Electronic Supplementary Materials

Practical Biocatalytic Desymmetrization of Meso *N*-Heterocyclic Dicarboxamides and Their Application in the Construction of Aza-sugar Containing Nucleoside Analogs

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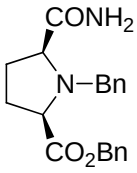
1. General Information

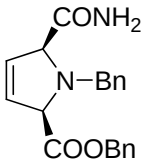
^{1}H and ^{13}C NMR spectra were recorded on 300MHz and 400MHz spectrometers. Chemical shifts are reported in ppm versus tetramethylsilane or the residual solvent resonance used as an internal standard. Melting points are uncorrected. Enantiomeric excess (ee) values of all compounds were obtained from HPLC analyses using chiral stationary phases.

2. General Procedure for Biocatalytic Desymmetrization

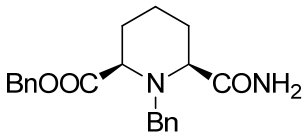
To an Erlenmeyer flask (150 mL) with a screw cap were added aqueous potassium phosphate buffer (0.1 M, pH 7.0, 250 mL) and *Rhodococcus erythropolis* AJ270 cells (2 g wet weight). The resting cells were activated at 30 ^{o}C for 0.5 h with orbital shaking. Dicarboxamide substrates **1** (1 mmol) was added in one portion to the flask, and the resulting mixture was incubated at 30 ^{o}C using an orbital shaker (200 rpm). The reaction, monitored TLC, was quenched after a period of time (see Table 1 and Scheme 1) by removing the biomass by filtration through a Celite pad, and the filtrate was freeze-dried. The residue was mixed with DMF (2 mL), BnBr (1 mL) and K_2CO_3 (1.38g, 10 mmol). After stirring for 24 h, water (10 mL) was added and the resulting mixture was extracted with ethyl acetate (3×100 mL), washed with brine (3×2 mL) and dried with anhydrous Na_2SO_4. After removal of solvent, the residue was chromatographed using a silica gel column with ethyl acetate as eluent to give pure products **2**.



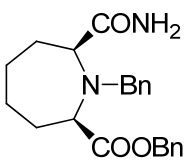
Benzyl *N*-benzyl-5-carbamoylpyrrolidine-2-carboxylate (2a): white solid; mp 58 ^{o}C; $[\alpha]^{25}_{D}$ +19.2^{o} (*c* 1, CH_2Cl_2); ee >99.5% (HPLC analysis using a Diacel-ADH column); IR (KBr) ν 3422, 3369, 1740, 1663 cm^{-1}; ^{1}H NMR (300 MHz/$CDCl_3$) δ 7.89 (br, s, 1H), 7.37-7.22 (m, 10H), 5.90 (br, s, 1H), 4.98 (s, 2H), 3.88 (d, *J* = 13.2 Hz, 1H), 3.79 (d, *J* = 13.2 Hz, 1H), 3.63 (t, *J* = 7.4 Hz, 1H), 3.54-3.50 (m, 1H), 2.19-1.88 (m, 4H); ^{13}C NMR (75MHz/$CDCl_3$) δ 177.1, 174.1, 136.4, 134.7, 128.5, 127.8, 127.6, 127.56, 127.3, 126.8, 67.1, 65.9, 65.5, 58.2, 29.8, 29.5; MS (ESI) *m/z* 339.1 (M+1, 86), 361.2 (M+23, 100%). Anal. Calcd. for $C_{20}H_{22}N_2O_3$: C, 70.99; H, 6.55; N, 8.28. Found: C, 70.65; H, 6.71; N, 8.53.



Benzyl *N*-benzyl-5-carbamoyl-2,5-dihydro-1H-pyrrole-2-carboxylate (2b): mp 127-128 ^{o}C; $[\alpha]^{25}_{D}$ -36.4^{o} (*c* 1, CH_2Cl_2); ee >99.5% (HPLC analysis using a Diacel-ADH column); IR (KBr) ν 3361, 3344, 3223, 2527, 1707, 1682, 1627, 1177 cm^{-1}; ^{1}H NMR (300 MHz/Acetone-d_6) δ 7.88 (br, s, 1H), 7.41-7.26 (m, 10H), 6.43 (br, s, 1H), 5.95-5.91 (m, 1H), 5.84-5.82 (m, 1H), 5.07 (d, *J* = 12.3 Hz, 1H), 5.04 (d, *J* = 12.3 Hz, 1H), 4.63-4.61 (m, 1H), 4.27-4.25 (m, 1H), 4.05 (d, *J* = 13.5 Hz, 1H), 3.97 (d, *J* = 13.5 Hz, 1H); ^{13}C NMR (75 MHz/Acetone-d_6) δ 173.9, 172.7, 137.9, 136.0, 130.9, 129.2, 128.5, 128.3, 128.1, 128.0, 127.3, 126.6, 76.2, 73.6, 66.4, 58.4; MS (ESI) *m/z* 338.3 (M+D, 90), 360.3 (M(D)+23, 100%). Anal. Calcd. for $C_{20}H_{20}N_2O_3$: C, 71.41; H, 5.99; N, 8.33. Found: C, 71.15; H, 5.98; N, 8.17.



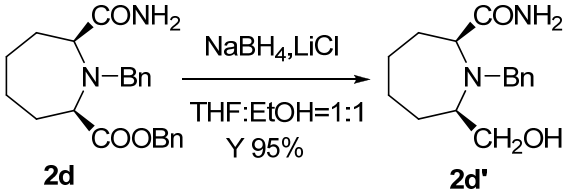
Benzyl *N*-benzyl-6-carbamoylpiperidine-2-carboxylate (2c): mp 105 ^{o}C; $[\alpha]^{25}_{D}$ -25.6^{o} (*c* 1, CH_2Cl_2); ee >99.5% (HPLC analysis using a Diacel-ADH column); IR (KBr) ν 3420, 1744, 1632 cm^{-1}; ^{1}H NMR (300 MHz/$CDCl_3$) δ 7.36-7.17 (m, 11 H), 5.71 (br, s, 0.5 H), 5.64 (br, s, 0.5H), 5.07 (s, 2 H), 3.77 (s, 2 H), 3.23 (dd, 1H, *J* = 10.3, 3.7 Hz), 3.09 (dd, 1H, *J* = 9.4, 3.7 Hz), 2.00-1.84 (m, 2H), 1.73-1.63 (m, 3H), 1.26-1.17 (m, 2H); ^{13}C NMR (75 MHz/$CDCl_3$) δ 177.3, 174.0, 135.6, 134.9, 130.3, 128.6, 128.5, 128.4, 128.2, 127.6, 66.7,. 63.3, 61.6, 58.3, 28.2, 28.1, 20.7; MS (ESI) *m/z* 353.2 (M+1,100%), 375.2 (M+23, 17%). Anal. Calcd. for $C_{21}H_{24}N_2O_3$: C, 71.57; H, 6.86; N, 7.95. Found: C, 71.58; H, 6.84; N, 7.96.



Benzyl 1-benzyl-7-carbamoylazepane-2-carboxylate (2d): oil; $[\alpha]^{25}_{D}$ -25.6 ^{o} (*c* 1,

CH_2Cl_2); IR (KBr) ν 3410, 1737, 1670 cm^{-1}; ^1H NMR (300 MHz/$CDCl_3$) δ 8.42 (br, s, 1 H), 7.38-7.23 (m, 10 H), 5.88 (br, s, 1 H), 5.15 (d, 1 H, *J* = 12.1 Hz), 5.07 (d, 1 H, *J* = 12.1 Hz), 3.75 (d, 1 H, *J* = 8.7 Hz), 3.72 (d, 1 H, *J* = 8.7 Hz), 3.62 (dd, 1 H, *J* = 8.7, 1.8 Hz), 3.42 (d, 1 H, *J* = 8.1 Hz), 2.02-1.46 (m, 8 H); ^{13}C NMR (75 MHz/$CDCl_3$) δ 178.4, 176.3, 138.0, 135.5, 129.0, 128.7, 128.54, 128.50, 128.3, 127.6, 67.0, 66.3, 60.6, 29.1, 28.2, 28.1, 26.8; MS (ESI) *m/z* 367.2 (M+1, 20%), 389.3 (M+23,100). Anal. Calcd. for $C_{22}H_{26}N_2O_3$: C, 72.11; H, 7.15; N, 7.64. Found: C, 72.07; H, 7.10; N, 7.79.

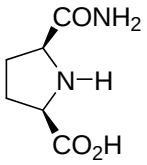
To determine the ee value of the product, **2d** was converted into **2d'.**



2d **2d'**

Preparation of 2d'. To a solution of **2d** (70 mg, 0.2 mmol) in a mixture of EtOH (5 mL) and THF (5 mL) was added consecutively $NaBH_4$ (15.2 mg, 0.4 mmol) and LiCl (15.2 mg, 0.4 mmol). After the resulting mixture was stirred for 3 h at ambient temperature, water (20 mL) was added and the resulting mixture was extracted with ethyl acetate (3×15 mL). Combined organic phase was washed with brine (3×5 mL) and dried with anhydrous Na_2SO_4. After removal of solvent, the residue was chromatographed using a silica gel column with ethyl acetate as an eluent to give pure products **2d'** (50 mg, 95%): mp 146 ^oC; $[\alpha]^{25}_D$ +22.9^o (*c* 0.35, CH_2Cl_2); ee 63% (HPLC analysis using a Diacel-OJH column); IR (KBr) ν 3364, 3274, 2943, 2919, 1664 cm^{-1}; ^1H NMR (300 MHz/ DMSO-d_6) δ 7.86 (br, s, 0.5 H), 7.85 (br, s, 0.5 H), 7.38-7.21 (m, 5 H), 7.02 (br, s, 1 H), 7.02 (br, s, 1 H), 4.98 (t, 1 H, *J* = 4.8 Hz), 3.81 (d, 1 H, *J* = 14.4 Hz), 3.67 (d, 1 H, *J* = 14.4 Hz), 3.53-3.47 (m, 2H), 3.17 (dd, 1 H, *J* = 15.3, 2.4 Hz), 2.67 (t, 1 H, *J* = 4.2 Hz), 1.98-1.91 (m, 1 H), 1.72-1.46 (m, 6 H), 1.34-1.17 (m, 1 H); ^{13}C NMR (75 MHz/ DMSO-d_6) δ 176.4, 140.5, 128.4, 128.1, 126.8, 66.6, 65.0, 63.2, 58.0, 29.2, 28.0, 26.3, 25.2; MS (ESI) *m/z* 263.4 (M+1, 75%), 285.3(M+23,100). Anal. Calcd. for $C_{15}H_{22}N_2O_2$: C, 68.67; H, 8.45; N, 10.68. Found: C, 68.60; H, 8.38; N, 10.72.

3. Procedure for large scale biocatalytic desymmetric hydrolysis of 1a. To an Erlenmeyer flask (500 mL) with a screw cap *Rhodococcus erythropolis* AJ270 cells (2 g wet weight) were suspended in aqueous potassium phosphate buffer (0.1 M, pH 7.0, 250 mL), and activated at 30 ^{o}C for 0.5 hour with orbital shaking. Dicarboxamide **1a** (20 g) was added in one portion to the flask, and the resulting mixture was incubated at 30 ^{o}C using an orbital shaker (200 rpm). The reaction, monitored by HPLC, was quenched after 12 h by removing the biomass by filtration through a Celite pad. The filtrate was concentrated to 100 mL using a rotary evaporator under reduced pressure, and product **3** (8.0 g) precipitated from solution. The mother liquid was subjected to an ion-exchange column and eluted with aqueous ammonia solution (1%) to give another portion of product **3** (11.0 g).

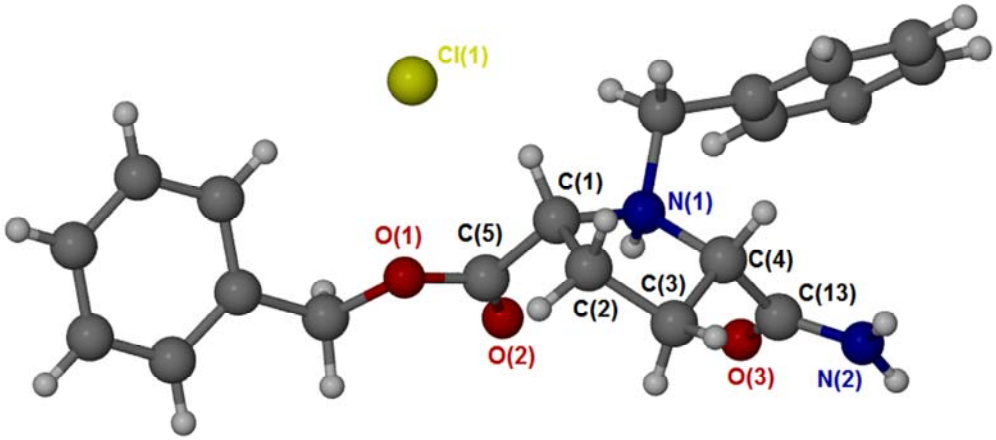


Product **3** (19.0 g, 94%): mp 234-233 ^{o}C; $[\alpha]^{25}_{D}$ -9.6°(*c* 1, H_2O); IR(KBr) ν 3308, 3153, 2361, 1696, 1642, 1576 cm^{-1}; ^{1}H NMR (D_2O/300MHz) 4.34 (t, *J* = 7.2 Hz, 1 H), 4.11 (t, *J* = 6.3 Hz, 1 H), 2.39-2.25 (m , 2 H), 2.05-1.91 (m , 2 H); ^{13}C NMR (75MHz /D_2O) 173.8, 171.4, 61.8, 60.31, 29.8, 29.2; MS (ESI) m/z 159 (M+1, 7), 181 (M+23, 100%). Anal. Calcd. for $C_6H_{10}N_2O_3$: C, 45.57; H, 6.37; N, 17.71. Found: C, 45.54; H, 6.53; N, 17.78.

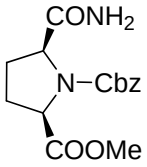
To determine the enantiomeric excess (ee) value and the absolute configuration of product **3**, transformation of **3** into **2a** was conducted. Thus, a mixture of **3** (158 mg), K_2CO_3 (1.38 g), benzyl bromide (1 mL) in dry DMF (2 mL) was stirred at ambient temperature for 24 h. Water (10 mL) was then added, and the mixture was extracted with ethyl acetate (3×10 mL). The combined organic layer was washed with brine (3×10 mL), and dried with anhydrous Na_2SO_4. After removal of organic solvent, the residue was chromatographed on a silica gel column eluted with ethyl acetate to give **2a** (320 mg, 95%). Slow vapor diffusion of diethyl ether into a mixture of **2a** (15.7

mg), concentrated hydrochloric acid (15 μL) and ethanol (0.5 mL) at 5 °C for 2 days led to the formation of a single crystal of **2a**·HCl.

X-ray structure:

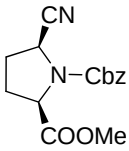


4. Synthesis of Aza sugar containing nucleoside Analogs



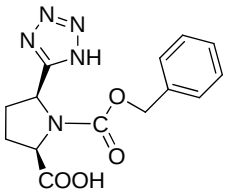
Preparation of 4. To a mixture of **3** (4.0 g, 25 mmol) in ethanol (20 mL) and saturated $NaHCO_3$ aqueous solution (20 mL) was added drop-wise CbzCl (6 mL) at room temperature while stirring. The resulting mixture was kept stirring overnight. The reaction was quenched by adding hydrochloric acid (2 N) until the pH was adjusted to 7. Under reduced pressure, the solvent was completely removed. The residue was mixed with methanol (100 mL) and $SOCl_2$ (4 mL) at ambient temperature. After stirring for another 4 h at ambient temperature, saturated $NaHCO_3$ aqueous solution (200 mL) was added. The mixture was extracted with ethyl acetate (3×100 mL). The combined organic layer was washed with brine (3×20 mL) and dried with anhydrous Na_2SO_4. After removal of organic solvent, the residue was chromatographed on a silica gel column eluted with ethyl acetate to give product **4** (6.9 g, 91%): mp 104 °C; $[\alpha]^{25}_D$ +46.6° (*c* 0.6, $CHCl_3$); IR (KBr) ν 3435, 3401, 1734,

1700, 1683 cm^{-1}; ^1H NMR (300 MHz/DMSO-d_6, 375 K) δ 7.35-7.25 (m, 5H), 6.97 (br, s, 2H), 5.09 (d, J = 12.6 Hz, 1H), 5.05 (d, J = 12.9 Hz, 1H) , 4.42 (t, J = 7.2 Hz, 1H), 4.20-4.16 (m, 1 H), 3.66 (s, 3 H), 2.31-2.17 (m, 2 H), 1.98-1.87 (m, 2 H); ^{13}C NMR (75 MHz/DMSO-d_6) δ 175.0, 174.8, 174.3, 174.0, 154.4, 154.1, 136.9, 136.7, 128.8, 128.4, 128.3, 127.7, 127.6, 67.2, 67.1, 62.5, 62.1, 60.5, 60.1, 53.1, 53.0, 30.6, 29.7,29.6, 28.8; MS (ESI) *m/z* 307 (M+1, 20), 329 (M+23, 100%). Anal. Calcd. for $C_{15}H_{18}N_2O_5$: C, 58.82; H, 5.92; N, 9.15. Found: C, 58.87; H, 5.99; N, 9.10.

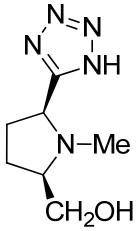


Synthesis of 5.

To a solution of **4** (3.06 g, 10 mmol) in dry DMF (4 mL) was added $SOCl_2$ (1 mL) at 0 ^oC. After stirring for another 1 h at room temperature, the reaction was quenched by the addition of saturated $NaHCO_3$ aqueous solution (10 mL). The mixture was extracted with ethyl acetate (3×20 mL). The combined organic layer was washed with brine (3×4mL) and dried with anhydrous Na_2SO_4. After removal of organic solvent, the residue was chromatographed on a silica gel column eluted with a mixture of ethyl acetate and petroleum ether (1:2) to give compound **5** (2.6 g, 90%): oil; $[\alpha]^{25}_D$ -14 ^{o} (*c* 1, $CHCl_3$) ; IR (KBr) ν 1746, 1715 cm^{-1}; ^1H NMR (300MHz/$CDCl_3$) δ 7.40-7.33 (m, 5H), 5.28-5.09 (m, 2H), 4.72-4.63 (m, 1H), 4.47-4.37 (m, 1H), 3.79 (s, 1.5H), 3.64 (s, 1.5H), 2.44-2.21 (m, 4H); ^1H NMR (300 MHz/DMSO-d_6, 375K) δ 7.39-7.28 (m, 5H), 5.18-5.06 (m, 2H), 4.84-4.80 (m, 1H), 4.42-4.37 (m, 1H), 3.64 (s, 3H), 2.42-2.30 (m, 2H), 2.24-2.12 (m, 1H), 2.10-2.02 (m, 1H); ^{13}C NMR (75 MHz/DMSO-d_6) δ 171.6, 171.4, 153.3, 135.6, 128.6, 128.4, 128.2, 128.1, 128.0, 127.8, 118.0, 117.8, 68.3, 68.0, 67.5, 59.6, 59.3, 52.7, 52.5, 48.1, 47.5, 30.6, 29.8, 29.7, 28.7; MS (ESI) *m/z* 311 (M+23, 100%). Anal. Calcd. for $C_{15}H_{16}N_2O_4$: C, 62.49; H, 5.59; N, 9.72. Found: C, 62.70; H, 5.62; N, 9.57.

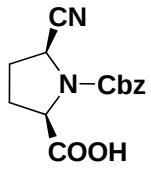


Synthesis of 6. A mixture of **5** (576 mg, 2 mmol), NaN_3 (260 mg,4 mmol), $ZnBr_2$ (225 mg,1 mmol) in water (6 mL) and 2-propanol (3 mL) was refluxed for 16 h. After cooling down to room temperature, hydrochloric acid (1 N, 10 mL) was added. The mixture was extracted with ethyl acetate (3×20 mL). The combined organic layer was washed with brine (3×4mL) and dried with anhydrous Na_2SO_4. After removal of organic solvent, the residue was chromatographed on a silica gel column eluted with a mixture of ethyl acetate and methanol (20:1) to give compound **6** (367 mg, 58%): mp 183-185 ^oC; oil; $[\alpha]^{25}_D$ -22.0° (*c* 0.5, $CHCl_3$); IR (KBr) ν 2960, 1707, 1451, 1422 cm^{-1}; ^1H NMR (300 MHz/DMSO-d_6, 373K) δ 7.31-7.23 (m, 5H), 5.33-5.31 (m, 1H), 5.05 (s, 2H), 4.41 (t, 1H, *J* = 8.0 Hz), 2.46-2.35 (m, 2H), 2.19-2.05 (m, 2H); ^{13}C NMR (75 MHz/ DMSO-d_6) δ 177.53, 177.05, 157.7, 157.3, 152.8, 134.4, 134.1, 127.6, 127.4, 126.9, 67.2, 67.1, 58.97, 58.5, 52.5, 52.1, 31.6, 30.5, 29.9, 28.7, 27.8; MS (ESI) *m/z* 340 (M^++23, 100%). Anal. Calcd. for $C_{14}H_{16}N_5O_4$ [M+H]: 318.1202. Found: 318.1192.



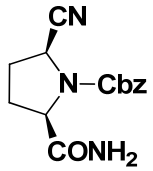
Synthesis of 7. Under protection of argon, a mixture of **6** (317 mg, 1 mmol) and $LiAlH_4$ (380 mg, 10 mmol) in dry THF (10 mL) was refluxed for 24 h. While the mixture was kept at -20℃, NaOH aqueous solution (2 N, 1 mL) was slowly injected through a syringe. The resulting mixture was filtrate through a Celite pad and washed thoroughly with a mixture of CH_2Cl_2 and MeOH (20:1). After removal of solvent, the

residue was mixed with hydrochloric acid (1 N) with pH value of the mixture being adjusted to pH 2. The resulting mixture was subjected to an ion-exchange column (nk 001×7) and then eluted with pure water. After the pH of the fraction was around 7, the column was eluted with aqueous ammonia solution (1%). After removal of solvent, product **7** was obtained. **7** (152 mg, 83%): mp 185 ^{o}C; $[\alpha]^{25}_{D}$ +10.3° (*c* 0.78, H_2O); IR (KBr) ν 3447, 2959, 2922, 1578, 1411, 1075, 1030 cm^{-1}; ^{1}H NMR (300 MHz/D_2O) δ 4.53 (t, *J* = 8.7 Hz, 1H), 3.77-3.64 (m, 2H), 3.54-3.45 (m, 1H), 2.72 (s, 3H), 2.38-2.26 (m, 2H), 2.23-2.14 (m, 1H), 1.94-1.83 (m, 1H); ^{13}C NMR (75MHz/D_2O) δ 157.1, 70.3, 64.2, 59.6, 39.1, 27.7, 24.9; MS (ESI) *m/z* 184.1 (M+1, 15%), 206.1 (M+23, 100%). Anal. Calcd. for $C_7H_{14}N_5O$ [M+H]: 184.1198. Found: 184.1193.

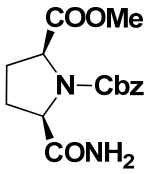


Preparation of 8. A mixture of **5** (100 mg, 0.33 mmol) and $LiOH·H_2O$ (23mg, 0.55 mmol) in THF (3 mL) and water (3 mL) was stirring at ambient temperature for 2 h. The mixture was then treated with hydrochloric acid (1 N) until the pH of the mixture was adjusted to 2, and extracted with ethyl acetate (3×10 mL). The combined organic layer was washed with brine (3×3 mL) and dried with anhydrous Na_2SO_4. After removal of organic solvent, the residue was chromatographed on a silica gel column eluted with a mixture of petroleum ether, ethyl acetate and acetic acid (200:100:0.5). The collected fractions were concentrated to about 10 mL at 30-40 ^{o}C under reduced pressure using a rotary evaporator. The resulting solution was mixed with ethyl acetate (50 mL) and washed with brine (3×10 mL). After drying with anhydrous Na_2SO_4 and removing solvent, pure **8** was obtained. **8** (90 mg, 95%): oil; $[\alpha]^{25}_{D}$ -24.6° (*c* 4.6, $CHCl_3$); IR (KBr) ν 3065, 3038, 2960, 1715, 1414, 1358 cm^{-1}; ^{1}H NMR (300MHz/DMSO-d_6, 375K) δ 7.36-7.28 (m, 5H), 5.14 (s, 2H), 4.82-4.78 (m, 1H), 4.34-4.30 (m, 1H), 2.42-2.29 (m, 2H), 2.24-2.11 (m, 1H), 2.09-2.00 (m, 1H); ^{13}C

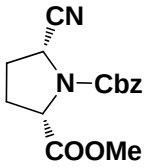
NMR (75 MHz/DMSO-d_6) δ 173.3, 173.0, 153.7, 153.4, 136.7, 128.8, 128.4, 128.3, 127.9, 127.7, 119.7, 119.4, 67.4, 67.3, 60.1, 59.6, 48.4, 47.8, 30.7, 29.9, 29.7, 28.9; MS (ESI) *m/z* 273.1 (M-1, 100%). Anal. Calcd. for $C_{14}H_{15}N_2O_4$ [M+H]: 275.1032. Found: 275.1022.



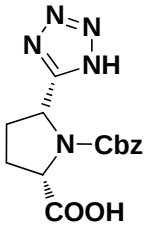
9: To a solution of **8** (66.1mg, 0.24 mmol) in CH_2Cl_2 (4 mL) was added consecutively 2-chloro-4,6-dimethoxy-1,3,5-triazine (CDMT, 50.5 mg, 0.29 mmol) and *N*-methylmorpholine (NMM, 83 μL,0.72 mmol). After stirring at room temperature for 2.5 h, an ammonia gas balloon (250 mL) was connected, and the reaction mixture was stirred for 1 h. After removal of the ammonia gas balloon, the mixture was kept stirring for another 1 h. The reaction was quenched by adding hydrochloric acid (1 N, 20 mL). After extraction with ethyl acetate (3×10 mL), the combined organic layer was dried with anhydrous Na_2SO_4. After removal of organic solvent, the residue was chromatographed on a silica gel column eluted with a mixture of petroleum ether and ethyl acetate (1:2) to afford **9** (44 mg, 67%): mp 44 ^oC; $[\alpha]^{25}_D$ -7.0° (*c* 0.58, $CHCl_3$); IR (KBr) ν 3428, 3352, 3200, 1708, 1412, 1356, 1119 cm^{-1}; ^1H NMR (300 MHz/DMSO-d_6, 375K) δ 7.38-7.29 (m, 5H), 6.87 (s, br, 1H), 5.13 (d, *J* = 12.9 Hz, 1H), 5.11 (d, *J* = 12.9 Hz, 1H), 4.76 (dd, *J* = 7.4, 4.8 Hz, 1H), 4.29 (dd, *J* = 7.4, 5.1 Hz, 1H), 2.32-2.14 (m, 3H), 2.02-1.96 (s, br, 1H); ^{13}C NMR (75MHz/DMSO-d_6) δ 173.0, 172.8, 153.9 153.5, 136.8, 128.8, 128.4, 128.2, 127.9, 127.6, 119.8, 119.5, 67.2, 67.1, 60.7, 60.2, 48.6, 48.0, 30.6, 29.7, 29.5; MS (ESI) *m/z* 296.2 (M+23, 100%). Anal. Calcd. for $C_{14}H_{16}N_3O_3$ [M+H]: 274.1192. Found: 274.1186. Anal. Calcd. for $C_{14}H_{15}N_3NaO_3$ [M+Na]: 296.1011. Found: 296.1004.



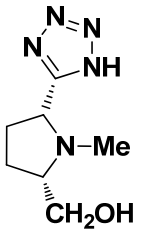
Synthesis of ent-4. To a solution of **9** (155mg, 0.57 mmol) in MeOH (4 mL) at -15 ^{o}C was bubbled with dry HCl (g) for 1 h. After the resulting solution was kept at -20 ^{o}C for 12 h, hydrochloric acid (6 N, 10 mL) was added. After extraction with ethyl acetate (3×100mL) and washing with brine (3×10 mL), the combined organic phase was dried with anhydrous Na_2SO_4. The solvent was removed and the residue was chromatographed on a silica gel column eluted with ethyl acetate to give ent-**4** (133 mg, 76%): $[\alpha]^{25}_{D}$ -47.3° (*c* 1.7, $CHCl_3$). Identical IR and ^{1}H NMR spectra as that of **4** were obtained.



Ent-**5** was synthesized from ent-**4** following the same procedure for the conversion of **4** to **5**. Ent-**5:** $[\alpha]^{25}_{D}$ +14.7°(*c* 3.0, $CHCl_3$). Identical IR and ^{1}H NMR spectra as that of **5** were obtained.



Ent-**6** was synthesized from ent-**5** following the same procedure for the transformation of **5** into **6**. Ent-**6:** $[\alpha]^{25}_{D}$ +24.0° (*c* 1.0, MeOH). Identical IR and ^{1}H NMR spectra as that of **6** were obtained.



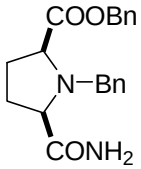
Ent-**7** was synthesized from ent-**6** following the same procedure for the transformation from **6** into **7**. Ent-**7:** mp 187 ^{o}C; $[\alpha]^{25}_{D}$ -11.0° (*c* 2.0, H_2O). Following identical IR, ^{1}H and ^{13}C NMR spectra as that of **7** were obtained. IR (KBr) ν 3447, 2958, 2921, 1577, 1409, 1077, 1025 cm^{-1}; ^{1}H NMR (300 MHz/D_2O) δ 4.53 (t, *J* = 8.7 Hz, 1H), 3.77-3.64 (m, 2H), 3.54-3.45 (m, 1H), 2.72 (s, 3H), 2.38-2.26 (m, 2H), 2.23-2.14 (m, 1H), 1.94-1.83 (m, 1H); ^{13}C NMR (75 MHz/D_2O) δ 157.1, 70.3, 64.2, 59.6, 39.1, 27.7, 24.9; MS (ESI) *m/z* 184.1 (M+1, 100%). Anal. Calcd. for $C_7H_{14}N_5O$ [M+H]: 184.1198. Found: 184.1190.

4. HPLC analysis of products.

A Shimadzu LC-10AVP HPLC system was used to analyze enantiomeric excess values of all products.

Table S1: HPLC analysis of amides 2a-d

Compound	Hexane / 2-propanol	Temperature (^{o}C)	Rate (mL/min)	t_1 (min)	t_2 (min)	Column
2a	9/1	15	0.5	41.9	49.1	Chiralcel ADH
2b	9/1	15	0.5	51.4	57.2	Chiralcel ADH
2c	9/1	15	0.5	26.4	27.9	Chiralcel ADH
2d	9/1	20	0.5	25.2	28.0	Chiralcel OJH



Racemic

cShimadzu CLASS-VP V6.13 SP2 ***Area % Report***

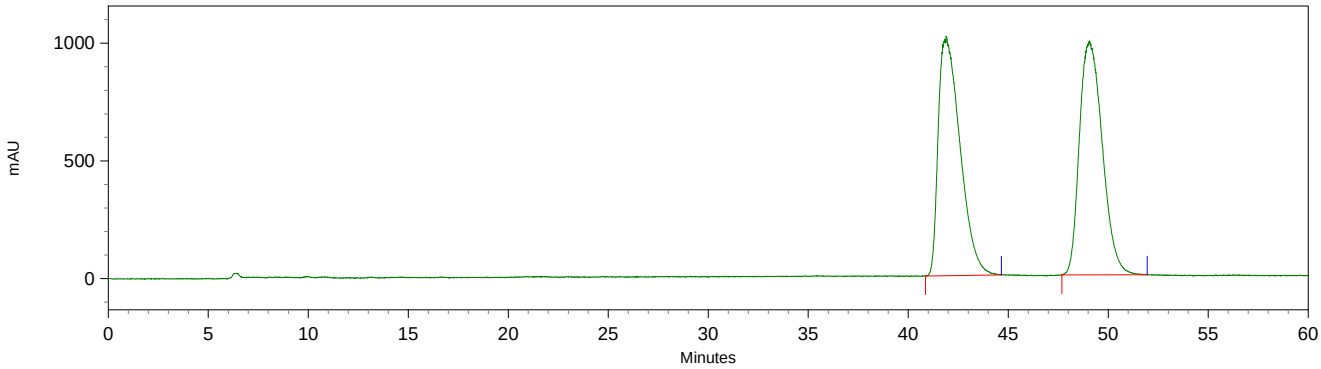
Method Name: D:\HPLCÊý¾Ý\yangluo\2006\method\¸´¼þ Gaoming212nm.met

Data Name: E:\chenpeng\ËÄÇâßÁ¿©\µªÇâ\2011-9-10 211b\rac-211b001

User: System

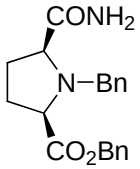
Acquired: 2011-9-10 18:16:06

Printed: 2011-9-19 18:38:04



Detector A-213
nm

Pk #	Retention Time	**Area**	**Area %**
1	41.899	76472298	49.2
2	49.067	78818336	50.8
Totals		155290634	100.0



cShimadzu CLASS-VP V6.13 SP2 ***Area % Report***

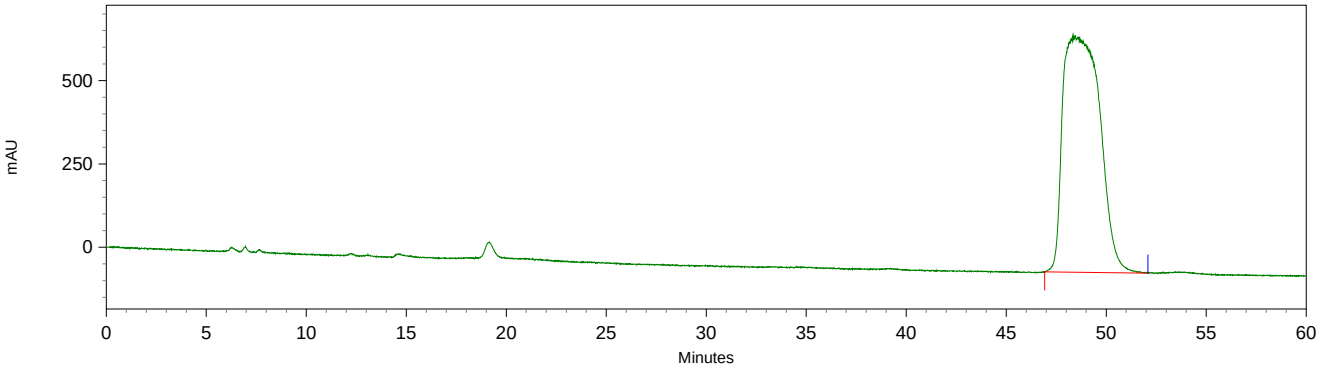
Method Name: **D:\HPLCÊý¾Ý\yangluo\2006\method\¸´¼þ Gaoming212nm.met**

Data Name: **E:\chenpeng\ËÄÇâßÁ¿©\µªÇâ\2011-9-10 211b\211b-16h001**

User: **System**

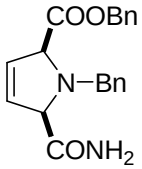
Acquired: **2011-9-11 13:16:57**

Printed: **2011-9-19 18:38:57**



Detector A-213 nm

Pk #	Retention Time	**Area**	**Area %**
1	48.459	91678707	100.0
Totals		91678707	100.0



Racemic

cShimadzu CLASS-VP V6.13 SP2 ***Area % Report***

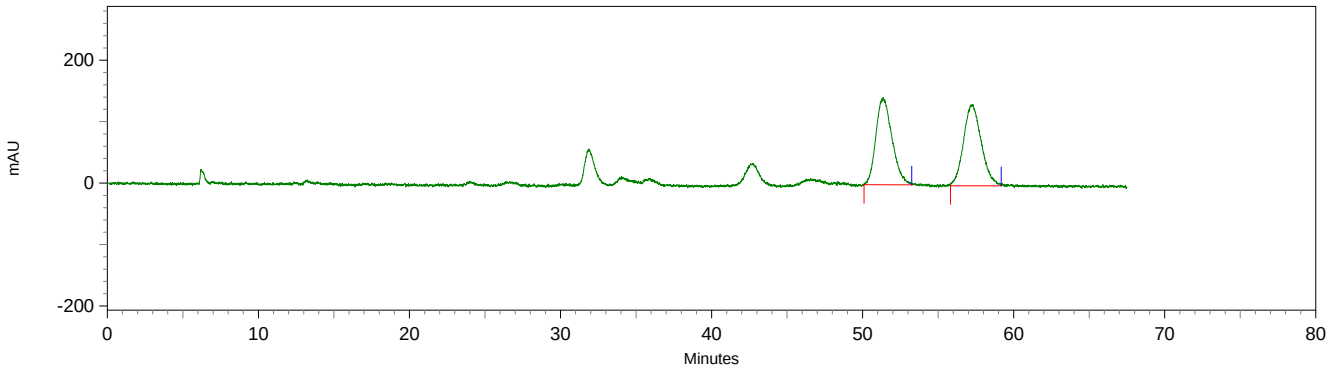
Method Name: **D:\HPLCÊý¾Ý\yangluo\2006\method\¸´¼þ Gaoming212nm.met**

Data Name: **E:\chenpeng\ËÄÇâßÁ¿©\µªÇâ\rac-d5-15c-0001.5-adh**

User: **System**

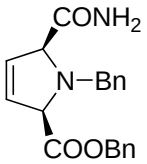
Acquired: **2009-12-19 19:12:10**

Printed: **2010-4-1 20:53:21**



Detector
A-207 nm

Pk #	Retention Time	**Area**	**Area %**
1	51.360	10488937	49.3
2	57.205	10770562	50.7
Totals		21259499	100.0



cShimadzu CLASS-VP V6.13 SP2 ***Area % Report***

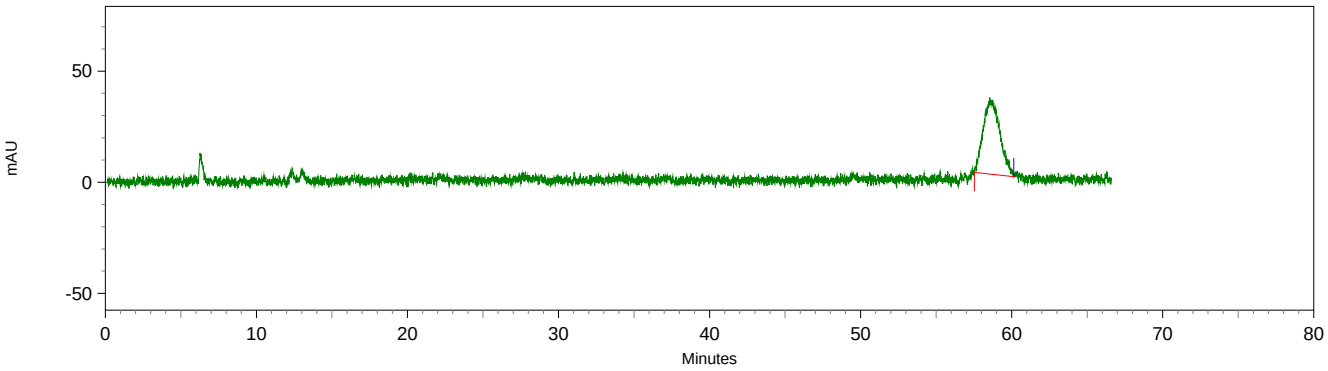
Method Name: **D:\HPLCÊý¾Ý\yangluo\2006\method\¸´¼þ Gaoming212nm.met**

Data Name: **E:\chenpeng\ËÄÇâßÁ¿©\µªÇâ\bio-d5-15c-0001.5-adh**

User: **System**

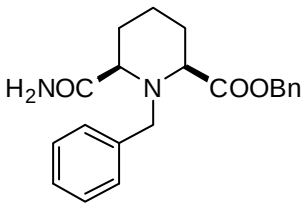
Acquired: **2009-12-31 12:38:04**

Printed: **2010-4-1 20:39:37**



Detector
A-207 nm

Pk #	Name	Retention Time	**Area**	**Area %**
1		58.549	2586761	100.0
Totals			2586761	100.0



Racemic

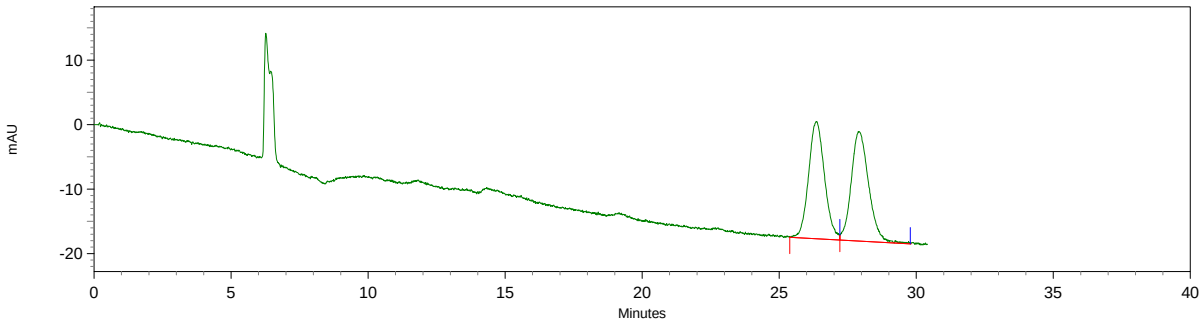
Shimadzu CLASS-VP V6.13 SP2 ***Area % Report***

Method Name: D:\HPLCÊý¾Ý\yangluo\2006\method\¸´¼þ Gaoming212nm.met

Data Name: E:\chenpeng\hexdiamide\rac-h-3-15c-0.5-adh'

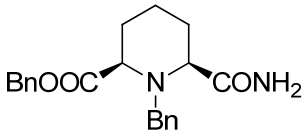
User: System

Acquired: 2008-7-9 20:33:29



1: 254 nm, 8 nm

Pk #	Retention Time	**Area**	**Area %**
1	26.368	735902	49.5
2	27.915	750097	50.5
Totals		1485999	100.0



cShimadzu CLASS-VP V6.13 SP2 ***Area % Report***

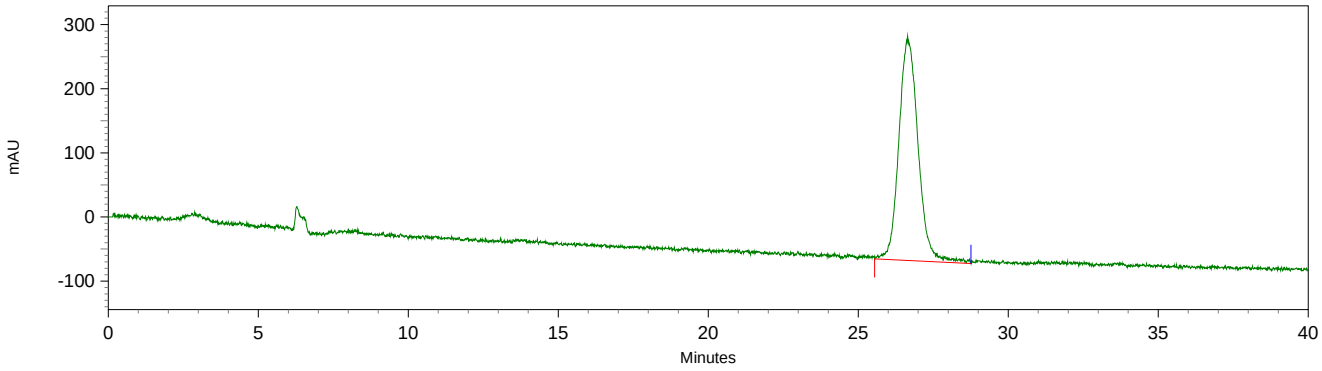
Method Name: D:\HPLCÊý¾Ý\yangluo\2006\method\¸´¼þ Gaoming212nm.met

Data Name: **E:\chenpeng\hexdiamide\h3-15c-0002.5-adh-a**

User: **System**

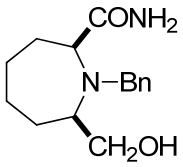
Acquired: **2010-6-25 17:25:06**

Printed: **2011-9-13 16:29:39**



Detector A-216 nm

Pk #	Retention Time	Area	Area %
1	26.645	15439731	100.0
Totals		15439731	100.0



Racemic

cShimadzu CLASS-VP V6.13 SP2 ***Area % Report***

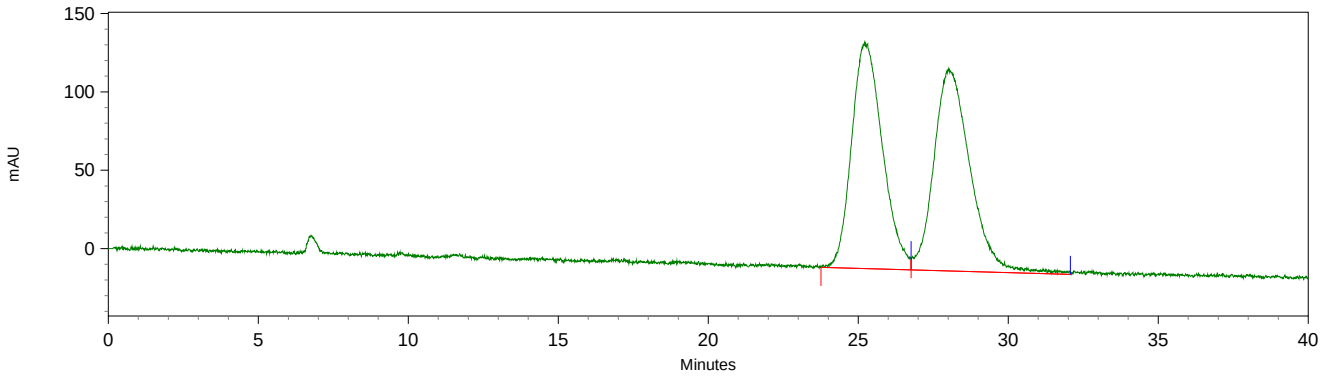
Method Name: D:\HPLCÊý¾Ý\yangluo\2006\method\¸´¼þ Gaoming212nm.met

Data Name: **E:\chenpeng\q\RAC-Q5-0001.5-20C-OJH'**

User: **System**

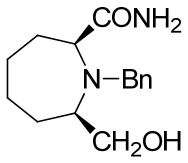
Acquired: **2009-7-18 16:18:44**

Printed: **2011-9-13 16:55:06**



Detector A-215 nm

Pk #	Retention Time	**Area**	**Area %**
1	25.216	10316827	48.8
2	28.021	10827528	51.2
Totals		21144355	100.0



cShimadzu CLASS-VP V6.13 SP2 ***Area % Report***

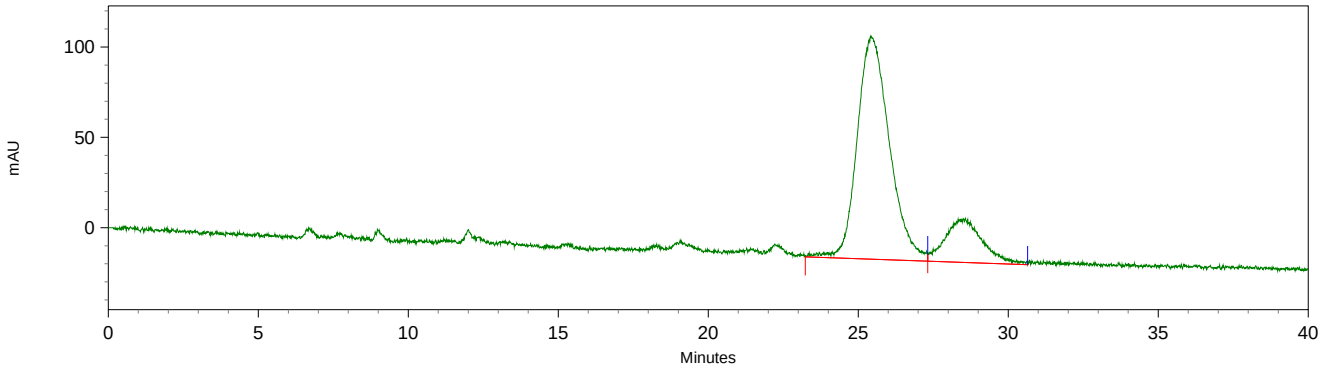
Method Name: D:\HPLCÊý¾Ý\yangluo\2006\method\¸´¼þ Gaoming212nm.met

Data Name: **E:\chenpeng\q\bio-q5-0002.5-20c-ojh**

User: **System**

Acquired: **2009-7-18 9:50:01**

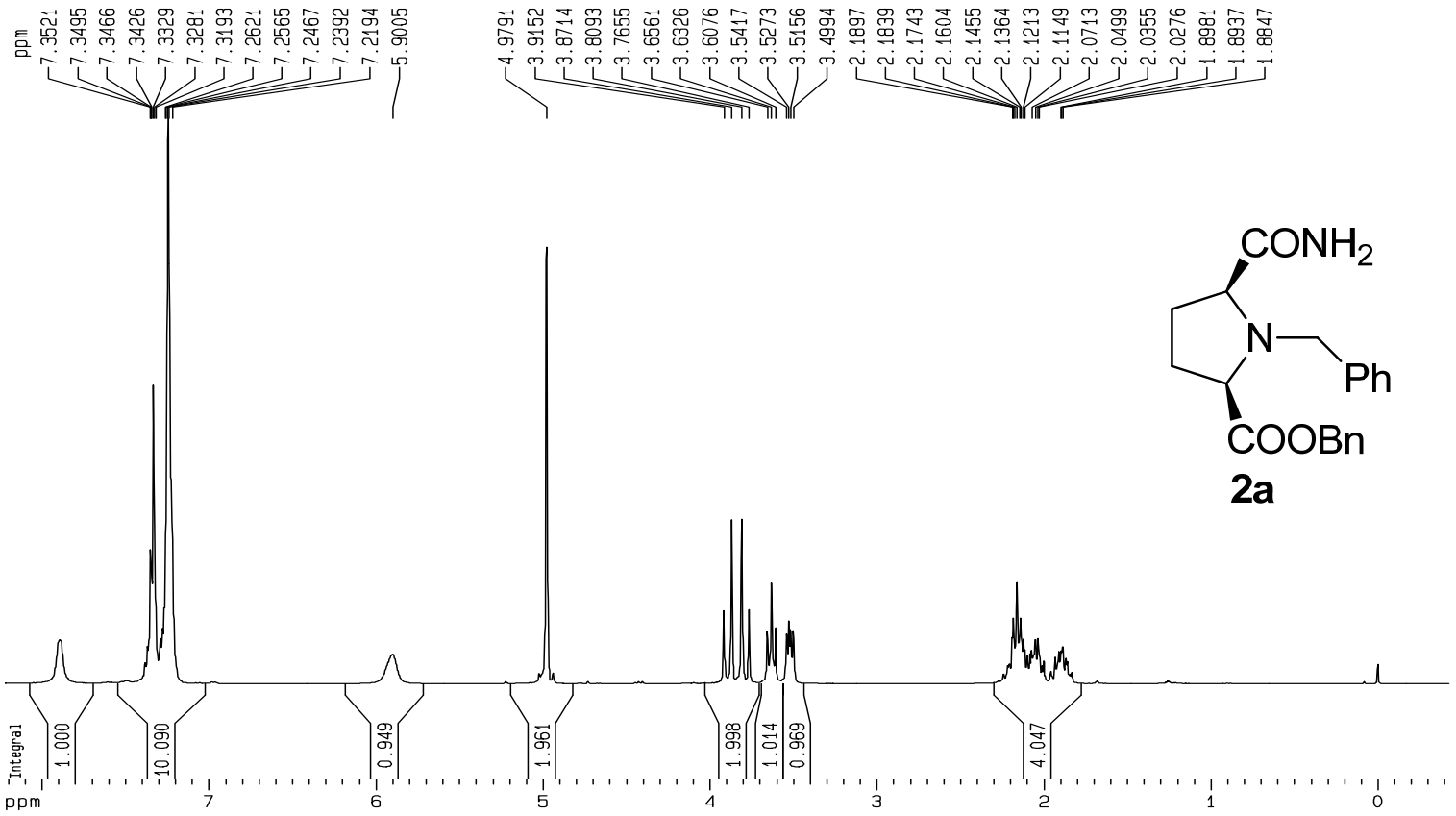
Printed: **2011-9-13 16:58:38**



Detector A-215 nm

Pk #	Retention Time	**Area**	**Area %**
1	25.419	9222160	81.7
2	28.512	2072085	18.3
Totals		11294245	100.0

5. ^{1}H and ^{13}C NMR spectra of all products



2a

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Current Data Parameters
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EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
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Time              20.33
INSTRUM           av300
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            8992.806 Hz
FIDRES        0.137219 Hz
AQ            3.6438515 sec
RG                   64
DW               55.600 usec
DE                6.00 usec
TE               295.2 K
D1            5.00000000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                10.10 usec
PL1               -1.00 dB
SFO1         300.1318534 MHz

F2 - Processing parameters
SI                32768
SF          300.1300064 MHz
WDW                  EM
SSB                   0
LB                0.35 Hz
GB                    0
PC                1.00

1D NMR plot parameters
CX                20.00 cm
CY                10.00 cm
F1P               8.223 ppm
F1              2467.99 Hz
F2P              -0.427 ppm
F2              -128.07 Hz
PPMCM           0.43249 ppm/cm
HZCM          129.80270 Hz/cm
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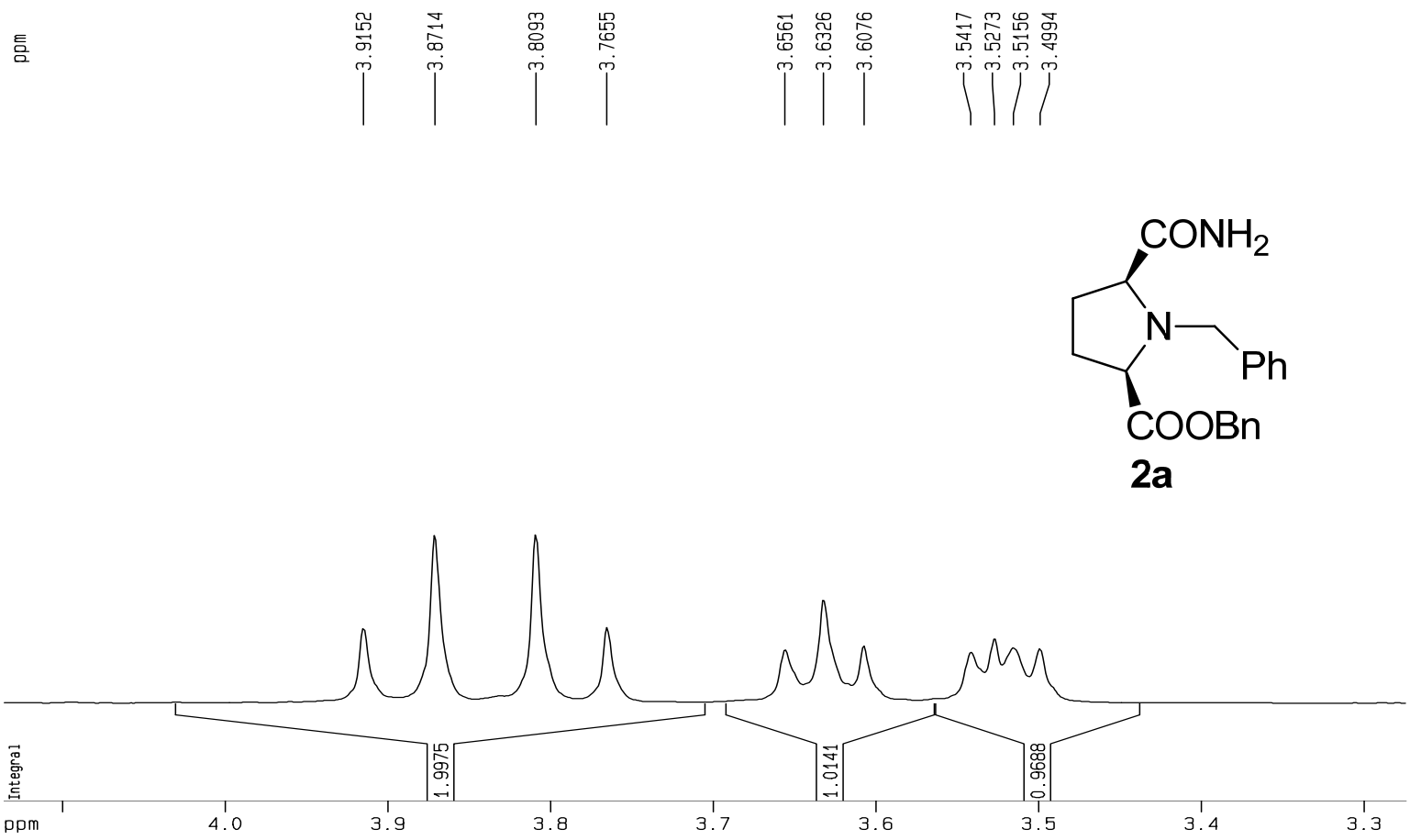


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Current Data Parameters
NAME      cp-211b-b4p9b
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_          20080123
Time              20.33
INSTRUM           av300
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            8992.806 Hz
FIDRES         0.137219 Hz
AQ             3.6438515 sec
RG                   64
DW                55.600 usec
DE                 6.00 usec
TE                295.2 K
D1             5.00000000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                10.10 usec
PL1               -1.00 dB
SFO1         300.1318534 MHz

F2 - Processing parameters
SI                32768
SF          300.1300064 MHz
WDW                  EM
SSB                   0
LB                 0.35 Hz
GB                    0
PC                 1.00

1D NMR plot parameters
CX                20.00 cm
CY                10.00 cm
F1P                4.136 ppm
F1               1241.40 Hz
F2P                3.274 ppm
F2                982.60 Hz
PPMCM          0.04311 ppm/cm
HZCM          12.93984 Hz/cm
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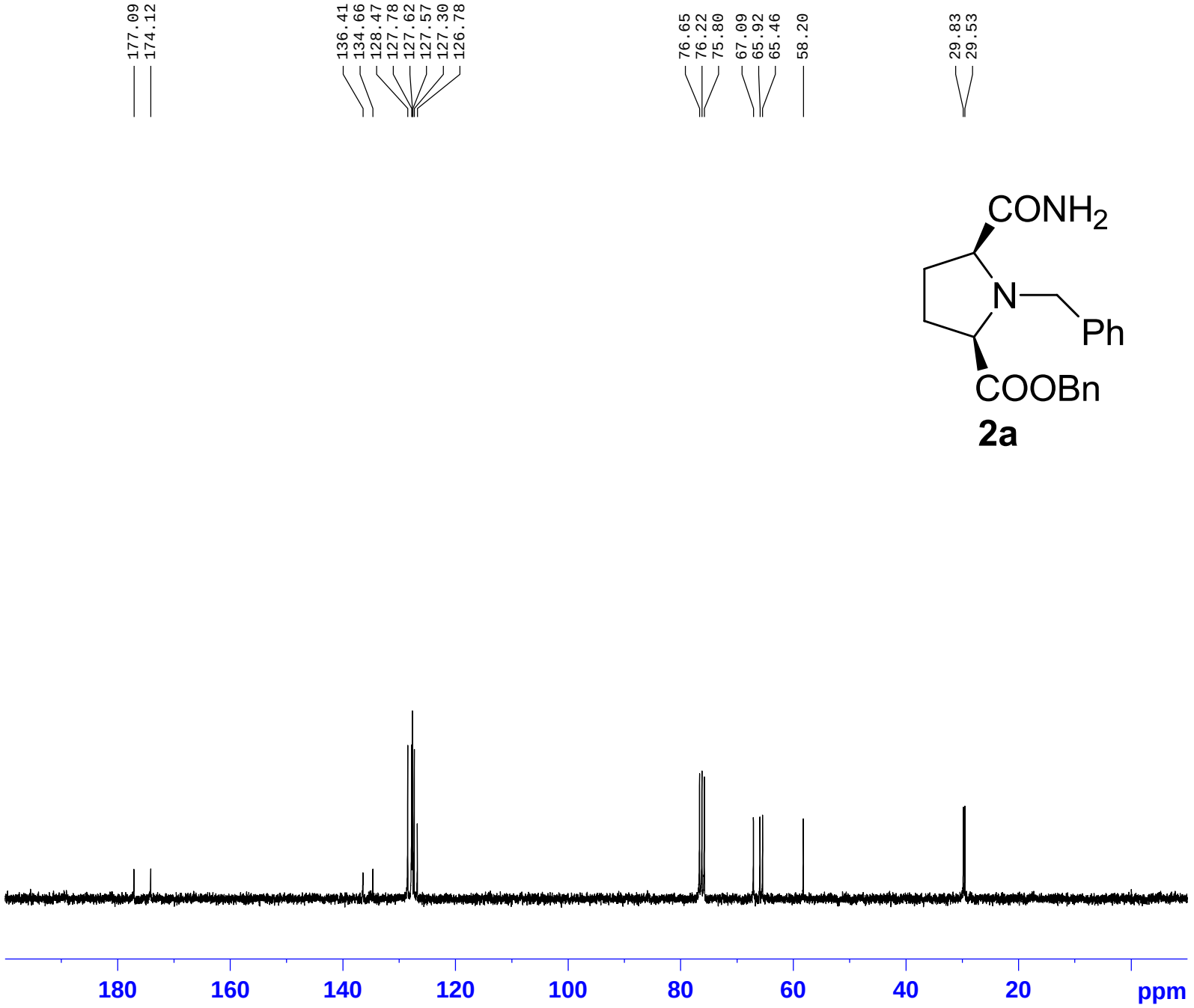


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Current Data Parameters
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EXPNO                   10
PROCNO                   1

F2 - Acquisition Parameters
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Time                  9.41
INSTRUM              spect
PROBHD   5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                      92
DS                       4
SWH              17985.611 Hz
FIDRES            0.274439 Hz
AQ                1.8219508 sec
RG                   1625.5
DW                  27.800 usec
DE                   6.00 usec
TE                  301.2 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                  12.50 usec
PL1                  2.00 dB
SFO1           75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                 -1.00 dB
PL12                20.16 dB
PL13                16.98 dB
SFO2          300.1312005 MHz

F2 - Processing parameters
SI                    32768
SF             75.4678131 MHz
WDW                      EM
SSB                       0
LB                   1.00 Hz
GB                        0
PC                   1.40
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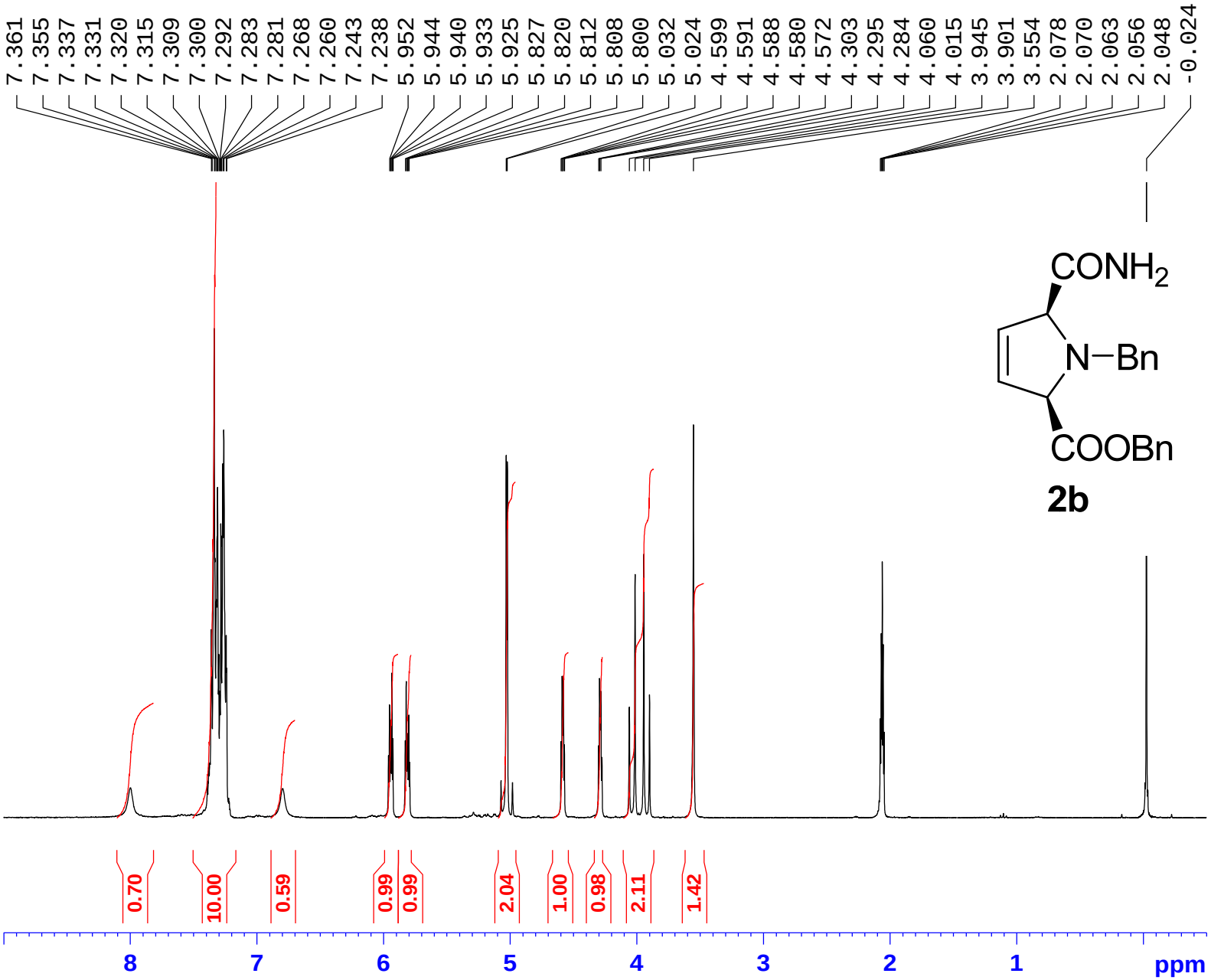


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Current Data Parameters
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EXPNO                     46
PROCNO                     1

F2 - Acquisition Parameters
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Time                   18.53
INSTRUM                spect
PROBHD    5 mm DUL 13C-1
PULPROG                zg30
TD                    32768
SOLVENT           Acetone/D2O
NS                        12
DS                         0
SWH                8992.806 Hz
FIDRES             0.274439 Hz
AQ                 1.8219508 sec
RG                       256
DW                    55.600 usec
DE                     8.00 usec
TE                    299.2 K
D1                 2.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     10.80 usec
PL1                     3.00 dB
SFO1            300.1318008 MHz

F2 - Processing parameters
SI                        32768
SF              300.1300000 MHz
WDW                       EM
SSB                        0
LB                     0.30 Hz
GB                         0
PC                     1.00
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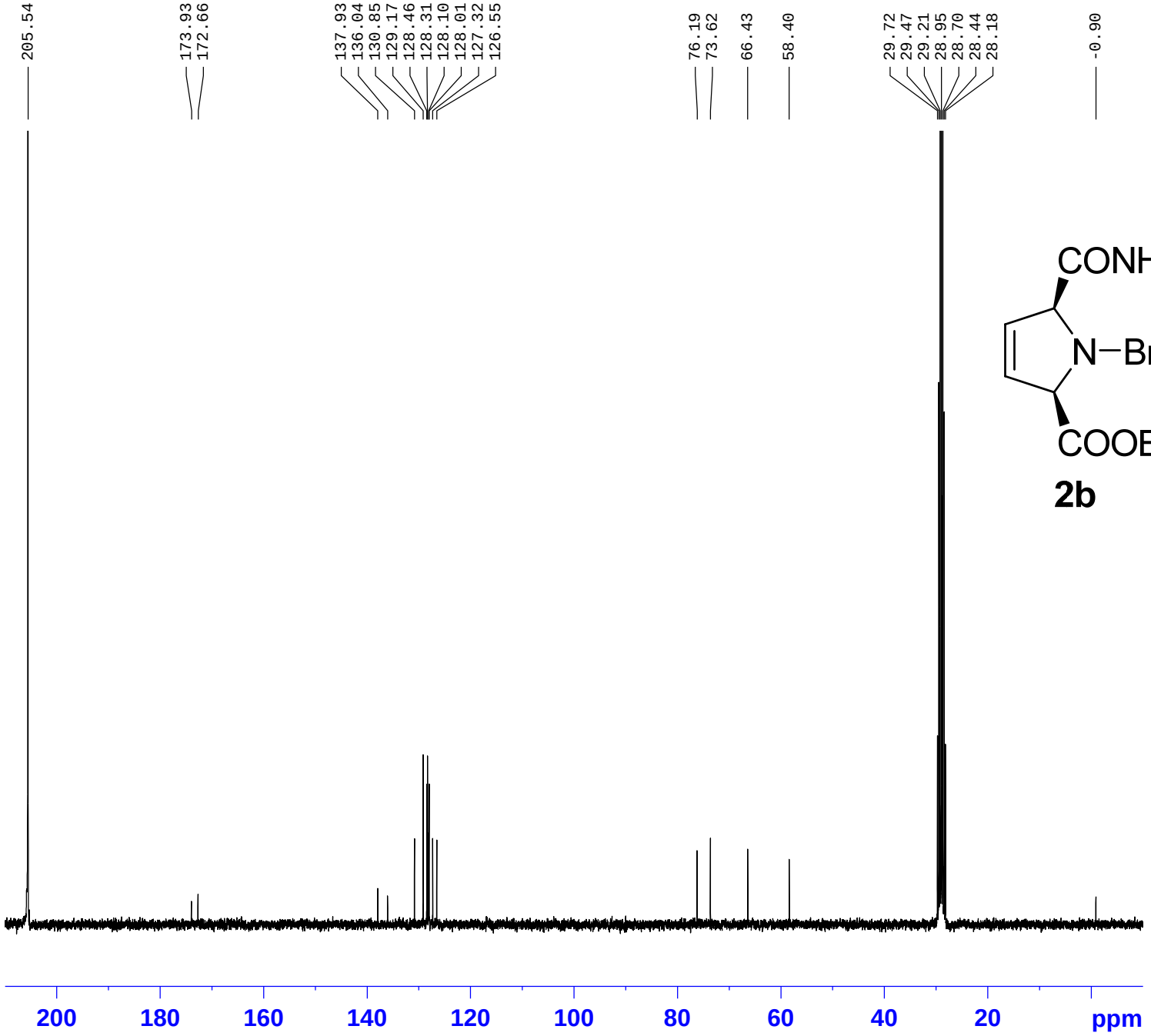

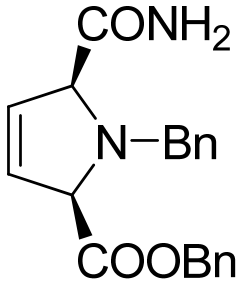

2b

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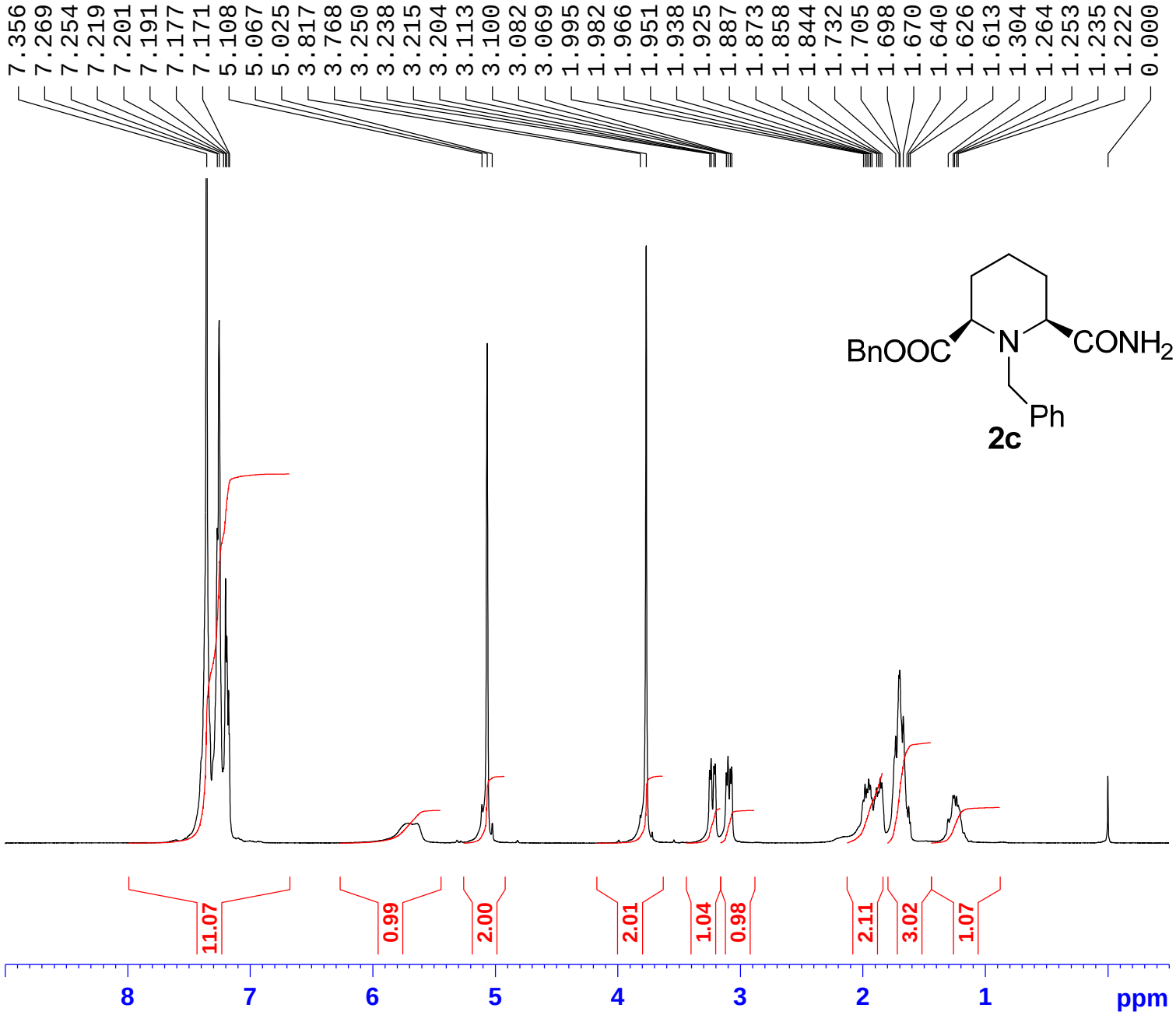
Current Data Parameters
NAME                  cp-d5'
EXPNO                     44
PROCNO                     1

F2 - Acquisition Parameters
Date_              20111006
Time                  17.53
INSTRUM               spect
PROBHD   5 mm DUL 13C-1
PULPROG              zgig30
TD                    32768
SOLVENT             Acetone
NS                      500
DS                        0
SWH              18832.393 Hz
FIDRES            0.574719 Hz
AQ               0.8700404 sec
RG                      256
DW                 26.550 usec
DE                  8.00 usec
TE                  299.7 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                   13C
P1                  12.50 usec
PL1                  2.00 dB
SFO1           75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                   1H
PCPD2               100.00 usec
PL2                  3.00 dB
PL12                22.33 dB
SFO2          300.1312005 MHz

F2 - Processing parameters
SI                    32768
SF             75.4677490 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

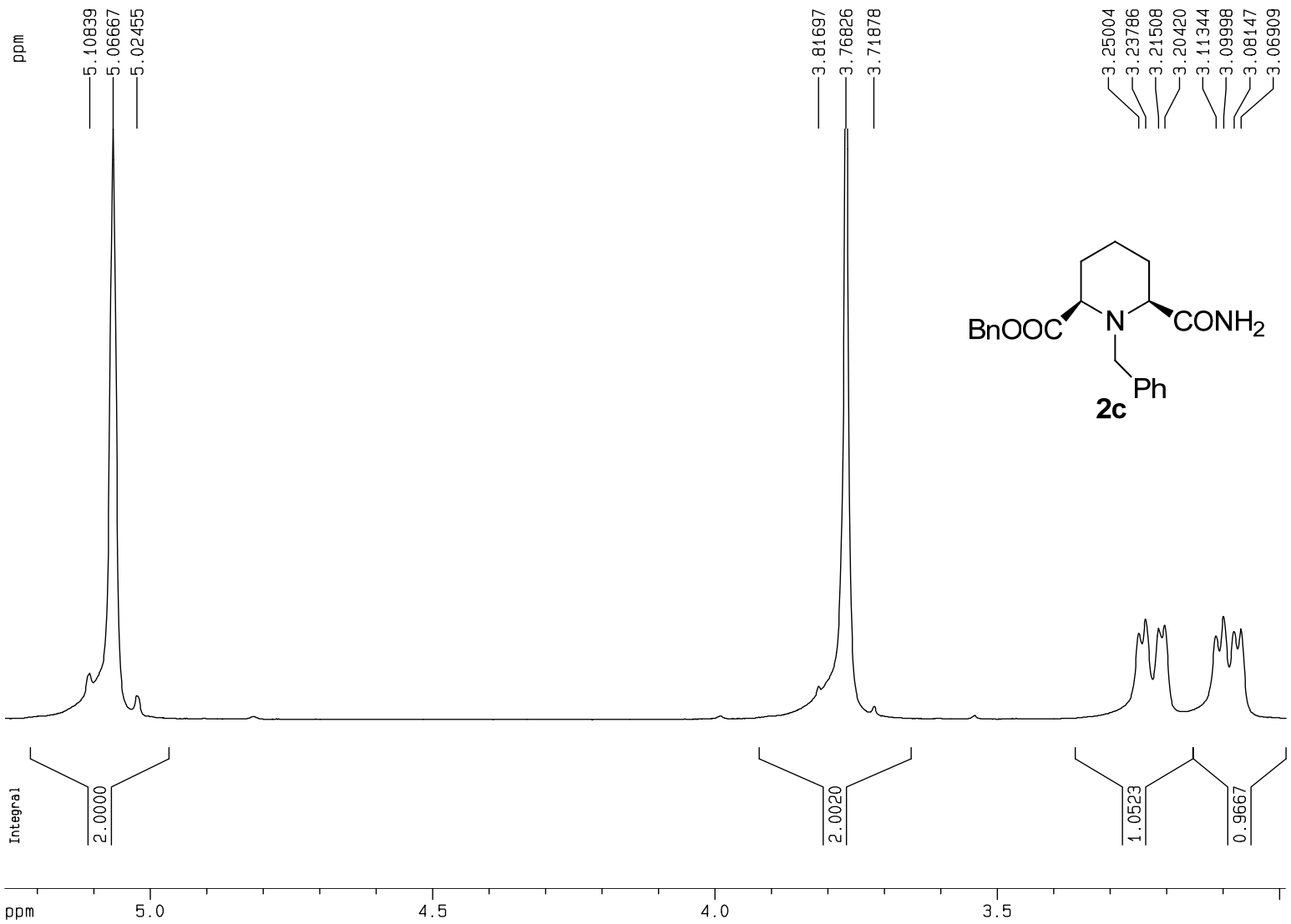



```
Current Data Parameters
NAME                cp-h3
EXPNO                  20
PROCNO                  1

F2 - Acquisition Parameters
Date_            20090717
Time                11.24
INSTRUM             spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     0
SWH              8992.806 Hz
FIDRES           0.137219 Hz
AQ              3.6438515 sec
RG                 101.6
DW                55.600 usec
DE                 6.00 usec
TE                302.0 K
D1             1.00000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                 7.00 usec
PL1               -1.00 dB
SFO1         300.1324010 MHz

F2 - Processing parameters
SI                 32768
SF           300.1300067 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```



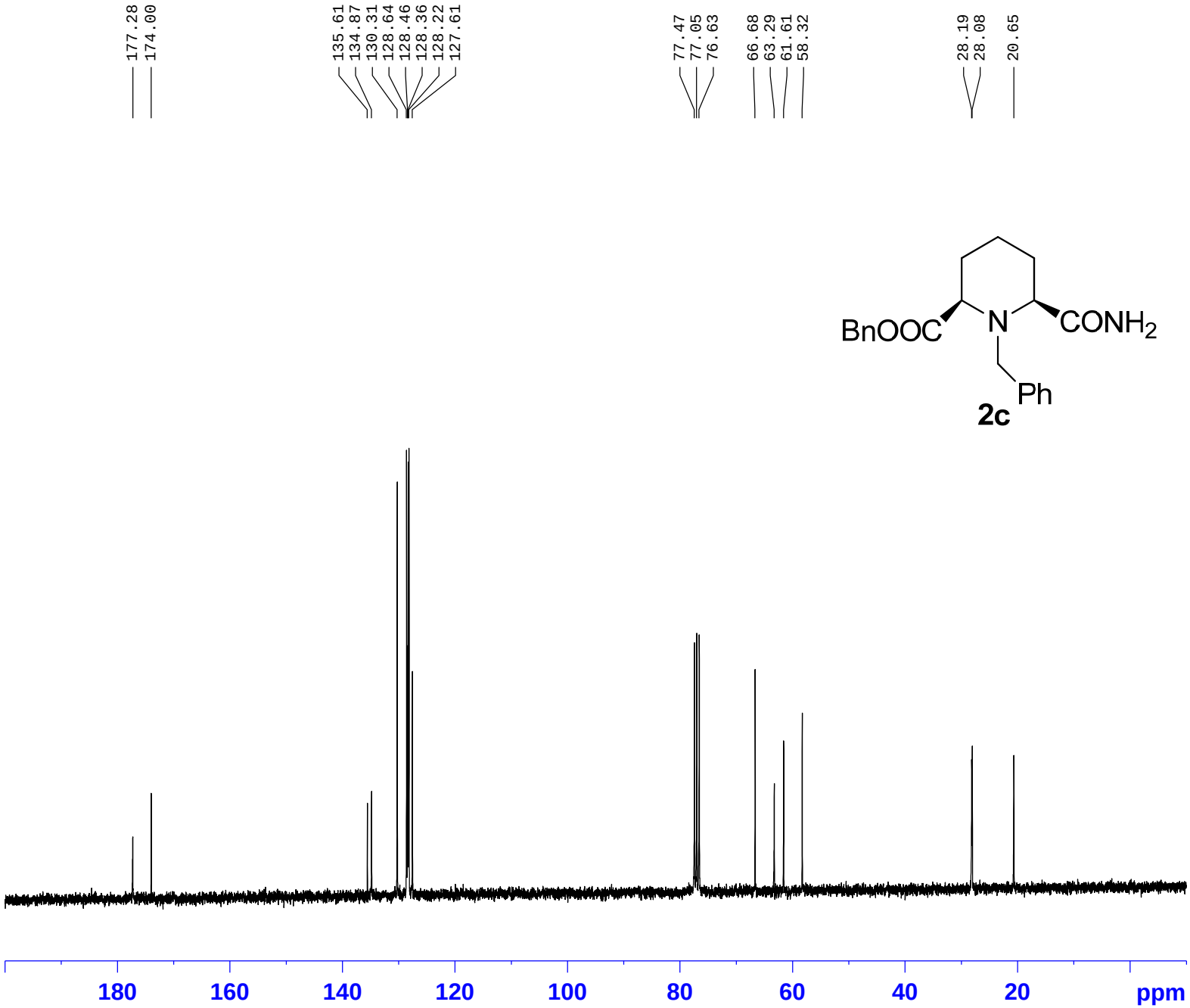

```
Current Data Parameters
NAME                  cp-h3
EXPNO                    20
PROCNO                    1

F2 - Acquisition Parameters
Date_              20090717
Time                  11.24
INSTRUM               spect
PROBHD   5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        0
SWH                8992.806 Hz
FIDRES             0.137219 Hz
AQ                 3.6438515 sec
RG                     101.6
DW                    55.600 usec
DE                     6.00 usec
TE                    302.0 K
D1              1.00000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                     1H
P1                     7.00 usec
PL1                   -1.00 dB
SFO1           300.1324010 MHz

F2 - Processing parameters
SI                    32768
SF             300.1300067 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00

1D NMR plot parameters
CX                    22.00 cm
CY                    20.00 cm
F1P                    5.258 ppm
F1                  1577.99 Hz
F2P                    2.990 ppm
F2                   897.25 Hz
PPMCM              0.10310 ppm/cm
HZCM              30.94262 Hz/cm
```



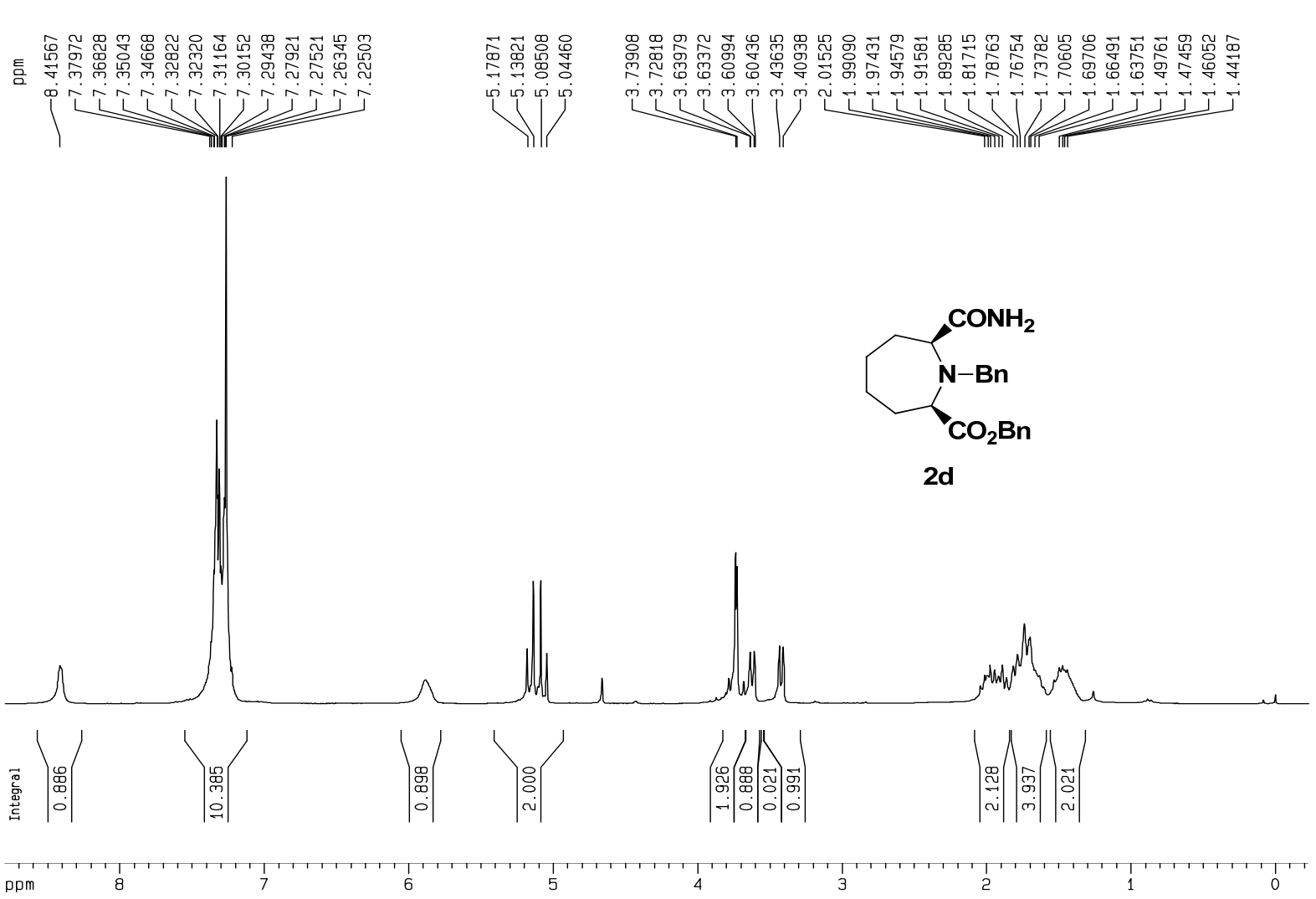

```
Current Data Parameters
NAME                  cp-h3
EXPNO                    21
PROCNO                    1

F2 - Acquisition Parameters
Date_              20090717
Time                  11.38
INSTRUM               spect
PROBHD    5 mm DUL 13C-1
PULPROG            zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      261
DS                        4
SWH               17985.611 Hz
FIDRES             0.274439 Hz
AQ                 1.8219508 sec
RG                    1149.4
DW                    27.800 usec
DE                     6.00 usec
TE                    302.1 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                    12.50 usec
PL1                    2.00 dB
SFO1            75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                 80.00 usec
PL2                   -1.00 dB
PL12                  20.16 dB
PL13                  16.98 dB
SFO2           300.1312005 MHz

F2 - Processing parameters
SI                     32768
SF              75.4677487 MHz
WDW                       EM
SSB                        0
LB                     1.00 Hz
GB                         0
PC                     1.40
```



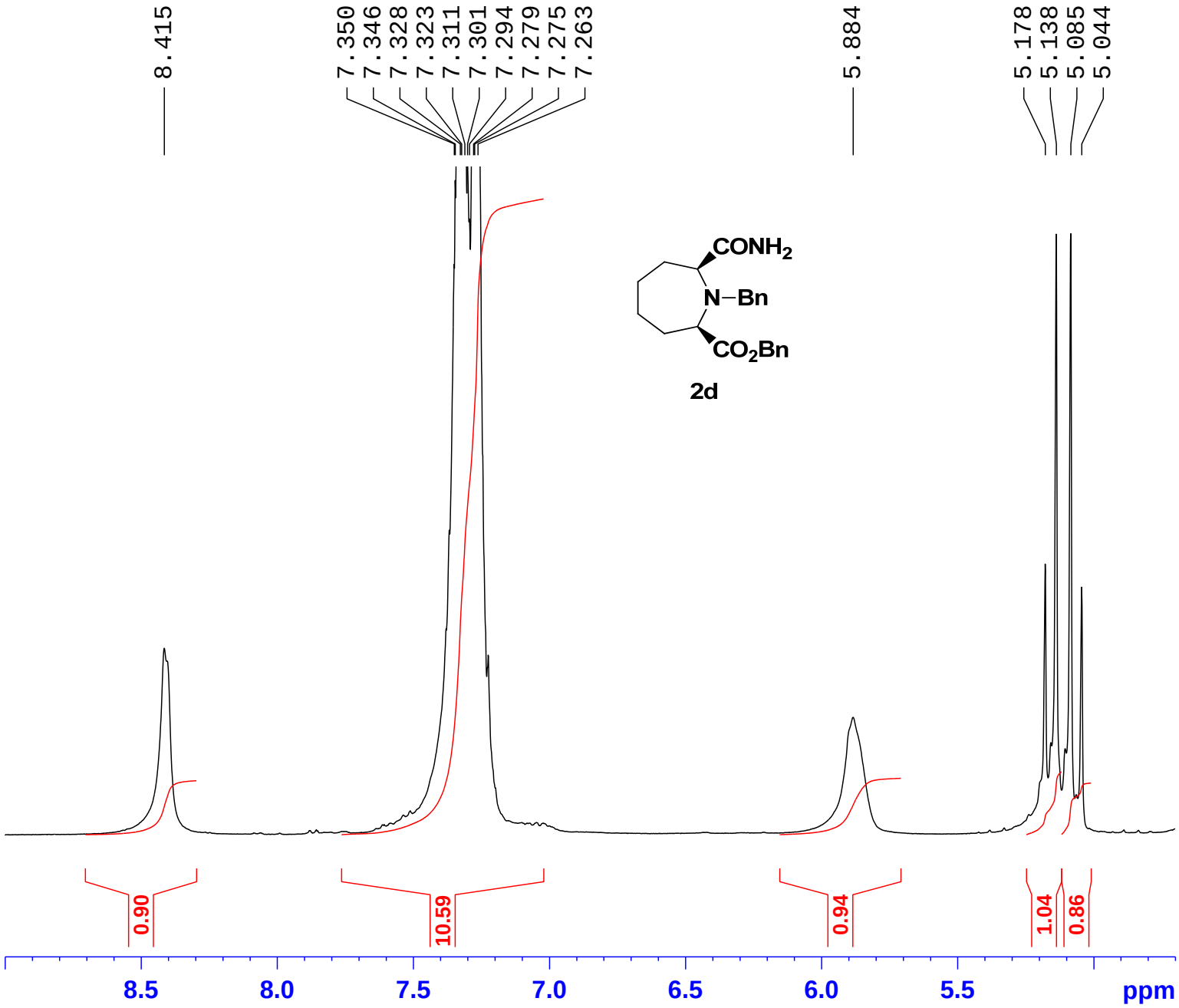

```
Current Data Parameters
NAME                  cp-q4
EXPNO                    60
PROCNO                    1

F2 - Acquisition Parameters
Date_              20090630
Time                 14.12
INSTRUM              spect
PROBHD   5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        0
SWH                8992.806 Hz
FIDRES             0.137219 Hz
AQ                 3.6438515 sec
RG                       57
DW                   55.600 usec
DE                    6.00 usec
TE                   299.7 K
D1                1.00000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                     1H
P1                    7.00 usec
PL1                  -1.00 dB
SFO1           300.1324010 MHz

F2 - Processing parameters
SI                    32768
SF             300.1300086 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                    1.00

1D NMR plot parameters
CX                   22.00 cm
CY                   10.00 cm
F1P                   8.796 ppm
F1                 2639.94 Hz
F2P                  -0.227 ppm
F2                   -68.17 Hz
PPMCM              0.41014 ppm/cm
HZCM             123.09608 Hz/cm
```

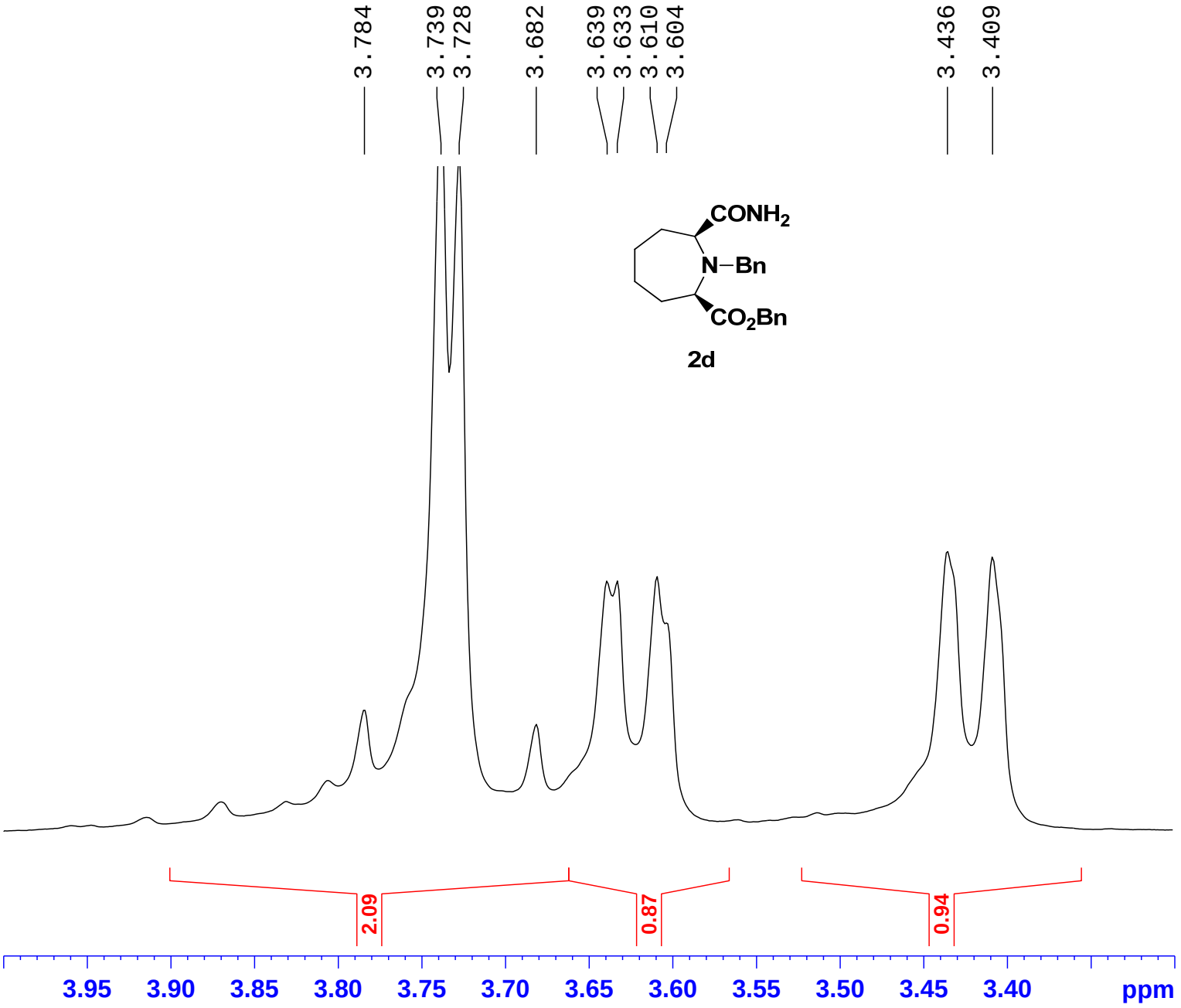



```
Current Data Parameters
NAME                  cp-q4
EXPNO                    60
PROCNO                    1

F2 - Acquisition Parameters
Date_              20090630
Time                  14.12
INSTRUM               spect
PROBHD   5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        0
SWH                8992.806 Hz
FIDRES             0.137219 Hz
AQ                 3.6438515 sec
RG                       57
DW                   55.600 usec
DE                    6.00 usec
TE                   299.7 K
D1              1.00000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                     1H
P1                    7.00 usec
PL1                  -1.00 dB
SFO1           300.1324010 MHz

F2 - Processing parameters
SI                    32768
SF             300.1300086 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                    1.00
```

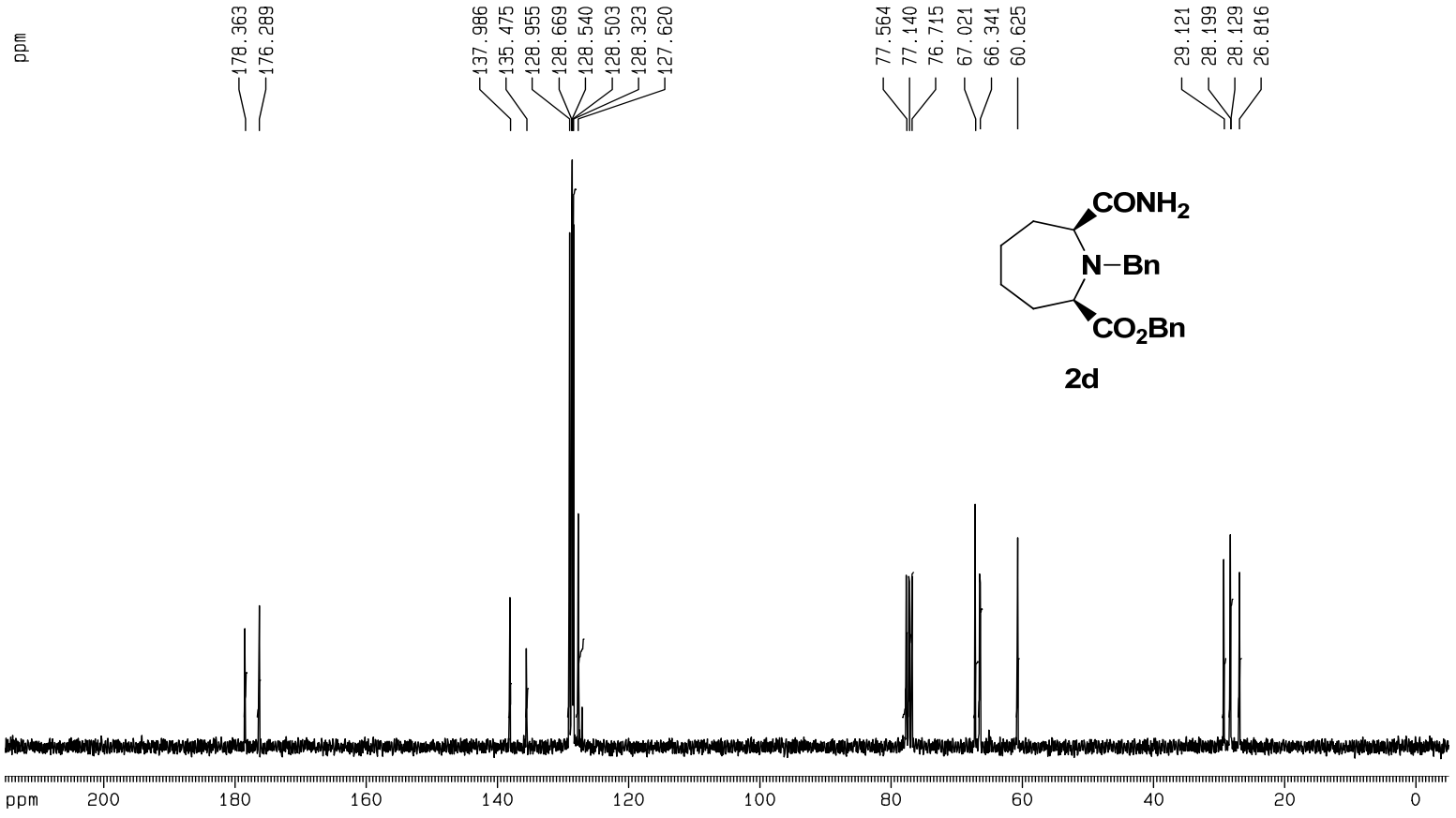



```
Current Data Parameters
NAME                  cp-q4
EXPNO                    60
PROCNO                    1

F2 - Acquisition Parameters
Date_              20090630
Time                  14.12
INSTRUM               spect
PROBHD   5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        0
SWH                8992.806 Hz
FIDRES             0.137219 Hz
AQ                 3.6438515 sec
RG                       57
DW                   55.600 usec
DE                    6.00 usec
TE                   299.7 K
D1                1.00000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                     1H
P1                    7.00 usec
PL1                  -1.00 dB
SFO1           300.1324010 MHz

F2 - Processing parameters
SI                    32768
SF             300.1300086 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                    1.00
```




```
Current Data Parameters
NAME                  cp-q4
EXPNO                    61
PROCNO                    1

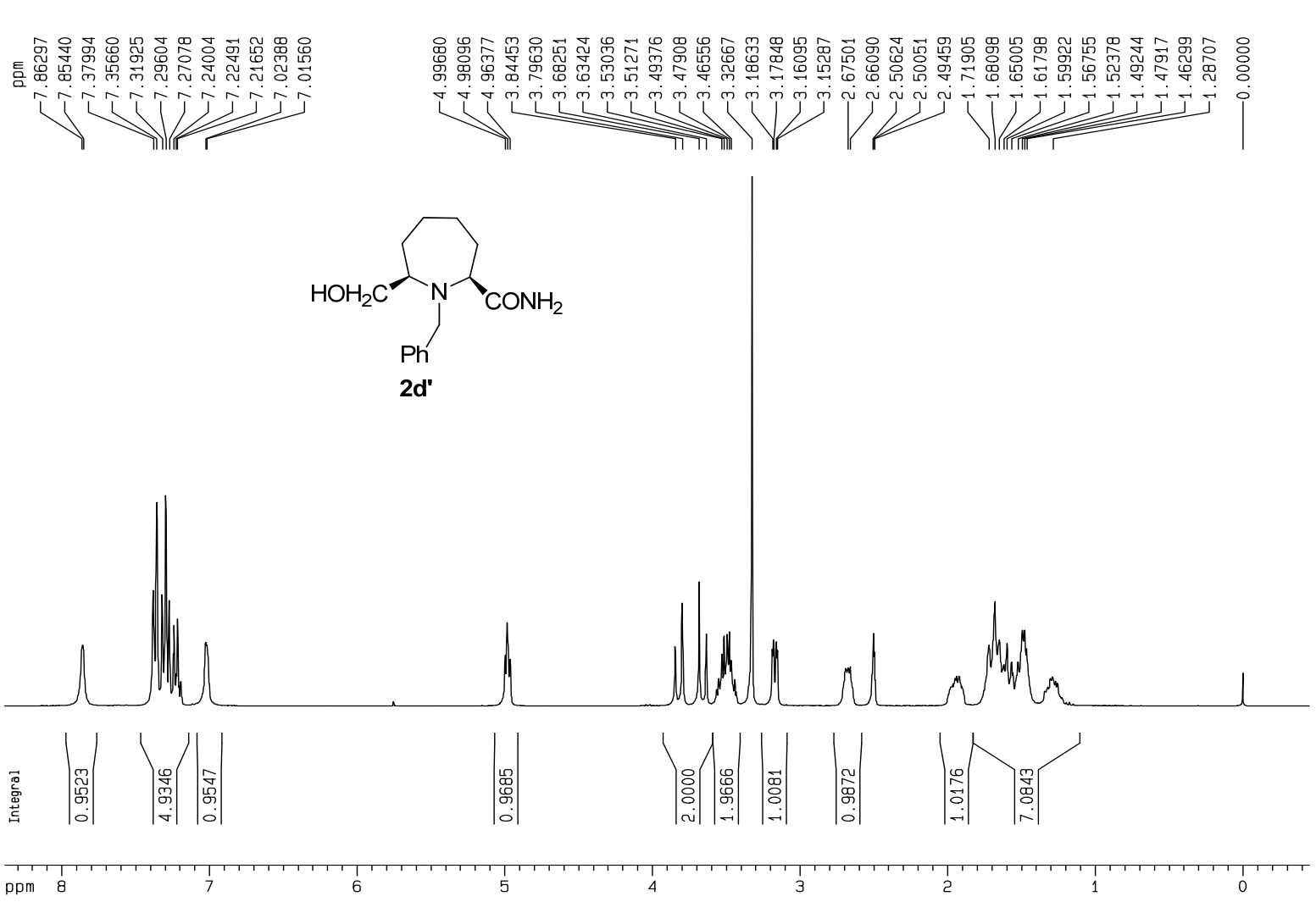
F2 - Acquisition Parameters
Date_              20090630
Time                  14.20
INSTRUM               spect
PROBHD   5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                      87
DS                       4
SWH              17985.611 Hz
FIDRES               0.274439 Hz
AQ                1.8219508 sec
RG                    8192
DW                   27.800 usec
DE                    6.00 usec
TE                   301.1 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                    12.50 usec
PL1                    2.00 dB
SFO1             75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                 80.00 usec
PL2                   -1.00 dB
PL12                  20.16 dB
PL13                  16.98 dB
SFO2            300.1312005 MHz

F2 - Processing parameters
SI                    32768
SF               75.4677490 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40

1D NMR plot parameters
CX                    22.00 cm
CY                    10.00 cm
F1P                  215.000 ppm
F1                 16225.57 Hz
F2P                   -5.000 ppm
F2                  -377.34 Hz
PPMCM                10.00000 ppm/cm
HZCM                754.67749 Hz/cm
```



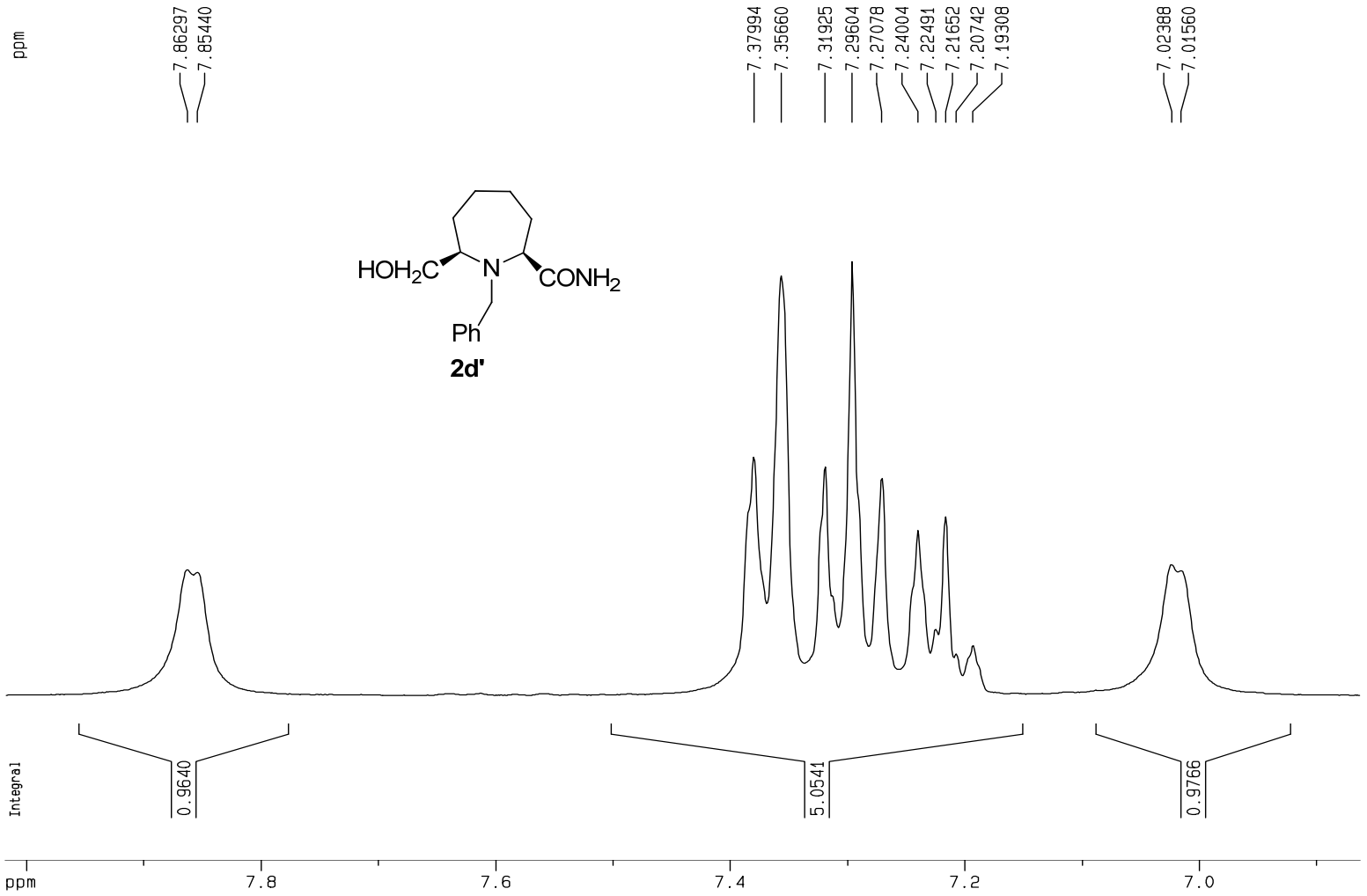

```
Current Data Parameters
NAME                  cp-q5
EXPNO                    10
PROCNO                    1

F2 - Acquisition Parameters
Date_              20090721
Time                 20.11
INSTRUM              spect
PROBHD    5 mm DUL 13C-1
PULPROG               zg30
TD                   65536
SOLVENT               DMSO
NS                       16
DS                        0
SWH                8992.806 Hz
FIDRES             0.137219 Hz
AQ                 3.6438515 sec
RG                     203.2
DW                    55.600 usec
DE                     6.00 usec
TE                    299.2 K
D1                 1.00000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                     1H
P1                    7.00 usec
PL1                  -1.00 dB
SFO1           300.1324010 MHz

F2 - Processing parameters
SI                    32768
SF             300.1300008 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00

1D NMR plot parameters
CX                    22.00 cm
CY                    10.00 cm
F1P                   8.386 ppm
F1                 2516.99 Hz
F2P                 -0.450 ppm
F2                 -135.10 Hz
PPMCM               0.40166 ppm/cm
HZCM              120.54928 Hz/cm
```



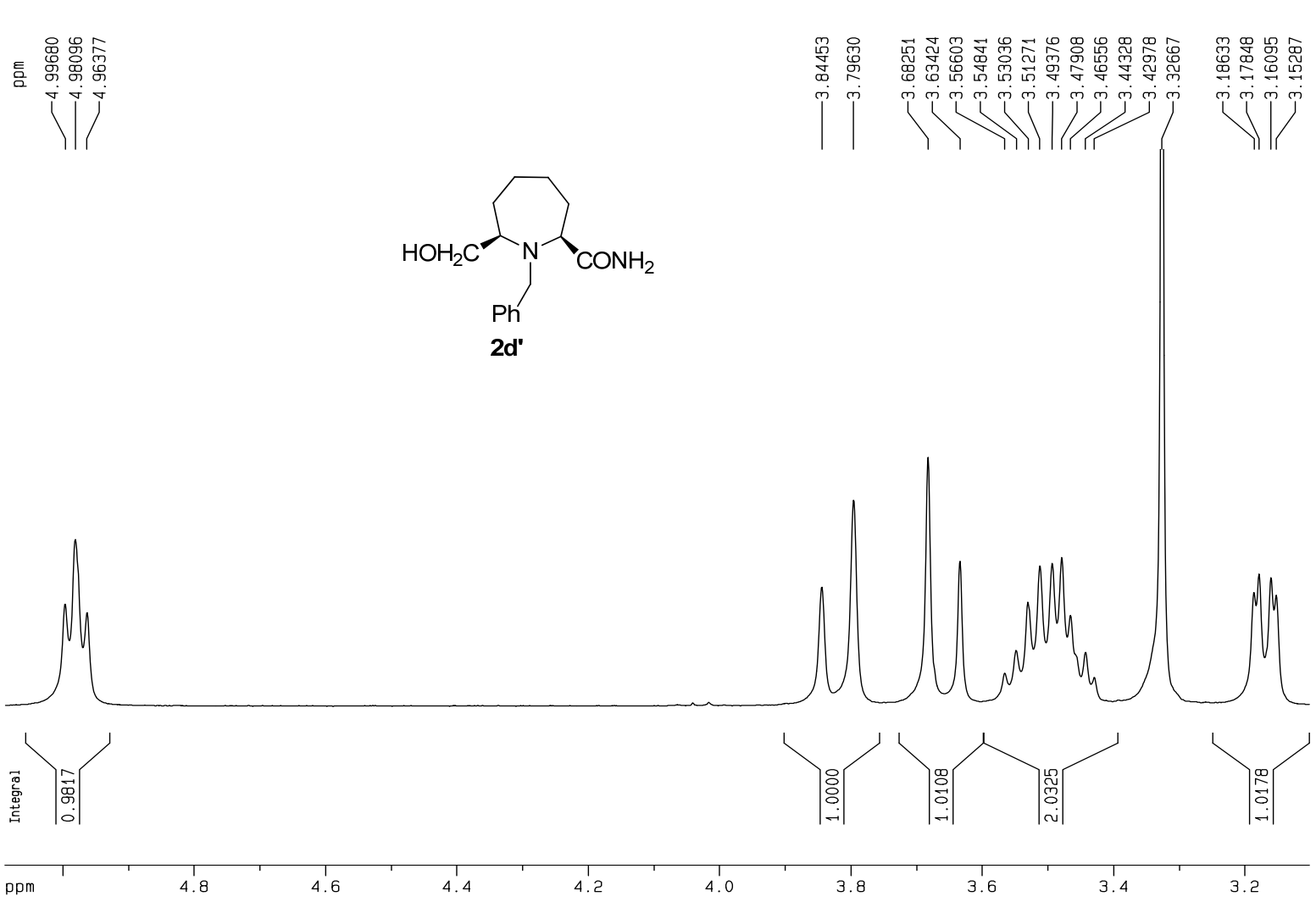

```
Current Data Parameters
NAME                  cp-q5
EXPNO                    10
PROCNO                    1

F2 - Acquisition Parameters
Date_              20090721
Time                 20.11
INSTRUM              spect
PROBHD    5 mm DUL 13C-1
PULPROG               zg30
TD                   65536
SOLVENT               DMSO
NS                       16
DS                        0
SWH                8992.806 Hz
FIDRES             0.137219 Hz
AQ                 3.6438515 sec
RG                     203.2
DW                    55.600 usec
DE                     6.00 usec
TE                    299.2 K
D1                 1.00000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                     1H
P1                    7.00 usec
PL1                  -1.00 dB
SFO1            300.1324010 MHz

F2 - Processing parameters
SI                    32768
SF               300.1300008 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00

1D NMR plot parameters
CX                    22.00 cm
CY                    20.00 cm
F1P                    8.018 ppm
F1                  2406.48 Hz
F2P                    6.863 ppm
F2                  2059.72 Hz
PPMCM                0.05252 ppm/cm
HZCM                15.76198 Hz/cm
```



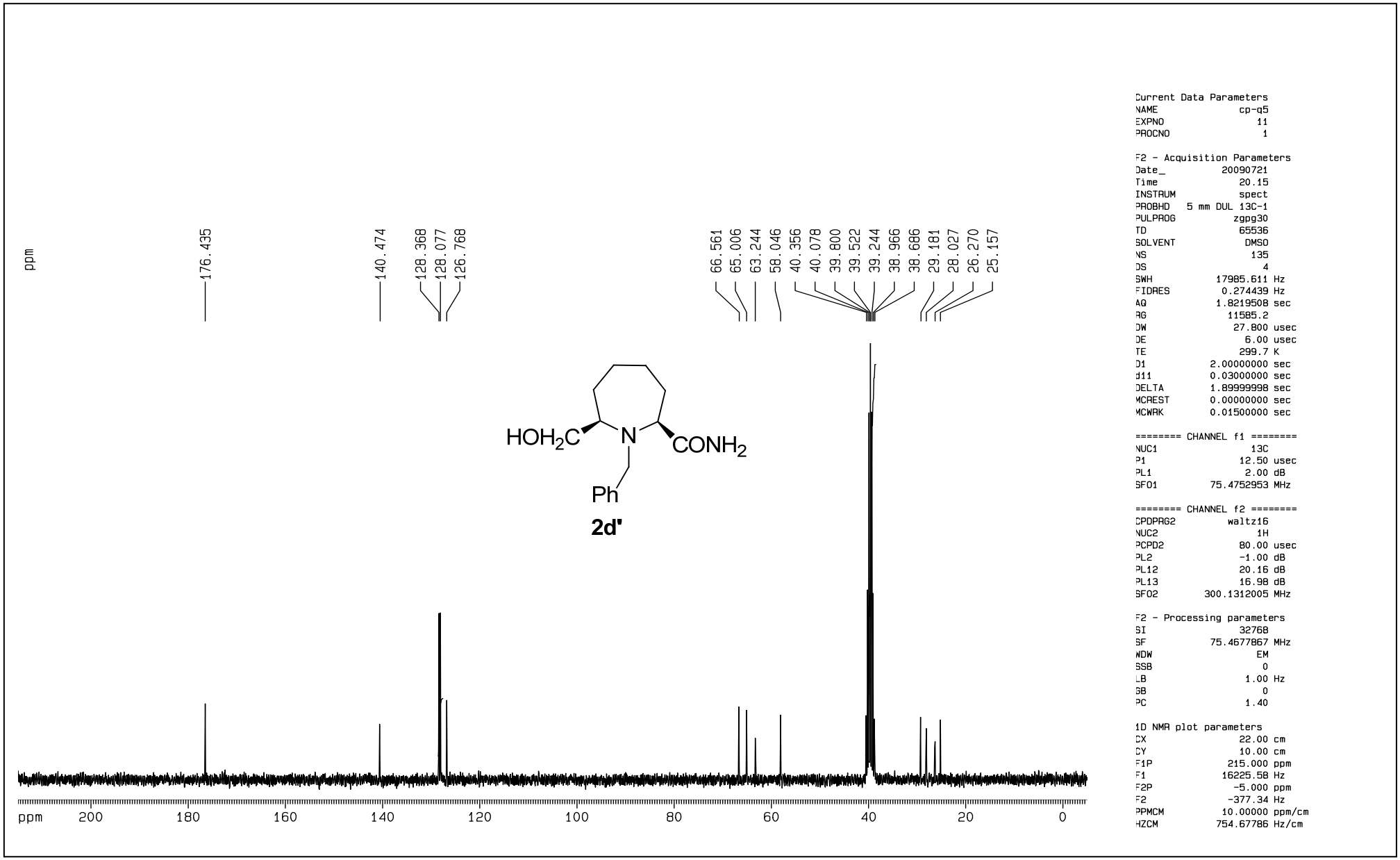

```
Current Data Parameters
NAME                  cp-q5
EXPNO                    10
PROCNO                    1

F2 - Acquisition Parameters
Date_              20090721
Time                 20.11
INSTRUM              spect
PROBHD    5 mm DUL 13C-1
PULPROG               zg30
TD                   65536
SOLVENT                DMSO
NS                       16
DS                        0
SWH                8992.806 Hz
FIDRES             0.137219 Hz
AQ                 3.6438515 sec
RG                     203.2
DW                    55.600 usec
DE                     6.00 usec
TE                    299.2 K
D1                 1.00000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                     1H
P1                    7.00 usec
PL1                  -1.00 dB
SFO1           300.1324010 MHz

F2 - Processing parameters
SI                    32768
SF             300.1300008 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00

1D NMR plot parameters
CX                    22.00 cm
CY                    20.00 cm
F1P                    5.088 ppm
F1                  1527.06 Hz
F2P                    3.101 ppm
F2                   930.83 Hz
PPMCM               0.09030 ppm/cm
HZCM               27.10176 Hz/cm
```




```
Current Data Parameters
NAME                  cp-q5
EXPNO                    11
PROCNO                    1

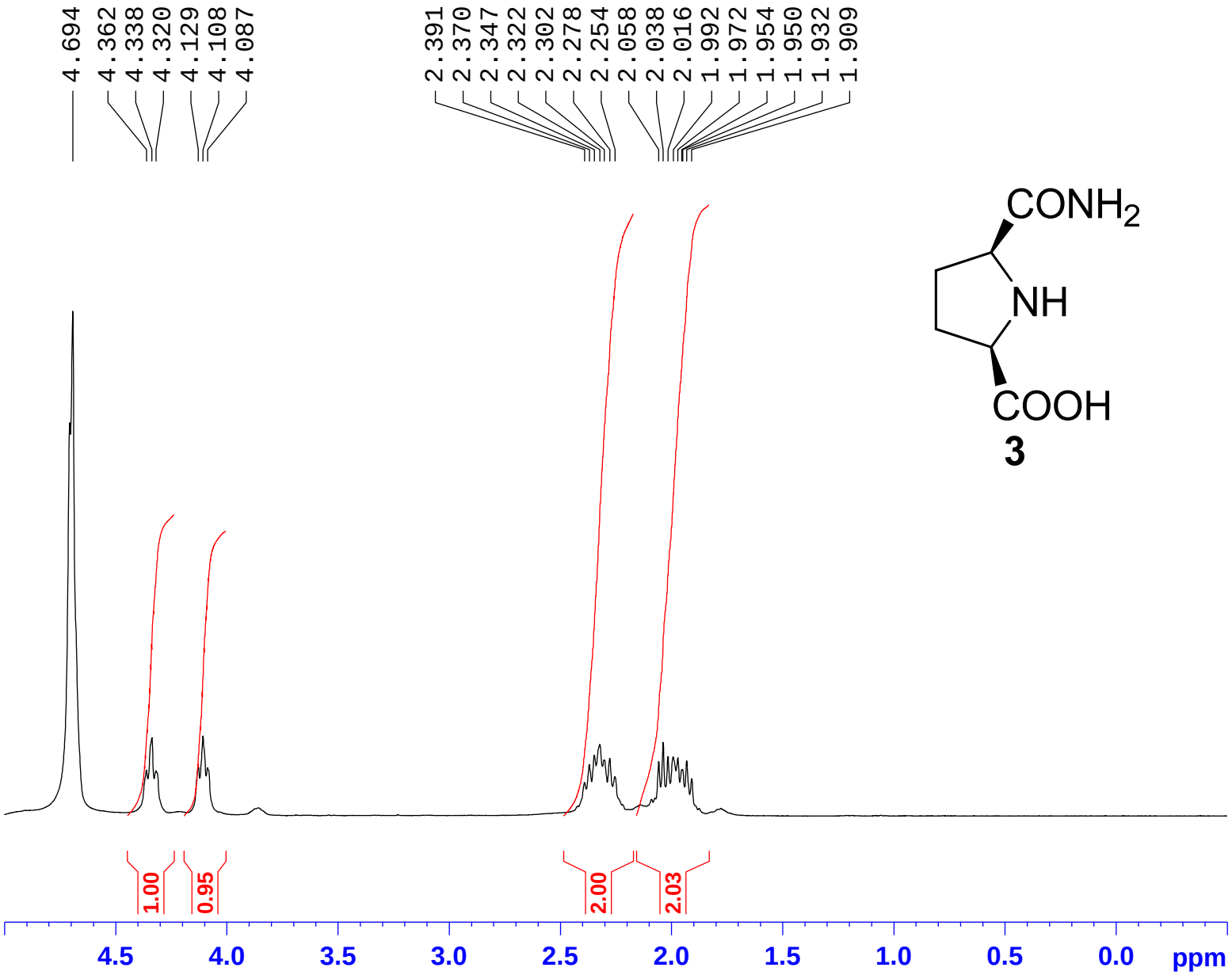
F2 - Acquisition Parameters
Date_              20090721
Time                 20.15
INSTRUM              spect
PROBHD   5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT                DMSO
NS                      135
DS                        4
SWH               17985.611 Hz
FIDRES            0.274439 Hz
AQ                1.8219508 sec
RG                  11585.2
DW                   27.800 usec
DE                    6.00 usec
TE                   299.7 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                   12.50 usec
PL1                   2.00 dB
SFO1            75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                   1H
PCPD2                80.00 usec
PL2                  -1.00 dB
PL12                 20.16 dB
PL13                 16.98 dB
SFO2           300.1312005 MHz

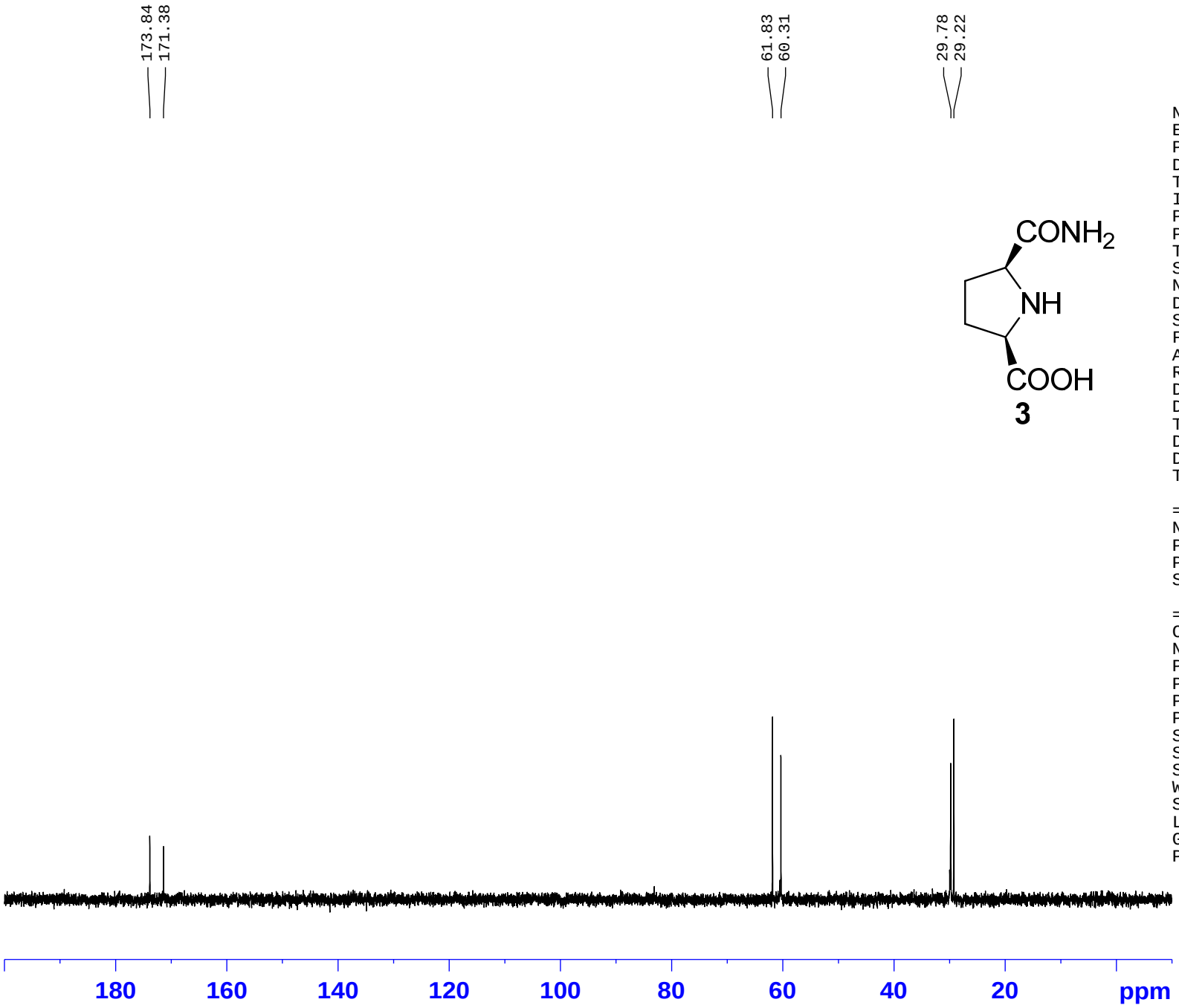
F2 - Processing parameters
SI                    32768
SF              75.4677867 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40

1D NMR plot parameters
CX                    22.00 cm
CY                    10.00 cm
F1P                215.000 ppm
F1                16225.58 Hz
F2P                 -5.000 ppm
F2                -377.34 Hz
PPMCM             10.00000 ppm/cm
HZCM             754.67786 Hz/cm
```



3

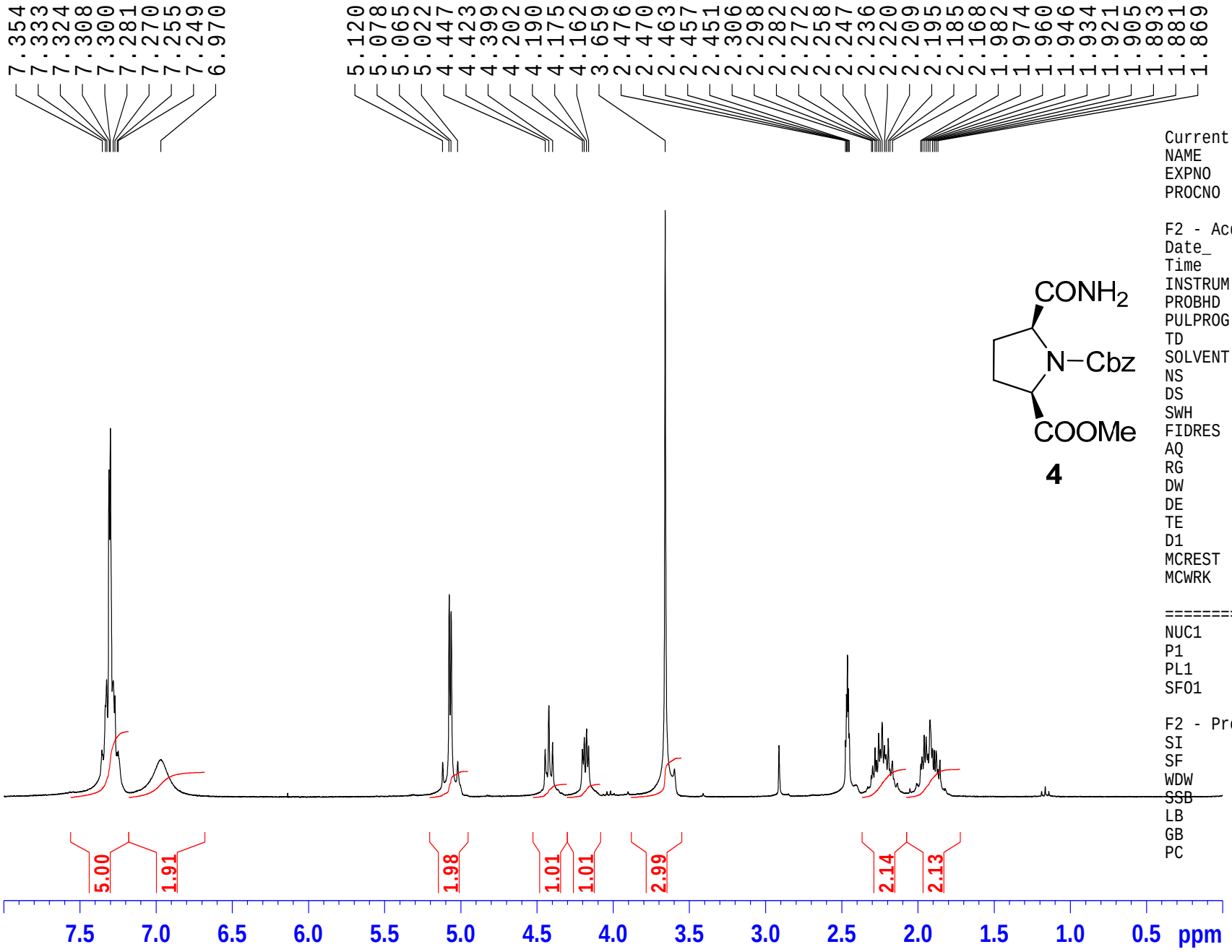
NAME	cp-p0
EXPNO	20
PROCNO	1
Date_	20101130
Time	20.09
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	65536
SOLVENT	D2O
NS	16
DS	0
SWH	8992.806 Hz
FIDRES	0.137219 Hz
AQ	3.6438515 sec
RG	128
DW	55.600 usec
DE	8.00 usec
TE	296.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.80 usec
PL1	3.00 dB
SFO1	300.1324010 MHz
SI	32768
SF	300.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00




```
NAME                cp-p0
EXPNO                  21
PROCNO                  1
Date_            20101130
Time                20.14
INSTRUM             spect
PROBHD    5 mm DUL 13C-1
PULPROG            zgpg30
TD                  65536
SOLVENT               D2O
NS                    262
DS                      4
SWH            17985.611 Hz
FIDRES          0.274439 Hz
AQ              1.8219508 sec
RG                14596.5
DW                 27.800 usec
DE                  8.00 usec
TE                 296.5 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                 12.50 usec
PL1                 2.00 dB
SFO1          75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2             100.00 usec
PL2                 3.00 dB
PL12                22.33 dB
PL13                23.00 dB
SFO2         300.1312005 MHz
SI                  32768
SF             75.4677490 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```



Current Data Parameters

NAME	cp-p13 375K
EXPNO	397
PROCNO	1

F2 - Acquisition Parameters

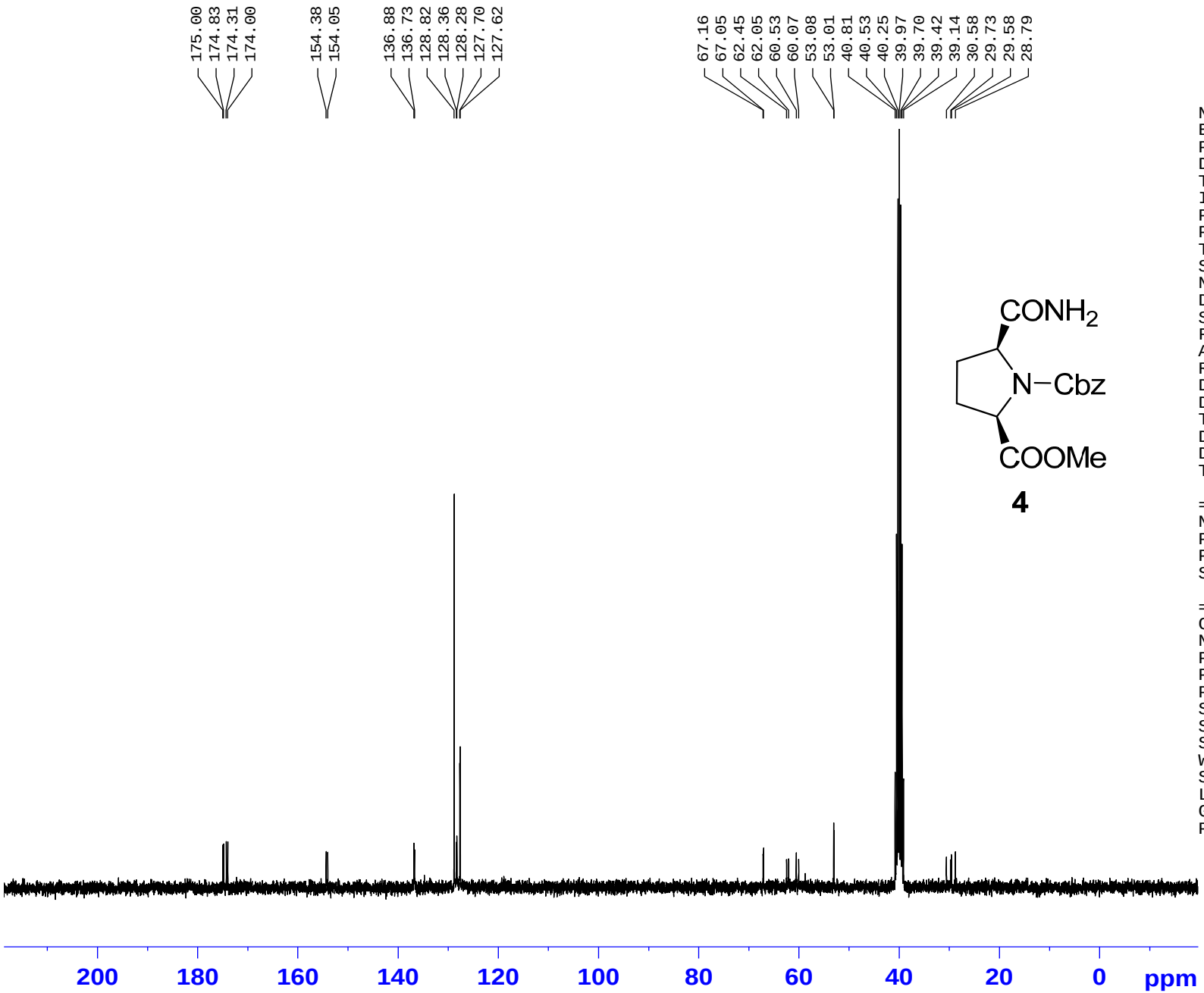
Date_	20110326
Time	18.48
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	0
SWH	6188.119 Hz
FIDRES	0.094423 Hz
AQ	5.2953587 sec
RG	8192
DW	80.800 usec
DE	6.00 usec
TE	375.1 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

======== CHANNEL f1 ========

NUC1	1H
P1	13.80 usec
PL1	3.00 dB
SFO1	300.1318534 MHz

F2 - Processing parameters

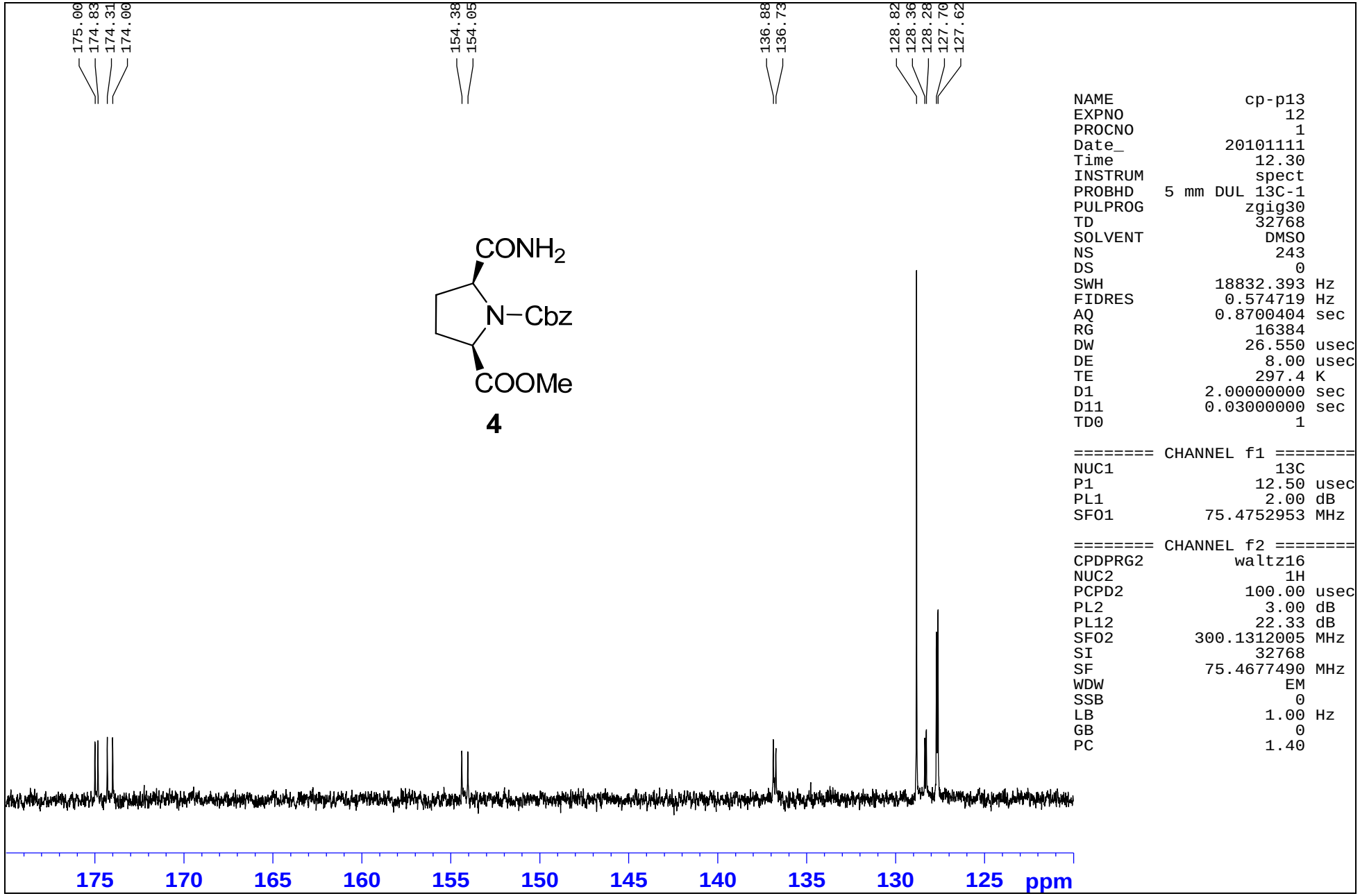
SI	32768
SF	300.1300114 MHz
WDW	EM
SSB	0
LB	0.20 Hz
GB	0
PC	1.00



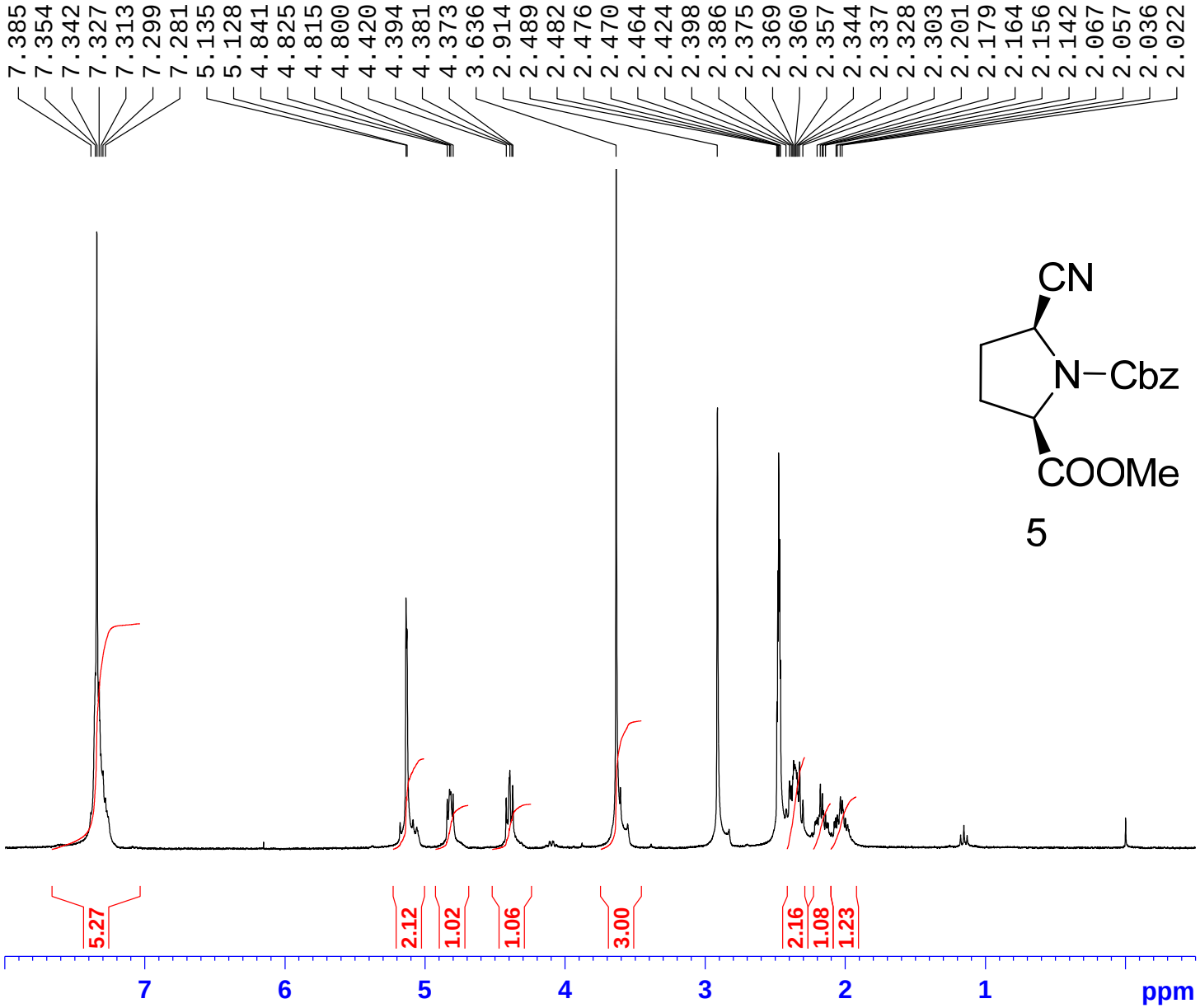

```
NAME                cp-p13
EXPNO                   12
PROCNO                   1
Date_             20101111
Time                 12.30
INSTRUM              spect
PROBHD    5 mm DUL 13C-1
PULPROG             zgig30
TD                   32768
SOLVENT                DMSO
NS                     243
DS                       0
SWH              18832.393 Hz
FIDRES            0.574719 Hz
AQ               0.8700404 sec
RG                   16384
DW                  26.550 usec
DE                   8.00 usec
TE                  297.4 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                  12.50 usec
PL1                  2.00 dB
SFO1           75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                   1H
PCPD2              100.00 usec
PL2                  3.00 dB
PL12                22.33 dB
SFO2          300.1312005 MHz
SI                   32768
SF             75.4677490 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```



cp-p35 375K

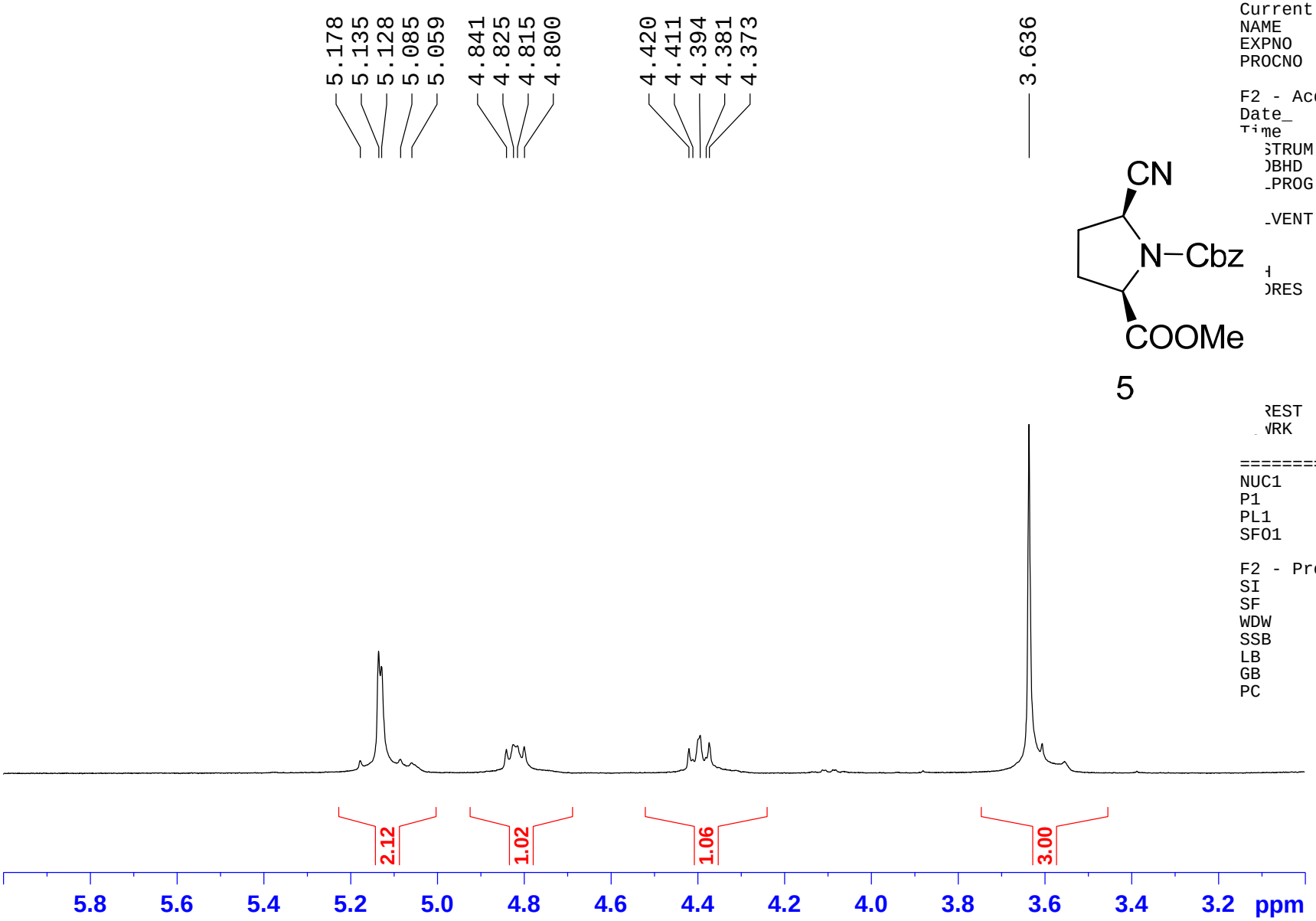



```
Current Data Parameters
NAME                 shengwen
EXPNO                     367
PROCNO                      1

F2 - Acquisition Parameters
Date_               20110226
Time                   16.54
INSTRUM                spect
PROBHD   5 mm BBO BB-1H
PULPROG                 zg30
TD                     65536
SOLVENT                 DMSO
NS                        27
DS                         0
SWH                 6188.119 Hz
FIDRES              0.094423 Hz
AQ                5.2953587 sec
RG                     16384
DW                   80.800 usec
DE                    6.00 usec
TE                   375.8 K
D1                1.00000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                      13.80 usec
PL1                      3.00 dB
SFO1             300.1318534 MHz

F2 - Processing parameters
SI                      32768
SF               300.1300075 MHz
WDW                        EM
SSB                         0
LB                       0.20 Hz
GB                          0
PC                       1.00
```

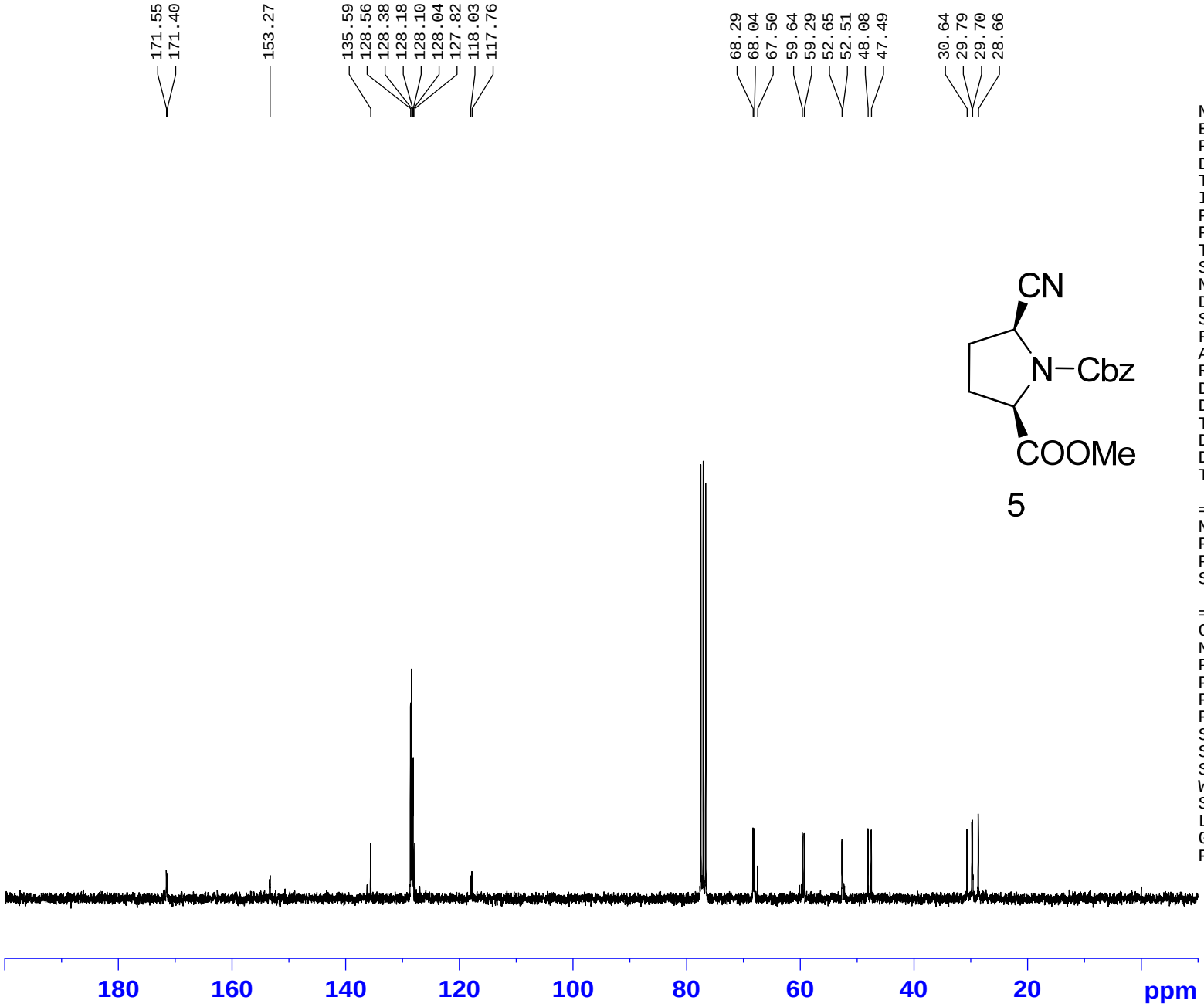



```
Current Data Parameters
NAME                  shengwen
EXPNO                      367
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20110226
Time                     16.54
   STRUM                 spect
   OBHD    5 mm BBO BB-1H
   _PROG                 zg30
                        65536
   _VENT                 DMSO
                           27
                            0
   H                 6188.119 Hz
   ORES              0.094423 Hz
                    5.2953587 sec
                        16384
                     80.800 usec
                      6.00 usec
                      375.8 K
                   1.00000000 sec
   REST            0.00000000 sec
   WRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                     13.80 usec
PL1                     3.00 dB
SFO1             300.1318534 MHz

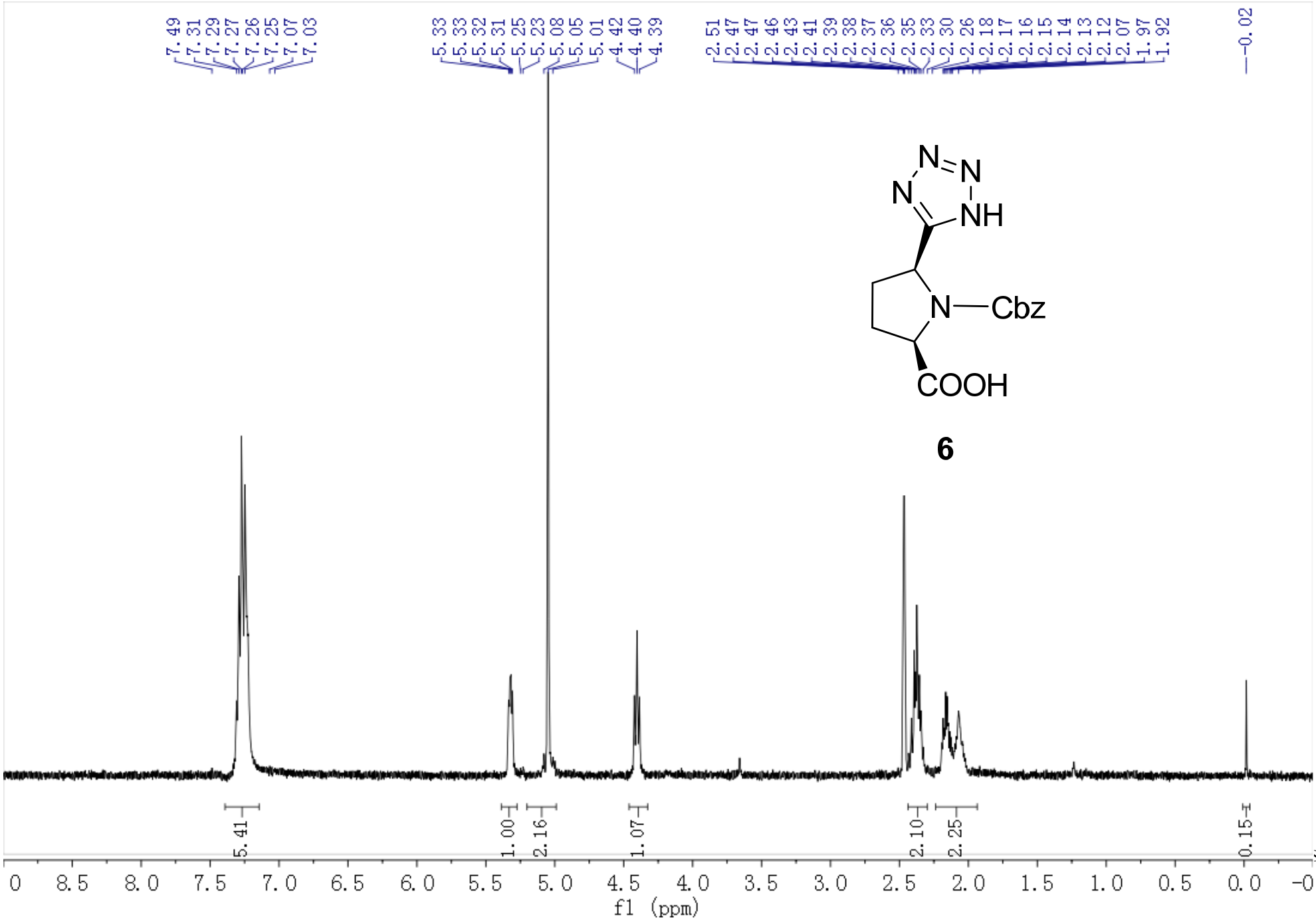
F2 - Processing parameters
SI                       32768
SF               300.1300075 MHz
WDW                         EM
SSB                          0
LB                      0.20 Hz
GB                           0
PC                      1.00
```

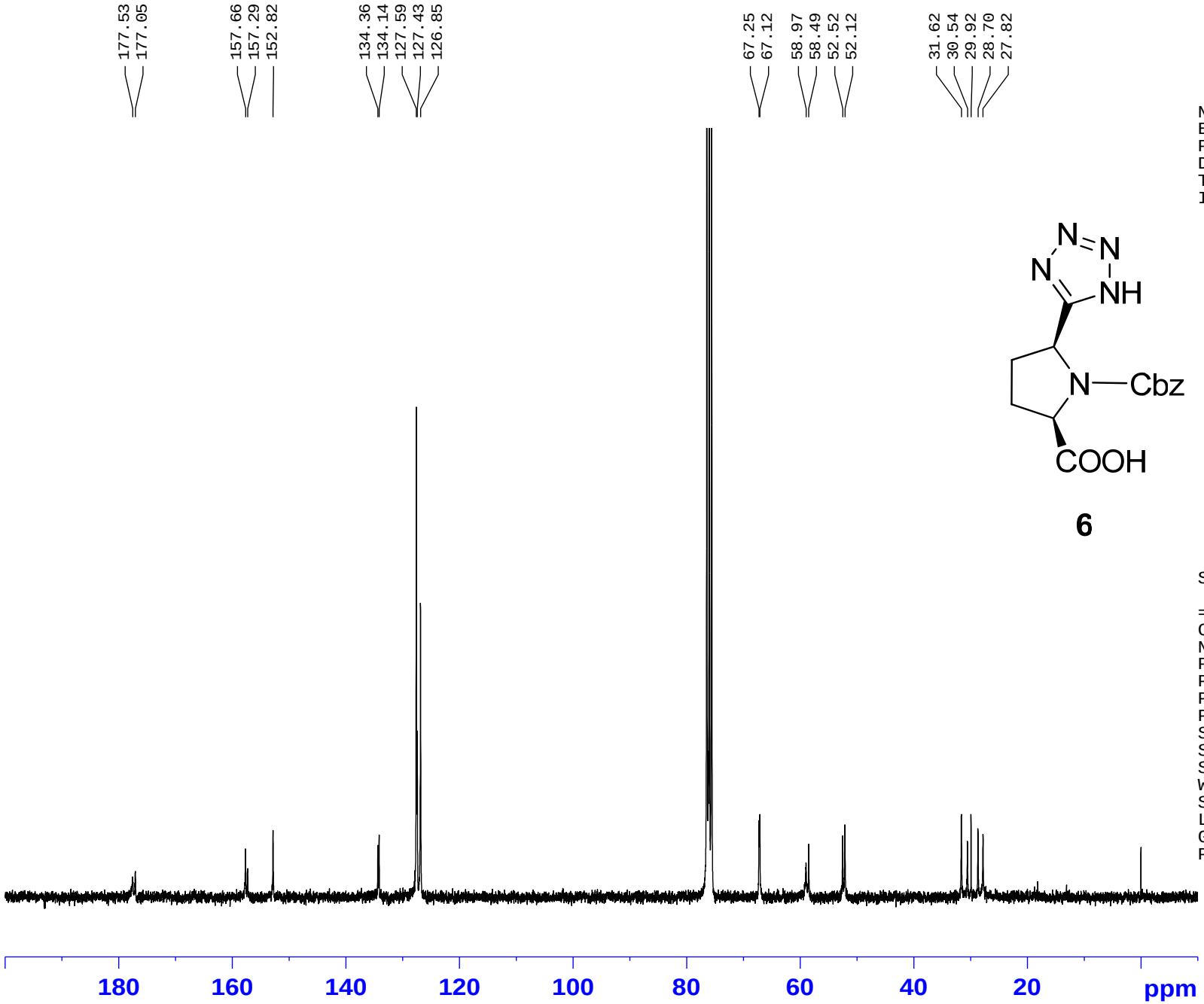



```
NAME              cp-p35
EXPNO                 11
PROCNO                 1
Date_           20100818
Time               20.20
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   398
DS                     4
SWH            17985.611 Hz
FIDRES          0.274439 Hz
AQ             1.8219508 sec
RG                 16384
DW                27.800 usec
DE                 8.00 usec
TE                301.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

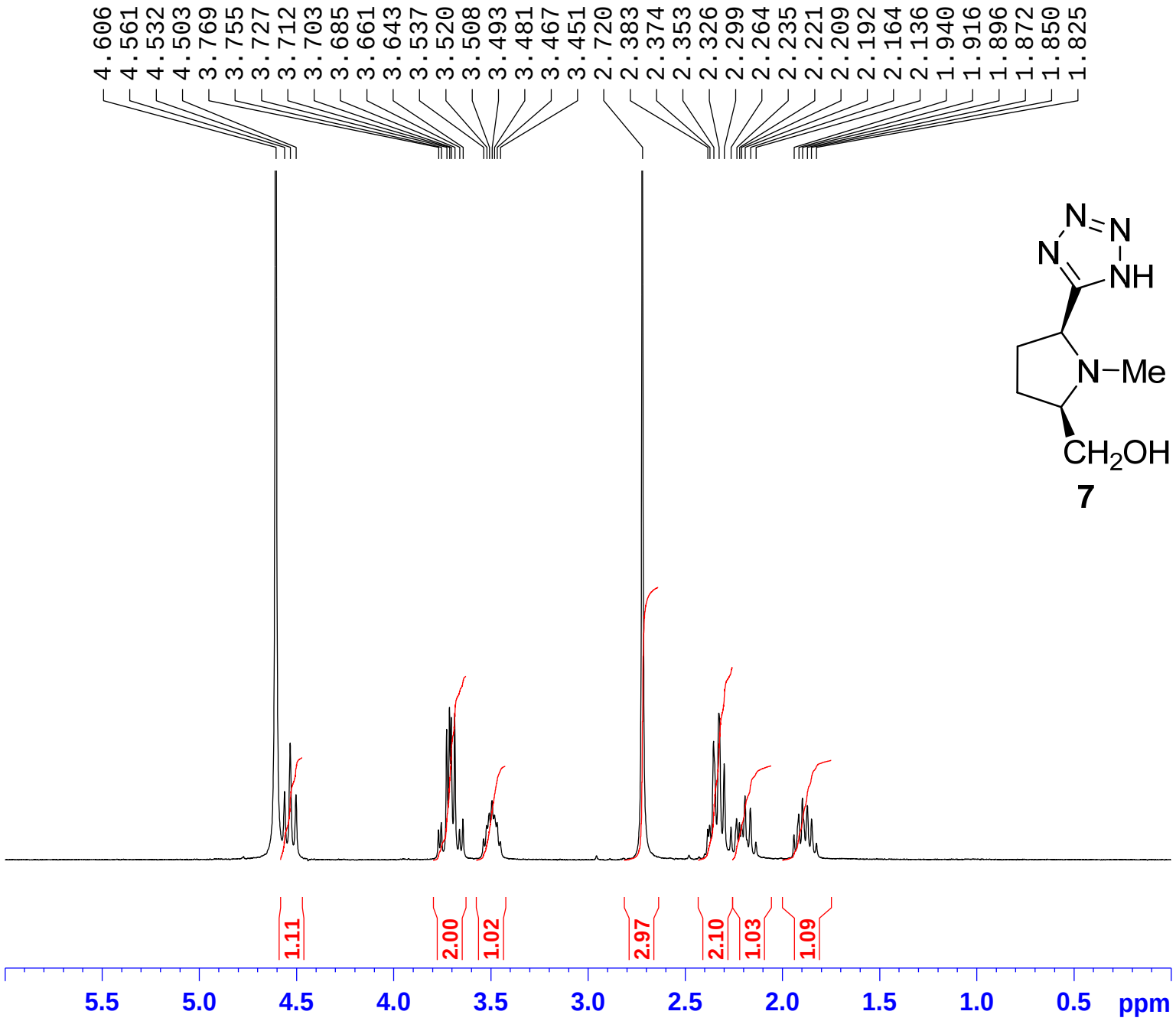
======== CHANNEL f1 ========
NUC1                13C
P1                12.50 usec
PL1                2.00 dB
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             100.00 usec
PL2                3.00 dB
PL12               22.33 dB
PL13               23.00 dB
SFO2        300.1312005 MHz
SI                 32768
SF           75.4677490 MHz
WDW                EM
SSB                 0
LB                1.00 Hz
GB                  0
PC                1.40
```





NAME	cp-p803
EXPNO	20
PROCNO	1
Date_	20101220
Time	8.20
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	9544
DS	4
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	9195.2
DW	27.800 usec
DE	8.00 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	12.50 usec
PL1	2.00 dB
SFO1	75.4752953 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	100.00 usec
PL2	3.00 dB
PL12	22.33 dB
PL13	23.00 dB
SFO2	300.1312005 MHz
SI	32768
SF	75.4678257 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



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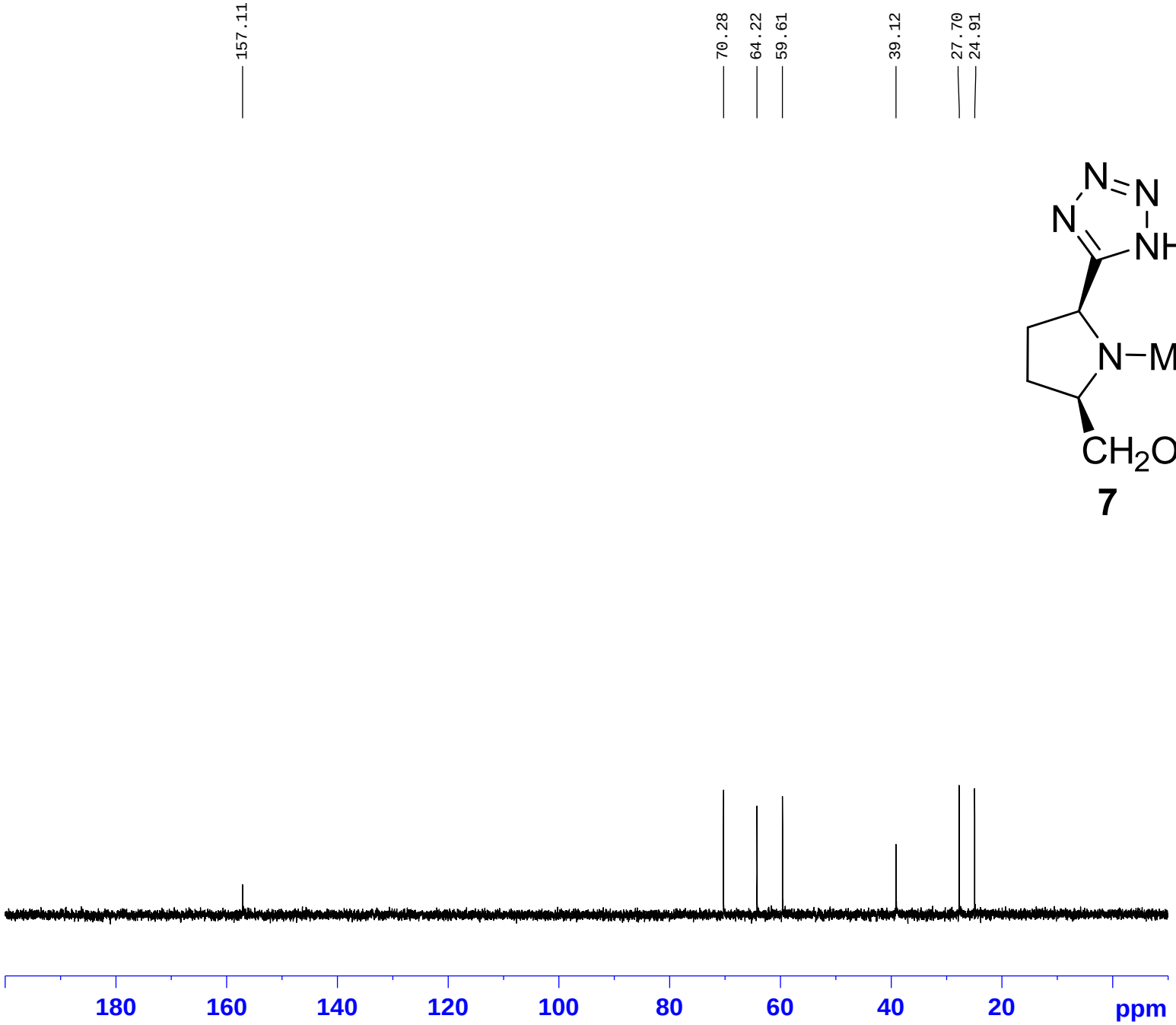
```
Current Data Parameters
NAME                 cp-p82
EXPNO                    80
PROCNO                    1

F2 - Acquisition Parameters
Date_              20111105
Time                   0.35
INSTRUM               spect
PROBHD   5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT                 D2O
NS                       16
DS                        0
SWH                8992.806 Hz
FIDRES             0.137219 Hz
AQ                 3.6438515 sec
RG                      256
DW                   55.600 usec
DE                    8.00 usec
TE                   296.8 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                   10.80 usec
PL1                   3.00 dB
SFO1          300.1324010 MHz

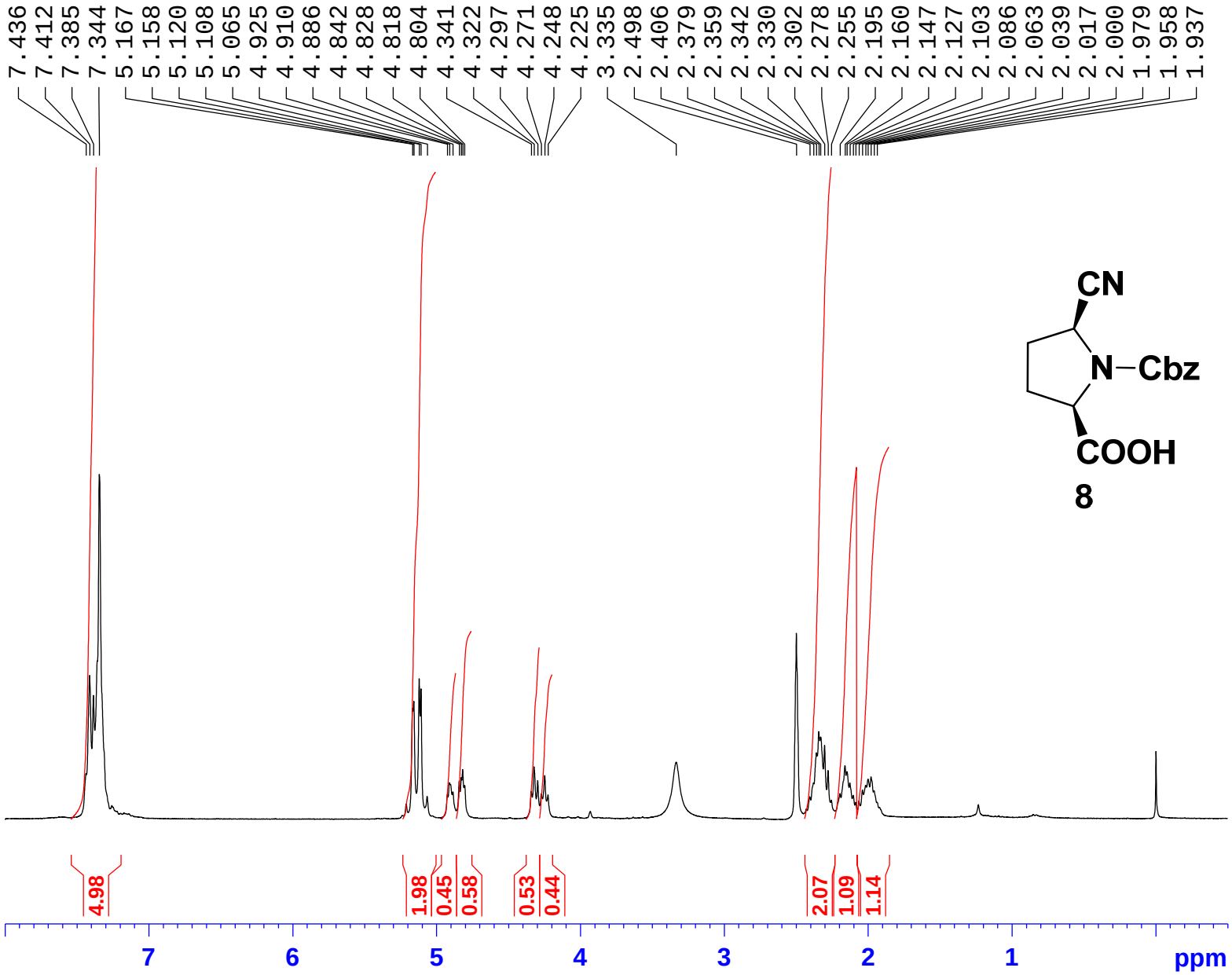
F2 - Processing parameters
SI                    32768
SF            300.1300268 MHz
WDW                      EM
SSB                       0
LB                   0.30 Hz
GB                        0
PC                    1.00
```




```
NAME              cp-p82
EXPNO                 11
PROCNO                 1
Date_           20111104
Time                10.54
INSTRUM             spect
PROBHD   5 mm DUL 13C-1
PULPROG            zgpg30
TD                  65536
SOLVENT               D2O
NS                     26
DS                      4
SWH            17985.611 Hz
FIDRES          0.274439 Hz
AQ              1.8219508 sec
RG                11585.2
DW                 27.800 usec
DE                  6.50 usec
TE                298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 12.50 usec
PL1                 2.00 dB
SFO1          75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              100.00 usec
PL2                  3.00 dB
PL12                22.33 dB
PL13                23.00 dB
SFO2         300.1312005 MHz
SI                 32768
SF            75.4677490 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

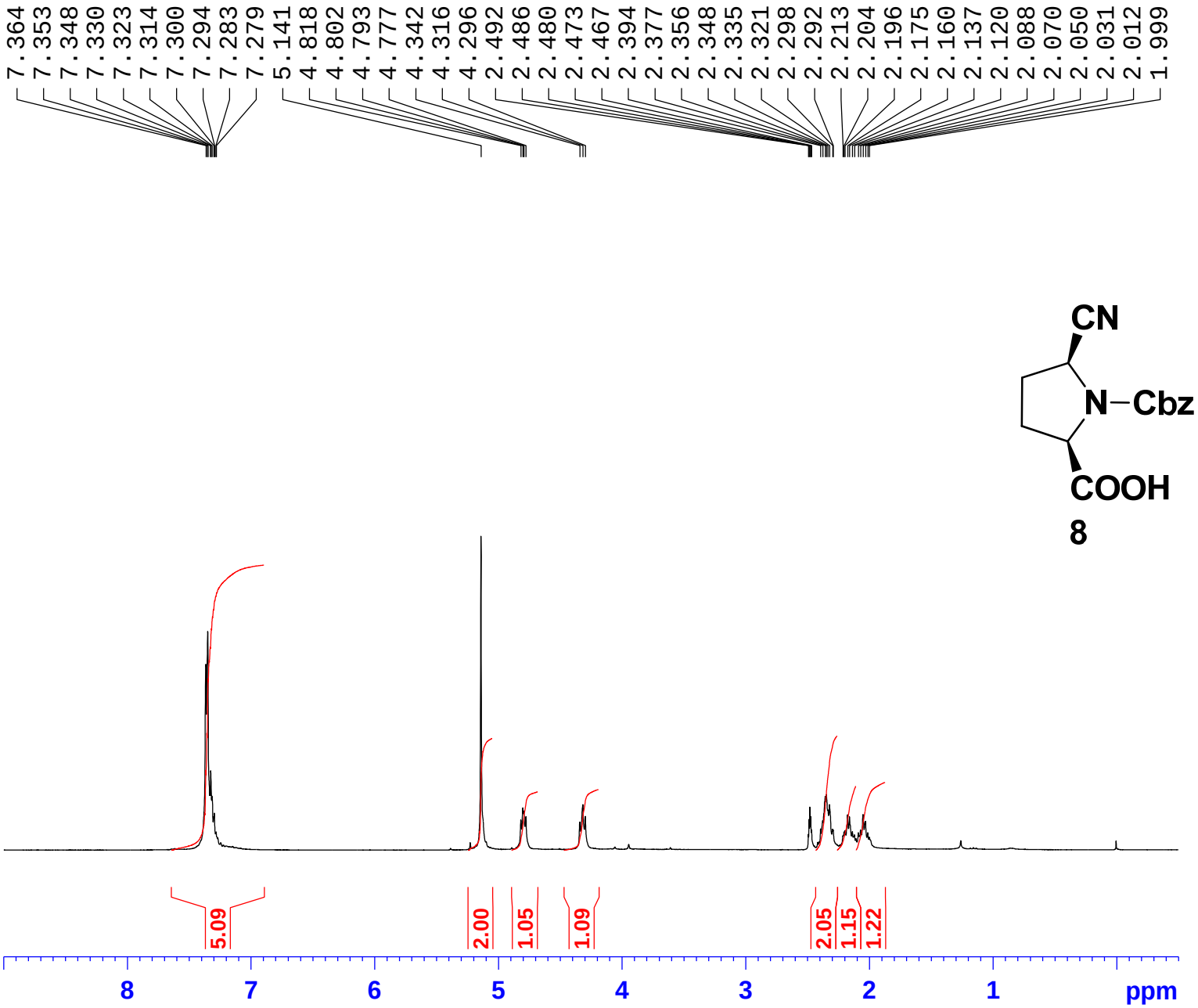



```
Current Data Parameters
NAME                  cp-p90
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20111022
Time                  10.55
INSTRUM               spect
PROBHD   5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                       16
DS                        0
SWH                8992.806 Hz
FIDRES             0.137219 Hz
AQ                 3.6438515 sec
RG                      256
DW                   55.600 usec
DE                    8.00 usec
TE                   297.5 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                   10.80 usec
PL1                   3.00 dB
SFO1           300.1324010 MHz

F2 - Processing parameters
SI                    32768
SF             300.1300012 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                    1.00
```

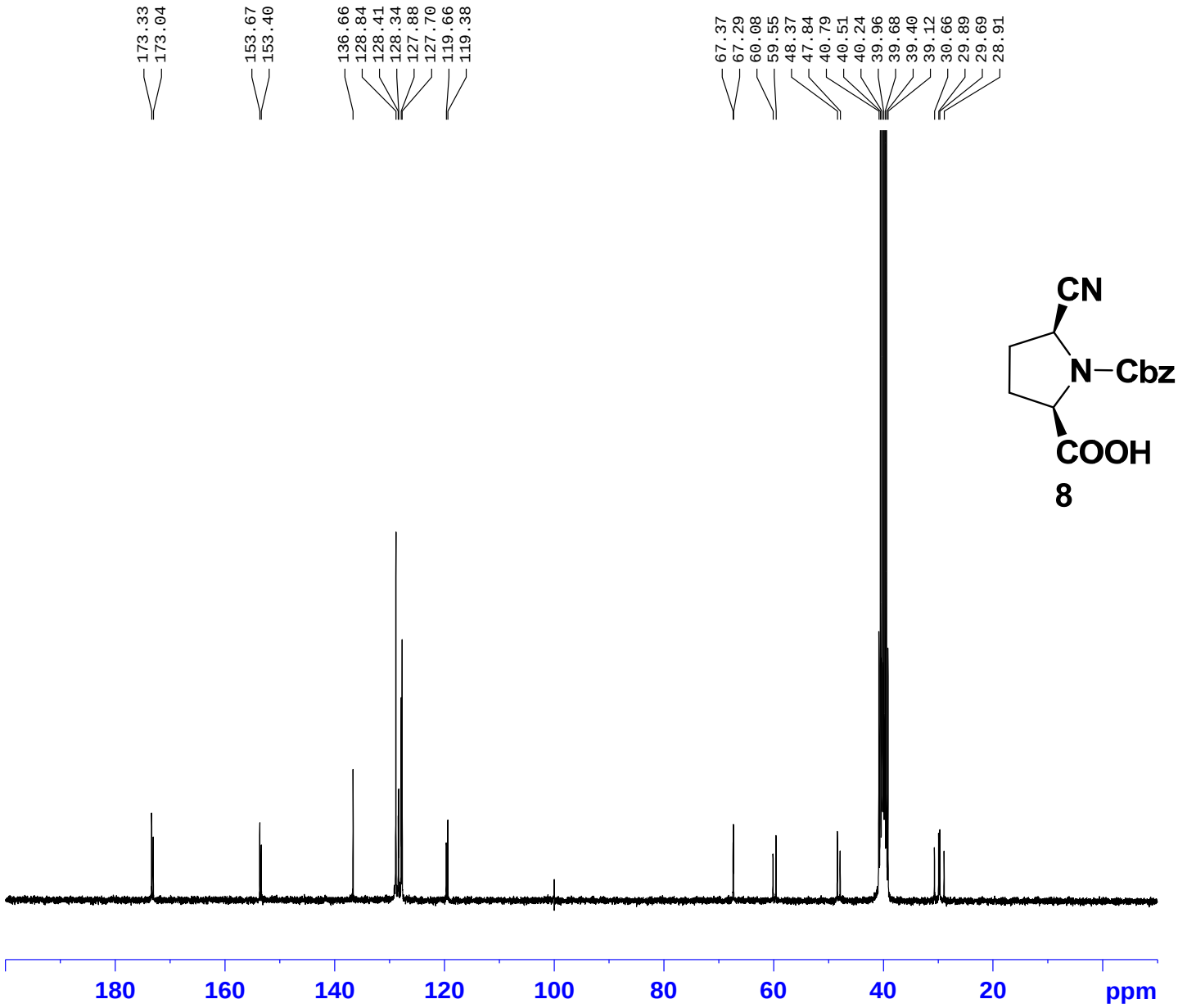



```
Current Data Parameters
NAME            p90 375K
EXPNO                415
PROCNO                 1

F2 - Acquisition Parameters
Date_           20111031
Time               17.02
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                    16
DS                     0
SWH             8992.806 Hz
FIDRES          0.274439 Hz
AQ             1.8219508 sec
RG                  2048
DW                55.600 usec
DE                 6.00 usec
TE                375.1 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 13.80 usec
PL1                 3.00 dB
SFO1         300.1315007 MHz

F2 - Processing parameters
SI                 32768
SF           300.1300071 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```



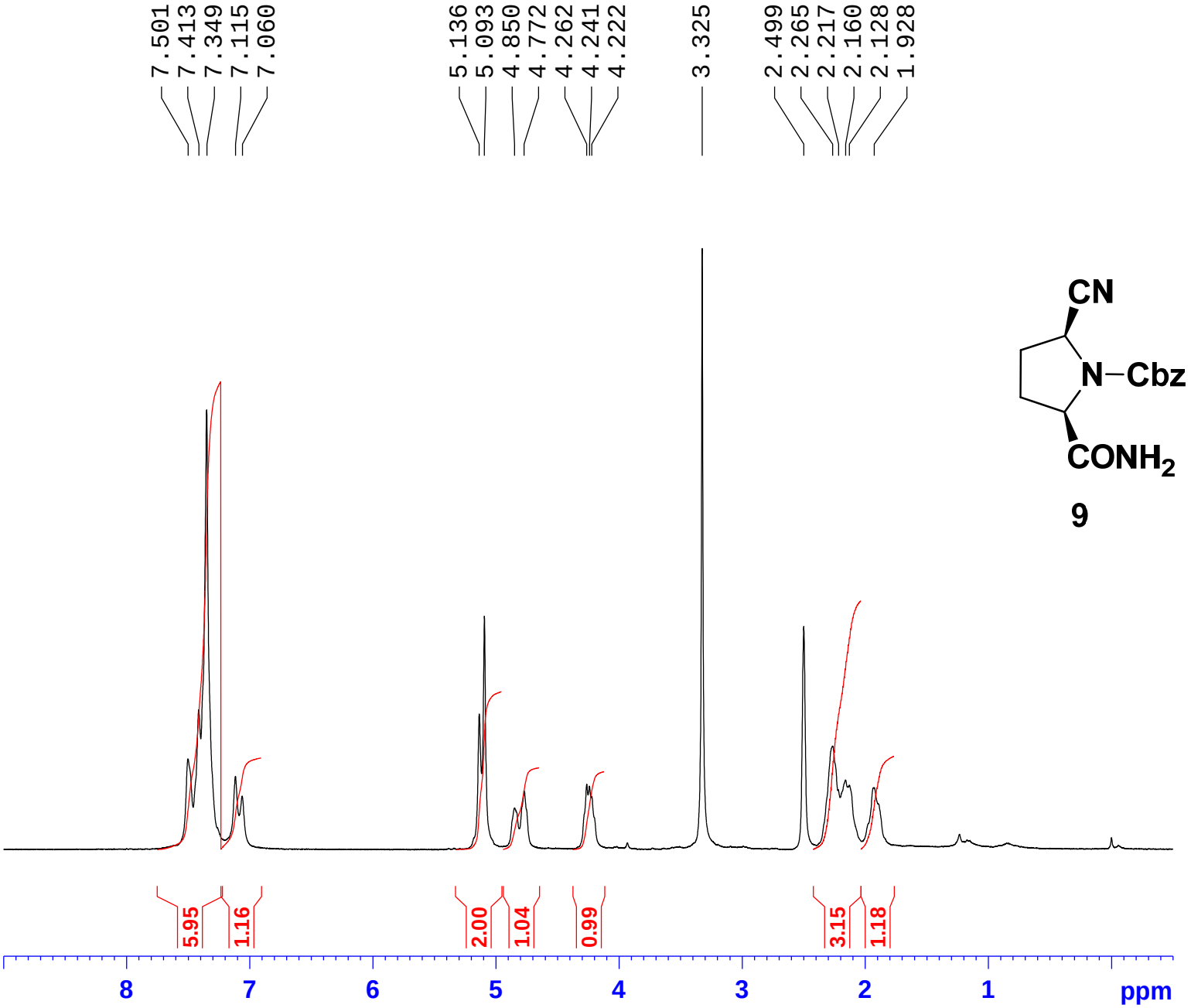

```
Current Data Parameters
NAME                  cp-p90
EXPNO                      3
PROCNO                     1

F2 - Acquisition Parameters
Date_              20111022
Time                  11.25
INSTRUM               spect
PROBHD   5 mm DUL 13C-1
PULPROG              zgig30
TD                    32768
SOLVENT                DMSO
NS                     3216
DS                        0
SWH              18832.393 Hz
FIDRES            0.574719 Hz
AQ                0.8700404 sec
RG                  11585.2
DW                   26.550 usec
DE                    8.00 usec
TE                   297.2 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                    12.50 usec
PL1                    2.00 dB
SFO1           75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               100.00 usec
PL2                    3.00 dB
PL12                  22.33 dB
SFO2          300.1312005 MHz

F2 - Processing parameters
SI                    32768
SF             75.4677490 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```



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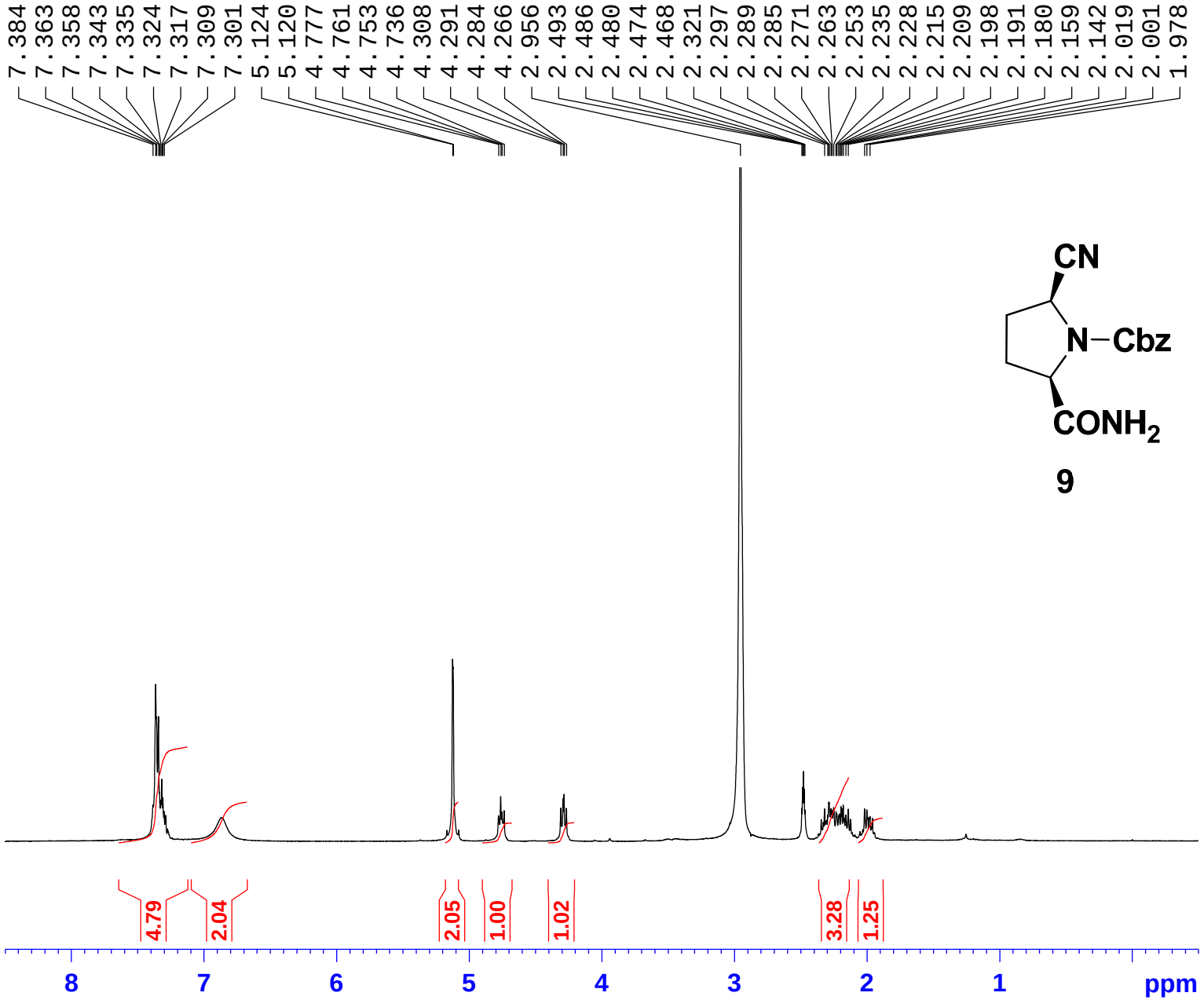
NAME	cp-p91
EXPNO	20
PROCNO	1
Date_	20111103
Time	19.57
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	0
SWH	8992.806 Hz
FIDRES	0.137219 Hz
AQ	3.6438515 sec
RG	256
DW	55.600 usec
DE	8.00 usec
TE	298.8 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.80 usec
PL1	3.00 dB
SFO1	300.1324010 MHz
SI	32768
SF	300.1300009 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



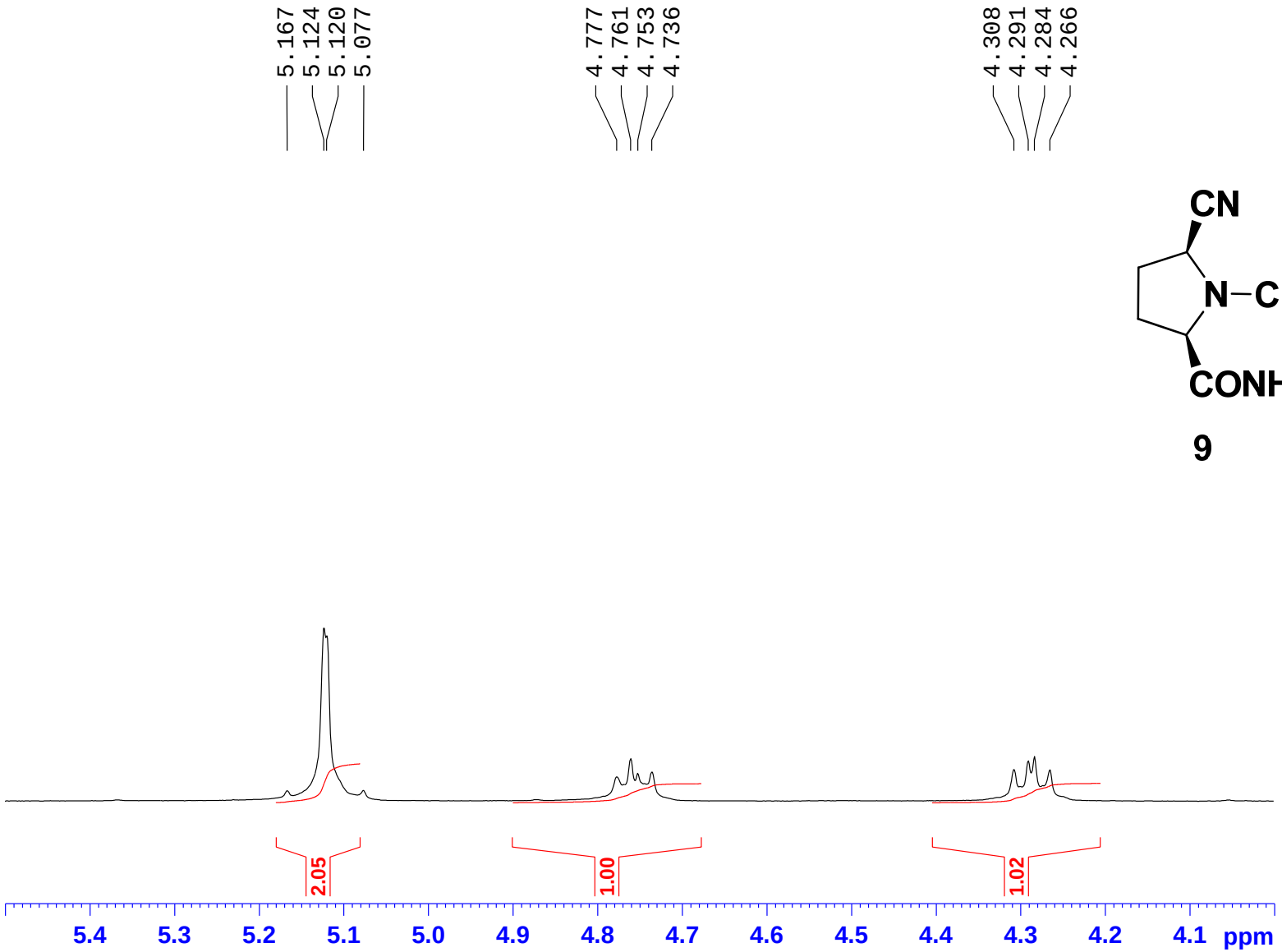
9

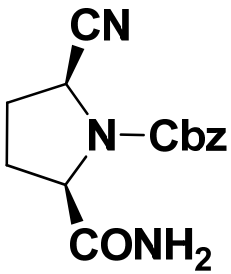
```
Current Data Parameters
NAME                 shengwen
EXPNO                     424
PROCNO                      1

F2 - Acquisition Parameters
Date_               20111110
Time                    8.35
INSTRUM                spect
PROBHD   5 mm BBO BB-1H
PULPROG                 zg30
TD                     32768
SOLVENT                 DMSO
NS                        16
DS                         0
SWH                 8992.806 Hz
FIDRES              0.274439 Hz
AQ                  1.8219508 sec
RG                      2048
DW                    55.600 usec
DE                     6.00 usec
TE                     372.9 K
D1                 2.00000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                      13.80 usec
PL1                      3.00 dB
SFO1             300.1315007 MHz

F2 - Processing parameters
SI                         32768
SF               300.1300071 MHz
WDW                        EM
SSB                         0
LB                       0.30 Hz
GB                          0
```





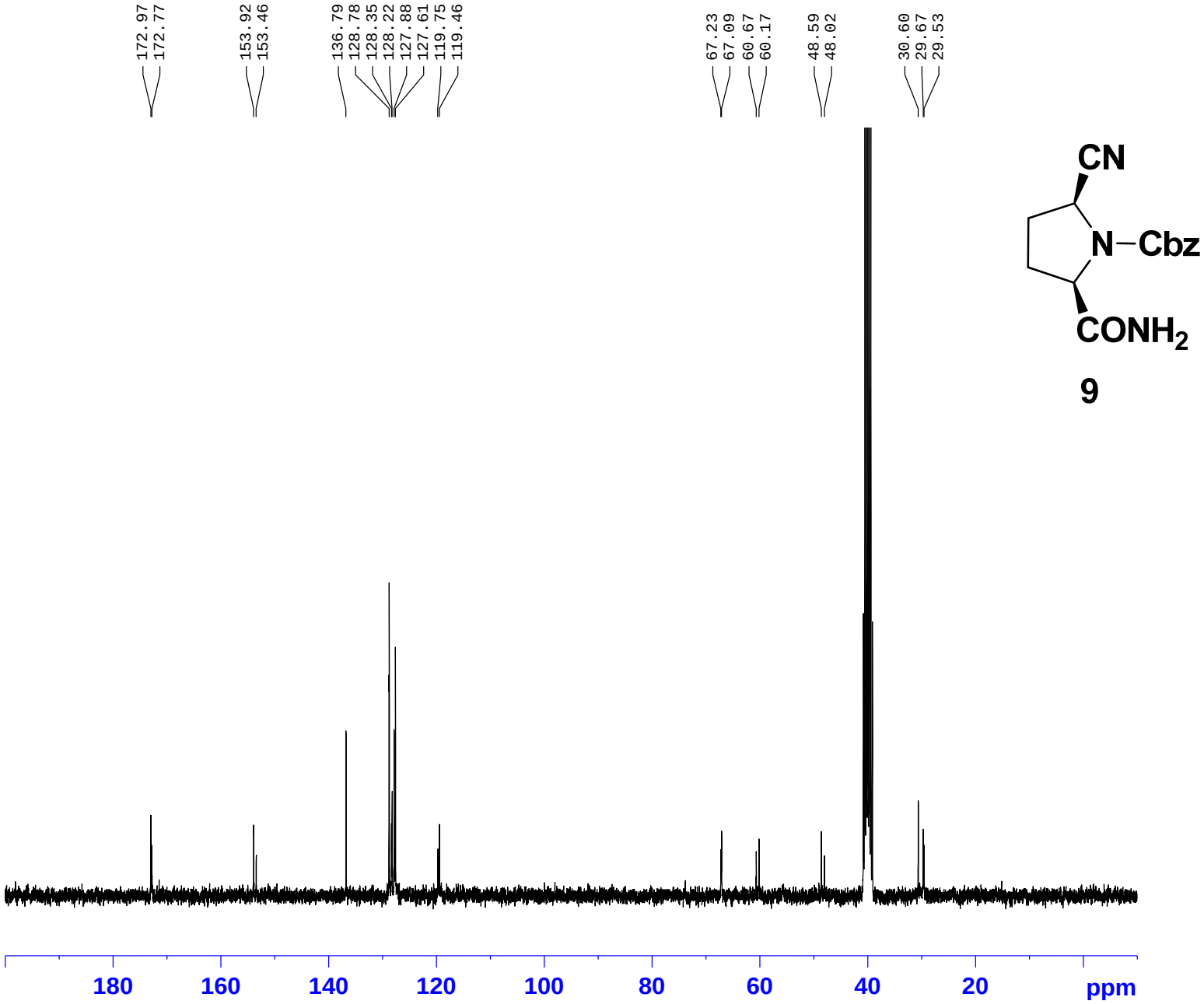
9

```
Current Data Parameters
NAME                  shengwen
EXPNO                      424
PROCNO                       1

F2 - Acquisition Parameters
   :e_                20111110
   ıe                     8.35
   ;TRUM                 spect
   )BHD   5 mm BBO BB-1H
   .PROG                  zg30
                         32768
   .VENT                  DMSO
                            16
                             0
   ł                8992.806 Hz
   )RES                0.274439 Hz
                     1.8219508 sec
                          2048
                        55.600 usec
                         6.00 usec
                         372.9 K
D1                  2.00000000 sec
MCREST              0.00000000 sec
MCWRK               0.01500000 sec

======== CHANNEL f1 ========
NUC1                        1H
P1                       13.80 usec
PL1                       3.00 dB
SFO1                300.1315007 MHz

F2 - Processing parameters
SI                         32768
SF                  300.1300071 MHz
WDW                           EM
SSB                            0
LB                          0.30 Hz
GB                             0
```



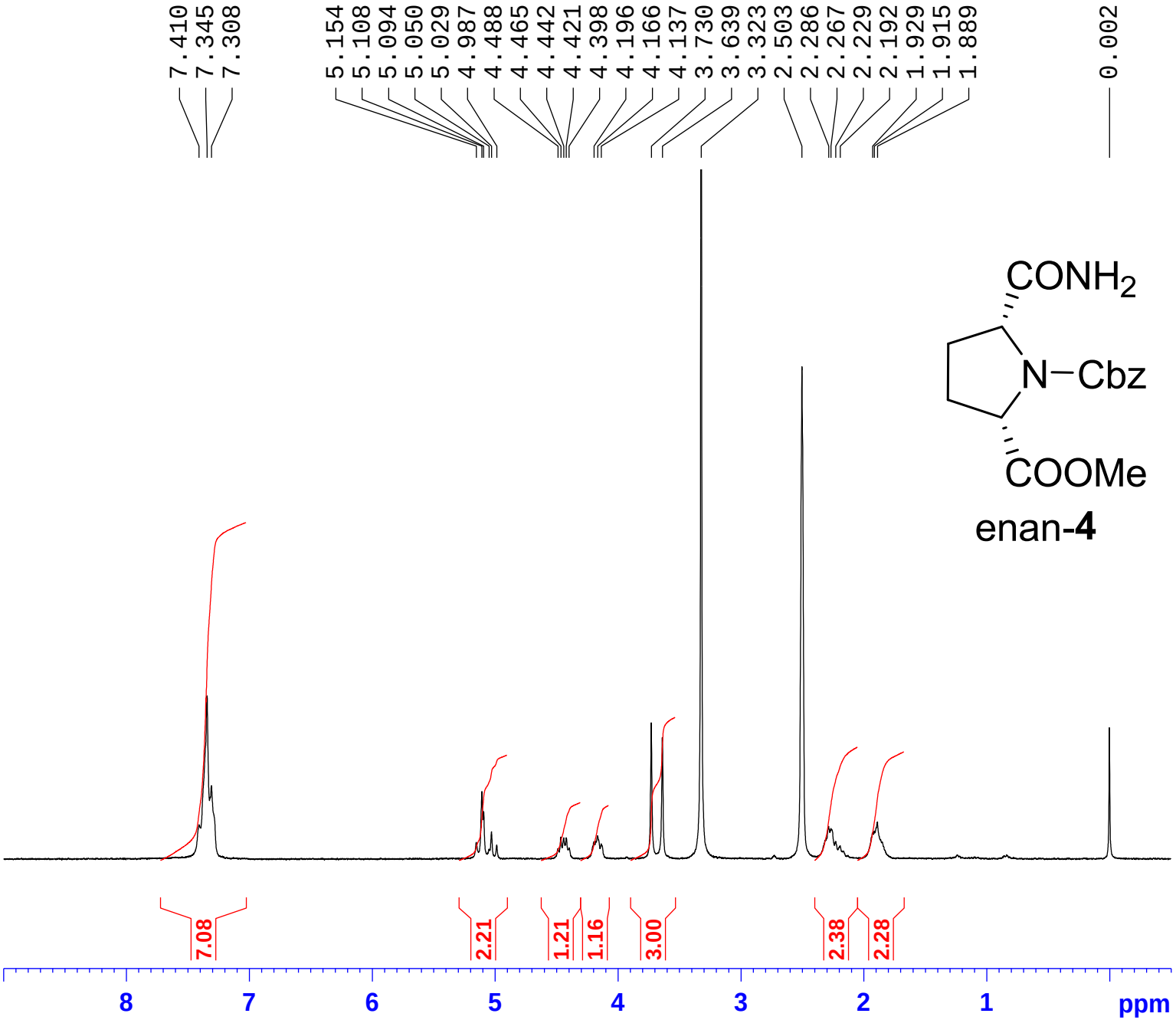

```
Current Data Parameters
NAME                  cp-p91
EXPNO                     13
PROCNO                     1

F2 - Acquisition Parameters
Date_              20111103
Time                   11.51
INSTRUM                spect
PROBHD   5 mm DUL 13C-1
PULPROG              zgig30
TD                    32768
SOLVENT                DMSO
NS                     1119
DS                        0
SWH               18832.393 Hz
FIDRES             0.574719 Hz
AQ                 0.8700404 sec
RG                      256
DW                    26.550 usec
DE                     8.00 usec
TE                    297.8 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                    12.50 usec
PL1                    2.00 dB
SFO1             75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                    1H
PCPD2                100.00 usec
PL2                    3.00 dB
PL12                  22.33 dB
SFO2            300.1312005 MHz

F2 - Processing parameters
SI                    32768
SF               75.4677490 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

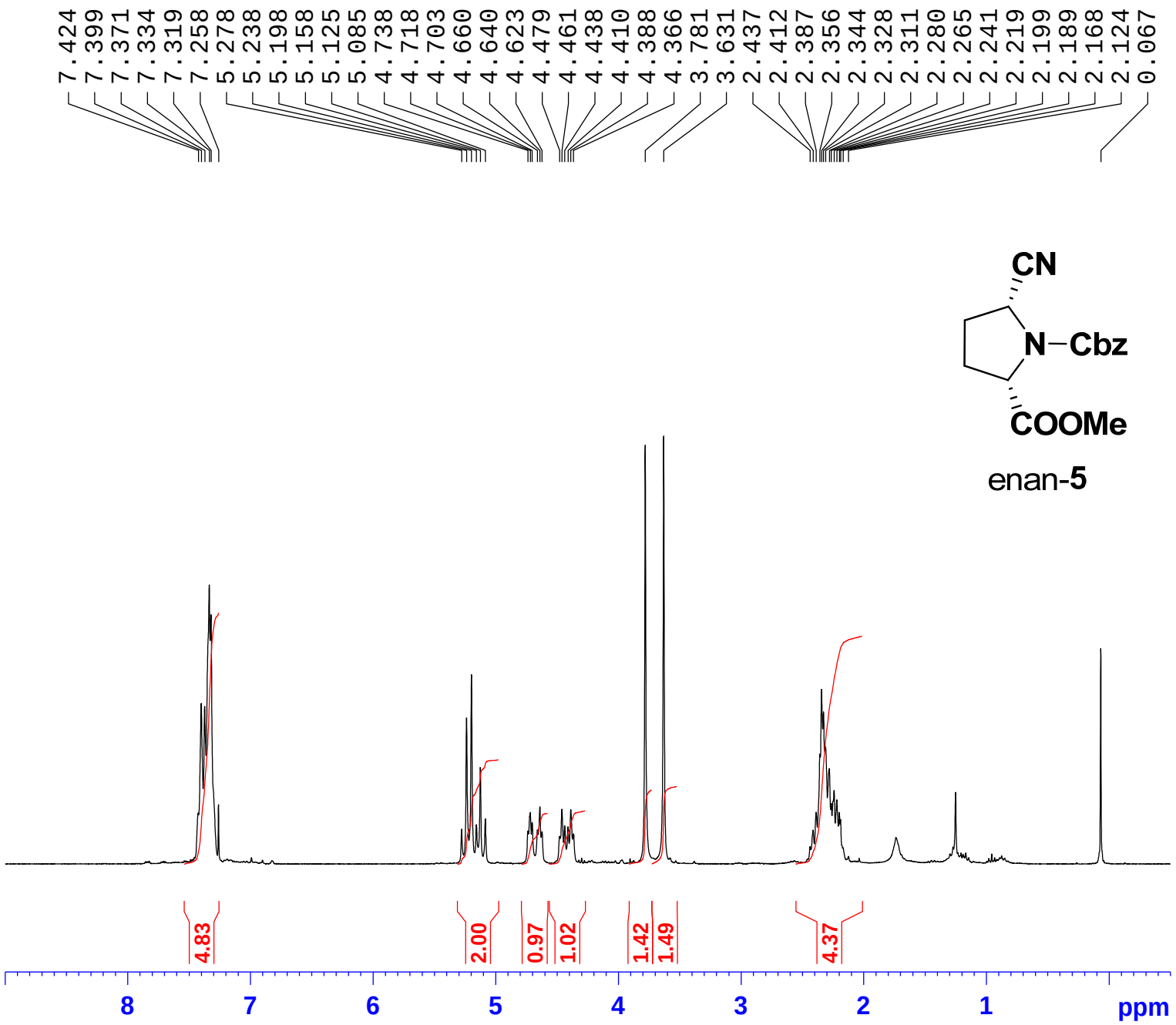



```
Current Data Parameters
NAME                  cp-p13e
EXPNO                     190
PROCNO                      1

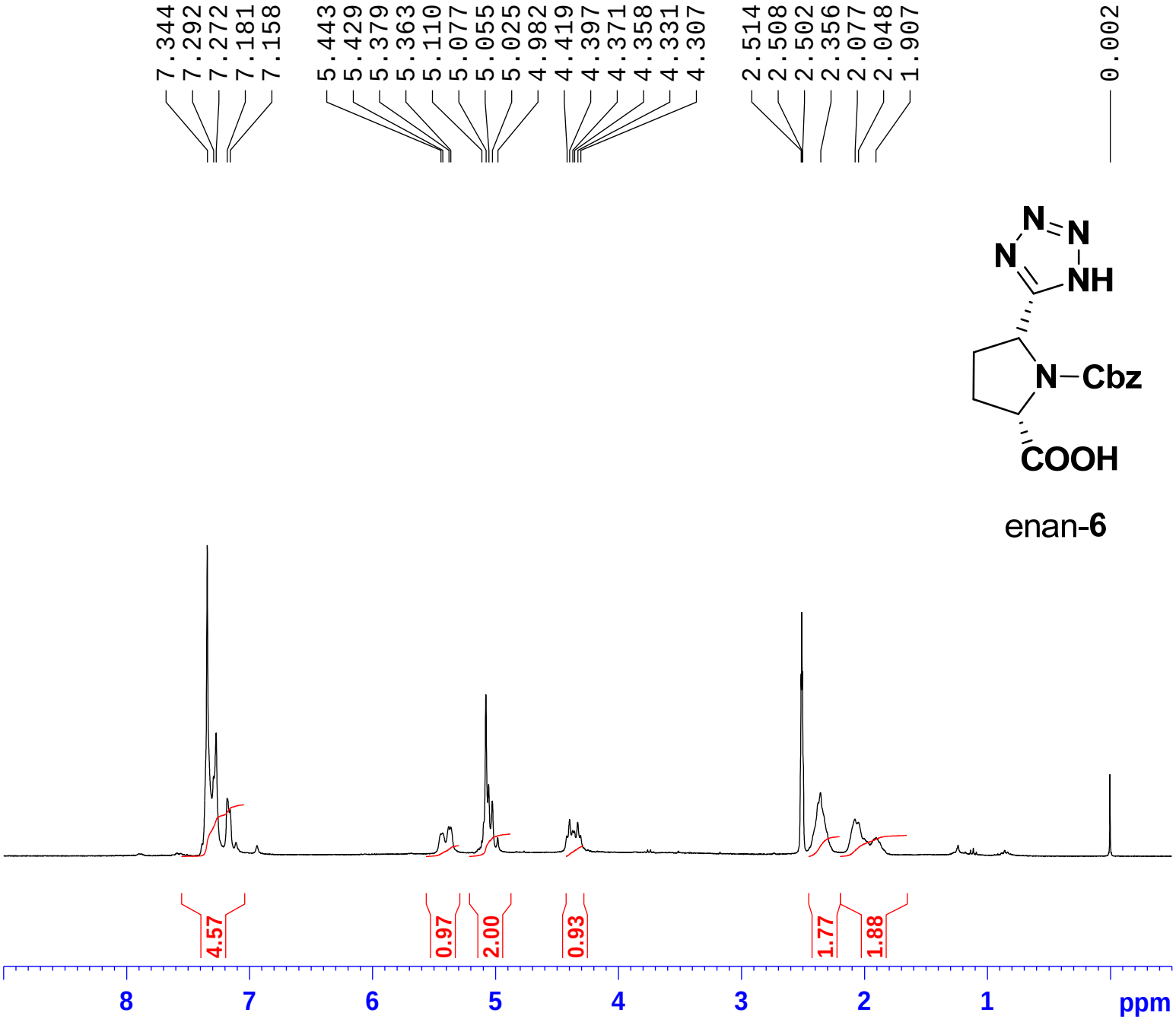
F2 - Acquisition Parameters
Date_                20111024
Time                    15.49
INSTRUM                 spect
PROBHD   5 mm DUL 13C-1
PULPROG                  zg30
TD                      32768
SOLVENT                  DMSO
NS                         16
DS                          0
SWH                  8992.806 Hz
FIDRES               0.274439 Hz
AQ                   1.8219508 sec
RG                        512
DW                     55.600 usec
DE                      8.00 usec
TE                     297.8 K
D1                2.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      10.80 usec
PL1                      3.00 dB
SFO1             300.1318008 MHz

F2 - Processing parameters
SI                      32768
SF               300.1300000 MHz
WDW                        EM
SSB                         0
LB                      0.30 Hz
GB                          0
PC                      1.00
```



NAME	cp-p35e	
EXPNO	10	
PROCNO	1	
Date_	20111104	
Time	19.21	
INSTRUM	spect	
PROBHD	5 mm DUL 13C-1	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	0	
SWH	8992.806	Hz
FIDRES	0.137219	Hz
AQ	3.6438515	sec
RG	181	
DW	55.600	usec
DE	8.00	usec
TE	297.0	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	10.80	usec
PL1	3.00	dB
SFO1	300.1324010	MHz
SI	32768	
SF	300.1300266	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

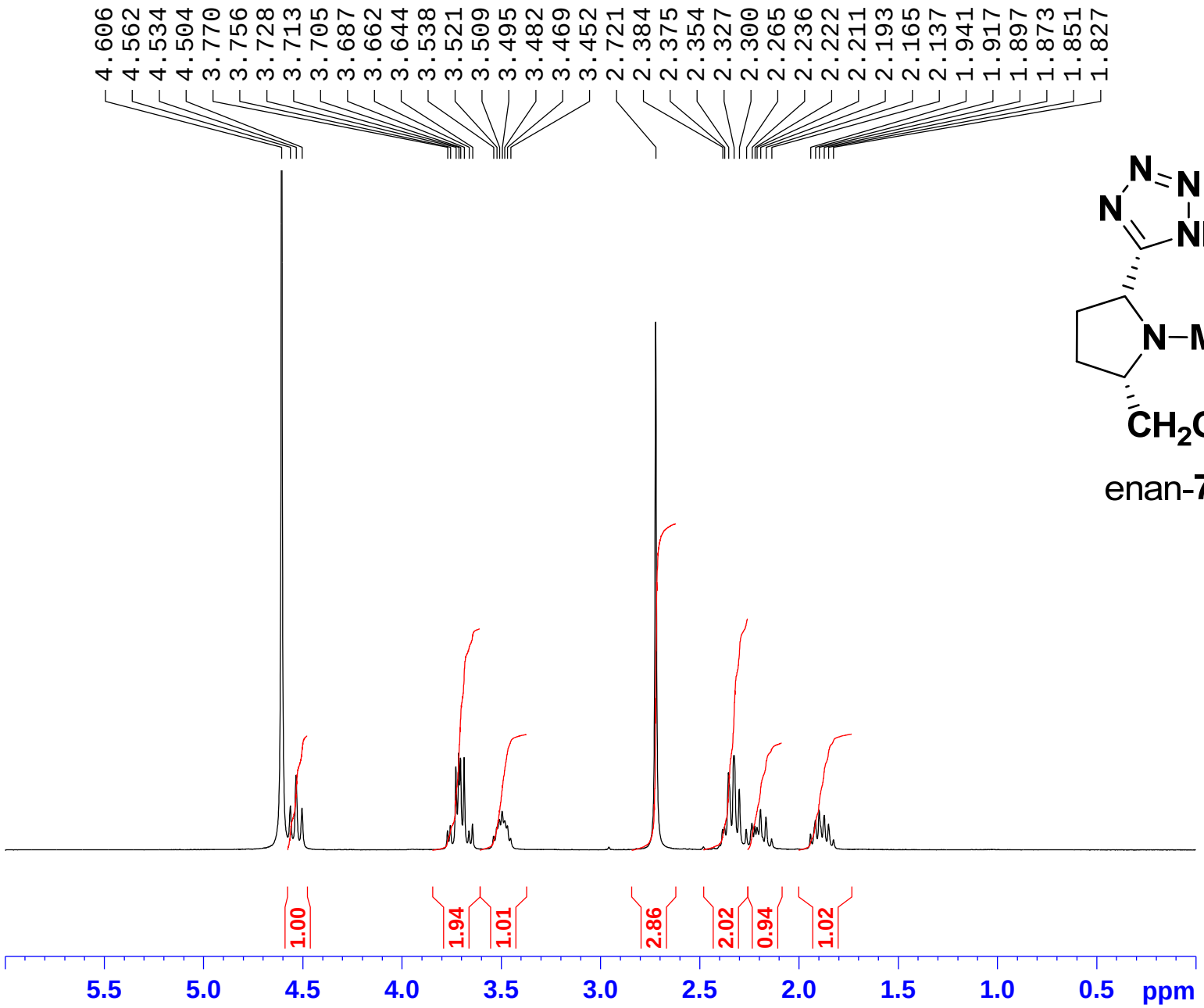


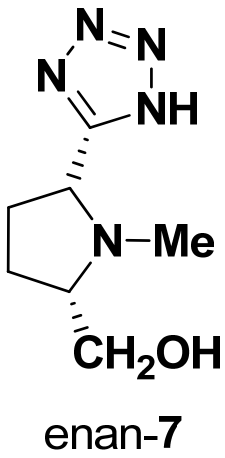

```
Current Data Parameters
NAME          cp-p80-3e
EXPNO                12
PROCNO                1

F2 - Acquisition Parameters
Date_          20111105
Time               1.57
INSTRUM           spect
PROBHD   5 mm DUL 13C-1
PULPROG            zg30
TD                65536
SOLVENT            DMSO
NS                   16
DS                    0
SWH            8992.806 Hz
FIDRES         0.137219 Hz
AQ            3.6438515 sec
RG                  256
DW               55.600 usec
DE                8.00 usec
TE               296.5 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                1H
P1              10.80 usec
PL1              3.00 dB
SFO1       300.1324010 MHz

F2 - Processing parameters
SI                 32768
SF         300.1299984 MHz
WDW                   EM
SSB                   0
LB               0.30 Hz
GB                    0
PC                 1.00
```





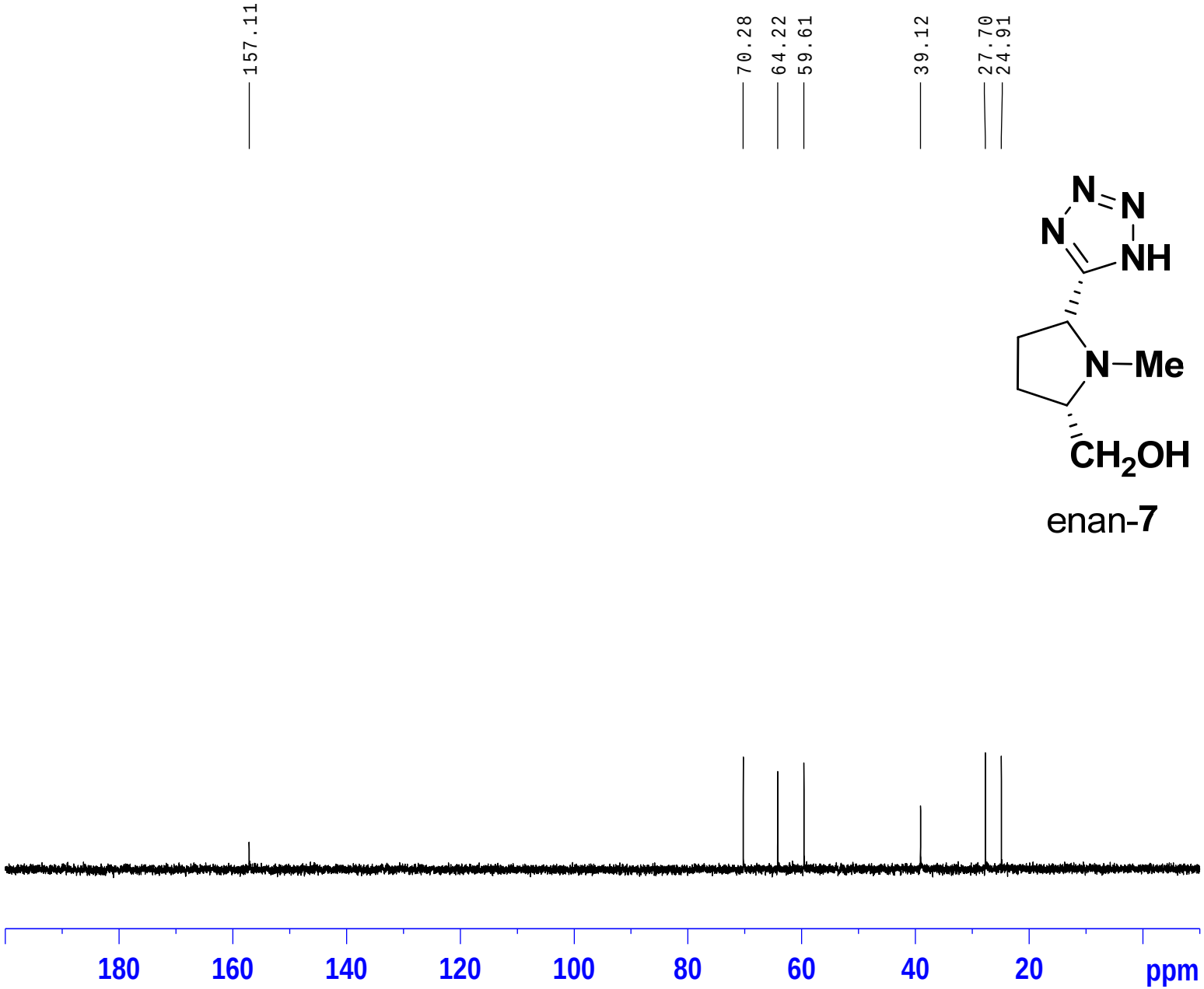
enan-7

```
Current Data Parameters
NAME                  cp-p82e
EXPNO                      14
PROCNO                      1

F2 - Acquisition Parameters
  te_                 20111105
  me                      0.32
  STRUM                 spect
  OBHD    5 mm DUL 13C-1
  LPROG                  zg30
                        65536
  LVENT                   D2O
                           16
                            0
  H                  8992.806 Hz
  DRES               0.137219 Hz
                    3.6438515 sec
                          256
                     55.600 usec
                      8.00 usec
                      296.9 K
                  1.00000000 sec
  0                         1

====== CHANNEL f1 ========
  C1                       1H
                     10.80 usec
PL1                   3.00 dB
SFO1          300.1324010 MHz

F2 - Processing parameters
SI                       32768
SF            300.1300268 MHz
WDW                         EM
SSB                          0
LB                    0.30 Hz
GB                           0
PC                    1.00
```



NAME	cp-p82e
EXPNO	11
PROCNO	1
Date_	20111103
Time	10.54
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	D2O
NS	26
DS	4
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	11585.2
DW	27.800 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	12.50 usec
PL1	2.00 dB
SFO1	75.4752953 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	100.00 usec
PL2	3.00 dB
PL12	22.33 dB
PL13	23.00 dB
SFO2	300.1312005 MHz
SI	32768
SF	75.4677490 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40