Supporting Information

A greener borrowing hydrogen methodology: palladium-catalyzed dehydrative N-benzylation of 2-aminopyridines in water

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General procedure: A mixture of aminopyridines **1** (1 mmol), palladium(II) acetate (12 mg, 0.05 mmol), sodium diphenylphosphinobenzene-3-sulfonate (TPPMS, 36 mg, 0.1 mmol) and benzyl alcohol **2** (5-10 mmol) in H_2O (4 mL) was heated for 16 h in a sealed tube under air. After cooling, the reaction mixture was poured into water and extracted with EtOAc. The organic layer was washed with brine, dried over $MgSO_4$ and concentrated in vacuo. The residue was purified by flash column chromatography (silica gel, hexanes/EtOAc) to give desired product **3**.

N-Benzylpyridin-2-amine **3a** [1]

Yield 165 mg (90%) as a white solid; mp 90-91 °C; IR (KBr) (cm^{-1}) 3226, 3029, 1600, 1575; ^{1}H NMR (400 MHz, $CDCl_3$): δ 4.50 (d, *J*=5.7 Hz, 2H), 4.95 (brs, 1H), 6.36 (dt, *J*=8.5, 0.9 Hz, 1H), 6.58 (ddd, *J*=7.1, 5.0, 0.9 Hz, 1H), 7.23-7.36 (m, 4H), 7.39 (dd, *J*=8.7, 7.1, 1.8 Hz, 1H), 8.09 (ddd, *J*=5.0, 1.8, 0.9 Hz, 2H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ: 46.3, 106.8, 113.1, 127.2, 127.4, 128.6, 137.5, 139.2, 148.2, 158.6; MS (FAB): *m/z* 185 $[M+H]^+$.

N-Benzyl-5-methylpyridin-2-amine **3b** [1]

Yield 158 mg (80%) as a pale yellow solid; mp 105-107 °C; IR (KBr) (cm^{-1}) 3234, 3027, 1610, 1535; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 2.17 (s, 3H), 4.47 (d, *J*=5.5 Hz, 2H), 4.77 (brs, 1H), 6.31 (d, *J*=8.2 Hz, 1H), 7.20-7.29 (m, 2H), 7.29-7.39 (m, 4H), 7.92 (d, *J*=2.3 Hz, 1H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 17.4, 46.5, 106.4, 121.9, 127.1, 127.4, 128.6, 138.5, 139.4, 147.7, 156.9; MS (FAB): *m/z* 199 $[M+H]^+$.

N-Benzyl-3-methylpyridin-2-amine **3c** [1]

Yield 163 mg (82%) as a colorless oil; IR (KBr) (cm^{-1}) 3443, 1601; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 2.09 (s, 3H), 4.35 (brs, 1H), 4.69 (d, *J*=5.5 Hz, 2H), 6.56 (dd, *J*=6.9, 5.0 Hz 1H), 7.22-7.26 (m, 1H), 7.28 (tt, *J*=6.9, 1.8 Hz 1H), 7.32-7.42 (m, 3H), 8.05 (dd, *J*=4.8, 1.4 Hz 1H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 17.1, 45.9, 113.1, 116.7, 127.3, 128.0, 128.7, 137.0, 140.2, 145.6, 156.8; MS (FAB): *m/z* 199 $[M+H]^+$.

N-Benzyl-5-fluoropyridin-2-amine **3d** [1]

Yield 113 mg (56%) as a white solid; mp 95-97 °C; IR (KBr) (cm^{-1}) 3239, 3031, 1618, 1585; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 4.47 (d, *J*=6.0 Hz 2H), 4.80 (brs, 1H), 6.33 (dd, *J*=9.1, 3.2 Hz 1H), 7.18 (d, *J*=9.2, 7.8, 2.8 Hz 1H), 7.24-7.38 (m, 5H), 7.97 (d, *J*=2.8 Hz 1H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 46.8, 107.1 (d, J_{CF}=3.8 Hz), 125.2 (d, J_{CF}=21.1 Hz), 127.3, 127.4, 128.7, 134.8 (d, J_{CF}=24.9 Hz), 139.0, 153.5 (d, J_{CF}=242 Hz), 155.3; MS (FAB): *m/z* 203 $[M+H]^+$.

Ethyl 2-(benzylamino)nicotinate **3e** [2]

Yield 213 mg (83%) as a colorless oil; IR (KBr) (cm^{-1}) 3367, 1686, 1594; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 1.37 (t, *J*=6.9 Hz, 3H), 4.31 (q, *J*=7.3 Hz, 2H), 4.76 (d, *J*=5.5 Hz, 2H), 6.55 (dd, *J*=7.8, 4.6 Hz, 1H), 7.22-7.28 (m, 1H), 7.30-7.40 (m, 3H), 8.15 (dd, *J*=7.8, 1.8 Hz, 1H), 8.29 (dd, *J*=4.6, 1.8 Hz, 1H), 8.32 (brs, 1H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 14.4, 45.0, 60.9, 106.3, 111.3, 127.1, 127.6, 128.7, 139.7, 140.0, 153.7, 158.6, 167.6; MS (FAB): *m/z* 257 $[M+H]^+$.

Methyl 6-(benzylamino)nicotinate **3f**

Yield 208 mg (86%) as a white solid; mp 147-149 °C; IR (KBr) (cm^{-1}) 3222, 1706, 1601; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 3.87 (s, 3H), 4.58 (d, *J*=6.0 Hz, 2H), 5.41 (brs, 1H), 6.36 (d, *J*=8.7 Hz, 1H), 7.27-7.38 (m, 5H), 7.99 (d, *J*=8.7, 2.3 Hz, 1H), 8.76 (d, *J*=1.8 Hz, 1H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 46.1, 51.7, 105.7, 115.5, 127.4, 127.6, 128.8, 138.1, 138.6, 151.5, 160.8, 166.4; MS (FAB): *m/z* 243 $[M+H]^+$; Anal. Calcd for $C_{14}H_{14}N_2O_2$: C, 69.41; H, 5.82; N, 11.56. Found: C, 69.41; H, 5.93; N, 11.45.

N-Benzyl-5-(trifluoromethyl)pyridin-2-amine **3g** [1]

Scale-up experiment (see Scheme 8): A mixture of 5-(trifluoromethyl)pyridin-2-amine (**1b**) (1.13 g, 7 mmol), $Pd(OAc)_2$ (78.6 mg, 0.35 mmol), sodium diphenylphosphinobenzene-3-sulfonate (TPPMS, 255.0 mg, 0.7 mmol) and benzyl alcohol (**2a**) (3.4 mL, 35 mmol) in H_2O (28 mL) was heated at 100 °C for 16 h under air. After cooling, the reaction mixture was poured into water and extracted with EtOAc. The organic layer was washed with brine, dried over $MgSO_4$ and concentrated in vacuo. The residue was purified by flash column chromatography (silica gel, hexanes/EtOAc) to give desired product **3g** (1.27 g, 5.0 mmol, 72%) as a white solid; mp 148-150 °C; IR (KBr) (cm^{-1}) 3233, 1616; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 4.57 (d, *J*=6.0 Hz, 2H), 5.20 (brs, 1H), 6.40 (d, *J*=8.7 Hz, 1H), 7.25-7.40 (m, 5H), 7.58 (dd, *J*=8.7, 2.8 Hz, 1H), 8.36 (s, 1H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 46.1, 106.1, 115.8 (q, J_{CF}=32.6 Hz), 124.6 (q, J_{CF}=270.3 Hz), 127.4, 127.6, 128.8, 134.5 (q, J_{CF}=2.9 Hz), 138.2, 146.1 (q, J_{CF}=3.8 Hz), 160.2; MS (FAB): *m/z* 253 $[M+H]^+$.

6-(Benzylamino)nicotinonitrile **3h** [3]

Yield 178 mg (85%) as a white solid; mp 118-120 °C; IR (KBr) (cm^{-1}) 3227, 2219, 1604; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 4.56 (d, *J*=5.5 Hz, 2H), 5.63 (brs, 1H), 6.38 (d, *J*=9.2 Hz, 1H), 7.27-7.39 (m, 4H), 7.56 (dd, *J*=8.7, 2.3 Hz, 1H), 8.29 (d, *J*=1.8 Hz, 1H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 46.0, 97.3, 106.6, 118.5, 127.5, 127.8, 128.9, 137.6, 139.8, 153.2, 159.7; MS (FAB): *m/z* 210 $[M+H]^+$.

6-(Benzylamino)nicotinamide **3i** [4]

Yield 205 mg (90%) as a white solid; mp 168-170 °C; IR (KBr) (cm^{-1}) 3411, 3178, 1648, 1603; ^{1}H-NMR (400 MHz, DMSO-d_6) δ 4.53 (d, *J*=6.0 Hz, 2H), 6.51 (d, *J*=8.7 Hz, 1H), 7.06 (brs, 1H), 7.18-7.27 (m, 1H), 7.28-7.35 (m, 4H), 7.60 (t, *J*=6.0 Hz, 1H), 7.67 (brs, 1H), 7.82 (dd, *J*=8.7, 2.3 Hz, 1H), 8.52 (d,

J=2.3 Hz, 1H); ^{13}C-NMR (100 MHz, DMSO-d_6) δ 44.5, 107.6, 118.4, 127.2, 127.8, 128.8, 136.6, 140.6, 149.1, 160.6, 167.5; MS (FAB): *m/z* 228 $[M+H]^+$.

N-Benzylpyridin-3-amine **3j** [5]

Yield 166 mg (90%) as a pale brow solid; mp 87-89 °C; IR (KBr) (cm^{-1}) 3263, 1591; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 4.14 (brs, 1H), 4.34 (d, *J*=5.0 Hz, 2H), 6.87 (dd, *J*=8.2, 3.2 1.4 Hz, 1H), 7.06 (dd, *J*=8.2, 4,6 Hz, 1H), 7.26-7.40 (m, 5H), 7.97 (dd, *J*=4.6, 1.4 Hz, 1H), 8.01 (d, *J*=3.2 Hz, 1H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 47.9, 118.6, 123.8, 127.5, 127.6, 128.9, 136.3, 138.6, 139.0, 144.1; MS (FAB): *m/z* 185 $[M+H]^+$.

N-Benzylpyrimidin-2-amine **3k** [6]

Yield 130 mg (70%) as a white solid; mp 78-80 °C; IR (KBr) (cm^{-1}) 3236, 1600; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 4.64 (d, *J*=5.5 Hz, 2H), 5.84 (brs, 1H), 6.52 (t, *J*=4.6 Hz, 1H), 7.24-7.38 (m, 5H), 8.22 (brd, *J*=4.1 Hz, 1H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 45.5, 110.9, 127.3, 127.6, 128.7, 139.2, 158.2, 162.4; MS (FAB): *m/z* 186 $[M+H]^+$.

N-(4-Methylbenzyl)pyridin-2-amine **3l** [1]

Yield 149 mg (75%) as a white solid; mp 72-74 °C; IR (KBr) (cm^{-1}) 3235, 1609; ^{1}H-NMR (400 MHz, $CDCl_3$): δ 2.34 (s, 3H), 4.45 (d, *J*=5.5 Hz, 2H), 4.83 (brs, 1H), 6.37 (d, *J*=8.9 Hz, 1H), 6.58 (dd, *J*=7.3, 5.0, 0.7 Hz, 1H), 7.15 (d, *J*=7.8 Hz, 2H), 7.25 (d, *J*=8.2 Hz, 2H), 7.39 (ddd, *J*=8.7, 7.3, 1.8 Hz, 1H), 8.10 (dd, *J*=5.0, 1.4 Hz, 1H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 21.1, 46.1, 106.7, 113.0, 127.4, 129.3, 136.1, 136.9, 137.4, 148.2, 158.7; MS (FAB): *m/z* 199 $[M+H]^+$.

N-(3-Methylbenzyl)pyridin-2-amine **3m** [1]

Yield 159 mg (80%) as a white solid; mp 95-97 °C; IR (KBr) (cm^{-1}) 3240, 1608; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 2.37 (s, 3H), 4.47 (d, *J*=5.5 Hz, 2H), 4.64 (brs, 1H), 6.38 (dt, *J*=8.2, 0.9 Hz, 1H), 6.60 (ddd, *J*=6.9, 5.0, 0.9 Hz, 1H), 7.15-7.23 (m, 3H), 7.32 (d, *J*=6.9 Hz, 1H), 7.41 (ddd, *J*=9.2, 7.3, 1.8 Hz, 1H), 8.12 (ddd, *J*=5.0, 1.8, 0.9 Hz, 1H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 19.1, 44.5, 106.9, 113.1, 126.2, 127.5, 128.1, 130.5, 136.4, 136.9, 137.5, 148.3, 158.7; MS (FAB): *m/z* 199 $[M+H]^+$.

N-(2-Methylbenzyl)pyridin-2-amine **3n** [1]

Yield 159 mg (80%) as a white solid; mp 74-76 °C; IR (KBr) (cm^{-1}) 3223, 1601; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 2.34 (s, 3H), 4.46 (d, *J*=6.0 Hz, 2H), 4.84 (brs, 1H), 6.37 (d, *J*=8.2 Hz, 1H), 6.59 (dd, *J*=7.3, 5.5 Hz, 1H), 7.08 (d, *J*=7.3 Hz, 1H), 7.13-7.20 (m, 2H), 7.23 (t, *J*=7.3 Hz, 1H), 7.40 (dd, *J*=6.9, 1.8 Hz, 1H), 8.11 (dt, *J*=5.0, 0.9 Hz, 1H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 21.4, 46.3, 106.7, 113.1, 124.4, 128.0, 128.1, 128.5, 137.4, 138.3, 139.1, 148.2, 158.7; MS (FAB): *m/z* 199 $[M+H]^+$.

N-(3-Methylbenzyl)-4-(trifluoromethyl)aniline **3o**

Yield 178 mg (67%) as a white solid; mp 110-112 °C; IR (KBr) (cm^{-1}) 3245, 1620; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 2.35 (s, 2H), 4.51 (d, *J*=5.5 Hz, 2H), 5.27 (brs, 1H), 6.39 (d, *J*=9.2 Hz, 1H), 7.08-7.18 (m, 3H), 7.24 (t, *J*=7.8 Hz, 1H), 7.57 (dd, *J*=8.7, 2.3 Hz, 1H), 8.33 (s, 1H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 21.4, 46.1, 105.9, 115.6 (q, J_{CF}=33.6 Hz), 124.5, 124.6 (q, J_{CF}=270.3 Hz), 128.2, 128.4, 128.7, 134.5 (q, J_{CF}=2.9 Hz), 138.1, 138.6, 146.1 (q, J_{CF}=4.8 Hz), 160.3; MS (FAB): *m/z* 267 $[M+H]^+$; HRMS-FAB: *m/z* (M^+) calcd for $C_{14}H_{13}F_3N_2$ 267.1109, found 267.1109.

N-(4-Methoxybenzyl)pyridin-2-amine **3p** [1]

Yield 176 mg (82%) as a white solid; mp 118-120 °C; IR (KBr) (cm^{-1}) 3234, 1604; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 3.80 (s, 3H), 4.43 (d, *J*=6.0 Hz, 2H), 4.78 (brs, 1H), 6.37 (d, *J*=8.2 Hz, 1H), 6.59 (ddd, *J*=7.3, 5.0, 0.9 Hz, 1H), 6.88 (d, *J*=8.7 Hz, 2H), 7.29 (d, *J*=8.7 Hz, 2H), 7.40 (d, *J*=8.7, 6.9, 1.8 Hz, 1H), 8.11 (dd, *J*=5.0, 1.4 Hz, 1H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 45.8, 55.3, 106.8, 113.1, 114.0, 128.7, 131.1, 137.4, 148.2, 158.6, 158.8; MS (FAB): *m/z* 215 $[M+H]^+$.

N-(4-Butoxybenzyl)pyridin-2-amine **3q** [7]

Yield 208 mg (81%) as a white solid; mp 83-85 °C; IR (KBr) (cm^{-1}) 3229, 1606; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 0.97 (t, *J*=7.3 Hz 1H), 1.48 (sext, *J*=7.8 Hz 1H), 1.76 (quin, *J*=7.3 Hz 1H), 3.95 (t, *J*=6.9 Hz 2H), 4.42 (d, *J*=5.5 Hz 2H), 4.77 (brs, 1H), 6.37 (d, *J*=8.7 Hz, 1H), 6.58 (dd, *J*=7.3, 5.0 Hz, 1H), 6.86 (d, *J*=8.0 Hz, 2H), 7.26 (d, *J*=8.0 Hz, 2H), 7.40 (dd, *J*=6.9, 1.8 Hz, 1H), 8.10 (dt, *J*=5.0, 0.9 Hz, 1H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 13.9, 19.3, 31.3, 45.9, 67.7, 106.8, 113.1, 114.6, 128.7, 130.9, 137.4, 148.2, 158.4, 158.6; MS (FAB): *m/z* 257 $[M+H]^+$; Anal. Calcd for $C_{16}H_{20}N_2O$: C, 74.97; H, 7.86; N, 10.93. Found: C, 74.73; H, 7.90; N, 10.79.

N-[1-(4-Methoxyphenyl)ethyl]pyridin-2-amine **3r** [8]

Yield 139 mg (61%) as a white solid; mp 89-91 °C; IR (KBr) (cm^{-1}) 3263, 2978, 1610; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 1.53 (d, *J*=6.9 Hz, 3H), 3.79 (s, 3H), 4.68 (quint, *J*=6.6 Hz, 1H), 4.88 (brd, *J*=5.5 Hz, 1H), 6.19 (d, *J*=8.7 Hz, 1H), 6.54 (dd, *J*=6.9, 5.0 Hz, 1H), 6.86 (d, *J*=8.7 Hz, 2H), 7.29 (d, *J*=8.7 Hz, 2H), 7.32 (dd, *J*=6.4, 2.3 Hz, 1H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 24.4, 51.3, 55.3, 106.7, 113.0, 114.0, 126.9, 136.7, 137.4, 148.2, 158.1, 158.6; MS (FAB): *m/z* 229 $[M+H]^+$.

N-(Naphthalen-2-ylmethyl)pyridin-2-amine **3s** [9]

Yield 176 mg (75%) as a white solid; mp 110-112 °C; IR (KBr) (cm^{-1}) 3228, 1600; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 4.67 (d, *J*=5.8 Hz, 2H), 4.98 (brs, 1H), 6.40 (d, *J*=8.2 Hz, 1H), 6.60 (dd, *J*=6.9, 5.0, 0.9 Hz,

1H), 7.36-7.52 (m, 3H), 7.76-7.86 (m, 4H), 8.13 (dd, *J*=5.0, 1.8, 0.9 Hz, 1H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 46.5, 106.8, 113.3, 125.7, 125.8, 126.2, 127.7, 128.4, 132.7, 133.4, 136.7, 137.5, 148.3, 158.6; MS (FAB): *m/z* 235 $[M+H]^+$.

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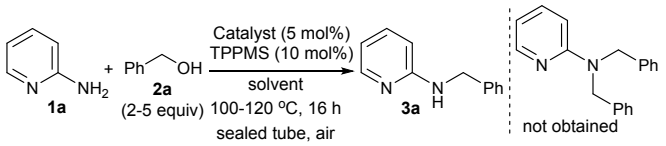
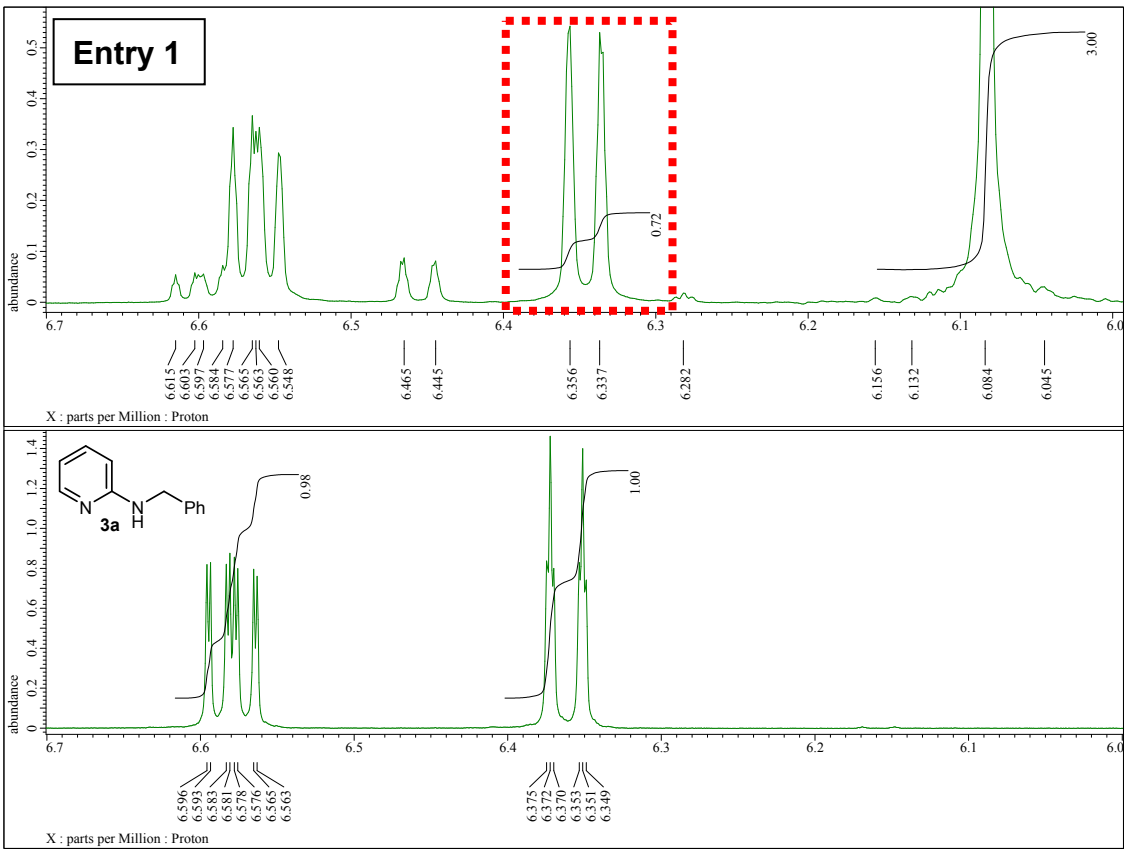
Table S1, Entry 1 (The yield was determined by ^{1}H NMR analysis of the crude product using 1,3,5-trimethoxybenzene as an internal standard.)



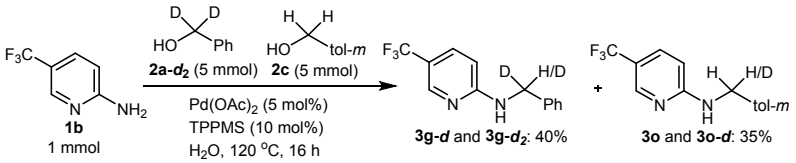
A mixture of 2-aminopyridine **1a** (94 mg, 1 mmol), $Pd(OAc)_2$ (11 mg, 0.05 mmol), sodium diphenylphosphinobenzene-3-sulfonate (TPPMS, 36 mg, 0.1 mmol), and benzyl alcohol **2a** (216 mg, 2 mmol), in H_2O (4 mL) was heated at 120 °C for 16 h in a sealed tube under air. After the reaction mixture was cooled, 1,3,5-trimethoxybenzene (168 mg, 1 mmol, internal standard) was added to the reaction mixture, which was extracted with AcOEt. The organic layer was concentrated in vacuo. The residue was was analyzed by ^{1}H-NMR spectroscopy.

Conversion yield was calculated by integration.

	desired **3a**	1,3,5-trimethoxybenzene, **internal standard**
Signal δ	6.34 (Ar-**H**)	6.08 (Ar-**H**)
Integral value	0.72 (1H)	3.00 (3H)
Calculated ratio	72% from **1a**	1 mmol



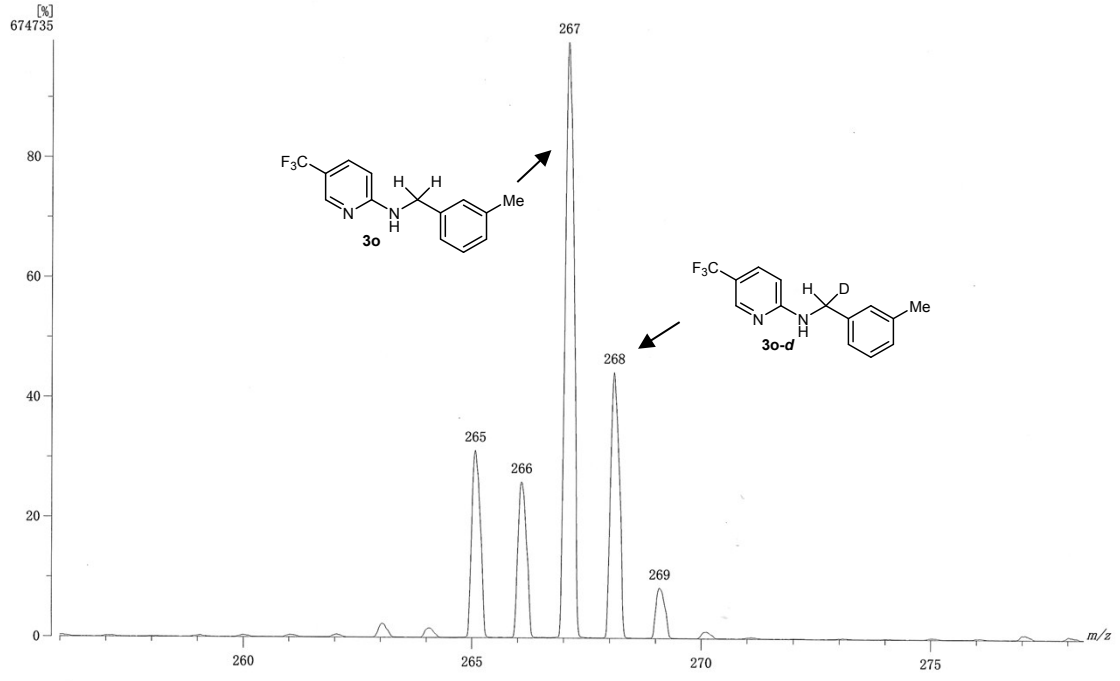
Scheme 3S. Crossover experiment.



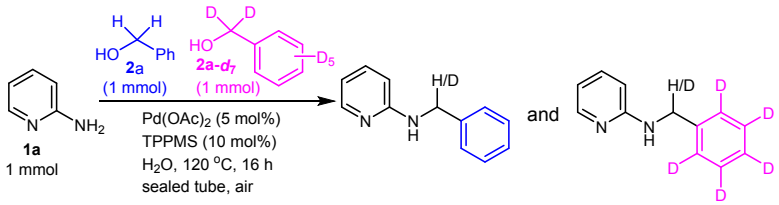
A mixture of **1b** (162 mg, 1 mmol), $Pd(OAc)_2$ (11 mg, 0.05 mmol), sodium diphenylphosphinobenzene-3-sulfonate (TPPMS, 36 mg, 0.1 mmol), benzyl-α,α-d_2 alcohol **2a-*d*$_2$** (5 mmol), and 3-methylbenzyl alcohol **2c** (5 mmol) in H_2O (4 mL) was heated at 120 °C for 16 h in a sealed tube under air. After cooling, the reaction mixture was poured into water and extracted with EtOAc. The organic layer was washed with brine, dried over $MgSO_4$ and concentrated in vacuo. The residue was purified by flash column chromatography (silica gel, hexanes/EtOAc) to give H/D scrambling products *N*-benzyl-5-(trifluoromethyl)pyridin-2-amine (**3g-*d*** and **3g-*d*$_2$** mixture) and *N*-(3-methylbenzyl)-5-(trifluoromethyl)pyridin-2-amine (**3o** and **3o-*d*** mixture) in 40% and 35% isolated yields, respectively.

N-(3-Methylbenzyl)-5-(trifluoromethyl)pyridin-2-amine (**3o** and **3o-*d*** mixture)

FAB-MS: *m/z* $[M+H]^+$ **3o**; 267, **3o-*d***; 268.

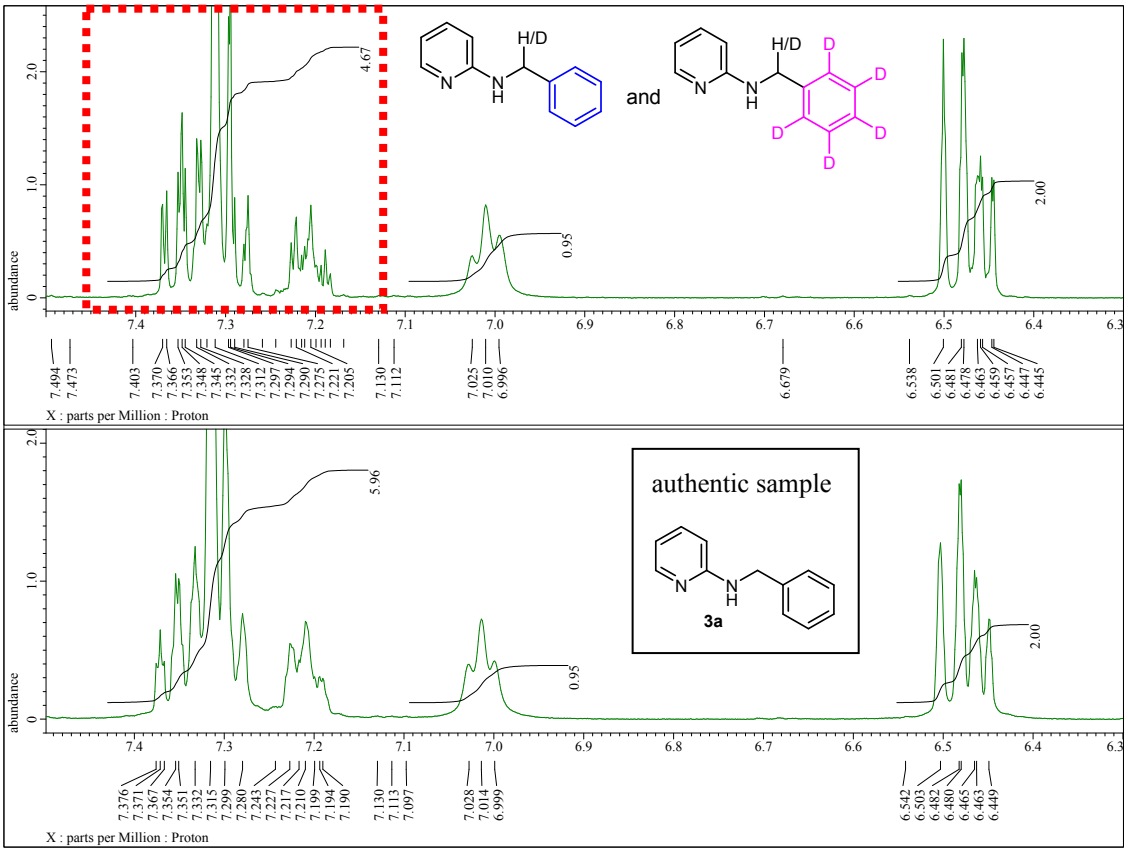


Scheme 4S. Kinetic isotope effects.

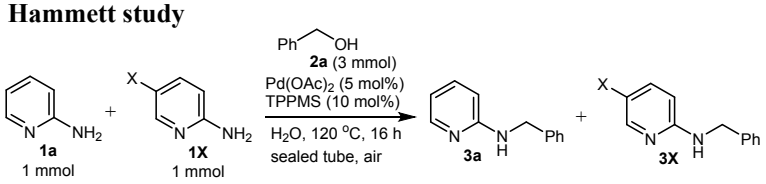


A mixture of 2-aminopyridine **1a** (94 mg, 1 mmol), $Pd(OAc)_2$ (11 mg, 0.05 mmol), sodium diphenylphosphinobenzene-3-sulfonate (TPPMS, 36 mg, 0.1 mmol), benzyl alcohol **2a** (108 mg, 1 mmol), and **2a-*d*$_7$** (115 mg, 1 mmol) in H_2O (2 mL) was heated at 120 °C for 16 h in a sealed tube under air. After cooling, the reaction mixture was poured into water and extracted with EtOAc. The organic layer was washed with brine, dried over $MgSO_4$ and concentrated in vacuo. The residue was purified by flash column chromatography (silica gel, hexanes/EtOAc). The product was analyzed by ^{1}H-NMR spectroscopy.

Signal δ	7.18-7.40 (Ph-**5H** and Py-**H**)	6.43-6.52 (Py-**2H**)
Integral value	4.67	2.00
	4.67-1.00 = 3.67 (Ph-**5H**), 5.00-3.67 = 1.33 (Ph-**5D**) KIE = 3.67/1.33 = 2.8	



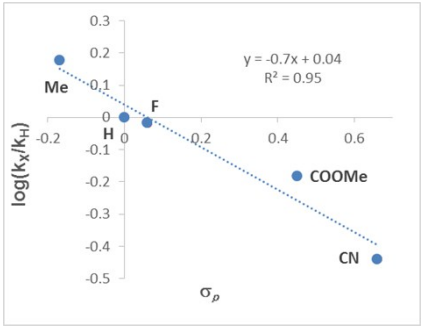
Hammett study



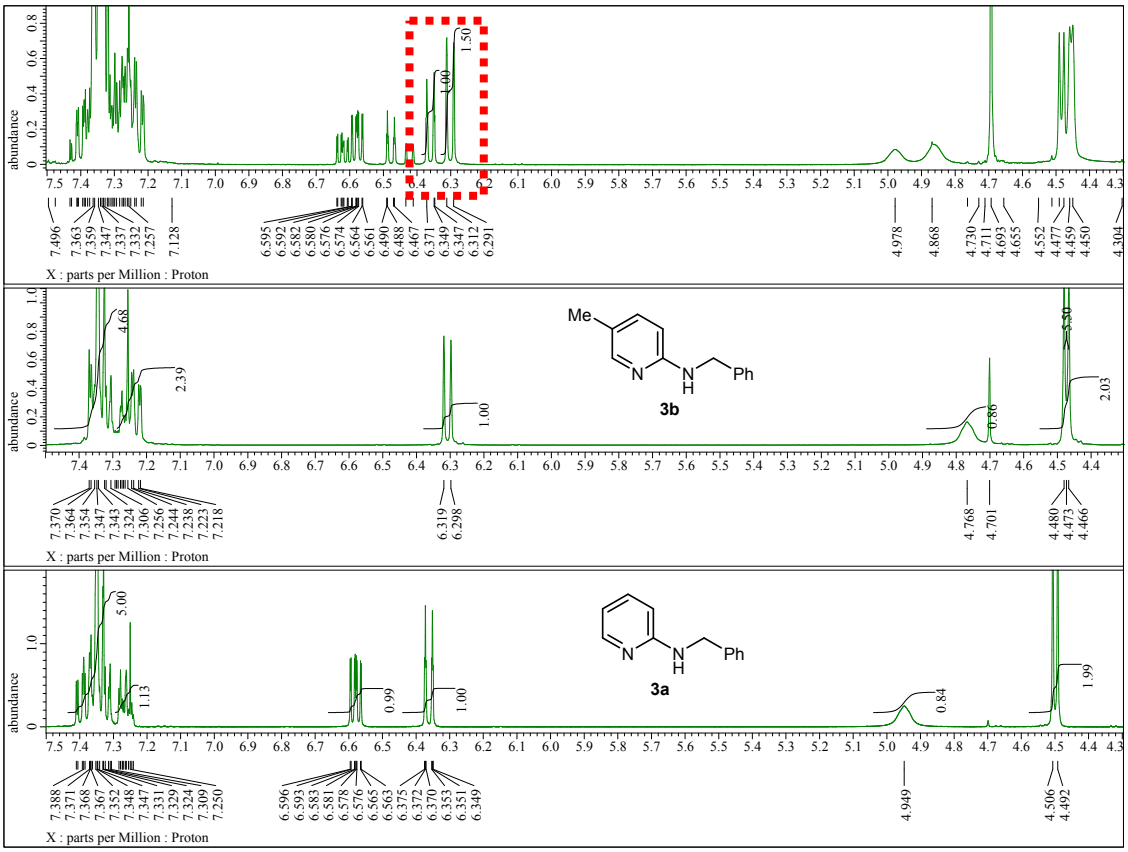
A mixture of 2-aminopyridine **1a** (94 mg, 1 mmol), **1X** (1 mmol), $Pd(OAc)_2$ (11 mg, 0.05 mmol), sodium diphenylphosphinobenzene-3-sulfonate (TPPMS, 36 mg, 0.1 mmol), and benzyl alcohol **2a** (310 μL, 2 mmol), in H_2O (4 mL) was heated at 120 °C for 16 h in a sealed tube under air. After cooling, the reaction mixture was poured into water and extracted with EtOAc. The organic layer was concentrated in vacuo. The residue was was analyzed by ^{1}H-NMR spectroscopy.

R =	σ	$\log(k_X/k_H)$
Me	-0.17	0.176
H	0	0
F	0.06	-0.018
COOMe	0.45	-0.182
CN	0.66	-0.44

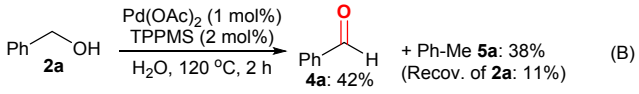
Figure S3



R = Me: $\log(k_X/k_H) = \log(1.50/1.00) = 0.176$



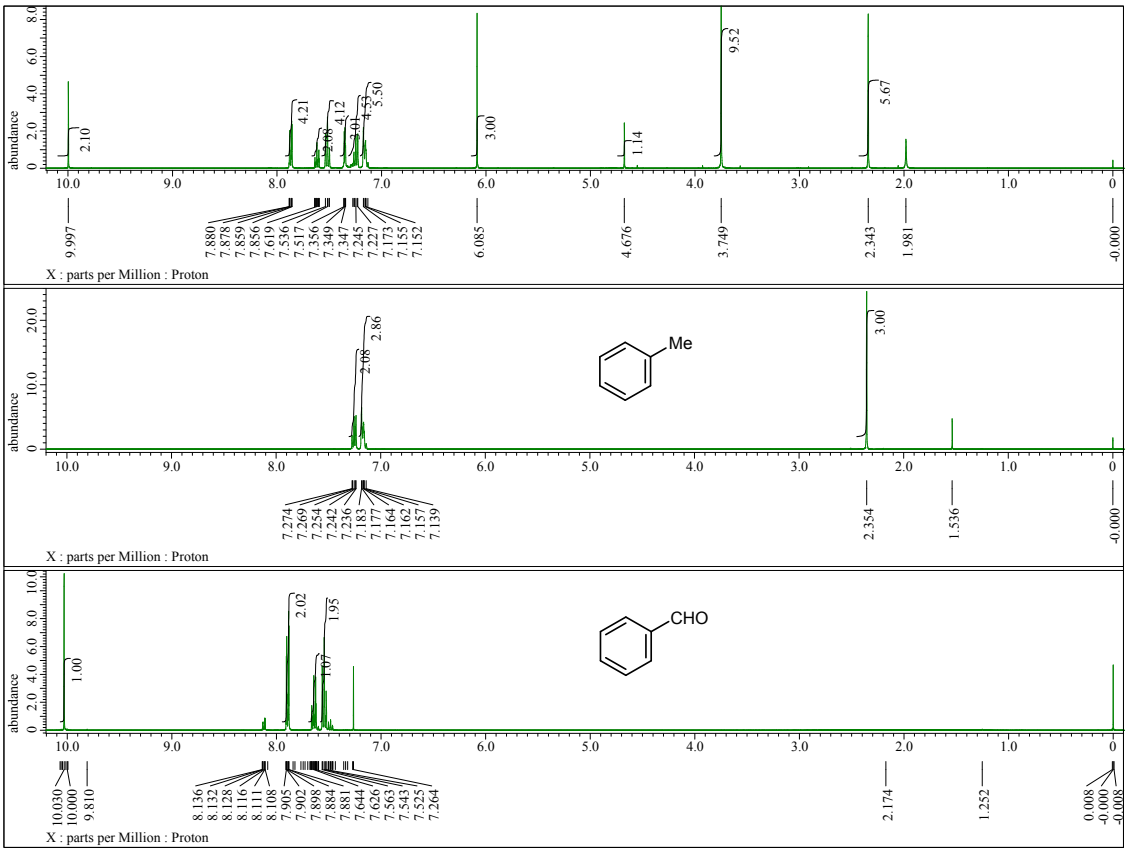
Scheme 6(B)S. Control experiments.



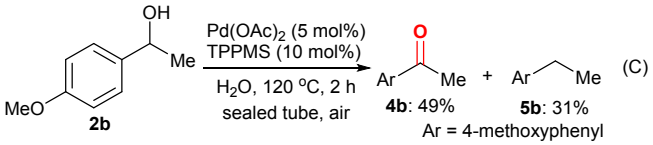
A mixture of benzyl alcohol **2a** (541 mg, 5 mmol), palladium(II) acetate (11 mg, 0.05 mmol), sodium diphenylphosphinobenzene-3-sulfonate (TPPMS, 36 mg, 0.1 mmol) in H_2O (4 mL) was heated for 2 h in sealed tube. After the reaction mixture was cooled, 1,3,5-trimethoxybenzene (168 mg, 1 mmol, internal standard) was added to the reaction mixture, which was extracted with $CDCl_3$ (8 mL), then the organic layer was analyzed by ^{1}H-NMR spectroscopy.

Conversion yield was calculated by integration.

	Ph-CHO **4a**	Ph-Me **5a**	1,3,5-trimethoxybenzene, **internal standard**
Signal δ	10.0 (Ph-C**H**O)	2.34 (Ph-C**H$_3$**)	6.09 (Ar-**H**)
Integral value	2.1 (1H)	5.67 (3H)	3.00 (3H)
Calculated ratio	42% from **2a**	38% from **2a**	1 mmol



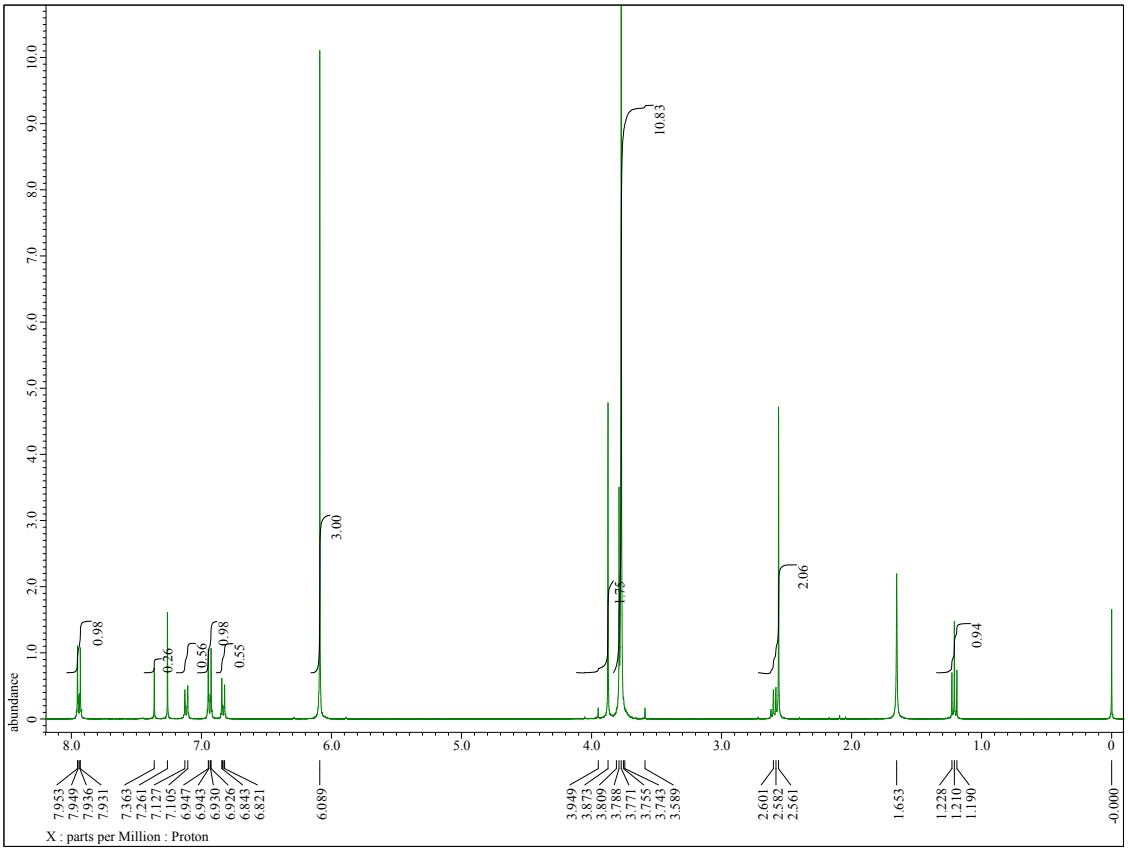
Scheme 6(C)S. Control experiments.

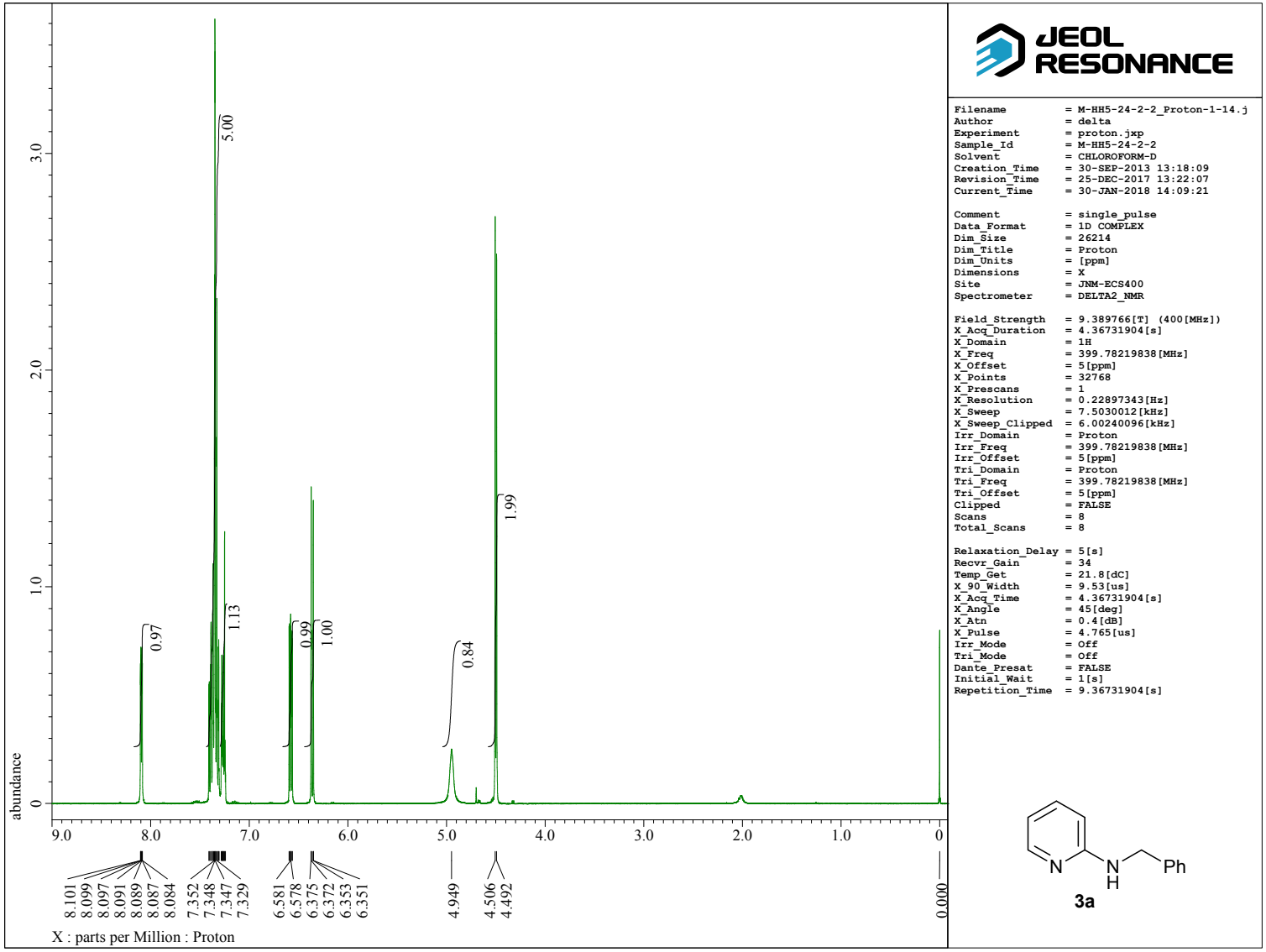


A mixture of benzyl alcohol **2b** (152 mg, 1 mmol), palladium(II) acetate (11 mg, 0.05 mmol), sodium diphenylphosphinobenzene-3-sulfonate (TPPMS, 36 mg, 0.1 mmol) in H_2O (4 mL) was heated for 2 h in sealed tube. After the reaction mixture was cooled, 1,3,5-trimethoxybenzene (168 mg, 1 mmol, internal standard) was added to the reaction mixture, which was extracted with $CDCl_3$ (8 mL), then the organic layer was analyzed by ^{1}H-NMR spectroscopy.

Conversion yield was calculated by integration.

	4b	**5b**	1,3,5-trimethoxybenzene, **internal standard**
Signal δ	7.94 (Ar-2**H**)	1.21 (Ar-CH_2C**H**$_3$)	6.09 (Ar-**H**)
Integral value	0.98 (2H)	0.94 (3H)	3.00 (3H)
Calculated ratio	49% from **2b**	31% from **2b**	1 mmol





JEOL RESONANCE

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Author	= delta
Experiment	= proton.jxp
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Solvent	= CHLOROFORM-D
Creation_Time	= 30-SEP-2013 13:18:09
Revision_Time	= 25-DEC-2017 13:22:07
Current_Time	= 30-JAN-2018 14:09:21
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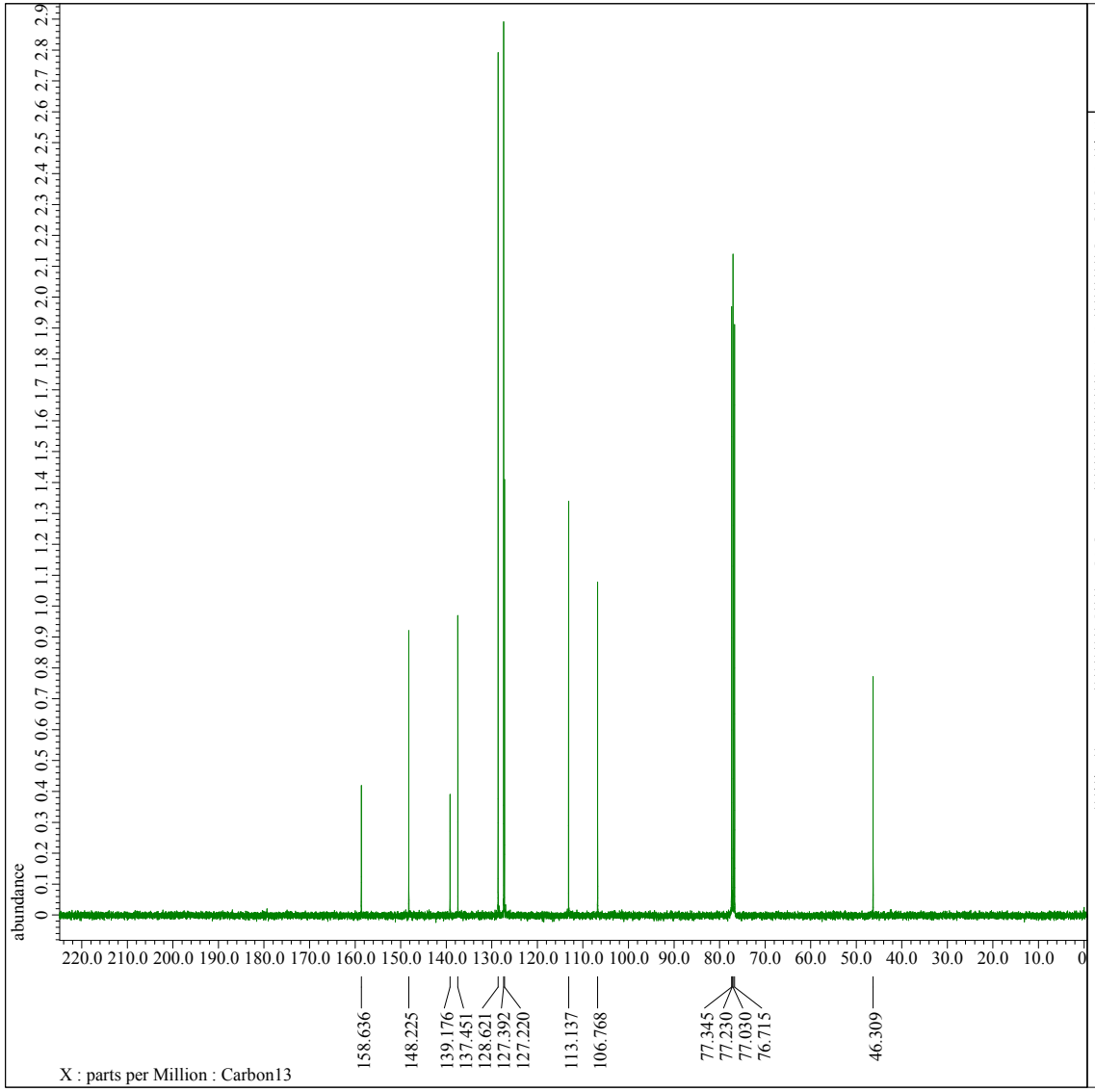
Dim_Size	= 26214
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.389766[T] (400[MHz])
X_Acq_Duration	= 4.36731904[s]
X_Domain	= 1H
X_Freq	= 399.78219838[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 0.22897343[Hz]
X_Sweep	= 7.5030012[kHz]
X_Sweep_Clipped	= 6.00240096[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.78219838[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 34
Temp_Get	= 21.8[dC]
X_90_Width	= 9.53[us]
X_Acq_Time	= 4.36731904[s]
X_Angle	= 45[deg]
X_Atn	= 0.4[dB]
X_Pulse	= 4.765[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 9.36731904[s]

3a



JEOL RESONANCE

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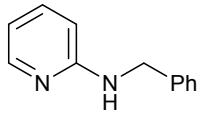
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = M-HH5-24-2-2
Solvent           = CHLOROFORM-D
Creation_Time     = 30-SEP-2013 13:22:00
Revision_Time     = 30-JAN-2018 14:10:42
Current_Time      = 30-JAN-2018 14:10:53

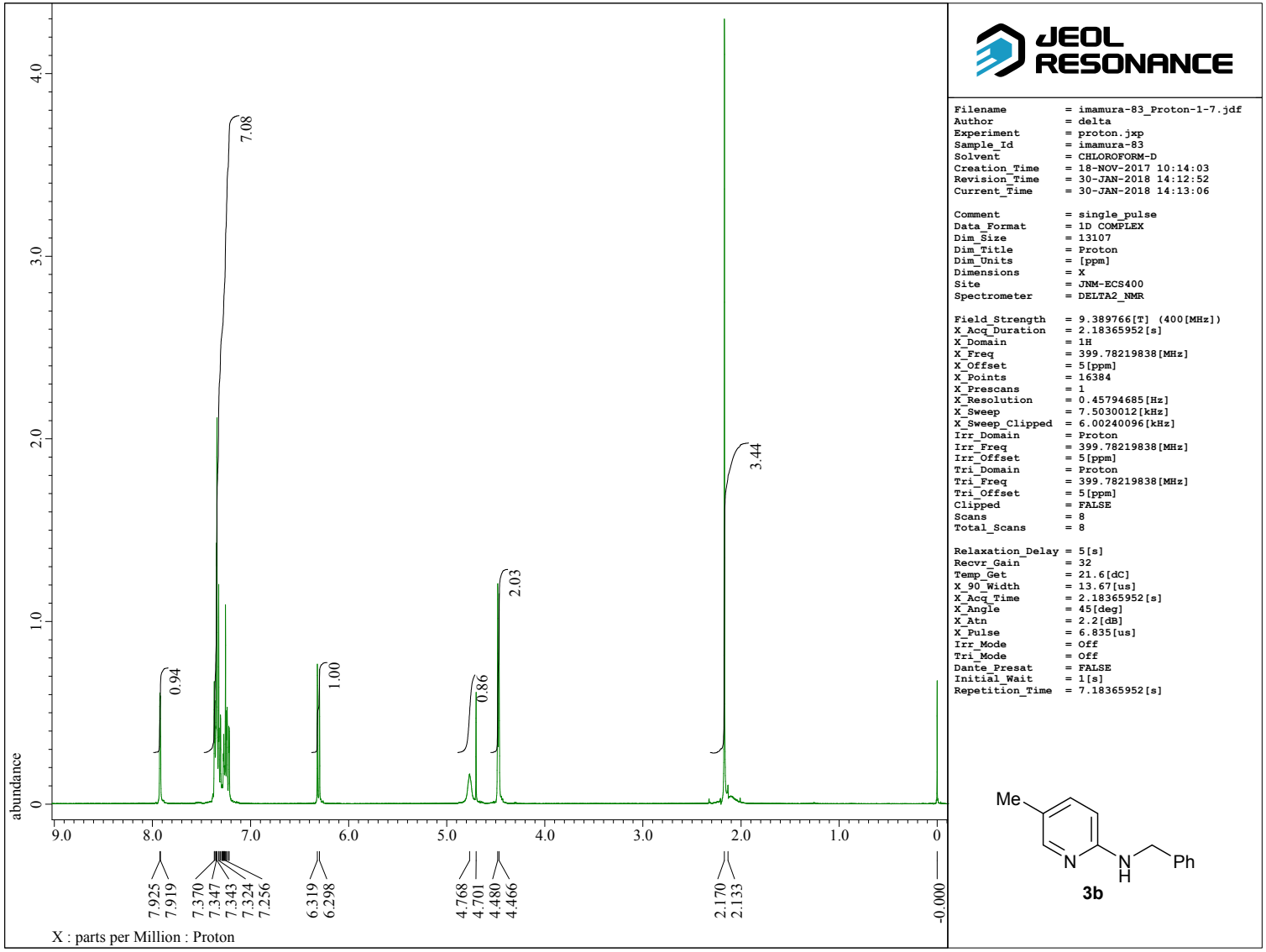
Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 699
Total_Scans       = 699

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 22[dC]
X_90_Width        = 8[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 4.1[dB]
X_Pulse           = 2.66666667[us]
Irr_Atn_Dec       = 21.763[dB]
Irr_Atn_Noe       = 21.763[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```



3a



JEOL RESONANCE

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Author            = delta
Experiment        = proton.jxp
Sample_Id         = imamura-83
Solvent           = CHLOROFORM-D
Creation_Time     = 18-NOV-2017 10:14:03
Revision_Time     = 30-JAN-2018 14:12:52
Current_Time      = 30-JAN-2018 14:13:06

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
X_Sweep_Clipped   = 6.00240096[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay = 5[s]
Recvr_Gain        = 32
Temp_Get          = 21.6[dC]
X_90_Width        = 13.67[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 2.2[dB]
X_Pulse           = 6.835[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.18365952[s]
```
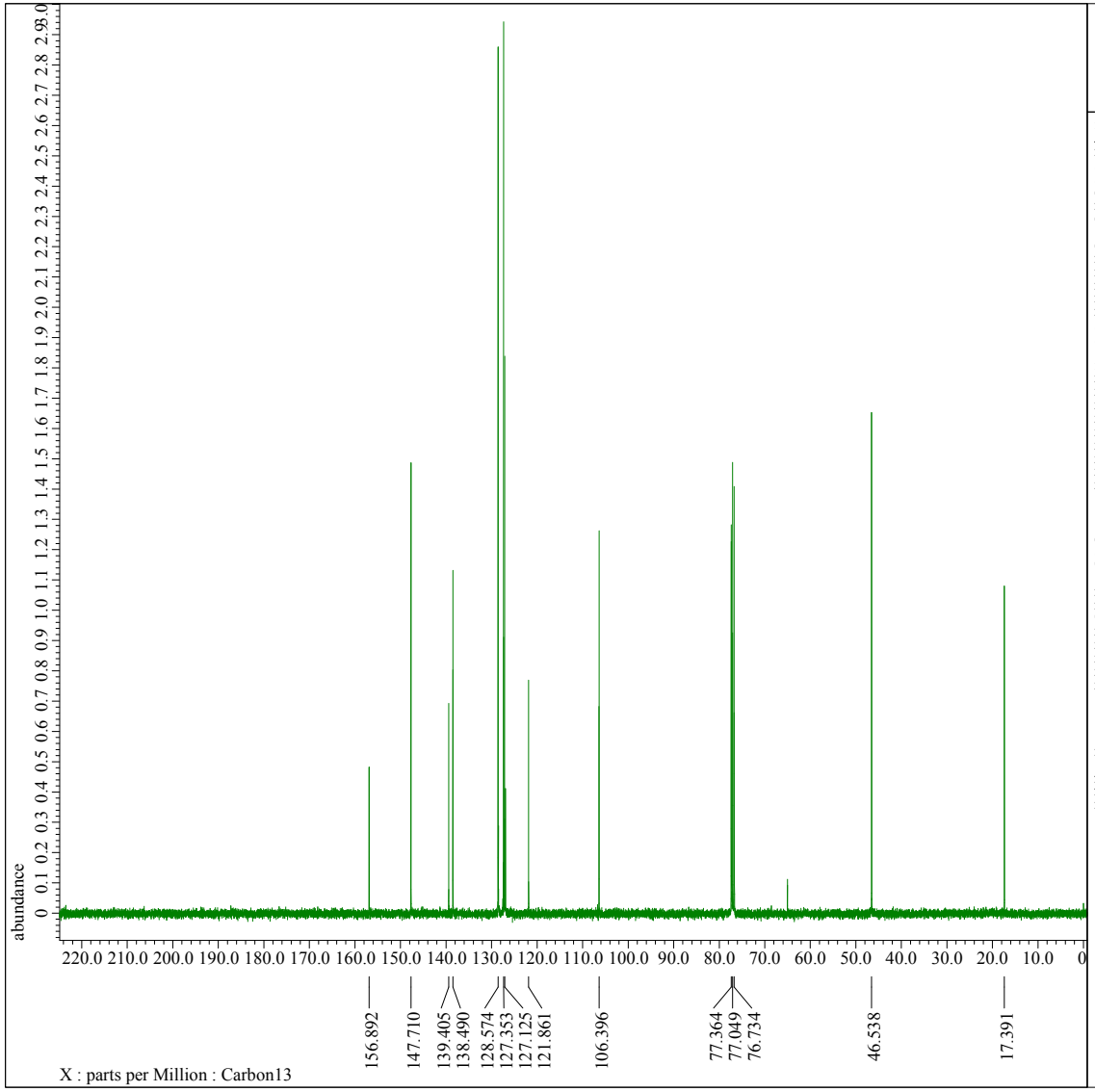


3b



JEOL RESONANCE

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Author            = delta
Experiment        = carbon.jxp
Sample_Id         = M-imamura-83-C
Solvent           = CHLOROFORM-D
Creation_Time     = 21-NOV-2017 09:31:10
Revision_Time     = 30-JAN-2018 14:14:34
Current_Time      = 30-JAN-2018 14:14:46

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 403
Total_Scans       = 403

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 21.7[dC]
X_90_Width        = 9.74[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 3.3[dB]
X_Pulse           = 3.24666667[us]
Irr_Atn_Dec       = 20.699[dB]
Irr_Atn_Noe       = 20.699[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
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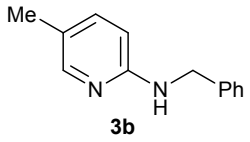
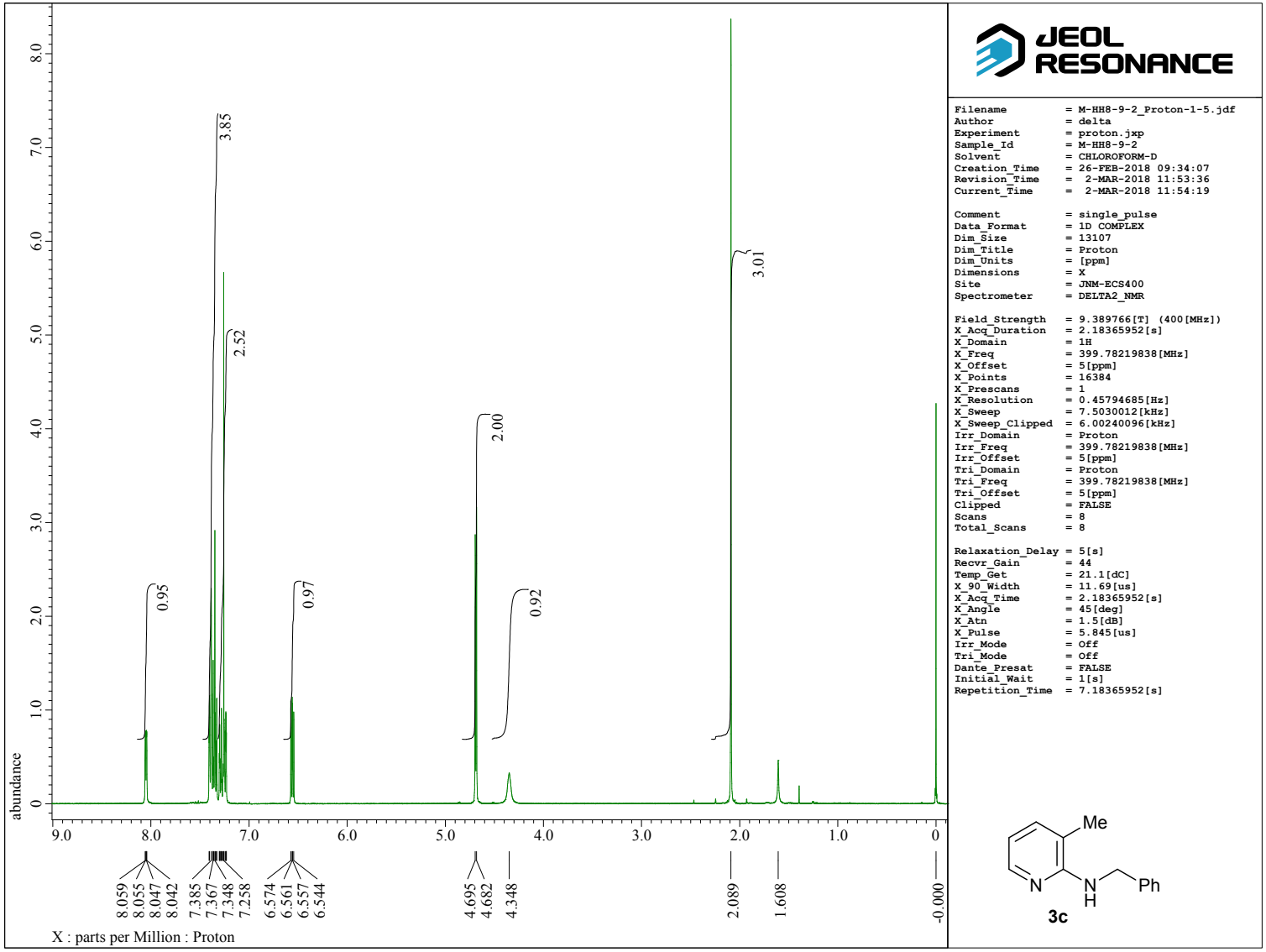


3b



JEOL RESONANCE

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Author	= delta
Experiment	= proton.jxp
Sample_Id	= M-HH8-9-2
Solvent	= CHLOROFORM-D
Creation_Time	= 26-FEB-2018 09:34:07
Revision_Time	= 2-MAR-2018 11:53:36
Current_Time	= 2-MAR-2018 11:54:19
Comment	= single_pulse
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Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.389766[T] (400[MHz])
X_Acq_Duration	= 2.18365952[s]
X_Domain	= 1H
X_Freq	= 399.78219838[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45794685[Hz]
X_Sweep	= 7.5030012[kHz]
X_Sweep_Clipped	= 6.00240096[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.78219838[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 44
Temp_Get	= 21.1[dC]
X_90_Width	= 11.69[us]
X_Acq_Time	= 2.18365952[s]
X_Angle	= 45[deg]
X_Atn	= 1.5[dB]
X_Pulse	= 5.845[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
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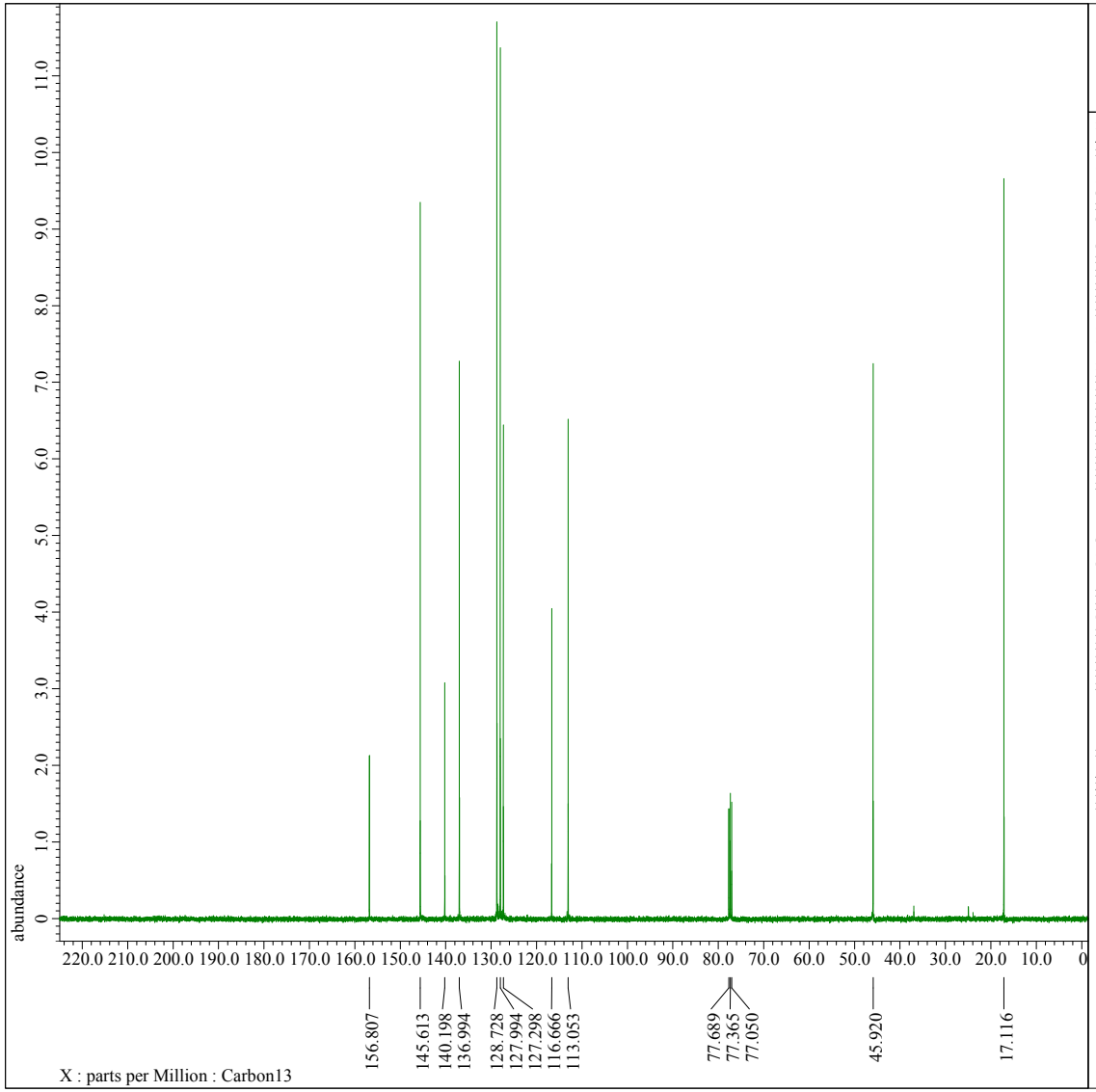
3c



JEOL RESONANCE

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Experiment        = carbon.jxp
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Solvent           = CHLOROFORM-D
Creation_Time     = 26-FEB-2018 09:53:19
Revision_Time     =  2-MAR-2018 11:55:24
Current_Time      =  2-MAR-2018 11:55:40

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 93
Total_Scans       = 93

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 21.4[dC]
X_90_Width        = 9.36[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 3.3[dB]
X_Pulse           = 3.12[us]
Irr_Atn_Dec       = 20.394[dB]
Irr_Atn_Noe       = 20.394[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
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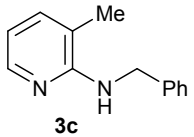
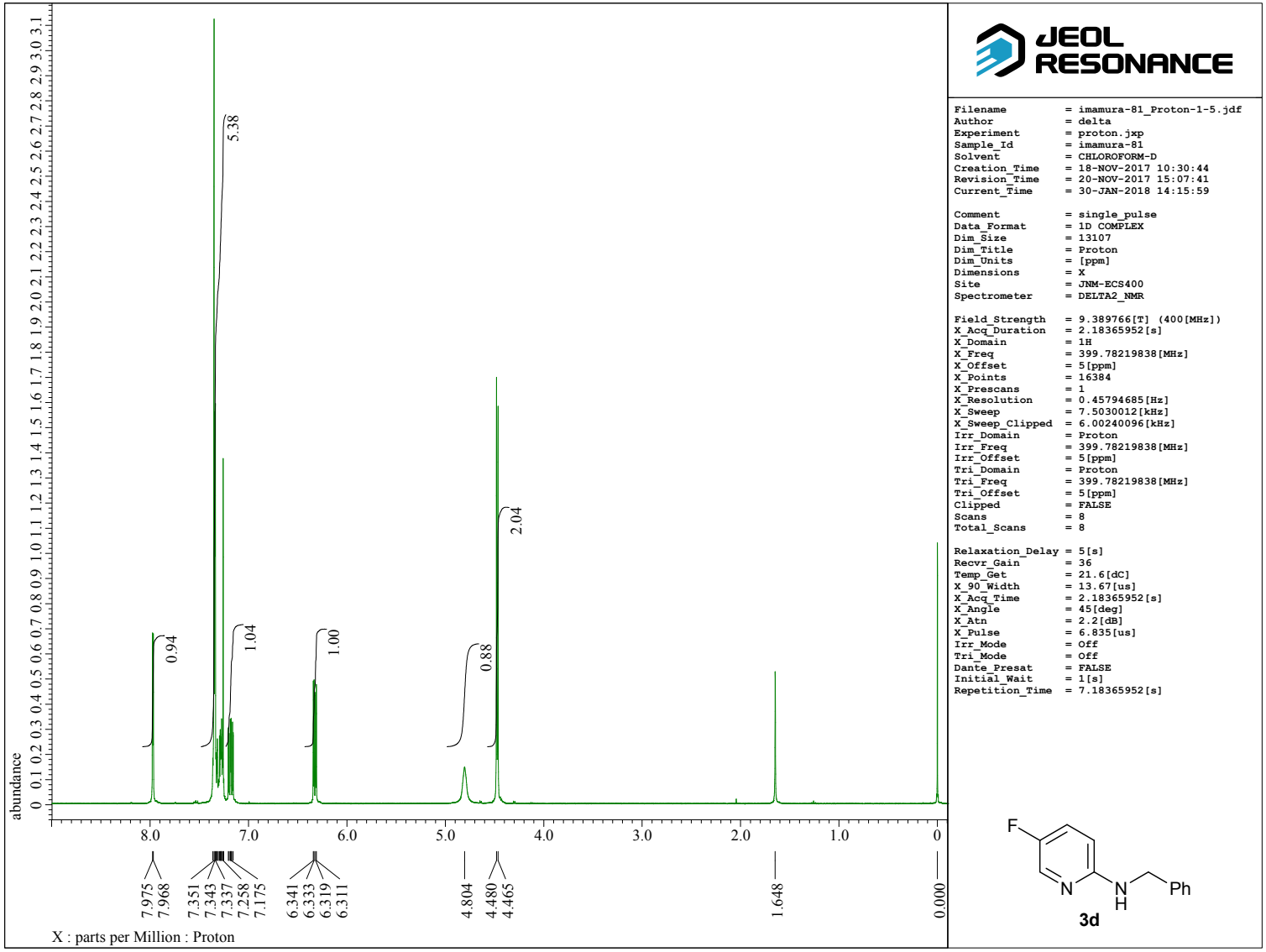


3c



JEOL RESONANCE

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Experiment	= proton.jxp
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Revision_Time	= 20-NOV-2017 15:07:41
Current_Time	= 30-JAN-2018 14:15:59
Comment	= single_pulse
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Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
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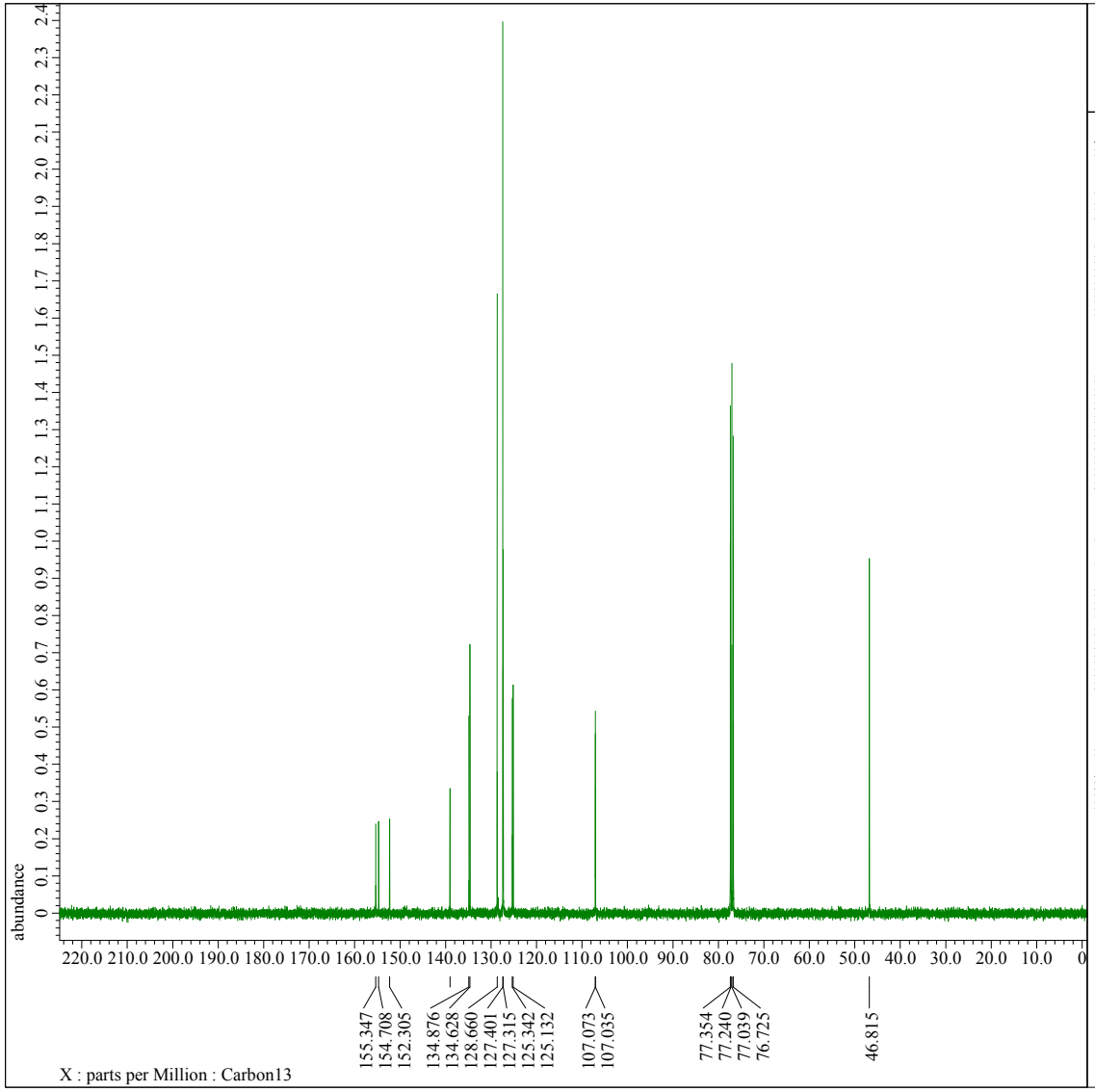
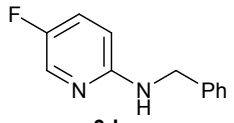
X_Acq_Duration	= 2.18365952[s]
X_Domain	= 1H
X_Freq	= 399.78219838[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45794685[Hz]
X_Sweep	= 7.5030012[kHz]
X_Sweep_Clipped	= 6.00240096[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.78219838[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 21.6[dC]
X_90_Width	= 13.67[us]
X_Acq_Time	= 2.18365952[s]
X_Angle	= 45[deg]
X_Atn	= 2.2[dB]
X_Pulse	= 6.835[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18365952[s]

3d

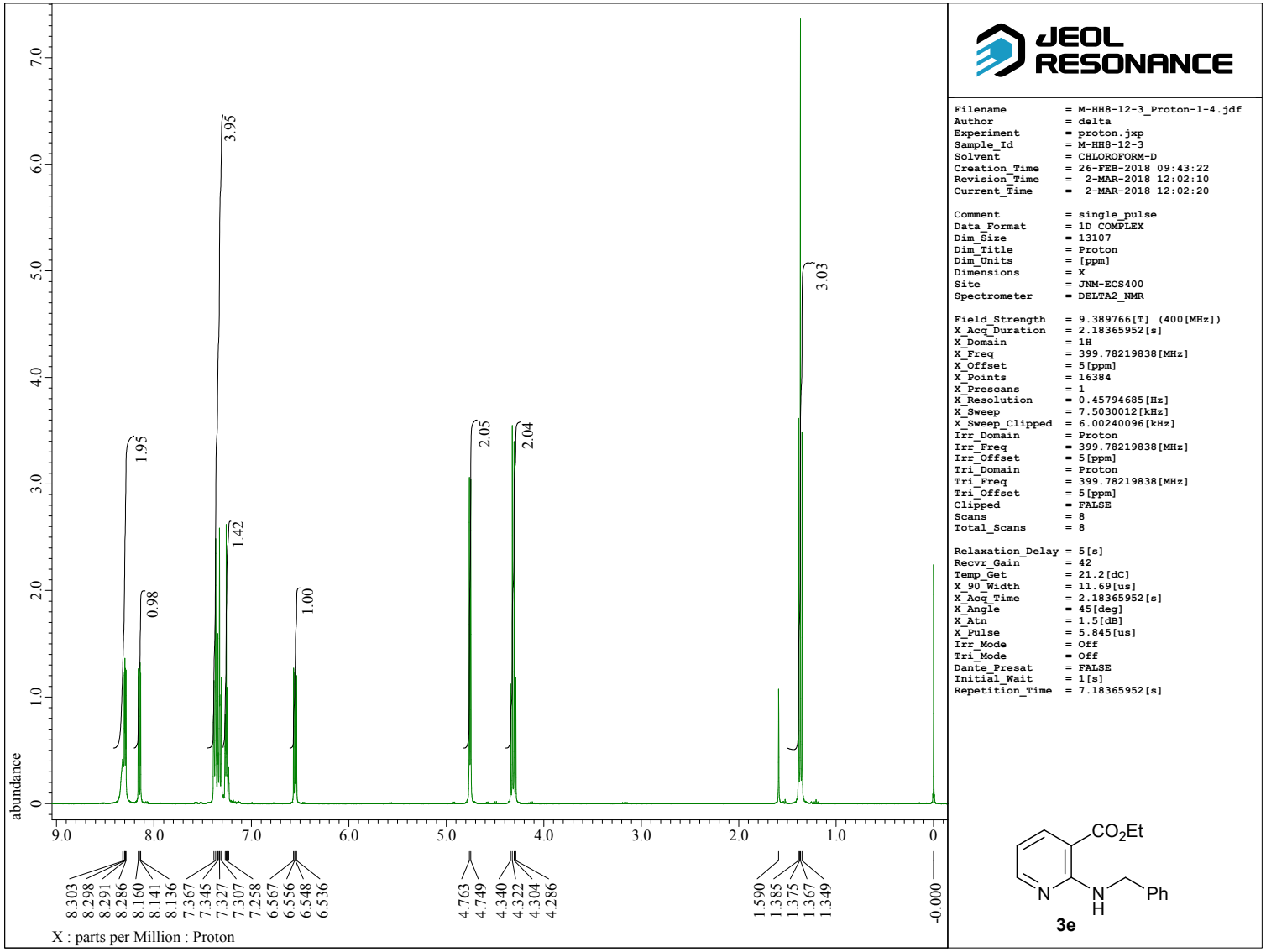


JEOL RESONANCE

```
Filename          = M-imamura-81-C_Carbon-1-4.
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = M-imamura-81-C
Solvent           = CHLOROFORM-D
Creation_Time     = 22-NOV-2017 11:32:19
Revision_Time     = 30-JAN-2018 14:17:06
Current_Time      = 30-JAN-2018 14:17:31

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 512
Total_Scans       = 512

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 21.8[dC]
X_90_Width        = 9.74[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 3.3[dB]
X_Pulse           = 3.24666667[us]
Irr_Atn_Dec       = 20.699[dB]
Irr_Atn_Noe       = 20.699[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```



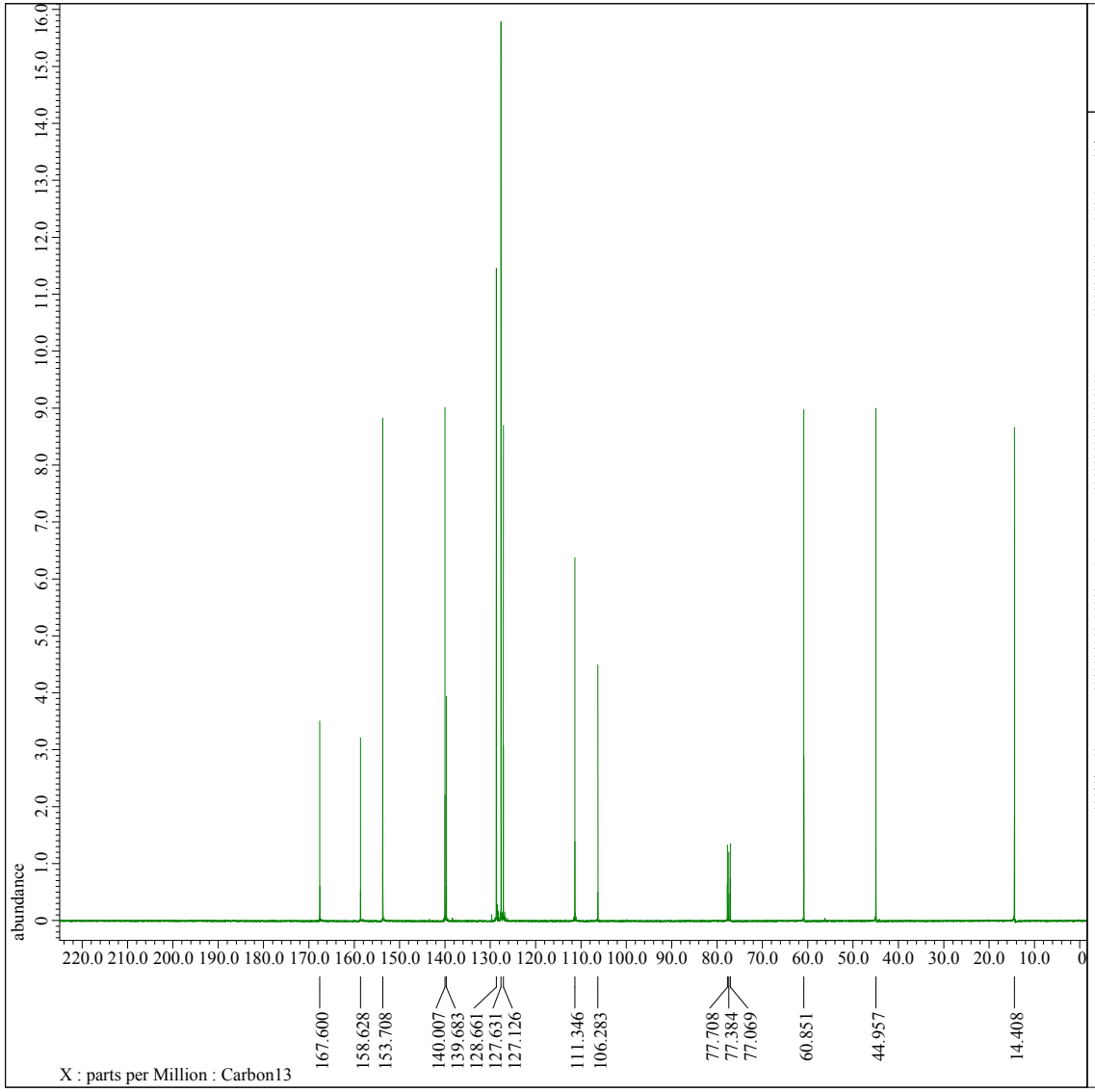
3d



JEOL RESONANCE

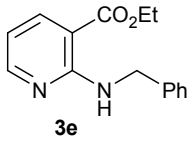
```
Filename          = M-HH8-12-3_Proton-1-4.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = M-HH8-12-3
Solvent           = CHLOROFORM-D
Creation_Time     = 26-FEB-2018 09:43:22
Revision_Time     =  2-MAR-2018 12:02:10
Current_Time      =  2-MAR-2018 12:02:20

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
X_Sweep_Clipped   = 6.00240096[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay = 5[s]
Recvr_Gain        = 42
Temp_Get          = 21.2[dC]
X_90_Width        = 11.69[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 1.5[dB]
X_Pulse           = 5.845[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.18365952[s]
```


3e

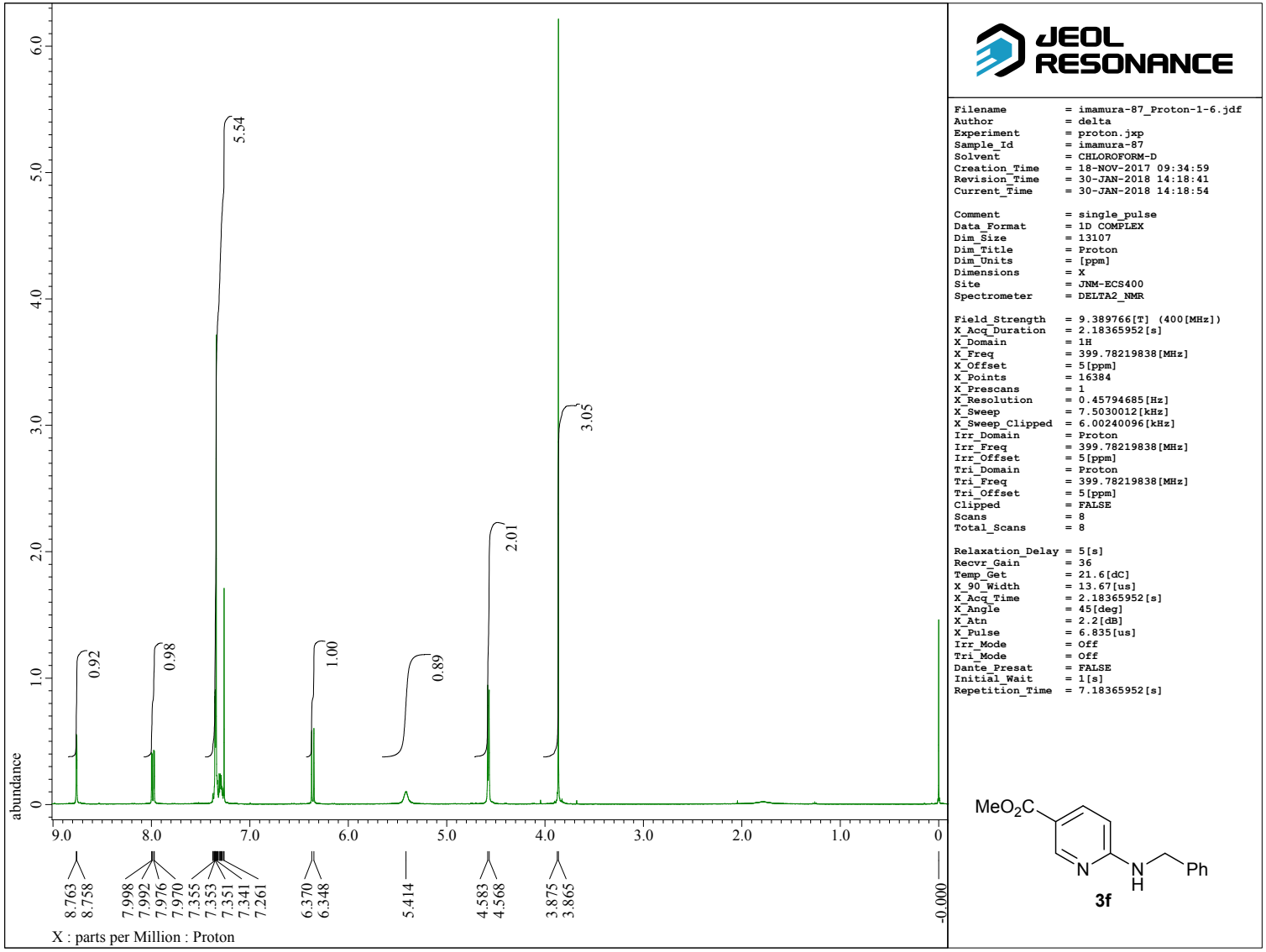


JEOL RESONANCE

```
Filename          = M-HH8-12-3-C_Carbon-1-3.jd
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = M-HH8-12-3-C
Solvent           = CHLOROFORM-D
Creation_Time     = 26-FEB-2018 10:06:30
Revision_Time     =  2-MAR-2018 12:03:36
Current_Time      =  2-MAR-2018 12:03:51

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 494
Total_Scans       = 494

Relaxation_Delay = 2[s]
Recvr_Gain        = 58
Temp_Get          = 21.5[dC]
X_90_Width        = 9.36[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 3.3[dB]
X_Pulse           = 3.12[us]
Irr_Atn_Dec       = 20.394[dB]
Irr_Atn_Noe       = 20.394[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```



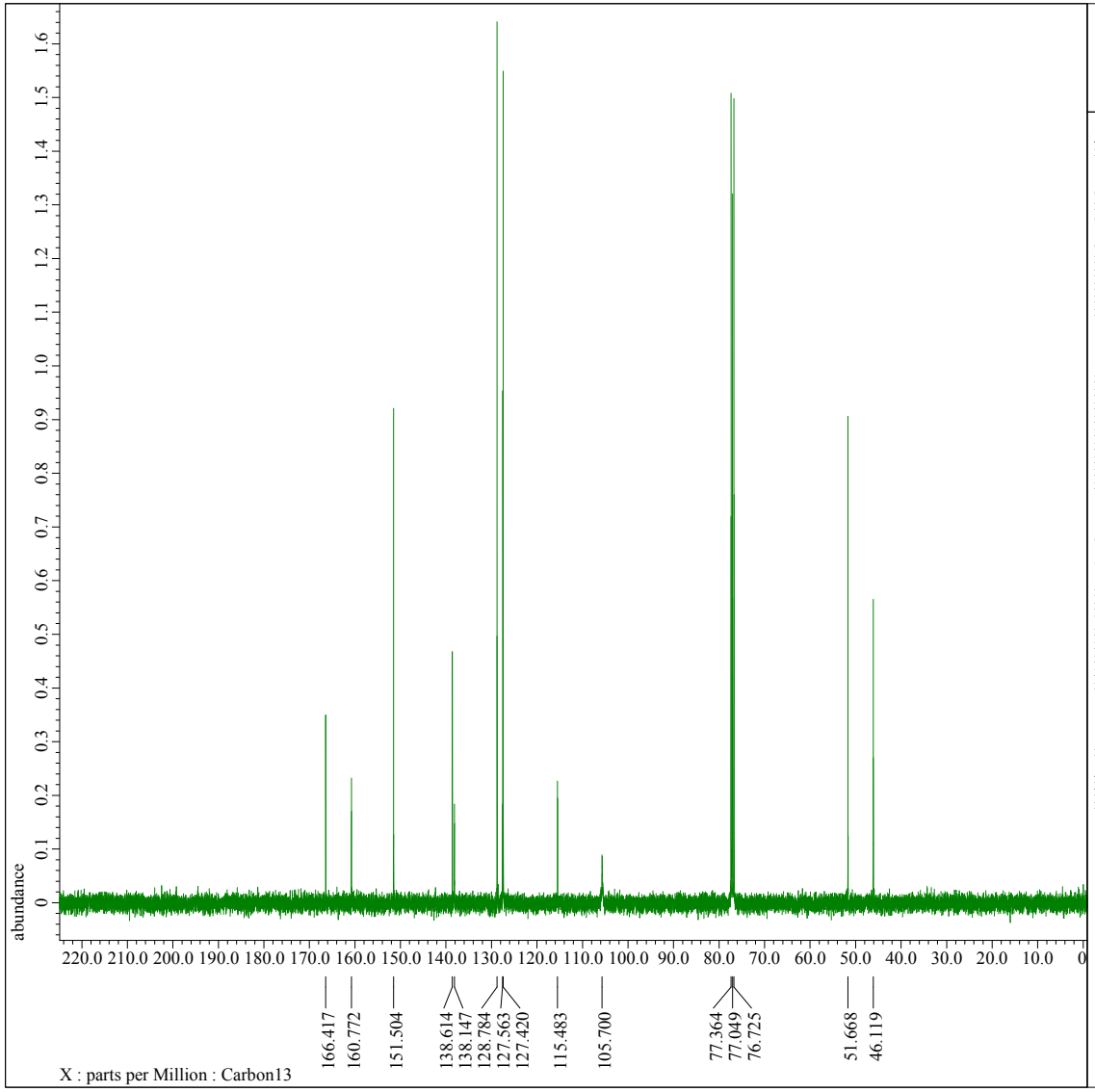
3e



JEOL RESONANCE

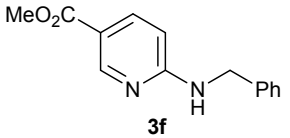
```
Filename          = imamura-87_Proton-1-6.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = imamura-87
Solvent           = CHLOROFORM-D
Creation_Time     = 18-NOV-2017 09:34:59
Revision_Time     = 30-JAN-2018 14:18:41
Current_Time      = 30-JAN-2018 14:18:54

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
X_Sweep_Clipped   = 6.00240096[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay = 5[s]
Recvr_Gain        = 36
Temp_Get          = 21.6[dC]
X_90_Width        = 13.67[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 2.2[dB]
X_Pulse           = 6.835[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.18365952[s]
```


3f

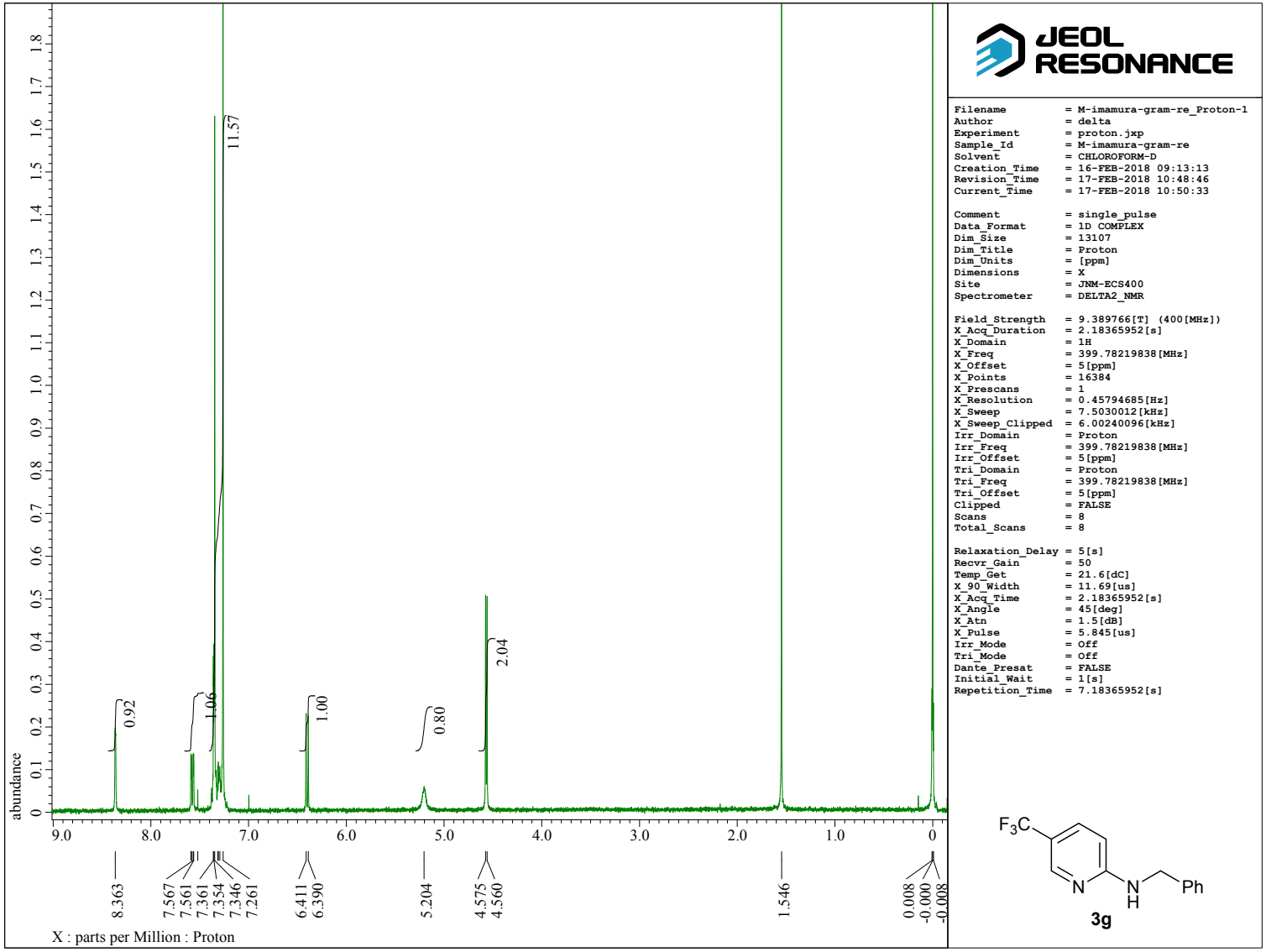


JEOL RESONANCE

```
Filename          = M-imamura-87-C_Carbon-1-3.
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = M-imamura-87-C
Solvent           = CHLOROFORM-D
Creation_Time     = 21-NOV-2017 10:00:15
Revision_Time     = 30-JAN-2018 14:19:34
Current_Time      = 30-JAN-2018 14:20:15

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 256
Total_Scans       = 256

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 21.8[dC]
X_90_Width        = 9.74[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 3.3[dB]
X_Pulse           = 3.24666667[us]
Irr_Atn_Dec       = 20.699[dB]
Irr_Atn_Noe       = 20.699[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```



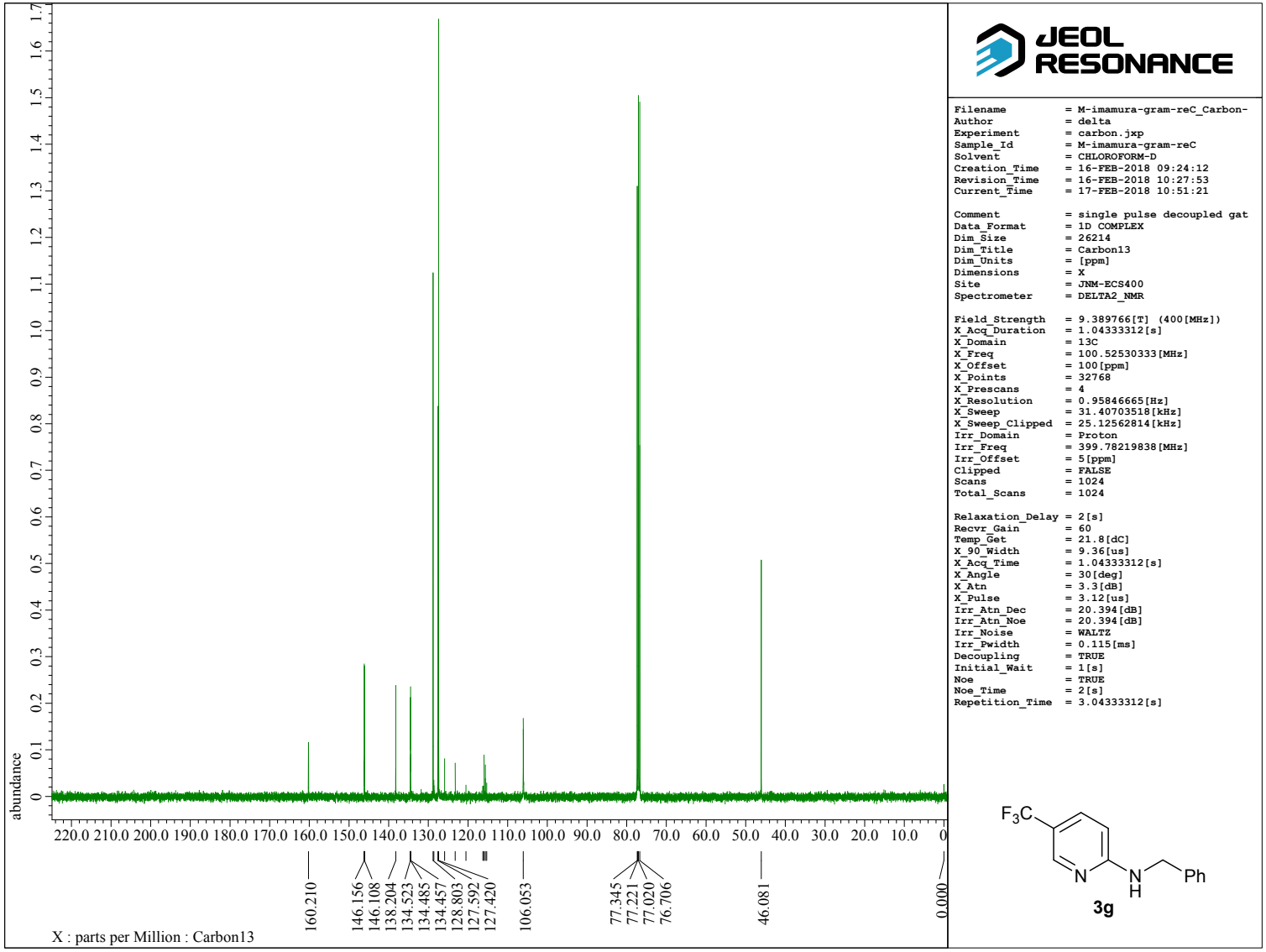
3f



JEOL RESONANCE

Filename	= M-imamura-gram-re_Proton-1
Author	= delta
Experiment	= proton.jxp
Sample_Id	= M-imamura-gram-re
Solvent	= CHLOROFORM-D
Creation_Time	= 16-FEB-2018 09:13:13
Revision_Time	= 17-FEB-2018 10:48:46
Current_Time	= 17-FEB-2018 10:50:33
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.389766[T] (400[MHz])
X_Acq_Duration	= 2.18365952[s]
X_Domain	= 1H
X_Freq	= 399.78219838[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45794685[Hz]
X_Sweep	= 7.5030012[kHz]
X_Sweep_Clipped	= 6.00240096[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.78219838[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 50
Temp_Get	= 21.6[dC]
X_90_Width	= 11.69[us]
X_Acq_Time	= 2.18365952[s]
X_Angle	= 45[deg]
X_Atn	= 1.5[dB]
X_Pulse	= 5.845[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18365952[s]

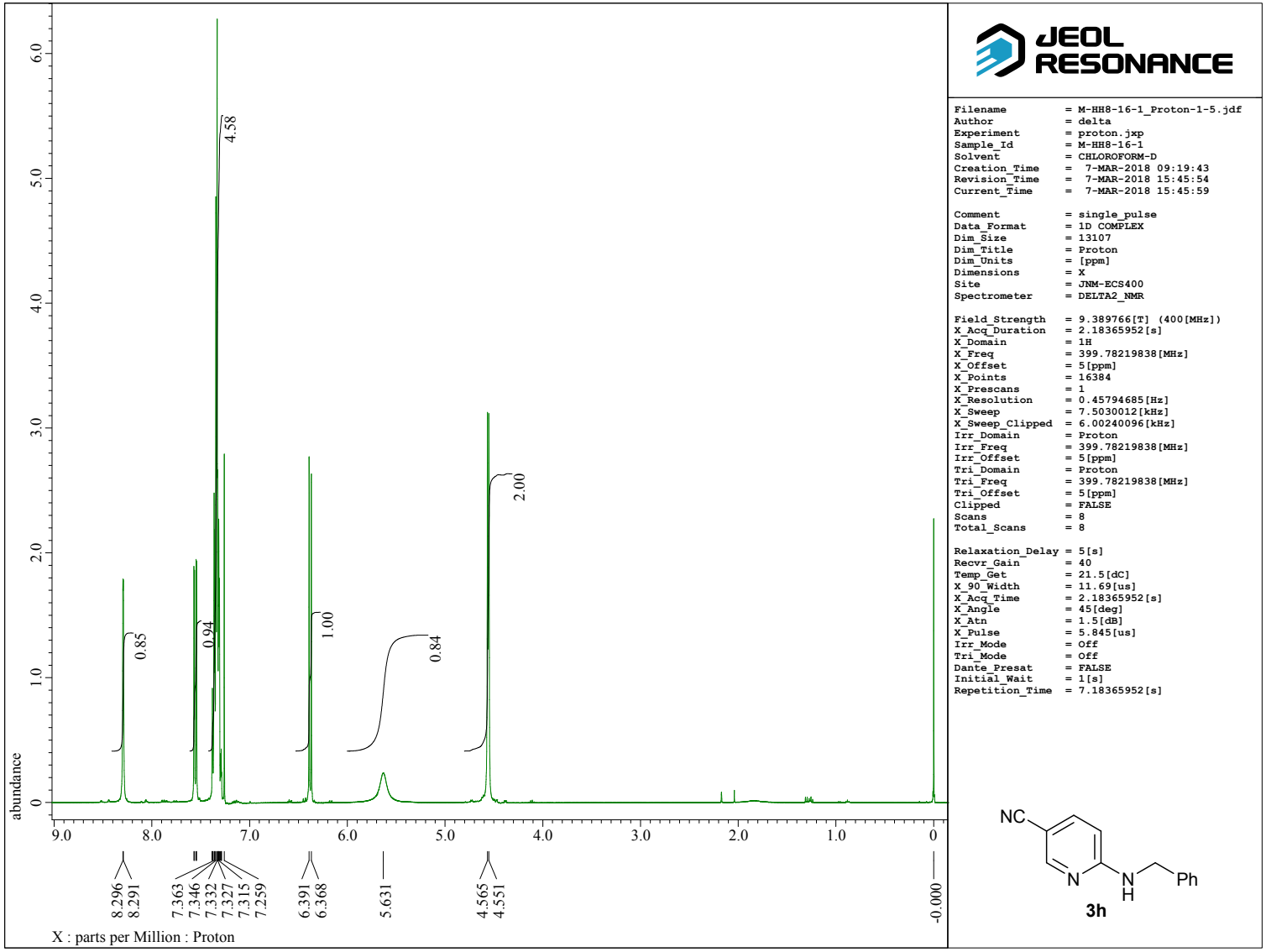
3g



JEOL RESONANCE

```
Filename          = M-imamura-gram-reC_Carbon-
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = M-imamura-gram-reC
Solvent           = CHLOROFORM-D
Creation_Time     = 16-FEB-2018 09:24:12
Revision_Time     = 16-FEB-2018 10:27:53
Current_Time      = 17-FEB-2018 10:51:21

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 1024
Total_Scans       = 1024

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 21.8[dC]
X_90_Width        = 9.36[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 3.3[dB]
X_Pulse           = 3.12[us]
Irr_Atn_Dec       = 20.394[dB]
Irr_Atn_Noe       = 20.394[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```

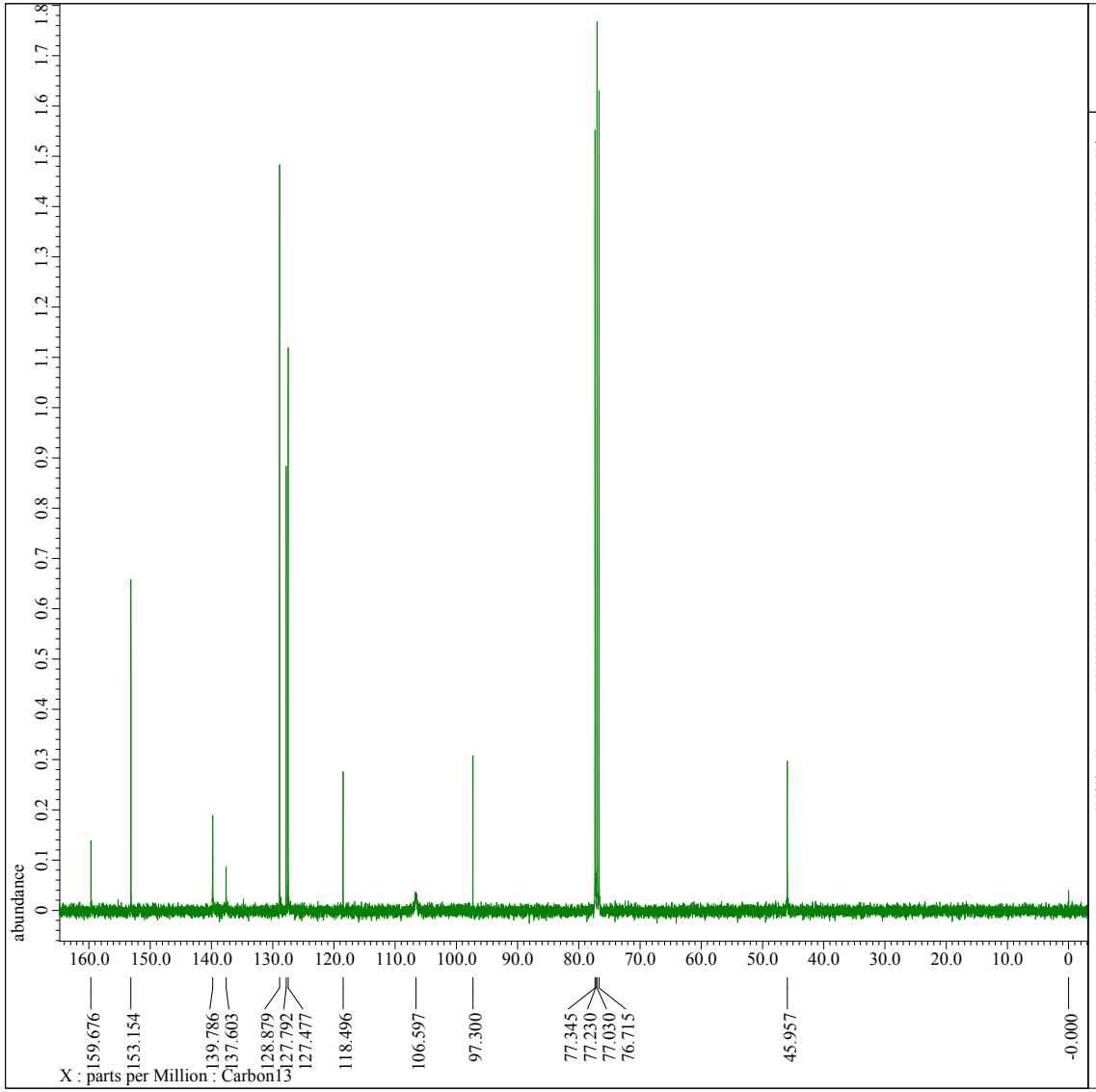

3g



JEOL RESONANCE

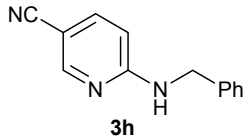
```
Filename          = M-HH8-16-1_Proton-1-5.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = M-HH8-16-1
Solvent           = CHLOROFORM-D
Creation_Time     =  7-MAR-2018 09:19:43
Revision_Time     =  7-MAR-2018 15:45:54
Current_Time      =  7-MAR-2018 15:45:59

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
X_Sweep_Clipped   = 6.00240096[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay = 5[s]
Recvr_Gain        = 40
Temp_Get          = 21.5[dC]
X_90_Width        = 11.69[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 1.5[dB]
X_Pulse           = 5.845[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.18365952[s]
```


3h

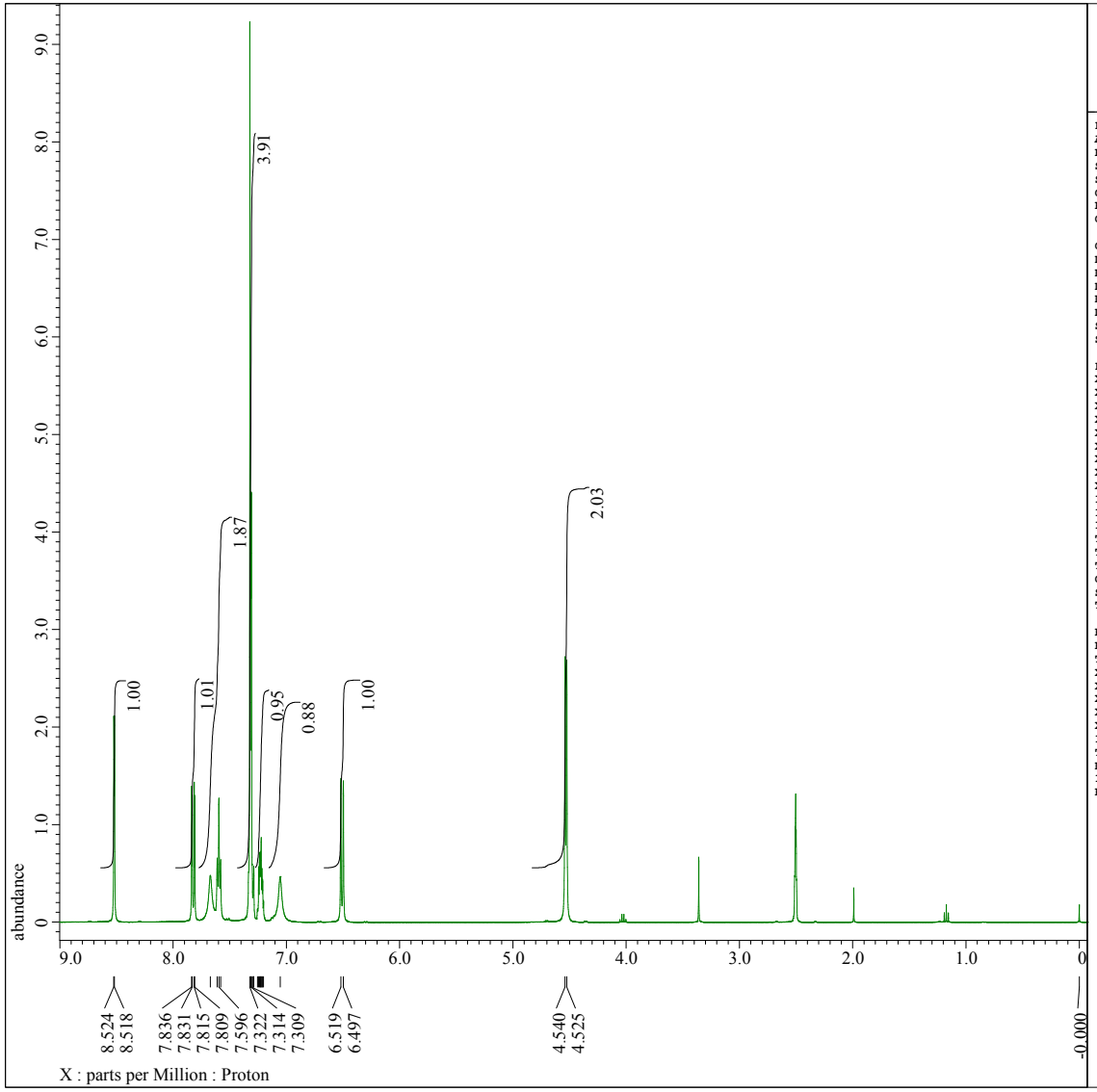


JEOL RESONANCE

```
Filename          = M-HH8-16-1_Carbon-1-6.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = M-HH8-16-1
Solvent           = CHLOROFORM-D
Creation_Time     =  7-MAR-2018 09:23:03
Revision_Time     =  7-MAR-2018 10:06:51
Current_Time      =  7-MAR-2018 15:51:34

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = TRUE
Scans             = 512
Total_Scans       = 512

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 21.7[dC]
X_90_Width        = 9.36[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 3.3[dB]
X_Pulse           = 3.12[us]
Irr_Atn_Dec       = 20.394[dB]
Irr_Atn_Noe       = 20.394[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```

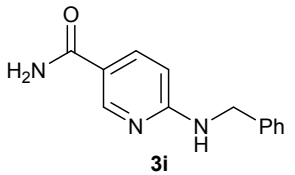


3h

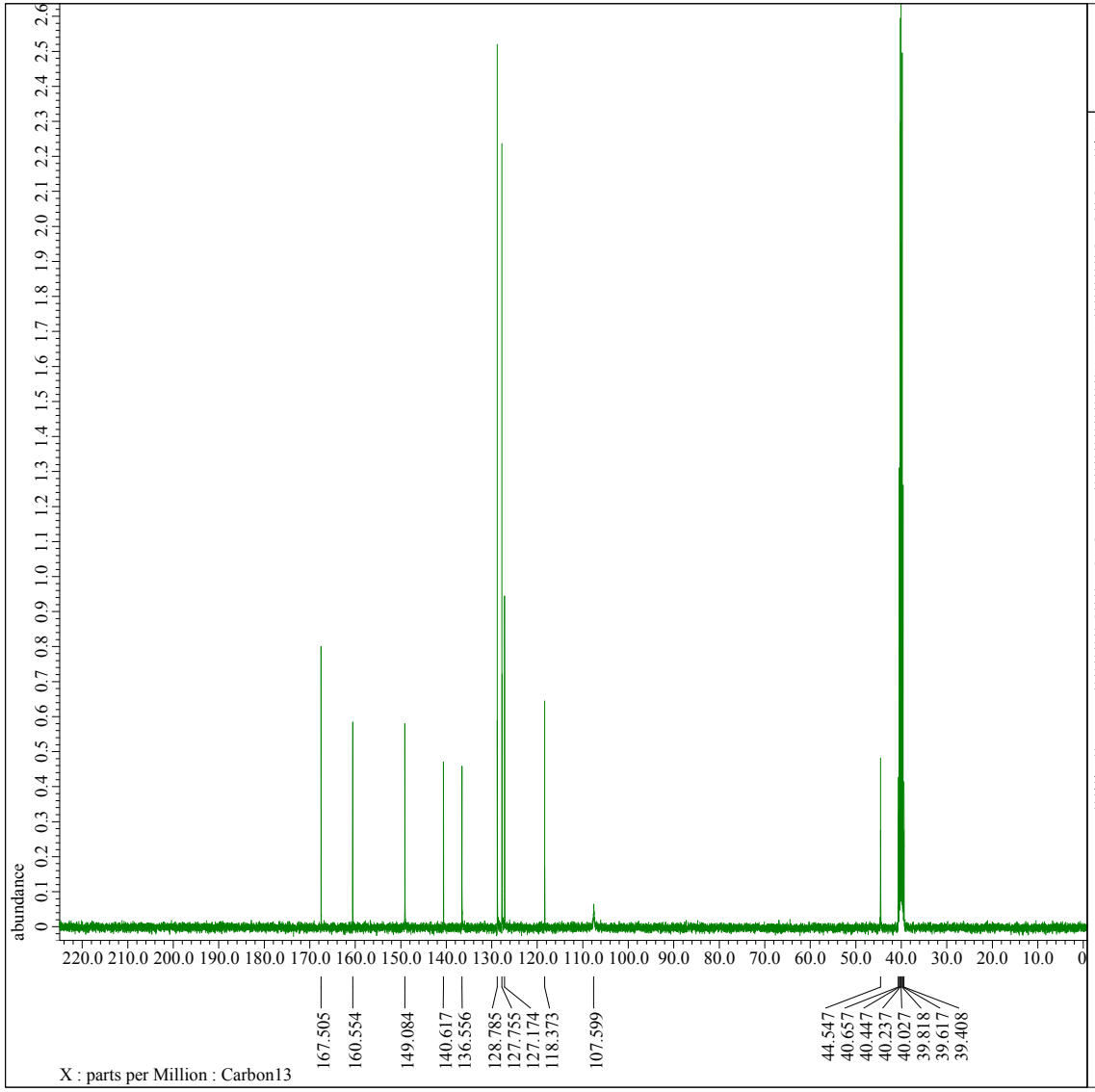


JEOL RESONANCE

```
Filename          = M-HH8-18-2-2_Proton-1-5.jd
Author            = delta
Experiment        = proton.jxp
Sample_Id         = M-HH8-18-2-2
Solvent           = DMSO-D6
Creation_Time     = 16-MAR-2018 09:42:25
Revision_Time     = 22-MAR-2018 13:40:38
Current_Time      = 22-MAR-2018 13:40:52

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
X_Sweep_Clipped   = 6.00240096[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay = 5[s]
Recvr_Gain        = 36
Temp_Get          = 21.5[dC]
X_90_Width        = 11.69[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 1.5[dB]
X_Pulse           = 5.845[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.18365952[s]
```

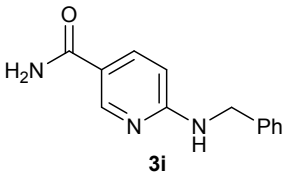


3i

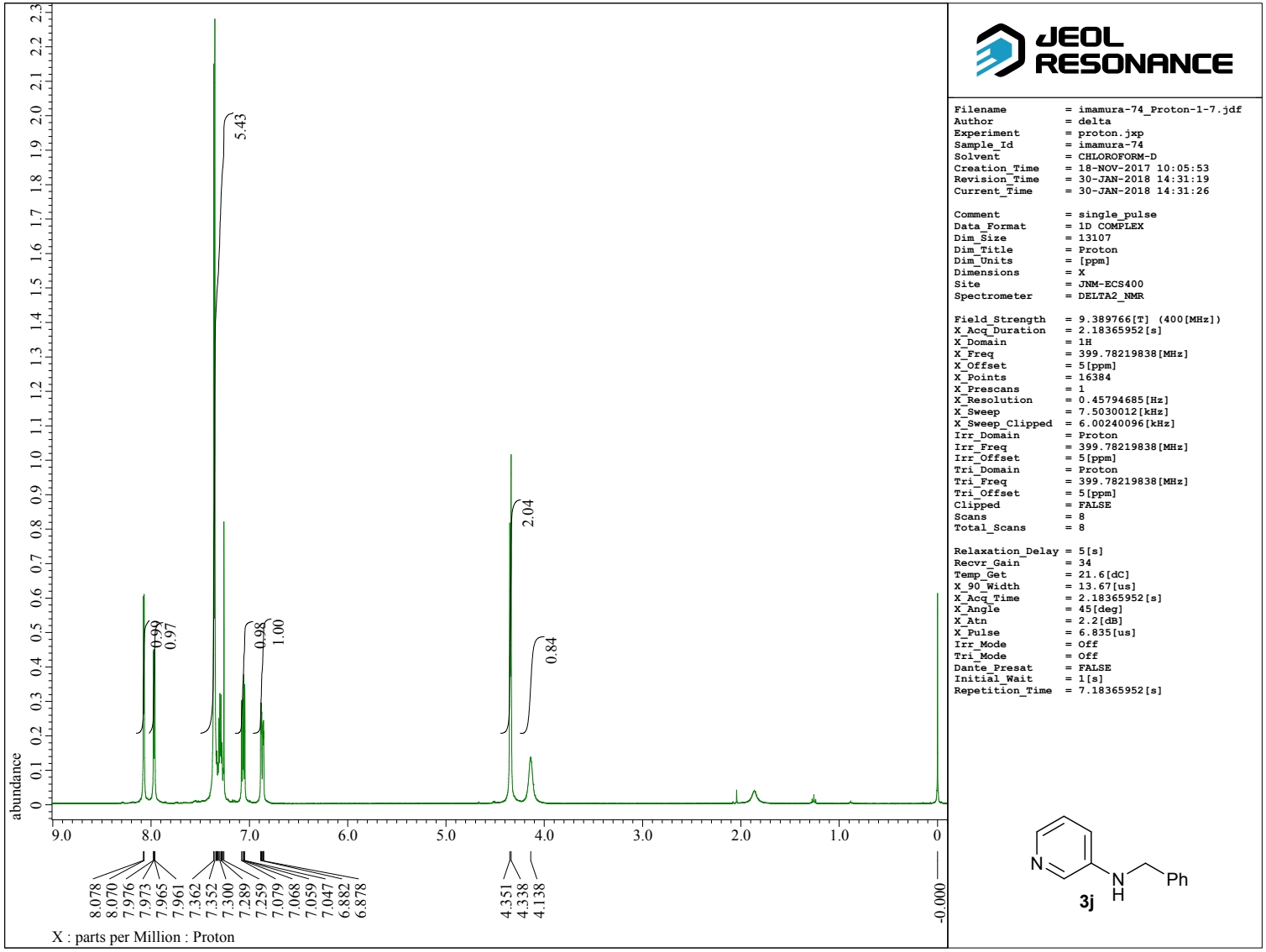


JEOL RESONANCE

```
Filename          = M-HH8-18-2-2_Carbon-1-2.jd
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = M-HH8-18-2-2
Solvent           = DMSO-D6
Creation_Time     = 16-MAR-2018 09:45:53
Revision_Time     = 16-MAR-2018 10:41:00
Current_Time      = 22-MAR-2018 13:45:20

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 512
Total_Scans       = 512

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 21.9[dC]
X_90_Width        = 9.36[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 3.3[dB]
X_Pulse           = 3.12[us]
Irr_Atn_Dec       = 20.394[dB]
Irr_Atn_Noe       = 20.394[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```



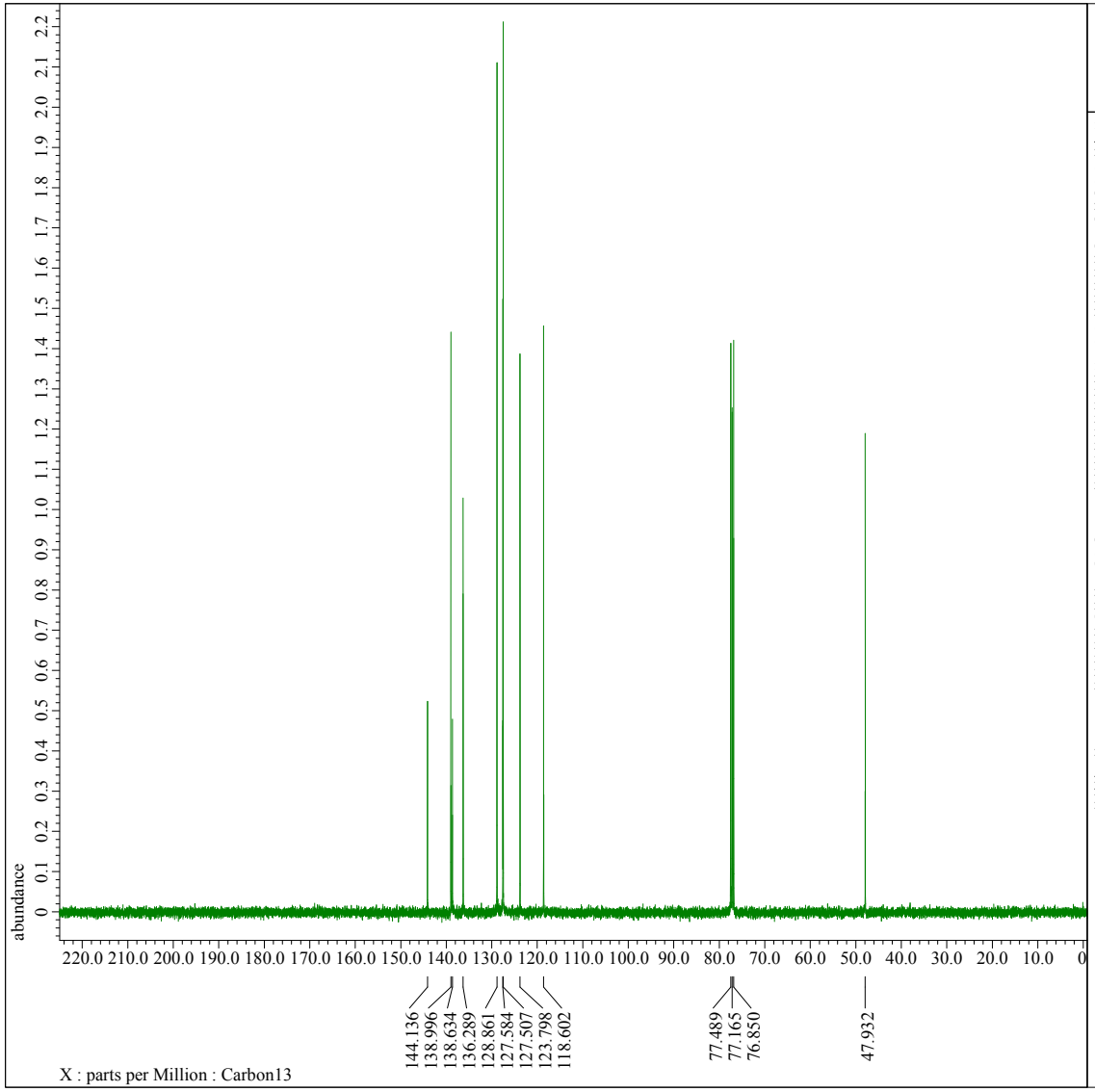
3i



JEOL RESONANCE

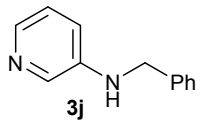
Filename	= imamura-74_Proton-1-7.jdf
Author	= delta
Experiment	= proton.jxp
Sample_Id	= imamura-74
Solvent	= CHLOROFORM-D
Creation_Time	= 18-NOV-2017 10:05:53
Revision_Time	= 30-JAN-2018 14:31:19
Current_Time	= 30-JAN-2018 14:31:26
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.389766[T] (400[MHz])
X_Acq_Duration	= 2.18365952[s]
X_Domain	= 1H
X_Freq	= 399.78219838[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45794685[Hz]
X_Sweep	= 7.5030012[kHz]
X_Sweep_Clipped	= 6.00240096[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.78219838[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 34
Temp_Get	= 21.6[dC]
X_90_Width	= 13.67[us]
X_Acq_Time	= 2.18365952[s]
X_Angle	= 45[deg]
X_Atn	= 2.2[dB]
X_Pulse	= 6.835[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18365952[s]

3j

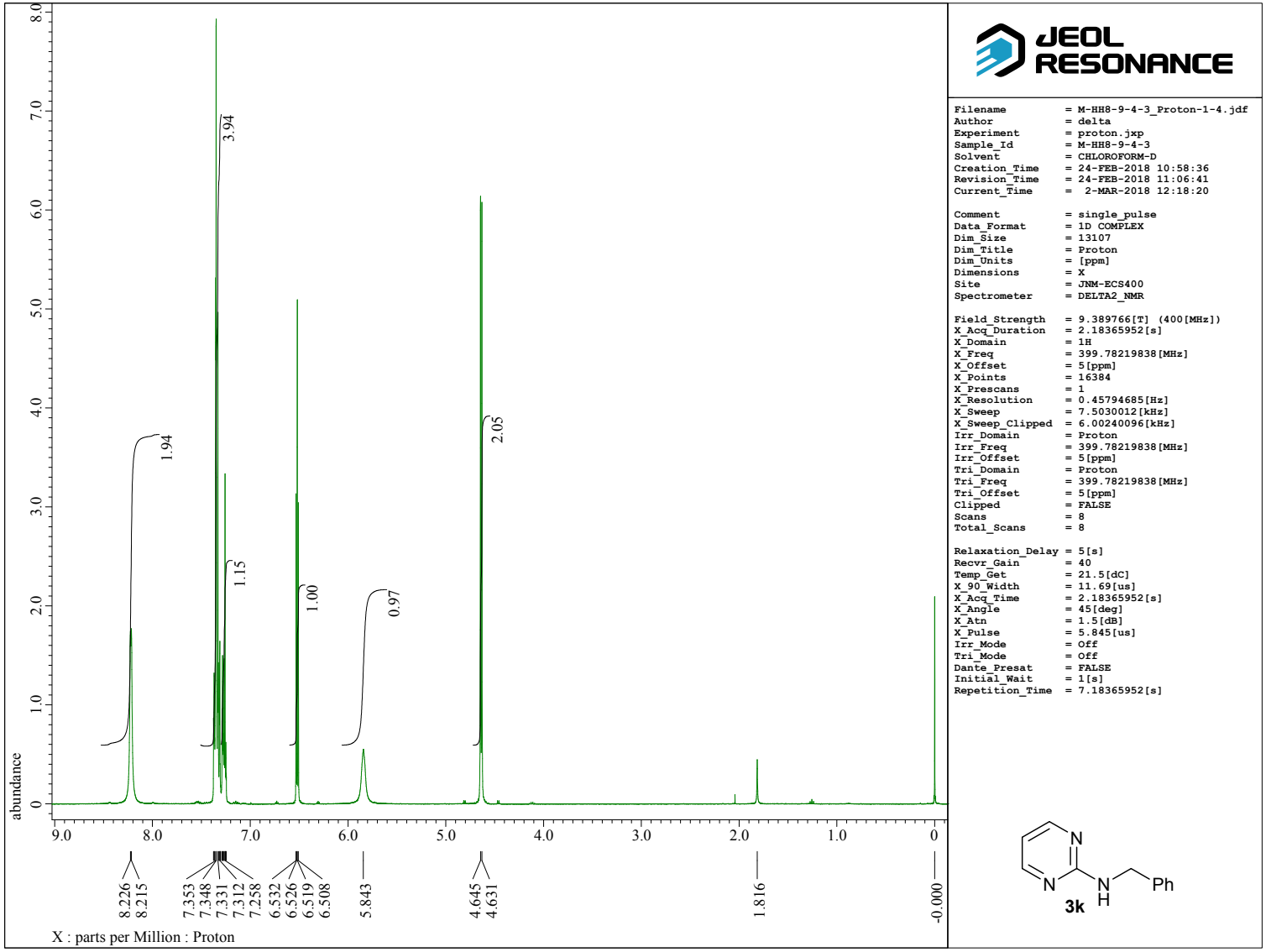


JEOL RESONANCE

```
Filename          = M-imamura-74-C_Carbon-1-2.
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = M-imamura-74-C
Solvent           = CHLOROFORM-D
Creation_Time     = 21-NOV-2017 11:44:27
Revision_Time     = 21-NOV-2017 12:16:58
Current_Time      = 30-JAN-2018 14:32:14

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 512
Total_Scans       = 512

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 21.9[dC]
X_90_Width        = 9.74[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 3.3[dB]
X_Pulse           = 3.24666667[us]
Irr_Atn_Dec       = 20.699[dB]
Irr_Atn_Noe       = 20.699[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```



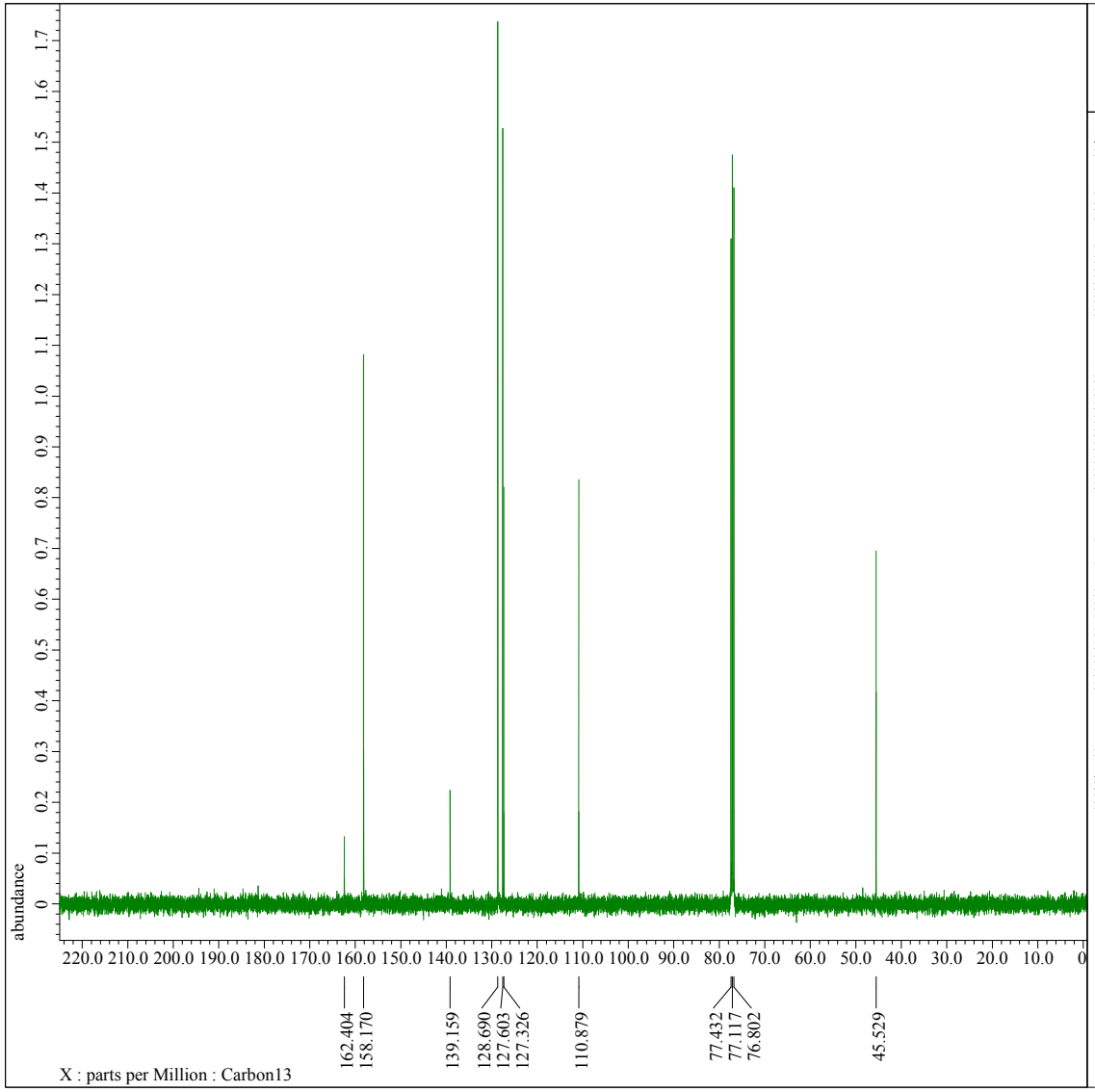
3j



JEOL RESONANCE

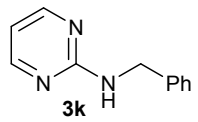
```
Filename          = M-HH8-9-4-3_Proton-1-4.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = M-HH8-9-4-3
Solvent           = CHLOROFORM-D
Creation_Time     = 24-FEB-2018 10:58:36
Revision_Time     = 24-FEB-2018 11:06:41
Current_Time      =  2-MAR-2018 12:18:20

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
X_Sweep_Clipped   = 6.00240096[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay = 5[s]
Recvr_Gain        = 40
Temp_Get          = 21.5[dC]
X_90_Width        = 11.69[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 1.5[dB]
X_Pulse           = 5.845[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.18365952[s]
```


3k

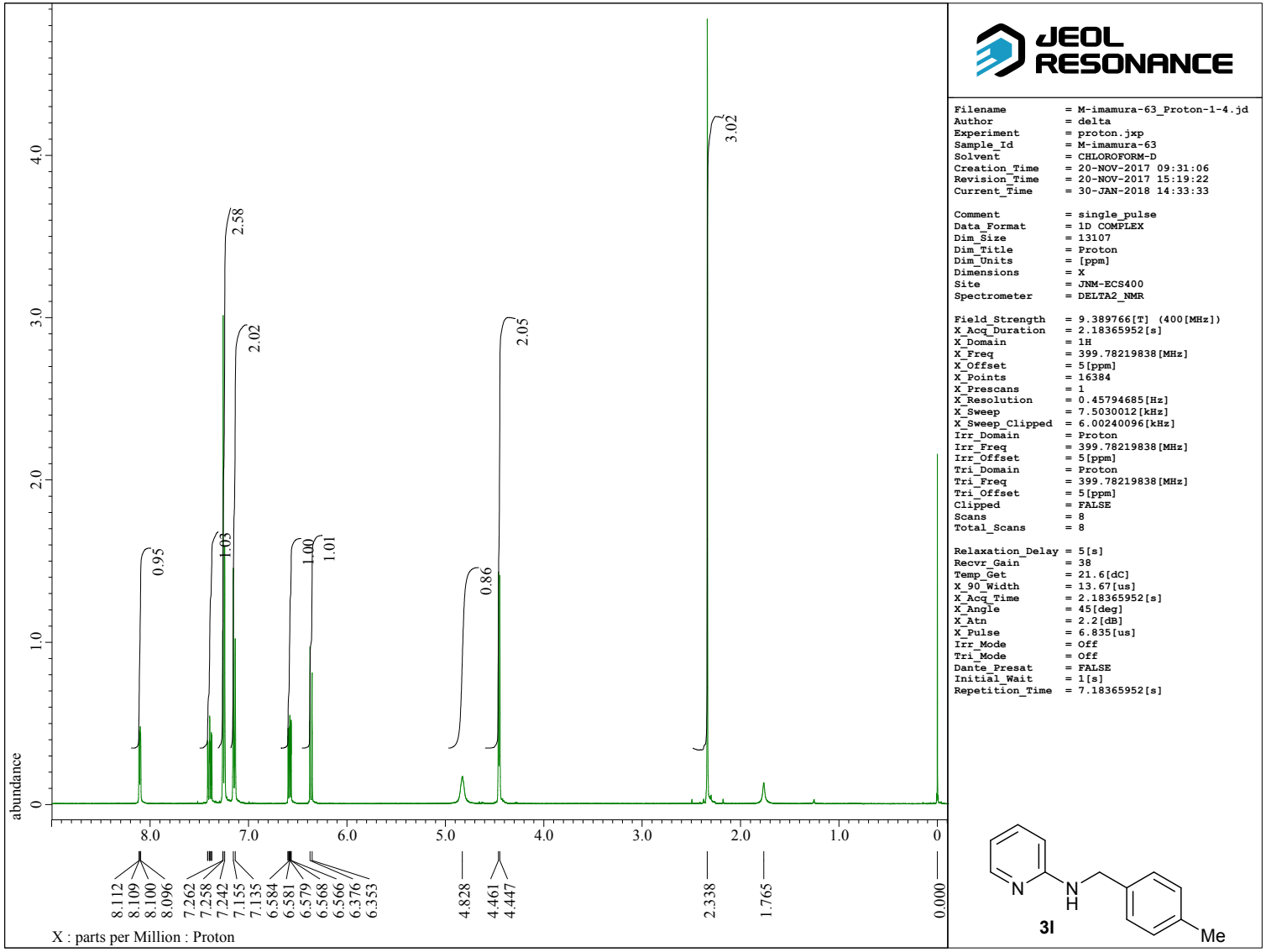


JEOL RESONANCE

```
Filename          = M-HH8-9-4-C_Carbon-1-2.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = M-HH8-9-4-C
Solvent           = CHLOROFORM-D
Creation_Time     = 24-FEB-2018 09:54:10
Revision_Time     = 24-FEB-2018 10:41:16
Current_Time      =  2-MAR-2018 14:13:18

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 279
Total_Scans       = 279

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 21.6[dC]
X_90_Width        = 9.36[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 3.3[dB]
X_Pulse           = 3.12[us]
Irr_Atn_Dec       = 20.394[dB]
Irr_Atn_Noe       = 20.394[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```



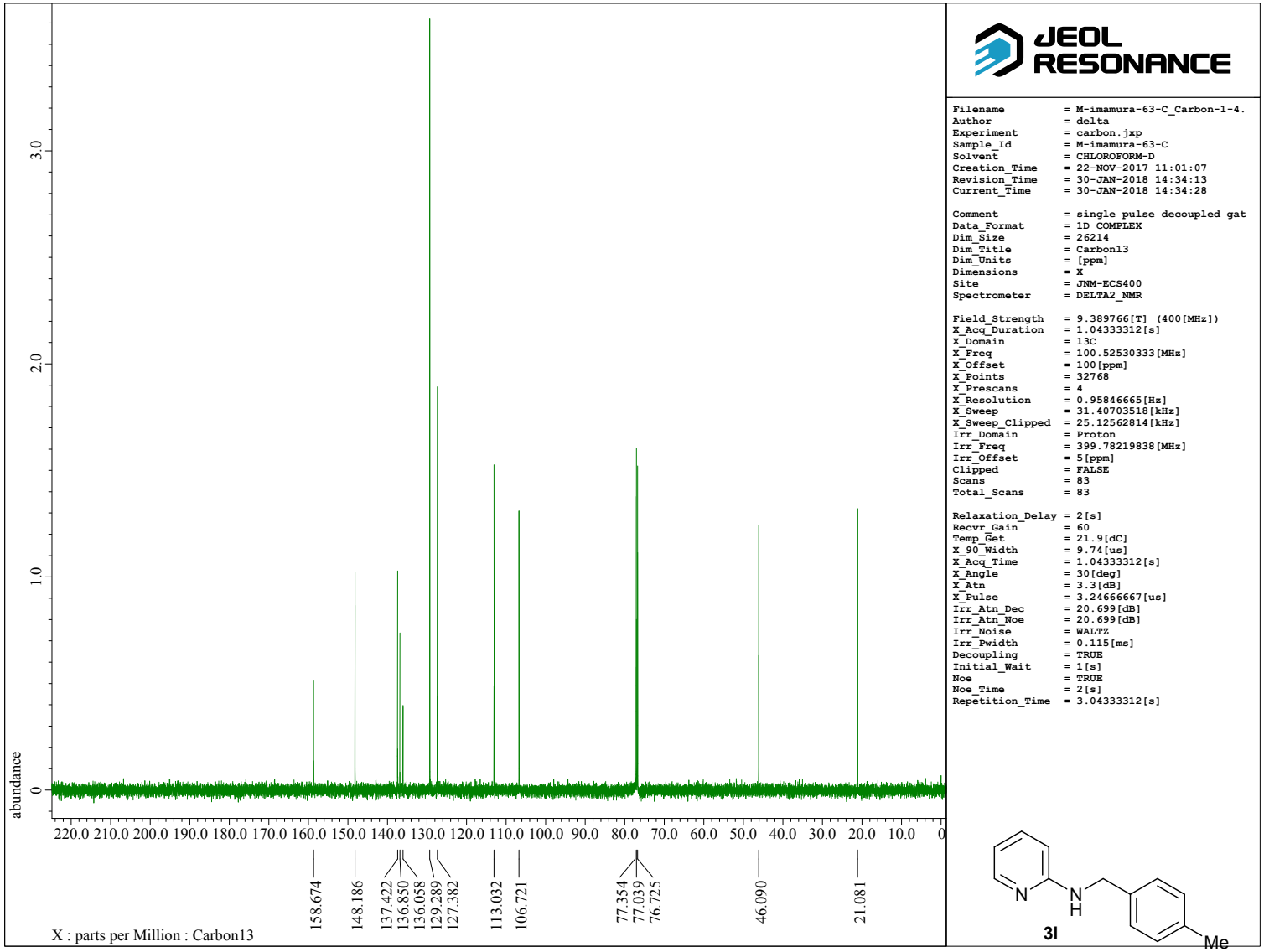
3k



JEOL RESONANCE

```
Filename          = M-imamura-63_Proton-1-4.jd
Author            = delta
Experiment        = proton.jxp
Sample_Id         = M-imamura-63
Solvent           = CHLOROFORM-D
Creation_Time     = 20-NOV-2017 09:31:06
Revision_Time     = 20-NOV-2017 15:19:22
Current_Time      = 30-JAN-2018 14:33:33

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
X_Sweep_Clipped   = 6.00240096[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 38
Temp_Get          = 21.6[dC]
X_90_Width        = 13.67[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 2.2[dB]
X_Pulse           = 6.835[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.18365952[s]
```

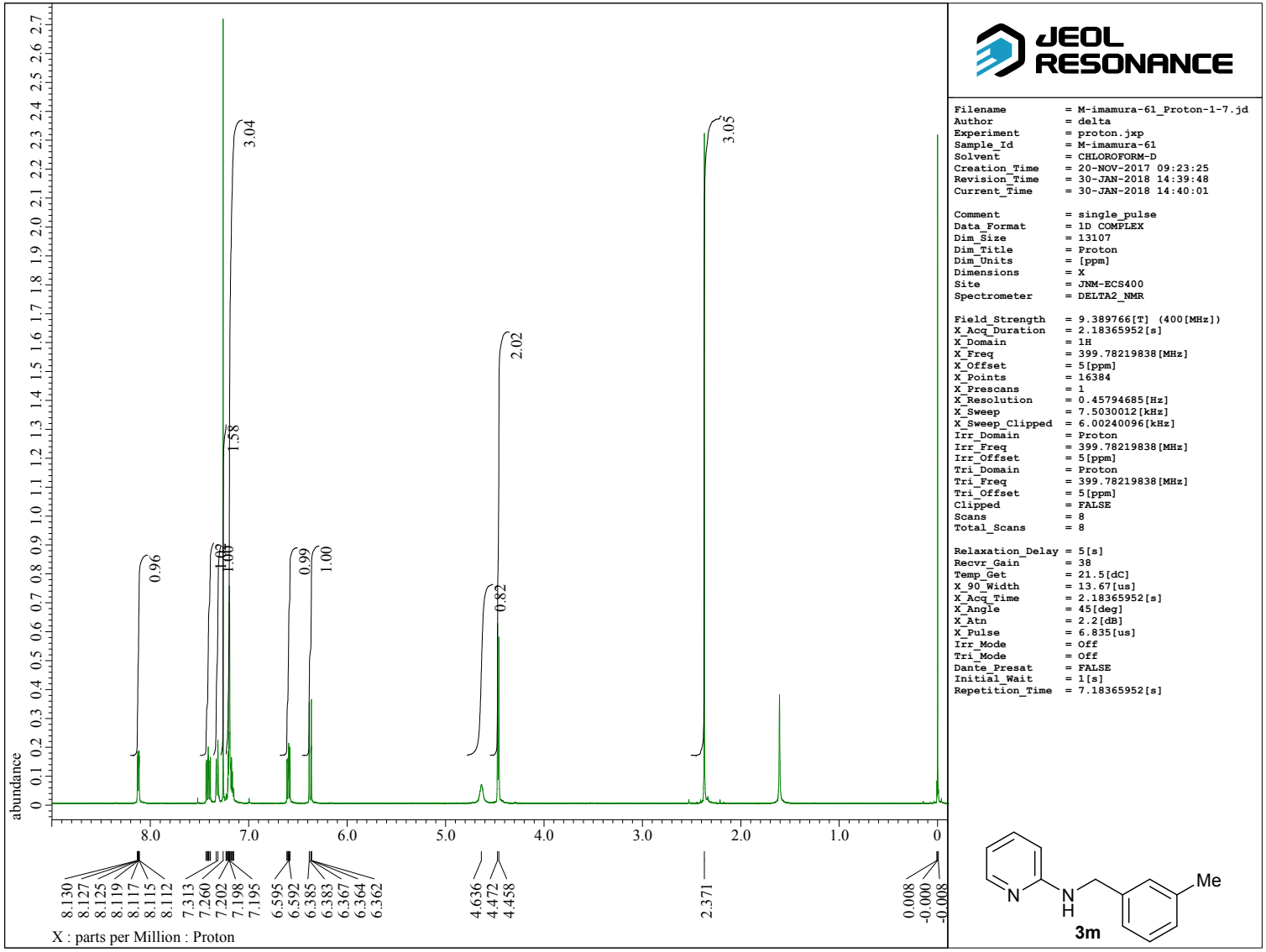

3l



JEOL RESONANCE

```
Filename          = M-imamura-63-C_Carbon-1-4.
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = M-imamura-63-C
Solvent           = CHLOROFORM-D
Creation_Time     = 22-NOV-2017 11:01:07
Revision_Time     = 30-JAN-2018 14:34:13
Current_Time      = 30-JAN-2018 14:34:28

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 83
Total_Scans       = 83

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 21.9[dC]
X_90_Width        = 9.74[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 3.3[dB]
X_Pulse           = 3.24666667[us]
Irr_Atn_Dec       = 20.699[dB]
Irr_Atn_Noe       = 20.699[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```

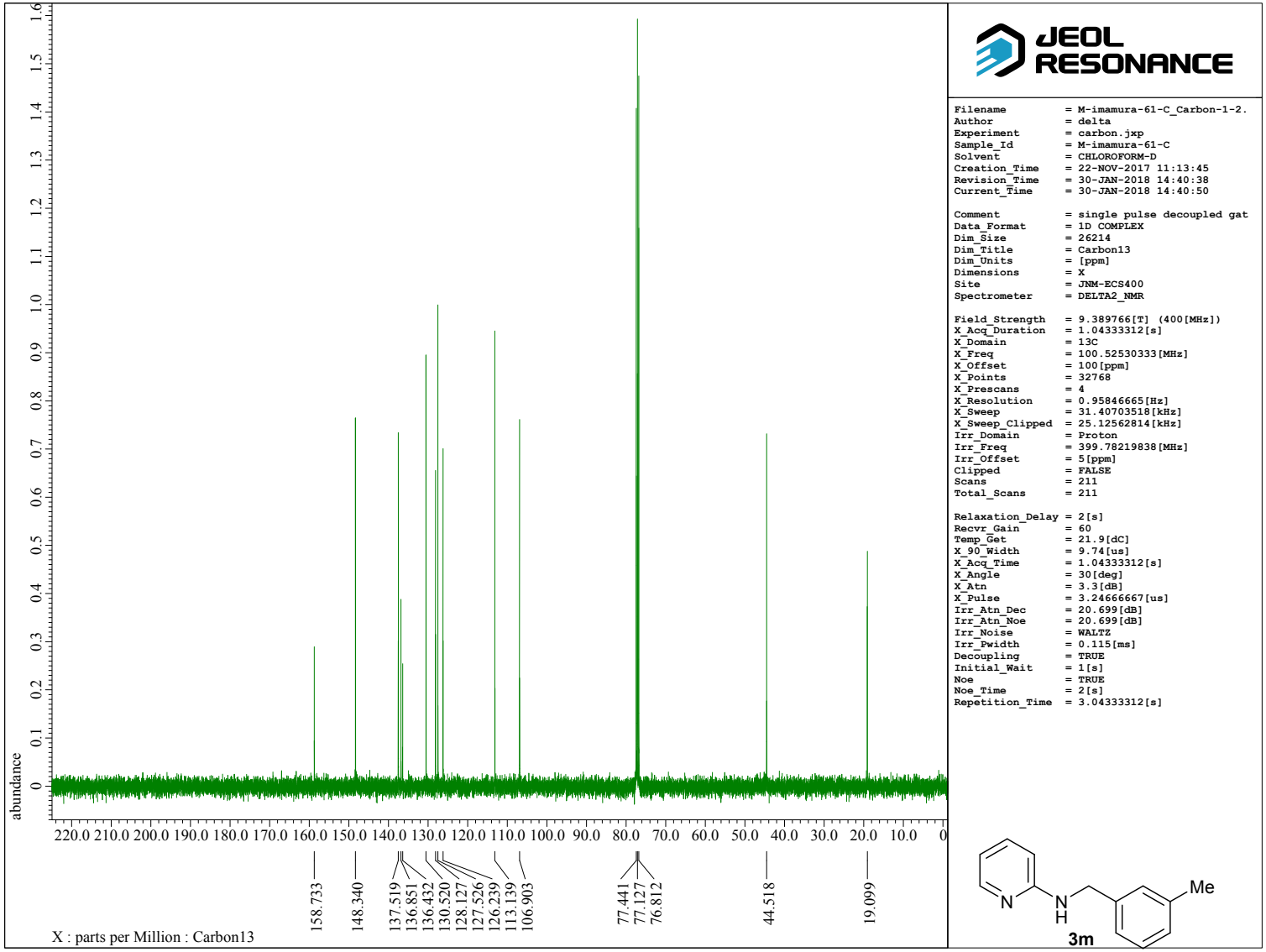

3l



JEOL RESONANCE

Filename	= M-imamura-61_Proton-1-7.jd
Author	= delta
Experiment	= proton.jxp
Sample_Id	= M-imamura-61
Solvent	= CHLOROFORM-D
Creation_Time	= 20-NOV-2017 09:23:25
Revision_Time	= 30-JAN-2018 14:39:48
Current_Time	= 30-JAN-2018 14:40:01
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.389766[T] (400[MHz])
X_Acq_Duration	= 2.18365952[s]
X_Domain	= 1H
X_Freq	= 399.78219838[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45794685[Hz]
X_Sweep	= 7.5030012[kHz]
X_Sweep_Clipped	= 6.00240096[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.78219838[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 38
Temp_Get	= 21.5[dC]
X_90_Width	= 13.67[us]
X_Acq_Time	= 2.18365952[s]
X_Angle	= 45[deg]
X_Atn	= 2.2[dB]
X_Pulse	= 6.835[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18365952[s]

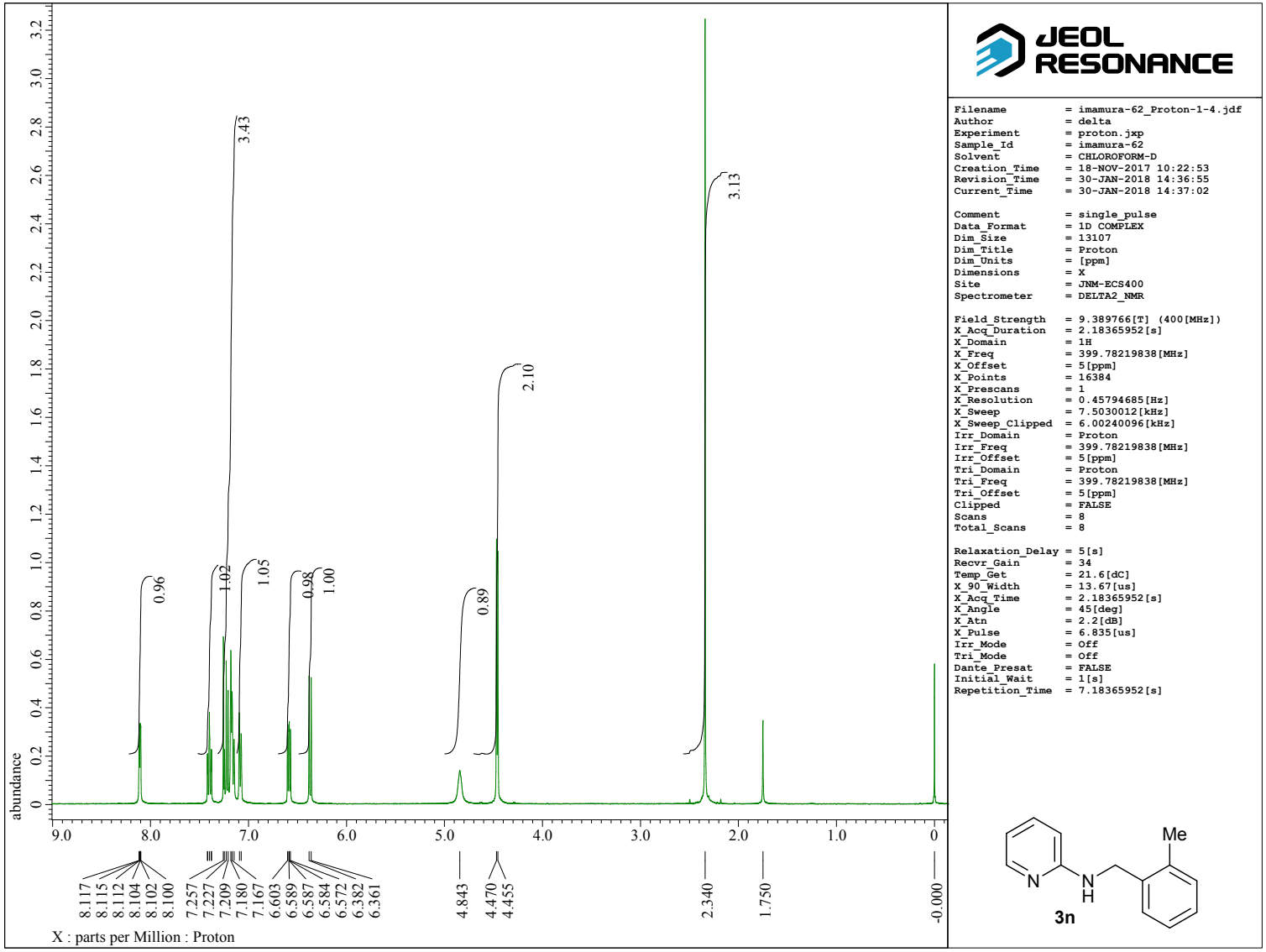
3m



JEOL RESONANCE

```
Filename          = M-imamura-61-C_Carbon-1-2.
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = M-imamura-61-C
Solvent           = CHLOROFORM-D
Creation_Time     = 22-NOV-2017 11:13:45
Revision_Time     = 30-JAN-2018 14:40:38
Current_Time      = 30-JAN-2018 14:40:50

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 211
Total_Scans       = 211

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 21.9[dC]
X_90_Width        = 9.74[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 3.3[dB]
X_Pulse           = 3.24666667[us]
Irr_Atn_Dec       = 20.699[dB]
Irr_Atn_Noe       = 20.699[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```

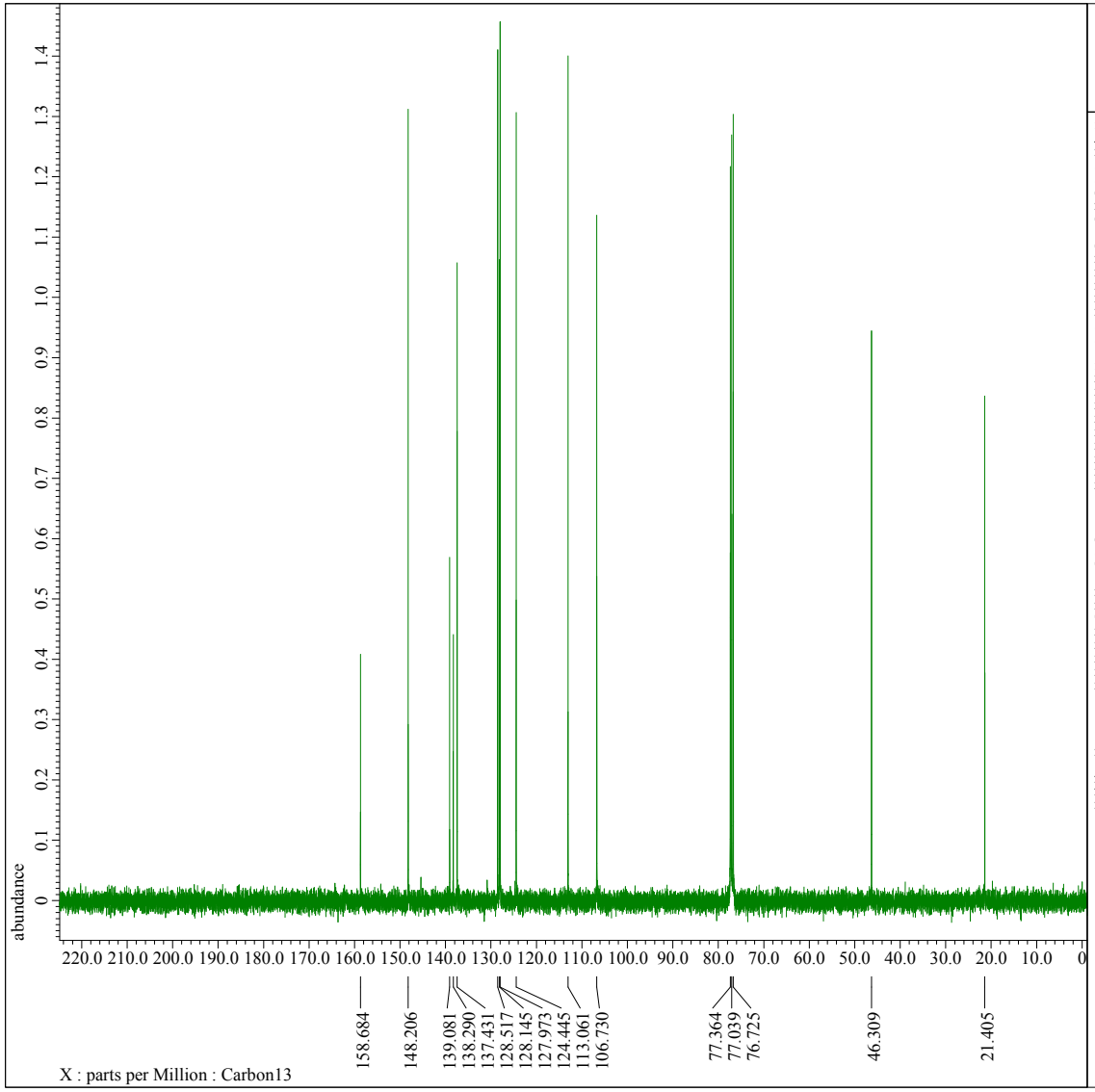

3m



JEOL RESONANCE

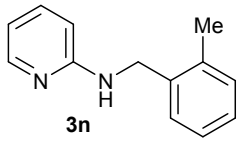
```
Filename          = imamura-62_Proton-1-4.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = imamura-62
Solvent           = CHLOROFORM-D
Creation_Time     = 18-NOV-2017 10:22:53
Revision_Time     = 30-JAN-2018 14:36:55
Current_Time      = 30-JAN-2018 14:37:02

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
X_Sweep_Clipped   = 6.00240096[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay = 5[s]
Recvr_Gain        = 34
Temp_Get          = 21.6[dC]
X_90_Width        = 13.67[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 2.2[dB]
X_Pulse           = 6.835[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.18365952[s]
```


3n

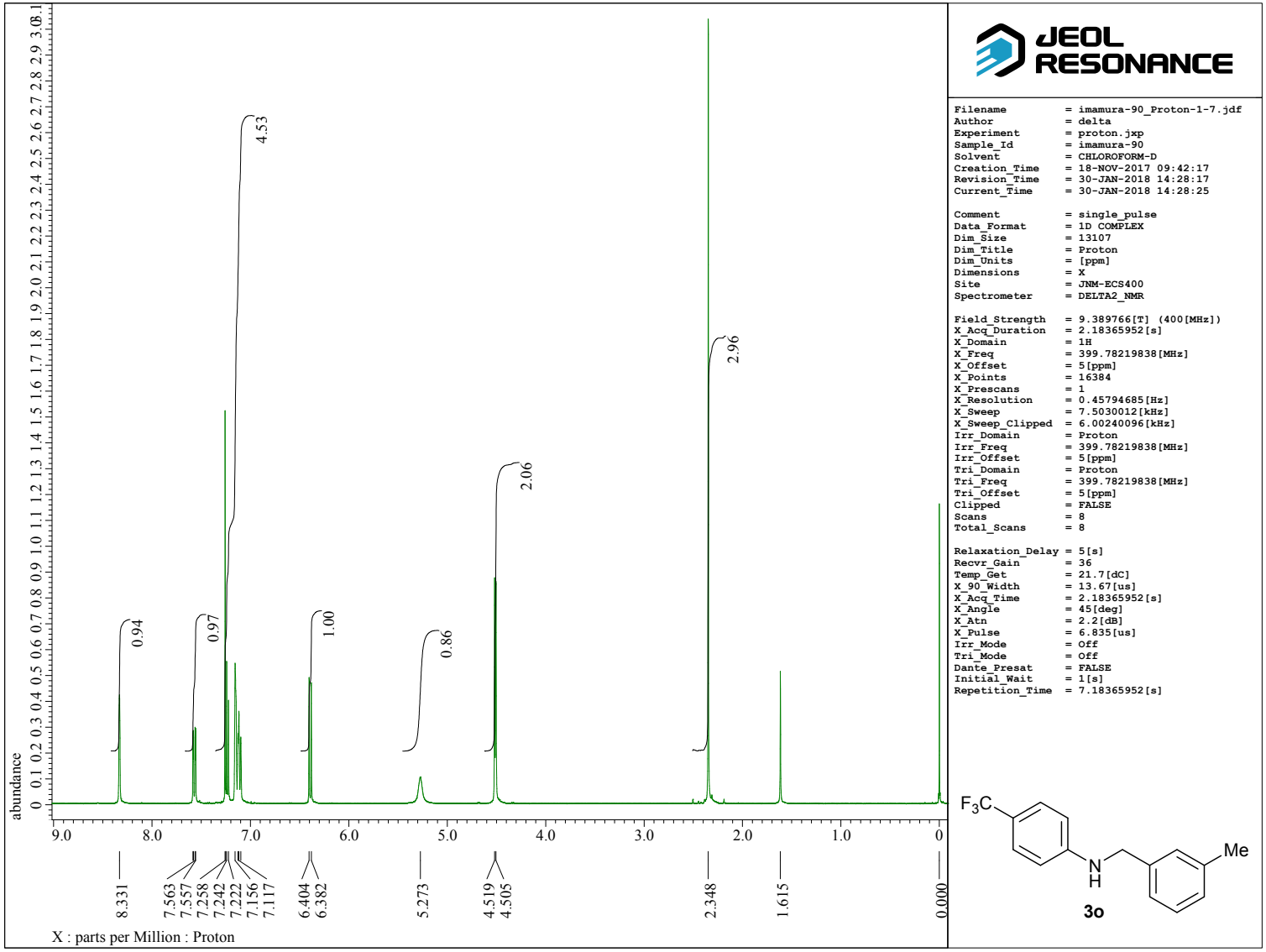


JEOL RESONANCE

```
Filename          = M-imamura-62-C_Carbon-1-3.
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = M-imamura-62-C
Solvent           = CHLOROFORM-D
Creation_Time     = 22-NOV-2017 10:40:10
Revision_Time     = 30-JAN-2018 14:37:48
Current_Time      = 30-JAN-2018 14:38:02

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 256
Total_Scans       = 256

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 21.9[dC]
X_90_Width        = 9.74[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 3.3[dB]
X_Pulse           = 3.24666667[us]
Irr_Atn_Dec       = 20.699[dB]
Irr_Atn_Noe       = 20.699[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```



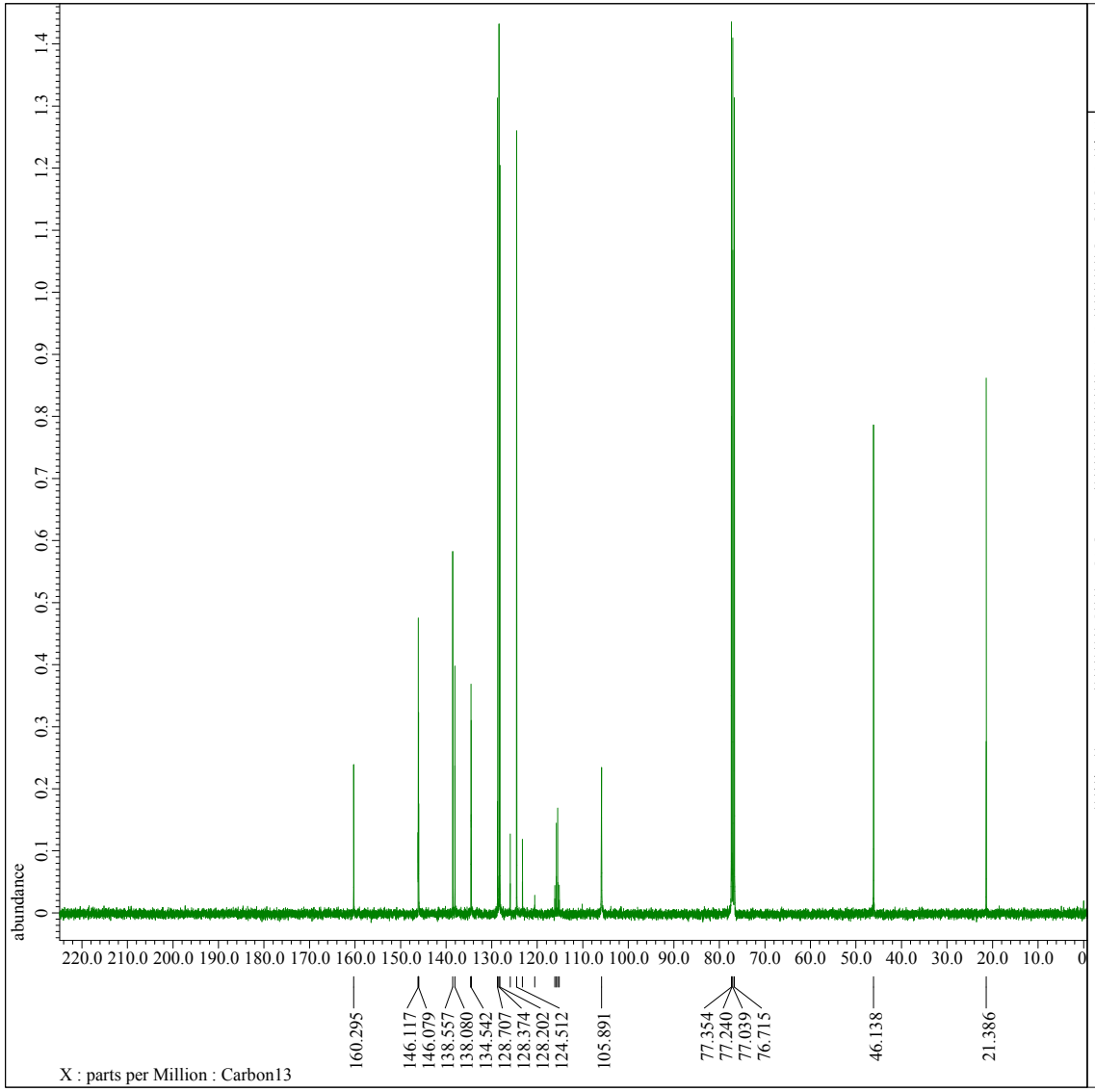
3n



JEOL RESONANCE

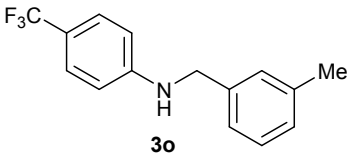
```
Filename          = imamura-90_Proton-1-7.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = imamura-90
Solvent           = CHLOROFORM-D
Creation_Time     = 18-NOV-2017 09:42:17
Revision_Time     = 30-JAN-2018 14:28:17
Current_Time      = 30-JAN-2018 14:28:25

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
X_Sweep_Clipped   = 6.00240096[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay = 5[s]
Recvr_Gain        = 36
Temp_Get          = 21.7[dC]
X_90_Width        = 13.67[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 2.2[dB]
X_Pulse           = 6.835[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.18365952[s]
```


3o

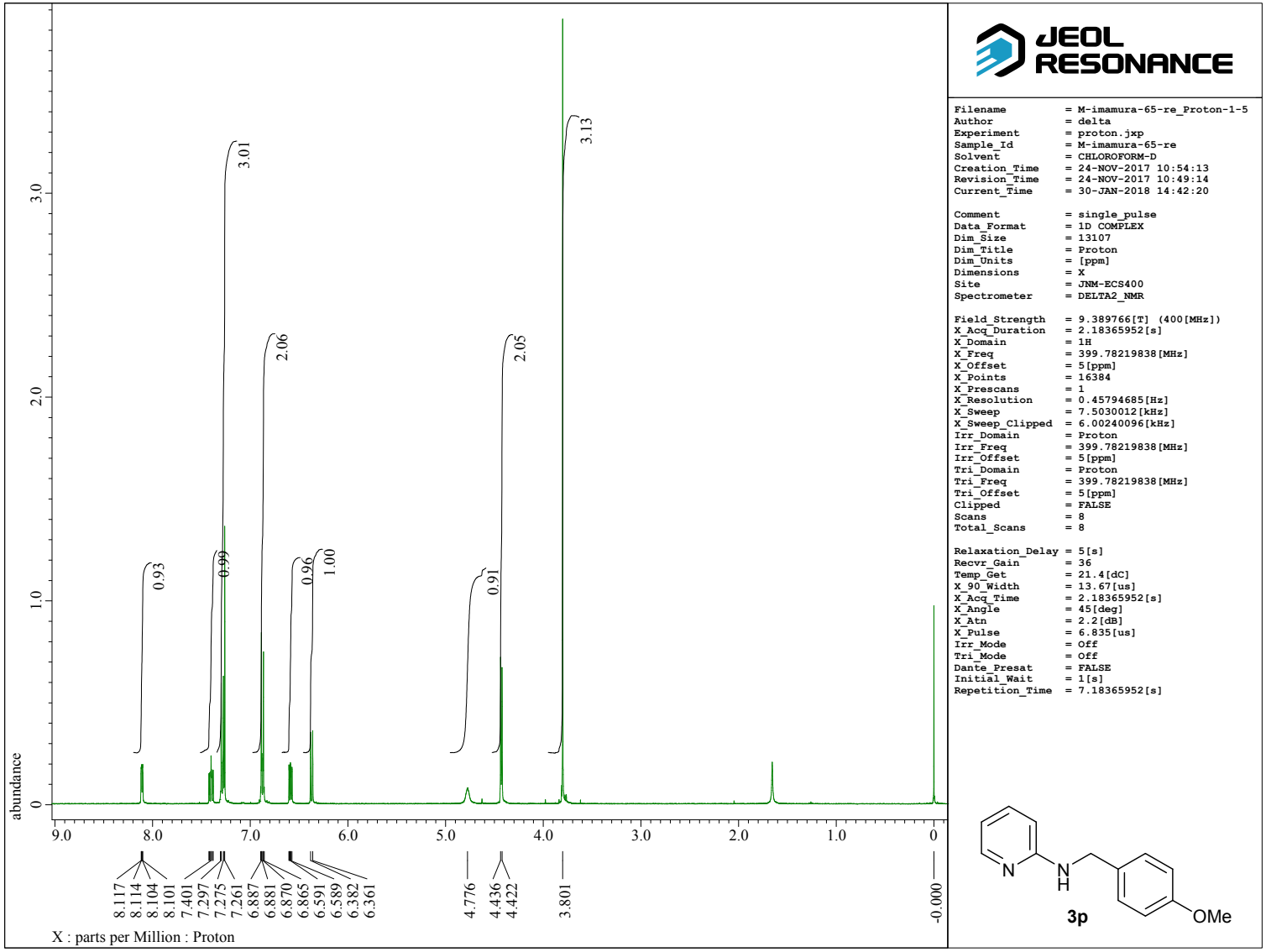


JEOL RESONANCE

```
Filename          = M-imamura-90-C_Carbon-1-6.
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = M-imamura-90-C
Solvent           = CHLOROFORM-D
Creation_Time     = 21-NOV-2017 10:21:13
Revision_Time     = 30-JAN-2018 14:29:08
Current_Time      = 30-JAN-2018 14:29:23

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 1489
Total_Scans       = 1489

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 21.8[dC]
X_90_Width        = 9.74[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 3.3[dB]
X_Pulse           = 3.24666667[us]
Irr_Atn_Dec       = 20.699[dB]
Irr_Atn_Noe       = 20.699[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```



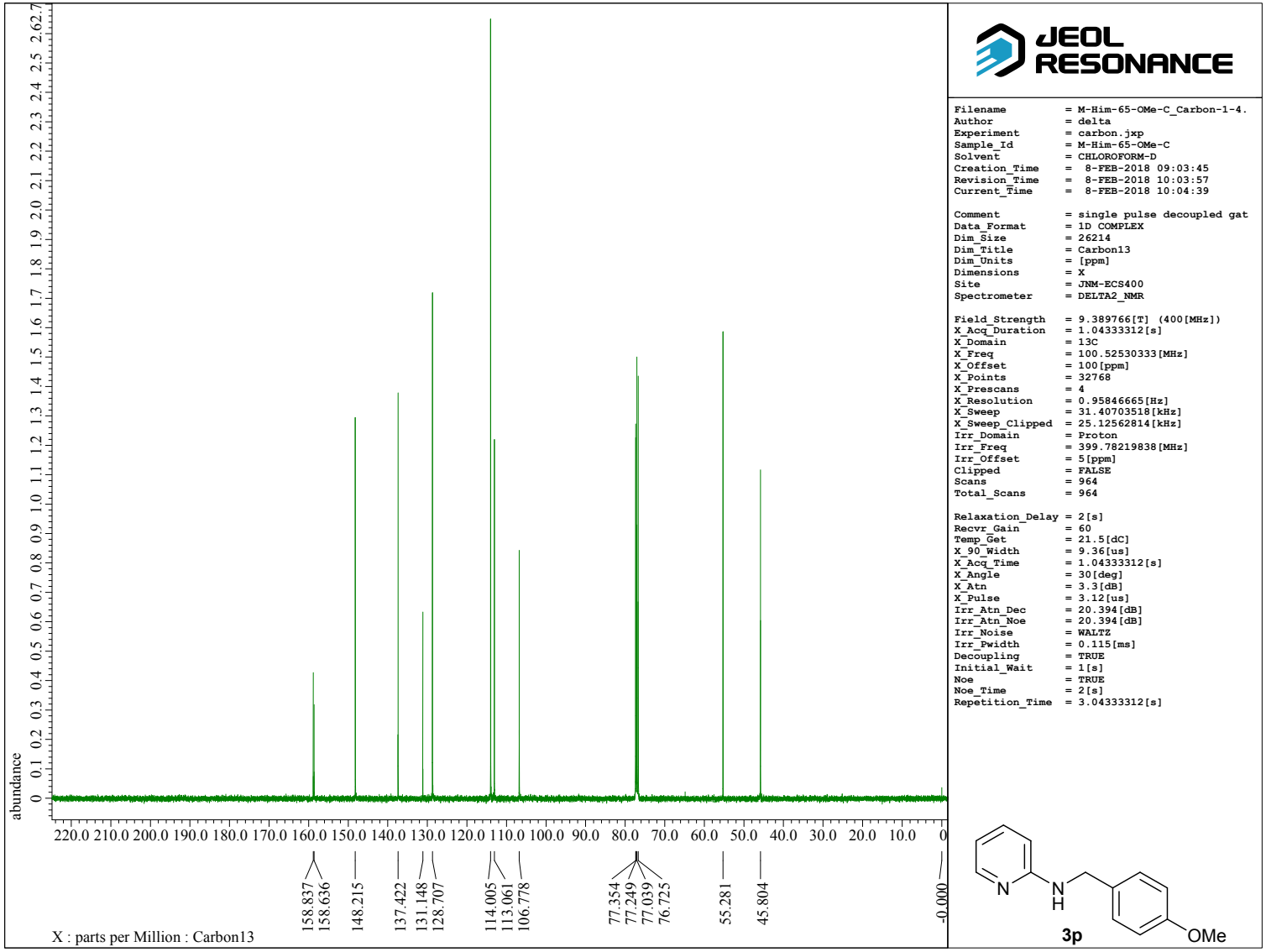
3o



JEOL RESONANCE

Filename	= M-imamura-65-re_Proton-1-5
Author	= delta
Experiment	= proton.jxp
Sample_Id	= M-imamura-65-re
Solvent	= CHLOROFORM-D
Creation_Time	= 24-NOV-2017 10:54:13
Revision_Time	= 24-NOV-2017 10:49:14
Current_Time	= 30-JAN-2018 14:42:20
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.389766[T] (400[MHz])
X_Acq_Duration	= 2.18365952[s]
X_Domain	= 1H
X_Freq	= 399.78219838[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45794685[Hz]
X_Sweep	= 7.5030012[kHz]
X_Sweep_Clipped	= 6.00240096[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.78219838[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 21.4[dC]
X_90_Width	= 13.67[us]
X_Acq_Time	= 2.18365952[s]
X_Angle	= 45[deg]
X_Atn	= 2.2[dB]
X_Pulse	= 6.835[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18365952[s]

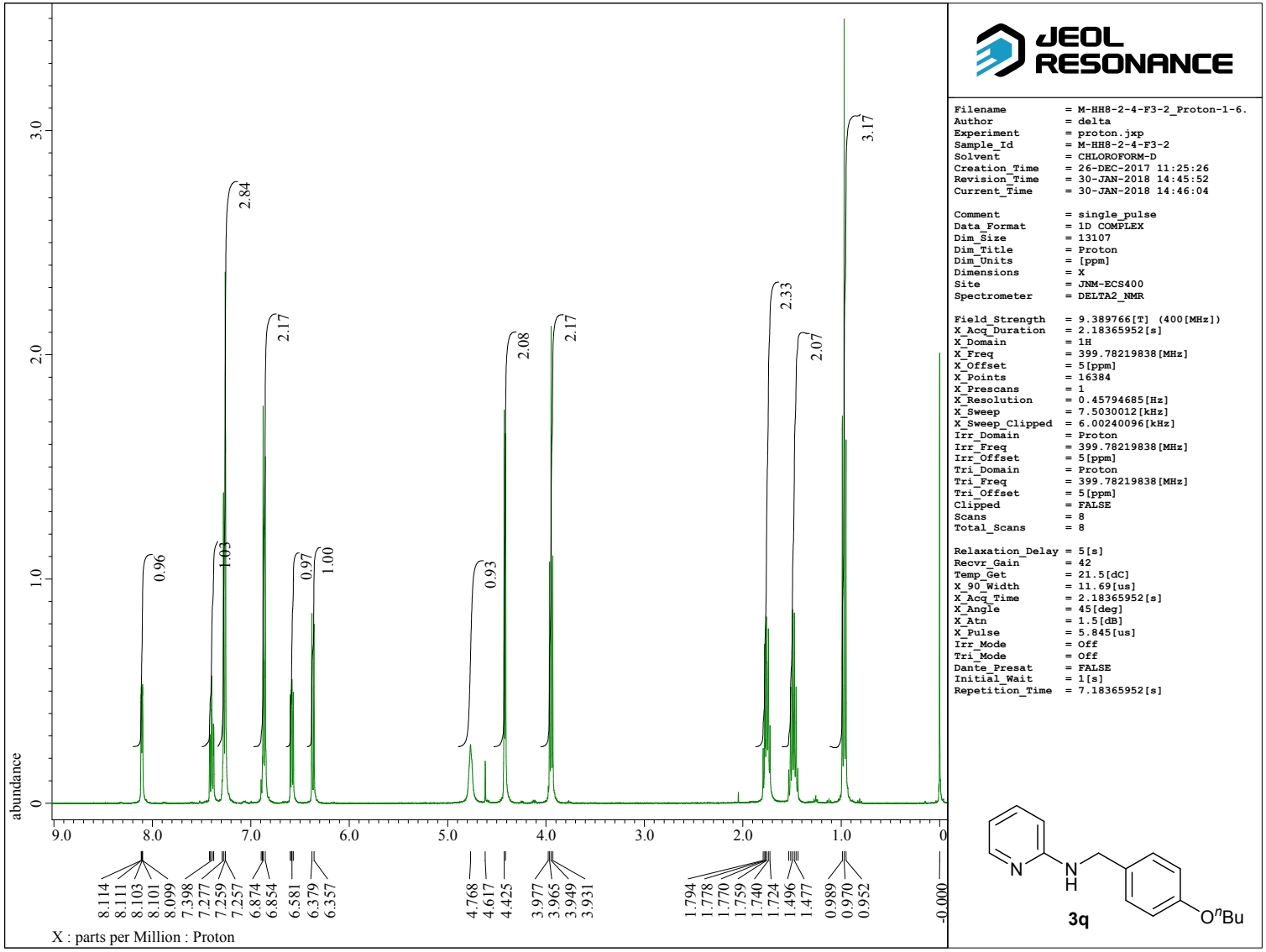
3p



JEOL RESONANCE

```
Filename          = M-Him-65-OMe-C_Carbon-1-4.
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = M-Him-65-OMe-C
Solvent           = CHLOROFORM-D
Creation_Time     =  8-FEB-2018 09:03:45
Revision_Time     =  8-FEB-2018 10:03:57
Current_Time      =  8-FEB-2018 10:04:39

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 964
Total_Scans       = 964

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 21.5[dC]
X_90_Width        = 9.36[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 3.3[dB]
X_Pulse           = 3.12[us]
Irr_Atn_Dec       = 20.394[dB]
Irr_Atn_Noe       = 20.394[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```

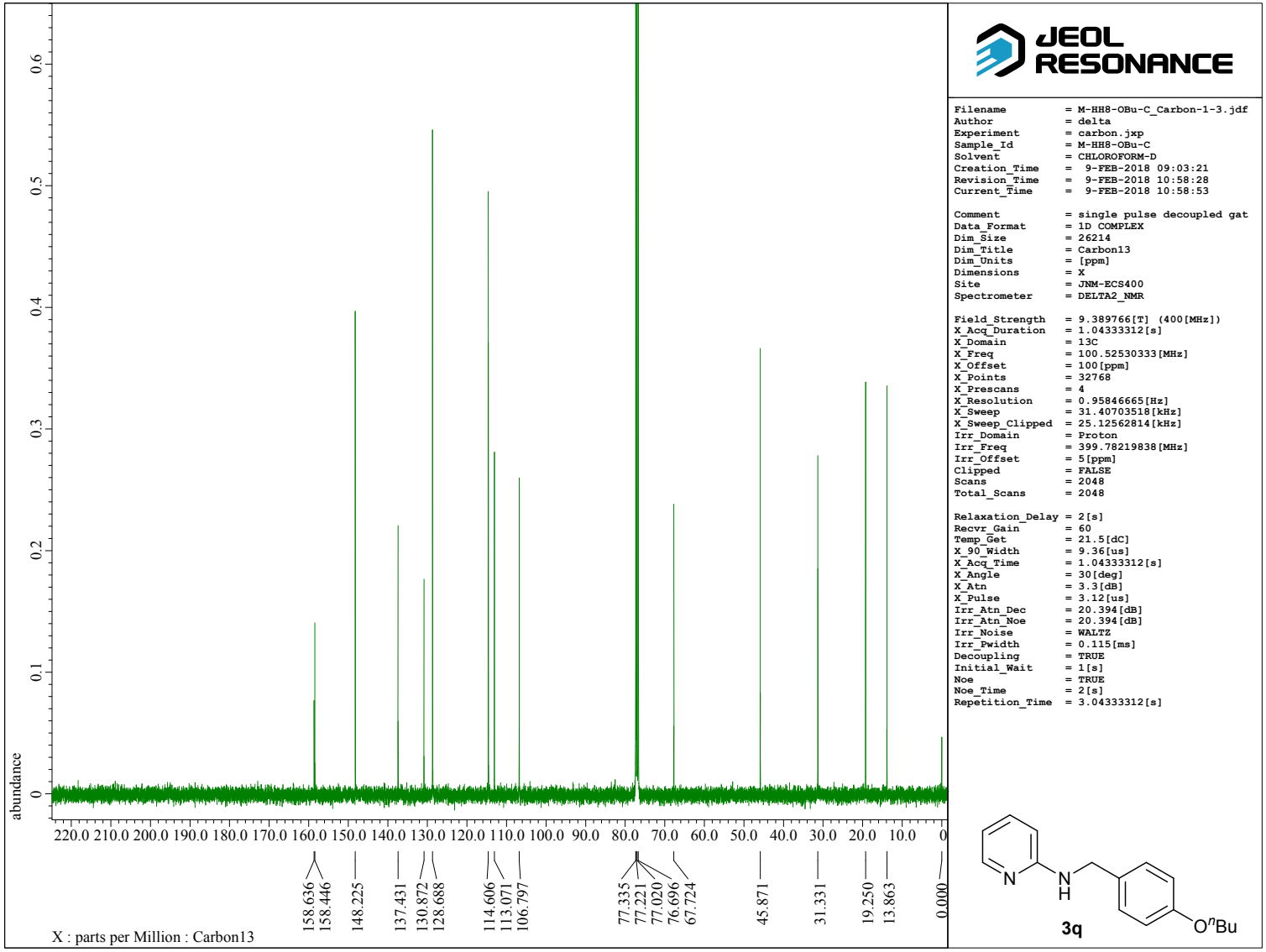

3p



JEOL RESONANCE

```
Filename          = M-HH8-2-4-F3-2_Proton-1-6.
Author            = delta
Experiment        = proton.jxp
Sample_Id         = M-HH8-2-4-F3-2
Solvent           = CHLOROFORM-D
Creation_Time     = 26-DEC-2017 11:25:26
Revision_Time     = 30-JAN-2018 14:45:52
Current_Time      = 30-JAN-2018 14:46:04

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
X_Sweep_Clipped   = 6.00240096[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 42
Temp_Get          = 21.5[dC]
X_90_Width        = 11.69[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 1.5[dB]
X_Pulse           = 5.845[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.18365952[s]
```

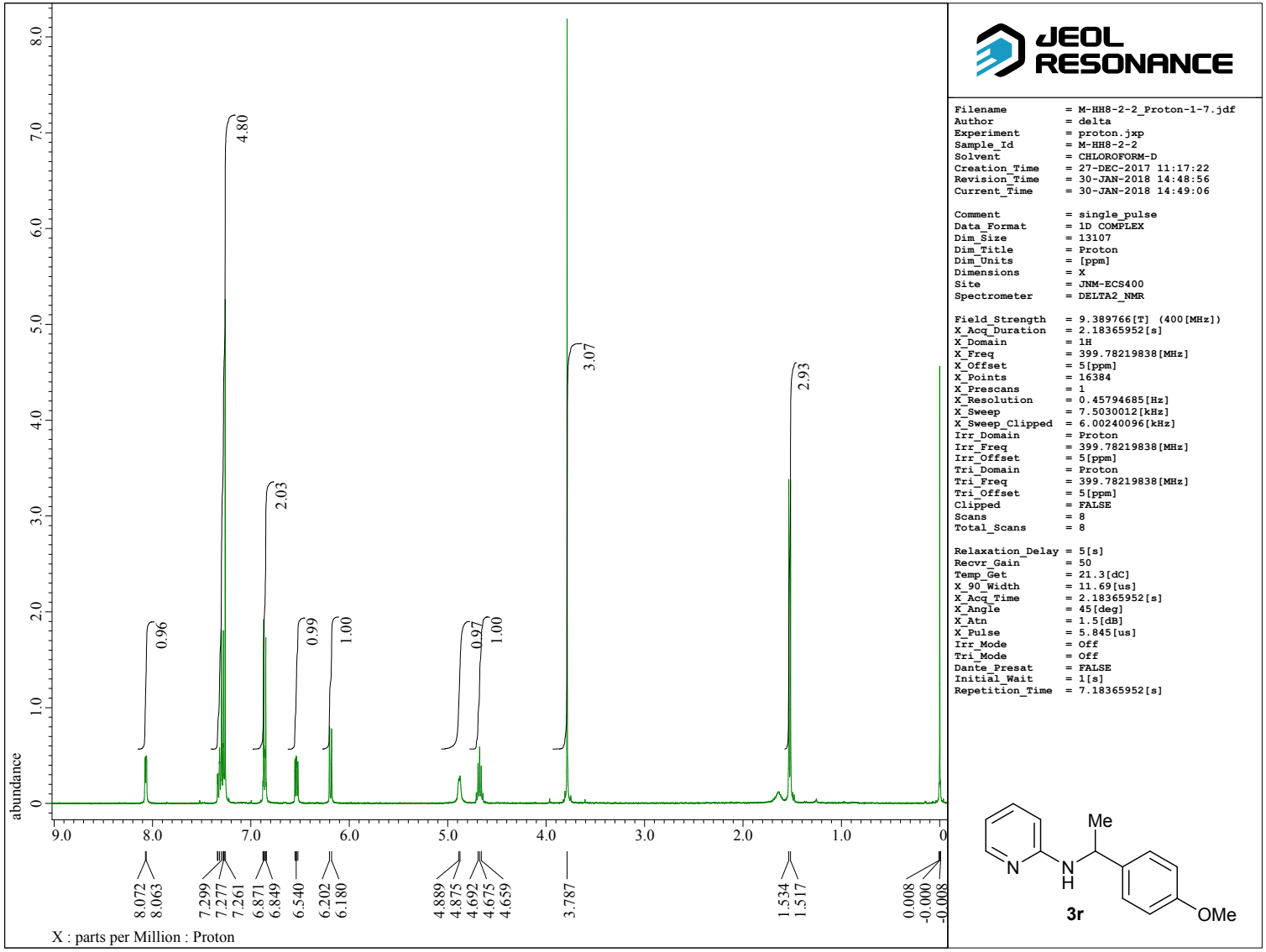

3q



JEOL RESONANCE

Filename	= M-HH8-OBu-C_Carbon-1-3.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= M-HH8-OBu-C
Solvent	= CHLOROFORM-D
Creation_Time	= 9-FEB-2018 09:03:21
Revision_Time	= 9-FEB-2018 10:58:28
Current_Time	= 9-FEB-2018 10:58:53
Comment	= single pulse decoupled gat
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.389766[T] (400[MHz])
X_Acq_Duration	= 1.04333312[s]
X_Domain	= 13C
X_Freq	= 100.52530333[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95846665[Hz]
X_Sweep	= 31.40703518[kHz]
X_Sweep_Clipped	= 25.12562814[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 2048
Total_Scans	= 2048
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 21.5[dC]
X_90_Width	= 9.36[us]
X_Acq_Time	= 1.04333312[s]
X_Angle	= 30[deg]
X_Atn	= 3.3[dB]
X_Pulse	= 3.12[us]
Irr_Atn_Dec	= 20.394[dB]
Irr_Atn_Noe	= 20.394[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.04333312[s]

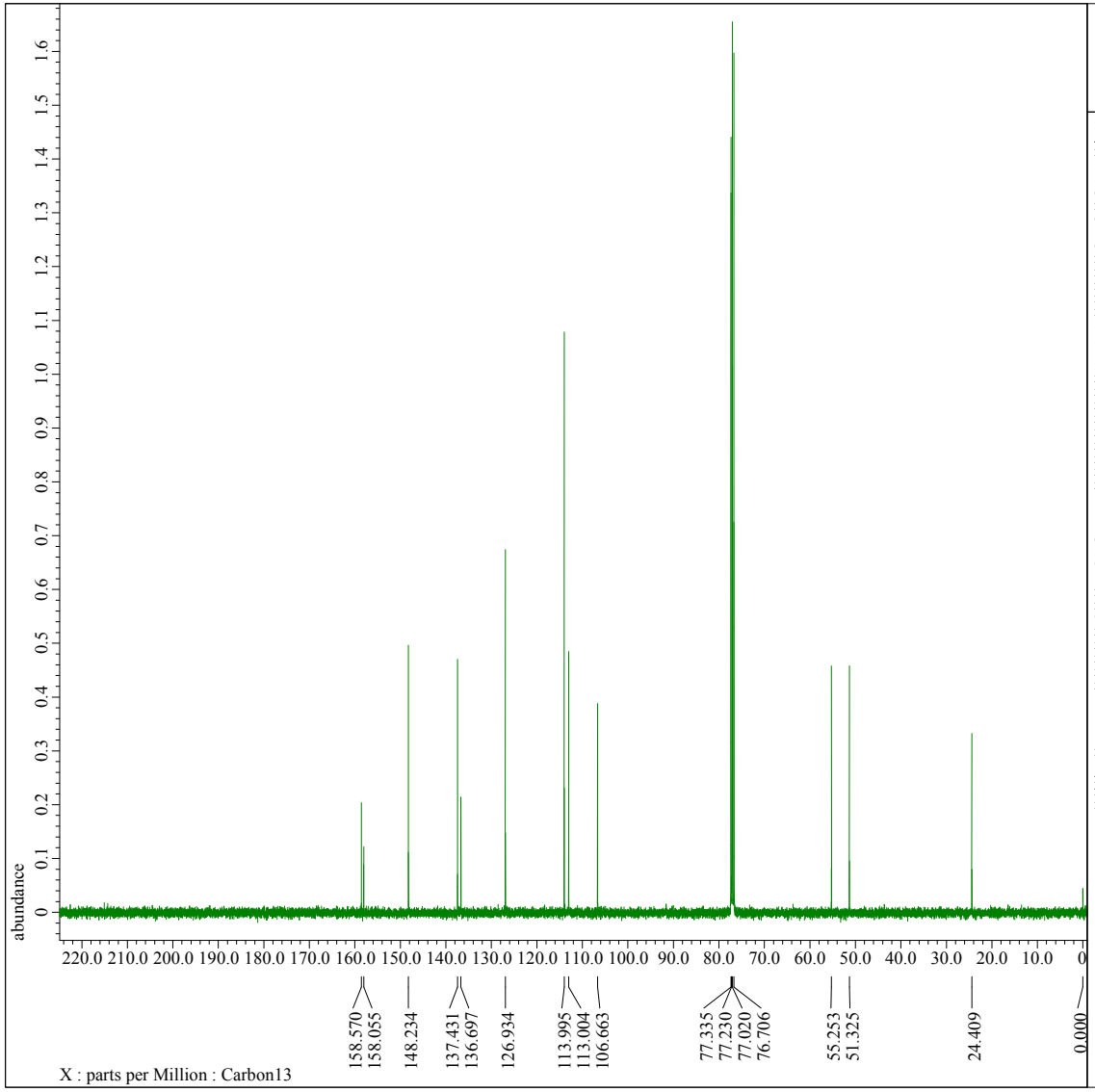
3q



JEOL RESONANCE

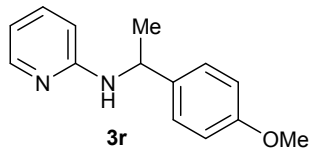
```
Filename          = M-HH8-2-2_Proton-1-7.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = M-HH8-2-2
Solvent           = CHLOROFORM-D
Creation_Time     = 27-DEC-2017 11:17:22
Revision_Time     = 30-JAN-2018 14:48:56
Current_Time      = 30-JAN-2018 14:49:06

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
X_Sweep_Clipped   = 6.00240096[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 50
Temp_Get          = 21.3[dC]
X_90_Width        = 11.69[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 1.5[dB]
X_Pulse           = 5.845[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.18365952[s]
```


3r

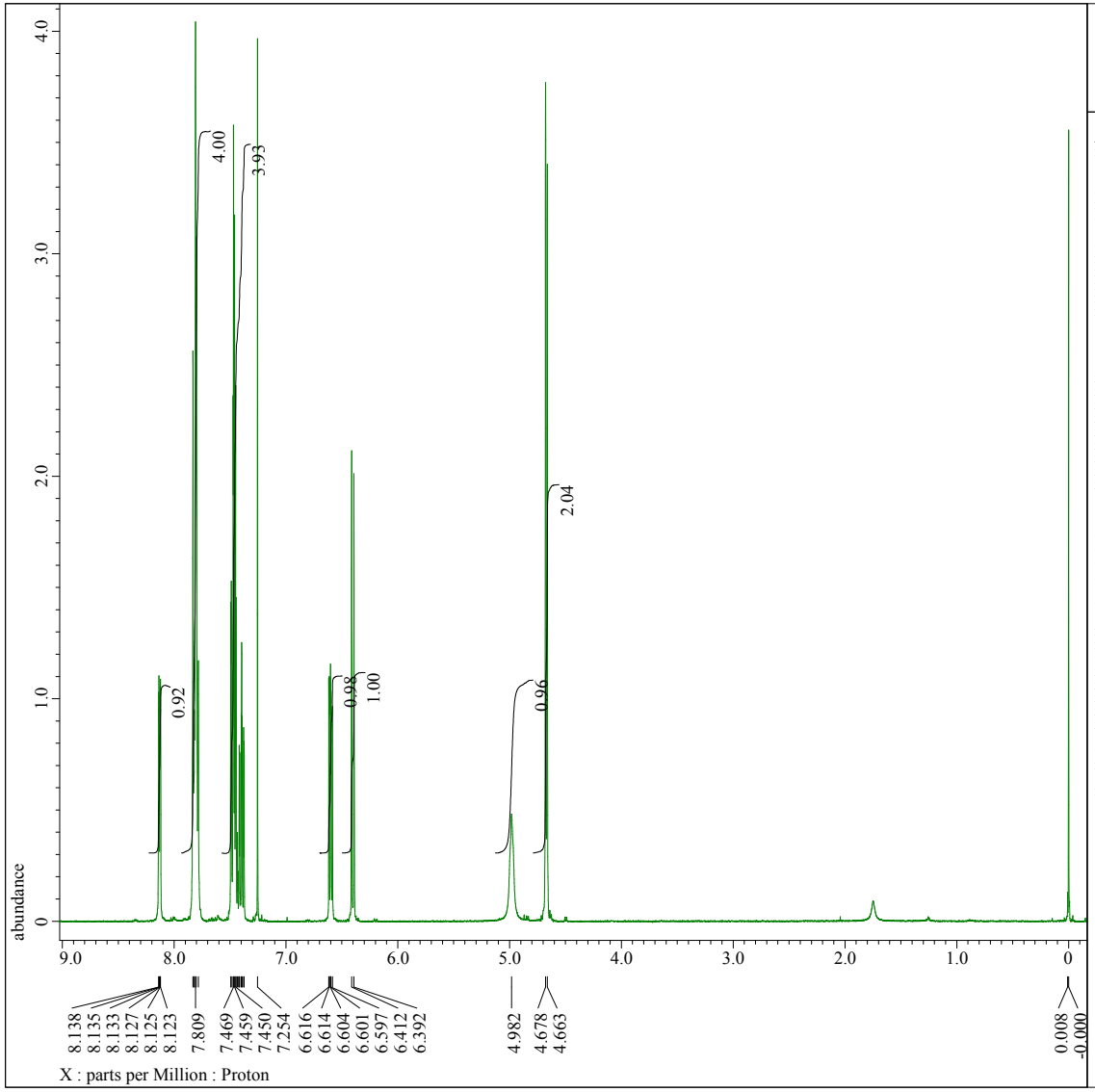


JEOL RESONANCE

```
Filename          = M-HH8-2-2-C_Carbon-1-3.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = M-HH8-2-2-C
Solvent           = CHLOROFORM-D
Creation_Time     =  7-FEB-2018 09:56:05
Revision_Time     =  7-FEB-2018 11:01:55
Current_Time      =  8-FEB-2018 10:07:15

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 1024
Total_Scans       = 1024

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 21.7[dC]
X_90_Width        = 9.36[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 3.3[dB]
X_Pulse           = 3.12[us]
Irr_Atn_Dec       = 20.394[dB]
Irr_Atn_Noe       = 20.394[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```

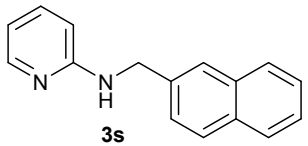


3r

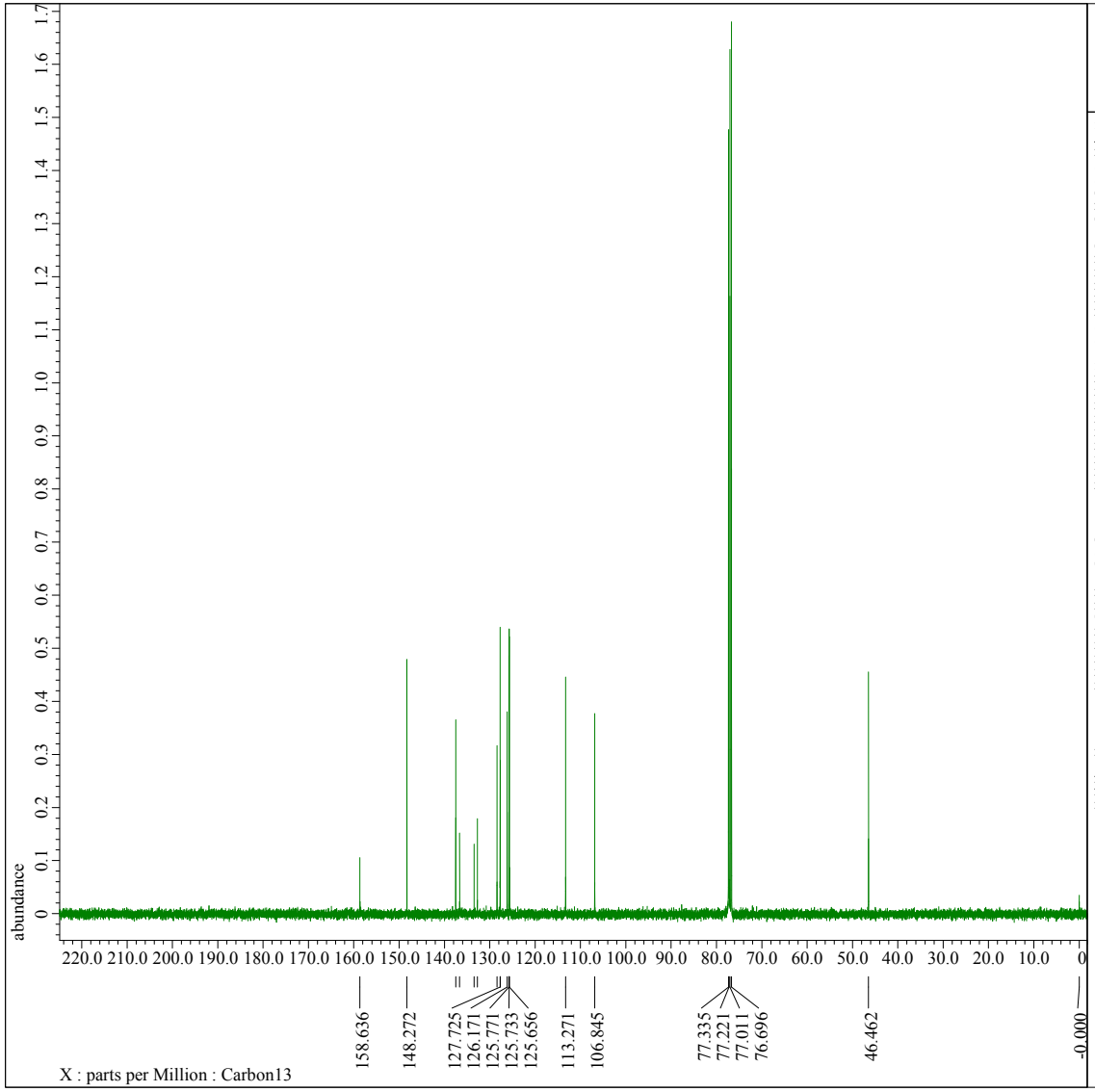


JEOL RESONANCE

```
Filename          = M-HH8-3-1_Proton-1-5.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = M-HH8-3-1
Solvent           = CHLOROFORM-D
Creation_Time     = 27-DEC-2017 11:29:12
Revision_Time     = 27-DEC-2017 12:50:33
Current_Time      = 30-JAN-2018 14:51:27

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
X_Sweep_Clipped   = 6.00240096[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay = 5[s]
Recvr_Gain        = 44
Temp_Get          = 21.3[dC]
X_90_Width        = 11.69[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 1.5[dB]
X_Pulse           = 5.845[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.18365952[s]
```

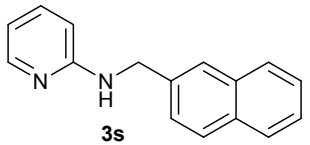


3s



JEOL RESONANCE

```
Filename          = M-HH8-3-1-C_Carbon-1-3.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = M-HH8-3-1-C
Solvent           = CHLOROFORM-D
Creation_Time     = 27-DEC-2017 13:03:32
Revision_Time     = 27-DEC-2017 14:03:11
Current_Time      = 30-JAN-2018 14:52:05

Comment           = single pulse decoupled gat
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 1024
Total_Scans       = 1024

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 21.8[dC]
X_90_Width        = 9.36[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 3.3[dB]
X_Pulse           = 3.12[us]
Irr_Atn_Dec       = 20.394[dB]
Irr_Atn_Noe       = 20.394[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.04333312[s]
```



3s