Supplementary Material (ESI) for Chemical Communications

Supplementary Information

"On-Water" Conjugate Additions of Anilines

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General Experimental:

Toluene was freshly distilled from sodium / benzophenone. All other solvents and reagents were used as received from commercial sources. Melting points were determined using a Stanford Research Systems Optimelt automated melting point system and are uncorrected. Infrared spectra were acquired on a Shimadzu FTIR-8400S or Bruker Alpha-E ATR spectrometer as a solution between sodium chloride plates, or neat. Absorption maxima are expressed in wavenumbers (cm^{-1}). ^{1}H and ^{13}C NMR spectra were recorded on a Bruker AVANCE DPX300, or Bruker DPX400 spectrometer (^{1}H frequencies 300, 400 MHz; ^{13}C frequencies 75 and 100 MHz respectively). ^{1}H chemical shifts are expressed as parts per million (ppm) with residual chloroform (δ 7.26) or tetramethylsilane as reference and are reported as chemical shift (δ_H); relative integral; multiplicity (s = singlet, br = broad, d = doublet, t = triplet, dd = doublet of doublets, dt = doublet of triplets, q = quartet, m = multiplet); and coupling constants (*J*) reported in Hz. ^{13}C NMR chemical shifts are expressed as parts per million (ppm) with residual chloroform (δ 77.1) as internal reference and are reported as chemical shift (δ_C); multiplicity (assigned from DEPT experiments). High resolution mass spectra were recorded on a Bruker ApexII Fourier Transform Ion Cyclotron Resonance mass spectrometer with a 7.0 T magnet, fitted with an off-axis Analytica electrospray source.

N-Acryloyl-2,5-dimethylpyrrole (**5**)

Acrylamide (500 mg, 7.03 mmol), 2,5-hexanedione (180 μL, 1.53 mmol) and *p*-toluenesulfonic acid (39 mg, 0.23 mmol) were dissolved in toluene (60 mL) and heated to reflux for 24 hours under continuous azeotropic distillation. The solution was washed with water (3 × 50 mL), dried over Na_2SO_4 and the solvent was removed. The residue was purified *via* column chromatography (5% diethyl ether in hexanes) to give the *title compound* (125 mg, 55%) as a bright yellow oil. R_f: 0.69 (10% ethyl acetate in hexanes); ν_{max} (neat)/cm^{-1} 2927, 1693, 1619, 1401, 1363, 1258, 976, 773; δ_H (300 MHz, $CDCl_3$): 6.69 (1 H, dd, *J* 9, 18), 6.45 (1 H, dd, *J* 3, 18), 5.94 (1 H, dd, *J* 3, 9), 5.84 (2 H, s), 2.34; δ_C (75 MHz, $CDCl_3$): 167.1 (C), 132.2 (CH), 131.3 (CH), 130.1 (C), 111.2 (CH), 15.7 (CH_3); *m/z* (APCI): 149 (M^+, 100%), 94 (62).

General "on-water" conditions

On-water reactions with methyl acrylate

Aniline (1.21 mmol, 1.1 equivalents) and methyl acrylate (100 μL, 1.11 mmol) were added to deionised water (4 mL) in a 21 mL screw-top vial and stirred vigorously for 24 hours. Dichloromethane (10 mL) was added, the phases were separated and the organic phase was dried over Na_2SO_4. The solvent was evaporated and the residue was purified by column chromatography.

On-water reactions with methyl vinyl ketone

Aniline (0.66 mmol, 1.1 equivalents) and methyl vinyl ketone (50 µL, 0.6 mmol) were added to deionised water (4 mL) in a 21 mL screw-top vial and stirred vigorously for 24 hours. Dichloromethane (10 mL) was added, the phases were separated and the organic phase was dried over Na_2SO_4. The solvent was evaporated and the residue was purified by column chromatography**.**

On-water reactions with N-acryloyl-2,5-dimethylpyrrole

Aniline (0.29 mmol, 1.1 equivalents) and *N*-acryloyl-2,5-dimethylpyrrole (**5**) (40 mg, 0.27 mmol) were added to deionised water (4 mL) in a 21 mL screw-top vial and stirred vigorously for 4 hours. Dichloromethane (10 mL) was added, the phases were separated and the organic phase was dried over Na_2SO_4. The solvent was evaporated and the residue was purified by column chromatography.

methyl 3-(phenylamino)propanoate[1]

R_f: 0.60 (50% ethyl acetate in hexanes); ν_{max} (neat)/cm^{-1} 3403, 2925, 1705, 1602, 1386, 1242, 750; δ_H (300 MHz, $CDCl_3$): 7.17 (2 H, t, *J* 6), 6.71 (1 H, t, *J* 6), 6.62 (2 H, d, *J* 6), 4.00 (1 H, br), 3.69 (3 H, s), 3.45 (2 H, t, *J* 6), 2.62 (2 H, t, *J* 6); δ_C (75 MHz, $CDCl_3$): 172.9 (C), 147.7 (C), 129.4 (CH), 117.9 (CH), 113.1 (CH), 51.8 (CH_3) 39.5 (CH_2), 33.8 (CH_2).

methyl 3-(*p*-tolylamino)propanoate[1]

R_f: 0.43 (20% ethyl acetate in hexanes); ν_{max} (neat)/cm^{-1} 3382, 2997, 1730, 1511, 1233, 831; δ_H (300 MHz, $CDCl_3$): 7.05 (2 H, d, *J* 9), 6.59 (2 H, d, *J* 9), 3.83 (1 H, br) 3.73 (3 H, s), 3.46 (2 H, t, *J* 6), 2.64 (2 H, t, *J* 6), 2.29 (3 H, s); δ_C (75 MHz, $CDCl_3$): 172.8 (C), 145.3 (C), 129.8 (CH), 126.9 (C), 115.0 (CH), 113.2 (CH), 51.6 (CH_3), 39.8 (CH_2), 33.7 (CH_2), 20.3 (CH_3).

methyl 3-(2,4-dimethylphenylamino)propanoate

HRMS (ESI) found: MH^+, 208.13321 $C_{12}H_{18}NO_2$ requires 208.13375; R_f: 0.60 (50% ethyl acetate in hexanes); ν_{max} (neat)/cm^{-1} 3401, 2953, 1735, 1619, 1176, 805; δ_H (300 MHz, $CDCl_3$): 6.92 (1 H, d, *J* 9), 6.88 (1 H, s), 6.53 (1 H, d, *J* 6), 3.79 (1 H, br), 3.68 (3 H, s), 3.46 (2 H, t, *J* 6), 2.64 (2 H, t, *J* 6), 2.21 (3 H, s), 2.09 (3 H, s); δ_C (75 MHz, $CDCl_3$): 173.5 (C), 143.6 (C), 131.3 (CH), 127.6 (CH), 126.7 (C), 123.1 (C), 110.4 (CH), 52.2 (CH_3), 39.9 (CH_2), 33.9 (CH_2), 20.5 (CH_3), 17.5 (CH_3); *m/z* (ESI): 209 (MH^+, 100%), 134 (37).

methyl 3-(4-methoxyphenylamino)propanoate[1]

R_f: 0.36 (50% ethyl acetate in hexanes); ν_{max} (neat)/cm^{-1} 3386, 2995, 1730, 1511, 1233, 819; δ_H (300 MHz, $CDCl_3$): 6.78 (2 H, d, *J* 9), 6.59 (2 H, d, *J* 9), 3.74 (3 H, s), 3.69 (3 H, s), 3.39 (2 H, t, *J* 6), 2.59 (2 H, t, *J* 6); δ_C (75 MHz,

$CDCl_3$): 172.9 (C), 152.5 (C), 141.8 (CH), 115.0 (CH), 114.6 (CH), 55.8 (CH_3), 51.7 (CH_3), 40.6 (CH_2), 33.8 (CH_2).

methyl 3-(4-bromophenylamino)propanoate

R_f: 0.81 (30% ethyl acetate in hexanes); v_{max} (neat)/cm^{-1} 3395, 2951, 1731, 1596, 1504, 1195, 815; δ_H (300 MHz, $CDCl_3$): 7.25 (2 H, d, *J* 9), 6.50 (2 H, d, *J* 9), 4.11 (1 H, br), 3.70 (3 H, s), 3.42 (2 H, t, *J* 6), 2.61 (2 H, t, *J* 6); δ_C (75 MHz, $CDCl_3$): (75 MHz, $CDCl_3$): 172.8 (C), 146.7 (C), 132.2 (CH), 114.7 (CH), 109.5 (C), 51.9 (CH_s), 39.6 (CH_2), 33.7 (CH_2); *m/z* (APCI): 258/260 (MH^+, 100%), 184/186 (75).

methyl 3-(4-hydroxyphenylamino)propanoate

HRMS (ESI) found: MH^+, 196.09682 $C_{10}H_{14}NO_3$ requires 196.09737; mp: 93.5 °C; R_f: 0.39 (50% ethyl acetate in hexanes); v_{max} (neat)/cm^{-1} 3305, 2953, 1719, 1514, 1177, 810; δ_H (300 MHz, $CDCl_3$): 6.68 (2 H, d, *J* 9), 6.55 (2 H, d, *J* 9), 4.41 (2 H, br), 3.70 (3 H, s), 3.38 (2 H, t, *J* 6), 2.60 (2 H, t, *J* 6); δ_C (75 MHz, $CDCl_3$): 173.3 (C), 148.5 (C), 141.5 (C), 116.4 (CH), 115.3 (CH), 51.9 (CH_3), 40.6 (CH_2), 33.8 (CH_2); *m/z* (ESI): 196 (MH^+, 100%), 122 (11).

dimethyl 3,3′-(4-hydroxyphenylazanediyl)dipropanoate

HRMS (ESI) found: MNa^+, 304.11554 $C_{14}H_{19}NO_5Na$ requires 304.11609; R_f: 0.53 (50% ethyl acetate in hexanes); v_{max} (neat)/cm^{-1} 3356, 2951, 1717, 1511, 1177, 810; δ_H (300 MHz, $CDCl_3$): 6.76 (2 H, d, *J* 9), 6.69 (2 H, d, *J,* 9), 4.81 (2 H, br), 3.66 (3 H, s), 3.51 (2 H, t, *J* 6), 2.52 (2 H, t, *J* 6); δ_C (75 MHz, $CDCl_3$): 172.9 (C), 148.8 (C), 141.6 (C), 117.2 (CH), 116.4 (CH), 51.8 (CH_3), 48.4 (CH_2), 32.6 (CH_2). *m/z* (ESI): 304 (MNa^+, 100%), 282 (MNa^+, 77), 208 (10).

methyl 3-(phenylthio)propanoate[2]

R_f: 0.37 (10% ethyl acetate in hexanes); v_{max} (neat)/cm^{-1} 2951, 1733, 1481, 1282, 893; δ_H (300 MHz, $CDCl_3$): 7.34-7.16 (5 H, m), 3.63 (3 H, s), 3.12 (2 H, t, *J* 6), 2.59 (2 H, t, *J* 6); δ_C (75 MHz, $CDCl_3$): 172.0 (C), 135.2 (C), 130.0 (CH), 129.0 (CH), 126.5 (CH), 51.7 (CH_3), 34.1 (CH_2), 29.0 (CH_2).

methyl 3-(*p*-tolylthio)propanoate[2]

R_f: 0.39 (10% ethyl acetate in hexanes); v_{max} (neat)/cm^{-1} 2951, 1733, 1435, 1282, 804; δ_H (300 MHz, $CDCl_3$): 7.27 (2 H, d, *J* 9), 7.09 (2 H, d, *J* 9), 3.65 (3 H, s), 3.09 (2 H, t, *J* 6), 2.58 (2 H, t, *J* 6), 2.30 (3 H, s); δ_C (75 MHz, $CDCl_3$): 172.3 (C), 136.9 (C), 131.4 (C), 131.1 (CH), 129.9 (CH), 51.8 (CH_3), 34.4 (CH_2), 29.9 (CH_2), 21.1 (CH_3).

methyl 3-(4-bromophenylthio)propanoate

HRMS (ESI) found: MNa^+, 296.95581/298.95380 $C_{10}H_{11}BrO_2SNa$ requires 296.95608/298.95404; mp: 49 – 50 °C; R_f: 0.65 (20% ethyl acetate in hexanes); v_{max} (neat)/cm^{-1} 2948, 1728, 1366, 1176, 809; δ_H (300 MHz,

$CDCl_3$): 7.25 (2 H, d, *J* 9), 7.06 (2 H, d, *J* 9), 3.52 (3 H, s), 2.98 (2 H, t, *J* 6), 2.45 (2 H, t, *J* 6); δ_C (75 MHz, $CDCl_3$): 172.0 (C), 134.6 (C), 132.1 (CH), 131.6 (CH), 120.5 (CH), 51.9 (CH_3), 34.1 (CH_2), 29.1 (CH_2); *m/z* (APCI): 273/275 (M^+, 15%), 214/216 (100), 188/186 (37), 149 (24), 119 (24).

4-(phenylamino)butan-2-one[1]

R_f: 0.19 (15% ethyl acetate in hexanes); v_{max} (neat)/cm^{-1} 3394 , 2900, 1708, 1601, 1504, 1168, 749; δ_H (300 MHz, $CDCl_3$): 7.21 (2 H, t, *J* 6), 6.73 (1 H, t, *J* 6), 6.62 (2 H, d, *J* 6), 3.98 (1 H, br), 3.42 (2 H, t, *J* 6), 2.73 (2 H, t, *J* 6), 2.16 (3 H, s); δ_C (75 MHz, $CDCl_3$): 208.1 (C), 147.8 (C), 129.3 (CH), 117.6 (CH), 113.0 (CH), 42.6 (CH_2), 38.4 (CH_2), 30.3 (CH_3).

4-(*p*-tolylamino)butan-2-one[1]

R_f: 0.28 (20% ethyl acetate in hexanes); v_{max} (neat)/cm^{-1} 3379 , 2918, 1708, 1518, 1168, 808; δ_H (300 MHz, $CDCl_3$): 7.01 (2 H, d, *J* 9), 6.56 (2 H, d, *J* 9), 3.64 (1 H, br), 3.39 (2 H, t, *J* 6), 2.72 (2 H, t, *J* 6), 2.26 (3 H, s), 2.16 (3 H, s); δ_C (75 MHz, $CDCl_3$): 208.1 (C), 145.4 (C), 129.8 (CH), 126.8 (C), 113.3 (CH), 42.6 (CH_2), 38.8 (CH_2), 30.2 (CH_3), 20.3(CH_3).

4,4′-(*p*-tolylazanediyl)dibutan-2-one[1]

R_f: 0.25 (20% ethyl acetate in hexanes); v_{max} (neat)/cm^{-1} 2918, 1708, 1518, 1168, 808; δ_H (300 MHz, $CDCl_3$): 7.05 (2 H, d, *J* 9), 6.61 (2 H, d, *J* 9), 3.54 (4 H, t, *J* 6), 2.69 (4 H, t, *J* 6), 2.25 (3 H, s), 2.14 (6 H, s); δ_C (75 MHz, $CDCl_3$): 208.0 (C), 145.1 (C), 130.1 (CH), 126.8 (C), 113.8 (CH), 46.3 (CH_2), 41.3 (CH_2), 30.7 (CH_3), 20.3 (CH_3).

4-(2,4-dimethylphenylamino)butan-2-one

HRMS (ESI) found: MH^+, 192.13829 $C_{12}H_{18}NO$ requires 192.13884; R_f: 0.34 (20% ethyl acetate in hexanes); v_{max} (neat)/cm^{-1} 3412, 2917, 1709, 1512, 1167, 804; δ_H (300 MHz, $CDCl_3$): 6.99 (1 H, d, *J* 9), 6.94 (1 H, s), 6.60 (1 H, d, *J* 9), 3.76 (1 H, br), 3.48 (2 H, t, *J* 6), 2.80 (2 H, t, *J* 6), 2.29 (3 H, s), 2.20 (3 H, s), 2.15 (3 H, s); δ_C (75 MHz, $CDCl_3$): 208.2 (C), 143.4 (C), 131.1 (CH), 127.3 (CH), 126.3 (C), 122.7 (C), 110.0 (CH), 42.6 (CH_2), 38.7 (CH_2), 30.2 (CH_3), 20.3 (CH_3), 17.3 (CH_3); *m/z* (ESI): 192 (MH^+, 100%), 88 (75).

4-(4-methoxyphenylamino)butan-2-one[1]

R_f: 0.28 (40% ethyl acetate in hexanes); v_{max} (neat)/cm^{-1} 3376, 2936, 1708, 1597, 1510, 1233, 820; δ_H (300 MHz, $CDCl_3$): 6.78 (2 H, d, *J* 9), 6.58 (2 H, d, *J* 9), 3.74 (3 H, s) 3.70 (1 H, br), 3.35 (2 H, t, *J* 6), 2.72 (2 H, t, *J* 6), 2.15 (3 H, s); δ_C (75 MHz, $CDCl_3$): 208.2 (C), 152.5 (C), 142.0 (C), 115.0 (CH), 114.7 (CH), 55.9 (CH_3), 42.8 (CH_2), 39.6 (CH_2), 30.3 (CH_3).

4,4′-(4-methoxyphenylaxanediyl)dibutan-2-one[1]

R_f: 0.25 (40% ethyl acetate in hexanes); ν_{max} (neat)/cm^{-1} 2930, 1708, 1597, 1510, 1233, 820; δ_H (300 MHz, $CDCl_3$): 6.84 (2 H, d, *J* 9), 6.72 (2 H, d, *J* 9), 3.76 (3 H, s), 3.45 (4 H, t, *J* 6), 2.64 (4 H, t, *J* 6), 2.13 (6 H, s); δ_C (75 MHz, $CDCl_3$): 208.3 (C), 153.6 (C), 142.3 (C), 117.4 (CH), 115.3 (CH), 56.1 (CH_3), 47.6 (CH_2), 41.7 (CH_2), 30.9 (CH_3).

4-(4-hydroxyphenylamino)butan-2-one and 4,4′-(4-hydroxyphenyl-azanediyl) dibutan-2-one

3 : 1 Mixture of mono- and bis- alkylation; R_f: 0.20 (50% ethyl acetate in hexanes); ν_{max} (neat)/cm^{-1} 3347, 1703, 1512, 1219, 823, 725; *4-(4-hydroxyphenylamino)-butan-2-one* HRMS (ESI): Found: MH^+, 180.10191 $C_{10}H_{14}$ N O_2 requires 180.10245; δ_H (300 MHz, $CDCl_3$): 6.68 (2 H, d, *J* 9), 6.53 (2 H, d, *J* 9), 4.90 (2 H, br), 3.32 (2 H, t, *J* 6), 2.69 (2 H, t, *J* 6), 2.15 (6 H, s); δ_C (75 MHz, $CDCl_3$): 209.1 (C), 148.4 (C), 141.3 (C), 116.4 (CH), 115.6 (CH), 42.6 (CH_2), 40.1 (CH_2), 30.4 (CH_s). *4,4'-(4-hydroxyphenylazanediyl)-dibutan-2-one* HRMS (ESI): Found: MNa^+, 272.12572 $C_{14}H_{19}NO_3Na$ requires 272.12626; δ_H (300 MHz, $CDCl_3$): 3.40 (4 H, t, *J* 6), 2.61 (4 H, t, *J* 6), 2.11 (6 H, s); δ_C (75 MHz, $CDCl_3$): 209.0 (C), 149.0 (C), 141.6 (C), 118.1 (CH), 117.3 (CH), 47.7 (CH_2), 41.4 (CH_2), 30.6 (CH_s); *m/z* (ESI): 250 (MH^+, 34%), 214 (100), 180 (MH^+, 29), 122 (15).

4-(4-bromophenylamino)butan-2-one

HRMS (ESI): Found: MH^+, 242.01762/244.01557 $C_{10}H_{11}BrO_2SNa$ requires 242.01750/244.01546; R_f: 0.35 (15% ethyl acetate in hexanes); ν_{max} (neat)/cm^{-1} 3380, 2892, 1702, 1597, 1503, 1313, 814; δ_H (300 MHz, $CDCl_3$): 7.20 (2 H, d, *J* 9), 6.44 (2 H, d, *J* 9), 4.02 (1 H, br), 3.31 (2 H, t, *J* 6), 2.68 (2 H, t, *J* 6), 2.12 (3 H, s); δ_C (75 MHz, $CDCl_3$): 173.3 (C), 148.5 (C), 141.5 (C), 116.4 (CH), 115.3 (CH), 51.9 (CH_3), 40.6 (CH_2), 33.8 (CH_2); *m/z* (APCI): 242/244 (M^+, 100%).

4-(2,4,5-trichlorophenylamino)butan-2-one

mp: 71.3 – 71.8 °C; R_f: 0.41 (20% ethyl acetate in hexanes); ν_{max} (neat)/cm^{-1} 3382, 2916, 1715, 1596, 1510, 1379; δ_H (300 MHz, $CDCl_3$): 7.31 (1 H, s), 6.70 (1 H, s), 4.64 (1 H, br), 3.43 (2 H, q, *J* 6), 2.78 (2 H, t, *J* 6), 2.20 (3 H, s); δ_C (75 MHz, $CDCl_3$): 207.1 (C), 143.3 (C), 131.8 (C), 130.2 (CH), 119.5 (C), 118.2 (C), 111.9 (CH), 42.3 (CH_2), 38.2 (CH_2), 30.4 (CH_3); *m/z* (APCI): 265/267 (MH^+, 45%), 201/203 (100).

4-(phenylthio)butan-2-one[2]

R_f: 0.27 (10% ethyl acetate in hexanes); ν_{max} (neat)/cm^{-1} 2951, 1712, 1480, 1359, 1158, 737; δ_H (300 MHz, $CDCl_3$): 7.33-7.14 (5 H, m), 3.10 (2 H, t, *J* 6), 2.72 (2 H, t, *J* 6), 2.10 (3 H, s); δ_C (75 MHz, $CDCl_3$): 206.4 (C), 135.7 (C), 129.3 (CH), 128.9 (CH), 126.2 (CH), 42.9 (CH_2), 29.9 (CH_3), 27.3 (CH_2).

4-(*p*-tolylthio)butan-2-one[2]

R_f: 0.33 (20% ethyl acetate in hexanes); ν_{max} (neat)/cm^{-1} 2925, 1716, 1493, 1361, 806; δ_H (300 MHz, $CDCl_3$): 7.27 (2 H, d, *J* 9), 7.12 (2 H, d, *J* 9), 3.09 (2 H, t, *J* 6), 2.73 (2 H, t, *J* 6), 2.33 (3 H, s), 2.14 (3 H, s); δ_C (75 MHz, $CDCl_3$): 206.8 (C), 136.6 (C), 131.9 (C), 130.5 (CH), 129.9 (CH), 43.3 (CH_2), 30.1 (CH_3), 28.3 (CH_2), 21.1 (CH_3).

4-(4-bromophenylthio)butan-2-one

HRMS (ESI) found: $MONa^+$, 296.95553/298.95372 $C_{10}H_{11}BrO_2SNa$ requires 296.95608/298.95404; mp: 62.1 °C; R_f: 0.25 (20% ethyl acetate in hexanes); ν_{max} (neat)/cm^{-1} 2925, 1712, 1472, 1092, 906, 728; δ_H (300 MHz, $CDCl_3$): 7.39 (2 H, d, *J* 9), 7.17 (2 H, d, *J* 9), 3.10 (2 H, t, *J* 6), 2.74 (2 H, t, *J* 6), 2.14 (3 H, s); δ_C (75 MHz, $CDCl_3$): 206.2 (C), 135.1 (C), 132.0 (CH), 130.9 (CH), 120.1 (C), 42.8 (CH_2), 30.1 (CH_3), 27.5 (CH_2); *m/z* (APCI): 273/275 (MO^+, 100%), 201/203 (63), 162/164 (17), 122 (24).

***N*-(3-(2,5-dimethyl-1*H*-pyrrol-1-yl)-3-oxo-prop-1-yl)-aniline**

HRMS (ESI) found: MH^+, 243.14919 $C_{15}H_{19}N_2O$ requires 243.14191; R_f: 0.21 (5% ethyl acetate in hexanes); ν_{max} (neat)/cm^{-1} 3403, 2925, 1705, 1602, 1386, 1242, 750; δ_H (300 MHz, $CDCl_3$): 7.16 (2 H, t, *J* 6), 6.70 (1 H, t, *J* 6), 6.61 (2 H, d, *J* 6), 5.81 (2 H, s), 4.12 (1 H, br), 3.58 (2 H, t, *J* 6), 3.04 (2 H, t, *J* 6), 2.37 (6 H, s); δ_C (75 MHz, $CDCl_3$): 173.5 (C), 147.6 (C), 130.7 (C), 129.5 (CH), 117.9 (CH), 113.2 (CH), 111.9 (CH), 39.5 (CH_2), 38.2 (CH_2), 17.1 (CH_3); *m/z* (APCI): 242 (M^+, 100%), 159 (44), 120 (16), 108 (20).

***N*-(3-(2,5-dimethyl-1*H*-pyrrol-1-yl)-3-oxo-prop-1-yl)-*p*-toluidine**

HRMS (ESI) found: MH^+, 257.16484 $C_{16}H_{21}N_2O$ requires 257.15756; R_f: 0.17 (5% ethyl acetate in hexanes); ν_{max} (neat)/cm^{-1} 3401, 2920, 1703, 1542, 1364, 1255, 980; δ_H (300 MHz, $CDCl_3$): 7.05 (2 H, d, *J* 9), 6.60 (2 H, d, *J* 9), 5.87 (2 H, s), 3.99 (1 H, br), 3.61 (2 H, t, *J* 6), 3.08 (2 H, t, *J* 6), 2.43 (6 H, s), 2.28 (3 H, s); δ_C (75 MHz, $CDCl_3$): 173.5 (C), 145.3 (C), 130.6 (C), 129.9 (CH), 127.1 (C), 113.4 (CH), 111.8 (CH), 39.8 (CH_2), 38.2 (CH_2), 20.4 (CH_3), 17.0 (CH_3); *m/z* (APCI): 257 (MH^+, 100%), 173 (12), 138 (29), 120 (100).

***N*-(3-(2,5-dimethyl-1*H*-pyrrol-1-yl)-3-oxo-prop-1-yl)-2,4-xylidine**

HRMS (ESI) found: MH^+, 271.18049 $C_{17}H_{23}N_2O$ requires 271.17321; R_f: 0.39 (10% ethyl acetate in hexanes); ν_{max} (neat)/cm^{-1} 3408, 2921, 1704, 1619, 1386, 1245; δ_H (300 MHz, $CDCl_3$): 6.92 (1 H, d, *J* 9), 6.87 (1 H, s), 6.56 (2 H, d, *J* 9), 5.81 (2 H, s), 3.61 (2 H, t, *J* 6), 3.04 (2 H, t, *J* 6), 2.38 (6 H, s), 2.21 (3 H, s), 2.08 (3 H, s); δ_C (75 MHz, $CDCl_3$): 173.7 (C), 143.2 (C), 131.4 (CH), 130.6 (C), 127.5 (CH), 126.6 (C), 122.9 (C), 111.9 (CH), 110.0 (CH), 39.7 (CH_2), 38.2 (CH_2), 20.4 (CH_3), 17.5 (CH_3), 17.0 (CH_3); *m/z* (APCI) 271 (M^+, 100%), 213 (19), 174 (25), 134 (87).

_N_-(3-(2,5-dimethyl-1_H_-pyrrol-1-yl)-3-oxo-prop-1-yl)-_p_-anisidine

HRMS (ESI) found: MH^+, 273.15975 $C_{16}H_{21}N_2O_2$ requires 273.15248; R_f: 0.18 (10% ethyl acetate in hexanes); ν_{max} (neat)/cm^{-1} 3397, 2929, 1705, 1513, 1331, 1239; δ_H (300 MHz, $CDCl_3$): 6.79 (2 H, d, *J* 9), 6.63 (2 H, d, *J* 9), 5.83 (2 H, s), 3.75 (3 H, s), 3.55 (2 H, t, *J* 6), 3.06 (2 H, t, *J* 6), 2.40 (6 H, s); δ_C (75 MHz, $CDCl_3$): 173.6 (C), 152.6 (C), 141.8 (C), 130.6 (C), 115.1 (CH), 114.8 (CH), 111.9 (CH), 55.0 (CH_3), 40.7 (CH_2), 38.3 (CH_2), 17.1 (CH_3); *m/z* (APCI): 273 (MH^+, 70%), 136 (100).

_N_-(3-(2,5-dimethyl-1_H_-pyrrol-1-yl)-3-oxo-prop-1-yl)-4-bromo-aniline

HRMS (ESI) found: MH^+, 321.05996/323.0596 $C_{15}H_{18}N_2OBr$ requires 321.05243/323.05038; R_f: 0.14 (5% ethyl acetate in hexanes); ν_{max} (neat)/cm^{-1} 3401, 2924, 1702, 1594, 1497, 1385, 1256, 813; δ_H (300 MHz, $CDCl_3$): 7.27 (2 H, d, *J* 9), 6.52 (2 H, d, *J* 9), 5.84 (2 H, s), 4.21 (1 H, br), 3.57 (2 H, t, *J* 6), 3.05 (2 H, t, *J* 6), 2.40 (6 H, s); δ_C (75 MHz, $CDCl_3$): 173.3 (C), 146.6 (C), 132.2 (CH), 130.7 (C), 114.7 (CH), 112.1 (CH), 109.5 (C), 39.5 (CH_2), 38.0 (CH_2), 17.1 (CH_3); *m/z* (APCI): 320/322 (M^+, 65%), 184/186 (100), 138 (70), 108 (11).

_N_-(3-(2,5-dimethyl-1_H_-pyrrol-1-yl)-3-oxo-prop-1-yl)-2,4,5-trichloro-aniline

HRMS (ESI) found: MH^+, 345.03246/347.02935 $C_{15}H_{16}N_2OCl_3$ requires 345.02500/345.02205; mp: 103 – 105.2 °C; R_f: 0.39 (10% ethyl acetate in hexanes); ν_{max} (neat)/cm^{-1} 3408, 2921, 1704, 1619, 1386, 1245; δ_H (300 MHz, $CDCl_3$): 7.32 (1 H, s), 6.75 (1 H, s), 5.85 (2 H, s), 4.82 (1 H, br), 3.63 (2 H, q, *J* 6), 3.09 (2 H, t, *J* 6), 2.41 (6 H, s); δ_C (75 MHz, $CDCl_3$): 172.7 (C), 143.3 (C), 131.9 (C), 130.8 (C), 130.3 (CH), 119.7 (C), 118.3 (C), 112.3 (CH), 111.9 (CH), 39.2 (CH_2), 38.0 (CH_2), 17.2 (CH_3); *m/z* (APCI): 345/347 (MH^+, 8%), 208/210 (100), 137 (22), 96 (33), 120 (11).

_N_-(3-(2,5-dimethyl-1_H_-pyrrol-1-yl)-3-oxo-prop-1-yl)-4-hydroxy-aniline

HRMS (ESI) found: MH^+, 259.14520 $C_{15}H_{19}N_2O_2$ requires 259.14465; R_f: 0.31 (25% ethyl acetate in hexanes); ν_{max} (neat)/cm^{-1} 3376, 2924, 1703, 1542, 1366, 1242; δ_H (300 MHz, $CDCl_3$): 6.68 (2 H, d, *J* 9), 6.57 (2 H, d, *J* 9), 5.83 (2 H, s), 4.69 (2 H, br), 3.52 (2 H, t, *J* 6), 3.04 (2 H, t, *J* 6), 2.39 (6 H, s); δ_C (75 MHz, $CDCl_3$): 173.8 (C), 148.7 (C), 141.2 (C), 130.7 (C), 116.5 (CH), 115.5 (CH), 112.0 (CH), 41.1 (CH_2), 38.0 (CH_2), 17.1 (CH_3); *m/z* (APCI): 259 (M^+, 100%), 162 (15), 122 (24).

_N,N'_-di-(3-(2,5-dimethyl-1_H_-pyrrol-1-yl)-3-oxo-prop-1-yl)-4-hydroxy-aniline

HRMS (ESI) found: MH^+, 408.22817 $C_{24}H_{30}N_3O_3$ requires 408.22872; mp: 136.4 °C; ν_{max} (neat)/cm^{-1} 2987, 1699, 1365, 1241, 777; δ_H (300 MHz, $CDCl_3$): 6.72 (4 H, dd, *J* 6, 9), 5.81 (2 H, s), 4.76 (1 H, br), 3.65 (4 H, t, *J* 6), 2.99 (2 H, t, *J* 6), 2.34 (6 H, s); δ_C (75 MHz, $CDCl_3$): 173.5 (C), 149.1 (C), 141.8 (C), 130.5 (C), 117.6 (CH), 116.5 (CH), 111.8 (CH), 48.9 (CH_2), 36.9 (CH_2), 16.8 (CH_3); *m/z* (APCI): 408 (M^+, 71%), 271 (100), 176 (19).

_S_-(3-(2,5-dimethyl-1_H_-pyrrol-1-yl)-3-oxo-prop-1-yl)-_p_-thiophenol

HRMS (ESI) found: MNa^+, 282.09231 $C_{15}H_{18}NOSNa$ requires 282.09285; mp: 53.2 – 54.0 °C; R_f: 0.40 (5% ethyl acetate in hexanes); ν_{max} (neat)/cm^{-1} 2928, 1709, 1367, 1265, 783; δ_H (300 MHz, $CDCl_3$): 7.37-7.20 (5 H, m), 5.81 (2 H, s), 3.29 (2 H, t, *J* 6), 3.08 (2 H, t, *J* 6), 2.34 (6 H, s); δ_C (75 MHz, $CDCl_3$): 172.8 (C), 135.3 (C), 130.6 (C), 130.4 (CH), 129.2 (CH), 126.9 (CH), 111.9 (CH), 38.9 (CH_2), 29.5 (CH_2), 16.9 (CH_3); *m/z* (APCI): 259 (M^+, 100%), 232 (95), 187 (39), 96 (30).

_S_-(3-(2,5-dimethyl-1_H_-pyrrol-1-yl)-3-oxo-prop-1-yl)-_p_-thiocresol

HRMS (ESI) found: MH^+, 274.12601 $C_{16}H_{20}NOS$ requires 274.11873; mp: 74.7 – 75.1 °C; R_f: 0.46 (5% ethyl acetate in hexanes); ν_{max} (neat)/cm^{-1} 2921, 1698, 1311 1276, 793; δ_H (300 MHz, $CDCl_3$): 7.28 (2 H, d, *J* 9), 7.10 (2 H, d, *J* 9), 5.80 (2 H, s), 3.26 (2 H, t, *J* 6), 3.03 (2 H, t, *J* 6), 2.33 (6 H, s), 2.31 (3 H, s); δ_C (75 MHz, $CDCl_3$): 172.9 (C), 137.2 (C), 131.4 (C), 131.3 (CH), 130.6 (C), 130.0 (CH), 111.8 (CH), 39.0 (CH_2), 30.2 (CH_2), 21.1 (CH_3), 16.9 (CH_3); *m/z* (APCI): 273 (M^+, 100%), 179 (41), 150 (24), 122 (16), 96 (10).

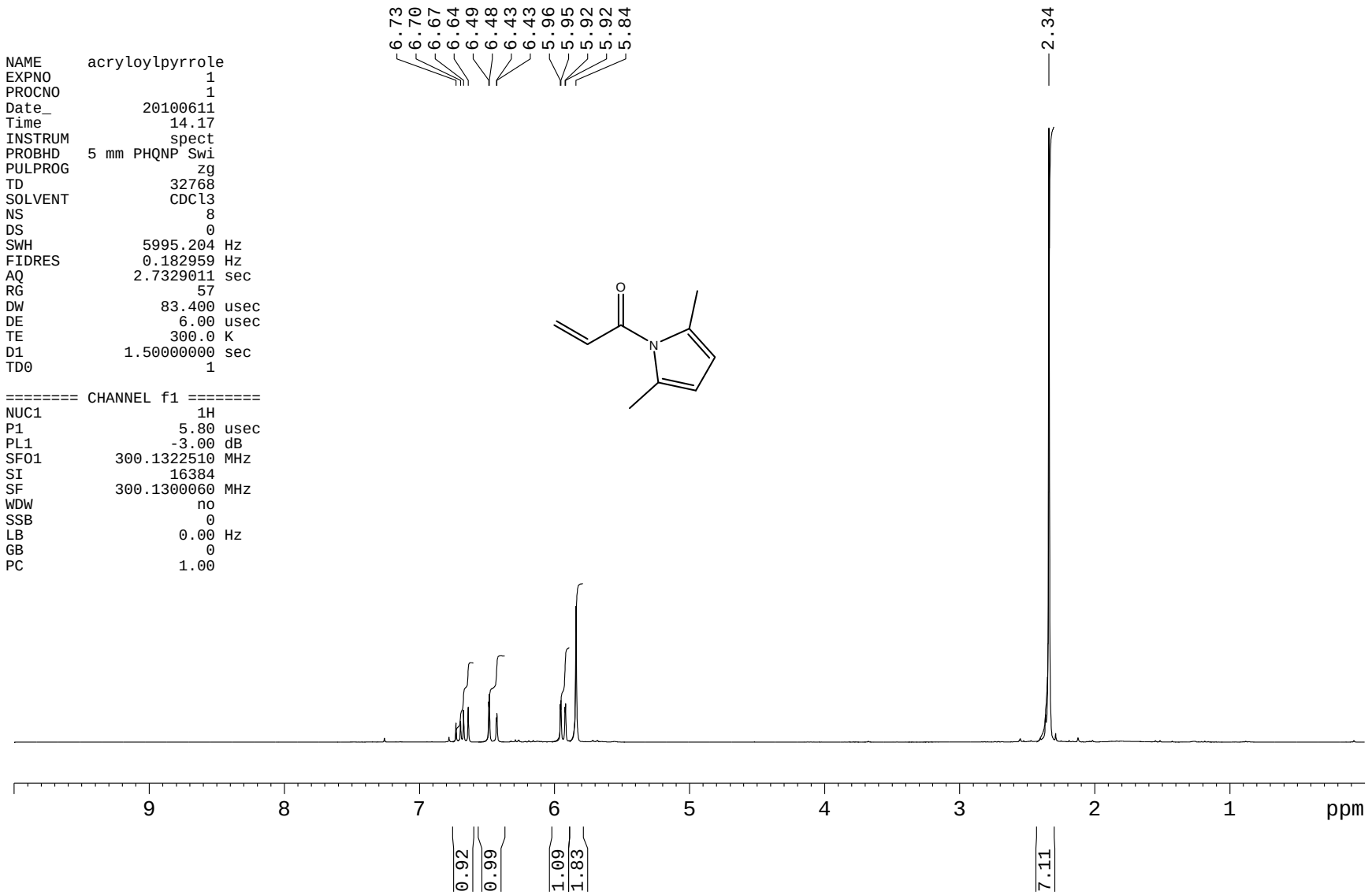
_S_-(3-(2,5-dimethyl-1_H_-pyrrol-1-yl)-3-oxo-prop-1-yl)-4-bromo-thiophenol

HRMS (ESI) found: MH^+, 338.02089/340.01878 $C_{15}H_{17}NOSBr$ requires 338.01360/340.01155; mp: 68.5 – 69 °C; R_f: 0.41 (5% ethyl acetate in hexanes); ν_{max} (neat)/cm^{-1} 2924, 1698, 1389 1278, 795; δ_H (300 MHz, $CDCl_3$): 7.40 (2 H, d, *J* 9), 7.20 (2 H, d, *J* 9), 5.81 (2 H, s), 3.27 (2 H, t, *J* 6), 3.05 (2 H, t, *J* 6), 2.34 (6 H, s); δ_C (75 MHz, $CDCl_3$): 172.5 (C), 134.7 (C), 132.2 (CH), 131.7 (CH), 130.6 (C), 120.7 (C), 112.0 (CH), 38.6 (CH_2), 29.5 (CH_2), 16.9 (CH_3); *m/z* (APCI): 337/339 (M^+, 100%), 215/217 (62), 201/203 (20), 150 (18), 112 (18).

References

[1] De, K.; Legros, J.; Crousse, B.; Bonnet-Delphon, D. *J. Org. Chem.* **2009**, *74*, 6260-6265

[2] Khatik, G. L.; Kumar, R.; Chakraborti, A. K. *Org. Lett.* **2006**, *8 (11)*, 2433-2436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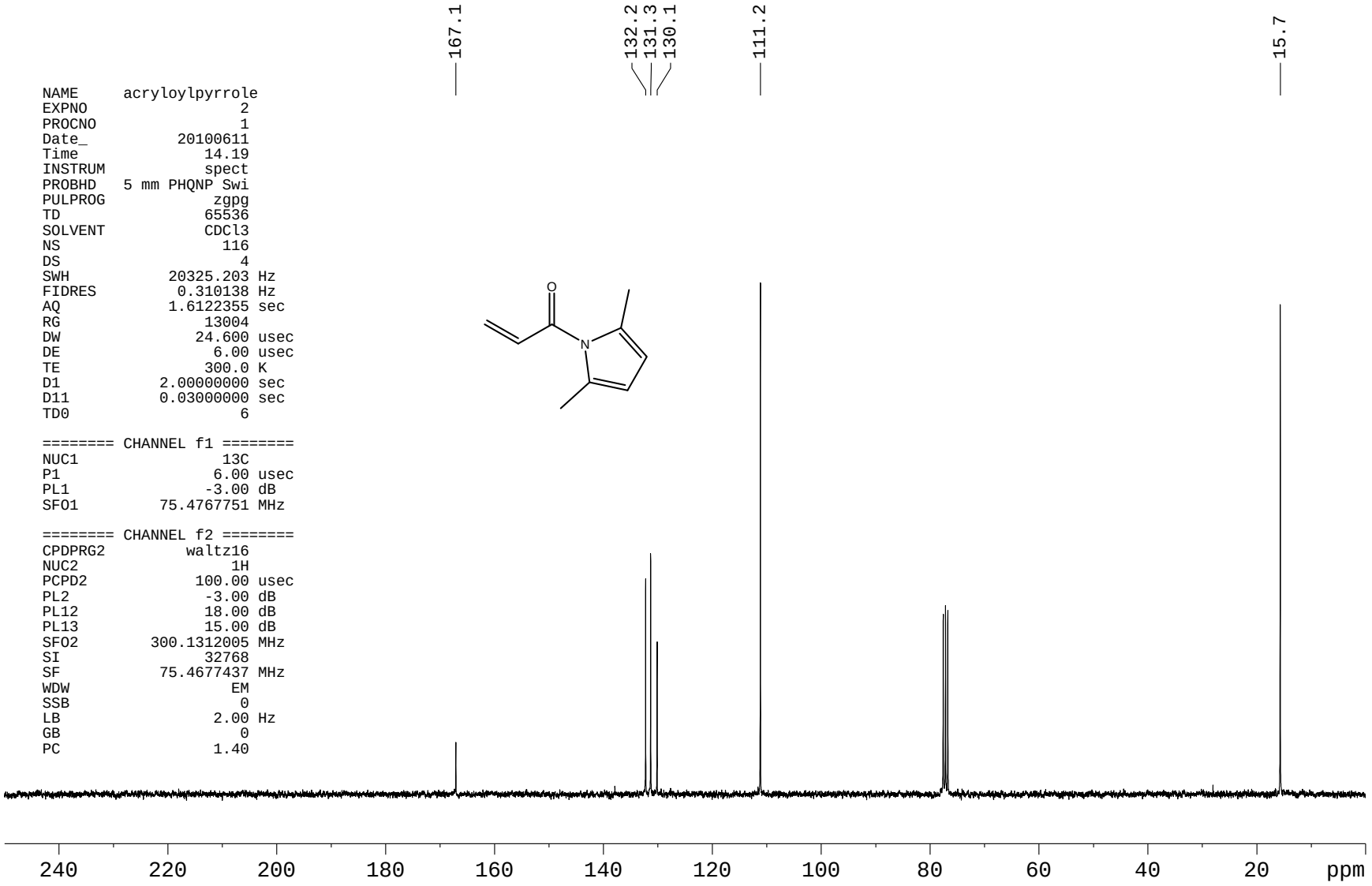


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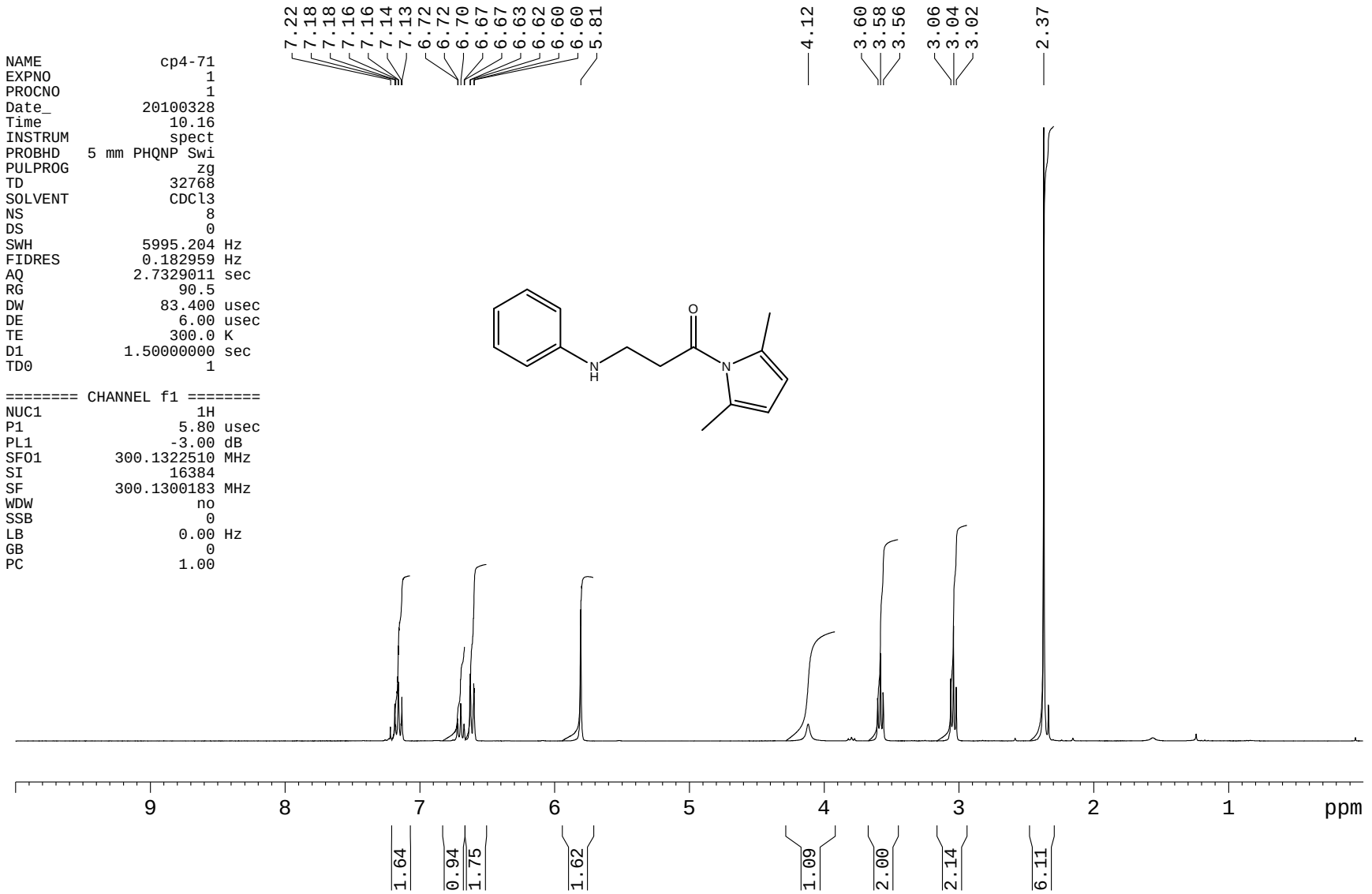
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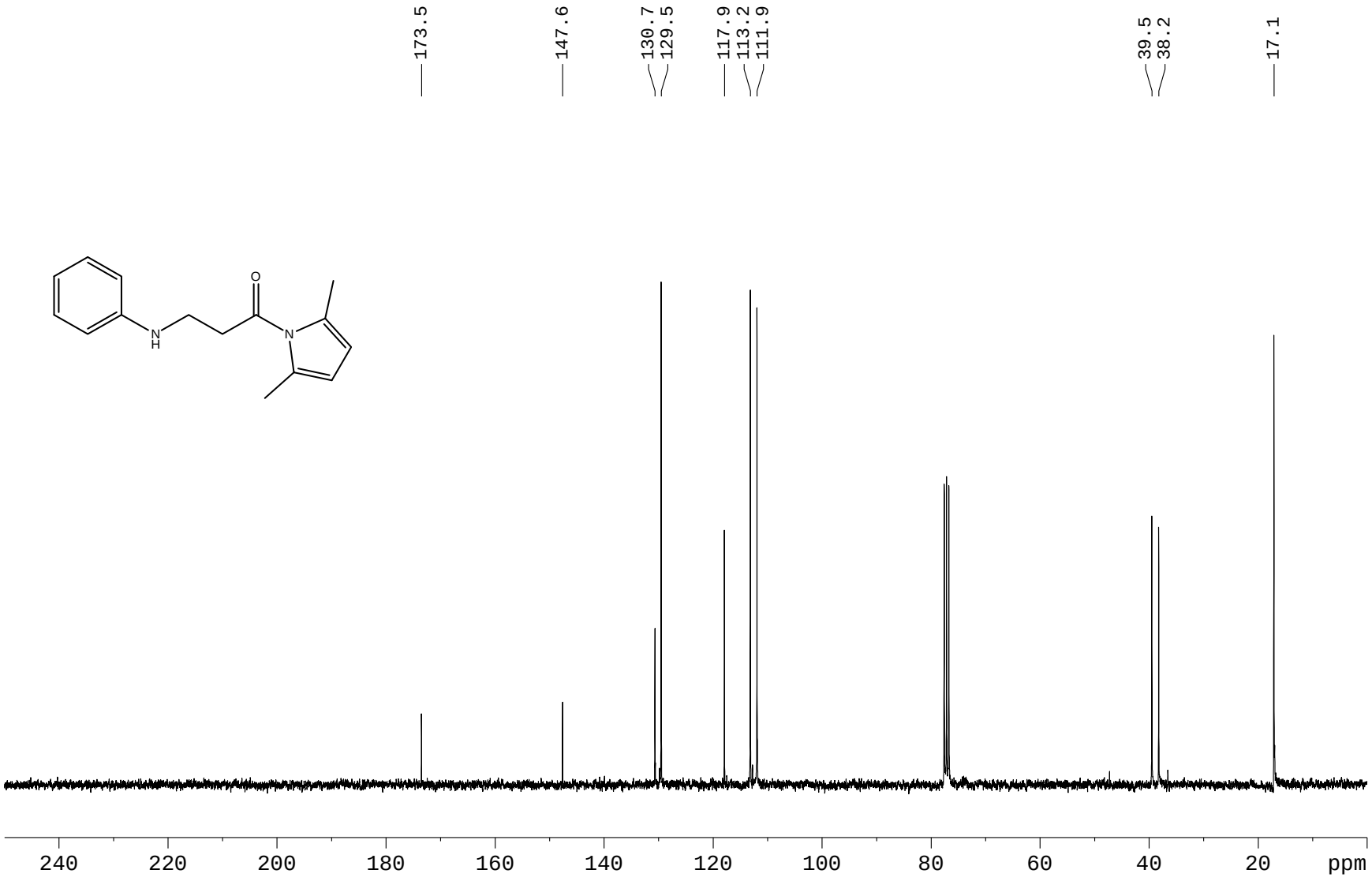
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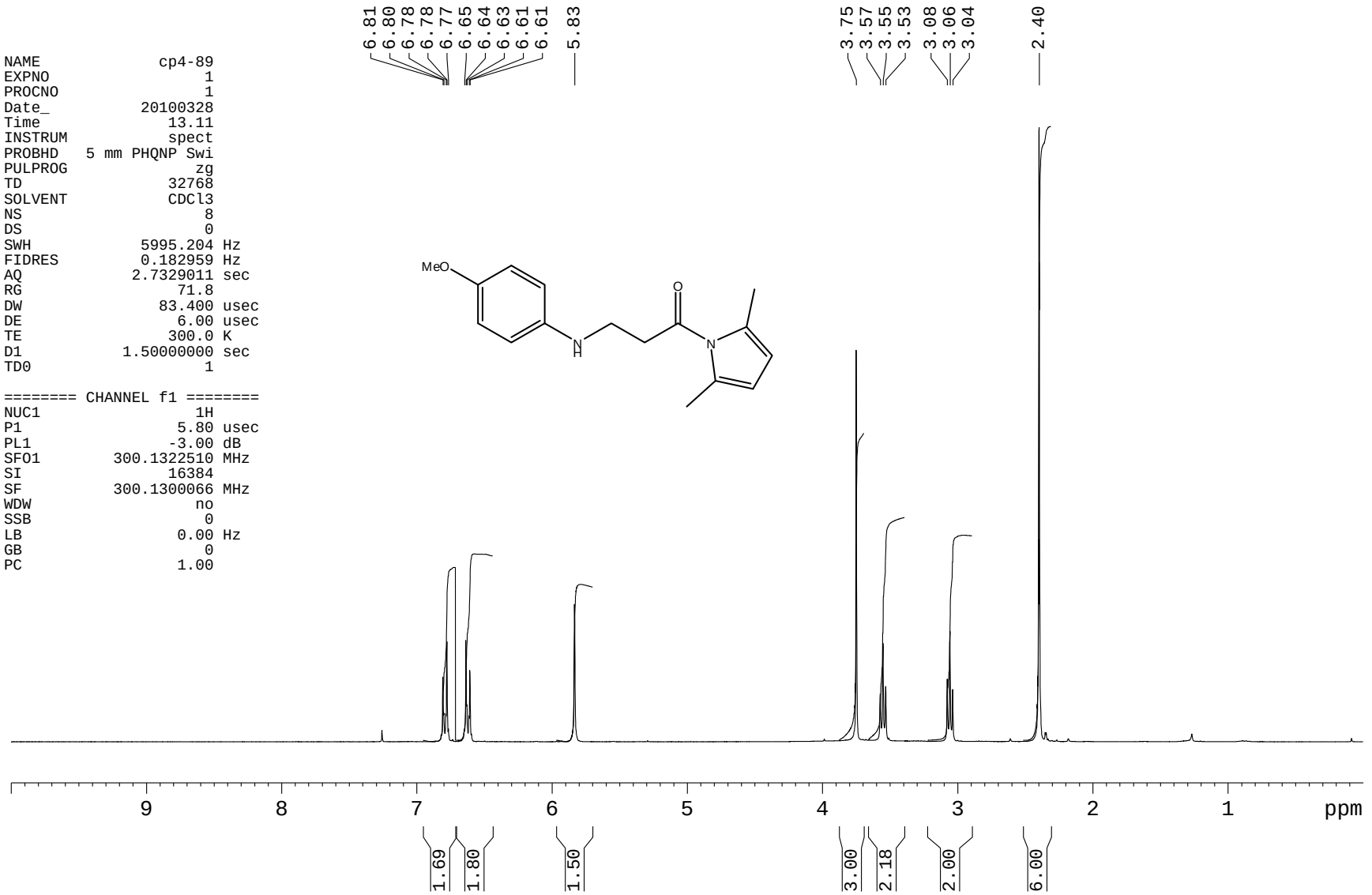
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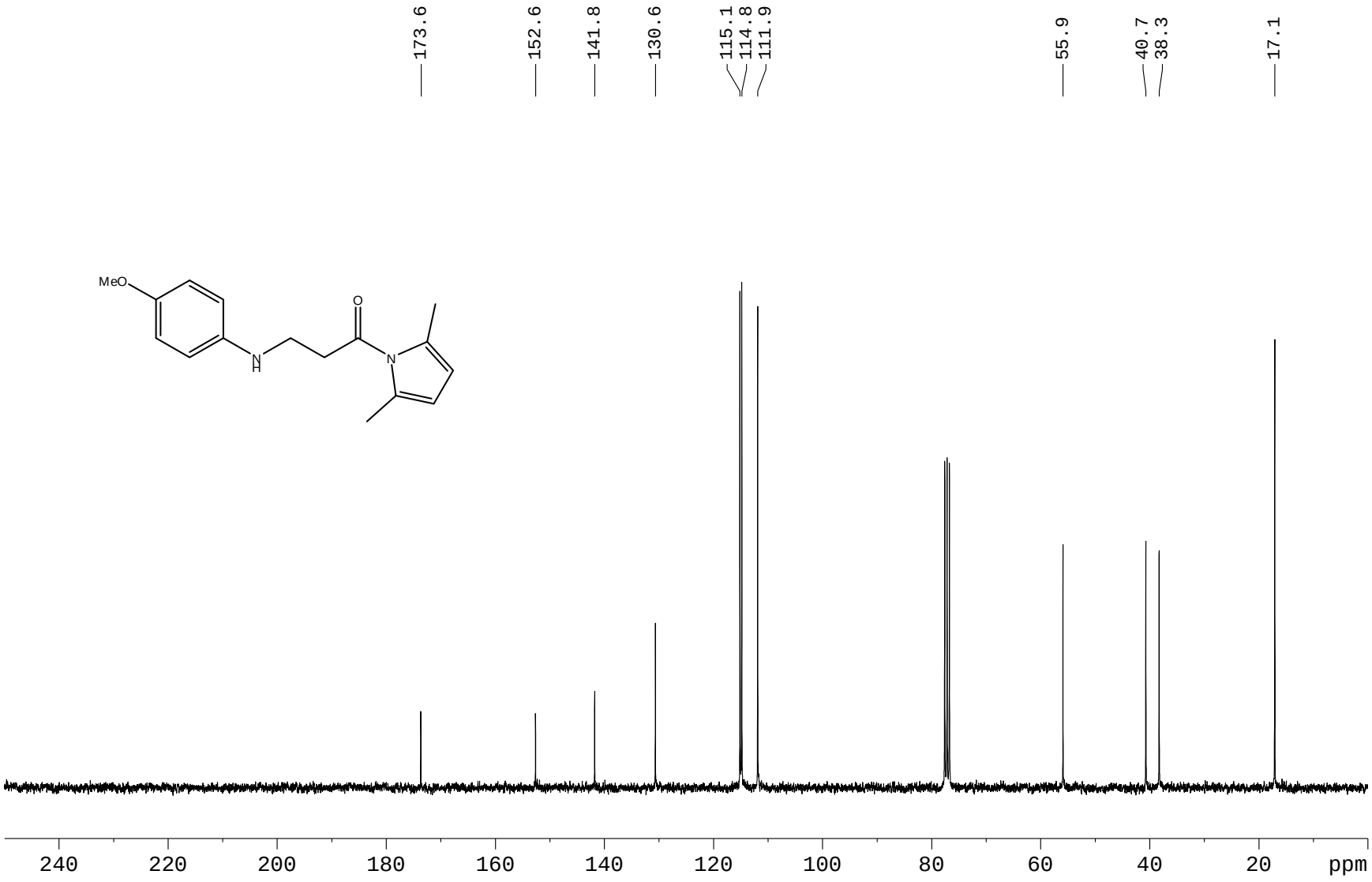
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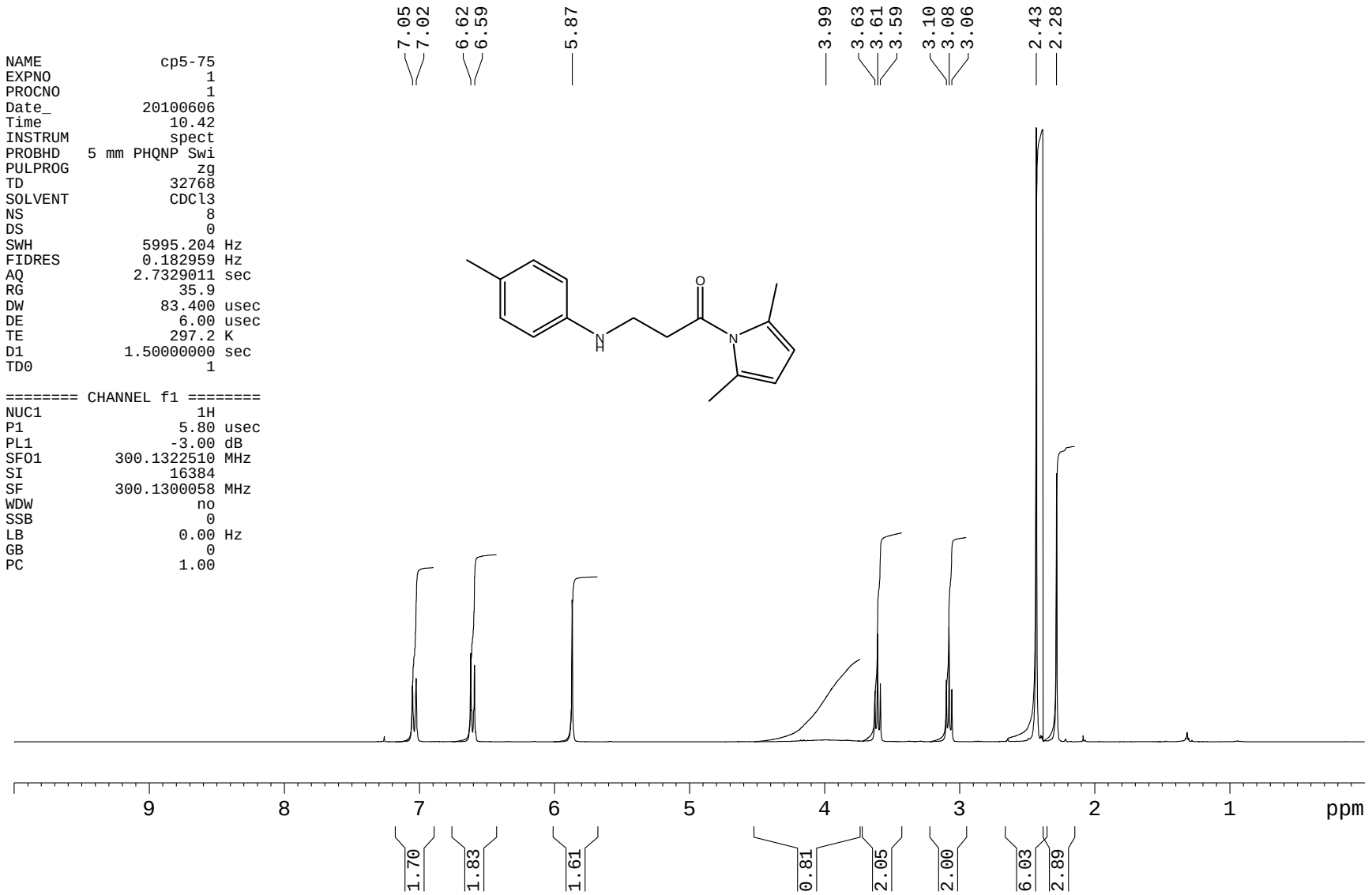
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H
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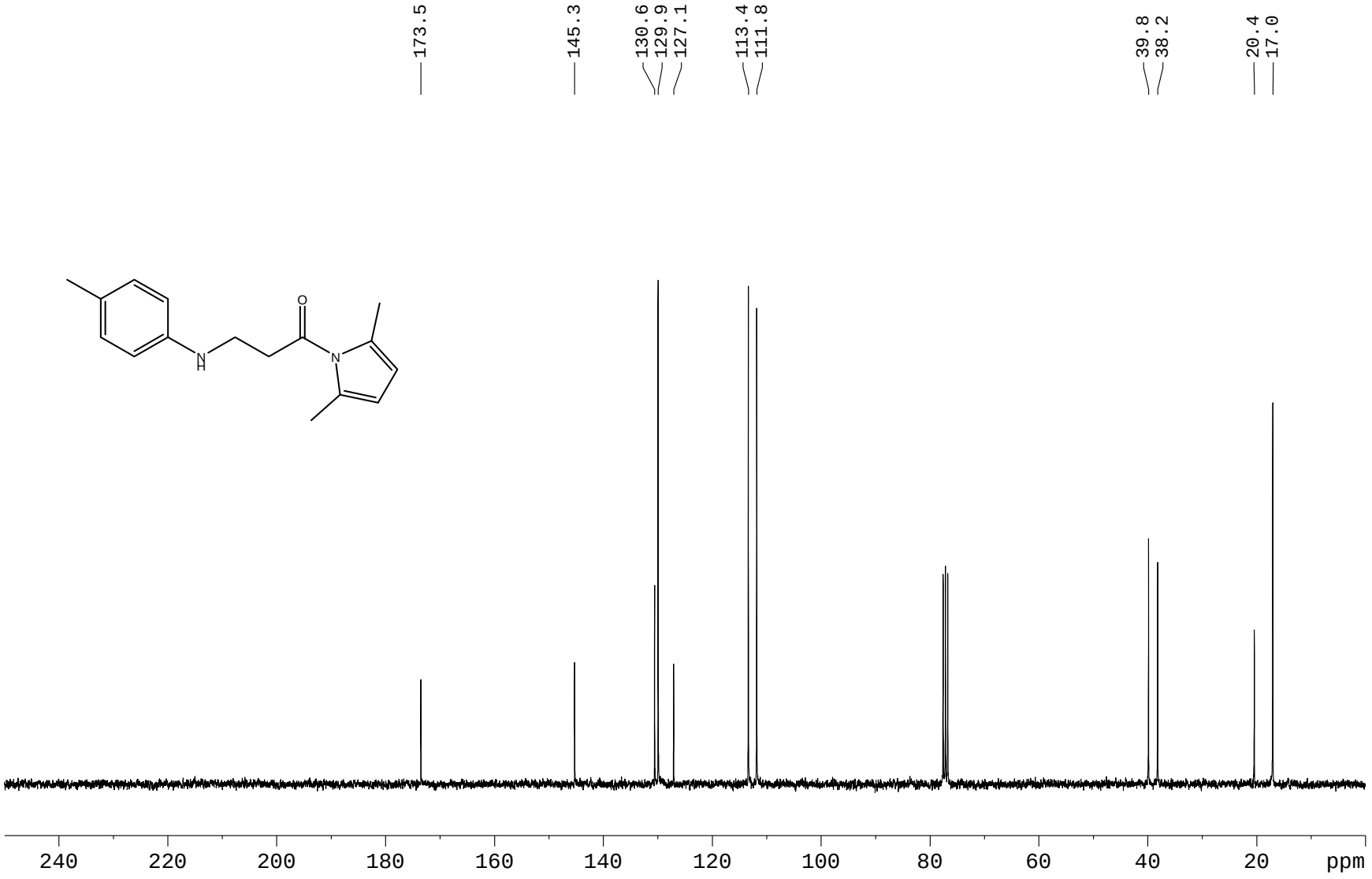
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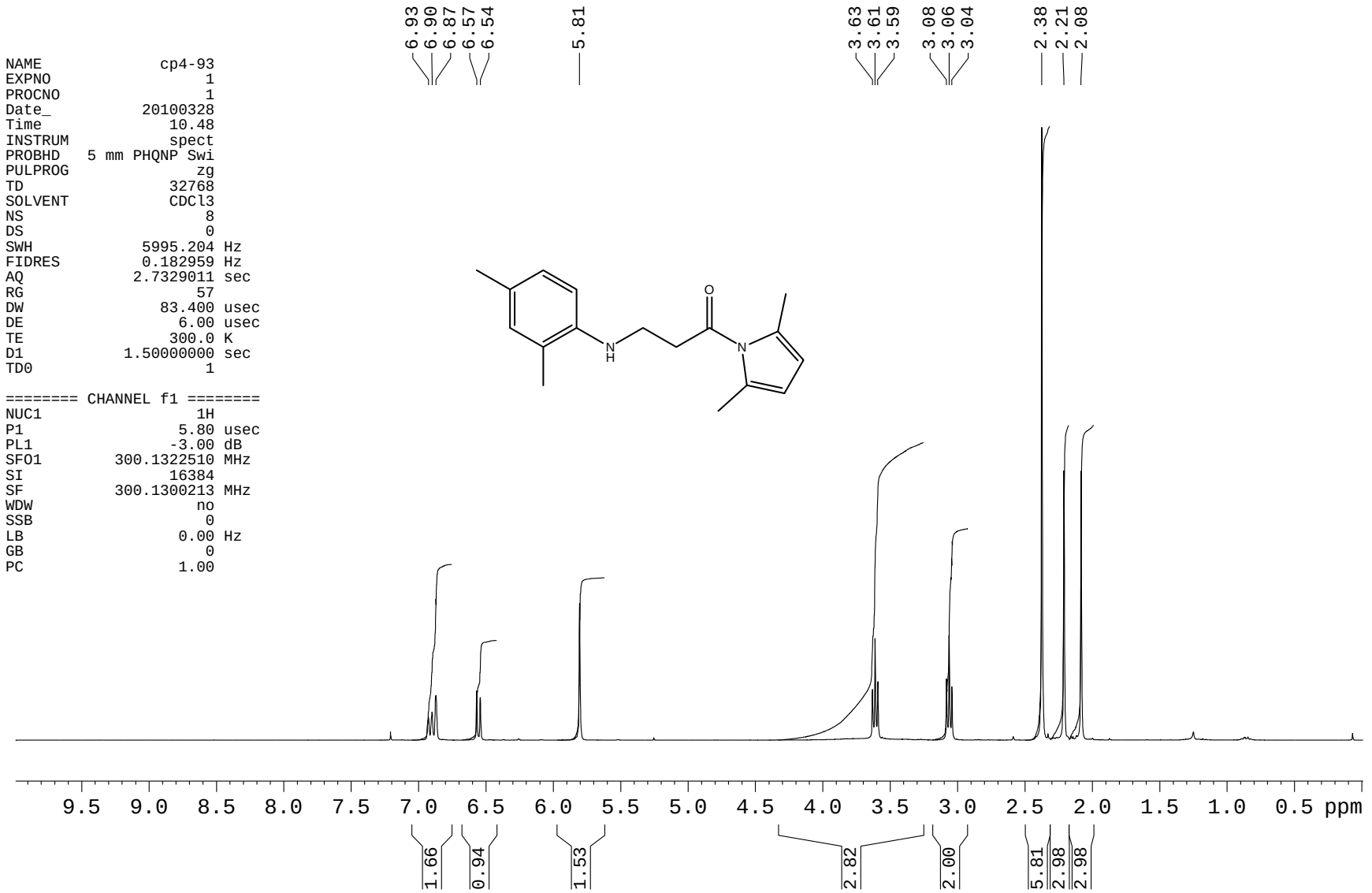
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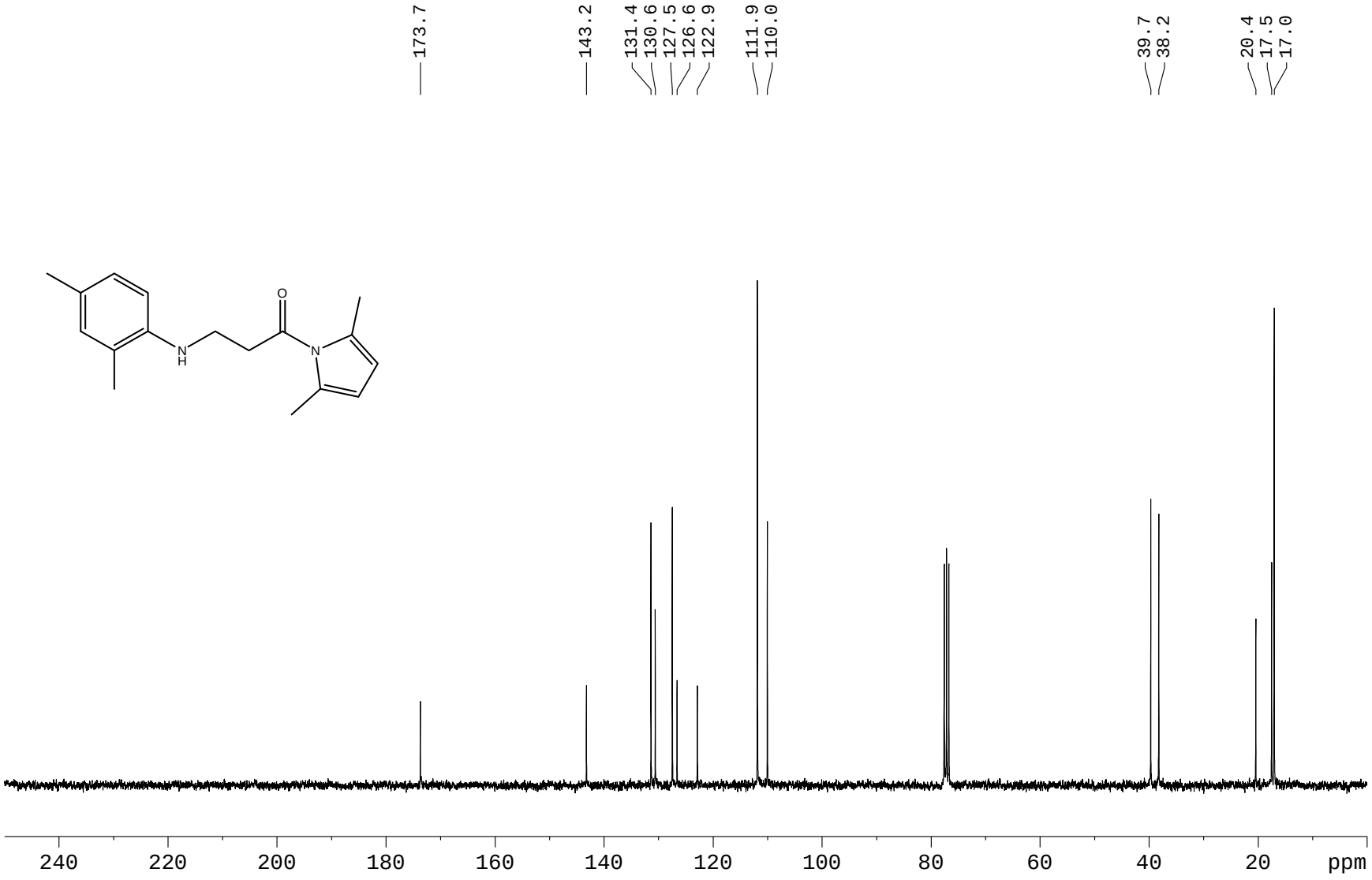
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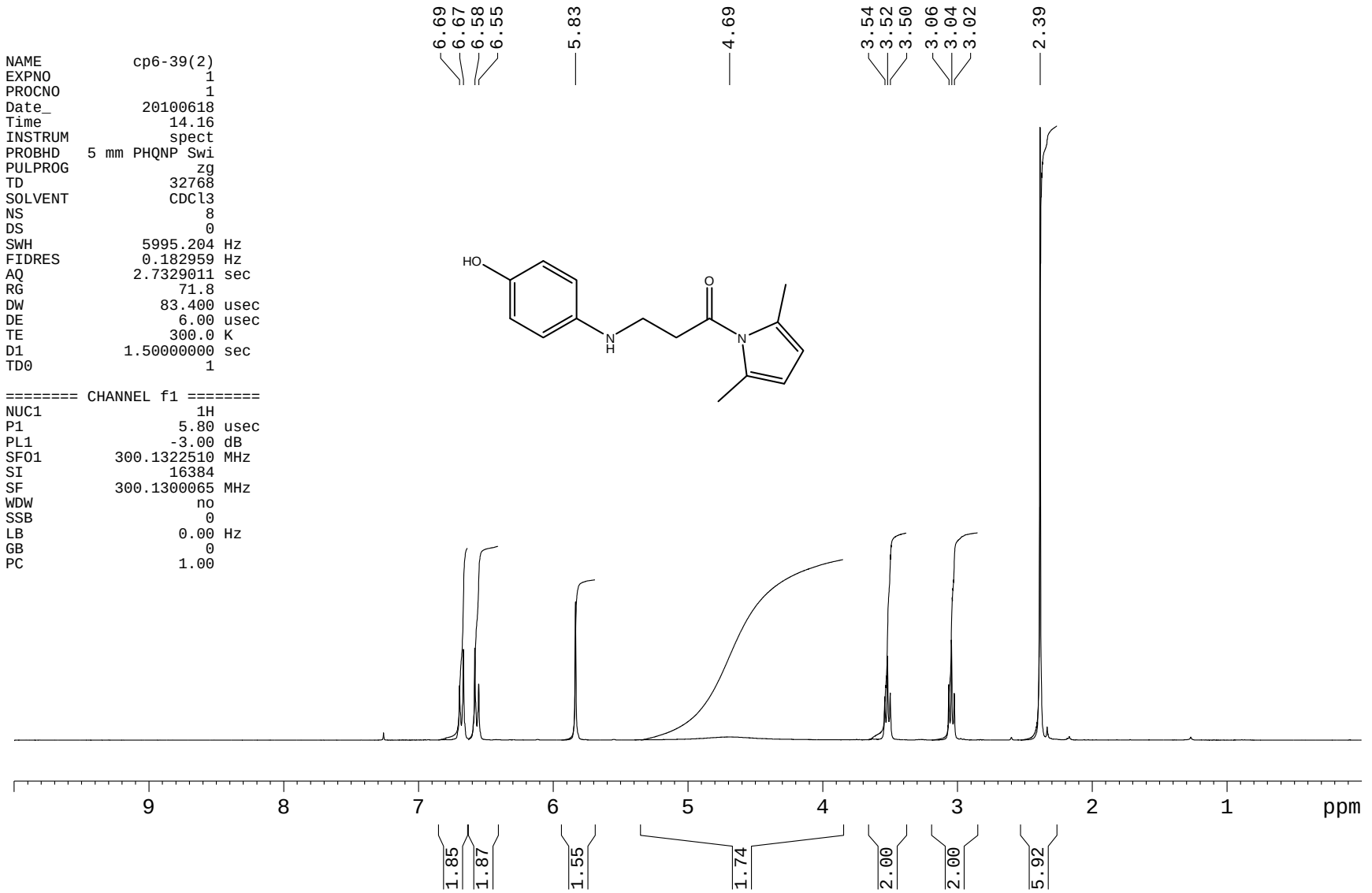
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DW 83.400 usec
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TE 300.0 K
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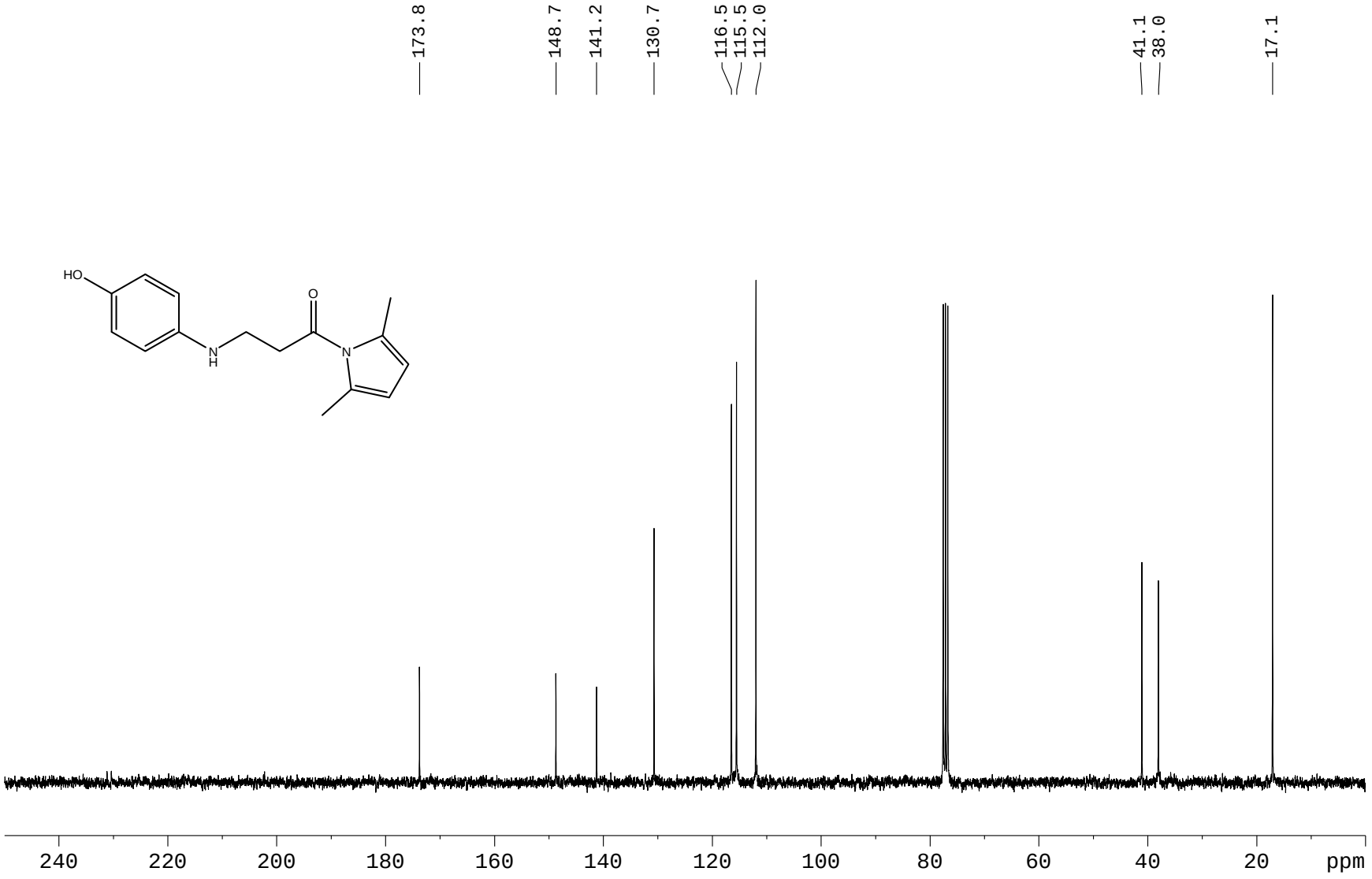
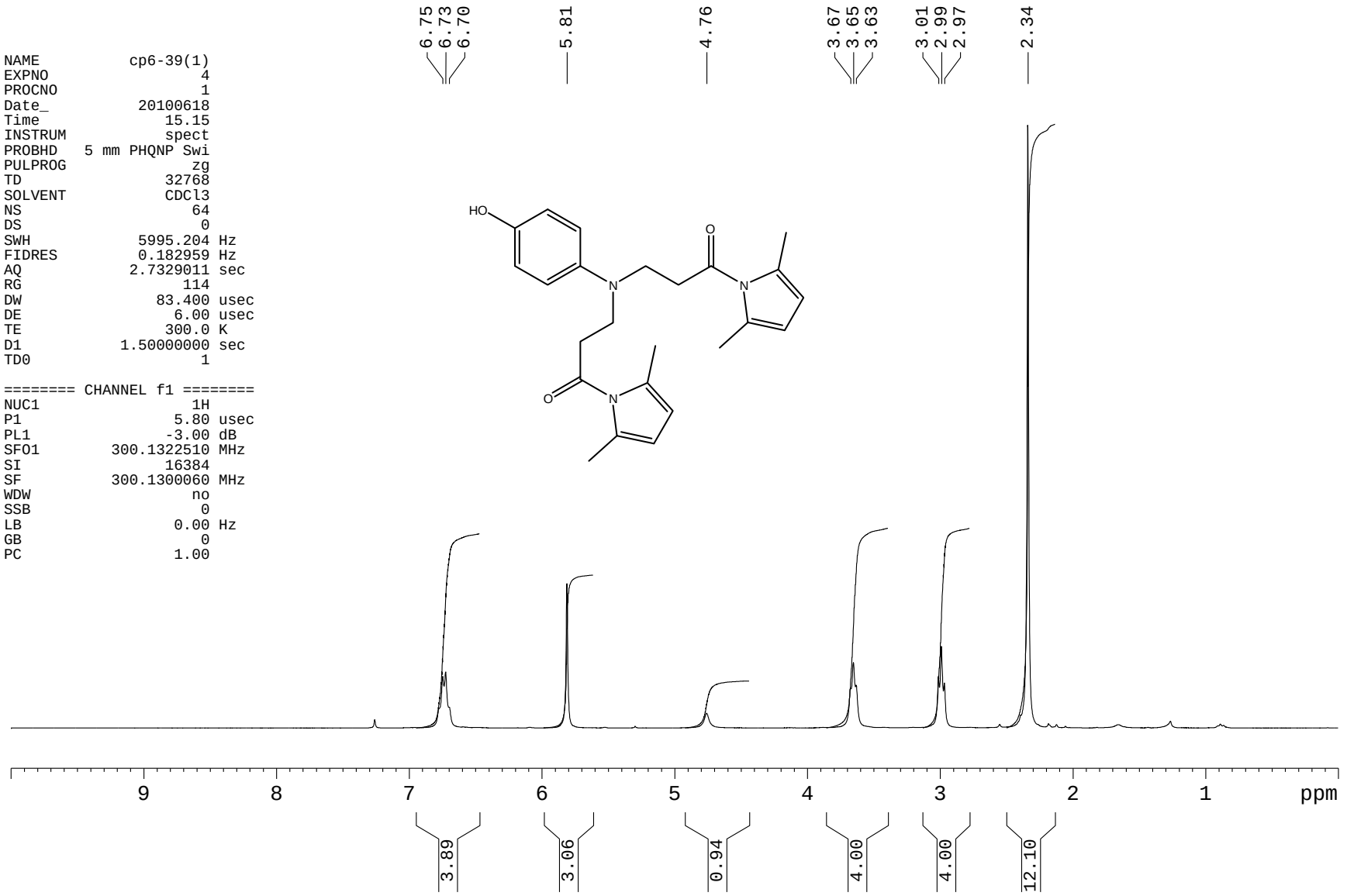
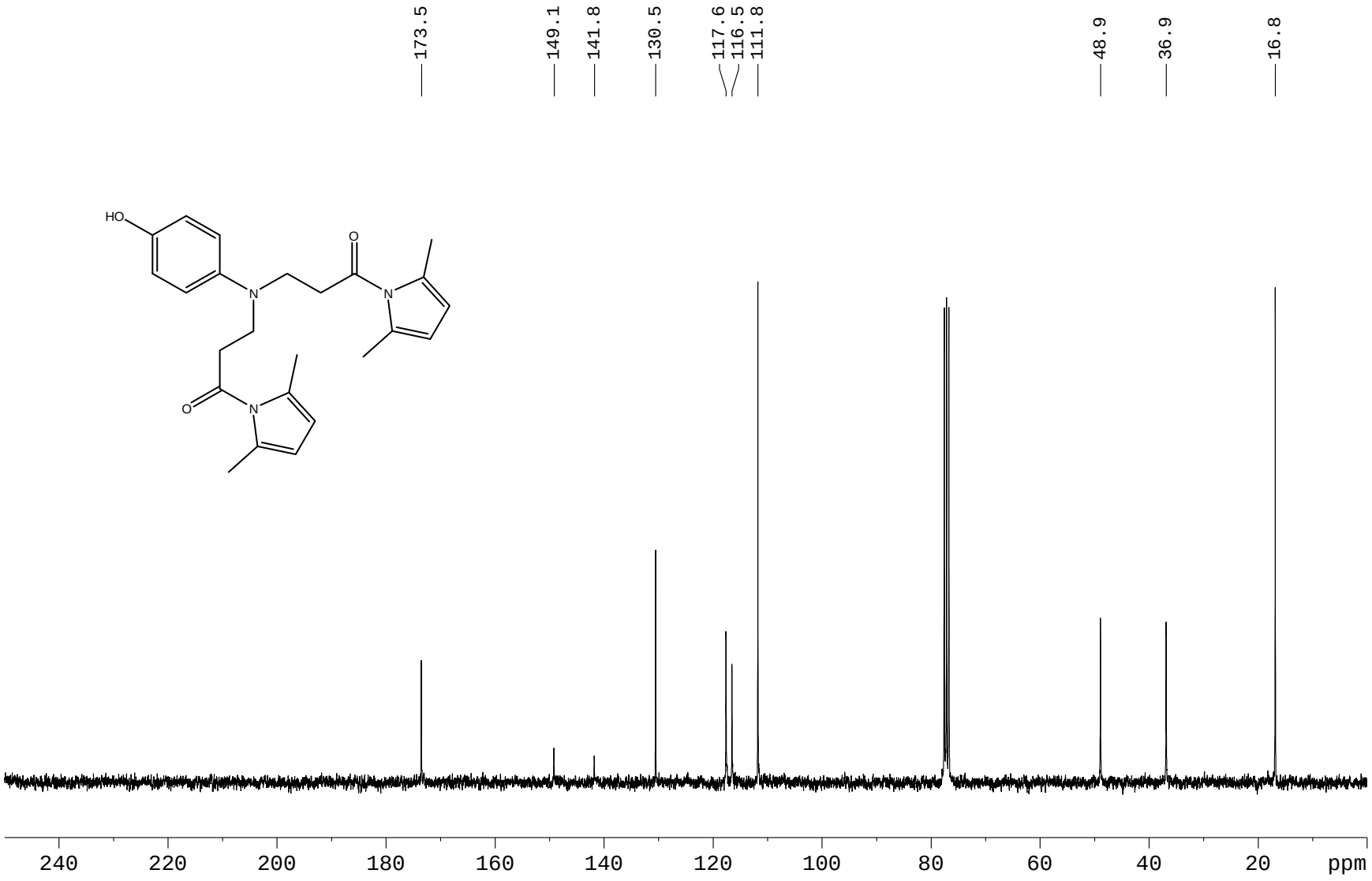
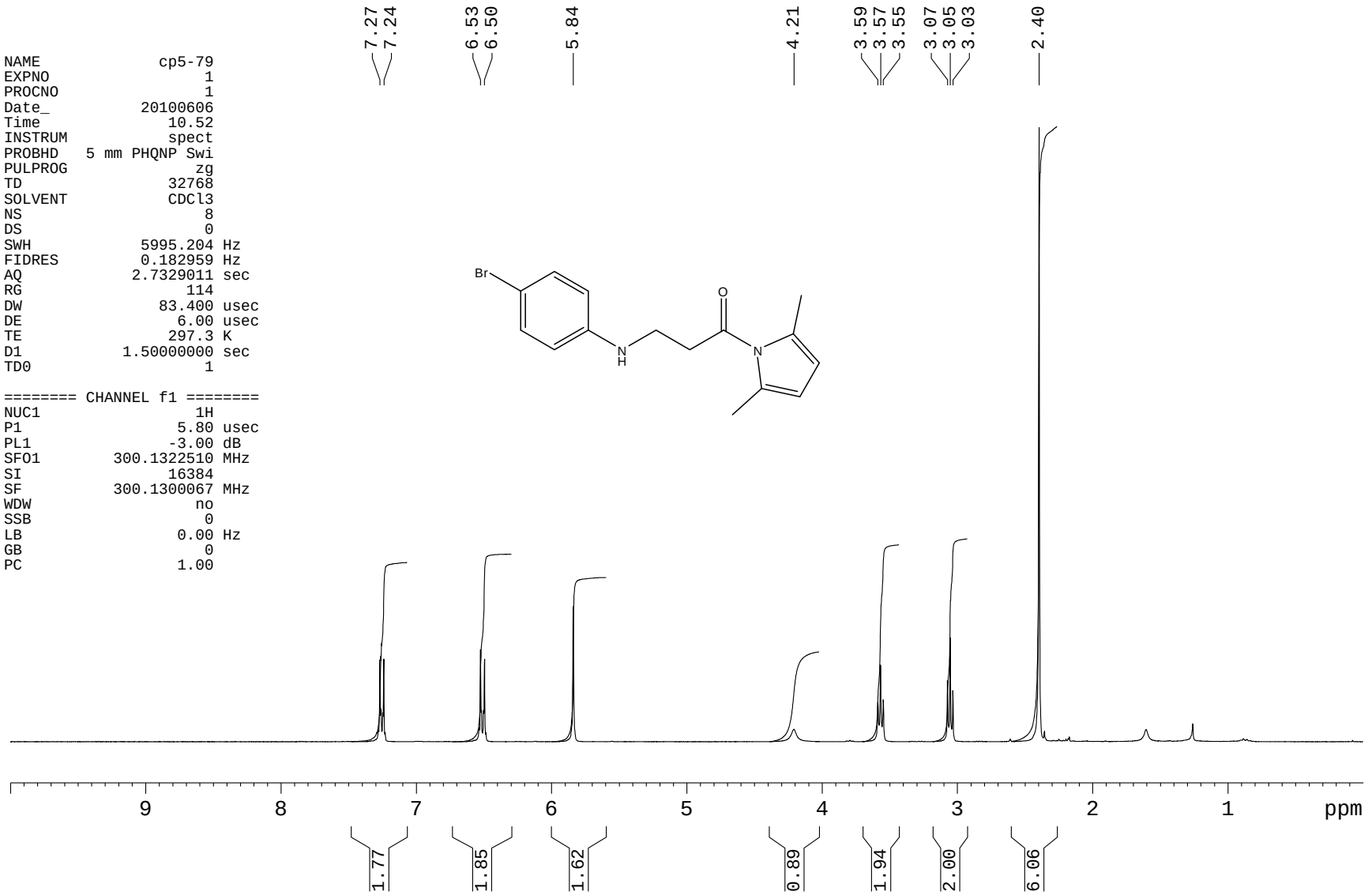
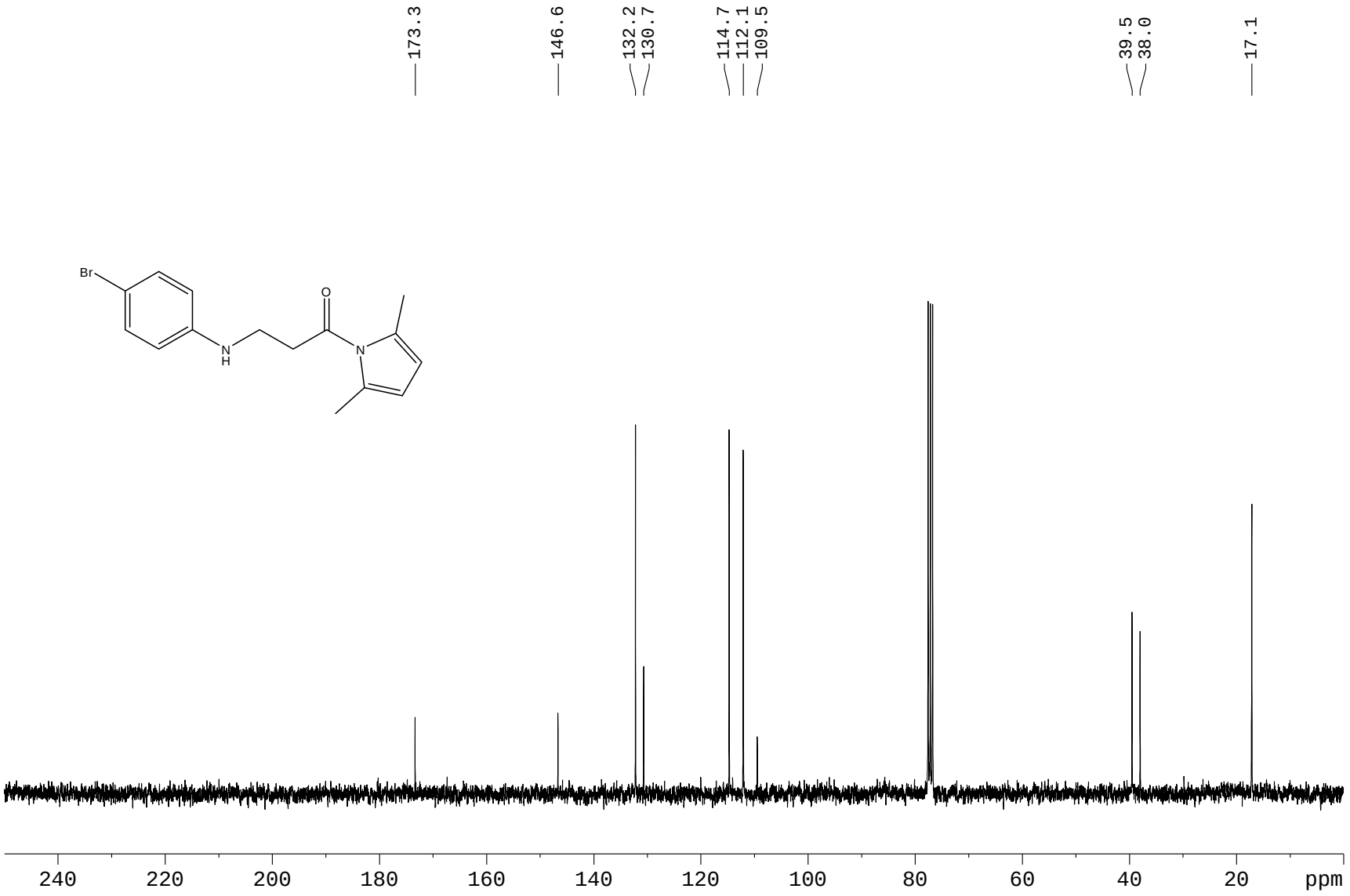
2.00
5.92

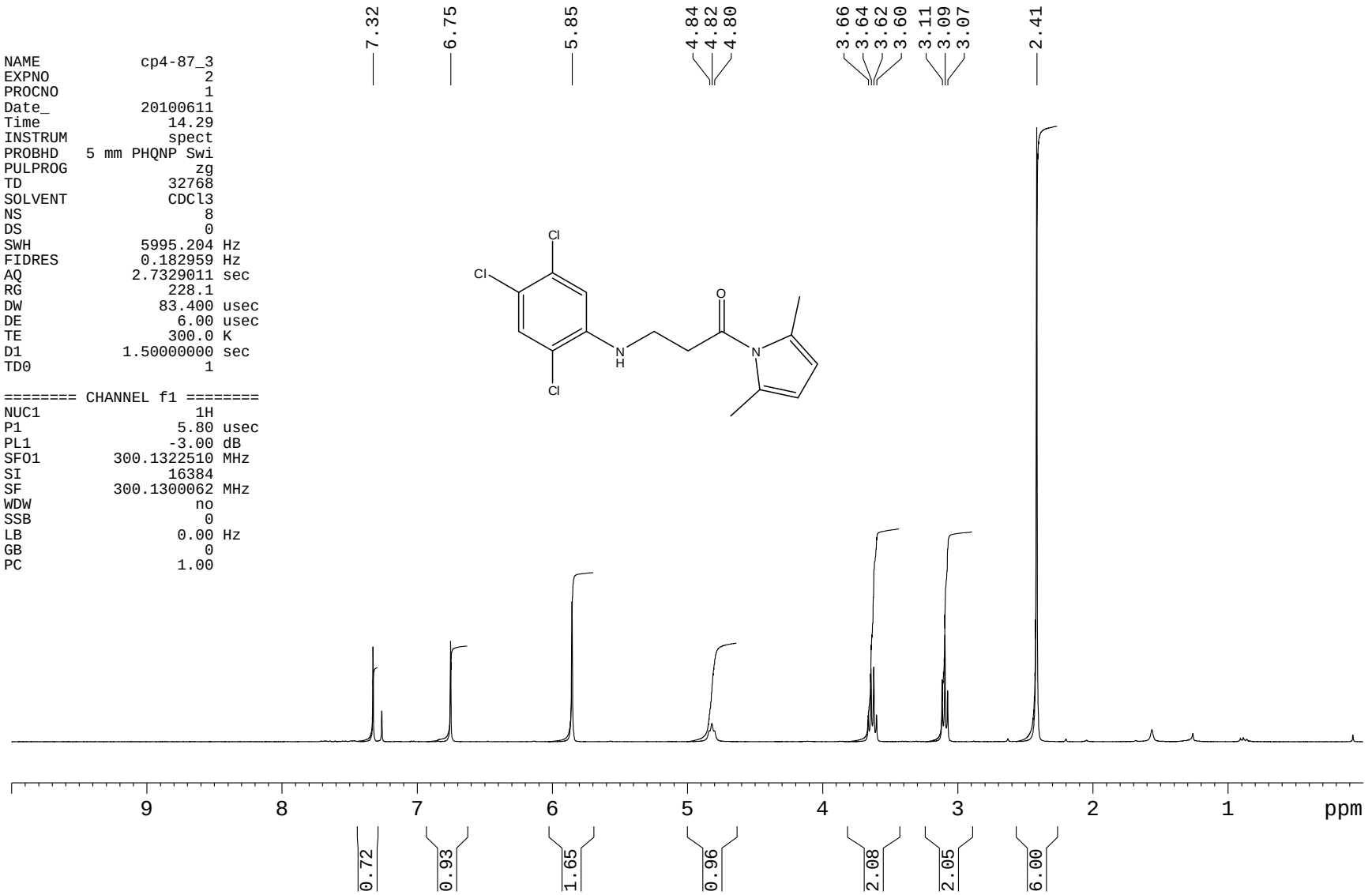

173.8
148.7
141.2
130.7
116.5
115.5
112.0
41.1
38.0
17.1
HO
O
N
H
N
240
220
200
180
160
140
120
100
80
60
40
20
ppm


6.75
6.73
6.70
5.81
4.76
3.67
3.65
3.63
3.01
2.99
2.97
2.34
HO
N
O
N
O
N
NAME cp6-39(1)
EXPNO 4
PROCNO 1
Date_ 20100618
Time 15.15
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 64
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 114
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 5.80 usec
PL1 -3.00 dB
SFO1 300.1322510 MHz
SI 16384
SF 300.1300060 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
ppm
3.89
3.06
0.94
4.00
4.00
12.10

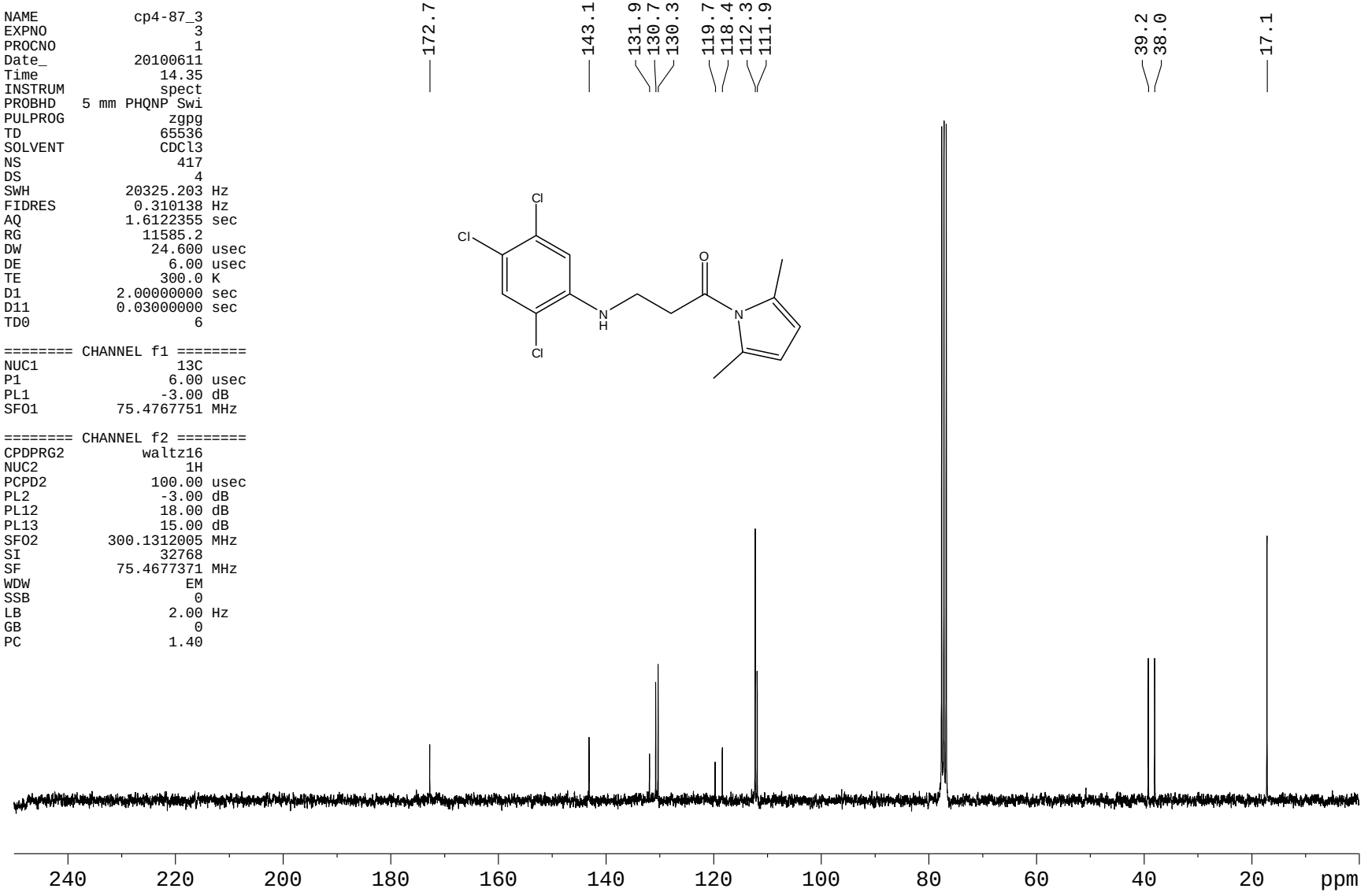

173.5
149.1
141.8
130.5
117.6
116.5
111.8
48.9
36.9
16.8
HO
O
N
N
O
N
240
220
200
180
160
140
120
100
80
60
40
20
ppm

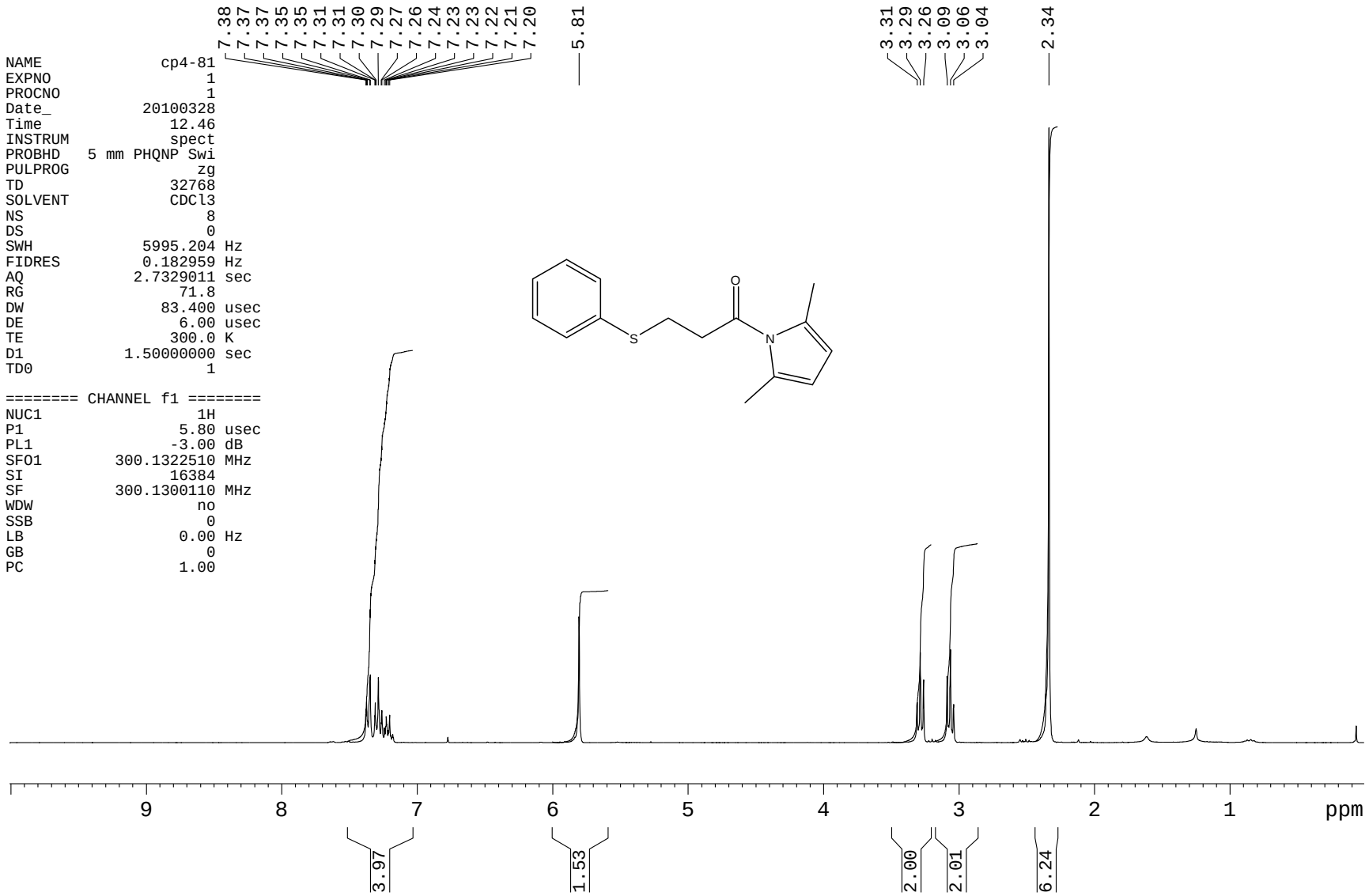

7.27
7.24
6.53
6.50
5.84
4.21
3.59
3.57
3.55
3.07
3.05
3.03
2.40
NAME cp5-79
EXPNO 1
PROCNO 1
Date_ 20100606
Time 10.52
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 114
DW 83.400 usec
DE 6.00 usec
TE 297.3 K
D1 1.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 5.80 usec
PL1 -3.00 dB
SFO1 300.1322510 MHz
SI 16384
SF 300.1300067 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Br
O
N
H
N
9
8
7
6
5
4
3
2
1
ppm
1.77
1.85
1.62
0.89
1.94
2.00
6.06

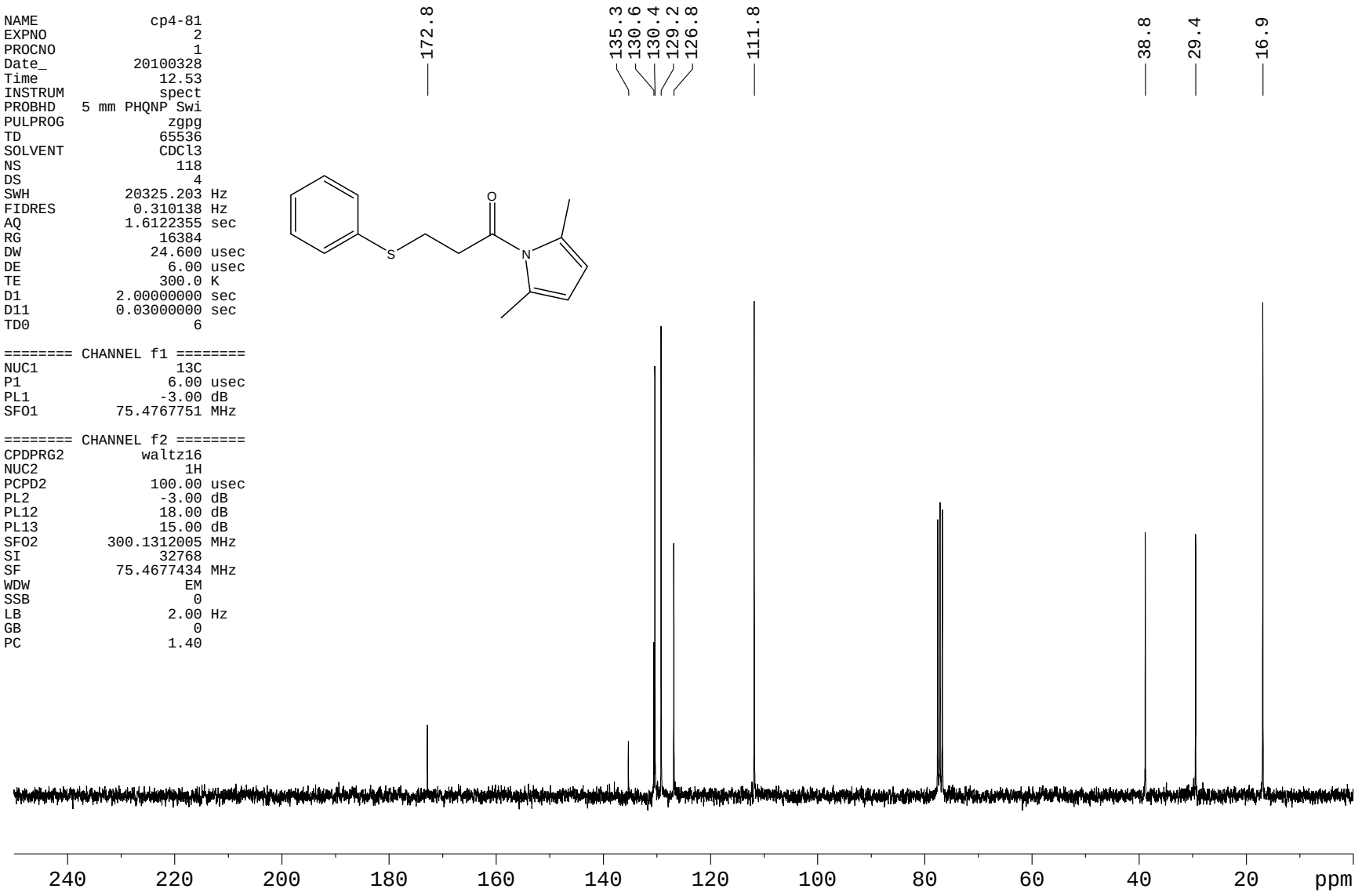

173.3
146.6
132.2
130.7
114.7
112.1
109.5
39.5
38.0
17.1
Br
O
N
H
N
240
220
200
180
160
140
120
100
80
60
40
20
ppm

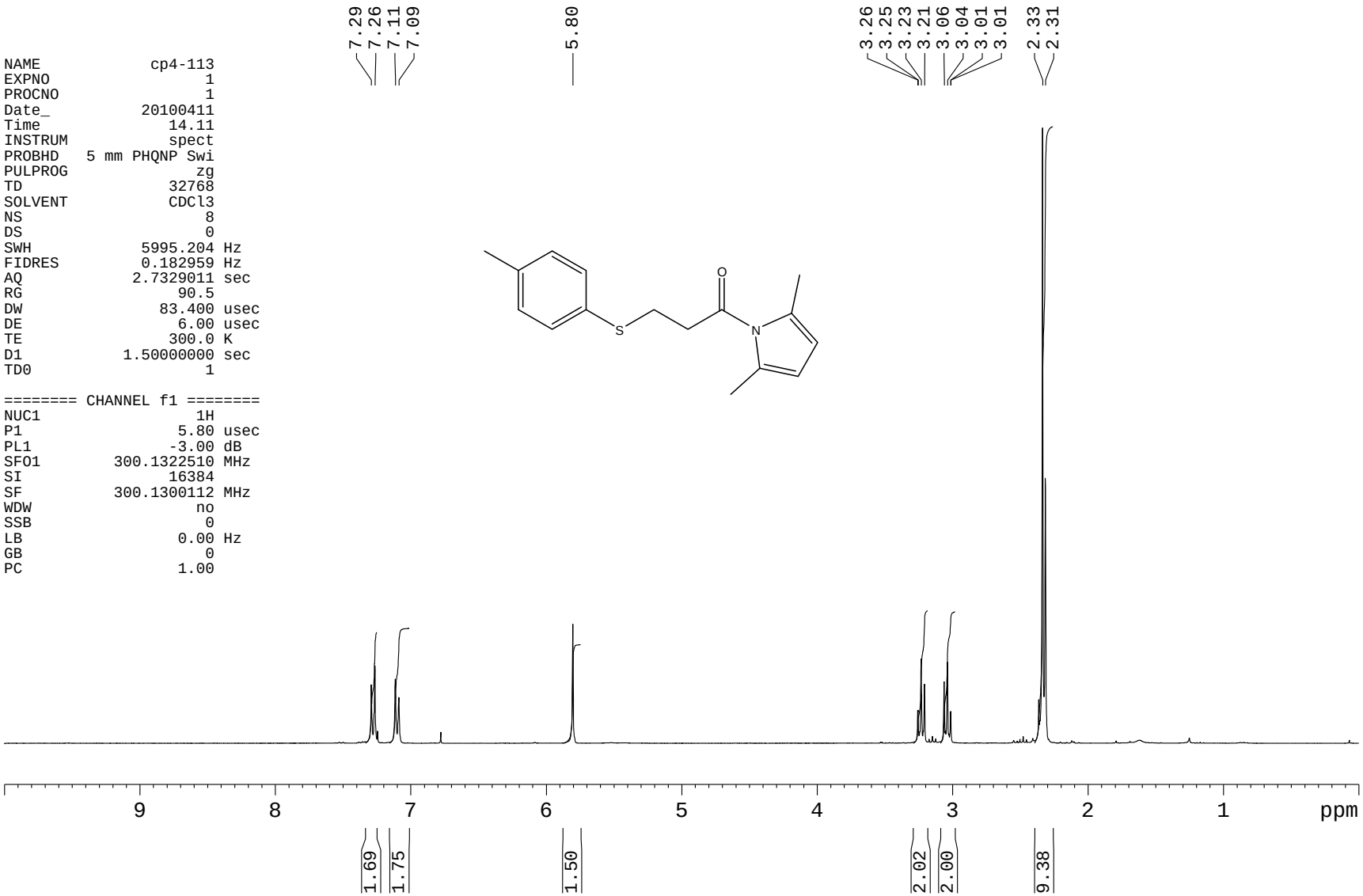

7.32
6.75
5.85
4.84
4.82
4.80
3.66
3.64
3.62
3.60
3.11
3.09
3.07
2.41
NAME cp4-87_3
EXPNO 2
PROCNO 1
Date_ 20100611
Time 14.29
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 228.1
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 5.80 usec
PL1 -3.00 dB
SFO1 300.1322510 MHz
SI 16384
SF 300.1300062 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Cl
Cl
Cl
O
N
H
N
9
8
7
6
5
4
3
2
1
ppm
0.72
0.93
1.65
0.96
2.08
2.05
6.00

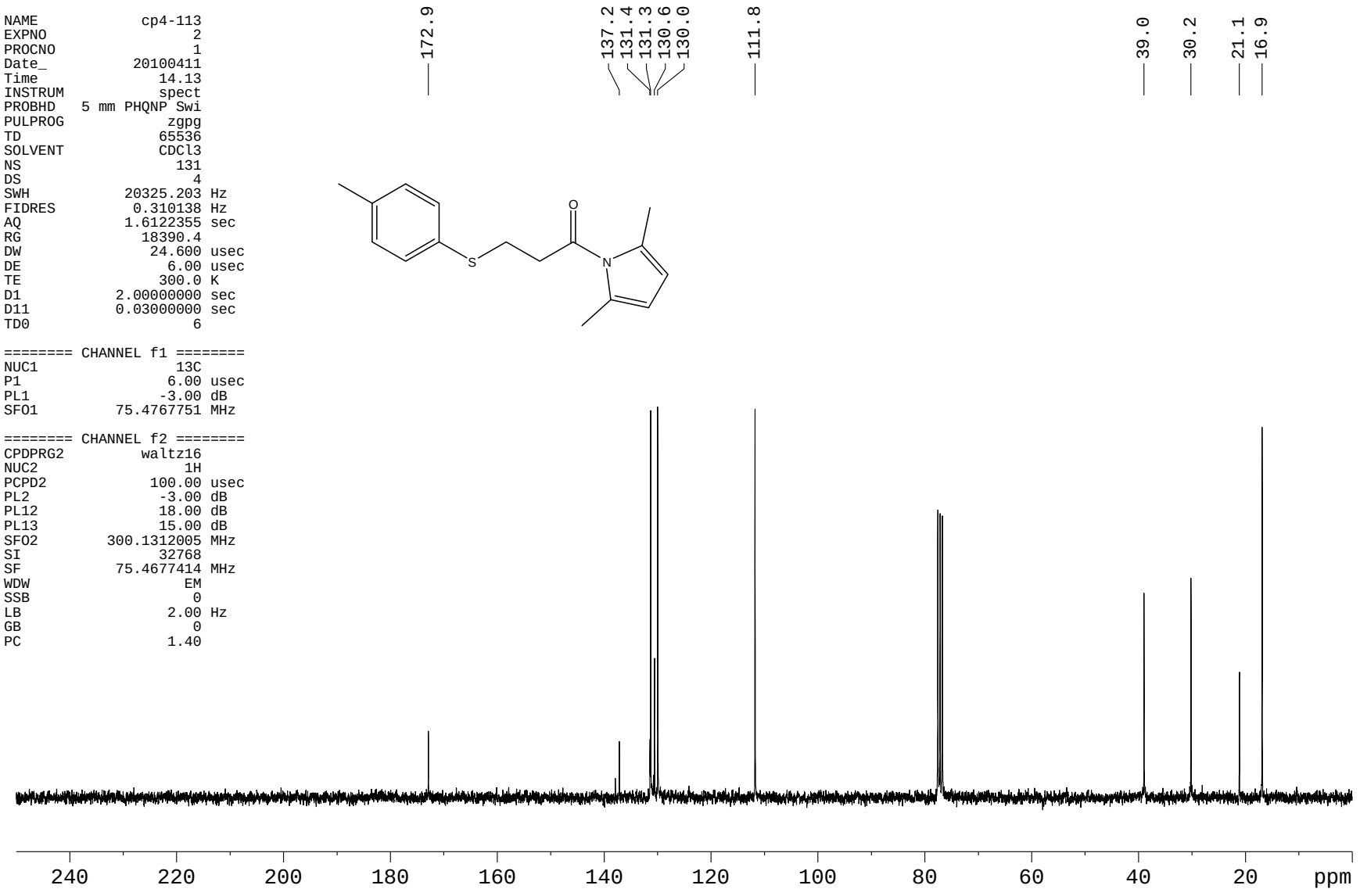
```
NAME            cp4-87_3
EXPNO                  3
PROCNO                 1
Date_           20100611
Time               14.35
INSTRUM            spect
PROBHD   5 mm PHQNP Swi
PULPROG             zgpg
TD                 65536
SOLVENT            CDCl3
NS                   417
DS                     4
SWH            20325.203 Hz
FIDRES          0.310138 Hz
AQ             1.6122355 sec
RG               11585.2
DW                24.600 usec
DE                 6.00 usec
TE                300.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    6

======== CHANNEL f1 ========
NUC1                 13C
P1                  6.00 usec
PL1                -3.00 dB
SFO1          75.4767751 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             100.00 usec
PL2                -3.00 dB
PL12               18.00 dB
PL13               15.00 dB
SFO2         300.1312005 MHz
SI                 32768
SF            75.4677371 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.40
```

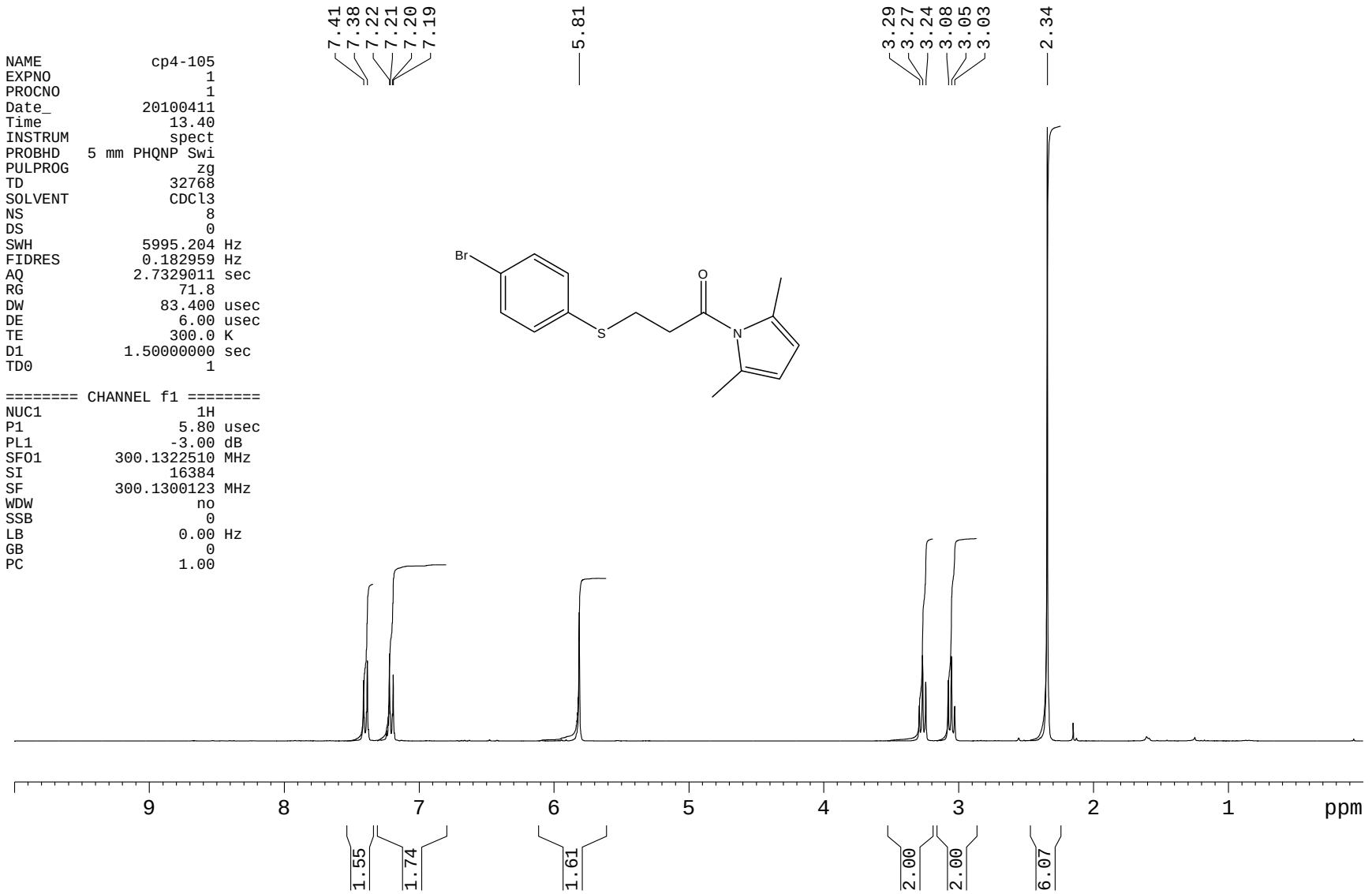


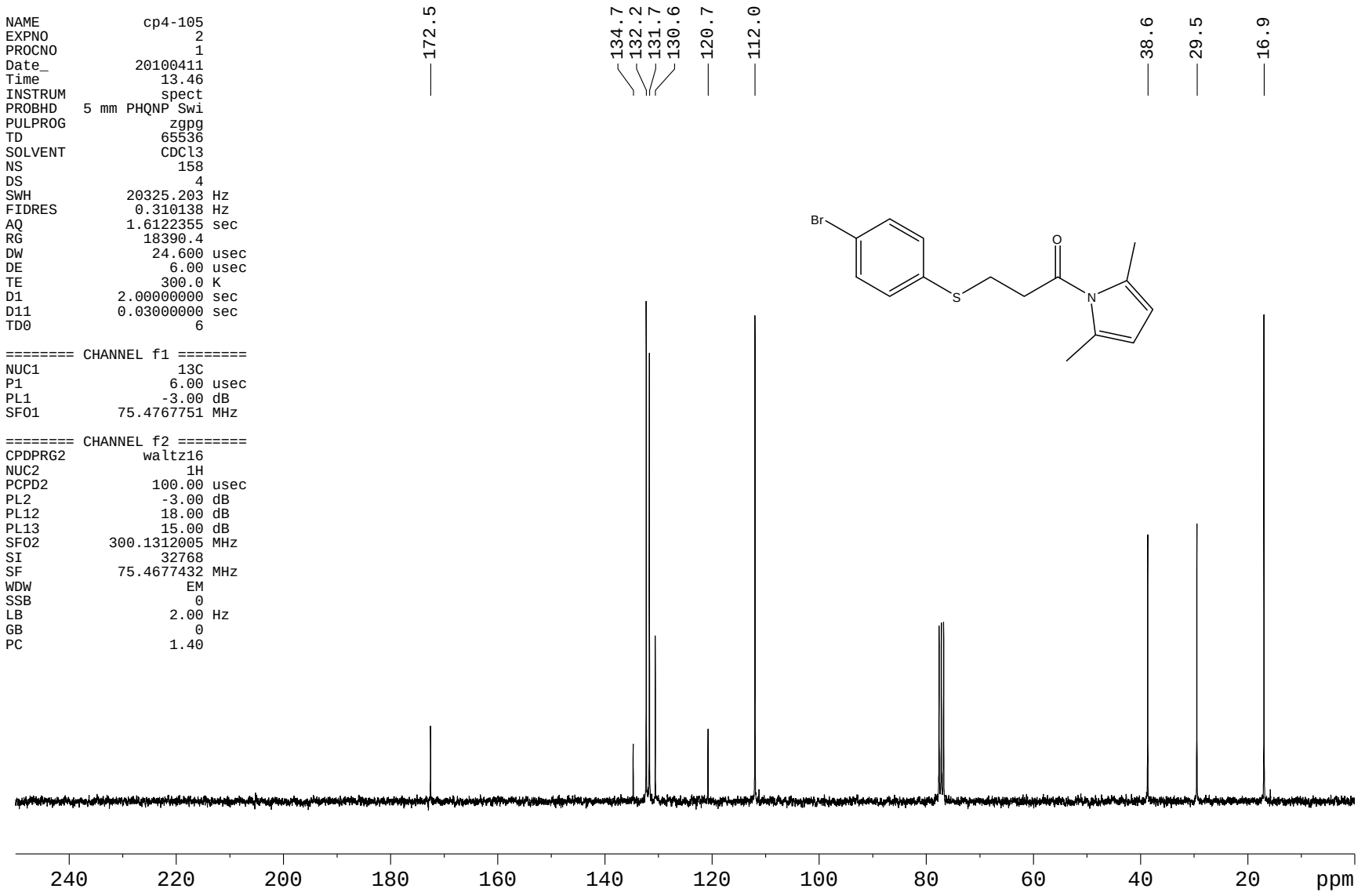

7.38
7.37
7.37
7.35
7.35
7.31
7.31
7.30
7.29
7.27
7.26
7.24
7.23
7.23
7.22
7.21
7.20
5.81
3.31
3.29
3.26
3.09
3.06
3.04
2.34
NAME cp4-81
EXPNO 1
PROCNO 1
Date_ 20100328
Time 12.46
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 71.8
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 5.80 usec
PL1 -3.00 dB
SFO1 300.1322510 MHz
SI 16384
SF 300.1300110 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
O
S
N
9
8
7
6
5
4
3
2
1
ppm
3.97
1.53
2.00
2.01
6.24

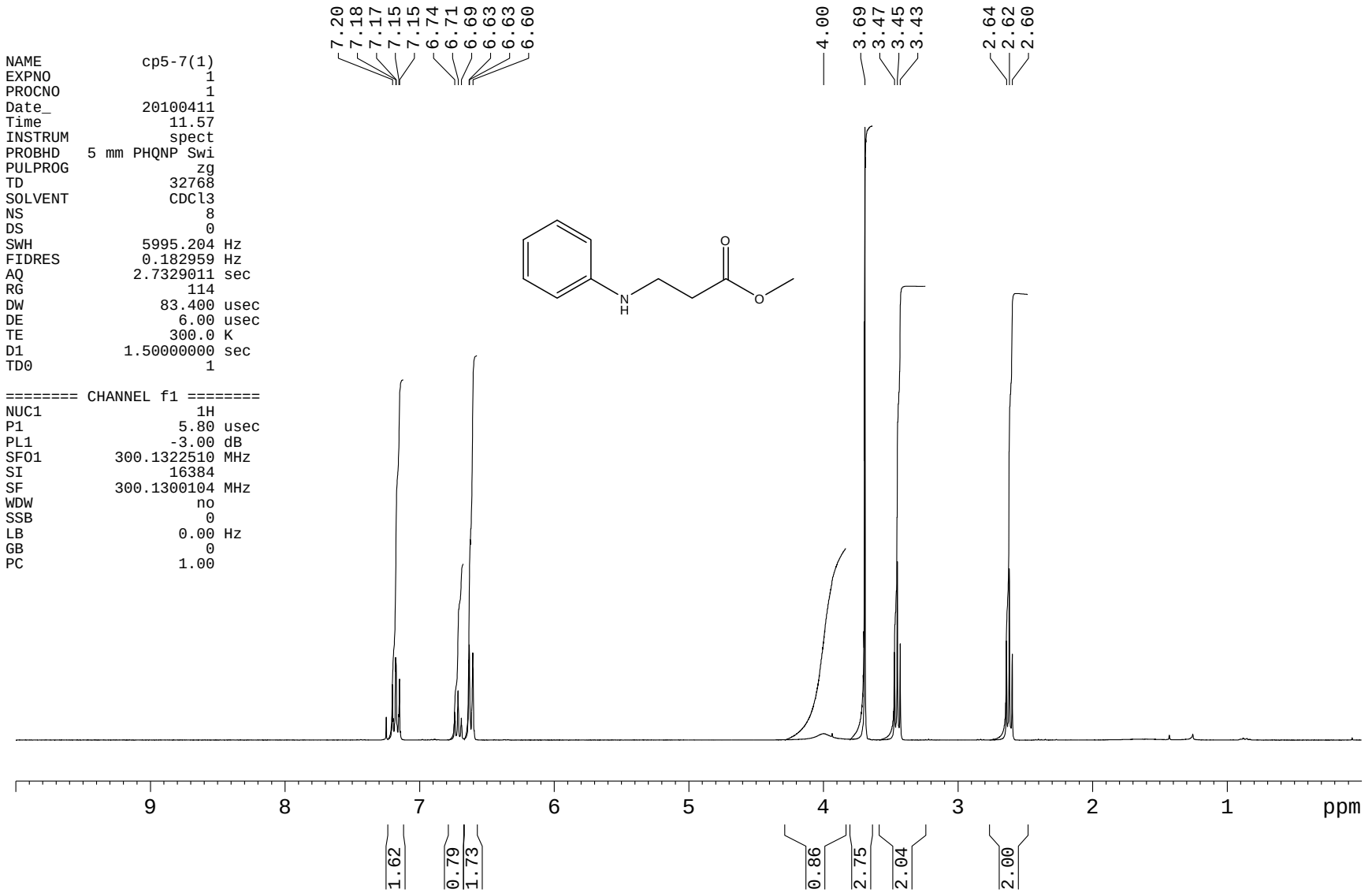

NAME cp4-81
EXPNO 2
PROCNO 1
Date_ 20100328
Time 12.53
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 118
DS 4
SWH 20325.203 Hz
FIDRES 0.310138 Hz
AQ 1.6122355 sec
RG 16384
DW 24.600 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 6
======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 -3.00 dB
SFO1 75.4767751 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -3.00 dB
PL12 18.00 dB
PL13 15.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677434 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
172.8
135.3
130.6
130.4
129.2
126.8
111.8
38.8
29.4
16.9
O
S
N
240
220
200
180
160
140
120
100
80
60
40
20
ppm

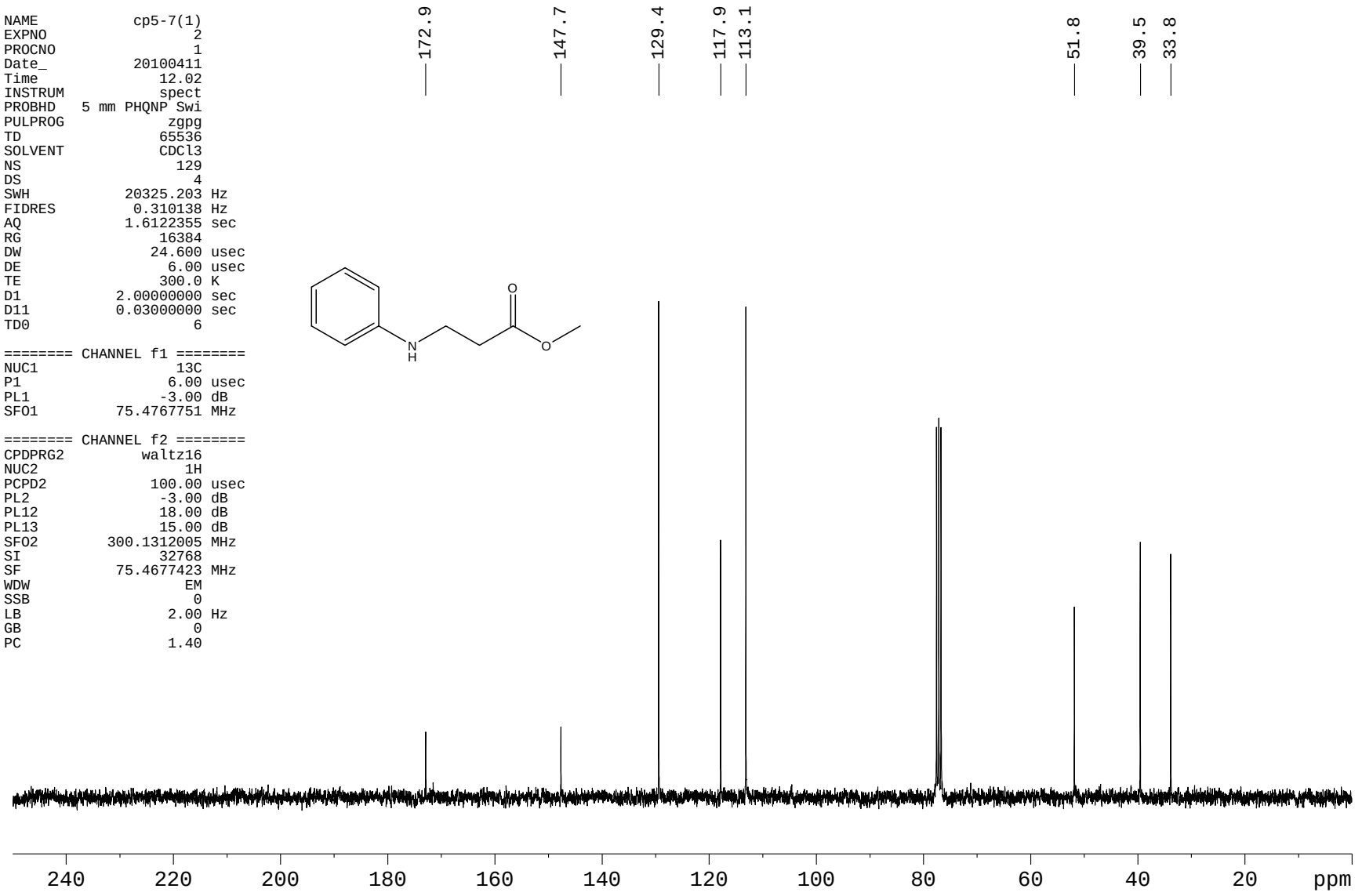

7.29
7.26
7.11
7.09
5.80
3.26
3.25
3.23
3.21
3.06
3.04
3.01
3.01
2.33
2.31
NAME cp4-113
EXPNO 1
PROCNO 1
Date_ 20100411
Time 14.11
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 90.5
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 5.80 usec
PL1 -3.00 dB
SFO1 300.1322510 MHz
SI 16384
SF 300.1300112 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
O
S
N
9
8
7
6
5
4
3
2
1
ppm
1.69
1.75
1.50
2.02
2.00
9.38

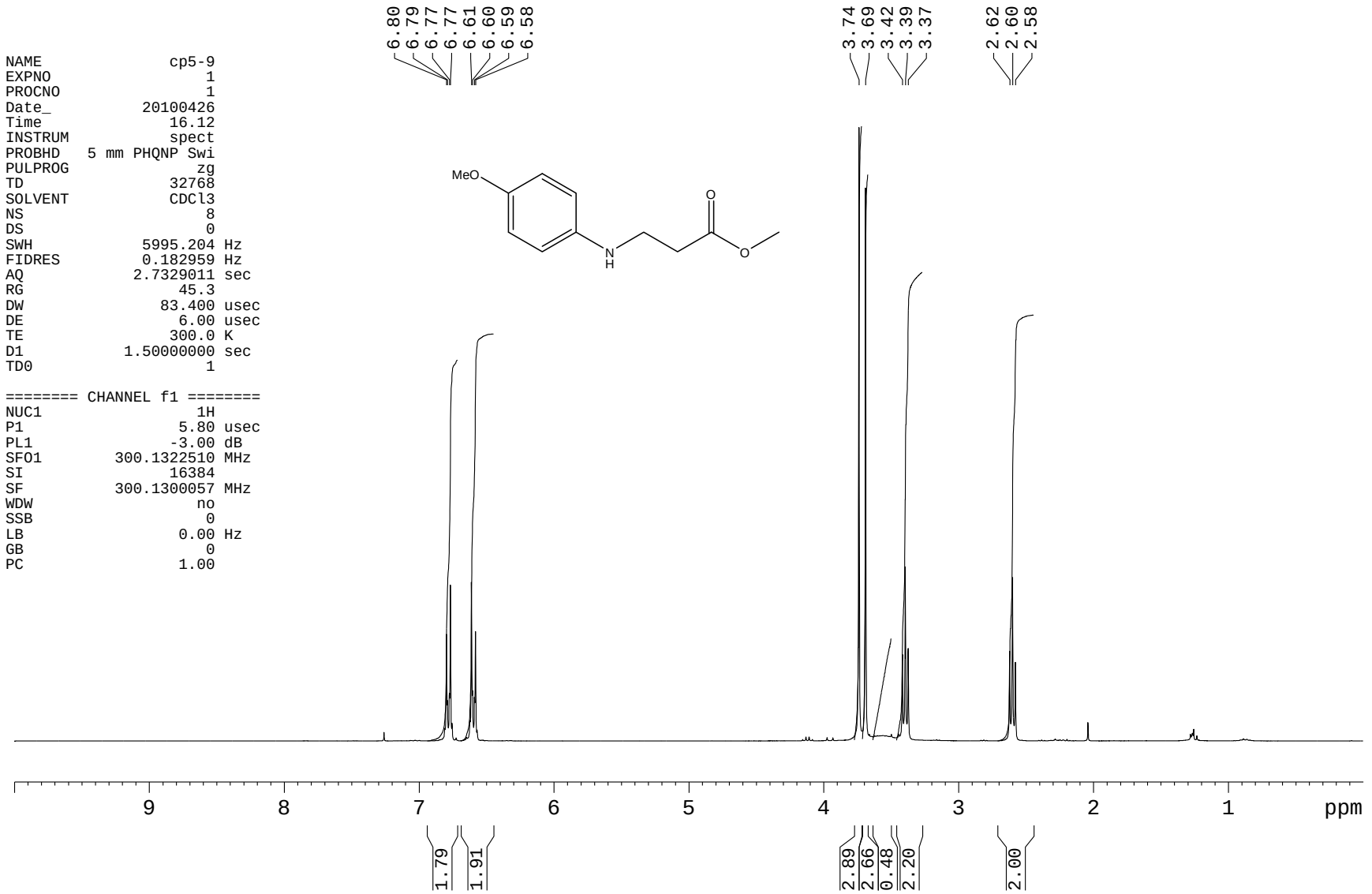

NAME cp4-113
EXPNO 2
PROCNO 1
Date_ 20100411
Time 14.13
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 131
DS 4
SWH 20325.203 Hz
FIDRES 0.310138 Hz
AQ 1.6122355 sec
RG 18390.4
DW 24.600 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 6
======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 -3.00 dB
SFO1 75.4767751 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -3.00 dB
PL12 18.00 dB
PL13 15.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677414 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
172.9
137.2
131.4
131.3
130.6
130.0
111.8
39.0
30.2
21.1
16.9
O
S
N
240
220
200
180
160
140
120
100
80
60
40
20
ppm

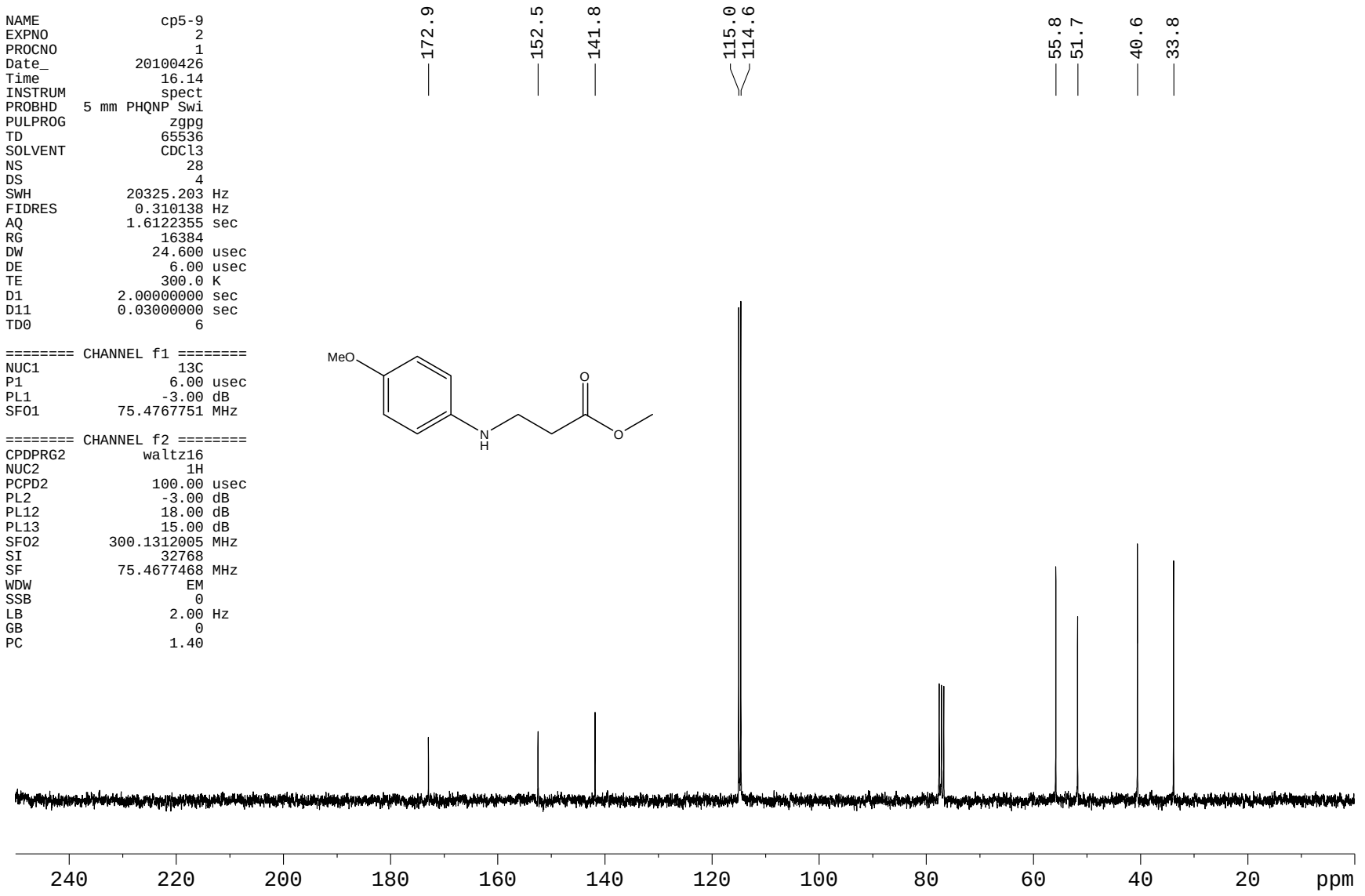

7.41
7.38
7.22
7.21
7.20
7.19
5.81
3.29
3.27
3.24
3.08
3.05
3.03
2.34
NAME cp4-105
EXPNO 1
PROCNO 1
Date_ 20100411
Time 13.40
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 71.8
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 5.80 usec
PL1 -3.00 dB
SFO1 300.1322510 MHz
SI 16384
SF 300.1300123 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Br
O
S
N
9
8
7
6
5
4
3
2
1
ppm
1.55
1.74
1.61
2.00
2.00
6.07

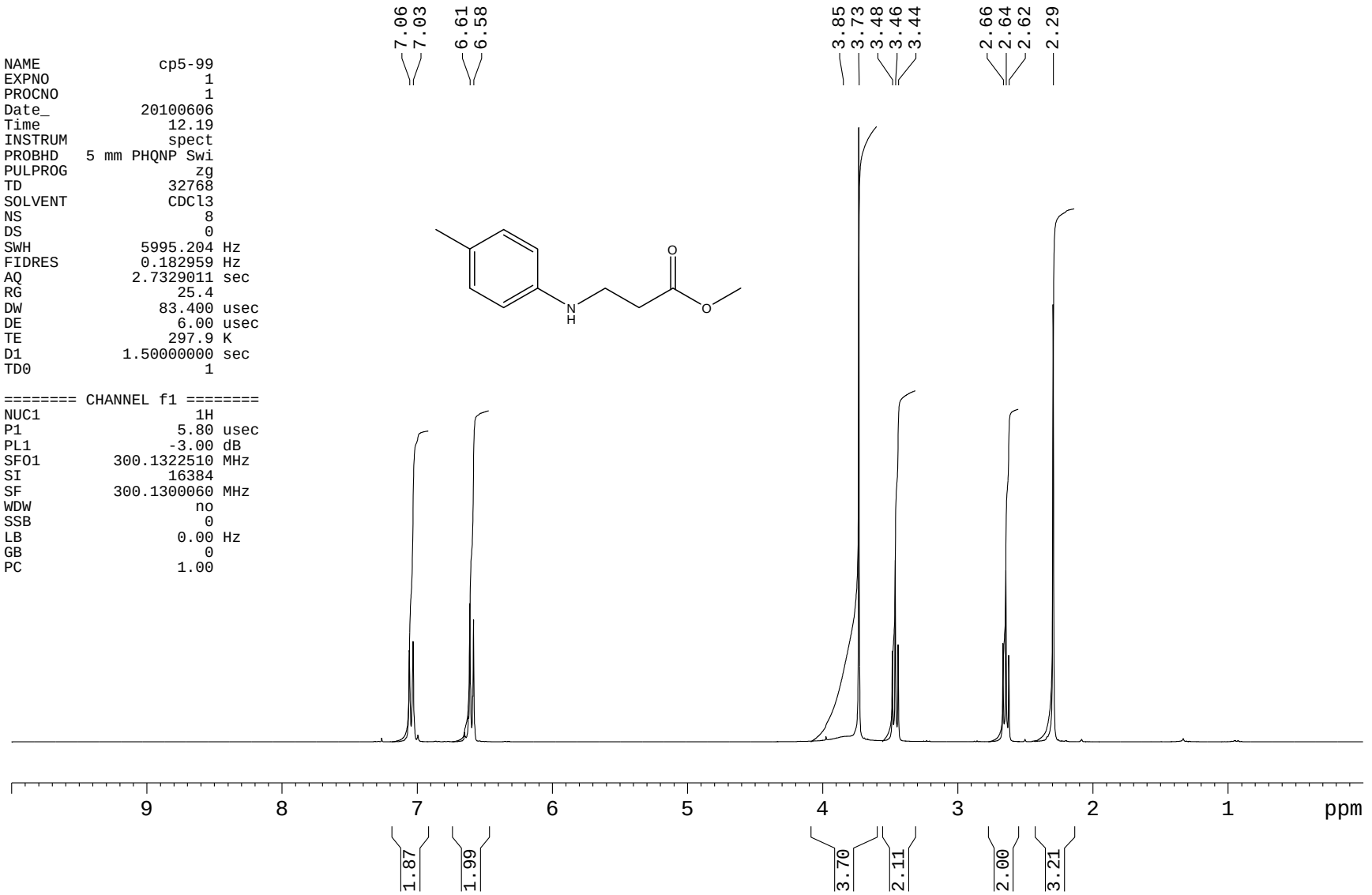

NAME cp4-105
EXPNO 2
PROCNO 1
Date_ 20100411
Time 13.46
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 158
DS 4
SWH 20325.203 Hz
FIDRES 0.310138 Hz
AQ 1.6122355 sec
RG 18390.4
DW 24.600 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 6
======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 -3.00 dB
SFO1 75.4767751 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -3.00 dB
PL12 18.00 dB
PL13 15.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677432 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
172.5
134.7
132.2
131.7
130.6
120.7
112.0
38.6
29.5
16.9
Br
S
O
N
240
220
200
180
160
140
120
100
80
60
40
20
ppm

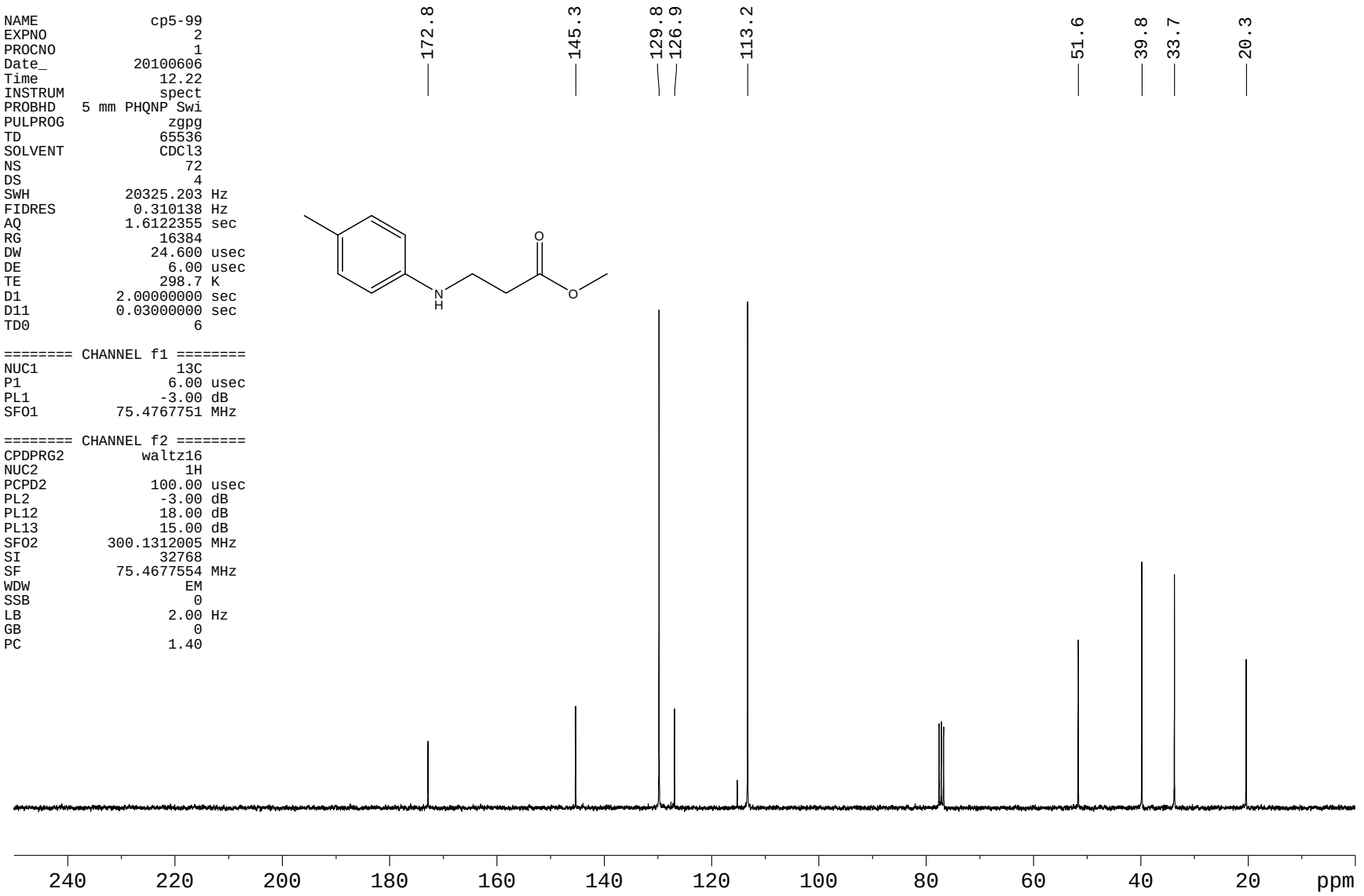

7.20
7.18
7.17
7.15
7.15
6.74
6.71
6.69
6.63
6.63
6.60
4.00
3.69
3.47
3.45
3.43
2.64
2.62
2.60
NAME cp5-7(1)
EXPNO 1
PROCNO 1
Date_ 20100411
Time 11.57
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 114
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 5.80 usec
PL1 -3.00 dB
SFO1 300.1322510 MHz
SI 16384
SF 300.1300104 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
O
N
H
O
9
8
7
6
5
4
3
2
1
ppm
1.62
0.79
1.73
0.86
2.75
2.04
2.00

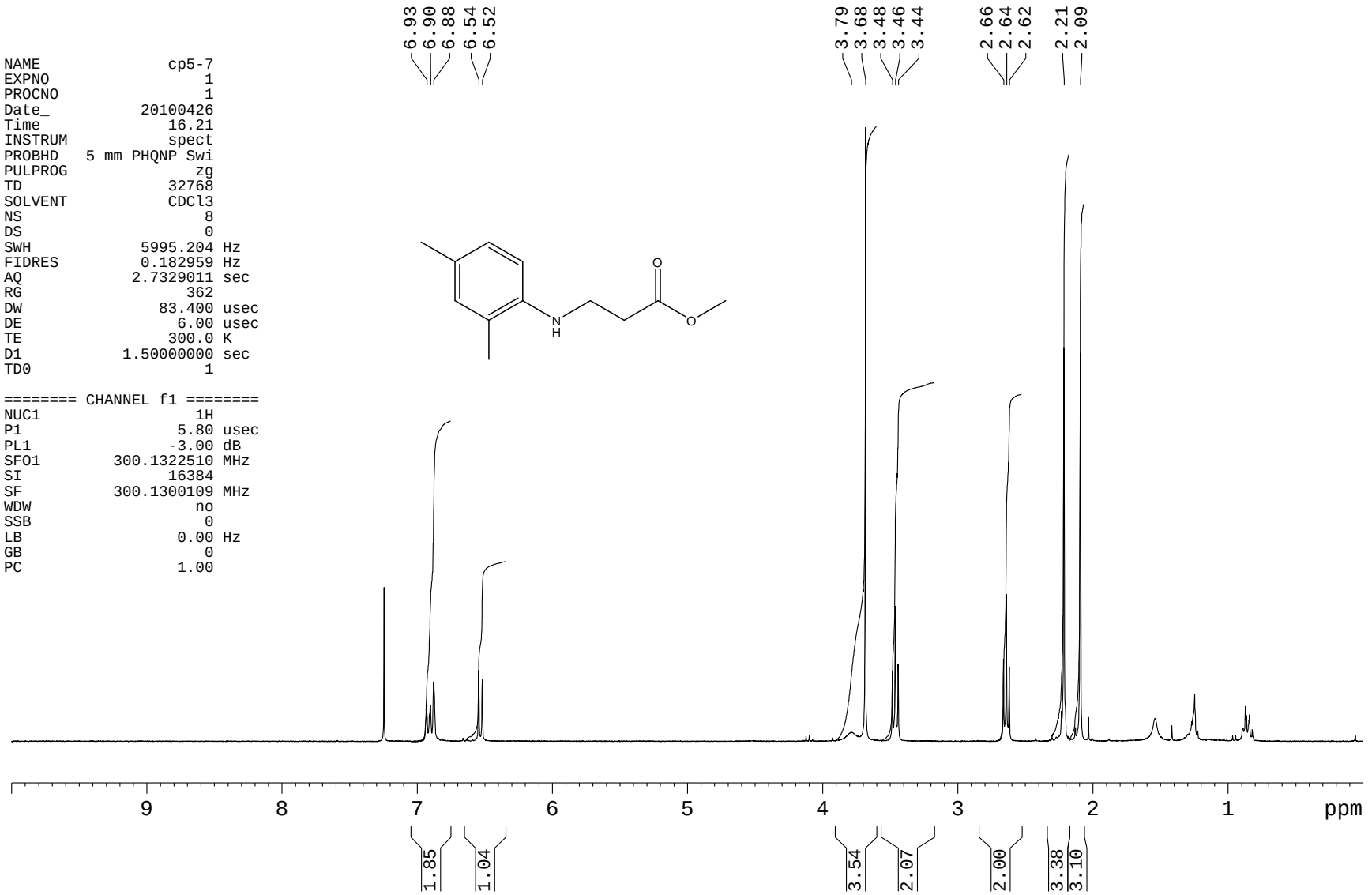

NAME cp5-7(1)
EXPNO 2
PROCNO 1
Date_ 20100411
Time 12.02
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 129
DS 4
SWH 20325.203 Hz
FIDRES 0.310138 Hz
AQ 1.6122355 sec
RG 16384
DW 24.600 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 6
======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 -3.00 dB
SFO1 75.4767751 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -3.00 dB
PL12 18.00 dB
PL13 15.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677423 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
172.9
147.7
129.4
117.9
113.1
51.8
39.5
33.8
O
N
H
O
240
220
200
180
160
140
120
100
80
60
40
20
ppm

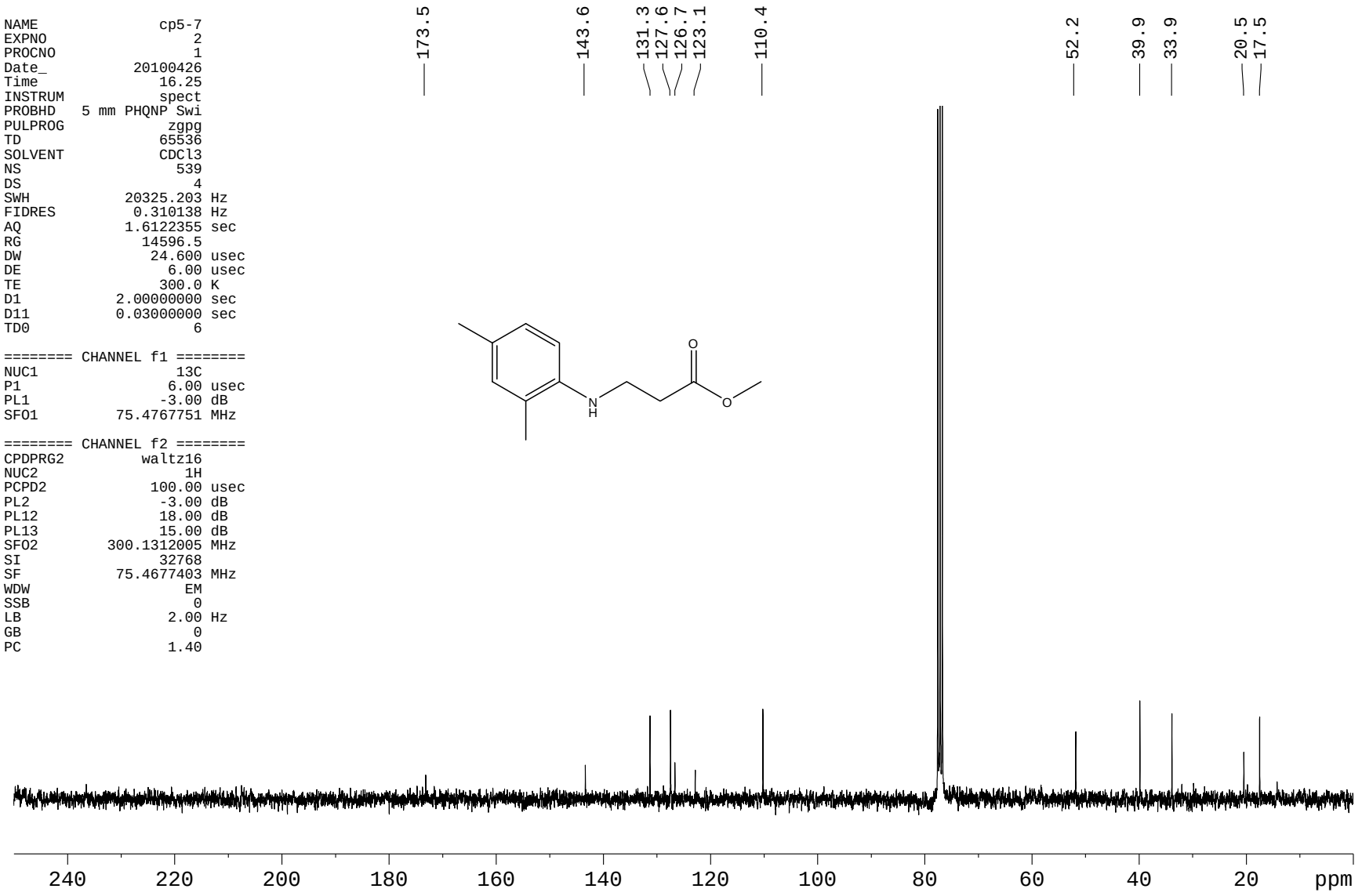

6.80
6.79
6.77
6.77
6.61
6.60
6.59
6.58
3.74
3.69
3.42
3.39
3.37
2.62
2.60
2.58
MeO
O
N
H
O
NAME cp5-9
EXPNO 1
PROCNO 1
Date_ 20100426
Time 16.12
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 45.3
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 5.80 usec
PL1 -3.00 dB
SFO1 300.1322510 MHz
SI 16384
SF 300.1300057 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
ppm
1.79
1.91
2.89
2.66
0.48
2.20
2.00

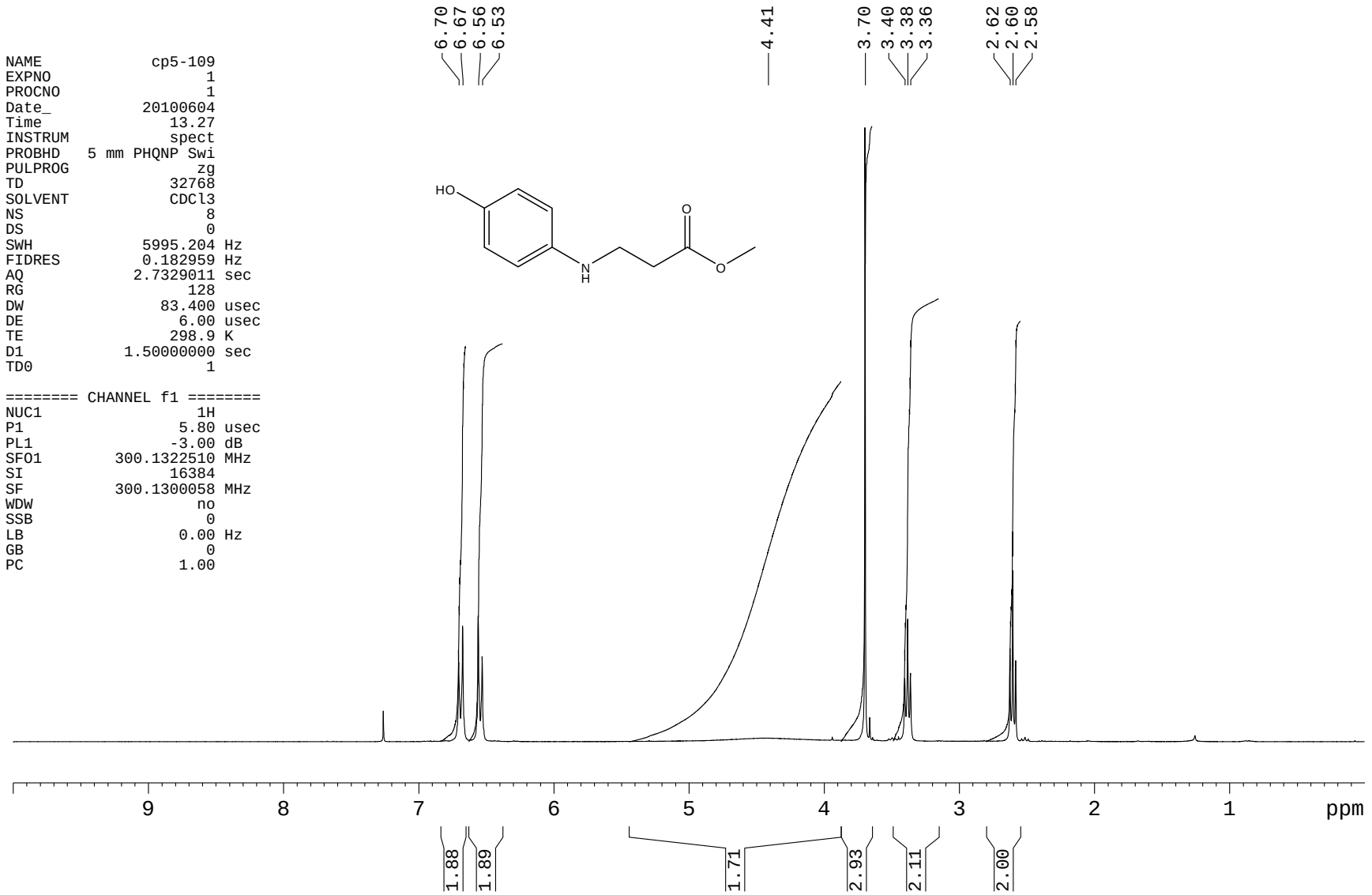

NAME cp5-9
EXPNO 2
PROCNO 1
Date_ 20100426
Time 16.14
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 28
DS 4
SWH 20325.203 Hz
FIDRES 0.310138 Hz
AQ 1.6122355 sec
RG 16384
DW 24.600 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 6
======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 -3.00 dB
SFO1 75.4767751 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -3.00 dB
PL12 18.00 dB
PL13 15.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677468 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
172.9
152.5
141.8
115.0
114.6
55.8
51.7
40.6
33.8
MeO
O
N
H
O
240
220
200
180
160
140
120
100
80
60
40
20
ppm


7.06
7.03
6.61
6.58
3.85
3.73
3.48
3.46
3.44
2.66
2.64
2.62
2.29
NAME cp5-99
EXPNO 1
PROCNO 1
Date_ 20100606
Time 12.19
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 25.4
DW 83.400 usec
DE 6.00 usec
TE 297.9 K
D1 1.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 5.80 usec
PL1 -3.00 dB
SFO1 300.1322510 MHz
SI 16384
SF 300.1300060 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
O
N
H
O
9
8
7
6
5
4
3
2
1
ppm
1.87
1.99
3.70
2.11
2.00
3.21


NAME cp5-99
EXPNO 2
PROCNO 1
Date_ 20100606
Time 12.22
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 72
DS 4
SWH 20325.203 Hz
FIDRES 0.310138 Hz
AQ 1.6122355 sec
RG 16384
DW 24.600 usec
DE 6.00 usec
TE 298.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 6
======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 -3.00 dB
SFO1 75.4767751 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -3.00 dB
PL12 18.00 dB
PL13 15.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677554 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
172.8
145.3
129.8
126.9
113.2
51.6
39.8
33.7
20.3
O
N
H
O
240
220
200
180
160
140
120
100
80
60
40
20
ppm

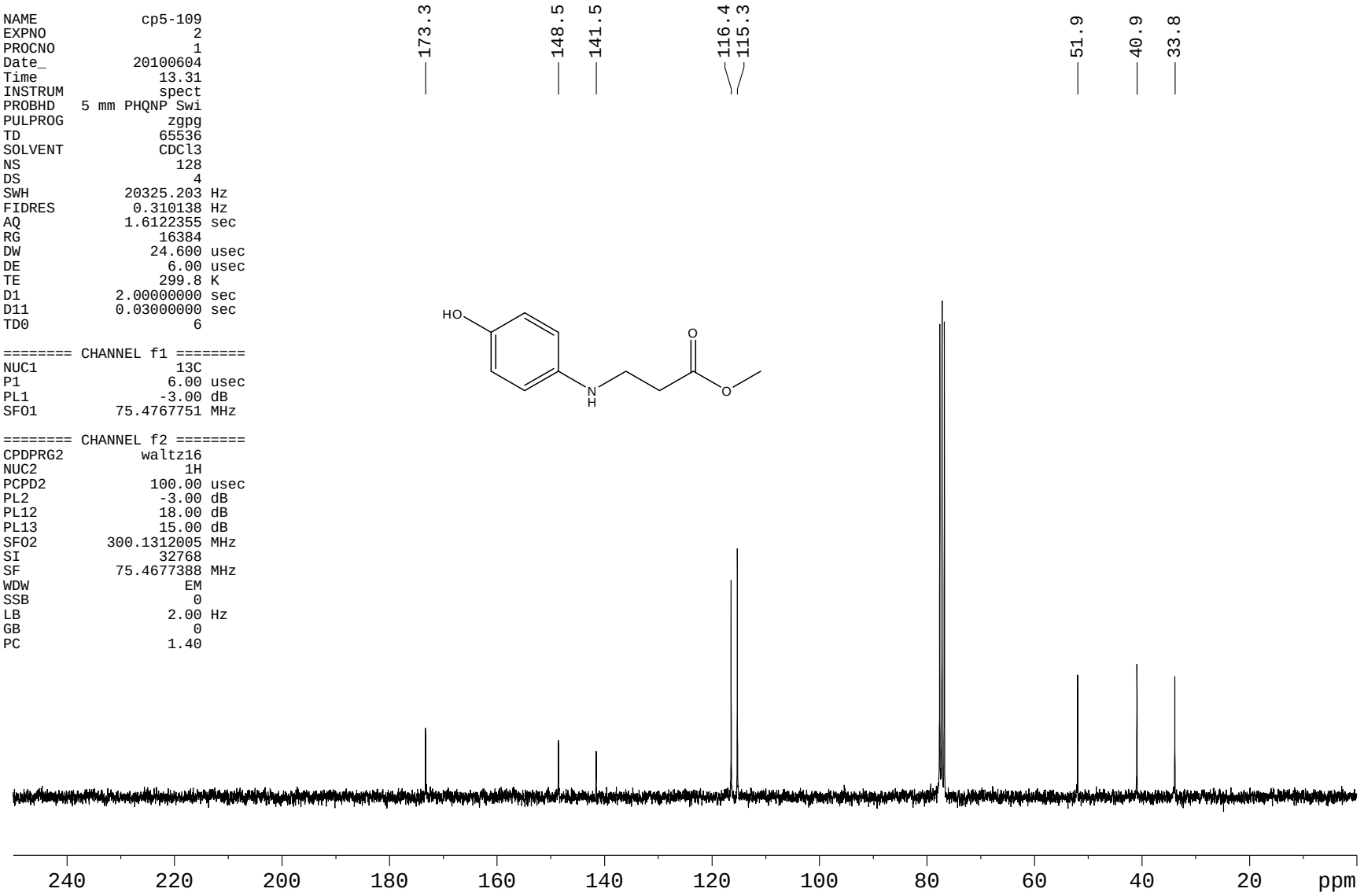

6.93
6.90
6.88
6.54
6.52
3.79
3.68
3.48
3.46
3.44
2.66
2.64
2.62
2.21
2.09
NAME cp5-7
EXPNO 1
PROCNO 1
Date_ 20100426
Time 16.21
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 362
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 5.80 usec
PL1 -3.00 dB
SFO1 300.1322510 MHz
SI 16384
SF 300.1300109 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
O
N
H
O
9
8
7
6
5
4
3
2
1
ppm
1.85
1.04
3.54
2.07
2.00
3.38
3.10

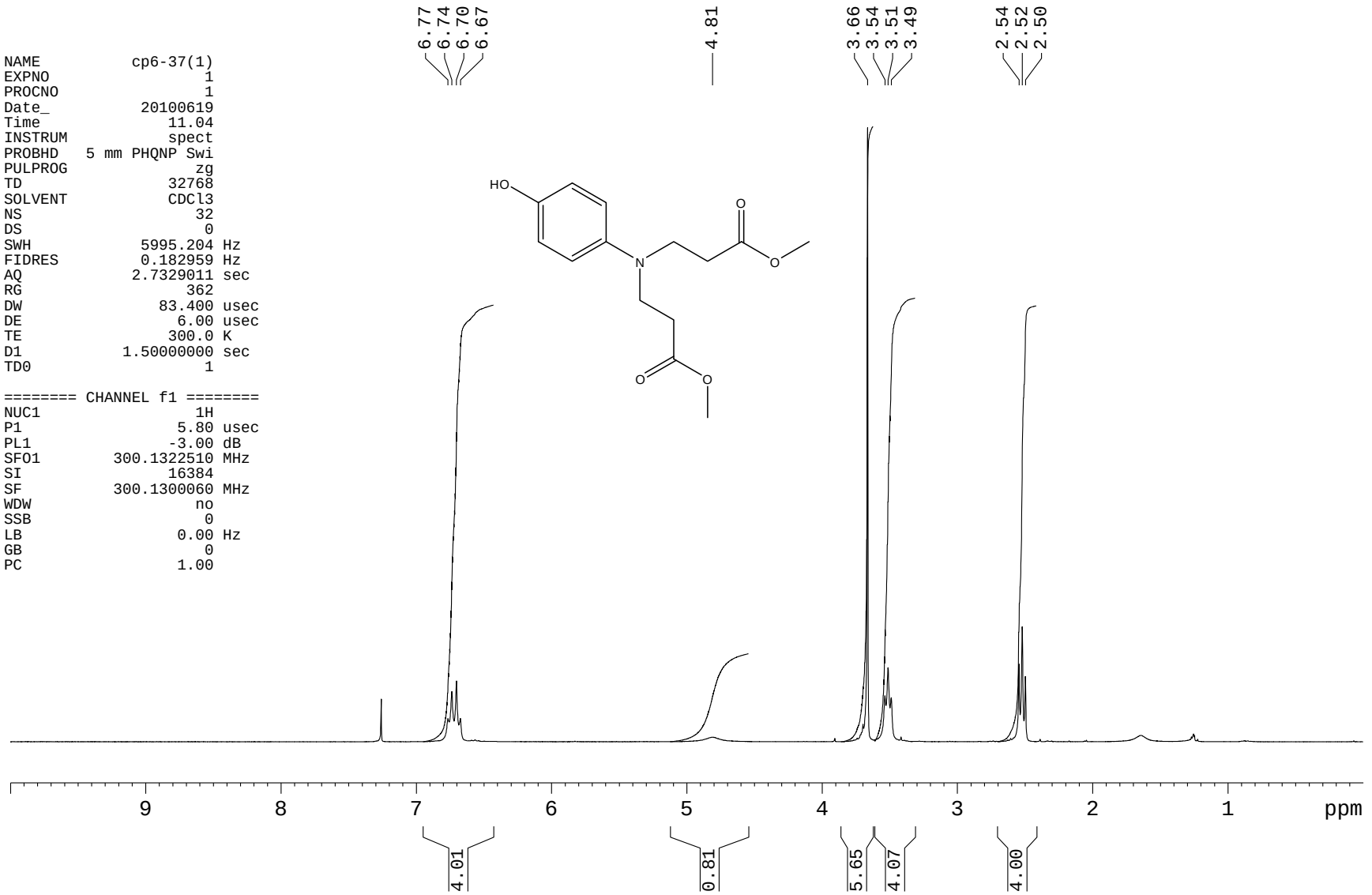

NAME cp5-7
EXPNO 2
PROCNO 1
Date_ 20100426
Time 16.25
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 539
DS 4
SWH 20325.203 Hz
FIDRES 0.310138 Hz
AQ 1.6122355 sec
RG 14596.5
DW 24.600 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 6
======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 -3.00 dB
SFO1 75.4767751 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -3.00 dB
PL12 18.00 dB
PL13 15.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677403 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
173.5
143.6
131.3
127.6
126.7
123.1
110.4
52.2
39.9
33.9
20.5
17.5
O
N
H
O
240
220
200
180
160
140
120
100
80
60
40
20
ppm

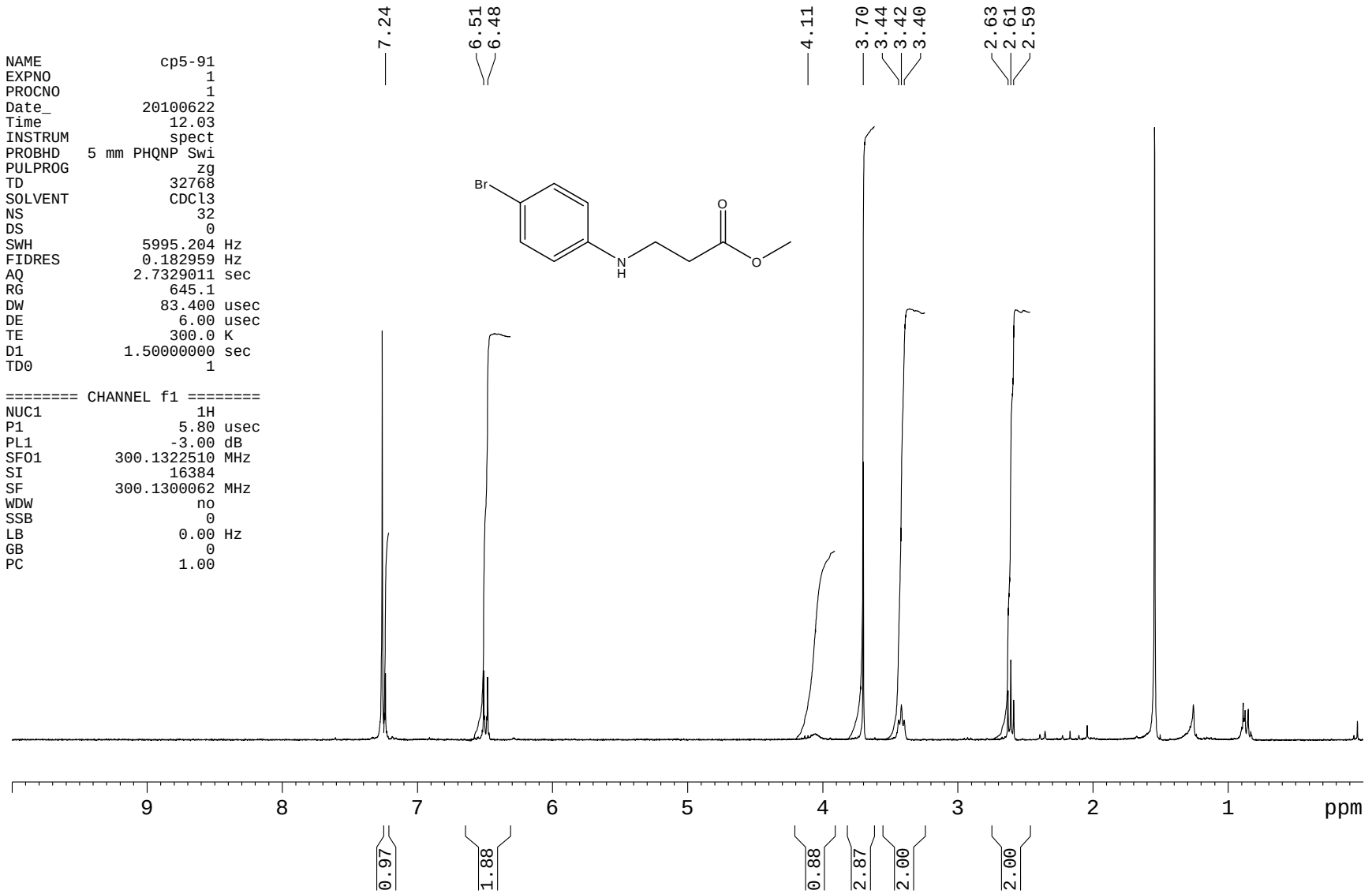


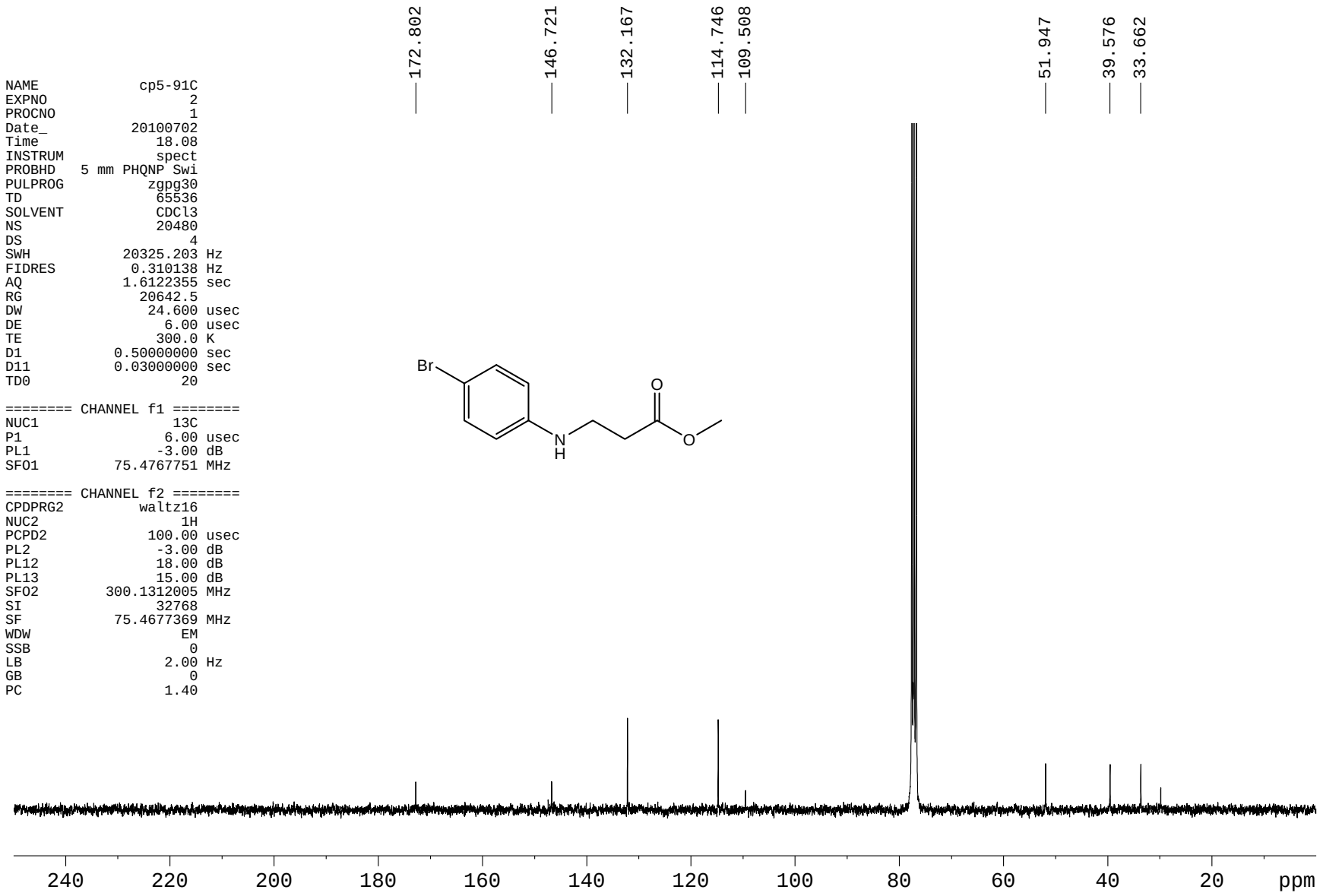

```
NAME            cp5-109
EXPNO                 1
PROCNO                1
Date_          20100604
Time              13.27
INSTRUM           spect
PROBHD   5 mm PHQNP Swi
PULPROG              zg
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    0
SWH            5995.204 Hz
FIDRES         0.182959 Hz
AQ            2.7329011 sec
RG                  128
DW                83.400 usec
DE                 6.00 usec
TE                298.9 K
D1           1.50000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                5.80 usec
PL1              -3.00 dB
SFO1        300.1322510 MHz
SI                16384
SF          300.1300058 MHz
WDW                  no
SSB                   0
LB                 0.00 Hz
GB                    0
PC                 1.00
```

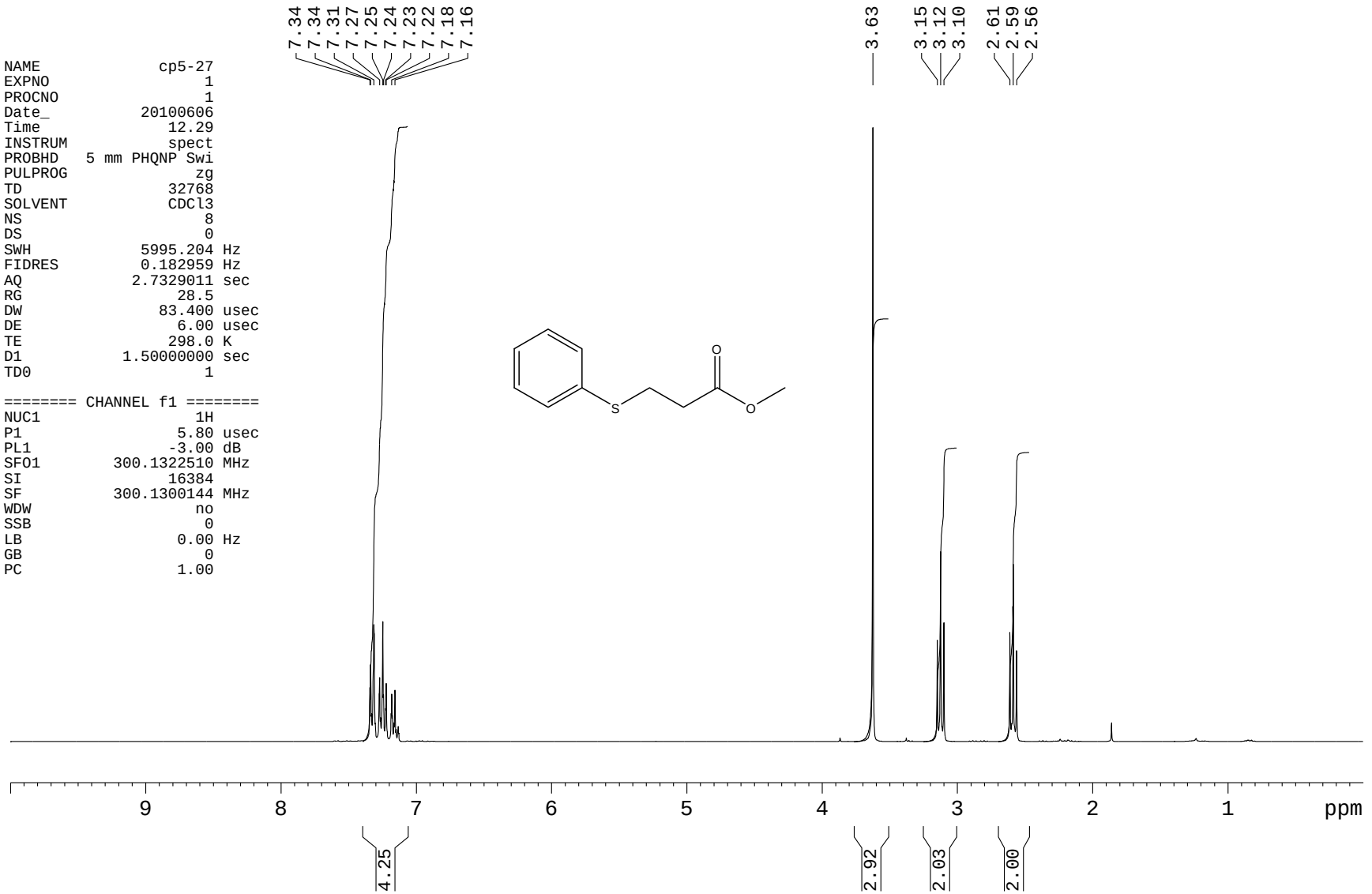
```
NAME            cp5-109
EXPNO                 2
PROCNO                1
Date_          20100604
Time              13.31
INSTRUM           spect
PROBHD   5 mm PHQNP Swi
PULPROG            zgpg
TD                65536
SOLVENT           CDCl3
NS                  128
DS                    4
SWH           20325.203 Hz
FIDRES         0.310138 Hz
AQ            1.6122355 sec
RG                16384
DW               24.600 usec
DE                6.00 usec
TE                299.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   6

======== CHANNEL f1 ========
NUC1                 13C
P1                  6.00 usec
PL1                -3.00 dB
SFO1          75.4767751 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             100.00 usec
PL2                -3.00 dB
PL12               18.00 dB
PL13               15.00 dB
SFO2         300.1312005 MHz
SI                32768
SF           75.4677388 MHz
WDW                  EM
SSB                   0
LB                 2.00 Hz
GB                    0
PC                 1.40
```



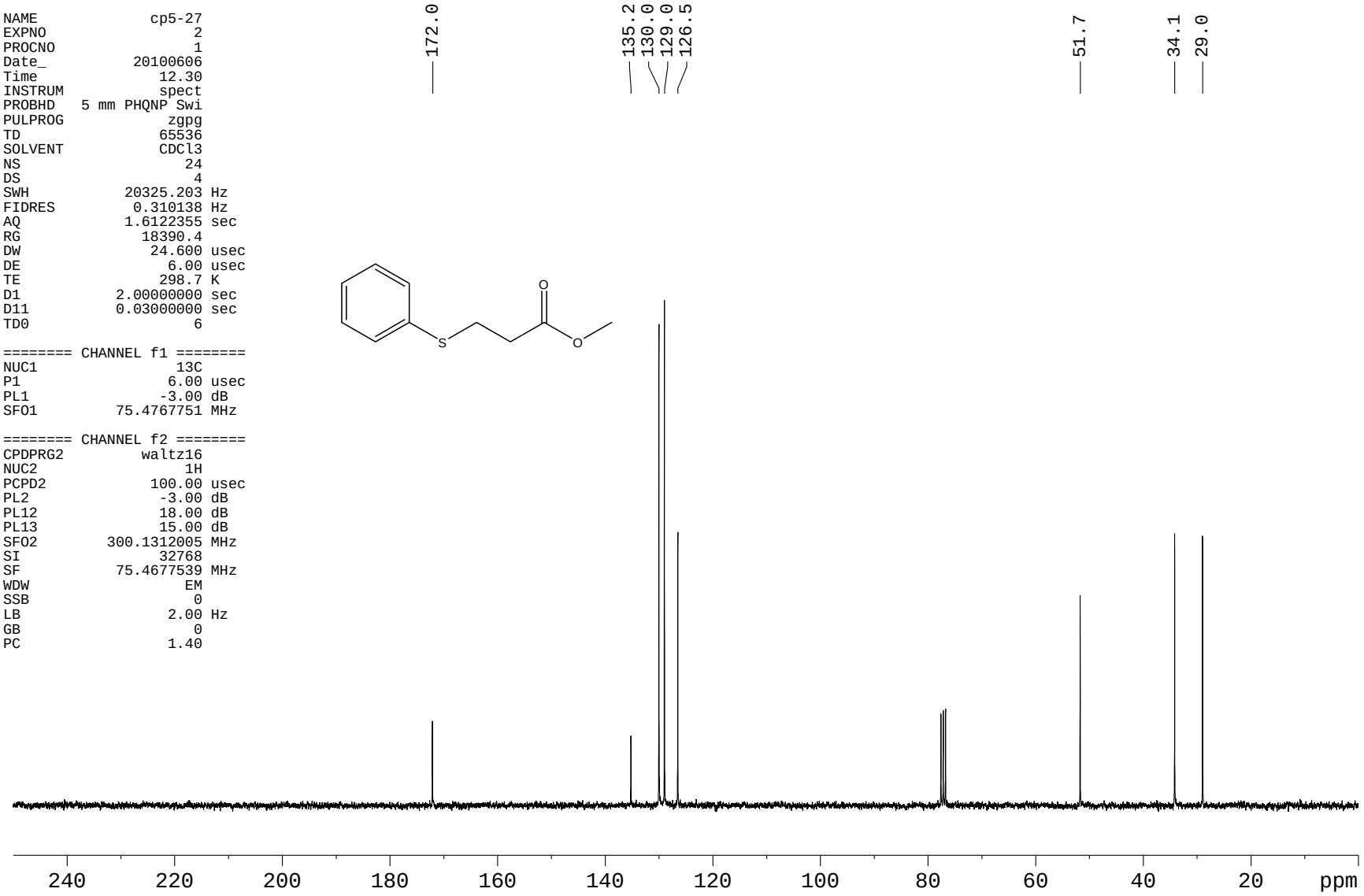

6.77
6.74
6.70
6.67
4.81
3.66
3.54
3.51
3.49
2.54
2.52
2.50
HO
N
O
O
O
O
NAME cp6-37(1)
EXPNO 1
PROCNO 1
Date_ 20100619
Time 11.04
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 362
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 5.80 usec
PL1 -3.00 dB
SFO1 300.1322510 MHz
SI 16384
SF 300.1300060 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
ppm
4.01
0.81
5.65
4.07
4.00

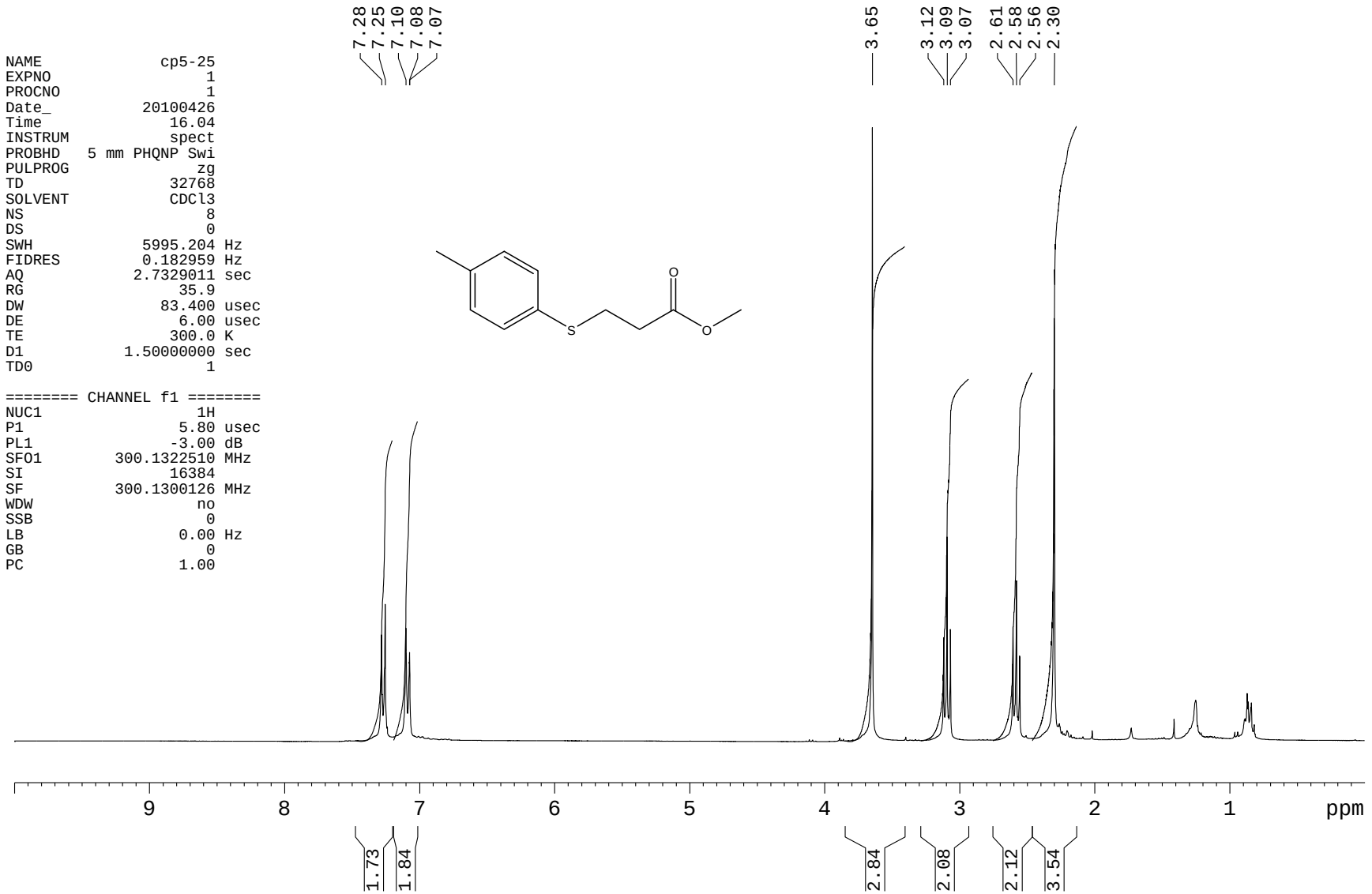

7.24
6.51
6.48
4.11
3.70
3.44
3.42
3.40
2.63
2.61
2.59
NAME cp5-91
EXPNO 1
PROCNO 1
Date_ 20100622
Time 12.03
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 645.1
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 5.80 usec
PL1 -3.00 dB
SFO1 300.1322510 MHz
SI 16384
SF 300.1300062 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Br
N
H
O
O
9
8
7
6
5
4
3
2
1
ppm
0.97
1.88
0.88
2.87
2.00
2.00

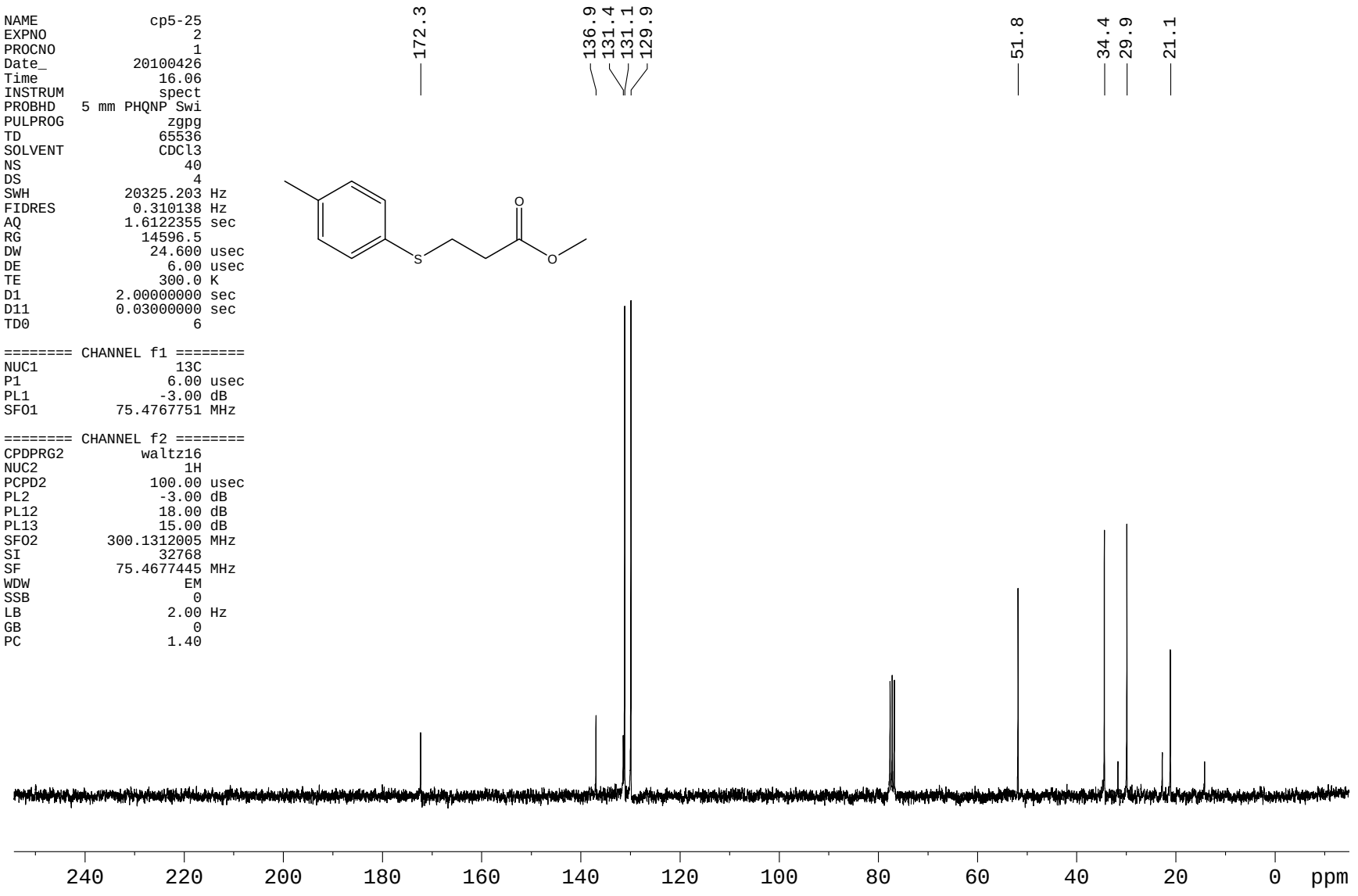

172.802
146.721
132.167
114.746
109.508
51.947
39.576
33.662
NAME cp5-91C
EXPNO 2
PROCNO 1
Date_ 20100702
Time 18.08
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 20480
DS 4
SWH 20325.203 Hz
FIDRES 0.310138 Hz
AQ 1.6122355 sec
RG 20642.5
DW 24.600 usec
DE 6.00 usec
TE 300.0 K
D1 0.50000000 sec
D11 0.03000000 sec
TD0 20
======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 -3.00 dB
SFO1 75.4767751 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -3.00 dB
PL12 18.00 dB
PL13 15.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677369 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
Br
O
N
H
O
240
220
200
180
160
140
120
100
80
60
40
20
ppm

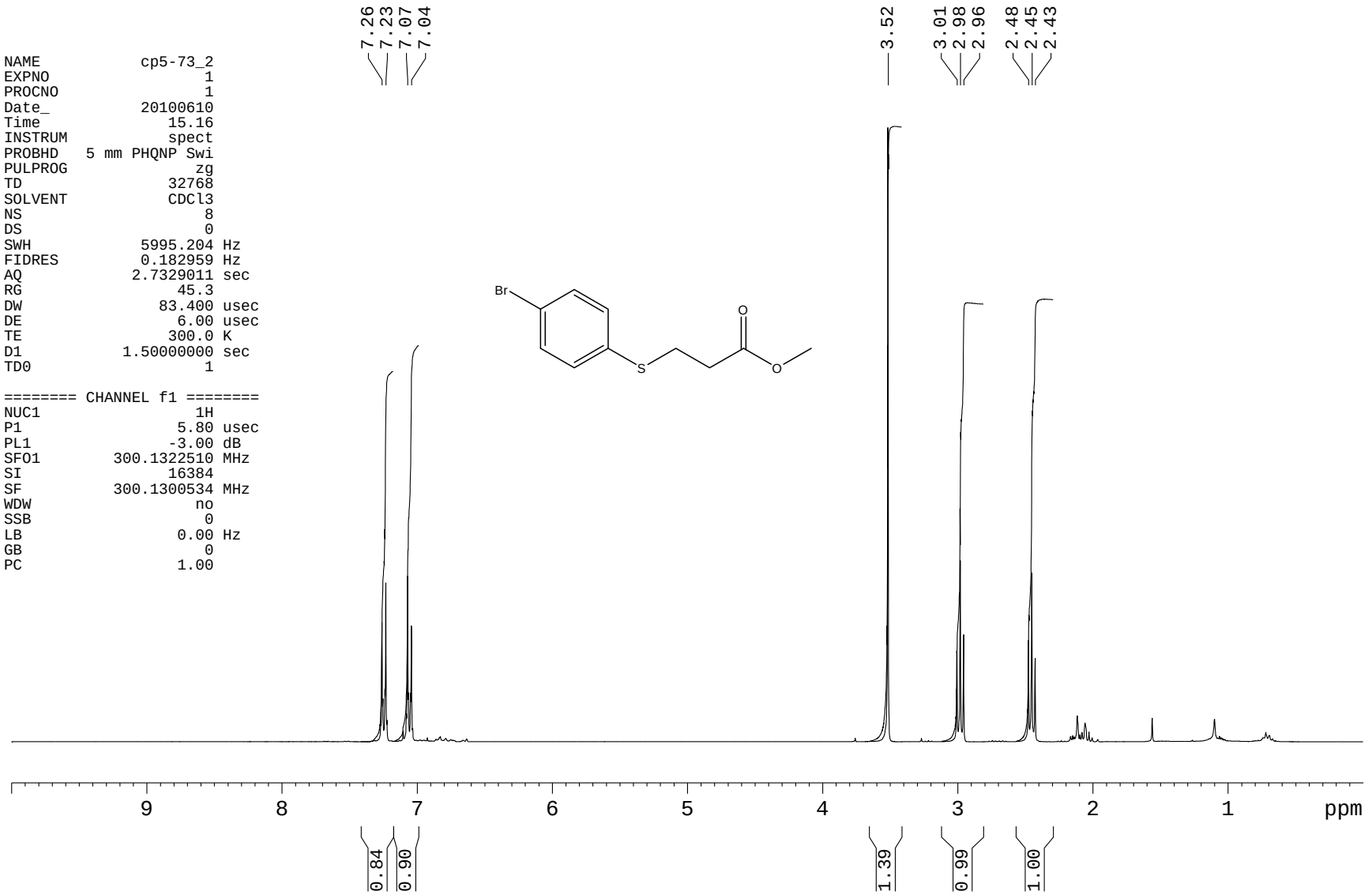

7.34
7.34
7.31
7.27
7.25
7.24
7.23
7.22
7.18
7.16
3.63
3.15
3.12
3.10
2.61
2.59
2.56
NAME cp5-27
EXPNO 1
PROCNO 1
Date_ 20100606
Time 12.29
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 28.5
DW 83.400 usec
DE 6.00 usec
TE 298.0 K
D1 1.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 5.80 usec
PL1 -3.00 dB
SFO1 300.1322510 MHz
SI 16384
SF 300.1300144 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
O
S
O
9
8
7
6
5
4
3
2
1
ppm
4.25
2.92
2.03
2.00

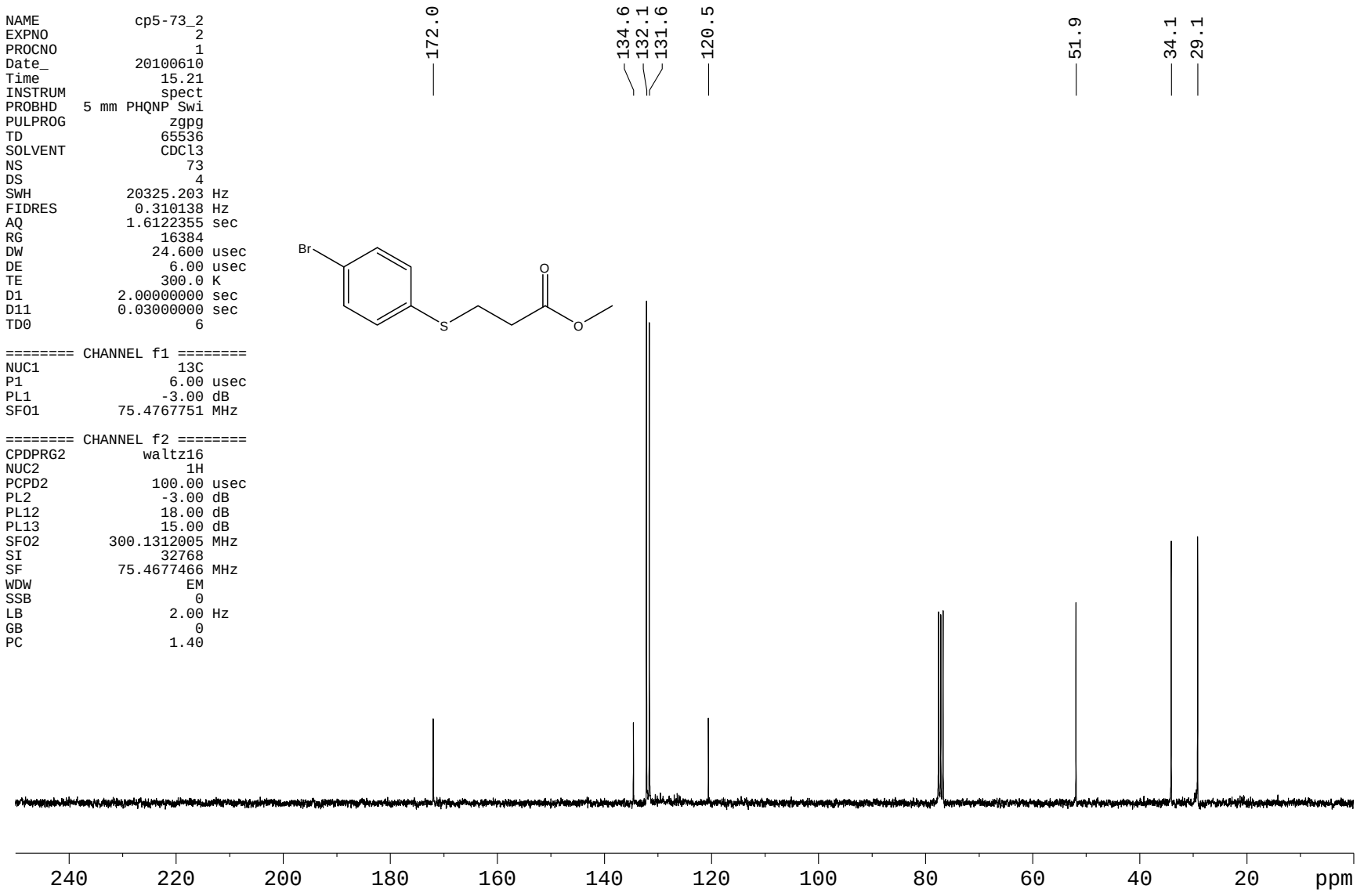
```
NAME             cp5-27
EXPNO                 2
PROCNO                1
Date_          20100606
Time              12.30
INSTRUM           spect
PROBHD   5 mm PHQNP Swi
PULPROG            zgpg
TD                65536
SOLVENT           CDCl3
NS                   24
DS                    4
SWH           20325.203 Hz
FIDRES         0.310138 Hz
AQ            1.6122355 sec
RG              18390.4
DW               24.600 usec
DE                6.00 usec
TE               298.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   6

======== CHANNEL f1 ========
NUC1                 13C
P1                  6.00 usec
PL1                -3.00 dB
SFO1         75.4767751 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             100.00 usec
PL2                -3.00 dB
PL12               18.00 dB
PL13               15.00 dB
SFO2        300.1312005 MHz
SI                 32768
SF           75.4677539 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.40
```

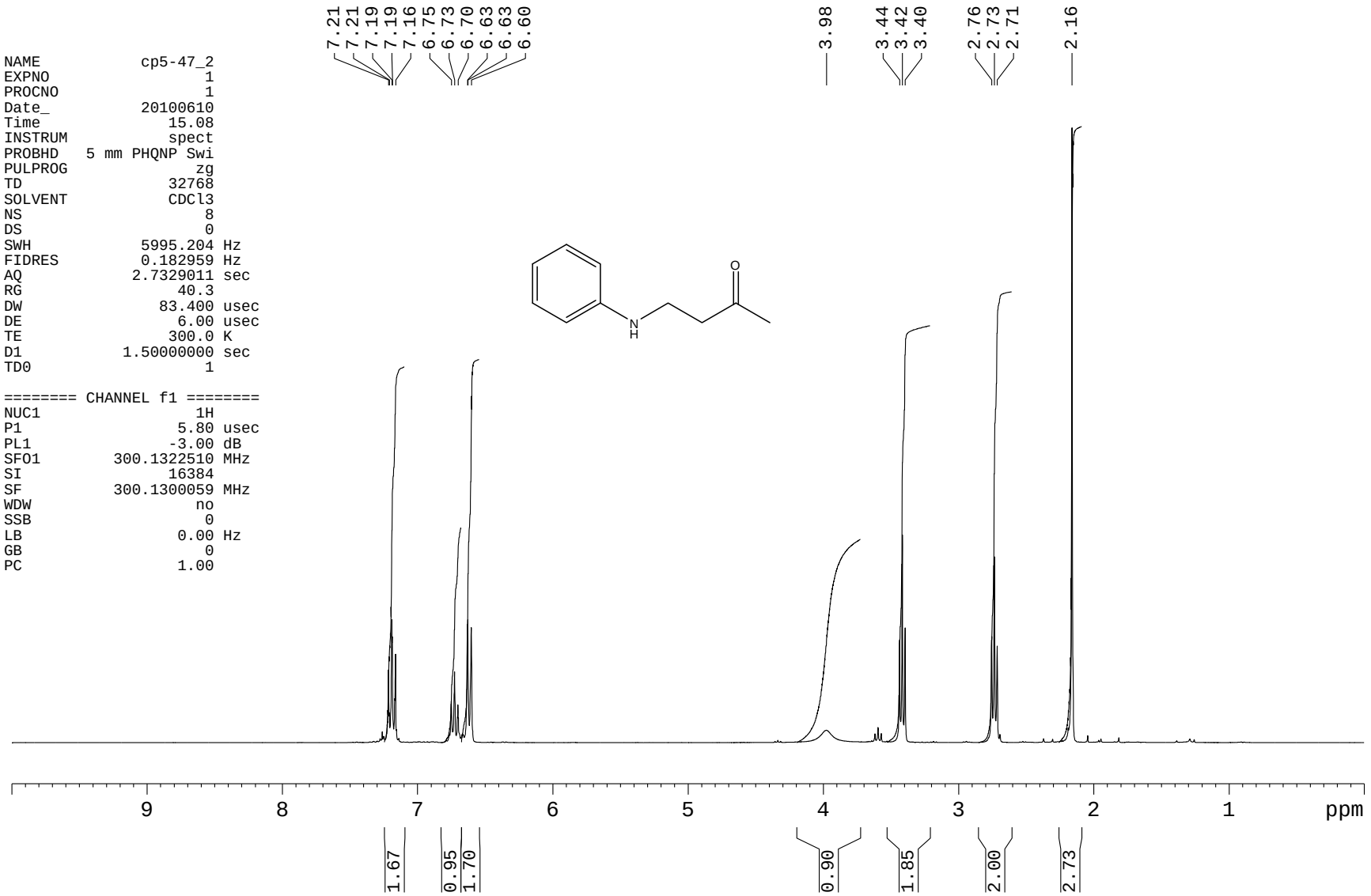


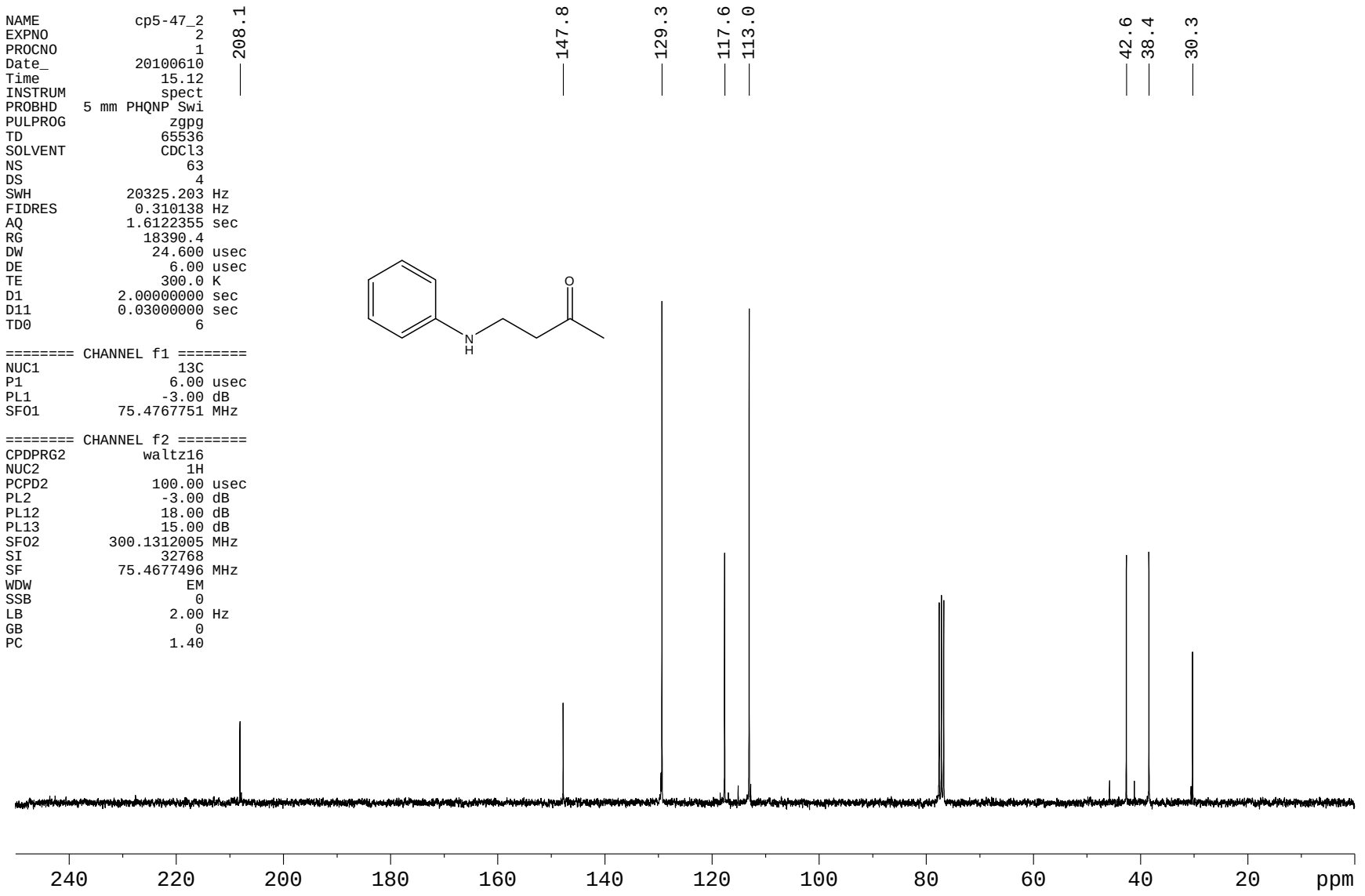

7.28
7.25
7.10
7.08
7.07
3.65
3.12
3.09
3.07
2.61
2.58
2.56
2.30
NAME cp5-25
EXPNO 1
PROCNO 1
Date_ 20100426
Time 16.04
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 35.9
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 5.80 usec
PL1 -3.00 dB
SFO1 300.1322510 MHz
SI 16384
SF 300.1300126 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
O
S
O
9
8
7
6
5
4
3
2
1
ppm
1.73
1.84
2.84
2.08
2.12
3.54

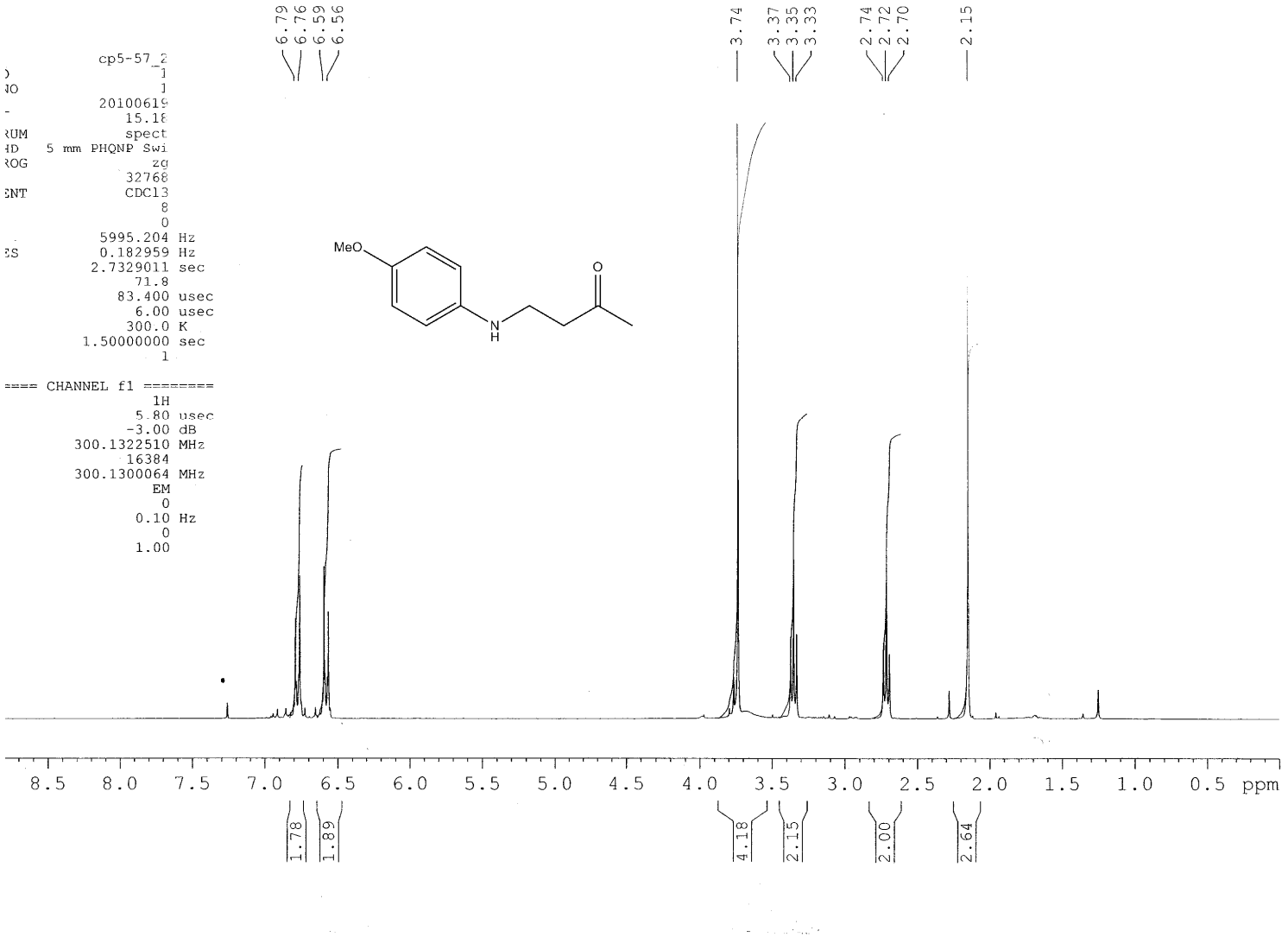

NAME cp5-25
EXPNO 2
PROCNO 1
Date_ 20100426
Time 16.06
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 40
DS 4
SWH 20325.203 Hz
FIDRES 0.310138 Hz
AQ 1.6122355 sec
RG 14596.5
DW 24.600 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 6
======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 -3.00 dB
SFO1 75.4767751 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -3.00 dB
PL12 18.00 dB
PL13 15.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677445 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
172.3
136.9
131.4
131.1
129.9
51.8
34.4
29.9
21.1
O
S
O
240
220
200
180
160
140
120
100
80
60
40
20
0
ppm

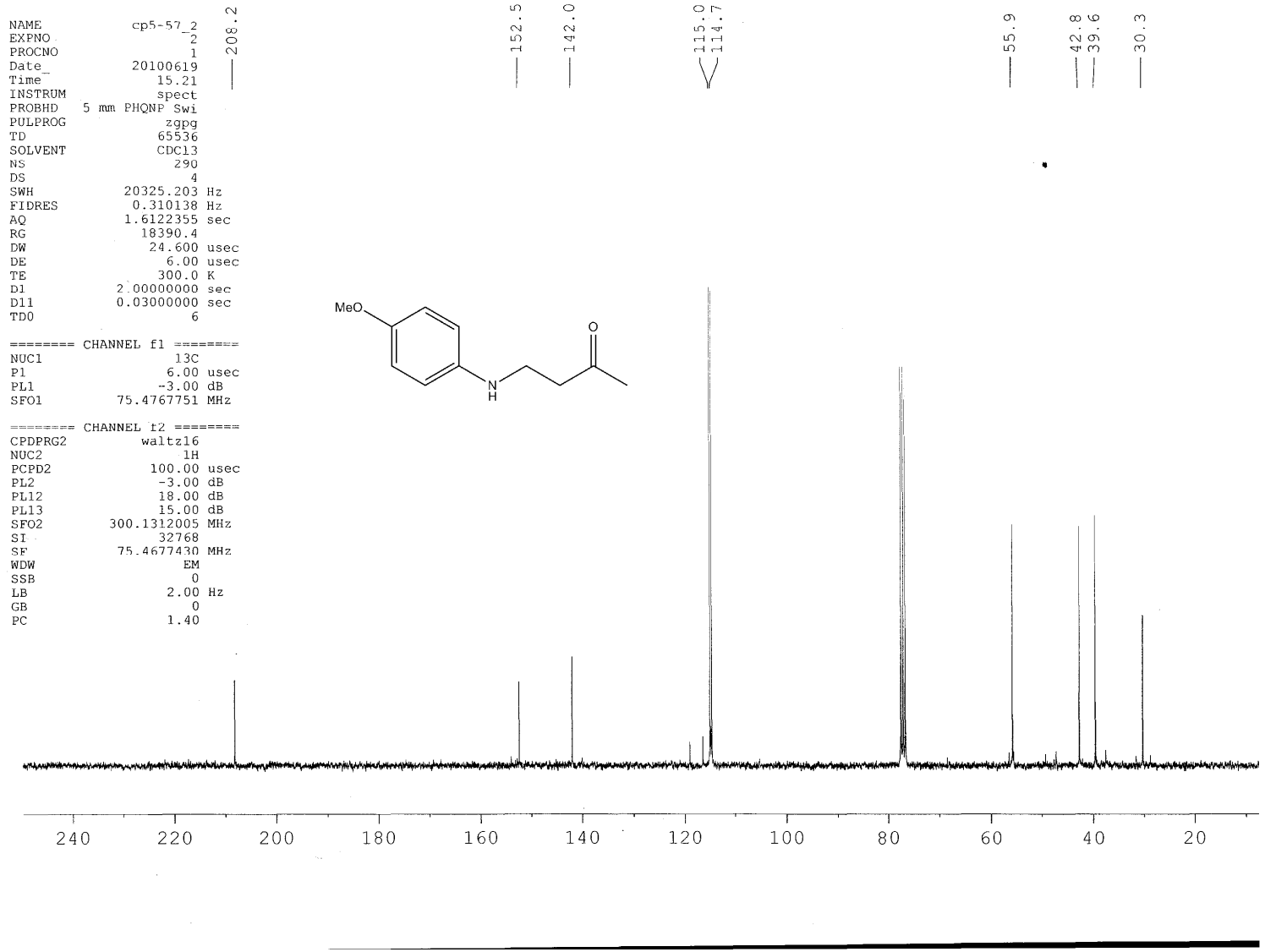

7.26
7.23
7.07
7.04
3.52
3.01
2.98
2.96
2.48
2.45
2.43
NAME cp5-73_2
EXPNO 1
PROCNO 1
Date_ 20100610
Time 15.16
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 45.3
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 5.80 usec
PL1 -3.00 dB
SFO1 300.1322510 MHz
SI 16384
SF 300.1300534 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Br
S
O
O
9
8
7
6
5
4
3
2
1
ppm
0.84
0.90
1.39
0.99
1.00

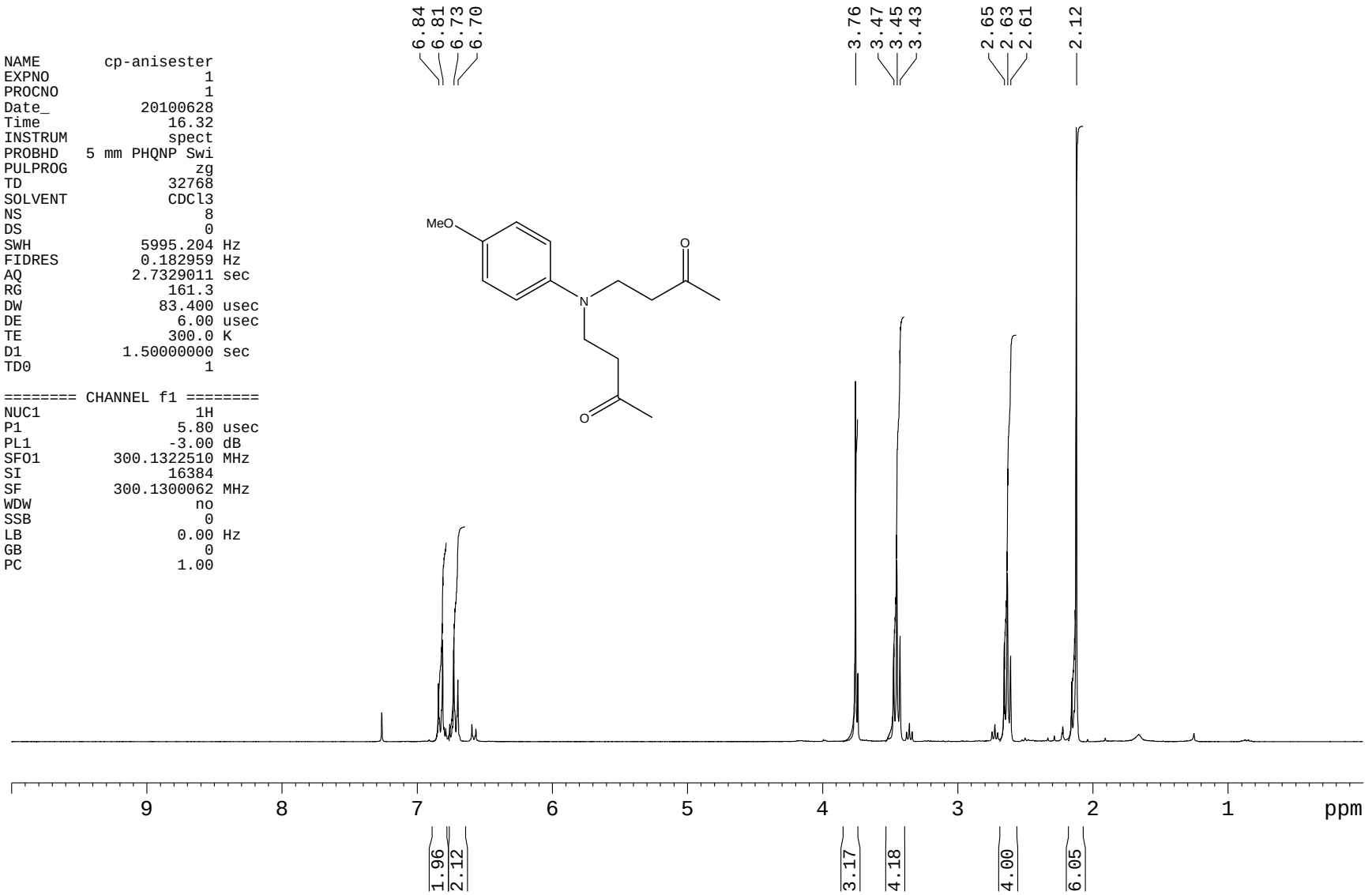

NAME cp5-73_2
EXPNO 2
PROCNO 1
Date_ 20100610
Time 15.21
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 73
DS 4
SWH 20325.203 Hz
FIDRES 0.310138 Hz
AQ 1.6122355 sec
RG 16384
DW 24.600 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 6
======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 -3.00 dB
SFO1 75.4767751 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -3.00 dB
PL12 18.00 dB
PL13 15.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677466 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
172.0
134.6
132.1
131.6
120.5
51.9
34.1
29.1
Br
S
O
O
240
220
200
180
160
140
120
100
80
60
40
20
ppm

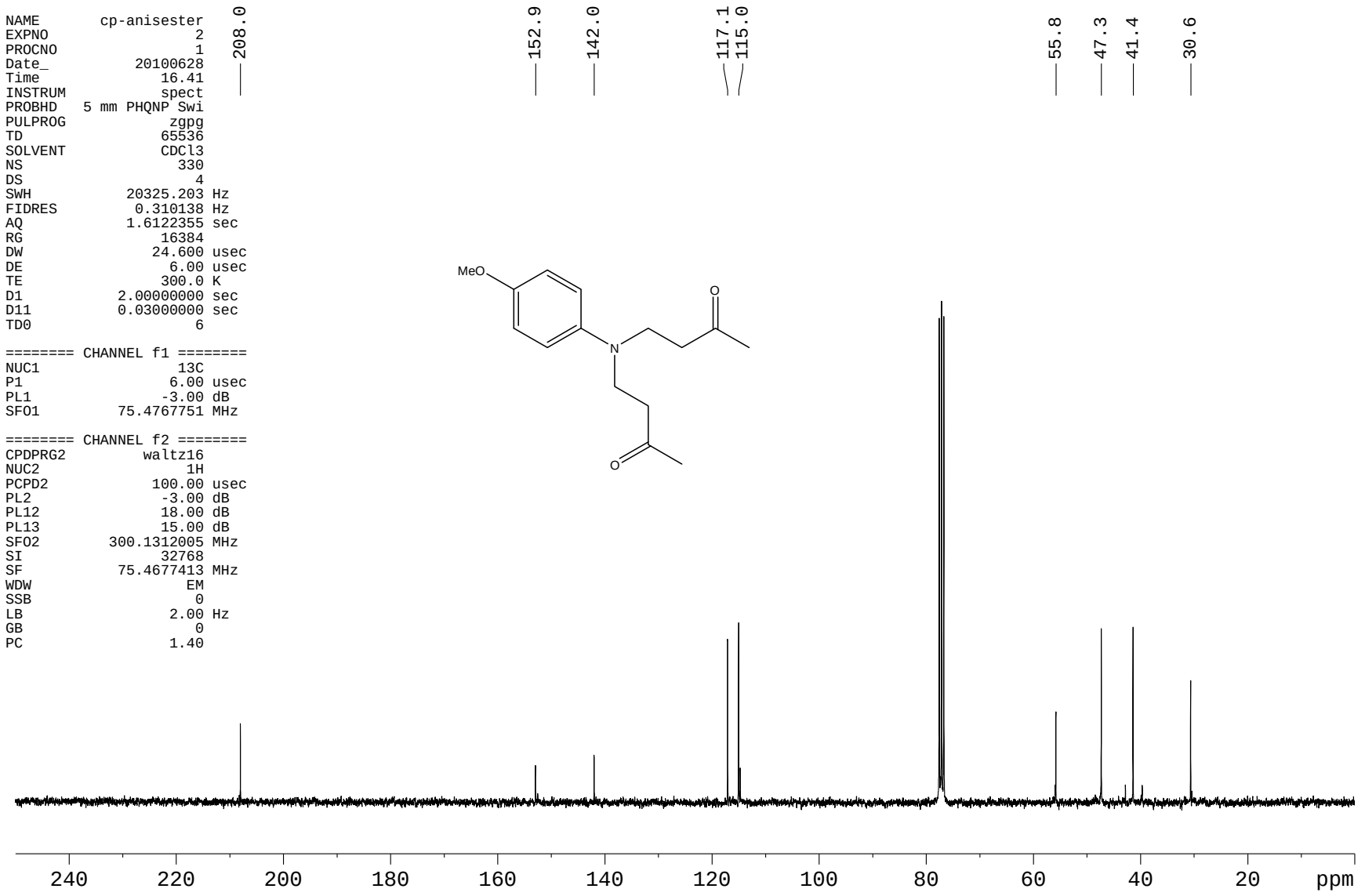

7.21
7.21
7.19
7.19
7.16
6.75
6.73
6.70
6.63
6.63
6.60
3.98
3.44
3.42
3.40
2.76
2.73
2.71
2.16
NAME cp5-47_2
EXPNO 1
PROCNO 1
Date_ 20100610
Time 15.08
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 40.3
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 5.80 usec
PL1 -3.00 dB
SFO1 300.1322510 MHz
SI 16384
SF 300.1300059 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
O
N
H
9
8
7
6
5
4
3
2
1
ppm
1.67
0.95
1.70
0.90
1.85
2.00
2.73


208.1
147.8
129.3
117.6
113.0
42.6
38.4
30.3
NAME cp5-47_2
EXPNO 2
PROCNO 1
Date_ 20100610
Time 15.12
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 63
DS 4
SWH 20325.203 Hz
FIDRES 0.310138 Hz
AQ 1.6122355 sec
RG 18390.4
DW 24.600 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 6
======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 -3.00 dB
SFO1 75.4767751 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -3.00 dB
PL12 18.00 dB
PL13 15.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677496 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
O
N
H
240
220
200
180
160
140
120
100
80
60
40
20
ppm

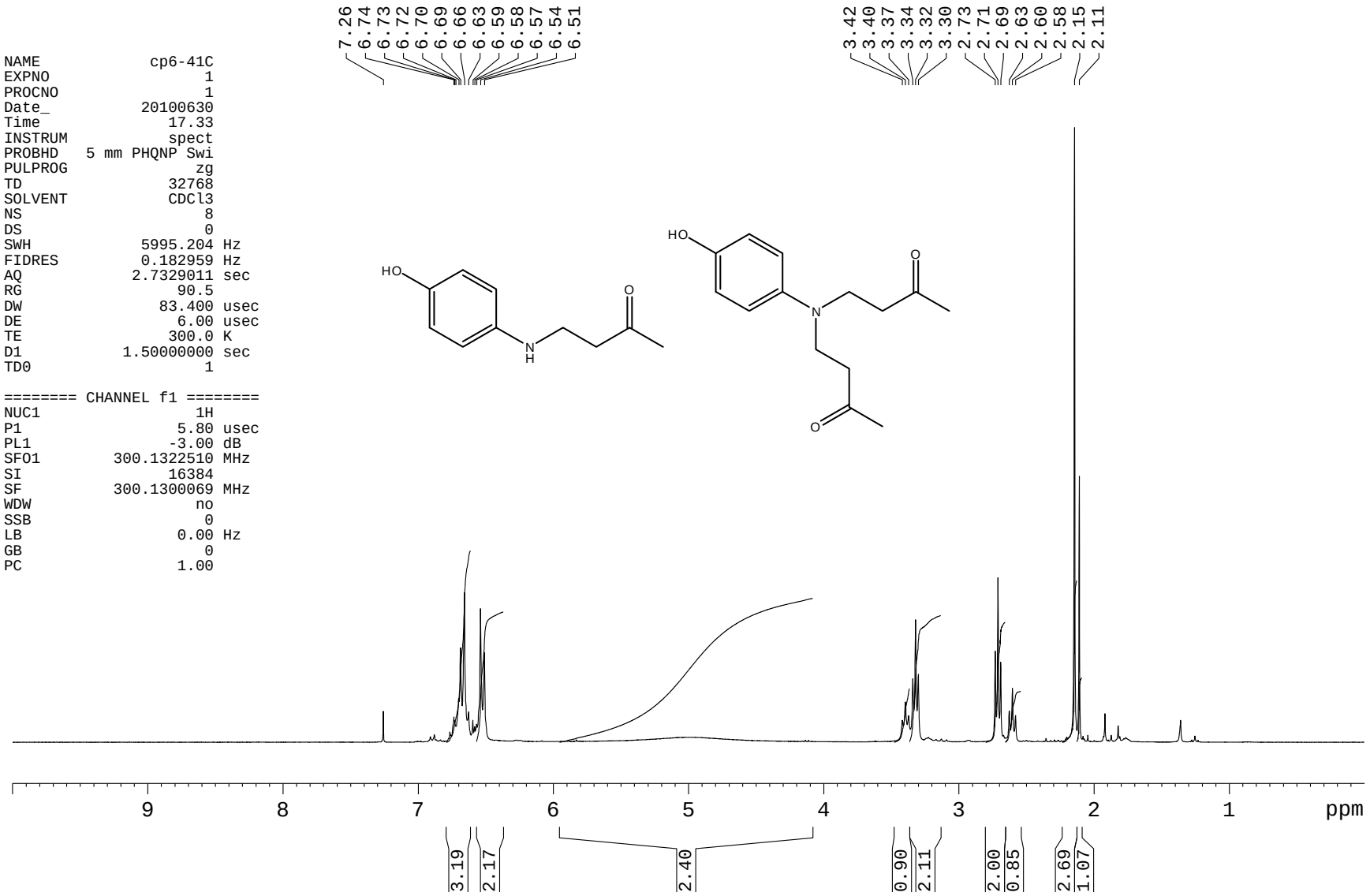

6.79
6.76
6.59
6.56
3.74
3.37
3.35
3.33
2.74
2.72
2.70
2.15
MeO
O
N
H
cp5-57_2
20100619
15.18
spect
5 mm PHQNP Swi
zg
32768
CDCl3
8
0
5995.204 Hz
0.182959 Hz
2.7329011 sec
71.8
83.400 usec
6.00 usec
300.0 K
1.50000000 sec
1
==== CHANNEL f1 ========
1H
5.80 usec
-3.00 dB
300.1322510 MHz
16384
300.1300064 MHz
EM
0
0.10 Hz
0
1.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.78
1.89
4.18
2.15
2.00
2.64

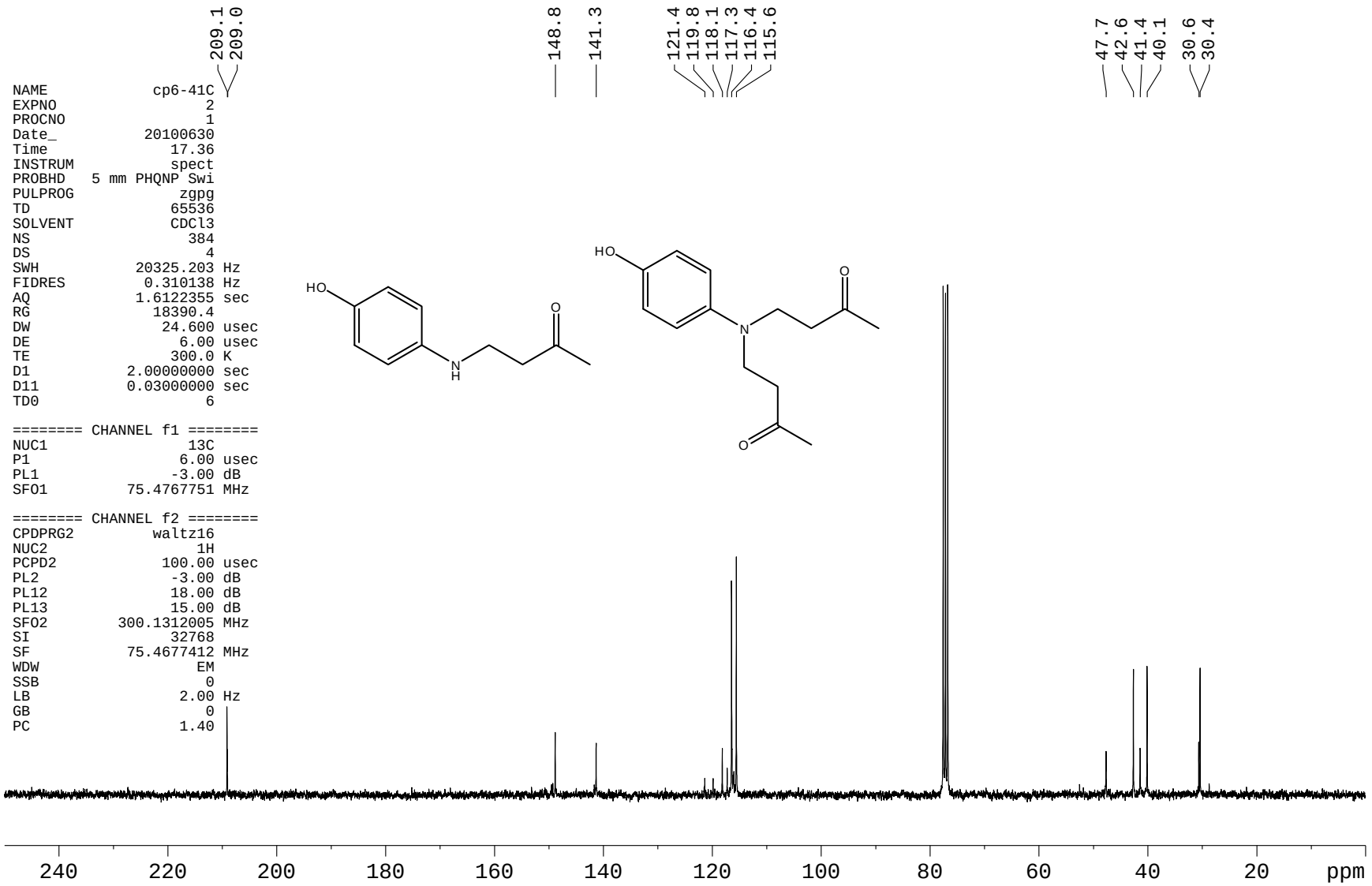

NAME cp5-57_2
EXPNO 2
PROCNO 1
Date_ 20100619
Time 15.21
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 290
DS 4
SWH 20325.203 Hz
FIDRES 0.310138 Hz
AQ 1.6122355 sec
RG 18390.4
DW 24.600 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 6
======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 -3.00 dB
SFO1 75.4767751 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -3.00 dB
PL12 18.00 dB
PL13 15.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677430 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
208.2
152.5
142.0
115.0
114.7
55.9
42.8
39.6
30.3
MeO
O
N
H
240
220
200
180
160
140
120
100
80
60
40
20

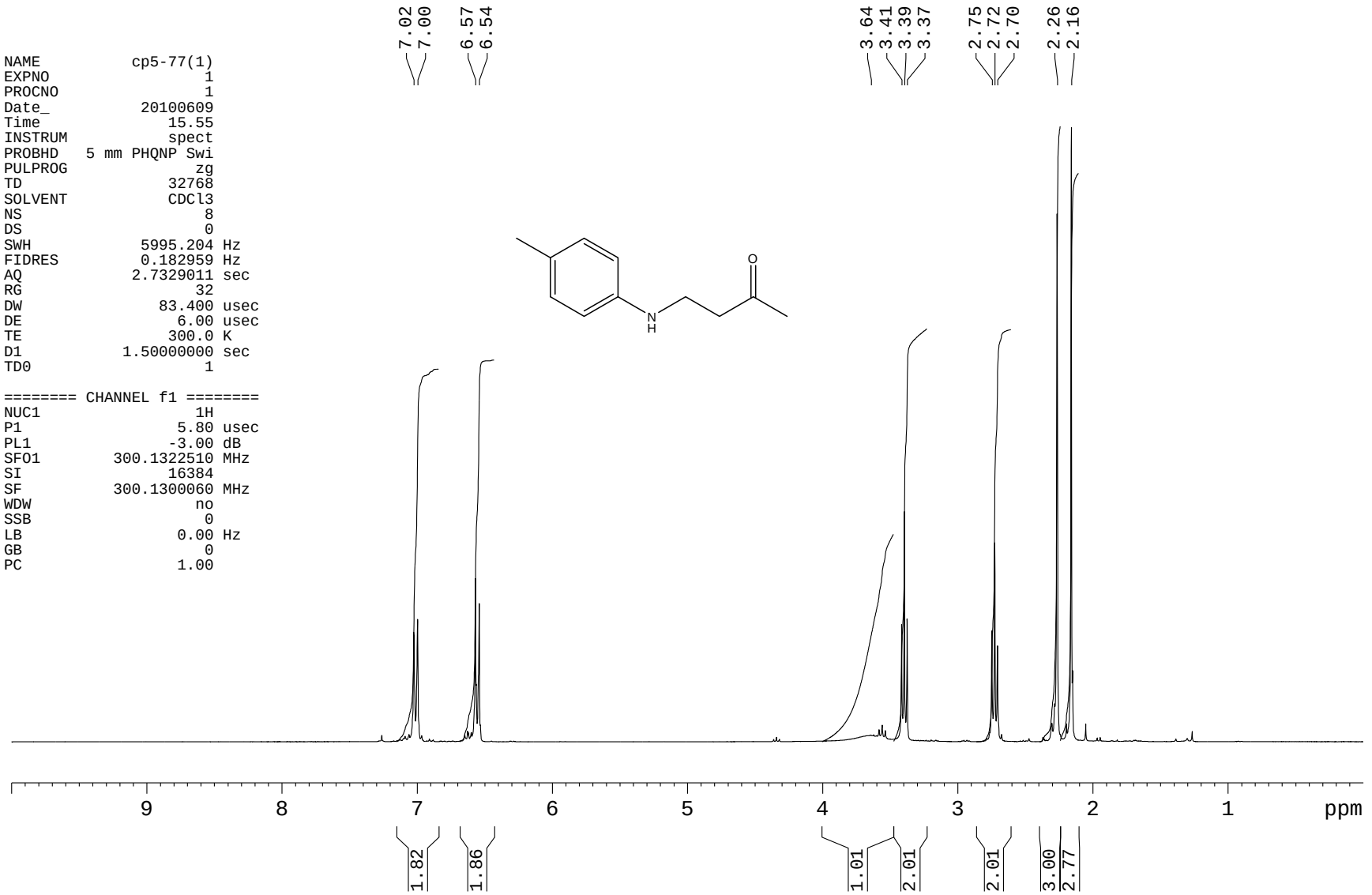

6.84
6.81
6.73
6.70
3.76
3.47
3.45
3.43
2.65
2.63
2.61
2.12
MeO
N
O
O
NAME cp-anisester
EXPNO 1
PROCNO 1
Date_ 20100628
Time 16.32
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 161.3
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 5.80 usec
PL1 -3.00 dB
SFO1 300.1322510 MHz
SI 16384
SF 300.1300062 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
ppm
1.96
2.12
3.17
4.18
4.00
6.05

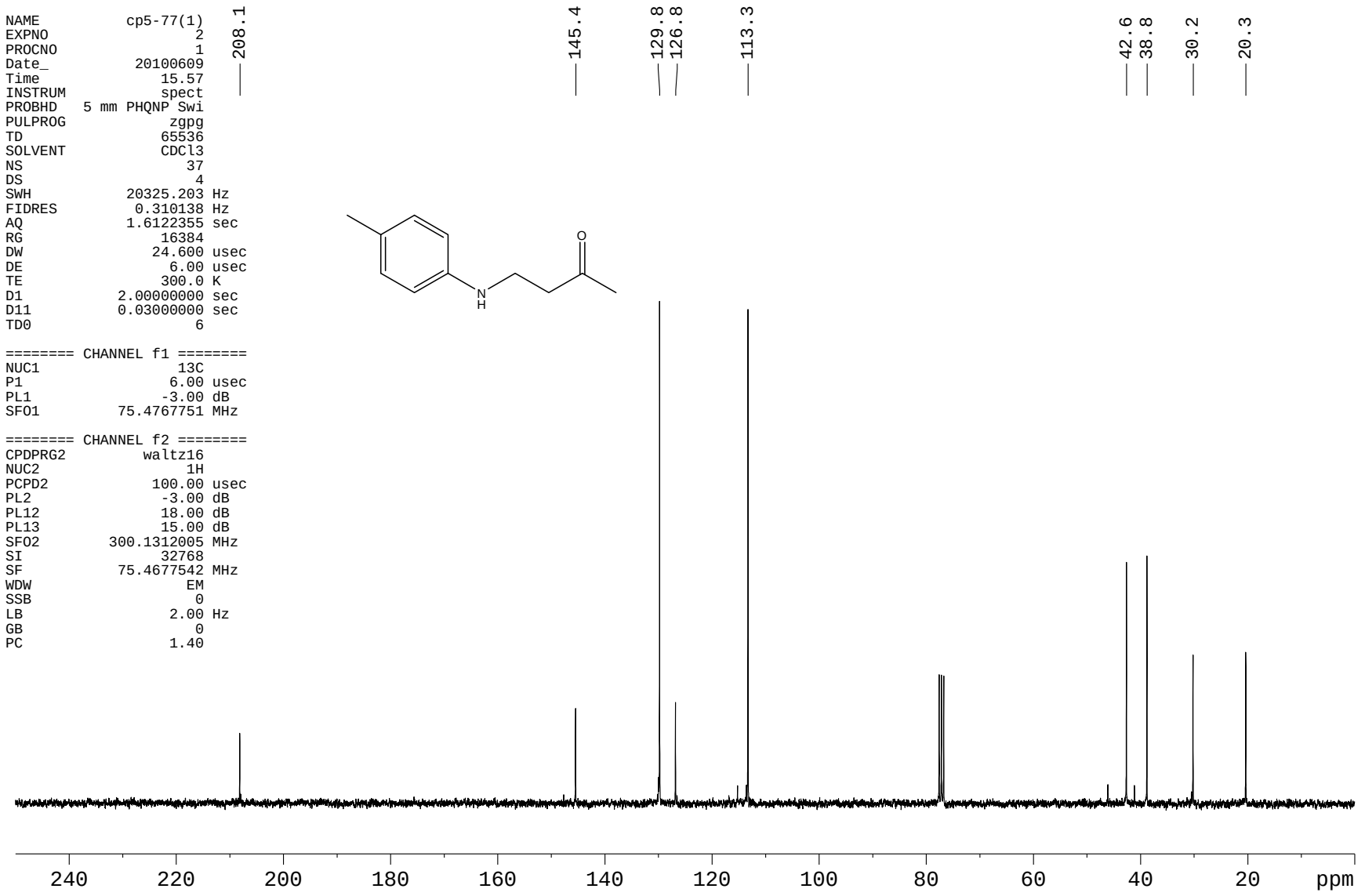


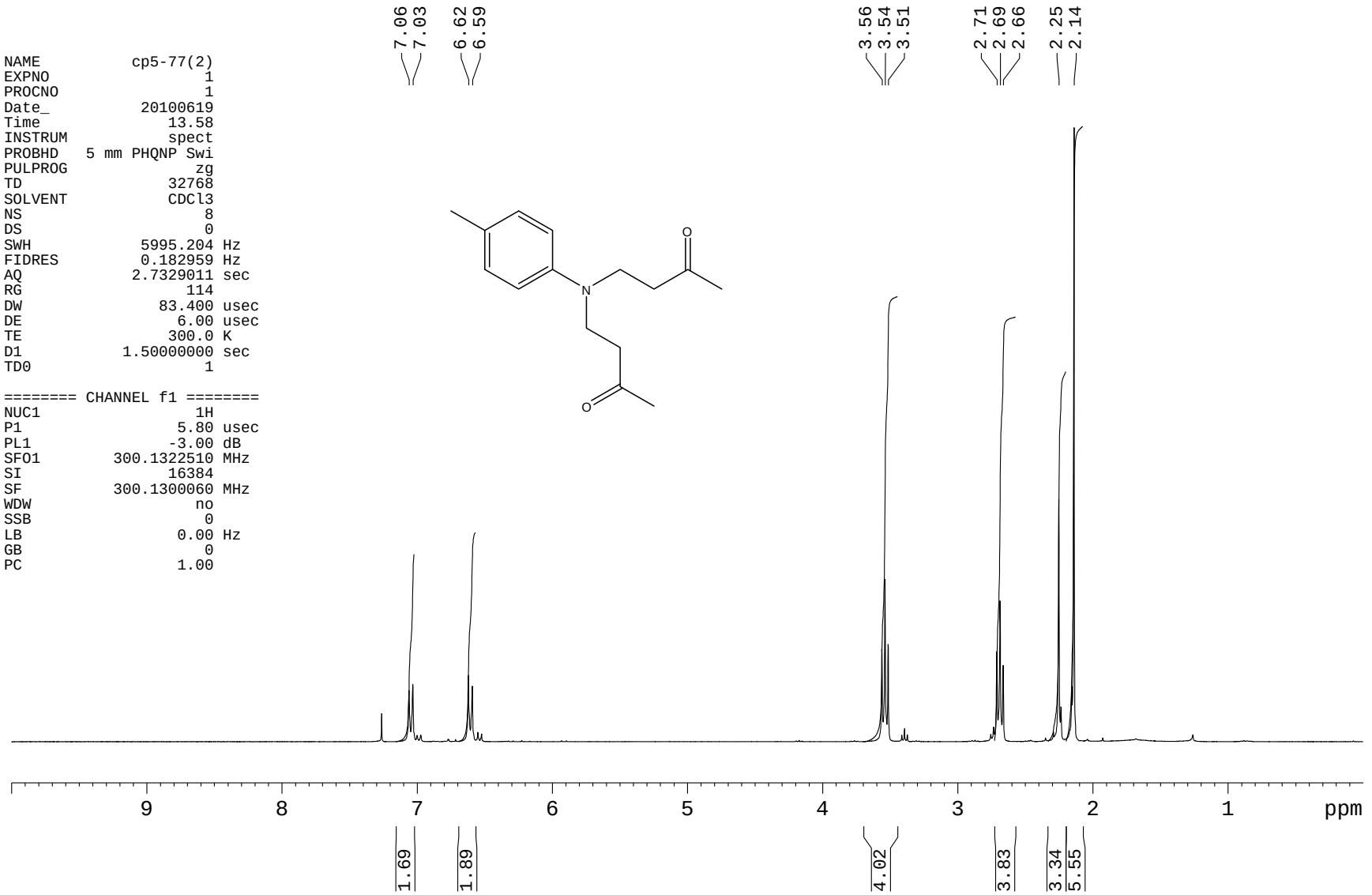

```
NAME        cp-anisester
EXPNO                2
PROCNO               1
Date_         20100628
Time             16.41
INSTRUM          spect
PROBHD   5 mm PHQNP Swi
PULPROG           zgpg
TD               65536
SOLVENT          CDCl3
NS                 330
DS                   4
SWH          20325.203 Hz
FIDRES        0.310138 Hz
AQ           1.6122355 sec
RG               16384
DW              24.600 usec
DE               6.00 usec
TE              300.0 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                  6

======== CHANNEL f1 ========
NUC1                13C
P1                 6.00 usec
PL1               -3.00 dB
SFO1         75.4767751 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            100.00 usec
PL2               -3.00 dB
PL12              18.00 dB
PL13              15.00 dB
SFO2        300.1312005 MHz
SI                32768
SF           75.4677413 MHz
WDW                 EM
SSB                  0
LB                2.00 Hz
GB                   0
PC                1.40
```

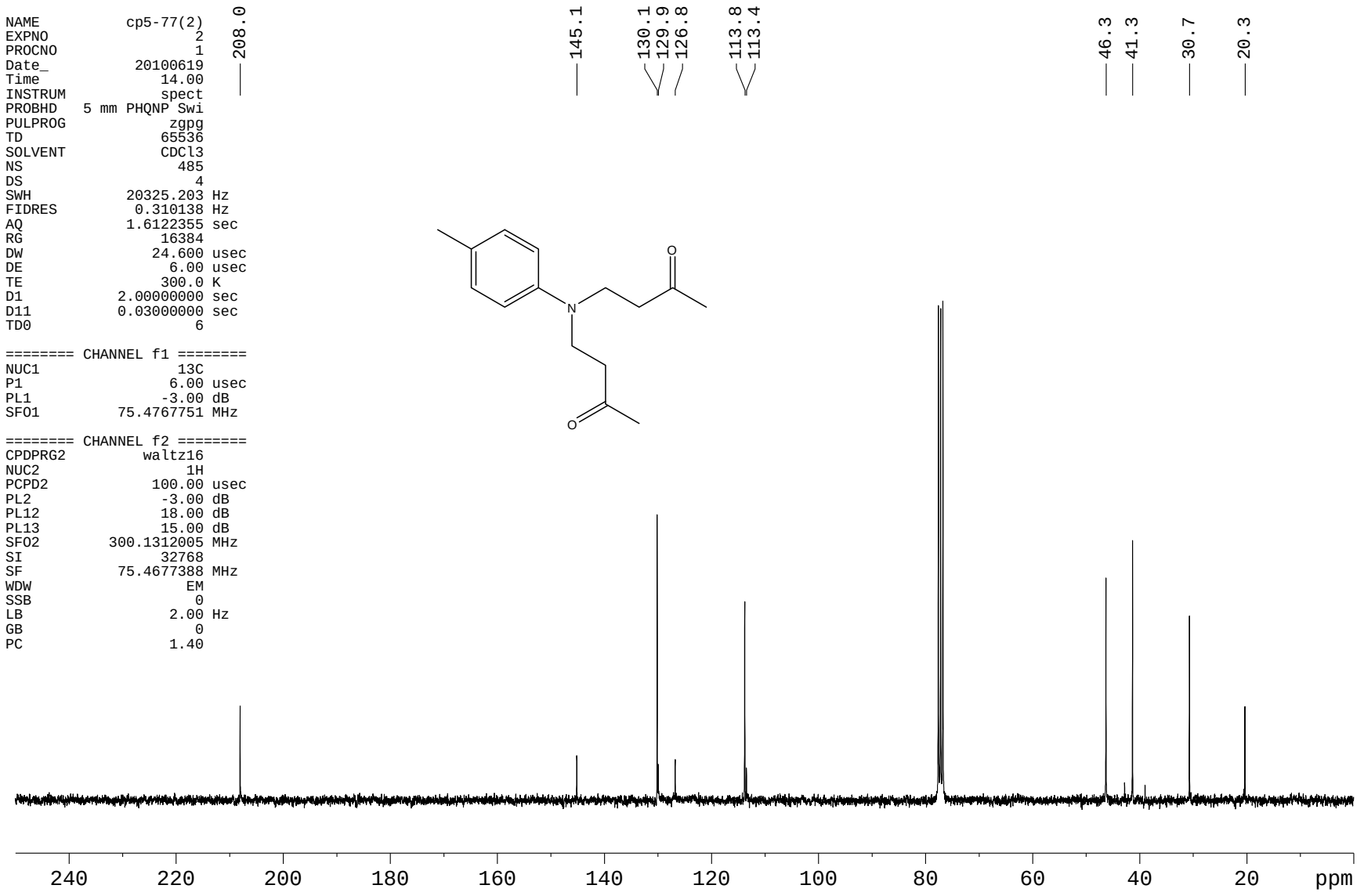

7.26
6.74
6.73
6.72
6.70
6.69
6.66
6.63
6.59
6.58
6.57
6.54
6.51
3.42
3.40
3.37
3.34
3.32
3.30
2.73
2.71
2.69
2.63
2.60
2.58
2.15
2.11
NAME cp6-41C
EXPNO 1
PROCNO 1
Date_ 20100630
Time 17.33
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 90.5
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 5.80 usec
PL1 -3.00 dB
SFO1 300.1322510 MHz
SI 16384
SF 300.1300069 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
HO
O
N
H
HO
O
N
O
9
8
7
6
5
4
3
2
1
ppm
3.19
2.17
2.40
0.90
2.11
2.00
0.85
2.69
1.07

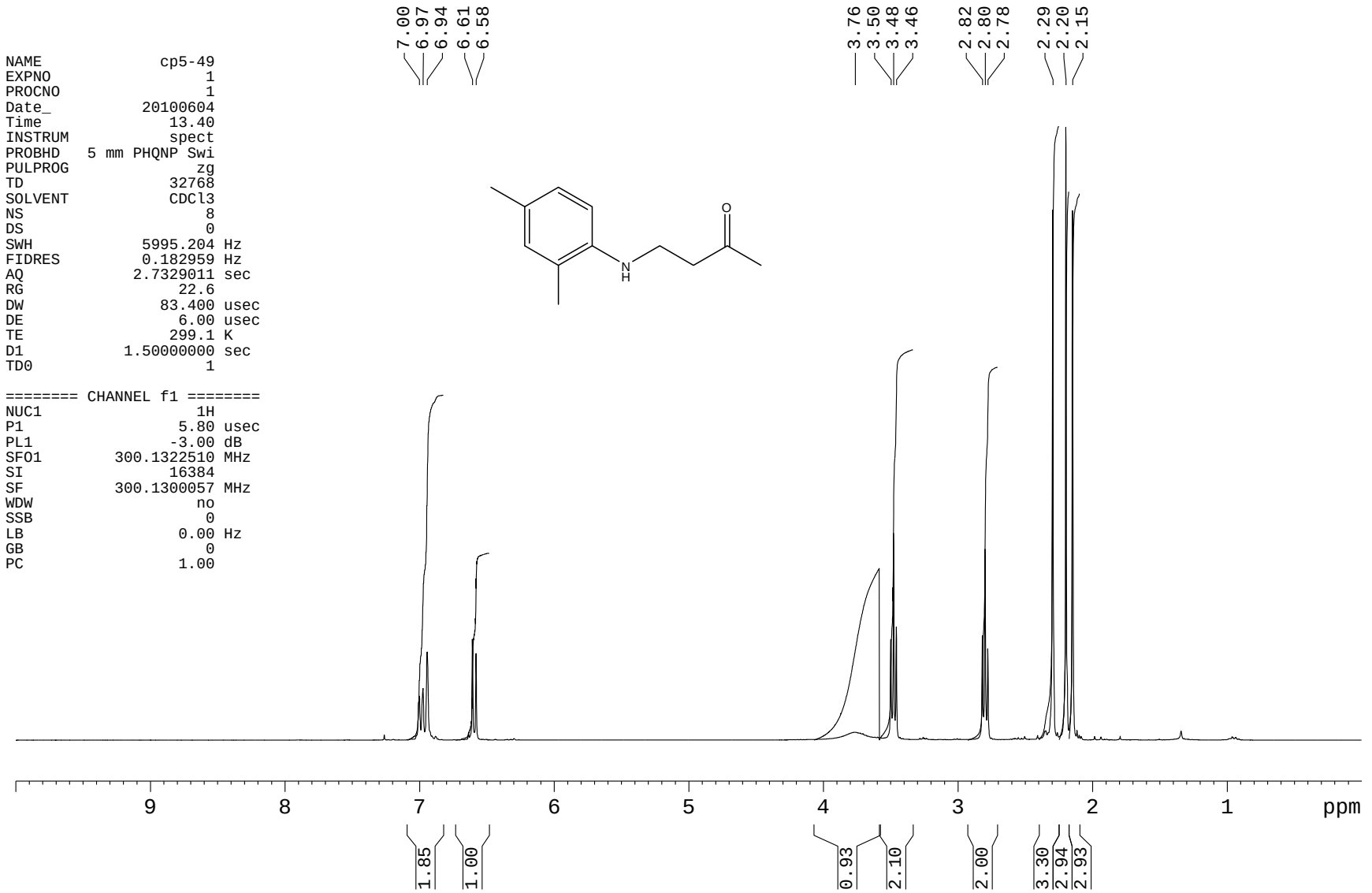

209.1
209.0
148.8
141.3
121.4
119.8
118.1
117.3
116.4
115.6
47.7
42.6
41.4
40.1
30.6
30.4
NAME cp6-41C
EXPNO 2
PROCNO 1
Date_ 20100630
Time 17.36
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 384
DS 4
SWH 20325.203 Hz
FIDRES 0.310138 Hz
AQ 1.6122355 sec
RG 18390.4
DW 24.600 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 6
======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 -3.00 dB
SFO1 75.4767751 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -3.00 dB
PL12 18.00 dB
PL13 15.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677412 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
HO
N
H
O
HO
N
O
O
240
220
200
180
160
140
120
100
80
60
40
20
ppm

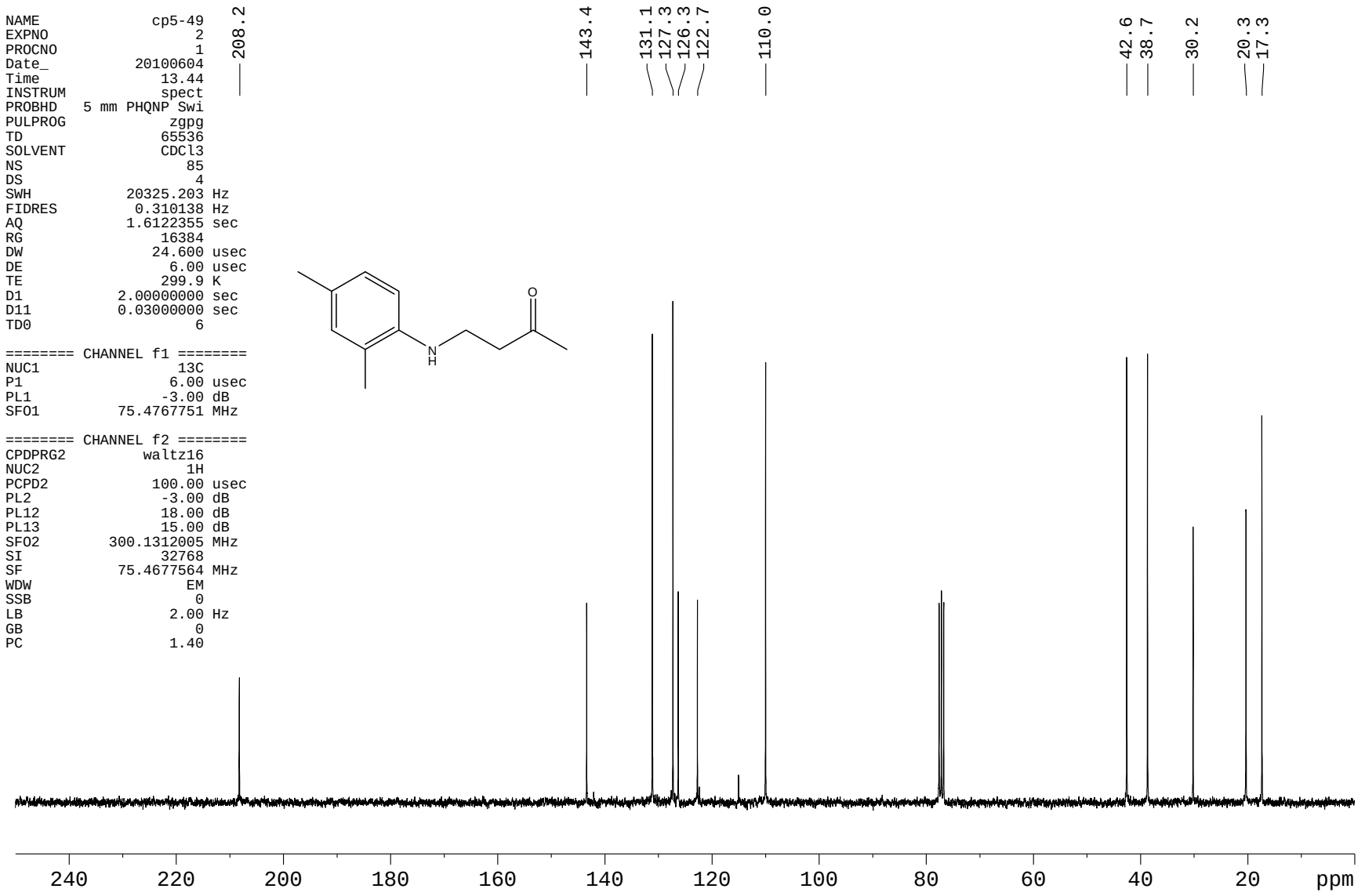

7.02
7.00
6.57
6.54
3.64
3.41
3.39
3.37
2.75
2.72
2.70
2.26
2.16
NAME cp5-77(1)
EXPNO 1
PROCNO 1
Date_ 20100609
Time 15.55
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 32
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 5.80 usec
PL1 -3.00 dB
SFO1 300.1322510 MHz
SI 16384
SF 300.1300060 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
N
H
O
9
8
7
6
5
4
3
2
1
ppm
1.82
1.86
1.01
2.01
2.01
3.00
2.77

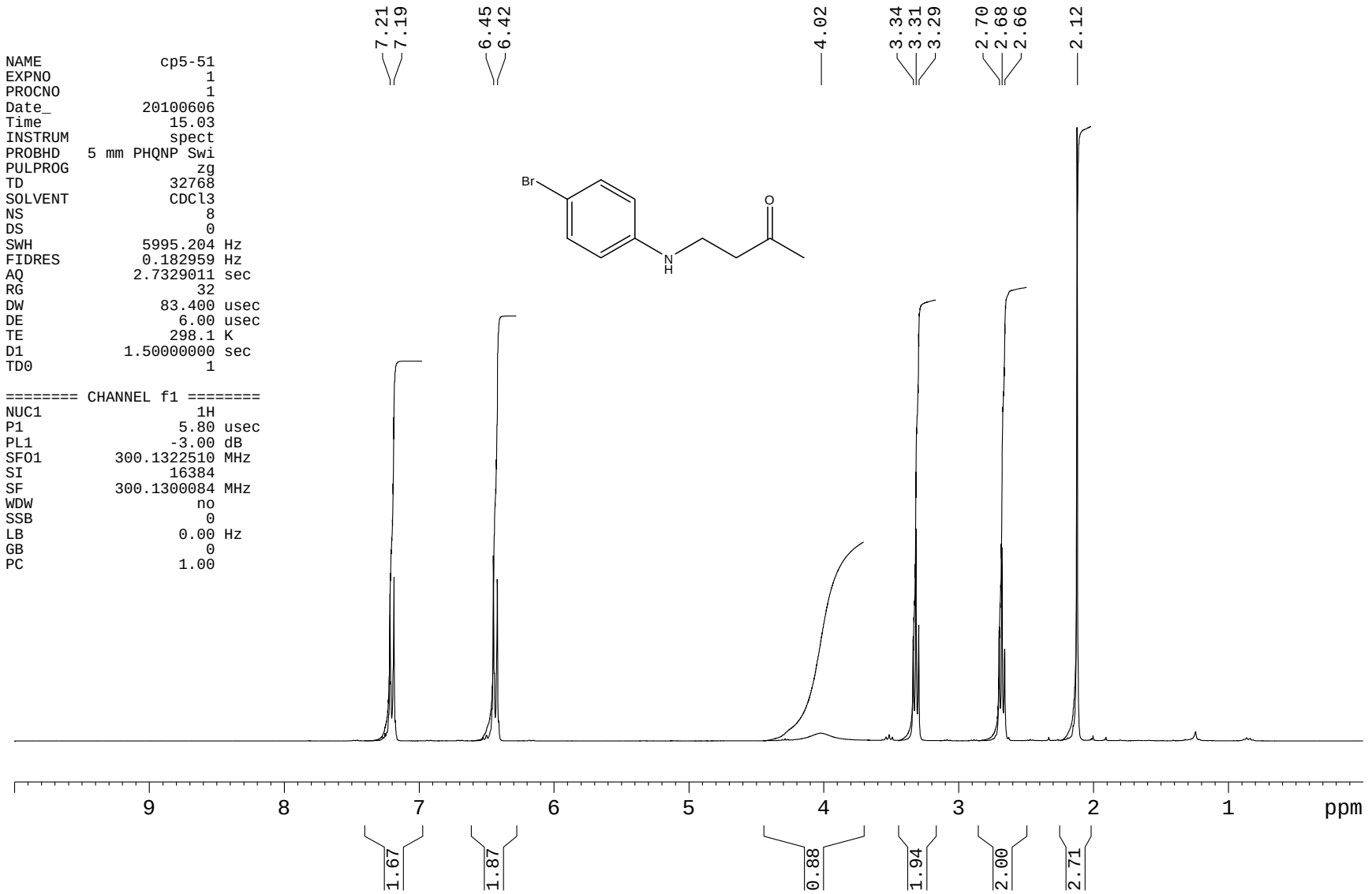

NAME cp5-77(1)
EXPNO 2
PROCNO 1
Date_ 20100609
Time 15.57
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 37
DS 4
SWH 20325.203 Hz
FIDRES 0.310138 Hz
AQ 1.6122355 sec
RG 16384
DW 24.600 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 6
======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 -3.00 dB
SFO1 75.4767751 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -3.00 dB
PL12 18.00 dB
PL13 15.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677542 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
208.1
145.4
129.8
126.8
113.3
42.6
38.8
30.2
20.3
O
N
H
240
220
200
180
160
140
120
100
80
60
40
20
ppm


7.06
7.03
6.62
6.59
3.56
3.54
3.51
2.71
2.69
2.66
2.25
2.14
NAME cp5-77(2)
EXPNO 1
PROCNO 1
Date_ 20100619
Time 13.58
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 114
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 5.80 usec
PL1 -3.00 dB
SFO1 300.1322510 MHz
SI 16384
SF 300.1300060 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
N
O
O
9
8
7
6
5
4
3
2
1
ppm
1.69
1.89
4.02
3.83
3.34
5.55

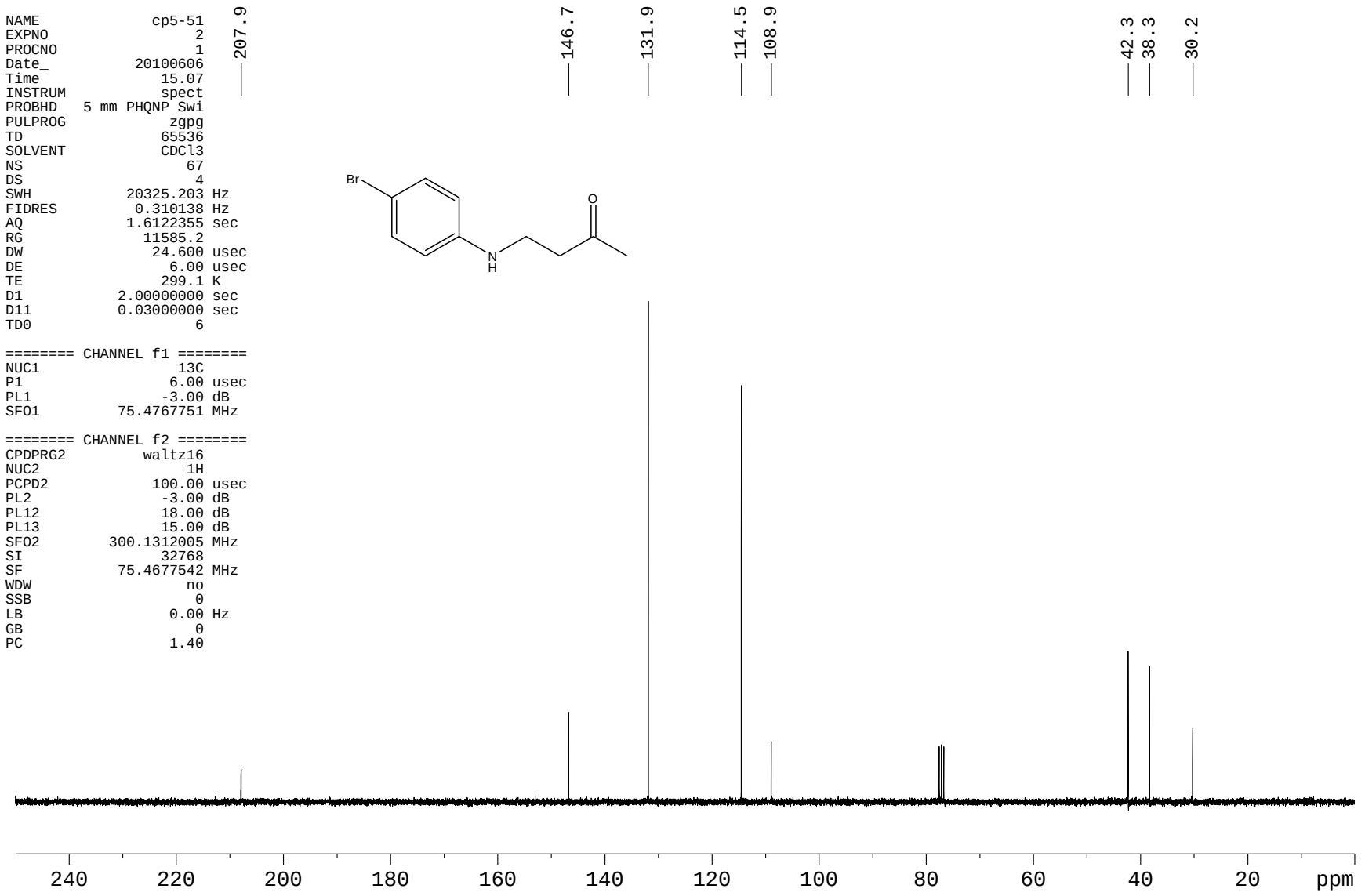

NAME cp5-77(2)
EXPNO 2
PROCNO 1
Date_ 20100619
Time 14.00
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 485
DS 4
SWH 20325.203 Hz
FIDRES 0.310138 Hz
AQ 1.6122355 sec
RG 16384
DW 24.600 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 6
======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 -3.00 dB
SFO1 75.4767751 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -3.00 dB
PL12 18.00 dB
PL13 15.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677388 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
208.0
145.1
130.1
129.9
126.8
113.8
113.4
46.3
41.3
30.7
20.3
N
O
O
240
220
200
180
160
140
120
100
80
60
40
20
ppm

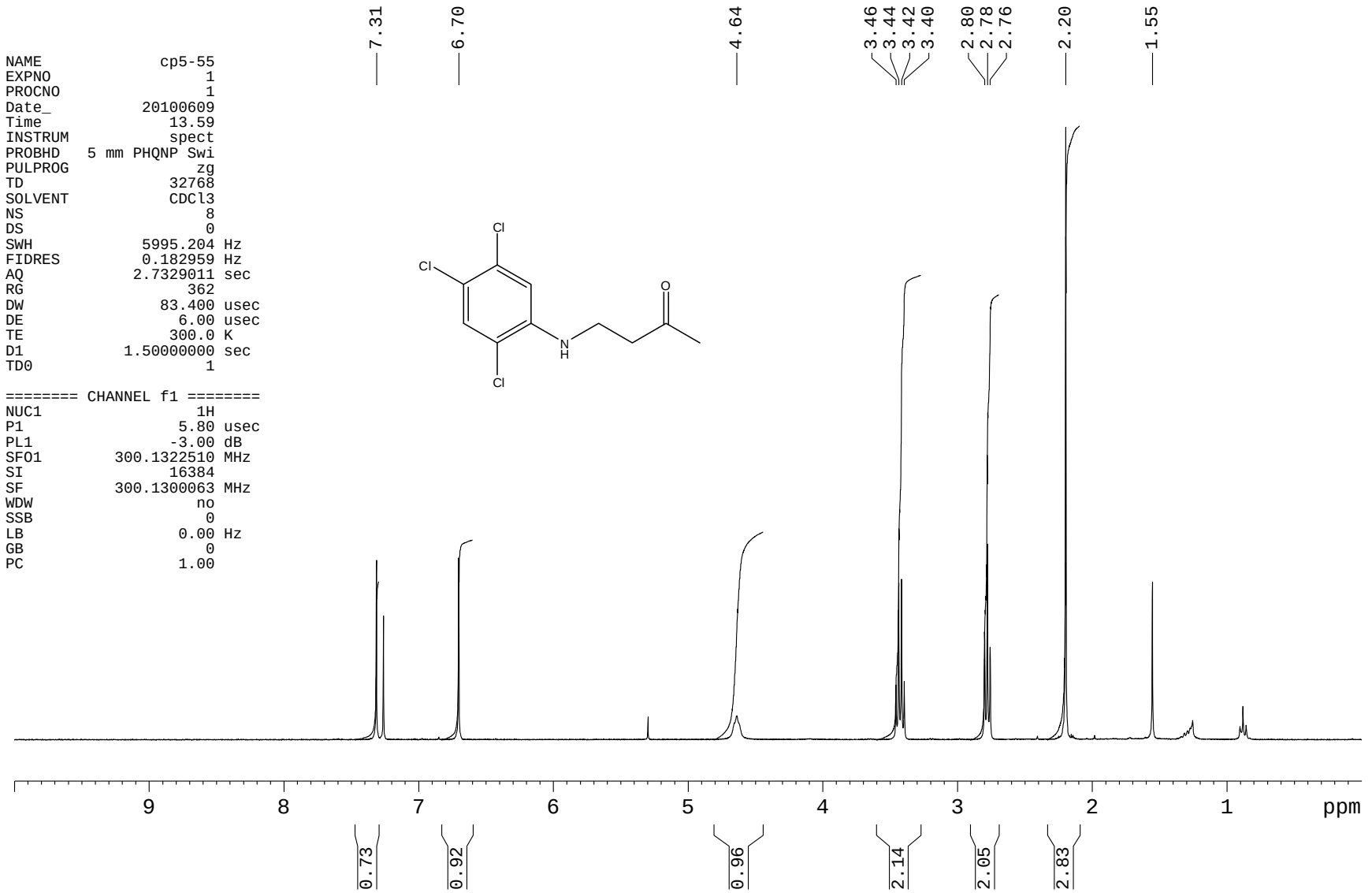

7.00
6.97
6.94
6.61
6.58
3.76
3.50
3.48
3.46
2.82
2.80
2.78
2.29
2.20
2.15
NAME cp5-49
EXPNO 1
PROCNO 1
Date_ 20100604
Time 13.40
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 22.6
DW 83.400 usec
DE 6.00 usec
TE 299.1 K
D1 1.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 5.80 usec
PL1 -3.00 dB
SFO1 300.1322510 MHz
SI 16384
SF 300.1300057 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
O
N
H
9
8
7
6
5
4
3
2
1
ppm
1.85
1.00
0.93
2.10
2.00
3.30
2.94
2.93

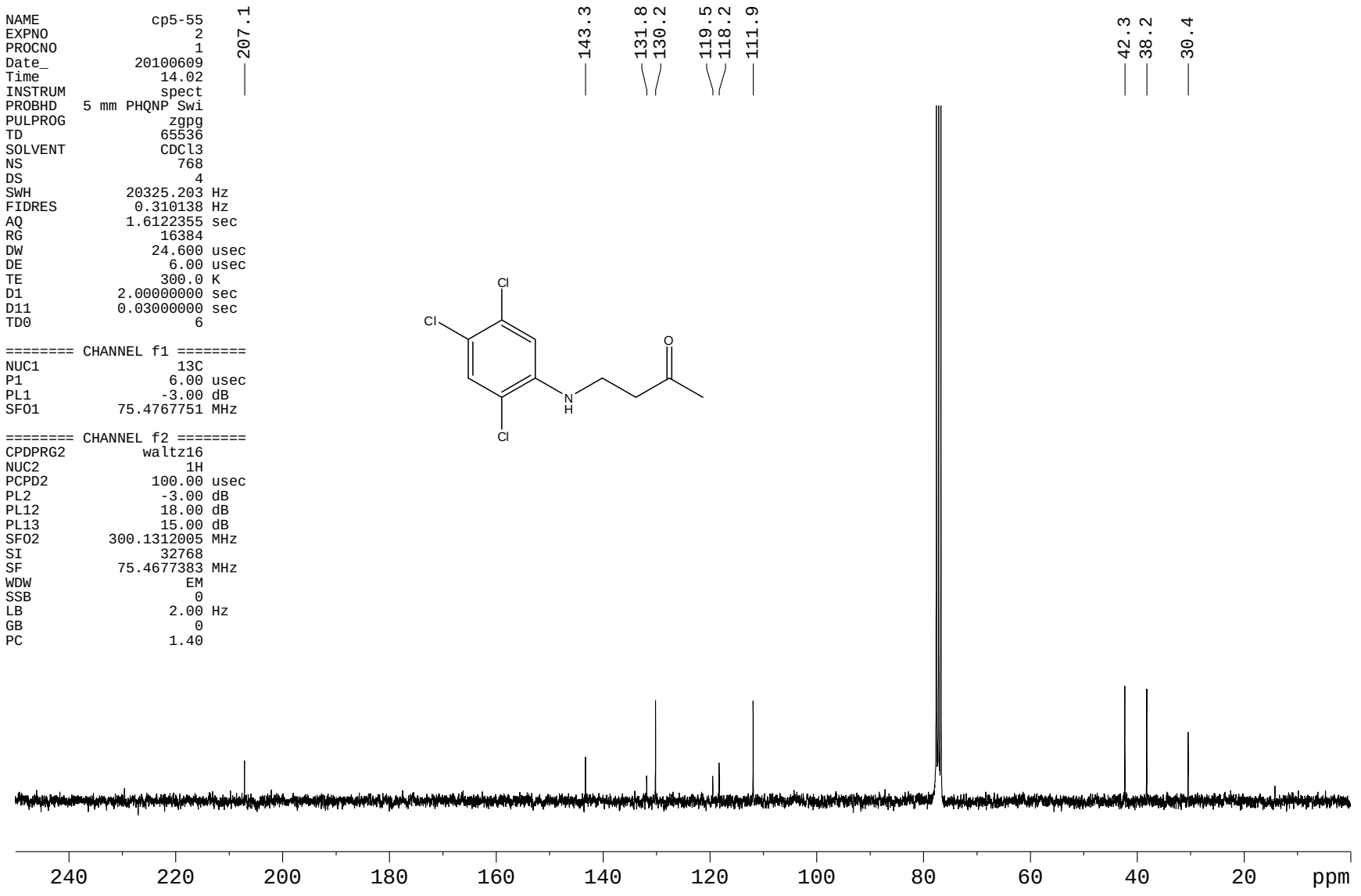

NAME cp5-49
EXPNO 2
PROCNO 1
Date_ 20100604
Time 13.44
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 85
DS 4
SWH 20325.203 Hz
FIDRES 0.310138 Hz
AQ 1.6122355 sec
RG 16384
DW 24.600 usec
DE 6.00 usec
TE 299.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 6
======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 -3.00 dB
SFO1 75.4767751 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -3.00 dB
PL12 18.00 dB
PL13 15.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677564 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
208.2
143.4
131.1
127.3
126.3
122.7
110.0
42.6
38.7
30.2
20.3
17.3
O
N
H
240
220
200
180
160
140
120
100
80
60
40
20
ppm

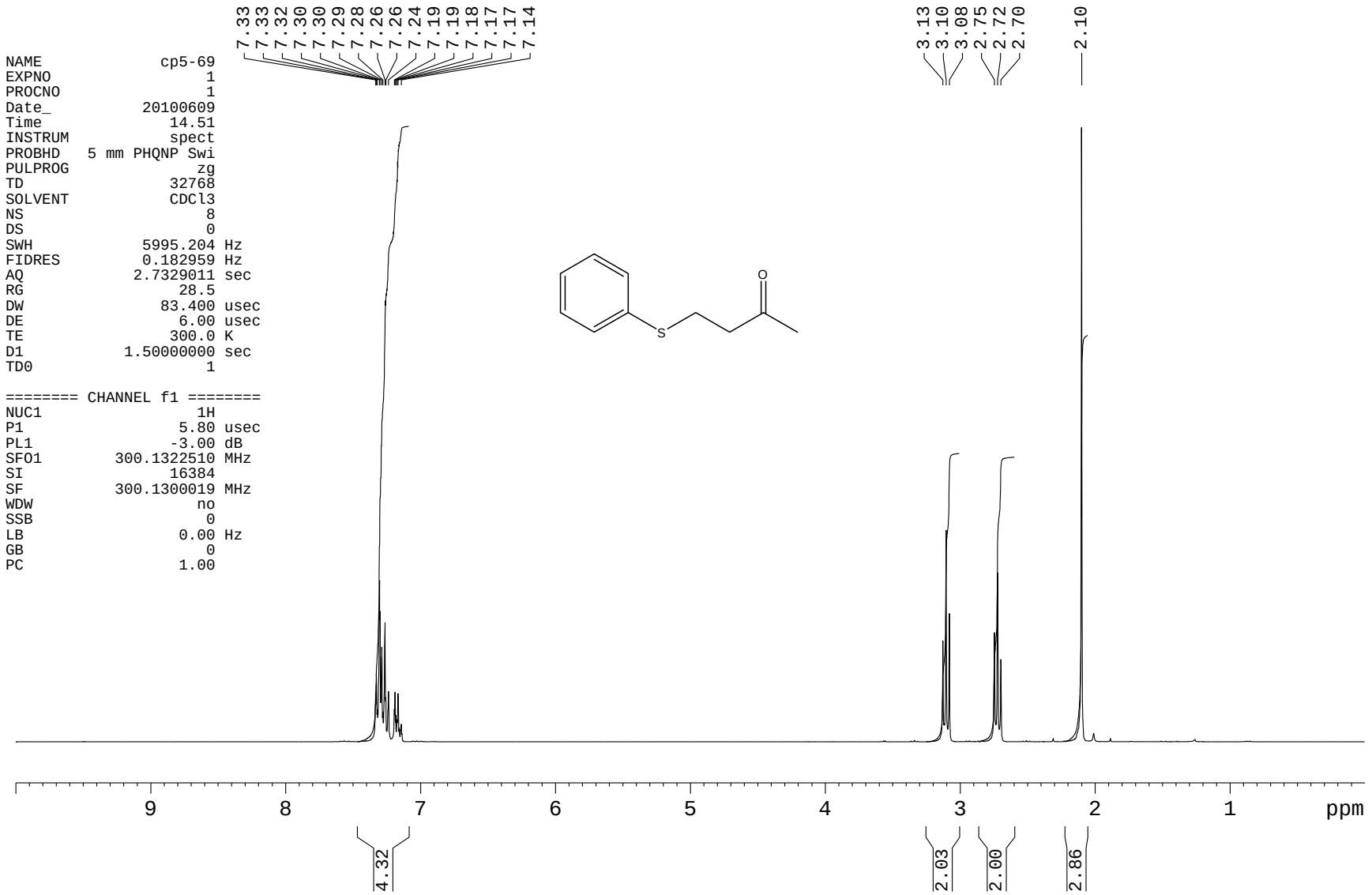



```
NAME              cp5-51
EXPNO                  1
PROCNO                 1
Date_           20100606
Time               15.03
INSTRUM            spect
PROBHD   5 mm PHQNP Swi
PULPROG               zg
TD                 32768
SOLVENT            CDCl3
NS                     8
DS                     0
SWH             5995.204 Hz
FIDRES          0.182959 Hz
AQ             2.7329011 sec
RG                    32
DW                83.400 usec
DE                 6.00 usec
TE                298.1 K
D1           1.50000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                  5.80 usec
PL1                -3.00 dB
SFO1         300.1322510 MHz
SI                 16384
SF           300.1300084 MHz
WDW                   no
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  1.00
```

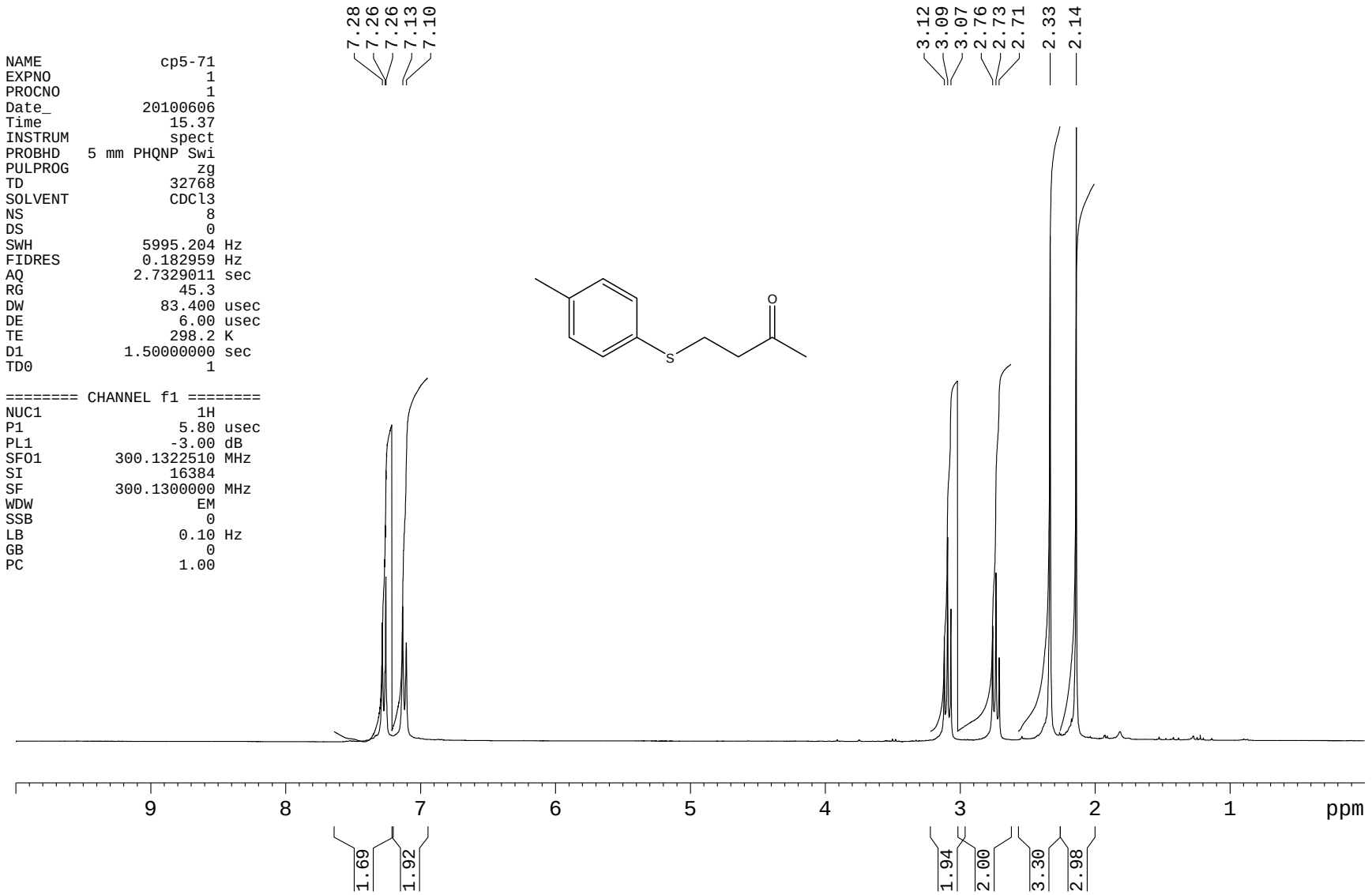

NAME cp5-51
EXPNO 2
PROCNO 1
Date_ 20100606
Time 15.07
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 67
DS 4
SWH 20325.203 Hz
FIDRES 0.310138 Hz
AQ 1.6122355 sec
RG 11585.2
DW 24.600 usec
DE 6.00 usec
TE 299.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 6
======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 -3.00 dB
SFO1 75.4767751 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -3.00 dB
PL12 18.00 dB
PL13 15.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677542 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
207.9
146.7
131.9
114.5
108.9
42.3
38.3
30.2
Br
O
N
H
240
220
200
180
160
140
120
100
80
60
40
20
ppm

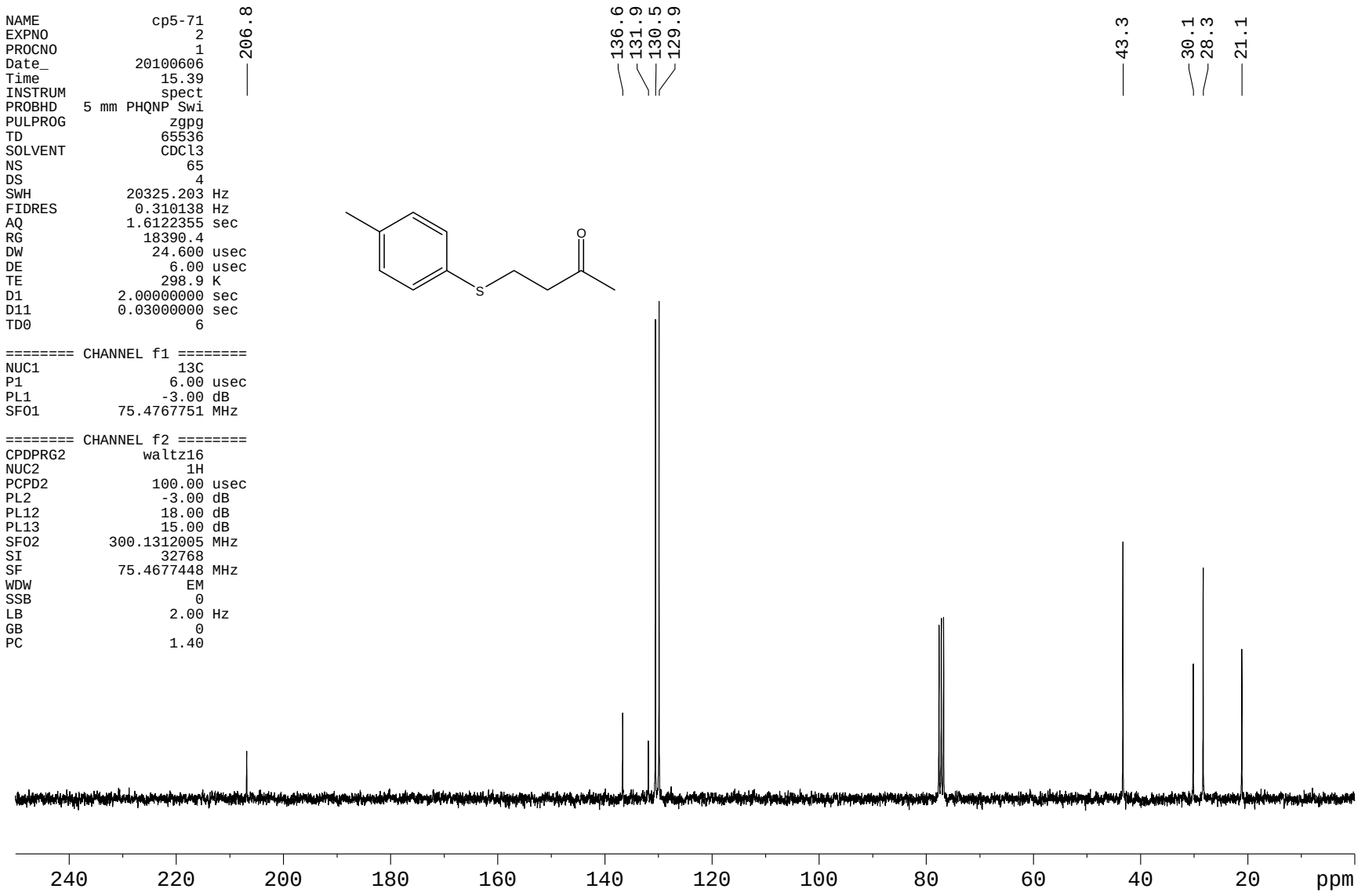

7.31
6.70
4.64
3.46
3.44
3.42
3.40
2.80
2.78
2.76
2.20
1.55
NAME cp5-55
EXPNO 1
PROCNO 1
Date_ 20100609
Time 13.59
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 362
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 5.80 usec
PL1 -3.00 dB
SFO1 300.1322510 MHz
SI 16384
SF 300.1300063 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Cl
Cl
Cl
N
H
O
9
8
7
6
5
4
3
2
1
ppm
0.73
0.92
0.96
2.14
2.05
2.83


NAME cp5-55
EXPNO 2
PROCNO 1
Date_ 20100609
Time 14.02
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 768
DS 4
SWH 20325.203 Hz
FIDRES 0.310138 Hz
AQ 1.6122355 sec
RG 16384
DW 24.600 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 6
======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 -3.00 dB
SFO1 75.4767751 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -3.00 dB
PL12 18.00 dB
PL13 15.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677383 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
207.1
143.3
131.8
130.2
119.5
118.2
111.9
42.3
38.2
30.4
Cl
Cl
Cl
N
H
O
240
220
200
180
160
140
120
100
80
60
40
20
ppm

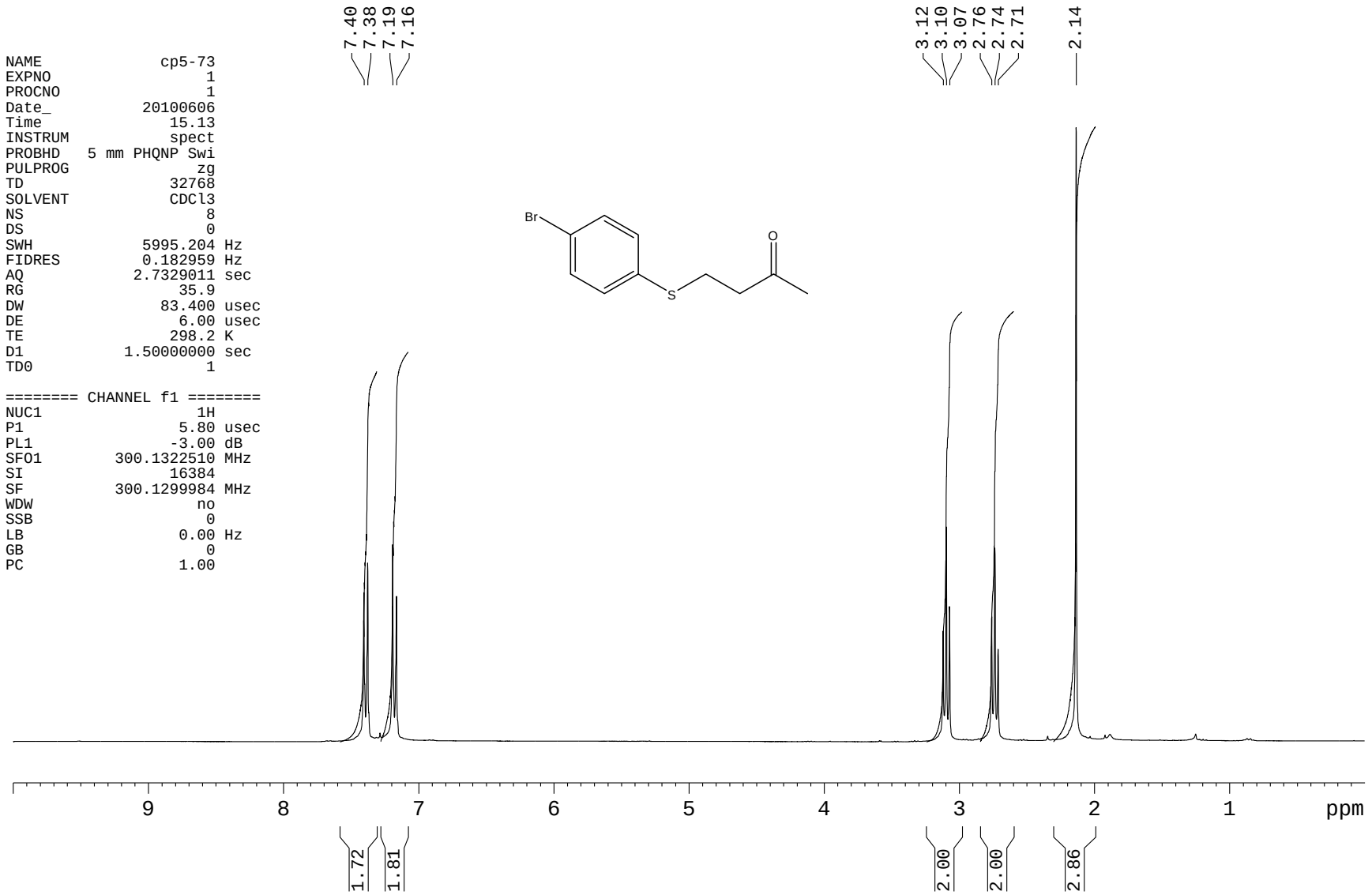

7.33
7.33
7.32
7.30
7.30
7.29
7.28
7.26
7.26
7.24
7.19
7.19
7.18
7.17
7.17
7.14
3.13
3.10
3.08
2.75
2.72
2.70
2.10
NAME cp5-69
EXPNO 1
PROCNO 1
Date_ 20100609
Time 14.51
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 28.5
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 5.80 usec
PL1 -3.00 dB
SFO1 300.1322510 MHz
SI 16384
SF 300.1300019 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
O
S
9
8
7
6
5
4
3
2
1
ppm
4.32
2.03
2.00
2.86

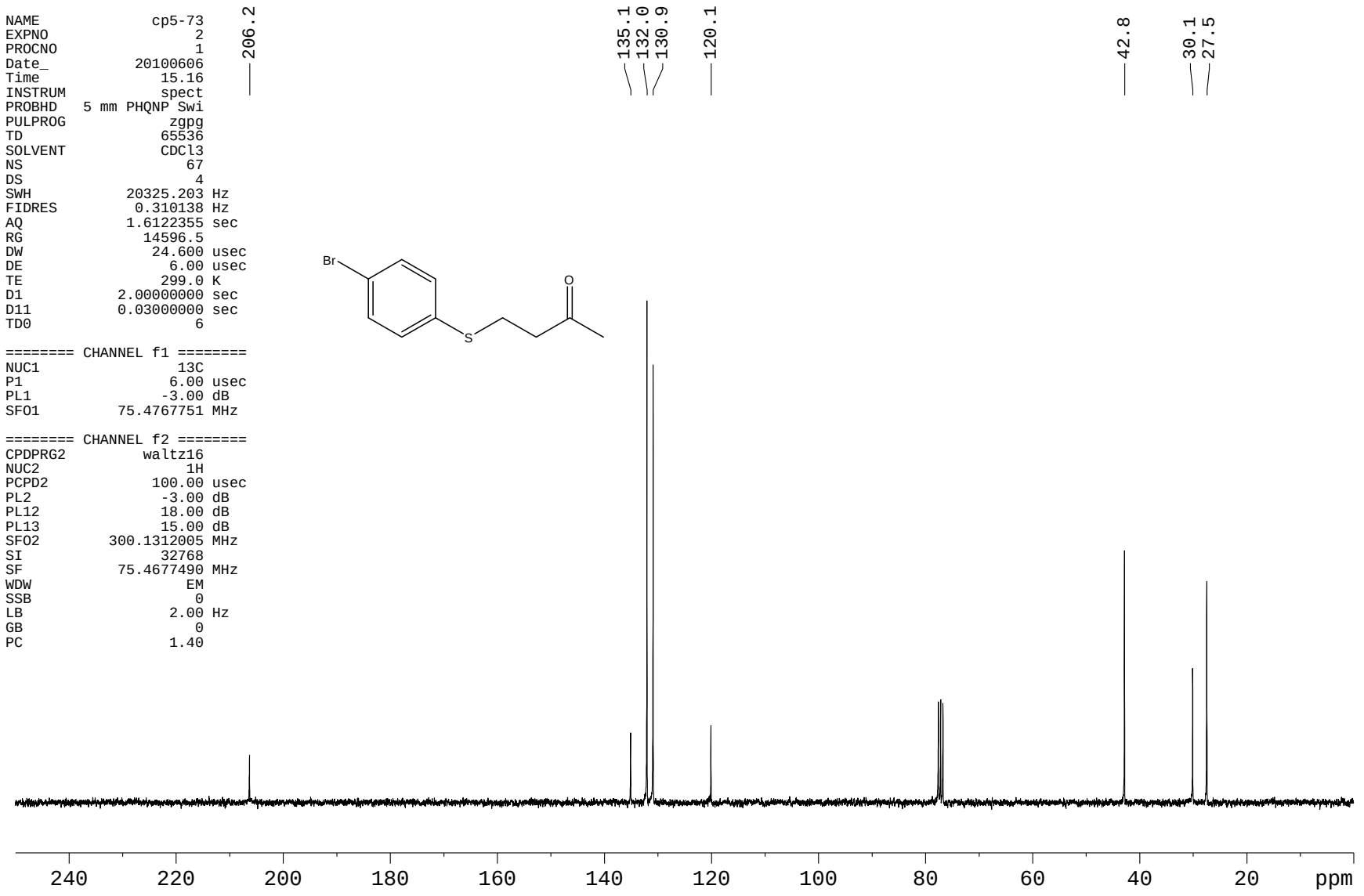
NAME	cp5-69
EXPNO	2
PROCNO	1
Date_	20100609
Time	14.54
INSTRUM	spect
PROBHD	5 mm PHQNP Swi
PULPROG	zgpg
TD	65536
SOLVENT	CDCl3
NS	52
DS	4
SWH	20325.203 Hz
FIDRES	0.310138 Hz
AQ	1.6122355 sec
RG	14596.5
DW	24.600 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	6
======== CHANNEL f1 ========	
NUC1	13C
P1	6.00 usec
PL1	-3.00 dB
SFO1	75.4767751 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	100.00 usec
PL2	-3.00 dB
PL12	18.00 dB
PL13	15.00 dB
SFO2	300.1312005 MHz
SI	32768
SF	75.4677568 MHz
WDW	EM
SSB	0
LB	2.00 Hz
GB	0
PC	1.40


7.28
7.26
7.26
7.13
7.10
3.12
3.09
3.07
2.76
2.73
2.71
2.33
2.14
NAME cp5-71
EXPNO 1
PROCNO 1
Date_ 20100606
Time 15.37
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 45.3
DW 83.400 usec
DE 6.00 usec
TE 298.2 K
D1 1.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 5.80 usec
PL1 -3.00 dB
SFO1 300.1322510 MHz
SI 16384
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
O
S
9
8
7
6
5
4
3
2
1
ppm
1.69
1.92
1.94
2.00
3.30
2.98




```
NAME              cp5-71
EXPNO                  2
PROCNO                 1
Date_           20100606
Time               15.39
INSTRUM            spect
PROBHD   5 mm PHQNP Swi
PULPROG             zgpg
TD                 65536
SOLVENT            CDCl3
NS                    65
DS                     4
SWH            20325.203 Hz
FIDRES          0.310138 Hz
AQ             1.6122355 sec
RG               18390.4
DW                24.600 usec
DE                 6.00 usec
TE                298.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    6

======== CHANNEL f1 ========
NUC1                  13C
P1                   6.00 usec
PL1                 -3.00 dB
SFO1          75.4767751 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              100.00 usec
PL2                 -3.00 dB
PL12                18.00 dB
PL13                15.00 dB
SFO2         300.1312005 MHz
SI                 32768
SF            75.4677448 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.40
```


7.40
7.38
7.19
7.16
3.12
3.10
3.07
2.76
2.74
2.71
2.14
NAME cp5-73
EXPNO 1
PROCNO 1
Date_ 20100606
Time 15.13
INSTRUM spect
PROBHD 5 mm PHQNP Swi
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 35.9
DW 83.400 usec
DE 6.00 usec
TE 298.2 K
D1 1.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 5.80 usec
PL1 -3.00 dB
SFO1 300.1322510 MHz
SI 16384
SF 300.1299984 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Br
O
S
9
8
7
6
5
4
3
2
1
ppm
1.72
1.81
2.00
2.00
2.86




```
NAME              cp5-73
EXPNO                  2
PROCNO                 1
Date_           20100606
Time               15.16
INSTRUM            spect
PROBHD   5 mm PHQNP Swi
PULPROG             zgpg
TD                 65536
SOLVENT            CDCl3
NS                    67
DS                     4
SWH            20325.203 Hz
FIDRES          0.310138 Hz
AQ             1.6122355 sec
RG               14596.5
DW                24.600 usec
DE                 6.00 usec
TE                299.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    6

======== CHANNEL f1 ========
NUC1                  13C
P1                   6.00 usec
PL1                 -3.00 dB
SFO1          75.4767751 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              100.00 usec
PL2                 -3.00 dB
PL12                18.00 dB
PL13                15.00 dB
SFO2         300.1312005 MHz
SI                 32768
SF            75.4677490 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.40
```