Mn(II)/O_2-Promoted Oxidative Annulation of Vinyl Isocyanides with Boronic Acids: Synthesis of Multi-substituted Isoquinolines

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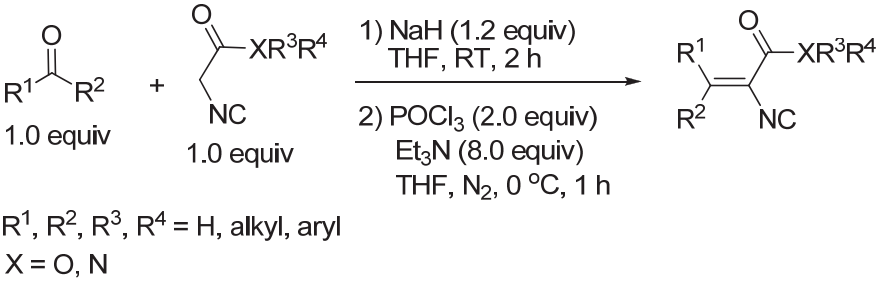
Supporting Information

CONTENTS:

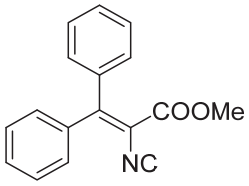
1. General Information

All reagents and metal catalysts were obtained from commercial sources without further purification, and commercially available solvents were purified before use. All new compounds were fully characterized. All melting points were taken on a WRS-1A or a WRS-1B Digital Melting Point Apparatus without correction. Infrared spectra were obtained using an AVATAR 370 FT-IR spectrometer. ^{1}H, ^{13}C and ^{19}F spectra were recorded with a Bruker AV-500 spectrometer operating at 500, 125 and 470 MHz, respectively, with chemical shift values being reported in ppm relative to chloroform (δ = 7.26 ppm) or TMS (δ = 0.00 ppm) for ^{1}H NMR, chloroform (δ = 77.16 ppm) for ^{13}C NMR, and C_6F_6 (δ = –164.9 ppm) for ^{19}F NMR. Mass spectra and high resolution mass spectra were recorded with an Agilent 5975N using an Electron impact (EI) or Electrospray ionization (ESI) techniques. Elemental analyses were carried out on an Elementar Vario EL elemental analyzer. Silica gel plate GF254 were used for thin layer chromatography (TLC) and silica gel H or 300–400 mesh were used for flash column chromatography. Yields refer to chromatographically and spectroscopically pure compounds, unless otherwise indicated.

2. Synthesis and Characterization for vinyl isocyanides 1a-1p:

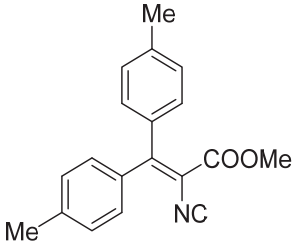


General Procedure[1-3]: To a suspension of NaH (12.0 mmol, 60% in oil) in THF (10.0 mL), a mixture of ketone or aldehyde (10.0 mmol) and isocyanide (10.0 mmol) in THF (10 mL) was added dropwise at room temperature. After stirring for 2 h at room temperature, 10% HOAc was added to the mixture at 0 °C until there is no hydrogen gas release. After removal of the solvent under reduced pressure, the residue was extracted with CH_2Cl_2 for three times and the extract was washed with H_2O, dried over Na_2SO_4 and concentrated under reduced pressure. Further recrystallization in MeOH afforded the corresponding formamide product as a white solid. To an ice cooled three necked flask containing prepared formamide (5.0 mmol), NEt_3 (40 mmol) and THF (10.0 mL) under N_2 atmosphere, $POCl_3$ (10.0 mmol) was added dropwise and the mixture was stirred for 1 h at 0 °C after addition was completed. Then the mixture was quenched by sat. Na_2CO_3 and stirred for another 1 h. The mixture was extracted with CH_2Cl_2 for three times, dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1) to give **1a-1p**.



1a

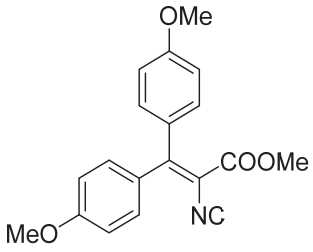
Methyl 2-isocyano-3,3-diphenylacrylate (1a)[1]**:** White solid (62% yield for 2 steps). M.p. 104–105 °C. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.44–7.38 (m, 4H), 7.38–7.34 (m, 4H), 7.16–7.12 (m, 2H), 3.68 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 169.78, 162.28, 154.60, 137.81, 137.39, 130.31, 129.88, 129.59, 129.09, 128.46, 128.25, 113.79, 52.92.



1a'

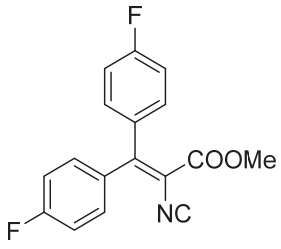
Methyl 2-isocyano-3,3-di-*p*-tolylacrylate (1a')[1]**:** Pale yellow solid (64% yield for 2 steps). M.p. 97–99 °C. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.25 (d, *J* = 7.5 Hz, 2H), 7.20

(d, *J* = 8.0 Hz, 2H), 7.16 (d, *J* = 8.0 Hz, 2H), 7.02 (d, *J* = 8.0 Hz, 2H), 3.70 (s, 3H), 2.39–2.37 (m, 6H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 169.14, 162.60, 155.10, 140.79, 139.89, 135.08, 134.75, 130.12, 129.32, 129.08, 128.92, 112.71, 52.83, 21.49, 21.45.



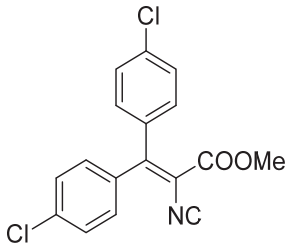
1b

Methyl 2-isocyano-3,3-bis(4-methoxyphenyl)acrylate (1b)[1]**:** Pale yellow solid (54% yield for 2 steps). M.p. 84–85 °C. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.31 (d, *J* = 9.0 Hz, 2H), 7.05 (d, *J* = 8.5 Hz, 2H), 6.90 (d, *J* = 8.5 Hz, 2H), 6.86 (d, *J* = 9.0 Hz, 2H), 3.83 (s, 3H), 3.82 (s, 3H), 3.69 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 168.57, 163.00, 161.36, 161.03, 154.68, 132.36, 131.40, 130.26, 129.88, 113.76, 113.63, 111.34, 55.43, 55.34, 52.76.



1c

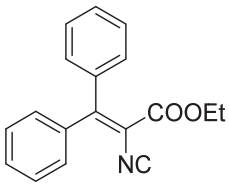
Methyl 3,3-bis(4-fluorophenyl)-2-isocyanoacrylate (1c)[1]**:** Pale yellow solid (48% yield for 2 steps). M.p. 97–98 °C. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.38–7.33 (m, 2H), 7.15–7.03 (m, 6H), 3.70 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 170.38, 163.74 (d, *J* = 251.2 Hz), 163.58 (d, *J* = 250.0 Hz), 162.00, 152.42, 133.47 (d, *J* = 3.5 Hz), 133.21 (d, *J* = 3.5 Hz), 132.23 (d, *J* = 9.0 Hz), 131.27 (d, *J* = 8.5 Hz), 115.82 (d, *J* = 21.8 Hz), 115.60 (d, *J* = 21.8 Hz), 113.80, 50.03; ^{19}F NMR ($CDCl_3$, 470 MHz): δ –108.57 (m, Ar–F), –110.17 (m, Ar–F).



1d

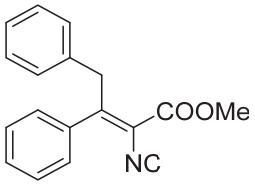
Methyl 3,3-bis(4-chlorophenyl)-2-isocyanoacrylate (1d): Pale yellow solid (68% yield for 2 steps). M.p. 111–112 °C. IR (KBr, cm^{-1}): 2117.1, 1734.5, 1580.0, 1484.5, 1246.2, 1083.5, 827.4, 770.8. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.37 (td, *J* = 9.5, 2.0 Hz, 2H), 7.32 (td, *J* = 9.5, 2.0 Hz, 2H), 7.26 (td, *J* = 9.5, 2.0 Hz, 2H), 7.04 (td, *J* = 9.0, 2.0 Hz, 2H), 3.69 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 171.06, 161.73, 152.05, 136.80, 136.12, 135.70, 135.40, 131.30, 130.55, 128.96, 128.73, 114.24, 53.16. EI-MS *m/z* (%): 331 (90) [M$^+$ (2×^{35}Cl)], 333 (60) [M$^+$ (^{35}Cl, ^{37}Cl)], 335 (11) [M$^+$

(2×^{37}Cl)], 237 (100), 300 (47), 296 (44). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{17}H_{11}Cl_2NO_2$: 332.0245; found: 332.0237.



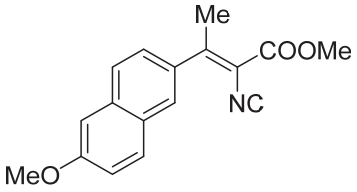
1e

Ethyl 2-isocyano-3,3-diphenylacrylate (1e): Pale yellow solid (72% yield for 2 steps). M.p. 104–105 °C. IR (KBr, cm^{-1}): 2112.4, 1721.4, 1444.8, 1323.7, 1260.4, 1116.0, 1009.1, 754.3, 697.5. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.44–7.38 (m, 4H), 7.38–7.33 (m, 4H), 7.16–7.12 (m, 2H), 4.11 (q, *J* = 7.5 Hz, 2H), 1.06 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 169.60, 161.95, 153.90, 138.03, 137.37, 130.24, 129.88, 129.45, 129.10, 128.44, 128.22, 114.35, 62.24, 13.58. EI-MS *m/z* (%): 277 (25) [M$^+$], 204 (100), 203 (46), 176 (28), 177 (21). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{18}H_{15}NO_2$: 278.1181; found: 278.1173.



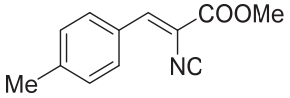
1f

Methyl (*Z*)-2-isocyano-3,4-diphenylbut-2-enoate (1f)[1]**:** Pale yellow solid (42% yield for 2 steps). M.p. 138–139 °C. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.38–7.33 (m, 3H), 7.23–7.14 (m, 5H), 7.05 (d, *J* = 6.5 Hz, 2H), 4.36 (s, 2H), 3.92 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 168.64, 161.70, 157.95, 137.81, 136.38, 129.32, 129.04, 128.53, 128.51, 127.48, 126.82, 115.36, 53.11, 39.47.



1g

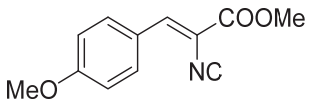
Methyl (*Z*)-2-isocyano-3-(6-methoxynaphthalen-2-yl)but-2-enoate (1g)[1]**:** White solid (44% yield for 2 steps). M.p. 62–63 °C. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.80 (s, 1H), 7.77 (t, *J* = 8.0 Hz, 2H), 7.44 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.18 (dd, *J* = 9.0, 2.5 Hz, 1H), 7.16–7.13 (m, 1H), 3.93 (s, 3H), 3.91 (s, 3H), 2.64 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 168.11, 162.10, 158.84, 156.14, 134.92, 134.35, 130.04, 128.23, 127.13, 127.08, 125.08, 119.66, 114.31, 105.70, 55.41, 52.86, 21.79.



1h

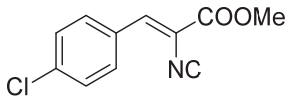
Methyl (*Z*)-2-isocyano-3-(*p*-tolyl)acrylate (1h): White solid (32% yield for 2 steps). M.p. 80–81 °C. IR (KBr, cm^{-1}): 2115.6, 1727.2, 1613.7, 1282.7, 1201.5, 1088.3, 812.4. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.77 (d, *J* = 8.0 Hz, 2H), 7.61 (s, 1H), 7.27 (d, *J* = 8.5 Hz, 2H), 3.91 (s, 3H), 2.40 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 173.58, 162.02, 143.03, 138.48, 131.10, 129.88, 128.35, 113.19, 53.40, 21.73. EI-MS *m/z* (%): 201

(32) [M^+], 143 (100), 142 (40), 170 (25), 140 (24). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{12}H_{11}NO_2$: 202.0868; found: 202.0857.



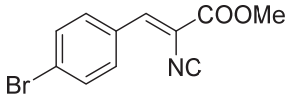
1i

Methyl (*Z*)-2-isocyano-3-(4-methoxyphenyl)acrylate (1i)[1]**:** Pale yellow solid (34% yield for 2 steps). M.p. 109–110 °C. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.85 (d, *J* = 9.0 Hz, 2H), 7.57 (s, 1H), 6.96 (d, *J* = 9.0 Hz, 2H), 3.89 (s, 3H), 3.86 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 173.16, 162.59, 162.27, 138.05, 133.24, 123.80, 114.62, 111.68, 55.53, 53.30.



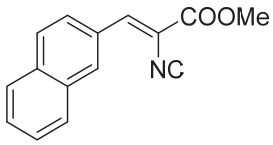
1j

Methyl (*Z*)-3-(4-chlorophenyl)-2-isocyanoacrylate (1j): White solid (39% yield for 2 steps). M.p. 89–90 °C. IR (KBr, cm^{-1}): 2111.0, 1727.0, 1623.9, 1437.6, 1281.3, 1194.4, 1078.5, 816.9, 756.9. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.81 (d, *J* = 8.5 Hz, 2H), 7.61 (s, 1H), 7.45 (d, *J* = 8.5 Hz, 2H), 3.93 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 174.63, 161.52, 138.11, 136.89, 132.08, 129.47, 129.43, 114.53, 53.59. EI-MS *m/z* (%): 221 (31) [M^+(^{35}Cl)], 223 (12) [M^+(^{37}Cl)], 186 (100), 162 (58), 127 (46). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{11}H_8ClNO_2$: 222.0322; found: 222.0311.



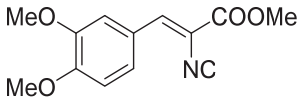
1k

Methyl (*Z*)-3-(4-bromophenyl)-2-isocyanoacrylate (1k): White solid (38% yield for 2 steps). M.p. 114–116 °C. IR (KBr, cm^{-1}): 2111.3, 1726.6, 1626.0, 1283.0, 1194.1, 1072.5, 813.4, 758.3. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.71 (d, *J* = 9.0 Hz, 2H), 7.61 (s, 1H), 7.58 (d, *J* = 7.0 Hz, 2H), 3.92 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 174.71, 161.54, 137.03, 132.47, 132.17, 129.83, 126.72, 114.65, 53.63. EI-MS *m/z* (%): 265 (33) [M^+ (^{79}Br)], 267 (31) [M^+ (^{81}Br)], 186 (100), 207 (32), 127 (94). HRMS (ESI) ([M+H]$^+$) Calcd. For $C_{11}H_8BrNO_2$: 265.9817; found: 265.9805.



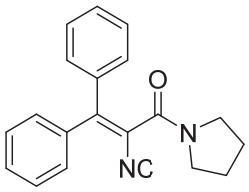
1l

Methyl (*Z*)-2-isocyano-3-(naphthalen-2-yl)acrylate (1l)[1]**:** White solid (45% yield for 2 steps). M.p. 120–121°C. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.31 (s, 1H), 8.01 (dd, *J* = 9.0, 2.0 Hz, 1H), 7.94–7.88 (m, 2H), 7.86 (d, *J* = 8.5 Hz, 1H), 7.80 (s, 1H), 7.59 (td, *J* = 7.0, 1.0 Hz, 1H), 7.55 (td, *J* = 7.0, 1.0 Hz, 1H), 3.95 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 174.03, 161.95, 138.50, 134.71, 132.97, 132.90, 129.14, 128.91, 128.56, 127.80, 127.05, 126.07, 114.07, 53.53.



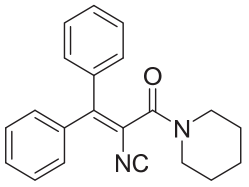
1m

Methyl (*Z*)-3-(3,4-dimethoxyphenyl)-2-isocyanoacrylate (1m)[1]**:** Pale yellow solid (43% yield for 2 steps). M.p. 109–111 °C. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.57 (d, *J* = 2.0 Hz, 1H), 7.52 (s, 1H), 7.34 (dd, *J* = 8.5, 2.0 Hz, 1H), 6.89 (d, *J* = 8.5 Hz, 1H), 3.90 (s, 3H), 3.89 (s, 3H), 3.87 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 173.21, 162.12, 152.39, 149.05, 138.29, 126.69, 123.97, 112.19, 111.61, 110.97, 56.01, 55.92, 53.27.



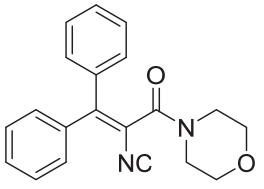
1n

2-Isocyano-3,3-diphenyl-1-(pyrrolidin-1-yl)prop-2-en-1-one (1n): Pale yellow solid (65% yield for 2 steps). M.p. 141–143 °C. IR (KBr, cm^{-1}): 2109.0, 1631.9, 1434.8, 1332.5, 1174.1, 771.2, 750.2, 702.8. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.40–7.26 (m, 8H), 7.22–7.18 (m, 2H), 3.33 (t, *J* = 6.5 Hz, 2H), 3.20 (t, *J* = 6.5 Hz, 2H), 1.71–1.65 (m, 4H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 169.37, 161.15, 145.48, 136.80, 136.74, 129.77, 129.75, 129.53, 129.46, 128.46, 128.40, 117.13, 47.12, 45.77, 25.58, 24.08. EI-MS *m/z* (%): 302 (100) [M^+], 77 (96), 204 (70), 178 (68), 176 (59). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{20}H_{18}N_2O$: 303.1497; found: 303.1488.



1o

2-Isocyano-3,3-diphenyl-1-(piperidin-1-yl)prop-2-en-1-one (1o)[1]**:** Pale yellow solid (69% yield for 2 steps). M.p. 143–144 °C. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.40–7.29 (m, 8H), 7.22 (d, *J* = 7.5 Hz, 2H), 3.45 (t, *J* = 5.5 Hz, 2H), 3.29 (t, *J* = 5.5 Hz, 2H), 1.50–1.43 (m, 2H), 1.43–1.35 (m, 2H), 1.30–1.00 (m, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 169.23, 161.49, 145.06, 136.78, 136.75, 129.72, 129.65, 129.58, 129.48, 128.45, 115.87, 47.55, 42.73, 25.49, 24.83, 24.10.

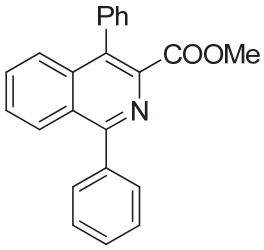


1p

2-Isocyano-1-morpholino-3,3-diphenylprop-2-en-1-one (1p): Pale yellow solid (54% yield for 2 steps). M.p. 131–132 °C. IR (KBr, cm^{-1}): 2111.5, 1633.0, 1433.2, 1257.7, 1105.4, 1015.6, 770.9, 697.3. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.45–7.30 (m, 8H), 7.21 (d, *J* = 8.0 Hz, 2H), 3.55–3.40 (m, 4H), 3.34–3.24 (m, 2H), 3.20–3.04 (m, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 169.60, 161.82, 146.06, 136.58, 136.42, 130.05, 129.78, 129.73, 129.60, 128.65, 128.53, 114.79, 65.94, 65.91, 46.73, 42.13. EI-MS *m/z* (%): 318 (80) [M^+], 204 (100), 203 (85), 232 (71), 178 (69). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{20}H_{18}N_2O_2$: 319.1447; found: 319.1436.

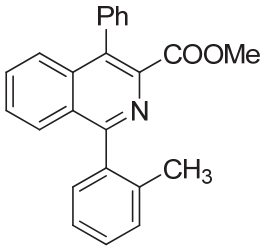
3. Synthesis and Characterization for Compounds 3 and 4.

General Procedure: An oxygen-purged schlenk tube was equipped with a rubber septum and magnetic stir bar and was charged with vinyl isocyanide **1** (0.5 mmol), boronic acid **2** (1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (1.0 mmol) in dry toluene (5.0 mL). The tube was evacuated and backfilled with O_2 for three times. The reaction mixture was stirred in a pre-heated oil bath at 80 ^oC for 2 h. The reaction was cooled to room temperature, filtered through a plug of celite and then washed with EtOAc (3×20 mL). The combined organic layers were dried over Na_2SO_4 and concentrated under reduced pressure after filtration. The crude reaction mixture was purified by chromatography on silica gel (eluent: hexane/EtOAc = 20:1 to 3:1) to give the desired product **3** or **4**.



3a

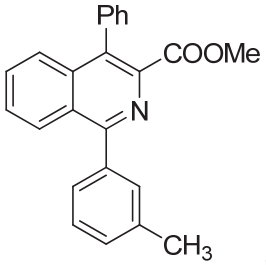
Methyl 1,4-diphenylisoquinoline-3-carboxylate (3a)[1]**:** Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (131.5 mg, 0.5 mmol), phenylboronic acid **2a** (122 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 ^oC for 2 h, to give **3a** (166.1 mg, 98%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1). M.p. 180–181 ^oC. IR (KBr, cm^{-1}): 1723.5, 1546.0, 1337.0, 1226.2, 1180.5, 997.2, 762.9, 699.4, 668.9. ^1H NMR ($CDCl_3$, 500 MHz): δ 8.18 (d, *J* = 8.0 Hz, 1H), 7.77 (d, *J* = 7.0 Hz, 2H), 7.71 (d, *J* = 7.5 Hz, 1H), 7.66 (t, *J* = 8.0 Hz, 1H), 7.60 (t, *J* = 7.5 Hz, 1H), 7.58–7.48 (m, 6H), 7.42 (d, *J* = 7.0 Hz, 2H), 3.70 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 167.69, 160.27, 141.41, 138.91, 136.52, 136.10, 132.76, 130.58, 130.24, 129.86, 128.95, 128.47, 128.32, 128.05, 127.75, 127.20, 126.74, 52.43. EI-MS *m/z* (%): 339 (44) [M^+], 280 (100), 278 (47), 281 (35), 279 (24).



3b

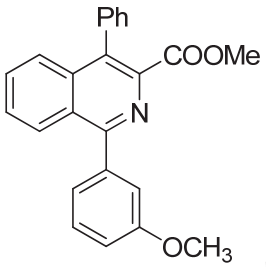
Methyl 4-phenyl-1-(*o*-tolyl)isoquinoline-3-carboxylate (3b): Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (131.5 mg, 0.5 mmol), *o*-tolylboronic acid **2b** (136.0 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 ^oC for 2 h, to give **3b** (148.3 mg, 84%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1). M.p. 146–147 ^oC. IR (KBr, cm^{-1}): 1731.2, 1440.7, 1381.3, 1328.7, 1225.3, 1167.0, 998.2, 765.5, 696.4. ^1H NMR ($CDCl_3$, 500 MHz): δ 7.74 (d, *J* = 8.0 Hz, 1H), 7.72 (d, *J* = 8.5 Hz,

1H), 7.64 (td, *J* = 5.5, 1.0 Hz, 1H), 7.58–7.49 (m, 4H), 7.49–7.45 (m, 1H), 7.45–7.38 (m, 3H), 7.38–7.32 (m, 2H), 3.70 (s, 3H), 2.16 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 167.65, 160.86, 141.35, 138.24, 136.76, 136.04, 132.83, 130.71, 130.45, 129.93, 129.89, 129.86, 128.79, 128.39, 128.34, 128.28, 128.07, 127.90, 127.66, 126.67, 125.74, 52.48, 20.04. EI-MS *m/z* (%): 353 (51) [M^+], 292 (100), 291 (64), 352 (45), 293 (38). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{24}H_{19}NO_2$: 354.1494; found: 354.1485.



3c

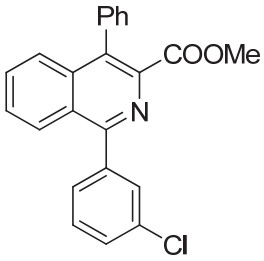
Methyl 4-phenyl-1-(*m*-tolyl)isoquinoline-3-carboxylate (3c): Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (131.5 mg, 0.5 mmol), *m*-tolylboronic acid **2c** (136 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 ^{o}C for 2 h, to give **3c** (174.7 mg, 99%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1). M.p. 156–158 ^{o}C. IR (KBr, cm^{-1}): 1716.5, 1435.1, 1380.7, 1327.3, 1227.7, 1163.0, 1003.5, 768.3, 692.5, 600.2. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.18 (d, *J* = 8.0 Hz, 1H), 7.70 (d, *J* = 8.0 Hz, 1H), 7.65 (td, *J* = 5.5, 1.0 Hz, 1H), 7.60 (td, *J* = 8.5, 1.5 Hz, 2H), 7.56–7.48 (m, 4H), 7.46–7.40 (m, 3H), 7.33 (d, *J* = 8.0 Hz, 1H), 3.70 (s, 3H), 2.47 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 167.68, 160.51, 141.35, 138.78, 138.29, 136.48, 136.12, 132.66, 130.80, 130.56, 129.86, 129.69, 128.30, 128.25, 128.20, 128.02, 127.88, 127.33, 127.25, 126.69, 52.41, 21.54. EI-MS *m/z* (%): 353 (51) [M^+], 294 (100), 77 (76), 271 (54), 225 (47). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{24}H_{19}NO_2$: 354.1494; found: 354.1486.



3d

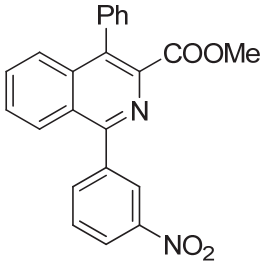
Methyl 1-(3-methoxyphenyl)-4-phenylisoquinoline-3-carboxylate (3d): Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (131.5 mg, 0.5 mmol), (3-methoxyphenyl)boronic acid **2d** (152.0 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 ^{o}C for 2 h, to give **3d** (182.6 mg, 99%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1). M.p. 115–116 ^{o}C. IR (KBr, cm^{-1}): 1721.4, 1432.9, 1327.3, 1266.0, 1227.8, 1171.6, 1110.6, 998.5, 768.1, 695.1. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.19 (d, *J* = 8.5 Hz, 1H), 7.70 (d, *J* = 8.0 Hz, 1H), 7.68–7.58 (m, 2H), 7.56–7.48 (m, 3H), 7.45 (t, *J* = 7.5 Hz, 1H), 7.41 (d, *J* = 7.0 Hz, 2H), 7.32 (d, *J* = 7.5 Hz, 2H), 7.07 (dd, *J* = 8.0, 2.0 Hz, 1H), 3.89 (s, 3H), 3.70 (s, 3H); ^{13}C NMR ($CDCl_3$, 125

MHz): δ 167.60, 160.08, 159.73, 141.30, 140.10, 136.50, 136.03, 132.84, 130.64, 129.84, 129.43, 128.33, 128.31, 128.06, 127.79, 127.21, 126.71, 122.71, 115.46, 114.98, 55.47, 52.44. EI-MS *m/z* (%): 369 (76) [M^+], 310 (100), 225 (63), 77 (54). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{24}H_{19}NO_3$: 370.1443; found: 370.1435.



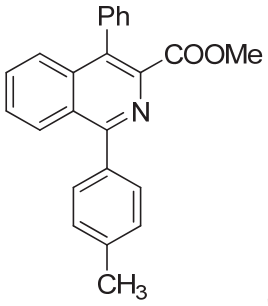
3e

Methyl 1-(3-chlorophenyl)-4-phenylisoquinoline-3-carboxylate (3e)[1]**:** Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (131.5 mg, 0.5 mmol), (3-chlorophenyl)boronic acid **2e** (156.3 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 ^oC for 2 h, to give **3e** (167.9 mg, 90%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1). M.p. 131–132 ^oC. IR (KBr, cm^{-1}): 1724.4, 1329.3, 1227.3, 762.8, 698.4. ^1H NMR ($CDCl_3$, 500 MHz): δ 8.12 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.77 (d, *J* = 2.0 Hz, 1H), 7.72 (dd, *J* = 7.5, 1.0 Hz, 1H), 7.69–7.62 (m, 3H), 7.56–7.45 (m, 5H), 7.43–7.38 (m, 2H), 3.70 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 167.50, 158.63, 141.39, 140.62, 136.55, 135.89, 134.55, 133.29, 130.76, 130.28, 129.78, 129.70, 129.07, 128.63, 128.41, 128.33, 128.13, 127.27, 127.04, 126.90, 52.49. EI-MS *m/z* (%): 373 (30) [M^+ (^{35}Cl)], 375 (16) [M^+ (^{37}Cl)], 314 (100), 315 (37), 316 (35).



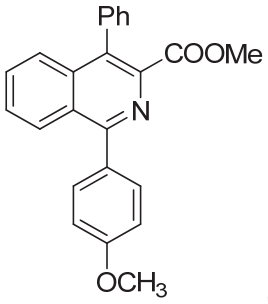
3f

Methyl 1-(3-nitrophenyl)-4-phenylisoquinoline-3-carboxylate (3f): Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (131.5 mg, 0.5 mmol), (3-nitrophenyl)boronic acid **2f** (167.0 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 ^oC for 2 h, to give **3f** (180.5 mg, 94%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1). M.p. 169–170 ^oC. IR (KBr, cm^{-1}): 1726.8, 1526.6, 1344.4, 1228.4, 774.9, 695.3. ^1H NMR ($CDCl_3$, 500 MHz): δ 8.66 (s, 1H), 8.38 (dd, *J* = 7.0, 1.0 Hz, 1H), 8.13 (d, *J* = 7.5 Hz, 1H), 8.07 (d, *J* = 7.5 Hz, 1H), 7.80–7.65 (m, 4H), 7.58–7.48 (m, 3H), 7.41 (d, *J* = 6.5 Hz, 2H), 3.70 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 167.35, 157.32, 148.36, 141.56, 140.53, 136.67, 136.26, 135.65, 133.83, 131.04, 129.75, 129.61, 129.09, 128.39, 128.28, 127.18, 126.85, 126.64, 125.27, 123.79, 52.54. EI-MS *m/z* (%): 384 (37) [M^+], 325 (100), 326 (44), 278 (44), 279 (37). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{23}H_{16}N_2O_4$: 385.1188; found: 385.1179.



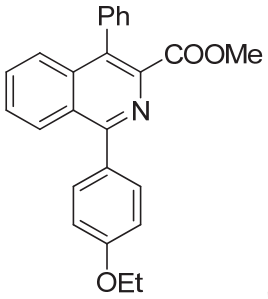
3g

Methyl 4-phenyl-1-(*p*-tolyl)isoquinoline-3-carboxylate (3g): Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (131.5 mg, 0.5 mmol), *p*-tolylboronic acid **2g** (136 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 ^oC for 2 h, to give **3g** (151.8 mg, 86%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1). M.p. 145–146 ^oC. IR (KBr, cm^{-1}): 1736.8, 1435.0, 1230.2, 1165.3, 1115.7, 768.0, 697.9, 504.7. ^1H NMR ($CDCl_3$, 500 MHz): δ 8.21 (d, *J* = 8.0 Hz, 1H), 7.75–7.57 (m, 5H), 7.55–7.46 (m, 3H), 7.41 (d, *J* = 7.0 Hz, 2H), 7.36 (d, *J* = 8.0 Hz, 2H), 3.70 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 167.74, 160.34, 141.42, 138.86, 136.52, 136.18, 136.09, 132.49, 130.47, 130.18, 129.87, 129.14, 128.29, 128.18, 127.99, 127.83, 127.23, 126.70, 52.38, 21.42. EI-MS *m/z* (%): 353 (86) [M^+], 294 (100), 293 (67). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{24}H_{19}NO_2$: 354.1494; found: 354.1486.



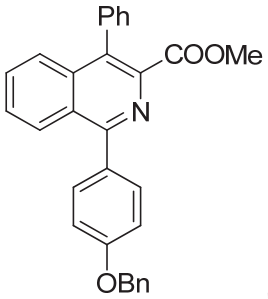
3h

Methyl 1-(4-methoxyphenyl)-4-phenylisoquinoline-3-carboxylate (3h)[1]: Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (131.5 mg, 0.5 mmol), (4-methoxyphenyl)boronic acid **2h** (152.0 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 ^oC for 2 h, to give **3h** (134.7 mg, 73%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1). M.p. 174–175 ^oC. IR (KBr, cm^{-1}): 1730.1, 1605.6, 1507.8, 1387.5, 1334.2, 1244.3, 1169.4, 1111.8, 1028.2, 843.2, 770.5, 699.9, 521.8. ^1H NMR ($CDCl_3$, 500 MHz): δ 8.22 (d, *J* = 8.5 Hz, 1H), 7.74 (td, *J* = 8.5, 2.0 Hz, 2H), 7.69 (d, *J* = 8.5 Hz, 1H), 7.67–7.58 (m, 2H), 7.55–7.48 (m, 3H), 7.43–7.38 (m, 2H), 7.09 (td, *J* = 9.0, 2.5 Hz, 2H), 3.90 (s, 3H), 3.70 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 167.71, 160.37, 159.89, 141.33, 136.60, 136.17, 132.32, 131.68, 131.40, 130.48, 129.87, 128.28, 128.20, 127.98, 127.81, 127.19, 126.72, 113.94, 55.47, 52.38. EI-MS *m/z* (%): 369 (74) [M^+], 310 (100), 225 (42).



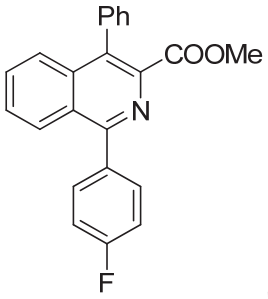
3i

Methyl 1-(4-ethoxyphenyl)-4-phenylisoquinoline-3-carboxylate (3i): Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (131.5 mg, 0.5 mmol), (4-ethoxyphenyl)boronic acid **2i** (166.0 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 ^oC for 2 h, to give **3i** (170.4 mg, 89%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1). M.p. 172–173 ^oC. IR (KBr, cm^{-1}): 1726.9, 1603.9, 1506.4, 1440.1, 1384.4, 1332.0, 1245.3, 1167.8, 1110.4, 769.2, 699.1. ^1H NMR ($CDCl_3$, 500 MHz): δ 8.23 (d, *J* = 7.5 Hz, 1H), 7.72 (d, *J* = 8.5 Hz, 2H), 7.69 (d, *J* = 8.5 Hz, 1H), 7.64 (td, *J* = 6.5, 1.0 Hz, 1H), 7.60 (td, *J* = 5.5, 1.0 Hz, 1H), 7.55–7.45 (m, 3H), 7.40 (dd, *J* = 8.0, 1.5 Hz, 2H), 7.07 (d, *J* = 9.0 Hz, 2H), 4.14 (q, *J* = 7.0 Hz, 2H), 3.79 (s, 3H), 1.47 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 167.64, 159.93, 159.77, 141.22, 136.62, 136.14, 132.32, 131.69, 131.10, 130.52, 129.87, 128.28, 128.21, 127.98, 127.88, 127.18, 126.72, 114.49, 63.64, 52.39, 14.86. EI-MS *m/z* (%): 383 (100) $[M^+]$, 324 (94). HRMS (ESI) ($[M+H]^+$) Calcd. for $C_{25}H_{21}NO_3$: 384.1600; found: 384.1591.



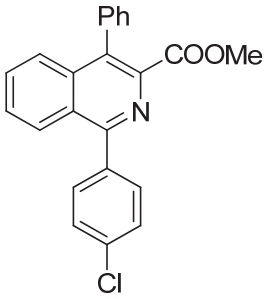
3j

Methyl 1-(4-(benzyloxy)phenyl)-4-phenylisoquinoline-3-carboxylate (3j): Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (131.5 mg, 0.5 mmol), (4-(benzyloxy)phenyl)boronic acid **2j** (228 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 ^oC for 2 h, to give **3j** (171.3 mg, 77%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1). M.p. 122–123 ^oC. IR (KBr, cm^{-1}): 1725.5, 1607.9, 1507.8, 1384.7, 1229.3, 1174.7, 1114.2, 1031.5, 772.6, 699.3. ^1H NMR ($CDCl_3$, 500 MHz): δ 8.23 (d, *J* = 8.5 Hz, 1H), 7.74 (td, *J* = 8.5, 2.0 Hz, 2H), 7.70 (d, *J* = 9.0, 1.0 Hz, 1H), 7.68–7.58 (m, 2H), 7.56–7.47 (m, 5H), 7.45–7.38 (m, 4H), 7.36 (t, *J* = 7.0 Hz, 1H), 7.16 (d, *J* = 8.5 Hz, 2H), 5.19 (s, 2H), 3.70 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 167.66, 159.83, 159.55, 141.28, 136.85, 136.61, 136.14, 132.38, 131.71, 131.59, 130.51, 129.87, 128.68, 128.29, 128.22, 128.07, 127.99, 127.83, 127.47, 127.17, 126.74, 114.90, 70.12, 52.40. EI-MS *m/z* (%): 445 (32) $[M^+]$, 91 (100), 224 (25). HRMS (ESI) ($[M+H]^+$) Calcd. for $C_{30}H_{23}NO_3$: 446.1756; found: 446.1748.



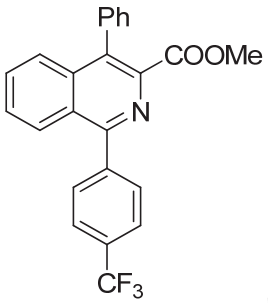
3k

Methyl 1-(4-fluorophenyl)-4-phenylisoquinoline-3-carboxylate (3k)[1]: Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (131.5 mg, 0.5 mmol), (4-fluorophenyl)boronic acid **2k** (140.0 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 ^{o}C for 2 h, to give **3k** (148.2 mg, 83%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1). M.p. 181–182 ^{o}C. IR (KBr, cm^{-1}): 1717.1, 1600.9, 1504.4, 1379.3, 1223.1, 1157.9, 1001.6, 845.6, 767.7, 696.2. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.14 (d, *J* = 8.0 Hz, 1H), 7.78–7.75 (m, 2H), 7.72 (d, *J* = 8.0 Hz, 1H), 7.70–7.60 (m, 2H), 7.56–7.48 (m, 3H), 7.41 (d, *J* = 7.0 Hz, 2H), 7.28–7.22 (m, 2H), 3.70 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 167.61, 163.35 (d, *J* = 247.5 Hz), 159.12, 141.39, 136.57, 135.99, 135.01 (d, *J* = 3.75 Hz), 132.89, 132.09 (d, *J* = 8.75 Hz), 130.64, 129.81, 128.46, 128.32, 128.08, 127.42, 127.13, 126.86, 115.50 (d, *J* = 21.2 Hz), 52.44; ^{19}F NMR ($CDCl_3$, 470 MHz): δ –112.5 (m, Ar–F). EI-MS *m/z* (%): 357 (36) [M^+], 298 (100), 299 (31).



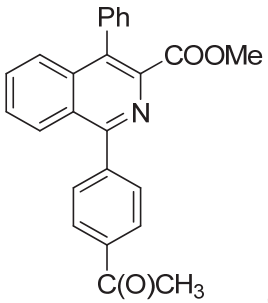
3l

Methyl 1-(4-chlorophenyl)-4-phenylisoquinoline-3-carboxylate (3l)[1]**:** Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (131.5 mg, 0.5 mmol), (4-chlorophenyl)boronic acid **2l** (156.3 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 ^{o}C for 2 h, to give **3l** (164.1 mg, 88%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1). M.p. 174–175 ^{o}C. IR (KBr, cm^{-1}): 1715.1, 1599.1, 1493.1, 1436.1, 1326.4, 1225.1, 1167.1, 1081.6, 1003.7, 968.4, 841.7, 770.2, 696.8. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.13 (d, *J* = 8.0 Hz, 1H), 7.72 (d, *J* = 8.0 Hz, 3H), 7.67 (td, *J* = 6.5, 1.0 Hz, 1H), 7.63 (td, *J* = 6.5, 1.5 Hz, 1H), 7.55–7.48 (m, 5H), 7.40 (dd, *J* = 8.0, 1.5 Hz, 2H), 3.70 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 167.49, 158.90, 141.35, 137.22, 136.59, 135.88, 135.23, 133.09, 131.61, 130.76, 129.80, 128.73, 128.57, 128.33, 128.13, 127.32, 127.04, 126.91, 52.47. EI-MS *m/z* (%): 373 (42) [M^+ (^{35}Cl)], 375 (20) [M^+ (^{37}Cl)], 314 (100), 315 (51), 316 (39).



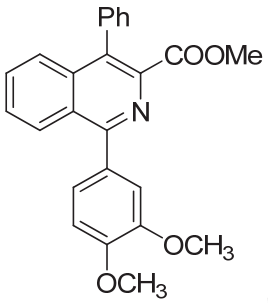
3m

Methyl 4-phenyl-1-(4-(trifluoromethyl)phenyl)isoquinoline-3-carboxylate (3m)[1]**:** Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (131.5 mg, 0.5 mmol), (4-(trifluoromethyl)phenyl)boronic acid **2m** (190.0 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 ^oC for 2 h, to give **3m** (160.8 mg, 79%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1). M.p. 164–166 ^oC. IR (KBr, cm^{-1}): 1719.6, 1325.7, 1228.3, 1164.8, 1116.6, 1063.8, 1009.3, 850.6, 772.7, 705.3, 604.8. ^1H NMR ($CDCl_3$, 500 MHz): δ 8.09 (d, *J* = 8.0 Hz, 1H), 7.90 (d, *J* = 8.0 Hz, 2H), 7.83 (d, *J* = 8.5 Hz, 2H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.69 (td, *J* = 5.5, 1.0 Hz, 1H), 7.64 (td, *J* = 7.0, 1.5 Hz, 1H), 7.57–7.49 (m, 3H), 7.41 (dd, *J* = 8.0, 1.0 Hz, 2H), 3.70 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 167.45, 158.61, 142.40 (q, *J* = 1.0 Hz), 141.48, 136.58, 135.79, 133.46, 131.27 (q, *J* = 32.5 Hz), 130.85, 130.61, 129.77, 128.73, 128.36, 128.19, 127.39, 127.09, 126.99, 125.47 (q, *J* = 3.75 Hz), 124.14 (q, *J* = 270.0 Hz), 52.49; ^{19}F NMR ($CDCl_3$, 470 MHz): δ –62.58 (s, Ar–CF_3). EI-MS *m/z*: 407 (34) [M^+], 348 (100), 349 (41), 346 (16), 278 (15).



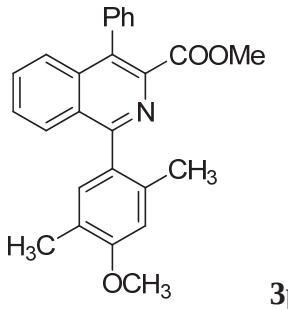
3n

Methyl 1-(4-acetylphenyl)-4-phenylisoquinoline-3-carboxylate (3n): Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (131.5 mg, 0.5 mmol), (4-acetylphenyl)boronic acid **2n** (164.0 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 ^oC for 2 h, to give **3n** (169.5 mg, 89%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 20:1 to 5:1). M.p. 209–210 ^oC. IR (KBr, cm^{-1}): 1727.0, 1683.2, 1265.2, 1231.8, 773.9. ^1H NMR ($CDCl_3$, 500 MHz): δ 8.15 (d, *J* = 7.5 Hz, 2H), 8.10 (d, *J* = 8.5 Hz, 1H), 7.88 (d, *J* = 8.0 Hz, 2H), 7.73 (d, *J* = 8.0 Hz, 1H), 7.68 (td, *J* = 6.5, 1.0 Hz, 1H), 7.63 (td, *J* = 8.5, 1.0 Hz, 1H), 7.56–7.48 (m, 3H), 7.40 (d, *J* = 7.0 Hz, 2H), 3.69 (s, 3H), 2.69 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 197.84, 167.49, 158.92, 143.39, 141.49, 137.23, 136.55, 135.83, 133.34, 130.80, 130.56, 129.78, 128.65, 128.46, 128.35, 128.17, 127.19, 127.02, 126.94, 52.48, 26.86. EI-MS *m/z* (%): 381 (43) [M^+], 322 (100), 225 (52), 323 (51), 278 (48). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{25}H_{19}NO_3$: 382.1443; found: 382.1434.



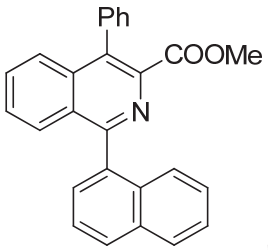
3o

Methyl 1-(3,4-dimethoxyphenyl)-4-phenylisoquinoline-3-carboxylate (3o): Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (131.5 mg, 0.5 mmol), (3,4-dimethoxyphenyl)boronic acid **2o** (182.0 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 ^oC for 2 h, to give **3o** (197.5 mg, 99%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1). M.p. 162–163 ^oC. IR (KBr, cm^{-1}): 1735.1, 1513.0, 1227.1, 1168.5, 766.4. ^1H NMR ($CDCl_3$, 500 MHz): δ 8.24 (d, *J* = 8.0 Hz, 1H), 7.71–7.58 (m, 3H), 7.55–7.45 (m, 3H), 7.40 (d, *J* = 6.5 Hz, 2H), 7.36–7.29 (m, 2H), 7.04 (d, *J* = 8.5 Hz, 1H), 3.97 (s, 3H), 3.96 (s, 3H), 3.69 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 167.64, 159.92, 149.90, 149.12, 141.29, 136.60, 136.03, 132.38, 131.47, 130.60, 129.86, 128.30, 128.26, 128.04, 127.85, 127.23, 126.71, 123.19, 113.43, 110.91, 56.11, 52.40. EI-MS *m/z* (%): 399 (96) [M^+], 225 (100), 77 (73). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{25}H_{11}NO_4$: 400.1549; found: 400.1539.



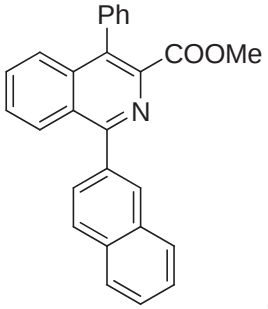
3p

Methyl 1-(4-methoxy-2,5-dimethylphenyl)-4-phenylisoquinoline-3-carboxylate (3p): Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (131.5 mg, 0.5 mmol), (4-methoxy-2,5-dimethylphenyl)boronic acid **2p** (180.0 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 ^oC for 2 h, to give **3p** (152.8 mg, 77%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1). M.p. 228–229 ^oC. IR (KBr, cm^{-1}): 1729.8, 1331.6, 1228.3, 1184.9, 772.4, 697.2. ^1H NMR ($CDCl_3$, 500 MHz): δ 7.81 (d, *J* = 8.5 Hz, 1H), 7.70 (d, *J* = 8.5 Hz, 1H), 7.63 (td, *J* = 7.0, 1.0 Hz, 1H), 7.59–7.47 (m, 4H), 7.46 (d, *J* = 7.5 Hz, 1H), 7.41 (d, *J* = 6.5 Hz, 1H), 7.19 (s, 1H), 6.81(s, 1H), 3.90 (s, 3H), 3.70 (s, 3H), 2.24 (s, 3H), 2.14 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 167.67, 161.02, 158.06, 141.33, 136.09, 136.01, 135.41, 132.47, 132.21, 130.61, 130.12, 129.89, 128.32, 128.26, 128.18, 128.02, 127.98, 126.58, 123.89, 111.93, 55.50, 52.43, 20.20, 15.77. EI-MS *m/z* (%): 397 (58) [M^+], 336 (100), 396 (69), 337 (26), 278 (18), 398 (10). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{26}H_{23}NO_3$: 398.1756; found: 398.1752.



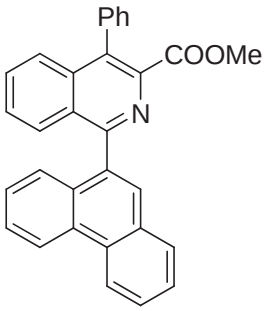
3q

Methyl 1-(naphthalen-1-yl)-4-phenylisoquinoline-3-carboxylate (3q)[1]**:** Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (131.5 mg, 0.5 mmol), naphthalen-1-ylboronic acid **2q** (172.0 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 ^oC for 2 h, to give **3q** (169.2 mg, 87%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1). M.p. 198–199 ^oC. IR (KBr, cm^{-1}): 1726.2, 1639.7, 1500.7, 1440.2, 1376.2, 1327.9, 1228.3, 1162.8, 1115.9, 774.0, 694.2, 615.5. ^1H NMR ($CDCl_3$, 500 MHz): δ 8.02 (d, *J* = 8.0 Hz, 1H), 7.96 (d, *J* = 8.5 Hz, 1H), 7.77 (d, *J* = 8.5 Hz, 1H), 7.71–7.62 (m, 4H), 7.59–7.44 (m, 8H), 7.37 (t, *J* = 8.0 Hz, 1H), 3.71 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 167.68, 159.97, 141.68, 136.33, 136.07, 136.06, 133.75, 133.16, 132.41, 130.80, 129.94, 129.88, 129.20, 128.73, 128.40, 128.36, 128.31, 128.14, 128.00, 126.63, 126.49, 126.09, 126.07, 125.31, 52.53. EI-MS *m/z* (%): 389 (62) [M^+], 328 (100), 225 (61), 329 (55).



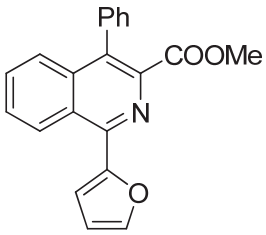
3r

Methyl 1-(naphthalen-2-yl)-4-phenylisoquinoline-3-carboxylate (3r): Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (131.5 mg, 0.5 mmol), naphthalen-2-ylboronic acid **2r** (172.0 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 ^oC for 2 h, to give **3r** (192.5 mg, 99%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1). M.p. 129–130 ^oC. IR (KBr, cm^{-1}): 1735.0, 1221.4, 1164.7, 1102.3, 764.3, 477.3. ^1H NMR ($CDCl_3$, 500 MHz): δ 8.28 (s, 1H), 8.24 (d, *J* = 8.5 Hz, 1H), 8.04 (d, *J* = 8.5 Hz, 1H), 7.98–7.94 (m, 2H), 7.91 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.76 (d, *J* = 8.5 Hz, 1H), 7.67 (td, *J* = 7.0, 1.5 Hz, 1H), 7.60 (td, *J* = 8.0, 1.5 Hz, 1H), 7.59–7.49 (m, 5H), 7.46 (d, *J* = 7.5 Hz, 2H), 3.73 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 167.74, 160.21, 141.55, 136.60, 136.34, 136.13, 133.49, 133.22, 132.81, 130.64, 129.94, 129.90, 128.57, 128.44, 128.36, 128.16, 128.10, 127.82, 127.74, 127.39, 126.82, 126.79, 126.50, 52.47. EI-MS *m/z* (%): 389 (71) [M^+], 330 (100), 328 (77), 164 (68), 329 (60). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{27}H_{19}NO_2$: 390.1494; found: 390.1487.



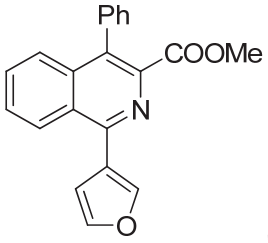
3s

Methyl 1-(phenanthren-9-yl)-4-phenylisoquinoline-3-carboxylate (3s): Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (131.5 mg, 0.5 mmol), phenanthren-9-ylboronic acid **2s** (222.0 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 ^oC for 2 h, to give **3s** (201.9 mg, 92%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1). M.p. 193–194 ^oC. IR (KBr, cm^{-1}): 1725.6, 1325.5, 1221.5, 1159.8, 998.1, 764.1, 711.1, 698.3. ^1H NMR ($CDCl_3$, 500 MHz): δ 8.83 (d, *J* = 8.5 Hz, 1H), 8.80 (d, *J* = 8.0 Hz, 1H), 7.97 (s, 1H), 7.95 (d, *J* = 8.0 Hz, 1H), 7.80–7.73 (m, 3H), 7.71–7.62 (m, 3H), 7.61–7.44 (m, 8H), 3.72 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 167.65, 159.93, 141.73, 136.10, 136.05, 135.09, 133.39, 131.41, 131.31, 130.90, 130.73, 130.62, 129.96, 129.87, 129.24, 129.09, 128.86, 128.46, 128.44, 128.37, 128.18, 128.01, 127.32, 127.06, 127.01, 126.85, 126.81, 126.69, 122.96, 122.68, 52.57. EI-MS *m/z* (%): 439 (26) [M^+], 378 (100), 379 (60), 377 (34), 380 (25). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{31}H_{21}NO_2$: 440.1651; found: 440.1646.



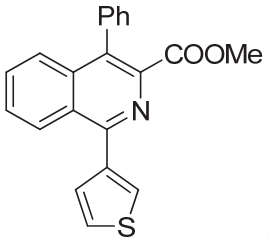
3t

Methyl 1-(furan-2-yl)-4-phenylisoquinoline-3-carboxylate (3t): Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (131.5 mg, 0.5 mmol), furan-2-ylboronic acid **2t** (112.0 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 ^oC for 2 h, to give **3t** (97.1 mg, 59%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 10:1 to 5:1). M.p. 202–203 ^oC. IR (KBr, cm^{-1}): 1721.7, 1332.8, 1237.9, 1197.9, 1005.9, 766.7, 698.4. ^1H NMR ($CDCl_3$, 500 MHz): δ 8.88 (d, *J* = 8.5 Hz, 1H), 7.77–7.62 (m, 4H), 7.55–7.44 (m, 3H), 7.37 (d, *J* = 7.0 Hz, 2H), 7.31 (d, *J* = 3.0 Hz, 1H), 6.65 (s, 1H), 3.71 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 167.38, 153.22, 148.46, 144.26, 141.34, 136.86, 136.09, 132.89, 130.58, 129.83, 128.79, 128.27, 128.01, 126.88, 126.86, 125.88, 113.82, 111.95, 52.41. EI-MS *m/z* (%): 329 (45) [M^+], 270 (100), 77 (23), 240 (19), 270 (19). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{21}H_{15}NO_3$: 330.1130; found: 330.1125.



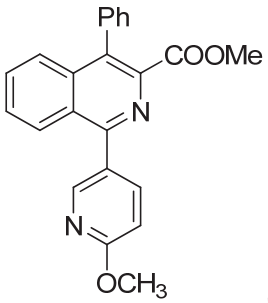
3u

Methyl 1-(furan-3-yl)-4-phenylisoquinoline-3-carboxylate (3u): Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (131.5 mg, 0.5 mmol), furan-2-ylboronic acid **2u** (112.0 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 ^oC for 2 h, to give **3u** (121.7 mg, 74%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1). M.p. 176–177 ^oC. IR (KBr, cm^{-1}): 1727.1, 1550.2, 1508.5, 1326.9, 1228.4, 1071.5, 771.8, 695.6. ^1H NMR ($CDCl_3$, 500 MHz): δ 8.42 (dd, *J* = 8.5, 2.5 Hz, 1H), 8.02 (s, 1H), 7.72–7.64 (m, 3H), 7.61 (t, *J* = 1.5 Hz, 1H), 7.55–7.45 (m, 3H), 7.38 (dd, *J* = 8.0, 1.5 Hz, 2H), 7.01 (d, *J* = 1.0 Hz, 1H), 3.70 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 167.56, 152.68, 143.20, 143.01, 141.46, 136.42, 136.04, 132.58, 130.64, 129.82, 128.58, 128.28, 128.01, 127.29, 126.93, 126.72, 124.82, 112.04, 52.38. EI-MS *m/z* (%): 329 (42) [M^+], 270 (100), 328 (44), 241 (43), 240 (30). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{21}H_{15}NO_3$: 330.1130; found: 330.1120.



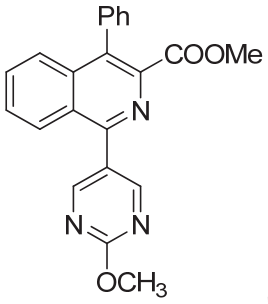
3v

Methyl 4-phenyl-1-(thiophen-3-yl)isoquinoline-3-carboxylate (3v): Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (131.5 mg, 0.5 mmol), thiophen-3-ylboronic acid **2v** (128.0 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 ^oC for 2 h, to give **3v** (162.1 mg, 94%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1). M.p. 196–198 ^oC. IR (KBr, cm^{-1}): 1722.6, 1328.6, 1230.4, 1164.4, 769.4, 704.7. ^1H NMR ($CDCl_3$, 500 MHz): δ 8.39–8.33 (m, 1H), 7.81 (d, *J* = 1.5 Hz, 1H), 7.74–7.64 (m, 3H), 7.60 (d, *J* = 4.0 Hz, 1H), 7.56–7.46 (m, 4H), 7.39 (d, *J* = 6.5 Hz, 2H), 3.70 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 167.52, 155.38, 141.28, 139.91, 136.55, 136.02, 132.74, 130.69, 129.83, 129.47, 128.54, 128.31, 128.05, 127.35, 127.33, 127.09, 126.80, 125.89, 52.43. EI-MS *m/z* (%): 345 (55) [M^+], 303 (100), 286 (77), 285 (77), 269 (75). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{21}H_{15}NO_2S$: 346.0902; found: 346.0894.



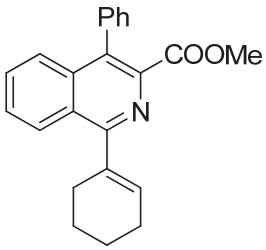
3w

Methyl 1-(6-methoxypyridin-3-yl)-4-phenylisoquinoline-3-carboxylate (3w): Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (131.5 mg, 0.5 mmol), (6-methoxypyridin-3-yl)boronic acid **2w** (153.0 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 ^oC for 2 h, to give **3w** (177.2 mg, 96%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1). M.p. 112–113 ^oC. IR (KBr, cm^{-1}): 1723.6, 1599.3, 1493.8, 1370.9, 1328.1, 1225.2, 1011.7, 841.0, 767.5, 698.3. ^1H NMR ($CDCl_3$, 500 MHz): δ 8.58 (d, *J* = 2.5 Hz, 1H), 8.18 (dd, *J* = 7.5, 1.5 Hz, 1H), 8.04 (dd, *J* = 8.5, 2.5 Hz, 1H), 7.75–7.59 (m, 3H), 7.55–7.45 (m, 3H), 7.39 (dd, *J* = 8.0, 1.5 Hz, 2H), 6.94 (d, *J* = 8.5 Hz, 1H), 4.03 (s, 3H), 3.69 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 167.55, 164.49, 157.19, 148.30, 141.54, 140.52, 136.60, 135.95, 132.90, 130.72, 129.80, 128.60, 128.32, 128.13, 128.09, 127.27, 127.12, 126.93, 110.90, 53.78, 52.43. EI-MS *m/z* (%): 370 (84) [M^+], 76 (100), 309 (86), 235 (66), 338 (54). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{23}H_{18}N_2O_3$: 371.1396; found: 371.1386.



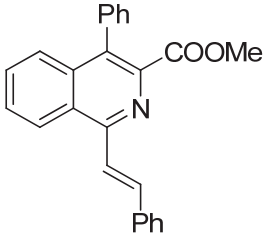
3x

Methyl 1-(2-methoxypyrimidin-5-yl)-4-phenylisoquinoline-3-carboxylate (3x): Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (131.5 mg, 0.5 mmol), (2-methoxypyrimidin-5-yl)boronic acid **2x** (154.0 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 ^oC for 2 h, to give **3x** (159.3 mg, 86%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 10:1 to 5:1). M.p. 180–181 ^oC. IR (KBr, cm^{-1}): 1735.1, 1593.6, 1546.4, 1482.0, 1384.4, 1331.6, 1227.4, 1180.8, 1037.5, 774.6, 695.7. ^1H NMR ($CDCl_3$, 500 MHz): δ 8.95 (s, 2H), 8.14–8.07 (m, 1H), 7.77–7.66 (m, 3H), 7.56–7.46 (m, 3H), 7.38 (dd, *J* = 8.0, 1.5 Hz, 2H), 4.12 (s, 3H), 3.69 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 167.26, 165.59, 160.29, 153.99, 141.70, 136.66, 135.57, 133.66, 131.10, 129.72, 129.16, 128.38, 128.27, 127.24, 127.21, 126.57, 126.29, 55.37, 52.53. EI-MS *m/z* (%): 371 (61) [M^+], 279 (100), 310 (68), 311 (46), 339 (49). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{22}H_{17}N_3O_3$: 372.1348; found: 372.1335.



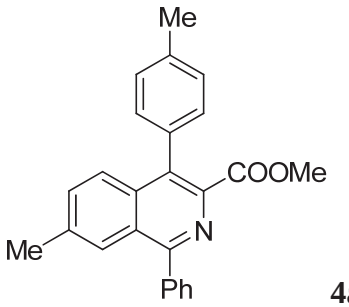
3y

Methyl 1-(cyclohex-1-en-1-yl)-4-phenylisoquinoline-3-carboxylate (3y): Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (131.5 mg, 0.5 mmol), cyclohex-1-en-1-ylboronic acid **2y** (126.0 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 ^oC for 2 h, to give **3y** (133.8 mg, 78%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1). M.p. 147–148 ^oC. IR (KBr, cm^{-1}): 2928.8, 1724.9, 1441.9, 1326.0, 1228.0, 1165.4, 997.7, 765.8, 698.4. ^1H NMR ($CDCl_3$, 500 MHz): δ 8.35–8.30 (m, 1H), 7.66–7.59 (m, 3H), 7.52–7.42 (m, 3H), 7.35 (d, *J* = 7.0 Hz, 2H), 6.06–6.03 (m, 1H), 3.67 (s, 3H), 2.64–2.61 (m, 2H), 2.36–2.31 (m, 2H), 1.96–1.88 (m, 2H), 1.87–1.79 (m, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 167.74, 162.86, 140.99, 136.41, 136.39, 136.20, 131.97, 131.29, 130.50, 129.84, 128.23, 127.90, 127.89, 127.51, 126.86, 126.60, 52.34, 29.03, 25.53, 22.78, 21.97. EI-MS *m/z* (%): 343 (100) [M^+], 282 (99), 282 (39), 270 (38), 225 (36). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{23}H_{21}NO_2$: 344.1651; found: 344.1644.



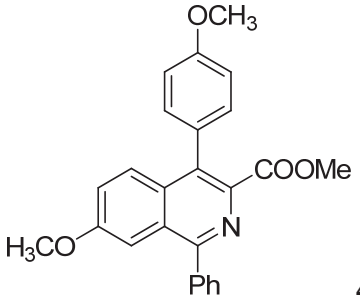
3z

Methyl (*E*)-4-phenyl-1-styrylisoquinoline-3-carboxylate (3z): Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (131.5 mg, 0.5 mmol), (*E*)-styrylboronic acid **2z** (148.0 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 ^oC for 2 h, to give **3z** (133.2 mg, 73%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 20:1). M.p. 171–172 ^oC. IR (KBr, cm^{-1}): 1720.3, 1640.3, 1550.1, 1221.8, 1023.5, 959.1, 757.7, 696.8. ^1H NMR ($CDCl_3$, 500 MHz): δ 8.47 (d, *J* = 8.0 Hz, 1H), 8.15–8.00 (m, 2H), 7.76–7.63 (m, 5H), 7.55–7.33 (m, 8H), 3.72 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 167.96, 154.17, 141.82, 137.43, 136.81, 136.34, 136.30, 132.36, 130.44, 129.91, 128.83, 128.80, 128.32, 128.28, 127.96, 127.63, 127.01, 126.94, 124.59, 122.22, 52.35. EI-MS *m/z* (%): 365 (27) [M^+], 304 (100), 350 (35), 77 (25), 152 (23), 280 (18). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{25}H_{19}NO_2$: 366.1494; found: 366.1487.



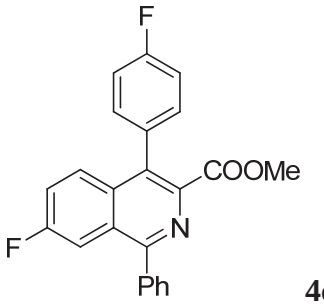
4a

Methyl 7-methyl-1-phenyl-4-(p-tolyl)isoquinoline-3-carboxylate (4a)[1]**:** Following the general procedure, methyl 2-isocyano-3,3-di-*p*-tolylacrylate **1a'** (145.5 mg, 0.5 mmol), phenylboronic acid **2a** (122.0 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 ^oC for 2 h, to give **4a** (154.1 mg, 84%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 20:1 to 5:1). M.p. 144–145 ^oC. IR (KBr, cm^{-1}): 1724.9, 1313.7, 1224.7, 1164.0, 1012.2, 770.8, 700.8, 523.8. ^1H NMR ($CDCl_3$, 500 MHz): δ 7.91 (s, 1H), 7.78–7.73 (m, 2H), 7.63 (d, *J* = 8.5 Hz, 1H), 7.59–7.45 (m, 4H), 7.35–7.27 (m, 4H), 3.73 (s, 3H), 2.48 (s, 3H), 2.47 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 167.75, 159.31, 140.51, 139.07, 138.59, 137.62, 134.93, 133.19, 133.01, 132.70, 130.19, 129.67, 129.03, 128.80, 128.44, 127.45, 126.71, 126.50, 52.43, 21.96, 21.45. EI-MS *m/z* (%): 367 (52) [M^+], 308 (100), 309 (30), 322 (14), 294 (69).



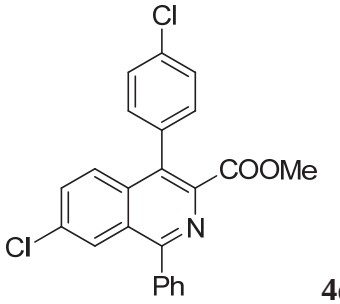
4b

Methyl 7-methoxy-4-(4-methoxyphenyl)-1-phenylisoquinoline-3-carboxylate (4b)[1]**:** Following the general procedure, methyl 2-isocyano-3,3-bis(4-methoxyphenyl)acrylate **1b** (161.5 mg, 0.5 mmol), phenylboronic acid **2a** (122.0 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 ^oC for 2 h, to give **4b** (186.1 mg, 93%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 10:1 to 5:1). M.p. 179–180 ^oC. IR (KBr, cm^{-1}): 1719.9, 1612.6, 1508.7, 1407.4, 1218.0, 1175.7, 1025.6, 846.8, 700.4. ^1H NMR ($CDCl_3$, 500 MHz): δ 7.77 (d, *J* = 7.0 Hz, 2H), 7.65 (d, *J* = 9.0 Hz, 1H), 7.55 (t, *J* = 7.0 Hz, 2H), 7.50 (d, *J* = 7.5 Hz, 1H), 7.44 (d, *J* = 2.5 Hz, 1H), 7.33–7.26 (m, 3H), 7.04 (d, *J* = 8.5 Hz, 2H), 3.90 (s, 3H), 3.81 (s, 3H), 3.72 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 167.83, 159.33, 159.22, 158.29, 139.78, 139.21, 132.87, 132.20, 130.93, 129.94, 128.81, 128.78, 128.56, 128.54, 128.34, 122.91, 113.76, 105.63, 55.47, 55.29, 52.41. EI-MS *m/z* (%): 399 (99) [M^+], 340 (100), 77 (38), 341 (47), 77 (38).



4c

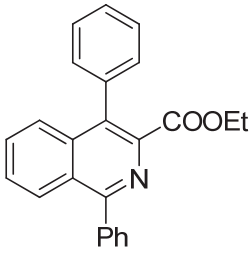
Methyl 7-fluoro-4-(4-fluorophenyl)-1-phenylisoquinoline-3-carboxylate (4c)[1]**:** Following the general procedure, methyl 3,3-bis(4-fluorophenyl)-2-isocyanoacrylate **1c** (149.5 mg, 0.5 mmol), phenylboronic acid **2a** (120.0 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 ^oC for 2 h, to give **4c** (168.3 mg, 90%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1). M.p. 189–190 ^oC. IR (KBr, cm^{-1}): 1726.1, 1621.6, 1508.0, 1408.0, 1225.7, 1191.9, 1157.7, 848.1, 709.9. ^1H NMR ($CDCl_3$, 500 MHz): δ 7.80 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.74 (d, *J* = 7.5 Hz, 2H), 7.69 (dd, *J* = 9.0, 5.5 Hz, 1H), 7.59–7.53 (m, 3H), 7.44 (td, *J* = 8.0, 2.0 Hz, 1H), 7.40–7.34 (m, 2H), 7.22 (t, *J* = 8.5 Hz, 2H), 3.73 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 167.26, 162.71 (d, *J* = 246.2 Hz), 161.72 (d, *J* = 248.7 Hz), 159.88 (d, *J* = 5.0 Hz), 141.05 (d, *J* = 2.5 Hz), 138.27, 133.72, 131.79 (d, *J* = 1.3 Hz), 131.62 (d, *J* = 3.7 Hz), 131.51 (d, *J* = 8.7 Hz) 129.99, 129.58 (d, *J* = 8.7 Hz), 129.28, 128.68, 128.41 (d, *J* = 8.7 Hz), 121.13 (d, *J* = 25.0 Hz), 115.56 (d, *J* = 21.2 Hz), 111.40 (d, *J* = 22.5 Hz), 52.56; ^{19}F NMR ($CDCl_3$, 470 MHz): δ –108.7 (m, Ar–F), –113.3 (m, Ar–F). EI-MS *m/z* (%): 375 (31) [M^+], 316 (100), 314 (44), 317 (33), 157 (15).



4d

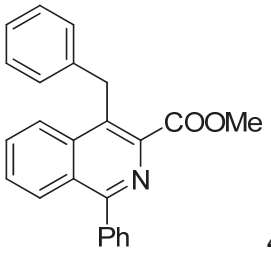
Methyl 7-chloro-4-(4-chlorophenyl)-1-phenylisoquinoline-3-carboxylate (4d): Following the general procedure, methyl 3,3-bis(4-chlorophenyl)-2-isocyanoacrylate **1d** (166.0 mg, 0.5 mmol), phenylboronic acid **2a** (122.0 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 ^oC for 2 h, to give **4d** (155.0 mg, 76%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1). M.p. 211–212 ^oC. IR (KBr, cm^{-1}): 1727.0, 1488.6, 1399.4, 1292.7, 1219.8, 1172.4, 1008.9, 974.3, 837.0, 705.2, 527.8. ^1H NMR ($CDCl_3$, 500 MHz): δ 8.15 (s, 1H), 7.76–7.72 (m, 2H), 7.62–7.48 (m, 7H), 7.35-7.31 (m, 2H), 3.74 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 167.08, 159.73, 141.47, 138.15, 134.83, 134.77, 134.46, 134.07, 131.73, 131.54, 131.13, 130.09, 129.35, 128.77, 128.72, 128.31, 127.88, 126.63, 52.63. EI-MS *m/z* (%): 407 (47) [M^+($2\times^{35}Cl$)], 409 (33) [M^+ (^{35}Cl, ^{37}Cl)], 411 (6) [M^+ ($2\times^{37}Cl$)], 348 (100), 350 (63), 314 (48). HRMS (ESI)

([M+H]$^+$) Calcd. for $C_{23}H_{15}Cl_2NO_3$: 408.0558; found: 408.0551.



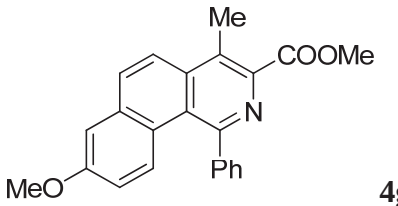
4e

Ethyl 1,4-diphenylisoquinoline-3-carboxylate (4e): Following the general procedure, ethyl 2-isocyano-3,3-diphenylacrylate **1e** (138.5 mg, 0.5 mmol), phenylboronic acid **2a** (122.0 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 ^{o}C for 2 h, to give **4e** (174.7 mg, 99%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1). M.p. 104–105 ^{o}C. IR (KBr, cm^{-1}): 1729.6, 1391.4, 1223.5, 1178.2, 1107.0, 1008.6, 770.1, 701.0. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.18 (d, *J* = 8.5 Hz, 1H), 7.80–7.75 (m, 2H), 7.73 (d, *J* = 8.0 Hz, 1H), 7.65 (td, *J* = 7.0, 1.5 Hz, 1H), 7.60 (td, *J* = 6.5, 1.0 Hz, 1H), 7.58–7.47 (m, 6H), 7.46–7.40 (m, 2H), 4.12 (q, *J* = 7.0 Hz, 2H), 0.98 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 167.54, 160.29, 142.22, 138.88, 136.40, 136.13, 131.96, 130.55, 130.26, 130.05, 128.90, 128.41, 128.27, 128.14, 128.02, 127.78, 127.07, 126.57, 61.30, 13.70. EI-MS *m/z* (%): 353 (21) [M$^+$], 280 (100), 281 (33), 277 (18), 279 (15). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{24}H_{19}NO_2$: 354.1494; found: 354.1488.



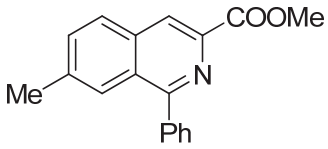
4f

Methyl 4-benzyl-1-phenylisoquinoline-3-carboxylate (4f)[1]**:** Following the general procedure, methyl (*Z*)-2-isocyano-3,4-diphenylbut-2-enoate **1f** (138.5 mg, 0.5 mmol), phenylboronic acid **2a** (122.0 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 ^{o}C for 2 h, to give **4f** (150.0 mg, 85%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1). M.p. 96–97 ^{o}C. IR (KBr, cm^{-1}): 1722.7, 1441.5, 1380.9, 1248.0, 1213.6, 1070.9, 990.9, 771.4, 703.0. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.02 (t, *J* = 8.5 Hz, 2H), 7.63 (d, *J* = 6.5 Hz, 2H), 7.57 (t, *J* = 7.5 Hz, 1H), 7.49–7.41 (m, 4H), 7.20–7.06 (m, 5H), 4.66 (s, 2H), 3.87 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 168.05, 159.76, 142.33, 139.91, 138.94, 136.50, 130.67, 130.23, 129.62, 128.87, 128.56, 128.44, 128.37, 128.15, 127.60, 126.18, 125.22, 52.82, 33.89. EI-MS *m/z* (%): 353 (67) [M$^+$], 321 (100), 320 (57), 292 (72), 293 (24).



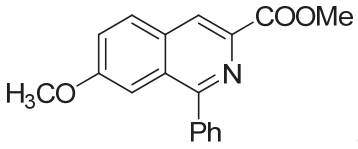
4g

Methyl 8-methoxy-4-methyl-1-phenylbenzo[h]isoquinoline-3-carboxylate (4g)[1]**:** Following the general procedure, methyl (*Z*)-2-isocyano-3-(6-methoxy-naphthalen-2-yl)but-2-enoate **1g** (140.5 mg, 0.5 mmol), phenylboronic acid **2a** (122.0 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 °C for 2 h, to give **4g** (137.4 mg, 77%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1). M.p. 181–182 °C. IR (KBr, cm^{-1}): 1708.6, 1609.2, 1504.4, 1448.2, 1346.8, 1219.9, 1206.8, 1137.4, 1021.5, 847.6, 708.5, 623.9. ^1H NMR ($CDCl_3$, 500 MHz): δ 8.02 (d, *J* = 9.0 Hz, 1H), 7.92 (d, *J* = 9.0 Hz, 1H), 7.66 (d, *J* = 9.5 Hz, 1H), 7.60–7.52 (m, 2H), 7.50–7.40 (m, 3H), 7.24–7.20 (m, 1H), 6.81 (dd, *J* = 9.0, 2.5 Hz, 1H), 4.01 (s, 3H), 3.90 (s, 3H), 2.90 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 168.00, 158.51, 155.83, 143.60, 141.49, 136.66, 135.13, 131.72, 130.08, 129.21, 129.13, 128.45, 127.65, 125.01, 123.71, 122.02, 116.50, 108.35, 55.36, 52.65, 14.78. EI-MS *m/z* (%): 357 (90) [M^+], 299 (100), 358 (24), 297 (73), 254 (36).



4h

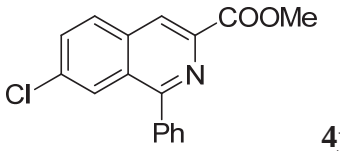
Methyl 7-methyl-1-phenylisoquinoline-3-carboxylate (4h): Following the general procedure, methyl (*Z*)-2-isocyano-3-(*p*-tolyl)acrylate **1h** (100.5 mg, 0.5 mmol), phenylboronic acid **2a** (122.0 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 °C for 2 h, to give **4h** (70.6 mg, 51%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1). M.p. 179–180 °C. IR (KBr, cm^{-1}): 1712.8, 1445.7, 1322.5, 1298.6, 1239.4, 1002.7, 815.0, 758.7, 699.5. ^1H NMR ($CDCl_3$, 500 MHz): δ 8.52 (s, 1H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.85 (s, 1H), 7.70–7.65 (m, 2H), 7.58 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.54–7.46 (m, 3H), 4.00 (s, 3H), 2.48 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 166.70, 160.48, 140.15, 139.94, 139.12, 134.78, 132.92, 130.12, 128.79, 128.49, 128.41, 128.29, 126.66, 123.25, 52.82, 22.24. EI-MS *m/z* (%): 277 (28) [M^+], 219 (100), 216 (33), 217 (30), 218 (24). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{18}H_{15}NO_2$: 278.1181; found: 278.1177.



4i

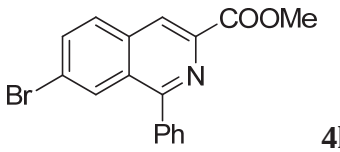
Methyl 7-methoxy-1-phenylisoquinoline-3-carboxylate (4i)[1]**:** Following the general procedure, methyl (*Z*)-2-isocyano-3-(4-methoxyphenyl)acrylate **1i** (108.5 mg, 0.5 mmol), phenylboronic acid **2a** (122.0 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 °C for 2 h, to give **4i** (92.3 mg, 63%) as a

white solid after purification on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1). M.p. 157–158 °C. IR (KBr, cm^{-1}): 1704.5, 1618.3, 1496.9, 1406.8, 1301.9, 1213.2, 1113.5, 1002.3, 708.4. ^1H NMR ($CDCl_3$, 500 MHz): δ 8.51 (s, 1H), 7.92 (d, *J* = 8.5 Hz, 1H), 7.73–7.71 (m, 2H), 7.54–7.48 (m, 3H), 7.43–7.38 (m, 2H), 4.02 (s, 3H), 3.81 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 166.71, 160.24, 159.46, 139.19, 131.93, 130.05, 129.87, 129.78, 128.83, 128.51, 123.40, 123.21, 105.83, 55.50, 52.76. EI-MS *m/z* (%): 293 (40) [M^+], 235 (100), 193 (33), 232 (20), 191 (21).



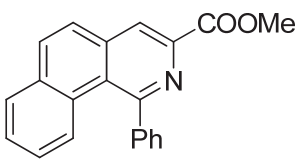
4j

Methyl 7-chloro-1-phenylisoquinoline-3-carboxylate (4j): Following the general procedure, methyl (*Z*)-3-(4-chlorophenyl)-2-isocyanoacrylate **1j** (110.5 mg, 0.5 mmol), phenylboronic acid **2a** (122.0 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 °C for 2 h, to give **4j** (62.4 mg, 42%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1). M.p. 196–197 °C. IR (KBr, cm^{-1}): 1715.8, 1283.3, 1237.8, 1076.2, 968.9, 819.3, 698.4. ^1H NMR ($CDCl_3$, 500 MHz): δ 8.54 (s, 1H), 8.10 (s, 1H), 7.96 (d, *J* = 9.0 Hz, 1H), 7.73–7.66 (m, 3H), 7.57–7.50 (m, 3H), 4.03 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 166.23, 160.40, 141.20, 138.25, 135.44, 134.90, 131.83, 130.04, 129.25, 128.79, 128.65, 126.79, 122.84, 52.97. EI-MS *m/z* (%): 297 (39) [$M^+(^{35}Cl)$], 299 (13) [$M^+(^{37}Cl)$], 239 (100), 203 (75), 204 (73), 202 (55). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{17}H_{12}ClNO_2$: 298.0635; found: 298.0627.



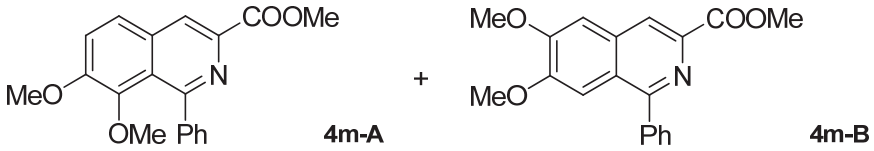
4k

Methyl 7-bromo-1-phenylisoquinoline-3-carboxylate (4k): Following the general procedure, methyl (*Z*)-3-(4-bromophenyl)-2-isocyanoacrylate **1k** (133.0 mg, 0.5 mmol), phenylboronic acid **2a** (122.0 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 °C for 2 h, to give **4k** (92.3 mg, 54%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1). M.p. 205–206 °C. IR (KBr, cm^{-1}): 1714.2, 1443.7, 1282.5, 1237.5, 1102.8, 1001.0, 810.1, 692.8. ^1H NMR ($CDCl_3$, 500 MHz): δ 8.52 (s, 1H), 8.27 (s, 1H), 7.90–7.81 (m, 2H), 7.68 (d, *J* = 6.5 Hz, 2H), 7.54 (d, *J* = 7.0 Hz, 3H), 4.03 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 166.23, 160.30, 141.27, 138.25, 135.09, 134.35, 130.05, 130.01, 129.25, 129.09, 128.66, 123.74, 122.88, 52.97. EI-MS *m/z* (%): 341 (32) [M^+ (^{79}Br)], 343 (28) [M^+ (^{81}Br)], 283 (100), 342 (20), 203 (62). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{17}H_{12}BrNO_2$: 342.0130; found: 342.0122.



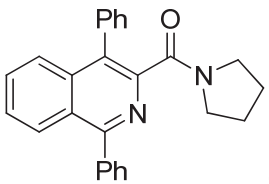
4l

Methyl 1-phenylbenzo[h]isoquinoline-3-carboxylate (4l)[1]**:** Following the general procedure, methyl (*Z*)-2-isocyano-3-(naphthalen-2-yl)acrylate **1l** (118.5 mg, 0.5 mmol), phenylboronic acid **2a** (122.0 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 °C for 2 h, to give **4l** (136.1 mg, 87%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1). M.p. 193–194 °C. IR (KBr, cm^{-1}): 1711.3, 1445.8, 1349.4, 1257.7, 1219.5, 992.4, 827.9, 756.9, 699.0. ^1H NMR ($CDCl_3$, 500 MHz): δ 8.52 (s, 1H), 7.95 (d, *J* = 8.5 Hz, 1H), 7.85 (d, *J* = 7.5 Hz, 1H), 7.76 (t, *J* = 9.0 Hz, 2H), 7.60–7.56 (m, 2H), 7.54–7.46 (m, 4H), 7.24–7.18 (m, 1H), 4.04 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 166.18, 159.32, 143.30, 141.55, 138.27, 134.29, 132.73, 129.22, 129.20, 129.11, 128.75, 128.74, 128.17, 127.69, 126.34, 126.12, 125.58, 123.01, 52.89. EI-MS *m/z* (%): 313 (41) [M^+], 255 (100), 252 (71), 254 (43), 105 (23).



4m-A **4m-B**

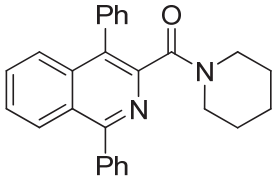
Methyl 7,8-dimethoxy-1-phenylisoquinoline-3-carboxylate (4m-A) and Methyl 6,7-dimethoxy-1-phenylisoquinoline-3-carboxylate (4m-B)[1]**:** Following the general procedure, methyl (*Z*)-3-(3,4-dimethoxyphenyl)-2-isocyanoacrylate **1m** (123.5 mg, 0.5 mmol), phenylboronic acid **2a** (122.0 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 °C for 2 h, to give **4m-A** (27.5 mg, 17%) and **4m-B** (93.7 mg, 58%) after purification on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1). Data for minor product **4m-A:** white solid. M.p. 175–177 °C. IR (KBr, cm^{-1}): 1705.3, 1509.3, 1420.5, 1256.4, 1009.3, 848.5, 707.1, 626.9. ^1H NMR ($CDCl_3$, 500 MHz): δ 8.50 (s, 1H), 7.82 (d, *J* = 8.5 Hz, 1H), 7.59 (d, *J* = 9.0 Hz, 1H), 7.55 (dd, *J* = 8.0, 2.0 Hz, 2H), 7.44–7.37 (m, 3H), 4.00 (s, 3H), 3.99 (s, 3H), 3.20 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 166.55, 158.63, 152.64, 144.59, 142.51, 138.47, 132.47, 129.07, 127.67, 127.13, 125.29, 123.79, 123.33, 119.10, 60.79, 56.68, 52.79. EI-MS *m/z* (%): 323 (23) [M^+], 348 (100), 265 (71), 266 (13), 349 (37). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{19}H_{17}NO_4$: 324.1236; found: 324.1224. Data for major product **4m-B:** white solid. M.p. 185–186 °C. IR (KBr, cm^{-1}): 1710.7, 1549.8, 1505.8, 1270.9, 1216.5, 1005.2, 697.3. ^1H NMR ($CDCl_3$, 500 MHz): δ 8.42 (s, 1H), 7.69 (d, *J* = 7.0 Hz, 2H), 7.53–7.44 (m, 3H), 7.36 (s, 1H), 7.22 (s, 1H), 4.03 (s, 3H), 3.99 (s, 3H), 3.85 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 166.78, 158.55, 153.04, 151.74, 139.94, 139.36, 133.33, 129.82, 128.75, 128.50, 124.43, 122.10, 106.26, 105.87, 56.23, 56.00, 52.73. EI-MS *m/z* (%): 323 (70) [M^+], 265 (100), 280 (75), 269 (59), 322 (51).



4n

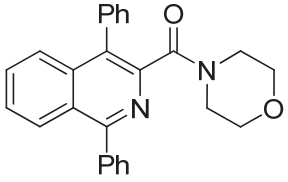
(1,4-Diphenylisoquinolin-3-yl)(pyrrolidin-1-yl)methanone (4n): Following the

general procedure, 2-isocyano-3,3-diphenyl-1-(pyrrolidin-1-yl)prop-2-en-1-one **1n** (151.0 mg, 0.5 mmol), phenylboronic acid **2a** (122.0 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 °C for 2 h, to give **4n** (151.2 mg, 80%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 10:1 to 2:1). M.p. 232–233 °C. IR (KBr, cm^{-1}): 1741.0, 1634.1, 1458.4, 1377.4, 1177.0, 765.7, 705.5. ^1H NMR ($CDCl_3$, 500 MHz): δ 8.13 (d, *J* = 8.5 Hz, 1H), 7.79 (d, *J* = 8.5 Hz, 1H), 7.74 (d, *J* = 7.0 Hz, 2H), 7.63 (t, *J* = 7.5 Hz, 1H), 7.58–7.43 (m, 9H), 3.87 (t, *J* = 7.0 Hz, 2H), 3.16 (t, *J* = 7.0 Hz, 2H), 1.72–1.63 (m, 4H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 167.24, 160.42, 146.87, 138.94, 136.22, 134.96, 130.52, 130.45, 130.16, 128.80, 128.60, 128.39, 128.36, 128.24, 127.81, 127.45, 126.51, 125.93, 47.44, 45.12, 25.74, 25.25. EI-MS *m/z* (%): 378 (4) [M^+], 280 (100), 281 (47), 309 (19), 277 (13). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{26}H_{22}N_2O$: 379.1810; found: 379.1804.



4o

(1,4-Diphenylisoquinolin-3-yl)(piperidin-1-yl)methanone (4o)[1]**:** Following the general procedure, 2-isocyano-3,3-diphenyl-1-(piperidin-1-yl)prop-2-en-1-one **1o** (158.0 mg, 0.5 mmol), phenylboronic acid **2a** (122.0 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 °C for 2 h, to give **4o** (150.9 mg, 77%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 5:1 to 3:1). M.p. 214–215 °C. IR (KBr, cm^{-1}): 1744.3, 1631.3, 1433.1, 1377.8, 1245.2, 1024.1, 985.9, 758.2, 698.0. ^1H NMR ($CDCl_3$, 500 MHz): δ 8.13 (d, *J* = 8.5 Hz, 1H), 7.79 (d, *J* = 8.5 Hz, 1H), 7.74 (d, *J* = 7.0 Hz, 2H), 7.62 (t, *J* = 7.5 Hz, 1H), 7.57–7.43 (m, 9H), 3.50 (t, *J* = 5.0 Hz, 2H), 3.10 (t, *J* = 5.0 Hz, 2H), 1.48–1.40 (m, 2H), 1.38–1.32 (m, 2H), 1.19–1.10 (m, 2H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 167.43, 160.40, 146.19, 138.98, 136.08, 134.90, 130.78, 130.49, 130.23, 128.78, 128.46, 128.36, 128.35, 128.24, 127.75, 127.36, 126.39, 125.91, 47.54, 42.09, 25.81, 25.14, 24.33. EI-MS *m/z* (%): 392 (9) [M^+], 280 (100), 281 (51), 208 (53), 256 (40).



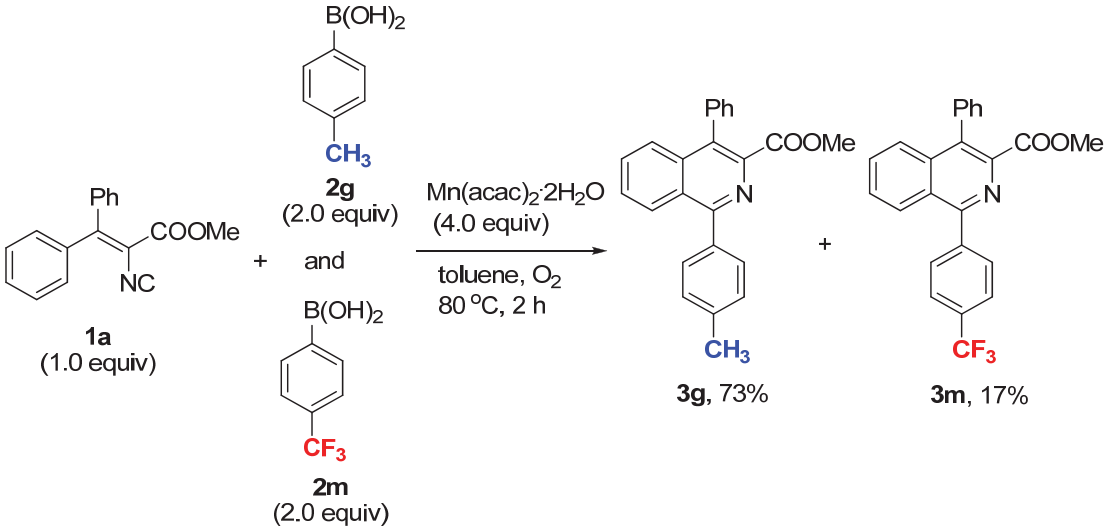
4p

(1,4-Diphenylisoquinolin-3-yl)(morpholino)methanone (4p): Following the general procedure, 2-isocyano-1-morpholino-3,3-diphenylprop-2-en-1-one **1p** (159.0 mg, 0.5 mmol), phenylboronic acid **2a** (122.0 mg, 1.0 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (253.0 mg, 1.0 mmol) in dry toluene (5.0 mL) at 80 °C for 2 h, to give **4p** (147.8 mg, 75%) as a white solid after purification on silica gel (eluent: hexane/EtOAc = 3:1 to 1:1). M.p. 243–244 °C. IR (KBr, cm^{-1}): 1637.7, 1432.7, 1272.2, 1230.5, 1109.1, 988.0, 778.3, 701.1. ^1H NMR ($CDCl_3$, 500 MHz): δ 8.16 (d, *J* = 8.5 Hz, 1H), 7.81 (d, *J* = 8.5 Hz,

1H), 7.75 (d, *J* = 7.0 Hz, 2H), 7.65 (t, *J* = 7.0 Hz, 1H), 7.60–7.48 (m, 9H), 3.58 (t, *J* = 4.5 Hz, 2H), 3.44 (t, *J* = 4.5 Hz, 2H), 3.25–3.09 (m, 4H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 167.59, 160.66, 144.98, 138.68, 125.97, 134.69, 130.76, 130.64, 130.21, 128.96, 128.88, 128.60, 128.55, 128.44, 127.88, 127.70, 126.56, 125.90, 66.43, 46.81, 41.61; EI-MS *m/z* (%): 394 (9) [M^+], 280 (100), 281 (54), 278 (12), 202 (12). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{26}H_{22}N_2O_2$: 395.1760; found: 395.1750.

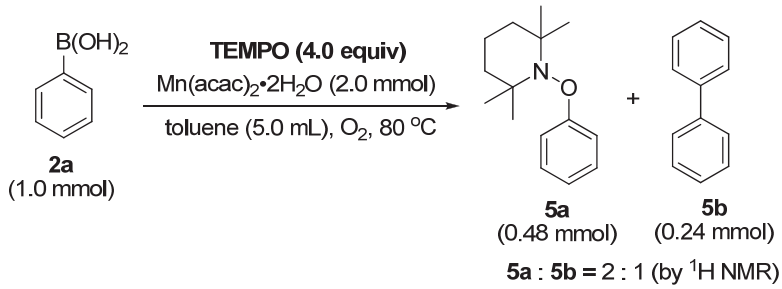
5. Mechanistic Studies

5.1 Intermolecular Competition Experiments.



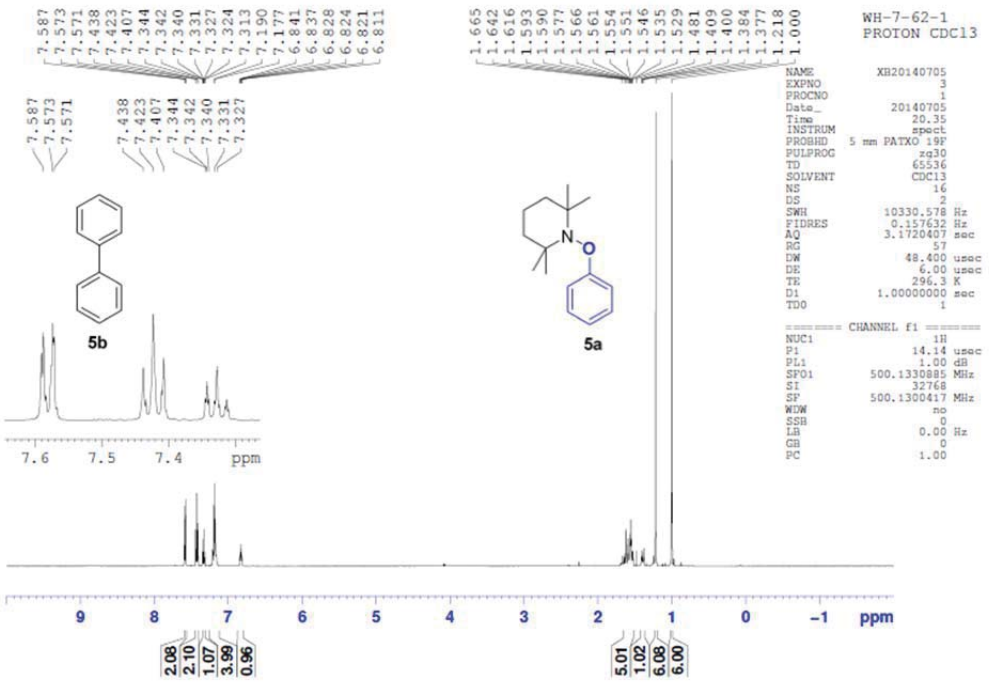
The mixture of methyl 2-isocyano-3,3-diphenylacrylate (**1a**) (78.9 mg, 0.3 mmol), *p*-tolylboronic acid) (**2g**) (81.6 mg, 0.6 mmol), (4-(trifluoromethyl)phenyl)boronic acid (**2m**) (114 mg, 0.6 mmol) and $Mn(acac)_2{\cdot}2H_2O$ (303.6 mg, 1.2 mmol) in dry toluene (5.0 mL). The tube was evacuated and backfilled with O_2 for three times. The reaction mixture was stirred in a pre-heated oil bath at 80 °C for 2 h. The reaction was cooled to room temperature, filtered through a plug of celite and then washed with EtOAc (3×20 mL). The combined organic layers were dried over Na_2SO_4 and concentrated under reduced pressure after filtration. The crude reaction mixture was purified by chromatography on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1) to give the desired product **3m** (21.2 mg, 17%) and **3g** (76.7 mg, 73%).

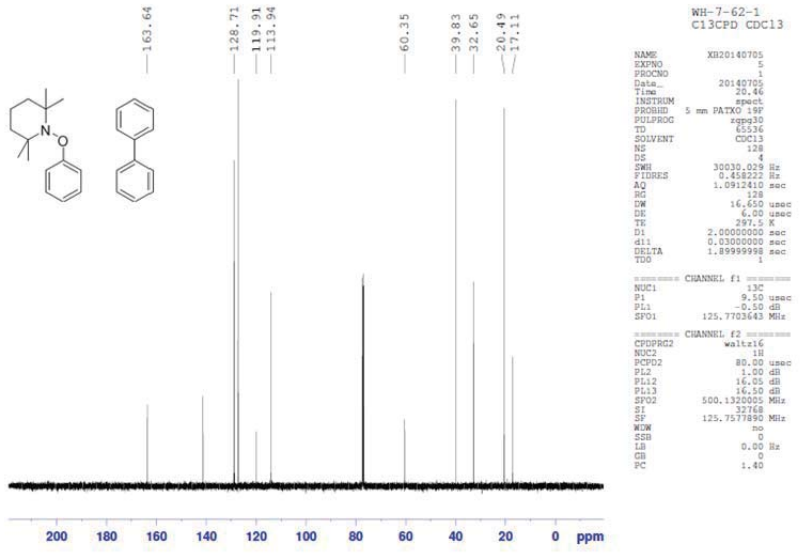
5.2 Capture of phenyl radical by TEMPO.



The tube containing a mixture of phenylboronic acid (**2a**) (122 mg, 1.0 mmol),

$Mn(acac)_2{\cdot}2H_2O$ (506 mg, 2.0 mmol), and 2,2,6,6-tetramethyl-piperidine-1-oxy (TEMPO) (624 mg, 4.0 mmol) in dry toluene (5.0 mL) was evacuated and backfilled with O_2 for three times. The reaction mixture was stirred in a pre-heated oil bath at 80 ^oC for 2 h. The reaction was cooled to room temperature, filtered through a plug of celite and then washed with EtOAc (3×20 mL). The combined organic layers were dried over Na_2SO_4 and concentrated under reduced pressure after filtration. The given crude was purified by chromatography on silica gel (eluent: hexane) to afford the product **5a** and **5b** (145.5 mg) as a mixture with a ratio at **5a**/**5b** = 2 : 1 by proton NMR analysis.



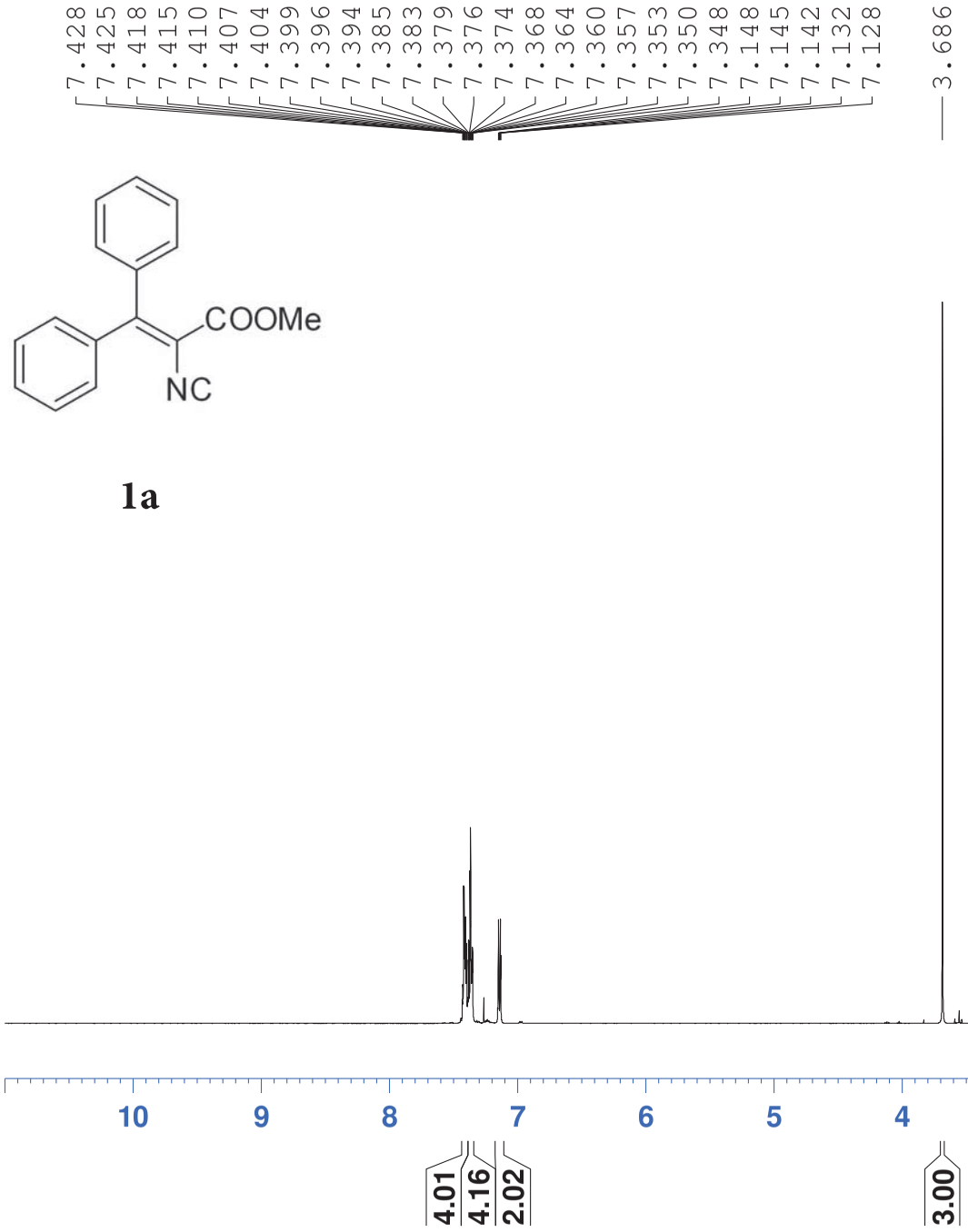


References:

(1) H. Jiang, Y. Cheng, R. Wang, Y. Zhang and S. Yu, *Chem. Comm.* 2014, **50**, 6164.

(2) M. Suzuki, K.-I. Nunami, K. Matsumoto, N. Yoneda, O. Kasuga, H. Yoshida and T. Yamaguchi, *Chem. Pharm. Bull.*1980, **28**, 2374.

(3) B. Beck, G. Larbig, B. Mejat, M. Magnin-Lachaux, A. Picard, E. Herdtweck and A. Dömling, *Org. Lett.* 2003, **5**, 1047.



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PROCNO	1
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DE	6.00 usec
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SSB	0
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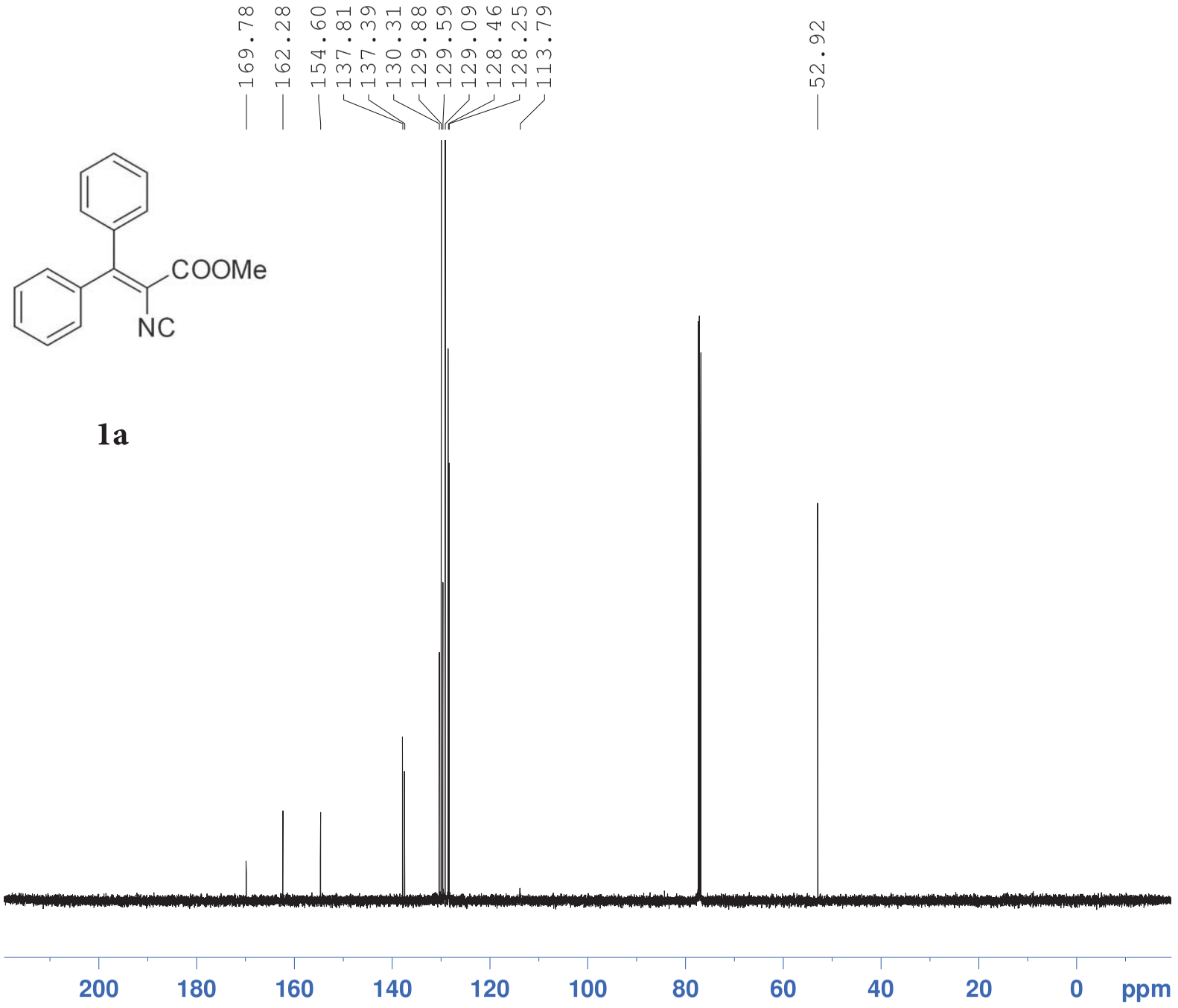
PC	1.00



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SFO1	125.7703643 MHz
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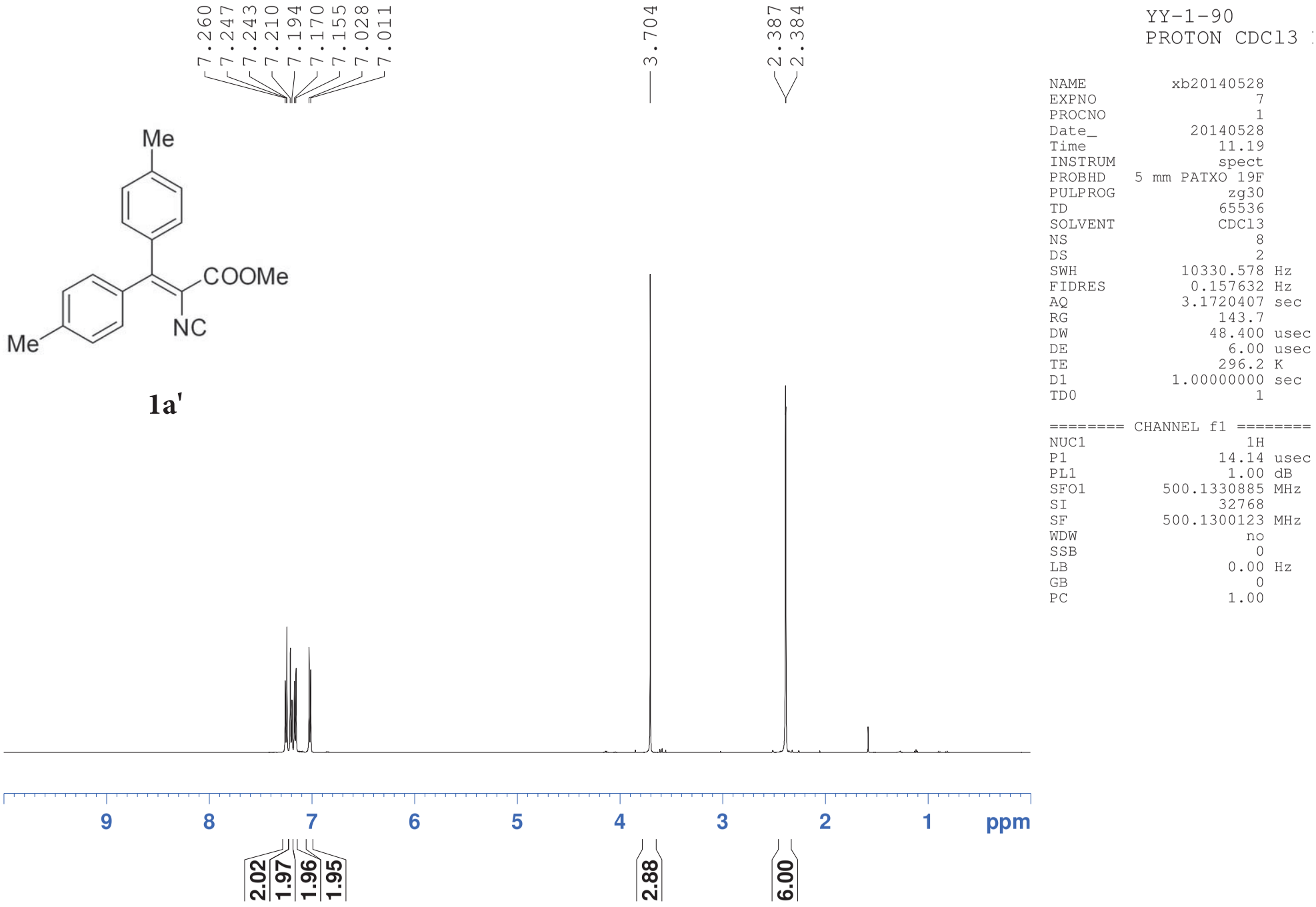
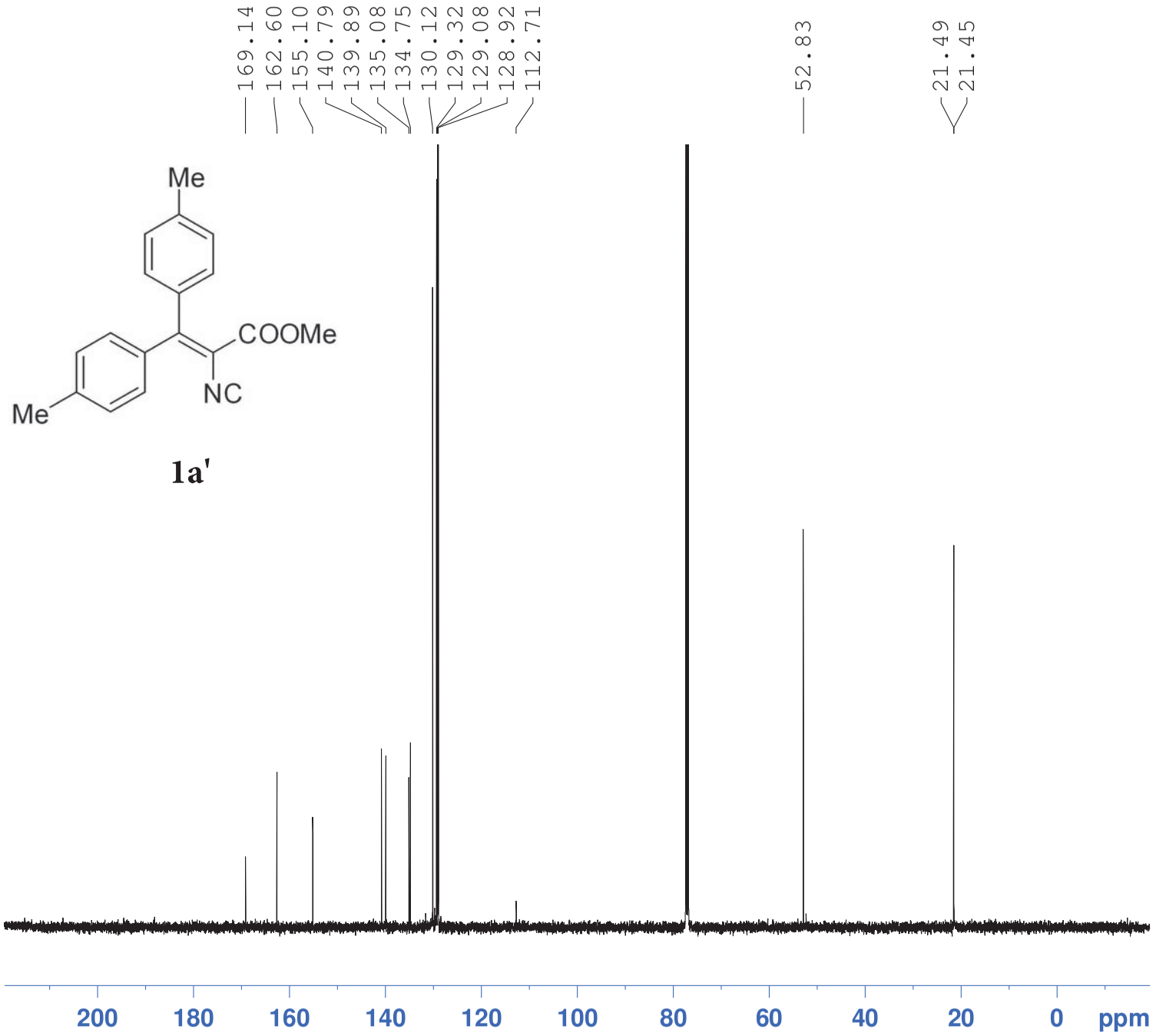
WDW	EM
SSB	0
LB	0.20 Hz
GB	0
PC	1.40



YY-1-90
PROTON CDCl3

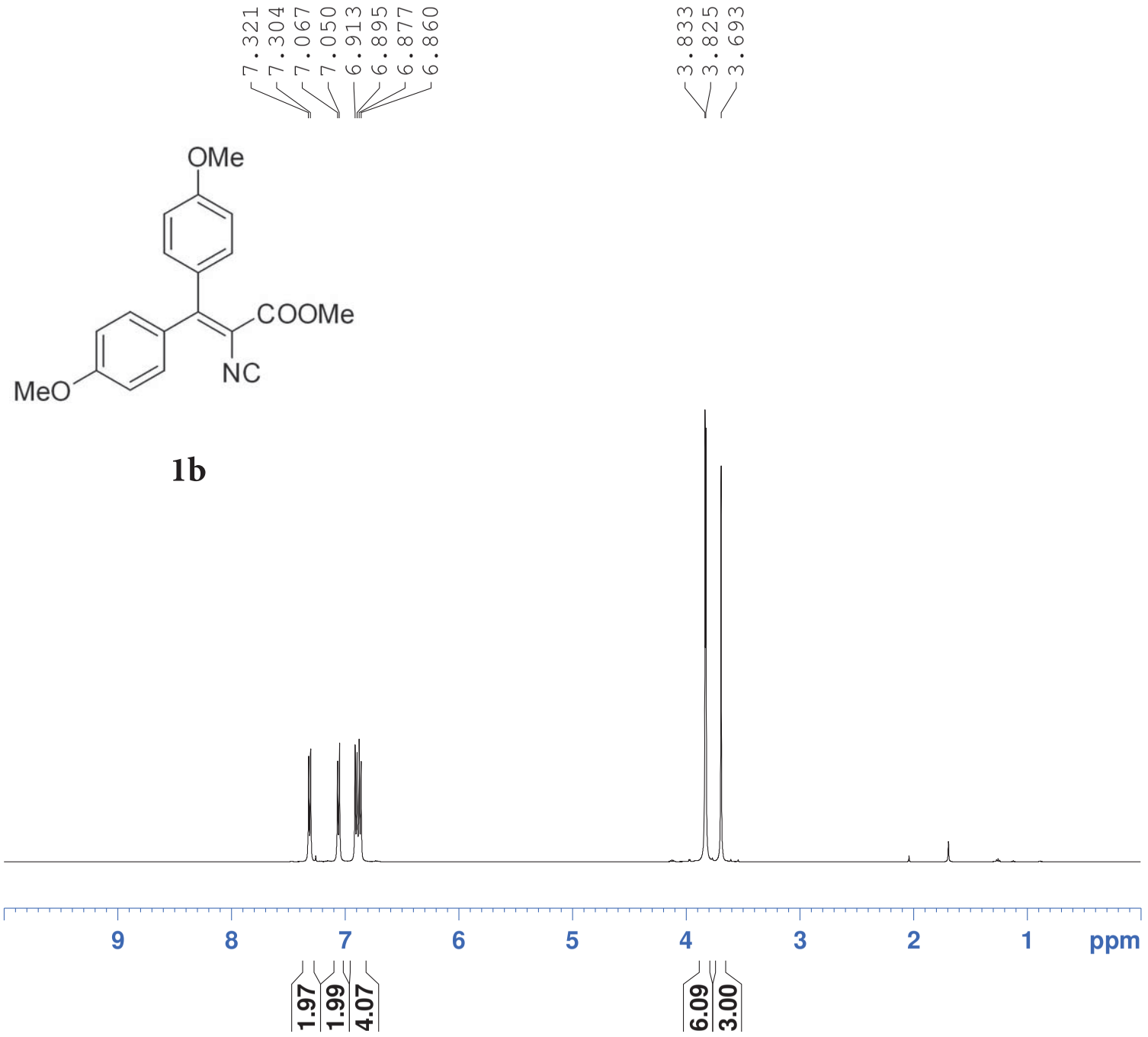
NAME	xb20140528
EXPNO	7
PROCNO	1
Date_	20140528
Time	11.19
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	143.7
DW	48.400 usec
DE	6.00 usec
TE	296.2 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300123 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



YY-1-90
C13CPD CDCl3

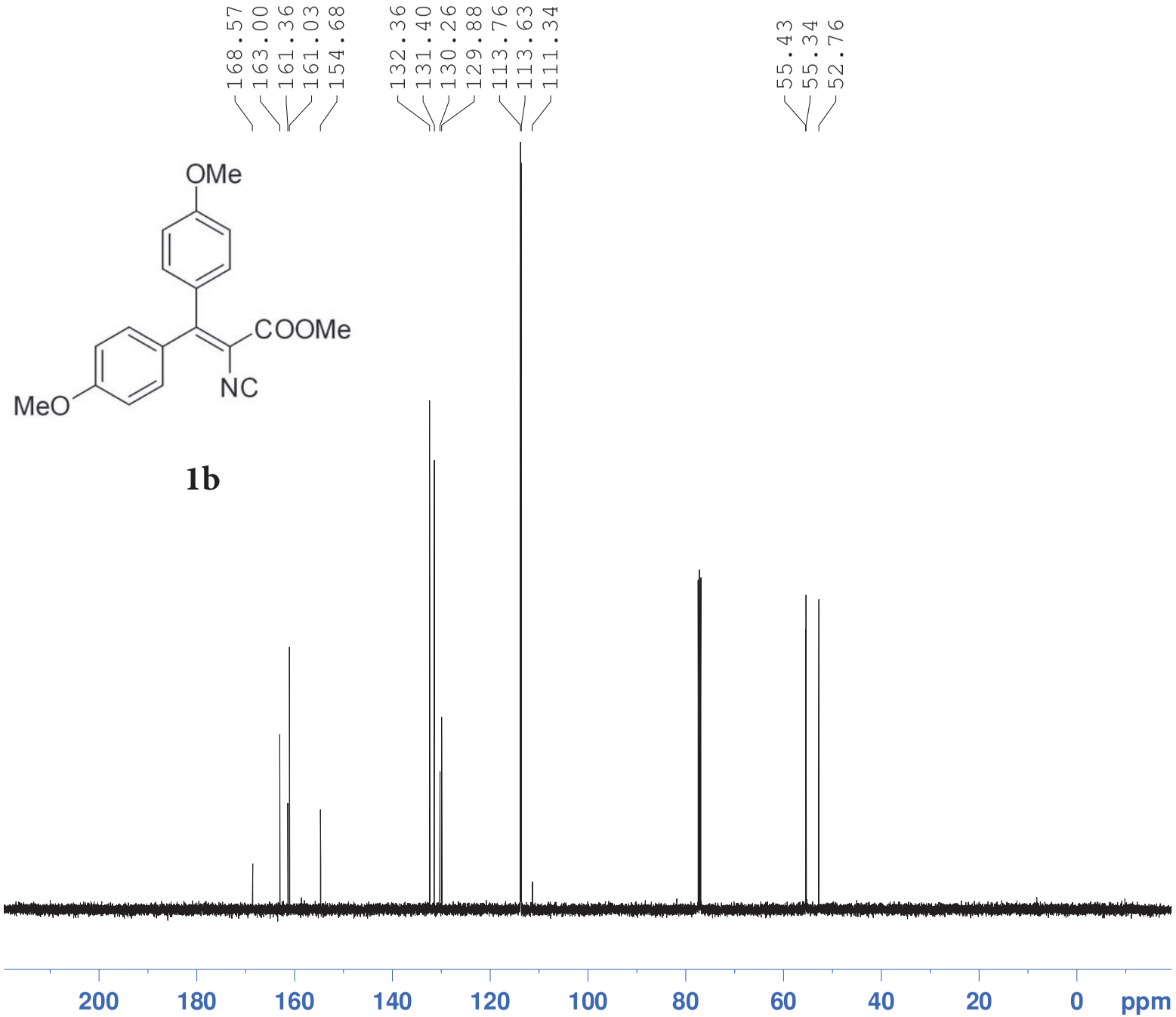
NAME	XB20140529
EXPNO	6
PROCNO	1
Date_	20140529
Time	16.25
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	512
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	322.5
DW	16.650 usec
DE	6.00 usec
TE	298.1 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



WH-6-132-S
PROTON CDCl3

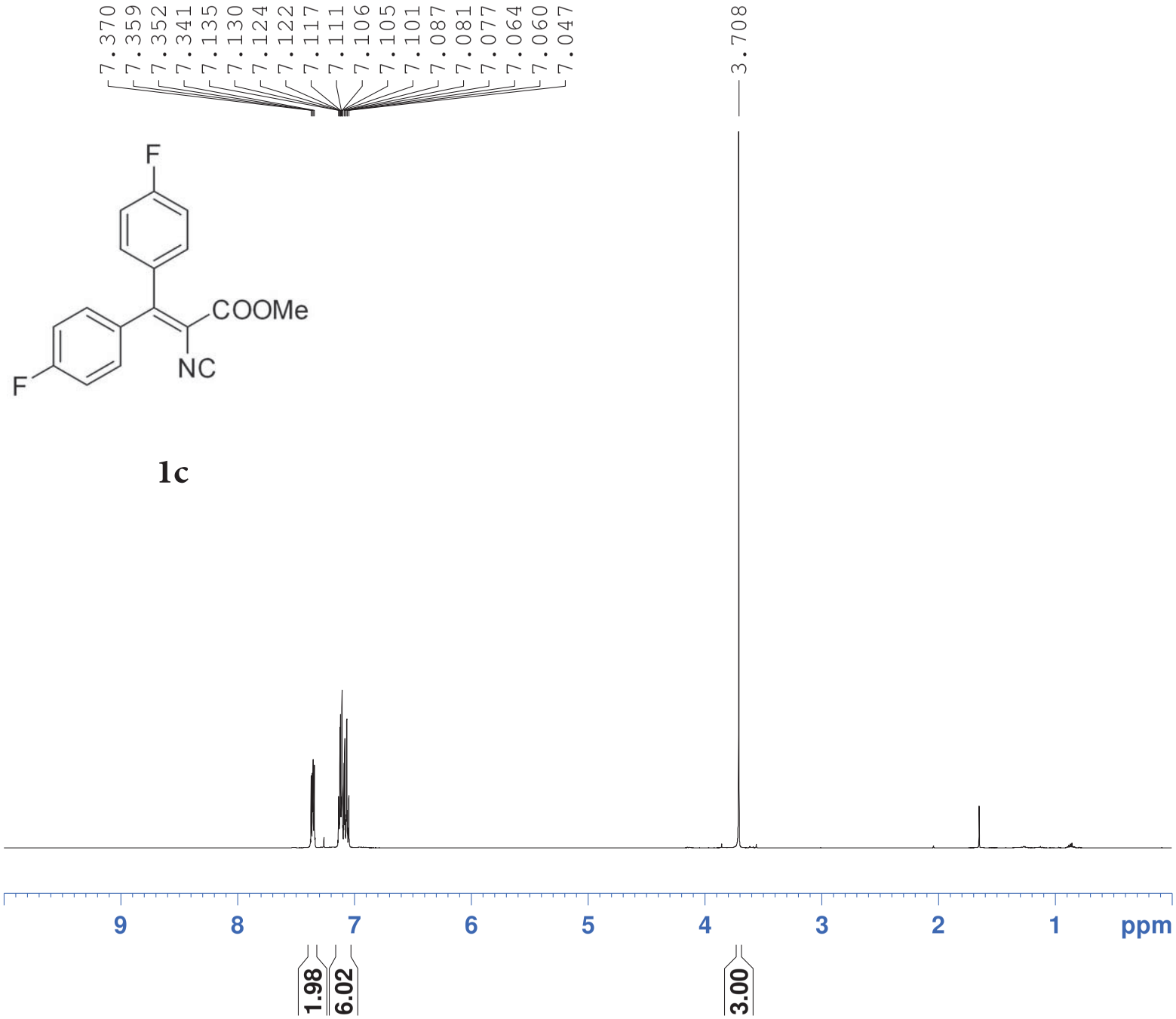
NAME	XB20140707
EXPNO	18
PROCNO	1
Date_	20140707
Time	15.05
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	64
DW	48.400 usec
DE	6.00 usec
TE	297.7 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300128 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



WH-6-132-S
C13CPD CDCl3

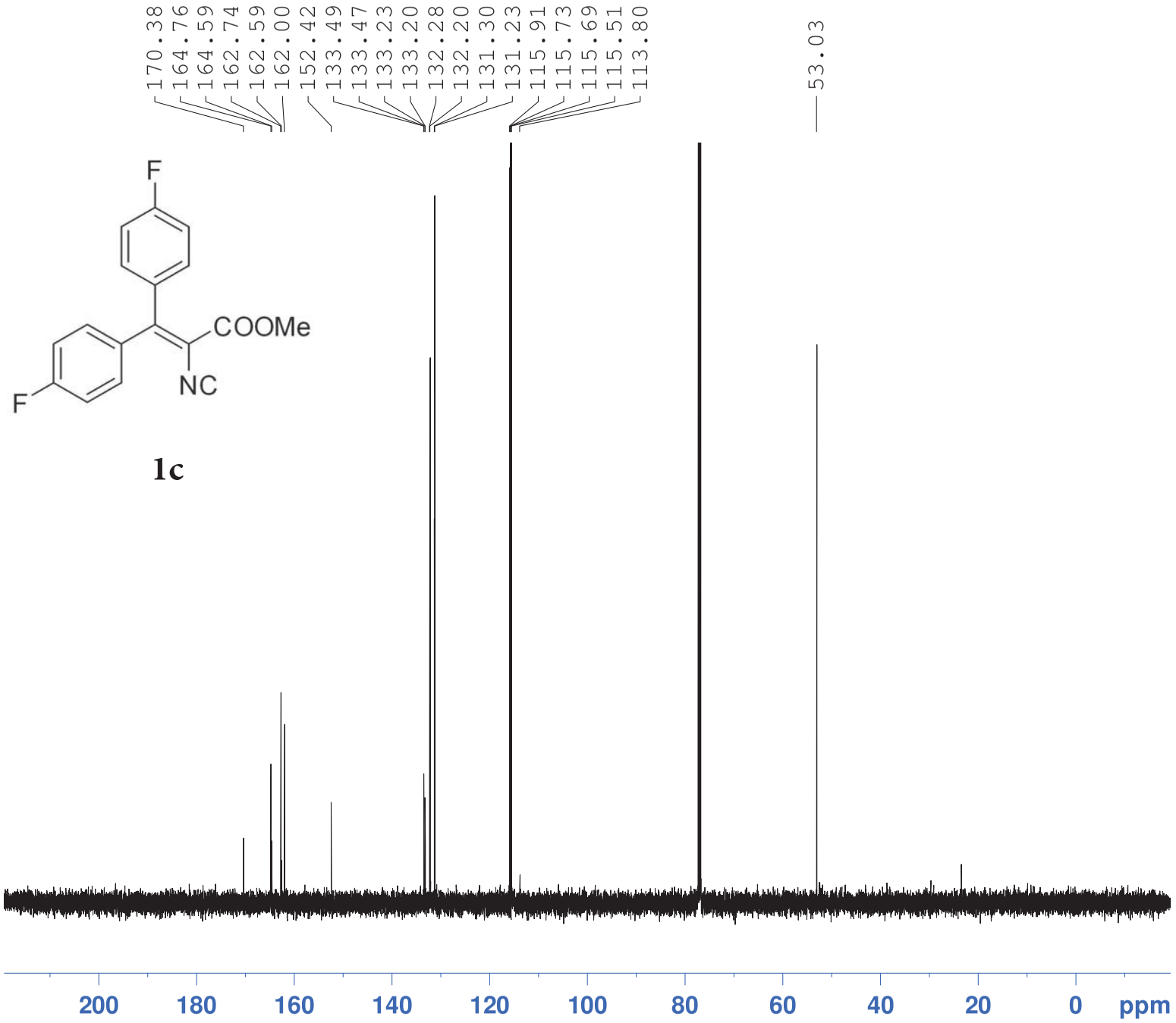
NAME	XB20140707
EXPNO	20
PROCNO	1
Date_	20140707
Time	15.22
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	256
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	203.2
DW	16.650 usec
DE	6.00 usec
TE	299.4 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577864 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40



1c

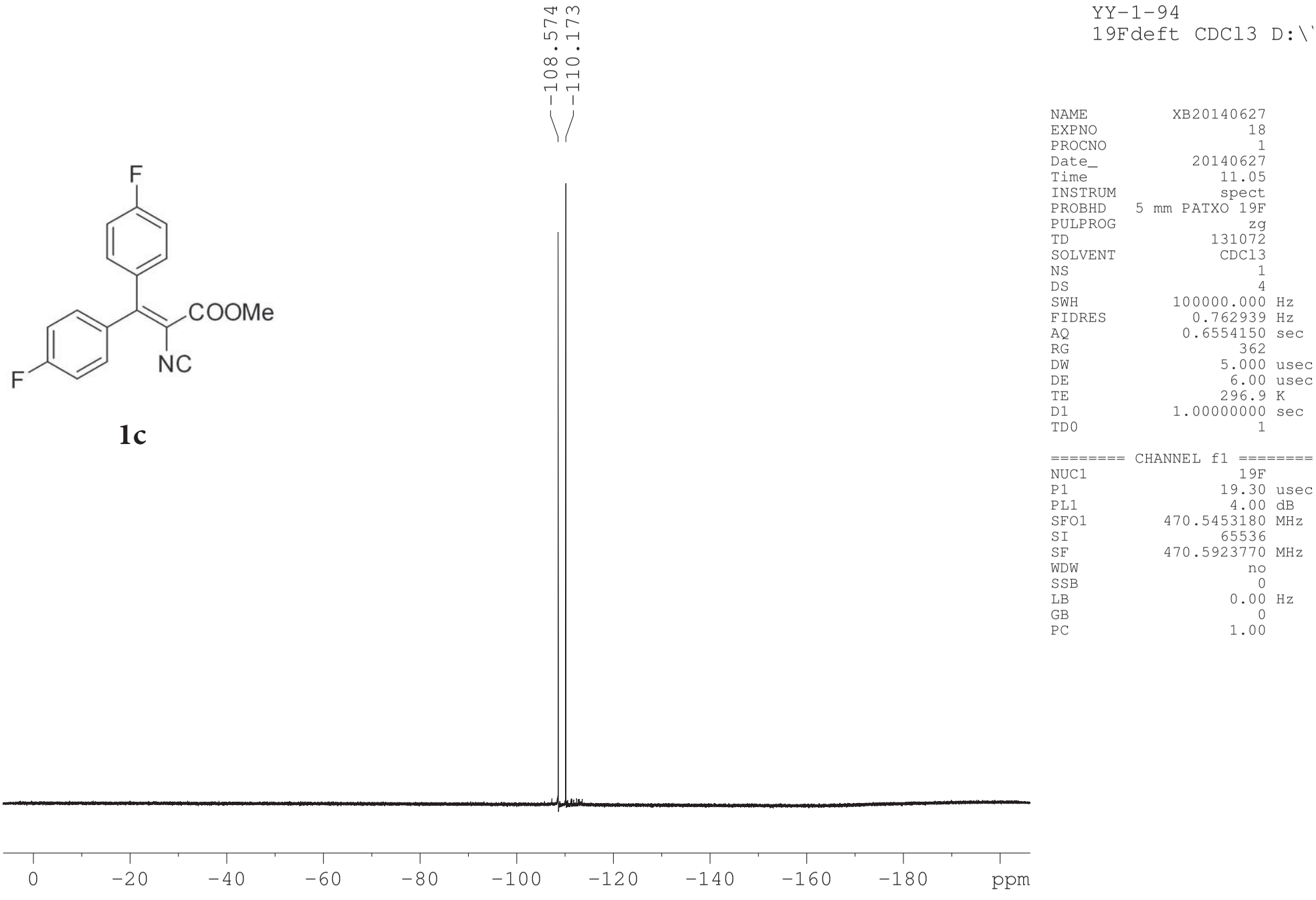
MH-2-44
PROTON CDCl3

NAME	XB20140702
EXPNO	1
PROCNO	1
Date_	20140702
Time	15.13
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	80.6
DW	48.400 usec
DE	6.00 usec
TE	295.9 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300126 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



YY-1-94
C13CPD CDCl3

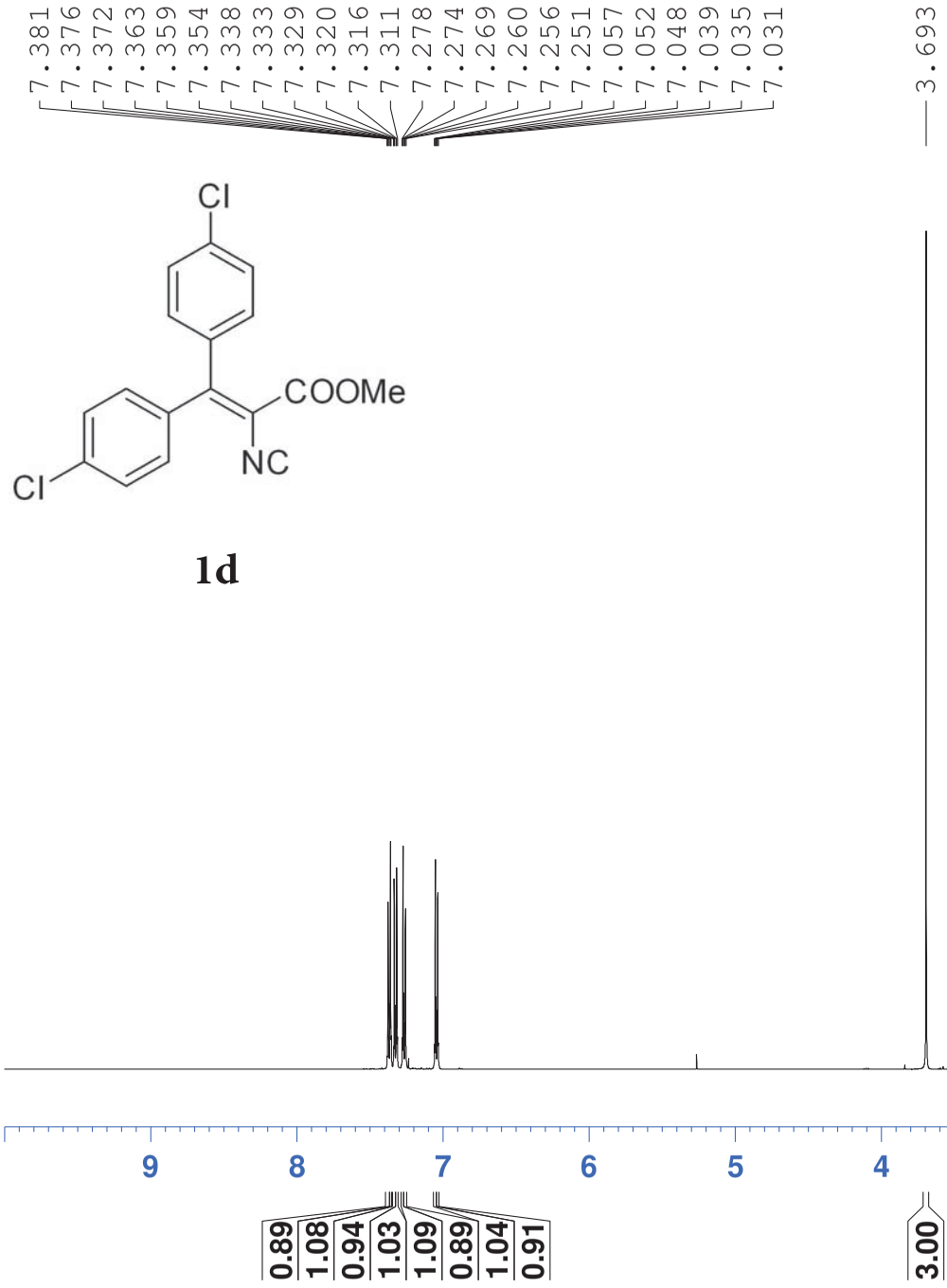
NAME	XB20140628
EXPNO	7
PROCNO	1
Date_	20140628
Time	15.10
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	128
DW	16.650 usec
DE	6.00 usec
TE	299.6 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40



1c

YY-1-94
19Fdeft CDCl3 D:\`

NAME	XB20140627
EXPNO	18
PROCNO	1
Date_	20140627
Time	11.05
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg
TD	131072
SOLVENT	CDCl3
NS	1
DS	4
SWH	100000.000 Hz
FIDRES	0.762939 Hz
AQ	0.6554150 sec
RG	362
DW	5.000 usec
DE	6.00 usec
TE	296.9 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	19F
P1	19.30 usec
PL1	4.00 dB
SFO1	470.5453180 MHz
SI	65536
SF	470.5923770 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

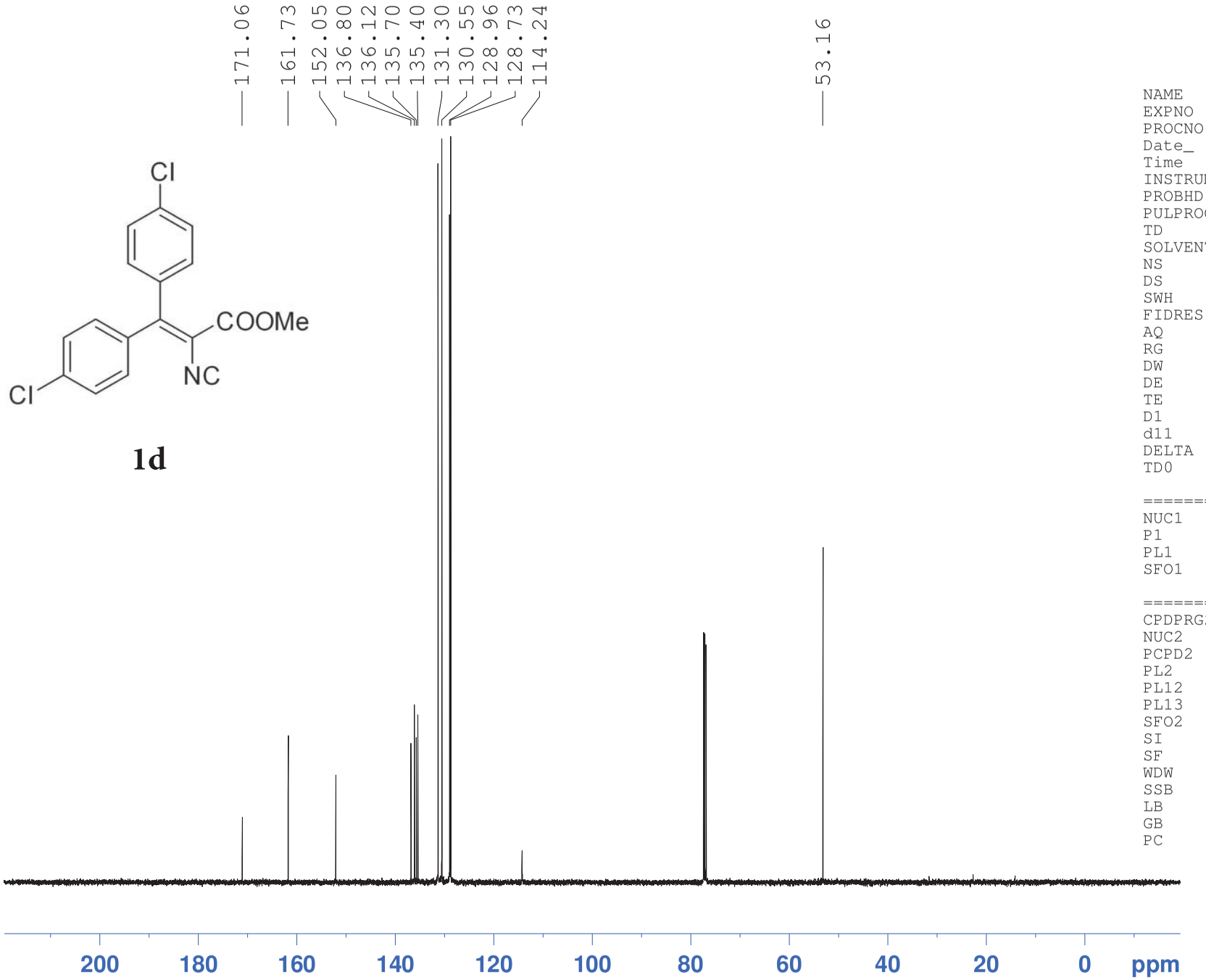


1d

YY-1-98
PROTON CDCl3

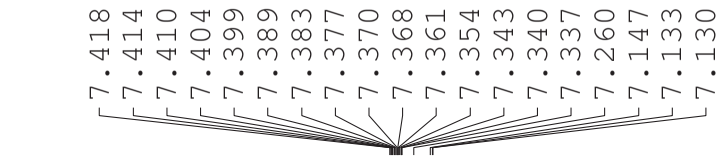
NAME	XB20140609
EXPNO	20
PROCNO	1
Date_	20140609
Time	11.53
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	71.8
DW	48.400 usec
DE	6.00 usec
TE	296.4 K
D1	1.00000000 sec
TD0	1

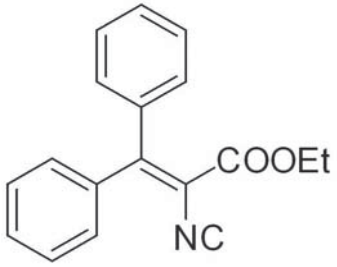
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300252 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



YY-1-98
C13CPD CDCl3 1

NAME	XB20140609
EXPNO	21
PROCNO	1
Date_	20140610
Time	3.56
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	256
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	181
DW	16.650 usec
DE	6.00 usec
TE	297.9 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

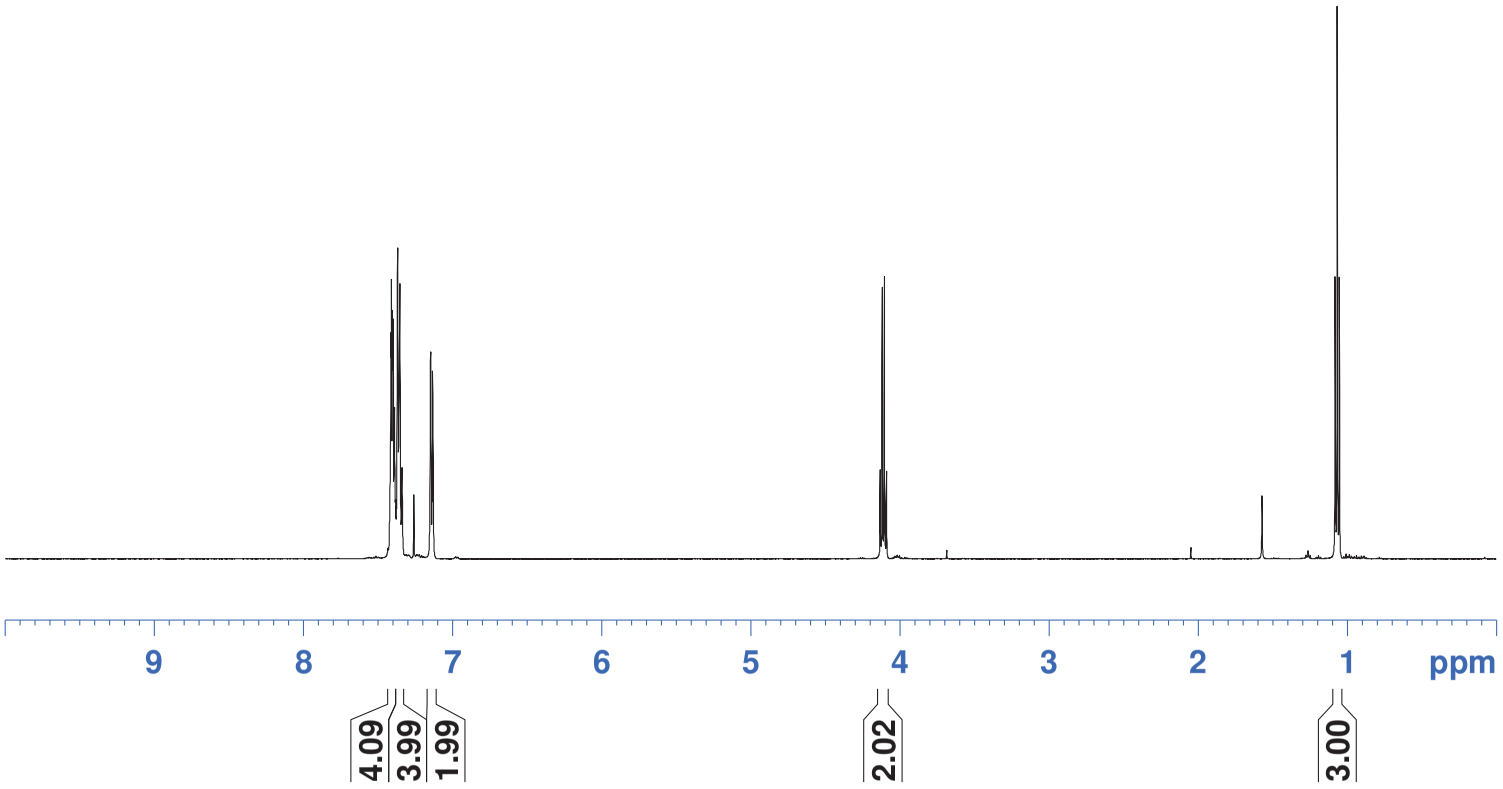


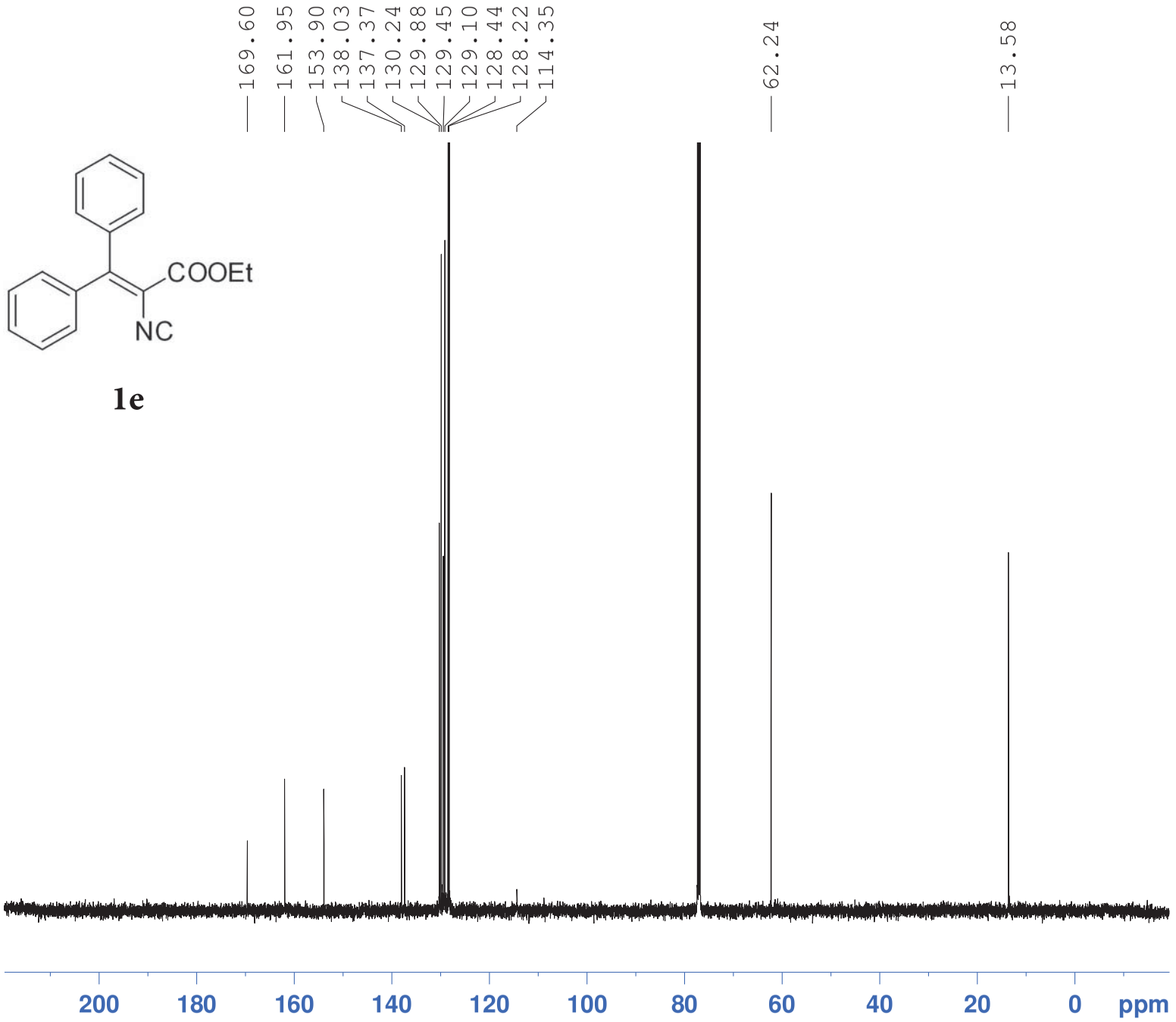


1e

WH-6-29-S
PROTON CDCl3

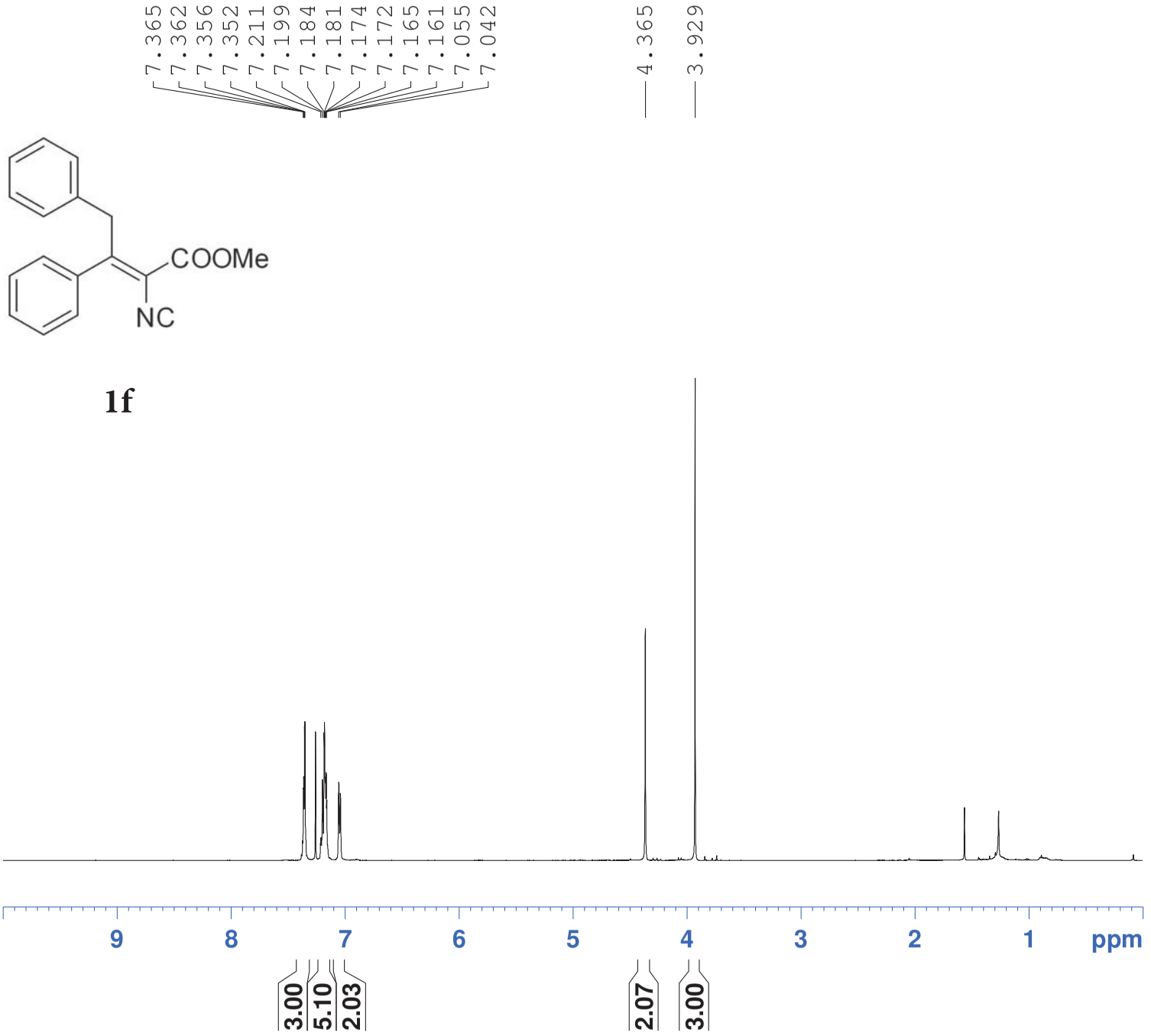
NAME	XB20140526
EXPNO	20
PROCNO	1
Date_	20140526
Time	17.24
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	256
DW	48.400 usec
DE	6.00 usec
TE	296.3 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300129 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00





WH-6-29-S
C13CPD CDCl3

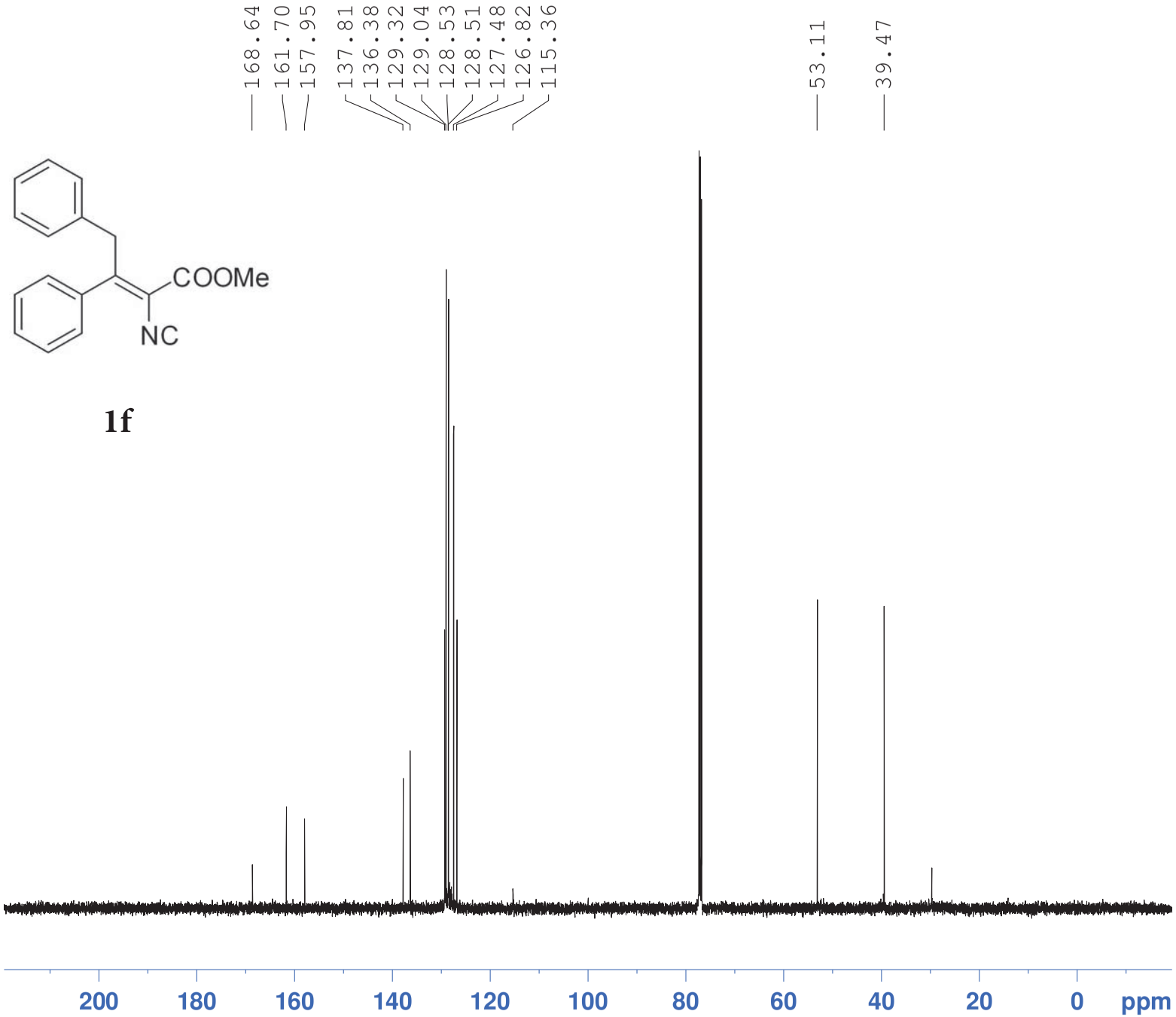
NAME	XB20140602
EXPNO	21
PROCNO	1
Date_	20140602
Time	21.57
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	512
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	181
DW	16.650 usec
DE	6.00 usec
TE	297.7 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



WH-7-40-S
PROTON CDCl3

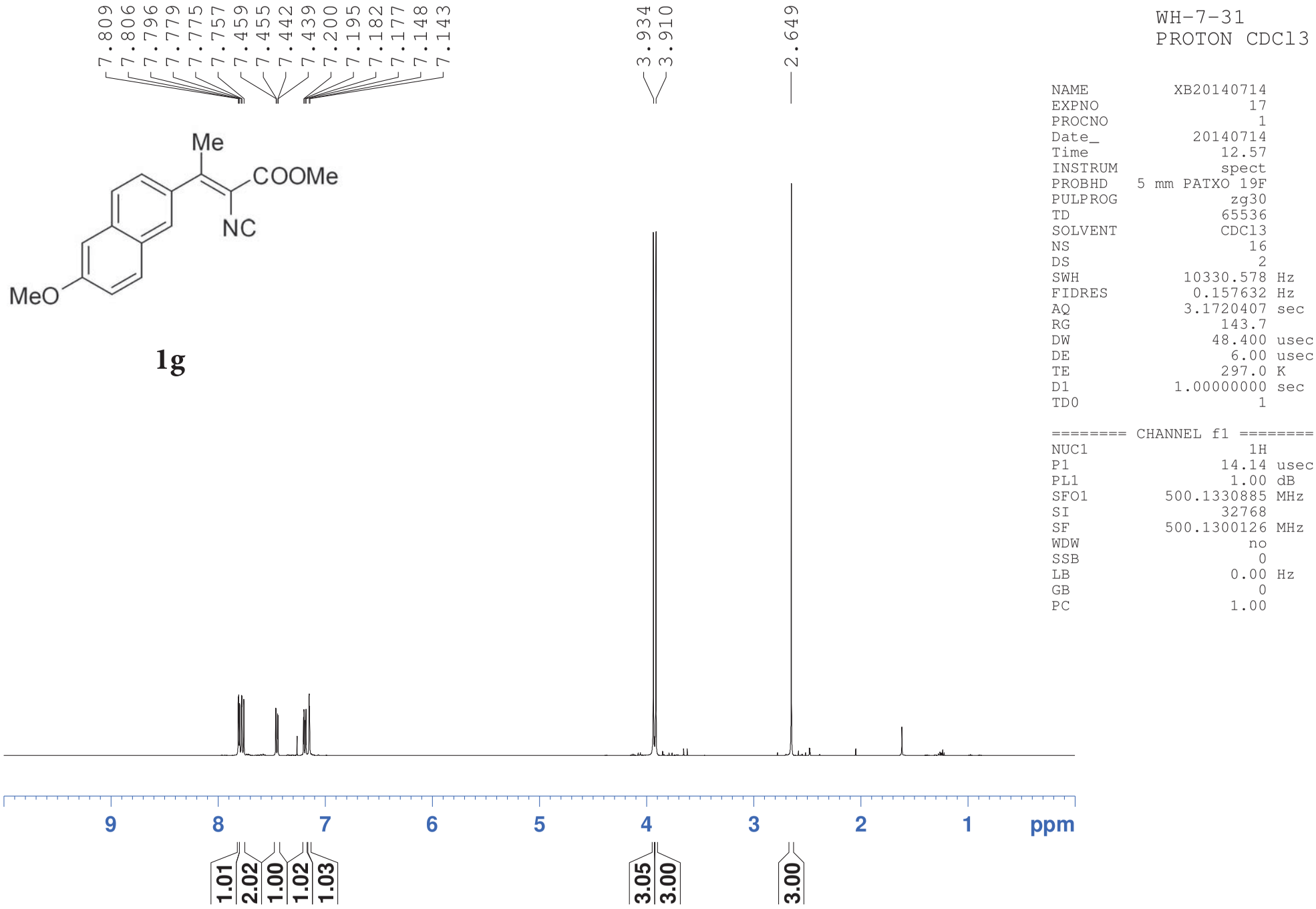
NAME	XB20140617
EXPNO	8
PROCNO	1
Date_	20140617
Time	12.44
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	203.2
DW	48.400 usec
DE	6.00 usec
TE	296.5 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300129 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



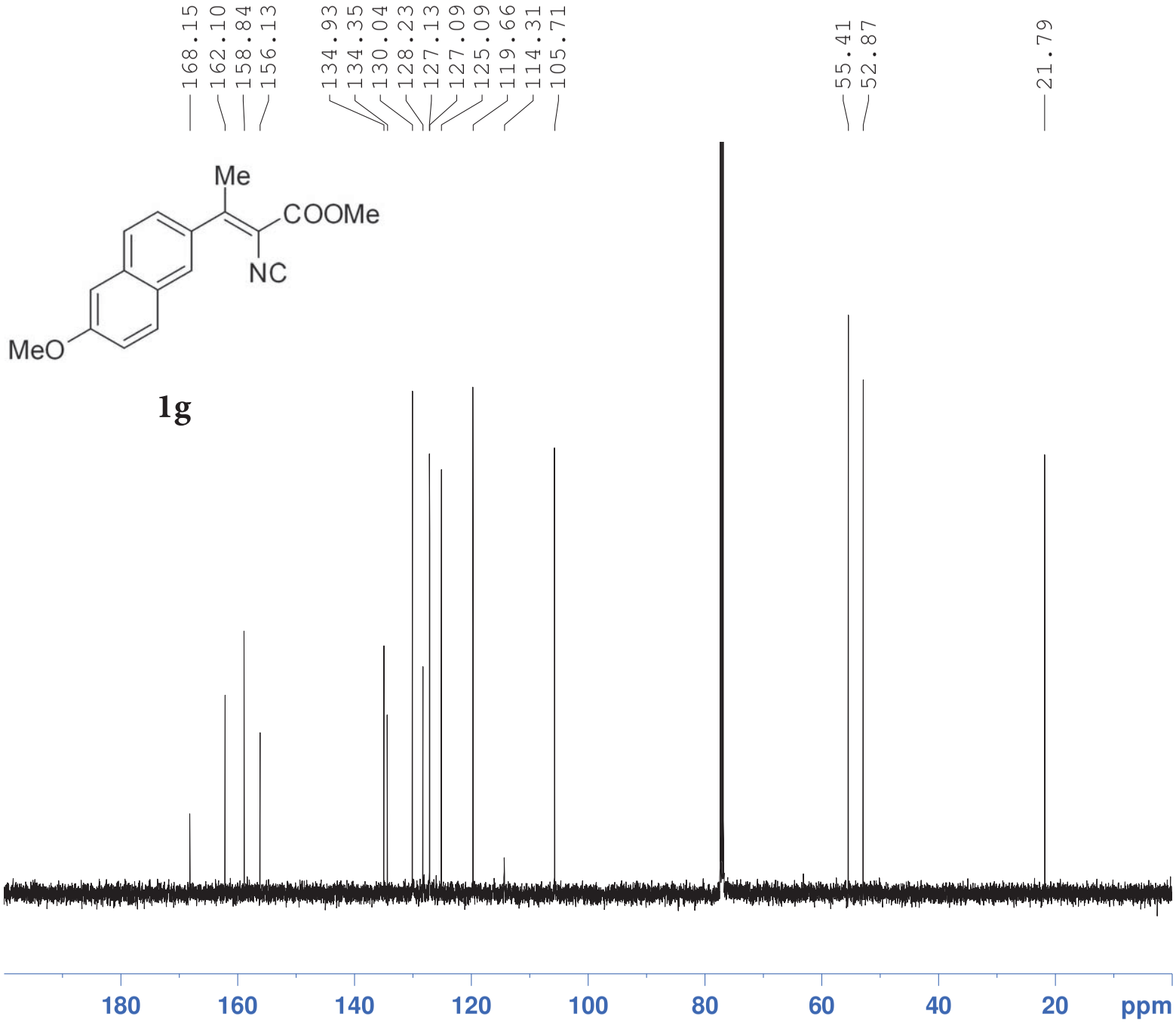
WH-7-40-S
C13CPD CDCl3

NAME	XB20140626
EXPNO	9
PROCNO	1
Date_	20140626
Time	10.49
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	440
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	228.1
DW	16.650 usec
DE	6.00 usec
TE	298.1 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



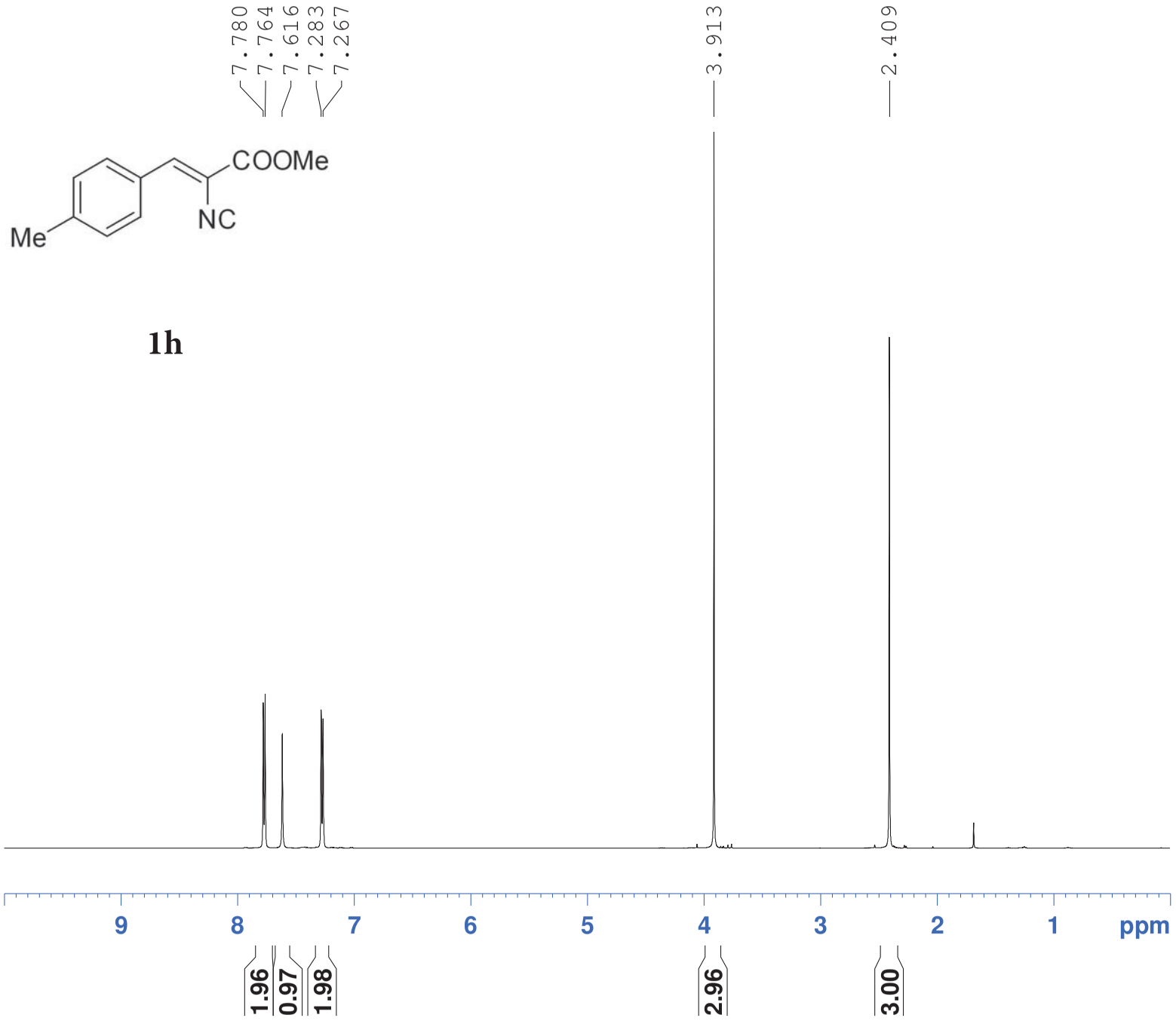
WH-7-31
PROTON CDCl3

NAME	XB20140714
EXPNO	17
PROCNO	1
Date_	20140714
Time	12.57
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	143.7
DW	48.400 usec
DE	6.00 usec
TE	297.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300126 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



WH-7-31
C13CPD CDCl3

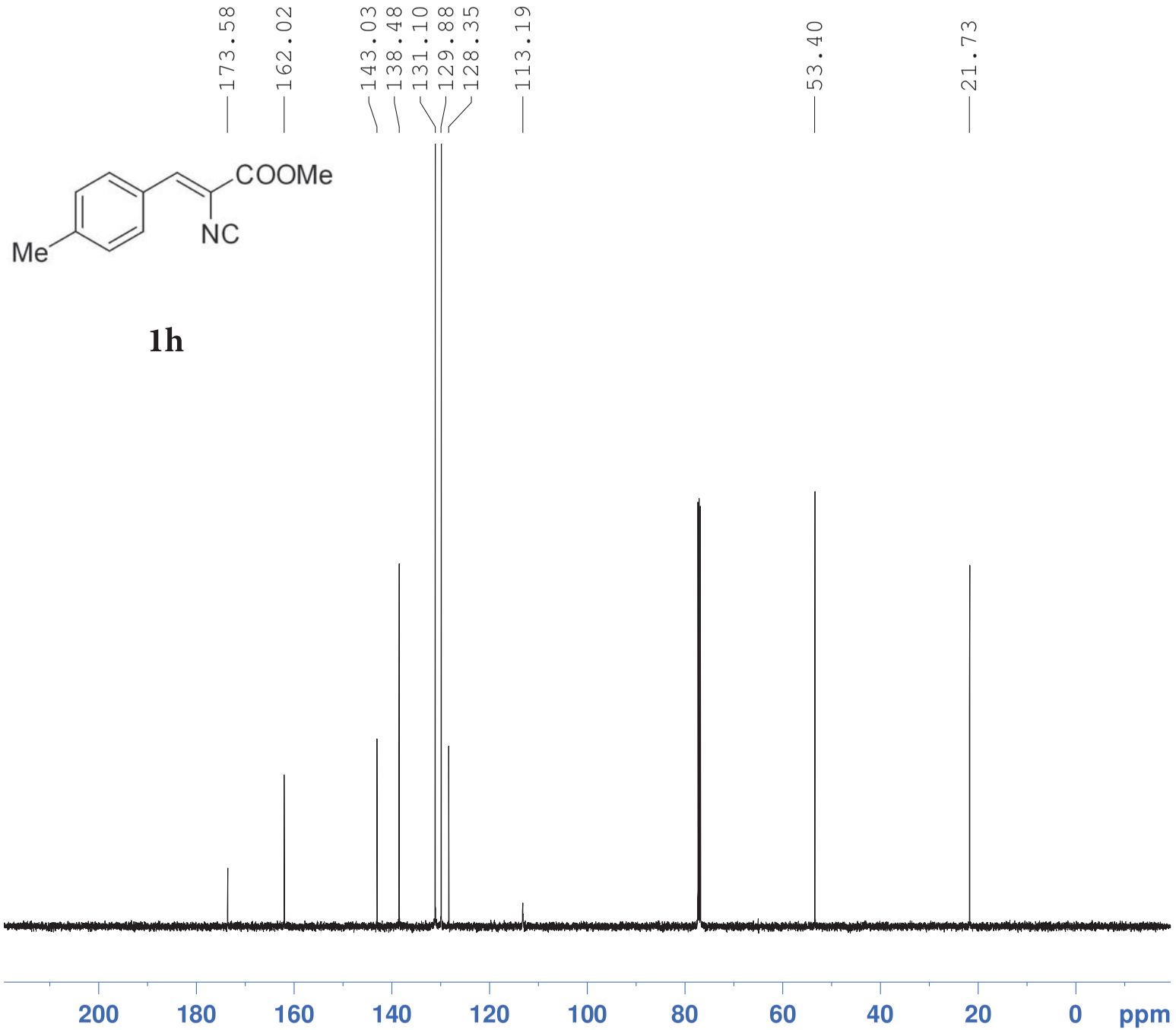
NAME	XB20140714
EXPNO	18
PROCNO	1
Date_	20140714
Time	13.12
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	256
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	114
DW	16.650 usec
DE	6.00 usec
TE	298.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



WH-7-35
PROTON CDCl3

NAME	XB20140617
EXPNO	21
PROCNO	1
Date_	20140617
Time	19.02
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	101.6
DW	48.400 usec
DE	6.00 usec
TE	296.6 K
D1	1.00000000 sec
TD0	1

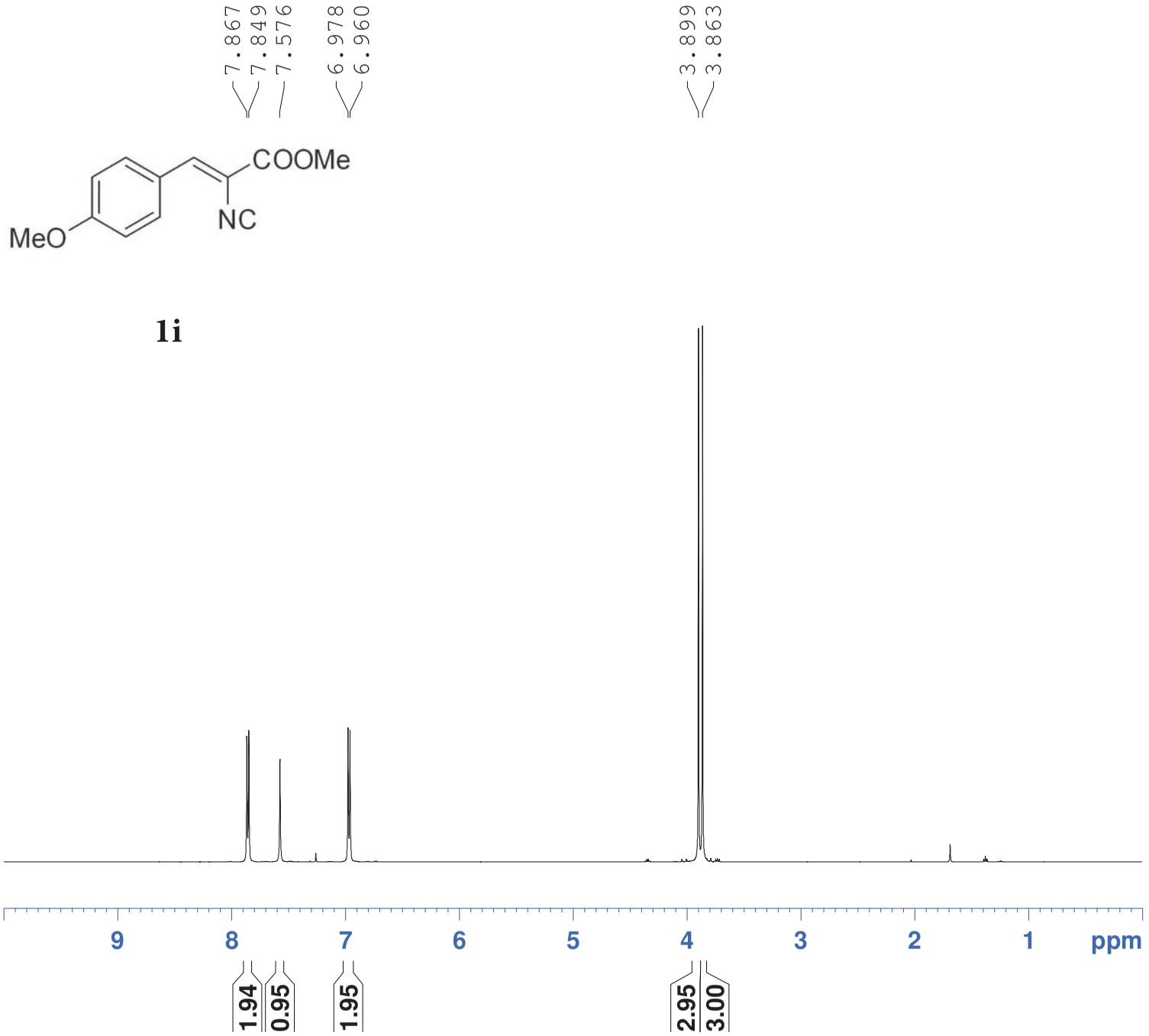
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300129 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



1h

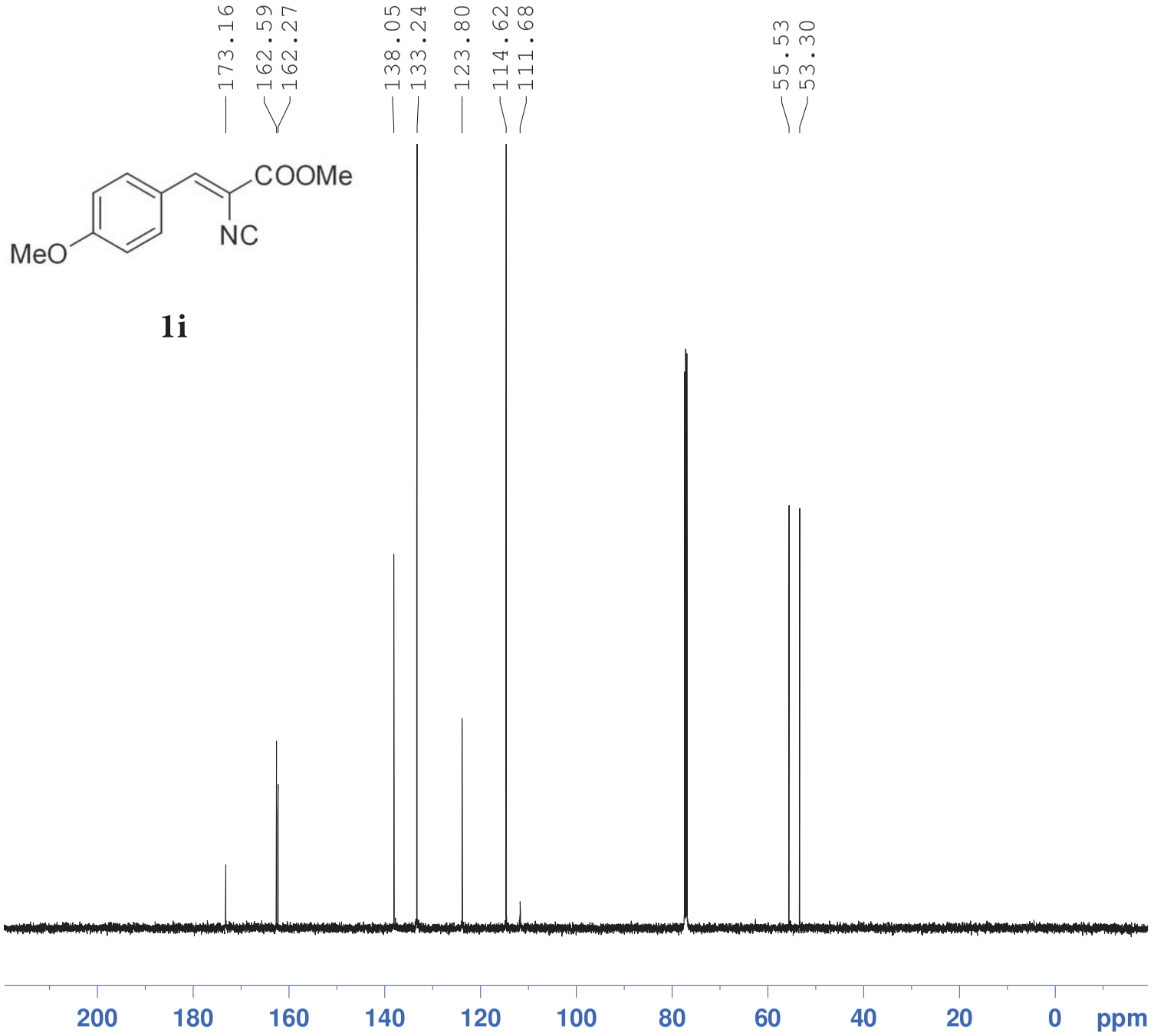
WH-7-35
C13CPD CDCl3

NAME	XB20140617
EXPNO	22
PROCNO	1
Date_	20140617
Time	19.19
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	256
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	228.1
DW	16.650 usec
DE	6.00 usec
TE	297.7 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



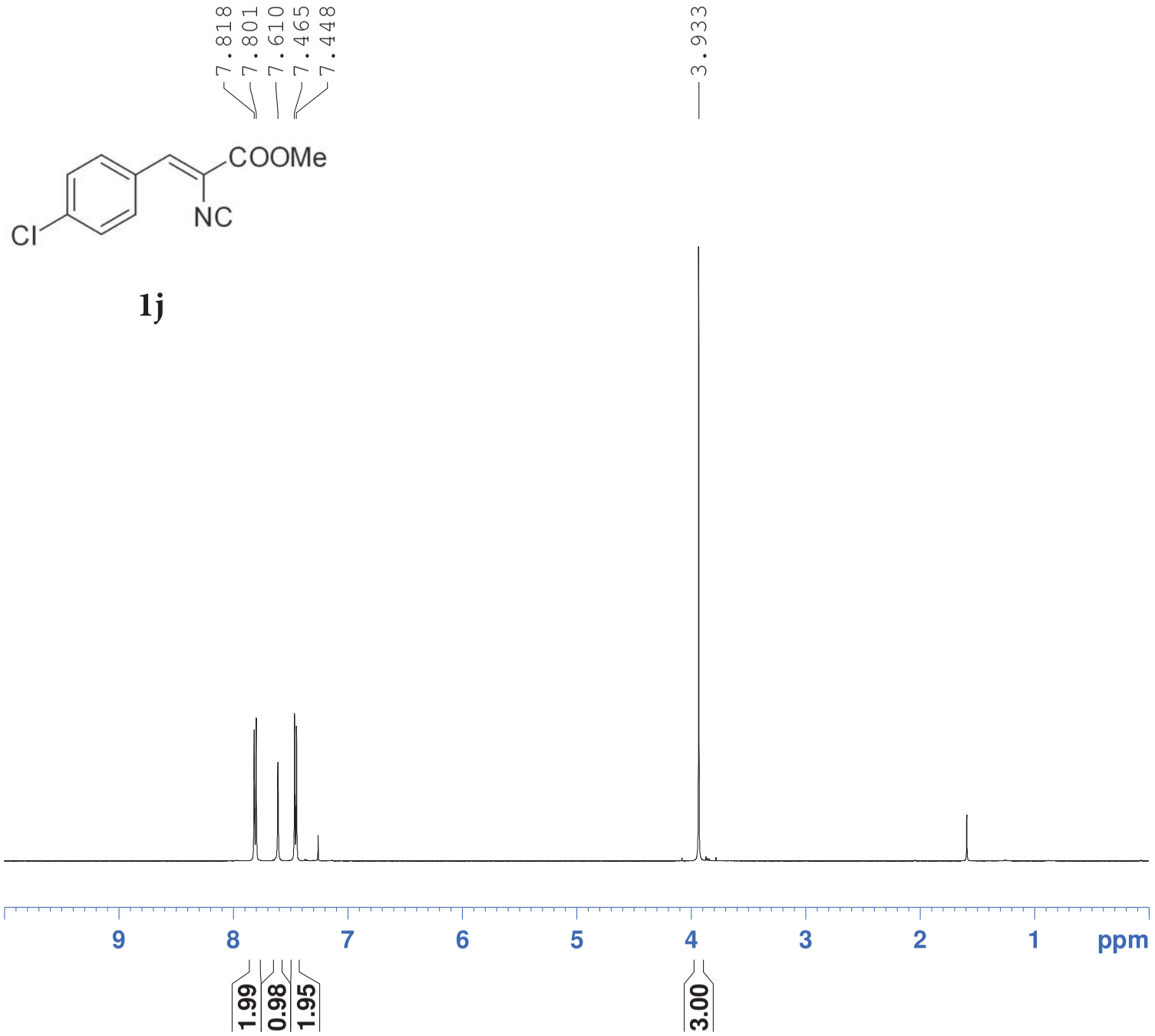
WH-7-36
PROTON CDCl3

NAME	XB20140617
EXPNO	23
PROCNO	1
Date_	20140617
Time	19.25
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	101.6
DW	48.400 usec
DE	6.00 usec
TE	296.5 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300126 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



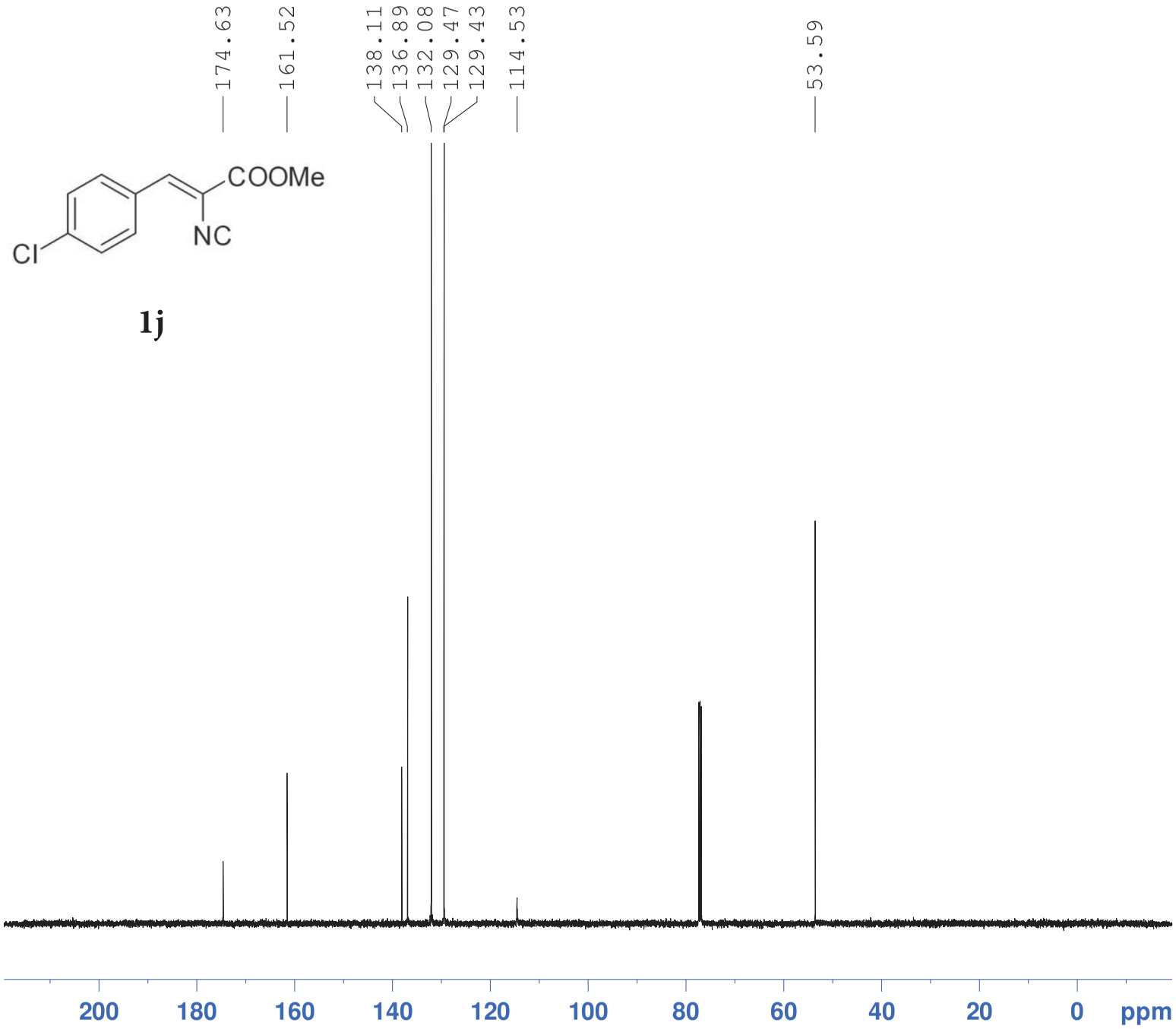
WH-7-36
C13CPD CDCl3

NAME	XB20140617
EXPNO	24
PROCNO	1
Date_	20140617
Time	19.40
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	256
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	114
DW	16.650 usec
DE	6.00 usec
TE	297.7 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



YY-1-101
PROTON CDCl3

NAME	XB20140617
EXPNO	12
PROCNO	1
Date_	20140617
Time	15.46
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	287.4
DW	48.400 usec
DE	6.00 usec
TE	296.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300129 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



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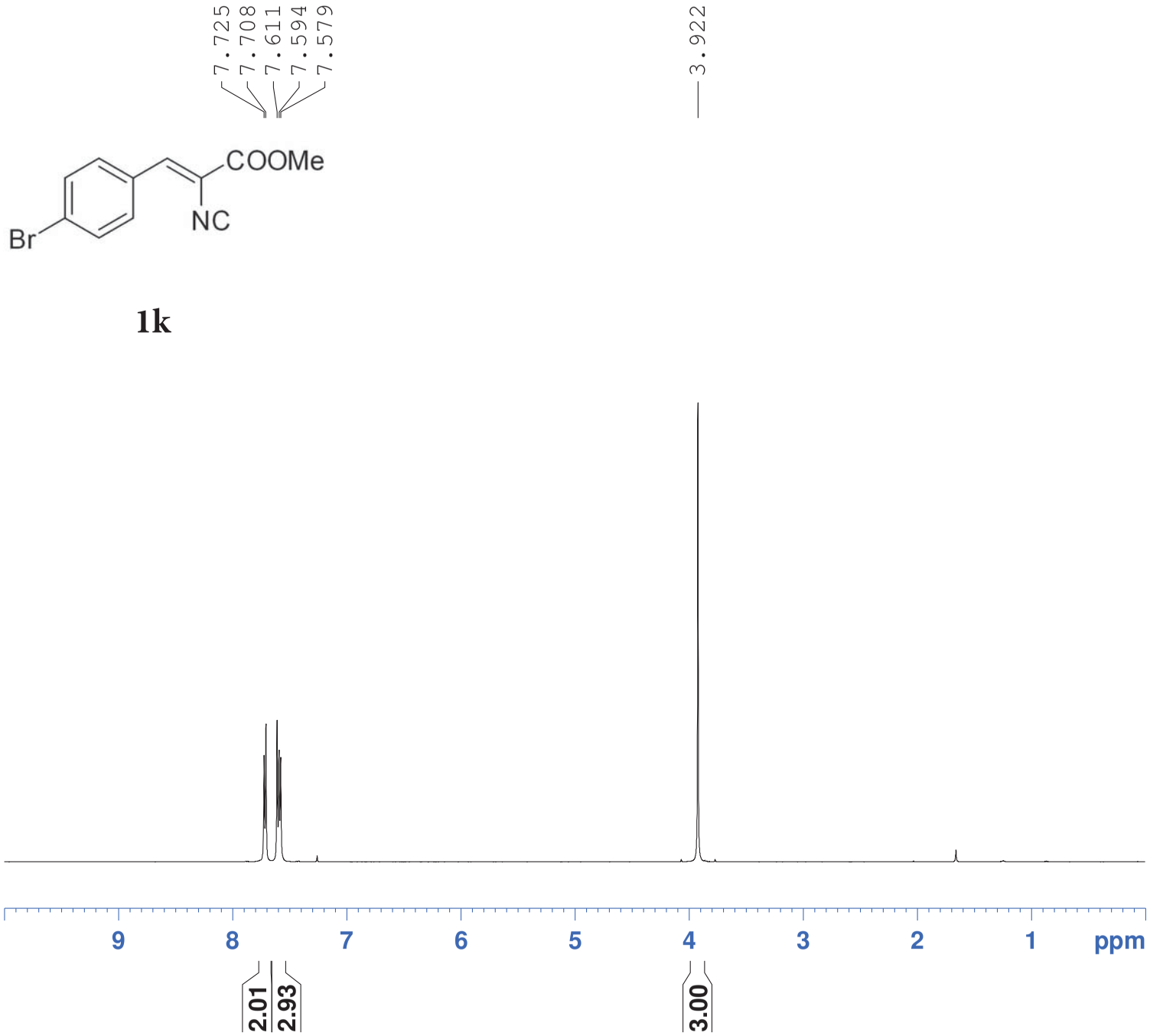
YY-1-101
C13CPD CDCl3

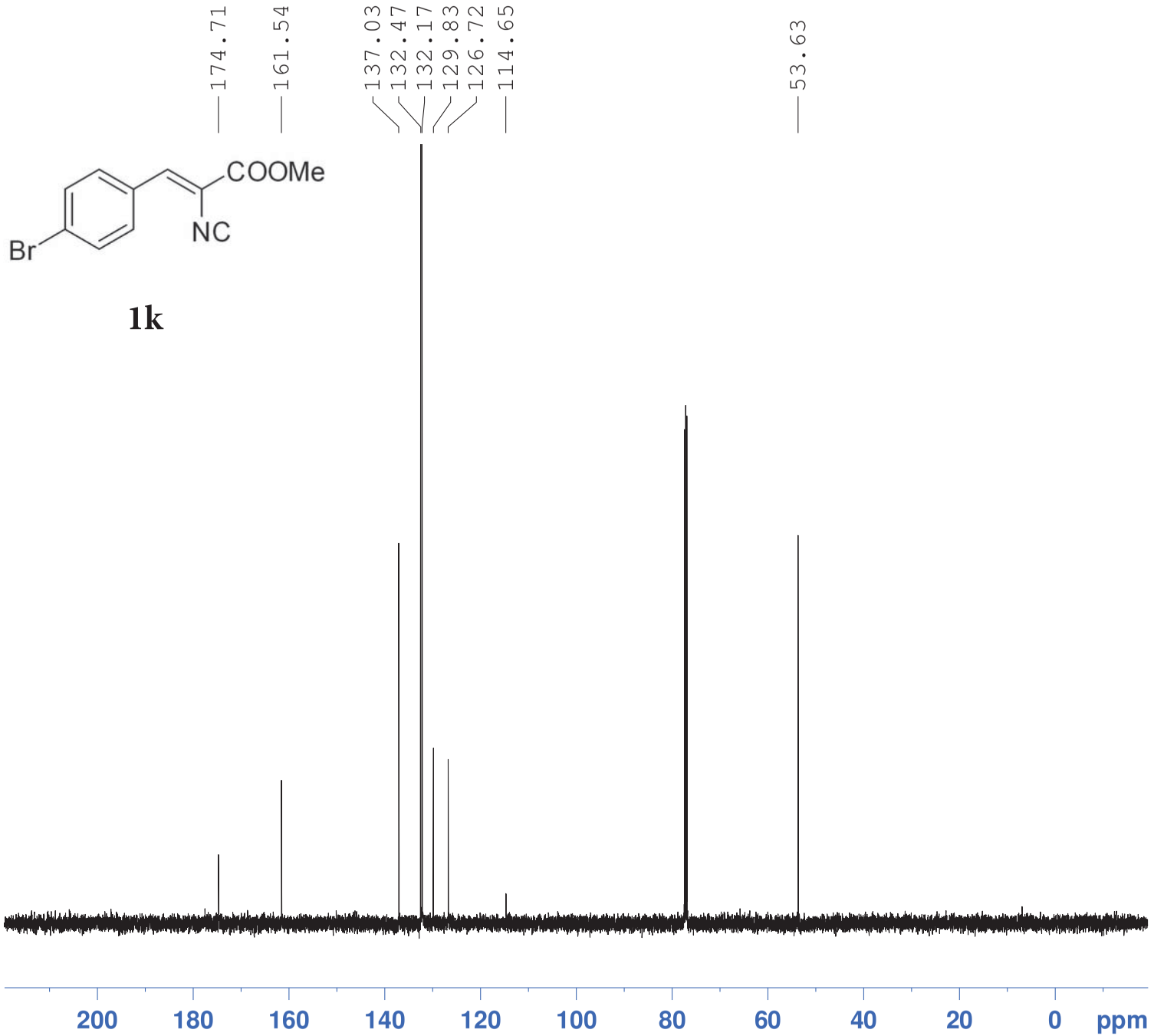
NAME	XB20140627
EXPNO	12
PROCNO	1
Date_	20140627
Time	10.05
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	127
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	181
DW	16.650 usec
DE	6.00 usec
TE	297.3 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



YY-1-100
PROTON CDCl3

NAME	XB20140617
EXPNO	10
PROCNO	1
Date_	20140617
Time	15.34
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	143.7
DW	48.400 usec
DE	6.00 usec
TE	296.1 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300126 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



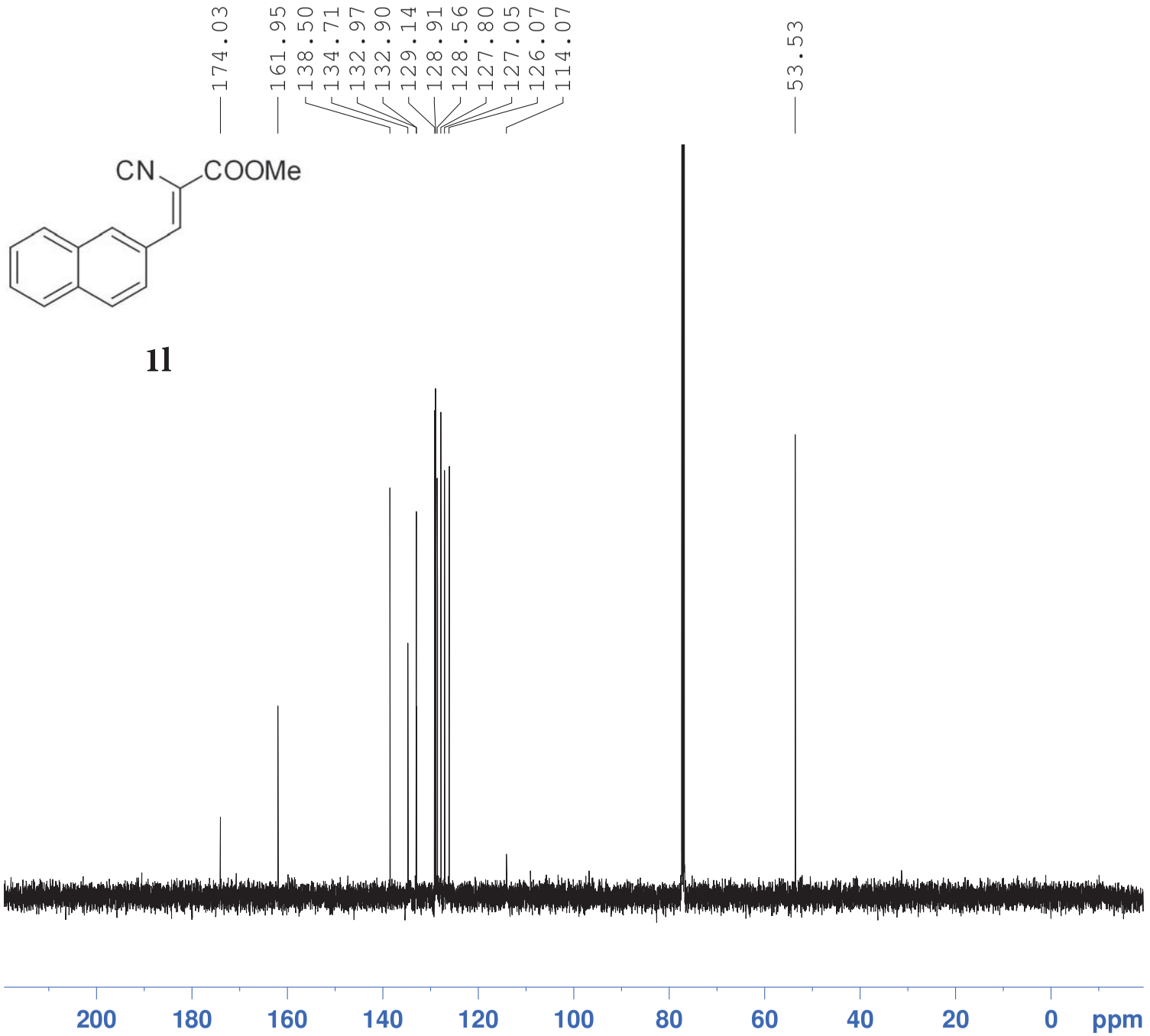
YY-1-100
C13CPD CDCl3

NAME	XB20140617
EXPNO	11
PROCNO	1
Date_	20140617
Time	15.37
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	78
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	406.4
DW	16.650 usec
DE	6.00 usec
TE	296.8 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1l

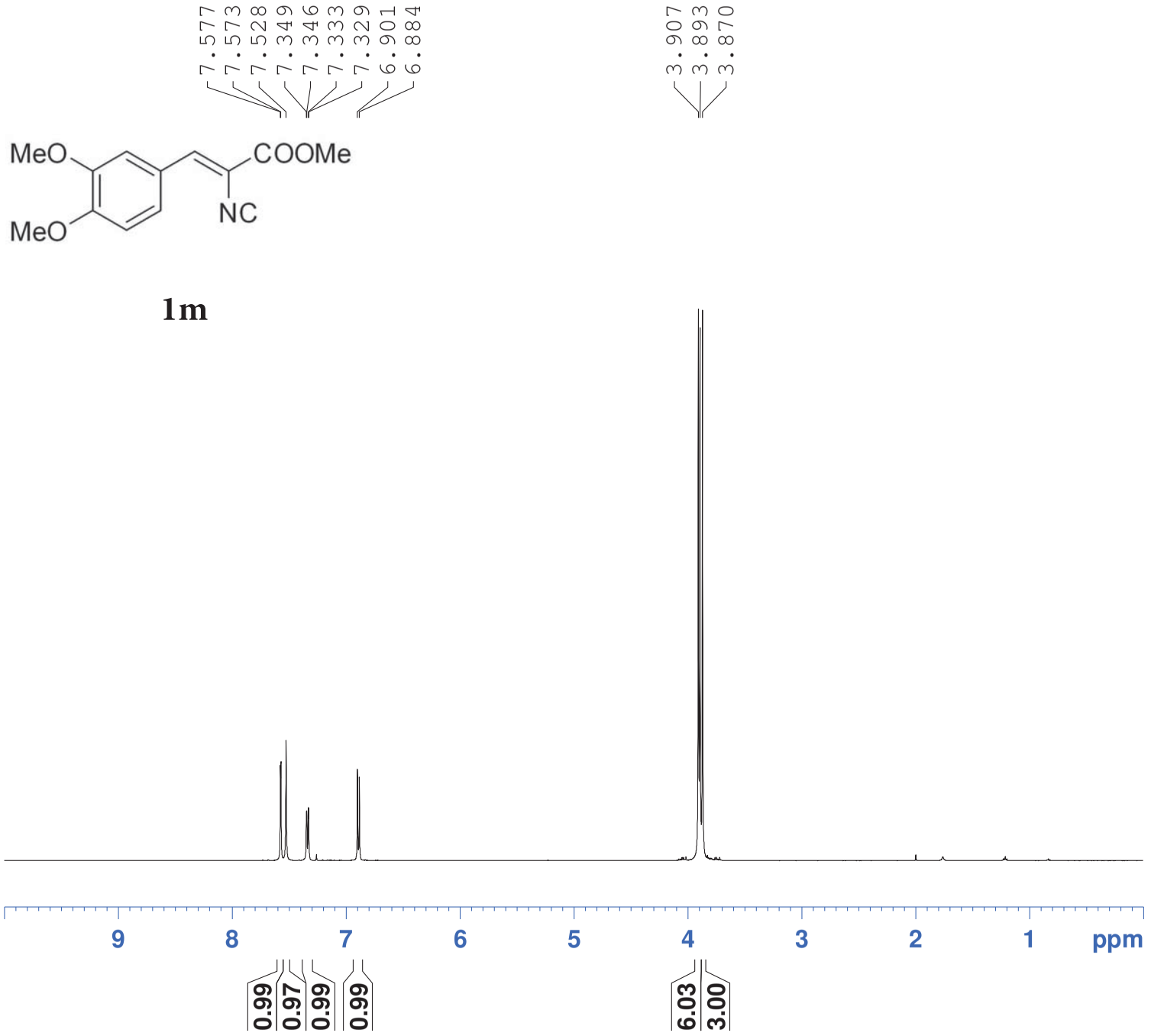
WH-7-29
PROTON CDCl3

NAME	XB20140613
EXPNO	5
PROCNO	1
Date_	20140613
Time	11.31
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	203.2
DW	48.400 usec
DE	6.00 usec
TE	296.5 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300126 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



WH-7-29
C13CPD CDCl3

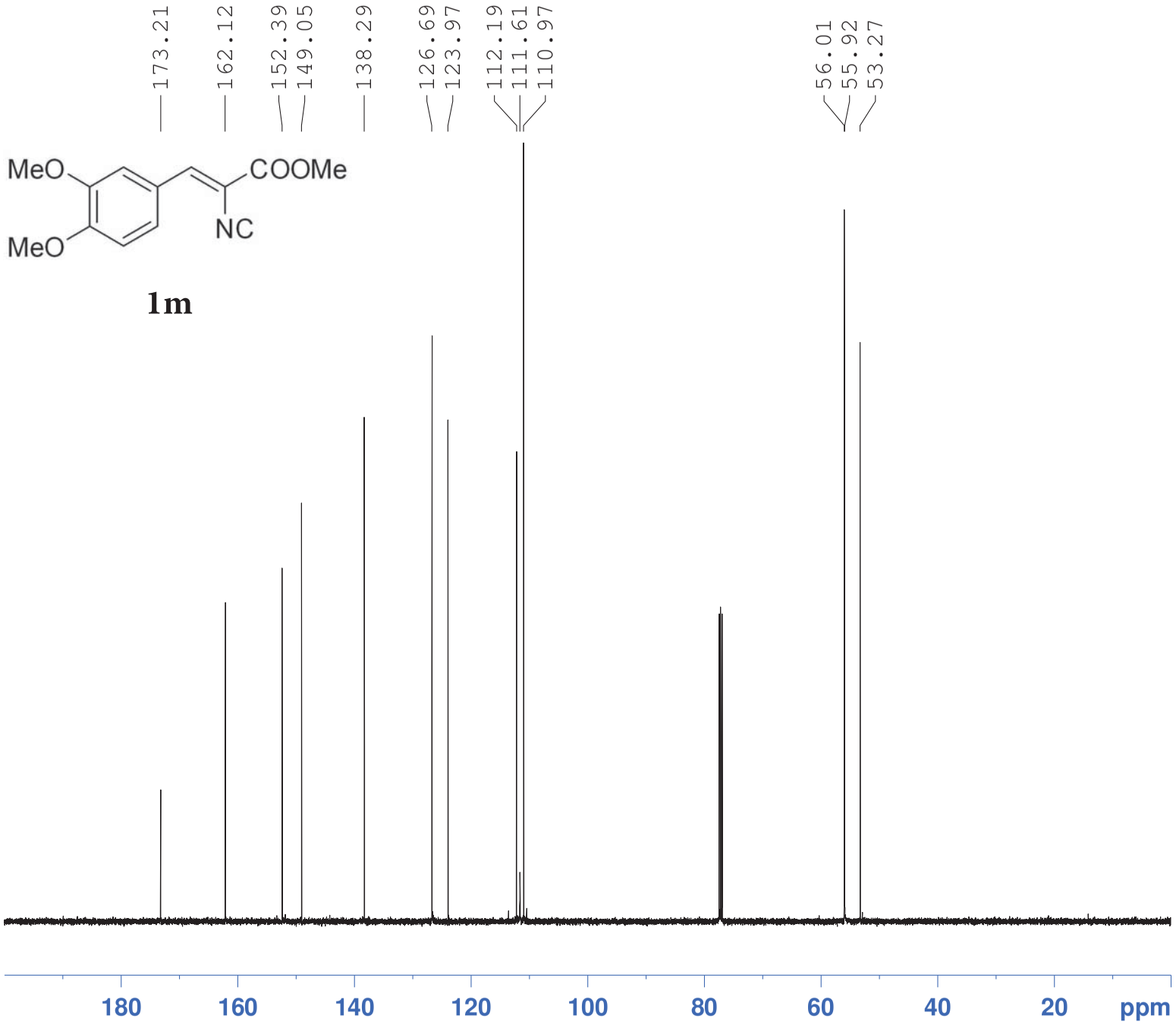
NAME	XB20140613
EXPNO	7
PROCNO	1
Date_	20140613
Time	11.42
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	128
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	322.5
DW	16.650 usec
DE	6.00 usec
TE	297.7 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



YY-1-96
PROTON CDCl3

NAME	XB20140630
EXPNO	1
PROCNO	1
Date_	20140630
Time	8.57
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	64
DW	48.400 usec
DE	6.00 usec
TE	296.1 K
D1	1.00000000 sec
TD0	1

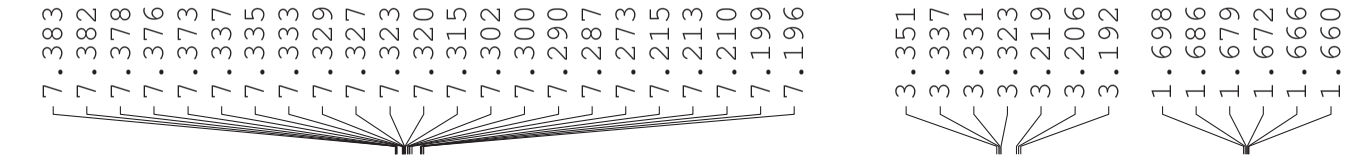
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300123 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

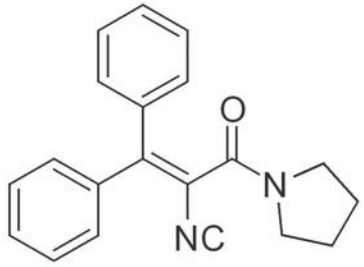


S59

YY-96
C13CPD CDCl3 I

NAME	XB20140706
EXPNO	15
PROCNO	1
Date_	20140706
Time	21.21
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	114
DW	16.650 usec
DE	6.00 usec
TE	298.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40





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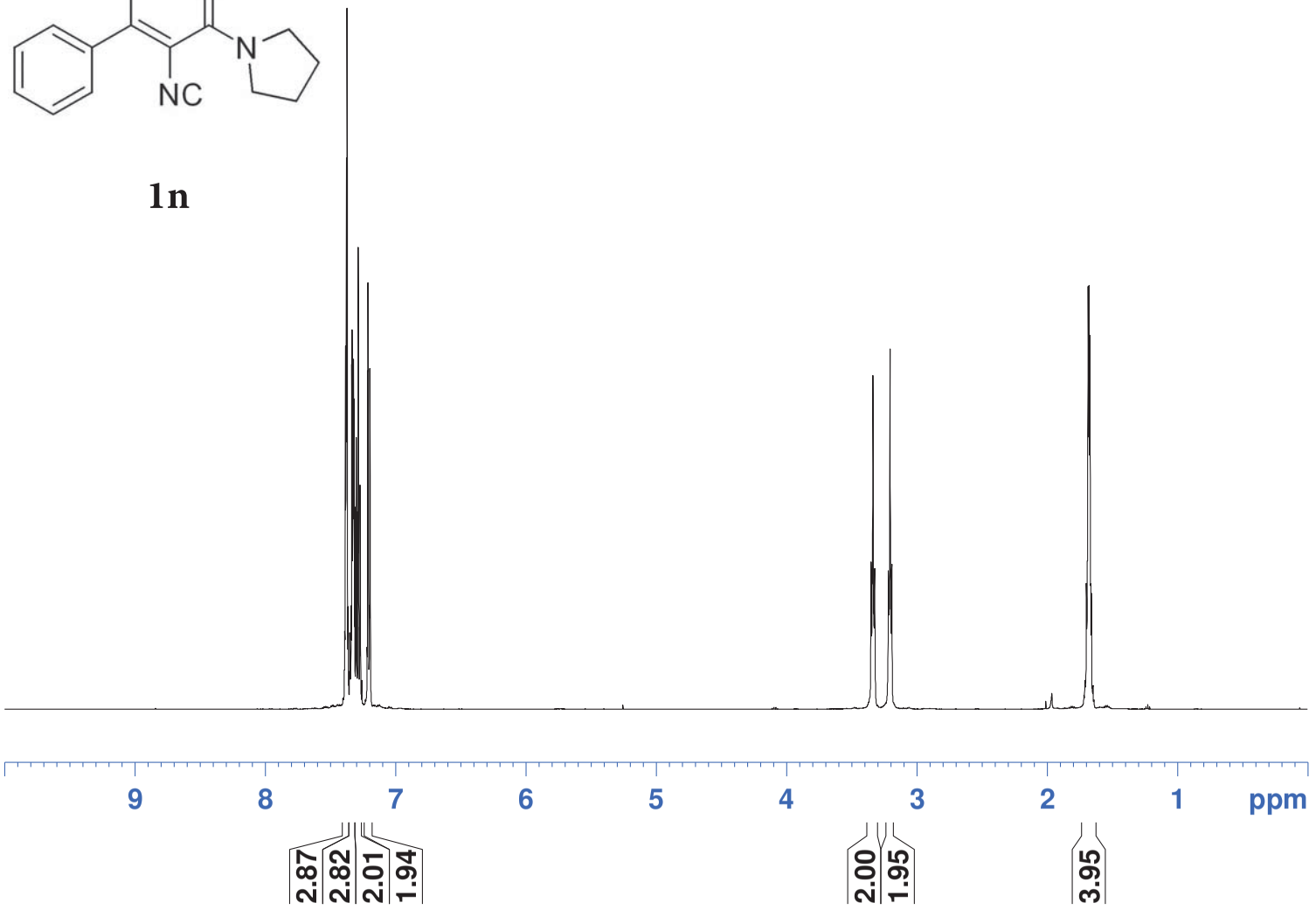
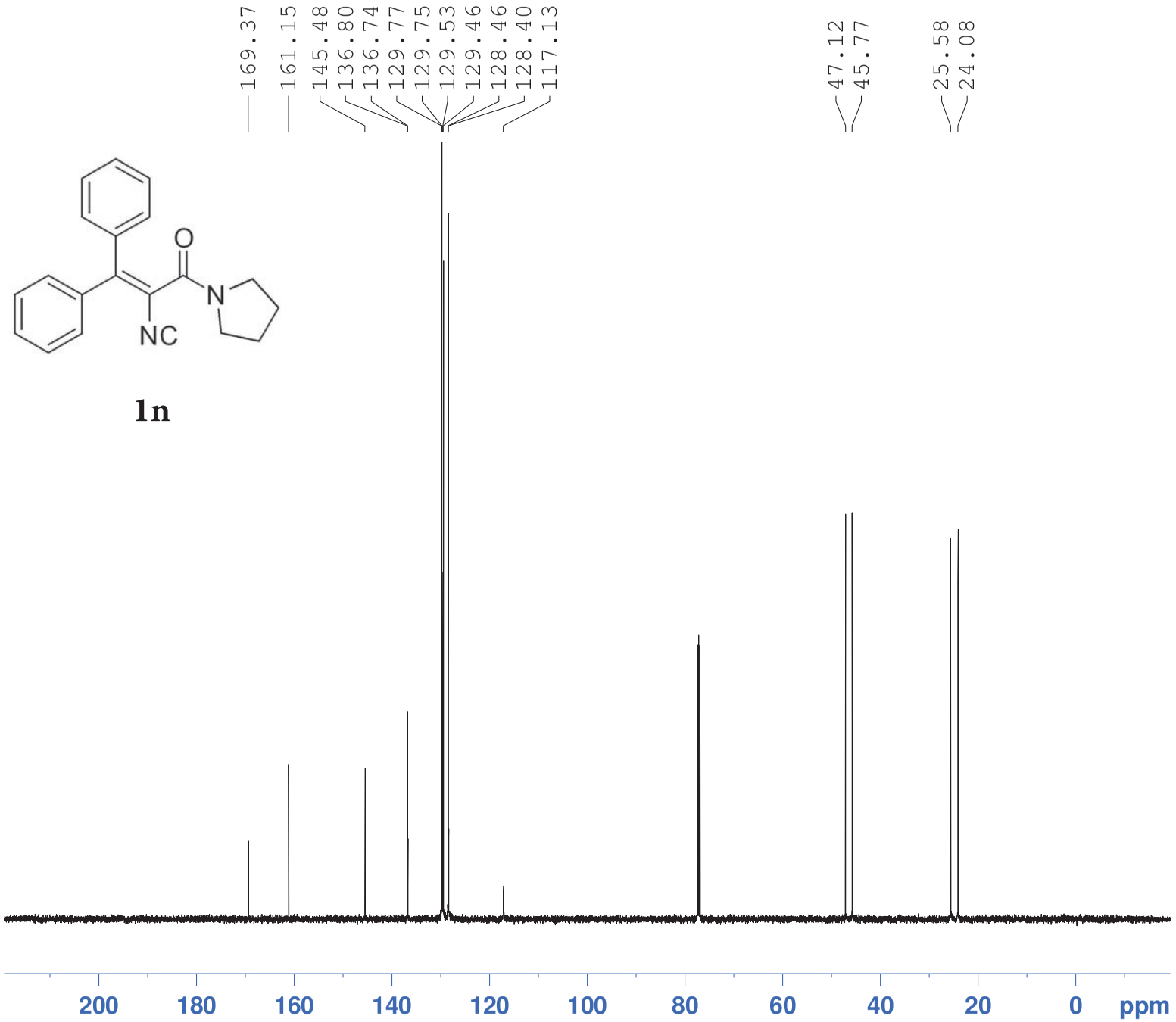


WH-7-23
PROTON CDCl3

NAME	XB20140609
EXPNO	22
PROCNO	1
Date_	20140610
Time	4.03
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	57
DW	48.400 usec
DE	6.00 usec
TE	296.7 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300126 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



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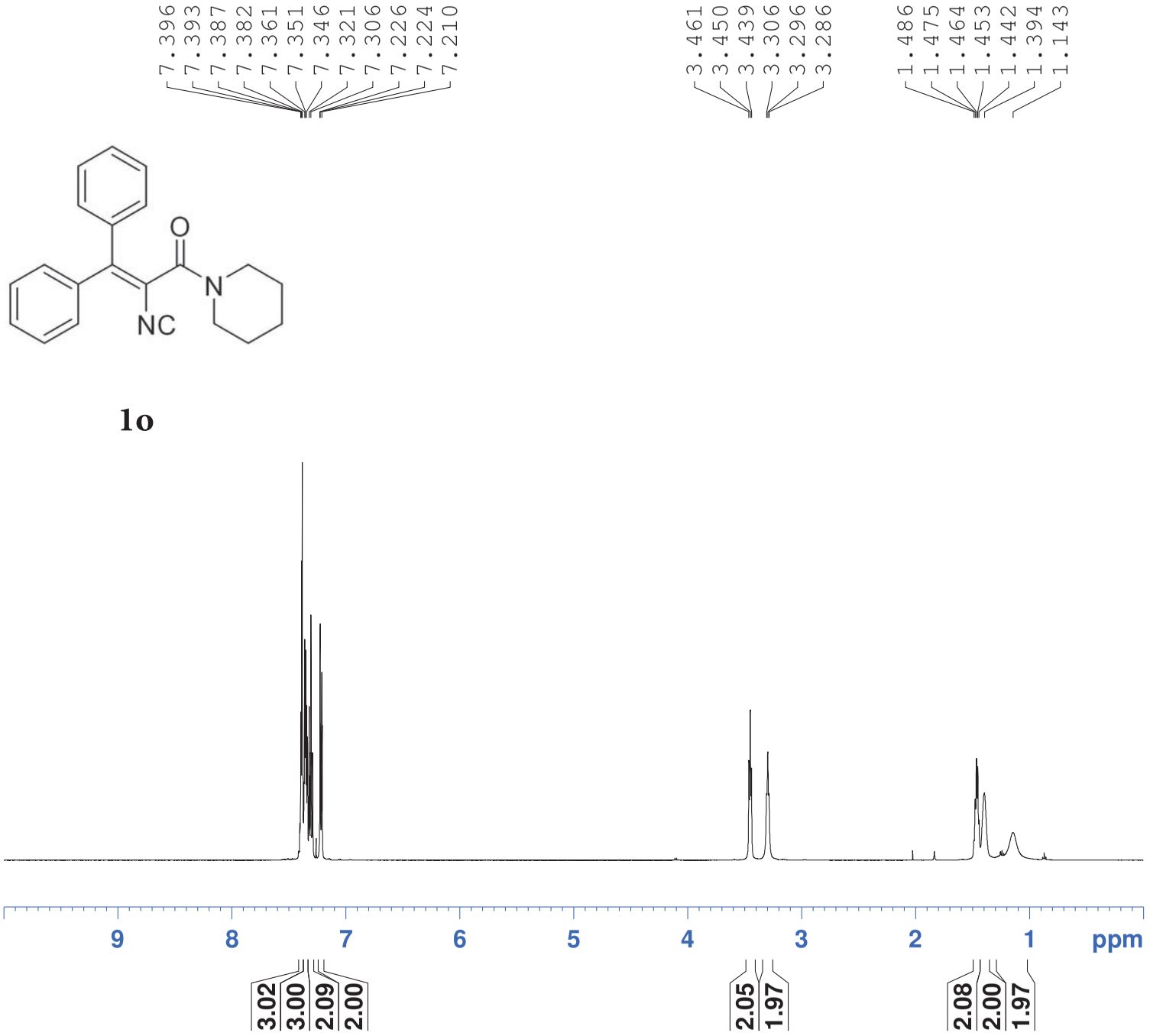
WH-7-23
C13CPD CDCl3

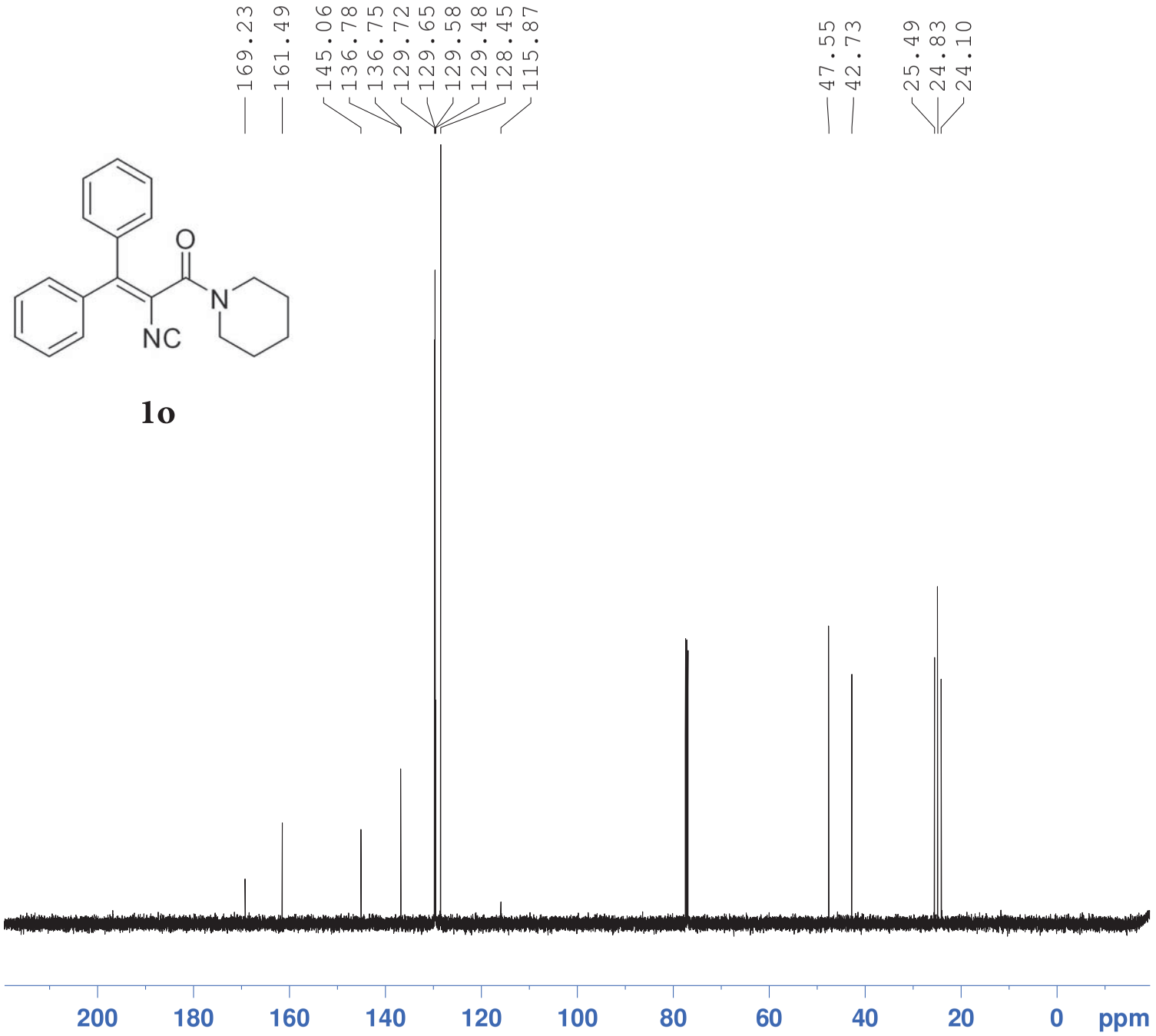
NAME	XB20140609
EXPNO	23
PROCNO	1
Date_	20140610
Time	4.18
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	256
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	114
DW	16.650 usec
DE	6.00 usec
TE	297.8 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



WH-7-7
PROTON CDCl3 I

NAME	XB20140603
EXPNO	5
PROCNO	1
Date_	20140603
Time	13.46
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	64
DW	48.400 usec
DE	6.00 usec
TE	295.9 K
D1	1.00000000 sec
TD0	1

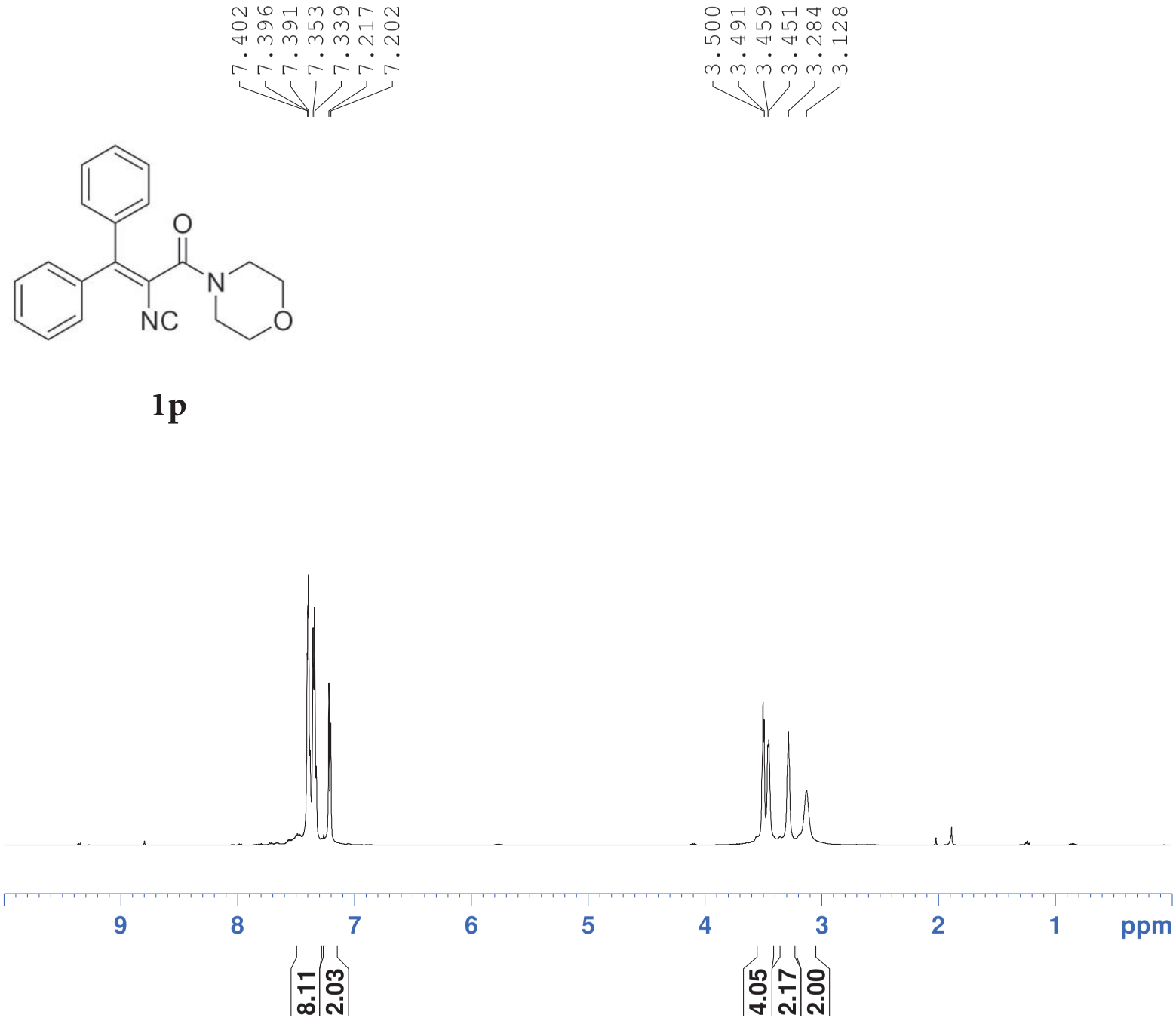
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300126 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



1o

WH-7-7
C13CPD CDCl3

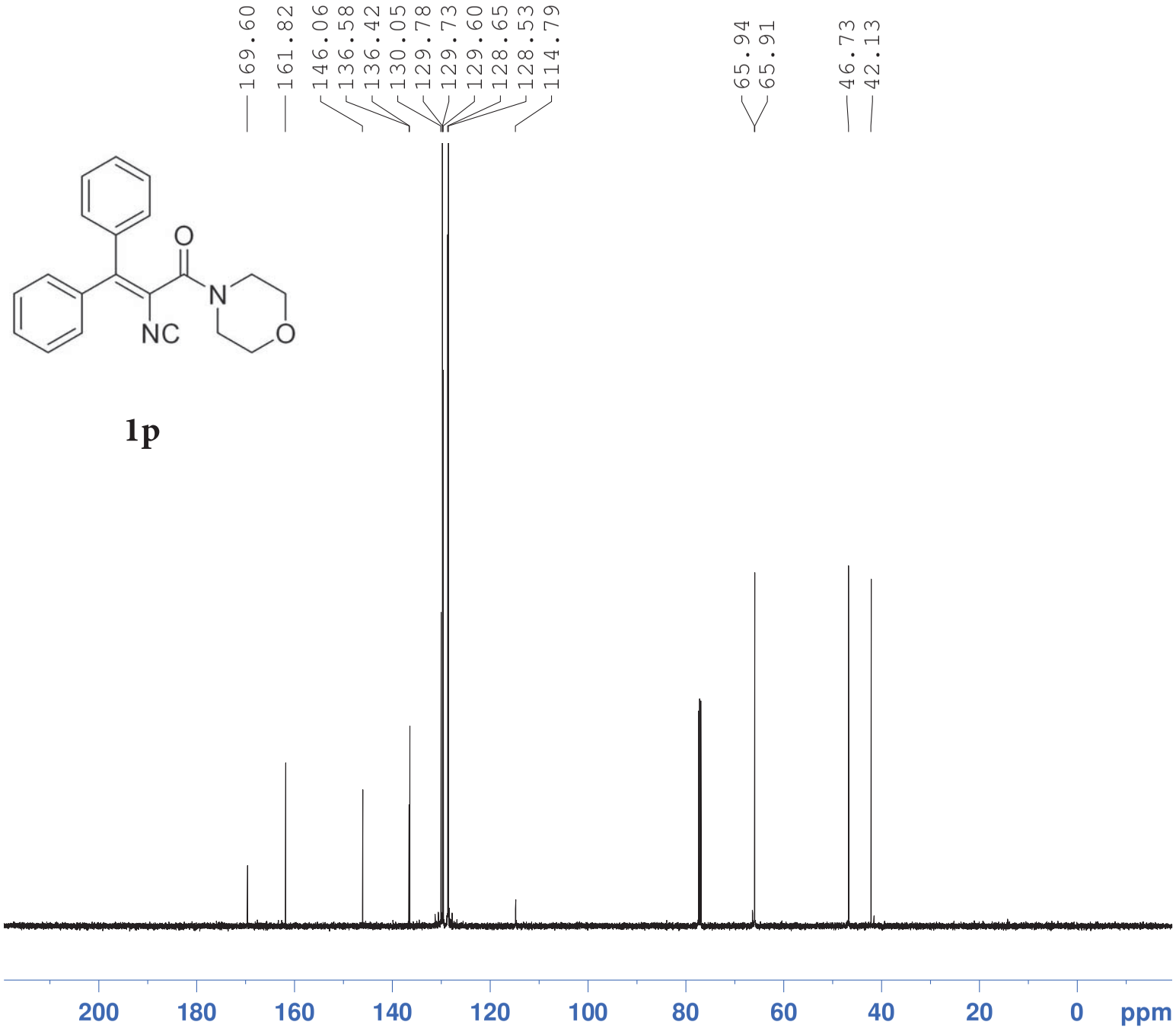
NAME	XB20140603
EXPNO	6
PROCNO	1
Date_	20140603
Time	13.50
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	145
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	114
DW	16.650 usec
DE	6.00 usec
TE	296.8 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40



WH-7-5
PROTON CDCl3 D

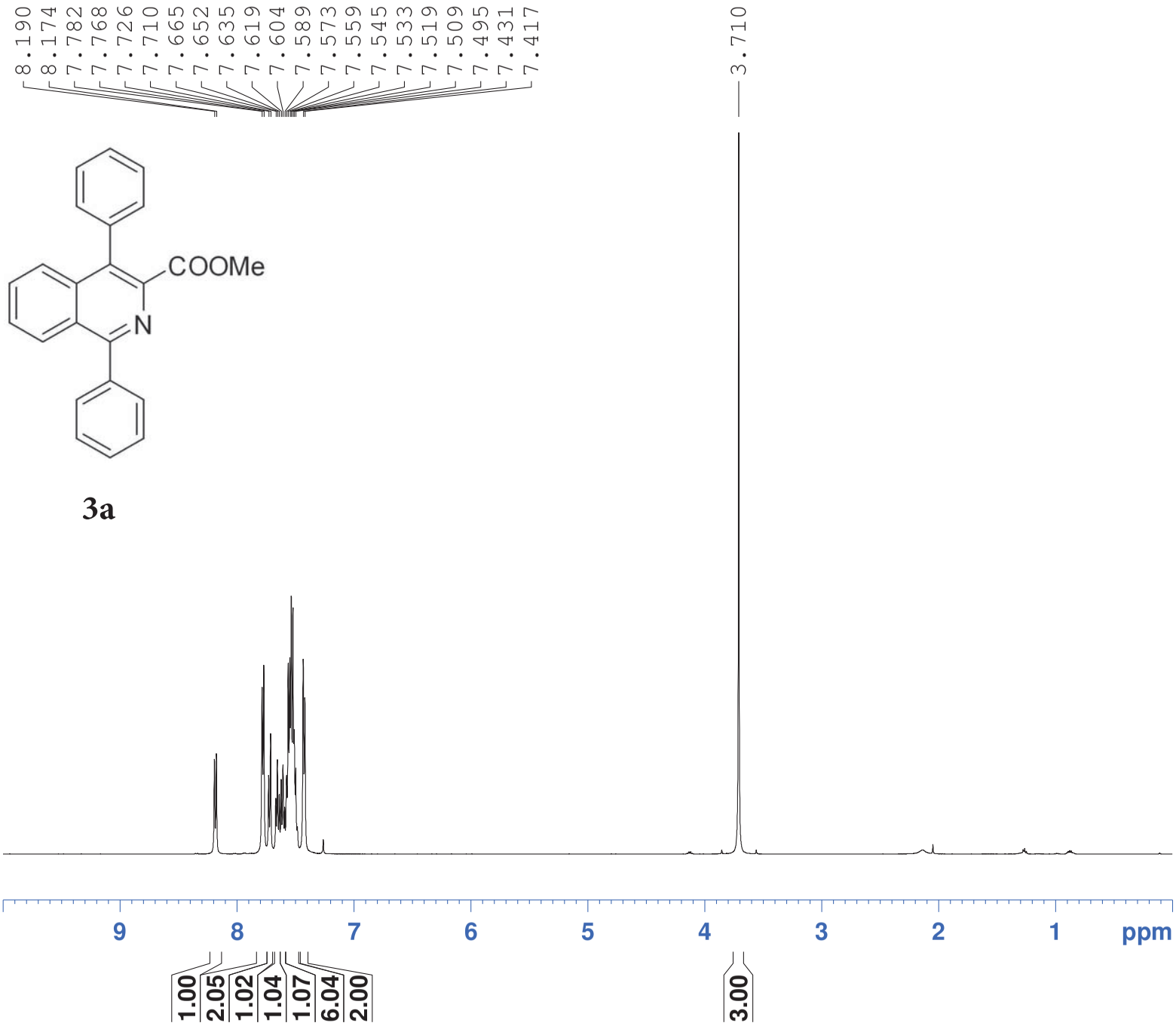
NAME	XB20140602
EXPNO	19
PROCNO	1
Date_	20140602
Time	20.29
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	57
DW	48.400 usec
DE	6.00 usec
TE	296.0 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300113 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



WH-7-5
C13CPD CDCl3

NAME	XB20140602
EXPNO	20
PROCNO	1
Date_	20140602
Time	21.25
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	181
DW	16.650 usec
DE	6.00 usec
TE	297.7 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40

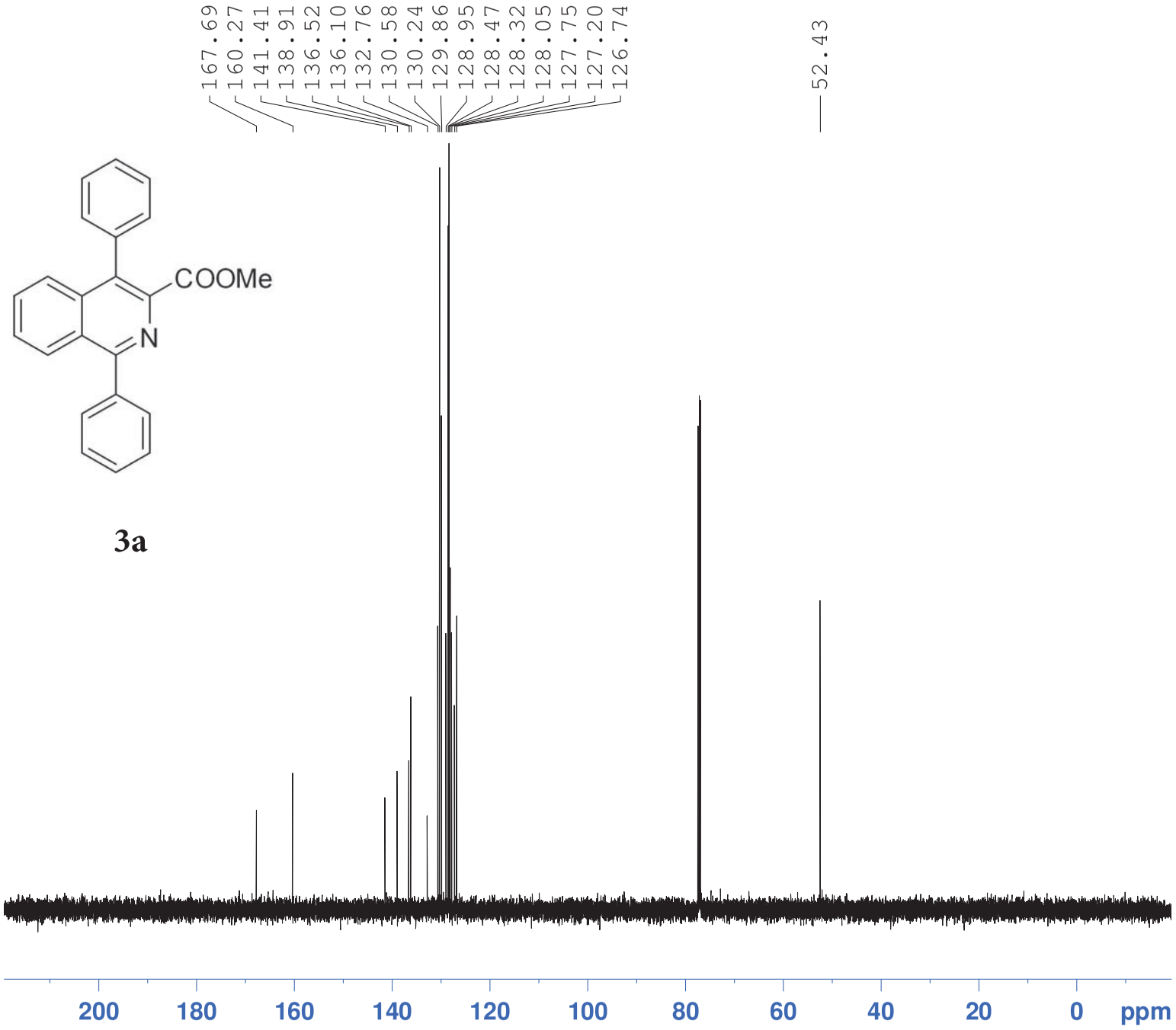


3a

WH-6-51
PROTON CDCl3

NAME	XB20140429
EXPNO	2
PROCNO	1
Date_	20140429
Time	9.42
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	90.5
DW	48.400 usec
DE	6.00 usec
TE	296.0 K
D1	1.00000000 sec
TD0	1

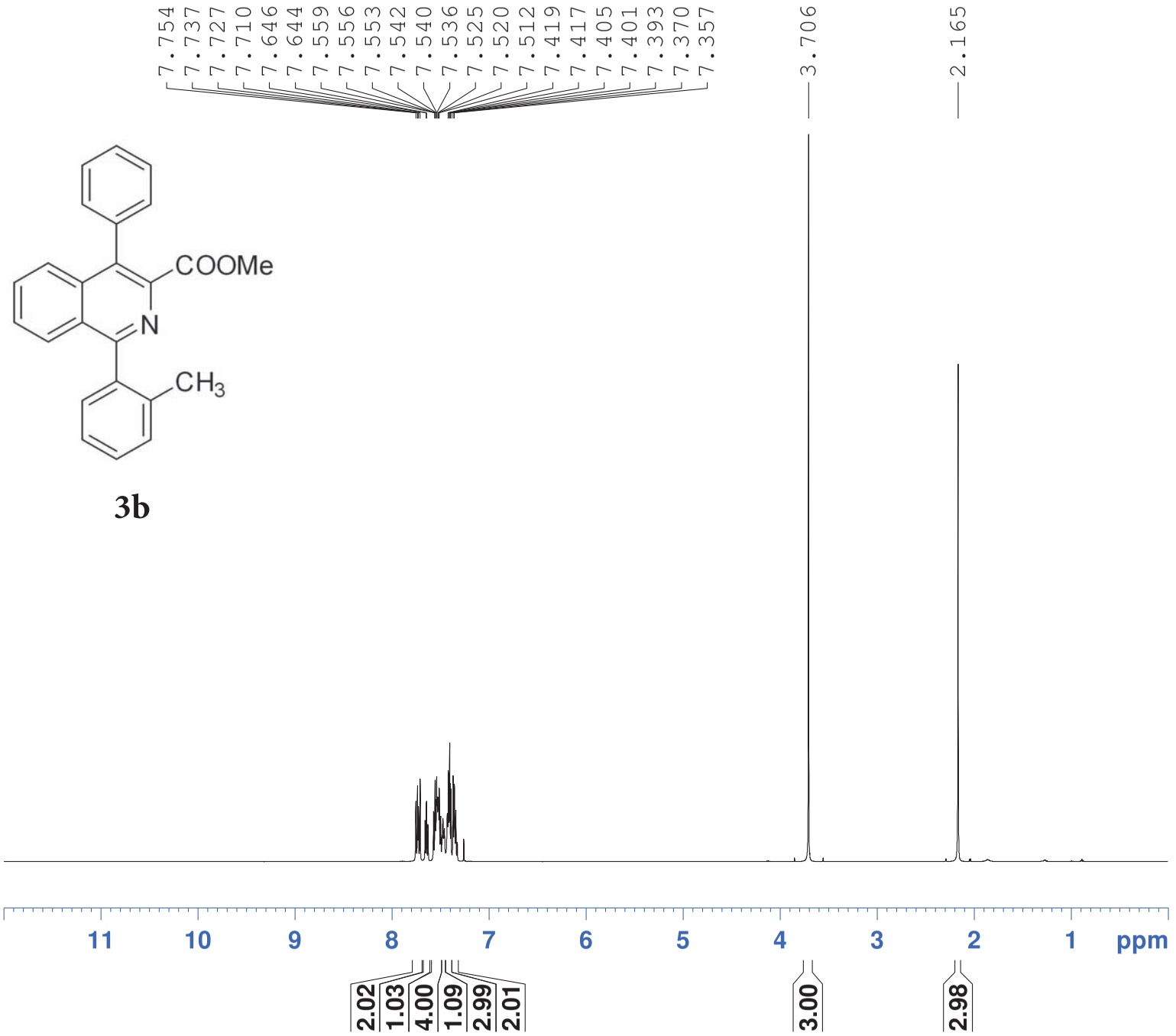
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300126 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



3a

WH-6-51
C13CPD CDCl3 D

NAME	XB20140429
EXPNO	3
PROCNO	1
Date_	20140429
Time	9.51
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	128
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	101.6
DW	16.650 usec
DE	6.00 usec
TE	297.3 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40

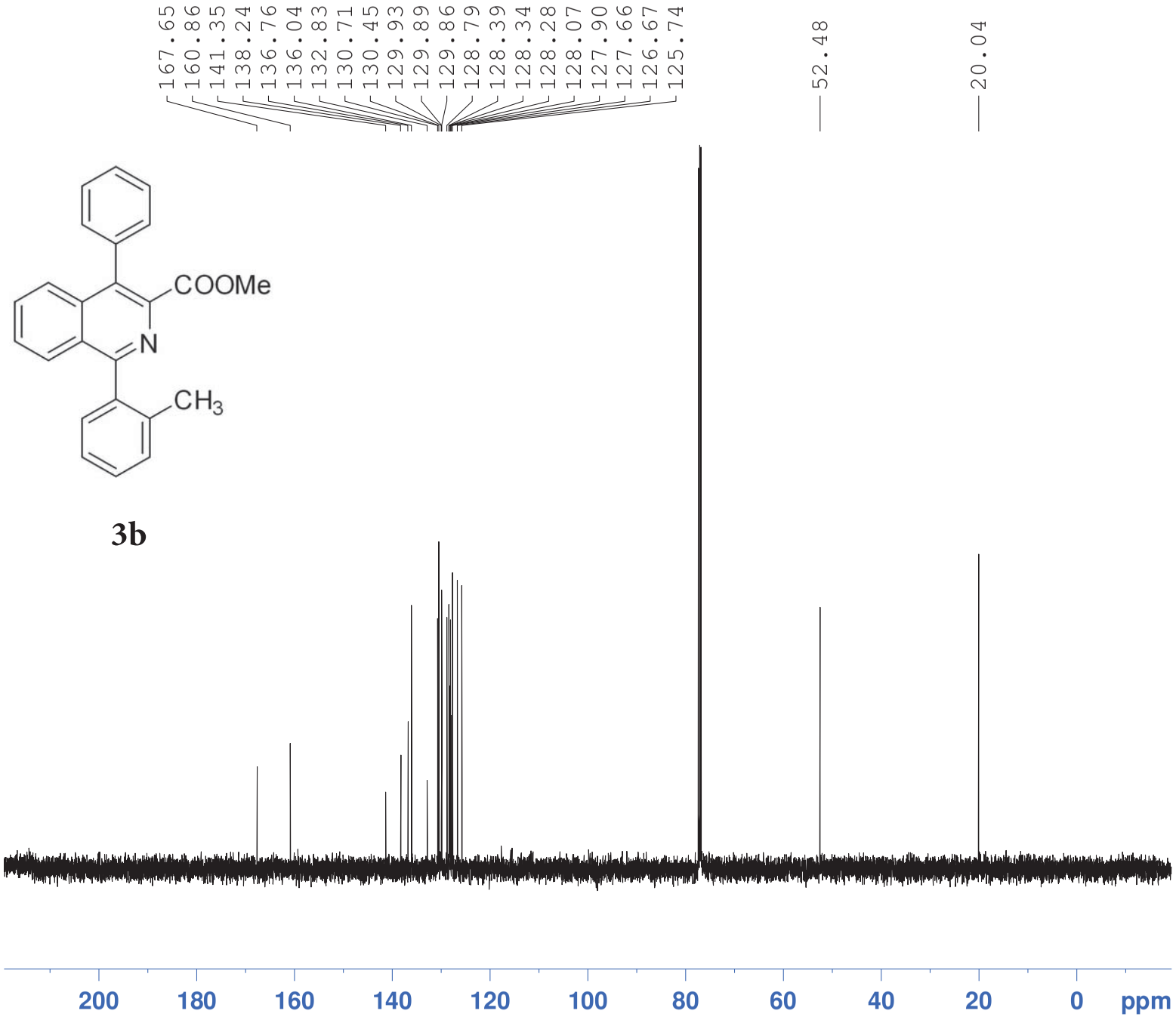


3b

WH-6-73
PROTON CDCl3

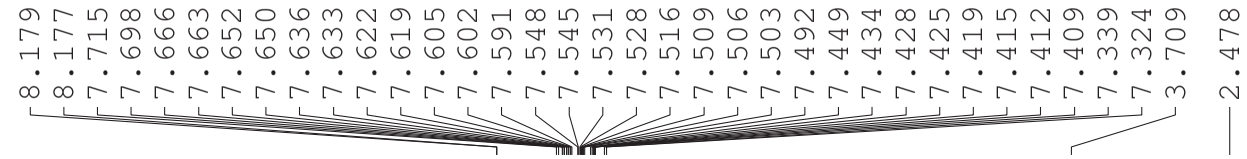
NAME	XB20140504
EXPNO	11
PROCNO	1
Date_	20140504
Time	9.29
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	114
DW	48.400 usec
DE	6.00 usec
TE	296.3 K
D1	1.00000000 sec
TD0	1

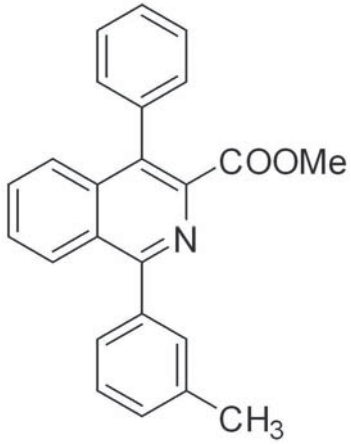
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300126 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



WH-6-73
C13CPD CDCl3

NAME	xb20140505
EXPNO	15
PROCNO	1
Date_	20140505
Time	10.53
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	63
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	287.4
DW	16.650 usec
DE	6.00 usec
TE	296.8 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



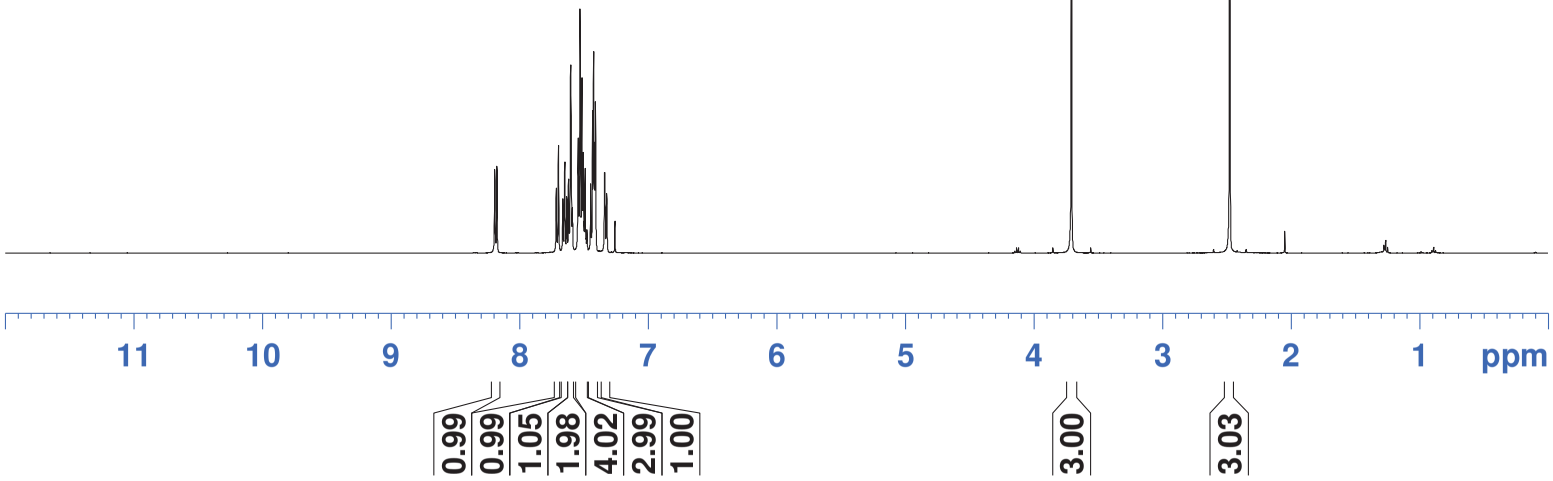


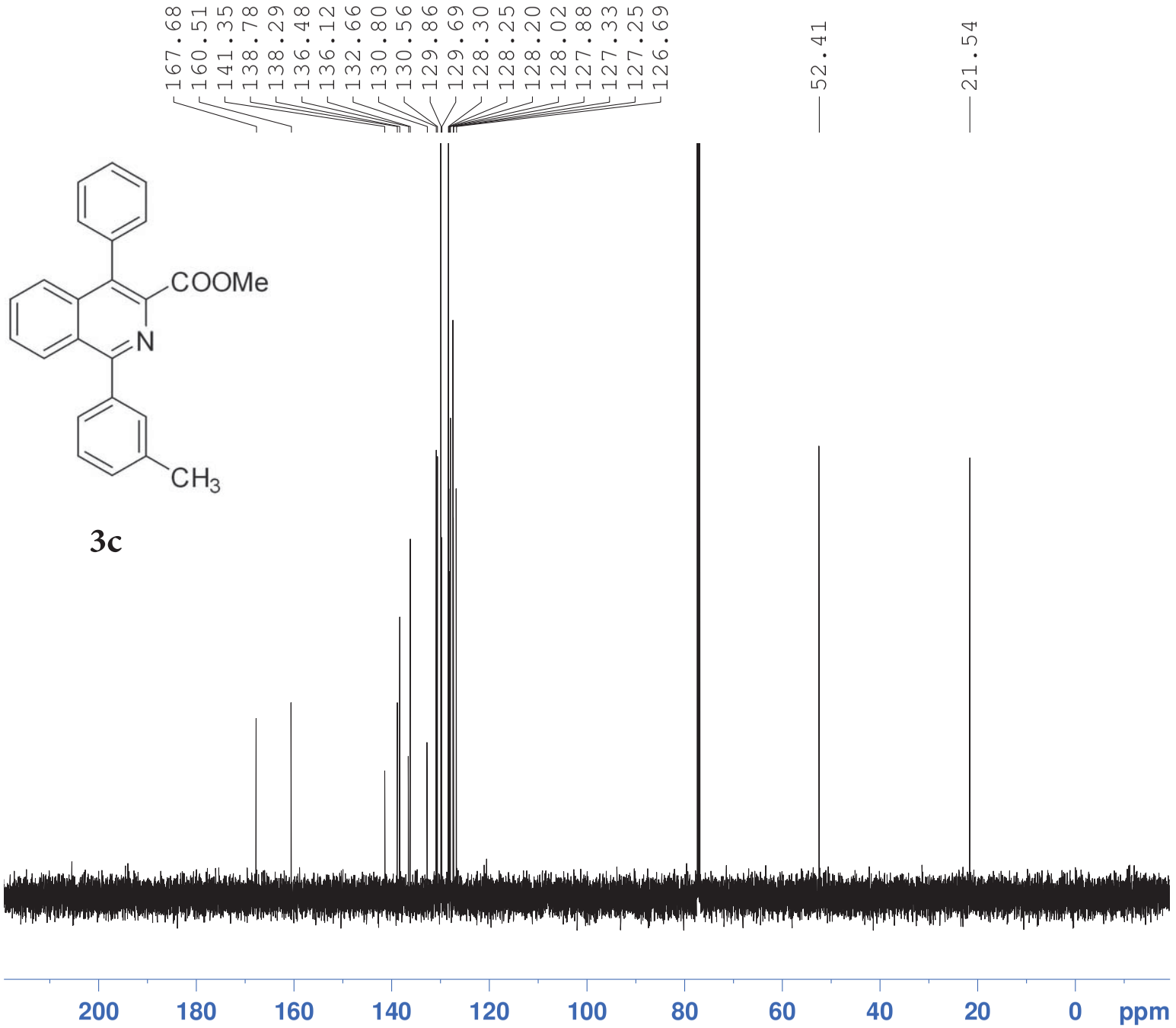
3c

WH-6-72
PROTON CDCl3

NAME	XB20140504
EXPNO	13
PROCNO	1
Date_	20140504
Time	9.43
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	114
DW	48.400 usec
DE	6.00 usec
TE	296.3 K
D1	1.00000000 sec
TD0	1

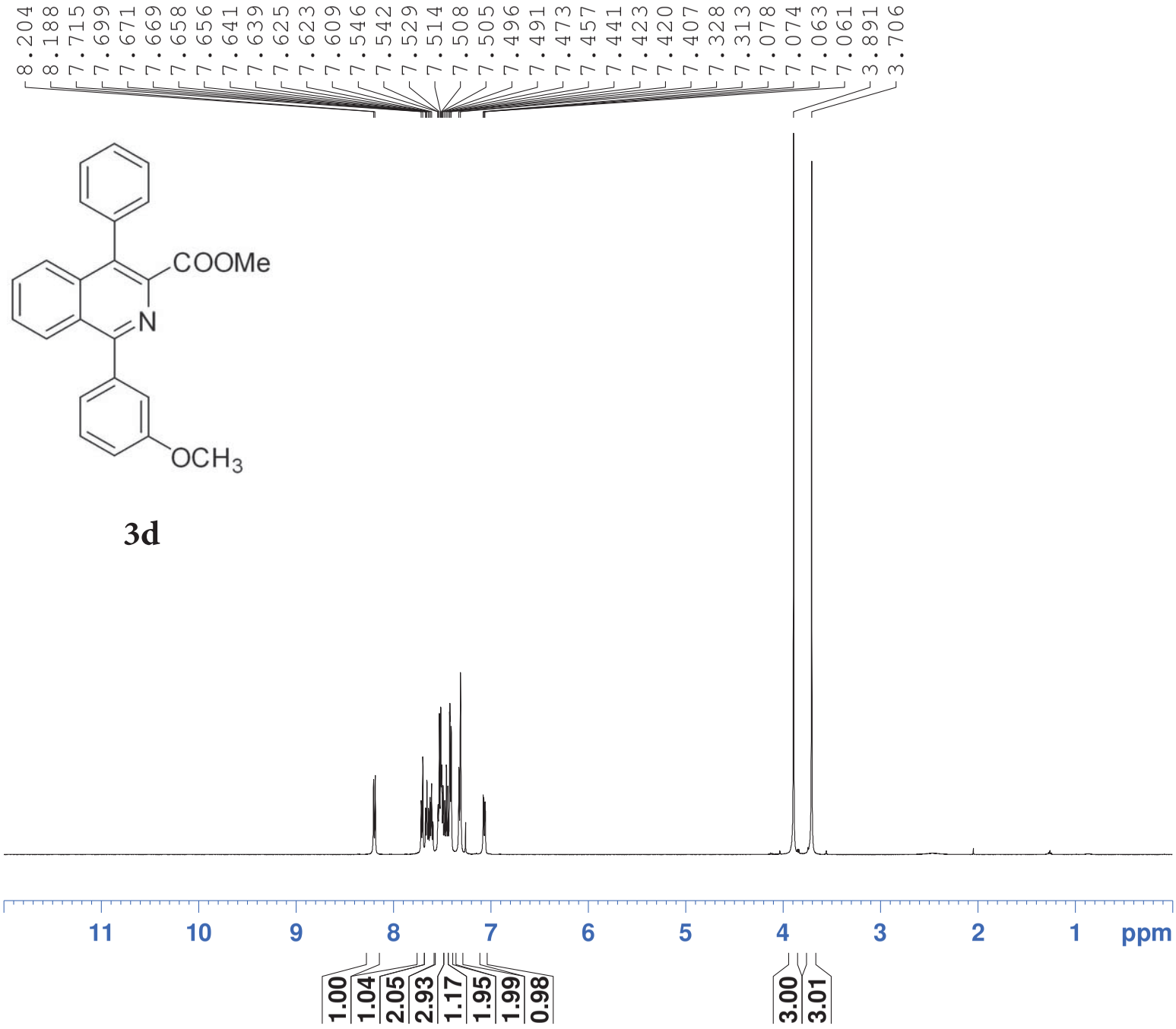
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300126 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00





WH-6-72
C13CPD CDCl3 I

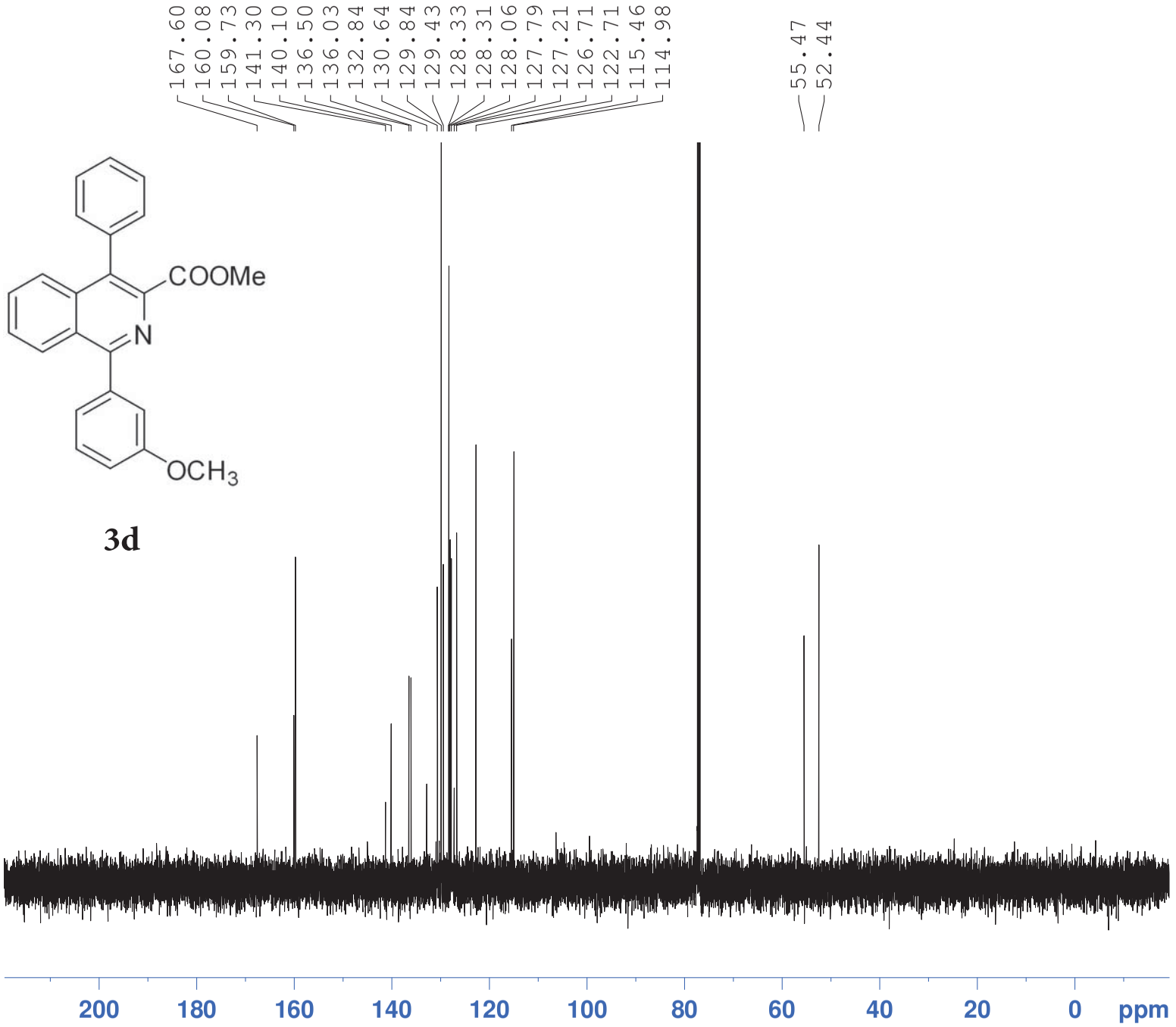
NAME	XB20140504
EXPNO	14
PROCNO	1
Date_	20140504
Time	9.52
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	128
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	101.6
DW	16.650 usec
DE	6.00 usec
TE	297.4 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40



3d

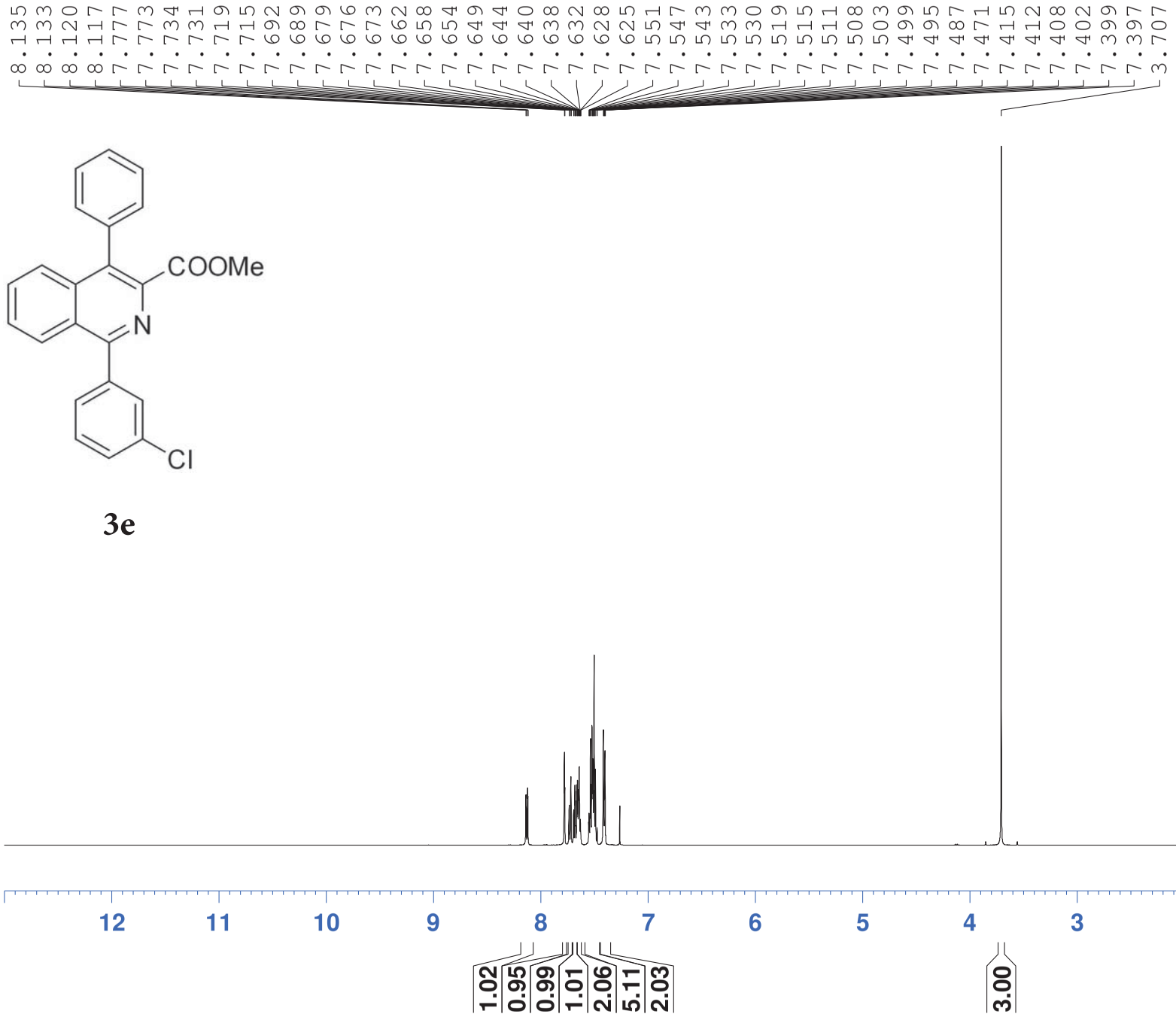
WH-6-63
PROTON CDCl3

NAME	XB20140504
EXPNO	17
PROCNO	1
Date_	20140504
Time	10.12
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	161.3
DW	48.400 usec
DE	6.00 usec
TE	296.4 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300126 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

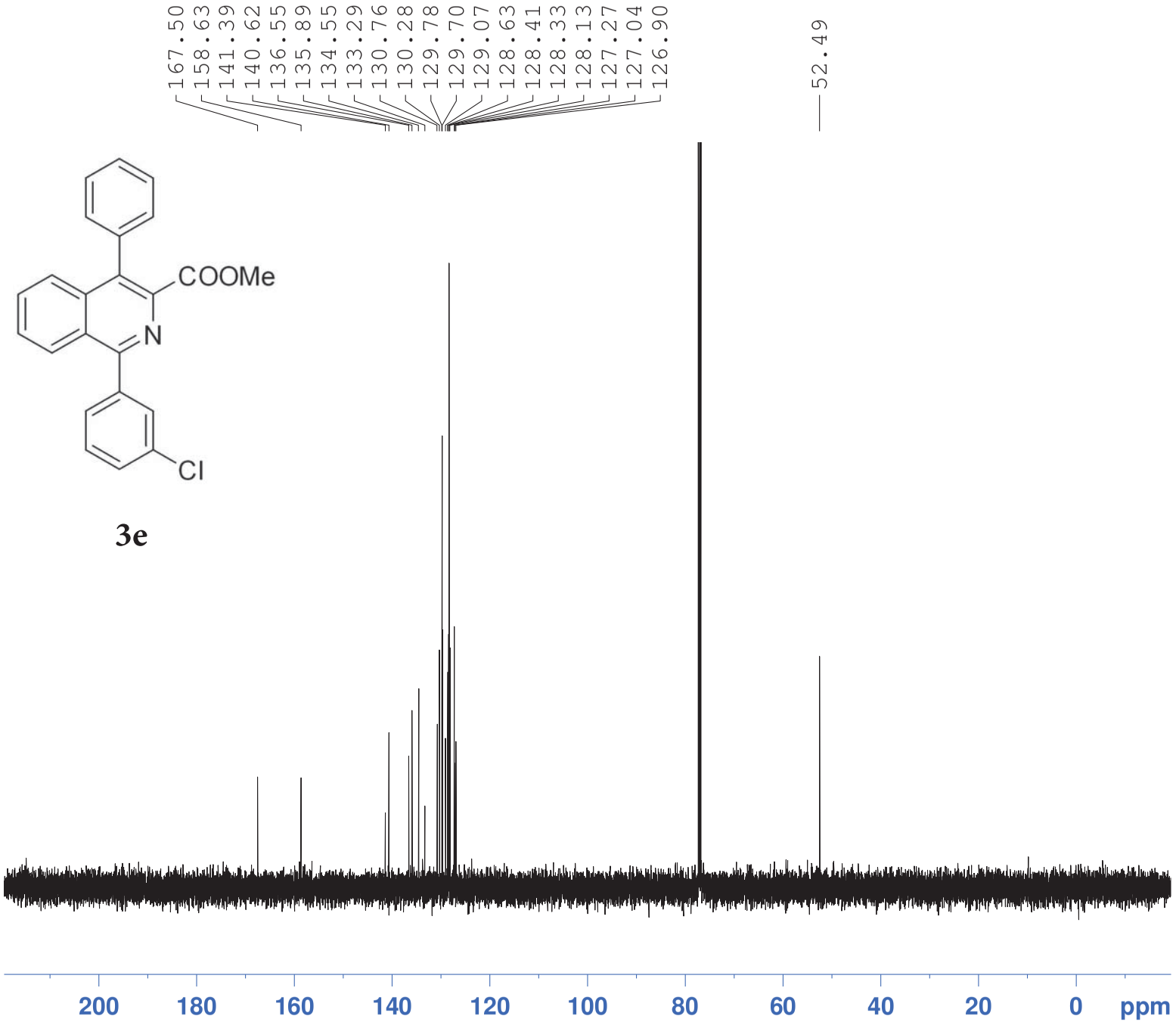


WH-6-63
C13CPD CDCl3

NAME	XB20140504
EXPNO	18
PROCNO	1
Date_	20140504
Time	10.21
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	128
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	101.6
DW	16.650 usec
DE	6.00 usec
TE	297.4 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40


8.135
8.133
8.120
8.117
7.777
7.773
7.734
7.731
7.719
7.715
7.692
7.689
7.679
7.676
7.673
7.662
7.658
7.654
7.649
7.644
7.640
7.638
7.632
7.628
7.625
7.551
7.547
7.543
7.533
7.530
7.519
7.515
7.511
7.508
7.503
7.499
7.495
7.487
7.471
7.415
7.412
7.408
7.402
7.399
7.397
3.707
COOMe
N
Cl
WH-6-83
PROTON CDCl3
NAME XB20140504
EXPNO 28
PROCNO 1
Date_ 20140504
Time 12.08
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 203.2
DW 48.400 usec
DE 6.00 usec
TE 296.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.14 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300126 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.02
0.95
0.99
1.01
2.06
5.11
2.03
3.00

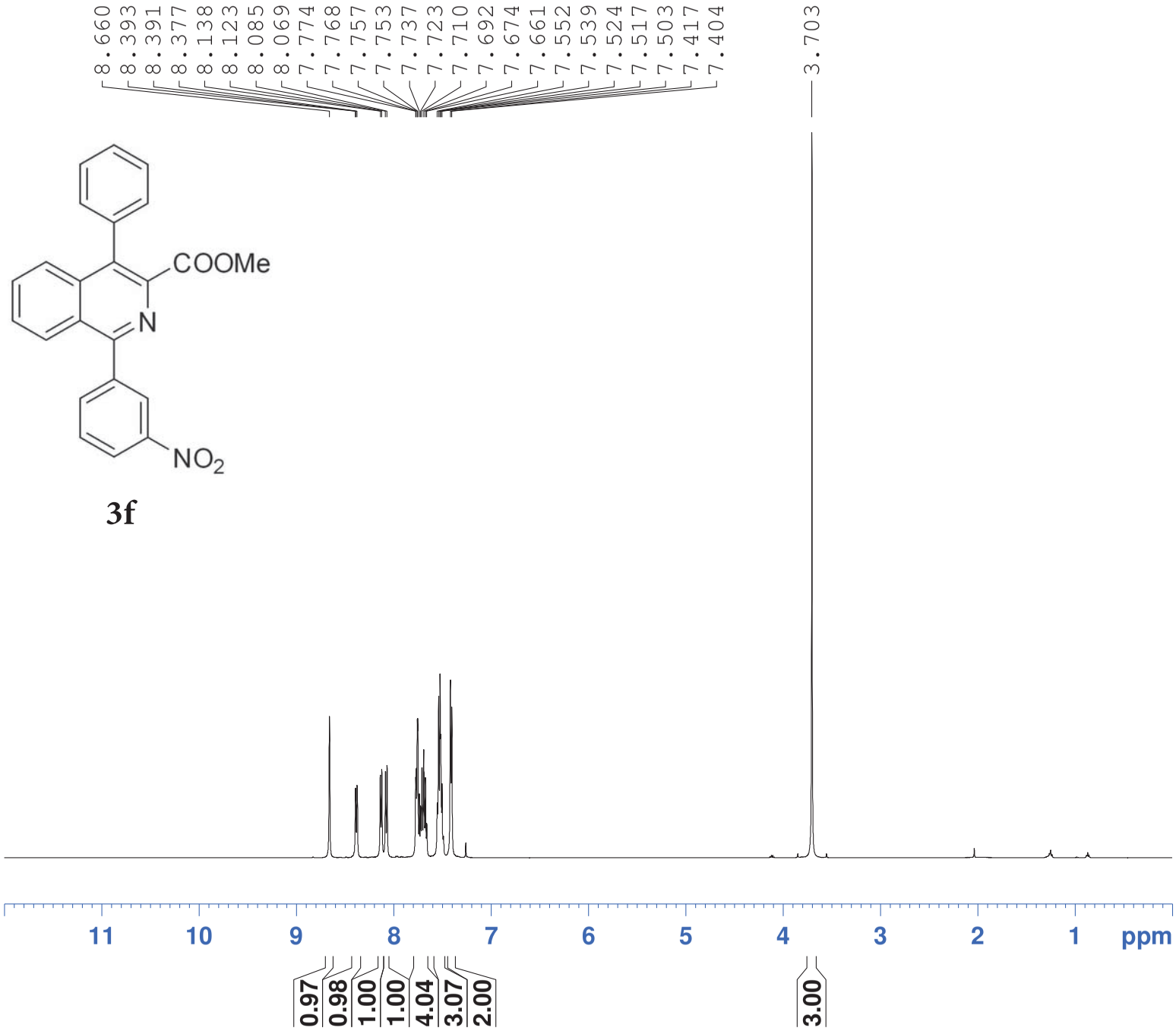
3e



3e

WH-6-83
C13CPD CDCl3

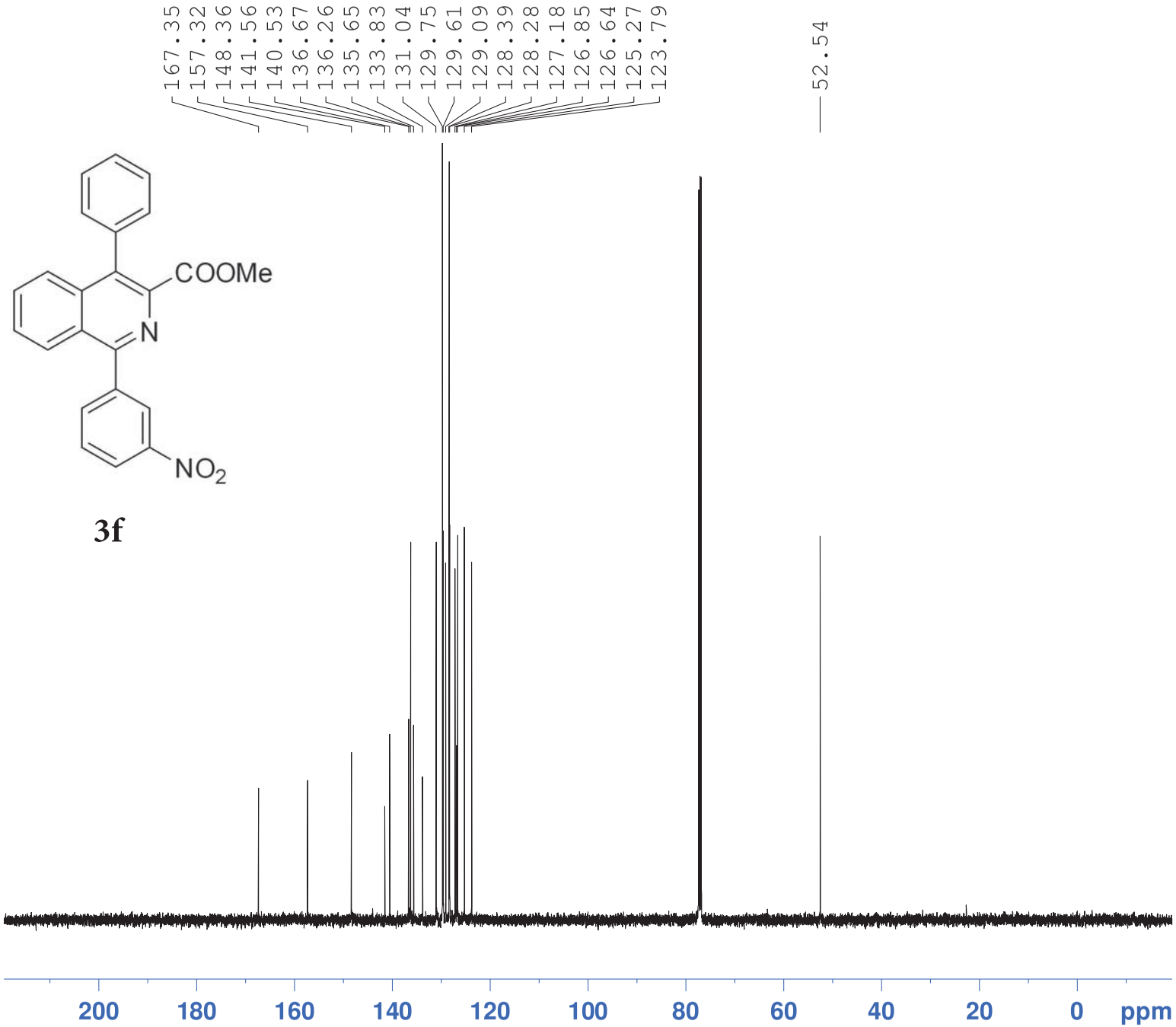
NAME	XB20140504
EXPNO	29
PROCNO	1
Date_	20140504
Time	12.17
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	128
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	287.4
DW	16.650 usec
DE	6.00 usec
TE	297.4 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40



3f

WH-6-96
PROTON CDCl3

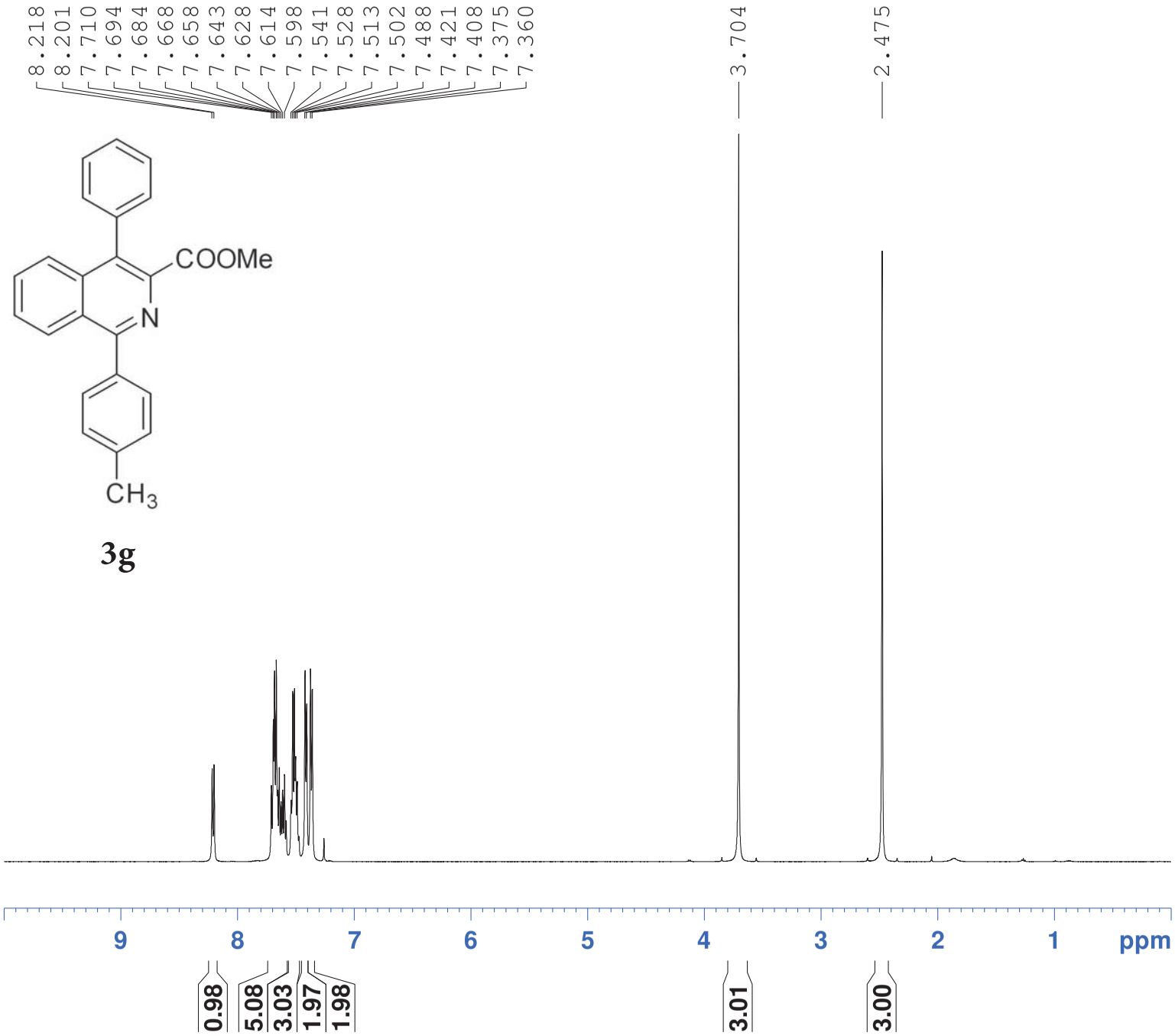
NAME	xb20140509
EXPNO	8
PROCNO	1
Date_	20140509
Time	9.56
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	90.5
DW	48.400 usec
DE	6.00 usec
TE	296.3 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300123 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



3f

WH-6-96
C13CPD CDCl3 I

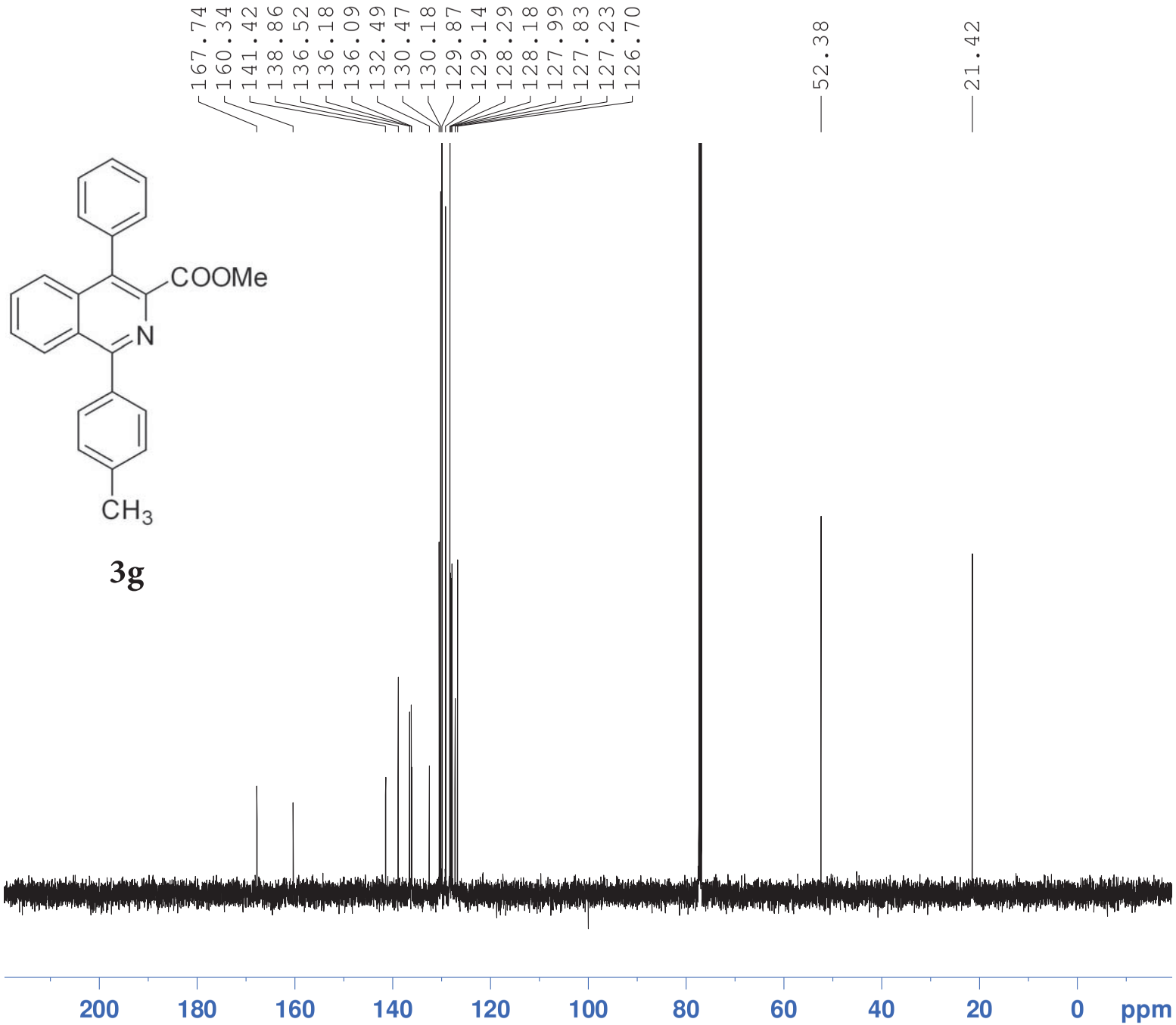
NAME	xb20140509
EXPNO	9
PROCNO	1
Date_	20140509
Time	10.11
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	256
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	228.1
DW	16.650 usec
DE	6.00 usec
TE	297.3 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



3g

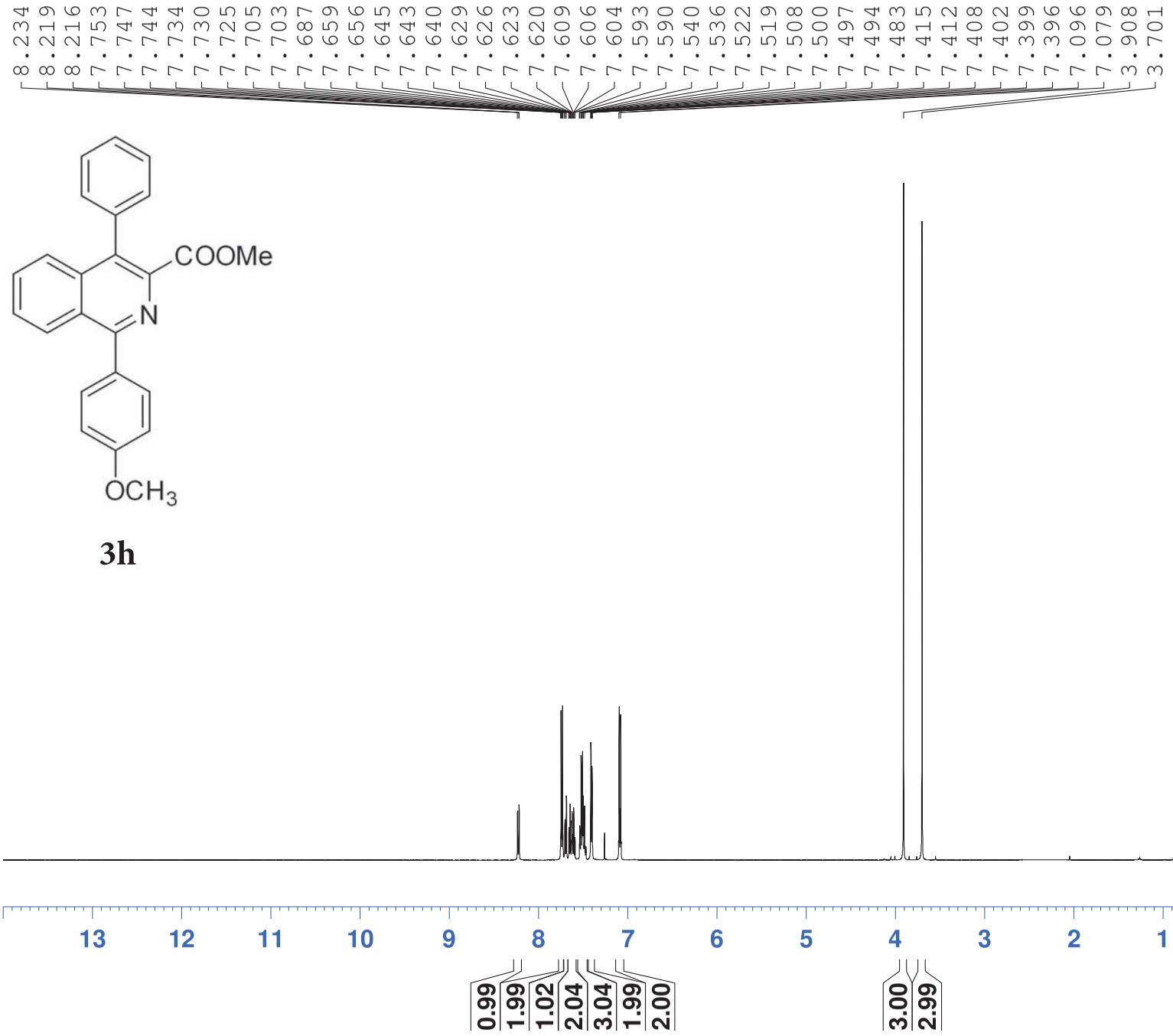
WH-6-59
PROTON CDC

NAME	XB20140430
EXPNO	2
PROCNO	1
Date_	20140430
Time	9.15
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	128
DW	48.400 usec
DE	6.00 usec
TE	295.9 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300123 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



WH-6-59
C13CPD CDCl3

NAME	XB20140430
EXPNO	4
PROCNO	1
Date_	20140430
Time	9.25
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	128
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	101.6
DW	16.650 usec
DE	6.00 usec
TE	297.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40


8.234
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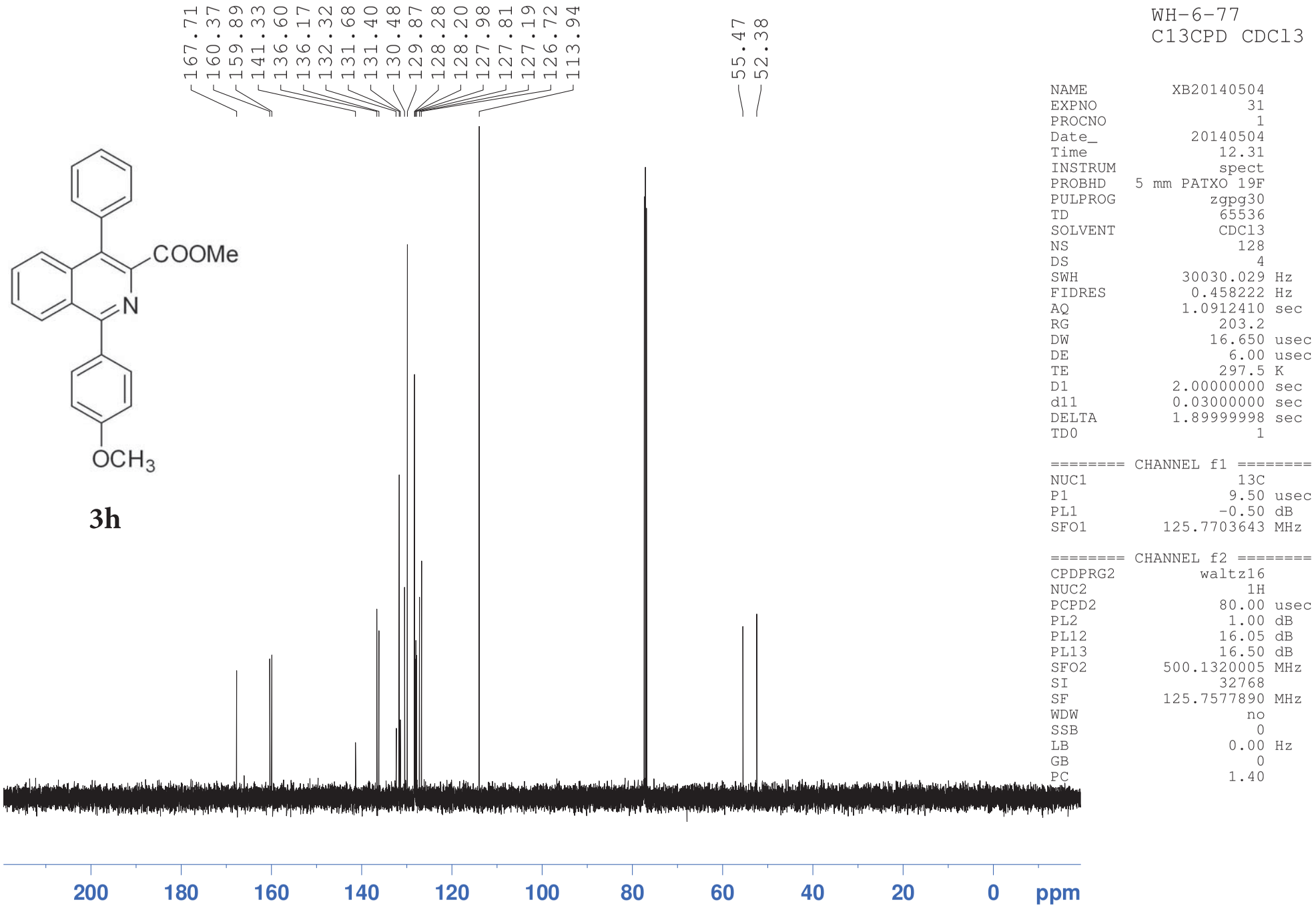
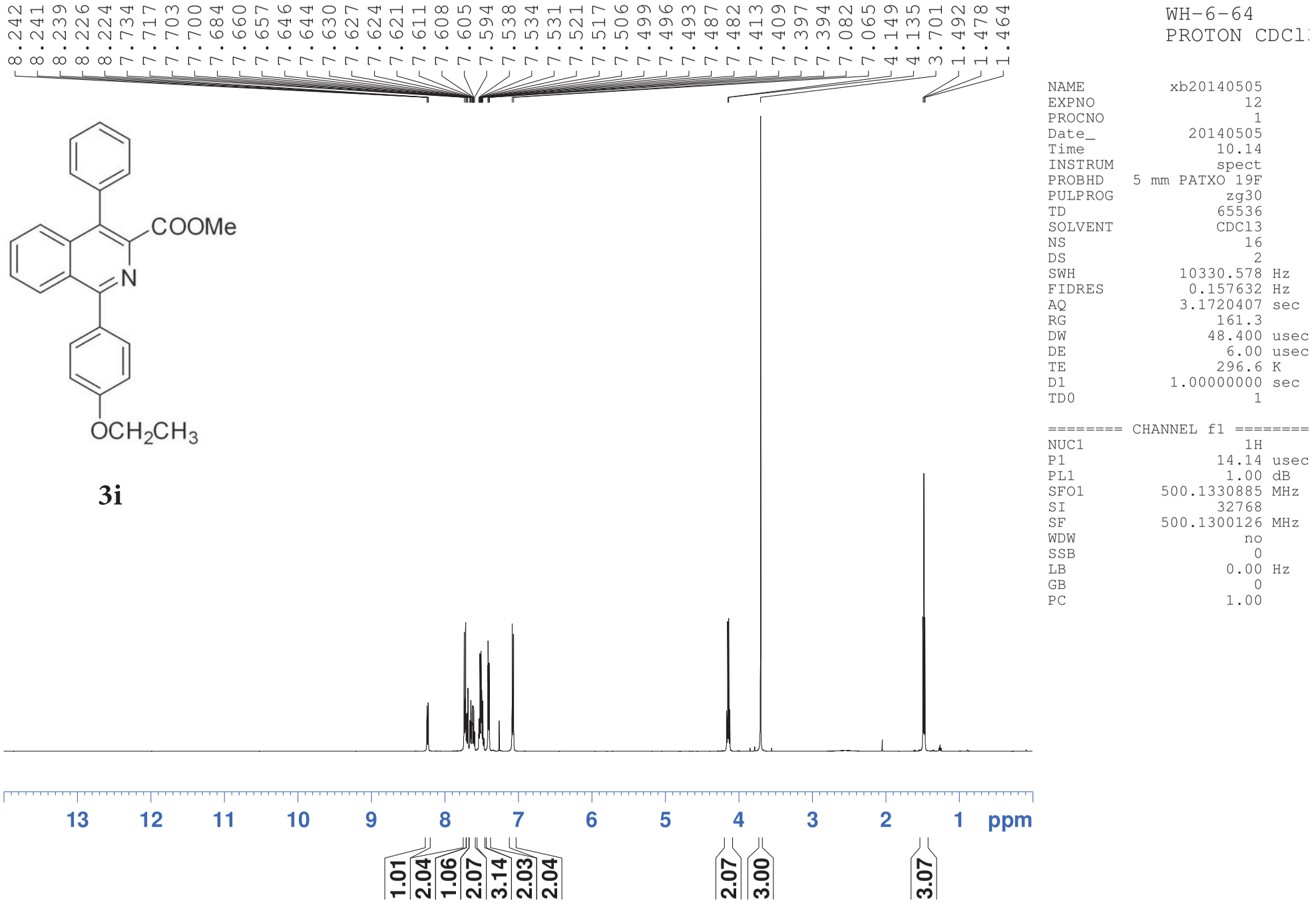
8.216
7.753
7.747
7.744
7.734
7.730
7.725
7.705
7.703
7.687
7.659
7.656
7.645
7.643
7.640
7.629
7.626
7.623
7.620
7.609
7.606
7.604
7.593
7.590
7.540
7.536
7.522
7.519
7.508
7.500
7.497
7.494
7.483
7.415
7.412
7.408
7.402
7.399
7.396
7.096
7.079
3.908
3.701
COOMe
N
OCH3
3h
WH-6-77
PROTON CDCl
NAME XB20140504
EXPNO 30
PROCNO 1
Date_ 20140504
Time 12.22
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 143.7
DW 48.400 usec
DE 6.00 usec
TE 296.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.14 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300126 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.99
1.99
1.02
2.04
3.04
1.99
2.00
3.00
2.99



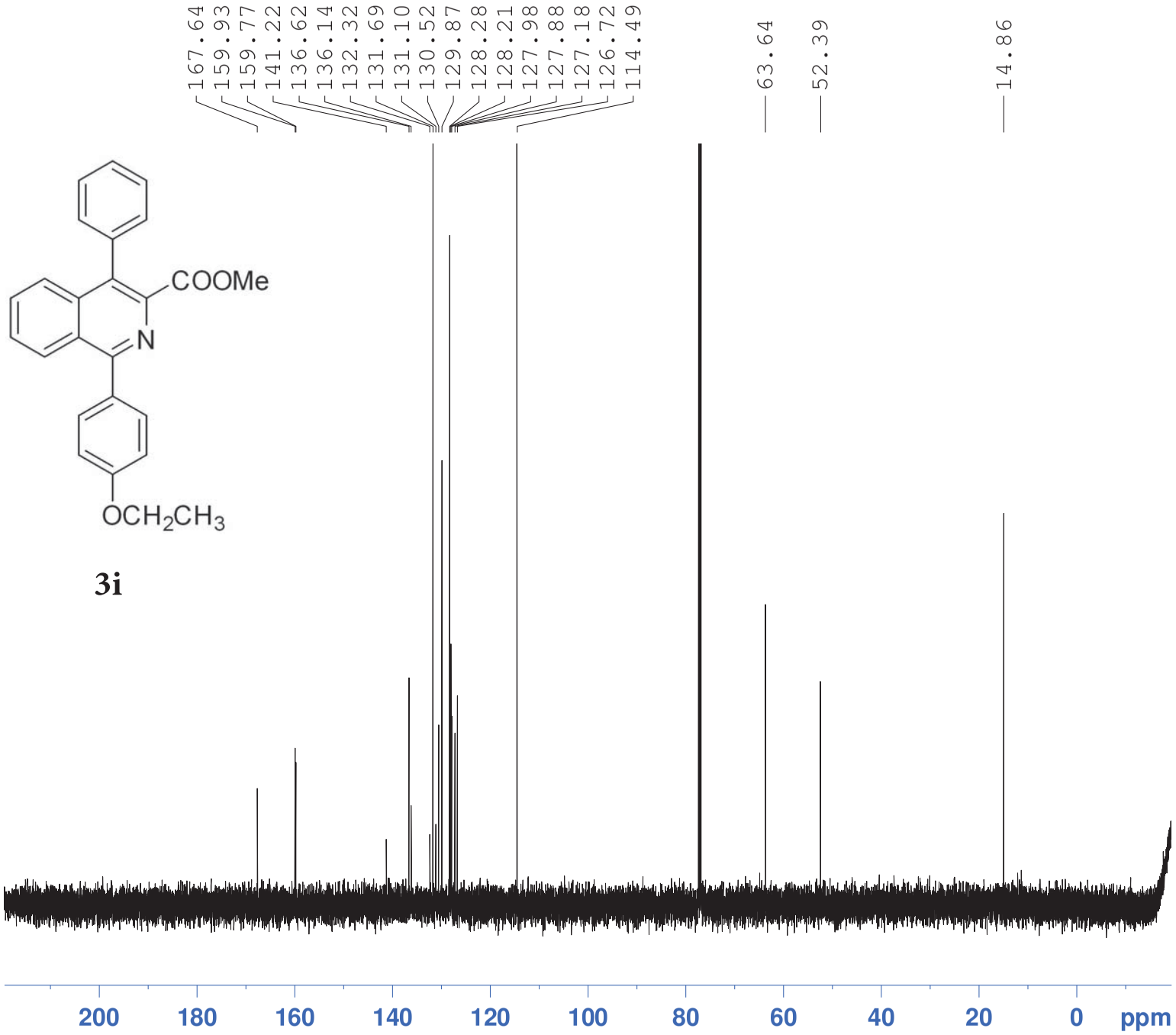
WH-6-77
C13CPD CDCl3

NAME	XB20140504
EXPNO	31
PROCNO	1
Date_	20140504
Time	12.31
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	128
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	203.2
DW	16.650 usec
DE	6.00 usec
TE	297.5 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40



WH-6-64
PROTON CDCl3

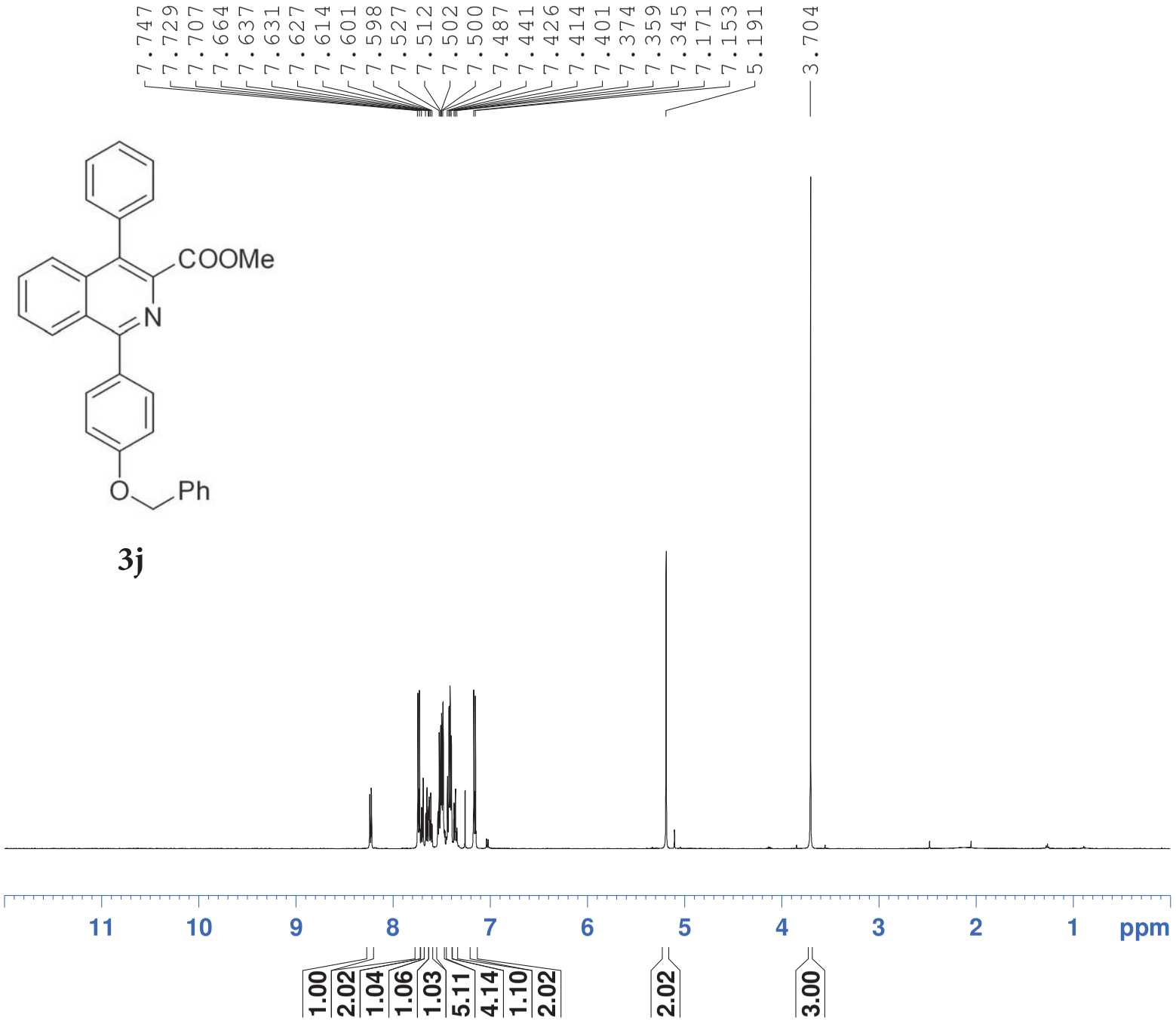
NAME	xb20140505
EXPNO	12
PROCNO	1
Date_	20140505
Time	10.14
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	161.3
DW	48.400 usec
DE	6.00 usec
TE	296.6 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300126 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



3i

WH-6-64
C13CPD CDCl3

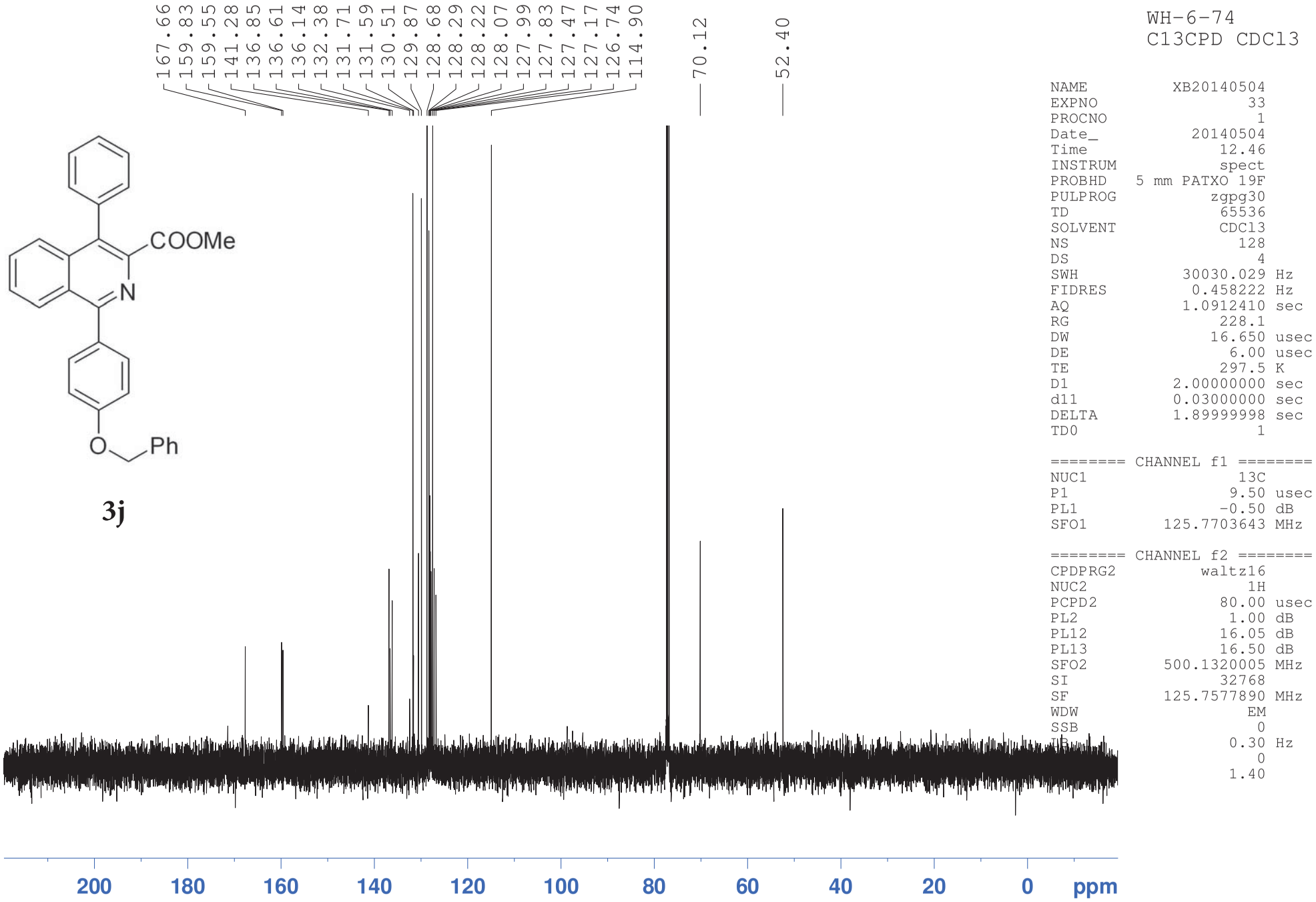
NAME	xb20140505
EXPNO	13
PROCNO	1
Date_	20140505
Time	10.23
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	128
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	203.2
DW	16.650 usec
DE	6.00 usec
TE	297.7 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40



3j

WH-6-74
PROTON CDCl3

NAME	XB20140504
EXPNO	32
PROCNO	1
Date_	20140504
Time	12.37
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	228.1
DW	48.400 usec
DE	6.00 usec
TE	296.3 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300126 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00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141.28
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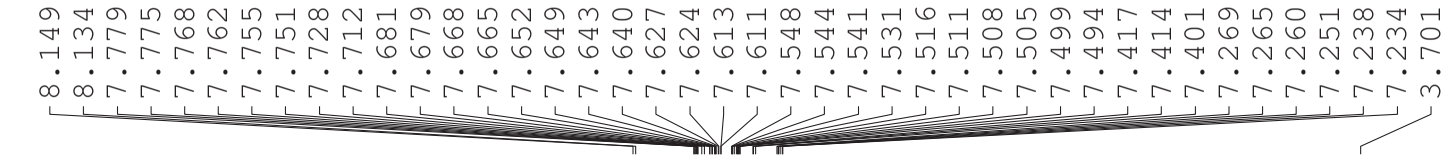
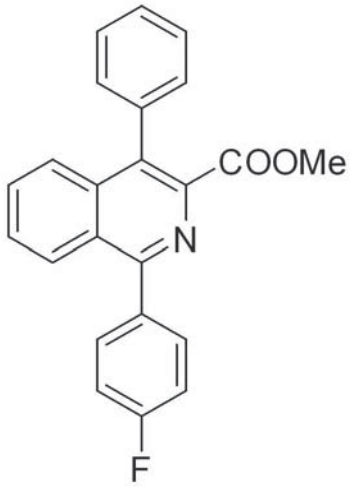
136.61
136.14
132.38
131.71
131.59
130.51
129.87
128.68
128.29
128.22
128.07
127.99
127.83
127.47
127.17
126.74
114.90
70.12
52.40
COOMe
N
O
Ph
3j
WH-6-74
C13CPD CDCl3
NAME XB20140504
EXPNO 33
PROCNO 1
Date_ 20140504
Time 12.46
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 228.1
DW 16.650 usec
DE 6.00 usec
TE 297.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.05 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 0.30 Hz
0
1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

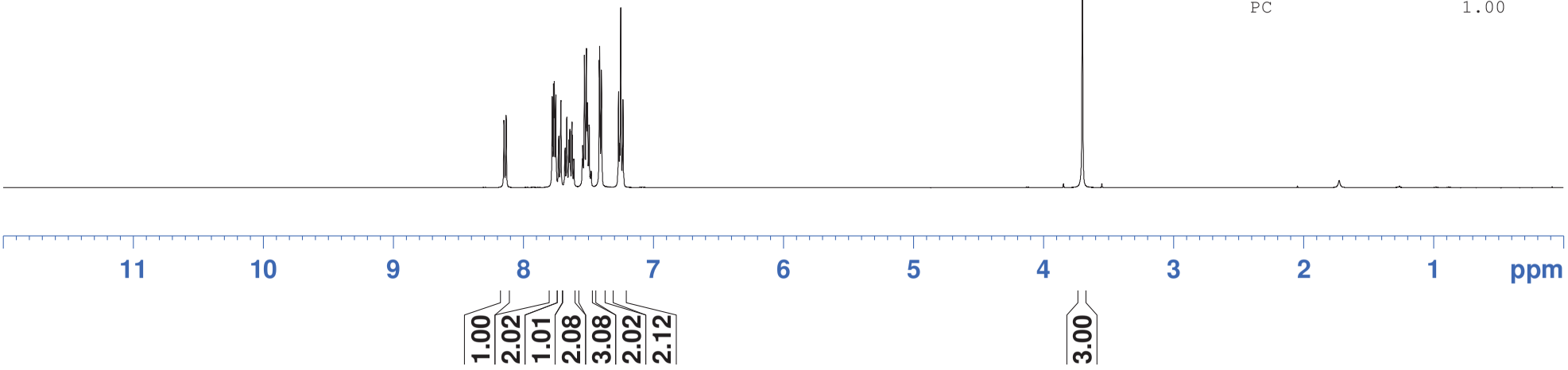


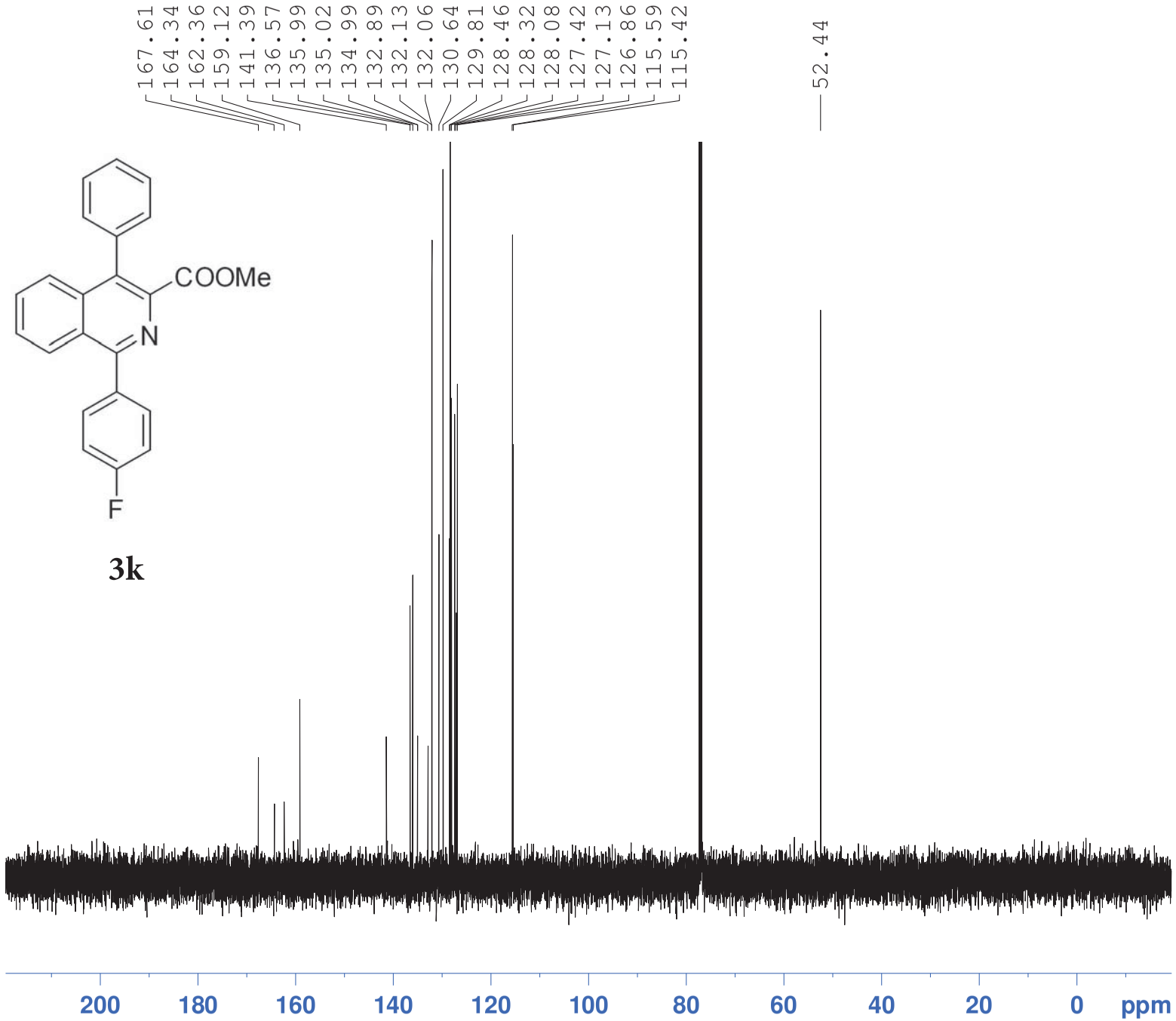


3k

WH-6-71
PROTON CDCl3 D:

NAME	XB20140504
EXPNO	5
PROCNO	1
Date_	20140504
Time	8.57
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	161.3
DW	48.400 usec
DE	6.00 usec
TE	295.9 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300126 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

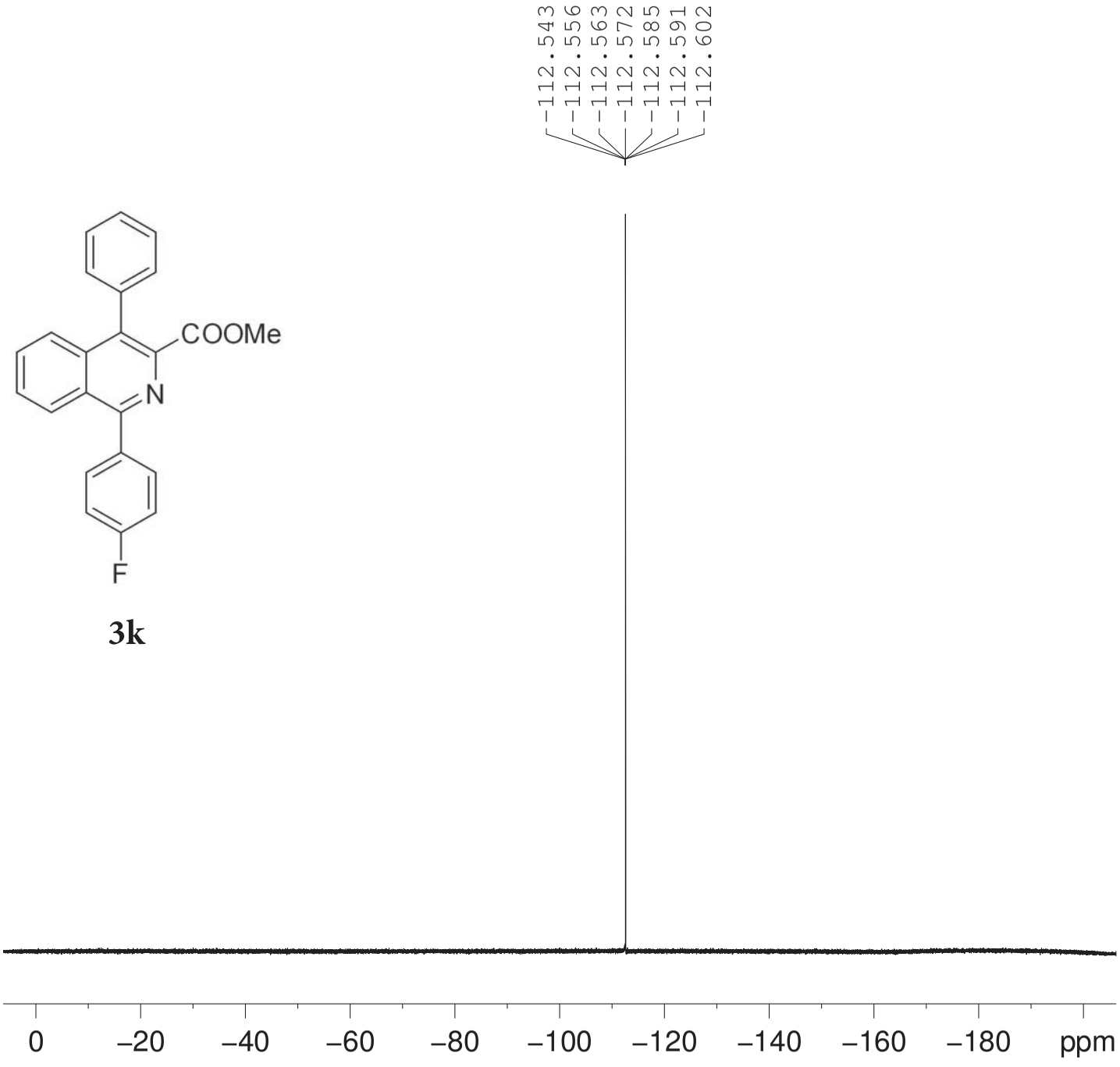




WH-6-71
C13CPD CDCl3

NAME	XB20140504
EXPNO	7
PROCNO	1
Date_	20140504
Time	9.07
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	128
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	181
DW	16.650 usec
DE	6.00 usec
TE	297.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40

3k

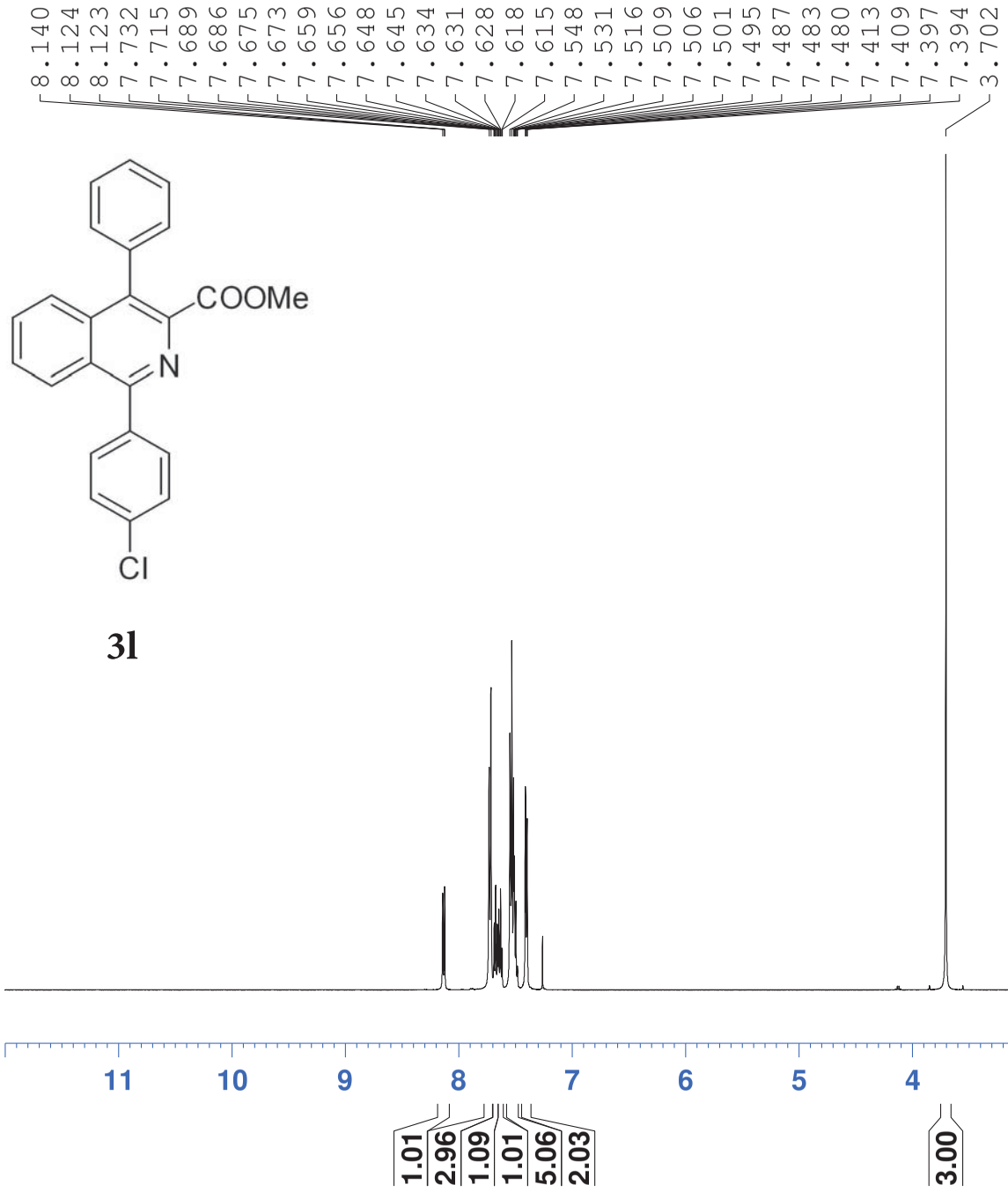


WH-6-71
19Fdeft CDCl3

NAME	XB20140504
EXPNO	6
PROCNO	1
Date_	20140504
Time	8.58
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg
TD	131072
SOLVENT	CDCl3
NS	1
DS	4
SWH	100000.000 Hz
FIDRES	0.762939 Hz
AQ	0.6554150 sec
RG	322.5
DW	5.000 usec
DE	6.00 usec
TE	295.9 K
D1	1.00000000 sec
TD0	1

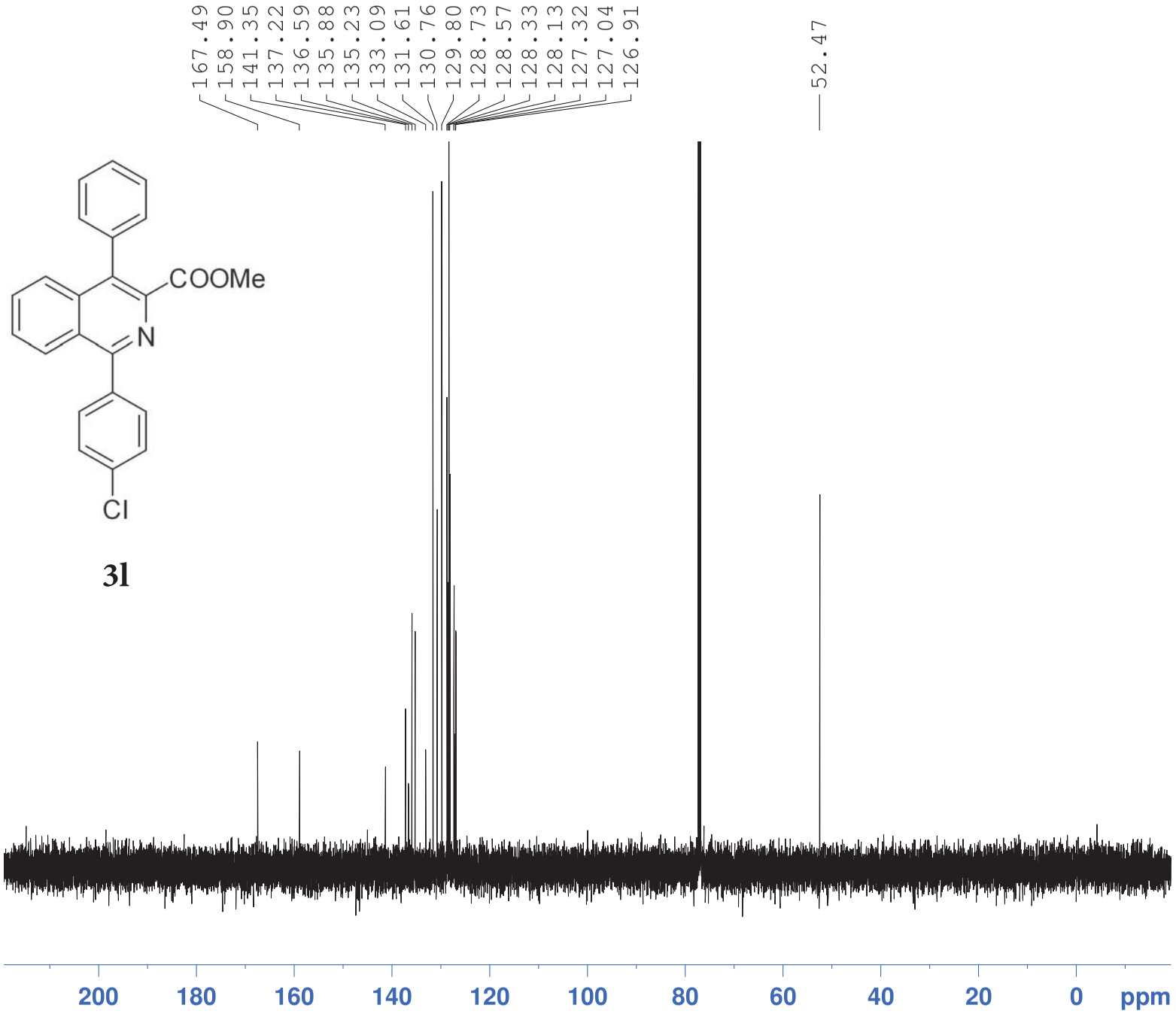
======== CHANNEL f1 ========

NUC1	19F
P1	19.30 usec
PL1	4.00 dB
SFO1	470.5453180 MHz
SI	65536
SF	470.5923770 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



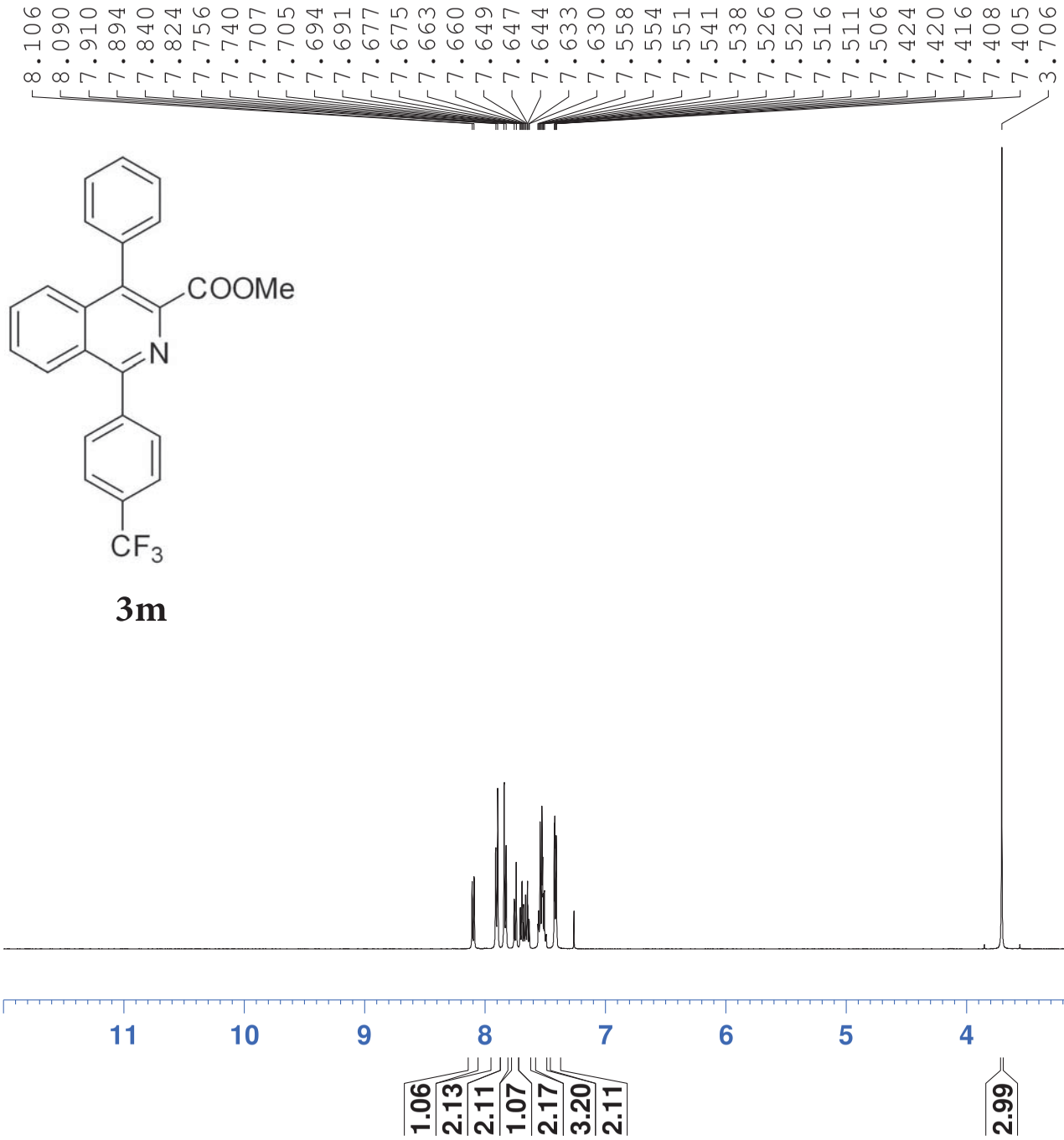
WH-6-80
PROTON CDCl3 D

NAME	xb20140505
EXPNO	10
PROCNO	1
Date_	20140505
Time	10.00
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	181
DW	48.400 usec
DE	6.00 usec
TE	296.5 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300126 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



WH-6-80
C13CPD CDCl3 1

NAME	xb20140505
EXPNO	11
PROCNO	1
Date_	20140505
Time	10.09
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	128
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	287.4
DW	16.650 usec
DE	6.00 usec
TE	297.5 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40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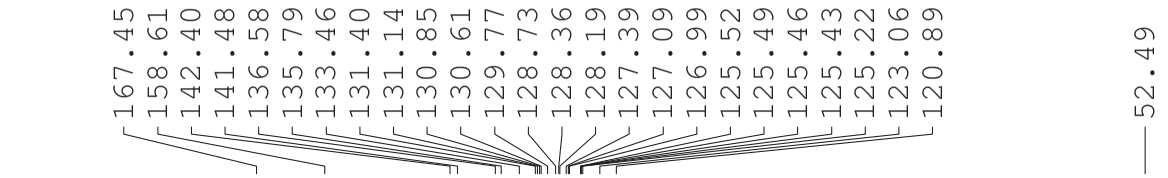
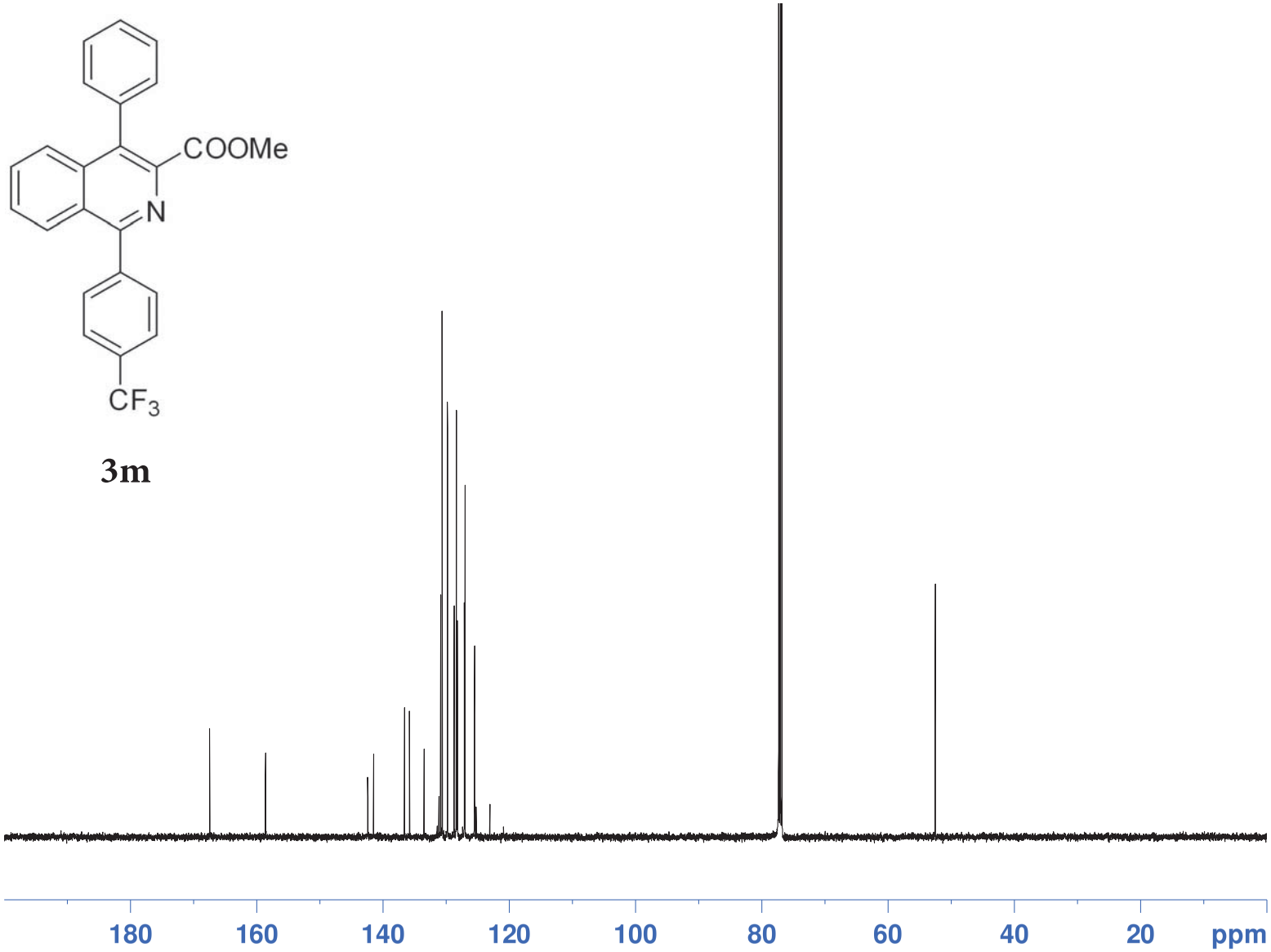
7.824
7.756
7.740
7.707
7.705
7.694
7.691
7.677
7.675
7.663
7.660
7.649
7.647
7.644
7.633
7.630
7.558
7.554
7.551
7.541
7.538
7.526
7.520
7.516
7.511
7.506
7.424
7.420
7.416
7.408
7.405
3.706
COOMe
N
CF3
3m
WH-6-76
PROTON CDCl3
NAME XB20140504
EXPNO 8
PROCNO 1
Date_ 20140504
Time 9.13
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 181
DW 48.400 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.14 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300126 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
11
10
9
8
7
6
5
4
3
2
1
ppm
1.06
2.13
2.11
1.07
2.17
3.20
2.11
2.99

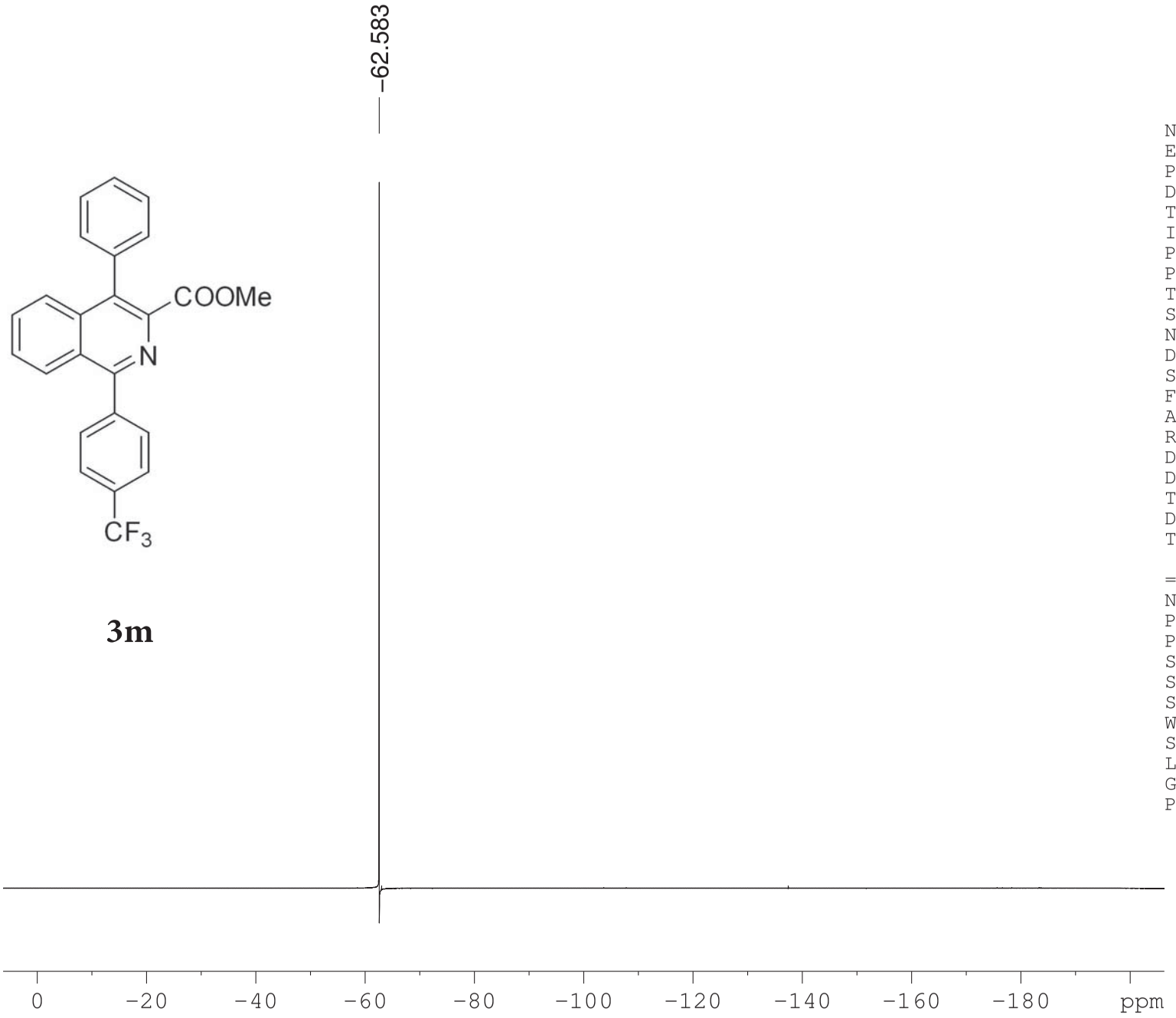


3m



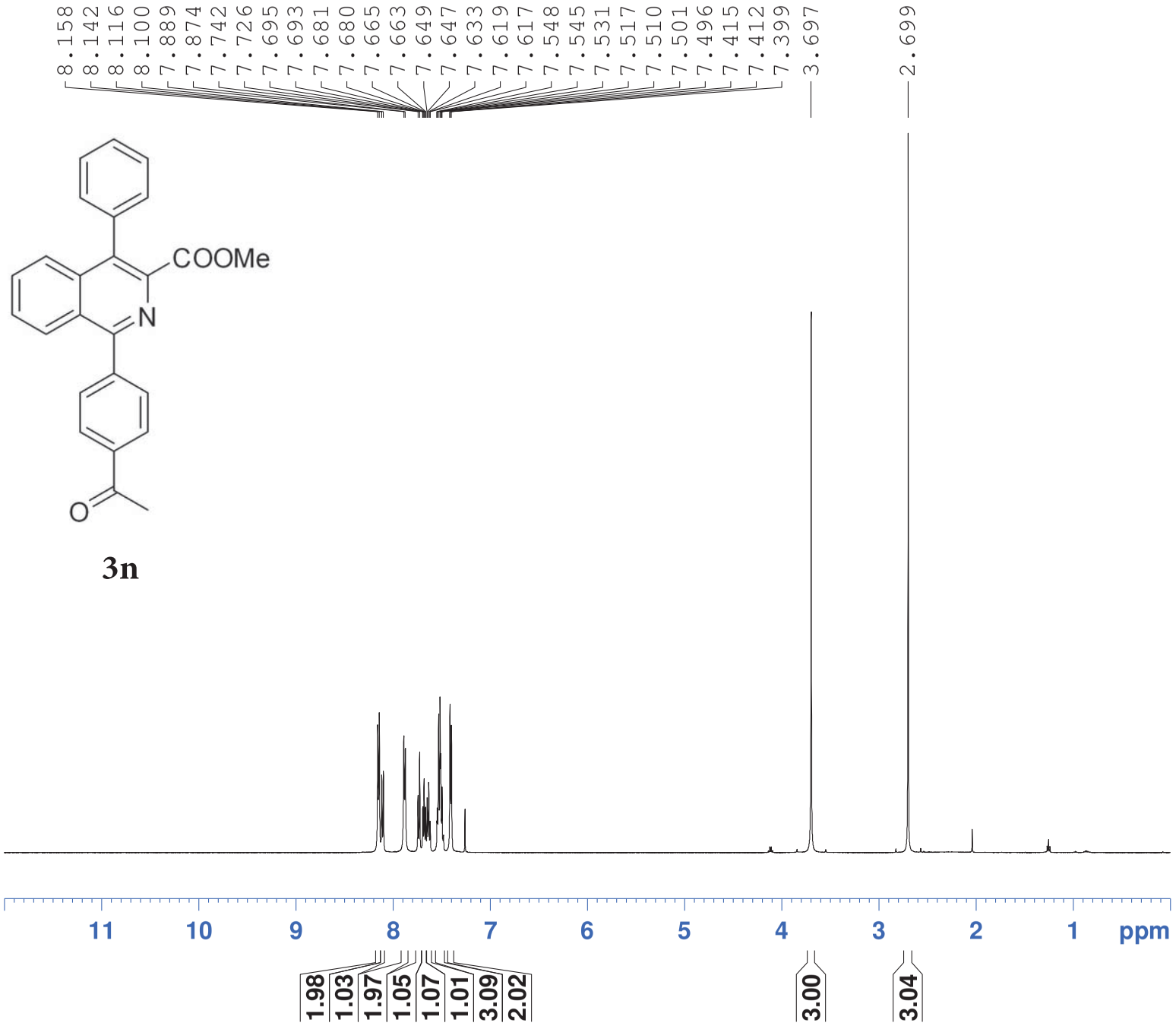
WH-6-76
C13CPD CDCl

NAME	xb20140505
EXPNO	21
PROCNO	1
Date_	20140505
Time	19.44
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	161.3
DW	16.650 usec
DE	6.00 usec
TE	297.7 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



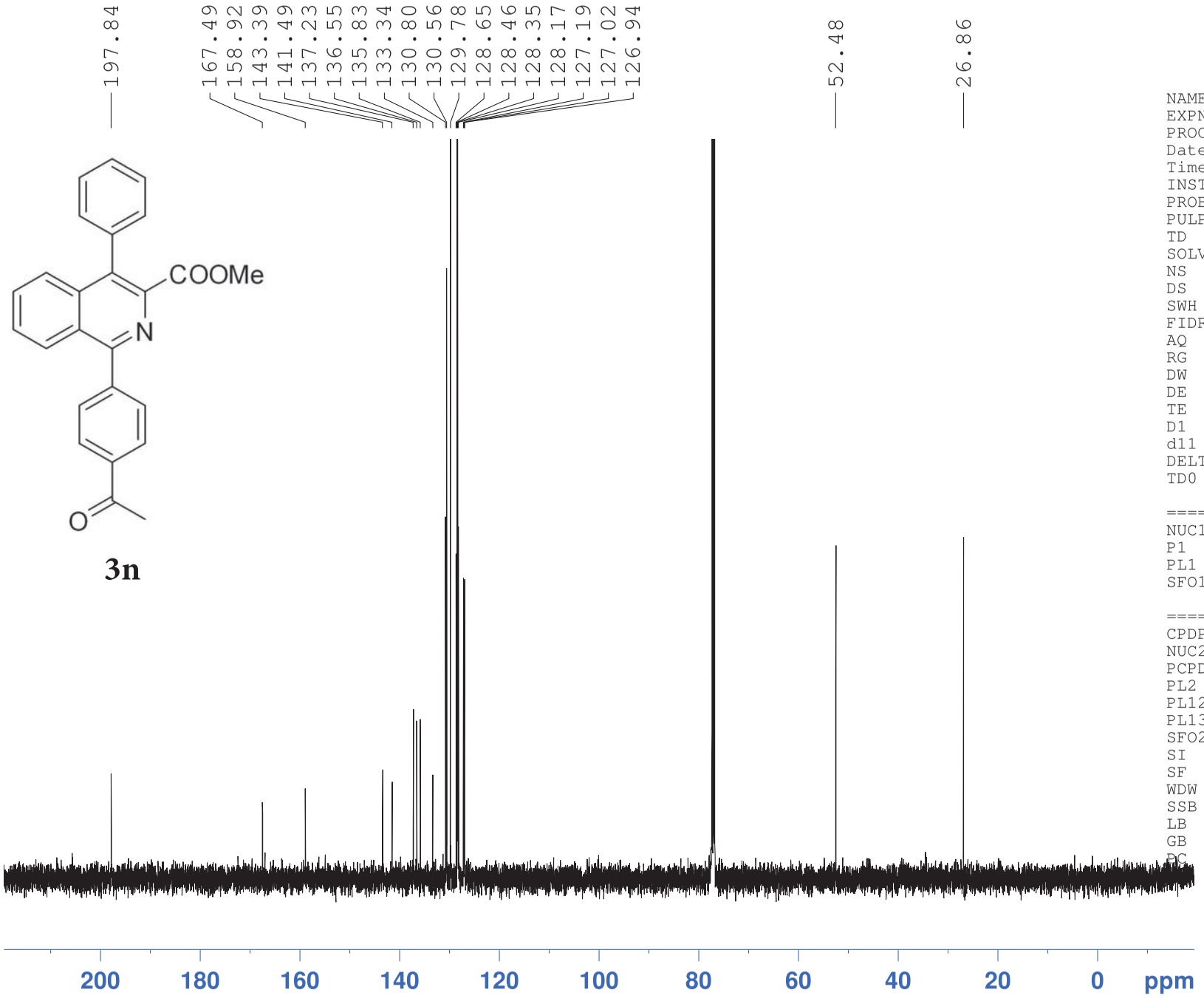
WH-6-76
19Fdeft CDCl3

NAME	XB20140504
EXPNO	9
PROCNO	1
Date_	20140504
Time	9.14
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg
TD	131072
SOLVENT	CDCl3
NS	1
DS	4
SWH	100000.000 Hz
FIDRES	0.762939 Hz
AQ	0.6554150 sec
RG	256
DW	5.000 usec
DE	6.00 usec
TE	296.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	19F
P1	19.30 usec
PL1	4.00 dB
SFO1	470.5453180 MHz
SI	65536
SF	470.5923770 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



WH-6-108
PROTON CDCl3

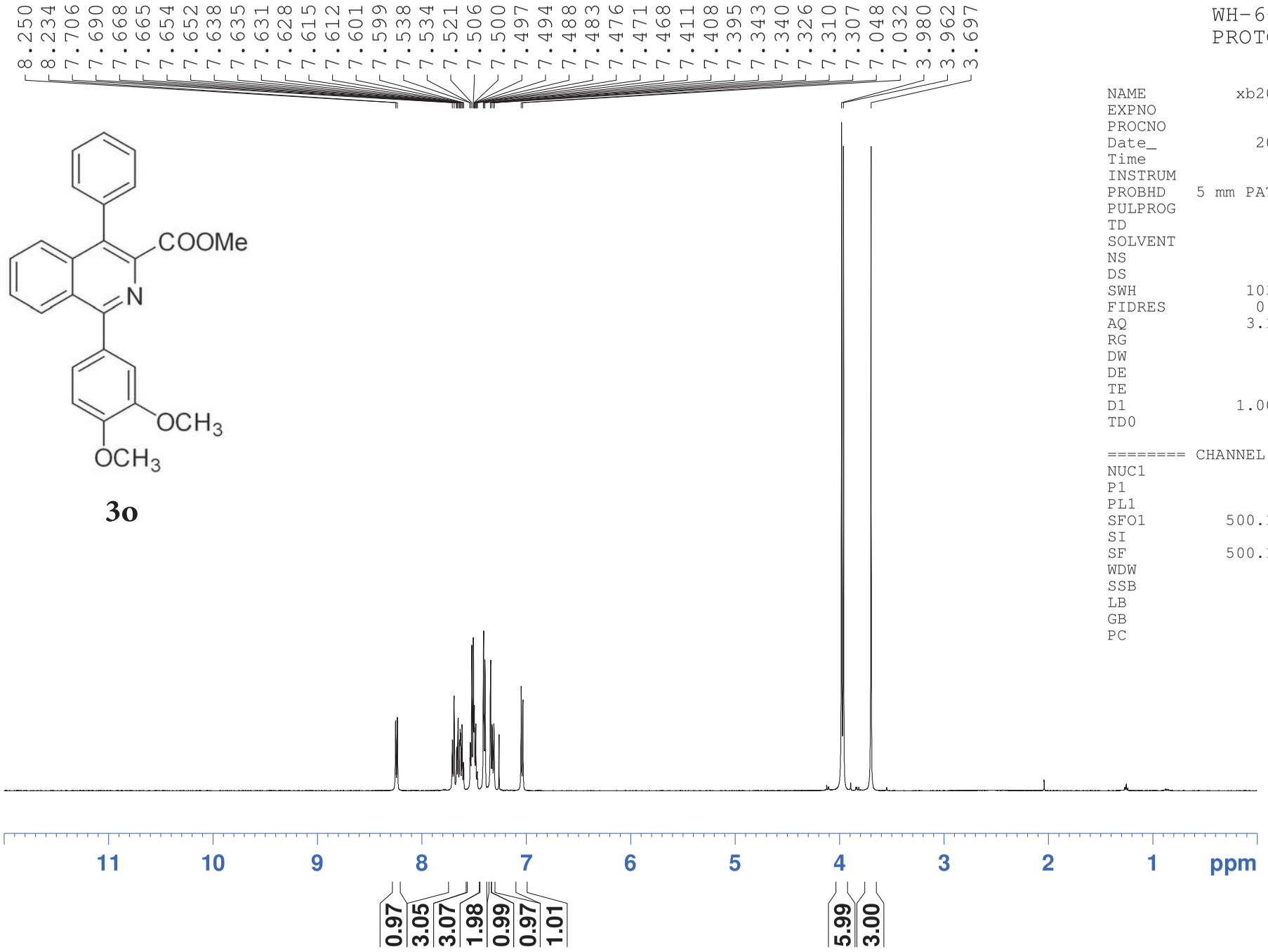
NAME	XB20140513
EXPNO	3
PROCNO	1
Date_	20140514
Time	4.20
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	181
DW	48.400 usec
DE	6.00 usec
TE	296.6 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300126 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



WH-6-108
C13CPD CDCl3

NAME	XB20140513
EXPNO	4
PROCNO	1
Date_	20140514
Time	4.36
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	256
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	228.1
DW	16.650 usec
DE	6.00 usec
TE	297.8 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

3o

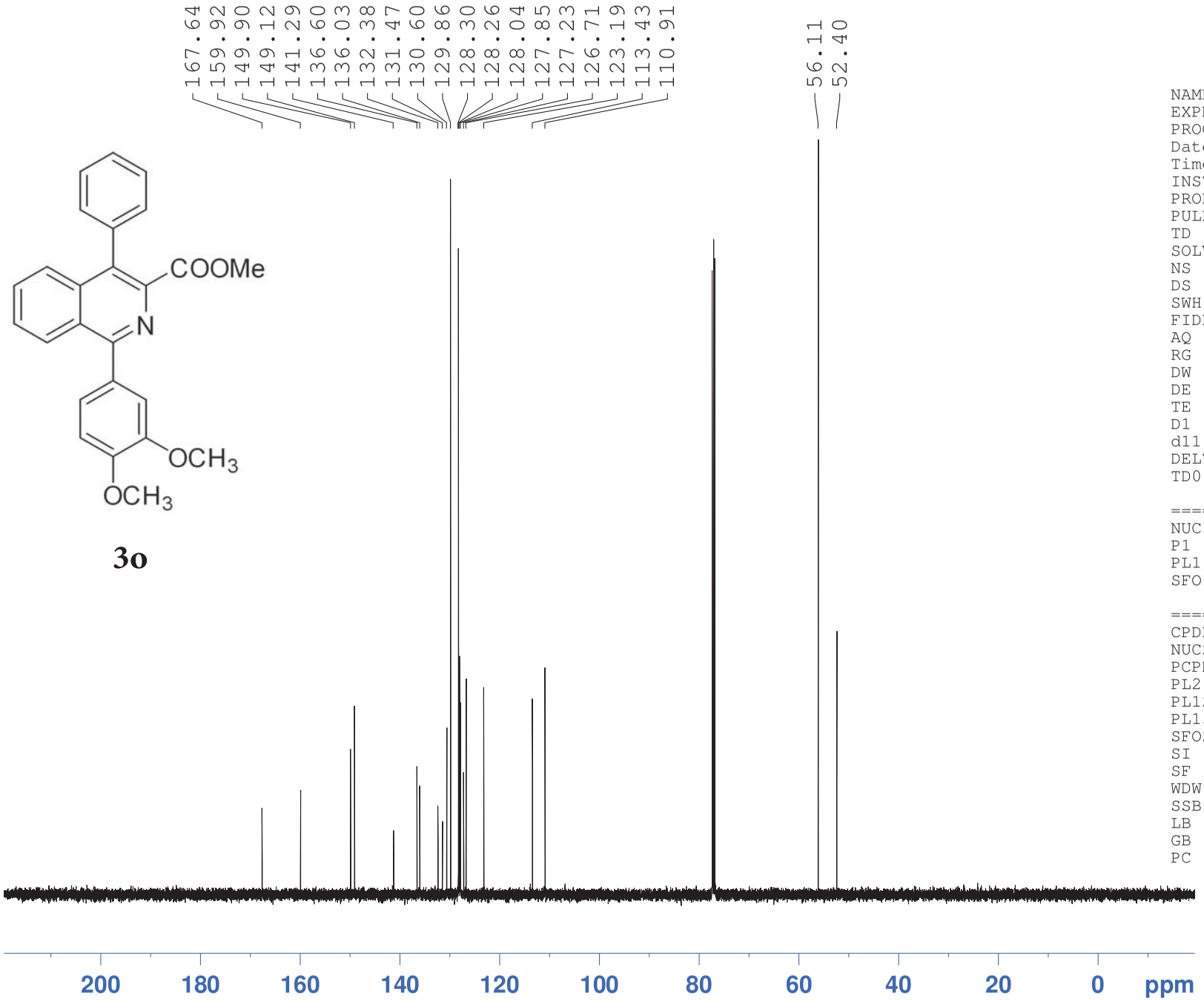


WH-6-88
PROTON CDCl3

NAME	xb20140505
EXPNO	6
PROCNO	1
Date_	20140505
Time	9.31
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	203.2
DW	48.400 usec
DE	6.00 usec
TE	296.2 K
D1	1.00000000 sec
TD0	1

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

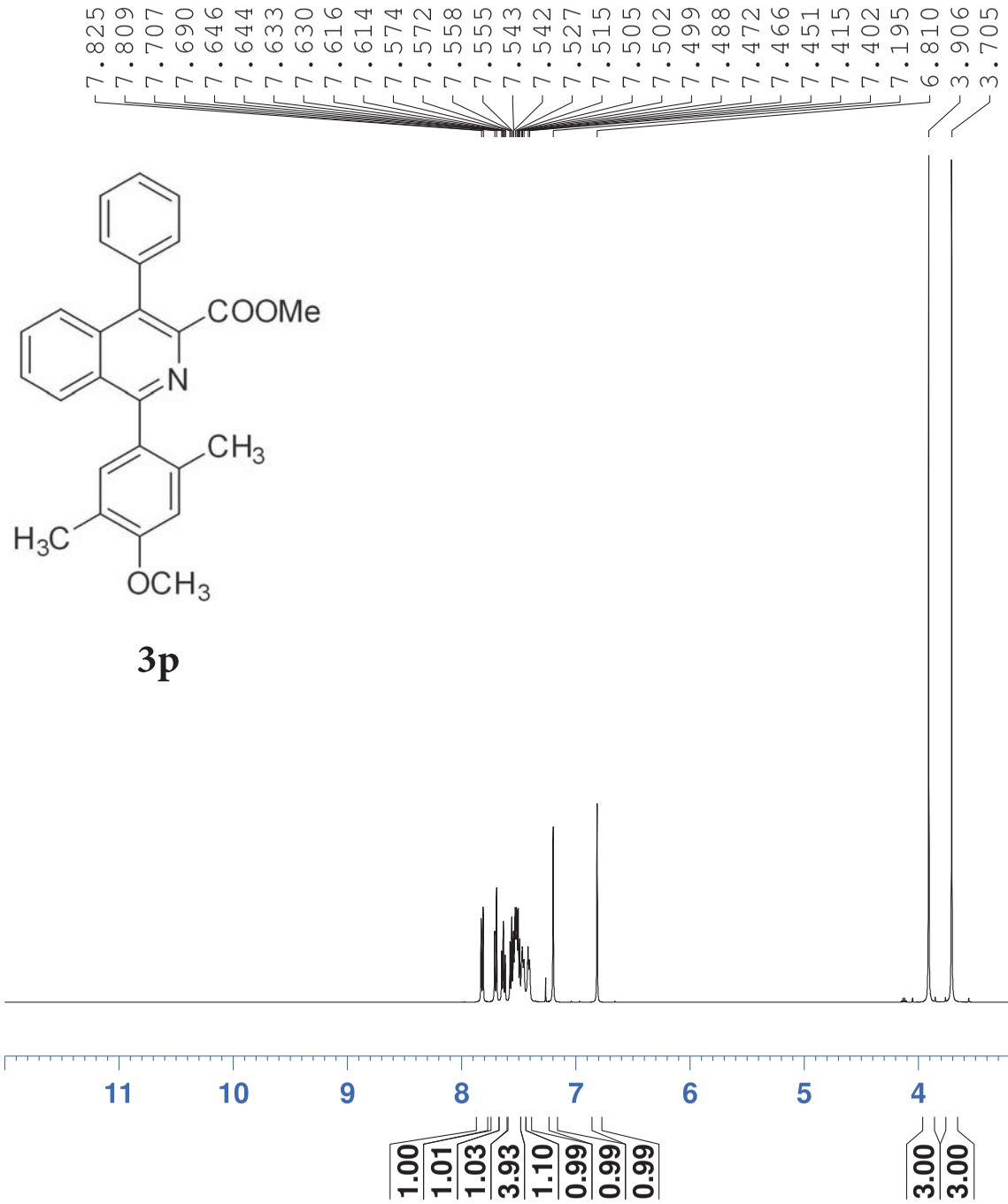
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300126 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



3o

WH-6-88
C13CPD CDCl3

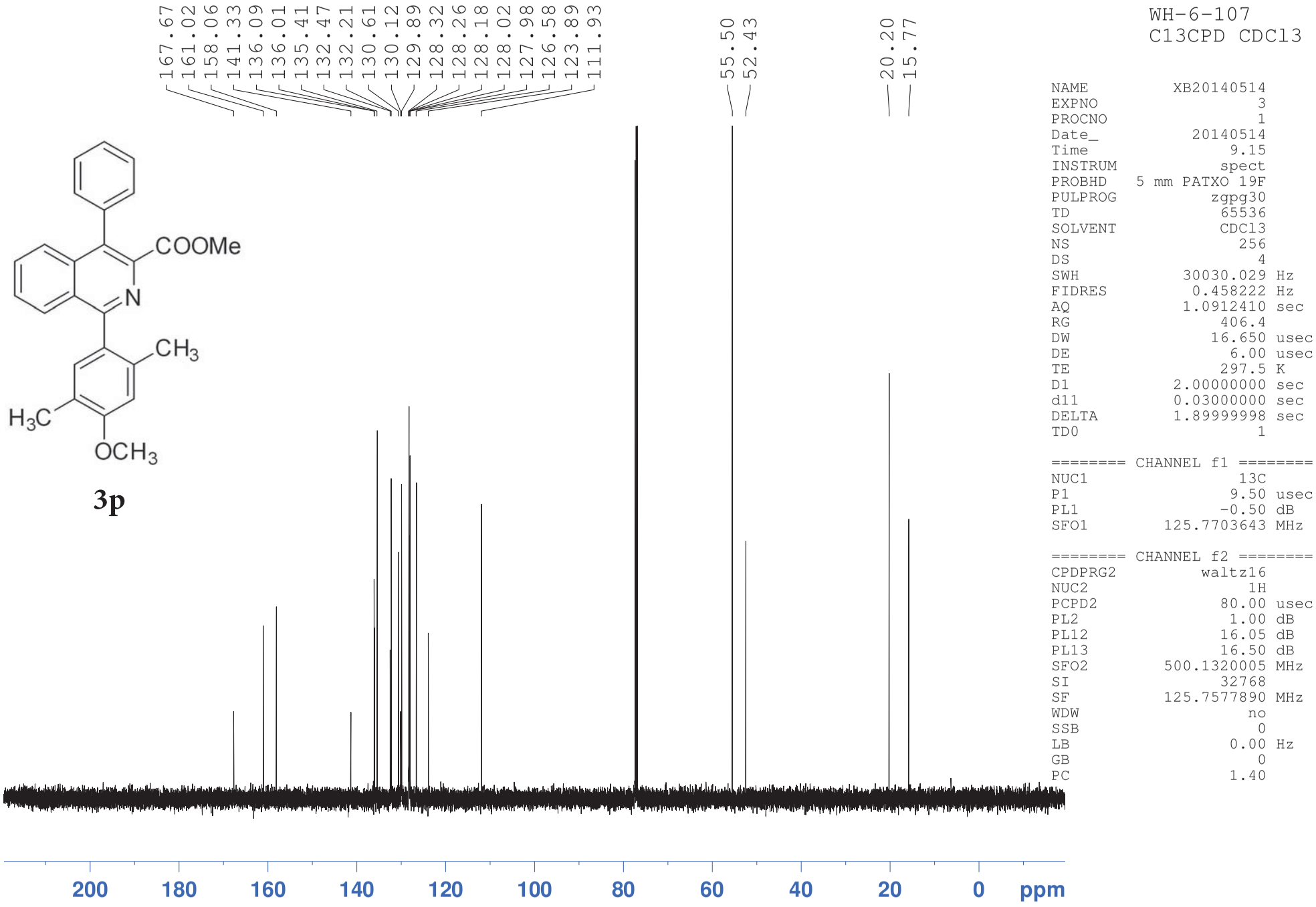
NAME	XB20140507
EXPNO	2
PROCNO	1
Date_	20140508
Time	8.15
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	512
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	161.3
DW	16.650 usec
DE	6.00 usec
TE	297.5 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40



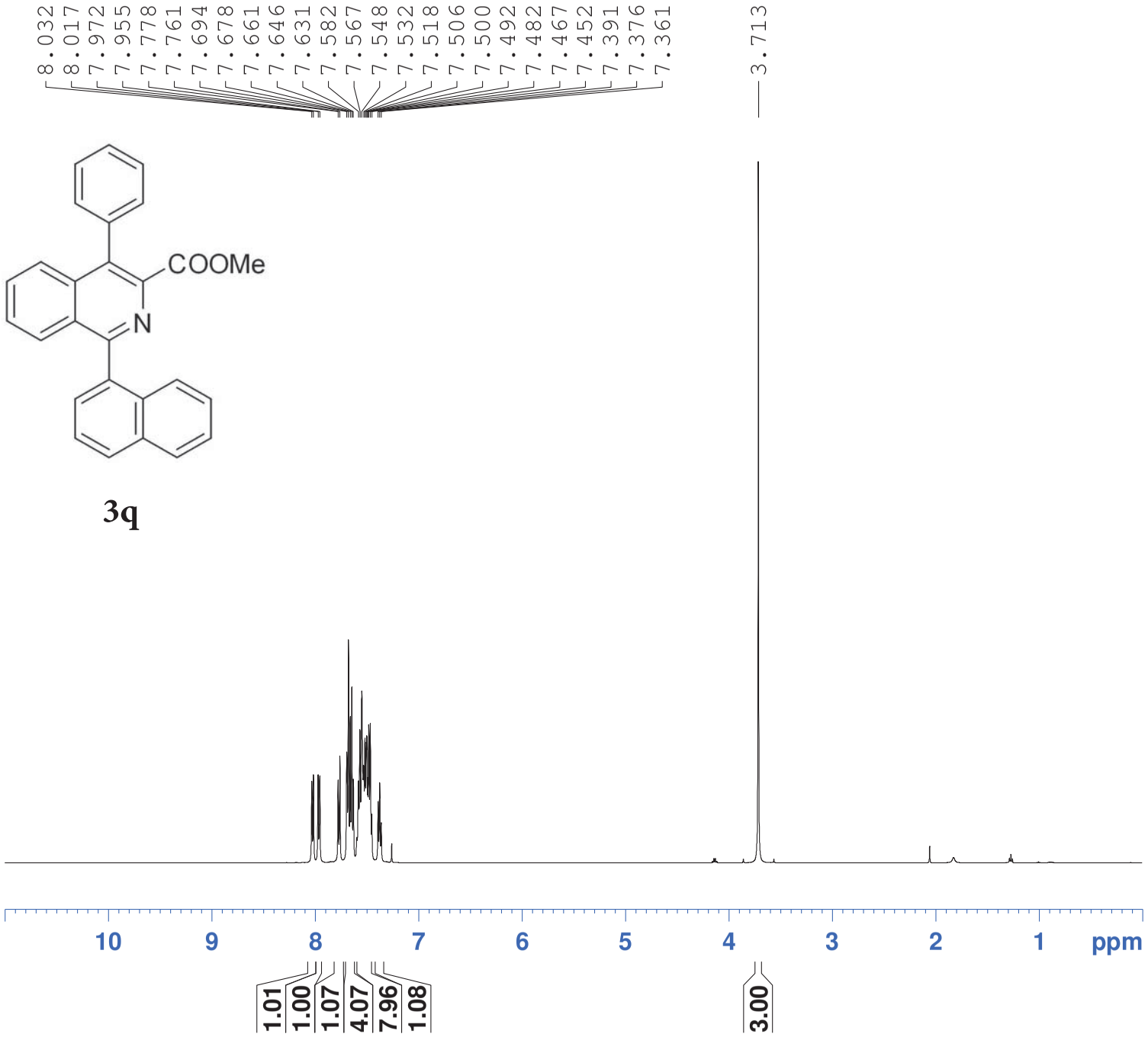
3p

WH-6-107
PROTON CDCl3 I

NAME	XB20140514
EXPNO	1
PROCNO	1
Date_	20140514
Time	8.57
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	90.5
DW	48.400 usec
DE	6.00 usec
TE	296.1 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300126 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



NAME	XB20140514
EXPNO	3
PROCNO	1
Date_	20140514
Time	9.15
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	256
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	406.4
DW	16.650 usec
DE	6.00 usec
TE	297.5 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40



3q

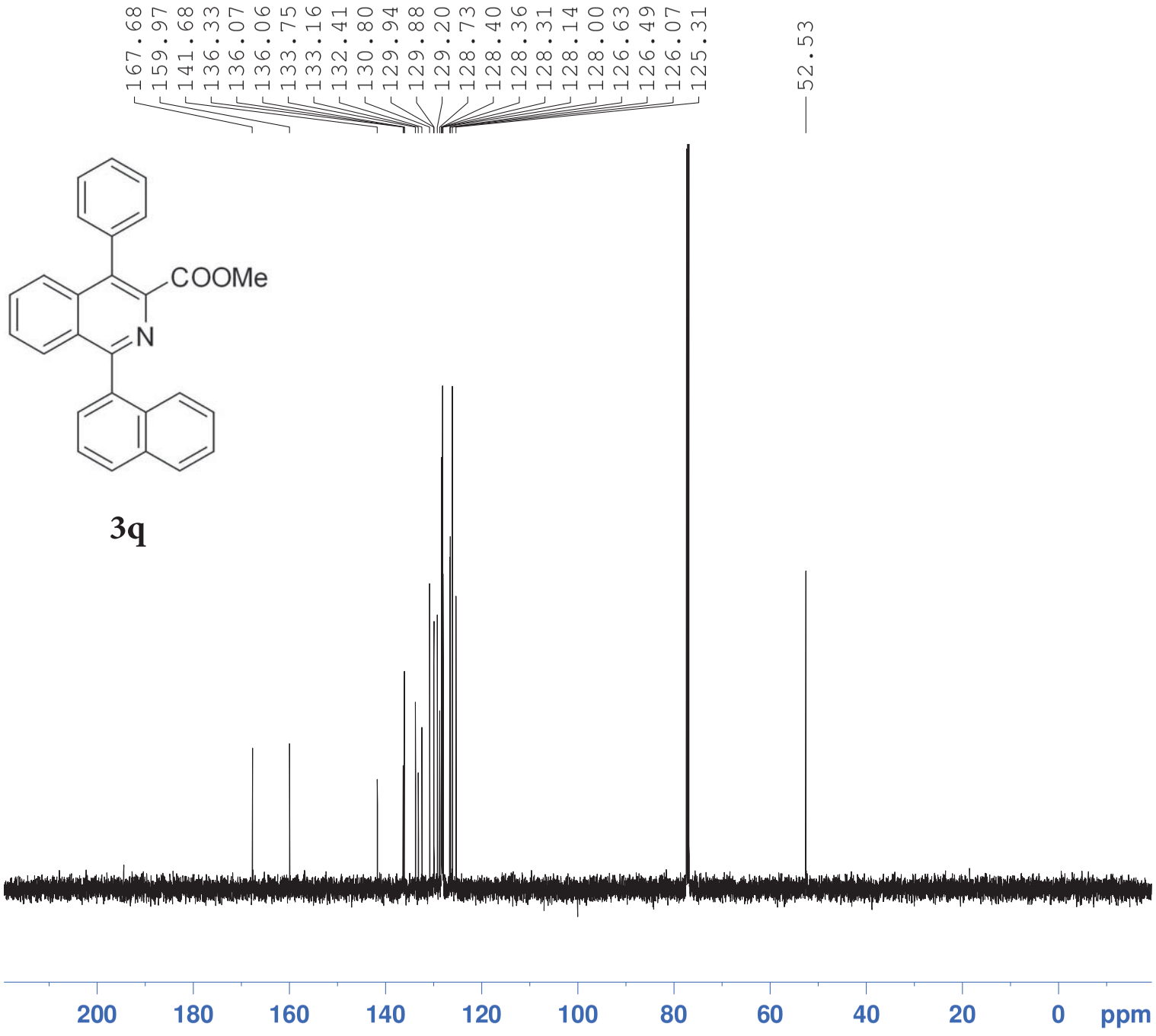
SI00

WH-6-62
PROTON CDC

NAME	XB20140430
EXPNO	5
PROCNO	1
Date_	20140430
Time	9.31
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	114
DW	48.400 usec
DE	6.00 usec
TE	296.1 K
D1	1.00000000 sec
TD0	1

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

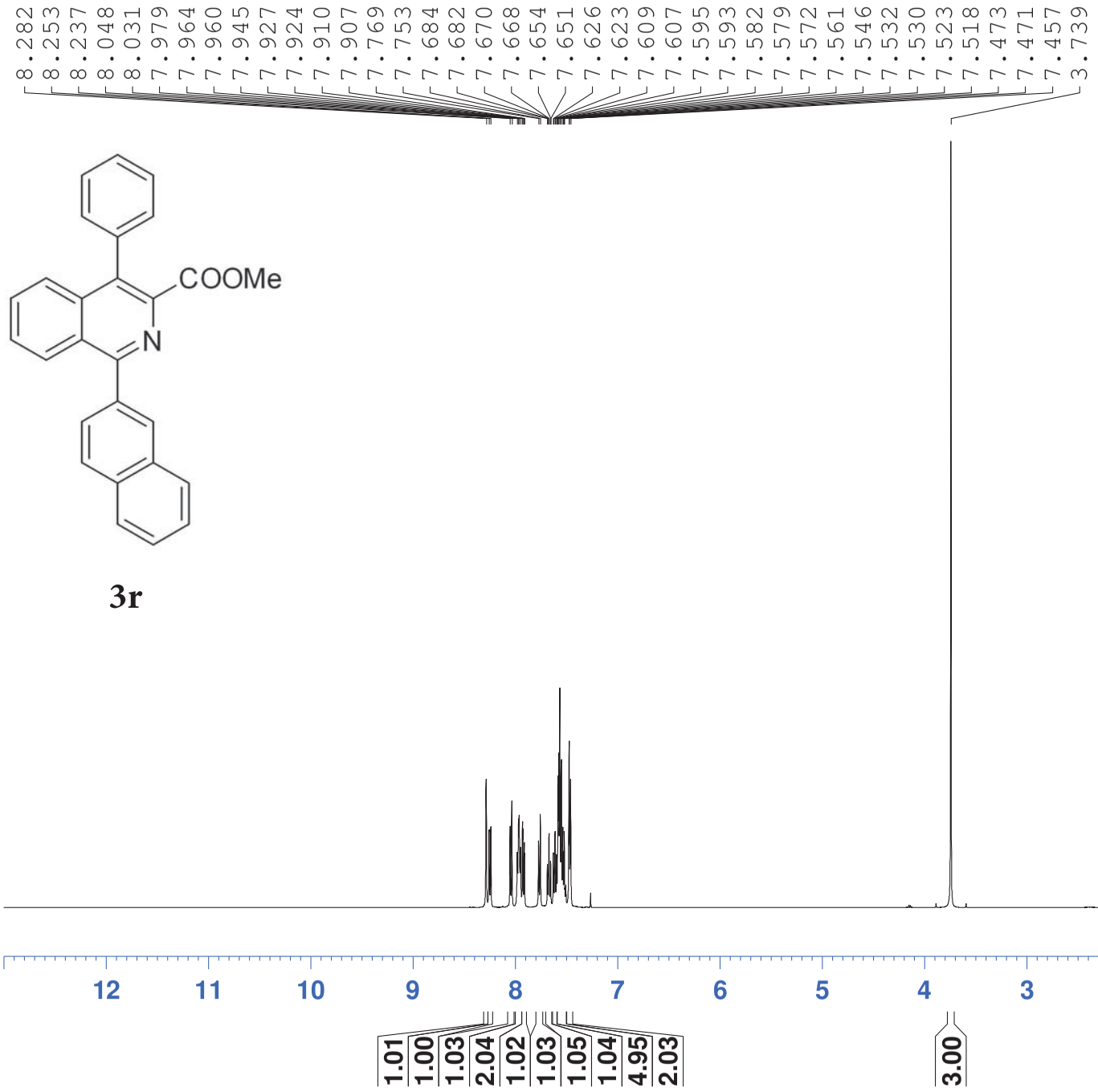
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300126 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



SI01

WH-6-62
C13CPD CDCl3

NAME	XB20140430
EXPNO	6
PROCNO	1
Date_	20140430
Time	9.36
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	90
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	101.6
DW	16.650 usec
DE	6.00 usec
TE	297.1 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

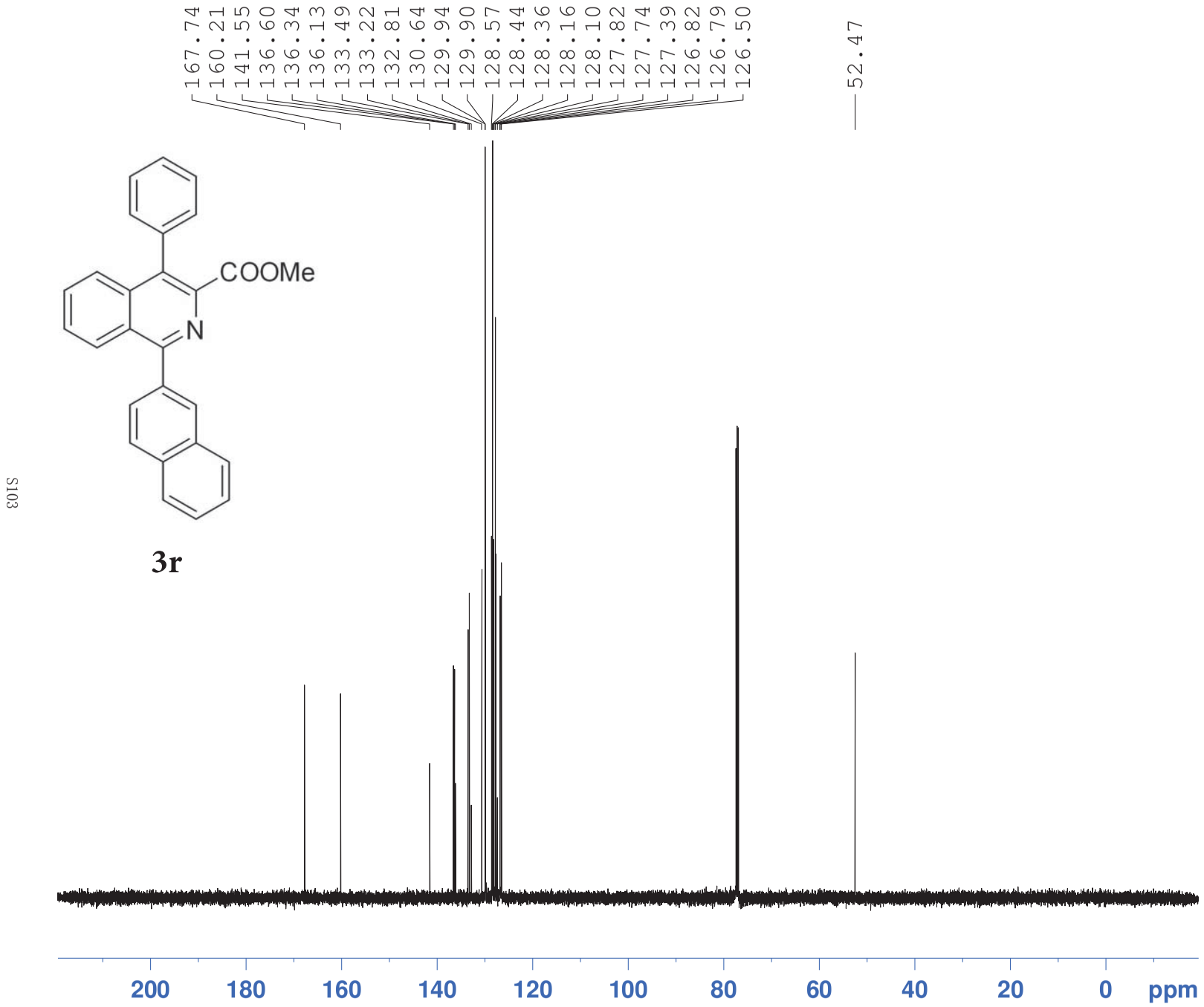


3r

WH-6-95
PROTON CDCl3 I

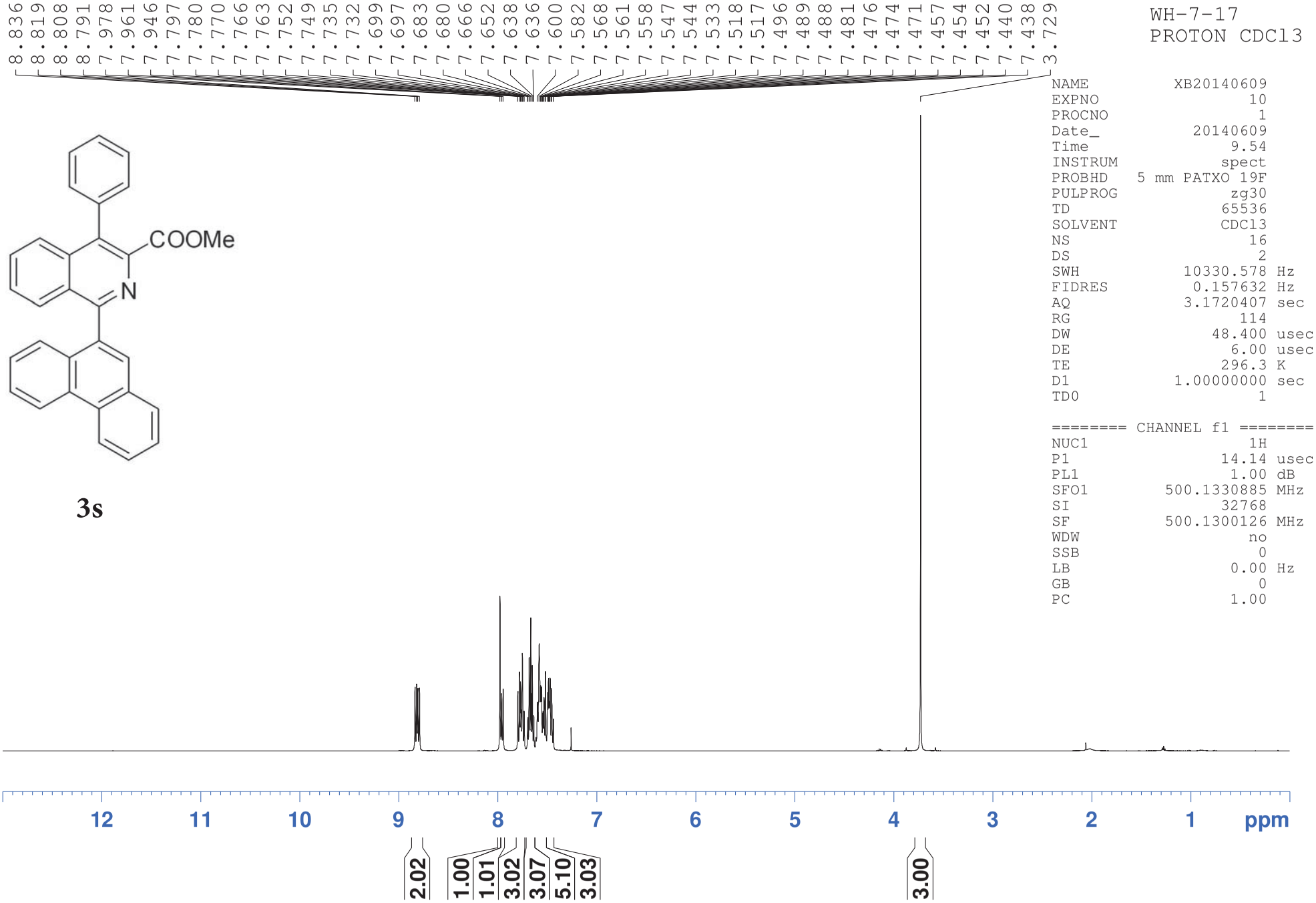
NAME	xb20140509
EXPNO	6
PROCNO	1
Date_	20140509
Time	9.35
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	71.8
DW	48.400 usec
DE	6.00 usec
TE	296.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300123 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

SI02



WH-6-95
C13CPD CDCl3

NAME	xb20140509
EXPNO	7
PROCNO	1
Date_	20140509
Time	9.44
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	256
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	114
DW	16.650 usec
DE	6.00 usec
TE	297.3 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40


8.836
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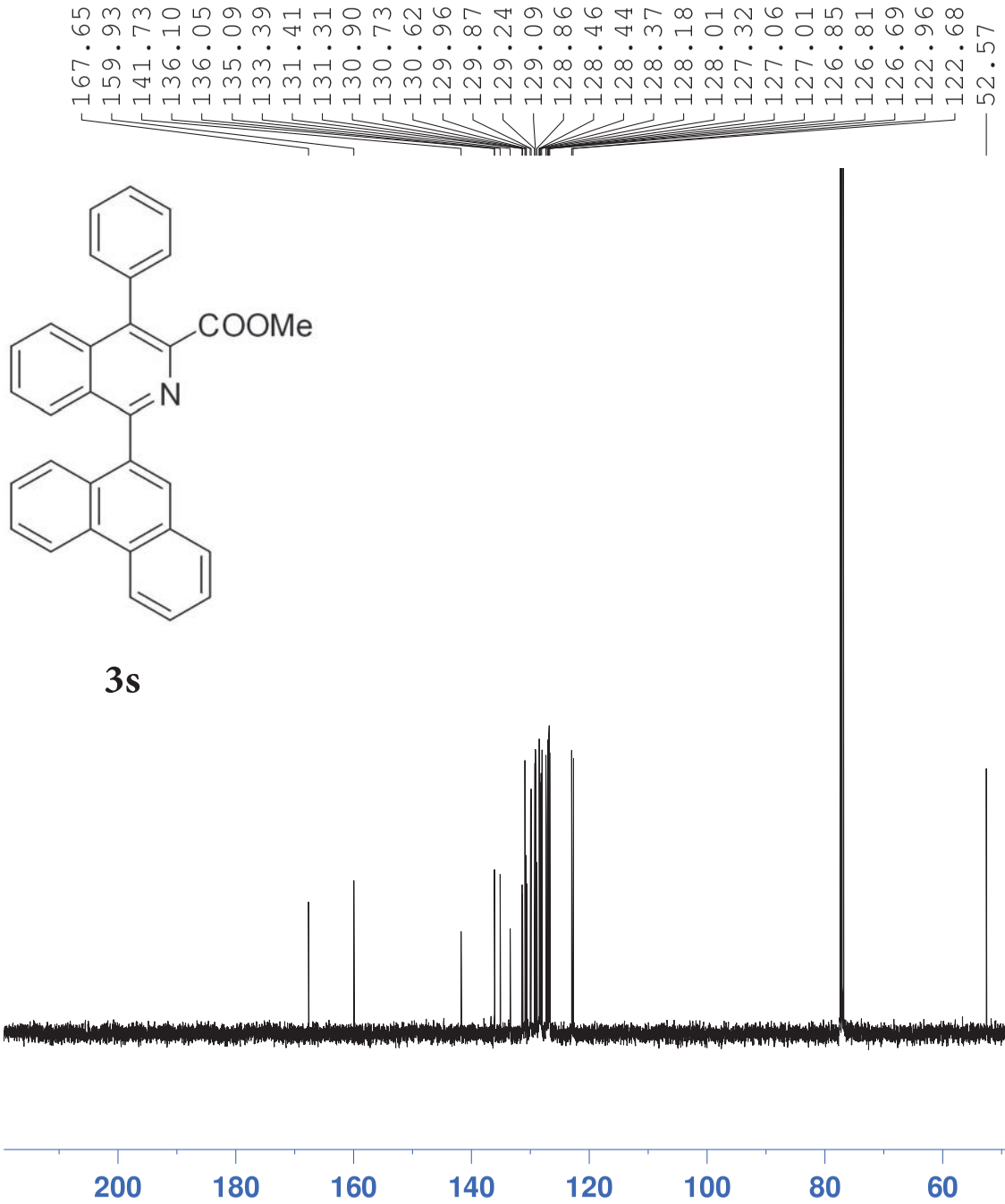
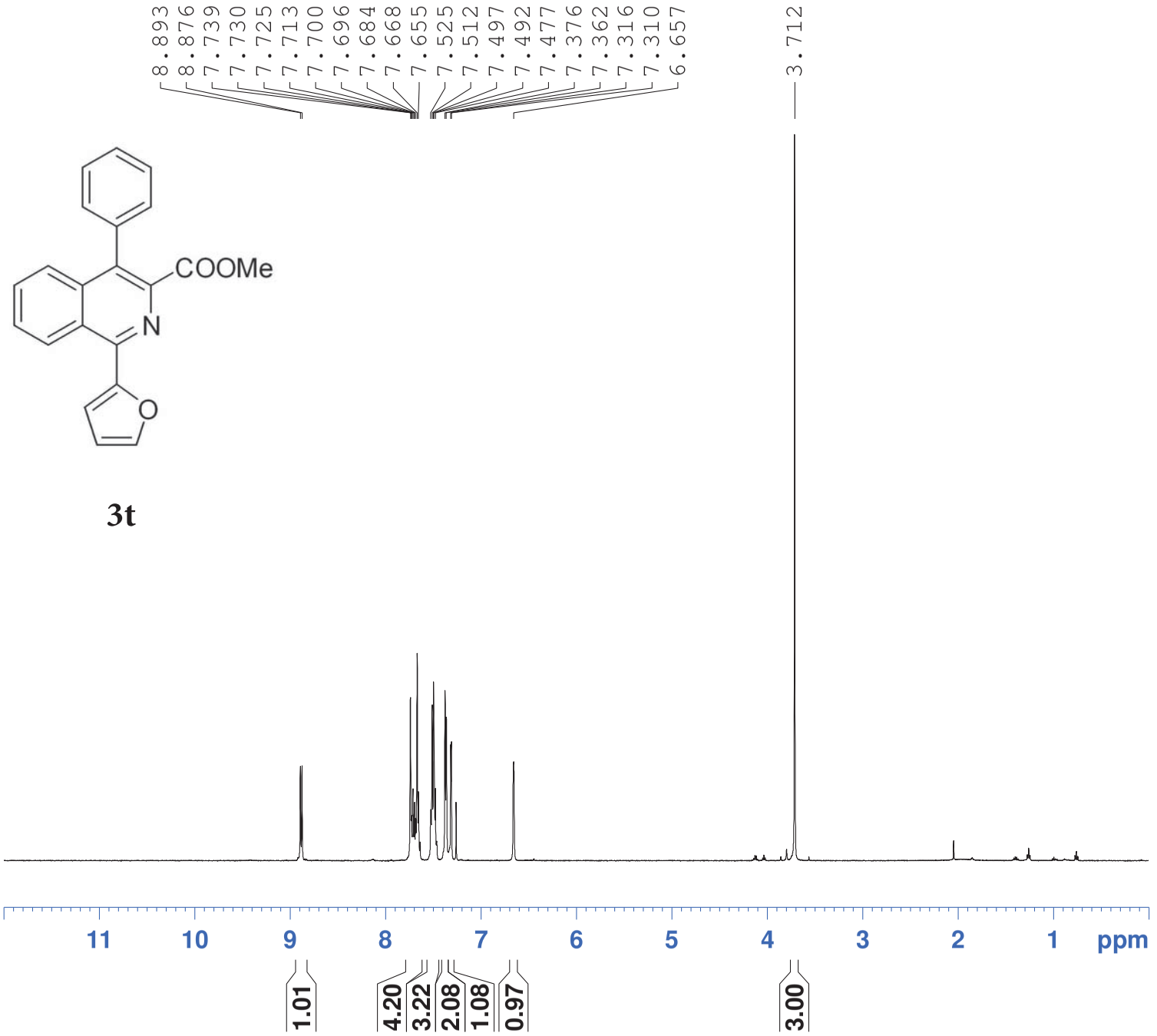
8.808
8.791
7.978
7.961
7.946
7.797
7.780
7.770
7.766
7.763
7.752
7.749
7.735
7.732
7.699
7.697
7.683
7.680
7.666
7.652
7.638
7.636
7.600
7.582
7.568
7.561
7.558
7.547
7.544
7.533
7.518
7.517
7.496
7.489
7.488
7.481
7.476
7.474
7.471
7.457
7.454
7.452
7.440
7.438
3.729
WH-7-17
PROTON CDCl3
NAME XB20140609
EXPNO 10
PROCNO 1
Date_ 20140609
Time 9.54
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 114
DW 48.400 usec
DE 6.00 usec
TE 296.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.14 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300126 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
COOMe
N
12
11
10
9
8
7
6
5
4
3
2
1
ppm
2.02
1.00
1.01
3.02
3.07
5.10
3.03
3.00

3s



WH-7-17
C13CPD CDCl3

NAME	XB20140609
EXPNO	11
PROCNO	1
Date_	20140609
Time	10.03
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	128
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	181
DW	16.650 usec
DE	6.00 usec
TE	297.6 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



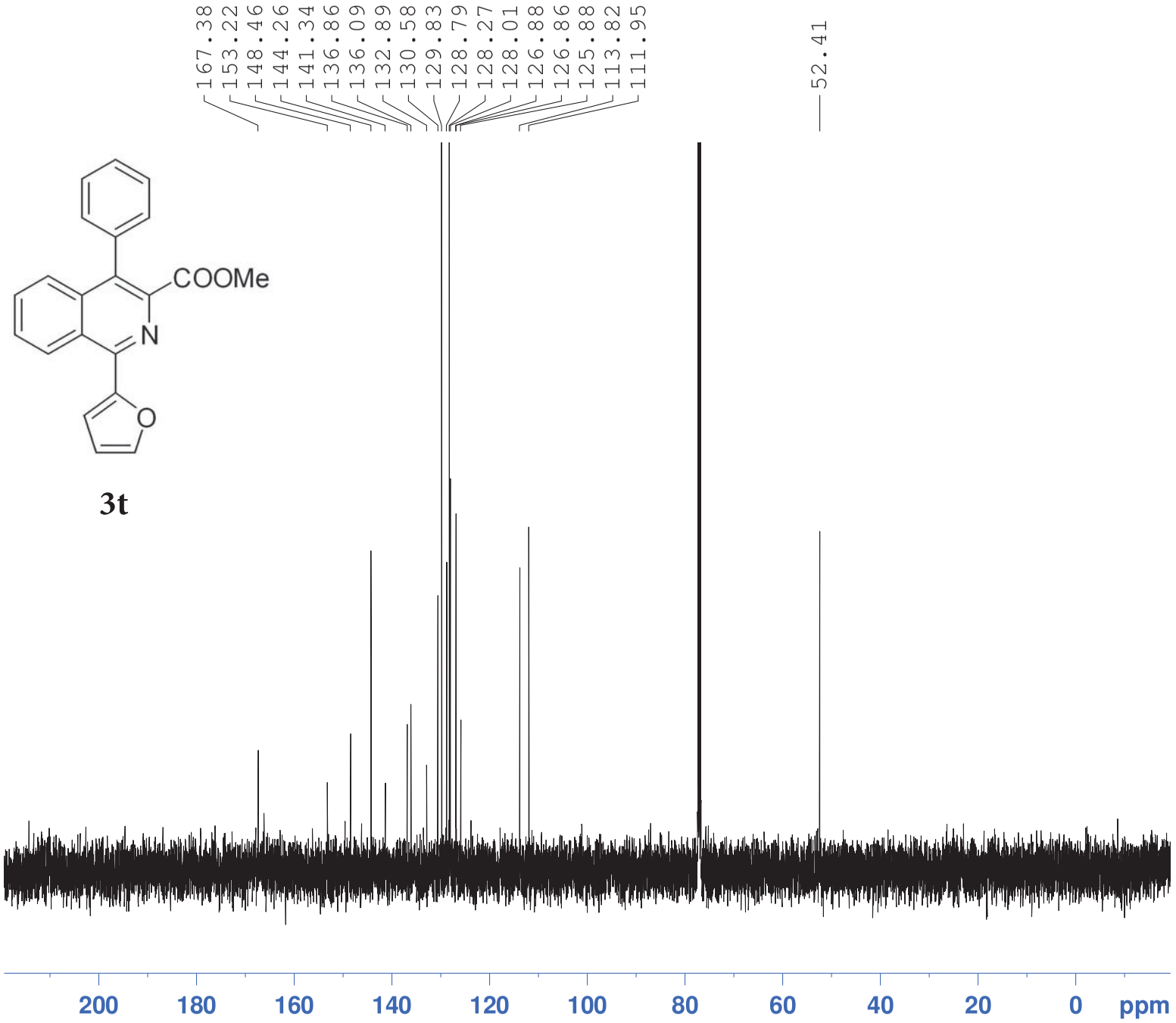
3t

SI06

WH-6-151
PROTON CDCl3

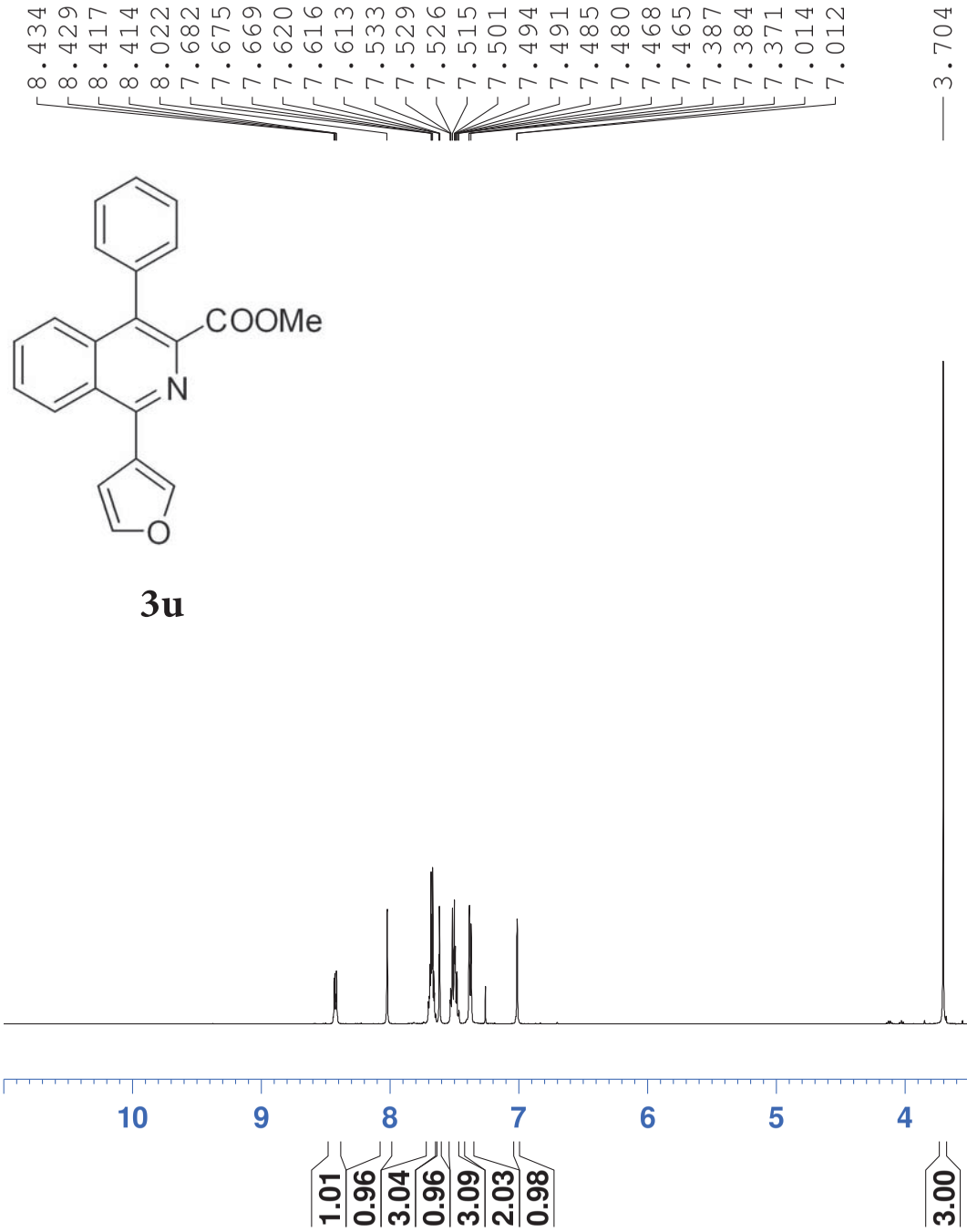
NAME	XB20140526
EXPNO	18
PROCNO	1
Date_	20140526
Time	16.38
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	256
DW	48.400 usec
DE	6.00 usec
TE	296.4 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300126 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



WH-6-151
C13CPD CDCl3

NAME	XB20140526
EXPNO	19
PROCNO	1
Date_	20140526
Time	17.20
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	128
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	512
DW	16.650 usec
DE	6.00 usec
TE	297.3 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

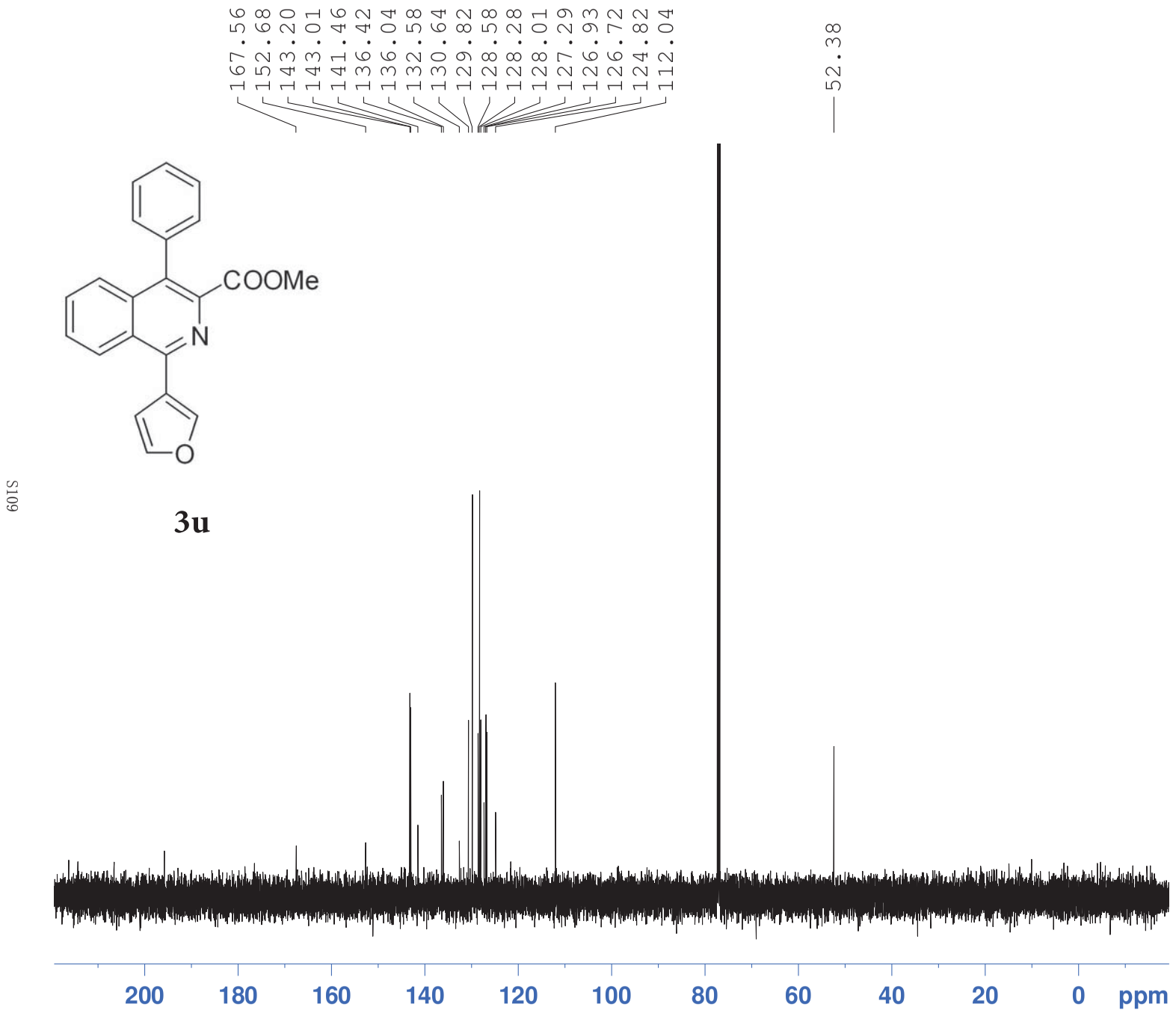


WH-6-150
PROTON CDCl3

NAME	XB20140526
EXPNO	16
PROCNO	1
Date_	20140526
Time	16.23
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	203.2
DW	48.400 usec
DE	6.00 usec
TE	296.3 K
D1	1.00000000 sec
TD0	1

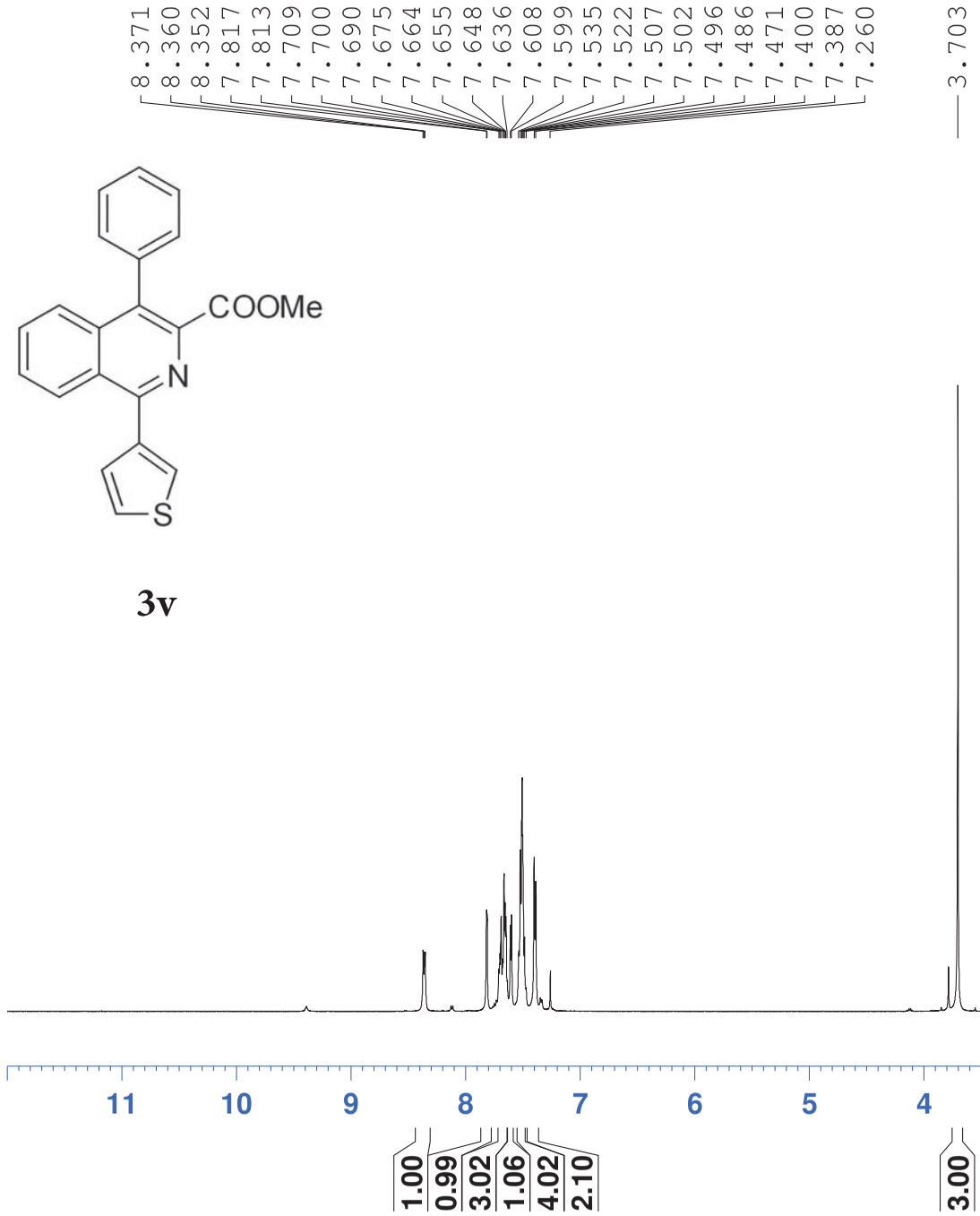
======== CHANNEL f1 ========

NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300129 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



WH-6-150
C13CPD CDCl3

NAME	XB20140526
EXPNO	17
PROCNO	1
Date_	20140526
Time	16.32
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	128
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	322.5
DW	16.650 usec
DE	6.00 usec
TE	297.5 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40

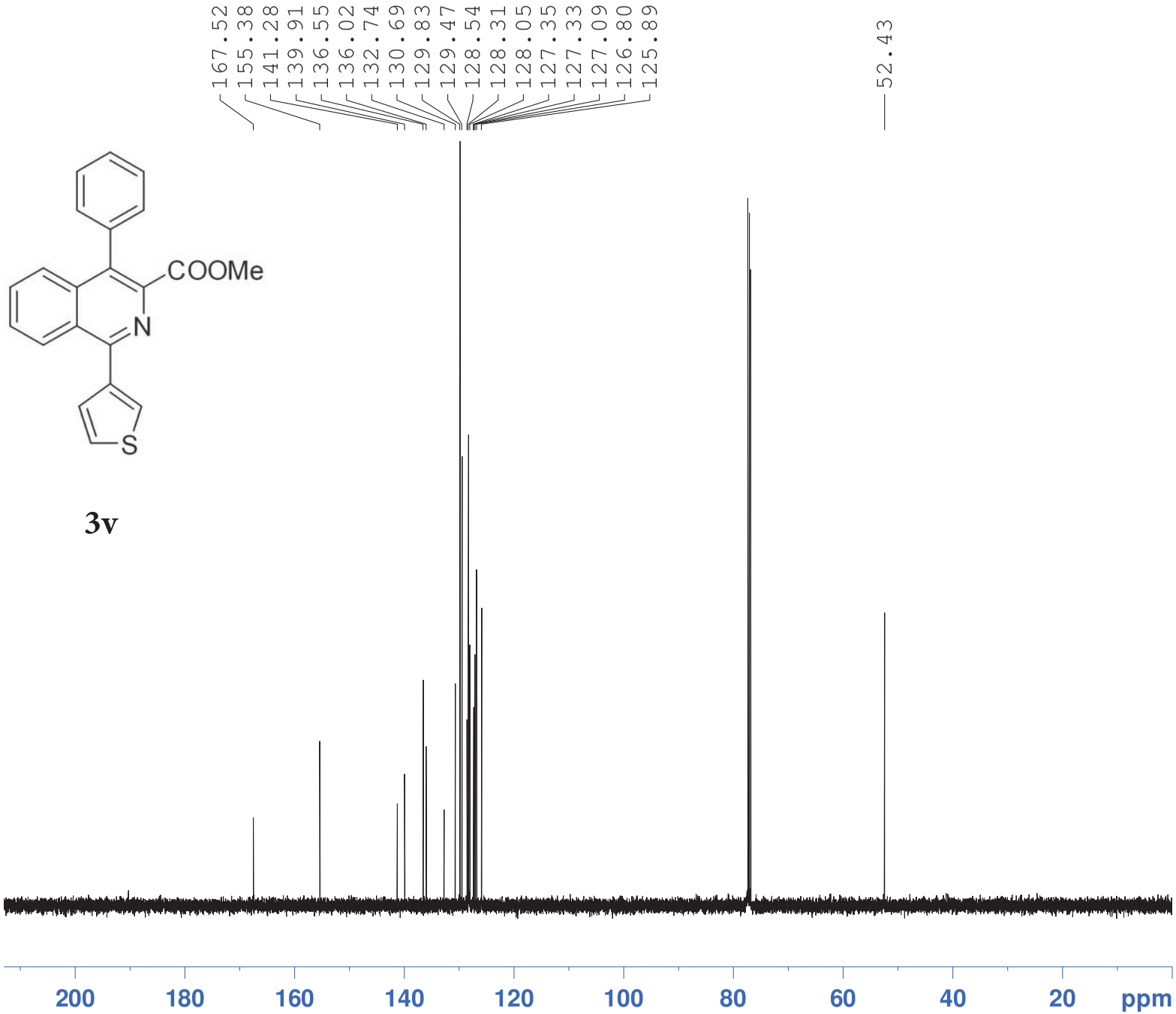


3v

WH-6-89
PROTON CDCl3

NAME	xb20140505
EXPNO	8
PROCNO	1
Date_	20140505
Time	9.46
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	228.1
DW	48.400 usec
DE	6.00 usec
TE	296.4 K
D1	1.00000000 sec
TD0	1

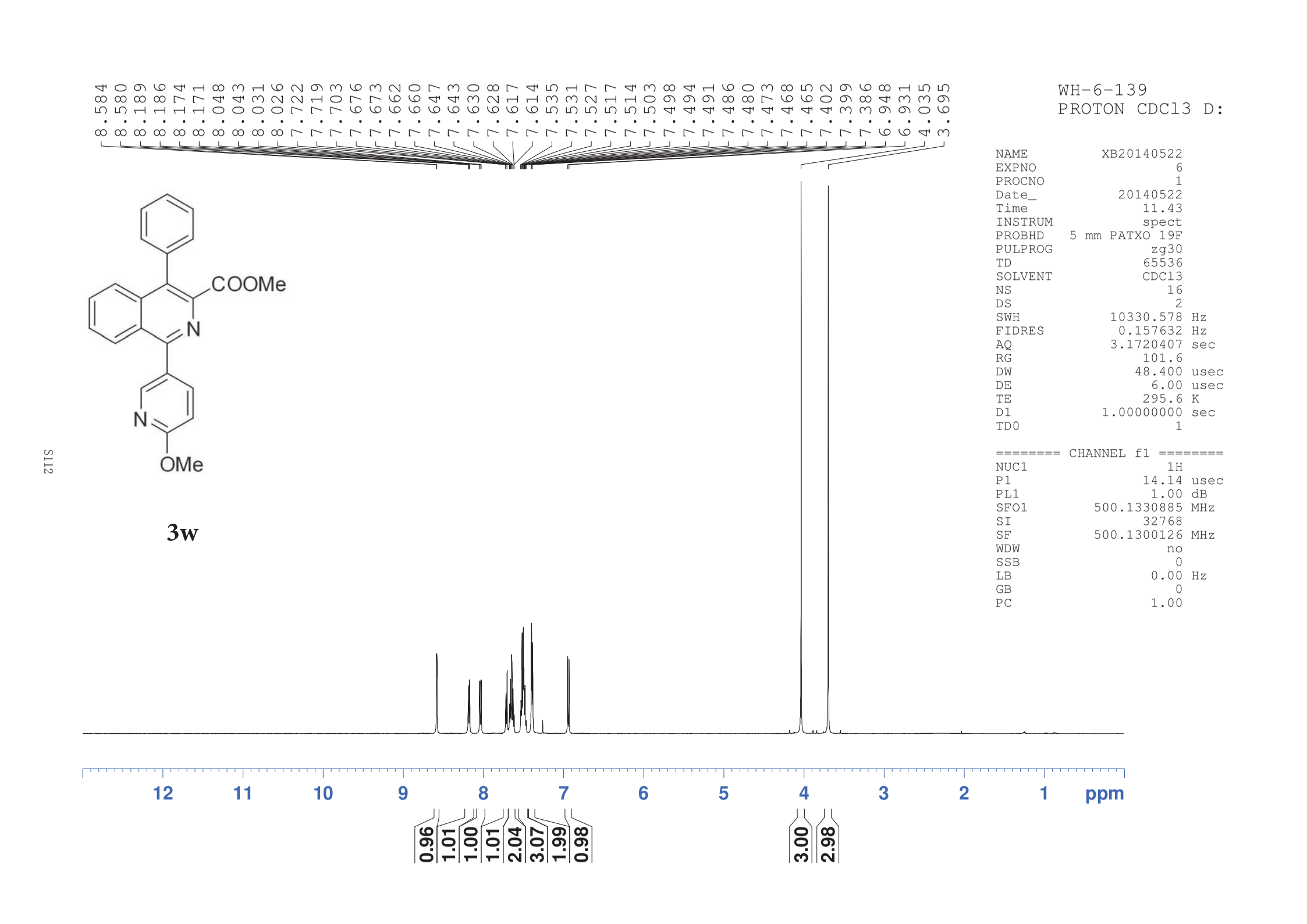
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300123 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



3v

WH-6-89
C13CPD CDCl3

NAME	XB20140508
EXPNO	5
PROCNO	1
Date_	20140508
Time	11.52
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	512
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	114
DW	16.650 usec
DE	6.00 usec
TE	297.4 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40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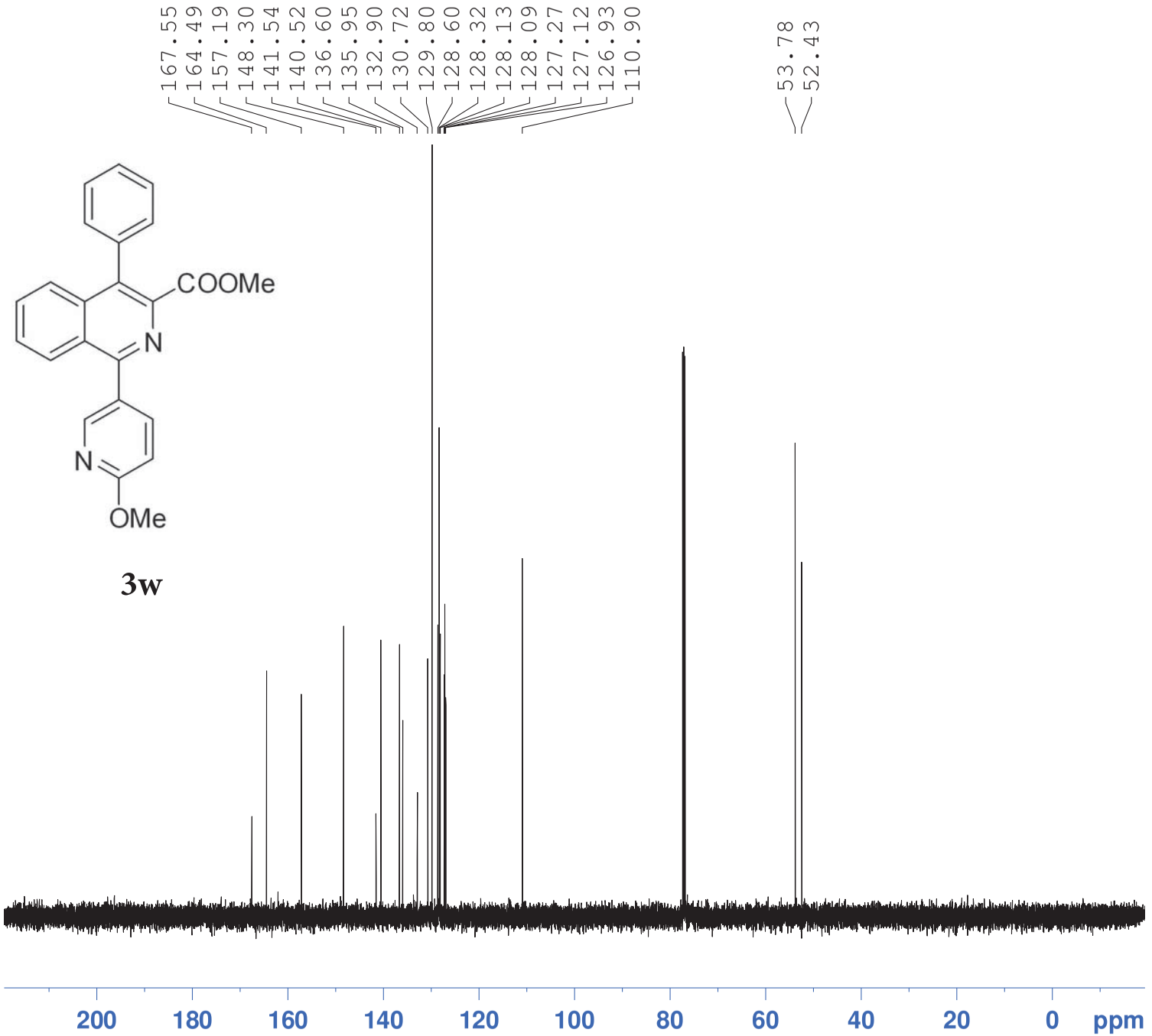
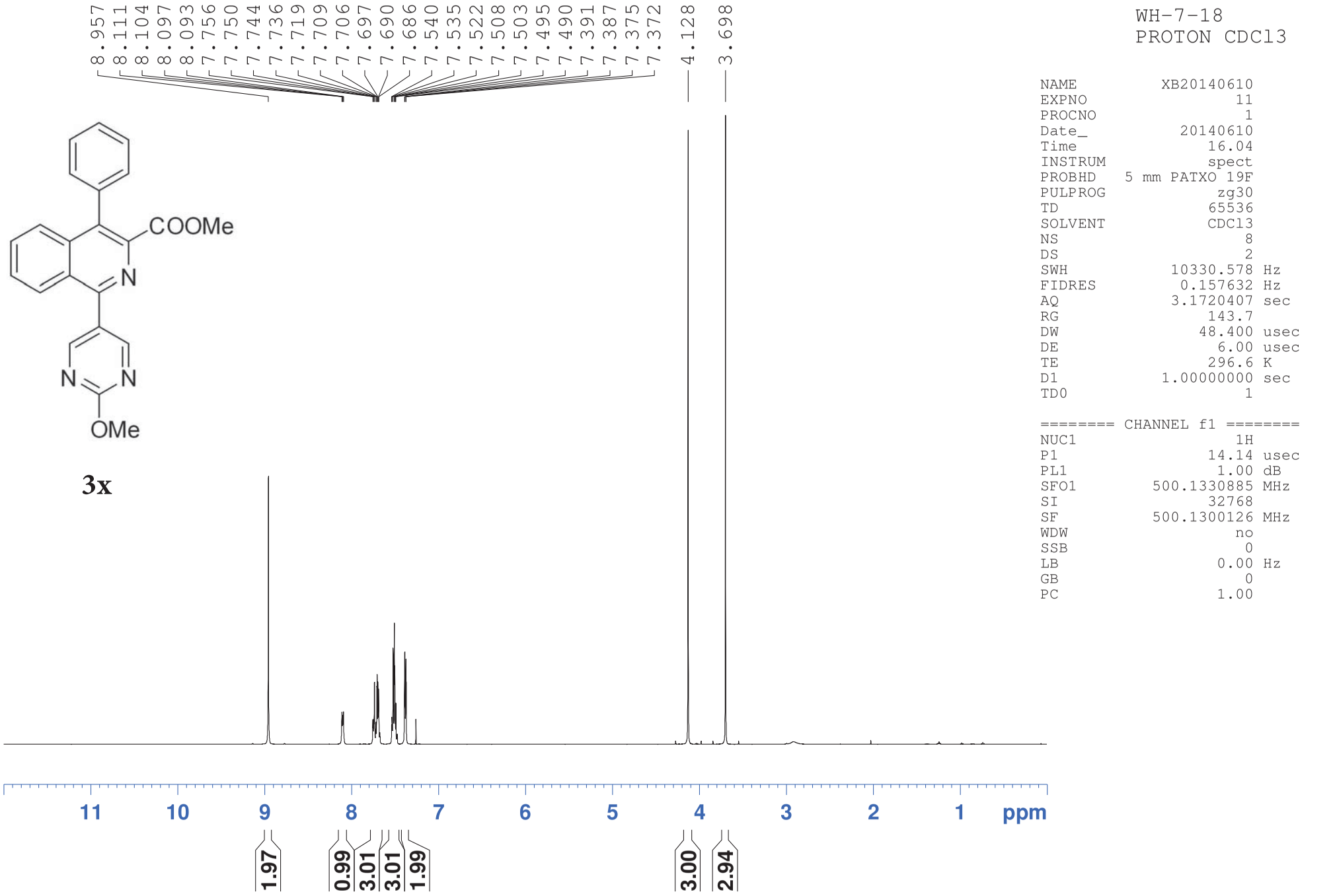
8.189
8.186
8.174
8.171
8.048
8.043
8.031
8.026
7.722
7.719
7.703
7.676
7.673
7.662
7.660
7.647
7.643
7.630
7.628
7.617
7.614
7.535
7.531
7.527
7.517
7.514
7.503
7.498
7.494
7.491
7.486
7.480
7.473
7.468
7.465
7.402
7.399
7.386
6.948
6.931
4.035
3.695
COOMe
N
N
OMe
3w
WH-6-139
PROTON CDCl3 D:
NAME XB20140522
EXPNO 6
PROCNO 1
Date_ 20140522
Time 11.43
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 101.6
DW 48.400 usec
DE 6.00 usec
TE 295.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.14 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300126 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
12
11
10
9
8
7
6
5
4
3
2
1
ppm
0.96
1.01
1.00
1.01
2.04
3.07
1.99
0.98
3.00
2.98

SI12



WH-6-139
C13CPD CDCl3 D

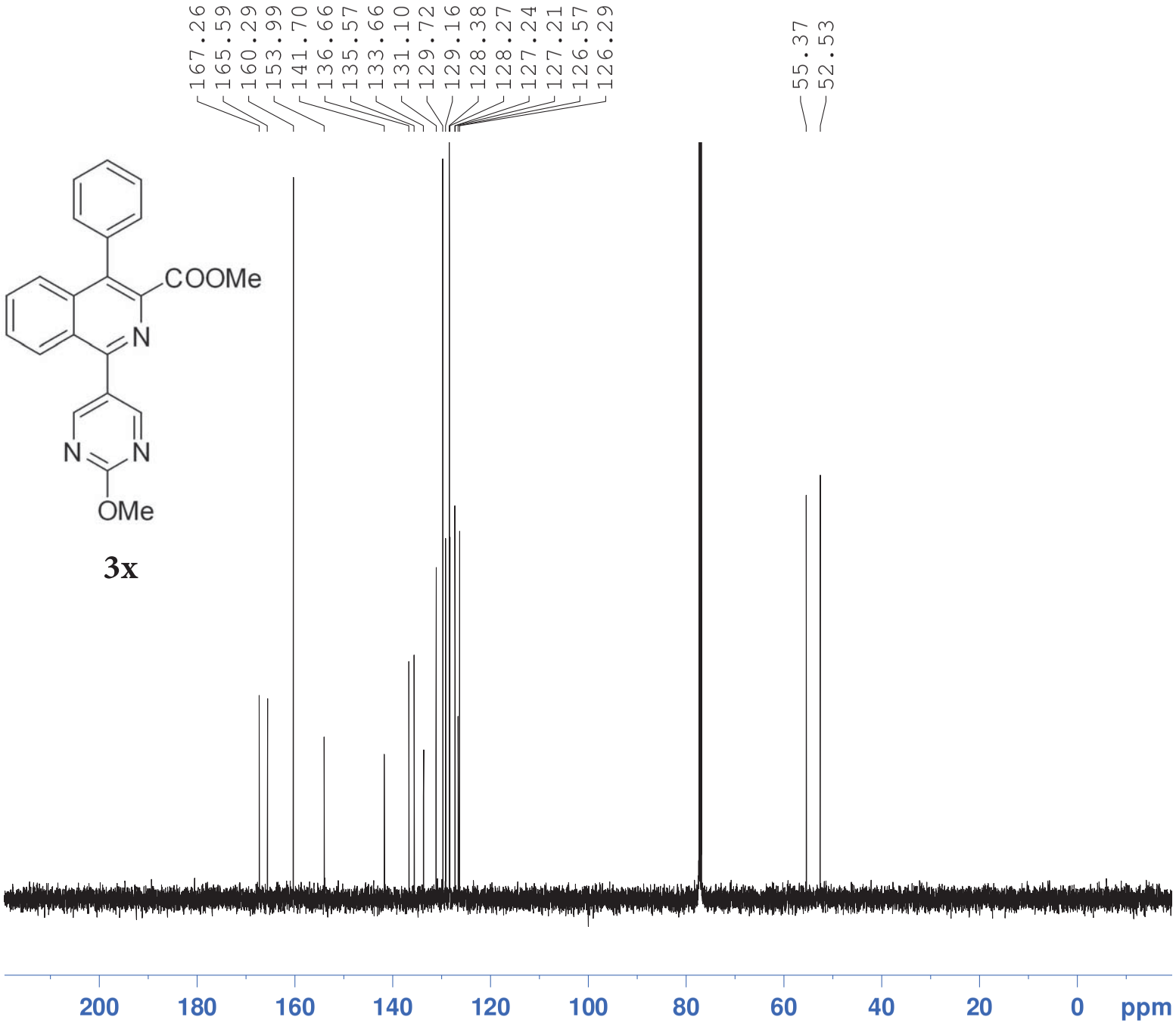
NAME	XB20140522
EXPNO	7
PROCNO	1
Date_	20140522
Time	11.52
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	128
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	181
DW	16.650 usec
DE	6.00 usec
TE	296.9 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40



WH-7-18
PROTON CDCl3

NAME	XB20140610
EXPNO	11
PROCNO	1
Date_	20140610
Time	16.04
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	143.7
DW	48.400 usec
DE	6.00 usec
TE	296.6 K
D1	1.00000000 sec
TD0	1

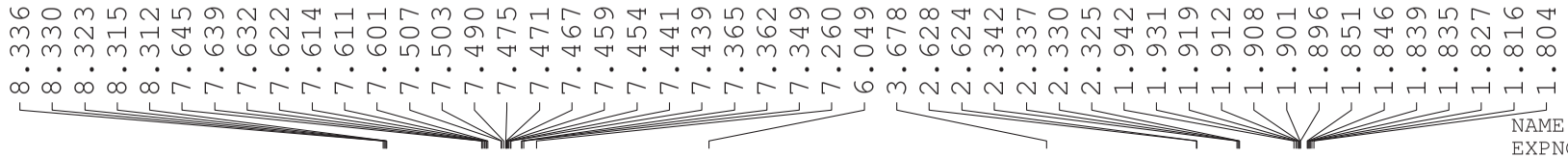
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300126 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

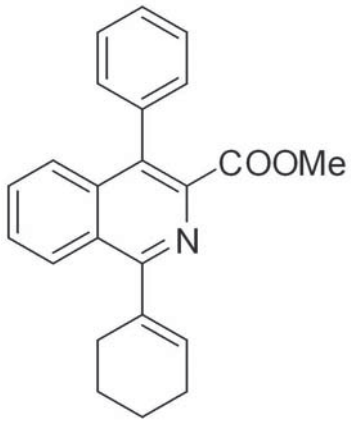


S116

WH-7-18
C13CPD CDCl3

NAME	XB20140610
EXPNO	12
PROCNO	1
Date_	20140610
Time	16.10
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	141
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	406.4
DW	16.650 usec
DE	6.00 usec
TE	297.5 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

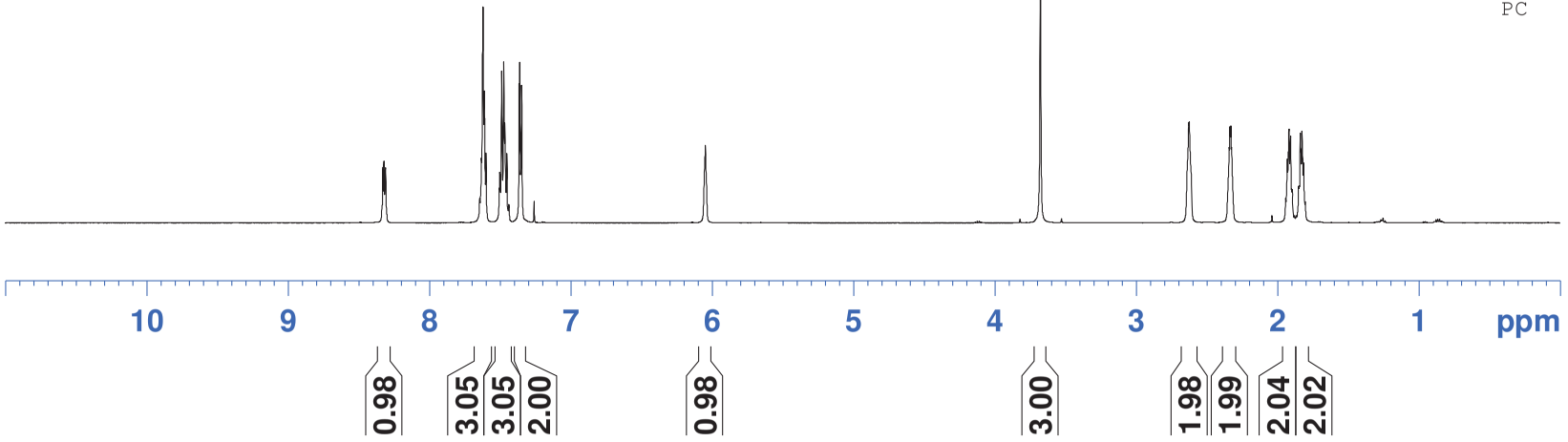


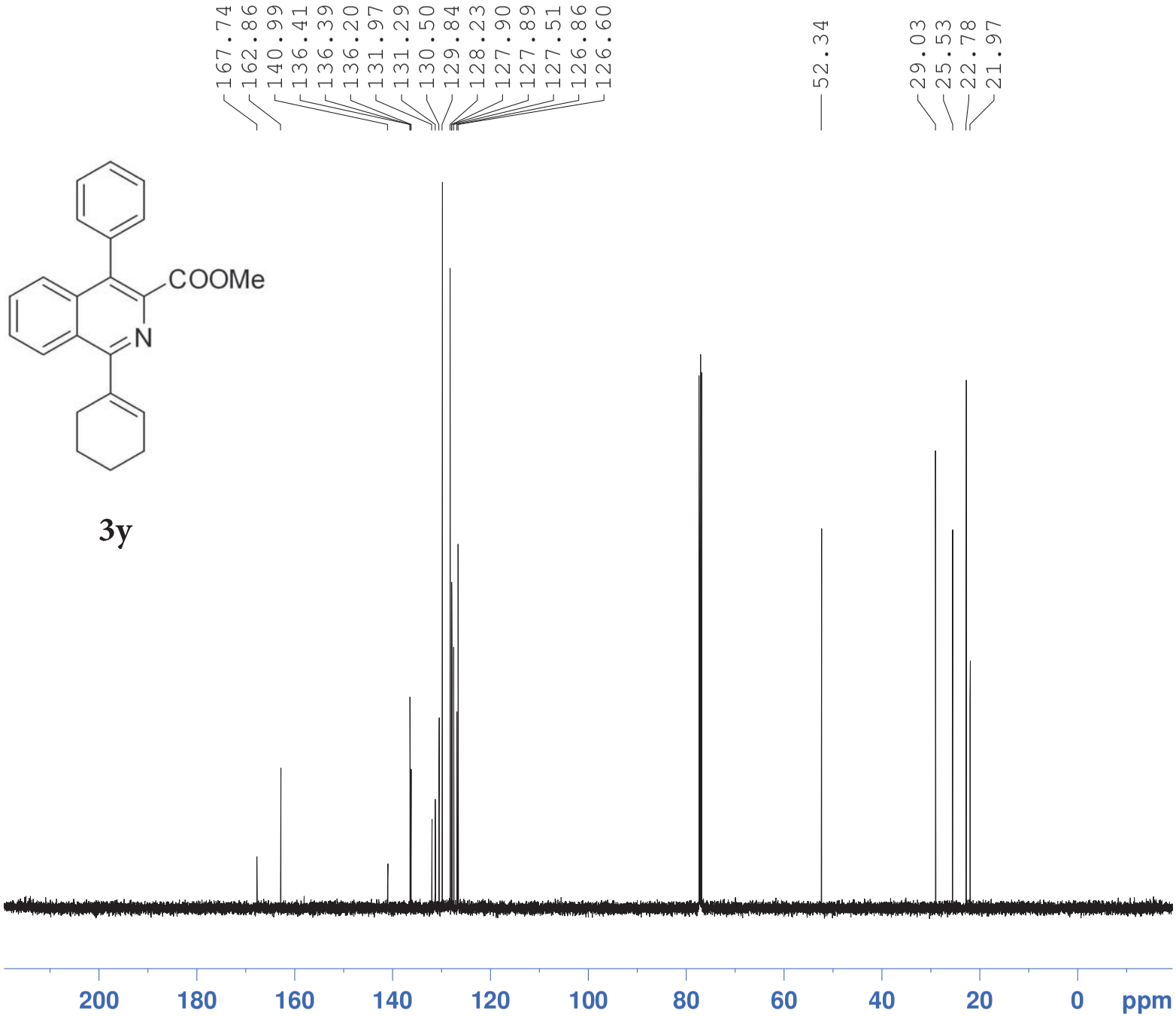


3y

WH-6-66
PROTON CDCl3

NAME	XB20140506
EXPNO	6
PROCNO	1
Date_	20140506
Time	9.32
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	101.6
DW	48.400 usec
DE	6.00 usec
TE	296.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300126 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



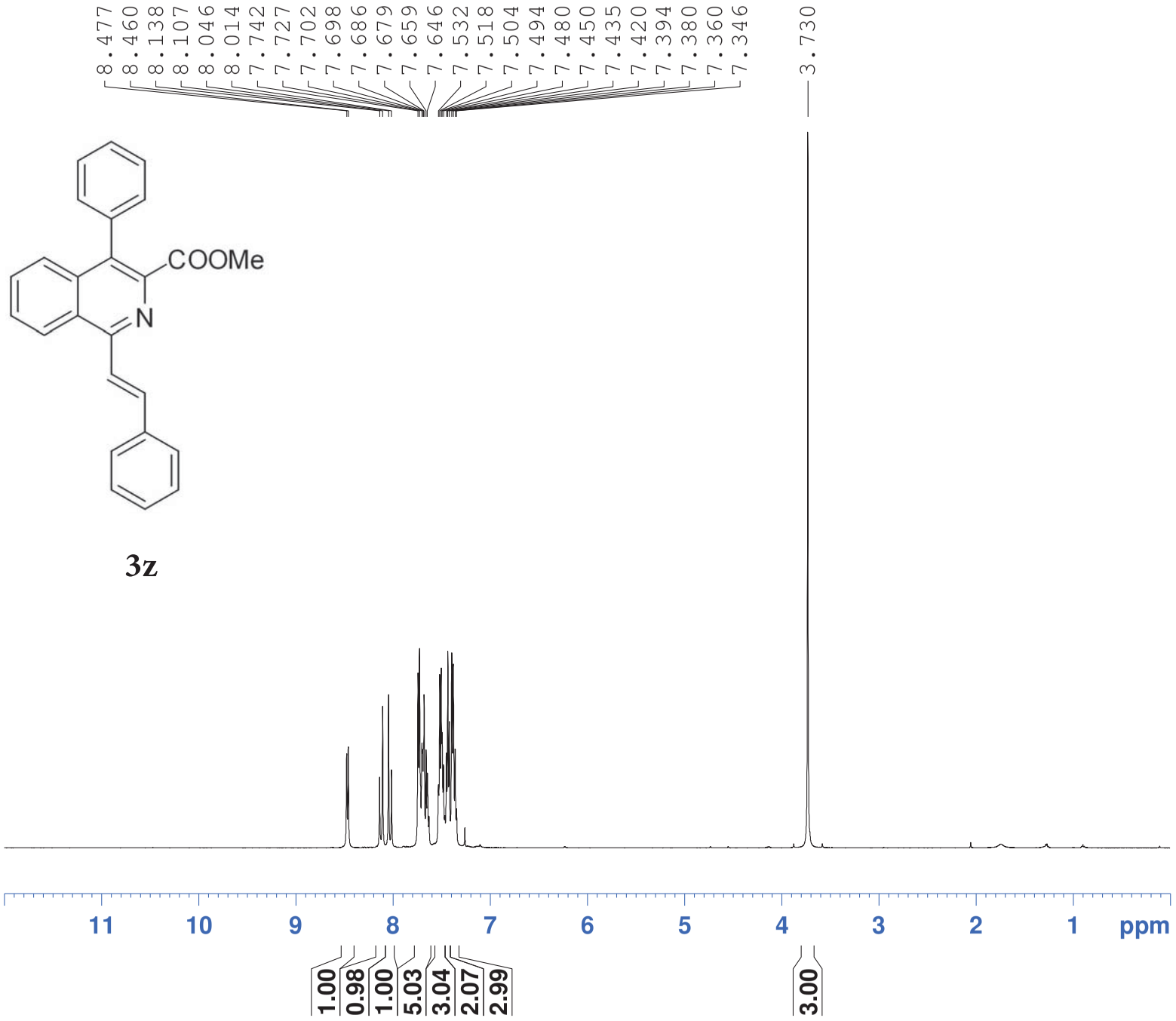


3y

S117

WH-6-66
C13CPD CDCl3

NAME	XB20140507
EXPNO	1
PROCNO	1
Date_	20140508
Time	7.43
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	512
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	114
DW	16.650 usec
DE	6.00 usec
TE	297.8 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40

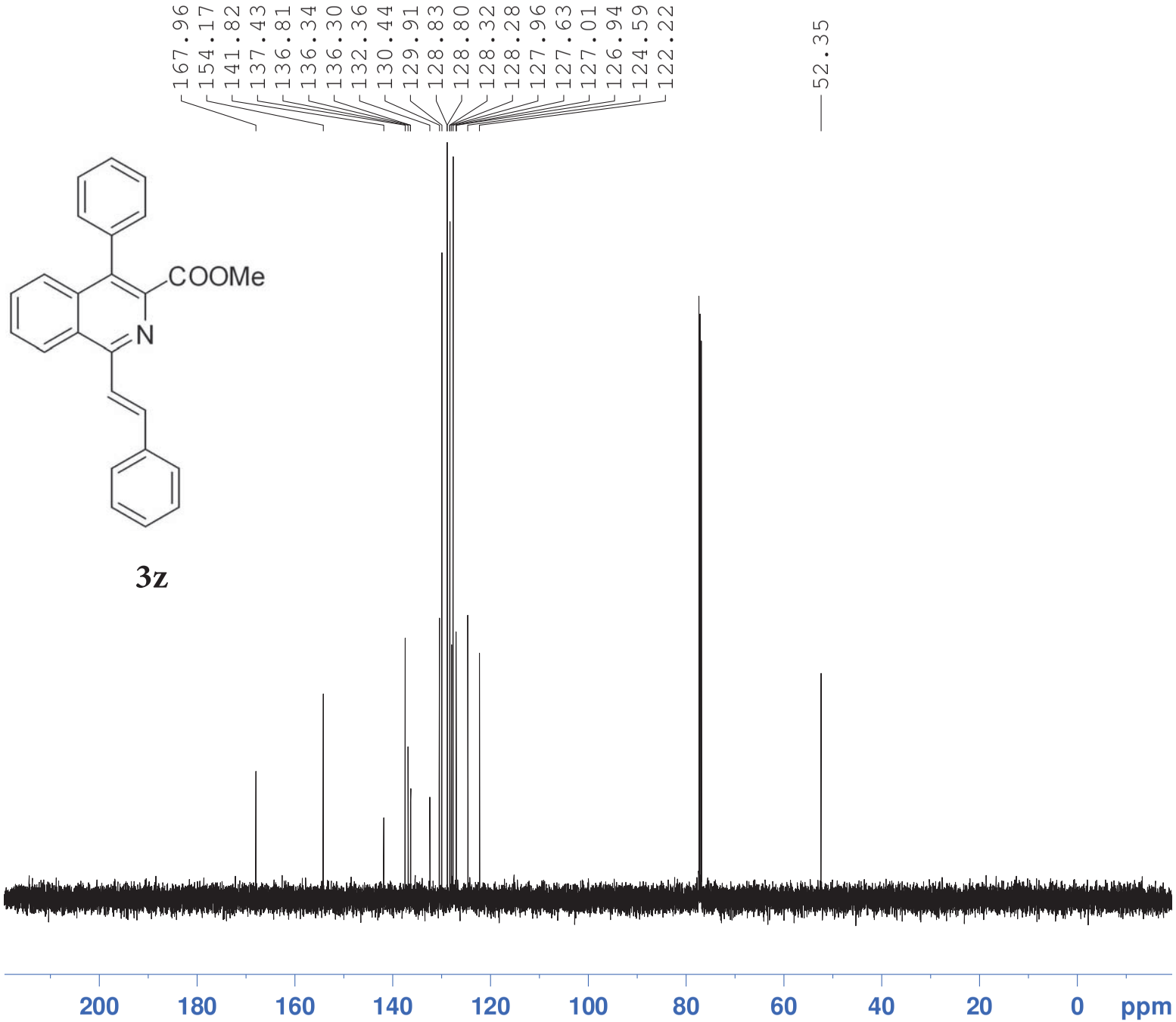


3z

WH-7-16
PROTON CDCl3

NAME	XB20140610
EXPNO	5
PROCNO	1
Date_	20140610
Time	10.37
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	114
DW	48.400 usec
DE	6.00 usec
TE	296.2 K
D1	1.00000000 sec
TD0	1

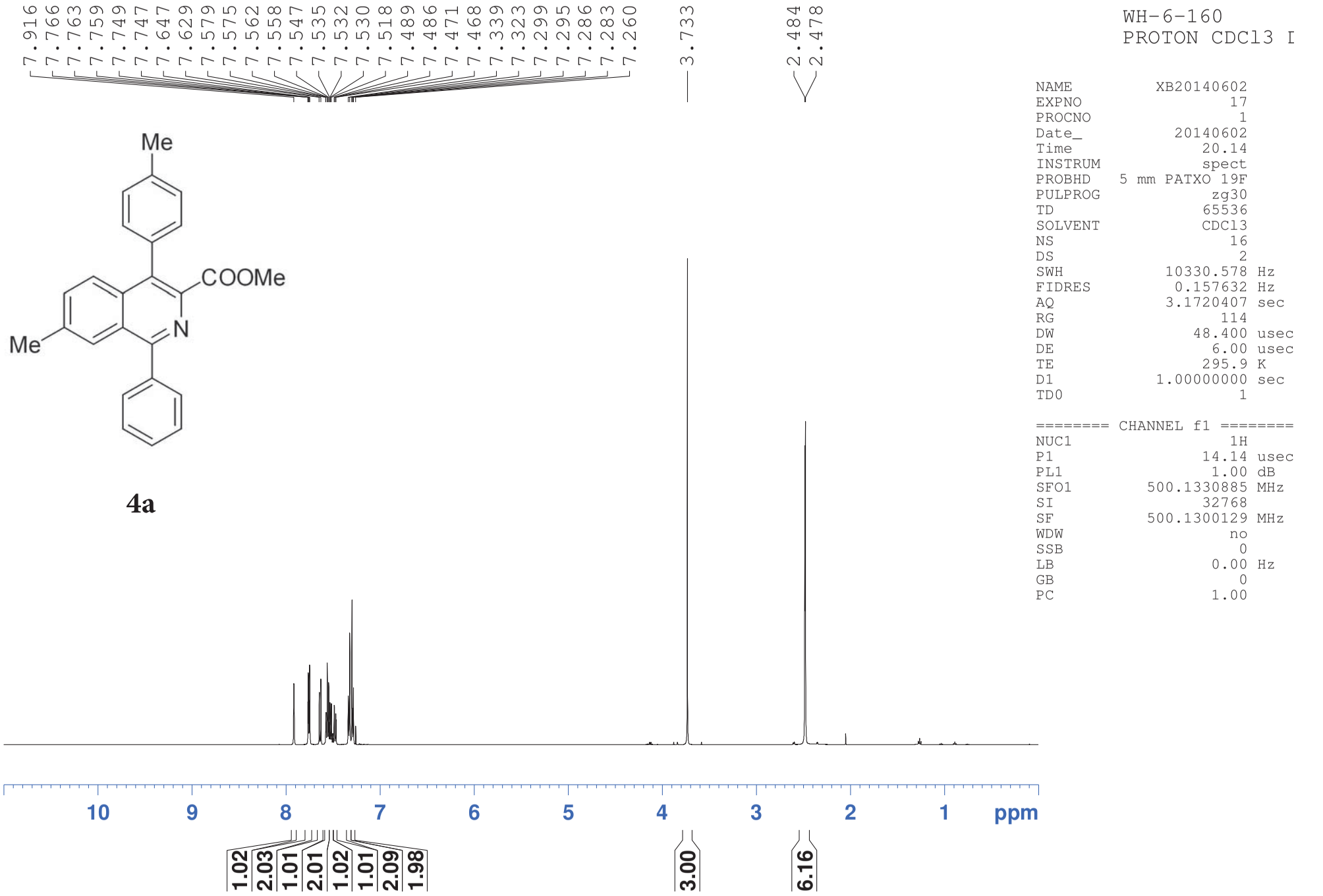
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300123 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



SII9

WH-7-16
C13CPD CDCl3 I

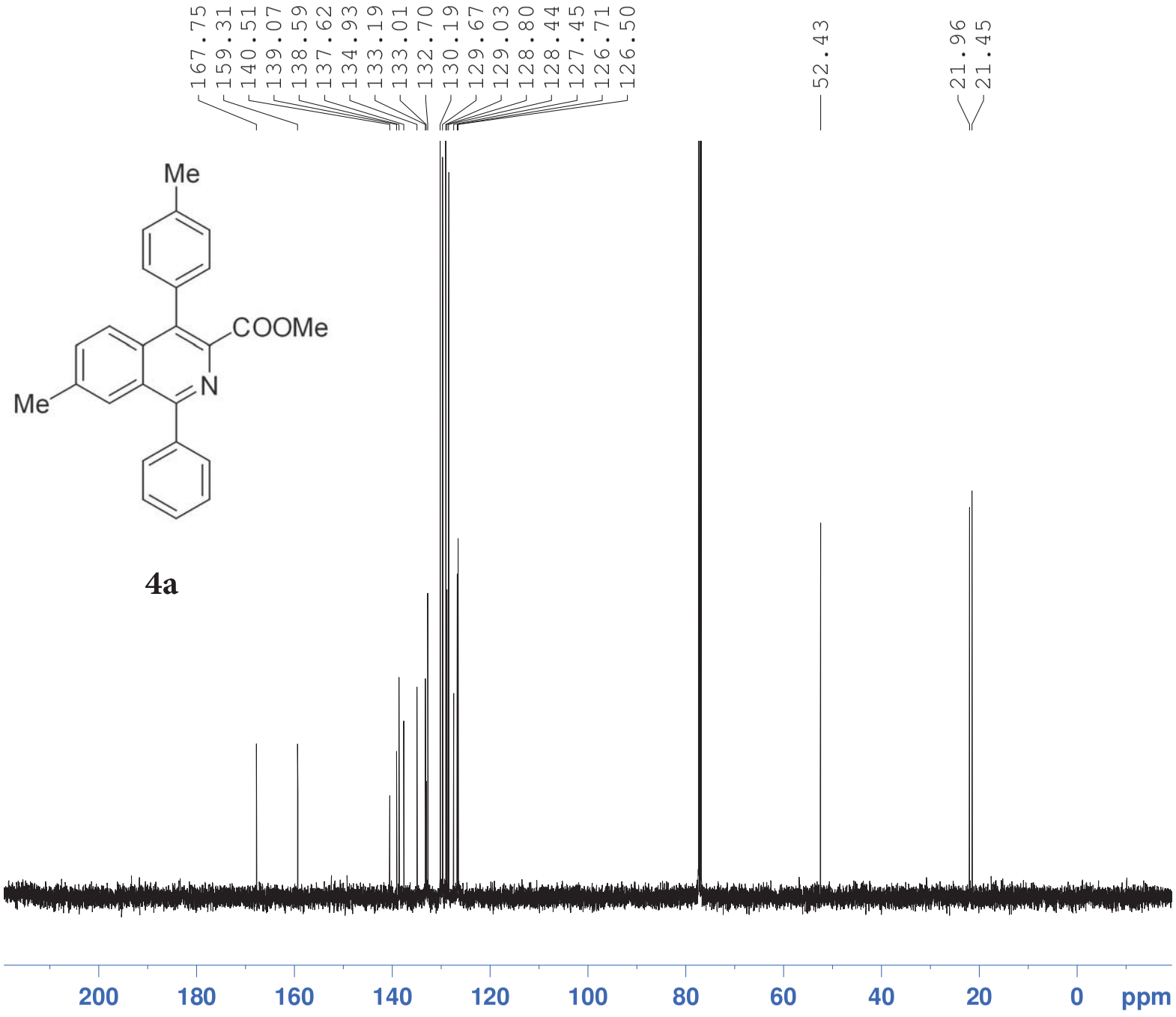
NAME	XB20140610
EXPNO	6
PROCNO	1
Date_	20140610
Time	10.46
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	128
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	228.1
DW	16.650 usec
DE	6.00 usec
TE	297.4 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40



WH-6-160
PROTON CDCl3 I

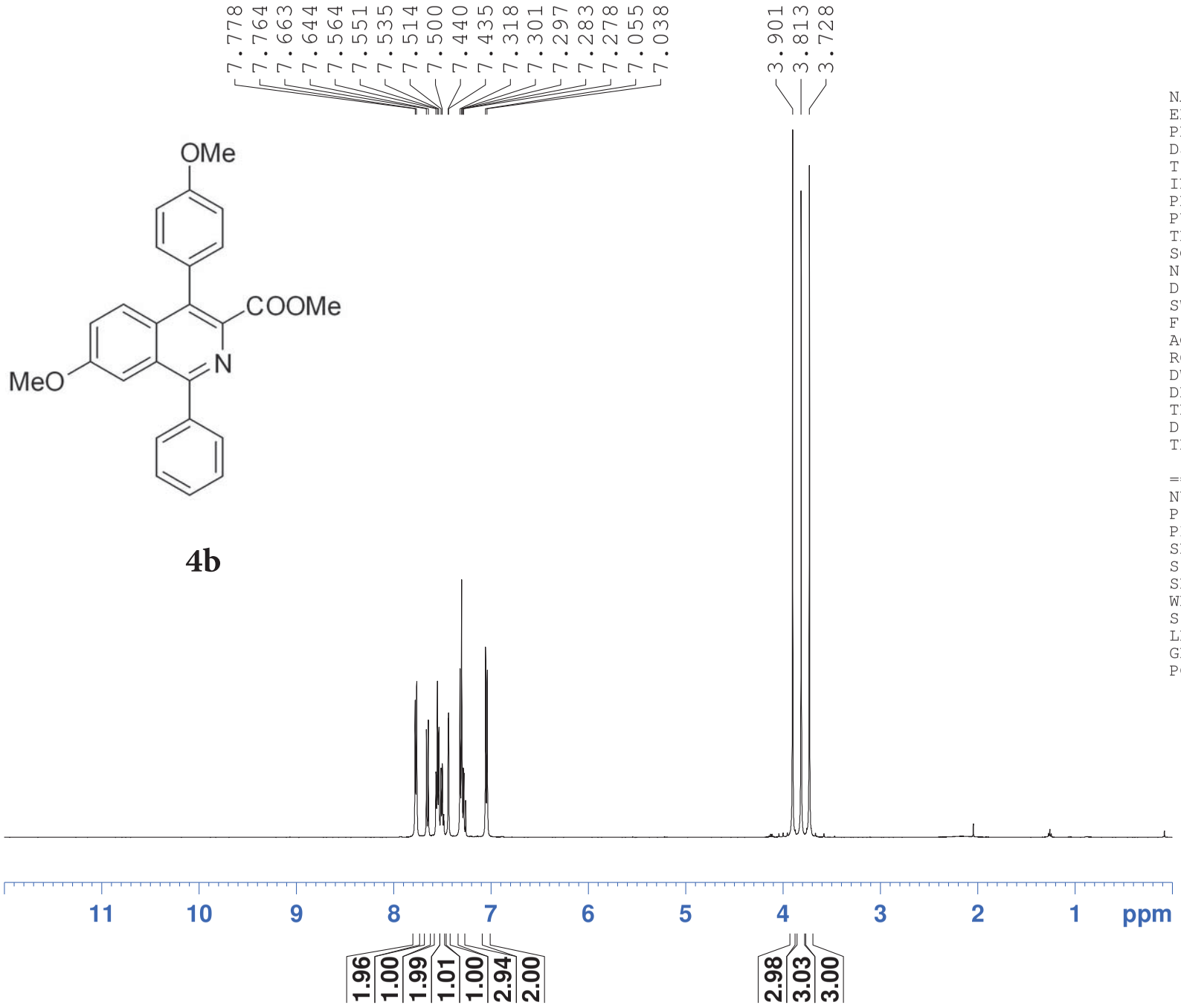
NAME	XB20140602
EXPNO	17
PROCNO	1
Date_	20140602
Time	20.14
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	114
DW	48.400 usec
DE	6.00 usec
TE	295.9 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300129 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



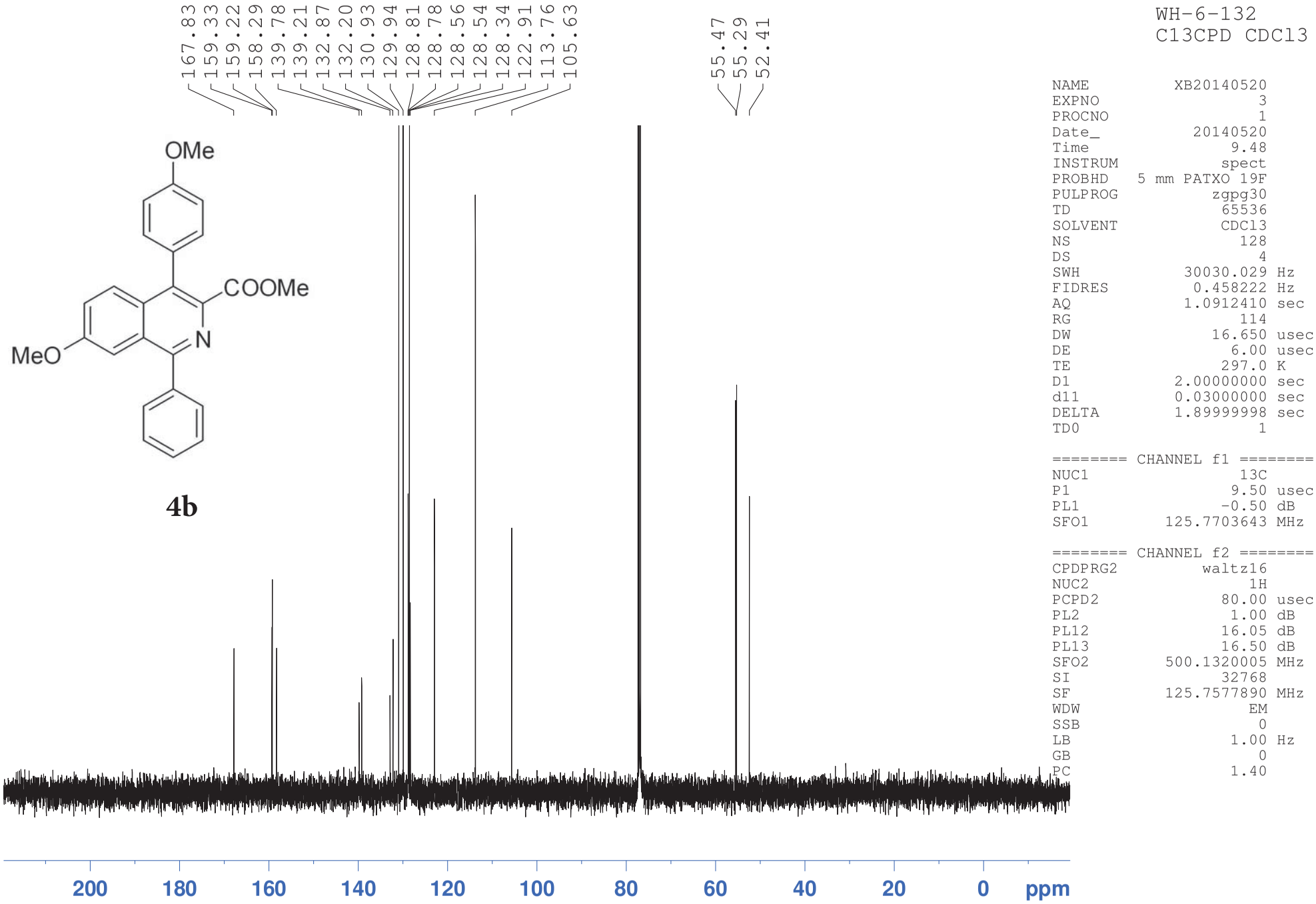
WH-6-160
C13CPD CDCl3 1

NAME	XB20140602
EXPNO	18
PROCNO	1
Date_	20140602
Time	20.23
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	128
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	362
DW	16.650 usec
DE	6.00 usec
TE	297.1 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



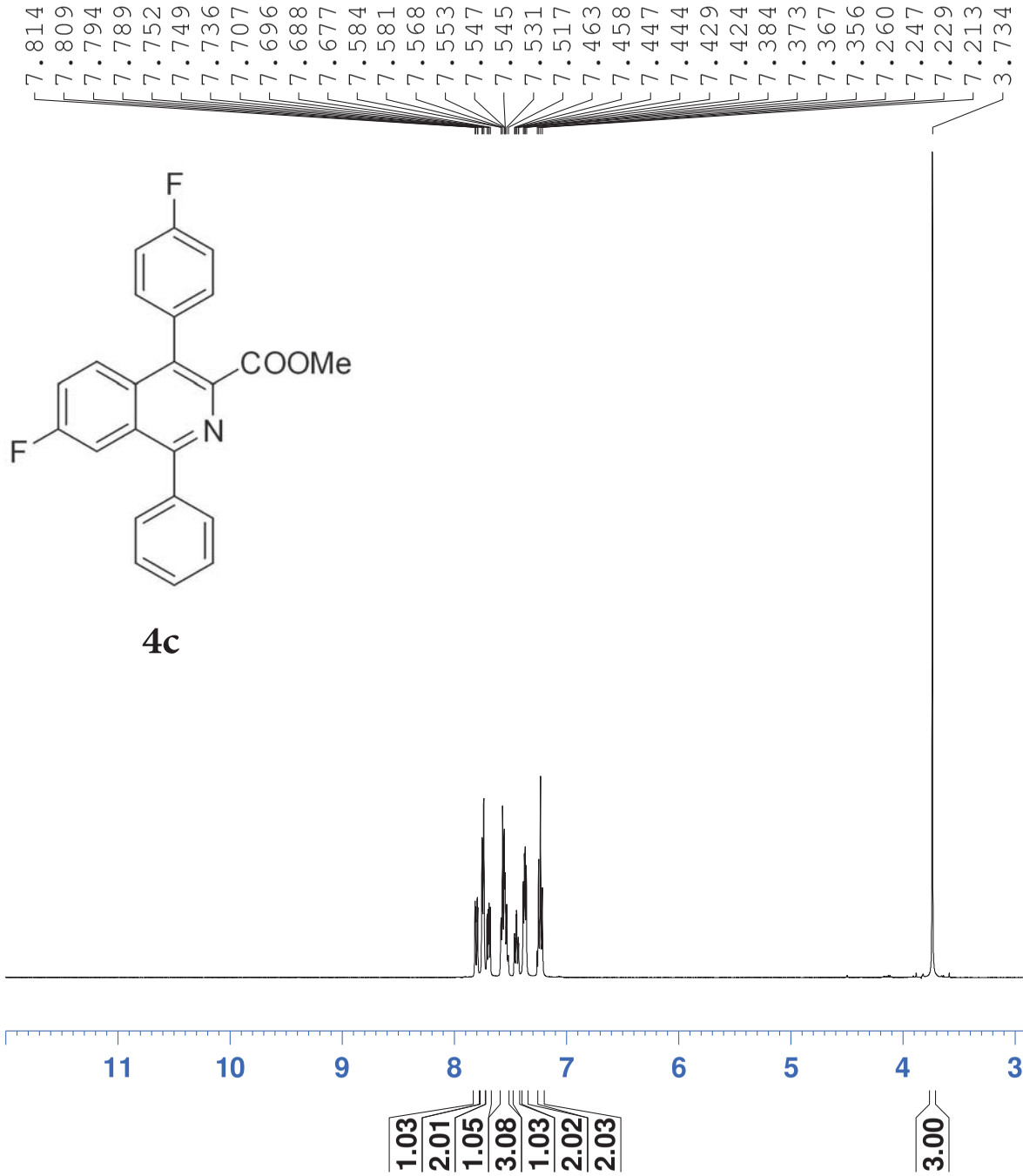
WH-6-132
PROTON CDCl3

NAME	XB20140520
EXPNO	1
PROCNO	1
Date_	20140520
Time	9.37
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	161.3
DW	48.400 usec
DE	6.00 usec
TE	295.7 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300126 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



WH-6-132
C13CPD CDCl3

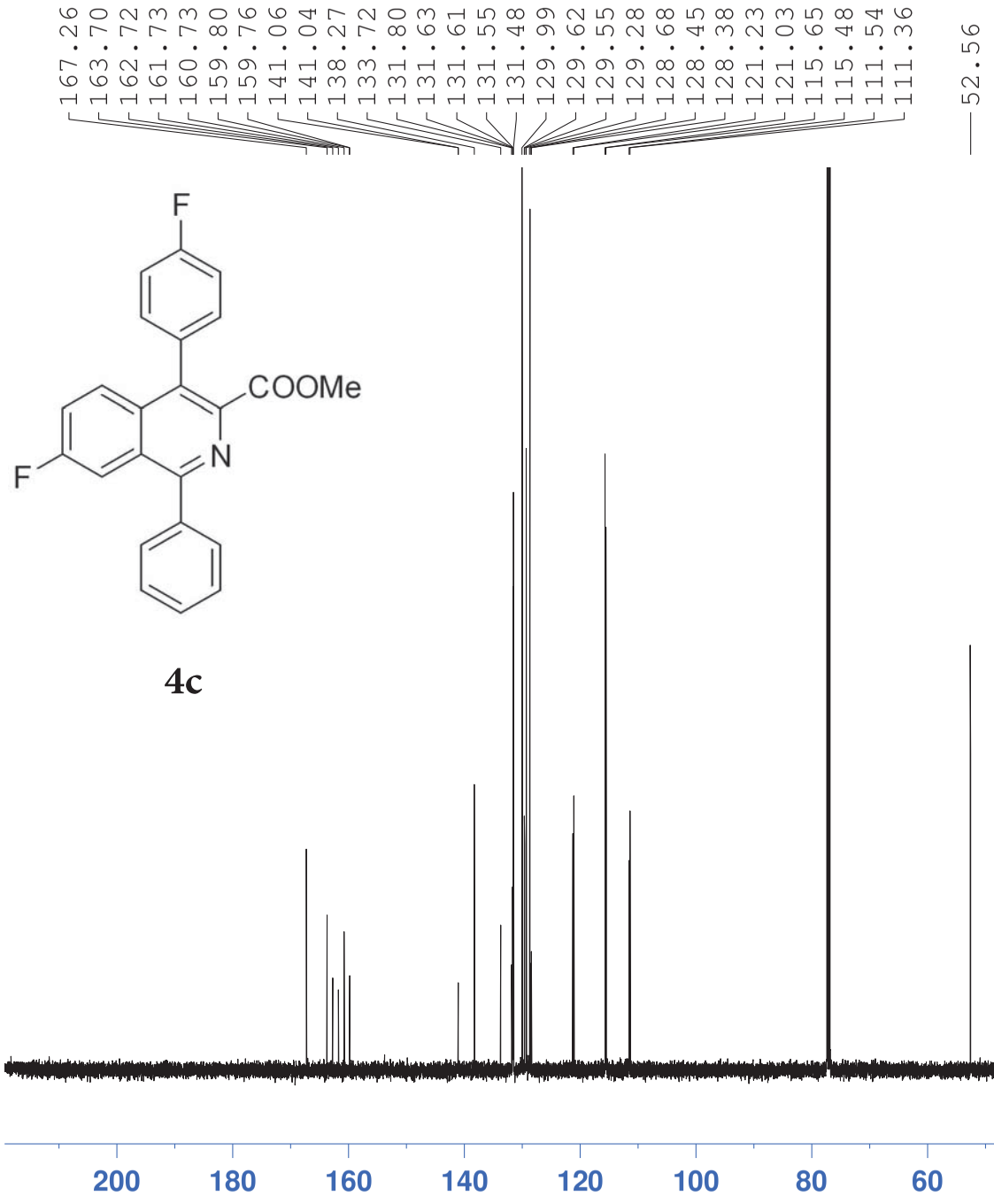
NAME	XB20140520
EXPNO	3
PROCNO	1
Date_	20140520
Time	9.48
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	128
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	114
DW	16.650 usec
DE	6.00 usec
TE	297.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



4c

WH-7-1
PROTON CDCl3

NAME	XB20140602
EXPNO	22
PROCNO	1
Date_	20140602
Time	23.02
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	114
DW	48.400 usec
DE	6.00 usec
TE	296.8 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300126 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



WH-7-1
C13CPD CDCl3

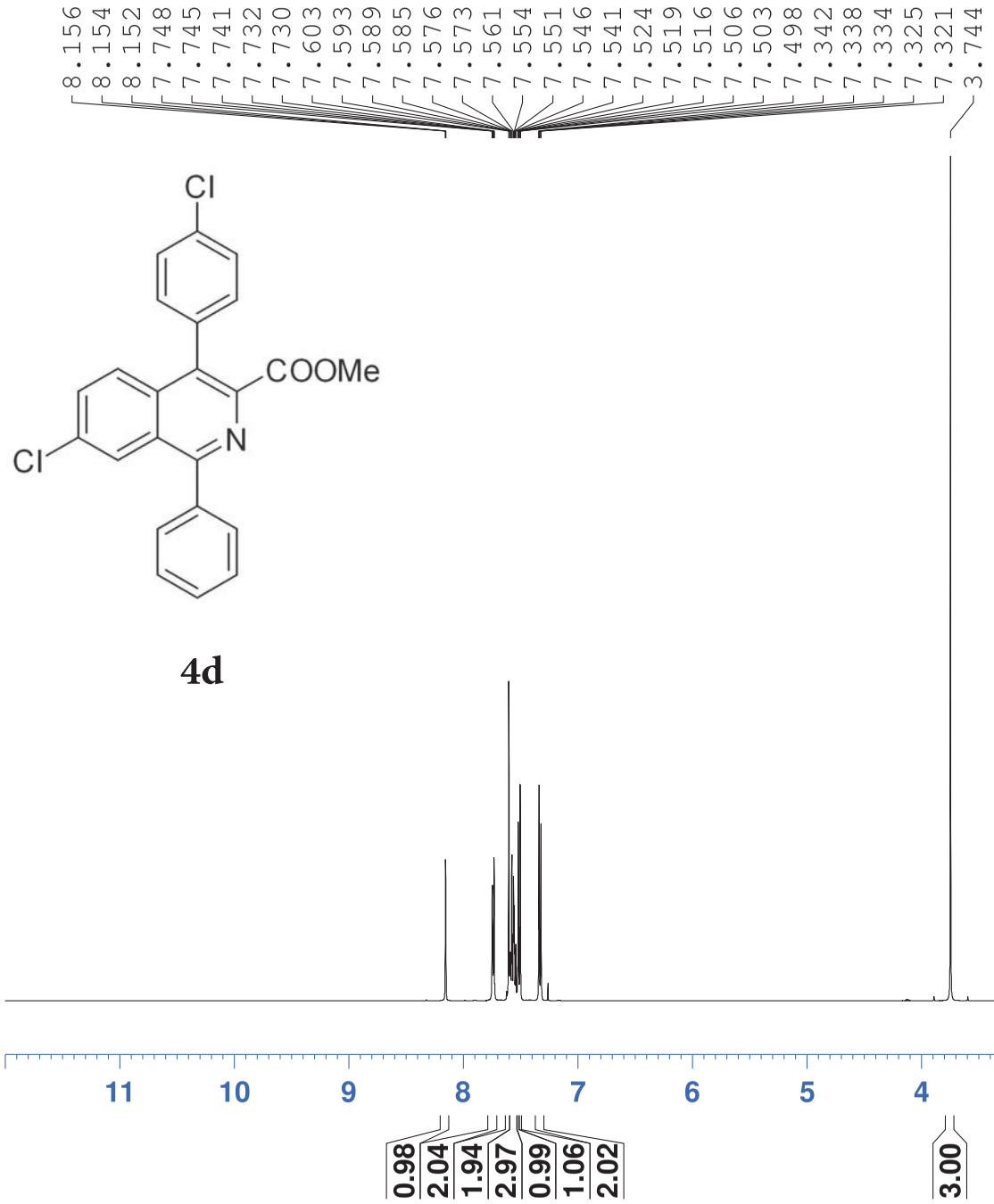
NAME	XB20140602
EXPNO	24
PROCNO	1
Date_	20140603
Time	0.00
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	114
DW	16.650 usec
DE	6.00 usec
TE	297.9 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40

4c

WH-7-1
19Fdeft CDCl3 D

NAME	XB20140602
EXPNO	23
PROCNO	1
Date_	20140602
Time	23.04
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg
TD	131072
SOLVENT	CDCl3
NS	16
DS	4
SWH	100000.000 Hz
FIDRES	0.762939 Hz
AQ	0.6554150 se
RG	406.4
DW	5.000 us
DE	6.00 us
TE	296.7 K
D1	1.00000000 se
TD0	1

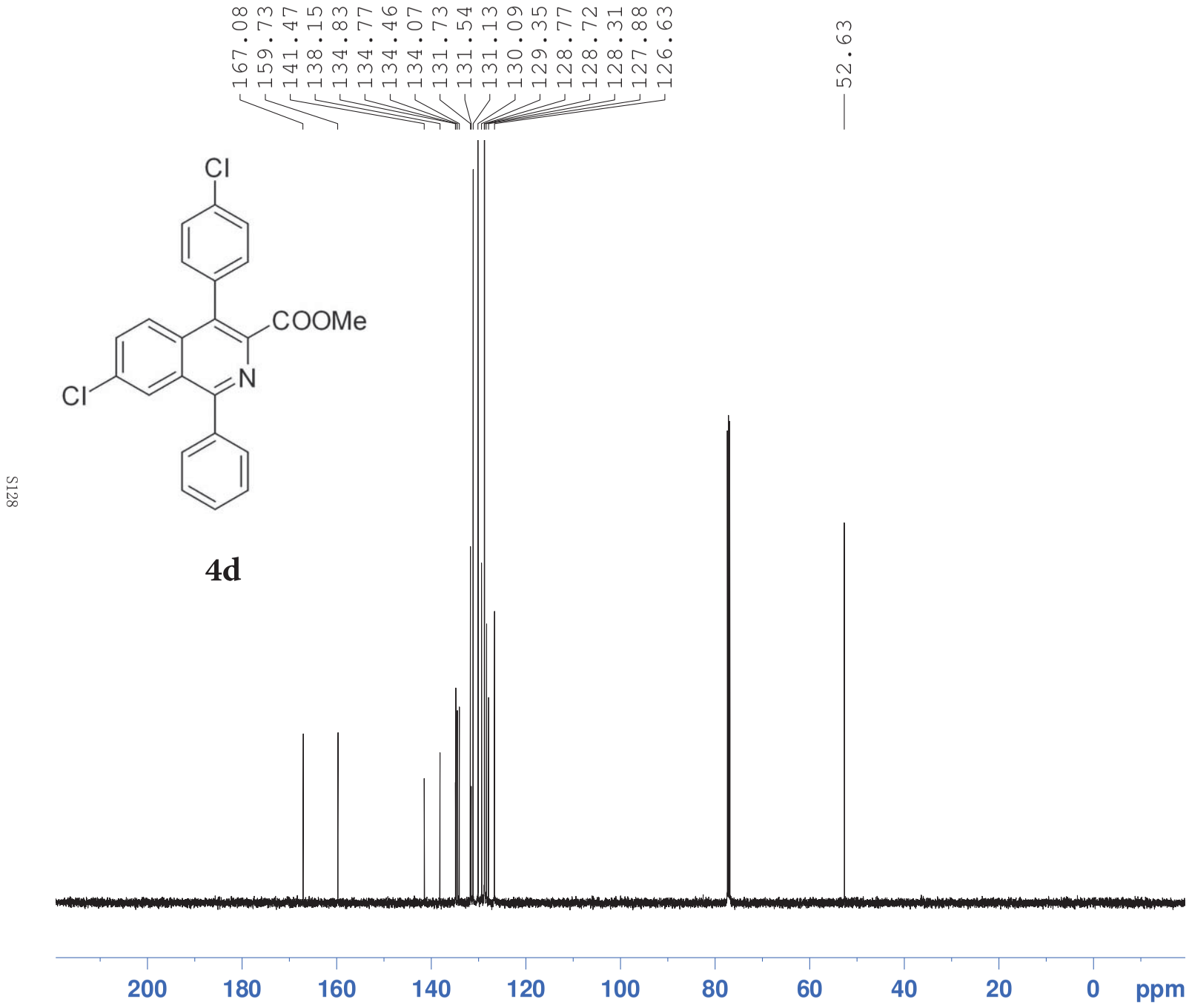
======== CHANNEL f1 ======	
NUC1	19F
P1	19.30 us
PL1	4.00 dB
SFO1	470.5453180 MH
SI	65536
SF	470.5923770 MH
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



WH-7-24
PROTON CDCl3 D

NAME	XB20140609
EXPNO	24
PROCNO	1
Date_	20140610
Time	4.24
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	90.5
DW	48.400 usec
DE	6.00 usec
TE	296.6 K
D1	1.00000000 sec
TD0	1

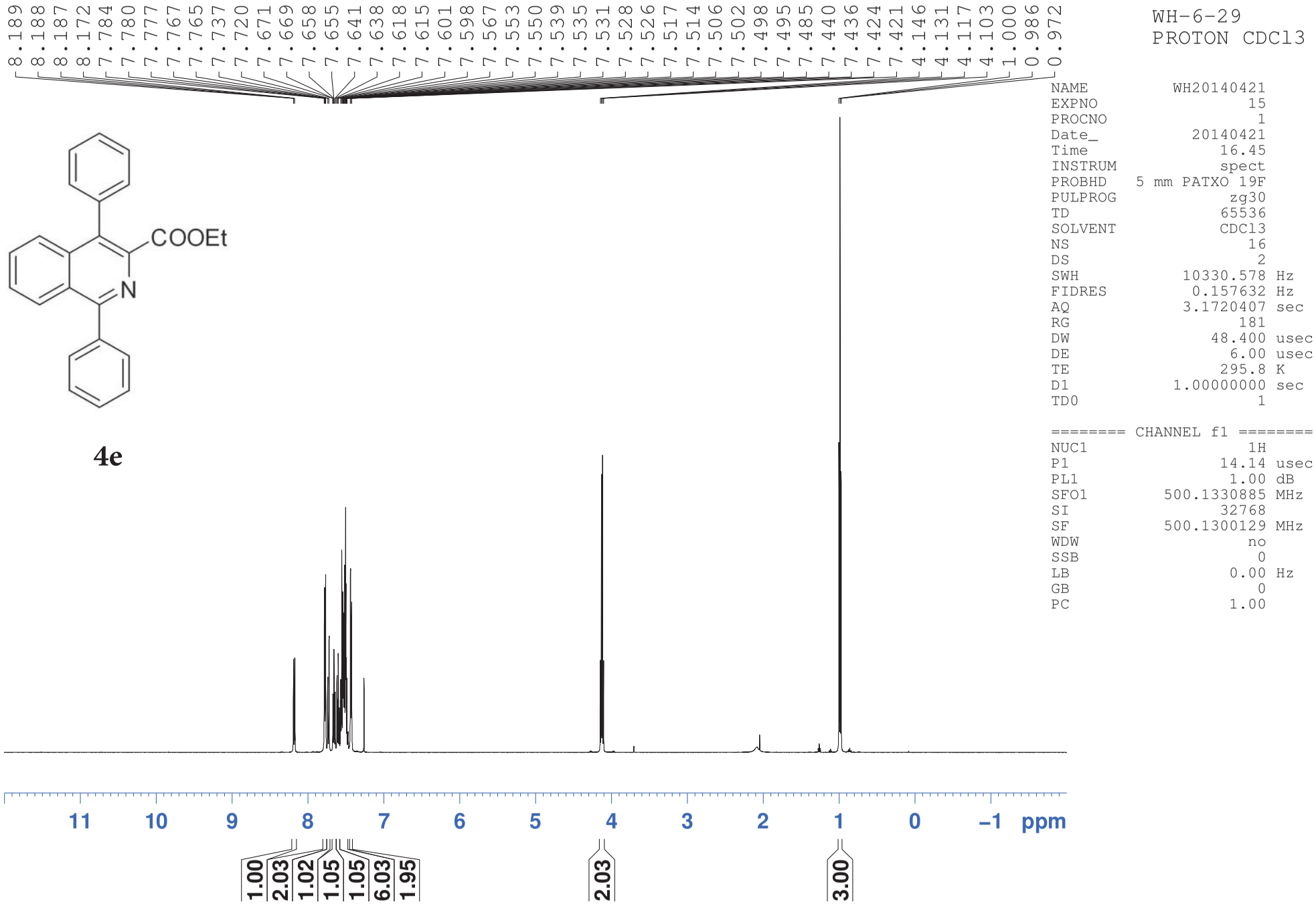
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300126 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

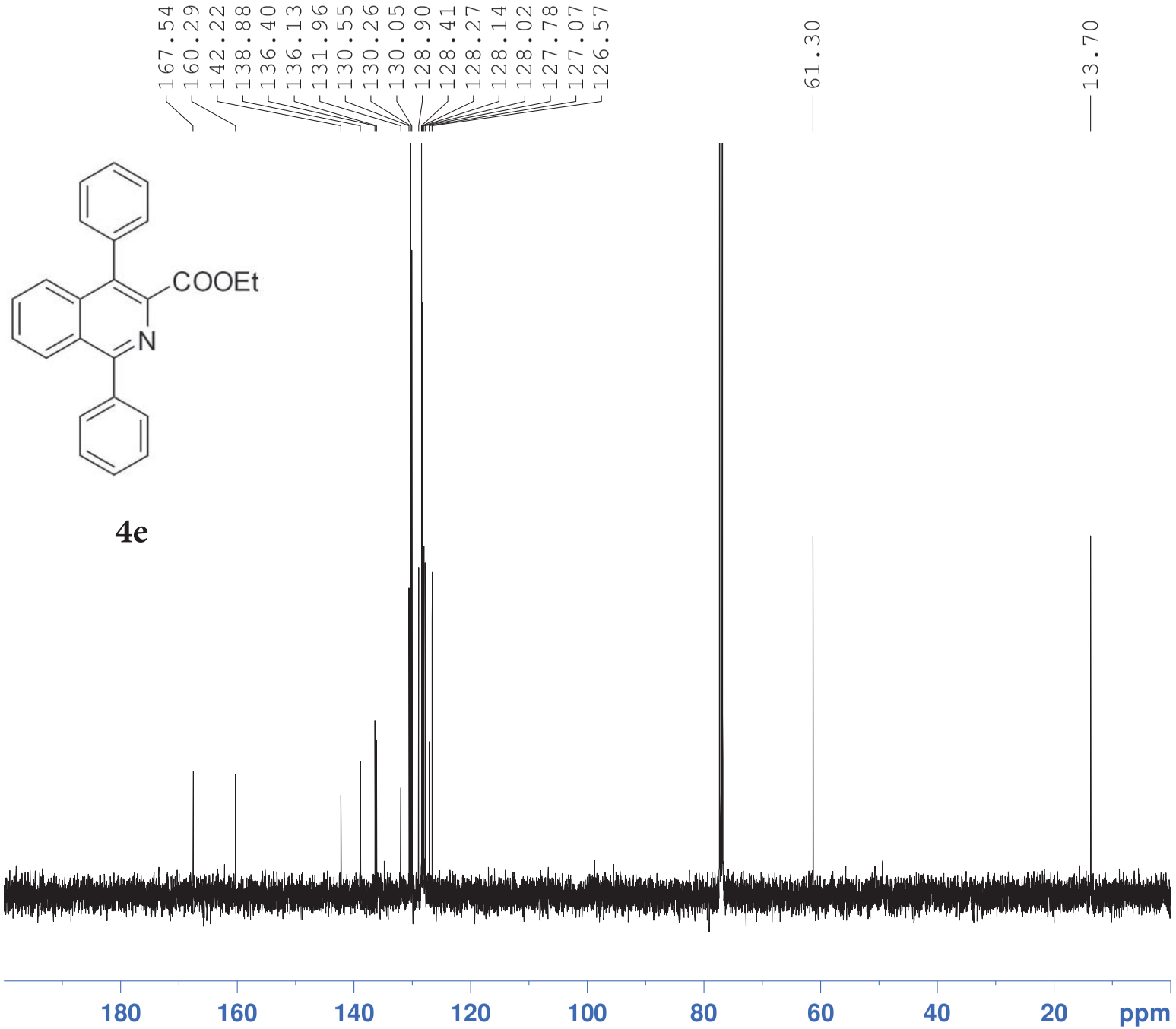


SI28

WH-7-24
C13CPD CDCl3

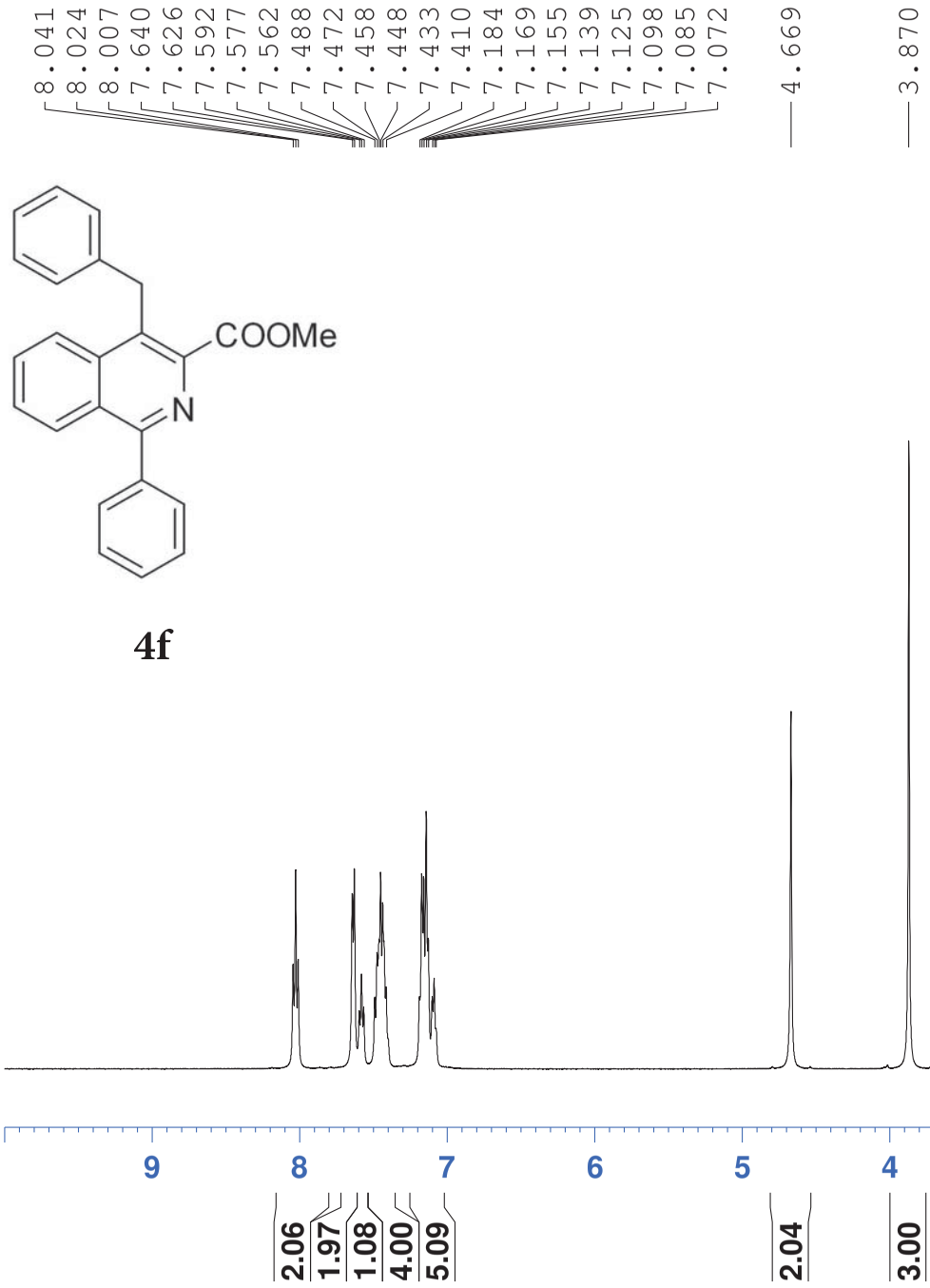
NAME	XB20140609
EXPNO	25
PROCNO	1
Date_	20140610
Time	4.40
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	256
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	203.2
DW	16.650 usec
DE	6.00 usec
TE	297.9 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40


8.189
8.188
8.187
8.172
7.784
7.780
7.777
7.767
7.765
7.737
7.720
7.671
7.669
7.658
7.655
7.641
7.638
7.618
7.615
7.601
7.598
7.567
7.553
7.550
7.539
7.535
7.531
7.528
7.526
7.517
7.514
7.506
7.502
7.498
7.495
7.485
7.440
7.436
7.424
7.421
4.146
4.131
4.117
4.103
1.000
0.986
0.972
COOEt
N
4e
WH-6-29
PROTON CDCl3
NAME WH20140421
EXPNO 15
PROCNO 1
Date_ 20140421
Time 16.45
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 181
DW 48.400 usec
DE 6.00 usec
TE 295.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.14 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300129 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm
1.00
2.03
1.02
1.05
1.05
6.03
1.95
2.03
3.00



WH-6-29
C13CPD CDCl3

NAME	WH20140421
EXPNO	16
PROCNO	1
Date_	20140421
Time	16.54
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	128
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	322.5
DW	16.650 usec
DE	6.00 usec
TE	297.1 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

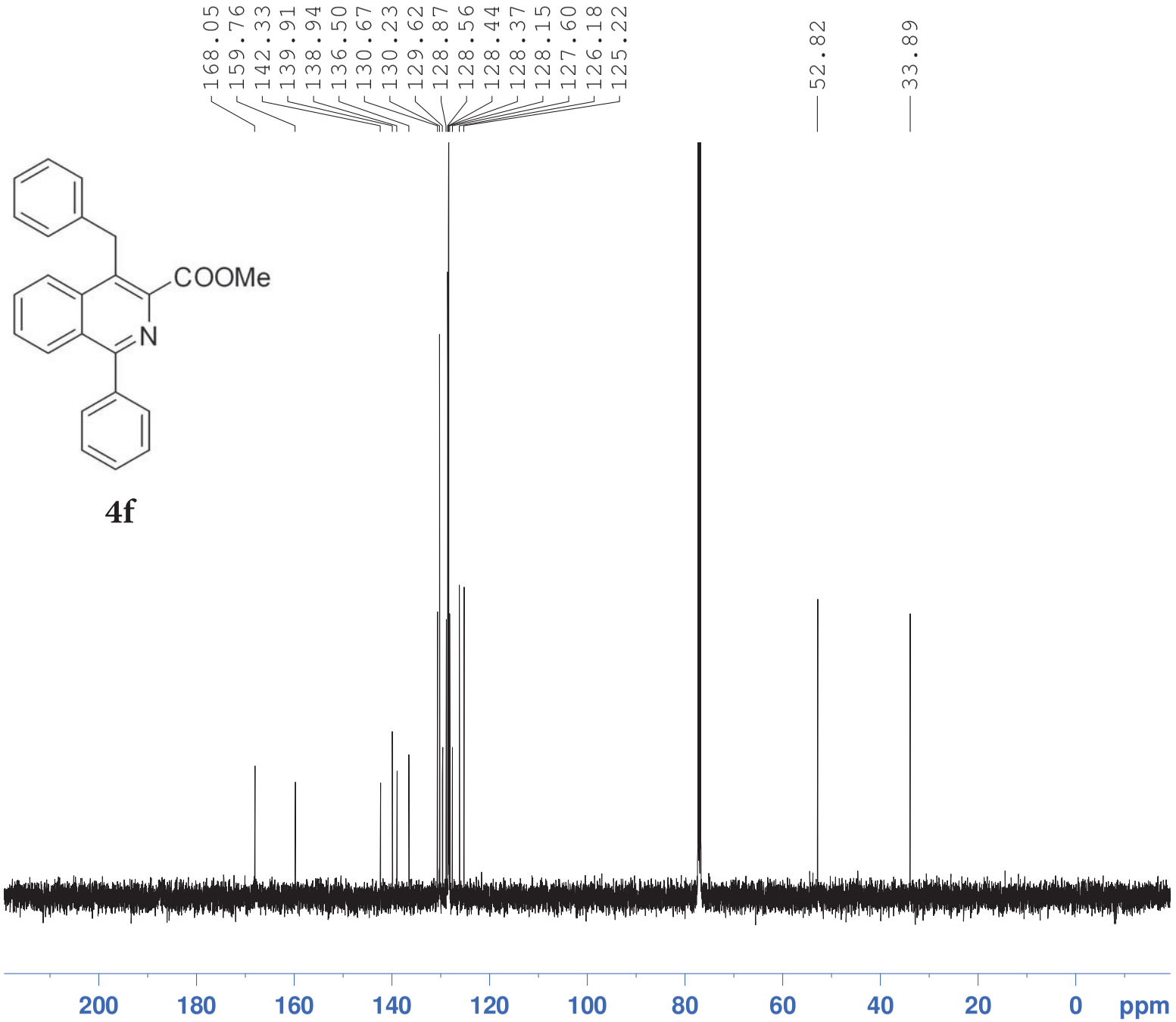


4f

WH-7-40
PROTON CDCl3 I

NAME	XB20140619
EXPNO	4
PROCNO	1
Date_	20140619
Time	11.23
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	181
DW	48.400 usec
DE	6.00 usec
TE	296.4 K
D1	1.00000000 sec
TD0	1

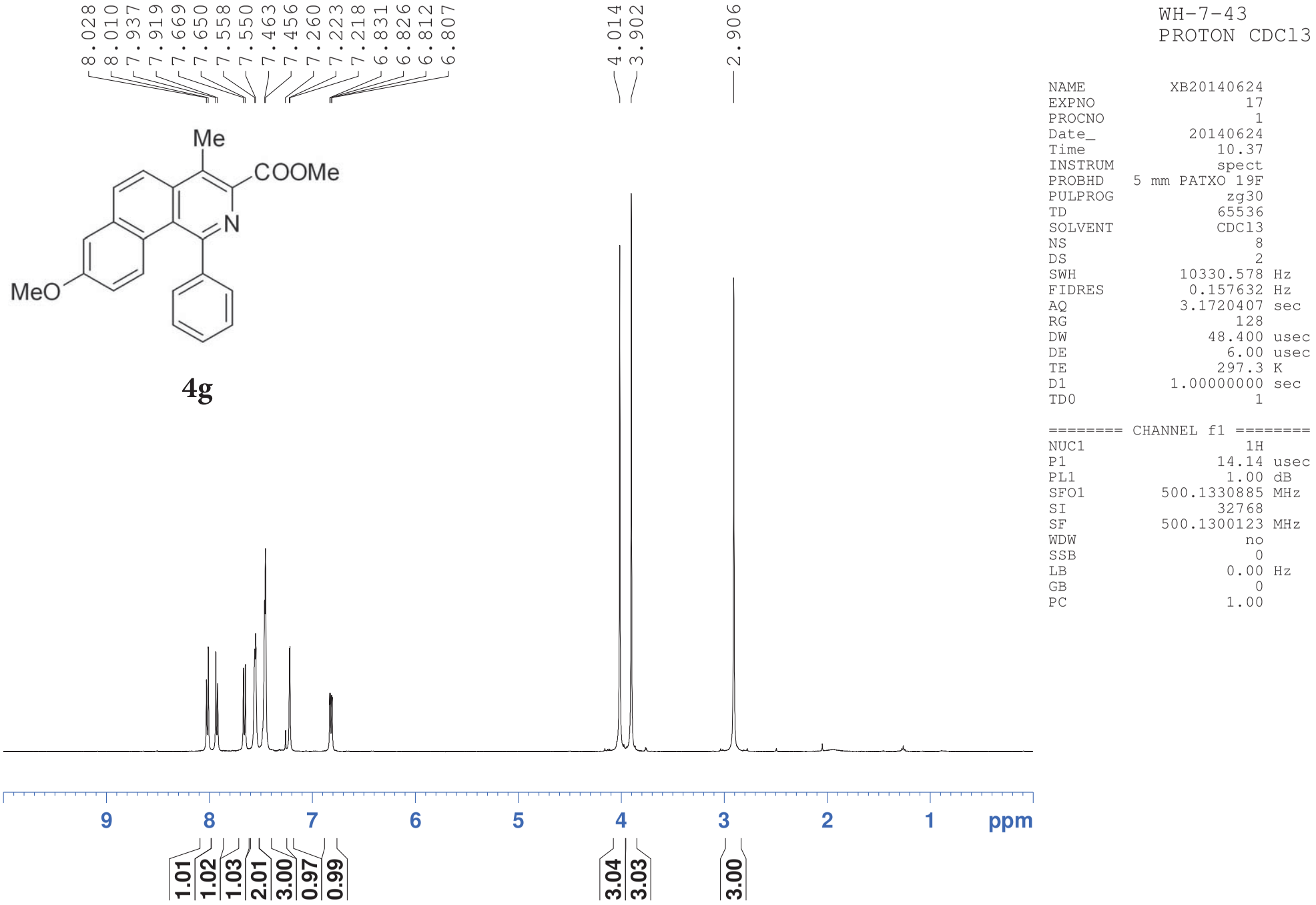
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300600 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



4f

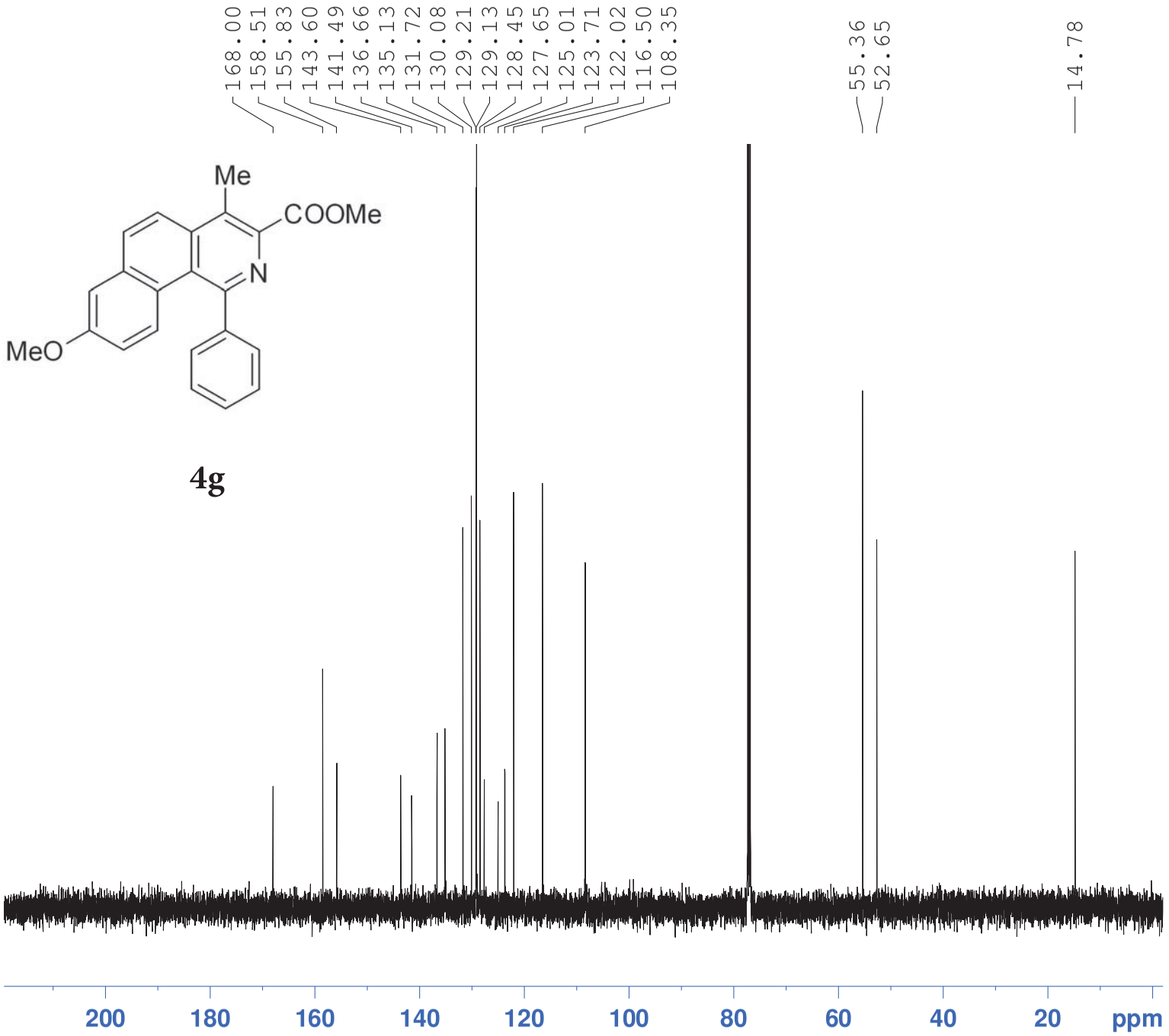
WH-7-40
C13CPD CDCl3

NAME	XB20140619
EXPNO	5
PROCNO	1
Date_	20140619
Time	11.28
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	225
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	322.5
DW	16.650 usec
DE	6.00 usec
TE	297.3 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



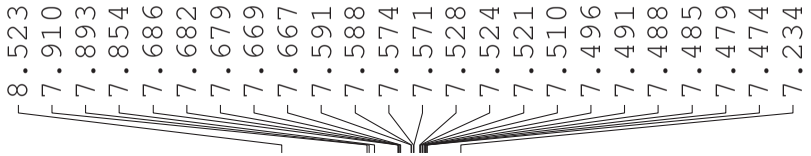
WH-7-43
PROTON CDCl3

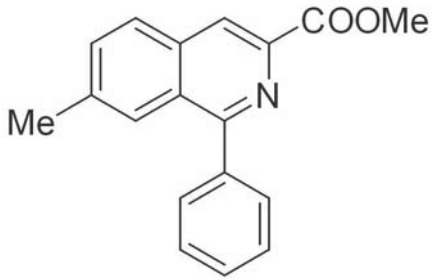
NAME	XB20140624
EXPNO	17
PROCNO	1
Date_	20140624
Time	10.37
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	128
DW	48.400 usec
DE	6.00 usec
TE	297.3 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300123 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



WH-7-43
C13CPD CDCl3

NAME	XB20140624
EXPNO	18
PROCNO	1
Date_	20140624
Time	10.46
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	128
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	406.4
DW	16.650 usec
DE	6.00 usec
TE	298.5 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



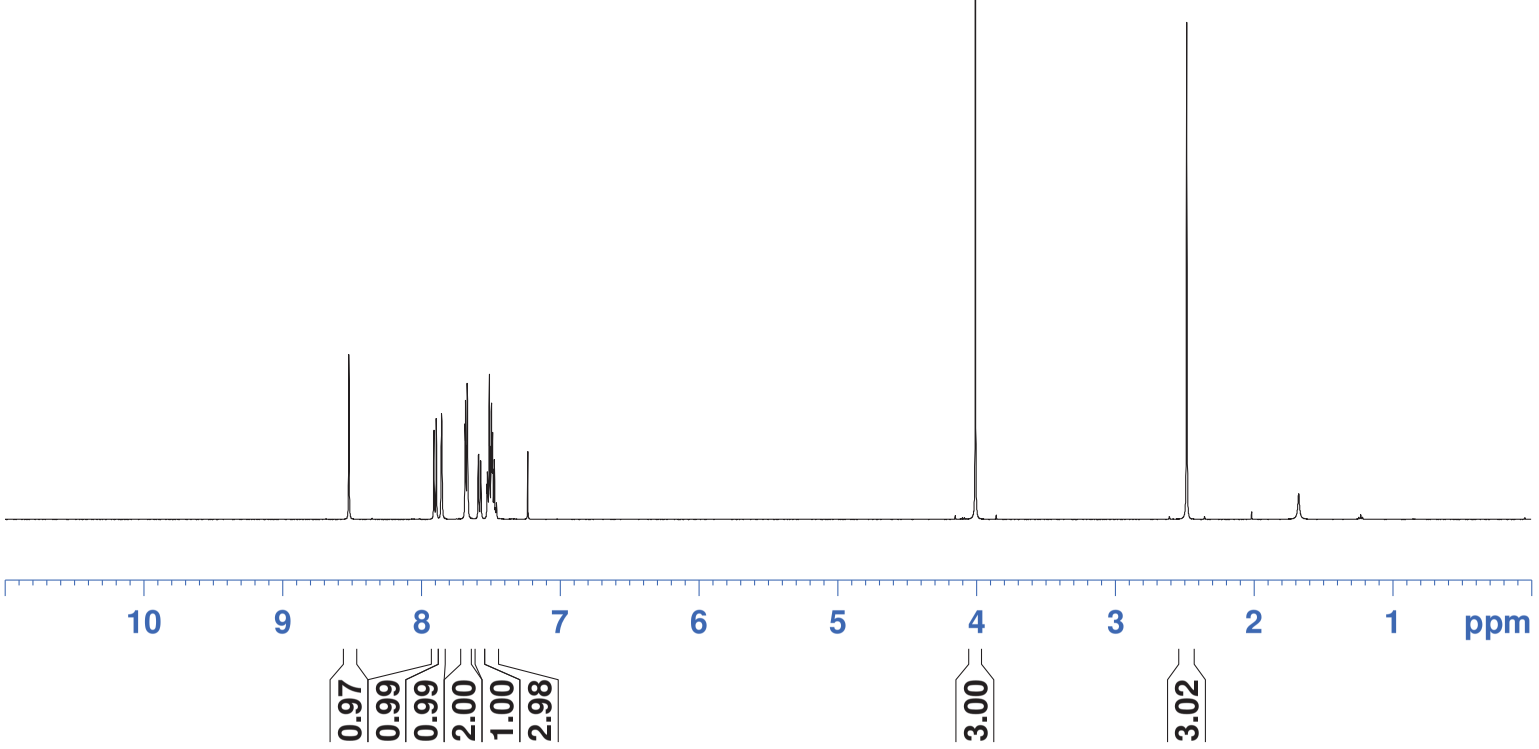


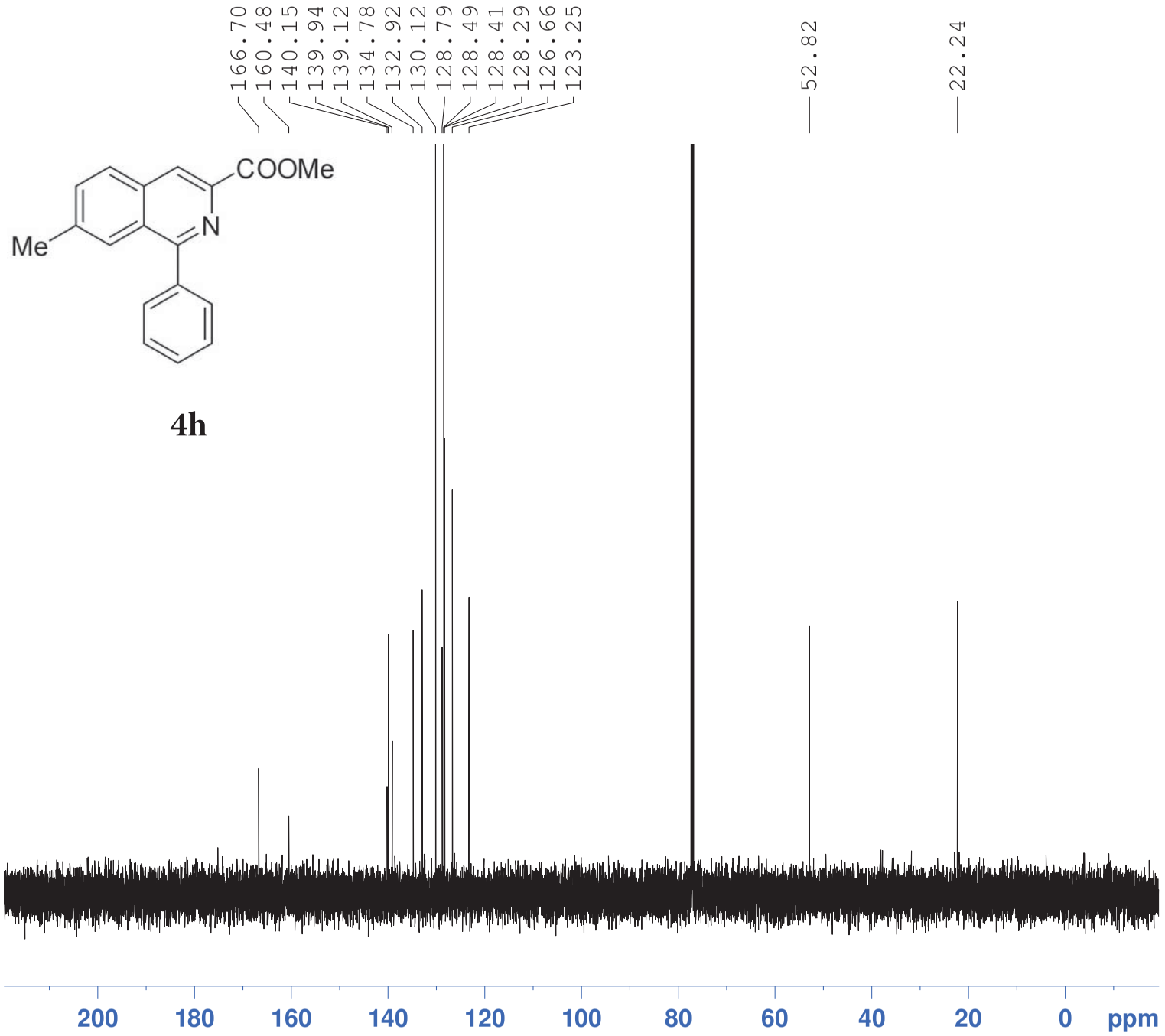
4h

WH-7-37
PROTON CDCl3

NAME	XB20140616
EXPNO	10
PROCNO	1
Date_	20140616
Time	10.05
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	287.4
DW	48.400 usec
DE	6.00 usec
TE	296.6 K
D1	1.00000000 sec
TD0	1

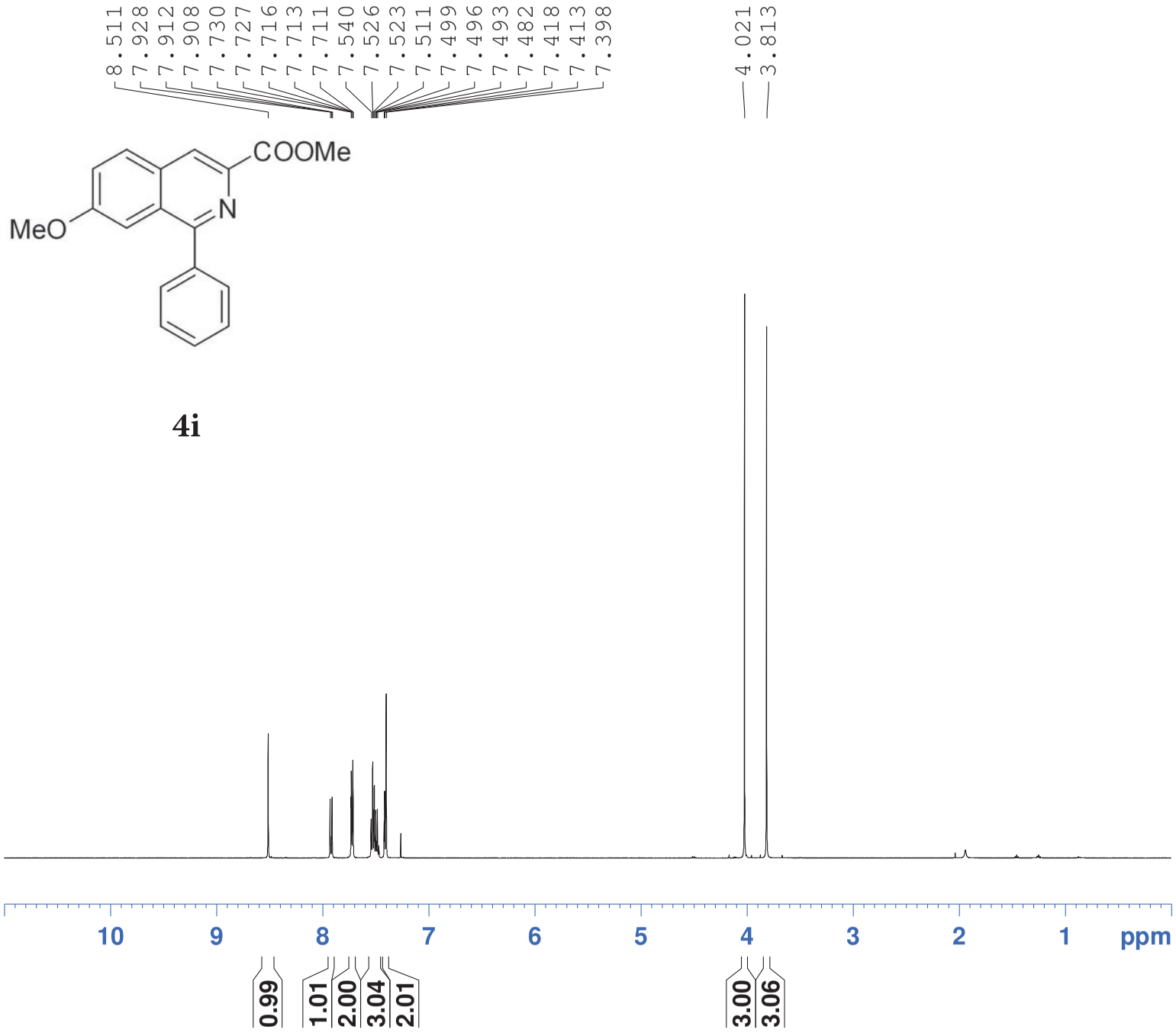
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300258 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00





WH-7-37
C13CPD CDCl3

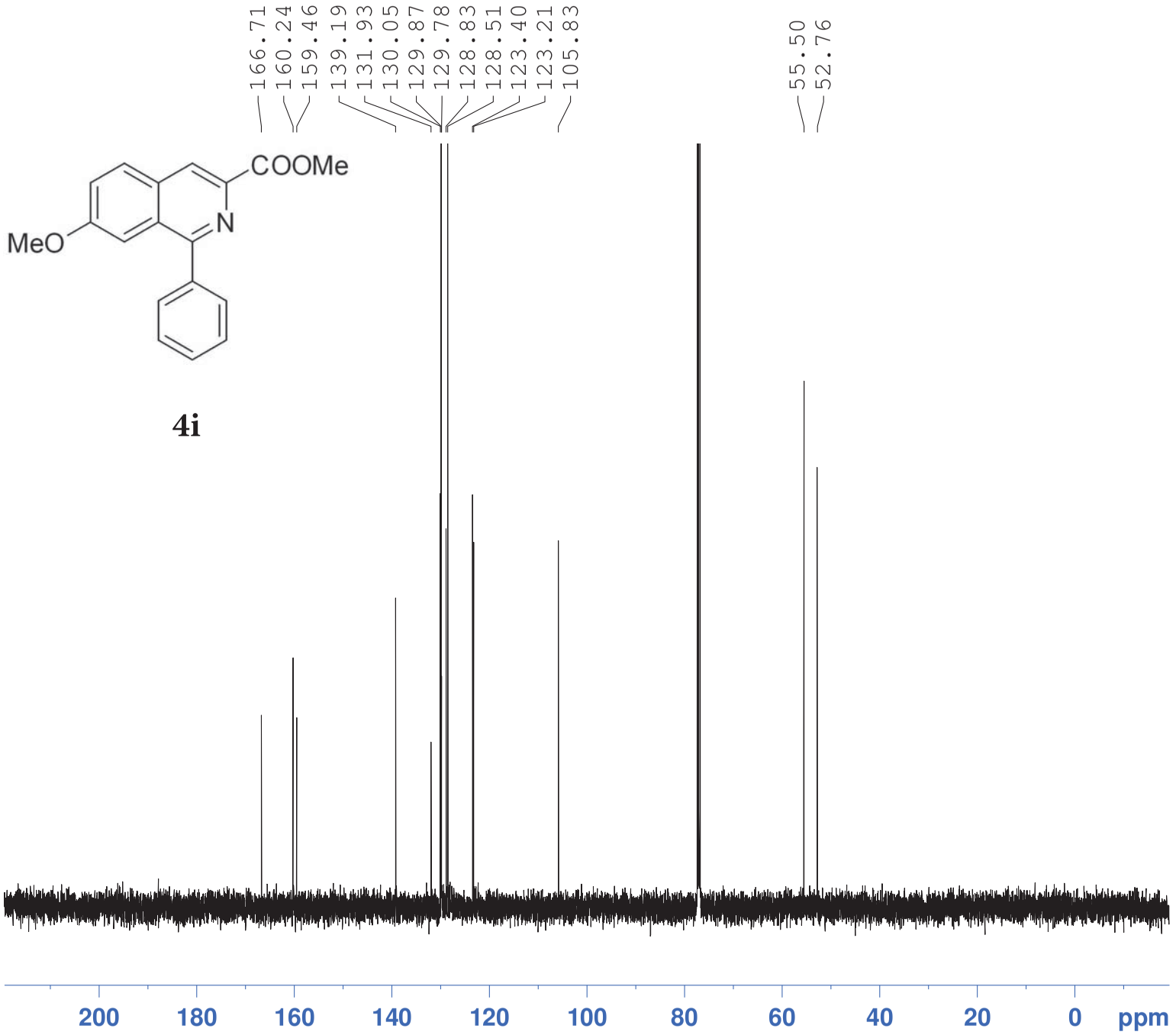
NAME	XB20140616
EXPNO	11
PROCNO	1
Date_	20140616
Time	10.10
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	213
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	181
DW	16.650 usec
DE	6.00 usec
TE	297.6 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40



4i

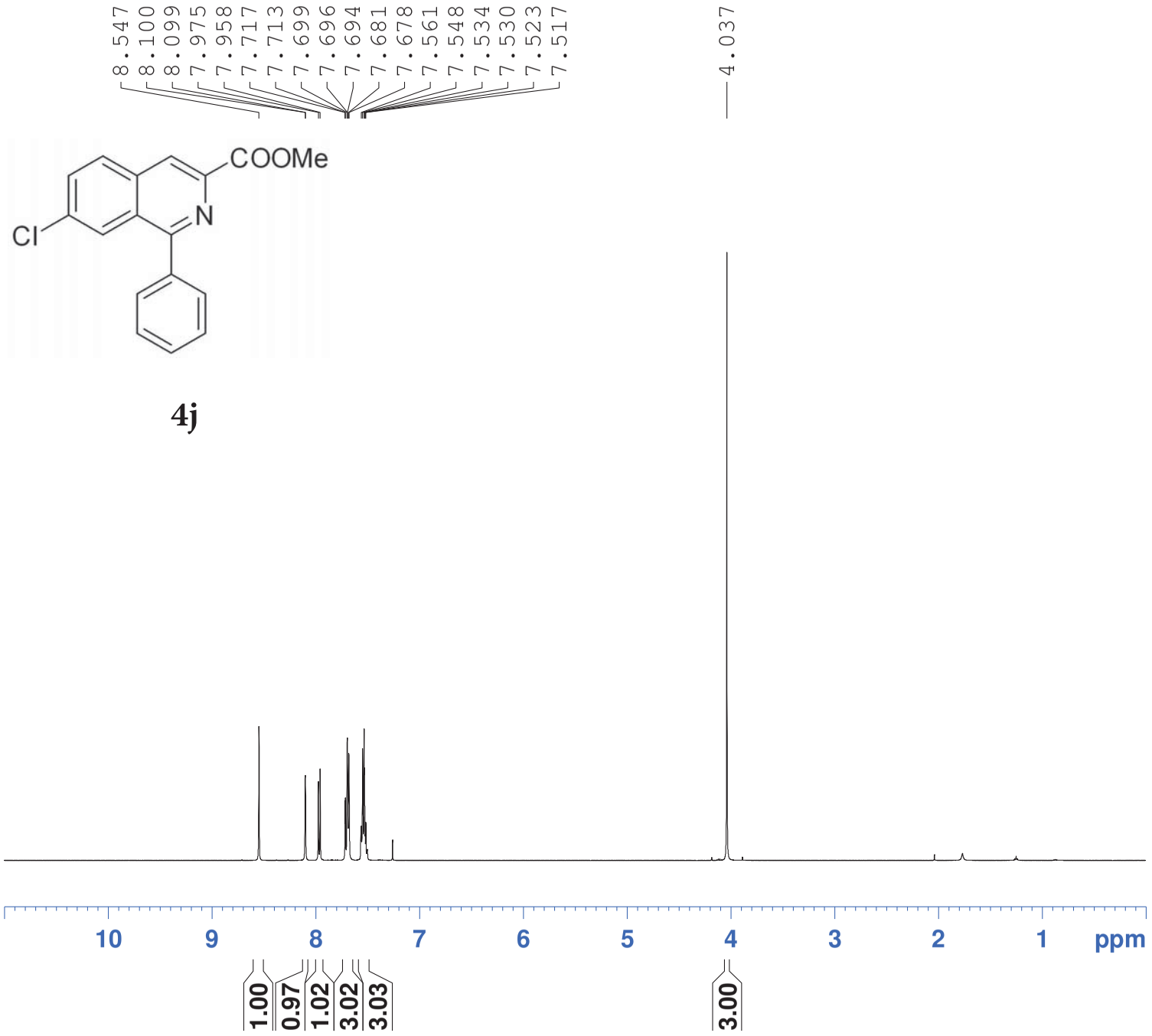
WH-7-38
PROTON CDCl3

NAME	XB20140616
EXPNO	12
PROCNO	1
Date_	20140616
Time	10.23
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	161.3
DW	48.400 usec
DE	6.00 usec
TE	296.7 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300126 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



WH-7-38
C13CPD CDCl3

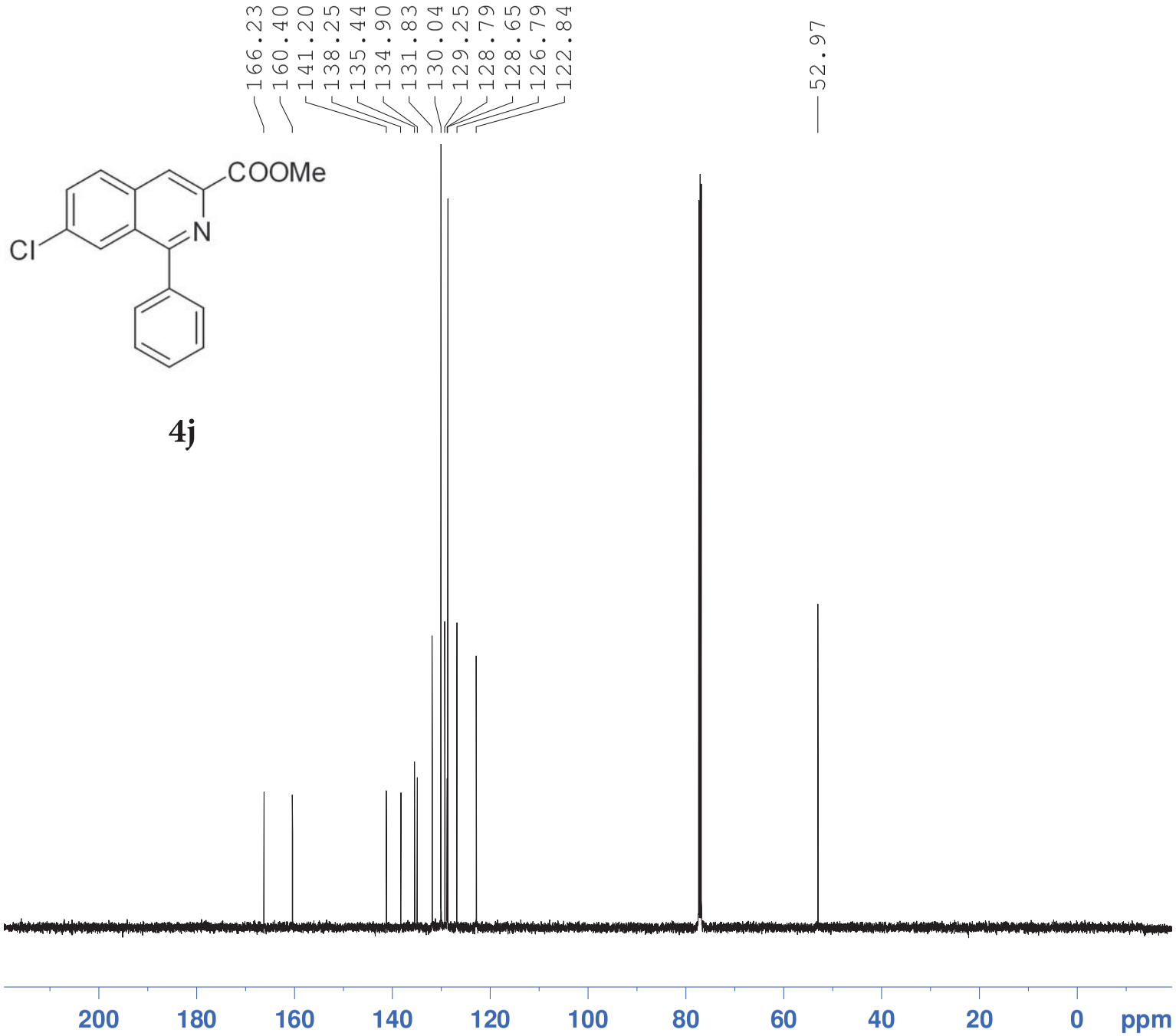
NAME	XB20140616
EXPNO	13
PROCNO	1
Date_	20140616
Time	10.29
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	110
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	256
DW	16.650 usec
DE	6.00 usec
TE	297.7 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



4j

WH-7-33
PROTON CDCl3

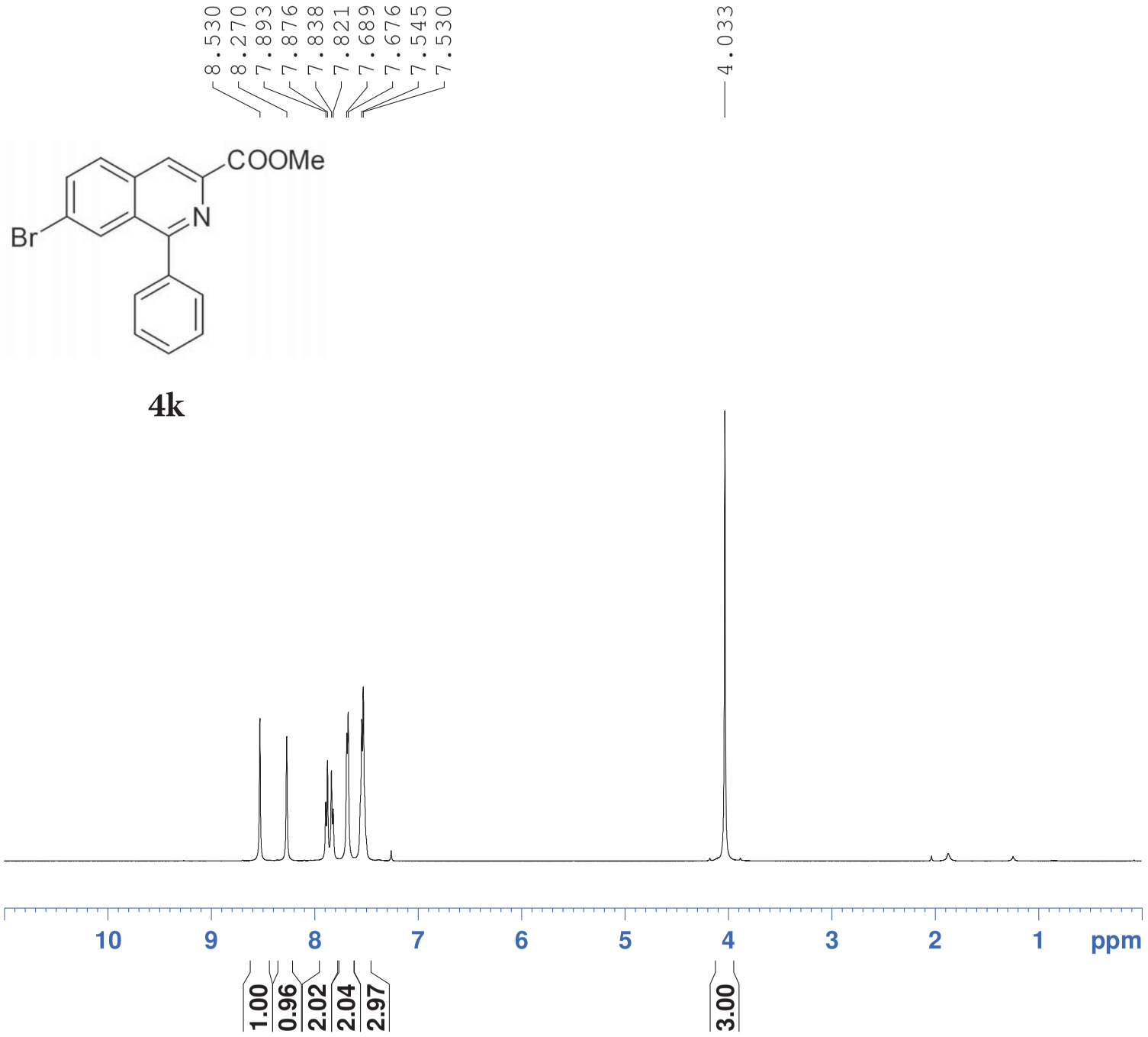
NAME	XB20140616
EXPNO	8
PROCNO	1
Date_	20140616
Time	9.51
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	181
DW	48.400 usec
DE	6.00 usec
TE	296.6 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300126 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



4j

WH-7-33
C13CPD CDCl3

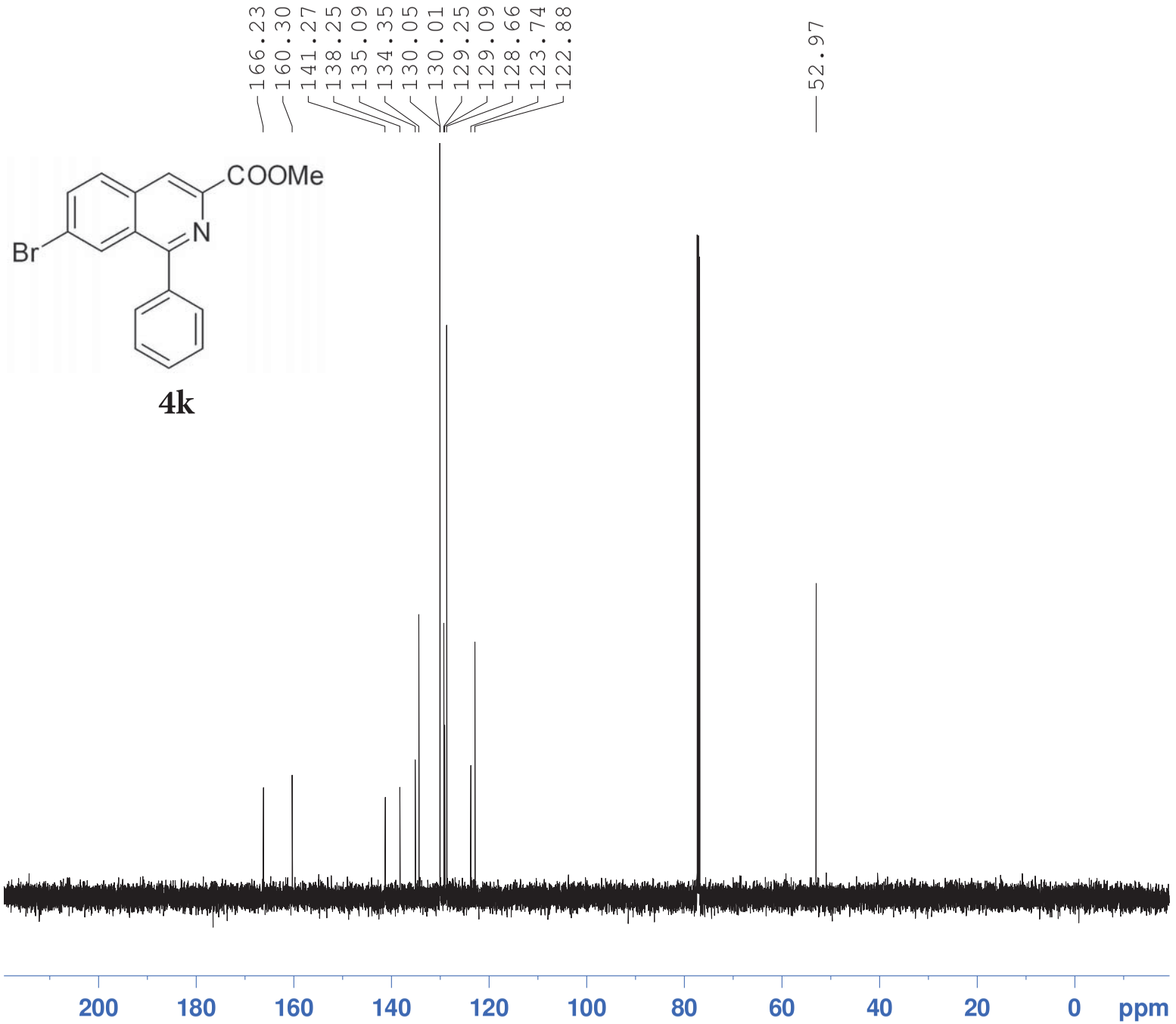
NAME	XB20140626
EXPNO	2
PROCNO	1
Date_	20140626
Time	9.47
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	440
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	228.1
DW	16.650 usec
DE	6.00 usec
TE	298.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



WH-7-32
PROTON CDCl3

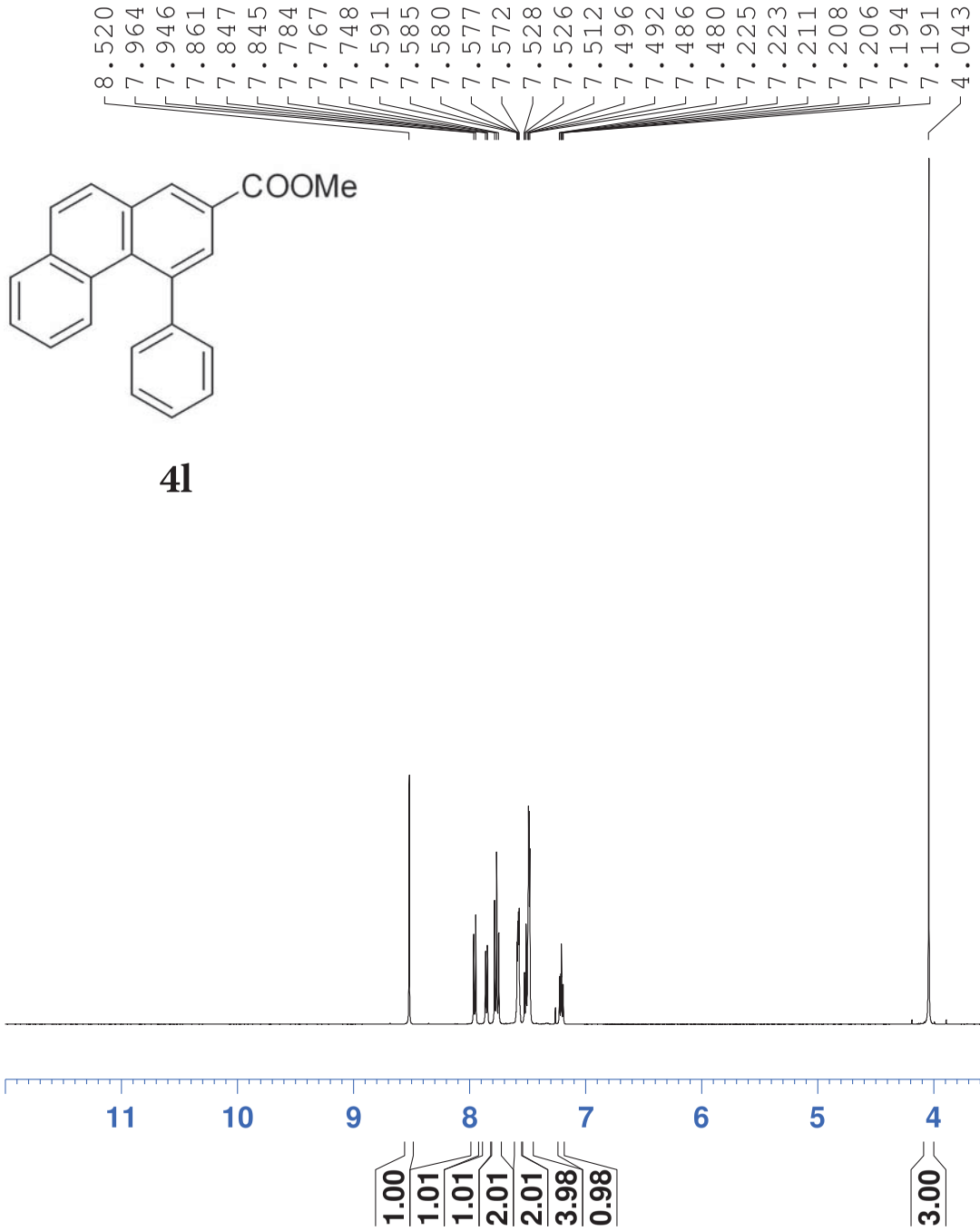
NAME	XB20140616
EXPNO	6
PROCNO	1
Date_	20140616
Time	9.35
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	143.7
DW	48.400 usec
DE	6.00 usec
TE	296.4 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300120 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



WH-7-32
C13CPD CDCl3

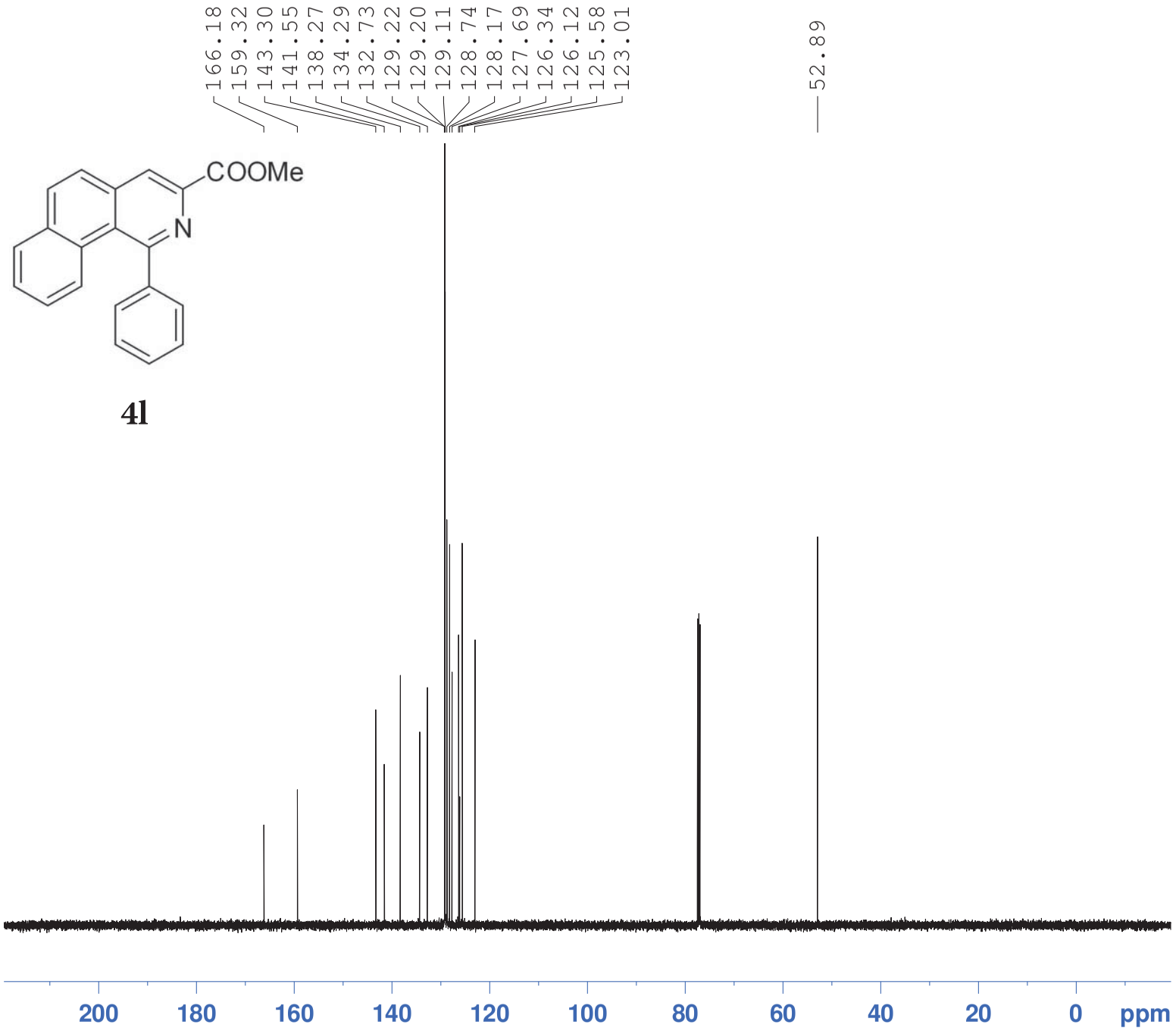
NAME	XB20140616
EXPNO	7
PROCNO	1
Date_	20140616
Time	9.37
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	152
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	406.4
DW	16.650 usec
DE	6.00 usec
TE	296.9 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40



4l

WH-7-30
PROTON CDCl3

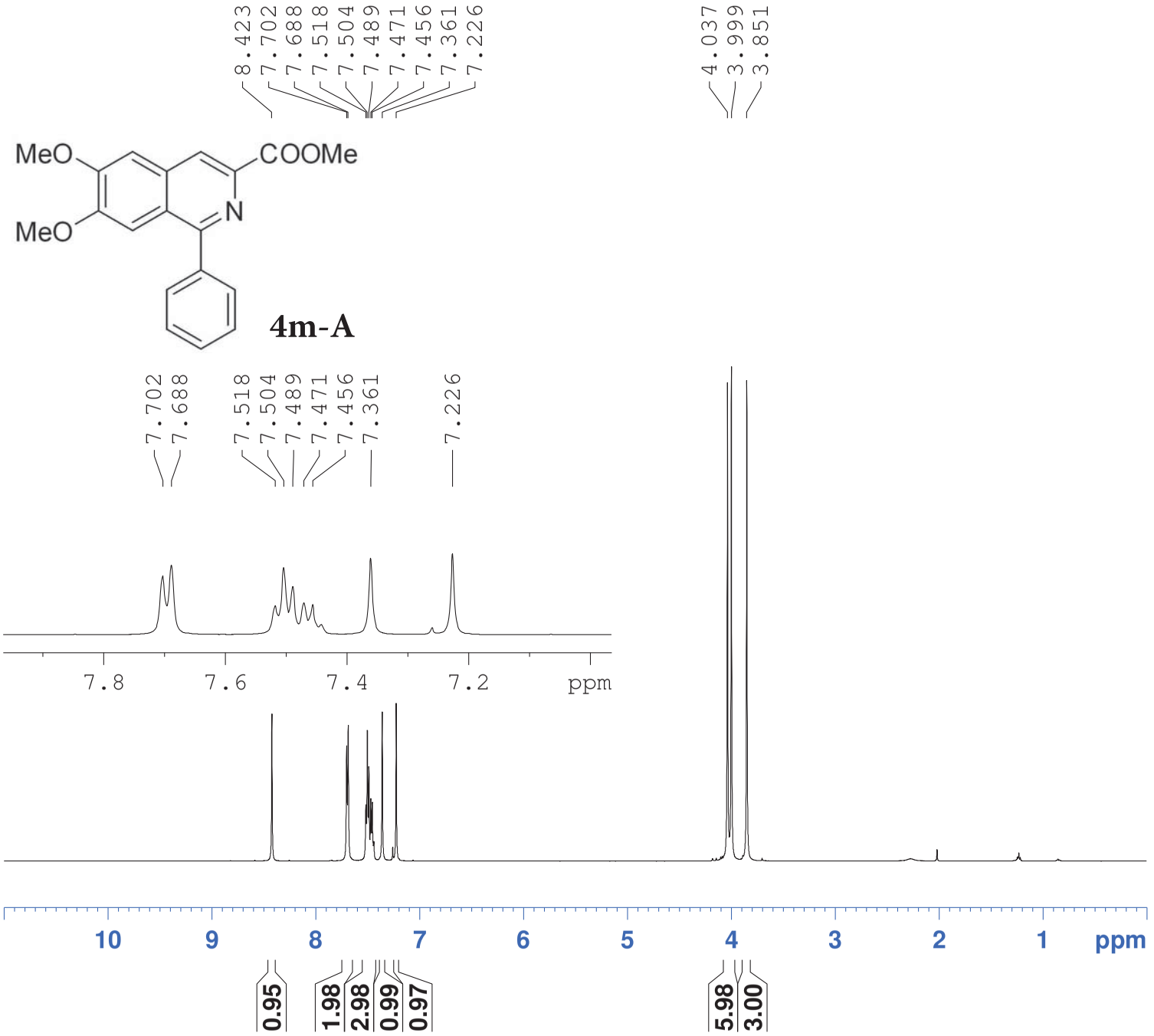
NAME	XB20140613
EXPNO	8
PROCNO	1
Date_	20140613
Time	11.47
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	80.6
DW	48.400 usec
DE	6.00 usec
TE	296.7 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300123 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



4l

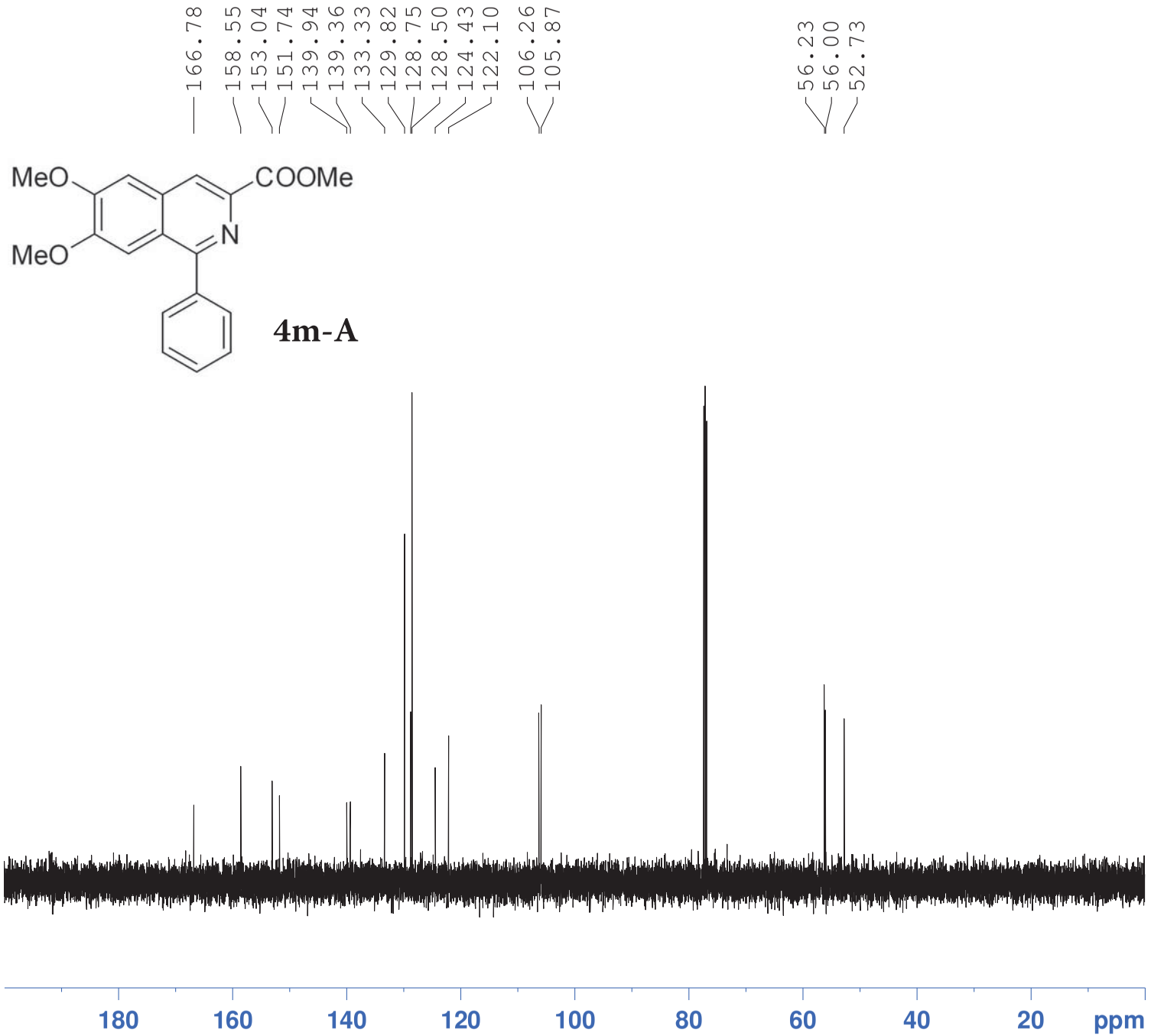
WH-7-30
C13CPD CDCl3

NAME	XB20140624
EXPNO	20
PROCNO	1
Date_	20140624
Time	11.00
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	128
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	256
DW	16.650 usec
DE	6.00 usec
TE	298.3 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	0.20 Hz
GB	0
PC	1.40



WH-7-31-2
PROTON CDCl3 I

NAME	XB20140616
EXPNO	4
PROCNO	1
Date_	20140616
Time	9.24
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	114
DW	48.400 usec
DE	6.00 usec
TE	296.4 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300123 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



WH-7-31-2
C13CPD CDCl3

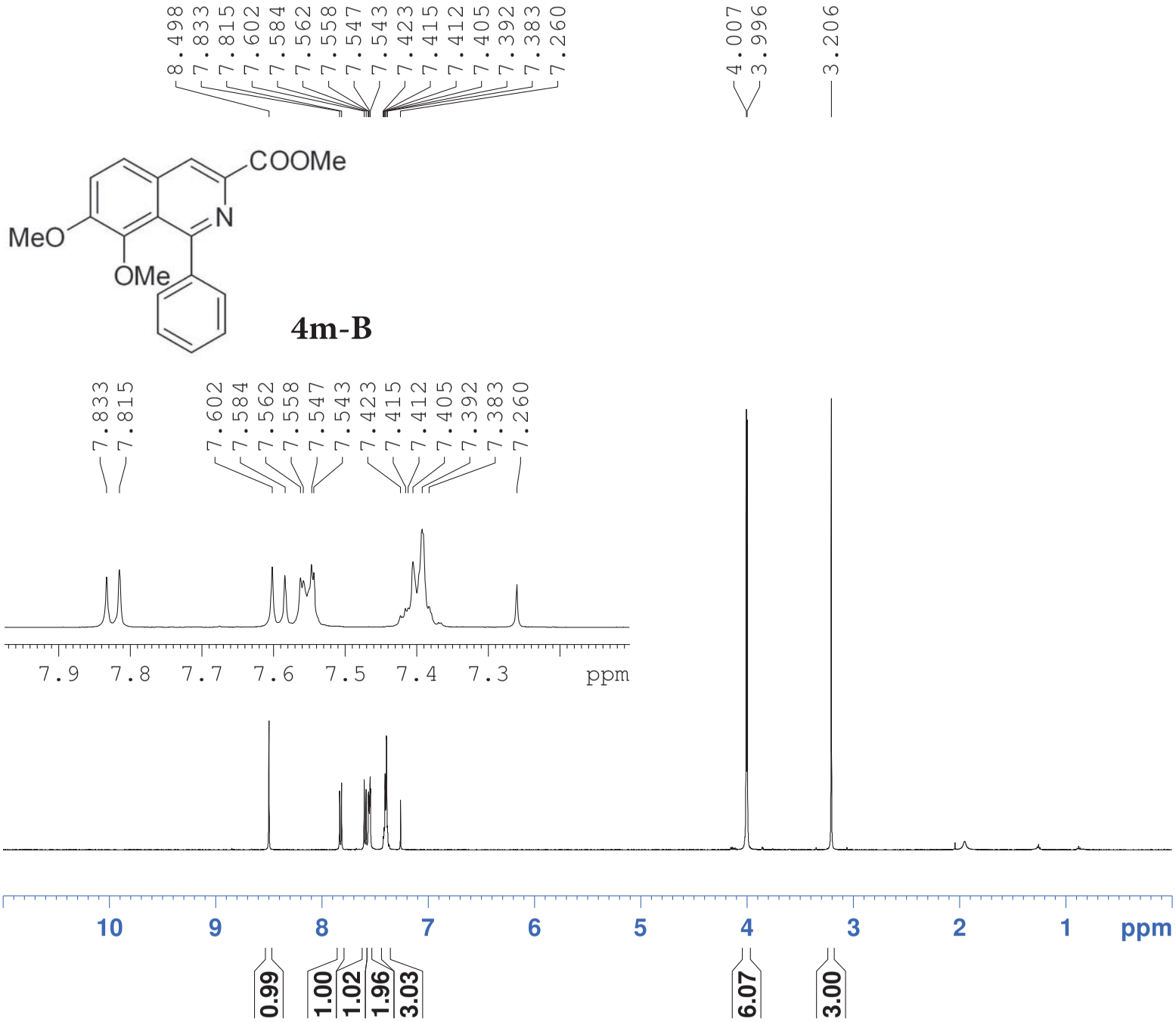
NAME	XB20140616
EXPNO	5
PROCNO	1
Date_	20140616
Time	9.27
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	53
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	114
DW	16.650 usec
DE	6.00 usec
TE	297.1 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40

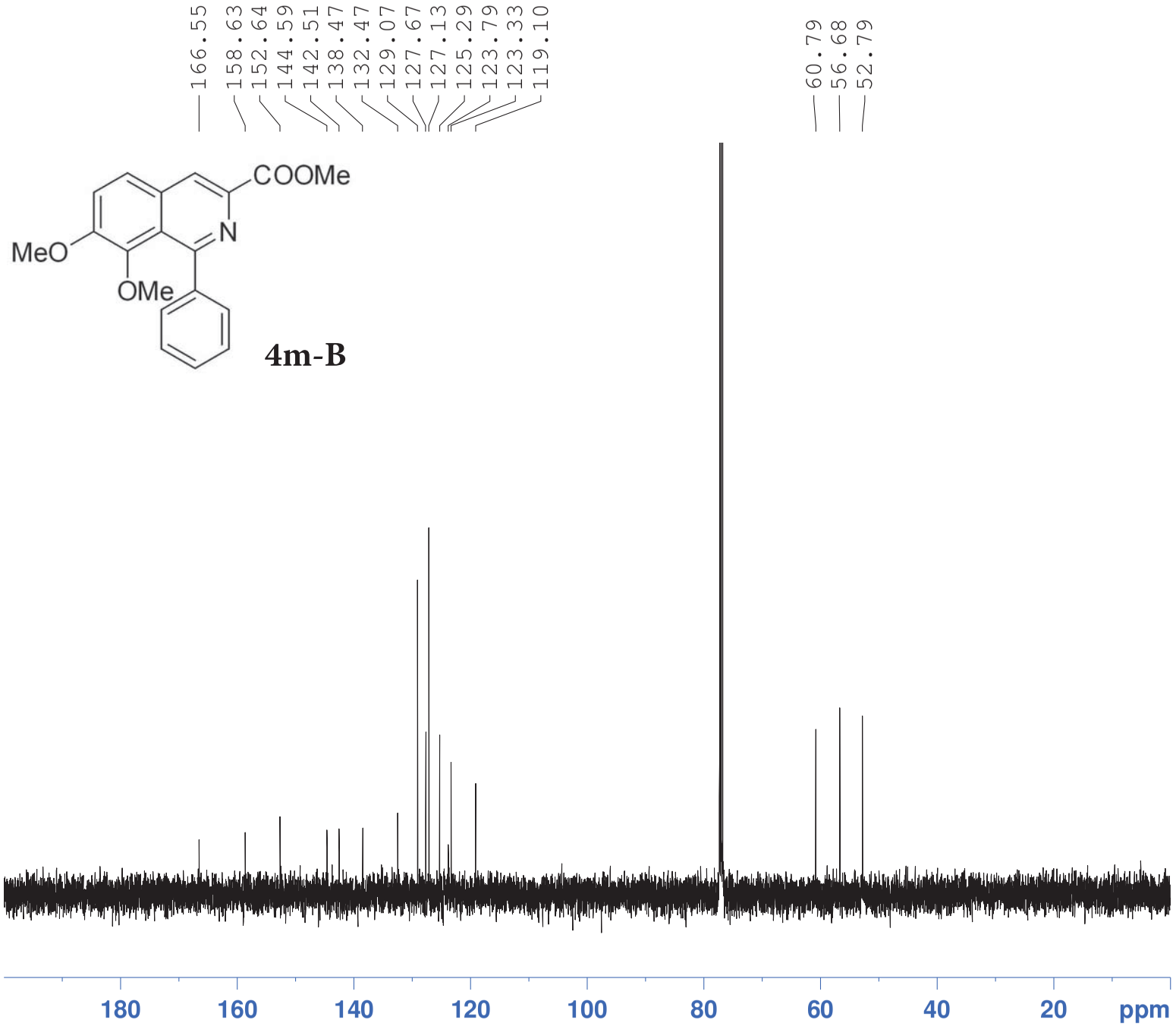
4m-B

WH-7-31-1
PROTON CDCl3

NAME	XB20140616
EXPNO	1
PROCNO	1
Date_	20140616
Time	9.08
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	322.5
DW	48.400 usec
DE	6.00 usec
TE	296.2 K
D1	1.00000000 sec
TD0	1

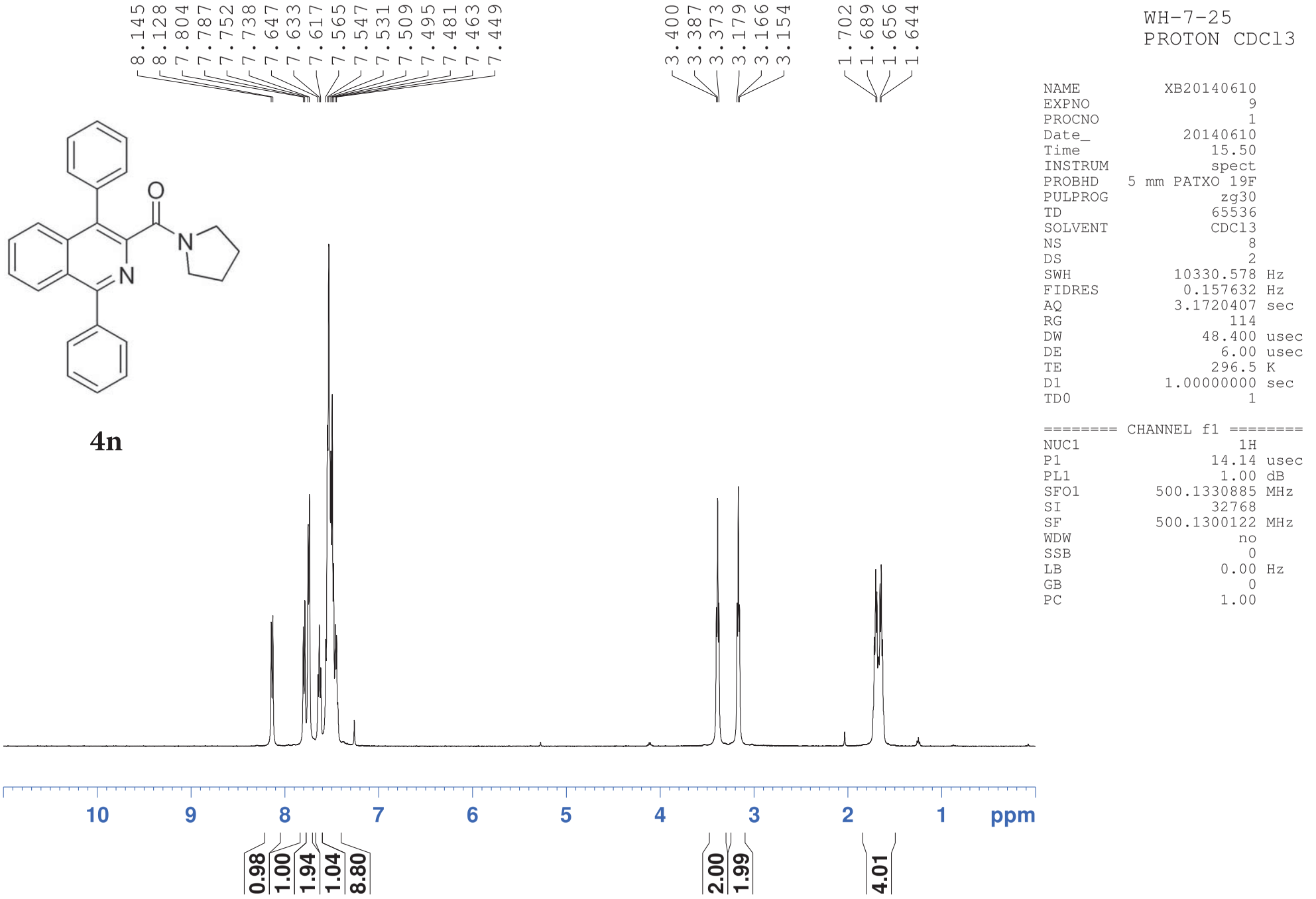
======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300126 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00





WH-7-31-1
C13CPD CDCl3 I

NAME	XB20140616
EXPNO	3
PROCNO	1
Date_	20140616
Time	9.13
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	123
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	228.1
DW	16.650 usec
DE	6.00 usec
TE	296.8 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

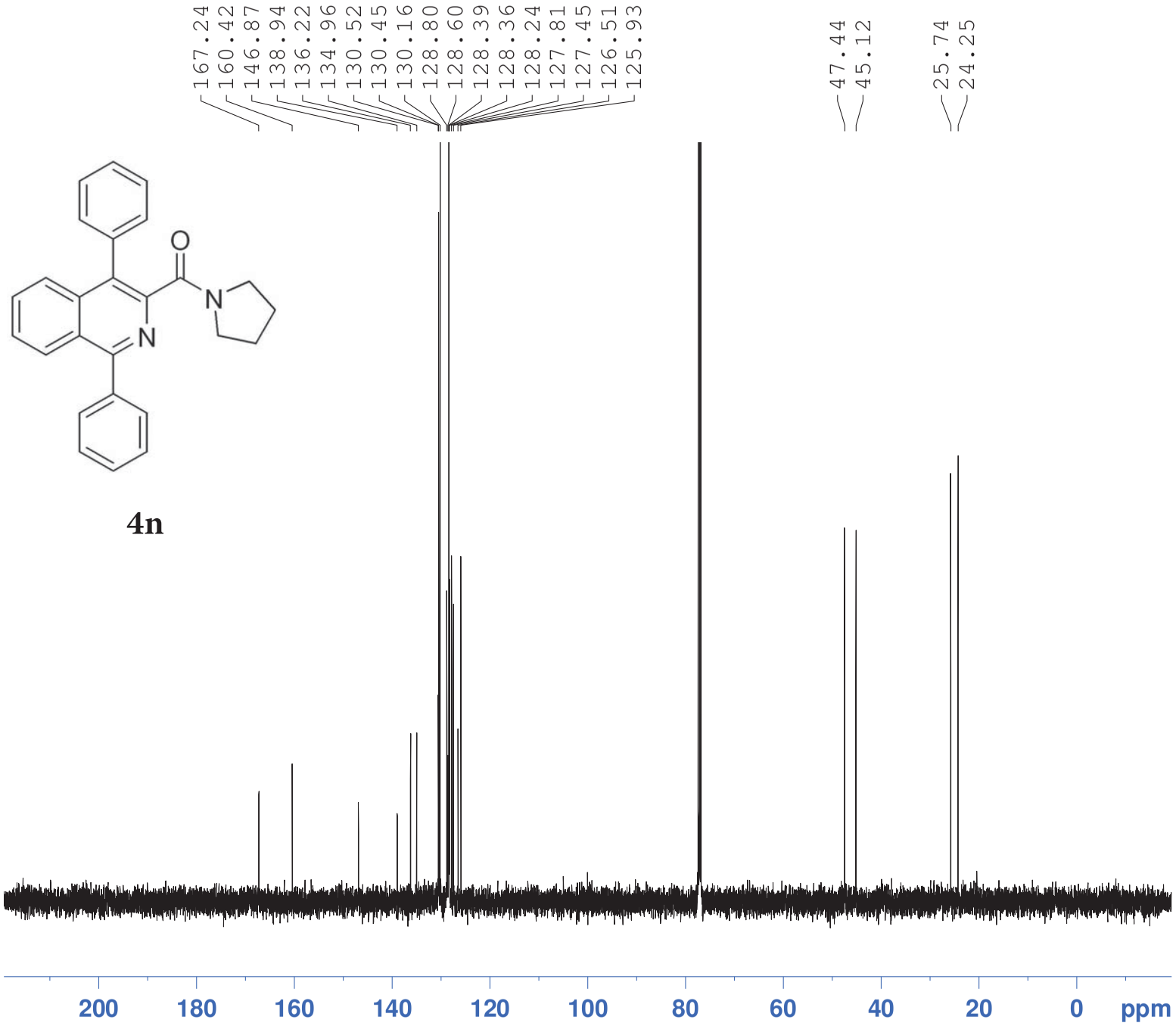


WH-7-25
PROTON CDCl3

NAME	XB20140610
EXPNO	9
PROCNO	1
Date_	20140610
Time	15.50
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	114
DW	48.400 usec
DE	6.00 usec
TE	296.5 K
D1	1.00000000 sec
TD0	1

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

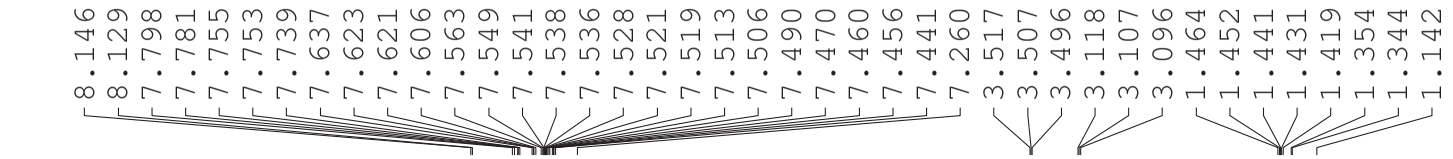
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300122 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

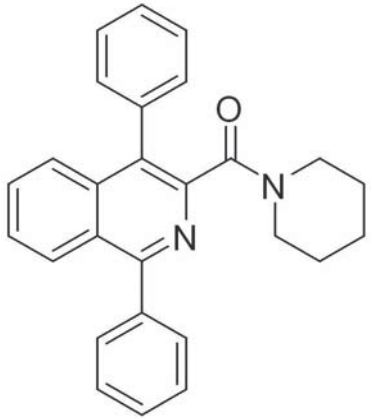


S160

WH-7-25
C13CPD CDCl3

NAME	XB20140610
EXPNO	10
PROCNO	1
Date_	20140610
Time	15.54
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	137
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	181
DW	16.650 usec
DE	6.00 usec
TE	297.4 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40





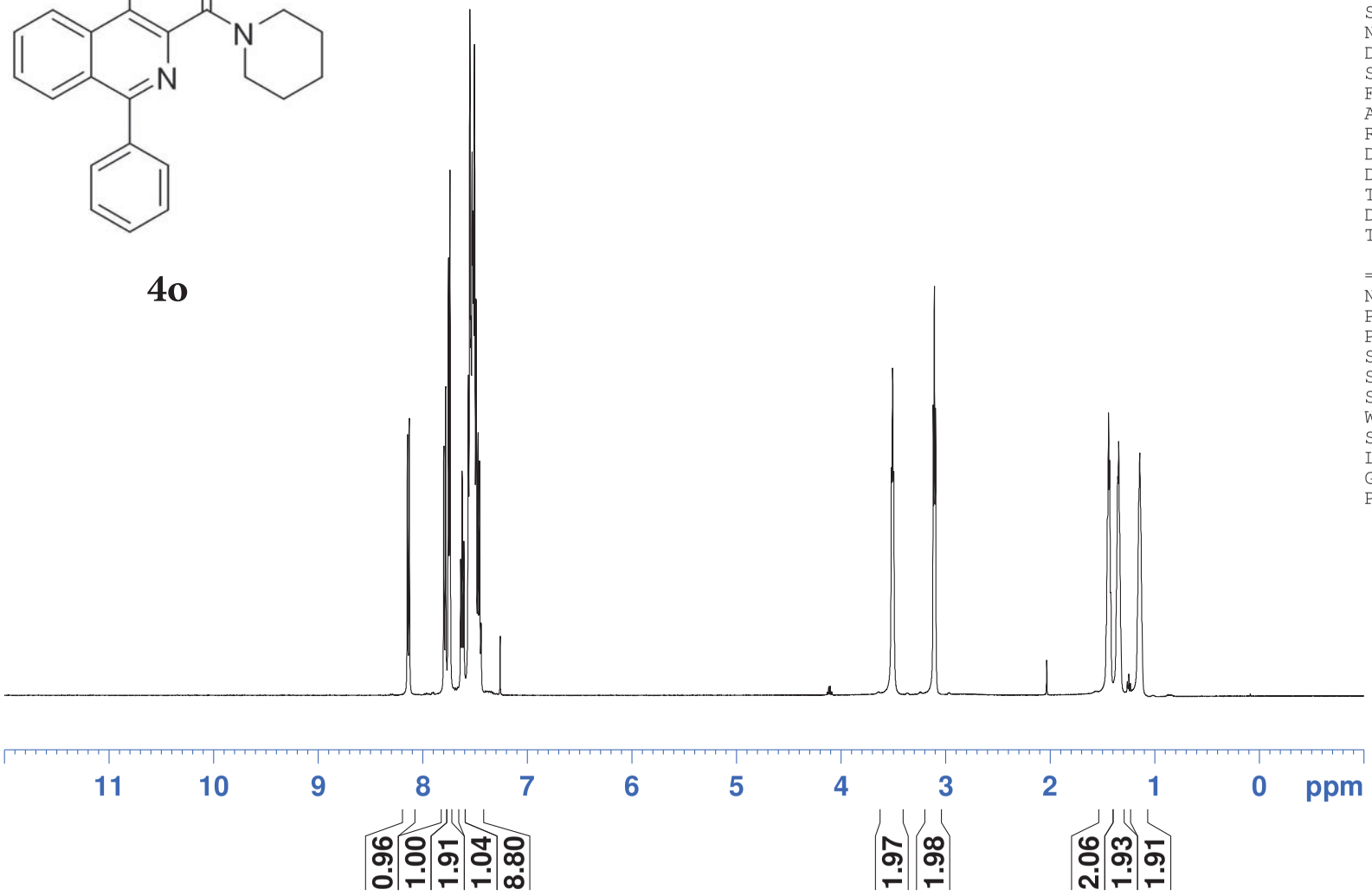
4o

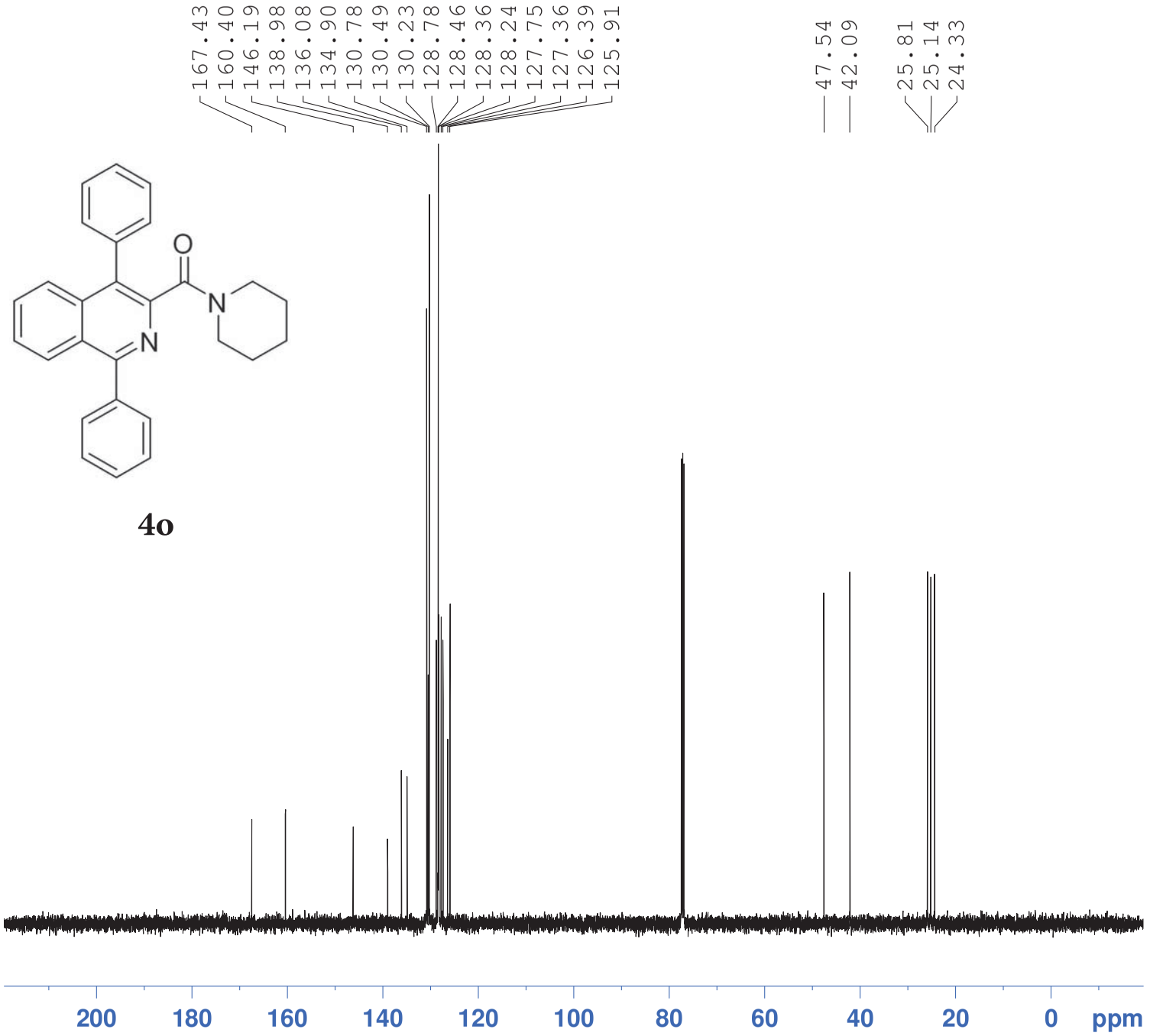
WH-7-14
PROTON CDCl3

NAME	XB20140610
EXPNO	7
PROCNO	1
Date_	20140610
Time	15.37
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	2
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	71.8
DW	48.400 usec
DE	6.00 usec
TE	296.5 K
D1	1.00000000 sec
TD0	1

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

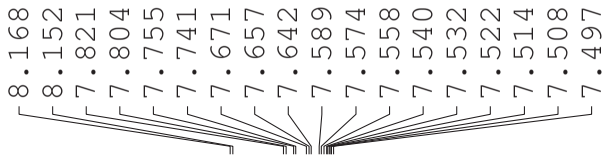
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300126 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

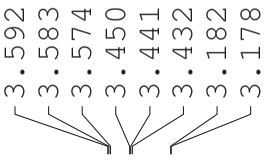




WH-7-14
C13CPD CDCl3

NAME	XB20140610
EXPNO	8
PROCNO	1
Date_	20140610
Time	15.41
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	108
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	322.5
DW	16.650 usec
DE	6.00 usec
TE	297.3 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

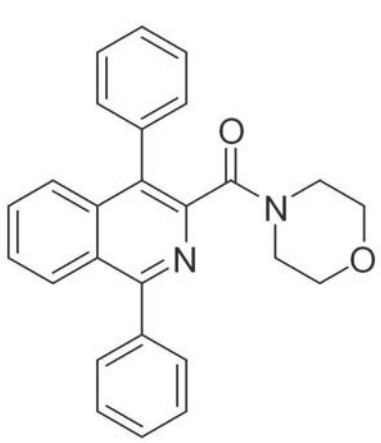




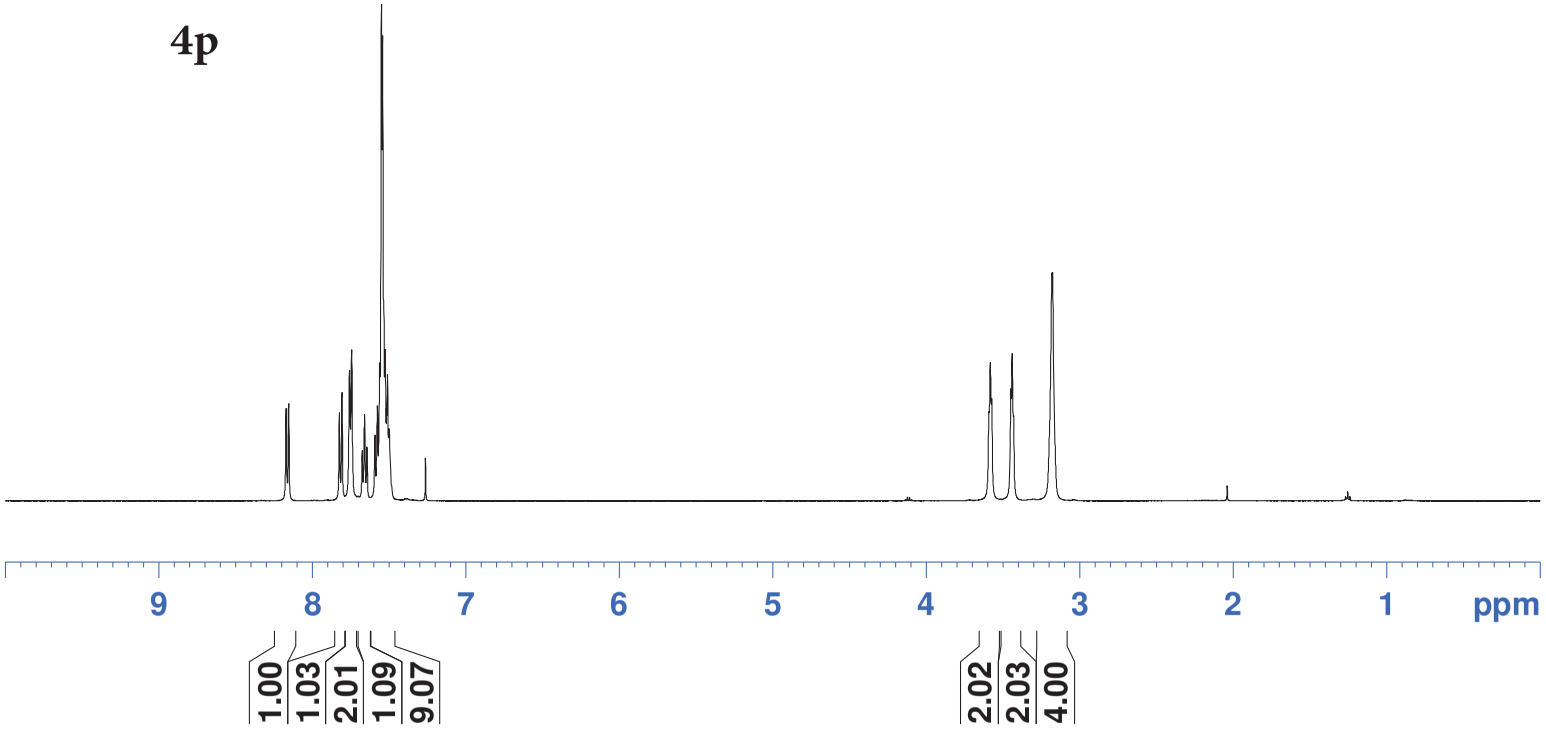
WH-7-6
PROTON CDCl3

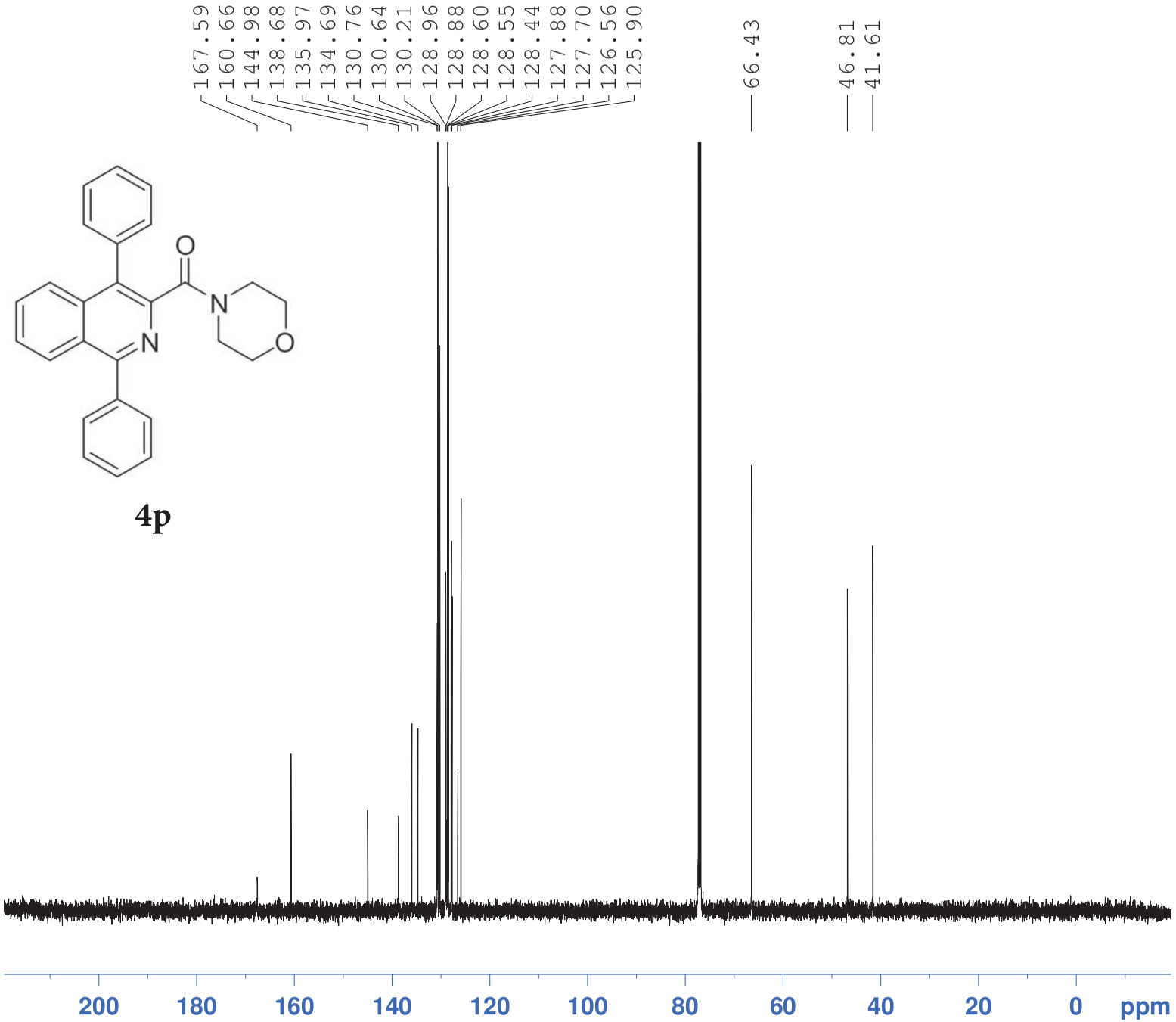
NAME	XB20140603
EXPNO	3
PROCNO	1
Date_	20140603
Time	13.31
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	143.7
DW	48.400 usec
DE	6.00 usec
TE	295.7 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300126 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



4p

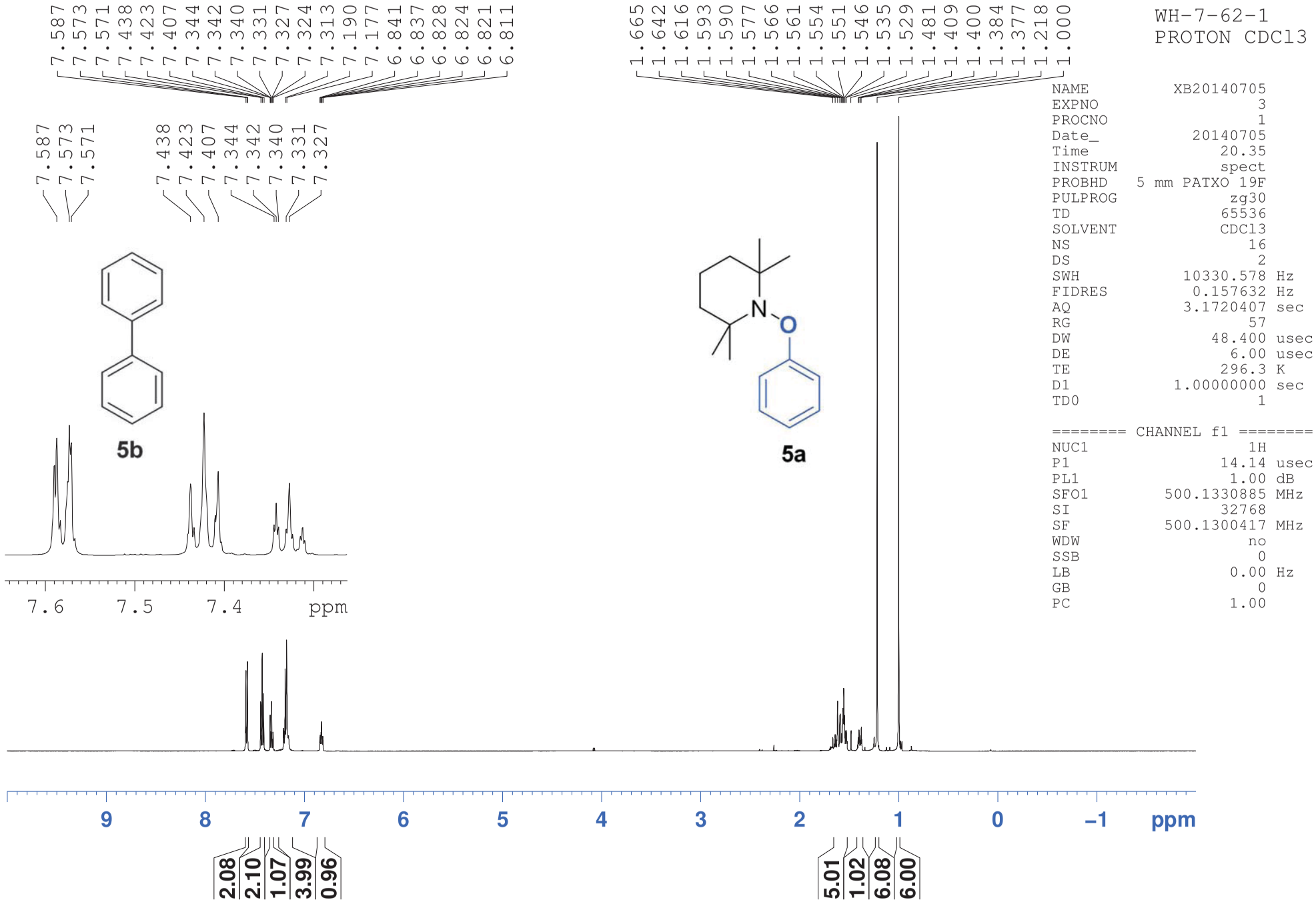


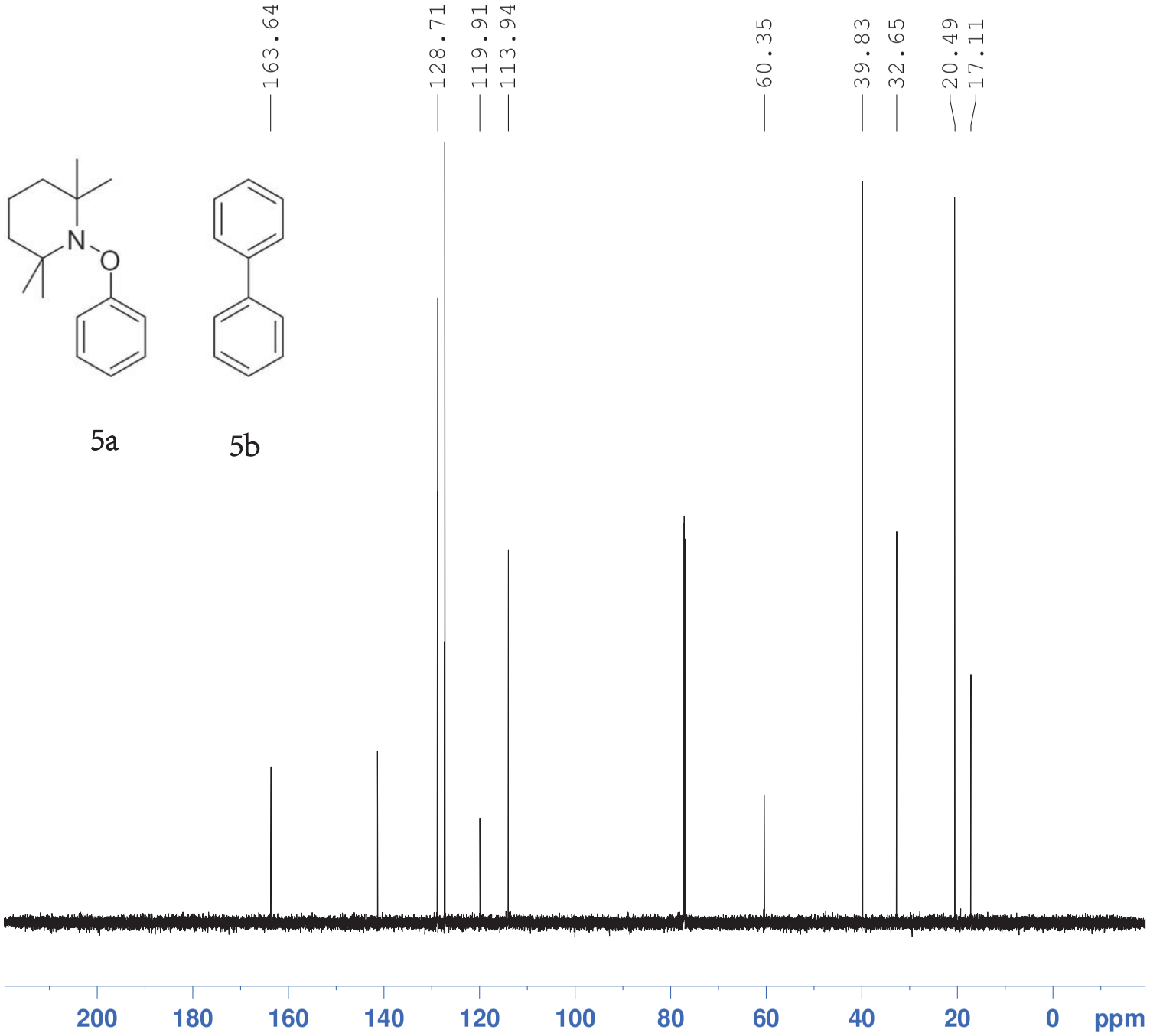


4p

WH-7-6
C13CPD CDCl3 D

NAME	XB20140604
EXPNO	8
PROCNO	1
Date_	20140604
Time	13.13
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	512
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	228.1
DW	16.650 usec
DE	6.00 usec
TE	297.4 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40


7.587
7.573
7.571
7.438
7.423
7.407
7.344
7.342
7.340
7.331
7.327
7.324
7.313
7.190
7.177
6.841
6.837
6.828
6.824
6.821
6.811
1.665
1.642
1.616
1.593
1.590
1.577
1.566
1.561
1.554
1.551
1.546
1.535
1.529
1.481
1.409
1.400
1.384
1.377
1.218
1.000
WH-7-62-1
PROTON CDCl3
NAME XB20140705
EXPNO 3
PROCNO 1
Date_ 20140705
Time 20.35
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 57
DW 48.400 usec
DE 6.00 usec
TE 296.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.14 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300417 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
5b
5a
N
O
7.6
7.5
7.4
ppm
9
8
7
6
5
4
3
2
1
0
−1
ppm
2.08
2.10
1.07
3.99
0.96
5.01
1.02
6.08
6.00



WH-7-62-1
C13CPD CDCl3

NAME	XB20140705
EXPNO	5
PROCNO	1
Date_	20140705
Time	20.46
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	128
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	128
DW	16.650 usec
DE	6.00 usec
TE	297.5 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	-0.50 dB
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.05 dB
PL13	16.50 dB
SFO2	500.1320005 MHz
SI	32768
SF	125.7577890 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40