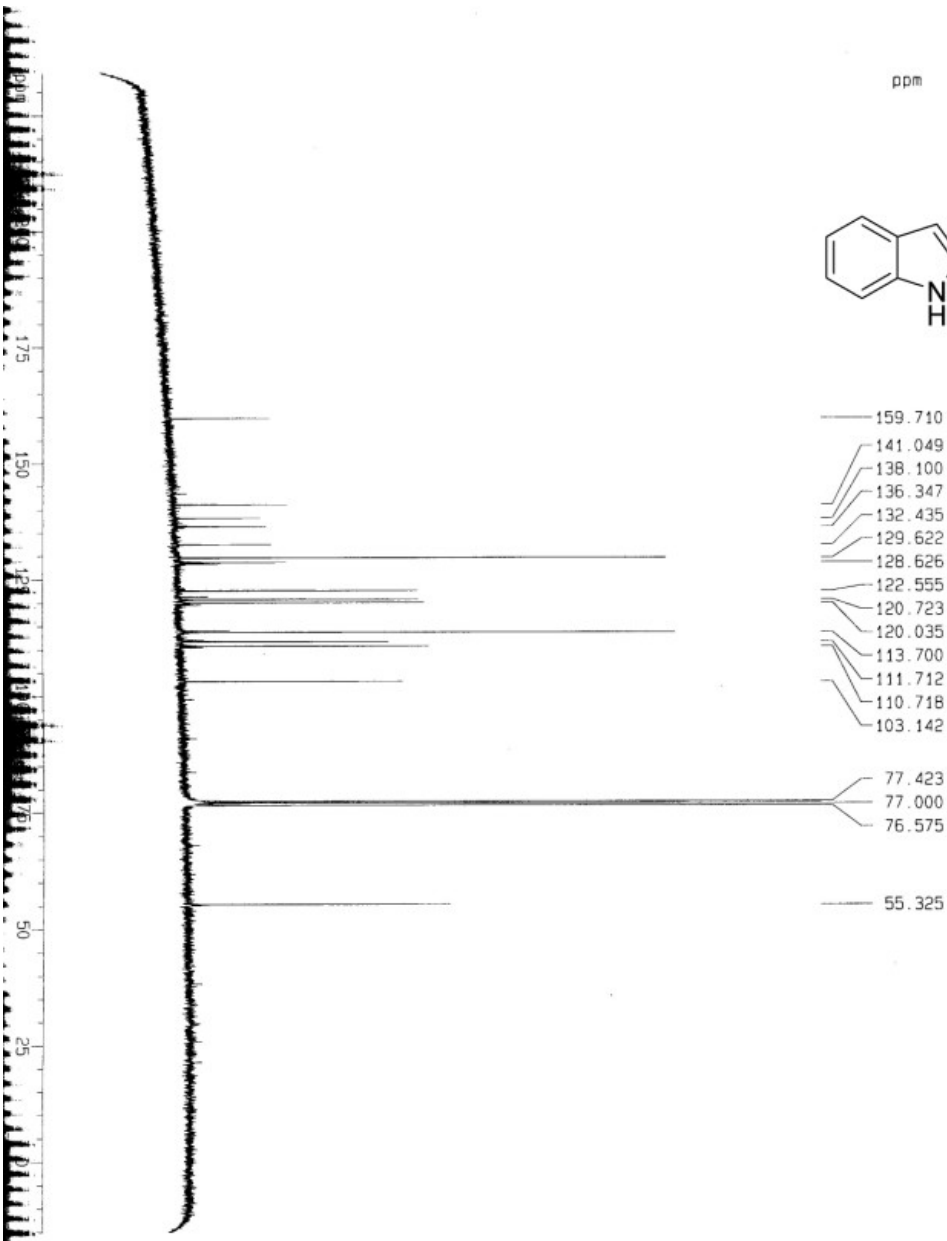
F2 - Processing parameters
SI         32768
SF         300.1300071 MHz
WDW        no
SSB        0
LB         0.00 Hz
GB         0
PC         1.00

1D NMR plot parameters
CX         20.00 cm
F1P        13.000 dpm
F1         3901.69 Hz
F2P        -1.000 dpm
F2         -300.13 Hz
PPOCKM    0.70000 dpm/cm
HZCM       210.09100 Hz/cm
  
```



DKH2-299 Product

- 159.710
- 141.049
- 138.100
- 136.347
- 132.435
- 129.622
- 128.626
- 122.555
- 120.723
- 120.035
- 113.700
- 111.712
- 110.718
- 103.142
- 77.423
- 77.000
- 76.575
- 55.325



```

Current Data Parameters
NAME      DKH2-299P
EXPNO    686
PROCNO   1

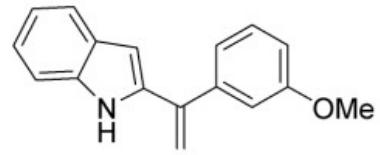
F2 - Acquisition Parameters
Date_    20060413
Time     15.26
INSTRUM spect
PROBHD   5 mm QNP 1H/1
PULPROG zgpg30
TD       65536
SOLVENT  CDCl3
NS       1119
DS       4
SMH      18736.992 Hz
FIDRES   0.286819 Hz
AQ       1.743076 sec
RG       1024
DM       26.600 usec
DE       6.00 usec
TE       300.0 K
O1       2.00000000 sec
D11      0.03000000 sec
D12      0.00002000 sec

***** CHANNEL f1 *****
NUC1     13C
P1       5.40 usec
PL1      -8.00 dB
SFO1     75.4106537 MHz

***** CHANNEL f2 *****
CPDPRG2  waltz16
NUC2     1H
P2       115.00 usec
PL2      0.00 dB
PL12     20.00 dB
PL13     20.00 dB
SFO2     299.8719995 MHz

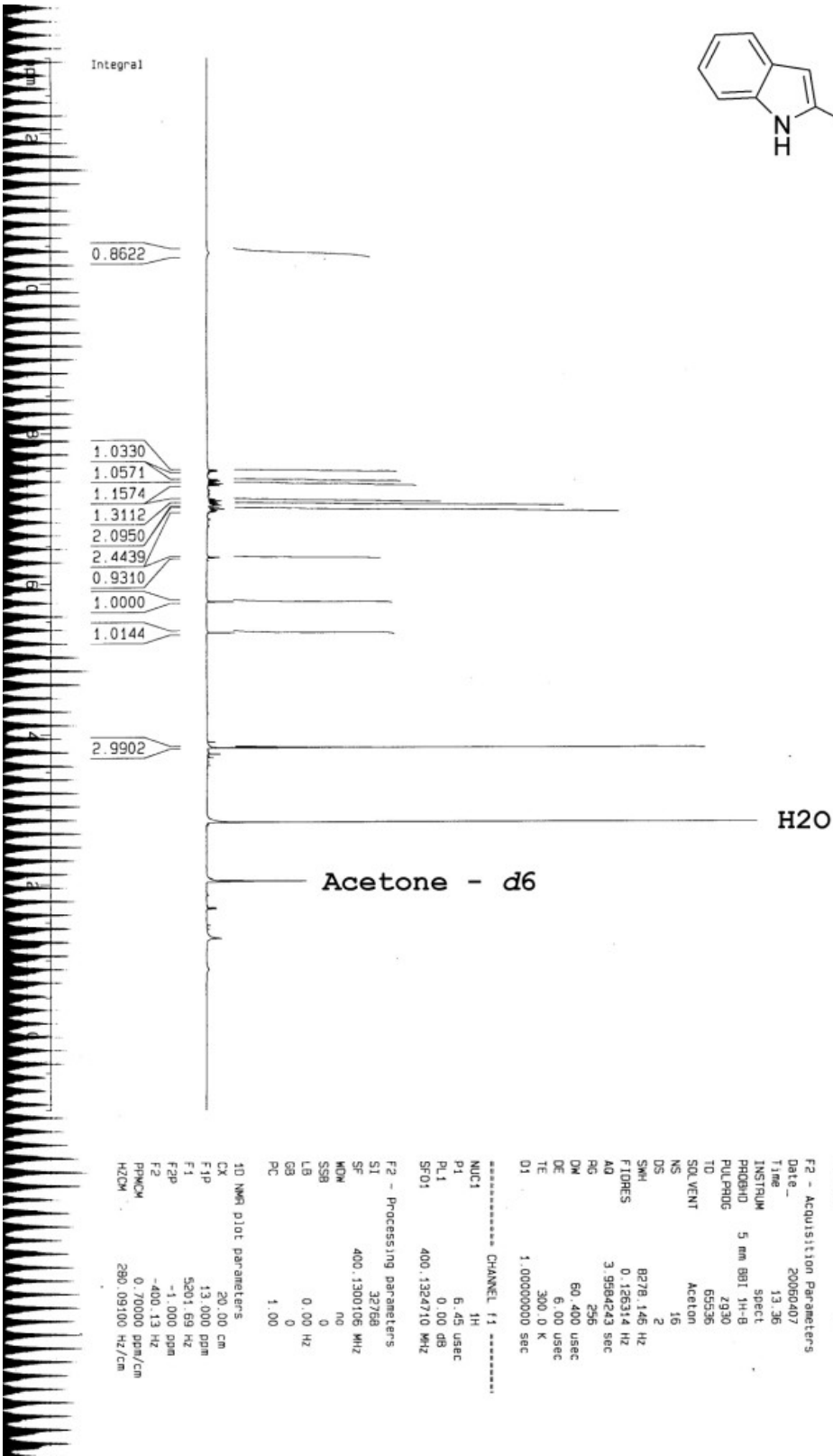
F2 - Processing parameters
SI       32768
SF       75.4023769 MHz
RG       64
SFO      299.8719995 MHz
PC       1.40

10 NMR plot parameters
CX       20.00 cm
FIP      234.175 ppm
F1       17657.36 Hz
F2P      -15.114 ppm
F3       -1139.83 Hz
F3P      12.48445 ppm/cm
SFO      939.84991 Hz/cm
  
```



14l

DKH2-129 Product



Current Data Parameters
 NAME DKH2-129P
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20060407
 Time 13.36
 INSTRUM spect
 PROBRID 5 mm BBI 1H-B
 PULPROG zg30
 TD 65536
 SOLVENT Aceton
 NS 16
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9586243 sec
 RG 296
 DM 60.400 usec
 DE 6.00 usec
 TE 300.0 K
 01 1.000000000 sec

***** CHANNEL f1 *****

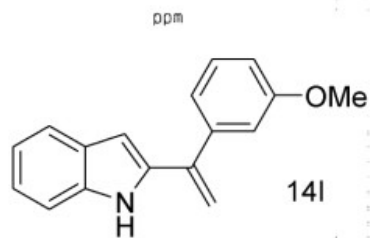
NUC1 1H
 P1 6.45 usec
 PL1 0.00 dB
 SF01 400.1324710 MHz

F2 - Processing parameters

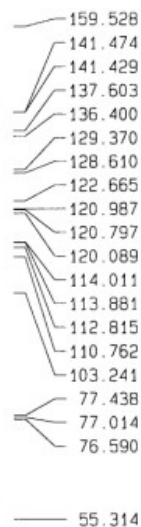
SF 32768
 SF 400.1300106 MHz
 MDM no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

10 MHz plot parameters

CX 20.00 cm
 F1P 13.000 ppm
 F1 5201.69 Hz
 F2P -1.000 ppm
 F2 -400.13 Hz
 PPM/CM 0.70000 ppm/cm
 HZ/CM 280.09100 Hz/cm



DKH3-18 Product (Yellow 011)



Current Data Parameters
NAME DKH3-18P
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

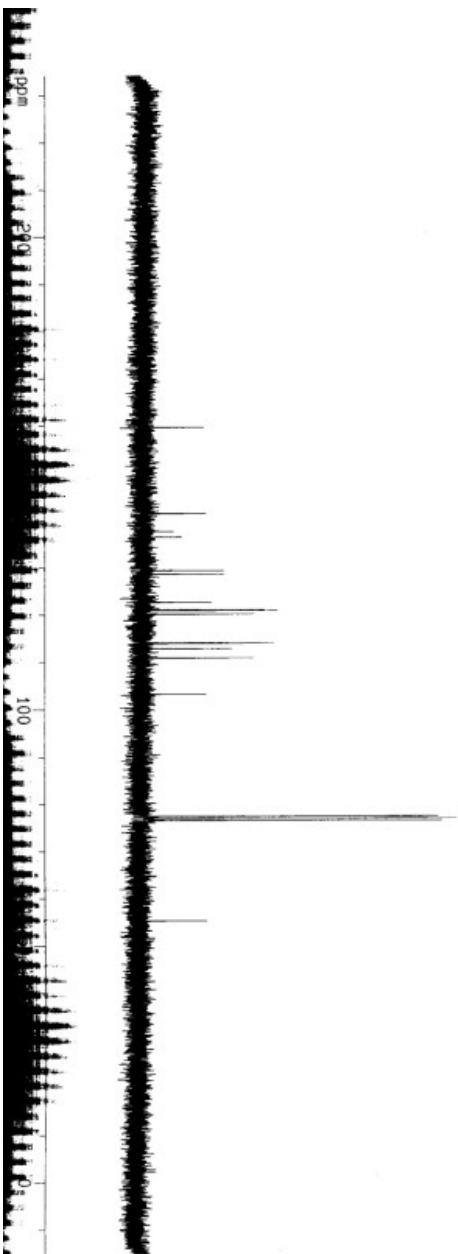
Date_ 20060417
Time 11:58
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 296
DS 4
SWH 18796.992 Hz
FIDRES 0.266819 Hz
AQ 1.743076 sec
RG 512
DM 26.600 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00020000 sec

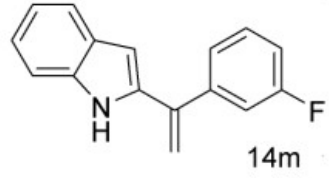
***** CHANNEL f1 *****
NUC1 13C
P1 5.40 usec
PL1 -6.00 dB
SFO1 75.4106357 MHz

***** CHANNEL f2 *****
CPDPRG2 maitz16
NUC2 1H
PCPRG2 115.00 usec
PL2 0.00 dB
PL12 20.00 dB
PL13 20.00 dB
SFO2 299.8711995 MHz

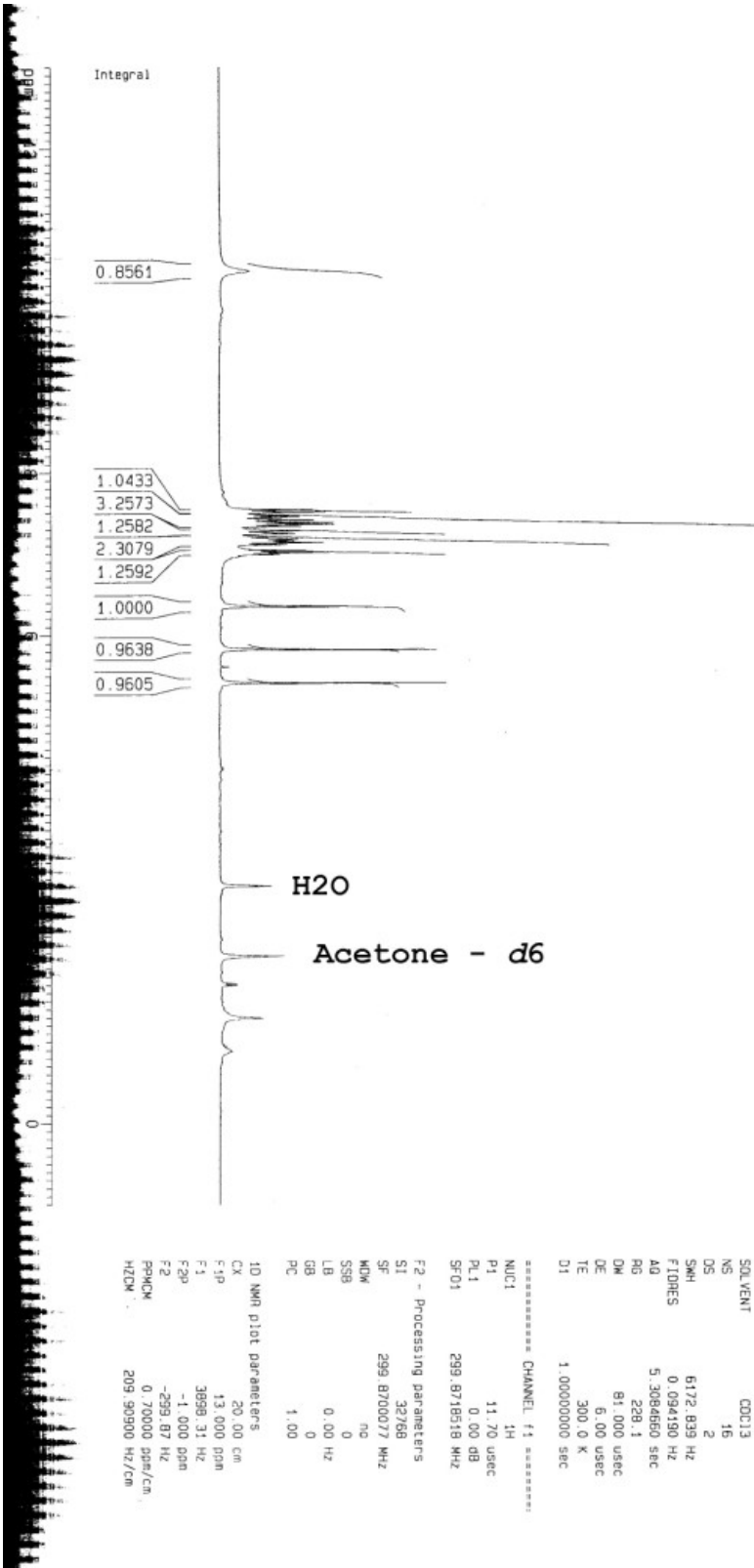
F2 - Processing parameters
S1 32768
SF 4023753 MHz
KTM no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

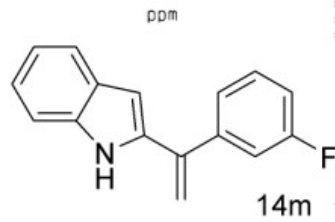
10 NMR plot parameters
CX 20.00 cm
F1P 234.196 dm
F1 17658.96 Hz
F2P -13.093 dm
F2 -1138.03 Hz





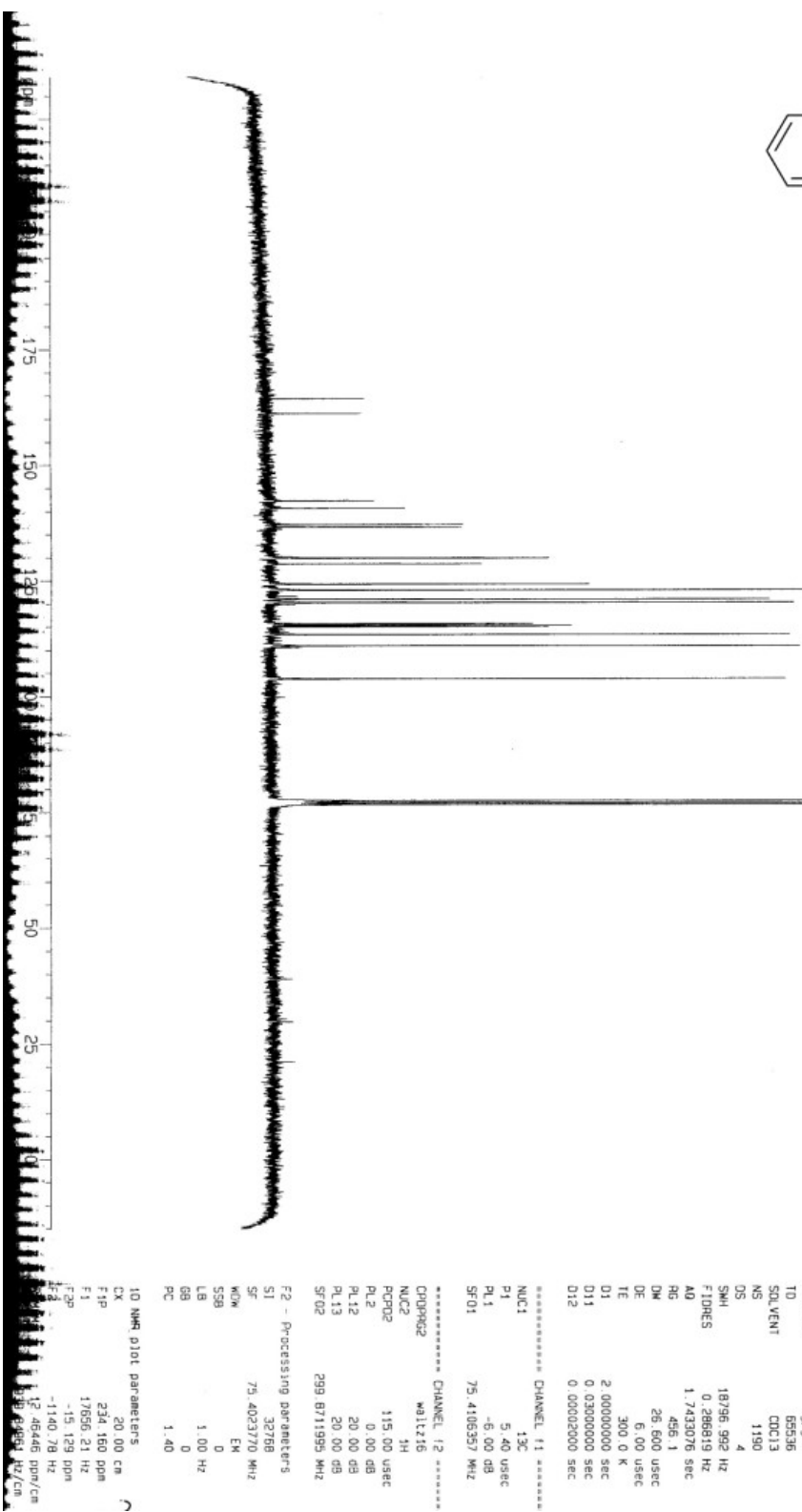
DKH 2-298 Product (Ye1)ow 0.11)





DKH2-298 Product

- 164.321
- 161.058
- 142.285
- 142.184
- 140.617
- 137.056
- 136.492
- 129.860
- 129.751
- 128.543
- 124.192
- 124.154
- 122.899
- 120.870
- 120.210
- 115.600
- 115.307
- 115.259
- 114.978
- 113.213
- 110.784
- 103.679
- 77.425
- 77.001
- 76.577



Current Data Parameters
 NAME DKH2-298P
 EXEND 666
 PROCDN 1

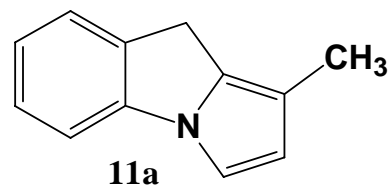
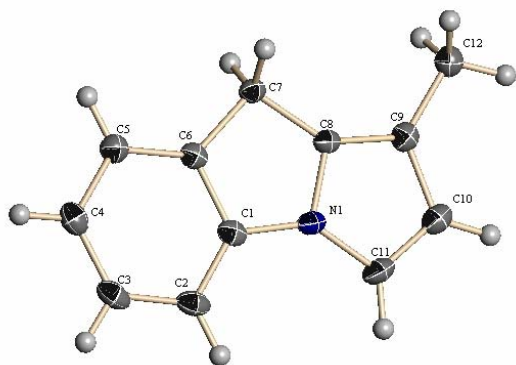
F2 - Acquisition Parameters
 Date 20060411
 Time 16:58
 INSTRUM Spect
 PROBHD 5 mm DNP 1H/1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1190
 DS 4
 SWH 18795.992 Hz
 FIDRES 0.286819 Hz
 AQ 1.7433078 sec
 RG 496.1
 DE 26.000 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec

***** CHANNEL f1 *****
 NUC1 13C
 P1 5.40 usec
 PL1 -6.00 dB
 SF01 75.4106337 MHz

***** CHANNEL f2 *****
 CPDPRG2 MALTZ16
 NUC2 1H
 PCPRG2 115.00 usec
 PL2 0.00 dB
 PL12 20.00 dB
 PL13 20.00 dB
 SF02 299.8711995 MHz

F2 - Processing parameters
 S1 32768
 SF 75.4023770 MHz
 KW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

10 NMR plot parameters
 CX 20.00 cm
 F1P 234.160 ppm
 F1 17856.21 Hz
 F2P -1140.78 Hz
 F2 12.6646 ppm/cm
 F3P 6956.42/cm

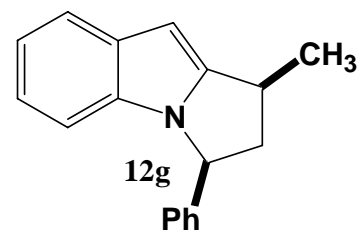
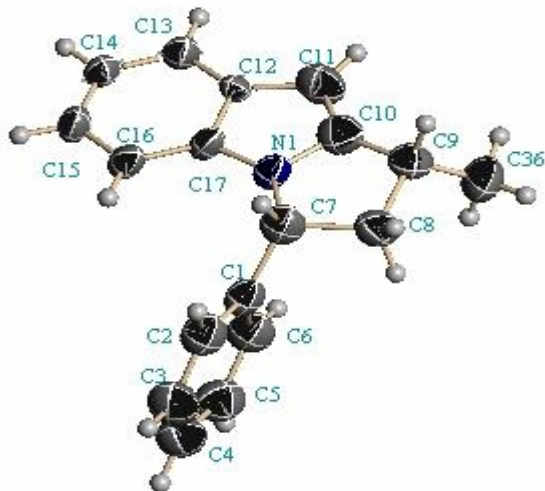


A yellow plate shaped crystal of **11a** (C₁₂ H₁₁ N) with approximate dimensions 0.10 x 0.30 x 0.40 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured at 108(2) K, cooled by Rigaku-MSX X-Stream 2000, on a Bruker SMART APEX CCD area detector system equipped with a graphite monochromator and a MoK α fine-focus sealed tube ($\lambda = 0.71073\text{\AA}$) operated at 1600 watts power (50 kV, 32 mA). The detector was placed at a distance of 5.8 cm from the crystal.

A total of 1850 frames were collected with a scan width of 0.3° in ω and an exposure time of 20 seconds/frame. The total data collection time was about 12 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame integration algorithm. The integration of the data using a Monoclinic unit cell yielded a total of 5358 reflections to a maximum θ angle of 28.28° (0.90\AA resolution), of which 2066 were independent, completeness = 94.9 %, $R_{\text{int}} = 0.0178$, $R_{\text{sig}} = 0.0245$ and 1729 were greater than $2\sigma(I)$. The final cell constants: $a = 11.907(4)\text{\AA}$, $b = 5.6848(16)\text{\AA}$, $c = 12.950(4)\text{\AA}$, $\alpha = 90^\circ$, $\beta = 92.517(5)^\circ$, $\gamma = 90^\circ$, volume = $875.7(4)\text{\AA}^3$, are based upon the refinement of the XYZ-centroids of 2113 reflections above $20\sigma(I)$ with $2.274^\circ < \theta < 28.242^\circ$. Analysis of the data showed negligible decay during data collection. Data were corrected for absorption effects using the multiscan technique (SADABS). The ratio of minimum to maximum apparent transmission was 0.849448.

The structure was solved and refined using the Bruker SHELXTL (Version 6.1) Software Package, using the space group P2(1)/n, with $Z = 4$ for the formula unit, C₁₂ H₁₁ N. The final anisotropic full-matrix least-squares refinement on F^2 with 119 variables converged at $R1 = 5.17\%$, for the observed data and $wR2 = 13.90\%$ for all data. The

goodness-of-fit was 1.072 . The largest peak on the final difference map was $0.403 \text{ e}^-/\text{\AA}^3$ and the largest hole was $-0.249 \text{ e}^-/\text{\AA}^3$. Based on the final model, the calculated density of the crystal is 1.283 g/cm^3 and F(000) amounts to 360 electrons.



A yellow needle shaped crystal of **12g** (C₁₈ H₁₇ N) (two molecules in the asymmetric unit) with approximate dimensions 0.04 x 0.08 x 0.35 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured at 298(2) K, on a Bruker SMART APEX CCD area detector system equipped with a graphite monochromator and a MoK α fine-focus sealed tube ($\lambda = 0.71073 \text{ \AA}$) operated at 1600 watts power (50 kV, 32 mA). The detector was placed at a distance of 5.8 cm from the crystal.

A total of 1850 frames were collected with a scan width of 0.3° in ω and an exposure time of 10 seconds/frame. The total data collection time was about 8 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame integration algorithm. The integration of the data using a Triclinic unit cell yielded a total of 8236 reflections to a maximum θ angle of 28.27° (0.90 \AA resolution), of which 6090 were independent, completeness = 89.6 %, $R_{\text{int}} = 0.0758$, $R_{\text{sig}} = 0.2293$ and 1717 were greater than $2\sigma(I)$. The final cell constants: $a = 5.538(3) \text{ \AA}$, $b = 9.573(5) \text{ \AA}$, $c = 25.815(14) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 87.270(12)^\circ$, $\gamma = 90^\circ$, volume = $1367.1(13) \text{ \AA}^3$, are based upon the refinement of the XYZ-centroids of 715 reflections above $20\sigma(I)$ with $2.269^\circ < \theta < 27.720^\circ$. Analysis of the data showed negligible decay during data collection. Data were corrected for absorption effects using the multiscan technique (SADABS). The ratio of minimum to maximum apparent transmission was 0.03821.

The structure was solved and refined using the Bruker SHELXTL (Version 6.1) Software

Package, using the space group P-1, with $Z = 2$ for the formula unit, C₃₆ H₃₄ N₂. The final anisotropic full-matrix least-squares refinement on F^2 with 345 variables converged at $R1 = 8.23\%$, for the observed data and $wR2 = 21.67\%$ for all data. The goodness-of-fit was 0.829. The largest peak on the final difference map was $0.233 \text{ e}^-/\text{\AA}^3$ and the largest hole was $-0.247 \text{ e}^-/\text{\AA}^3$. Based on the final model, the calculated density of the crystal is 1.202 g/cm^3 and $F(000)$ amounts to 528 electrons.