Supporting Information

One-Pot Synthesis of Polysubstituted 3-Acylpyrroles Using Cooperative Catalysis

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1. General

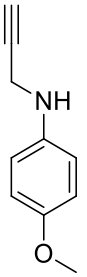
TLC was performed using Merck silica gel 60 F254 TLC aluminum sheets. Flash column chromatography was performed using Merck silica gel 60 (230-400 mesh). ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker Avance 400. Chemical shifts are reported in ppm from $CDCl_3$ as an internal standard. High-resolution mass spectra were recorded on a Thermo Scientific LTQ Orbitrap mass spectrometer. Melting points were measured on a Yanaco MP J3 melting point apparatus and recorded in °C.

α,α,α-Trifluorotoluene was purchased from TCI and stored over molecular sieves 4Å under argon. Solvents used for reactions were purchased as anhydrous or low water content and used as such. All other chemicals were purchased and used without further purification.

2. Synthesis of Propargylated Amines

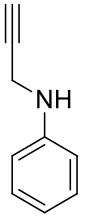
Propargylated amines were synthesized by reported procedures.[1-6]

4-Methoxy-*N*-(prop-2-yn-1-yl)aniline (2a)[1]



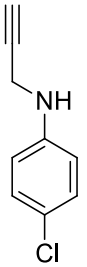
Prepared by the reported procedure[2] and purified by flash column chromatography (Hexane/EtOAc = 6:1); yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.85-6.81 (m, 2H), 6.71-6.67 (m, 2H), 3.91 (d, *J* = 2.4 Hz, 2H), 3.77 (s, 3H), 3.64 (brs, 1H), 2.23 (t, *J* = 2.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.0, 140.9, 115.1, 114.8, 81.4, 71.2, 55.7, 34.6.

N-(Prop-2-yn-1-yl)aniline[2]



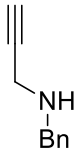
Prepared by the reported procedure[2] and purified by flash column chromatography (Hexane/EtOAc = 8:1); yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.26-7.21 (m, 2H), 6.83-6.79 (m, 1H), 6.72-6.69 (m, 2H), 3.96 (d, *J* = 2.4 Hz, 2H), 3.89 (brs, 1H), 2.23 (t, *J* = 2.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 146.9, 129.3, 118.7, 113.5, 81.0, 71.3, 33.7.

4-Chloro-*N*-(prop-2-yn-1-yl)aniline[3]



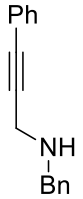
Prepared by the reported procedure[1] and purified by flash column chromatography (Hexane/EtOAc = 8:1); yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.19-7.17 (m, 2H), 6.64-6.62 (m, 2H), 3.93-3.92 (m, 3H), 2.23 (t, *J* = 2.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.4, 129.1, 123.4, 114.7, 80.5, 71.5, 33.7.

***N*-Benzylprop-2-yn-1-amine**[4]



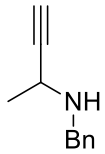
Prepared by the reported procedure[4] and purified by flash column chromatography (Hexane/EtOAc = 6:1); pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38-7.26 (m, 5H), 3.90 (s, 2H), 3.45 (d, *J* = 2.4 Hz, 2H), 2.28 (t, *J* = 2.4 Hz, 1H), 1.60 (brs, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.4, 128.5, 128.4, 127.2, 82.1, 71.6, 60.4, 37.3.

***N*-Benzyl-3-phenylprop-2-yn-1-amine**[5]



Prepared by the reported procedure[4] and purified by flash column chromatography (Hexane/EtOAc = 4:1); pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.47-7.29 (m, 10H), 3.98 (s, 2H), 3.69 (s, 2H), 1.70 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.5, 131.7, 128.5, 128.2, 128.1, 127.2, 123.2, 87.5, 83.8, 52.5, 38.3.

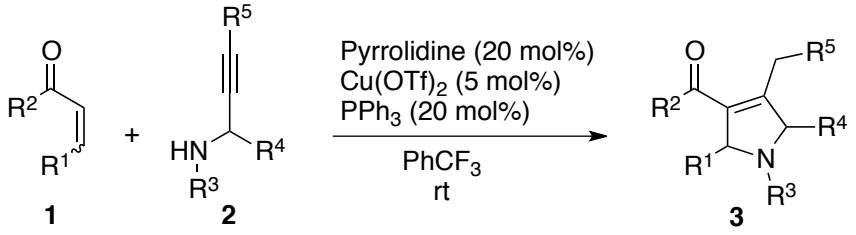
***N*-Benzylbut-3-yn-2-amine**[6]



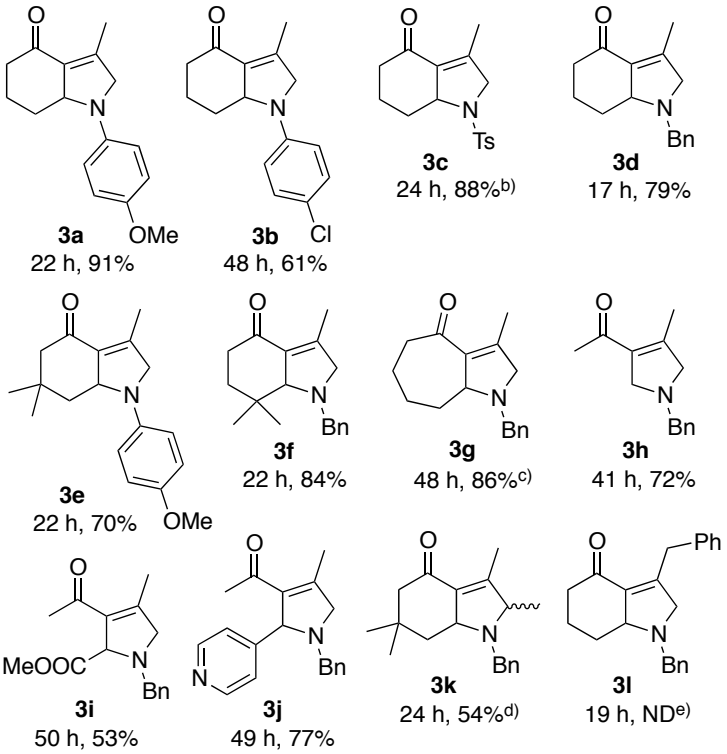
Prepared by the reported procedure[6] and purified by flash column chromatography (Hexane/EtOAc = 4:1); pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.39-7.25 (m, 5H), 4.04 (d, *J* = 12.8 Hz, 1H), 3.83 (d, *J* = 12.8 Hz, 1H), 3.51 (dq, *J* = 6.8, 2.4 Hz, 1H), 2.34 (d, *J* = 2.0 Hz, 1H), 1.44 (brs, 1H), 1.40 (d, *J* = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.8, 128.43, 128.40, 127.1, 86.3, 70.8, 51.4, 44.3, 22.3.

3. Synthesis of 2,5-Dihydropyrroles

General Procedure for the aza-Michael/Carbocyclization.

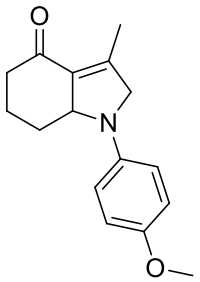


A mixture of $Cu(OTf)_2$ (0.01 mmol, 3.6 mg) and PPh_3 (0.04 mmol, 10.5 mg) in $PhCF_3$ (0.2 mL) was stirred at room temperature (25 °C) for 5 min under Ar. To the mixture, enone **1** (0.2 mmol), propargylated amine **2** (0.3 mmol) and pyrrolidine (0.04 mmol, 3.4 μL) were added. The resulting mixture was stirred at the same room temperature under Ar until enone **1** was consumed (monitored by TLC). The reaction mixture was directly purified by flash column chromatography on silica gel (Hexane/EtOAc or Hexane/Acetone) to give **3**.



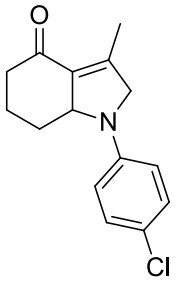
[a] Reaction of **1** (0.2 mmol) and **2** (0.3 mmol) was performed using pyrrolidine (0.04 mmol, 20 mol% to **1**), PPh_3 (0.04 mmol, 20 mol% to **1**), and $Cu(OTf)_2$ (0.01 mmol, 5 mol% to **1**) in $PhCF_3$ (0.2 mL, concentration of **1**: 1 M) at rt (25 °C). [b] Reaction in $PhCF_3$ (1.0 mL, concentration of **1**: 0.2 M). [c] Reaction in MeOH instead of in $PhCF_3$. [d] Reaction at 40 °C. [e] Reaction at 60 °C. ND = not detected.

Compound 3a



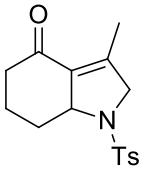
Purified by flash column chromatography (Hexane/EtOAc = 7:1); yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.89-6.86 (m, 2H), 6.64-6.60, (m, 2H), 4.49-4.41 (m, 1H), 4.31 (dd, *J* = 15.6 Hz, 6.0 Hz, 1H), 4.05 (ddq, *J* = 15.6 Hz, 4.0 Hz, 0.8 Hz, 1H), 3.78 (s, 3H), 2.66-2.53 (m, 2H), 2.36-2.27 (m, 1H), 2.09 (s, 3H), 2.08-2.01 (m, 1H), 1.92-1.80 (m, 1H), 1.51-1.42 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 199.3, 151.7, 144.0, 141.9, 133.5, 115.1, 113.3, 67.3, 62.3, 55.9, 40.8, 31.8, 20.9, 13.3. ESI-HRMS: calcd for $C_{16}H_{20}NO_2$ ($[M+H]^+$) 258.1489, found 258.1494.

Compound 3b



Purified by flash column chromatography (Hexane/EtOAc = 9:1); pale yellow solid; mp 136-138. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.25-7.18 (m, 2H), 6.57-6.53, (m, 2H), 4.52-4.40 (m, 1H), 4.28 (dd, *J* = 15.6 Hz, 6.0 Hz, 1H), 4.06 (ddq, *J* = 15.6 Hz, 3.6 Hz, 1.2 Hz, 1H), 2.65-2.54 (m, 2H), 2.36-2.27 (m, 1H), 2.09-2.02 (m, 4H), 1.92-1.82 (m, 1H), 1.45 (dt, *J* = 12.8 Hz, 3.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 199.2, 145.5, 143.3, 133.5, 129.1, 121.8, 113.4, 67.0, 61.5, 40.7, 31.3, 20.8, 13.2. ESI-HRMS: calcd for $C_{15}H_{17}ClNO$ ($[M+H]^+$) 262.0993, found 262.0970.

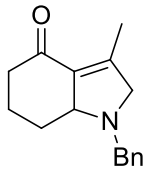
Compound 3c



Purified by flash column chromatography (Hexane/EtOAc = 3:1 to 2:1); colorless solid; mp 188-190. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72 (d, *J* = 8.0 Hz, 2H), 7.34 (d, *J* = 8.0 Hz, 2H), 4.31-4.24 (m, 1H), 4.13 (dd, *J* = 16.0 Hz, 5.6 Hz, 1H), 4.10-3.97 (m, 1H), 2.72-2.62 (m, 1H), 2.49-2.43 (m, 1H), 2.45 (s, 3H), 2.29-2.17 (m, 1H), 2.07-1.98 (m, 1H), 1.90 (d, *J* = 0.8 Hz, 2H), 1.79-1.66 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 198.5, 144.0, 142.2, 133.2, 131.9, 129.9,

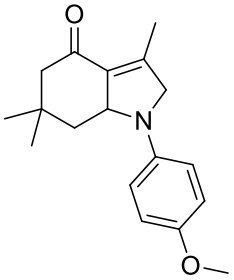
127.7, 67.6, 59.3, 40.5, 33.2, 21.5, 20.9, 12.9. ESI-HRMS: calcd for $C_{16}H_{20}NO_3S$ ($[M+H]^+$) 306.1158, found 306.1165.

Compound 3d



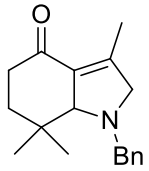
Purified by flash column chromatography (Hexane/EtOAc = 5:1); yellow gum; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.28-7.17 (m, 5H), 3.98 (d, *J* = 12.8 Hz, 1H), 3.58-3.50 (m, 1H), 3.48-3.43 (m, 2H), 3.17 (ddq, *J* = 15.6 Hz, 6.0 Hz, 1.6 Hz, 1H), 2.41-2.33 (m, 1H), 2.23-2.13 (m, 1H), 2.06-2.00 (m, 1H), 1.95 (d, *J* = 0.8 Hz, 3H), 1.93-1.87 (m, 1H), 1.68-1.56 (m, 1H), 1.45-1.35 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 199.1, 148.6, 139.0, 133.1, 128.8, 128.4, 127.2, 70.9, 64.4, 58.3, 40.6, 31.2, 21.2, 14.0. ESI-HRMS: calcd for $C_{16}H_{20}NO$ ($[M+H]^+$) 242.1539, found 242.1538.

Compound 3e



Purified by flash column chromatography (Hexane/Acetone = 9:1); pale yellow solid; mp 123-125. ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.90-6.86 (m, 2H), 6.63-6.59, (m, 2H), 4.68-4.60 (m, 1H), 4.32 (dd, *J* = 15.6 Hz, 5.6 Hz, 1H), 4.04 (dd, *J* = 15.2 Hz, 3.6 Hz, 1H), 3.78 (s, 3H), 2.42-2.33 (m, 2H), 2.22 (d, *J* = 16.4 Hz, 1H), 2.06 (s, 3H), 1.48 (t, *J* = 12.0 Hz, 1H), 1.16 (s, 3H), 1.08 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 199.3, 151.8, 143.4, 142.1, 132.8, 115.1, 113.5, 64.3, 62.8, 55.9, 54.9, 44.8, 33.0, 31.9, 27.3, 13.1. ESI-HRMS: calcd for $C_{18}H_{24}NO_2$ (($[M+H]^+$) 286.1804, found 286.1784.

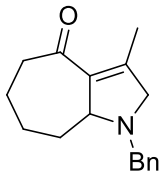
Compound 3f



Purified by flash column chromatography (Hexane/EtOAc = 10:1); pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.41-7.24, (m, 5H), 4.23 (d, *J* = 14.0 Hz, 1H), 3.71-3.65 (m, 2H), 3.59 (d, *J* =

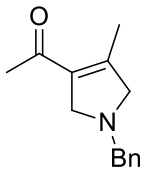
14.0 Hz, 1H), 3.29-3.22 (m, 1H), 2.39-2.35 (m, 2H), 1.97 (s, 3H), 1.74-1.56 (m, 2H), 1.13 (s, 3H), 1.01 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 200.1, 147.7, 140.4, 131.5, 129.4, 127.9, 126.8, 80.1, 66.7, 61.9, 37.2, 36.4, 35.7, 28.4, 18.5, 13.4. ESI-HRMS: calcd for $C_{18}H_{24}NO$ ($[M+H]^+$) 270.1858, found 270.1853.

Compound 3g



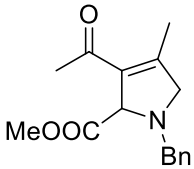
Purified by flash column chromatography (Hexane/EtOAc = 8:1); colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.34-7.25 (m, 5H), 4.10 (d, *J* = 13.2 Hz, 1H), 3.83-3.75 (m, 1H), 3.63 (dd, *J* = 16.4 Hz, 4.4 Hz, 1H), 3.51 (d, *J* = 13.2 Hz, 1H), 3.28 (ddd, *J* = 16.4 Hz, 4.8 Hz, 0.8 Hz, 1H), 2.55-2.42 (m, 2H), 2.14-2.07 (m, 1H), 2.04 (s, 3H), 2.02-1.92 (m, 2H), 1.62-1.43 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 200.6, 150.9, 139.2, 136.3, 128.6, 128.4, 127.1, 71.7, 64.6, 58.0, 46.0, 36.5, 28.4, 25.6, 14.4. ESI-HRMS: calcd for $C_{17}H_{22}NO$ ($[M+H]^+$) 256.1696, found 256.1698.

Compound 3h



Purified by flash column chromatography (Hexane/EtOAc = 1:1); yellow gum. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.35-7.26, (m, 5H), 3.78 (s, 2H), 3.76-3.73 (m, 2H), 3.60-3.57 (m, 2H), 2.23 (s, 3H), 2.07 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 195.9, 150.0, 138.8, 133.6, 128.6, 128.5, 127.2, 66.3, 60.7, 60.0, 30.1, 14.7. ESI-HRMS: calcd for $C_{14}H_{18}NO$ ($[M+H]^+$) 216.1383, found 216.1381.

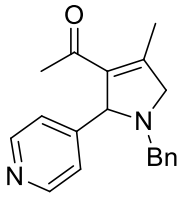
Compound 3i



Purified by flash column chromatography (Hexane/EtOAc = 3:1); yellow gum. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.35-7.24, (m, 5H), 4.58-4.55 (m, 1H), 3.97 (d, *J* = 13.2 Hz, 1H), 3.91-3.85 (m, 1H), 3.78 (d, *J* = 13.2 Hz, 1H), 3.69 (s, 3H), 3.54 (ddq, *J* = 16.4 Hz, 3.2 Hz, 0.8 Hz, 1H), 2.32 (s, 3H), 2.10 (d, *J* = 0.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 195.1, 172.6, 151.7, 138.2, 134.3, 128.7, 128.4, 127.3, 73.1, 65.9, 57.6, 52.0, 30.0, 14.7. ESI-HRMS: calcd for $C_{16}H_{20}NO_3$ ($[M+H]^+$)

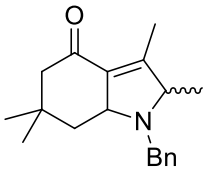
274.1438, found 274.1437.

Compound 3j



Purified by flash column chromatography (Hexane/Acetone = 1:1); brown solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.55 (d, *J* = 6.0 Hz, 2H), 7.30-7.16, (m, 7H), 4.86-4.84 (m, 1H), 3.82 (dd, *J* = 16.4, 4.8 Hz, 1H), 3.78 (d, *J* = 13.0 Hz, 1H), 3.53 (d, *J* = 13.0 Hz, 1H), 3.48 (ddq, *J* = 16.4, 4.4, 0.8 Hz, 1H), 2.11 (d, *J* = 0.8 Hz, 3H), 2.06 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 195.9, 151.4, 150.0, 149.7, 138.4, 137.3, 128.5, 128.3, 127.2, 123.8, 74.2, 64.8, 56.8, 30.5, 14.6. ESI-HRMS: calcd for $C_{19}H_{21}N_2O$ ($[M+H]^+$) 293.1648, found 293.1648.

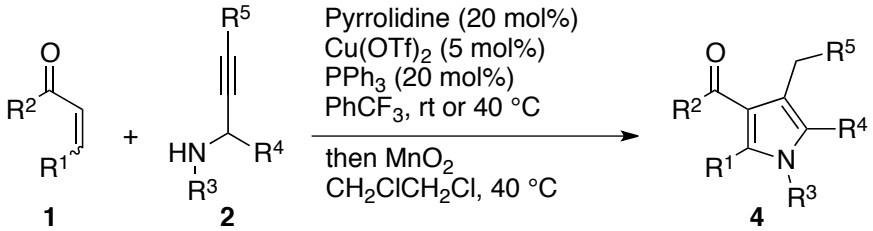
Compound 3k



Purified by flash column chromatography (Hexane/EtOAc = 3:1); 8.7:1 dr; colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.42-7.40 (m, 2H), 7.35-7.32 (m, 2H), 7.28-7.24 (m, 1H), 3.95-3.91 (m, 2H), 3.78-3.74 (m, 2H), 2.25 (dd, *J* = 16.4 Hz, 2.0 Hz, 1H), 2.20 (dd, *J* = 16.4 Hz, 2.0 Hz, 1H), 2.00 (d, *J* = 1.6 Hz, 3H), 1.94-1.87 (m, 1H), 1.47 (t, *J* = 12.0 Hz, 1H), 1.05 (s, 3H), 1.02 (d, *J* = 6.8 Hz, 3H), 1.00 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 199.8, 153.0, 139.4, 133.6, 128.4, 128.3, 126.9, 65.6, 64.2, 54.7, 51.4, 43.9, 33.1, 32.0, 26.7, 13.4, 11.7. ESI-HRMS: calcd for $C_{19}H_{26}NO$ ($[M+H]^+$) 284.2014, found 284.2007.

4. One-Pot Synthesis of 3-Acylpyrroles

General Procedure for the One-Pot aza-Michael/Carbocyclization-Oxidation (Table 2).

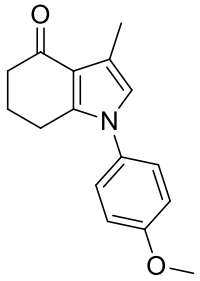


1 **2** **4**

A mixture of $Cu(OTf)_2$ (3.6 mg, 0.01 mmol) and PPh_3 (10.5 mg, 0.04 mmol) in $PhCF_3$ (0.2 mL) was stirred at room temperature (25 °C) for 5 min under Ar. To the mixture, enone **1** (0.2 mmol),

propargylated amine **2** (0.3 mmol), and pyrrolidine (3.4 μL, 0.04 mmol) were added. The resulting mixture was stirred at the same room temperature or 40 °C as indicated under Ar until enone **1** was consumed (monitored by TLC). To the mixture, MnO_2 (4.0 mmol) and CH_2ClCH_2Cl (DCE) (2 mL) were added. The mixture was stirred at 40 °C until dihydropyrrole **3** was consumed. The mixture was filtered through Celite. The filtrate was concentrated in vacuo and purified by flash column chromatography on silica gel to give product **4**. When the dihydropyrrole was synthesized in MeOH, the solvent was removed before addition of MnO_2 and DCE.

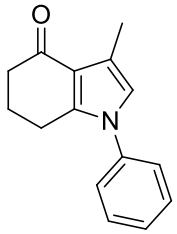
Compound 4a



Synthesis of dihydropyrrole at rt for 23 h; oxidation in CH_2Cl_2 at rt for 5 h; flash column chromatography (Hexane/EtOAc = 3:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.22-7.19 (m, 2H), 6.99-6.96 (m, 2H), 6.50 (m, 1H), 3.86 (s, 3H), 2.69 (t, *J* = 6.4 Hz, 2H), 2.48 (t, *J* = 6.4 Hz, 2H), 2.35 (d, *J* = 0.8 Hz, 3H), 2.08 (pentet, *J* = 6.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 195.5, 158.9, 143.5, 131.8, 126.2, 121.0, 119.7, 119.5, 114.5, 55.6, 38.5, 24.0, 23.1, 11.5. ESI-HRMS: calcd for $C_{16}H_{18}NO_2$ ($[M+H]^+$) 256.1332, found 256.1313.

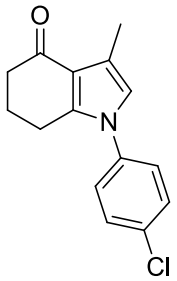
Gram-scale synthesis of **4a**: A mixture of $Cu(OTf)_2$ (180.8 mg, 0.5 mmol) and PPh_3 (524.6 mg, 2.0 mmol) in $PhCF_3$ (10.0 mL) was stirred at room temperature (25 °C) for 5 min under Ar. To the mixture, cyclohexanone (0.971 mL, 10.0 mmol), propargylated amine **2a** (1.93 g, 12.0 mmol), and pyrrolidine (165.4 μL, 2.0 mmol) were added. The resulting mixture was stirred at the room temperature until the enone was consumed (monitored by TLC, 51 h). To the mixture, MnO_2 (2.6 g, 30.0 mmol) and CH_2ClCH_2Cl (DCE) (30.0 mL) was added. The mixture was stirred at 40 °C until dihydropyrrole was consumed (68 h). The mixture was cooled to rt, diluted with EtOAc and filtered through Celite. The filtrate was washed with water (x 2) and brine (x 2), dried over Na_2SO_4, concentrated in vacuo, and purified by flash column chromatography on silica gel (Hexane/EtOAc = 3:1) to give **4a** (1.69 g, 66%) as a pink solid. Recrystallization (Hexane/EtOAc = 16 mL/6 mL) gave **4a** (1.24 g) as pale pink crystals; mp 106-108.

Compound 4b



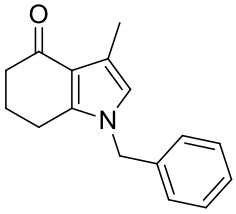
Synthesis of dihydropyrrole at rt for 45 h; oxidation at 40 °C for 44 h; flash column chromatography (Hexane/EtOAc = 3:1); pale yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.49-7.46 (m, 2H), 7.40-7.36 (m, 1H), 7.31-7.28 (m, 2H), 6.57 (m, 1H), 2.75 (t, *J* = 6.4 Hz, 2H), 2.49 (dd, *J* = 6.4 Hz, 6.0 Hz, 2H), 2.36 (d, *J* = 0.8 Hz, 3H), 2.09 (dq, *J* = 6.0 Hz, 6.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 195.6, 143.2, 138.8, 129.4, 127.5, 124.8, 120.7, 120.1, 119.9, 38.6, 24.1, 23.4, 11.5. ESI-HRMS: calcd for $C_{15}H_{16}NO$ ($[M+H]^+$) 226.1226, found 226.1230.

Compound 4c



Synthesis of dihydropyrrole at rt for 67 h; oxidation at 40 °C for 31 h; flash column chromatography (Hexane/EtOAc = 2:1); yellow gum. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.47-7.43 (m, 2H), 7.26-7.22 (m, 2H), 6.53 (q, *J* = 0.8 Hz, 1H), 2.73 (t, *J* = 6.0 Hz, 2H), 2.49 (dd, *J* = 7.2 Hz, 6.0 Hz, 2H), 2.35 (d, *J* = 0.8 Hz, 3H), 2.10 (dq, *J* = 7.2 Hz, 6.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 195.5, 143.1, 137.3, 133.3, 129.6, 126.0, 120.5, 120.3, 38.5, 24.0, 23.3, 11.5. ESI-HRMS: calcd for $C_{15}H_{15}NOCl$ ($[M+H]^+$) 260.0837, found 260.0844.

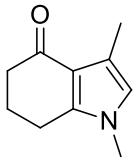
Compound 4d



Synthesis of dihydropyrrole at rt for 24 h; oxidation at 40 °C for 24 h; flash column chromatography (Hexane/EtOAc = 2:1); pale yellow gum. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.37-7.28 (m, 3H), 7.06-7.05 (m, 2H), 6.36 (s, 1H), 4.97 (s, 2H), 2.64 (t, *J* = 6.0 Hz, 2H), 2.43 (dd, *J* = 6.4 Hz, 6.0 Hz, 2H), 2.31 (d, *J* = 1.2 Hz, 3H), 2.10 (dq, *J* = 6.0 Hz, 6.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 195.1, 143.4, 136.8, 128.9, 127.9, 126.6, 120.4, 119.4, 119.3, 50.2,

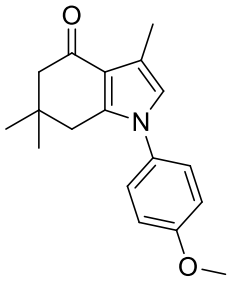
38.4, 23.7, 22.0, 11.6. ESI-HRMS: calcd for $C_{16}H_{18}NO$ ($[M+H]^+$) 240.1383, found 240.1382.

Compound 4e[7]



Synthesis of dihydropyrrole at 40 °C for 22 h; oxidation at 40°C for 66 h; flash column chromatography (Hexane/EtOAc = 1:1); colorless solid; mp 124-126. ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.28 (s, 1H), 3.48 (s, 3H), 2.69 (t, *J* = 6.0 Hz, 2H), 2.42 (dd, *J* = 6.8 Hz, 6.2 Hz, 2H), 2.28 (d, *J* = 0.8 Hz, 3H), 2.12 (dq, *J* = 6.8 Hz, 6.2 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 194.9, 143.5, 120.8, 118.96, 118.93, 38.3, 33.1, 23.6, 21.7, 11.4. ESI-HRMS: calcd for $C_{10}H_{14}NO$ ($[M+H]^+$) 164.1070, found 164.1070.

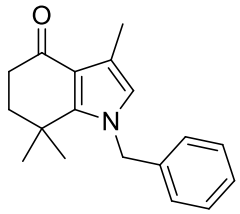
Compound 4f



Synthesis of dihydropyrrole at rt for 24 h; oxidation in CH_2Cl_2 at rt for 25 h; flash column chromatography (Hexane/EtOAc = 4:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.20-7.18 (m, 2H), 6.99-6.49 (m, 2H), 6.49 (m, 1H), 3.86 (s, 3H), 2.55 (s, 2H), 2.34 (s, 2H), 2.34 (s, 3H), 1.06 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 194.8, 158.9, 142.4, 131.8, 126.3, 121.3, 119.3, 118.6, 114.5, 55.6, 52.6, 37.0, 35.5, 28.5, 11.4. ESI-HRMS: calcd for $C_{18}H_{22}NO_2$ ($[M+H]^+$) 284.1645, found 284.1646.

Gram-scale synthesis of **4f**: A mixture of $Cu(OTf)_2$ (180.8 mg, 0.5 mmol) and PPh_3 (524.6 mg, 2.0 mmol) in $PhCF_3$ (10.0 mL) was stirred at room temperature (25 °C) for 5 min under Ar. To the mixture, 3,3-dimethylcyclohexenone (1.24 g, 10.0 mmol), propargylated amine **2a** (1.93 g, 12.0 mmol), and pyrrolidine (165.4 μL, 2.0 mmol) were added. The resulting mixture was stirred at the room temperature until the enone was consumed (monitored by TLC, 54 h). To the mixture, MnO_2 (2.6 g, 30.0 mmol) and CH_2ClCH_2Cl (DCE) (30.0 mL) was added. The mixture was stirred at 40 °C until dihydropyrrole was consumed (50 h). The mixture was cooled to rt, diluted with EtOAc, and filtered through Celite. The filtrate was washed with water (x 2) and brine (x 2), dried over Na_2SO_4, concentrated in vacuo, and purified by flash column chromatography on silica gel (Hexane/EtOAc = 4:1) to give **4f** (2.30 g, 80%) as an orange solid. Recrystallization (Hexane/EtOAc = 20 mL/5 mL) gave **4f** (1.46 g) as pale yellow crystals; mp: 160-162.

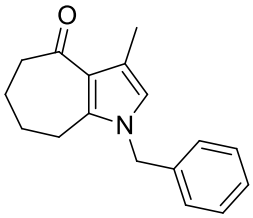
Compound 4g



Synthesis of dihydropyrrole at rt for 20 h; oxidation at 40°C for 43 h; flash column chromatography (Hexane/EtOAc = 4:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.37-7.26 (m, 3H), 7.05-7.04 (m, 2H), 6.22 (m, 1H), 5.19 (s, 2H), 2.50 (t, *J* = 6.4 Hz, 2H), 2.28 (d, *J* = 0.8 Hz, 3H), 1.95 (t, *J* = 6.4 Hz, 2H), 1.32 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 195.4, 148.9, 137.5, 128.8, 127.7, 126.4, 122.3, 119.2, 118.4, 51.5, 41.2, 35.6, 32.6, 27.4, 11.7. ESI-HRMS: calcd for $C_{18}H_{22}NO$ ($[M+H]^+$) 268.1701, found 268.1695.

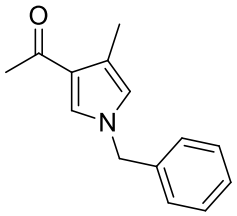
Gram-scale synthesis of **4g**: A mixture of $Cu(OTf)_2$ (180.8 mg, 0.5 mmol) and PPh_3 (524.6 mg, 2.0 mmol) in $PhCF_3$ (10.0 mL) was stirred at room temperature (25 °C) for 5 min under Ar. To the mixture, 4,4-dimethylcyclohexenone (1.3 mL, 10.0 mmol), *N*-benzylprop-2-yn-1-amine (1.74 g, 12.0 mmol), and pyrrolidine (165.4 μL, 2.0 mmol) were added. The resulting mixture was stirred at the room temperature until the enone was consumed (monitored by TLC, 69 h). To the mixture, MnO_2 (4.3 g, 50.0 mmol) and CH_2ClCH_2Cl (DCE) (30.0 mL) was added. The mixture was stirred at 40 °C. After 72 h, another portion of MnO_2 (4.3 g, 50.0 mmol) was added. The mixture was stirred at 60 °C for 24 h, then cooled to rt, diluted with EtOAc, and filtered through Celite. The filtrate was washed with water (x 2) and brine (x 2), dried over Na_2SO_4, concentrated in vacuo, and purified by flash column chromatography on silica gel (Hexane/EtOAc = 4:1) to give **4g** (1.64 g, 61%) as a yellow solid. Recrystallization (Hexane/EtOAc/Toluene = 5 mL/1 mL/1 mL) gave **4g** (1.04 g) as pale yellow crystals; mp: 79-81.

Compound 4h



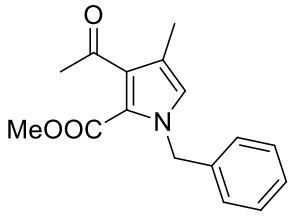
Synthesis of dihydropyrrole in MeOH at rt for 55 h; oxidation at 40 °C for 24 h; flash column chromatography (Hexane/EtOAc = 4:1); pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.36-7.28 (m, 3H), 7.01-7.00 (m, 2H), 6.39 (q, *J* = 0.8 Hz, 1H), 5.02 (s, 2H), 2.74 (t, *J* = 6.0 Hz, 2H), 2.69-2.66 (m, 2H), 2.28 (d, *J* = 0.8 Hz, 3H), 1.85-1.75 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 198.8, 139.9, 137.3, 128.9, 127.7, 126.2, 122.6, 121.0, 120.6, 50.5, 43.1, 25.1, 24.8, 22.1, 12.4. ESI-HRMS: calcd for $C_{17}H_{20}NO$ ($[M+H]^+$) 254.1539, found 254.1539.

Compound 4i



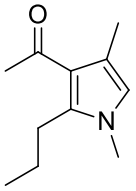
Synthesis of dihydropyrrole at rt for 47 h; oxidation at 40 °C for 7 h; flash column chromatography (Hexane/EtOAc = 4:1); pale yellow gum. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.39-7.33 (m, 3H), 7.24 (d, *J* = 2.0 Hz, 1H), 7.17-7.15 (m, 2H), 6.43 (m, 1H), 5.00 (s, 2H), 2.36 (s, 3H), 2.29 (d, *J* = 0.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 194.0, 136.7, 128.9, 128.1, 127.7, 127.2, 124.2, 121.7, 121.6, 53.7, 27.8, 12.3 ppm; ESI-HRMS: calcd for $C_{14}H_{16}NO$ ($[M+H]^+$) 214.1226, found 214.1229.

Compound 4j



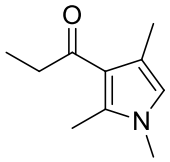
Synthesis of dihydropyrrole at rt for 48 h; oxidation at 40 °C for 30 h; flash column chromatography (Hexane/EtOAc = 4:1); pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.35-7.27 (m, 3H), 7.13-7.11 (m, 2H), 6.61 (d, *J* = 0.8 Hz, 1H), 5.41 (s, 2H), 3.77 (s, 3H), 2.44 (s, 3H), 2.06 (d, *J* = 0.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 200.8, 161.0, 137.4, 132.4, 128.7, 127.7, 127.0, 126.6, 120.2, 118.4, 52.0, 51.5, 31.9, 10.4. ESI-HRMS: calcd for $C_{16}H_{18}NO_3$ ($[M+H]^+$) 272.1281, found 272.1292.

Compound 4k



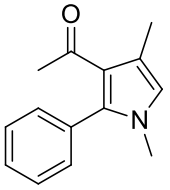
Synthesis of dihydropyrrole at 40 °C for 22 h; oxidation at 40 °C for 66 h; flash column chromatography (Hexane/EtOAc = 3:1); yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.26 (q, *J* = 0.8 Hz, 1H), 3.49 (s, 3H), 2.88-2.84 (m, 2H), 2.42 (s, 3H), 2.25 (d, *J* = 0.8 Hz, 3H), 1.60-1.54 (m, 2H), 0.99 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 195.2, 140.9, 120.9, 120.6, 118.8, 33.1, 31.0, 27.8, 22.6, 14.2, 13.8. ESI-HRMS: calcd for $C_{11}H_{18}NO$ ($[M+H]^+$) 180.1383, found 180.1385.

Compound 4l



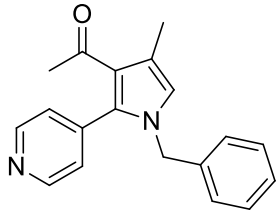
Synthesis of dihydropyrrole in MeOH at 40 °C for 52 h; oxidation at 40 °C for 42 h; flash column chromatography (Hexane/EtOAc = 5:1); colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.28 (brq, J = 0.8 Hz, 1H), 3.47 (s, 3H), 2.74 (q, J = 7.2 Hz, 2H), 2.48 (s, 3H), 2.26 (d, J = 0.8 Hz, 3H), 1.17 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 198.6, 136.0, 121.1, 120.4, 118.5, 35.5, 33.3, 13.8, 12.2, 8.4. ESI-HRMS: calcd for $C_{10}H_{16}NO$ ($[M+H]^+$) 166.1226, found 166.1227.

Compound 4m



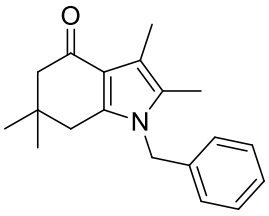
Synthesis of dihydropyrrole at 40 °C for 20 h; oxidation at 40 °C for 46 h; flash column chromatography (Hexane/EtOAc = 8:1); colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.49-7.46 (m, 3H), 7.35-7.32 (m, 2H), 6.45 (brq, J = 0.8 Hz, 1H), 3.32 (s, 3H), 2.32 (d, J = 0.8 Hz, 3H), 1.86 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 195.7, 138.7, 133.1, 130.7, 128.8, 128.6, 122.9, 121.3, 121.0, 34.3, 30.3, 12.7. ESI-HRMS: calcd for $C_{14}H_{16}NO$ ($[M+H]^+$) 214.1232, found 214.1236.

Compound 4n



Synthesis of dihydropyrrole at rt for 49 h; oxidation at 40 °C for 25 h; flash column chromatography (Hexane/Acetone = 1:1); pale yellow solid; mp 106-108. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.64 (m, 2H), 7.29-7.26 (m, 3H), 7.17 (m, 2H), 6.90-6.88 (m, 2H), 6.56 (m, 1H), 4.81 (s, 2H), 2.32 (d, J = 0.4 Hz, 3H), 2.01 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 195.2, 149.9, 141.2, 136.9, 135.1, 128.8, 127.9, 126.5, 125.5, 123.9, 122.0, 121.4, 50.8, 30.7, 12.6. ESI-HRMS: calcd for $C_{19}H_{19}N_2O$ ($[M+H]^+$) 291.1492, found 291.1496.

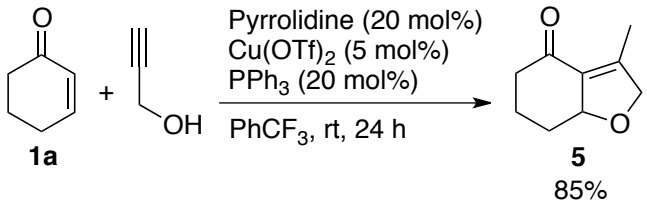
Compound 4o



Synthesis of dihydropyrrole at rt for 24 h; oxidation at 50 °C for 38 h; flash column chromatography (Hexane/EtOAc = 2:1); colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.34-7.25 (m, 3H), 6.92-6.90 (m, 2H), 5.01 (s, 2H), 2.50 (s, 2H), 2.32 (s, 2H), 2.28 (s, 3H), 1.73 (s, 3H), 1.07 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 194.3, 141.6, 137.1, 128.9, 127.5, 126.4, 125.6, 117.4, 114.4, 52.7, 47.0, 36.1, 35.1, 10.4, 9.1. ESI-HRMS: calcd for $C_{19}H_{24}NO$ ($[M+H]^+$) 282.1858, found 282.1853.

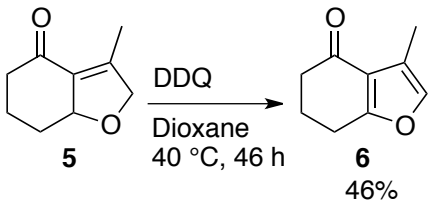
5. Synthesis of 2,5-Dihydrofuran and 3-Acylfuran

Synthesis of 5 (Scheme 1)



A mixture of $Cu(OTf)_2$ (3.6 mg, 0.01 mmol) and PPh_3 (10.5 mg, 0.04 mmol) in $PhCF_3$ (0.2 mL) was stirred at room temperature (25 °C) for 5 min under Ar. To the mixture, enone **1a** (19.4 μL, 0.2 mmol), propargyl alcohol (23.6 μL, 0.4 mmol), and pyrrolidine (3.4 μL, 0.04 mmol) were added. The resulting mixture was stirred at the same room temperature under Ar for 24 h until **1a** was consumed (monitored by TLC). The mixture was directly purified by flash column chromatography on silica gel (Hexane/EtOAc = 4:1) to give **5** as a colorless solid (26.0 mg, 85%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 4.91-4.84 (m, 1H), 4.67-4.61 (m, 1H), 4.57-4.50 (m, 1H), 2.51-2.45 (m, 1H), 2.32-2.20 (m, 2H), 2.03 (m, 3H), 2.03-1.98 (m, 1H), 1.77-1.65 (m, 1H), 1.63-1.53 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 198.7, 146.1, 132.8, 86.0, 78.1, 40.5, 32.2, 19.7, 11.6. ESI-HRMS: calcd for $C_9H_{13}O_2$ ($[M+H]^+$) 153.0910, found 153.0911.

Synthesis of 6 (Scheme 1)

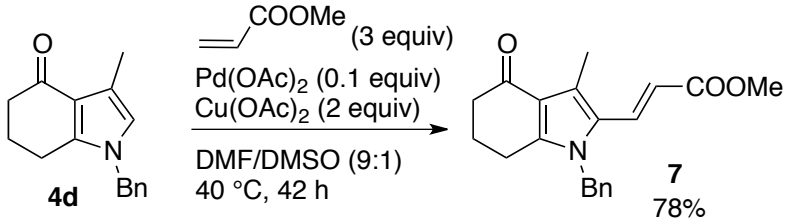


To a mixture of **5** (60.8 mg, 0.4 mmol) in dioxane (2.0 mL, anhydrous) was added a solution of DDQ (136.2 mg, 0.6 mmol) in dioxane. The mixture was stirred at 40 °C for 46 h under Ar. The mixture was diluted with CH_2Cl_2, washed with 1 M NaOH, water and brine. The organic layer was dried over Na_2SO_4, filtered, concentrated, and purified by flash column chromatography on silica gel (Hexane/EtOAc = 4:1) to give **6** as a colorless solid (27.3 mg, 46%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.07 (m, 1H), 2.84 (t, *J* = 6.4 Hz, 2H), 2.49-2.46 (m, 2H), 2.20 (d, *J* = 1.6 Hz, 3H), 2.19-2.12 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 195.7, 167.4, 138.9, 120.4, 119.1, 38.3, 23.6, 22.7, 9.1. ESI-HRMS: calcd for $C_9H_{11}O_2$ ($[M+H]^+$) 151.0759, found 151.0752.

6. Transformations of 3-Acylpyrroles

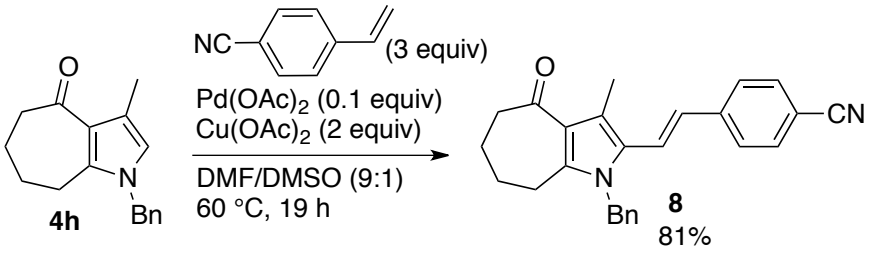
According to the reported indole C-H functionalization procedure,[8] 3-acylpyrroles **4d** and **4h** were transformed to **7** and **8**, respectively.

Synthesis of 7 (Scheme 2)



A mixture of 3-acylpyrrole **4d** (20.0 mg, 0.084 mmol, 1 equiv), methyl acrylate (22.8 μL, 0.25 mmol, 3 equiv to **4d**), $Cu(OAc)_2$ (30.5 mg, 0.17 mmol, 2 equiv), and $Pd(OAc)_2$ (1.9 mg, 0.008 mmol, 0.1 equiv) in DMF/DMSO (9:1, concentration of **4d**: 0.4 M) was stirred at 40 °C for 42 h. The mixture was cooled to rt, diluted with AcOEt, added to water, and extracted with EtOAc. Organic layers were combined, washed with brine, dried over Na_2SO_4, filtered, concentrated, and purified by flash column chromatography on silica gel (Acetone/Hexane = 1/2) to gave **7** as a pale yellow solid (21.1 mg, 78%); mp: 114-116. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.59 (d, *J* = 16.0 Hz, 1H), 7.37-7.29 (m, 3H), 6.97-6.96 (m, 2H), 6.03 (d, *J* = 16.0 Hz, 1H), 5.20 (s, 2H), 3.73 (s, 3H), 2.70 (t, *J* = 6.4 Hz, 2H), 2.57 (s, 3H), 2.49 (t, *J* = 6.4 Hz, 2H), 2.11 (pentet, *J* = 6.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 194.1, 166.9, 145.4, 134.9, 130.6, 128.1, 126.9, 125.8, 124.6, 124.1, 116.9, 113.8, 50.5, 46.7, 37.8, 22.0, 21.3, 11.2. ESI-HRMS: calcd for $C_{20}H_{22}NO_3$ ($[M+H]^+$) 324.1594, found 324.1594.

Synthesis of 8 (Scheme 2)



Compound **8** was synthesized from **4h** (19.0 mg, 0.075 mmol) by the procedure used for the synthesis of **7** from **4d** but at 60 °C for 19 h. Purification by flash column chromatography on silica gel (EtOAc/Hexane = 1/2) gave **8** as a pale green solid (23.2 mg, 81%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.56-7.54 (m, 2H), 7.39-7.31 (m, 5H), 7.01-6.99 (m, 2H), 6.95 (d, *J* = 16.0 Hz, 1H), 6.62 (d, *J* = 16.0 Hz, 1H), 5.23 (s, 2H), 2.82-2.79 (m, 2H), 2.73-2.70 (m, 2H), 2.50 (s, 3H), 1.91-1.98 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 199.1, 142.2, 141.8, 136.9, 132.4, 129.2, 128.2, 127.8, 127.6, 126.3, 125.5, 123.4, 122.1, 120.3, 119.1, 110.0, 47.7, 43.1, 25.0, 24.8, 21.9, 12.6. ESI-HRMS: calcd for $C_{26}H_{25}N_2O$ ($[M+H]^+$) 381.1961, found 381.1958.

7. References

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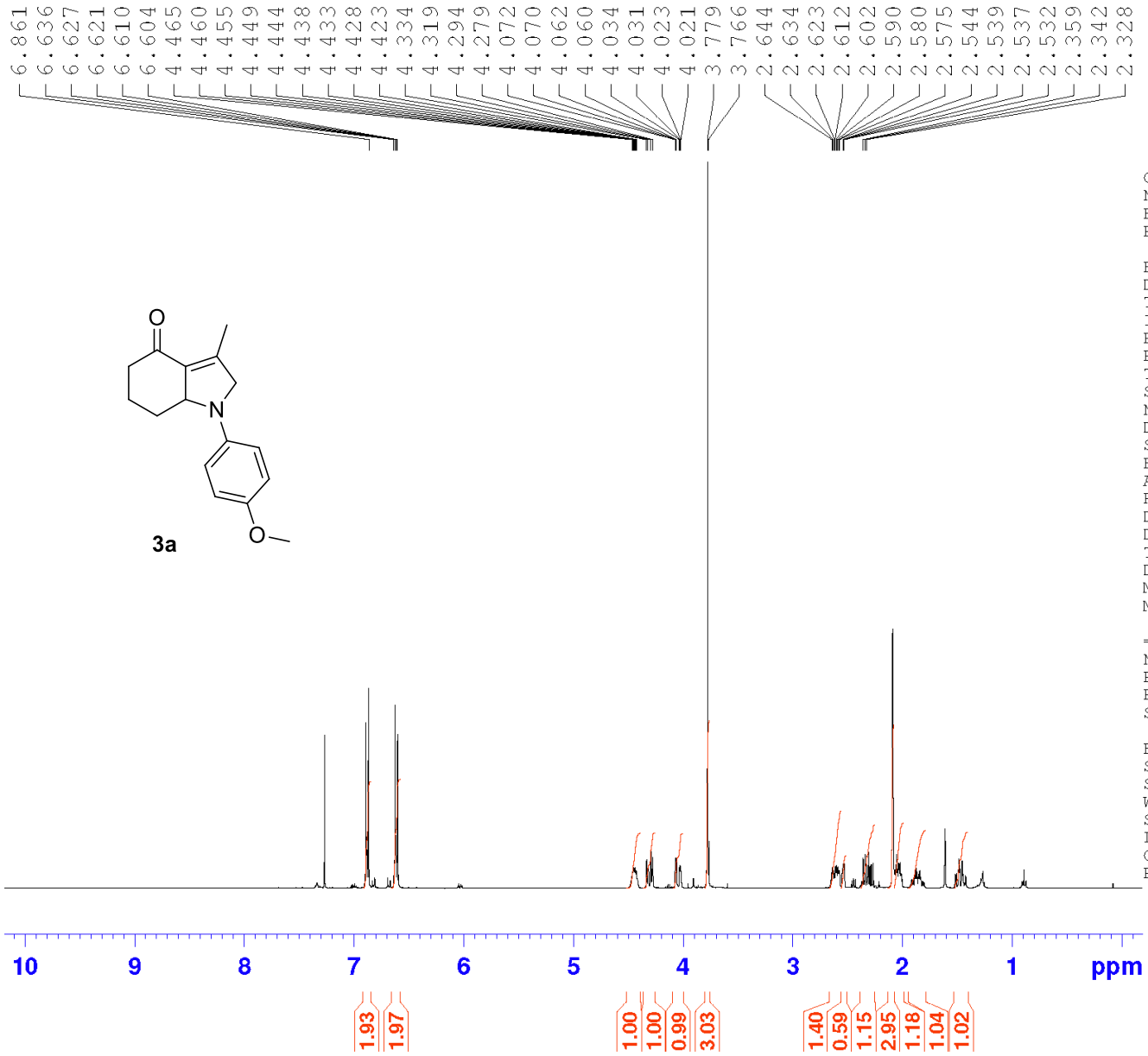


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MCREST        0.00000000 sec
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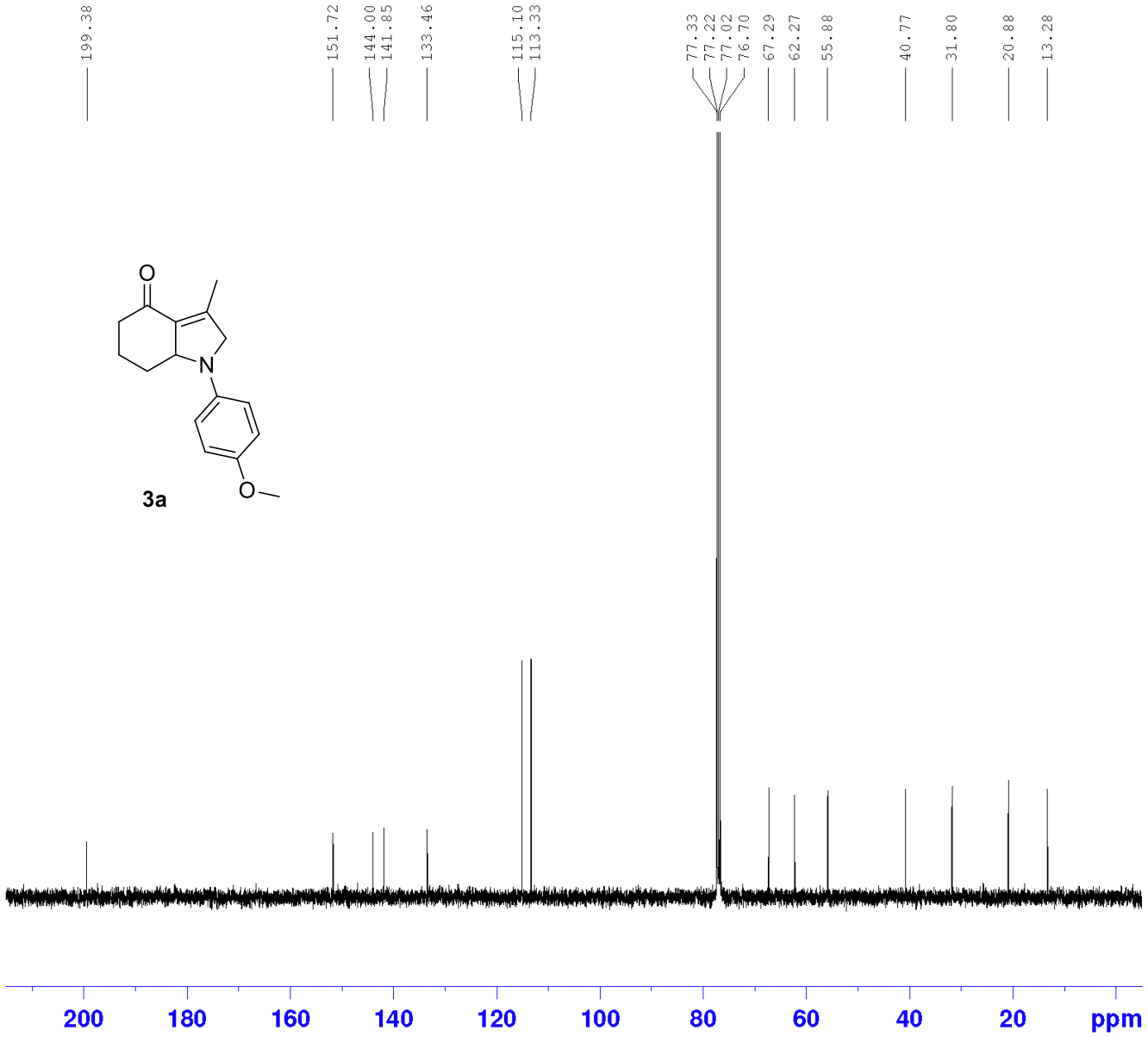


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PROCNO                 1

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TD                65536
SOLVENT           CDCl3
NS                  400
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3632196 sec
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DW               20.800 usec
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TE                298.9 K
D1           2.00000000 sec
d11          0.03000000 sec
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MCREST       0.00000000 sec
MCWRK        0.01500000 sec

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P1                10.00 usec
PL1               -2.00 dB
SFO1        100.6479773 MHz

======== CHANNEL f2 ========
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NUC2                 1H
PCPD2             80.00 usec
PL2                2.70 dB
PL12              17.10 dB
PL13              17.10 dB
SFO2        400.2316009 MHz

F2 - Processing parameters
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WDW                  EM
SSB                   0
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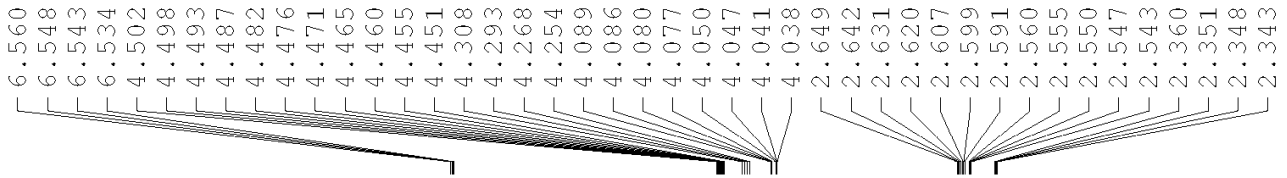

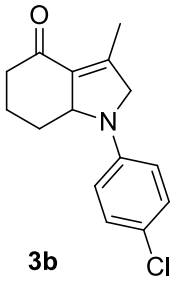

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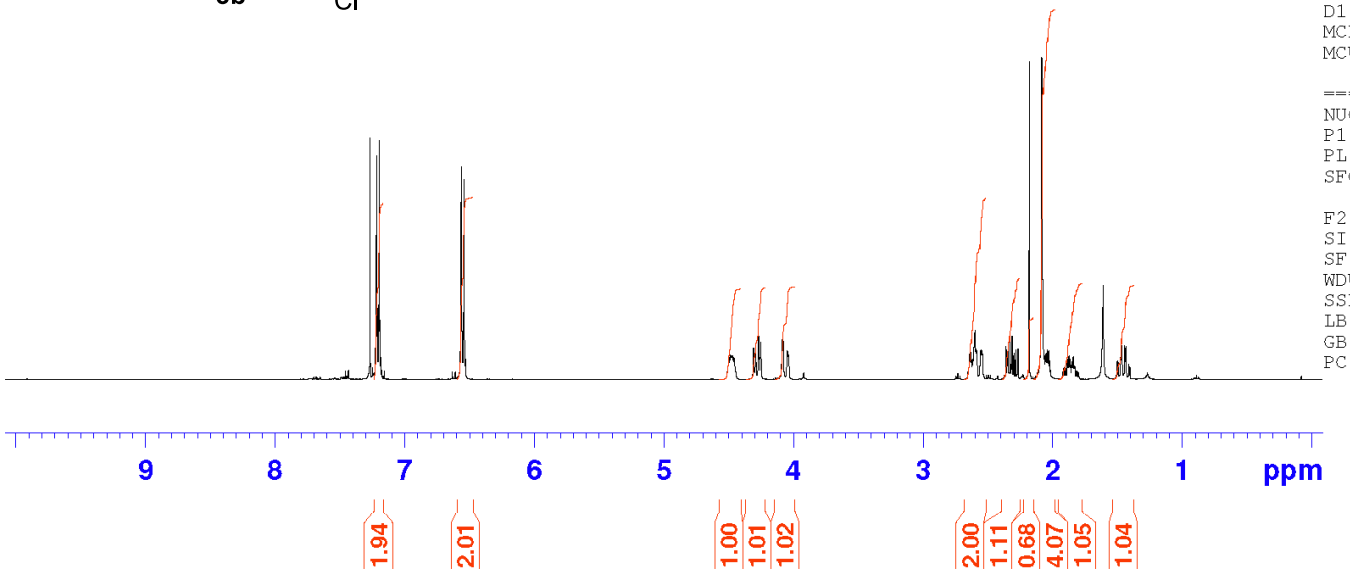


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SOLVENT            CDCl3
NS                    16
DS                     2
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FIDRES          0.125898 Hz
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TE                297.7 K
D1           1.00000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
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P1                15.00 usec
PL1                2.70 dB
SFO1        400.2324716 MHz

F2 - Processing parameters
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SF          400.2300015 MHz
WDW                   EM
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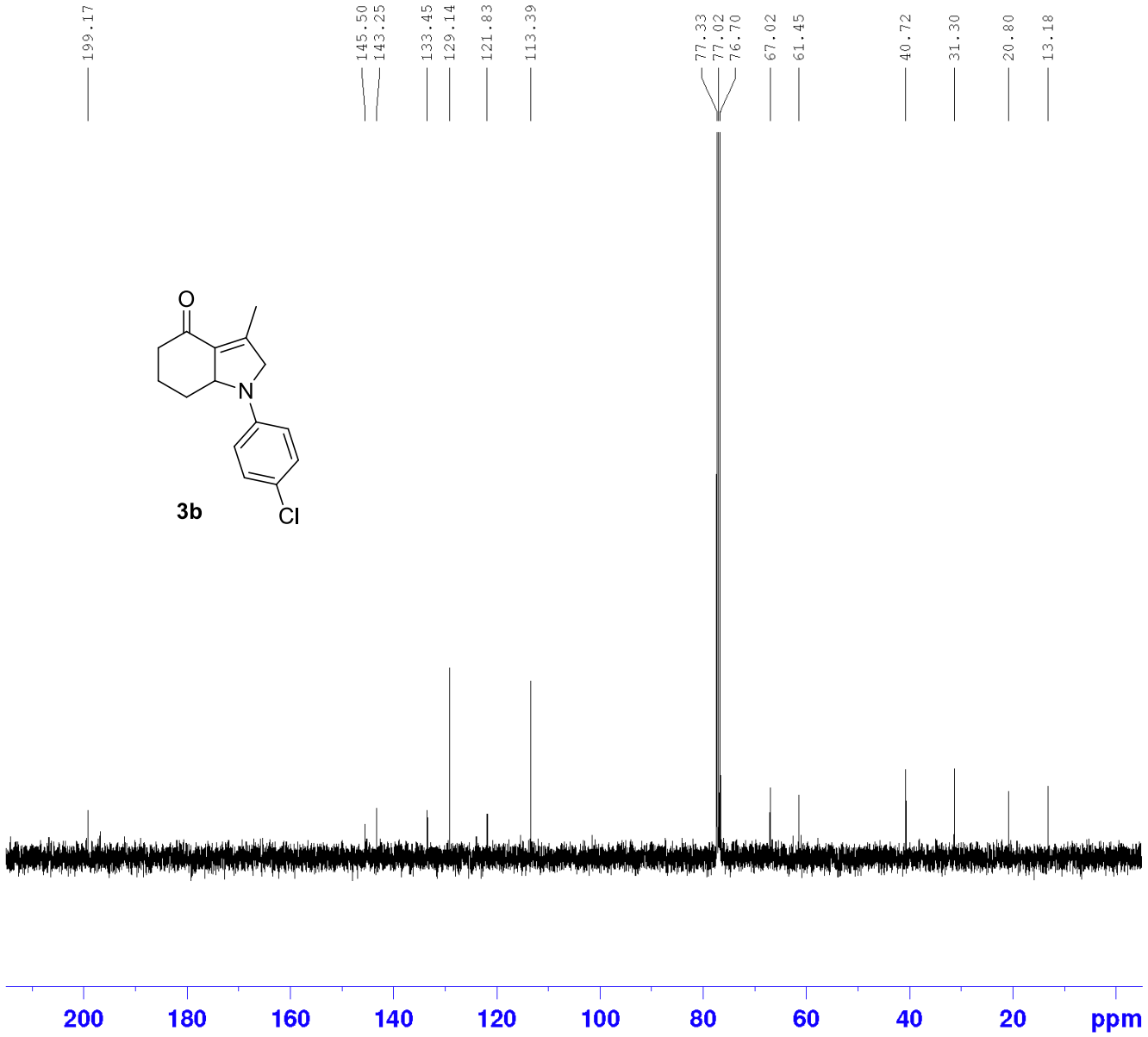


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PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  400
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3632196 sec
RG                32768
DW               20.800 usec
DE                6.00 usec
TE                298.7 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1               -2.00 dB
SFO1        100.6479773 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             80.00 usec
PL2                2.70 dB
PL12              17.10 dB
PL13              17.10 dB
SFO2        400.2316009 MHz

F2 - Processing parameters
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PC                 1.40
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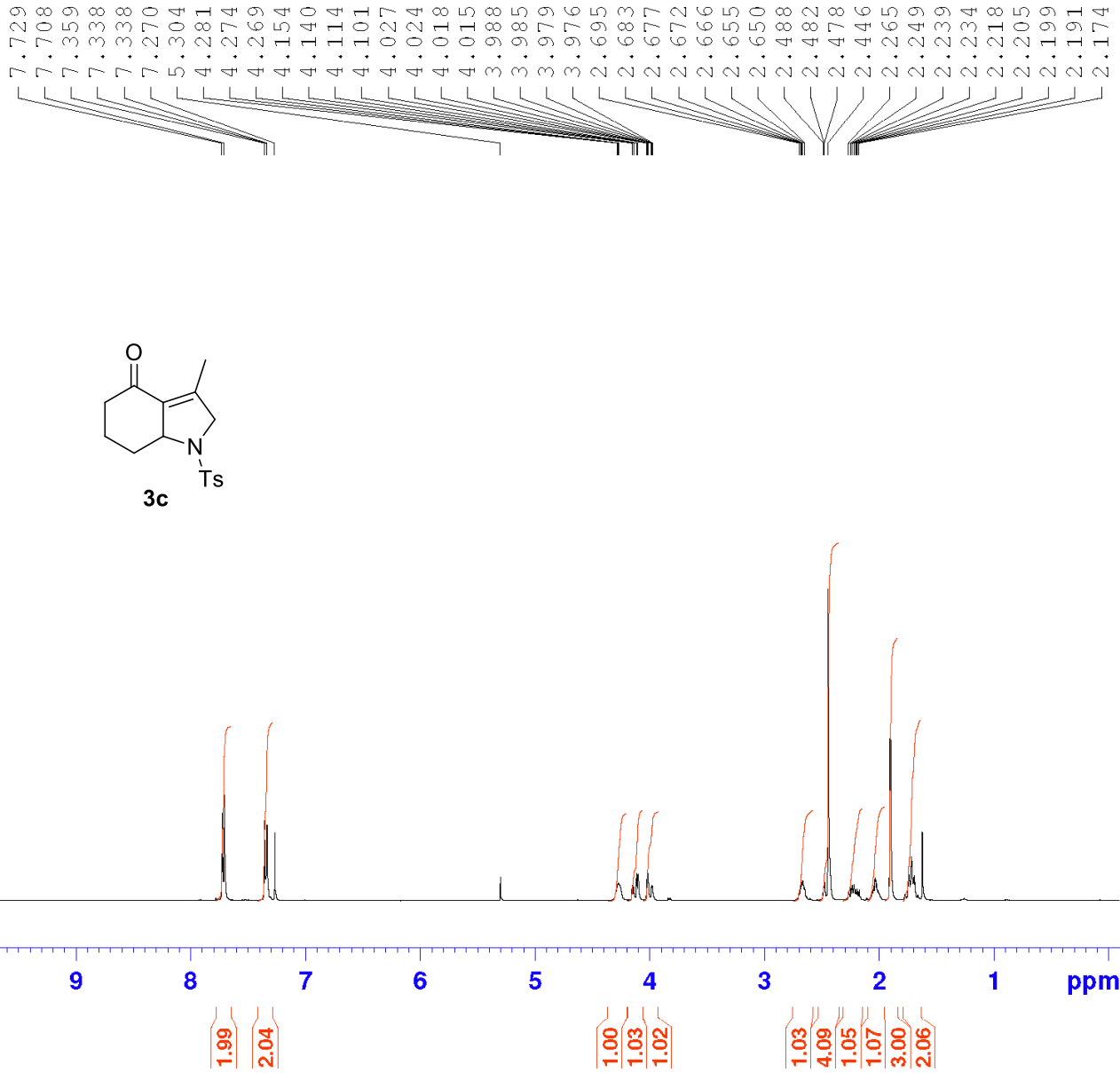


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PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8250.825 Hz
FIDRES          0.125898 Hz
AQ             3.9715922 sec
RG                 203.2
DW                60.600 usec
DE                 6.00 usec
TE                297.6 K
D1            1.00000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                2.70 dB
SFO1         400.2324716 MHz

F2 - Processing parameters
SI                 32768
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LB                0.30 Hz
GB                     0
PC                1.00
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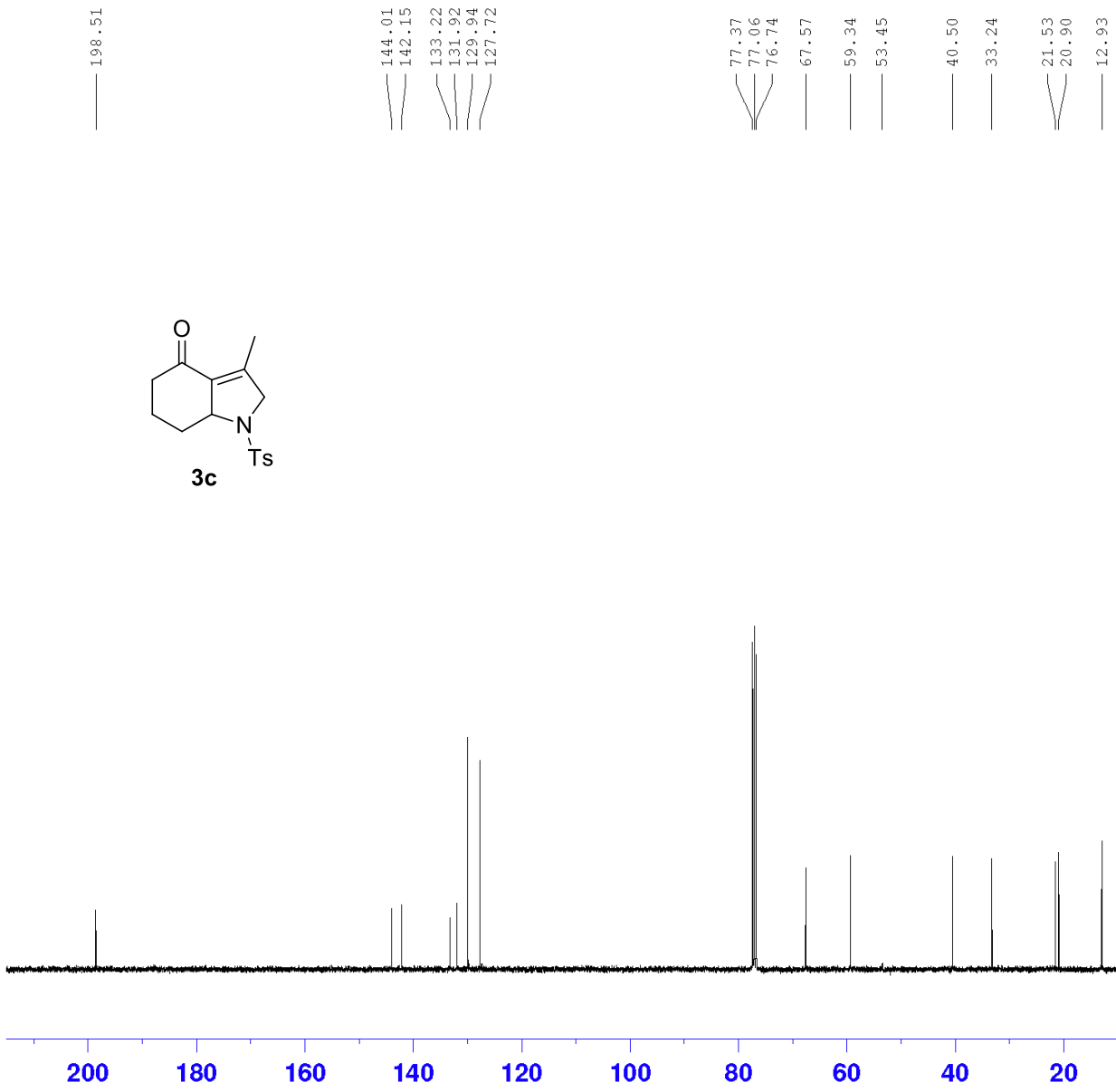


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SOLVENT           CDCl3
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SWH           24038.461 Hz
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MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1               -2.00 dB
SFO1        100.6479773 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2                2.70 dB
PL12              17.10 dB
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SFO2        400.2316009 MHz

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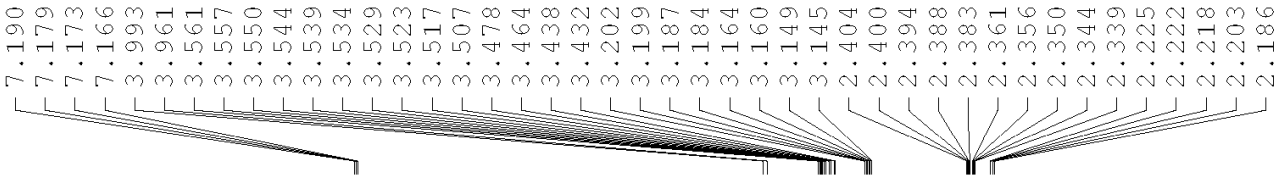

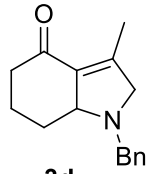

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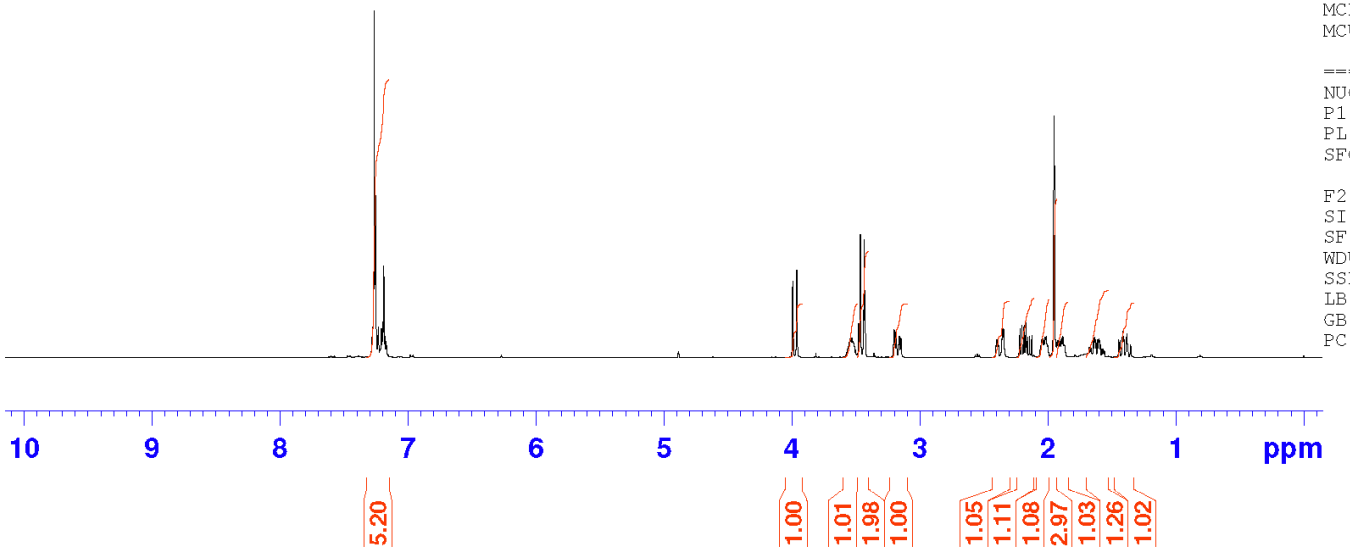


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PROCNO                 1

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TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8250.825 Hz
FIDRES          0.125898 Hz
AQ             3.9715922 sec
RG                   128
DW                60.600 usec
DE                 6.00 usec
TE                297.3 K
D1           1.00000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                2.70 dB
SFO1        400.2324716 MHz

F2 - Processing parameters
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SF          400.2300337 MHz
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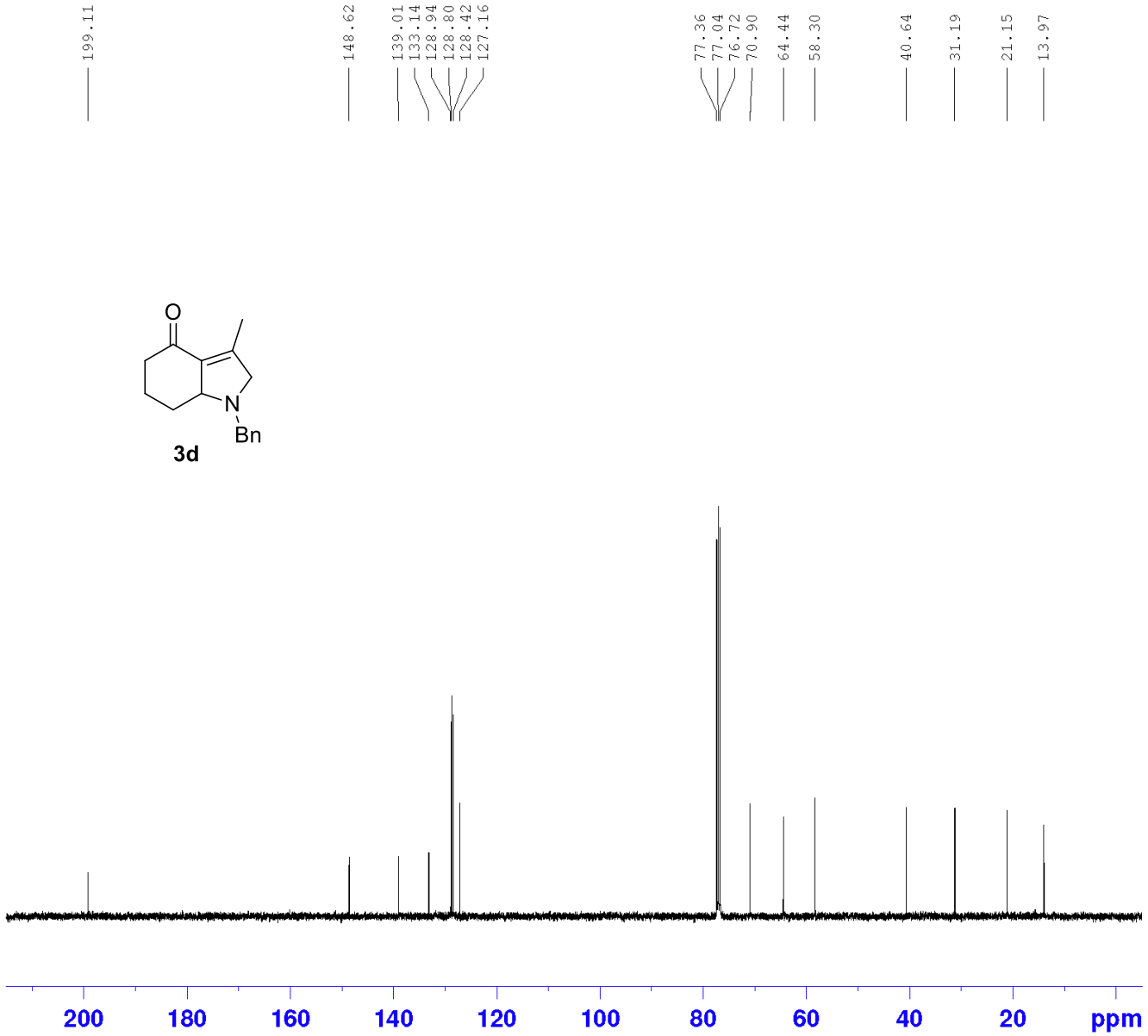


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PROCNO                1

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TD                65536
SOLVENT           CDCl3
NS                  300
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3632196 sec
RG               2896.3
DW               20.800 usec
DE                6.00 usec
TE               298.5 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1               -2.00 dB
SFO1        100.6479773 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2            80.00 usec
PL2               2.70 dB
PL12             17.10 dB
PL13             17.10 dB
SFO2        400.2316009 MHz

F2 - Processing parameters
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SF          100.6379140 MHz
WDW                   EM
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LB                 1.00 Hz
GB                     0
PC                 1.40
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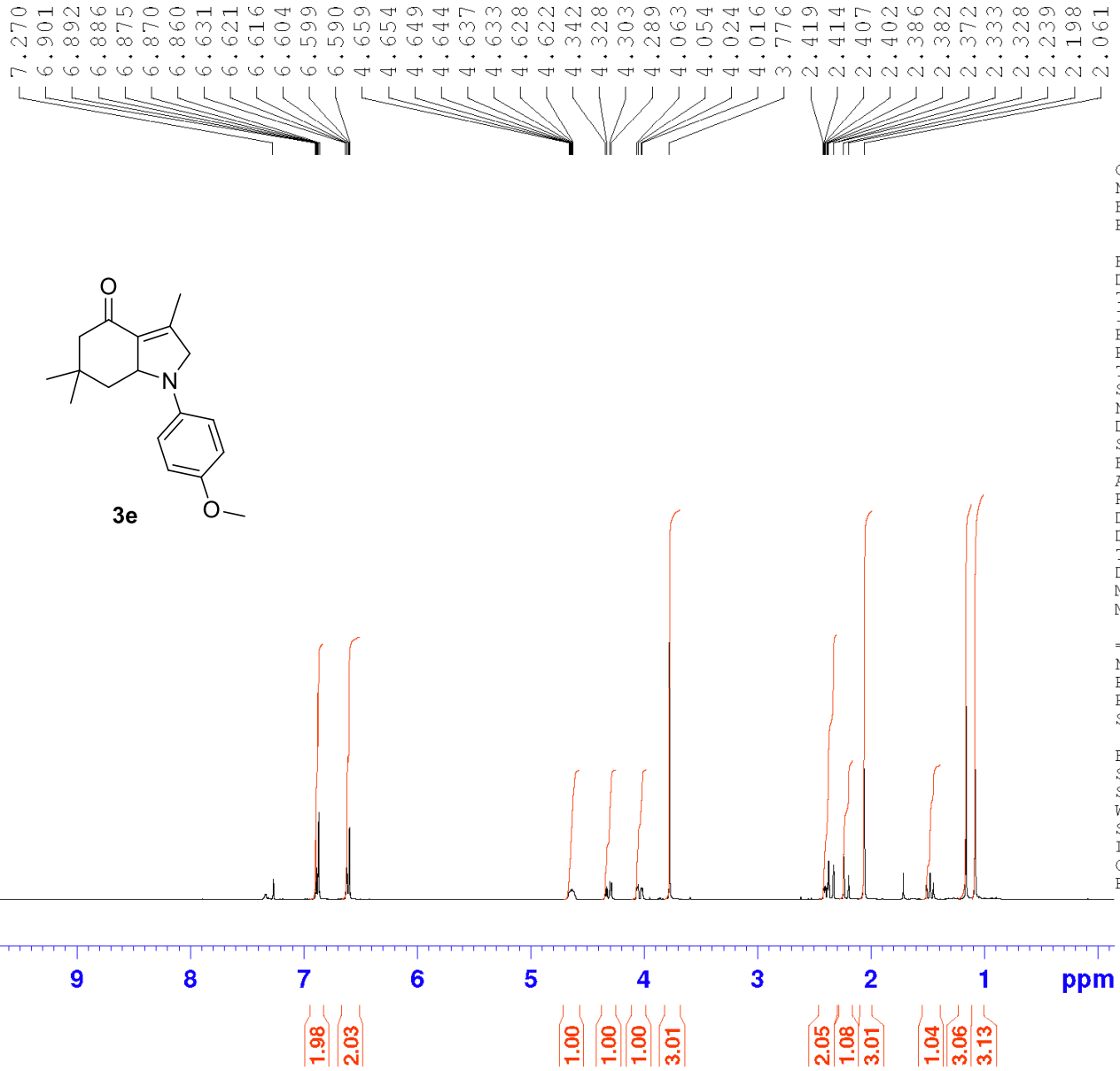


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TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
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FIDRES          0.125898 Hz
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DE                 6.00 usec
TE                297.6 K
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MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                2.70 dB
SFO1         400.2324716 MHz

F2 - Processing parameters
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LB                0.30 Hz
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PC                1.00
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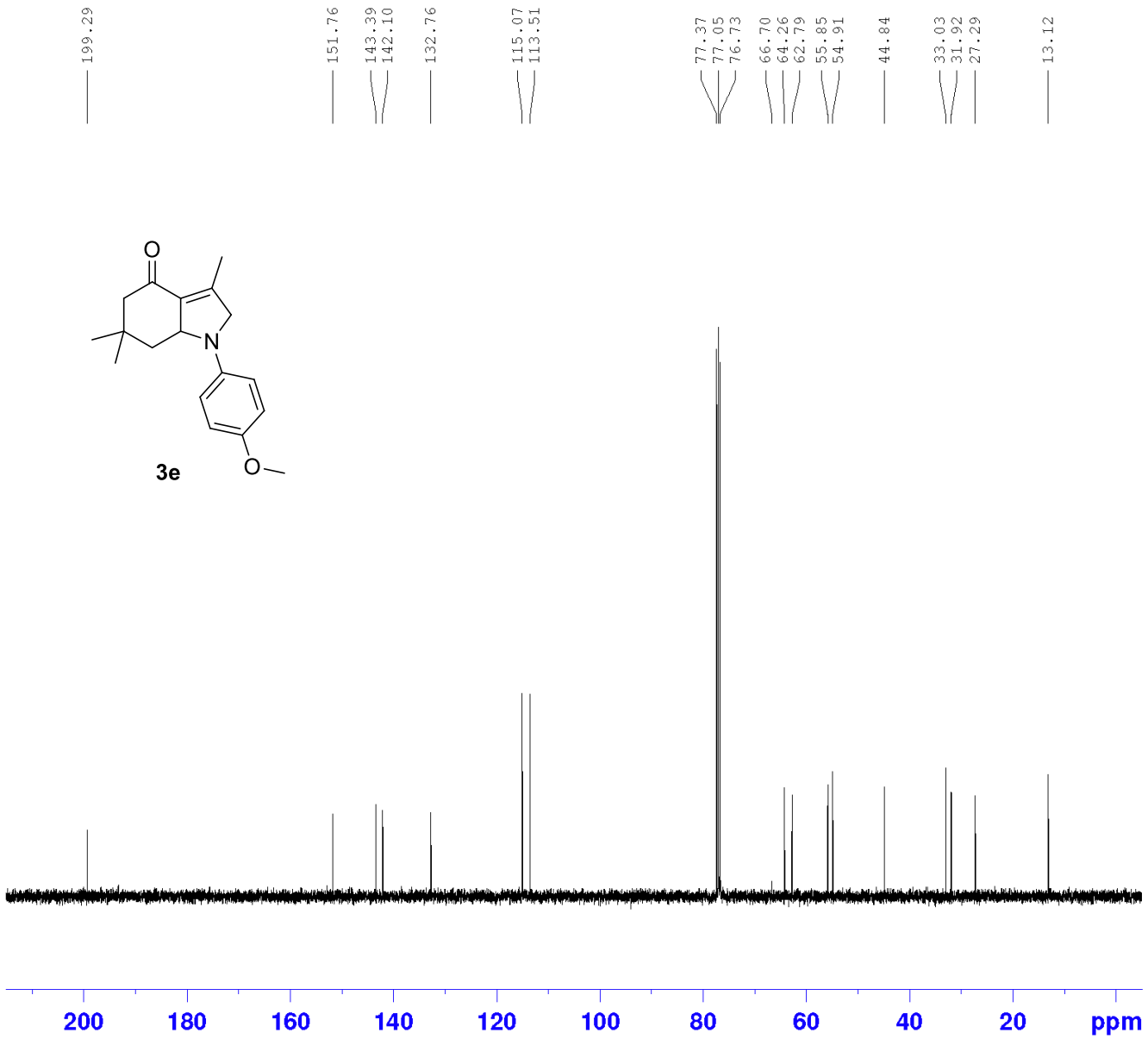


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DE                6.00 usec
TE                298.6 K
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d11          0.03000000 sec
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MCREST       0.00000000 sec
MCWRK        0.01500000 sec

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======== CHANNEL f2 ========
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NUC2                 1H
PCPD2             80.00 usec
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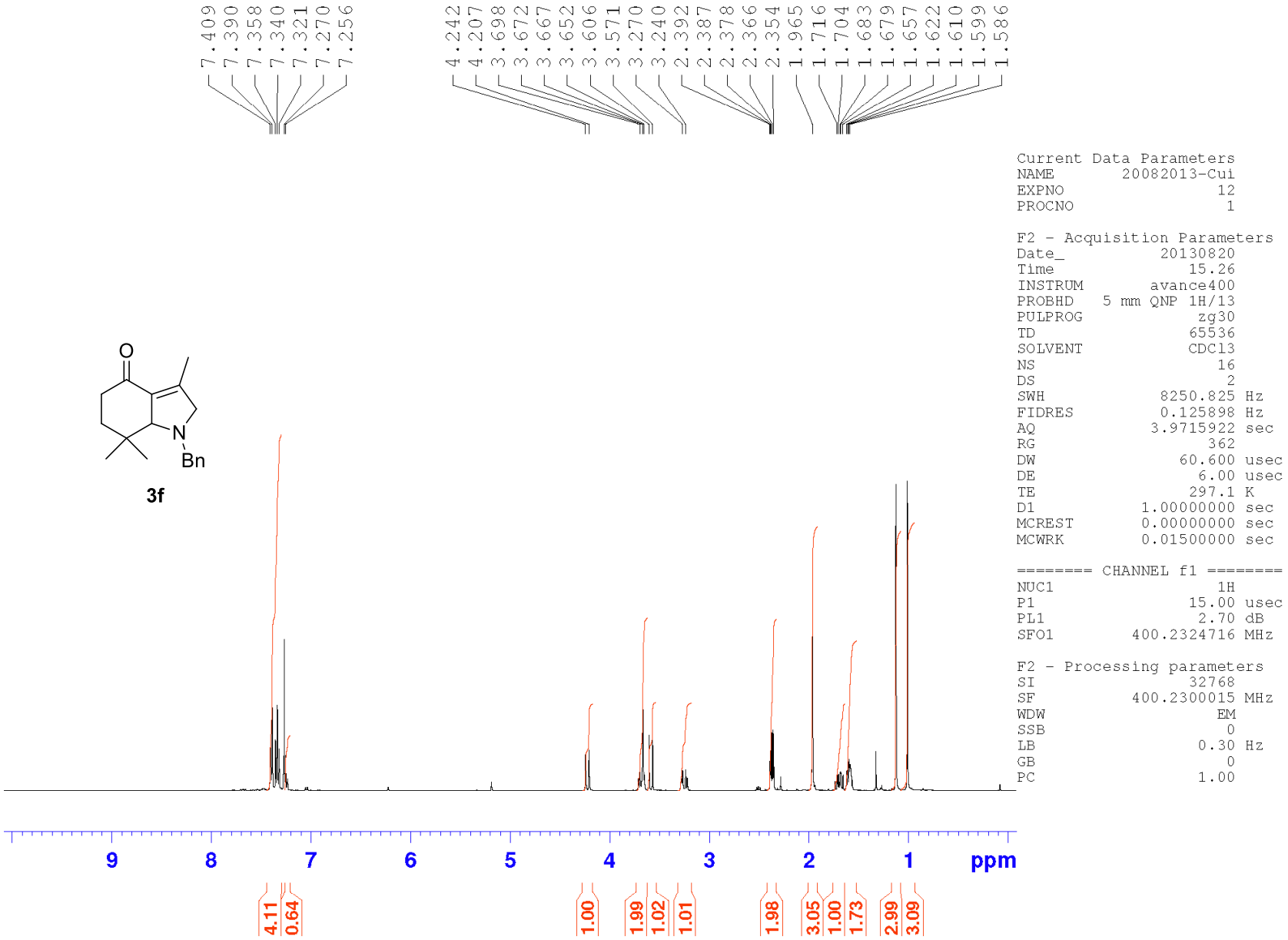
PL12              17.10 dB
PL13              17.10 dB
SFO2        400.2316009 MHz

F2 - Processing parameters
SI                32768
SF          100.6379140 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

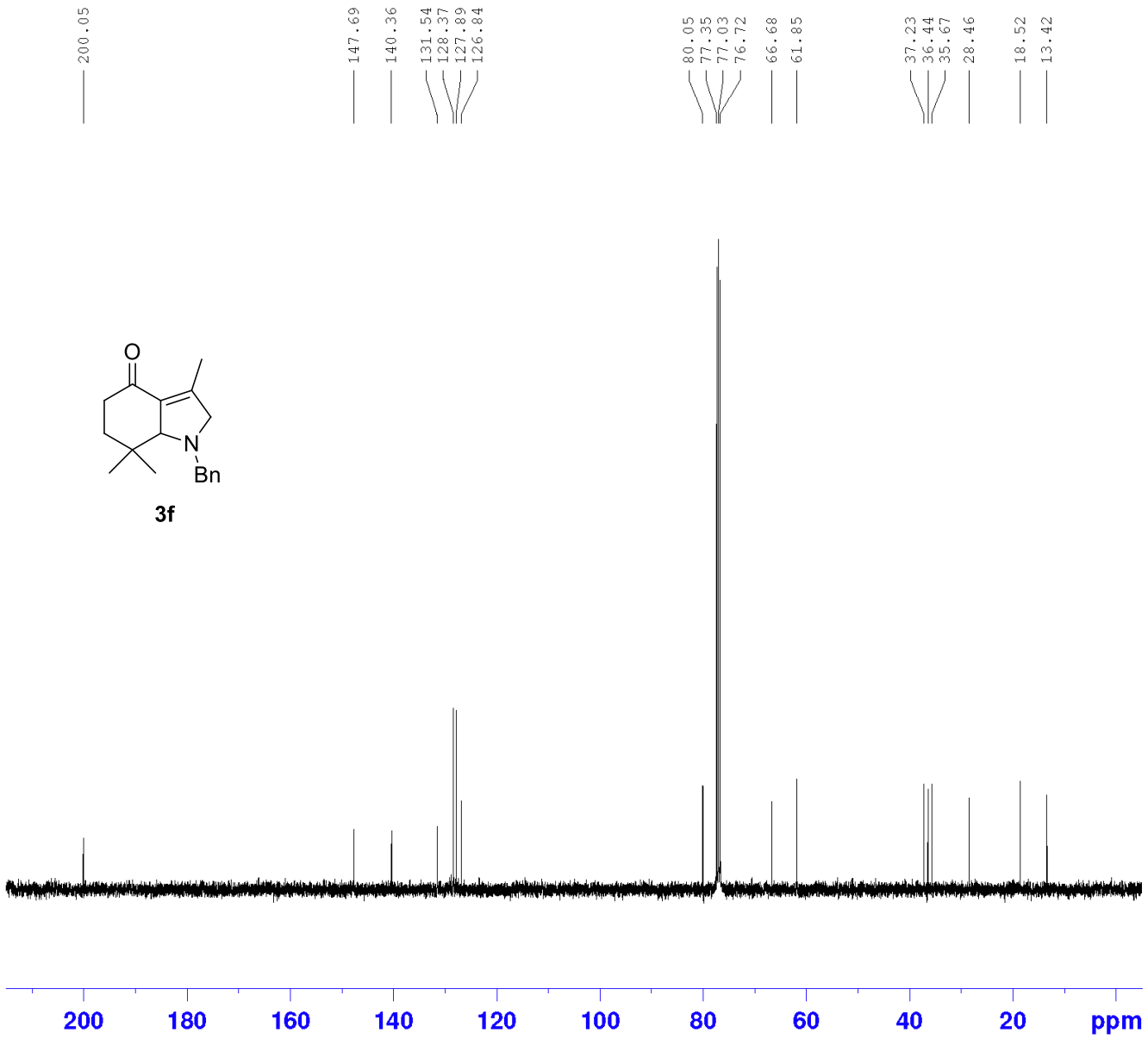



```
Current Data Parameters
NAME        20082013-Cui
EXPNO                 12
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130820
Time               15.26
INSTRUM        avance400
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8250.825 Hz
FIDRES          0.125898 Hz
AQ             3.9715922 sec
RG                   362
DW                60.600 usec
DE                 6.00 usec
TE                297.1 K
D1           1.00000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                2.70 dB
SFO1        400.2324716 MHz

F2 - Processing parameters
SI                 32768
SF          400.2300015 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```



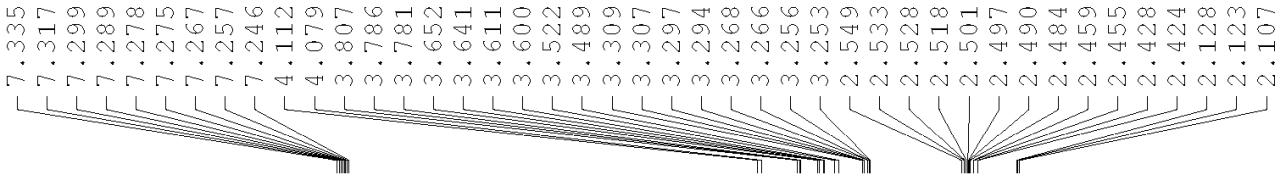

```
Current Data Parameters
NAME       20082013-Cui
EXPNO                11
PROCNO                1

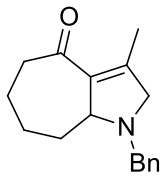
F2 - Acquisition Parameters
Date_          20130820
Time              14.58
INSTRUM       avance400
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  300
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3632196 sec
RG               5792.6
DW               20.800 usec
DE                6.00 usec
TE                297.8 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1               -2.00 dB
SFO1        100.6479773 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            80.00 usec
PL2               2.70 dB
PL12             17.10 dB
PL13             17.10 dB
SFO2        400.2316009 MHz

F2 - Processing parameters
SI                32768
SF          100.6379140 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```





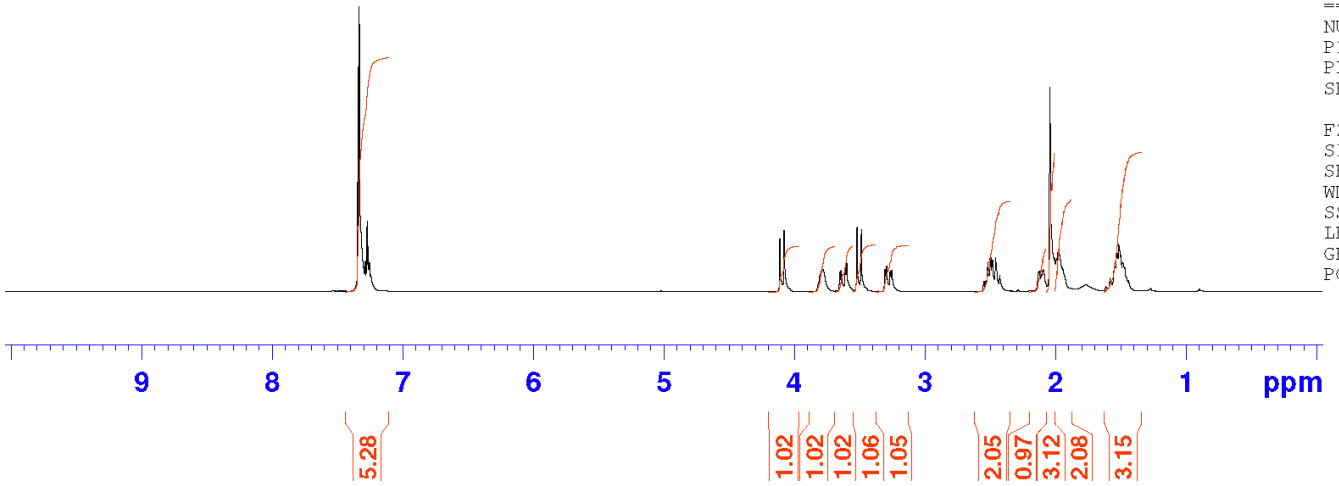
3g

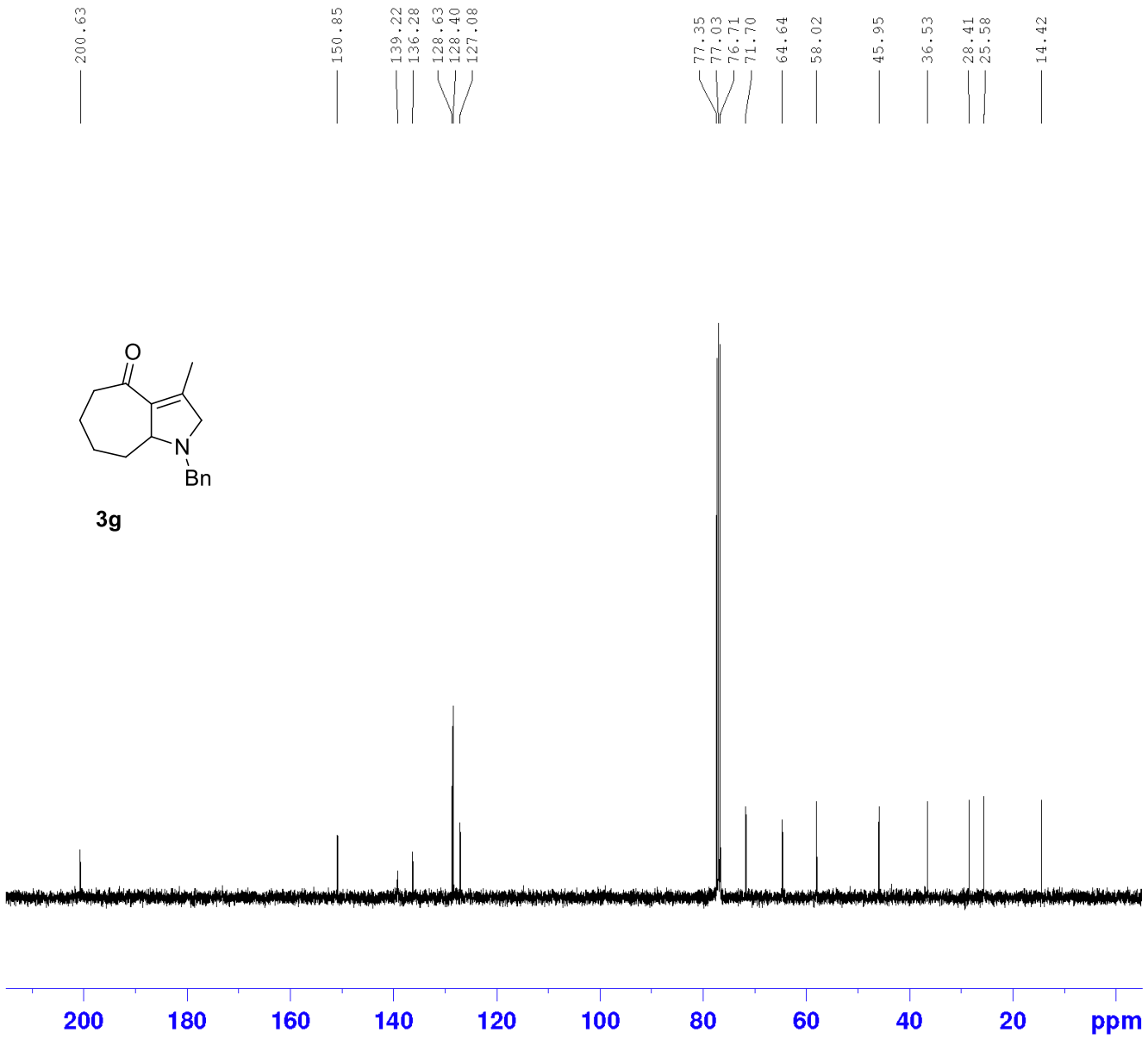
```
Current Data Parameters
NAME        01082013-Cui
EXPNO                 12
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130801
Time               11.36
INSTRUM        avance400
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8250.825 Hz
FIDRES          0.125898 Hz
AQ             3.9715922 sec
RG                 161.3
DW                60.600 usec
DE                 6.00 usec
TE                297.4 K
D1             1.00000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                 15.00 usec
PL1                 2.70 dB
SFO1         400.2324716 MHz

F2 - Processing parameters
SI                 32768
SF           400.2300000 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```





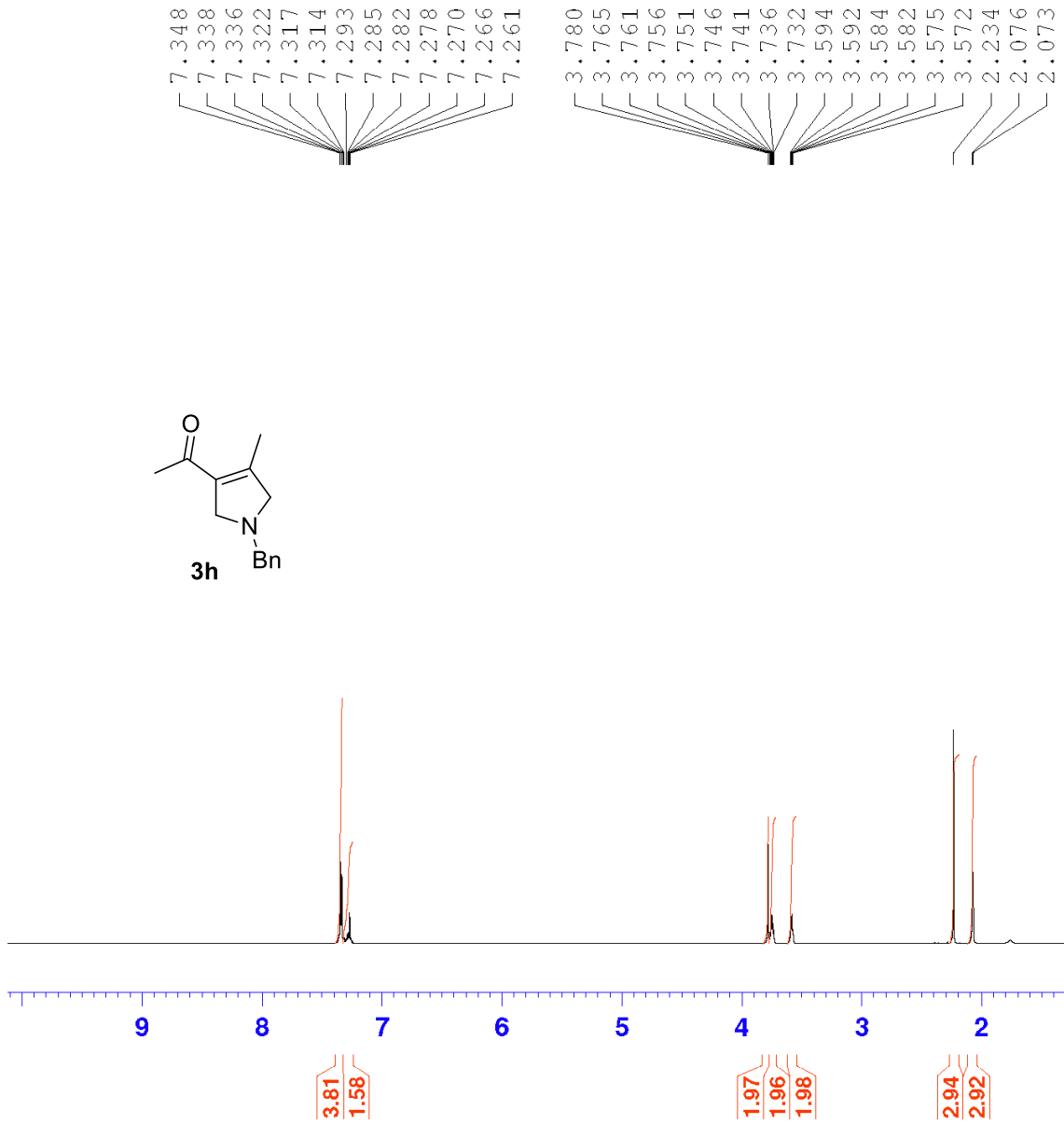

```
Current Data Parameters
NAME       01082013-Cui
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_          20130801
Time              11.31
INSTRUM       avance400
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  300
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3632196 sec
RG               3649.1
DW               20.800 usec
DE                6.00 usec
TE               297.9 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1               -2.00 dB
SFO1        100.6479773 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            80.00 usec
PL2               2.70 dB
PL12             17.10 dB
PL13             17.10 dB
SFO2        400.2316009 MHz

F2 - Processing parameters
SI                32768
SF          100.6379140 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

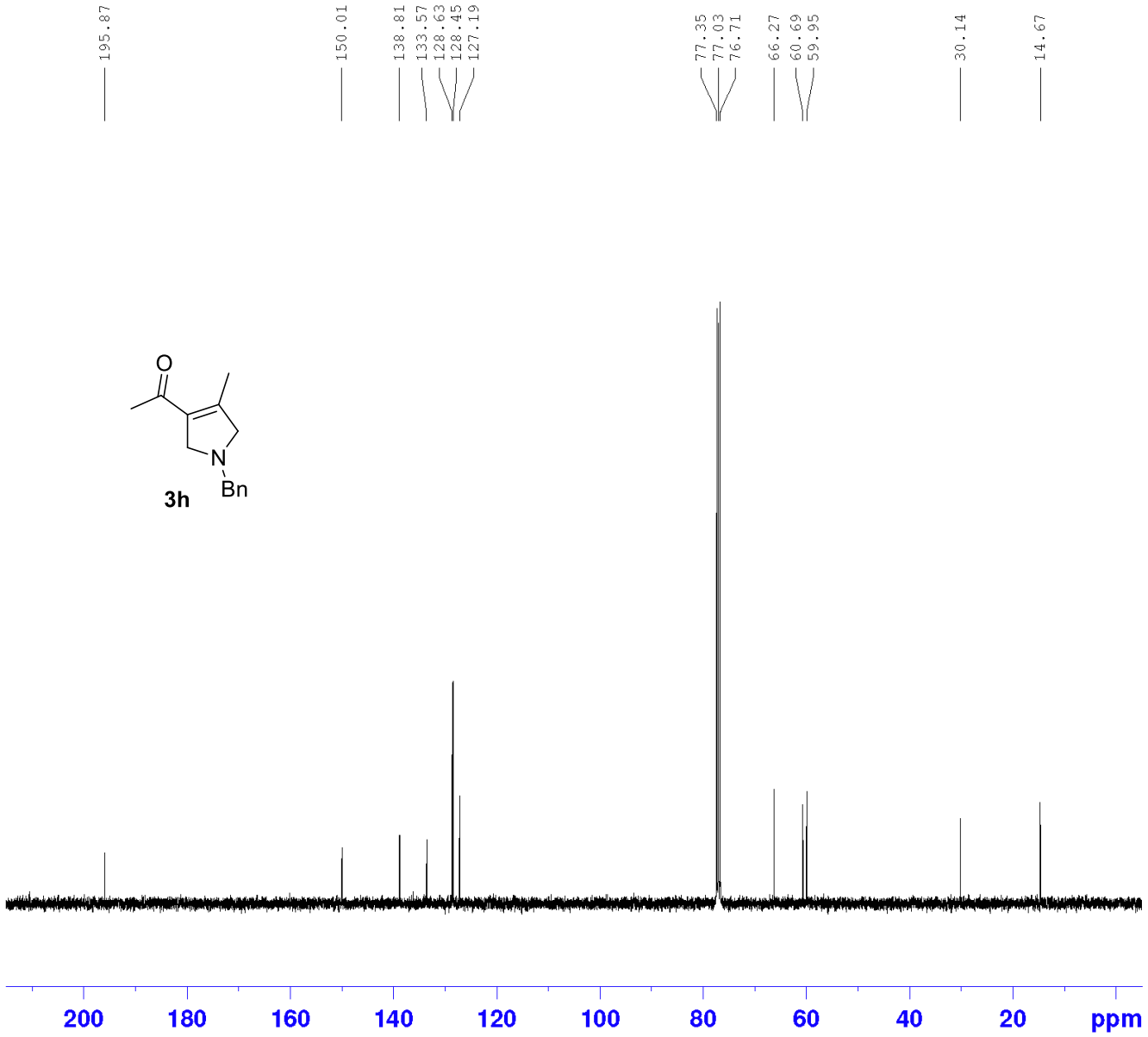



```
Current Data Parameters
NAME        12072013-Cui
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130712
Time                11.34
INSTRUM         avance400
PROBHD    5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8250.825 Hz
FIDRES          0.125898 Hz
AQ             3.9715922 sec
RG                   181
DW                60.600 usec
DE                 6.00 usec
TE                297.4 K
D1            1.00000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                2.70 dB
SFO1         400.2324716 MHz

F2 - Processing parameters
SI                 32768
SF           400.2300015 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```



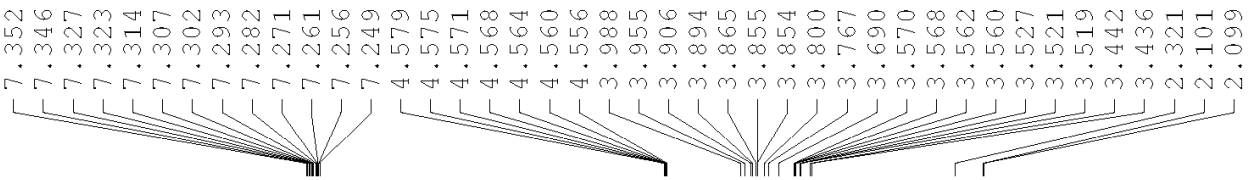

```
Current Data Parameters
NAME       12072013-Cui
EXPNO                11
PROCNO                1

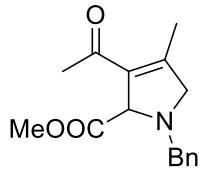
F2 - Acquisition Parameters
Date_          20130712
Time               12.05
INSTRUM       avance400
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  300
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3632196 sec
RG               2896.3
DW                20.800 usec
DE                 6.00 usec
TE                298.5 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1               -2.00 dB
SFO1        100.6479773 MHz

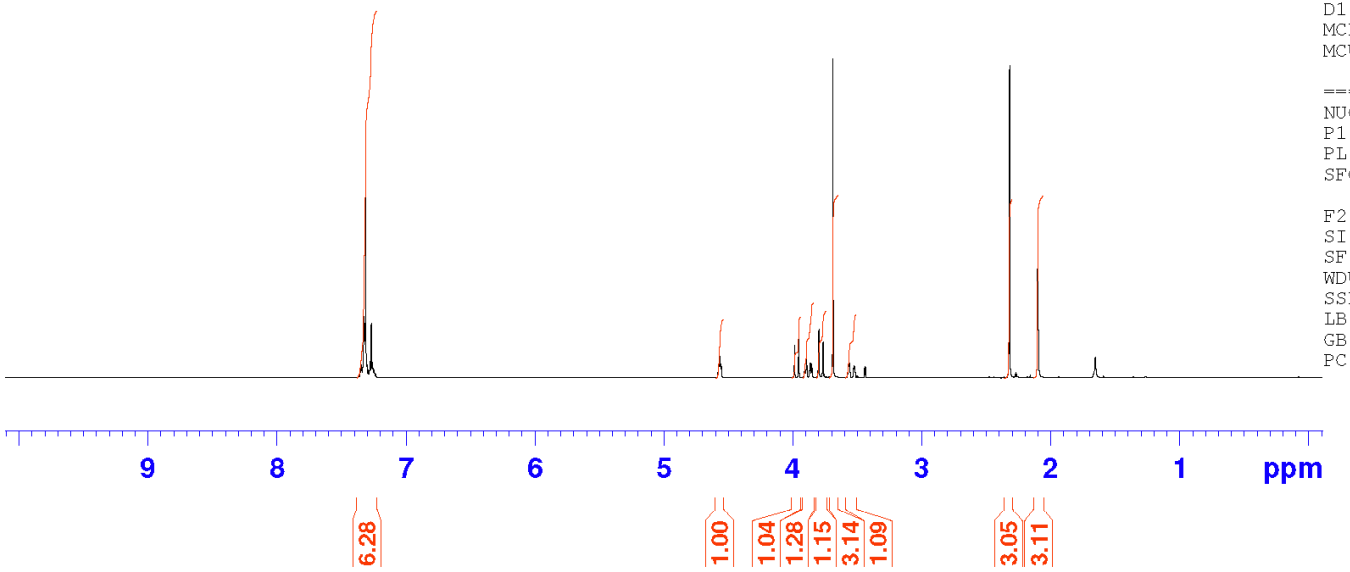
======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            80.00 usec
PL2               2.70 dB
PL12             17.10 dB
PL13             17.10 dB
SFO2        400.2316009 MHz

F2 - Processing parameters
SI                32768
SF          100.6379140 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```





3i

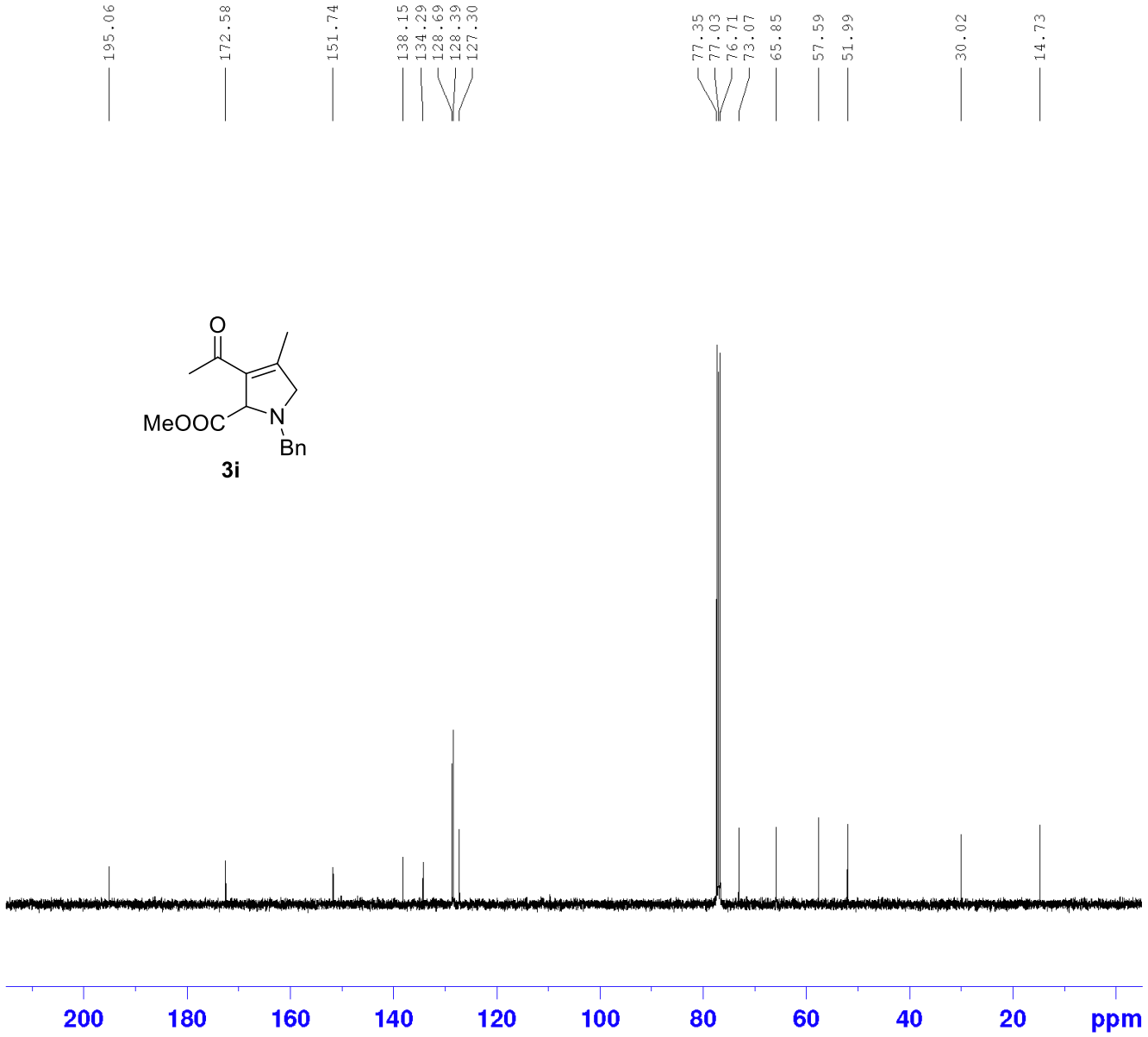



```
Current Data Parameters
NAME        18072013-Cui
EXPNO                 21
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130718
Time               15.16
INSTRUM        avance400
PROBHD   5 mm QNP 1H/13
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8250.825 Hz
FIDRES        0.125898 Hz
AQ            3.9715922 sec
RG                  181
DW               60.600 usec
DE                6.00 usec
TE                297.4 K
D1           1.00000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                1H
P1              15.00 usec
PL1              2.70 dB
SFO1        400.2324716 MHz

F2 - Processing parameters
SI                 32768
SF          400.2300013 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```



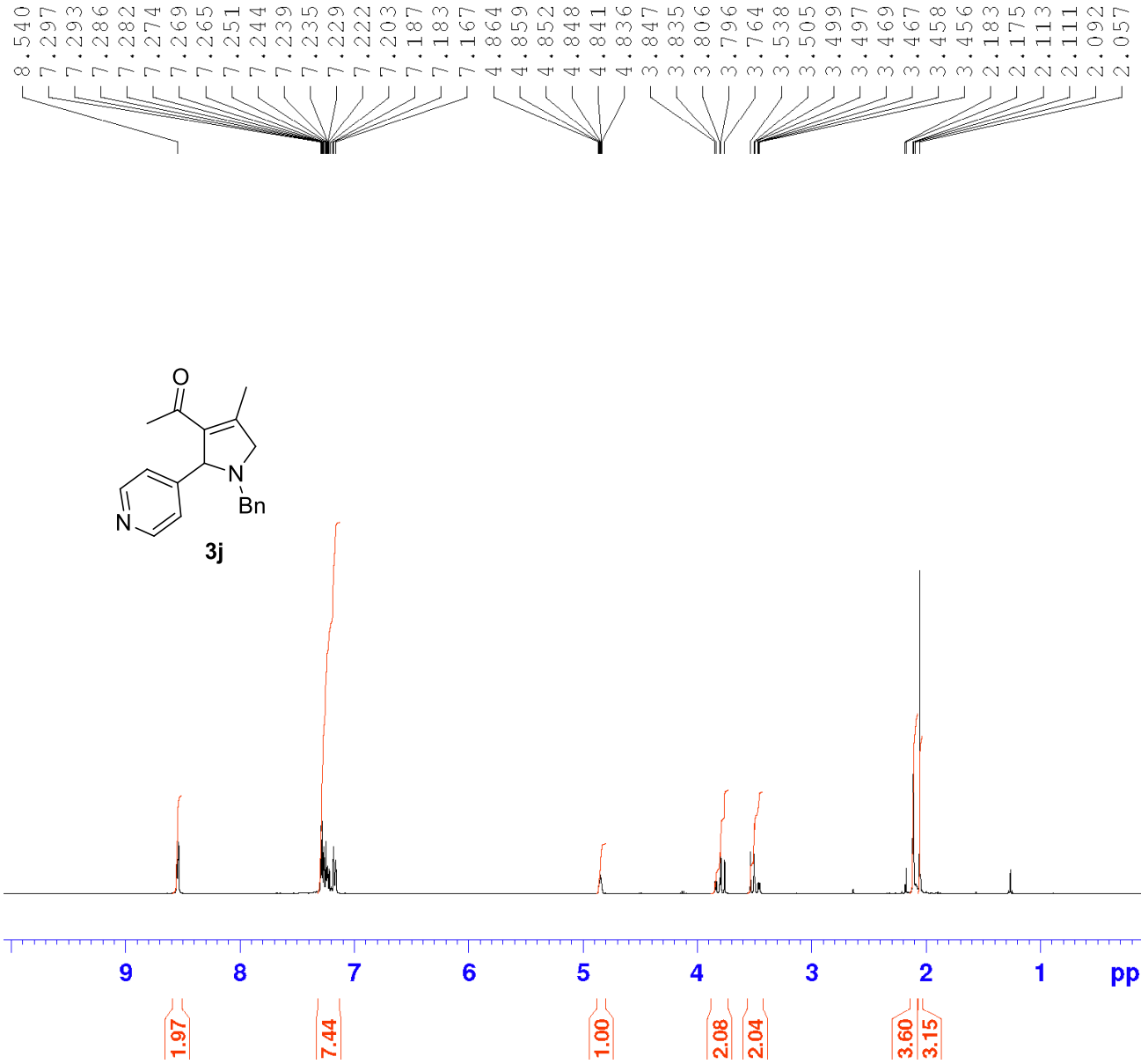

```
Current Data Parameters
NAME       18072013-Cui
EXPNO                22
PROCNO                1

F2 - Acquisition Parameters
Date_          20130718
Time               15.44
INSTRUM       avance400
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  300
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3632196 sec
RG               2896.3
DW                20.800 usec
DE                 6.00 usec
TE                298.3 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1               -2.00 dB
SFO1        100.6479773 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            80.00 usec
PL2               2.70 dB
PL12             17.10 dB
PL13             17.10 dB
SFO2        400.2316009 MHz

F2 - Processing parameters
SI                 32768
SF          100.6379140 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

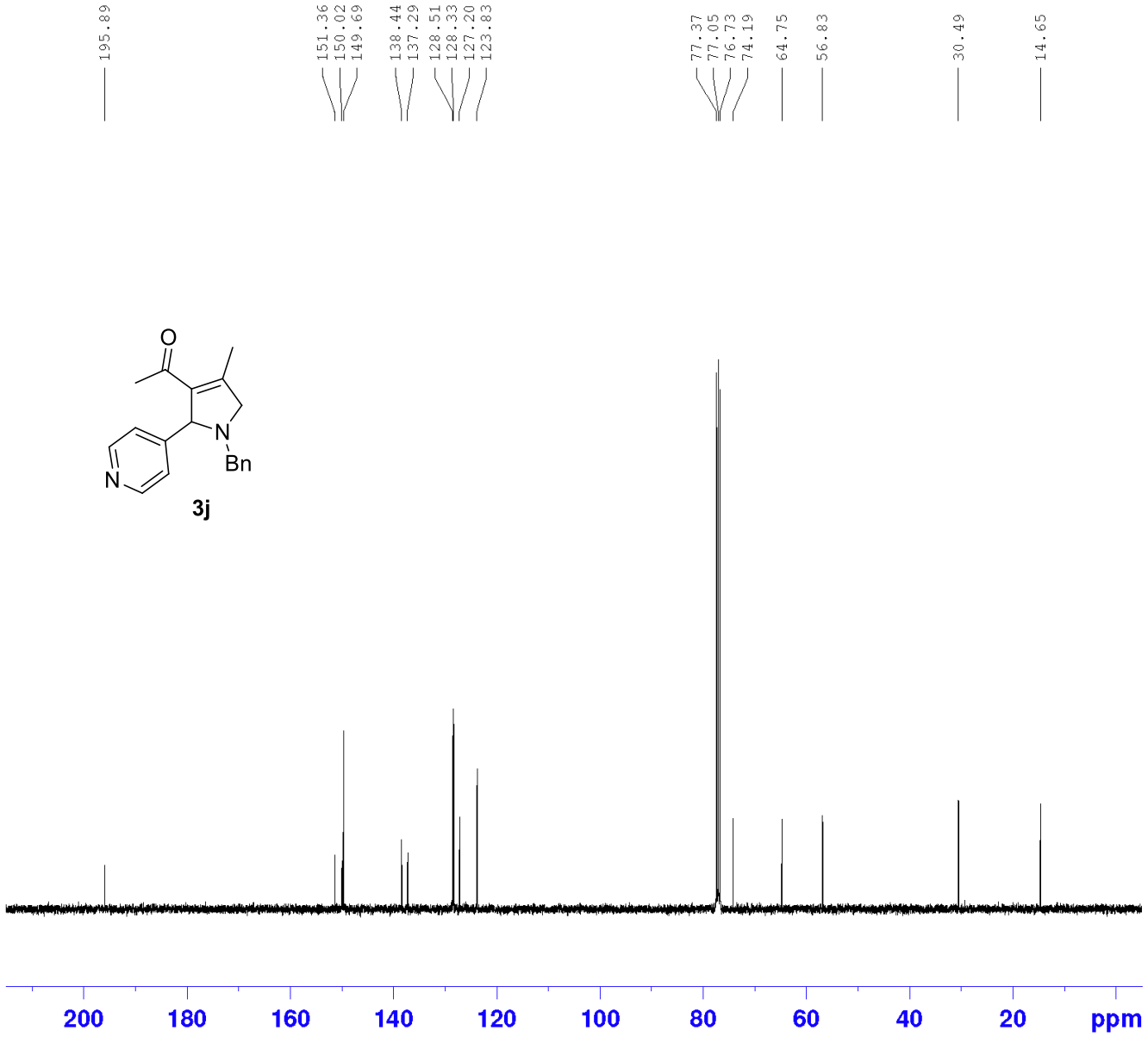



```
Current Data Parameters
NAME        29072013-Cui
EXPNO                 20
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130729
Time               11.57
INSTRUM        avance400
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8250.825 Hz
FIDRES          0.125898 Hz
AQ             3.9715922 sec
RG                 143.7
DW                60.600 usec
DE                 6.00 usec
TE                297.3 K
D1           1.00000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                2.70 dB
SFO1        400.2324716 MHz

F2 - Processing parameters
SI                 32768
SF          400.2300000 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                 1.00
```



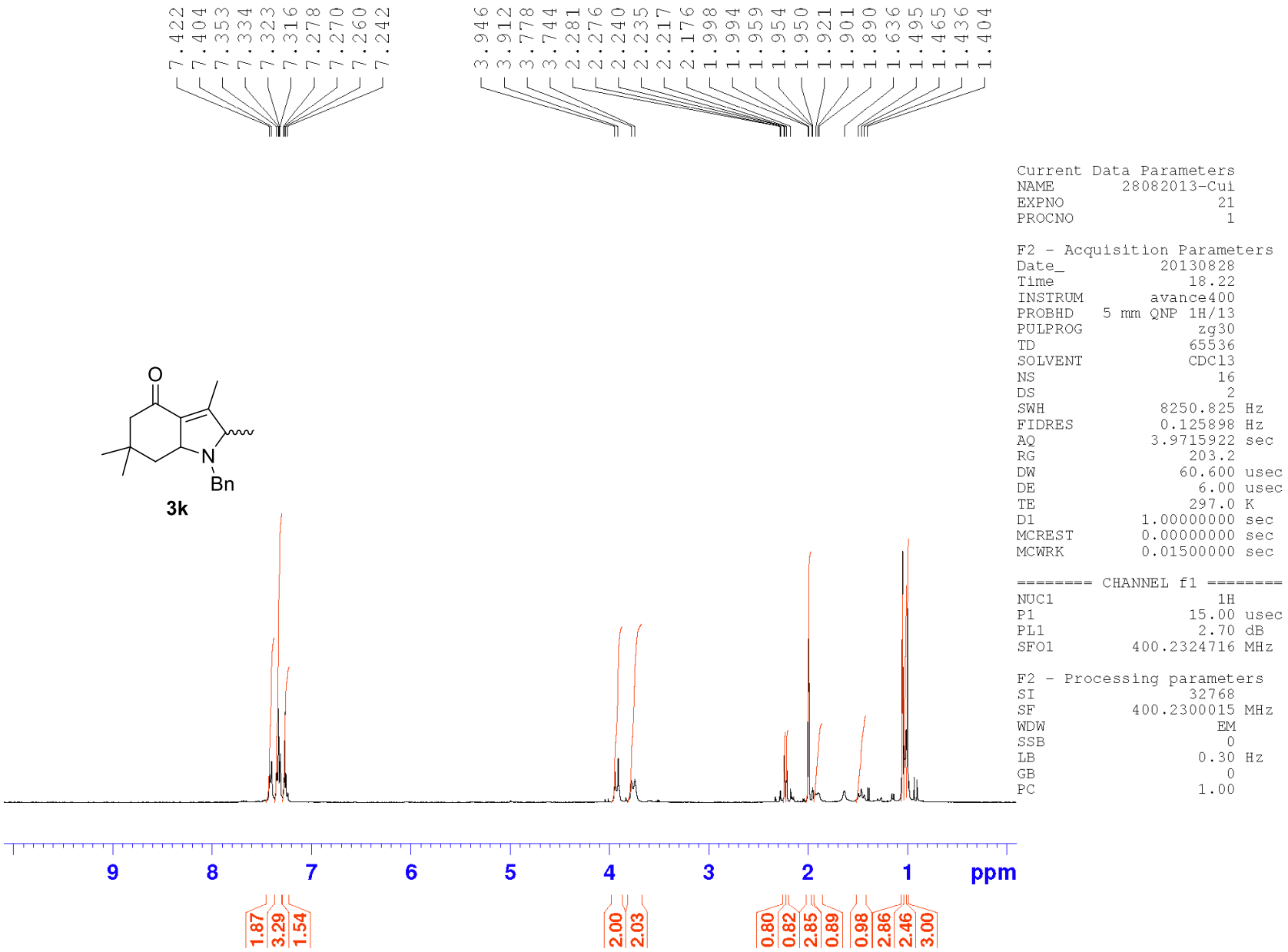

```
Current Data Parameters
NAME       29072013-Cui
EXPNO                21
PROCNO                1

F2 - Acquisition Parameters
Date_          20130729
Time              12.32
INSTRUM       avance400
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  400
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3632196 sec
RG               4597.6
DW               20.800 usec
DE                6.00 usec
TE                298.1 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1               -2.00 dB
SFO1        100.6479773 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2            80.00 usec
PL2               2.70 dB
PL12             17.10 dB
PL13             17.10 dB
SFO2        400.2316009 MHz

F2 - Processing parameters
SI                32768
SF          100.6379140 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

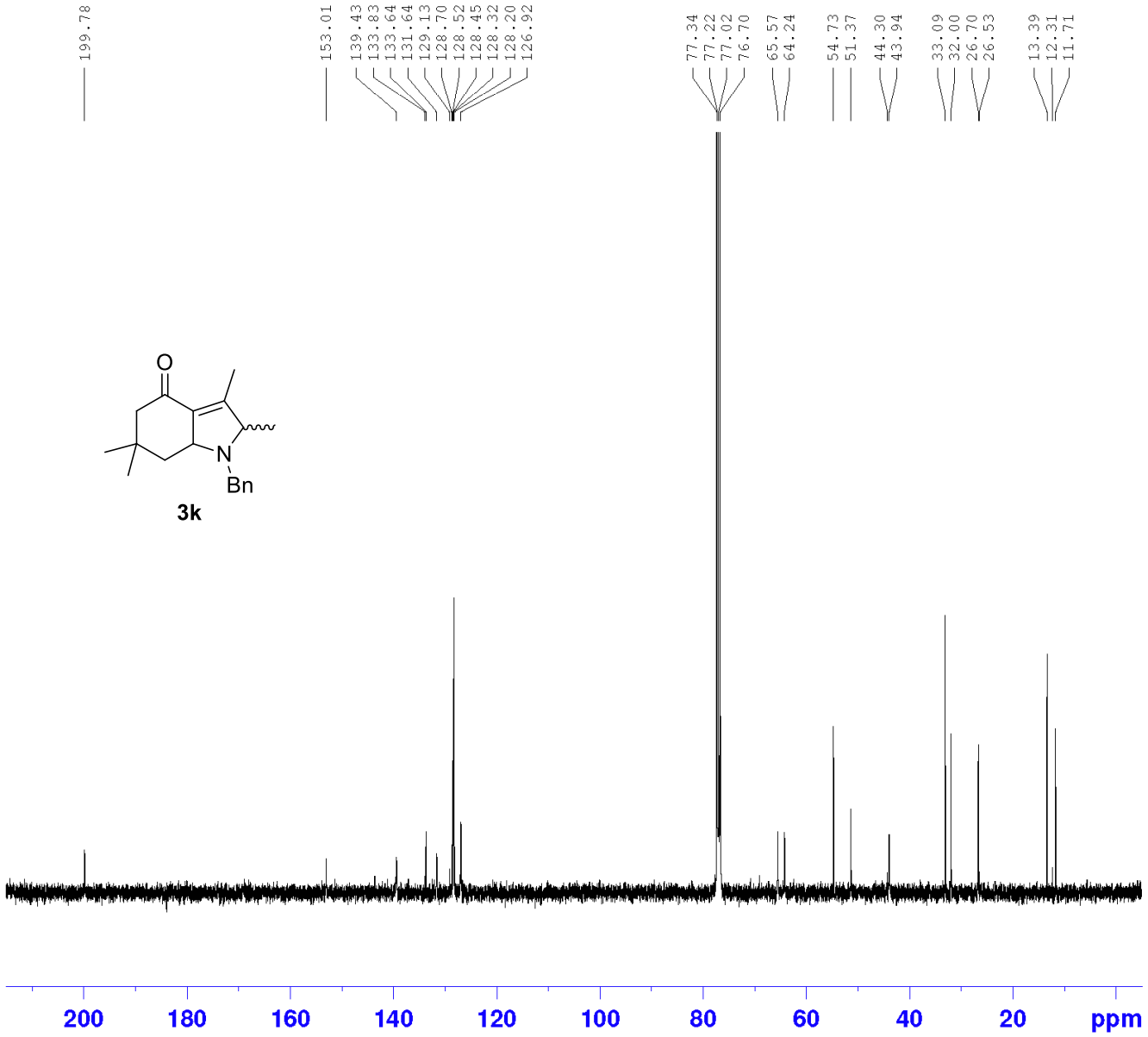



```
Current Data Parameters
NAME        28082013-Cui
EXPNO                 21
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130828
Time               18.22
INSTRUM        avance400
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8250.825 Hz
FIDRES          0.125898 Hz
AQ             3.9715922 sec
RG                 203.2
DW                60.600 usec
DE                 6.00 usec
TE                297.0 K
D1             1.00000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                 15.00 usec
PL1                 2.70 dB
SFO1         400.2324716 MHz

F2 - Processing parameters
SI                 32768
SF           400.2300015 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



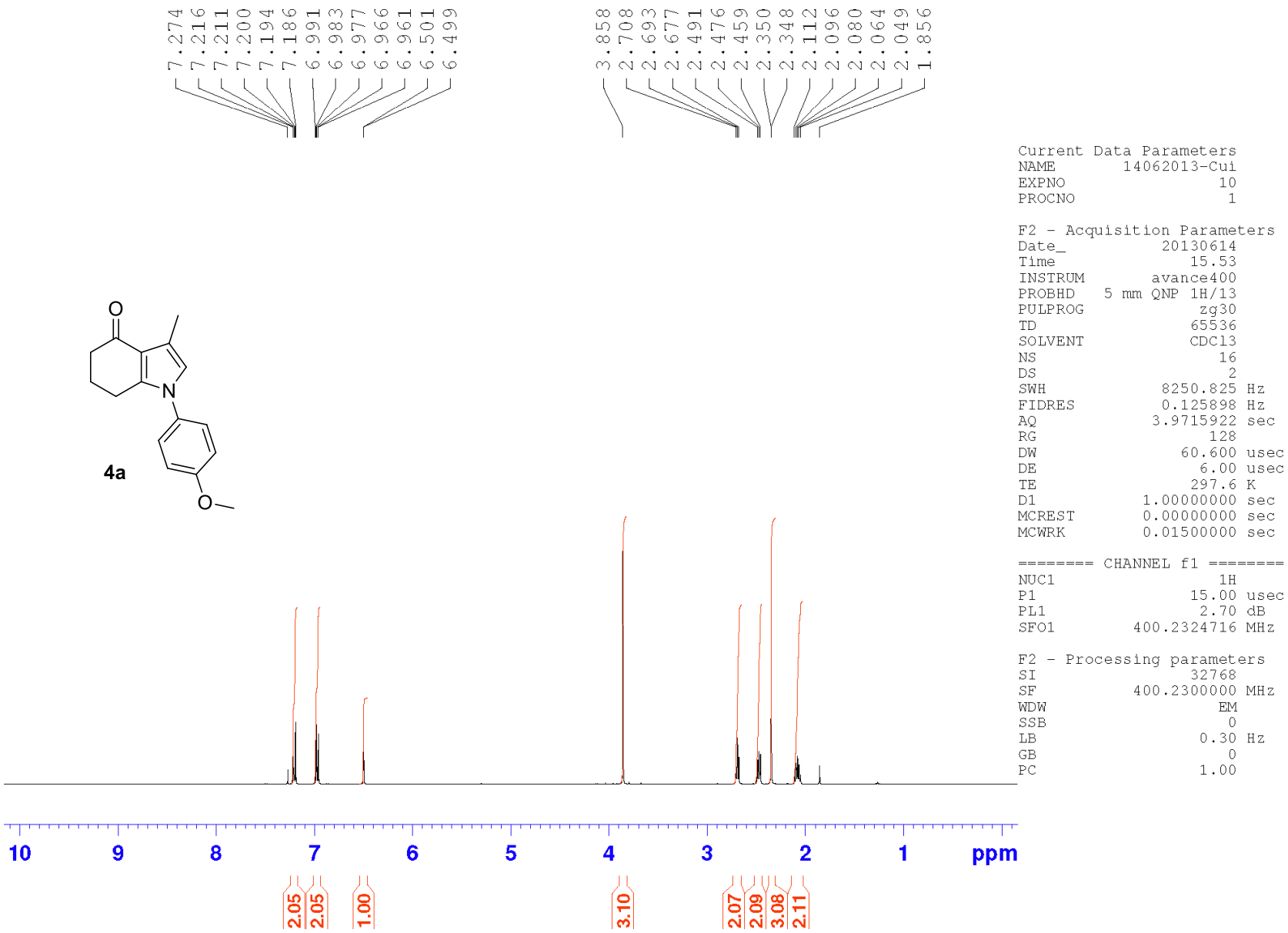

```
Current Data Parameters
NAME       28082013-Cui
EXPNO                23
PROCNO                1

F2 - Acquisition Parameters
Date_          20130828
Time              23.44
INSTRUM       avance400
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 5024
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3632196 sec
RG                7298.2
DW                20.800 usec
DE                 6.00 usec
TE                298.1 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1               -2.00 dB
SFO1         100.6479773 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2             80.00 usec
PL2                2.70 dB
PL12              17.10 dB
PL13              17.10 dB
SFO2         400.2316009 MHz

F2 - Processing parameters
SI                 32768
SF          100.6379140 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```

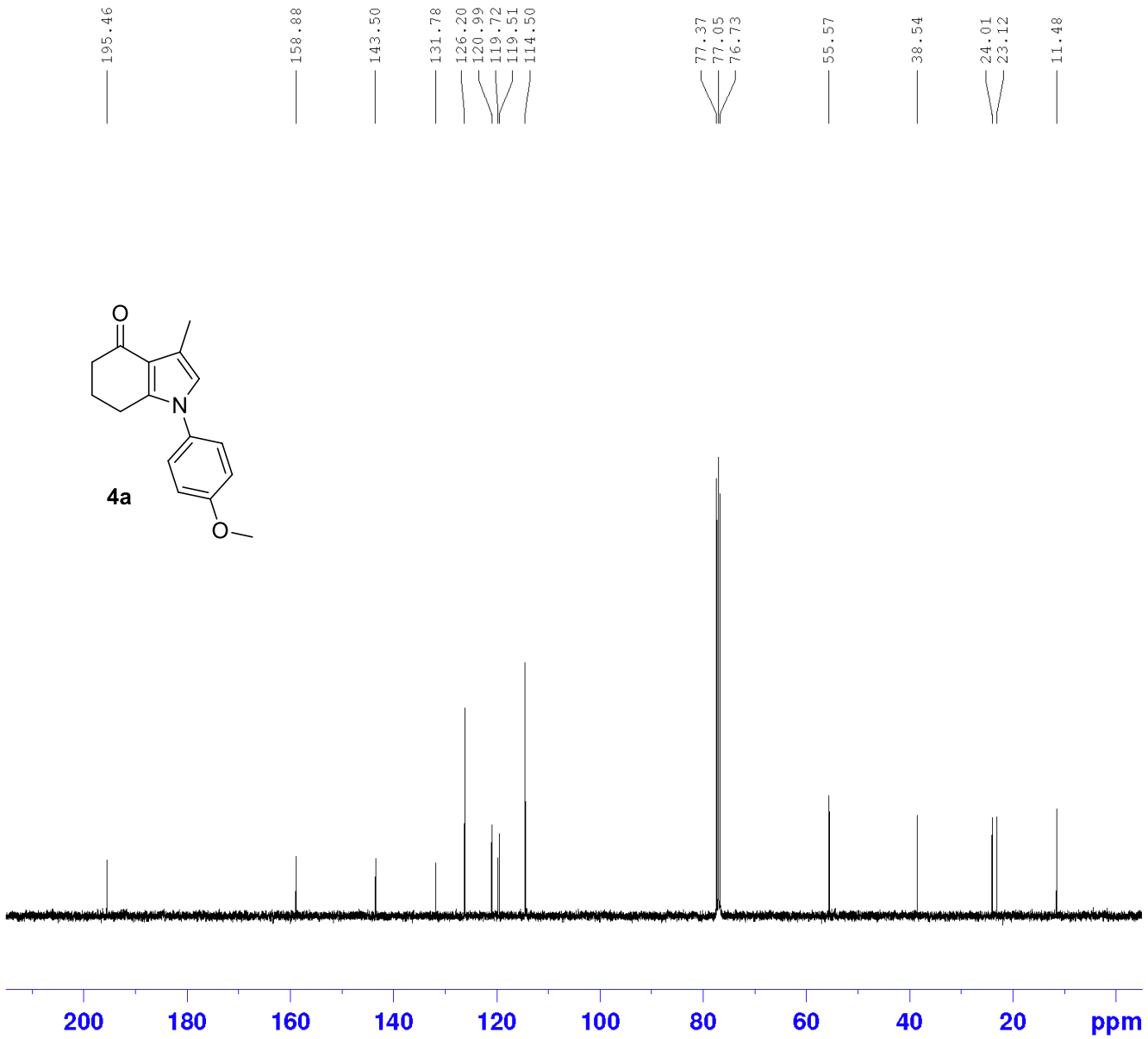



```
Current Data Parameters
NAME        14062013-Cui
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130614
Time               15.53
INSTRUM        avance400
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8250.825 Hz
FIDRES          0.125898 Hz
AQ             3.9715922 sec
RG                   128
DW                60.600 usec
DE                 6.00 usec
TE                297.6 K
D1            1.00000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                2.70 dB
SFO1         400.2324716 MHz

F2 - Processing parameters
SI                 32768
SF          400.2300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



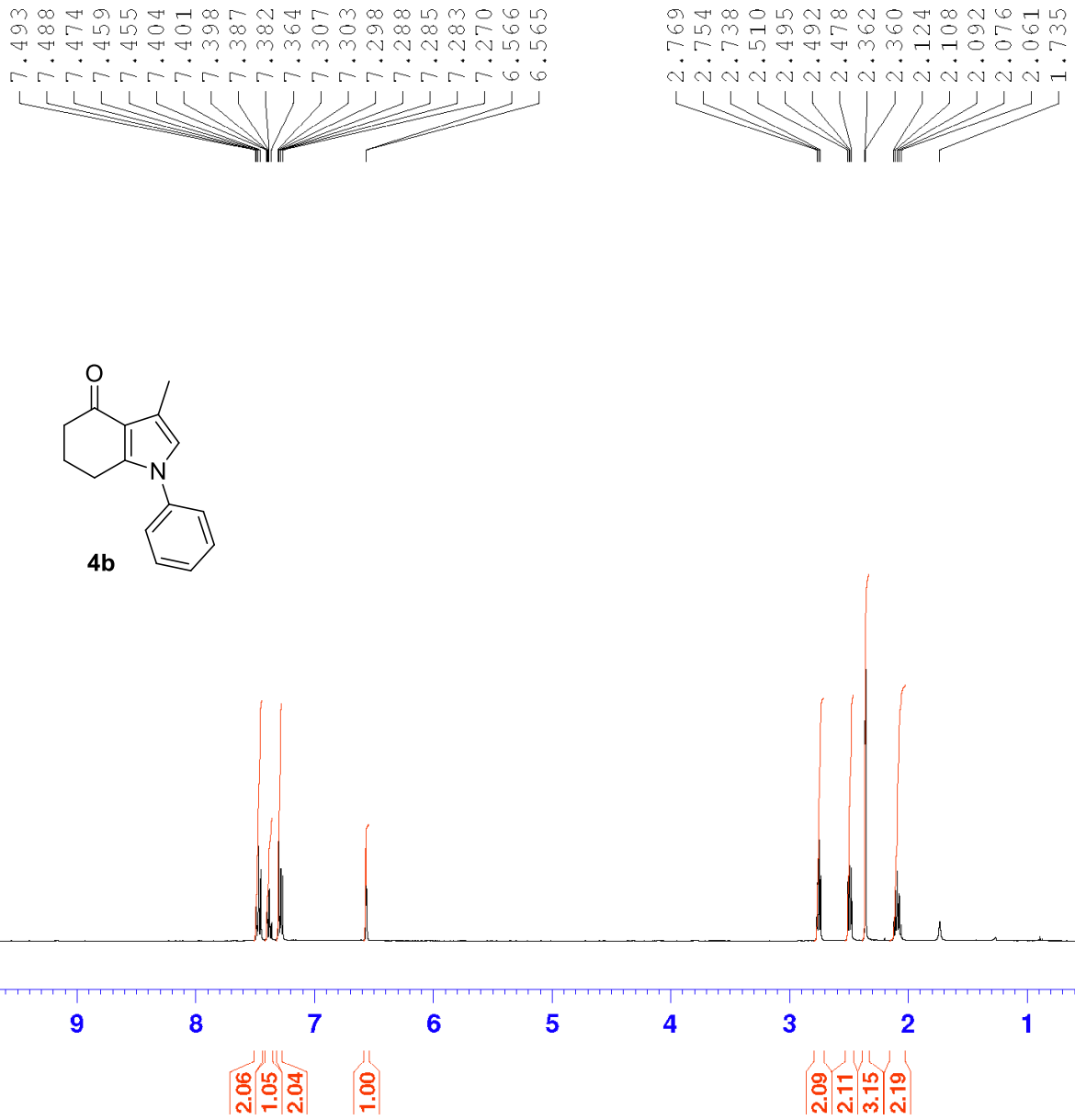

```
Current Data Parameters
NAME       14062013-Cui
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_          20130614
Time              16.21
INSTRUM       avance400
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  300
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3632196 sec
RG               5792.6
DW               20.800 usec
DE                6.00 usec
TE               298.6 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1               -2.00 dB
SFO1        100.6479773 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            80.00 usec
PL2               2.70 dB
PL12             17.10 dB
PL13             17.10 dB
SFO2        400.2316009 MHz

F2 - Processing parameters
SI                32768
SF          100.6379140 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

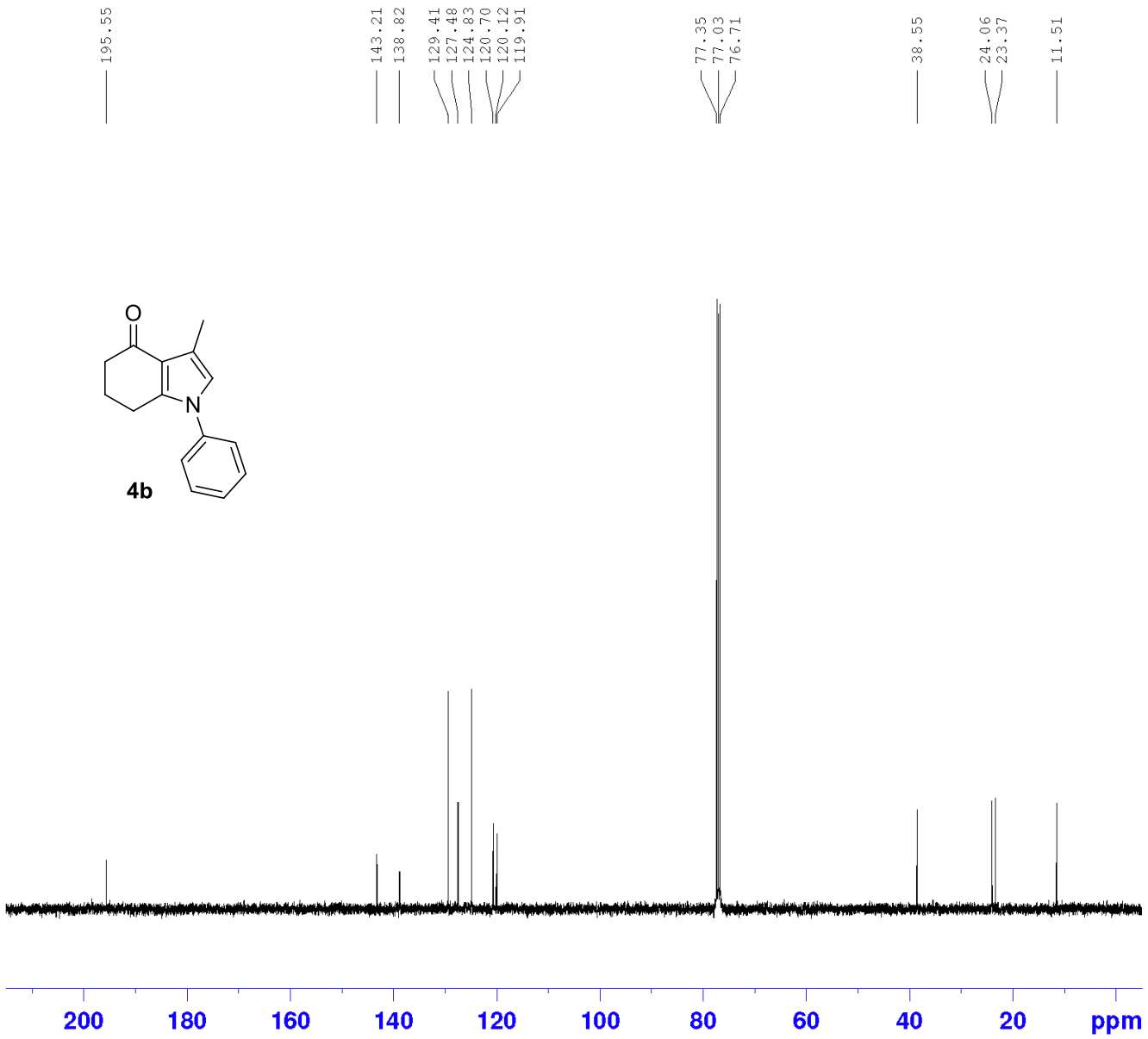



```
Current Data Parameters
NAME        20072013-Cui
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130720
Time               10.57
INSTRUM        avance400
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8250.825 Hz
FIDRES          0.125898 Hz
AQ             3.9715922 sec
RG                 203.2
DW                60.600 usec
DE                 6.00 usec
TE                297.6 K
D1           1.00000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                2.70 dB
SFO1        400.2324716 MHz

F2 - Processing parameters
SI                 32768
SF          400.2300018 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```



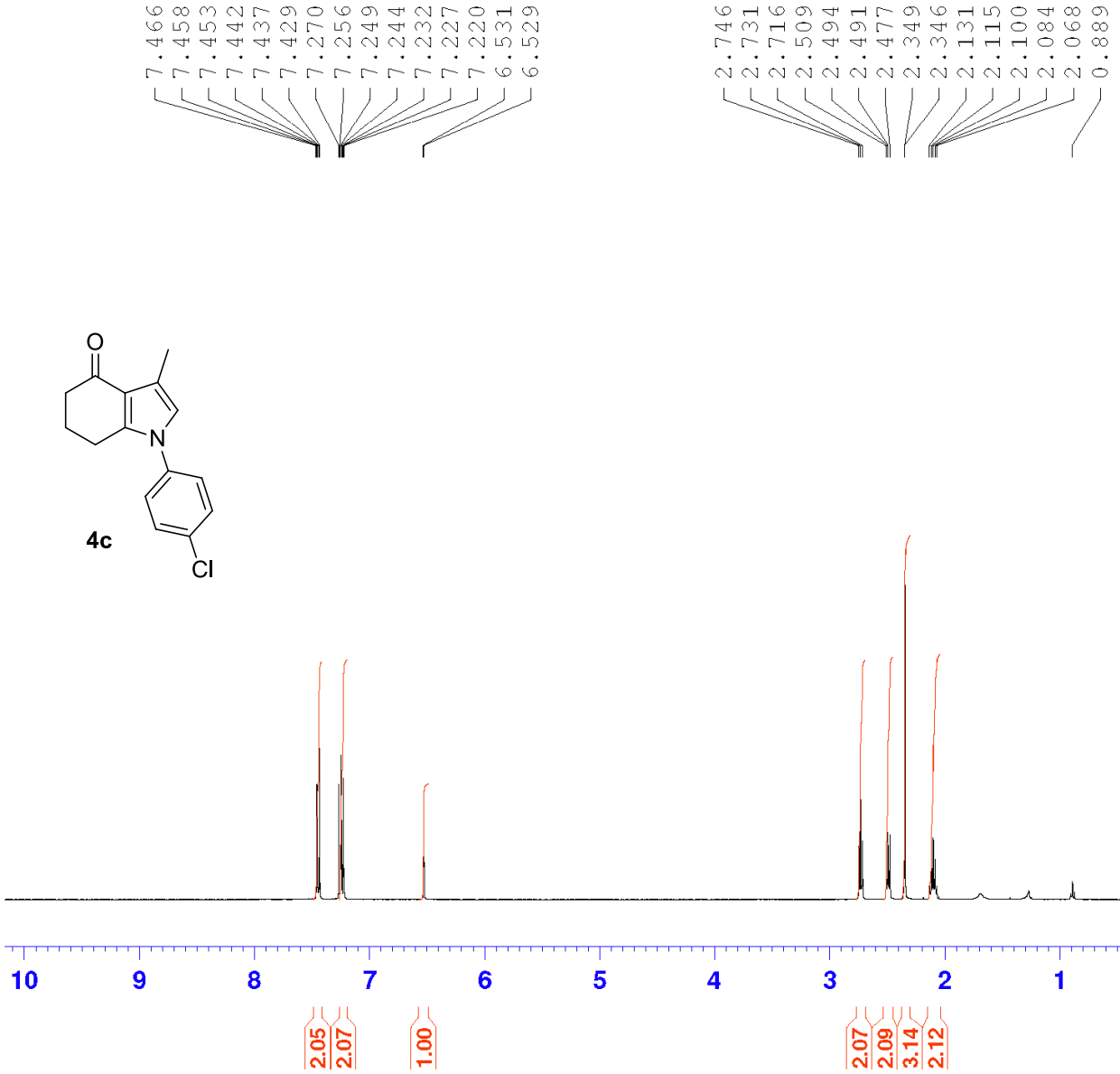

```
Current Data Parameters
NAME       20072013-Cui
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_          20130720
Time              11.29
INSTRUM       avance400
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  300
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3632196 sec
RG               5160.6
DW               20.800 usec
DE                6.00 usec
TE               298.6 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1               -2.00 dB
SFO1        100.6479773 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            80.00 usec
PL2               2.70 dB
PL12             17.10 dB
PL13             17.10 dB
SFO2        400.2316009 MHz

F2 - Processing parameters
SI                32768
SF          100.6379140 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

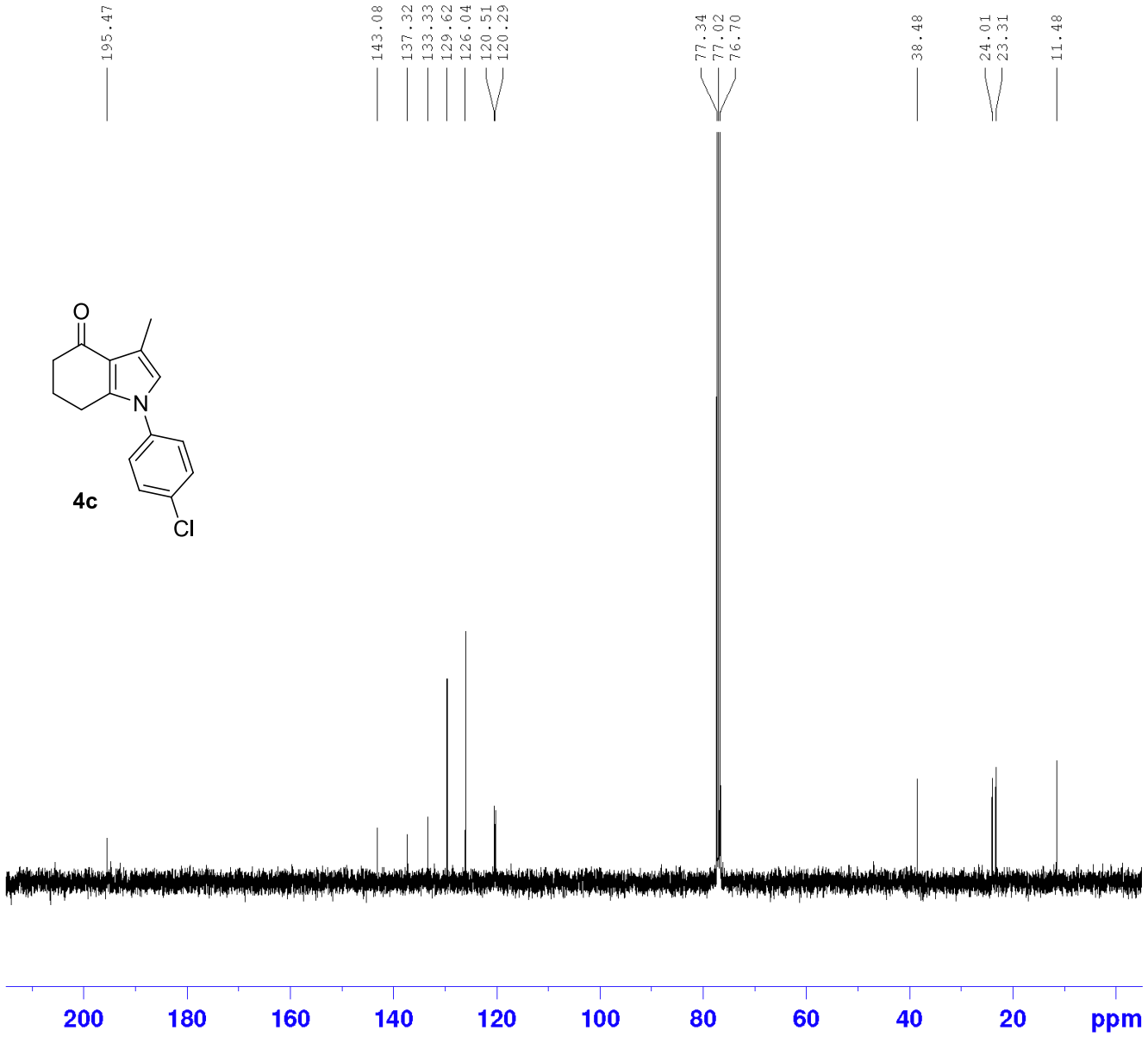



```
Current Data Parameters
NAME        13082013-Cui
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130813
Time               18.25
INSTRUM        avance400
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8250.825 Hz
FIDRES          0.125898 Hz
AQ             3.9715922 sec
RG                 322.5
DW                60.600 usec
DE                 6.00 usec
TE                297.2 K
D1            1.00000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                2.70 dB
SFO1         400.2324716 MHz

F2 - Processing parameters
SI                 32768
SF          400.2300018 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```



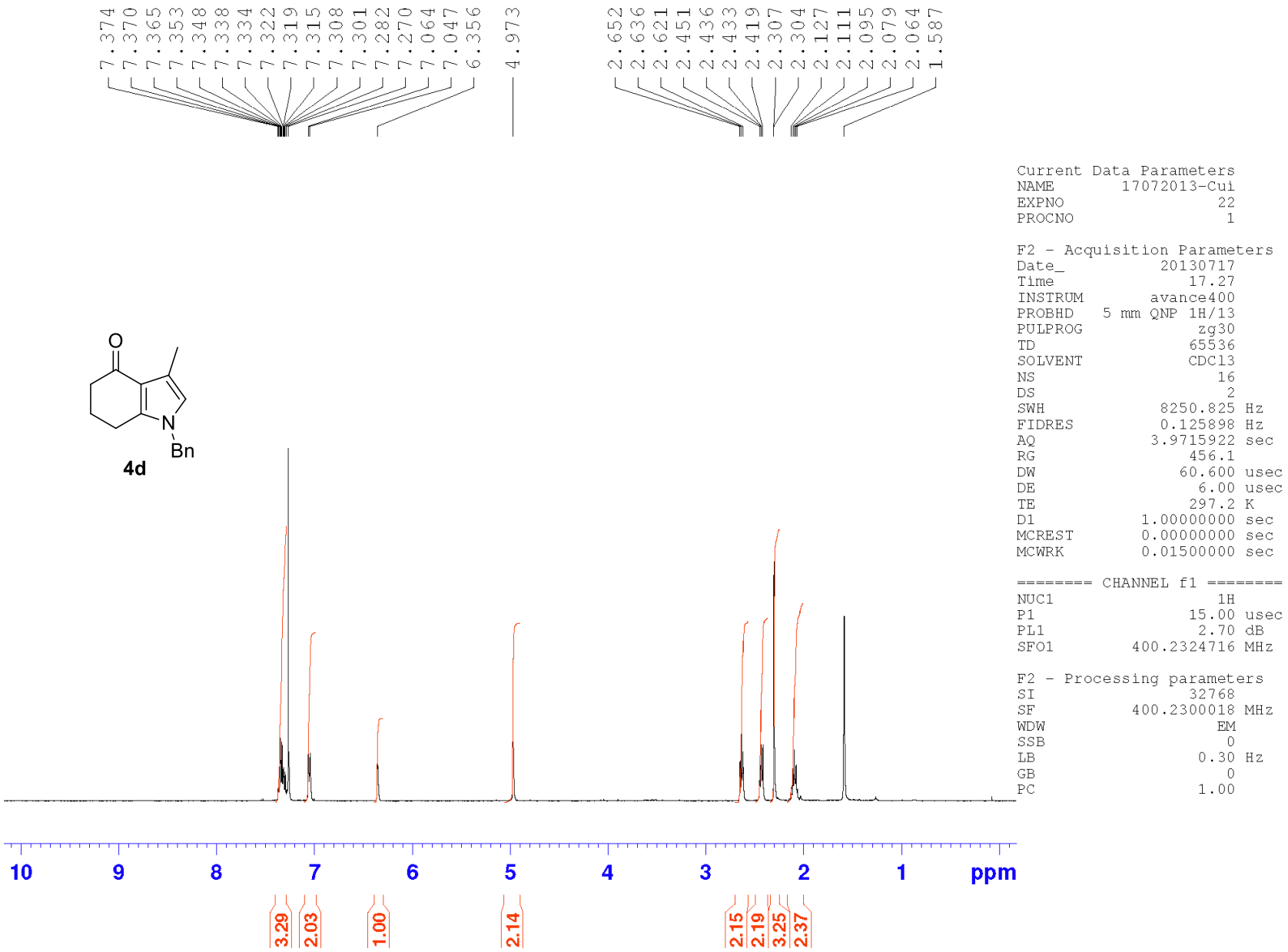

```
Current Data Parameters
NAME       13082013-Cui
EXPNO                11
PROCNO                1

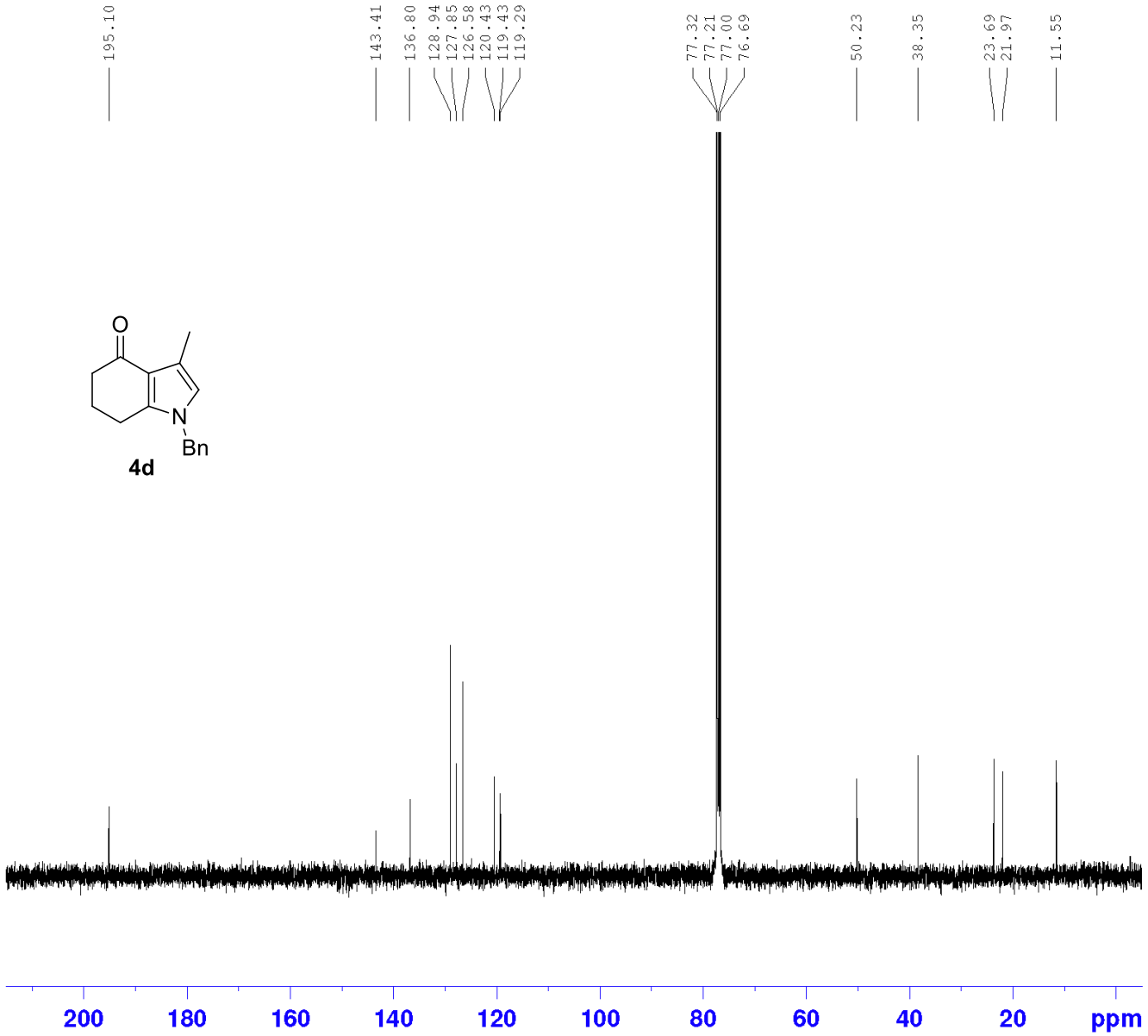
F2 - Acquisition Parameters
Date_           20130813
Time               18.56
INSTRUM       avance400
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  400
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3632196 sec
RG                4597.6
DW                20.800 usec
DE                 6.00 usec
TE                297.9 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1               -2.00 dB
SFO1        100.6479773 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2             80.00 usec
PL2                2.70 dB
PL12              17.10 dB
PL13              17.10 dB
SFO2        400.2316009 MHz

F2 - Processing parameters
SI                 32768
SF          100.6379140 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```


7.374
7.370
7.365
7.353
7.348
7.338
7.334
7.322
7.319
7.315
7.308
7.301
7.282
7.270
7.064
7.047
6.356
4.973
2.652
2.636
2.621
2.451
2.436
2.433
2.419
2.307
2.304
2.127
2.111
2.095
2.079
2.064
1.587
O
N
Bn
4d
Current Data Parameters
NAME 17072013-Cui
EXPNO 22
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130717
Time 17.27
INSTRUM avance400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8250.825 Hz
FIDRES 0.125898 Hz
AQ 3.9715922 sec
RG 456.1
DW 60.600 usec
DE 6.00 usec
TE 297.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PL1 2.70 dB
SFO1 400.2324716 MHz
F2 - Processing parameters
SI 32768
SF 400.2300018 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
3.29
2.03
1.00
2.14
2.15
2.19
3.25
2.37



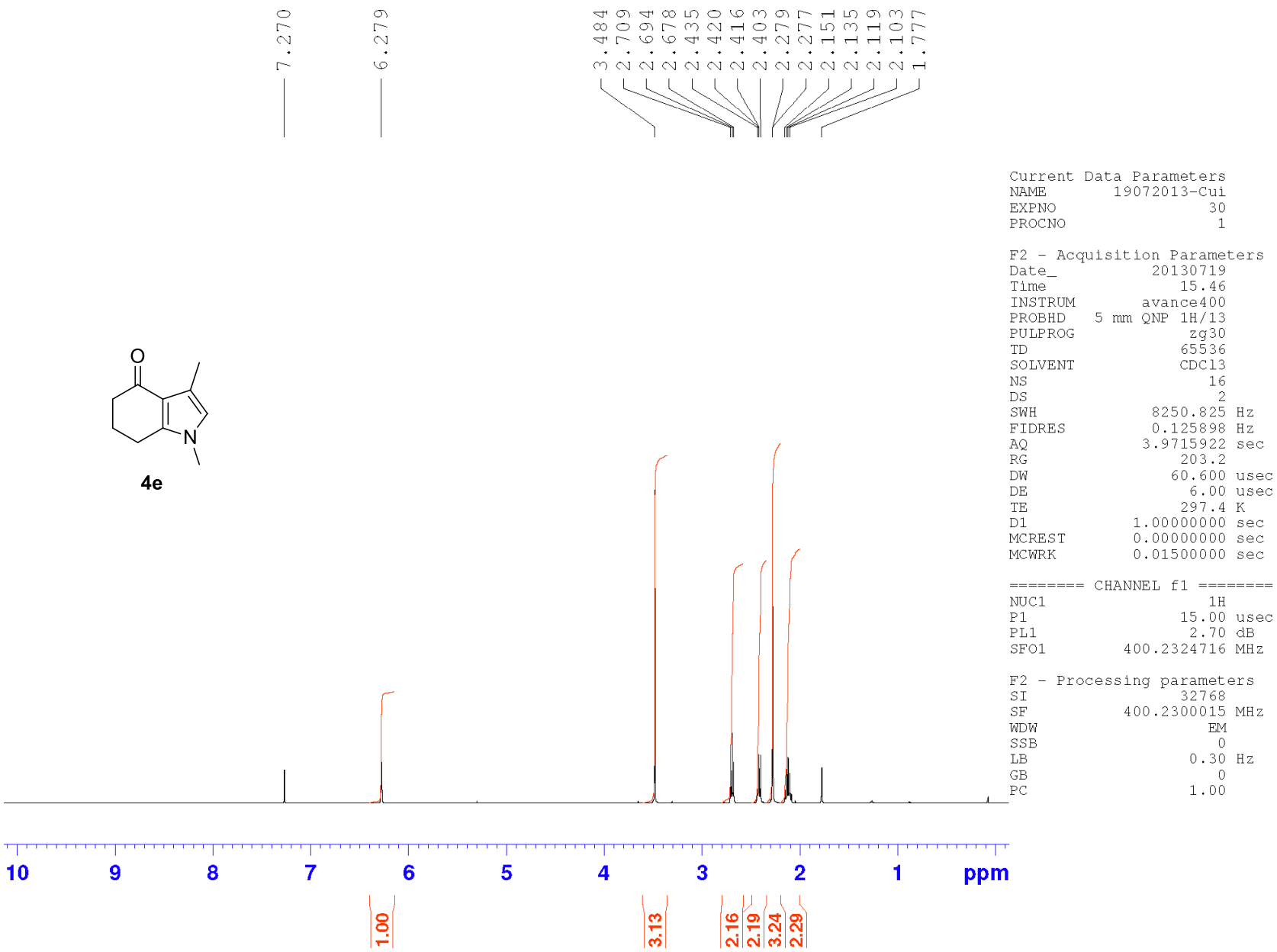

```
Current Data Parameters
NAME       17072013-Cui
EXPNO                23
PROCNO                1

F2 - Acquisition Parameters
Date_          20130717
Time              22.36
INSTRUM       avance400
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 5000
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3632196 sec
RG               2896.3
DW               20.800 usec
DE                6.00 usec
TE                298.6 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1               -2.00 dB
SFO1        100.6479773 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            80.00 usec
PL2               2.70 dB
PL12             17.10 dB
PL13             17.10 dB
SFO2        400.2316009 MHz

F2 - Processing parameters
SI                32768
SF          100.6379140 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

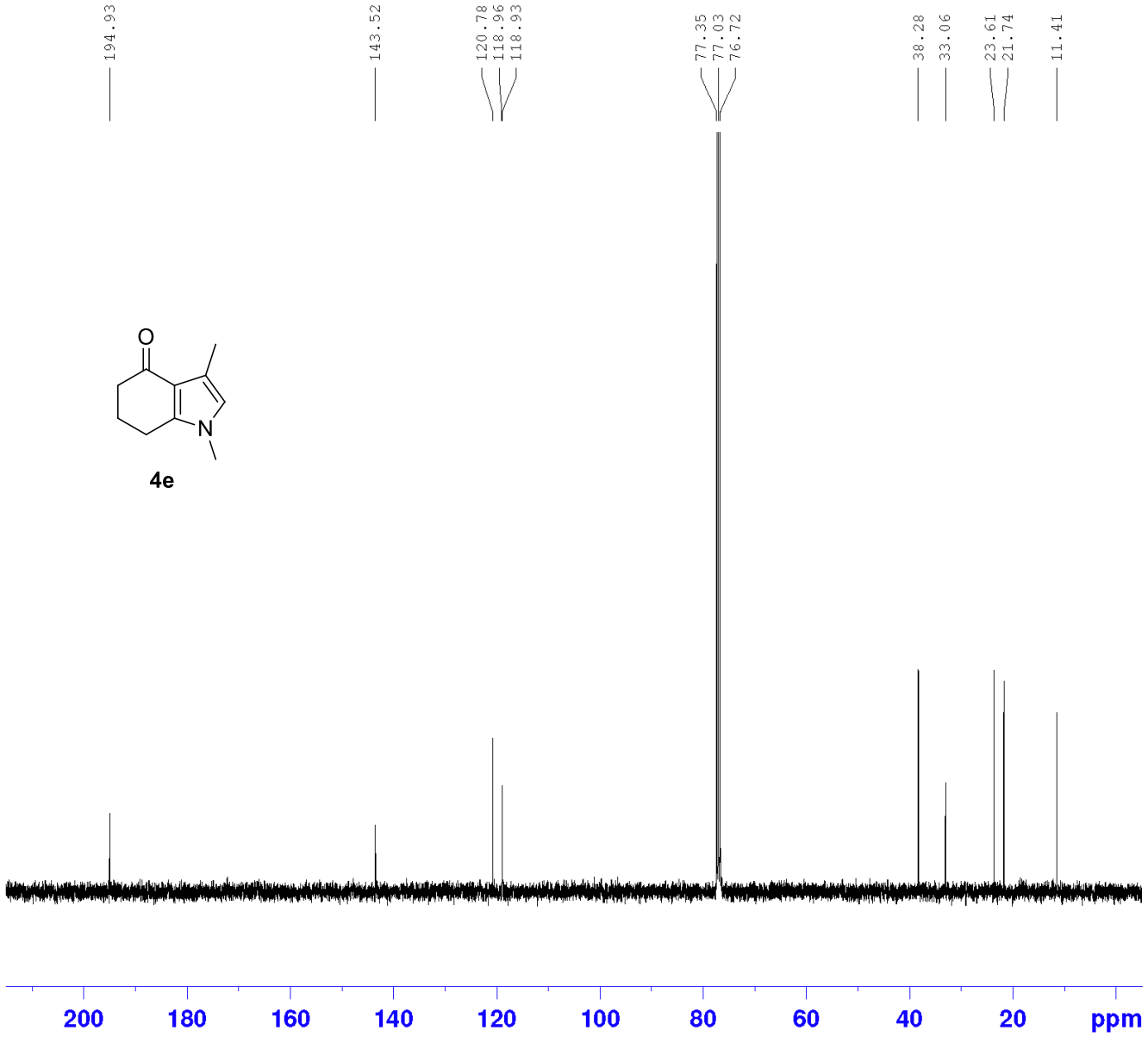



```
Current Data Parameters
NAME        19072013-Cui
EXPNO                 30
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130719
Time               15.46
INSTRUM        avance400
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8250.825 Hz
FIDRES          0.125898 Hz
AQ             3.9715922 sec
RG                 203.2
DW                60.600 usec
DE                 6.00 usec
TE                297.4 K
D1            1.00000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                2.70 dB
SFO1         400.2324716 MHz

F2 - Processing parameters
SI                 32768
SF          400.2300015 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```



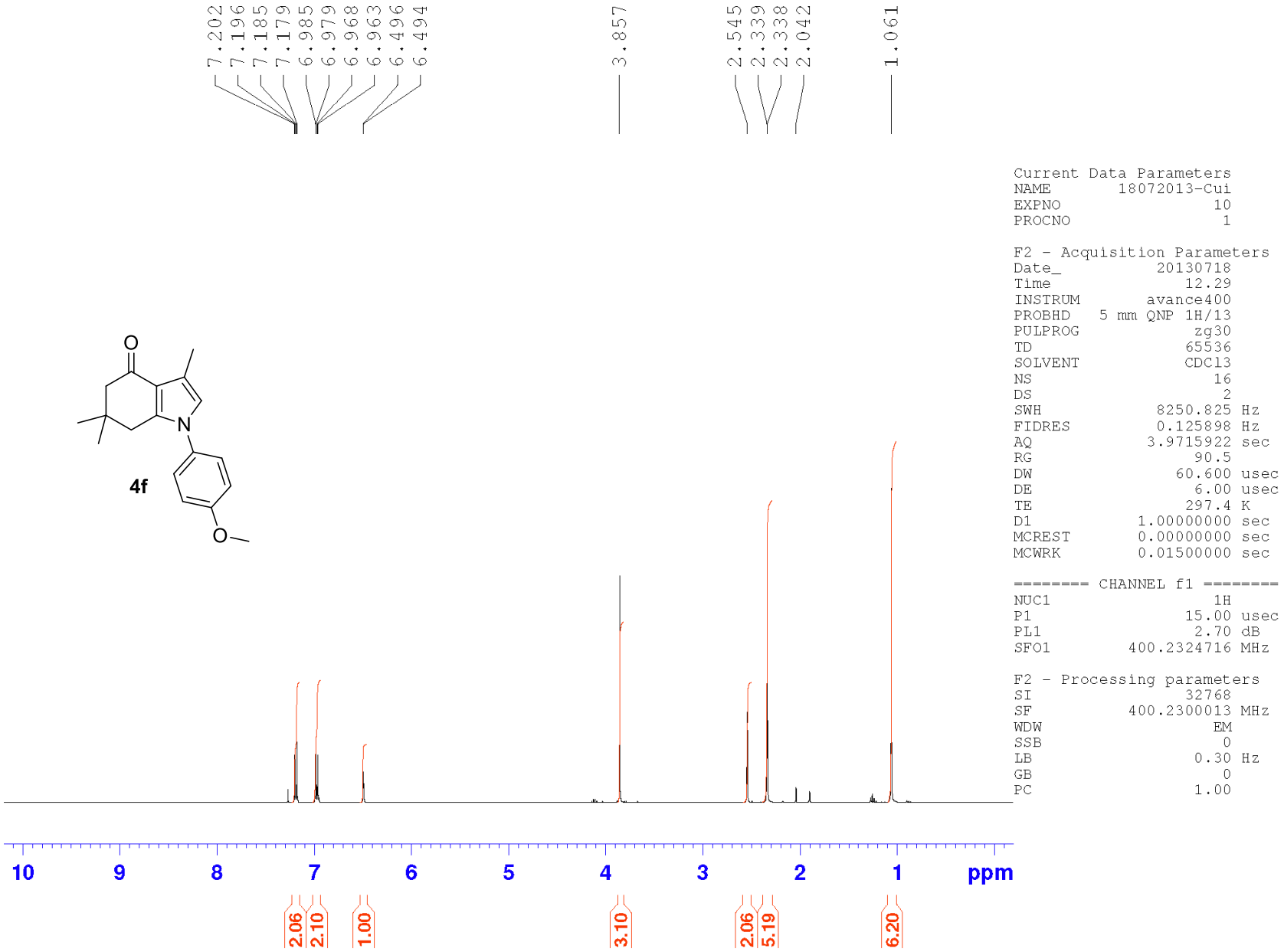

```
Current Data Parameters
NAME       19072013-Cui
EXPNO                31
PROCNO                1

F2 - Acquisition Parameters
Date_          20130719
Time              16.09
INSTRUM       avance400
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  300
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3632196 sec
RG               3649.1
DW                20.800 usec
DE                 6.00 usec
TE                298.5 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1               -2.00 dB
SFO1        100.6479773 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2             80.00 usec
PL2                2.70 dB
PL12              17.10 dB
PL13              17.10 dB
SFO2        400.2316009 MHz

F2 - Processing parameters
SI                32768
SF          100.6379140 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

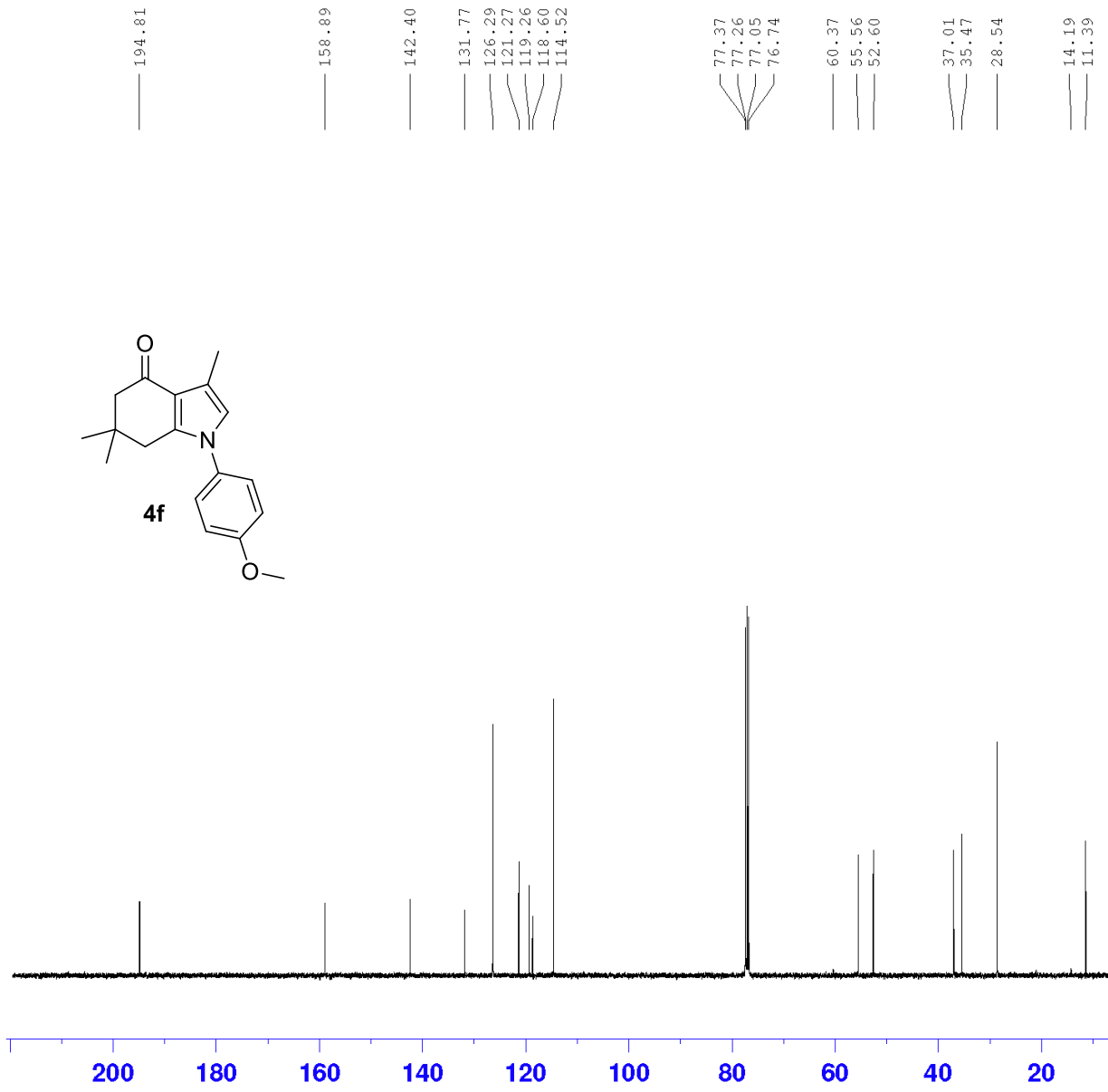



```
Current Data Parameters
NAME        18072013-Cui
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130718
Time               12.29
INSTRUM        avance400
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8250.825 Hz
FIDRES          0.125898 Hz
AQ             3.9715922 sec
RG                  90.5
DW                60.600 usec
DE                 6.00 usec
TE                297.4 K
D1            1.00000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.00 usec
PL1                 2.70 dB
SFO1         400.2324716 MHz

F2 - Processing parameters
SI                 32768
SF          400.2300013 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



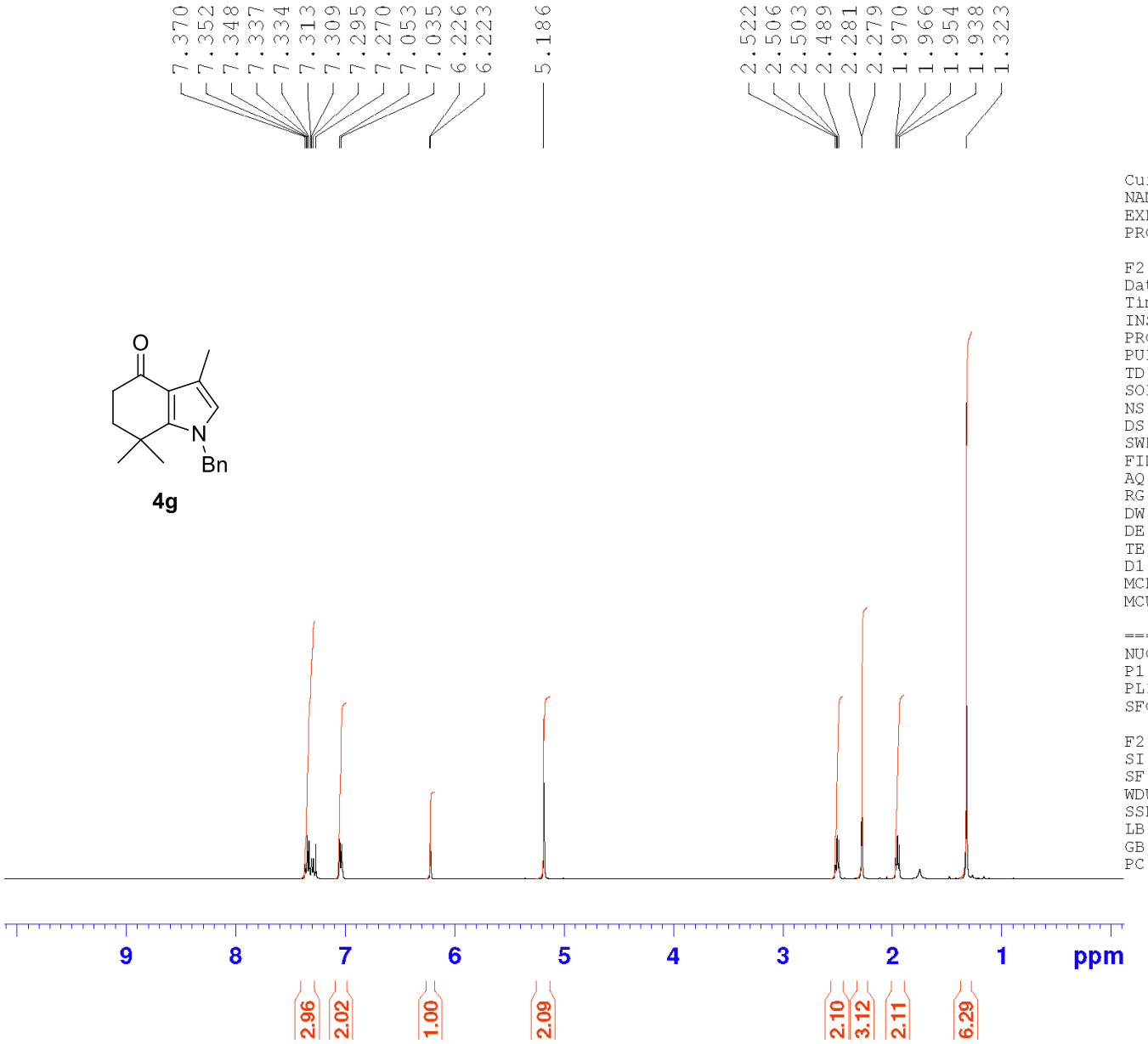

```
Current Data Parameters
NAME       18072013-Cui
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_          20130718
Time              13.05
INSTRUM       avance400
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  600
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3632196 sec
RG               5792.6
DW               20.800 usec
DE                6.00 usec
TE                298.5 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1               -2.00 dB
SFO1        100.6479773 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2            80.00 usec
PL2               2.70 dB
PL12             17.10 dB
PL13             17.10 dB
SFO2        400.2316009 MHz

F2 - Processing parameters
SI                32768
SF          100.6379140 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

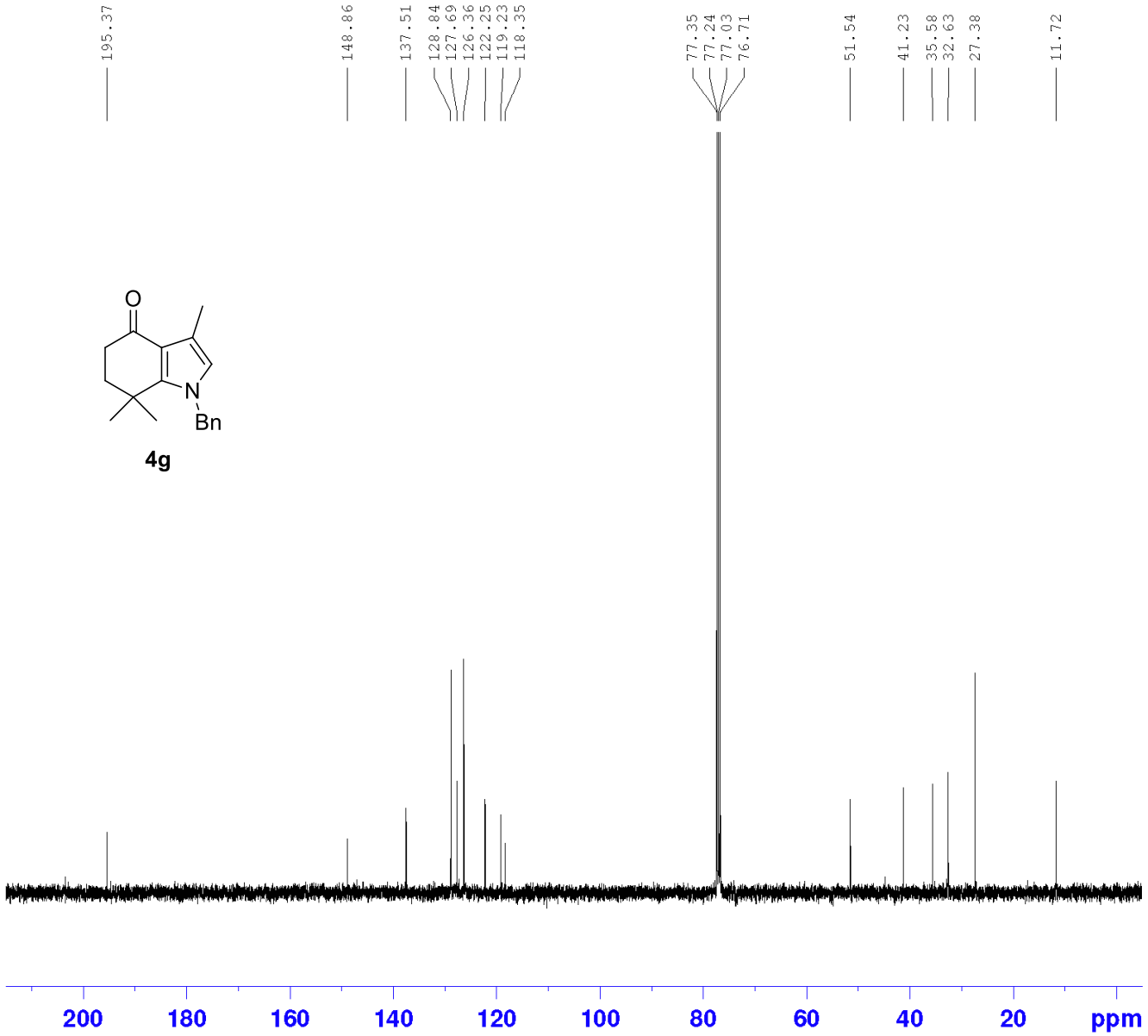



```
Current Data Parameters
NAME        22082013-Cui
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130822
Time               10.50
INSTRUM        avance400
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8250.825 Hz
FIDRES          0.125898 Hz
AQ             3.9715922 sec
RG                 203.2
DW                60.600 usec
DE                 6.00 usec
TE                297.2 K
D1            1.00000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                2.70 dB
SFO1         400.2324716 MHz

F2 - Processing parameters
SI                 32768
SF          400.2300018 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```



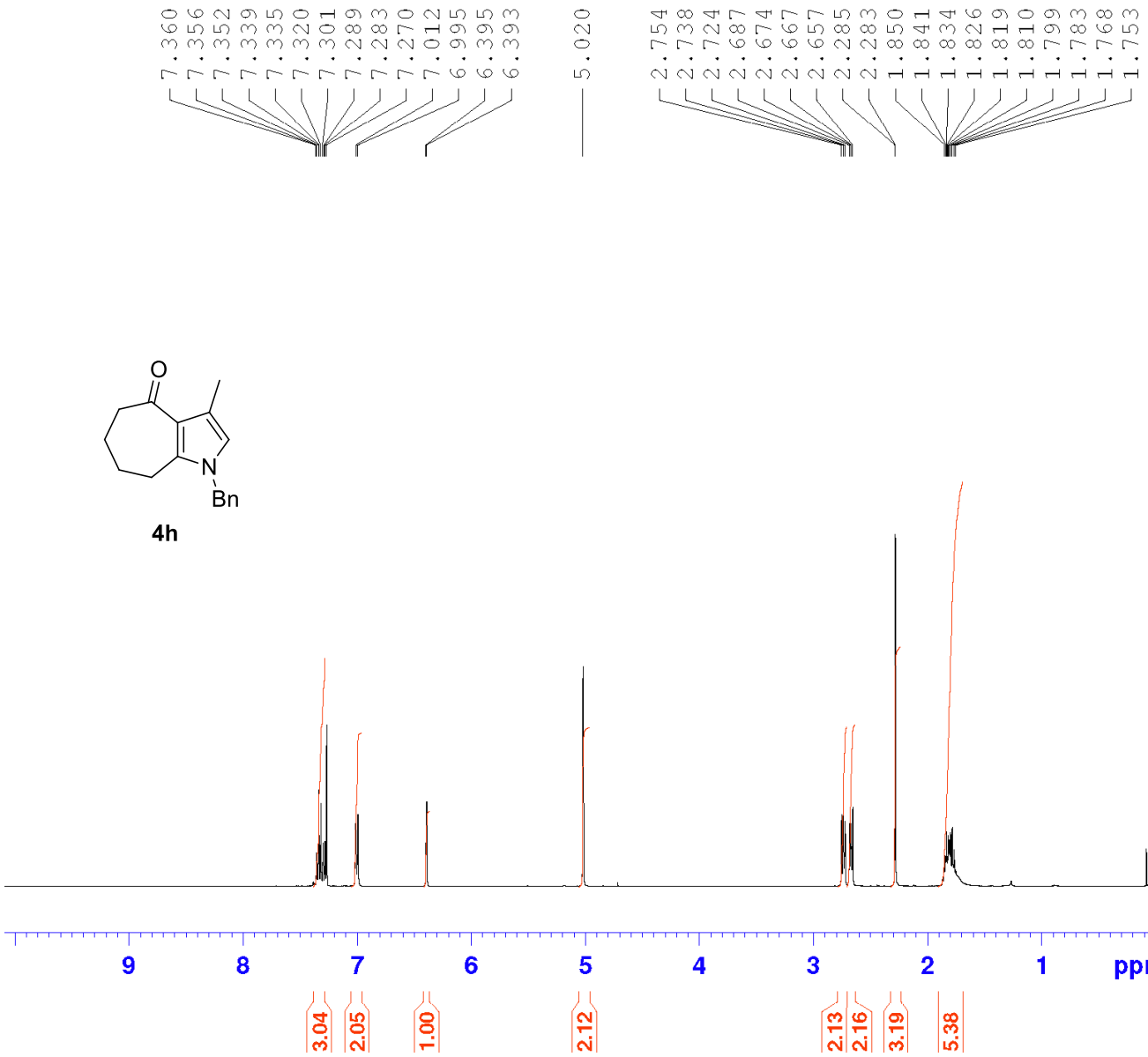

```
Current Data Parameters
NAME       22082013-Cui
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_          20130822
Time              11.14
INSTRUM       avance400
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  400
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3632196 sec
RG               5792.6
DW               20.800 usec
DE                6.00 usec
TE                298.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1               -2.00 dB
SFO1        100.6479773 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            80.00 usec
PL2               2.70 dB
PL12             17.10 dB
PL13             17.10 dB
SFO2        400.2316009 MHz

F2 - Processing parameters
SI                32768
SF          100.6379140 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

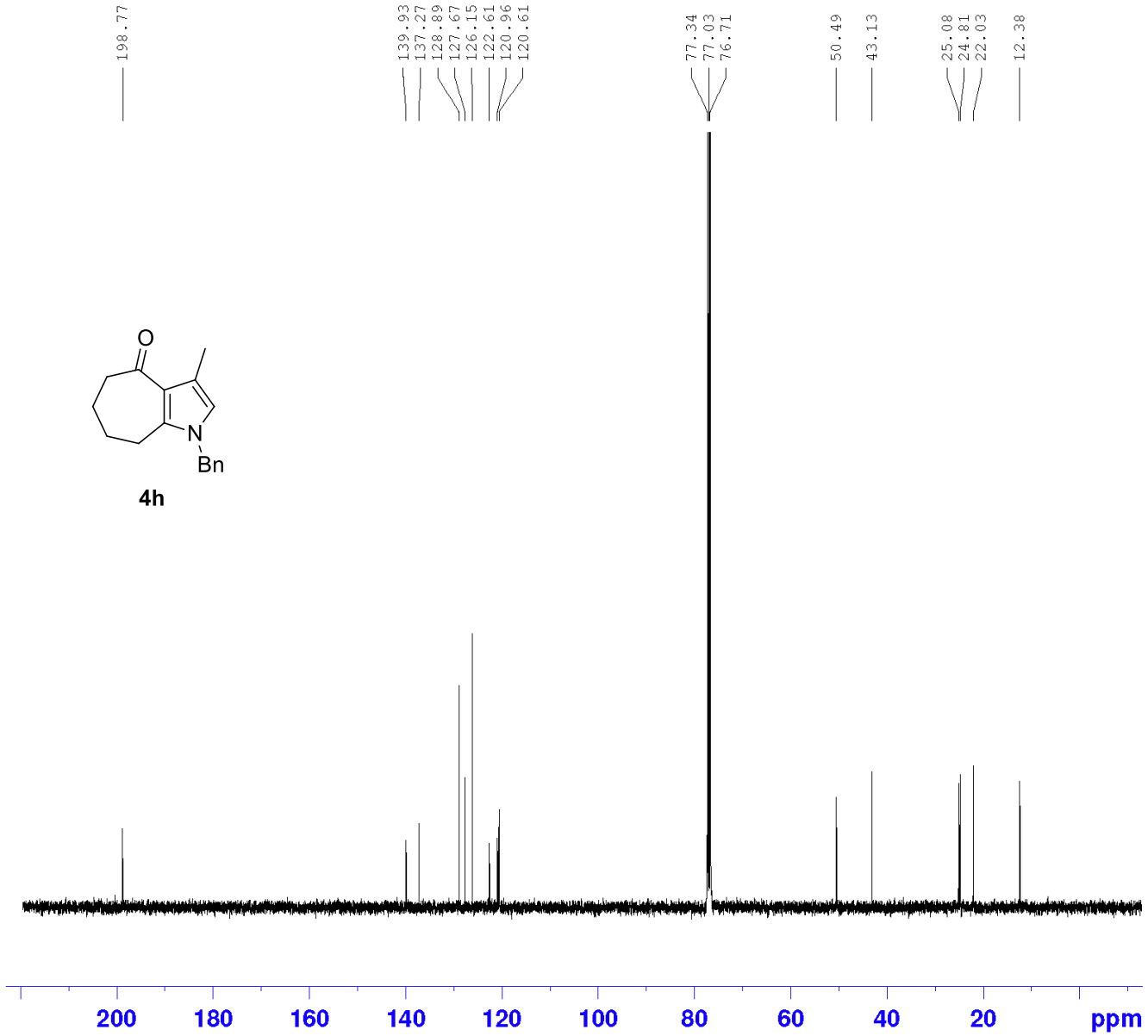



```
Current Data Parameters
NAME        14082013-Cui
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130814
Time               10.45
INSTRUM        avance400
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8250.825 Hz
FIDRES          0.125898 Hz
AQ             3.9715922 sec
RG                 322.5
DW                60.600 usec
DE                 6.00 usec
TE                297.4 K
D1           1.00000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                 15.00 usec
PL1                 2.70 dB
SFO1         400.2324716 MHz

F2 - Processing parameters
SI                 32768
SF          400.2300015 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



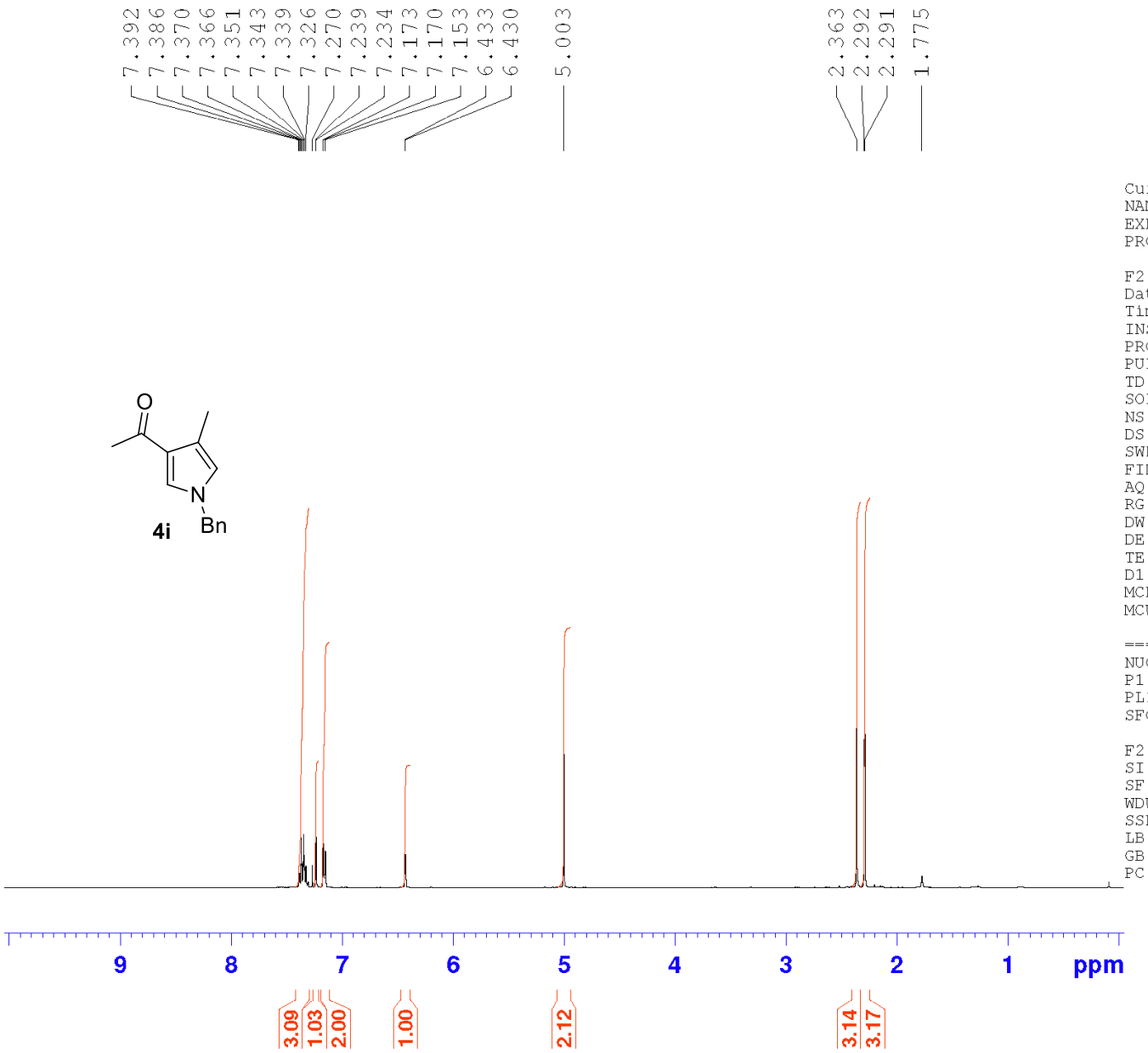

```
Current Data Parameters
NAME       31072013-Cui
EXPNO                21
PROCNO                1

F2 - Acquisition Parameters
Date_          20130731
Time              13.40
INSTRUM       avance400
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3632196 sec
RG               5160.6
DW               20.800 usec
DE                6.00 usec
TE                298.1 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1               -2.00 dB
SFO1        100.6479773 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            80.00 usec
PL2               2.70 dB
PL12             17.10 dB
PL13             17.10 dB
SFO2        400.2316009 MHz

F2 - Processing parameters
SI                32768
SF          100.6379140 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

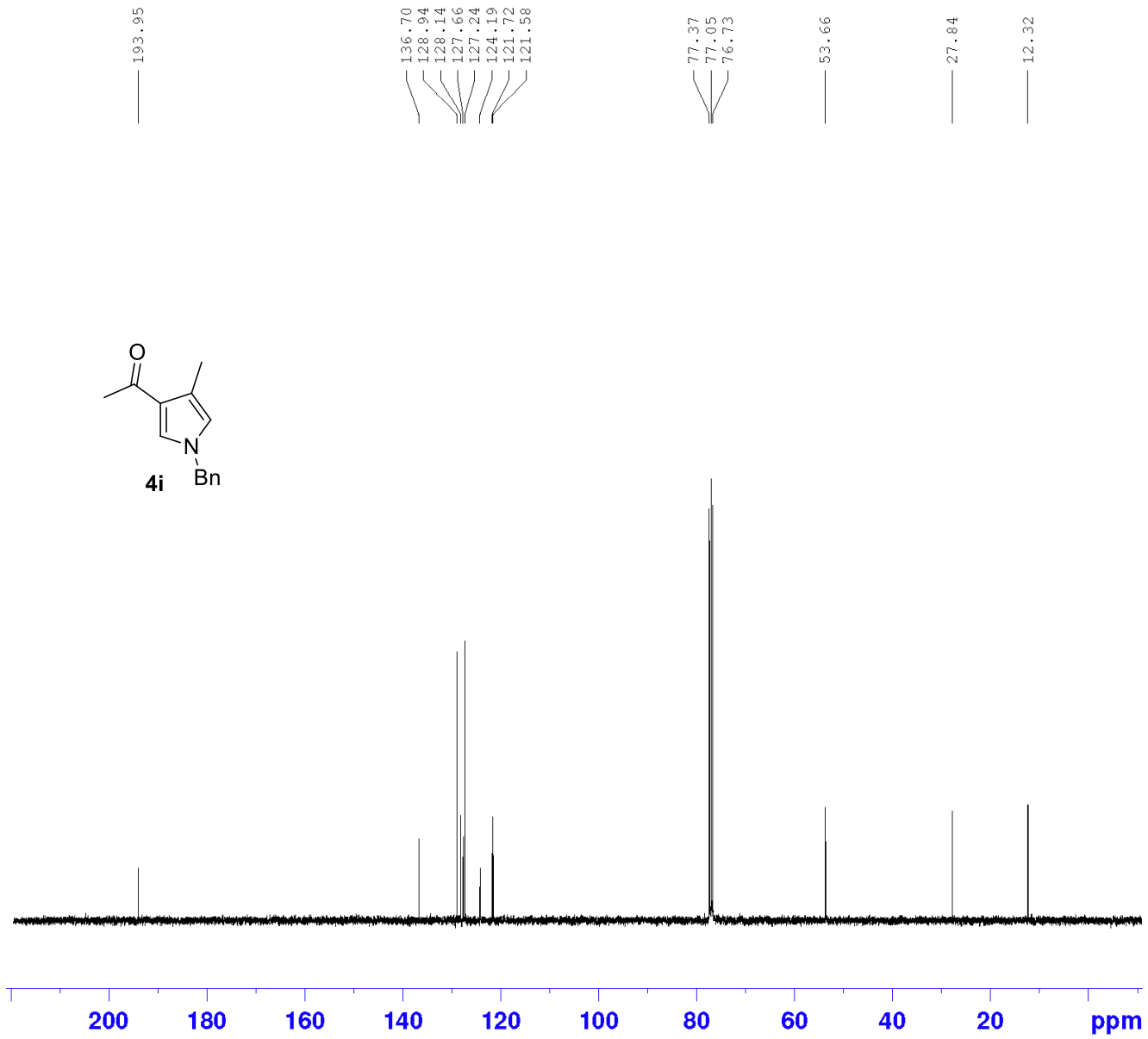



```
Current Data Parameters
NAME        19072013-Cui
EXPNO                 40
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130719
Time               18.17
INSTRUM        avance400
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8250.825 Hz
FIDRES          0.125898 Hz
AQ             3.9715922 sec
RG                 143.7
DW                60.600 usec
DE                 6.00 usec
TE                297.5 K
D1            1.00000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                2.70 dB
SFO1         400.2324716 MHz

F2 - Processing parameters
SI                 32768
SF          400.2300015 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



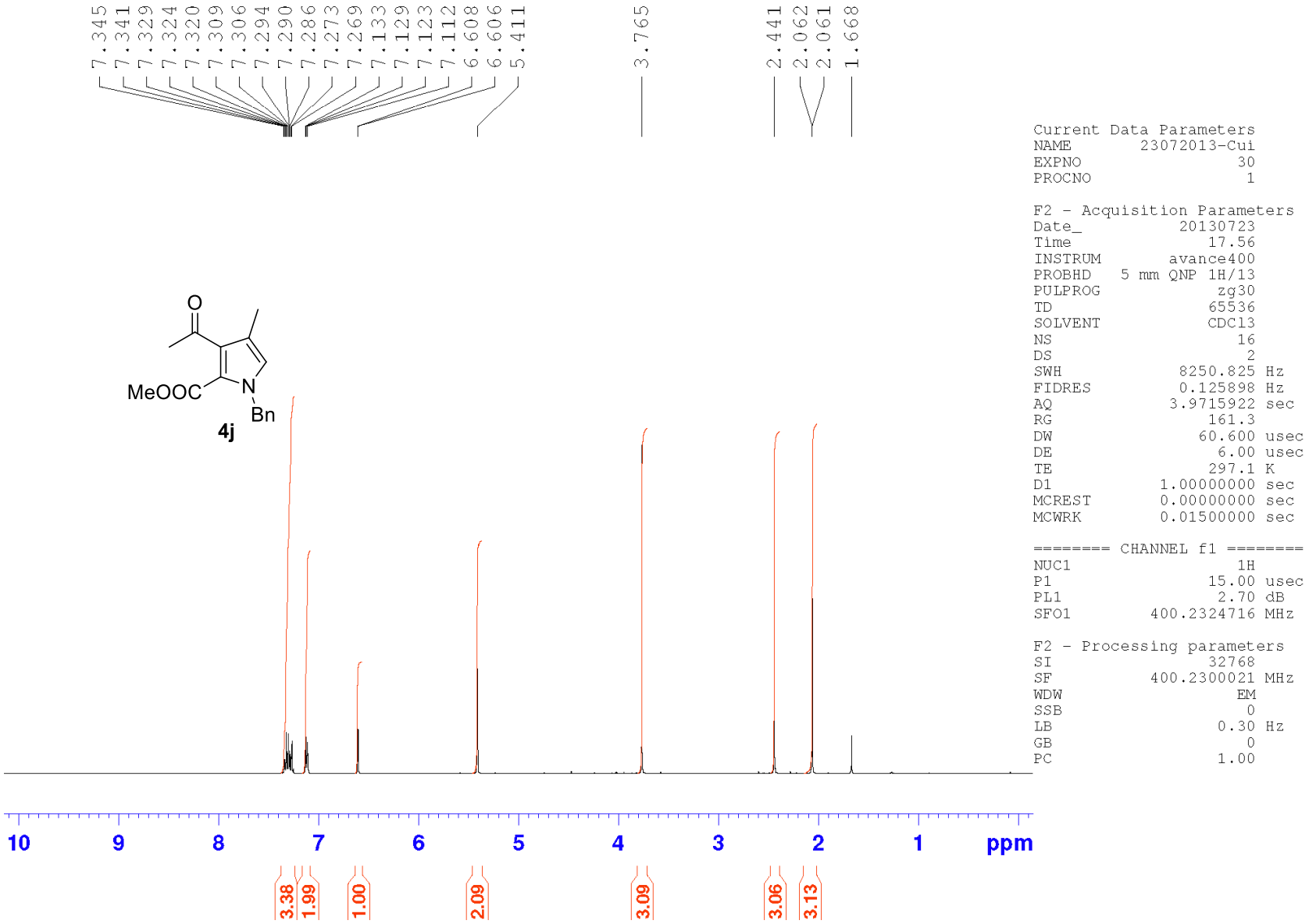

```
Current Data Parameters
NAME       19072013-Cui
EXPNO                41
PROCNO                1

F2 - Acquisition Parameters
Date_          20130719
Time              18.35
INSTRUM       avance400
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  300
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3632196 sec
RG                 3251
DW               20.800 usec
DE                6.00 usec
TE                298.6 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1               -2.00 dB
SFO1        100.6479773 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2             80.00 usec
PL2                2.70 dB
PL12              17.10 dB
PL13              17.10 dB
SFO2        400.2316009 MHz

F2 - Processing parameters
SI                 32768
SF          100.6379140 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

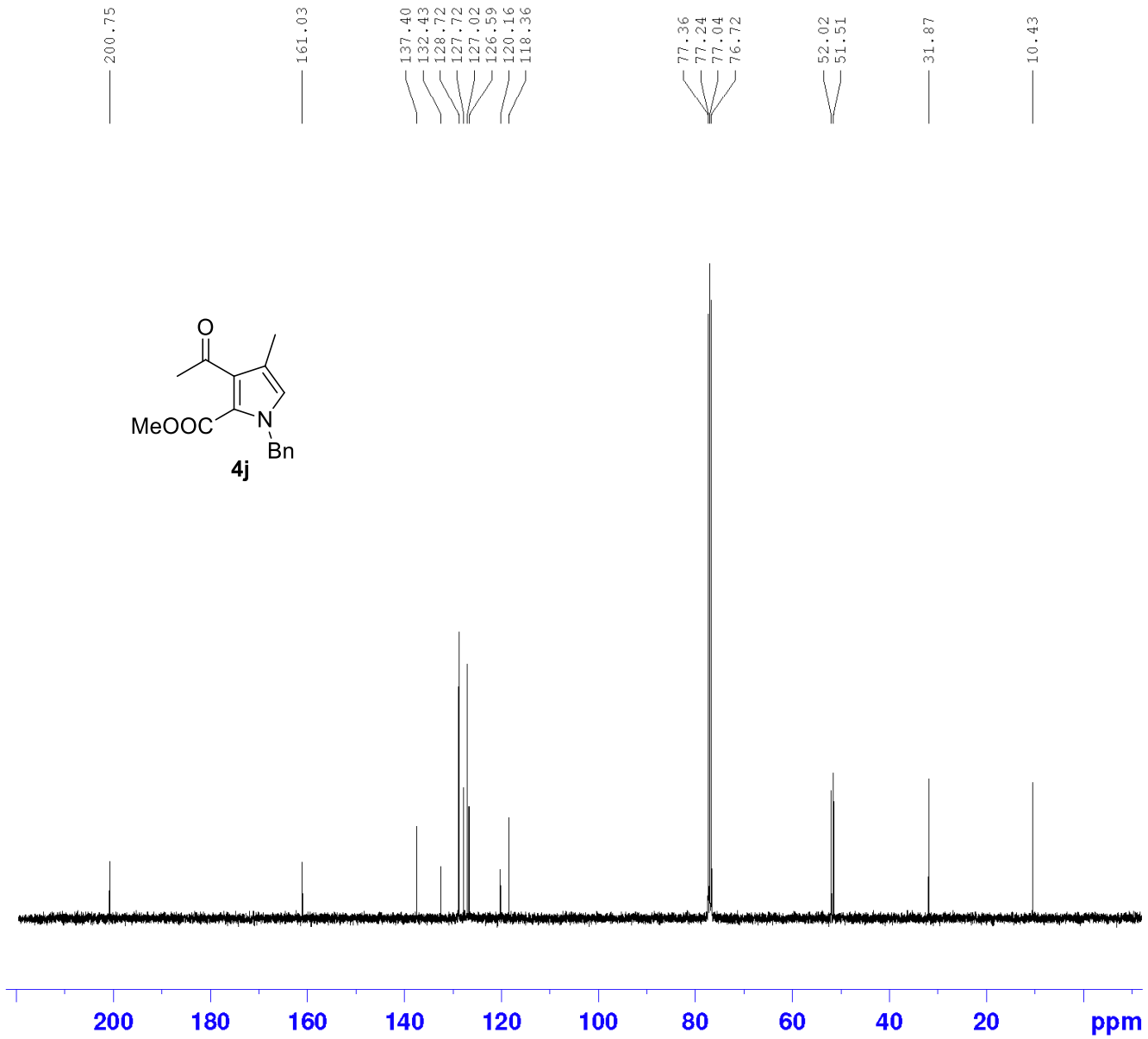



```
Current Data Parameters
NAME        23072013-Cui
EXPNO                 30
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130723
Time               17.56
INSTRUM        avance400
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8250.825 Hz
FIDRES          0.125898 Hz
AQ             3.9715922 sec
RG                 161.3
DW                60.600 usec
DE                 6.00 usec
TE                297.1 K
D1             1.00000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                 15.00 usec
PL1                 2.70 dB
SFO1         400.2324716 MHz

F2 - Processing parameters
SI                 32768
SF          400.2300021 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



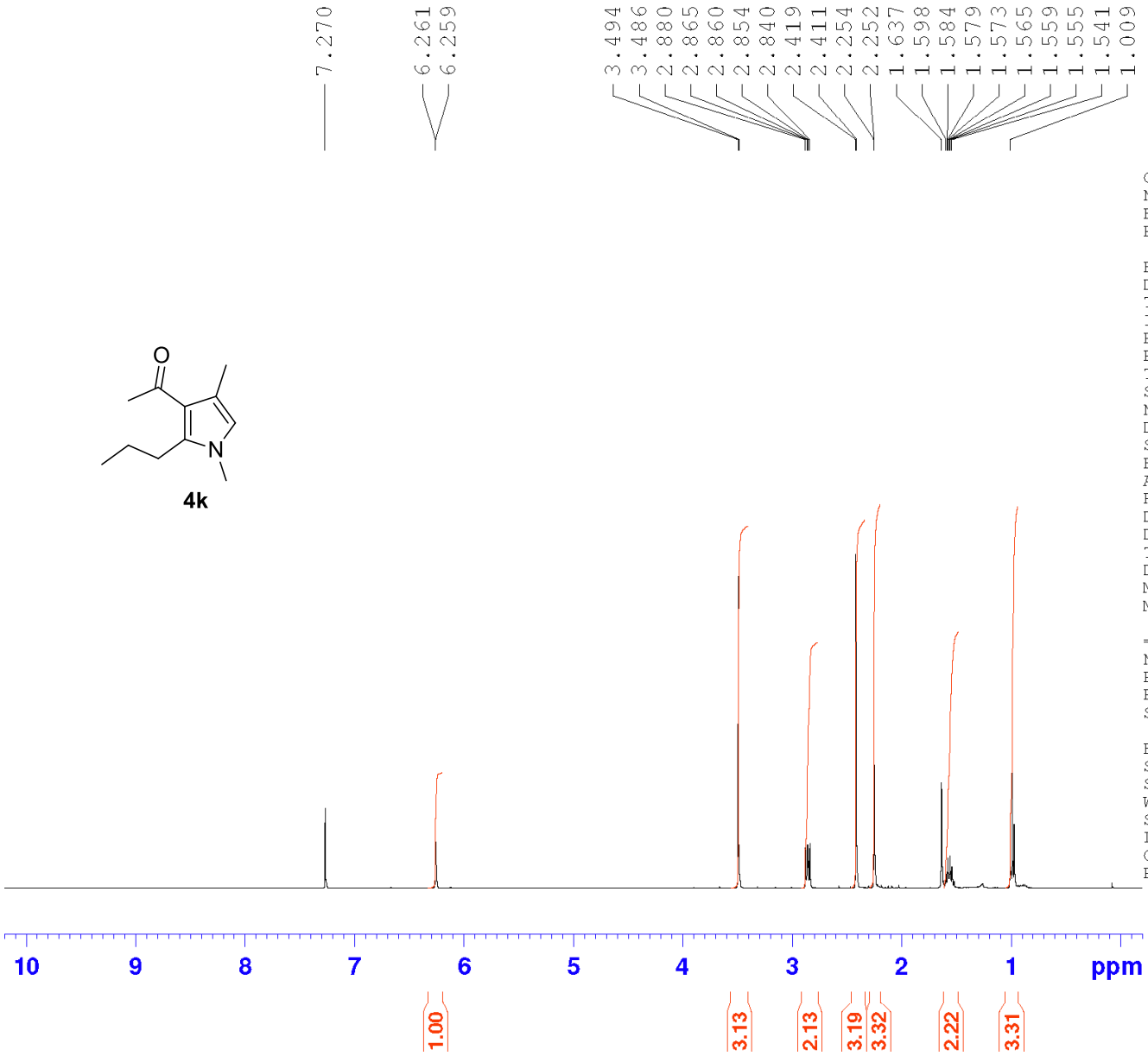

```
Current Data Parameters
NAME       23072013-Cui
EXPNO                32
PROCNO                1

F2 - Acquisition Parameters
Date_          20130723
Time               19.12
INSTRUM       avance400
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  400
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3632196 sec
RG               3649.1
DW                20.800 usec
DE                 6.00 usec
TE                298.1 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1               -2.00 dB
SFO1        100.6479773 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            80.00 usec
PL2               2.70 dB
PL12             17.10 dB
PL13             17.10 dB
SFO2        400.2316009 MHz

F2 - Processing parameters
SI                32768
SF          100.6379140 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

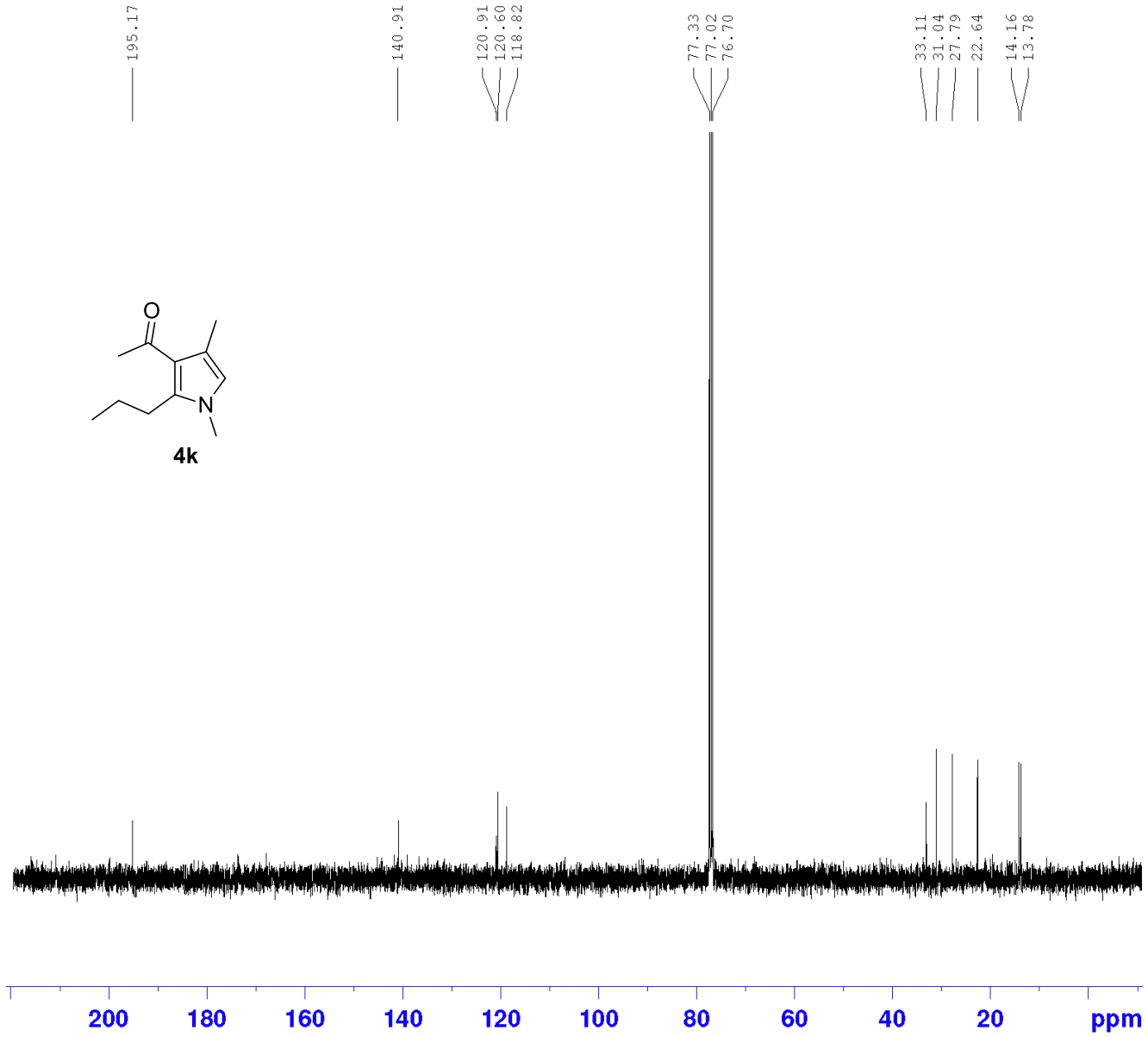



```
Current Data Parameters
NAME        23072013-Cui
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130723
Time               10.55
INSTRUM        avance400
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8250.825 Hz
FIDRES          0.125898 Hz
AQ             3.9715922 sec
RG                 287.4
DW                60.600 usec
DE                 6.00 usec
TE                297.1 K
D1            1.00000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                2.70 dB
SFO1         400.2324716 MHz

F2 - Processing parameters
SI                 32768
SF          400.2300018 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```



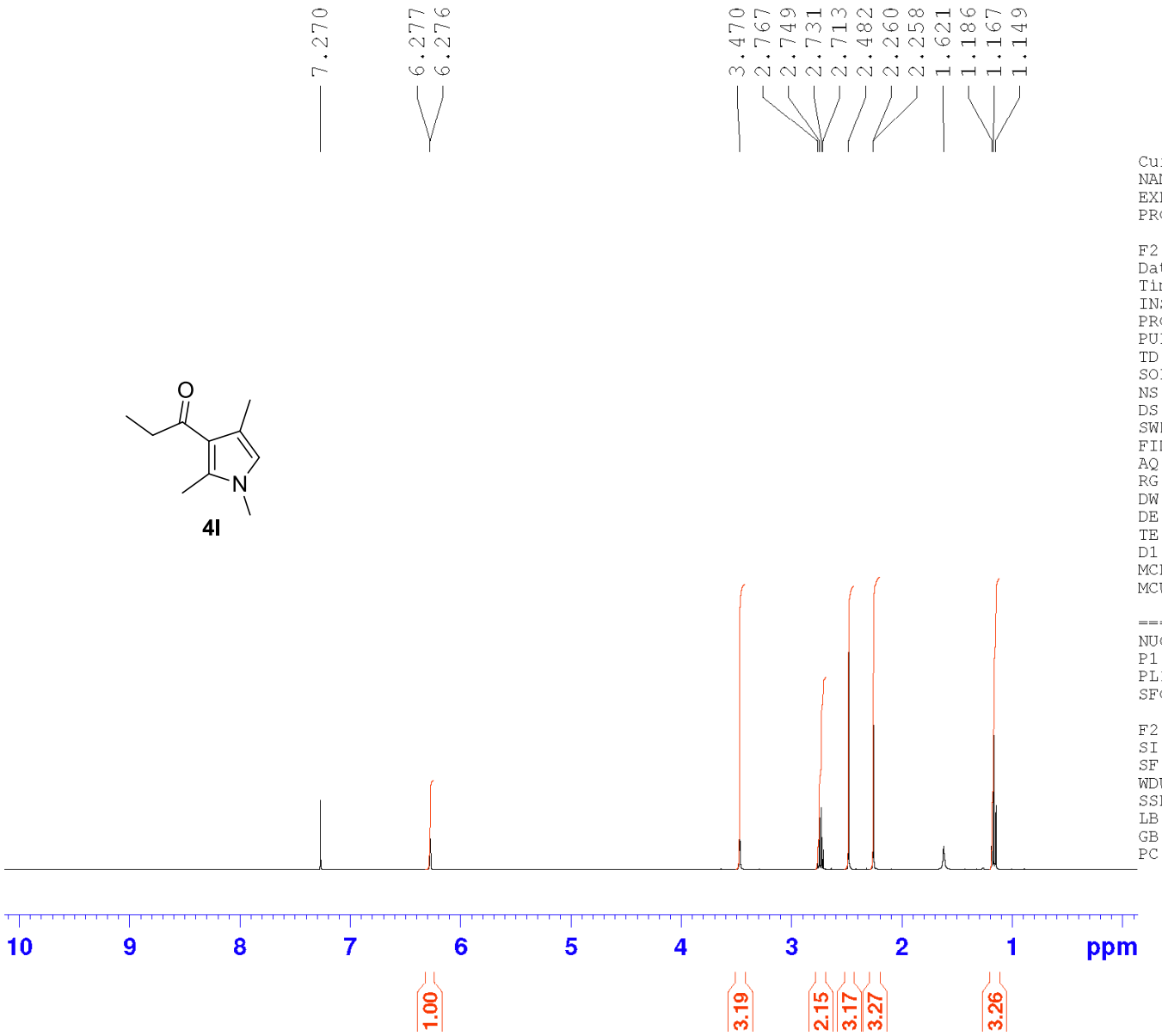

```
Current Data Parameters
NAME       23072013-Cui
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_           20130723
Time               11.26
INSTRUM       avance400
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  300
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3632196 sec
RG                 4096
DW               20.800 usec
DE                6.00 usec
TE                297.9 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1               -2.00 dB
SFO1        100.6479773 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2             80.00 usec
PL2                2.70 dB
PL12              17.10 dB
PL13              17.10 dB
SFO2        400.2316009 MHz

F2 - Processing parameters
SI                 32768
SF          100.6379140 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

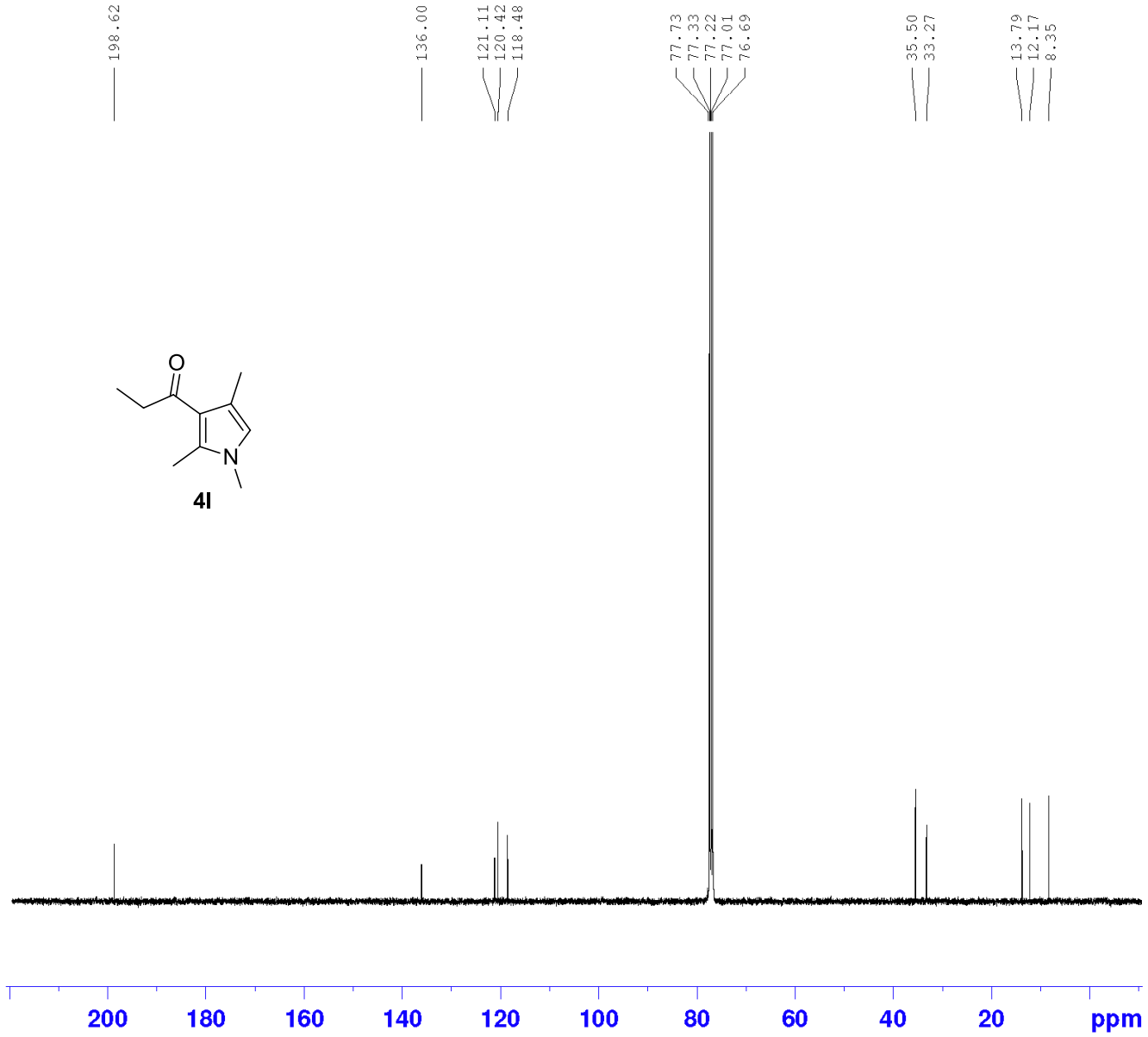



```
Current Data Parameters
NAME        31072013-Cui
EXPNO                 15
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130801
Time                9.41
INSTRUM        avance400
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8250.825 Hz
FIDRES          0.125898 Hz
AQ             3.9715922 sec
RG                   362
DW                60.600 usec
DE                 6.00 usec
TE                297.2 K
D1           1.00000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                2.70 dB
SFO1        400.2324716 MHz

F2 - Processing parameters
SI                 32768
SF          400.2300015 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```



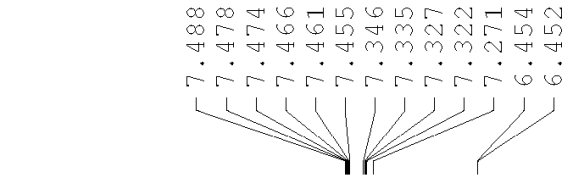

```
Current Data Parameters
NAME       31072013-Cui
EXPNO                14
PROCNO                1

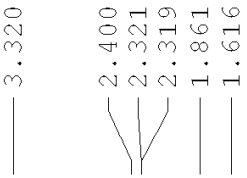
F2 - Acquisition Parameters
Date_          20130801
Time               3.33
INSTRUM       avance400
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                10000
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3632196 sec
RG               3649.1
DW                20.800 usec
DE                 6.00 usec
TE                298.3 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

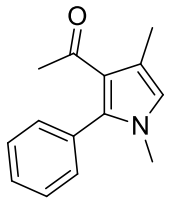
======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1               -2.00 dB
SFO1        100.6479773 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2             80.00 usec
PL2                2.70 dB
PL12              17.10 dB
PL13              17.10 dB
SFO2        400.2316009 MHz

F2 - Processing parameters
SI                32768
SF          100.6379140 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```







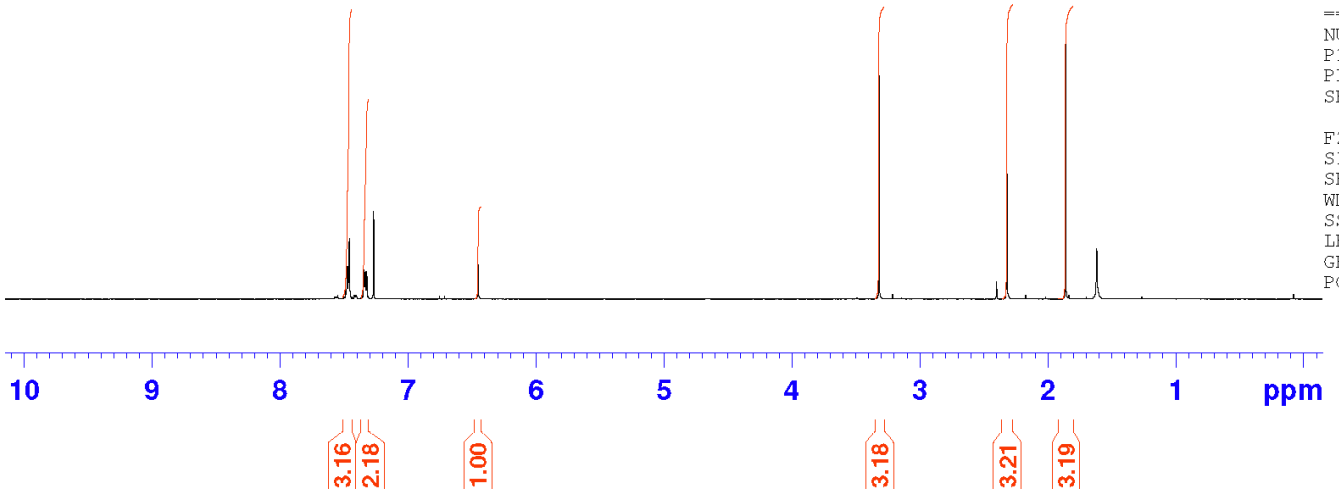
4m

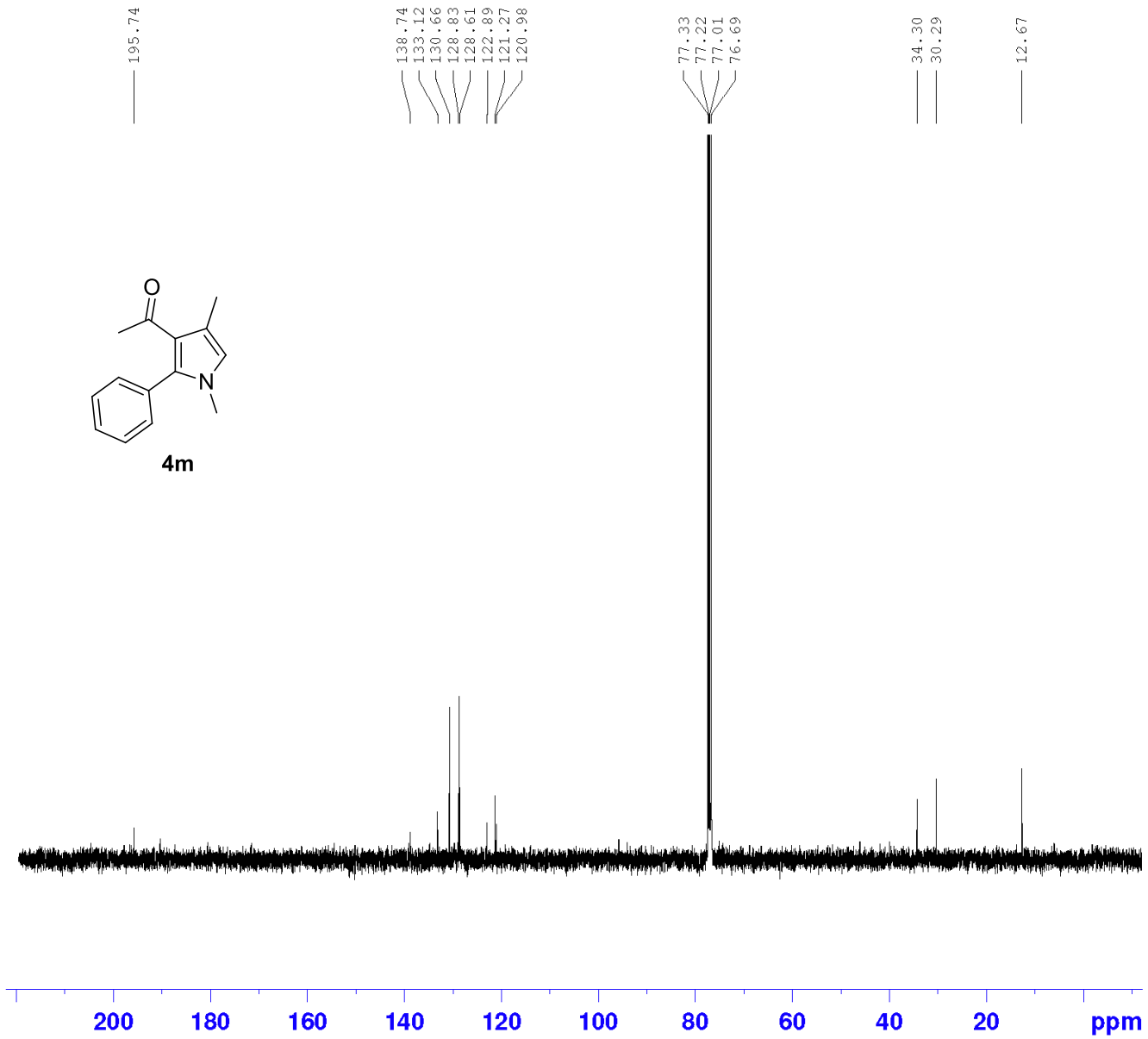
```
Current Data Parameters
NAME        23082013-Cui
EXPNO                 12
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130823
Time               14.19
INSTRUM        avance400
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8250.825 Hz
FIDRES          0.125898 Hz
AQ             3.9715922 sec
RG                   256
DW                60.600 usec
DE                 6.00 usec
TE                297.5 K
D1           1.00000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                2.70 dB
SFO1        400.2324716 MHz

F2 - Processing parameters
SI                 32768
SF          400.2300015 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```





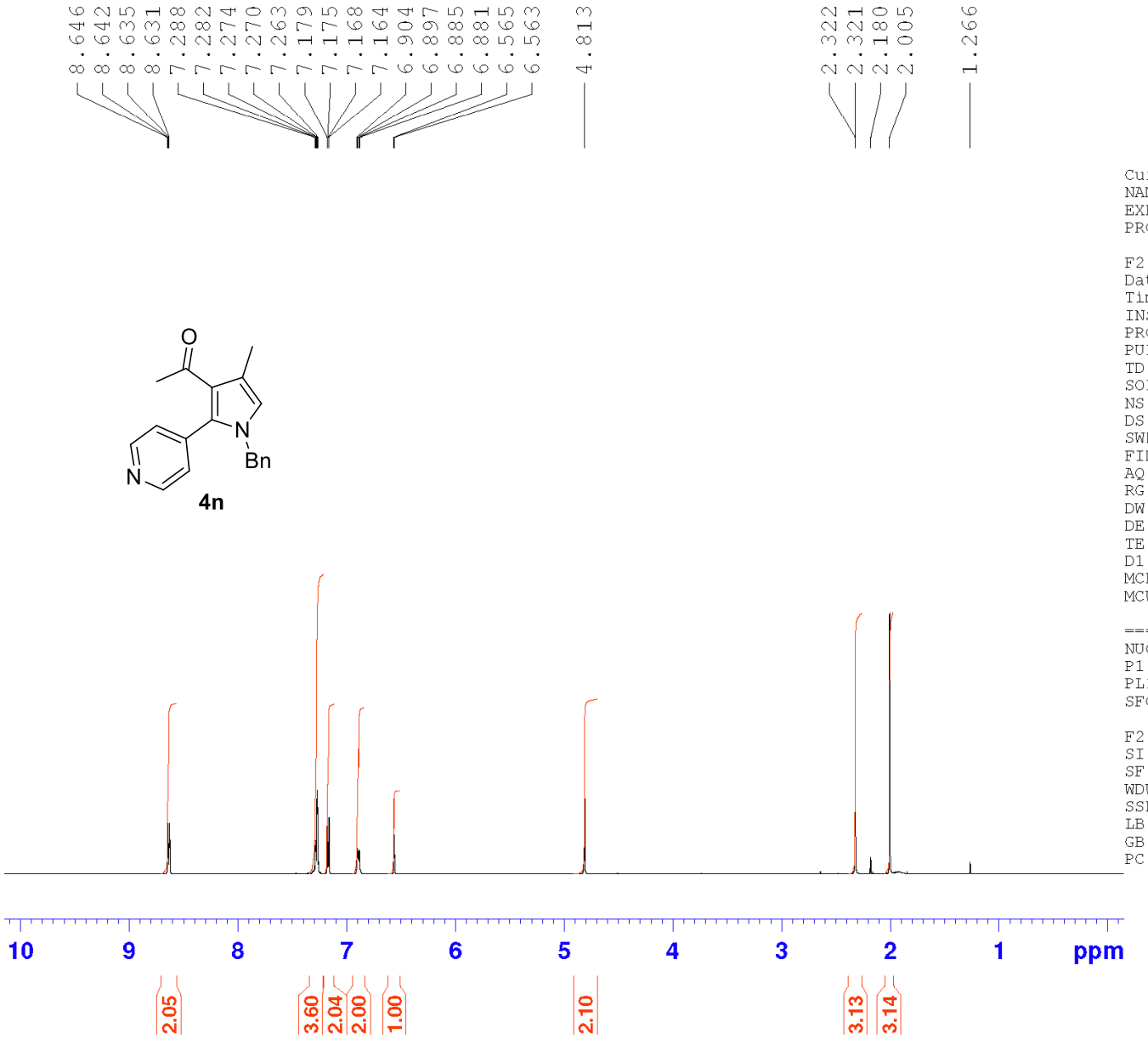

```
Current Data Parameters
NAME       23082013-Cui
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_          20130823
Time              13.38
INSTRUM       avance400
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3632196 sec
RG                 6502
DW               20.800 usec
DE                6.00 usec
TE                298.4 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1               -2.00 dB
SFO1        100.6479773 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            80.00 usec
PL2               2.70 dB
PL12             17.10 dB
PL13             17.10 dB
SFO2        400.2316009 MHz

F2 - Processing parameters
SI                 32768
SF          100.6379140 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                1.40
```

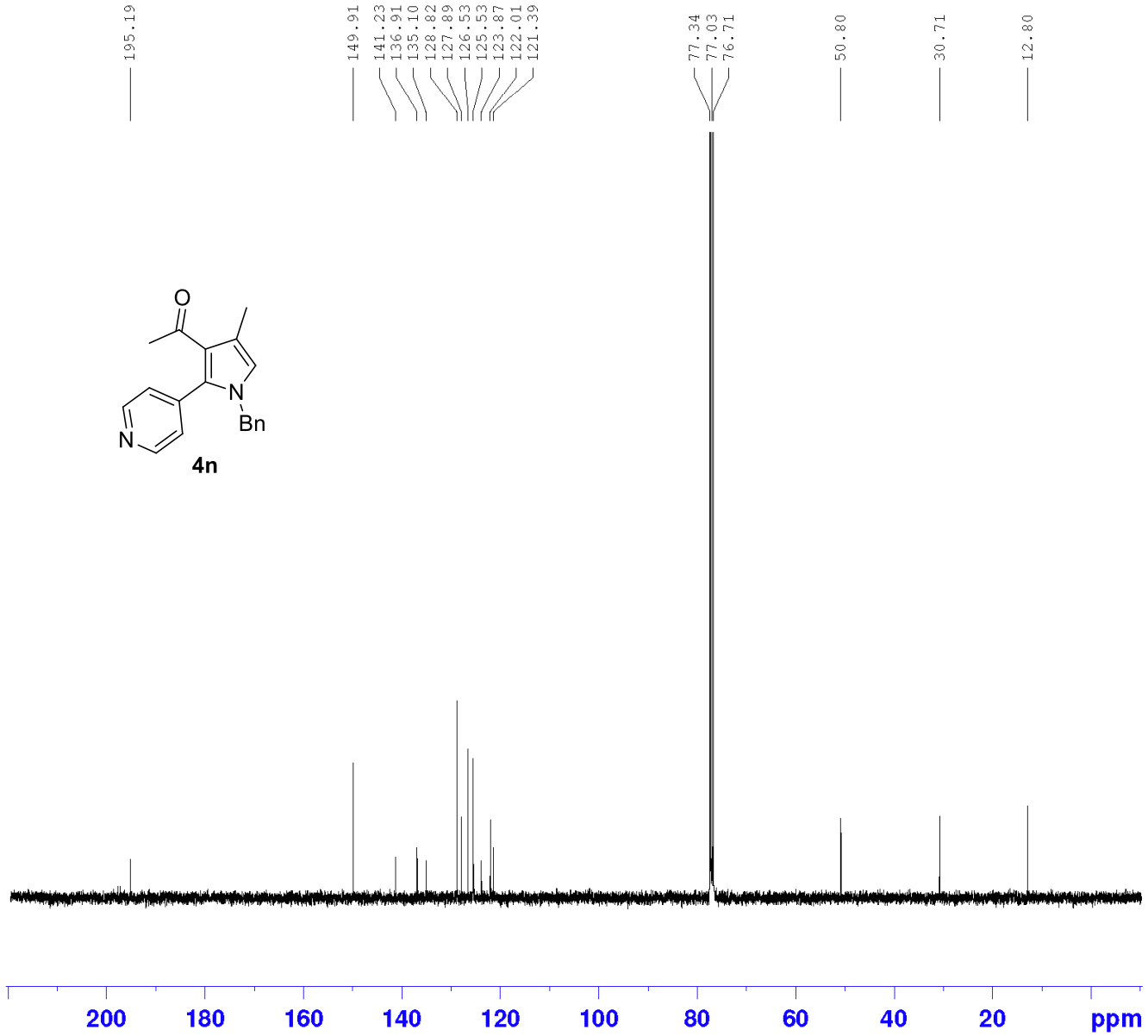



```
Current Data Parameters
NAME        26072013-Cui
EXPNO                 22
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130727
Time               10.03
INSTRUM        avance400
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8250.825 Hz
FIDRES          0.125898 Hz
AQ             3.9715922 sec
RG                   256
DW                60.600 usec
DE                 6.00 usec
TE                297.5 K
D1            1.00000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                2.70 dB
SFO1         400.2324716 MHz

F2 - Processing parameters
SI                 32768
SF          400.2300005 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```



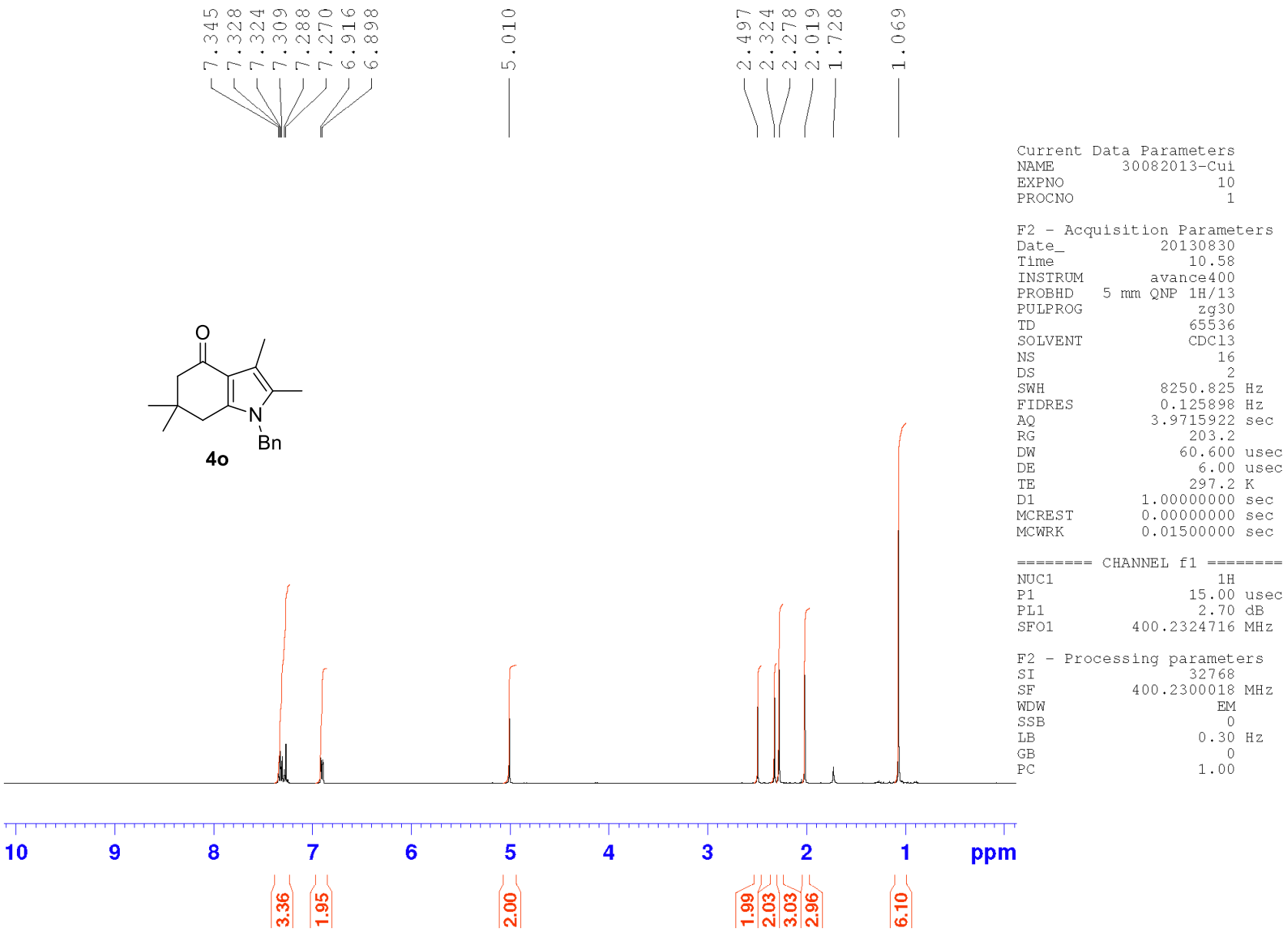

```
Current Data Parameters
NAME       26072013-Cui
EXPNO                23
PROCNO                1

F2 - Acquisition Parameters
Date_          20130727
Time              10.43
INSTRUM       avance400
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  500
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3632196 sec
RG               4597.6
DW                20.800 usec
DE                 6.00 usec
TE                298.3 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1               -2.00 dB
SFO1        100.6479773 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2                2.70 dB
PL12              17.10 dB
PL13              17.10 dB
SFO2        400.2316009 MHz

F2 - Processing parameters
SI                32768
SF          100.6379140 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

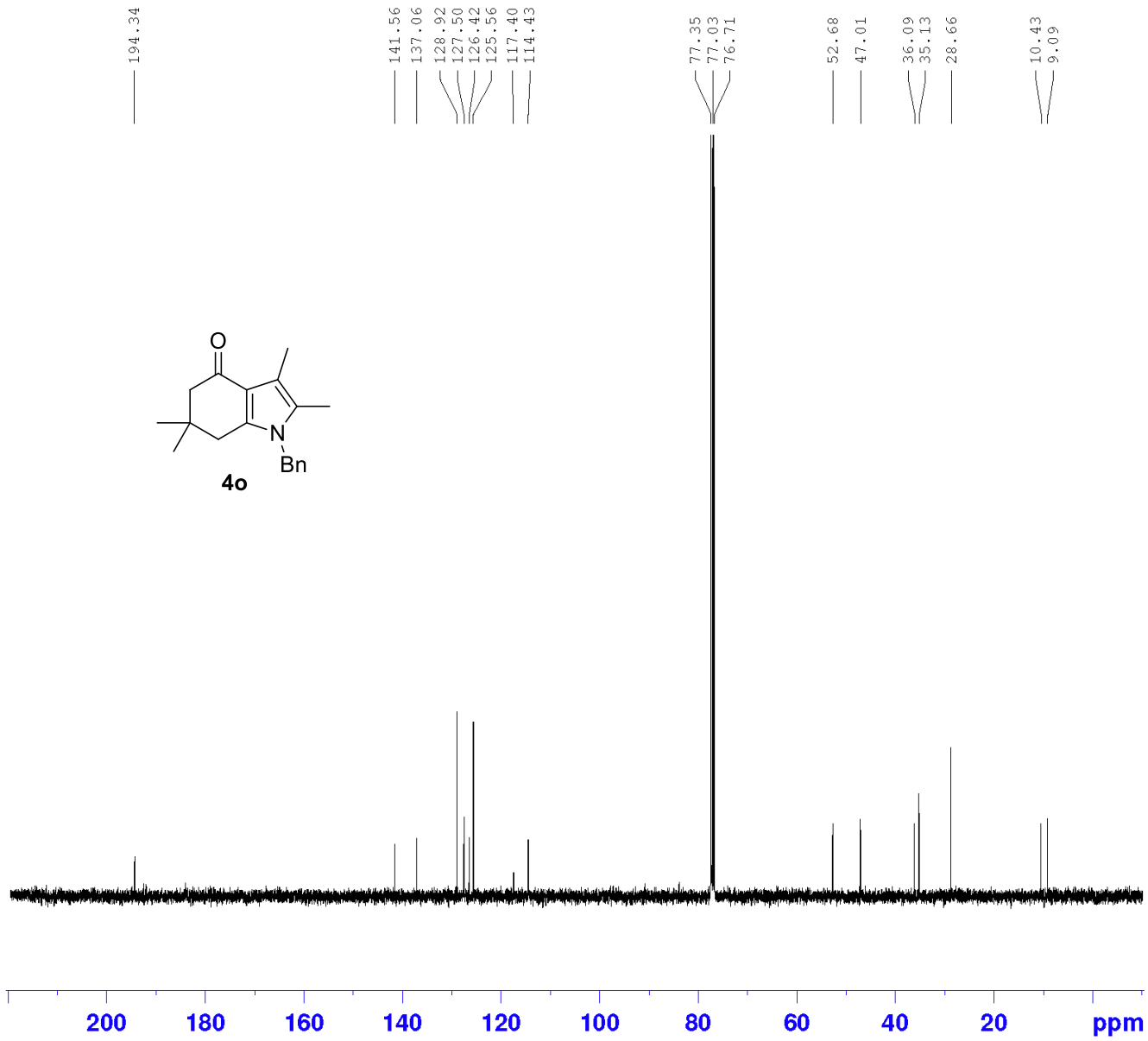



```
Current Data Parameters
NAME        30082013-Cui
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130830
Time               10.58
INSTRUM        avance400
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8250.825 Hz
FIDRES          0.125898 Hz
AQ             3.9715922 sec
RG                 203.2
DW                60.600 usec
DE                 6.00 usec
TE                297.2 K
D1            1.00000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                2.70 dB
SFO1         400.2324716 MHz

F2 - Processing parameters
SI                 32768
SF          400.2300018 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```



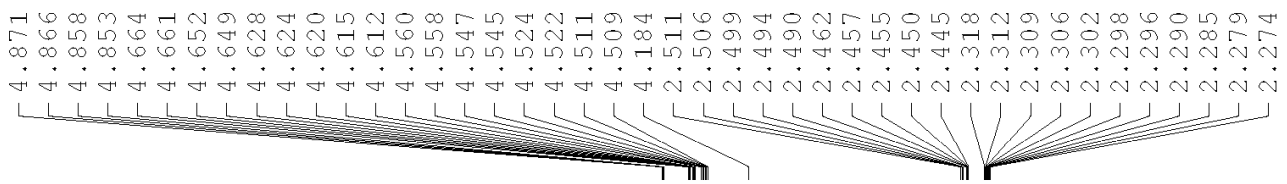

```
Current Data Parameters
NAME       30082013-Cui
EXPNO                11
PROCNO                1

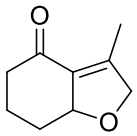
F2 - Acquisition Parameters
Date_          20130830
Time              11.27
INSTRUM       avance400
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  400
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3632196 sec
RG               5160.6
DW               20.800 usec
DE                6.00 usec
TE                297.8 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1               -2.00 dB
SFO1        100.6479773 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2                2.70 dB
PL12              17.10 dB
PL13              17.10 dB
SFO2        400.2316009 MHz

F2 - Processing parameters
SI                32768
SF          100.6379140 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```





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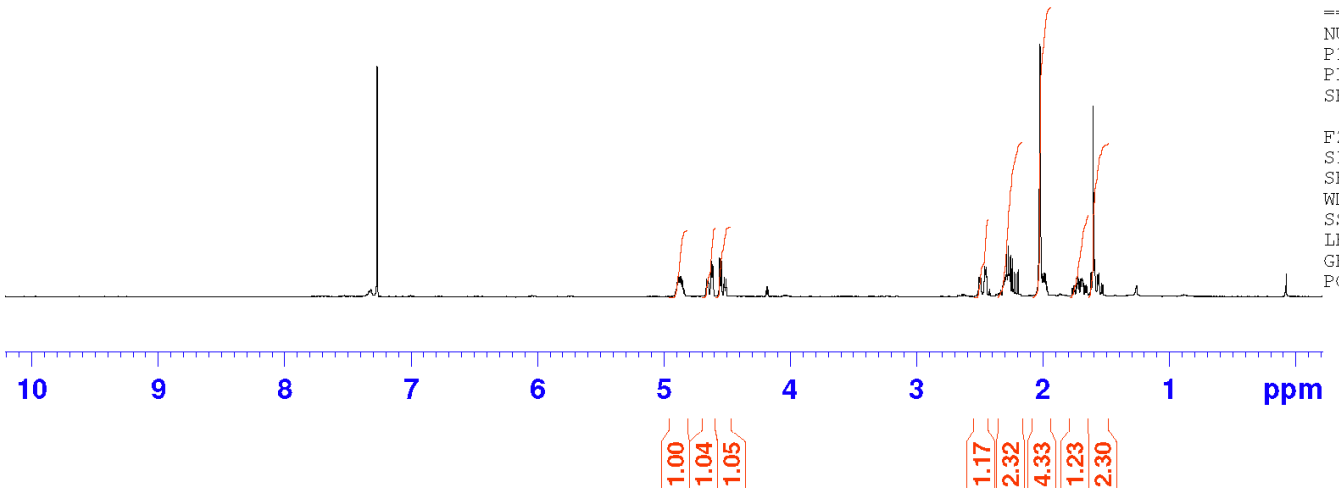
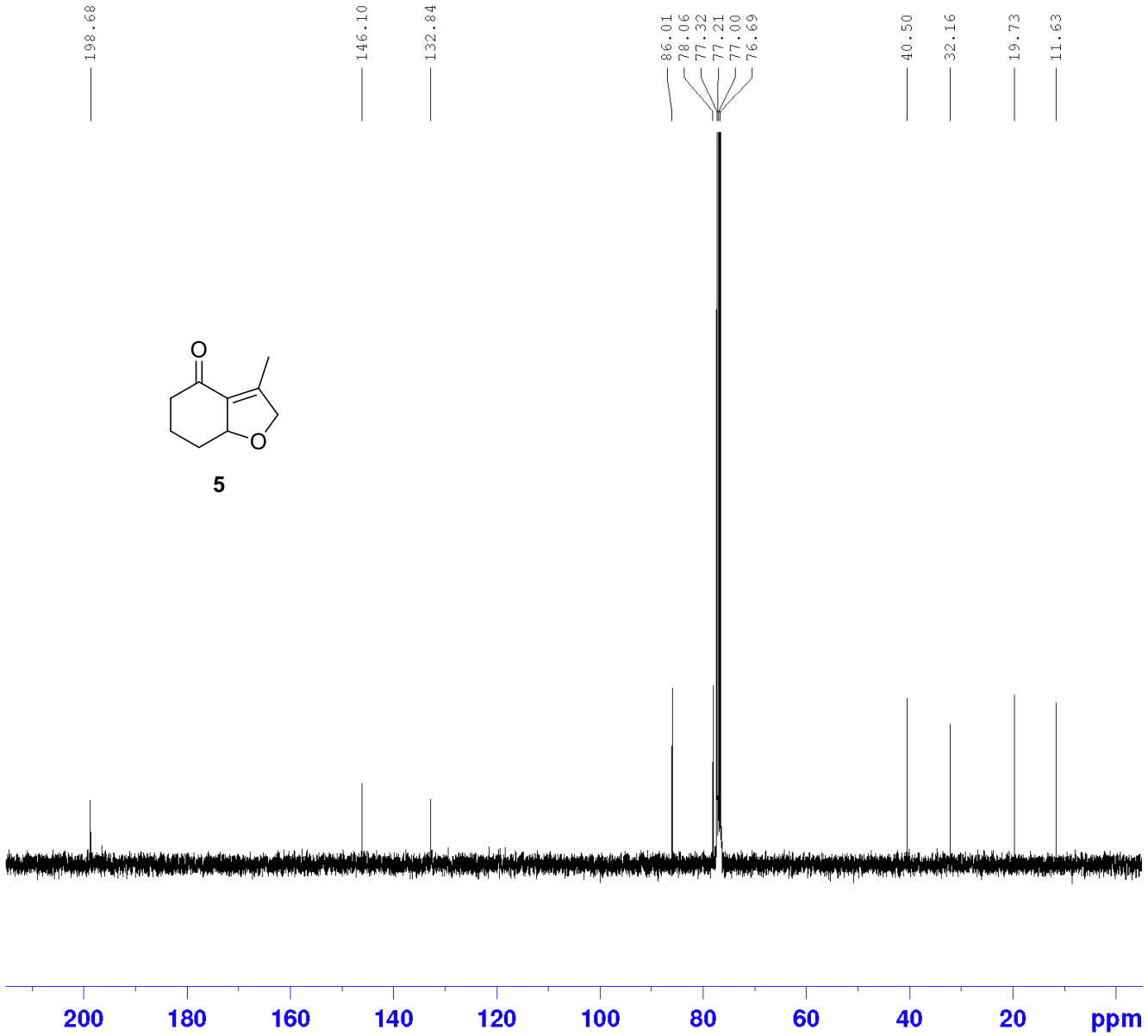



```
Current Data Parameters
NAME        16052013-Cui
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130516
Time               11.41
INSTRUM        avance400
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8250.825 Hz
FIDRES          0.125898 Hz
AQ             3.9715922 sec
RG                   362
DW                60.600 usec
DE                 6.00 usec
TE                297.5 K
D1           1.00000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                2.70 dB
SFO1        400.2324716 MHz

F2 - Processing parameters
SI                 32768
SF          400.2300015 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```



5

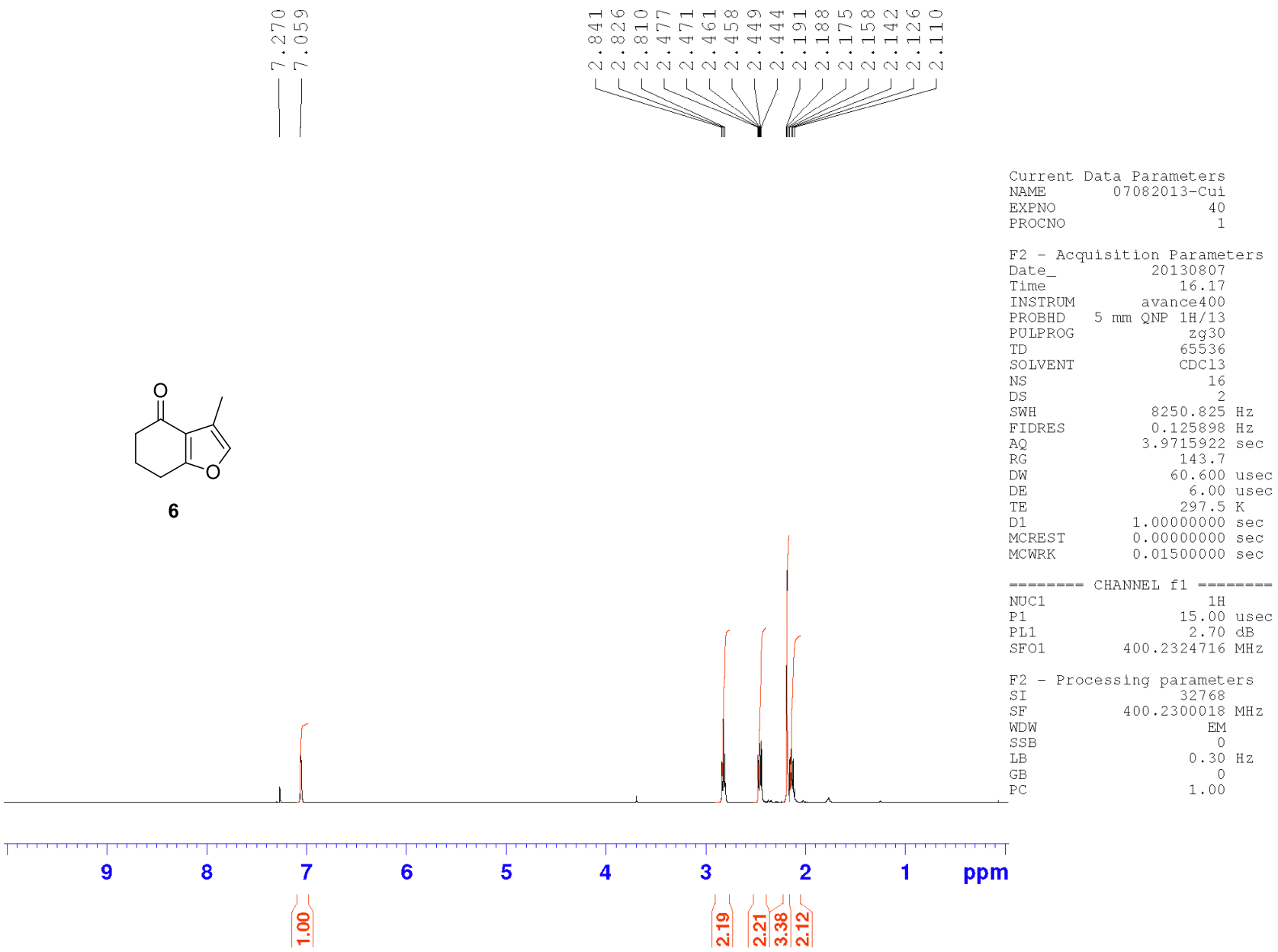
```
Current Data Parameters
NAME       16052013-Cui
EXPNO                12
PROCNO                1

F2 - Acquisition Parameters
Date_          20130516
Time              13.34
INSTRUM       avance400
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3632196 sec
RG               2896.3
DW               20.800 usec
DE                6.00 usec
TE                298.9 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1               -2.00 dB
SFO1        100.6479773 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2                2.70 dB
PL12              17.10 dB
PL13              17.10 dB
SFO2        400.2316009 MHz

F2 - Processing parameters
SI                32768
SF          100.6379140 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

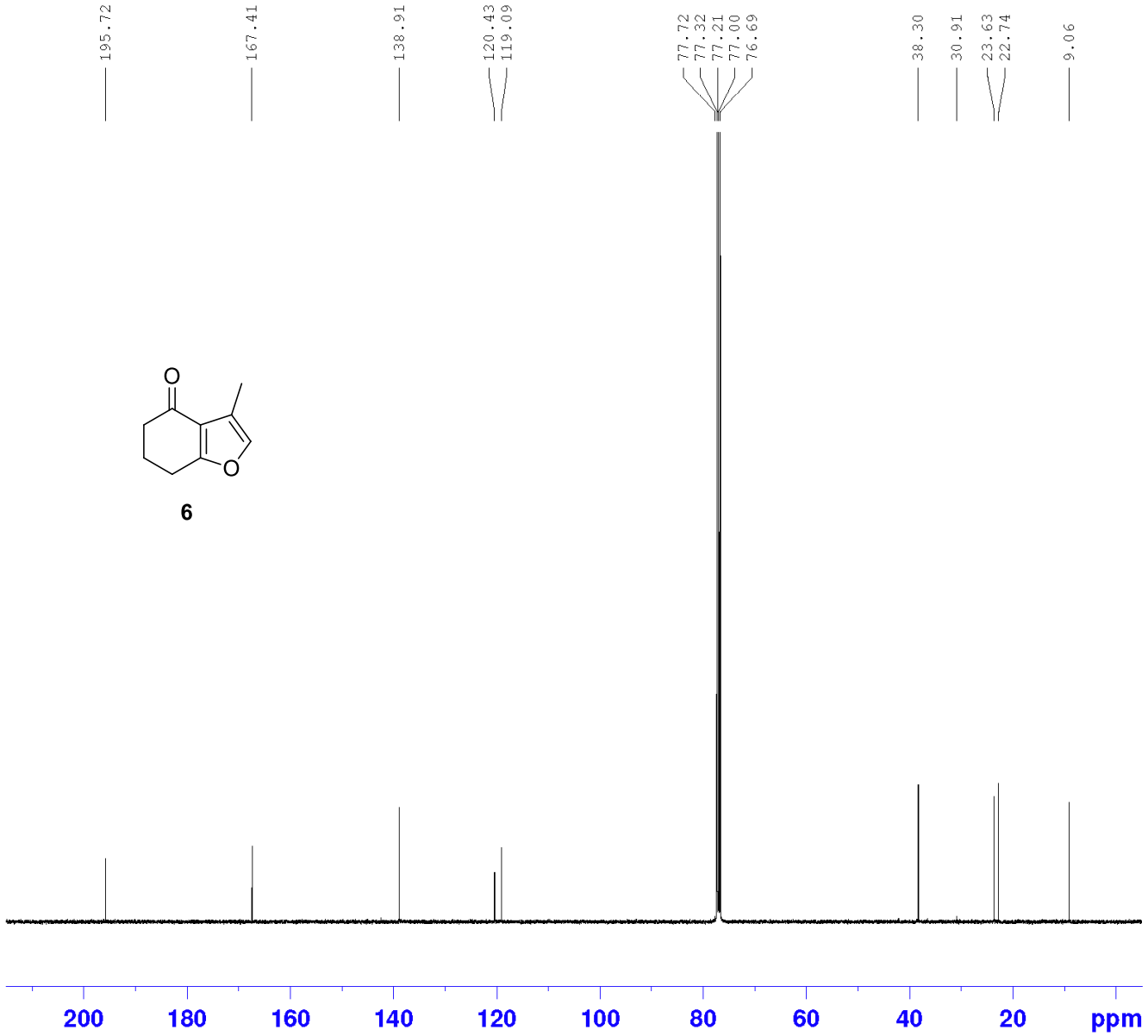



```
Current Data Parameters
NAME        07082013-Cui
EXPNO                 40
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130807
Time               16.17
INSTRUM        avance400
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8250.825 Hz
FIDRES          0.125898 Hz
AQ              3.9715922 sec
RG                 143.7
DW                60.600 usec
DE                 6.00 usec
TE                297.5 K
D1           1.00000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                2.70 dB
SFO1        400.2324716 MHz

F2 - Processing parameters
SI                 32768
SF          400.2300018 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                 1.00
```



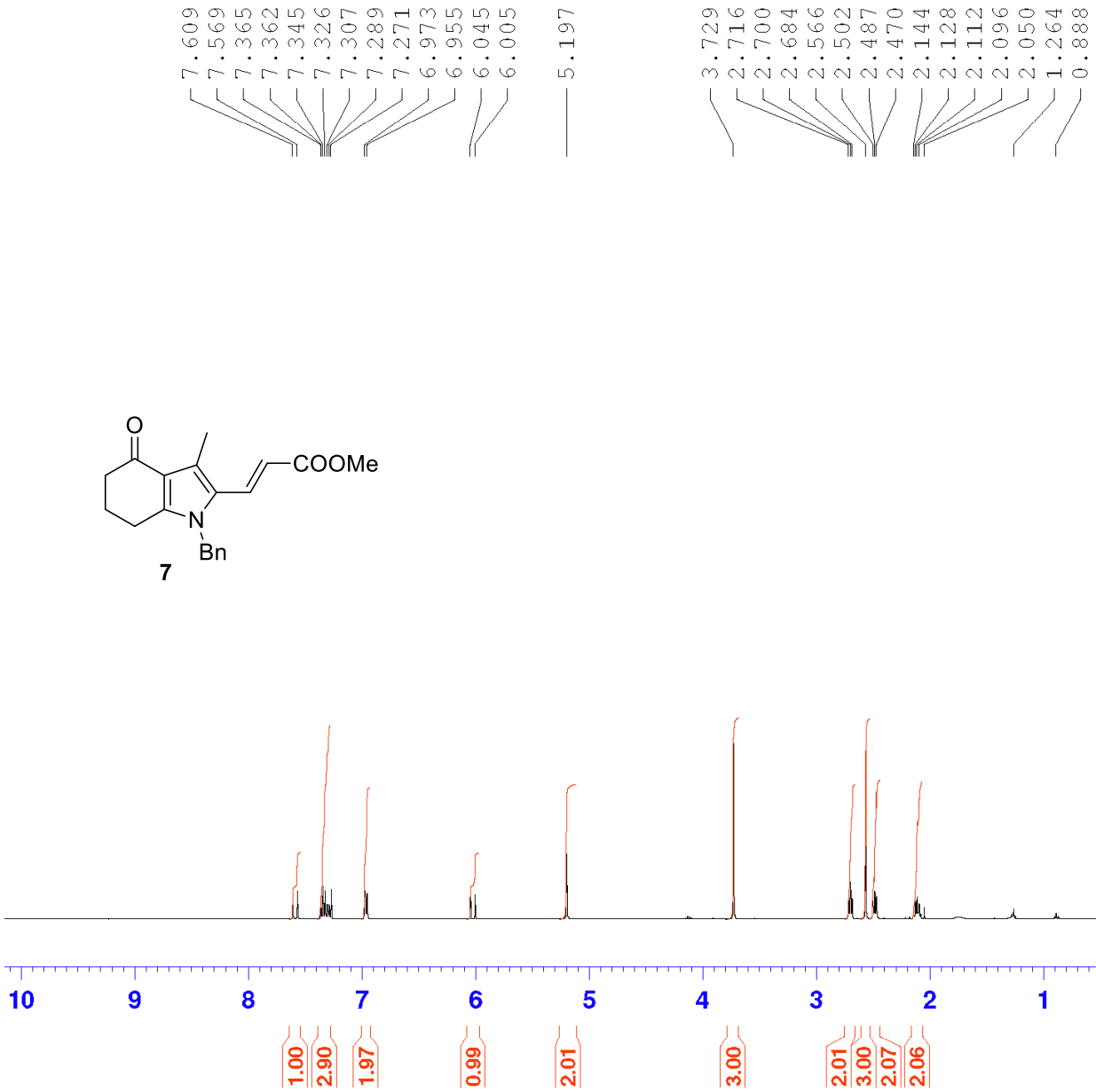

```
Current Data Parameters
NAME       03082013-Cui
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_          20130804
Time               1.58
INSTRUM       avance400
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                10000
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3632196 sec
RG               5160.6
DW               20.800 usec
DE                6.00 usec
TE               298.6 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1               -2.00 dB
SFO1        100.6479773 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2            80.00 usec
PL2               2.70 dB
PL12             17.10 dB
PL13             17.10 dB
SFO2        400.2316009 MHz

F2 - Processing parameters
SI                32768
SF          100.6379140 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

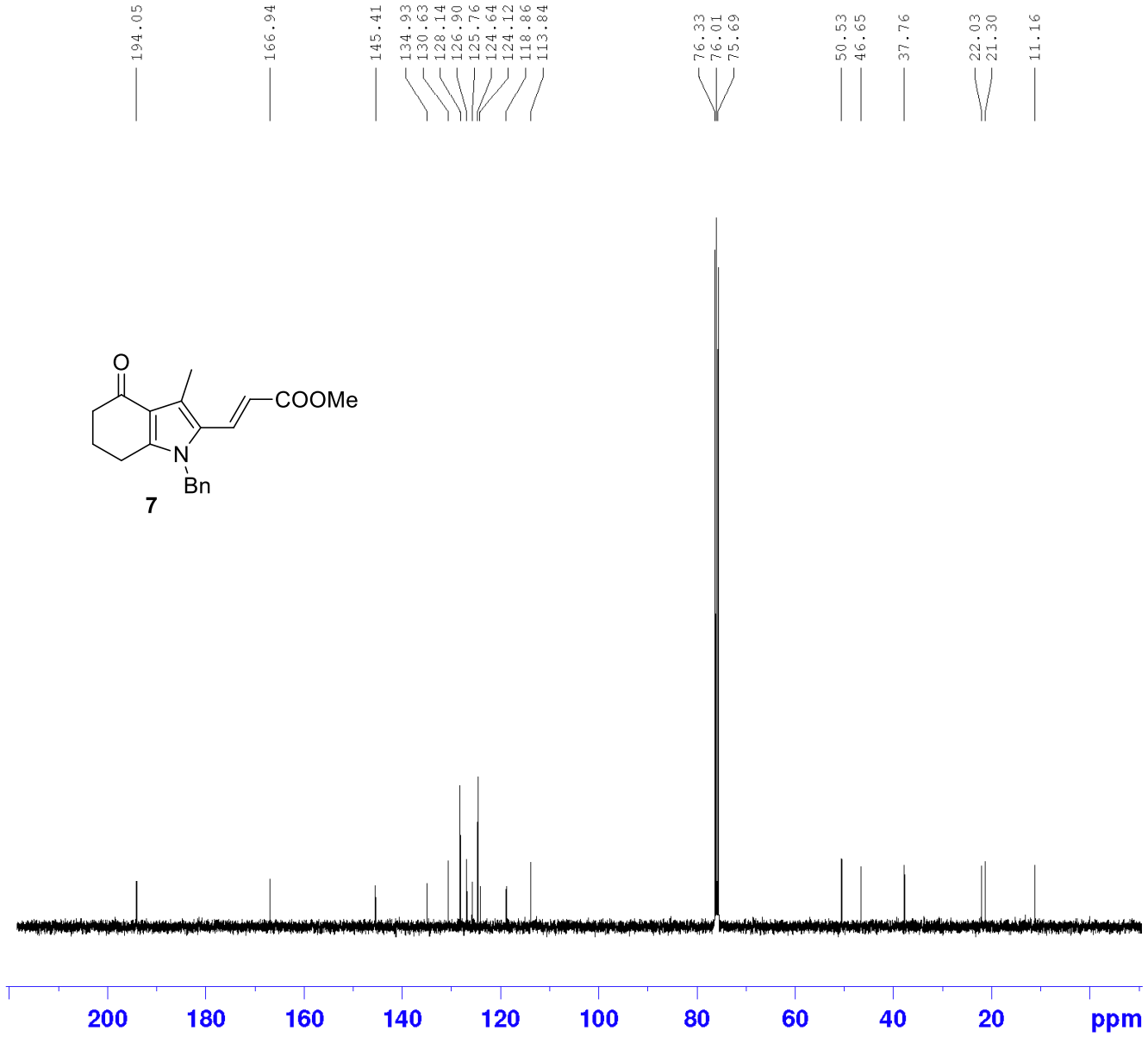



```
Current Data Parameters
NAME        01082013-Cui
EXPNO                 32
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130801
Time              17.04
INSTRUM        avance400
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8250.825 Hz
FIDRES          0.125898 Hz
AQ             3.9715922 sec
RG                 203.2
DW                60.600 usec
DE                 6.00 usec
TE                297.4 K
D1            1.00000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                2.70 dB
SFO1         400.2324716 MHz

F2 - Processing parameters
SI                 32768
SF          400.2300013 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```



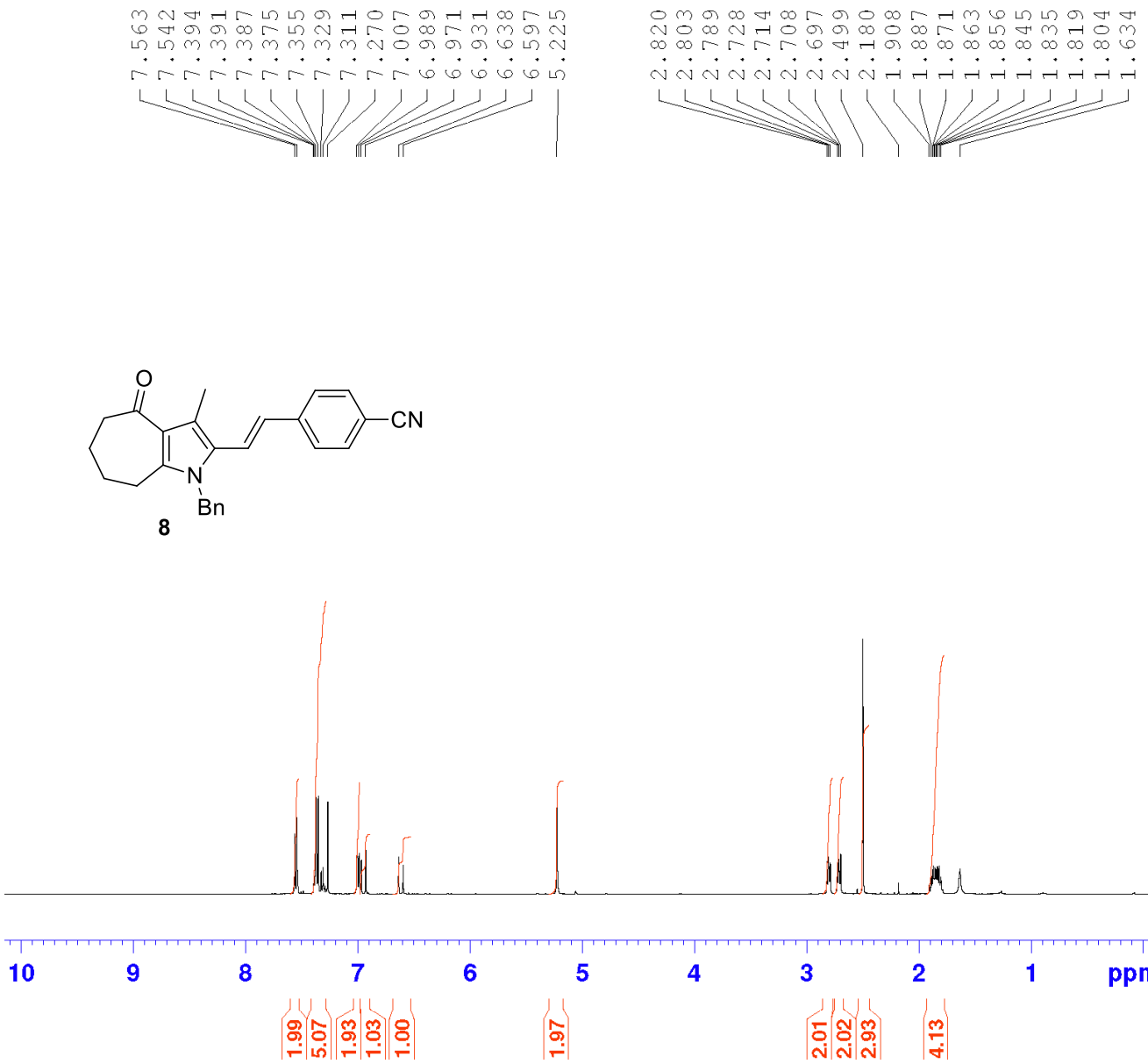

```
Current Data Parameters
NAME       01082013-Cui
EXPNO                31
PROCNO                1

F2 - Acquisition Parameters
Date_          20130801
Time              16.55
INSTRUM       avance400
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  400
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3632196 sec
RG                4597.6
DW                20.800 usec
DE                 6.00 usec
TE                298.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1               -2.00 dB
SFO1        100.6479773 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            80.00 usec
PL2               2.70 dB
PL12             17.10 dB
PL13             17.10 dB
SFO2        400.2316009 MHz

F2 - Processing parameters
SI                32768
SF          100.6380166 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

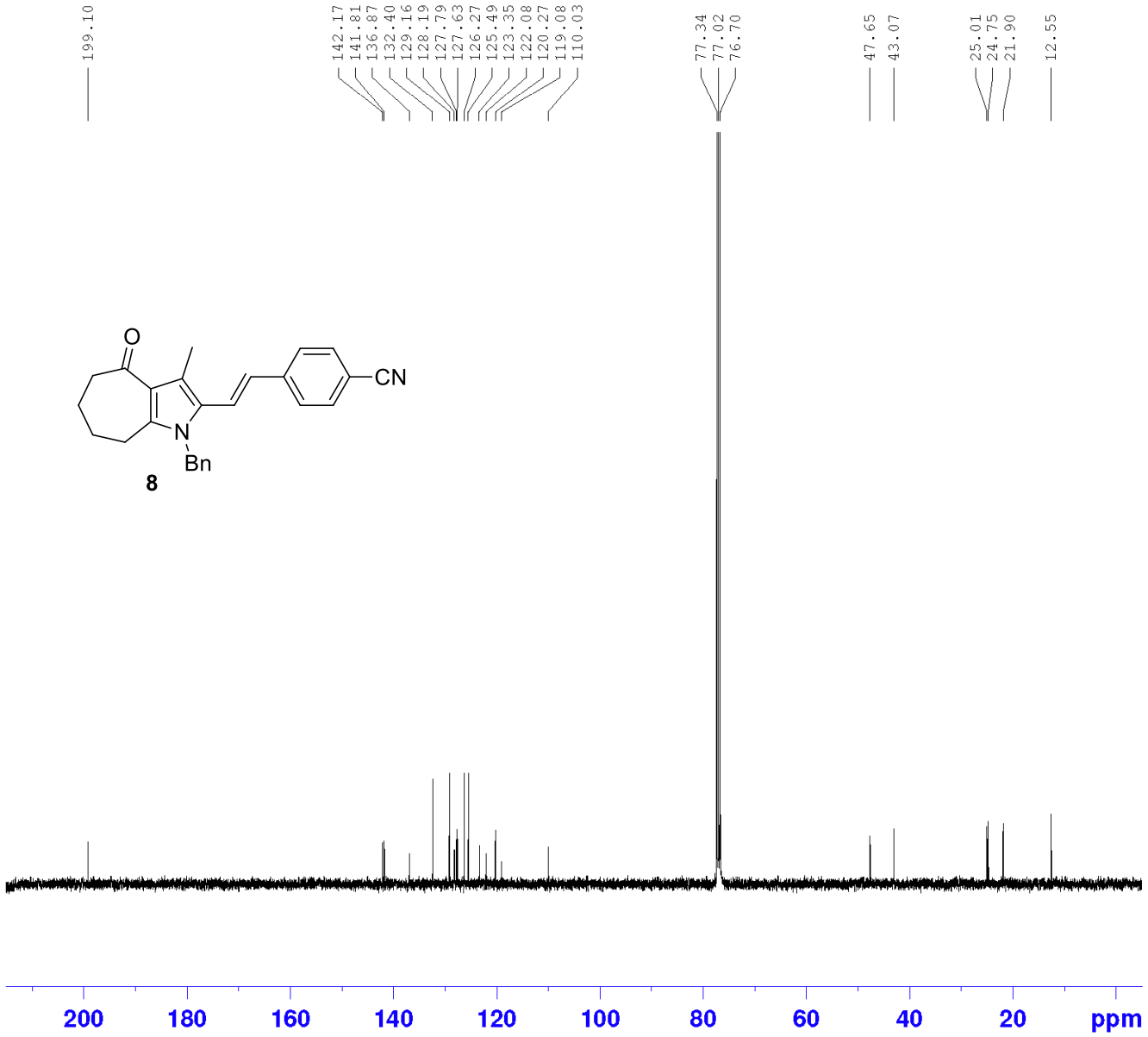



```
Current Data Parameters
NAME        15082013-Cui
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130815
Time               11.17
INSTRUM        avance400
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8250.825 Hz
FIDRES          0.125898 Hz
AQ             3.9715922 sec
RG                 287.4
DW                60.600 usec
DE                 6.00 usec
TE                297.4 K
D1           1.00000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                2.70 dB
SFO1        400.2324716 MHz

F2 - Processing parameters
SI                 32768
SF          400.2300015 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```




```
Current Data Parameters
NAME       15082013-Cui
EXPNO                12
PROCNO                1

F2 - Acquisition Parameters
Date_          20130815
Time              15.13
INSTRUM       avance400
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1290
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3632196 sec
RG                 8192
DW               20.800 usec
DE                6.00 usec
TE                298.9 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1               -2.00 dB
SFO1        100.6479773 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2                2.70 dB
PL12              17.10 dB
PL13              17.10 dB
SFO2        400.2316009 MHz

F2 - Processing parameters
SI                32768
SF          100.6379140 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```