Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.


# Manganese(II)-catalyzed modular synthesis of isoquinolines from vinyl isocyanides and hydrazines

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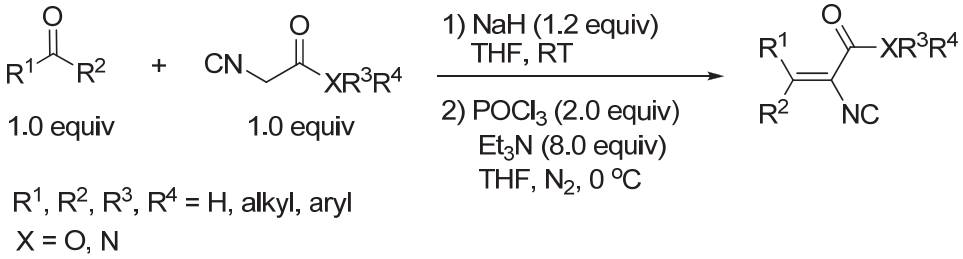
# Supporting Information

## CONTENTS:

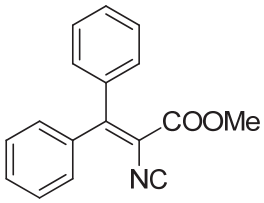
## 1. General Information

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 ($\delta$ = 7.26 ppm) or TMS ($\delta$ = 0.00 ppm) for $^{1}H$ NMR, chloroform ($\delta$ = 77.16 ppm) for $^{13}C$ NMR, and $C_6F_6$ ($\delta$ = -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. Silica gel plate GF254 was used for thin layer chromatography (TLC) and silica gel H or 300-400 mesh was used for flash column chromatography. Yields refer to chromatographically and spectroscopically pure compounds, unless otherwise indicated.

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

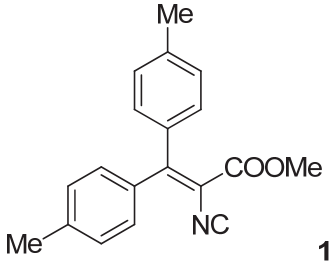



**General Procedure**[1]: A mixture of ketone or aldehyde (10.0 mmol) and isocyanide (10.0 mmol) in THF (10.0 mL) was added dropwise to a suspension of NaH (12.0 mmol, 60% in oil) in THF (10.0 mL) at room temperature. After stirring for 2 h at room temperature, 10% AcOH was added to the mixture at 0 °C until there was 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 organic layer 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 the addition was completed. Then the mixture was quenched by saturated $Na_2CO_3$ aqueous 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 to give **1a-1m**.




**1a**

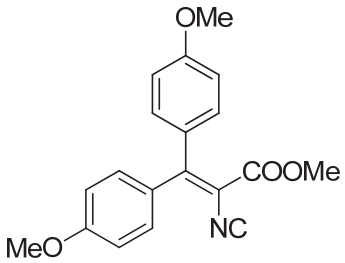
**Methyl 2-isocyano-3,3-diphenylacrylate (1a)**[1]**:** White solid (62% yield for 2 steps). M.p. 104–105 °C. $^1$H NMR ($CDCl_3$, 500 MHz): δ 7.44–7.38 (m, 4H), 7.38–7.34 (m, 4H), 7.16–7.12 (m, 2H), 3.69 (s, 3H); $^{13}$C NMR ($CDCl_3$, 125 MHz): δ 169.78, 162.28, 154.60, 137.81, 137.39, 130.31, 129.88, 129.59, 129.09, 128.46, 128.25, 52.92.




**1a'**

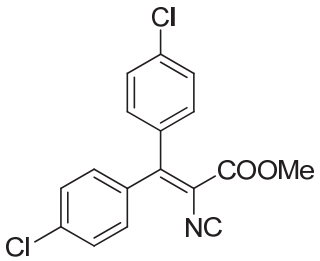
**Methyl 2-isocyano-3,3-di-*p*-tolylacrylate (1a')**[1]**:** Pale yellow solid (64% yield for 2 steps). M.p. 97–99 °C. $^1$H NMR ($CDCl_3$, 500 MHz): δ 7.25 (d, *J* = 7.5 Hz, 2H), 7.20

(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), 2.38–2.39 (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.



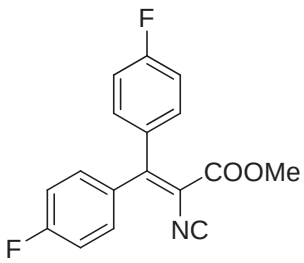
**1b**

**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**

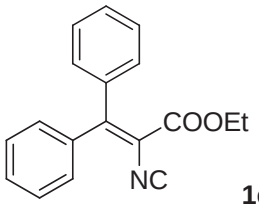
**Methyl 3,3-bis(4-chlorophenyl)-2-isocyanoacrylate (1c)**[1]**:** Pale yellow solid (68% yield for 2 steps). M.p. 111-112 °C. IR (KBr, cm$^{-1}$): 2117.1, 1734.5, 1580.0, 1484.5, 1246.2, 1083.5, 827.4, 770.8. $^1$H NMR ($CDCl_3$, 500 MHz): δ 7.37 (td, *J* = 9.5, 2.0 Hz, 2H), 7.32 (td, *J* = 9.5, 2.0 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* (%): 335 (11) [$M^+$ (2×$^{37}$Cl)], 333 (60) [$M^+$ ($^{35}$Cl, $^{37}$Cl)], 331 (90) [$M^+$ (2×$^{35}$Cl)], 300 (47), 296 (44), 237 (100). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{17}H_{12}Cl_2NO_2$: 332.0245; found: 332.0237.



**1d**,

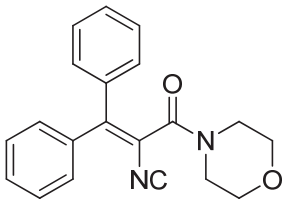
**Methyl 3,3-bis(4-fluorophenyl)-2-isocyanoacrylate (1d)**[1]**:** Pale yellow solid (48% for 2 steps). M.p. 97-98 °C. $^1$H NMR ($CDCl_3$, 500 MHz): δ 7.38-7.33 (m, 2H), 7.15-7.03 (m, 6H), 3.71 (s, 3H); $^{13}$C NMR ($CDCl_3$, 125 MHz): δ 170.38, 163.74 (d, *J* = 251.2 Hz), 163.58 (d, *J* = 250.0 Hz), 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).



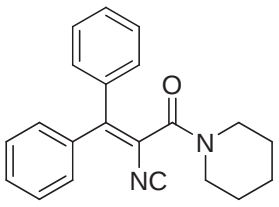

**1e**

**Ethyl 2-isocyano-3,3-diphenylacrylate (1e)**[1]**:** 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), 177 (21), 176 (28). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{18}H_{16}NO_2$: 278.1181; found: 278.1173.



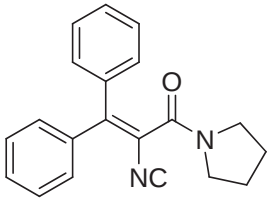

**1f**

**2-Isocyano-1-morpholino-3,3-diphenylprop-2-en-1-one (1f)**[1]**:** 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) [$M^+$], 232 (71), 204 (100), 203 (85), 178 (69). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{20}H_{19}N_2O_2$: 319.1447; found: 319.1436.



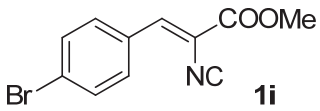

**1g**

**2-Isocyano-3,3-diphenyl-1-(piperidin-1-yl)prop-2-en-1-one (1g)**[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.



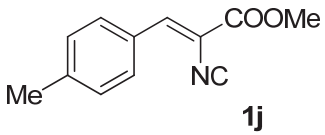

**1h**

**2-Isocyano-3,3-diphenyl-1-(pyrrolidin-1-yl)prop-2-en-1-one (1h)**[1]**:** 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) [$M^+$], 204 (70), 178 (68), 176 (59), 77 (96). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{20}H_{19}N_2O$: 303.1497; found: 303.1488.



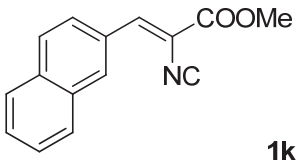

**1i**

**Methyl (*Z*)-3-(4-bromophenyl)-2-isocyanoacrylate (1i)**[1]**:** 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* (%): 267 (31) [$M^+$ ($^{81}$Br)], 265 (33) [$M^+$ ($^{79}$Br)], 207 (32), 186 (100), 127 (94). HRMS (ESI) ([M+H]$^+$) Calcd. For $C_{11}H_9BrNO_2$: 265.9817; found: 265.9805.




**1j**

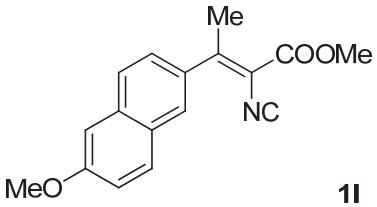
**Methyl (*Z*)-2-isocyano-3-(*p*-tolyl)acrylate (1j)**[1]**:** White solid (32% yield for 2 steps). M.p. 80-81 °C. IR (KBr, $cm^{-1}$): 2115.6, 1727.2, 1613.7, 1282.7, 1201.5, 1088.3, 812.4. $^1$H NMR ($CDCl_3$, 500 MHz): δ 7.77 (d, *J* = 8.0 Hz, 2H), 7.61 (s, 1H), 7.27 (d, *J* = 8.5 Hz, 2H), 3.91 (s, 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) [$M^+$], 170 (25), 143 (100), 142 (40), 140 (24). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{12}H_{12}NO_2$: 202.0868; found: 202.0857.




**1k**

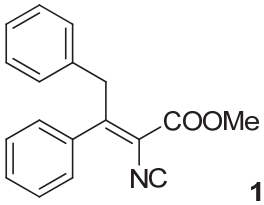
**Methyl (*Z*)-2-isocyano-3-(naphthalen-2-yl)acrylate (1k)**[1]**:** White solid (45% yield for 2 steps). M.p. 120-121°C. $^1$H NMR ($CDCl_3$, 500 MHz): δ 8.31 (s, 1H), 8.01 (dd, *J* = 9.0, 2.0 Hz, 1H), 7.94-7.88 (m, 2H), 7.86 (d, *J* = 8.5 Hz, 1H), 7.80 (s, 1H), 7.59 (td,

*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.



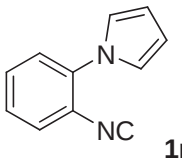

**1l**

**Methyl (*Z*)-2-isocyano-3-(6-methoxynaphthalen-2-yl)but-2-enoate (1l)[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), 2.65 (s, 3H); $^{13}$C NMR ($CDCl_3$, 125 MHz): δ 168.16, 162.10, 158.84, 156.13, 134.93, 134.35, 130.04, 128.23, 127.13, 127.09, 125.09, 119.66, 105.71, 55.42, 52.87, 21.79.



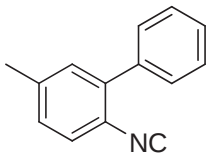

**1m**

**Methyl (*Z*)-2-isocyano-3,4-diphenylbut-2-enoate (1m)[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), 4.37 (s, 2H), 3.93 (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.




**1n**

**1-(2-isocyanophenyl)-1H-pyrrole (1n)[2]:** Yellow oil. $^1$H NMR ($CDCl_3$, 500 MHz): δ 7.54-7.45 (m, 2H), 7.40-7.32 (m, 2H), 7.06-7.02 (m, 2H), 6.44-6.39 (m, 2H); $^{13}$C NMR ($CDCl_3$, 125 MHz): δ 169.76, 137.17, 130.42, 128.73, 127.29, 126.25, 121.40, 110.62.

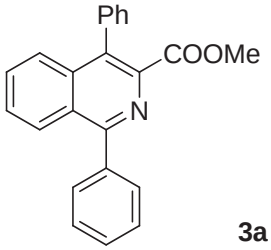



**1o**

**2-isocyano-5-methyl-1,1'-biphenyl (1o)[3]:** Yellow solid. M.p. 95-96 °C. $^1$H NMR ($CDCl_3$, 500 MHz): δ 7.55-7.48 (m, 4H), 7.46-7.42 (m, 1H), 7.40-7.36 (m, 1H), 7.27-7.23 (m, 1H), 7.19-7.16 (m, 1H), 2.43 (s, 3H); $^{13}$C NMR ($CDCl_3$, 125 MHz): δ 165.93, 139.94, 138.59, 137.22, 131.20, 129.00, 128.85, 128.56, 128.31, 127.70, 21.41.

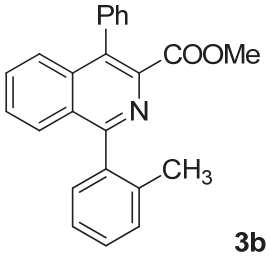
## 3. Synthesis and Characterization for Compounds 3-5.

**General Procedure:** A test tube equipped with a rubber septum and magnetic stir bar was charged with vinyl isocyanide **1** (0.4 mmol, 1.0 equiv), hydrazines **2** (1.6 mmol, 4.0 equiv), $Mn(OAc)_2{\cdot}4H_2O$ (0.08 mmol, 20 mol%) and TBPB (0.448 mL, 6.0 equiv) in dry MeCN (3.0 mL). The tube was evacuated and backfilled with $N_2$ for three times. The reaction mixture was stirred in a pre-heated oil bath at 70 $^oC$. The reaction was cooled to room temperature, washed with saturated sodium bicarbonate solution (50 mL) and then extracted with EtOAc (3×20 mL). The combined organic layer was dried over anhydrous $Na_2SO_4$ and concentrated under reduced pressure after filtration. The crude reaction mixture was purified by column chromatography on silica gel to give the desired products **3-5**.




**3a**

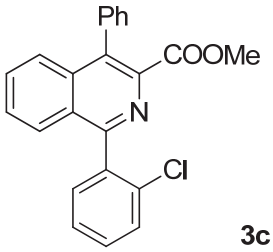
**Methyl 1,4-diphenylisoquinoline-3-carboxylate (3a)**[1]**:** Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (105.2 mg, 0.4 mmol), phenyl hydrazine **2a** (0.157 mL, 1.6 mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 $^oC$ for 23 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 20:1) to give **3a** (111.2 mg, 82%) as a light yellow solid. M.p. 181-182 $^oC$. IR (KBr, $cm^{-1}$): 1723.8, 1545.8, 1336.8, 1225.8, 1178.3, 996.3, 761.9, 698.7, 665.7. $^1H$ NMR ($CDCl_3$, 500 MHz): δ 8.18 (d, *J* = 8.0 Hz, 1H), 7.78-7.75 (m, 2H), 7.71 (d, *J* = 8.0 Hz, 1H), 7.68-7.64 (m, 1H), 7.64-7.59 (m, 1H), 7.58-7.47 (m, 6H), 7.43-7.40 (m, 2H), 3.71 (s, 3H); $^{13}C$ NMR ($CDCl_3$, 125 MHz): δ 167.69, 160.35, 141.40, 138.88, 136.67, 136.15, 132.92, 130.75, 130.36, 129.97, 129.10, 128.58. 128.45, 128.42, 128.17, 127.91, 127.32, 126.87, 52.55. EI-MS *m/z* (%): 339 (44) [$M^+$], 281 (35), 280 (100), 279 (24), 278 (47).




**3b**

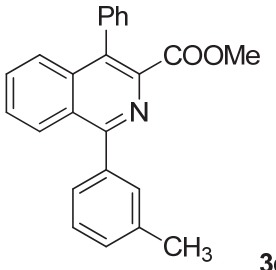
**Methyl 4-phenyl-1-(*o*-tolyl)isoquinoline-3-carboxylate (3b)**[1]**:** Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (105.2 mg, 0.4 mmol), *o*-tolylhydrazine **2b** (195.2 mg, 1.6 mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 $^oC$ for 19 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1) to give **3b**

(91.8 mg, 65%) as a yellow solid. M.p. 144-145 °C. IR (KBr, $cm^{-1}$): 1730.3, 1440.0, 1379.5, 1326.6, 1223.9, 1165.5, 996.8, 767.3, 692.9. $^1$H NMR ($CDCl_3$, 500 MHz): δ 7.76-7.71 (m, 2H) 7.67-7.63 (m, 1H), 7.58-7.49 (m, 4H), 7.48-7.45 (m, 1H), 7.43-7.39 (m, 3H), 7.38-7.32 (m, 2H), 3.71 (s, 3H), 2.16 (s, 3H); $^{13}$C NMR ($CDCl_3$, 125 MHz): δ 167.58, 160.83, 141.24, 138.13, 136.76, 136.06, 135.99, 132.89, 130.78, 130.46, 129.92, 129.88, 129.85, 128.83, 128.43, 128.35, 128.29, 128.09, 127.89, 127.68, 126.68, 125.75, 52.50, 20.04. EI-MS *m/z* (%): 353 (51) [$M^+$], 352 (45), 293 (38), 292 (100), 291 (64).




**3c**

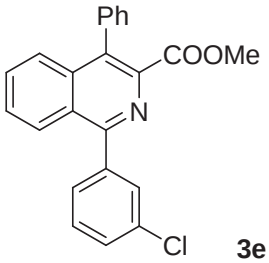
**Methyl 1-(2-chlorophenyl)-4-phenylisoquinoline-3-carboxylate (3c):** Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (105.2 mg, 0.4 mmol), (2-chlorophenyl)-hydrazine **2c** (227.2 mg, 1.6 mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 °C for 18 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1) to give **3c** (89.5 mg, 60%) as a yellow solid. M.p. 160-161 °C. IR (KBr, $cm^{-1}$): 1723.2, 1439.3, 1381.6, 1329.6, 1229.9, 1177.7, 998.1, 758.2, 690.5. $^1$H NMR ($CDCl_3$, 500 MHz): δ 7.72 (d, *J* = 8.5 Hz, 2H), 7.68-7.63 (m, 1H), 7.61-7.58 (m, 1H), 7.58-7.53 (m, 3H), 7.52-7.49 (m, 2H), 7.48-7.44 (m, 3H), 7.41-7.38 (m, 1H), 3.70 (s, 3H). $^{13}$C NMR ($CDCl_3$, 125 MHz): δ 167.41, 158.18, 141.24, 137.67, 135.99, 135.92, 133.80, 133.57, 131.69, 130.87, 130.24, 129.91, 129.77, 129.72, 128.62, 128.31, 128.14, 127.67, 127.46, 127.03, 126.76, 52.55. EI-MS *m/z* (%): 375 (11) [$M^+$ ($^{37}$Cl)], 373 (23) [$M^+$ ($^{35}$Cl)], 316 (39), 315 (42), 314 (100). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{23}H_{17}ClNO_2$: 374.0948; found: 374.0943.




**3d**

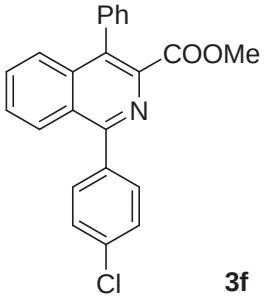
**Methyl 4-phenyl-1-(*m*-tolyl)isoquinoline-3-carboxylate (3d)**[1]**:** Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (105.2 mg, 0.4 mmol), *m*-tolylhydrazine **2d** (195.2 mg, 1.6 mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 °C for 23 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1) to give **3d** (105.3 mg, 75%) as a yellow solid. M.p. 151-152 °C. IR (KBr, $cm^{-1}$): 1715.3, 1436.5, 1379.1, 1325.4, 1226.3, 1161.3, 1000.0, 767.1, 689.0, 599.6. $^1$H NMR ($CDCl_3$, 500 MHz): δ 8.20-8.17 (m, 1H), 7.72-7.69 (m, 1H), 7.67-7.63 (m, 1H), 7.63-7.58 (m, 2H),

7.55-7.47 (m, 4H), 7.45-7.40 (m, 3H), 7.33 (d, *J* = 7.5 Hz, 1H), 3.71 (s, 3H), 2.48 (s, 3H); $^{13}$C NMR ($CDCl_3$, 125 MHz): δ 167.73, 160.58, 141.39, 138.81, 138.37, 136.58, 136.18, 132.76, 130.89, 130.66, 129.94, 129.79, 128.38, 128.34, 128.29, 128.11, 127.98, 127.42, 127.34, 126.78, 52.51, 21.62. EI-MS *m/z* (%): 353 (37) [$M^+$], 294 (100), 278 (39), 105 (77), 77 (72).




**3e**

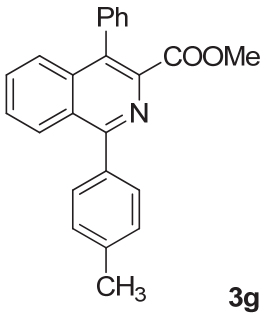
**Methyl 1-(3-chlorophenyl)-4-phenylisoquinoline-3-carboxylate (3e)**[1]**:** Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (105.2 mg, 0.4 mmol), (3-chlorophenyl)-hydrazine **2e** (227.2 mg, 1.6 mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 °C for 16 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1) to give **3e** (111 mg, 74%) as a yellow solid. M.p. 130-131 °C. IR (KBr, $cm^{-1}$): 1724.4, 1329.3, 1227.3, 762.8, 698.4. $^1$H NMR ($CDCl_3$, 500 MHz): δ 8.14-8.11 (m, 1H), 7.78-7.76 (m, 1H), 7.74-7.71 (m, 1H), 7.70-7.62 (m, 3H), 7.55-7.47 (m, 5H), 7.42-7.38 (m, 2H), 3.70 (s, 3H); $^{13}$C NMR ($CDCl_3$, 125 MHz): δ 167.56, 158.72, 141.44, 140.64, 136.68, 135.97, 134.67, 133.43, 130.91, 130.39, 129.90, 129.82, 129.22, 128.76, 128.53, 128.45, 128.26, 127.41, 127.15, 127.02, 52.61. EI-MS *m/z* (%): 375 (10) [$M^+$ ($^{37}$Cl)], 373 (26) [$M^+$ ($^{35}$Cl)], 314 (100), 278 (32), 57 (30).




**3f**

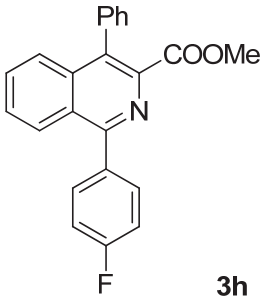
**Methyl 1-(4-chlorophenyl)-4-phenylisoquinoline-3-carboxylate (3f)**[1]**:** Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (105.2 mg, 0.4 mmol), (4-chlorophenyl)-hydrazine **2f** (227.2 mg, 1.6 mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 °C for 18 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1) to give **3f** (103.4 mg, 69%) as a yellow solid. M.p. 174-175 °C. IR (KBr, $cm^{-1}$): 1715.6, 1597.4, 1491.0, 1437.7, 1326.2, 1225.7, 1170.7, 1086.1, 1003.5, 970.2, 841.7, 767.3, 694.9. $^1$H NMR ($CDCl_3$, 500 MHz): δ 8.14-8.11 (m, 1H), 7.73-7.71 (m, 3H), 7.69-7.65 (m, 1H), 7.65-7.61 (m, 1H), 7.56-7.48 (m, 5H), 7.42-7.39 (m, 2H), 3.70 (s, 3H); $^{13}$C NMR ($CDCl_3$, 125 MHz): δ 167.55, 158.92, 141.41, 137.30, 136.58, 135.91, 135.19, 133.06, 131.60, 130.72, 129.80, 128.73, 128.55, 128.33, 128.12, 127.30, 127.04, 126.90, 52.46. EI-MS *m/z* (%): 375 (20) [$M^+$ ($^{37}$Cl)], 373 (42) [$M^+$ ($^{35}$Cl)],

316 (39), 315 (51), 314 (100).



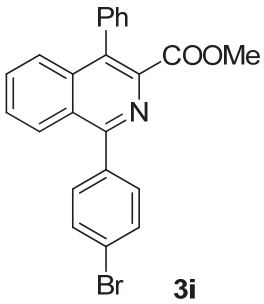

**3g**

**Methyl 4-phenyl-1-(*p*-tolyl)isoquinoline-3-carboxylate (3g)**[1]**:** Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (105.2mg, 0.4 mmol), *p*-tolylhydrazine **2g** (195.2 mg, 1.6 mmol), $Mn(OAc)_2 \cdot 4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 $^oC$ for 20 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1) to give **3g** (84.8 mg, 60%) as a yellow solid. M.p. 144-145 $^oC$. IR (KBr, $cm^{-1}$): 1732.1, 1437.0, 1227.0, 1176.3, 1111.6, 999.1, 769.7, 696.4. $^1H$ NMR ($CDCl_3$, 500 MHz): δ 8.22-8.19 (m, 1H), 7.71-7.58 (m, 5H), 7.55-7.46 (m, 3H), 7.42-7.39 (m, 2H), 7.36 (d, *J* = 8.0 Hz, 2H), 3.70 (s, 3H), 2.47 (s, 3H); $^{13}C$ NMR ($CDCl_3$, 125 MHz): δ 167.68, 160.32, 141.34, 138.92, 136.54, 136.13, 135.96, 132.52, 130.54, 130.19, 129.88, 129.15, 128.30, 128.23, 128.01, 127.86, 127.23, 126.71, 52.39, 21.42. EI-MS *m/z* (%): 353 (53) [$M^+$], 294 (100), 293 (20).



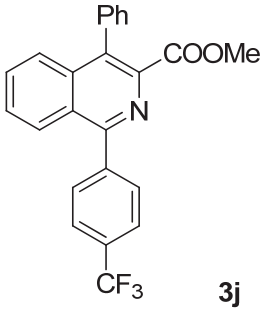

**3h**

**Methyl 1-(4-fluorophenyl)-4-phenylisoquinoline-3-carboxylate (3h)**[1]: Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (105.2mg, 0.4 mmol), (4-fluorophenyl)-hydrazine **2h** (201.6 mg, 1.6 mmol), $Mn(OAc)_2 \cdot 4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 $^oC$ for 16 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1) to give **3h** (94.4 mg, 66%) as a yellow solid. M.p. 179-180 $^oC$. IR (KBr, $cm^{-1}$): 1721.8, 1504.9, 1380.9, 1224.6, 1163.0, 1001.6, 845.1, 766.7, 693.0. $^1H$ NMR ($CDCl_3$, 500 MHz): δ 8.15-8.12 (m, 1H), 7.78-7.74 (m, 2H), 7.73-7.70 (m, 1H), 7.69-7.61 (m, 2H), 7.55-7.49 (m, 3H), 7.42-7.39 (m, 2H), 7.27-7.23 (m, 2H), 3.70 (s, 3H); $^{13}C$ NMR ($CDCl_3$, 125 MHz): δ 167.57, 163.36 (d, $^1J_{C\text{-}F}$ = 247.5 Hz), 159.11, 141.32, 136.58, 135.95, 134.92 (d, $^4J_{C\text{-}F}$ = 3.75 Hz), 132.92, 132.10 (d, $^3J_{C\text{-}F}$ = 8.75 Hz), 130.67, 129.81, 128.48, 128.32, 128.09, 127.44, 127.13, 126.87, 115.52 (d, $^2J_{C\text{-}F}$ = 21.3 Hz), 52.45; $^{19}F$ NMR ($CDCl_3$, 470 MHz): δ -112.5 (m, Ar-F). EI-MS *m/z* (%): 357 (45) [$M^+$], 299 (31), 298 (100).



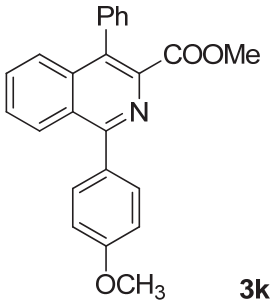

**3i**

**Methyl 1-(4-bromophenyl)-4-phenylisoquinoline-3-carboxylate (3i)**: Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (105.2mg, 0.4 mmol), (4-bromophenyl)-hydrazine **2i** (297.6 mg, 1.6mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 $^oC$ for 23 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1) to give **3i** (116.8 mg, 70%) as a yellow solid. M.p. 169-170 $^oC$. IR (KBr, $cm^{-1}$): 1713.1, 1433.5, 1385.5, 1224.2, 1169.5, 1002.2, 967.9, 766.4, 693.8. $^1H$ NMR ($CDCl_3$, 500 MHz): δ 8.14-8.11 (m, 1H), 7.73-7.61 (m, 7H), 7.55-7.47 (m, 3H), 7.41-7.38 (m, 2H), 3.70 (s, 3H); $^{13}C$ NMR ($CDCl_3$, 125 MHz): δ 167.52, 158.92, 141.42, 137.73, 136.58, 135.90, 133.09, 131.88, 131.69, 130.77, 129.80, 128.59, 128.35, 128.14, 127.28, 126.98, 126.91, 123.49, 52.47. LC-MS (ESI) m/z: 420 $[(M+H)^+$ ($^{81}Br$)], 418 $[(M+H)^+$ ($^{79}Br$)]. HRMS (ESI) ($[M+H]^+$) Calcd. for $C_{23}H_{17}BrNO_2$: 418.0443; found: 418.0438.



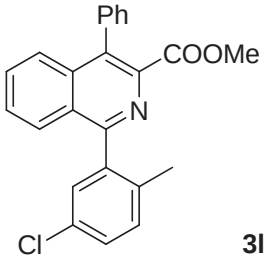

**3j**

**Methyl 4-phenyl-1-(4-(trifluoromethyl)phenyl)isoquinoline-3-carboxylate (3j)**[1]: Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (105.2 mg, 0.4 mmol), (4-(trifluoromethyl)phenyl)hydrazine **2j** (281.6 mg, 1.6 mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 $^oC$ for 23 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1) to give **3j** (113 mg, 69%) as a yellow solid. M.p. 164-165 $^oC$. IR (KBr, $cm^{-1}$): 1719.9, 1439.9, 1325.8, 1228.9, 1165.4, 1117.0, 1064.6, 1009.4, 851.1, 772.8, 705.4. $^1H$ NMR ($CDCl_3$, 500 MHz): δ 8.11-8.07 (m, 1H), 7.90 (d, $J$ = 8.0 Hz, 2H), 7.83 (d, $J$ = 8.0 Hz, 2H), 7.76-7.73 (m, 1H), 7.71-7.67 (m, 1H), 7.66-7.62 (m, 1H), 7.56-7.50 (m, 3H), 7.44-7.39 (m, 2H), 3.70 (s, 3H); $^{13}C$ NMR ($CDCl_3$, 125 MHz): δ 167.46, 158.61, 142.40, 141.47, 136.58, 135.79, 133.46, 131.14, 130.88, 130.85, 130.61, 129.77, 128.75, 128.36, 128.19, 127.39, 127.09, 126.99, 125.48 (q, $^2J_{C\text{-}F}$ = 3.5 Hz), 124.14 (q, $^1J_{C\text{-}F}$ = 270.0 Hz ), 120.89, 52.49; $^{19}F$ NMR ($CDCl_3$, 470 MHz): δ -62.58 (s, Ar-$CF_3$). EI-MS *m/z*: 407 (26) $[M^+]$, 349 (41), 348 (100), 346 (11), 278 (23).



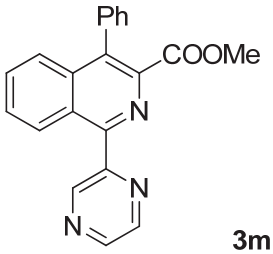

**3k**

**Methyl 1-(4-methoxyphenyl)-4-phenylisoquinoline-3-carboxylate (3k)**[1]: Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (105.2 mg, 0.4 mmol), (4-methoxy-phenyl)hydrazine **2k** (220.8 mg, 1.6 mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 $^oC$ for 20 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1) to give **3k** (78.2 mg, 53%) as a yellow solid. M.p. 173-174 $^oC$. IR (KBr, $cm^{-1}$): 1730.7, 1604.9, 1507.0, 1386.5, 1334.2, 1244.1, 1170.2, 1111.8, 1028.7, 843.2, 769.6, 699.7, 522.0. $^1H$ NMR ($CDCl_3$, 500 MHz): δ 8.24-8.21 (m, 1H), 7.75-7.72 (m, 2H), 7.71-7.68 (m, 1H), 7.67-7.59 (m, 2H), 7.54-7.48 (m, 3H), 7.42-7.38 (m, 2H), 7.11-7.06 (m, 2H), 3.91 (s, 3H), 3.70 (s, 3H); $^{13}C$ NMR ($CDCl_3$, 125 MHz): δ 167.57, 160.42, 159.85, 141.14, 136.64, 136.07, 132.41, 131.71, 131.16, 130.59, 129.86, 128.30, 128.27, 128.01, 127.87, 127.18, 126.74, 113.95, 55.47, 52.42. EI-MS *m/z* (%): 369 (84) [$M^+$], 310 (100), 308 (34), 265 (26).



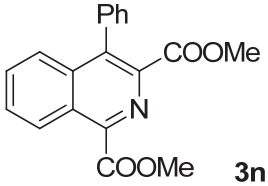

**3l**

**Methyl 1-(5-chloro-2-methylphenyl)-4-phenylisoquinoline-3-carboxylate (3l)**: Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (105.2 mg, 0.4 mmol), (5-chloro-2-methylphenyl)hydrazine **2l** (249.6 mg, 1.6 mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 $^oC$ for 18 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1) to give **3l** (107.8 mg, 70%) as a yellow solid. M.p. 119-120 $^oC$. IR (KBr, $cm^{-1}$): 1731.9, 1440.9, 1323.5, 1229.3, 1178.2, 1111.5, 999.0, 772.1, 696.7. $^1H$ NMR ($CDCl_3$, 500 MHz): δ 7.74-7.70 (m, 2H), 7.69-7.64 (m, *J* = 7.5, 1H), 7.61-7.51 (m, 1H), 7.56-7.49 (m, 3H), 7.46-7.43 (m, 1H), 7.42-7.36 (m, 3H), 7.29 (d, *J* = 8.0 Hz, 1H), 3.71 (s, 3H), 2.11 (s, 3H); $^{13}C$ NMR ($CDCl_3$, 125 MHz): δ 167.57, 159.36, 141.46, 139.91, 136.18, 135.96, 135.45, 133.42, 131.86, 131.61, 130.99, 129.92, 129.90, 128.92, 128.79, 128.47, 128.38, 128.24, 127.71, 127.31, 126.92, 52.62, 19.57. EI-MS *m/z* (%): 389 (25) [$M^+(^{37}Cl)$], 387 (65) [$M^+(^{35}Cl)$], 326 (100), 292 (46), 291 (57). HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{24}H_{19}ClNO_2$: 388.1104; found: 388.1099.



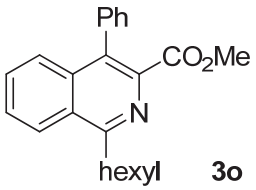

**3m**

**Methyl 4-phenyl-1-(pyrazin-2-yl)isoquinoline-3-carboxylate (3m)**: Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (105.2 mg, 0.4 mmol), 2-hydrazinyl-pyrazine **2m** (176 mg, 1.6 mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 $^oC$ for 23 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1) to give **3m** (71 mg, 52%) as a yellow solid. M.p. 187-188 $^oC$. IR (KBr, $cm^{-1}$): 1725.5, 1450.1, 1366.7, 1228.7, 1182.3, 1002.9, 762.7, 696.2, 406.7. $^1H$ NMR ($CDCl_3$, 500 MHz): δ 9.44 (s, 1H), 8.79-8.72 (m, 3H), 7.75-7.68 (m, 3H), 7.56-7.49 (m, 3H), 7.41-7.38 (m, 2H), 3.73 (s, 3H); $^{13}C$ NMR ($CDCl_3$, 125 MHz): δ 167.37, 153.82, 153.41, 146.96, 144.10, 143.00, 141.29, 137.19, 135.89, 135.13, 131.04, 129.83, 129.34, 128.46, 128.37, 127.36, 127.12, 52.64. EI-MS m/z (%): 341 (40) $[M^+]$, 282 (48), 281 (90), 280 (100). HRMS (ESI) ($[M+H]^+$) Calcd. for $C_{21}H_{16}N_3O_2$: 342.1243; found: 342.1236.




**3n**

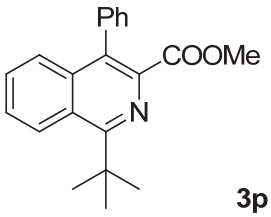
**Dimethyl 4-phenylisoquinoline-1,3-dicarboxylate (3n)**: Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (105.2 mg, 0.4 mmol), methyl hydrazinecarboxylate **2n** (144 mg, 1.6 mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 $^oC$ for 15 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 10:1 to 5:1) to give **3n** (38.9 mg, 30%) as a white solid. M.p. 118-119 $^oC$. IR (KBr, $cm^{-1}$): 1731.4, 1434.8, 1368.8, 1236.5, 1198.0, 1154.5, 988.5, 762.7, 698.7. $^1H$ NMR ($CDCl_3$, 500 MHz): δ 8.85-8.82 (m, 1H), 7.79-7.75 (m, 1H), 7.71-7.68 (m, 2H), 7.52-7.50 (m, 3H), 7.35-7.31 (m, 2H), 4.12 (s, 3H), 3.72 (s, 3H); $^{13}C$ NMR ($CDCl_3$, 125 MHz): δ 166.56, 165.86, 148.17, 140.48, 137.37, 136.80, 135.48, 131.21, 129.87, 129.45, 128.36, 128.32, 127.01, 126.95, 126.42, 53.25, 52.62. EI-MS *m/z* (%): 321 (298) $[M^+]$, 231 (826), 203 (815), 202 (552). HRMS (ESI) ($[M+H]^+$) Calcd. for $C_{19}H_{16}NO_4$: 322.1079; found: 322.1074.




**3o**

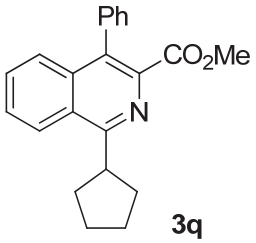
**Methyl 1-hexyl-4-phenylisoquinoline-3-carboxylate (3o):** Following the general

procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (105.2 mg, 0.4 mmol), hexylhydrazine **2o** (186 mg, 1.6 mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 $^oC$ for 23 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 30:1) to give **3o** (79.8 mg, 57%) as a white solid. M.p. 57-58 $^oC$. IR (KBr, $cm^{-1}$): 1719.1, 1446.6, 1433.4, 1384.8, 1228.9, 1196.2, 1161.8, 1007.8.5, 769.3, 701.5. $^1H$ NMR ($CDCl_3$, 500 MHz): δ 8.24 (d, *J* = 8.5 Hz, 1H), 7.68-7.57 (m, 3H), 7.50-7.42 (m, 3H), 7.35-7.31 (m, 2H), 3.68 (s, 3H), 3.41-3.36 (m, 2H), 1.95-1.86 (m, 2H), 1.57-1.49 (m, 2H), 1.41-1.30 (m, 4H), 0.93-0.88 (m, 3H); $^{13}C$ NMR ($CDCl_3$, 125 MHz): δ 167.98, 162.27, 141.05, 136.35, 135.85, 132.08, 130.29, 129.83, 128.19, 128.16, 127.83, 127.27, 127.14, 125.44, 52.35, 35.91, 31.76, 30.11, 29.70, 22.65, 14.13. LC-MS (ESI) m/z: 348 [$(M+H)^+$]. HRMS (ESI) ([$M+H]^+$) Calcd. for $C_{23}H_{26}NO_2$: 348.1964; found: 348.1959.




**3p**

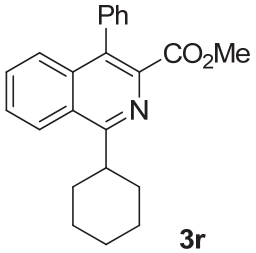
**Methyl 1-(*tert*-butyl)-4-phenylisoquinoline-3-carboxylate (3p)**: Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (105.2 mg, 0.4 mmol), *tert*-butylhydrazine hydrochloride **2p** (198.4 mg, 1.6 mmol), sodium bicarbonate (168 mg, 2.0 mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 $^oC$ for 18 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 60:1) to give **3p** (108.9 mg, 85%) as a white solid. M.p. 118-119 $^oC$. IR (KBr, $cm^{-1}$): 1729.9, 1441.6, 1361.5, 1235.6, 1160.4, 987.4, 771.6, 697.3, 556.9. $^1H$ NMR ($CDCl_3$, 500 MHz): δ 8.63 (d, *J* = 8.5 Hz, 1H), 7.69-7.65 (m, 1H), 7.64-7.60 (m, 1H), 7.59-7.55 (m, 1H), 7.51-7.43 (m, 3H), 7.36-7.30 (m, 2H), 3.67 (s, 3H), 1.73 (s, 9H); $^{13}C$ NMR ($CDCl_3$, 125 MHz): δ 168.28, 166.75, 139.95, 136.90, 136.50, 131.87, 129.89, 129.25, 128.17, 127.81, 127.78, 127.12, 126.80, 126.57, 52.12, 40.11, 31.19. EI-MS *m/z* (%): 319 (100) [$M^+$], 318 (44), 304 (52), 277 (82), 258 (84). HRMS (ESI) ([$M+H]^+$) Calcd. for $C_{21}H_{22}NO_2$: 320.1651; found: 320.1645.




**3q**

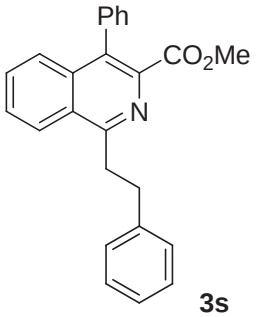
**Methyl 1-cyclopentyl-4-phenylisoquinoline-3-carboxylate (3q):** Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (105.2 mg, 0.4 mmol), cyclopentyl-hydrazine hydrochloride **2q** (218 mg, 1.6 mmol), sodium bicarbonate (168 mg, 2.0 mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 $^oC$ for 22 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 30:1) to give **3q** (71 mg, 54%) as a light yellow

solid. M.p. 98-99 °C. IR (KBr, $cm^{-1}$): 1732.2, 1433.6, 1393.6, 1232.2, 1165.2, 991.6, 771.9, 705.6. $^1$H NMR ($CDCl_3$, 500 MHz): δ 8.35-8.32 (m, 1H), 7.67-7.63 (m, 2H), 7.62-7.58 (m, 1H), 7.52-7.44 (m, 3H), 7.38-7.34 (m, 2H), 4.11-4.03 (m, 1H), 3.67 (s, 3H), 2.30-2.16 (m, 4H), 1.99-1.91 (m, 2H), 1.85-1.75 (m, 2H); $^{13}$C NMR ($CDCl_3$, 125 MHz): δ 168.36, 164.13, 141.16, 136.51, 135.79, 131.37, 130.01, 129.93, 128.20, 127.90, 127.79, 127.47, 127.04, 125.25, 52.14, 43.39, 32.58, 26.04. LC-MS (ESI) m/z: 332 [$(M+H)^+$]. HRMS (ESI) ([$M+H]^+$) Calcd. for $C_{22}H_{22}NO_2$: 332.1651; found: 332.1645.




**3r**

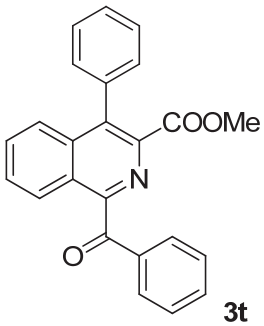
**Methyl 1-cyclohexyl-4-phenylisoquinoline-3-carboxylate (3r):** Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (105.2 mg, 0.4 mmol), cyclohexylhydrazine **2r** (182 mg, 1.6 mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 °C for 18 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 30:1) to give **3r** (102 mg, 74%) as a white solid. M.p. 147-148 °C. IR (KBr, $cm^{-1}$): 1727.9, 1444.3, 1393.6, 1332.6, 1230.3, 1163.8, 996.4, 765.6, 698.9, 599.5, 539.3. $^1$H NMR ($CDCl_3$, 500 MHz): δ 8.33-8.29 (m, 1H), 7.67-7.62 (m, 2H), 7.62-7.57 (m, 1H), 7.51-7.41 (m, 3H), 7.37-7.32 (m, 2H), 3.66 (s, 3H), 3.65-3.57 (m, 1H), 2.10-2.03 (m, 2H), 2.00-1.90 (m, 4H), 1.85-1.80 (m, 1H), 1.61-1.51 (m, 2H), 1.47-1.36 (m, 1H); $^{13}$C NMR ($CDCl_3$, 125 MHz): δ 168.42, 165.13, 141.46, 136.50, 135.82, 131.17, 129.94, 129.93, 128.18, 127.88, 127.77, 127.17, 126.61, 124.72, 52.15, 41.82, 32.35, 26.83, 26.16. LC-MS (ESI) m/z: 346 [$(M+H)^+$]. HRMS (ESI) ([$M+H]^+$) Calcd. for $C_{23}H_{24}NO_2$: 346.1807; found: 346.1802.




**3s**

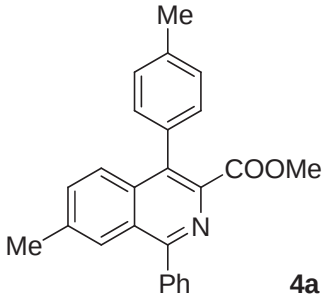
**Methyl 1-phenethyl-4-phenylisoquinoline-3-carboxylate (3s):** Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (105.2 mg, 0.4 mmol), phenethylhydrazine **2s** (218 mg, 1.6 mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 °C for 22 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 20:1) to give **3s** (85 mg, 58%) as a white solid. M.p. 117-118 °C. IR (KBr, $cm^{-1}$): 1721.5, 1647.5, 1554.8, 1510.1, 1226.7, 1162.2, 1009.7, 763.3, 701.6, 427.7. $^1$H NMR ($CDCl_3$, 500 MHz): δ

8.28-8.22 (m, 1H), 7.70-7.60 (m, 3H), 7.54-7.46 (m, 3H), 7.41-7.32 (m, 6H), 7.28-7.22 (m, 1H), 3.76-3.68 (m, 5H), 3.32-3.25 (m, 2H); $^{13}$C NMR ($CDCl_3$, 125 MHz): δ 168.03, 160.78, 141.83, 141.17, 136.28, 135.86, 132.37, 130.42, 129.87, 128.56, 128.55, 128.37, 128.26, 127.94, 127.33, 127.23, 126.17, 125.14, 52.39, 37.31, 35.41. LC-MS (ESI) m/z: 368 [$(M+H)^+$]. HRMS (ESI) ([$M+H]^+$) Calcd. for $C_{25}H_{22}NO_2$: 368.1651; found: 368.1639.




**3t**

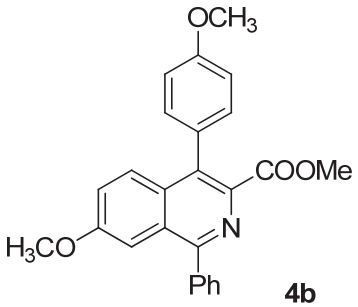
**Methyl 1-benzoyl-4-phenylisoquinoline-3-carboxylate (3t)**: Following the general procedure, methyl 2-isocyano-3,3-diphenylacrylate **1a** (105.2 mg, 0.4 mmol), benzylhydrazine **2t** (195 mg, 1.6 mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 $^o$C for 23 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1) to give **3t** (29.4 mg, 20%) as a yellow solid. M.p. 139-140 $^o$C. IR (KBr, $cm^{-1}$): 1735.5, 1671.0, 1443.2, 1387.0, 1232.0, 1162.9, 995.0, 768.9, 699.9, 634.0. $^1$H NMR ($CDCl_3$, 500 MHz): δ 8.25-8.20 (m, 1H), 8.09-8.04 (m, 2H), 7.76-7.61 (m, 4H), 7.57-7.48 (m, 5H), 7.43-7.40 (m, 2H), 3.67 (s, 3H); $^{13}$C NMR ($CDCl_3$, 125 MHz): δ 193.92, 167.14, 155.94, 140.56, 136.44, 136.15, 135.52, 135.29, 134.01, 131.29, 131.05, 129.65, 129.33, 128.57, 128.38, 128.36, 126.91, 126.61, 126.28, 52.52. LC-MS (ESI) m/z: 368 [$(M+H)^+$]. HRMS (ESI) ([$M+H]^+$) Calcd. for $C_{24}H_{18}NO_3$: 368.1287; found: 368.1291.




**4a**

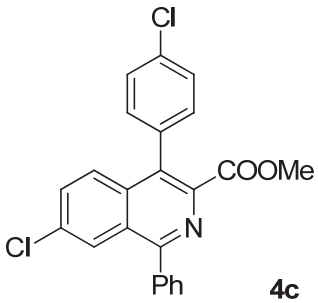
**Methyl 7-methyl-1-phenyl-4-(p-tolyl)isoquinoline-3-carboxylate (4a)**[1]**:** Following the general procedure, methyl 2-isocyano-3,3-di-*p*-tolylacrylate **1a'** (116.4 mg, 0.4 mmol), phenylhydrazine **2a** (0.157 mL, 1.6 mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 $^o$C for 17 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 20:1 to 5:1) to give **4a** (100.3 mg, 68%) as a yellow solid. M.p. 143-144 $^o$C. IR (KBr, $cm^{-1}$): 1724.9, 1313.7, 1224.7, 1164.0, 1012.2, 770.8, 700.8, 523.8. $^1$H NMR ($CDCl_3$, 500 MHz): δ 7.90 (s, 1H), 7.76-7.73 (m, 2H), 7.63 (d, *J* = 8.5 Hz, 1H), 7.58-7.46 (m, 4H), 7.35-7.26 (m, 4H), 3.72 (s, 3H), 2.48 (d, *J* = 6.0 Hz, 6H); $^{13}$C NMR ($CDCl_3$, 125

MHz): δ 167.57, 159.24, 140.28, 138.78, 138.69, 137.68, 134.98, 133.11, 133.06, 132.84, 130.21, 129.67, 129.03, 128.89, 128.45, 127.44, 126.73, 126.57, 52.47, 21.95, 21.43. EI-MS *m/z* (%): 367 (52) [$M^+$], 322 (14), 309 (30), 308 (100), 294 (69).




**4b**

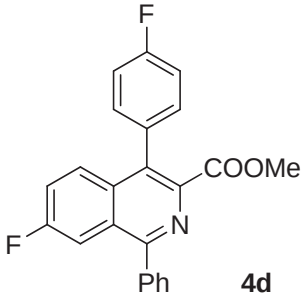
**Methyl 7-methoxy-4-(4-methoxyphenyl)-1-phenylisoquinoline-3-carboxylate (4b)**[1]**:** Following the general procedure, methyl 2-isocyano-3,3-bis(4-methoxyphenyl)acrylate **1b** (129.2 mg, 0.4 mmol), phenylhydrazine **2a** (0.157 mL, 1.6 mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 °C for 16 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 10:1 to 5:1) to give **4b** (100.8 mg, 63%) as a yellow solid. M.p. 179-180 °C. IR (KBr, $cm^{-1}$): 1719.9, 1612.6, 1508.7, 1407.4, 1218.0, 1175.7, 1025.6, 846.8, 700.4. $^1$H NMR ($CDCl_3$, 500 MHz): δ 7.79-7.75 (m, 2H), 7.65 (d, *J* = 9.0 Hz, 1H), 7.58-7.49 (m, 3H), 7.43 (d, *J* = 2.5 Hz, 1H), 7.32-7.28 (m, 3H), 7.06-7.03 (m, 2H), 3.90 (s, 3H), 3.81 (s, 3H), 3.73 (s, 3H); $^{13}$C NMR ($CDCl_3$, 125 MHz): δ 167.83, 159.47, 159.36, 158.35, 139.79, 139.15, 133.00, 132.34, 131.04, 130.06, 128.97, 128.89, 128.67, 128.64, 128.37, 123.10, 113.88, 105.79, 55.59, 55.40, 52.52. EI-MS *m/z* (%): 399 (99) [$M^+$], 341 (47), 340 (100), 77 (38).




**4c**

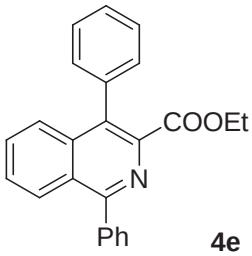
**Methyl 7-chloro-4-(4-chlorophenyl)-1-phenylisoquinoline-3-carboxylate (4c)**[1]**:** Following the general procedure, methyl 3,3-bis(4-chlorophenyl)-2-isocyanoacrylate **1c** (132.8 mg, 0.4 mmol), phenylhydrazine **2a** (0.157 mL, 1.6 mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 °C for 18 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1) to give **4c** (122.1 mg, 75%) as a yellow solid. M.p. 211-212 °C. 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. $^1$H NMR ($CDCl_3$, 500 MHz): δ 8.15 (t, *J* = 1.5 Hz, 1H), 7.75-7.71 (m, 2H), 7.61-7.50 (m, 7H), 7.34-7.31 (m, 2H), 3.74 (s, 3H); $^{13}$C NMR ($CDCl_3$, 125 MHz): δ 167.08, 159.75, 141.44, 138.13, 134.83, 134.78, 134.46, 134.06, 131.73, 131.55, 131.11, 130.08, 129.35, 128.76, 128.71, 128.29, 127.89, 126.64, 52.63; EI-MS *m/z* (%): 411 (6) [$M^+$ ($2\times^{37}$Cl)], 409 (33) [$M^+$ ($^{35}$Cl, $^{37}$Cl)], 407 (47) [$M^+$

(2×$^{35}$Cl)], 350 (63), 348 (100), 314 (48).




**4d**

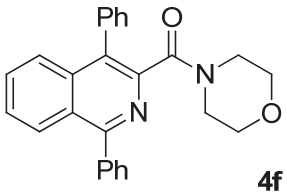
**Methyl 7-fluoro-4-(4-fluorophenyl)-1-phenylisoquinoline-3-carboxylate (4d)[1]:** Following the general procedure, methyl 3,3-bis(4-fluorophenyl)-2-isocyanoacrylate **1d** (119.6 mg, 0.4 mmol), phenylhydrazine **2a** (0.157 mL, 1.6 mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 $^oC$ for 18 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1) to give **4d** (117.5 mg, 78%) as a yellow solid. 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* = 10.0, 2.5 Hz, 1H), 7.76-7.71 (m, 2H), 7.69 (q, *J* = 5.5 Hz, 1H), 7.60-7.51 (m, 3H), 7.47-7.42 (m, 1H), 7.39-7.34 (m, 2H), 7.27-7.20 (m, 2H), 3.73 (s, 3H); $^{13}C$ NMR ($CDCl_3$, 125 MHz):δ 167.31, 162.70 (d, $^1J_{C\text{-}F}$ = 246.2 Hz), 161.72 (d, $^1J_{C\text{-}F}$ = 250.0 Hz), 159.80 (d, $^4J_{C\text{-}F}$ = 5.0 Hz), 141.09, 138.33, 133.70, 131.79, 131.64 (d, $^4J_{C\text{-}F}$ = 3.8 Hz), 131.50 (d, $^3J_{C\text{-}F}$ = 7.5 Hz) 129.97, 129.57 (d, $^3J_{C\text{-}F}$ = 8.7 Hz), 129.26, 128.67, 128.41 (d, $^3J_{C\text{-}F}$ = 8.7 Hz), 121.10 (d, $^2J_{C\text{-}F}$ = 25.0 Hz), 115.56 (d, $^2J_{C\text{-}F}$ = 21.2 Hz), 111.43 (d, $^2J_{C\text{-}F}$ = 22.5 Hz), 52.55; $^{19}F$ NMR ($CDCl_3$, 470 MHz): δ -108.8 (m, Ar-F), -113.4 (m, Ar-F). EI-MS *m/z* (%): 375 (31) [$M^+$], 317 (33), 316 (100), 314 (44), 157 (15).




**4e**

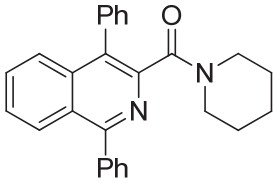
**Ethyl 1,4-diphenylisoquinoline-3-carboxylate (4e)[1]:** Following the general procedure, ethyl 2-isocyano-3,3-diphenylacrylate **1e** (110.8 mg, 0.4 mmol), phenylhydrazine **2a** (0.157 mL, 1.6 mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 $^oC$ for 21 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1) to give **4e** (95 mg, 67%) as a yellow solid. M.p. 104-105 $^oC$. IR (KBr, $cm^{-1}$): 1729.6, 1391.4, 1223.5, 1178.2, 1107.0, 1008.6, 770.1, 701.0. $^1H$ NMR ($CDCl_3$, 500 MHz): δ 8.19-8.16 (m, 1H), 7.79-7.76 (m, 2H), 7.73 (d, *J* = 8.0 Hz, 1H), 7.68-7.63 (m, 1H), 7.62-7.58 (m, 1H), 7.58-7.46 (m, 6H), 7.44-7.42 (m, 2H), 4.12 (q, *J* = 7.0 Hz, 2H), 0.99 (t, *J* = 7.0 Hz, 3H); $^{13}C$ NMR ($CDCl_3$, 125 MHz): δ 167.48, 160.27, 142.14, 138.78, 136.42, 136.09, 132.00, 130.60, 130.27, 130.05, 128.93, 128.41, 128.28, 128.18, 128.04, 127.80, 127.07, 126.58, 61.32, 13.70; EI-MS *m/z* (%): 353 (21) [$M^+$], 281 (33), 280

(100), 279 (15), 277 (18).



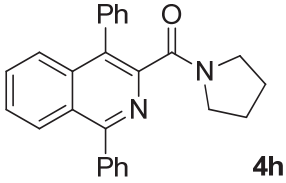

**4f**

**(1,4-Diphenylisoquinolin-3-yl)(morpholino)methanone (4f)**[1]**:** Following the general procedure, 2-isocyano-1-morpholino-3,3-diphenylprop-2-en-1-one **1f** (127.2 mg, 0.4 mmol), phenylhydrazine **2a** (0.157 mL, 1.6 mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 $^oC$ for 23 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 3:1 to 1:1) to give **4f** (115.8 mg, 73%) as a yellow solid after. M.p. 243-244 $^oC$. 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), 7.77-7.73 (m, 2H), 7.69-7.64 (m, 1H), 7.60-7.48 (m, 9H), 3.58 (t, *J* = 4.5 Hz, 2H), 3.44 (t, *J* = 4.5 Hz, 2H), 3.19-3.18 (m, 4H); $^{13}C$ NMR ($CDCl_3$, 125 MHz): δ 167.64, 160.69, 145.03, 138.75, 135.96, 134.72, 130.72, 130.64, 130.19, 128.94, 128.86, 128.60, 128.54, 128.43, 127.87, 127.68, 126.56, 125.89, 66.44, 66.42, 46.80, 41.61; EI-MS *m/z* (%): 394 (9) [$M^+$], 281 (54), 280 (100), 278 (12), 202 (12).




**4g**

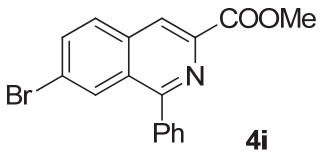
**(1,4-Diphenylisoquinolin-3-yl)(piperidin-1-yl)methanone (4g)**[1]**:** Following the general procedure, 2-isocyano-3,3-diphenyl-1-(piperidin-1-yl)prop-2-en-1-one **1g** (126.4 mg, 0.4 mmol), phenylhydrazine **2a** (0.157 mL, 1.6 mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 $^oC$ for 19 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 5:1 to 3:1) to give **4g** (112 mg, 71%) as a yellow solid. M.p. 214-215 $^oC$. 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 8.14 (d, *J* = 8.5 Hz, 1H), 7.79 (d, *J* = 8.5 Hz, 1H), 7.77-7.73 (m, 2H), 7.66-7.66 (m, 1H), 7.58-7.45 (m, 9H), 3.51 (t, *J* = 5.0 Hz, 2H), 3.11 (t, *J* = 5.0 Hz, 2H), 1.48-1.41 (m, 2H), 1.38-1.34 (m, 2H), 1.20-1.10 (m, 2H); $^{13}C$ NMR ($CDCl_3$, 125 MHz): δ 167.35, 160.38, 146.11, 138.88, 136.11, 134.87, 130.77, 130.52, 130.24, 128.81, 128.50, 128.36, 128.24, 127.79, 127.37, 126.40, 125.93, 47.54, 42.10, 25.81, 25.13, 24.32. EI-MS *m/z* (%): 392 (9) [$M^+$], 281 (51), 280 (100), 208 (53), 256 (40).




**4h**

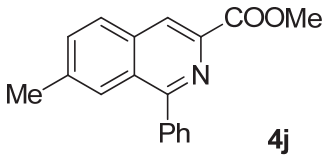
**(1,4-diphenylisoquinolin-3-yl)(pyrrolidin-1-yl)methanone (4h)**[1]**:** Following the general procedure, 2-isocyano-3,3-diphenyl-1-(pyrrolidin-1-yl)prop-2-en-1-one **1h**

(120.8 mg, 0.4 mmol), phenylhydrazine **2a** (0.157 mL, 1.6 mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 °C for 19 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 10:1 to 2:1) to give **4h** (98 mg, 65%) as a yellow solid. 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), 7.76-7.72 (m, 2H), 7.64-7.59 (m, 1H), 7.56-7.42 (m, 9H), 3.38 (t, *J* = 6.5 Hz, 2H), 3.16 (t, *J* = 6.0 Hz, 2H), 1.73-1.61 (m, 4H); $^{13}C$ NMR ($CDCl_3$, 125 MHz): δ 167.40, 160.48, 147.01, 139.13, 136.17, 135.02, 130.46, 130.43, 130.14, 128.74, 128.52, 128.38, 128.36, 128.22, 127.76, 127.40, 126.52, 125.91, 47.44, 45.11, 25.75, 24.25. EI-MS *m/z* (%): 378 (4) [$M^+$], 309 (19), 281 (47), 280 (100), 277 (13).



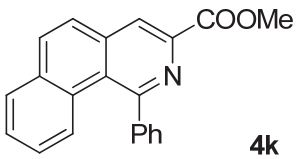

**4i**

**Methyl 7-bromo-1-phenylisoquinoline-3-carboxylate (4i)**[1]**:** Following the general procedure, methyl (*Z*)-3-(4-bromophenyl)-2-isocyanoacrylate **1i** (106.4 mg, 0.4 mmol), phenylhydrazine **2a** (0.157 mL, 1.6 mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 °C for 14 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1) to give **4i** (42.4 mg, 31%) as a yellow solid. 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 8.55 (s, 1H), 8.28 (s, 1H), 7.90 (d, *J* = 8.5 Hz, 1H), 7.85 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.71-7.68 (m, 2H), 7.58-7.52 (m, 3H), 4.04 (s, 3H); $^{13}C$ NMR ($CDCl_3$, 125 MHz): δ 166.26, 160.34, 141.28, 138.25, 135.12, 134.38, 130.10, 130.06, 130.01, 129.26, 129.13, 128.67, 123.75, 122.90, 52.98. EI-MS *m/z* (%): 343 (28) [$M^+$ ($^{81}Br$)], 341 (32) [$M^+$ ($^{79}Br$)], 342 (20), 283 (100), 203 (62).



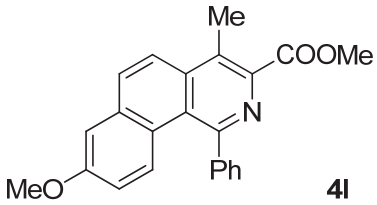

**4j**

**Methyl 7-methyl-1-phenylisoquinoline-3-carboxylate (4j)**[1]**:** Following the general procedure, methyl (*Z*)-2-isocyano-3-(*p*-tolyl)acrylate **1j** (80.4 mg, 0.4 mmol), phenylhydrazine **2a** (0.157 mL, 1.6 mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 °C for 21 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1) to give **4j** (45.7 mg, 41%) as a yellow solid. 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 8.55 (s, 1H), 7.94 (d, *J* = 8.5 Hz, 1H), 7.88 (s, 1H), 7.72-7.70 (m, 2H), 7.62 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.59-7.50 (m, 3H), 4.04 (s, 3H), 2.52 (s, 3H); $^{13}C$ NMR ($CDCl_3$, 125 MHz): δ 166.72, 160.49, 140.15, 139.95, 139.13, 134.78, 132.93, 130.11, 128.79, 128.49, 128.41, 128.29, 126.66, 123.26, 52.82, 22.24. EI-MS *m/z* (%): 277 (28) [$M^+$], 219 (100), 218 (24), 217 (30), 216 (33).



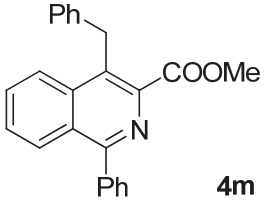

**4k**

**Methyl 1-phenylbenzo[h]isoquinoline-3-carboxylate (4k)**[1]**:** Following the general procedure, methyl (*Z*)-2-isocyano-3-(naphthalen-2-yl)acrylate **1k** (94.8 mg, 0.4 mmol), phenylhydrazine **2a** (0.157 mL, 1.6 mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 $^oC$ for 21 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1) to give **4k** (56.6 mg, 45%) as a yellow solid. M.p. 193-194 $^oC$. 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 8.55 (s, 1H), 8.0 (d, *J* = 8.5 Hz, 1H), 7.89 (d, *J* = 7.5 Hz, 1H), 7.82 (d, *J* = 9.0 Hz, 1H), 7.77 (d, *J* = 8.5 Hz, 1H), 7.60-7.58 (m, 2H), 7.55-7.52 (m, 1H), 7.49 (t, *J* = 3.0 Hz, 3H), 7.24-7.21 (m, 1H), 4.05 (s, 3H); $^{13}C$ NMR ($CDCl_3$, 125 MHz): δ 166.26, 159.40, 143.33, 141.61, 138.34, 134.34, 132.77, 129.30, 129.21, 129.11, 128.76, 128.74, 128.22, 127.70, 126.35, 126.21, 125.63, 123.03, 52.92. EI-MS *m/z* (%): 313 (41) [$M^+$], 255 (100), 254 (43), 252 (71), 105 (23).




**4l**

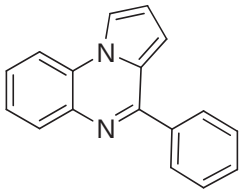
**Methyl 8-methoxy-4-methyl-1-phenylbenzo[h]isoquinoline-3-carboxylate (4l)**[1]**:** Following the general procedure, methyl (*Z*)-2-isocyano-3-(6-methoxy-naphthalen-2-yl)but-2-enoate **1l** (112.4 mg, 0.4 mmol), phenylhydrazine **2a** (0.157 mL, 1.6 mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 $^oC$ for 23 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1) to give **4l** (85.4 mg, 60%) as a yellow solid. M.p. 181-182 $^oC$. 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), 7.93 (d, *J* = 9.0 Hz, 1H), 7.66 (d, *J* = 9.5 Hz, 1H), 7.57-7.54 (m, 2H), 7.47-7.45 (m, 3H), 7.23-7.21 (m, 1H), 6.82 (dd, *J* = 9.5, 2.5 Hz, 1H), 4.01 (s, 3H), 3.90 (s, 3H), 2.91 (s, 3H); $^{13}C$ NMR ($CDCl_3$, 125 MHz): δ 168.02, 158.50, 155.84, 143.63, 141.50, 136.66, 135.13, 131.71, 130.08, 129.21, 129.13, 128.45, 127.67, 125.01, 123.70, 122.02, 116.50, 108.34, 55.36, 52.66, 14.79. EI-MS *m/z* (%): 357 (90) [$M^+$], 299 (100), 297 (73), 254 (36).




**4m**

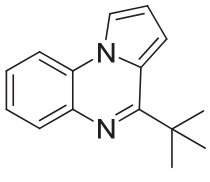
**Methyl 4-benzyl-1-phenylisoquinoline-3-carboxylate (4m)**[1]**:** Following the general procedure, methyl (*Z*)-2-isocyano-3,4-diphenylbut-2-enoate **1m** (110.8 mg,

0.4 mmol), phenylhydrazine **2a** (0.157 mL, 1.6 mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 °C for 22 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 20:1 to 10:1) to give **4m** (75.7 mg, 54%) as a yellow solid. M.p. 96-97 °C. IR (KBr, $cm^{-1}$): 1722.7, 1441.5, 1380.9, 1248.0, 1213.6, 1070.9, 990.9, 771.4, 703.0. $^1H$ NMR ($CDCl_3$, 500 MHz): δ 8.12 (t, *J* = 8.5 Hz, 2H), 7.74-7.71 (m, 2H), 7.69-7.65 (m, 1H), 7.59-7.48 (m, 4H), 7.28-7.21 (m, 4H), 7.20-7.16 (m, 1H), 4.76 (s, 2H), 3.96 (s, 3H); $^{13}C$ NMR ($CDCl_3$, 125 MHz): δ 168.06, 159.77, 142.34, 139.91, 138.95, 136.50, 130.67, 130.23, 129.63, 128.87, 128.56, 128.44, 128.36, 128.15, 127.61, 126.18, 125.22, 52.83, 33.89. EI-MS *m/z* (%): 353 (67) [$M^+$], 321 (100), 320 (57), 293 (24), 292 (72).



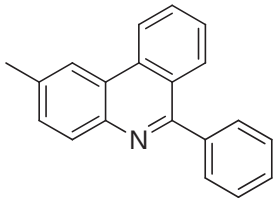
**5a**

**4-Phenylpyrrolo[1,2-*a*]quinoxaline (5a)**[4]**:** Following the general procedure, 1-(2-isocyano-phenyl)-1*H*-pyrrole **1n** (67.2 mg, 0.4 mmol), phenylhydrazine **2a** (0.157 mL, 1.6 mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 °C for 21 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 30:1) to give **5a** (43.1 mg, 44%) as a yellow solid. M.p. 96-97 °C. IR (KBr, $cm^{-1}$): 1524.3, 1462.9, 1363.7, 1317.3, 751.6, 698.9. $^1H$ NMR ($CDCl_3$, 500 MHz): δ 8.07-8.03 (m, 1H), 8.02-7.98 (m, 3H), 7.91-7.86 (m, 1H), 7.58-7.50 (m, 4H), 7.49-7.44 (m, 1H), 7.02-6.98 (m, 1H), 6.92-6.88 (m, 1H); $^{13}C$ NMR ($CDCl_3$, 125 MHz): δ 154.44, 138.50, 136.30, 130.28, 129.81, 128.63, 128.60, 127.49, 127.19, 125.42, 125.29, 114.61, 113.99, 113.65, 108.71. LC-MS (ESI) m/z: 245 [$(M+H)^+$].



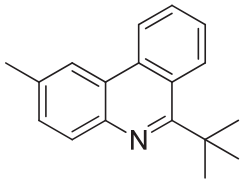
**5b**

**4-(*tert*-Butyl)pyrrolo[1,2-*a*]quinoxaline (5b)**[2]**:** Following the general procedure, 1-(2-isocyano-phenyl)-1*H*-pyrrole **1n** (67.2 mg, 0.4 mmol), *tert*-butylhydrazine hydrochloride **2p** (198.4 mg, 1.6 mmol), sodium bicarbonate (168 mg, 2.0 mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 °C for 27 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 200:1) to give **5b** (32 mg, 36%) as a light yellow oil. IR (KBr, $cm^{-1}$): 1712.2, 1604.8, 1478.1, 1454.5, 1359.7, 1325.6, 1193.1, 1106.4, 1043.4, 943.5, 754.3, 712.4, 405.6. $^1H$ NMR ($CDCl_3$, 500 MHz): δ 7.97-7.93 (m, 1H), 7.90-7.86 (m, 1H), 7.84-7.80 (m, 1H), 7.49-7.38 (m, 2H), 7.07-7.03 (m, 1H), 6.86-6.83 (m, 1H), 1.60 (s, 9H); $^{13}C$ NMR ($CDCl_3$, 125 MHz): δ 162.95, 135.38, 130.11, 127.12, 127.10, 124.83, 123.93, 113.34, 113.04, 112.72, 108.33, 39.32, 29.51. LC-MS (ESI) m/z: 225 [$(M+H)^+$].



**5c**

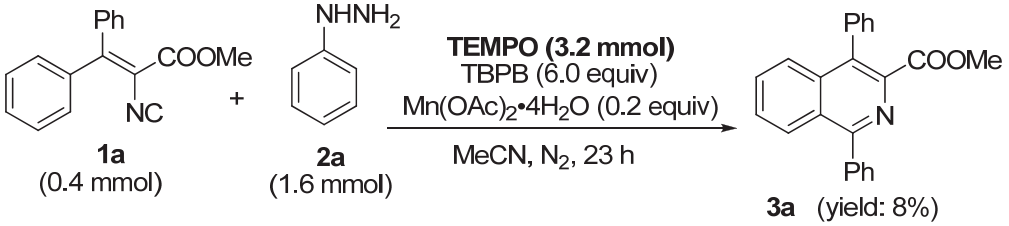
**2-Methyl-6-phenylphenanthridine (5c)**[3]**:** Following the general procedure, 2-isocyano-5-methyl-1,1'-biphenyl **1o** (77.2 mg, 0.4 mmol), phenylhydrazine **2a** (0.157 mL, 1.6 mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 $^oC$ for 25 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 30:1) to give **5c** (60.6 mg, 56%) as a yellow solid. M.p. 86-87 $^oC$. IR (KBr, $cm^{-1}$): 1551.3, 1359.1, 826.2, 767.9, 699.3, 578.6. $^1H$ NMR ($CDCl_3$, 500 MHz): δ 8.68 (d, *J* = 8.5 Hz, 1H), 8.39 (s, 1H), 8.15 (d, *J* = 8.5 Hz, 1H), 8.12-8.07 (m, 1H), 7.86-7.80 (m, 1H), 7.76-7.71 (m, 2H), 7.62-7.50 (m, 5H), 2.65 (s, 3H); $^{13}C$ NMR ($CDCl_3$, 125 MHz): δ 160.32, 142.13, 139.93, 136.83, 133.19, 130.59, 130.33, 130.09, 129.78, 128.84, 128.61, 128.43, 126.97, 125.31, 123.58, 122.17, 121.58, 22.05. LC-MS (ESI) m/z: 270 [$(M+H)^+$].



**5d**

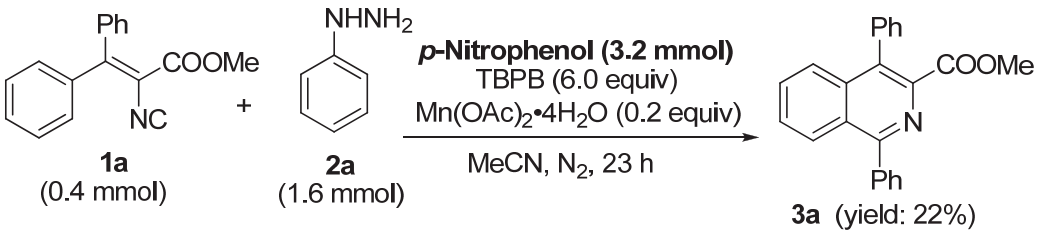
**6-(*tert*-butyl)-2-methylphenanthridine (5d)**[5]**:** Following the general procedure, 2-isocyano-5-methyl-1,1'-biphenyl **1o** (77.2 mg, 0.4 mmol), *tert*-butylhydrazine hydrochloride **2p** (198.4 mg, 1.6 mmol), sodium bicarbonate (168 mg, 2.0 mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 20 mol%) and TBPB (0.448 mL) were stirred in dry MeCN (3.0 mL) at 70 $^oC$ for 27 h. Purification by chromatography on silica gel (eluent: hexane/EtOAc = 200:1) to give **5d** (77.5 mg, 78%) as a light yellow oil. IR (KBr, $cm^{-1}$): 1711.8, 1523.9, 1482.7, 1446.6, 1360.1, 1190.9, 1103.6, 1043.1, 945.4, 756.1, 711.5. $^1H$ NMR ($CDCl_3$, 500 MHz): δ 8.67 (q, 2H), 8.33 (s, 1H), 8.09 (d, *J* = 8.0 Hz, 1H), 7.74-7.80 (m, 1H), 7.69-7.62 (m, 1H), 7.58-7.54 (m, 1H), 2.64 (s, 3H), 1.80 (s, 9H); $^{13}C$ NMR ($CDCl_3$, 125 MHz): δ 165.64, 141.34, 136.19, 133.86, 130.11, 130.10, 129.06, 128.24, 125.81, 124.44, 123.27, 122.99, 121.32, 40.14, 31.30, 22.05. LC-MS (ESI) m/z: 250 [$(M+H)^+$].

## 4. Mechanistic Studies




The tube containing a mixture of methyl 2-isocyano-3,3-diphenylacrylate (**1a**) (105.2

mg, 0.4 mmol), phenyl hydrazine (**2a**) (0.157 mL, 1.6 mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 0.2 equiv) and 2,2,6,6-tetramethyl-piperidine-1-oxy (TEMPO) (500.0 mg, 3.2 mmol) in dry MeCN (3.0 mL) was evacuated and backfilled with $N_2$ for three times. The reaction mixture was stirred in a pre-heated oil bath at 70 $^oC$ for 23 h. The reaction was cooled to room temperature, washed with saturated sodium bicarbonate solution (50 mL) and then extracted with EtOAc (3×20 mL). The combined organic layers were dried over $Na_2SO_4$ and then purified by chromatography on silica gel (eluent: PE/EA = 20:1) to give the product **3a** (10.8 mg, 8%).




The tube containing a mixture of methyl 2-isocyano-3,3-diphenylacrylate (**1a**) (105.2 mg, 0.4 mmol), Phenyl hydrazine (**2a**) (0.157 mL, 1.6 mmol), $Mn(OAc)_2{\cdot}4H_2O$ (19.6 mg, 0.2 equiv.) and *p*-nitrophenol (445.2 mg, 3.2 mmol) in dry MeCN (3.0 mL) was evacuated and backfilled with $N_2$ for three times. The reaction mixture was stirred in a pre-heated oil bath at 70 $^oC$ for 23 h. The reaction was cooled to room temperature, washed with saturated sodium bicarbonate solution (50 mL) and then extracted with EtOAc (3×20 mL). The combined organic layers were dried over $Na_2SO_4$ and then purified by chromatography on silica gel (eluent: PE/EA = 10:1) to give the product **3a** (29.9 mg, 22%).

## 5. References:

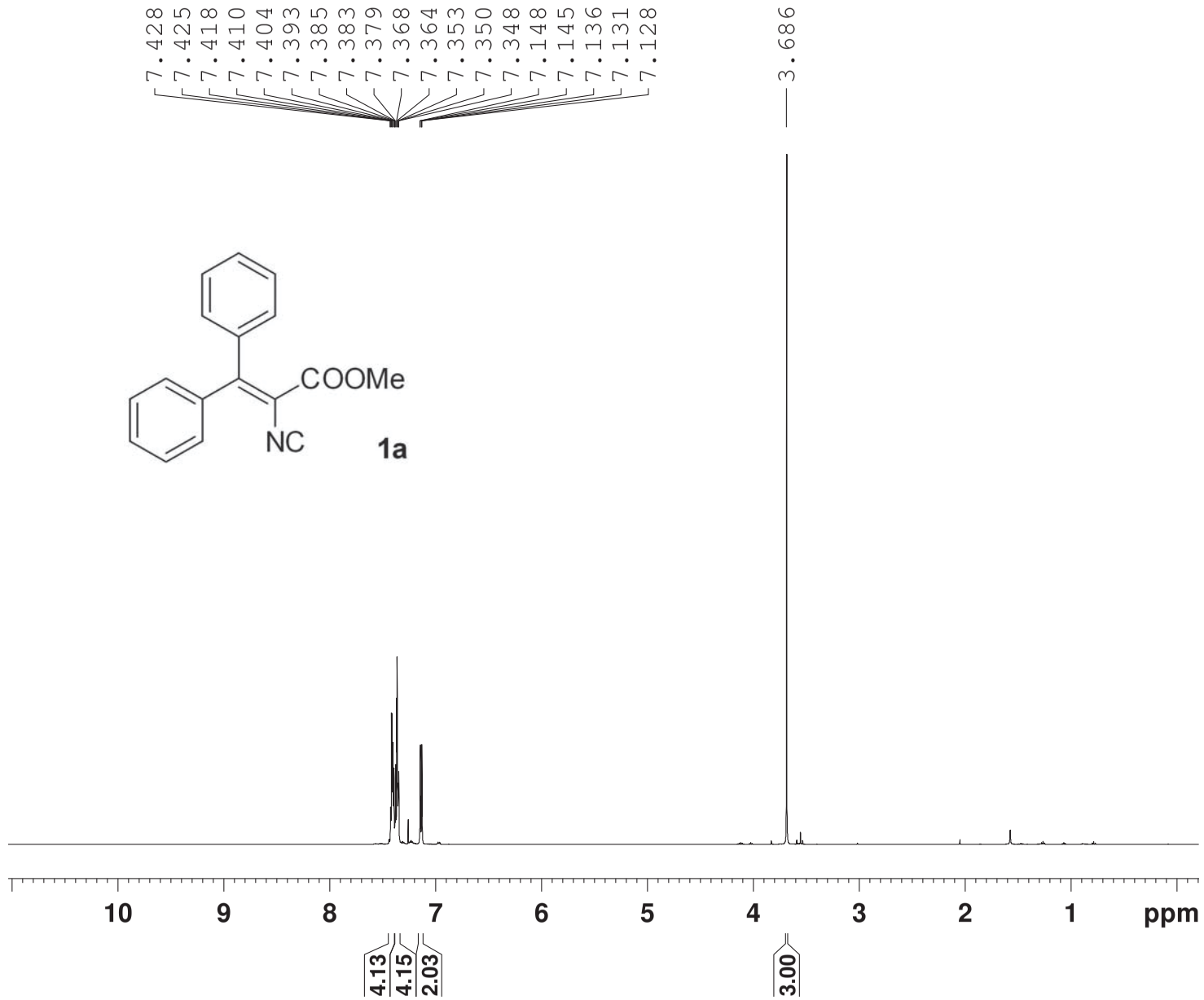

(1) H. Wang, Y. Yu, X. Hong, Y. Zhang and B. Xu, *Chem. Commun.*, 2014, **50**, 13485.

(2) Z. He, M. Bae, J. Wu, and T. F. Jamison, *Angew. Chem., Int. Ed.*, 2014, **53**, 14451.

(3) M. Tobisu, K. Koh, T. Furukawa and N. Chatani, *Angew. Chem. Int. Ed.*, 2012, **51**, 11363.

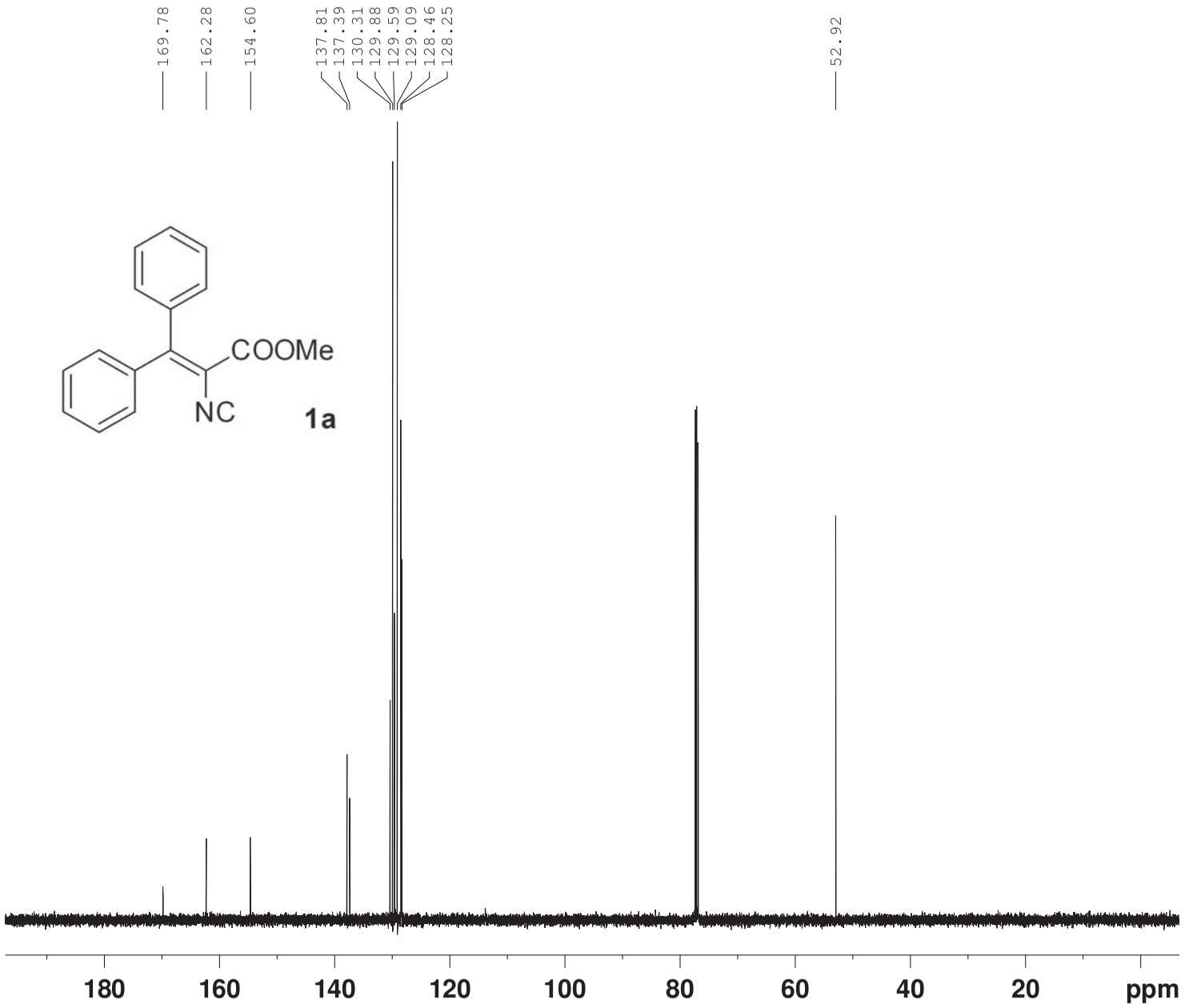
(4) Z. Zhang, J. Li, G. Zhang, N. Ma, Q. Liu and T. Liu, *J. Org. Chem.*, 2015, **80**, 6875.

(5) R. Haridharan, K. Muralirajan and C. H. Cheng, *Adv. Synth. Catal.*, 2015, **357**, 366.



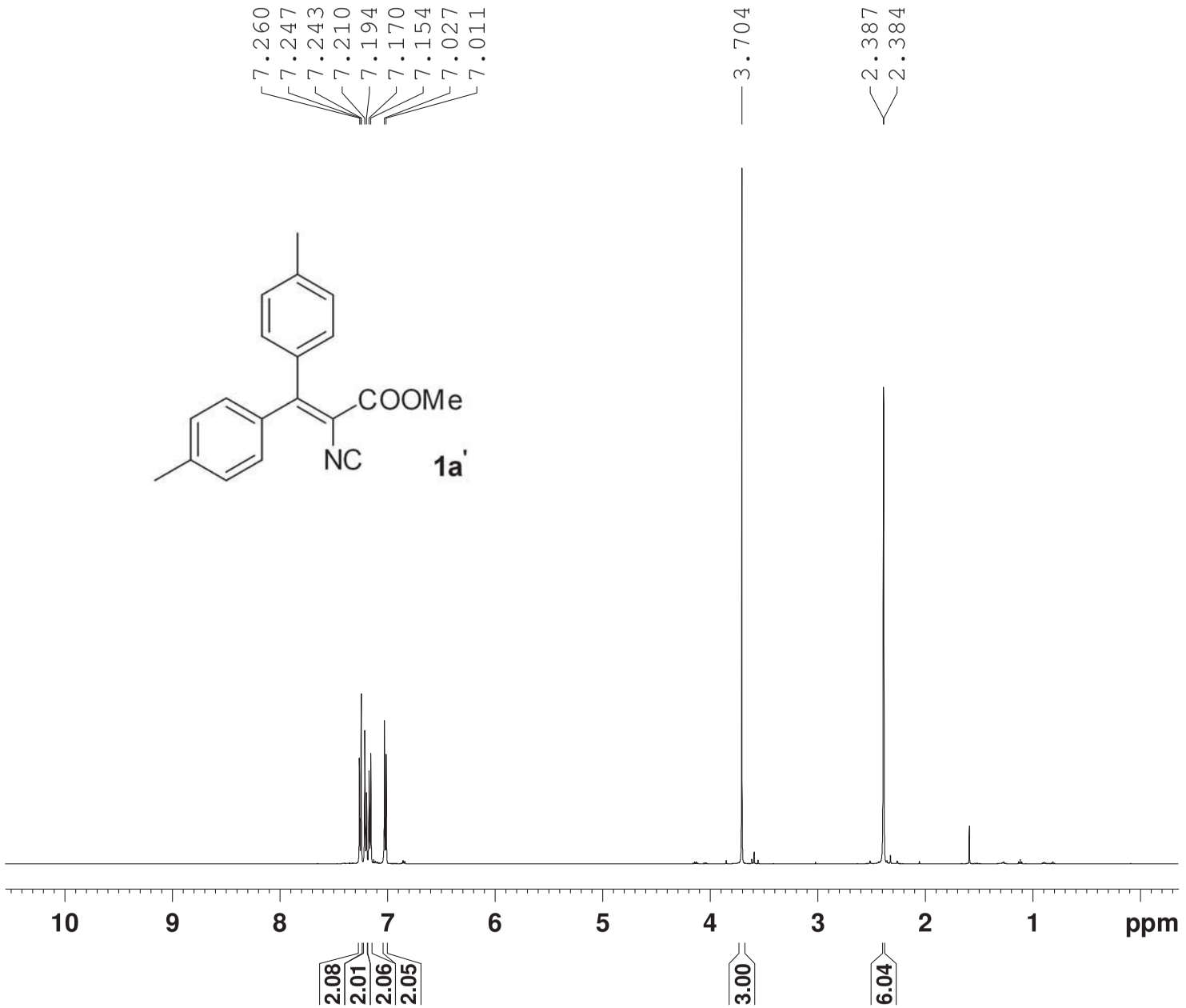

WH-6-51-S
PROTON CDCl3

| | |
|---|---|
| NAME | XB20140527 |
| EXPNO | 6 |
| PROCNO | 1 |
| Date_ | 20140527 |
| Time | 11.19 |
| 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 |



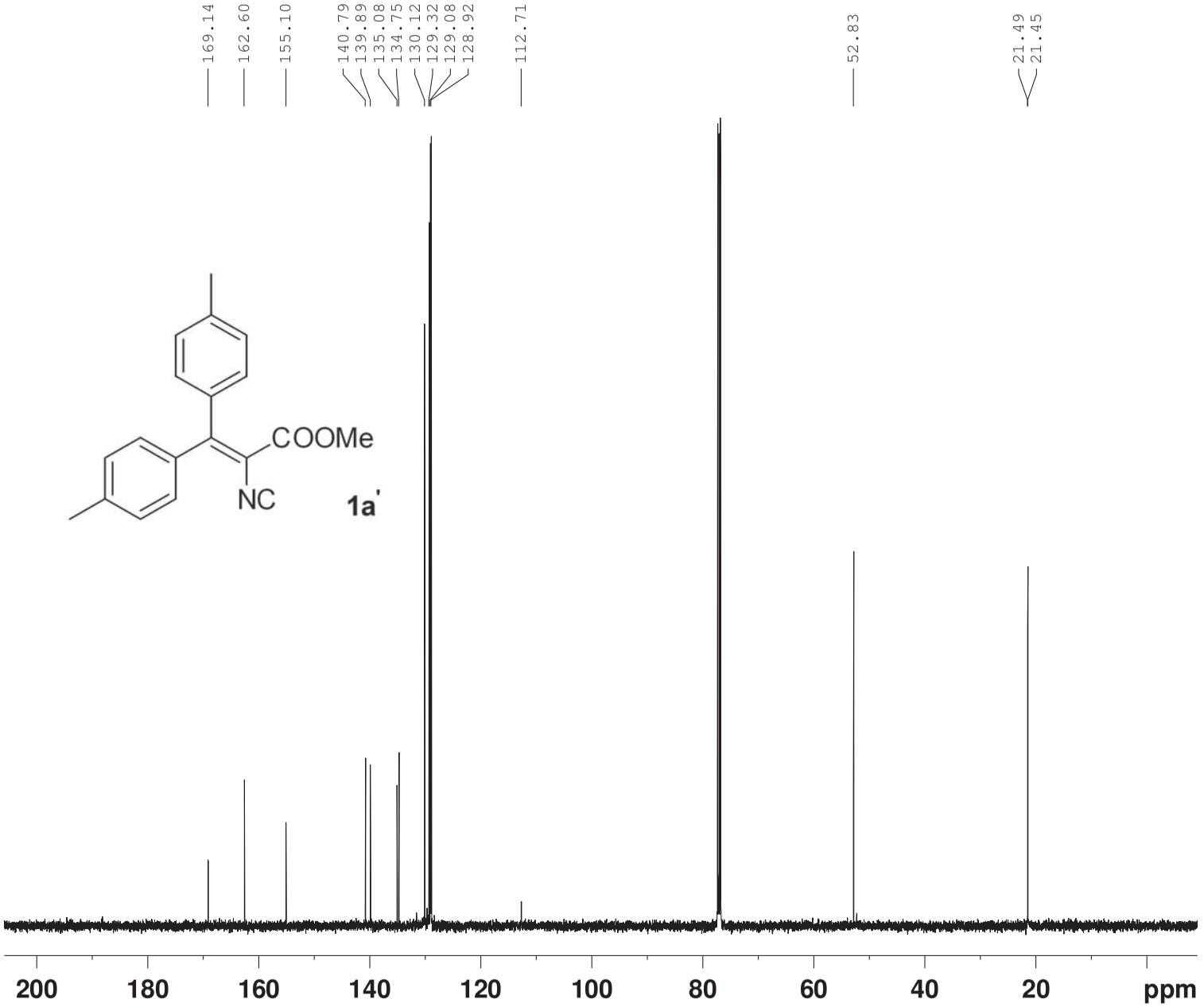

WH-6-51-S
C13CPD CDCl3

| | |
|---|---|
| NAME | XB20140529 |
| EXPNO | 9 |
| PROCNO | 1 |
| Date_ | 20140529 |
| Time | 18.09 |
| 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 | 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 | no |
| SSB | 0 |
| LB | 0.00 Hz |
| GB | 0 |
| PC | 1.40 |



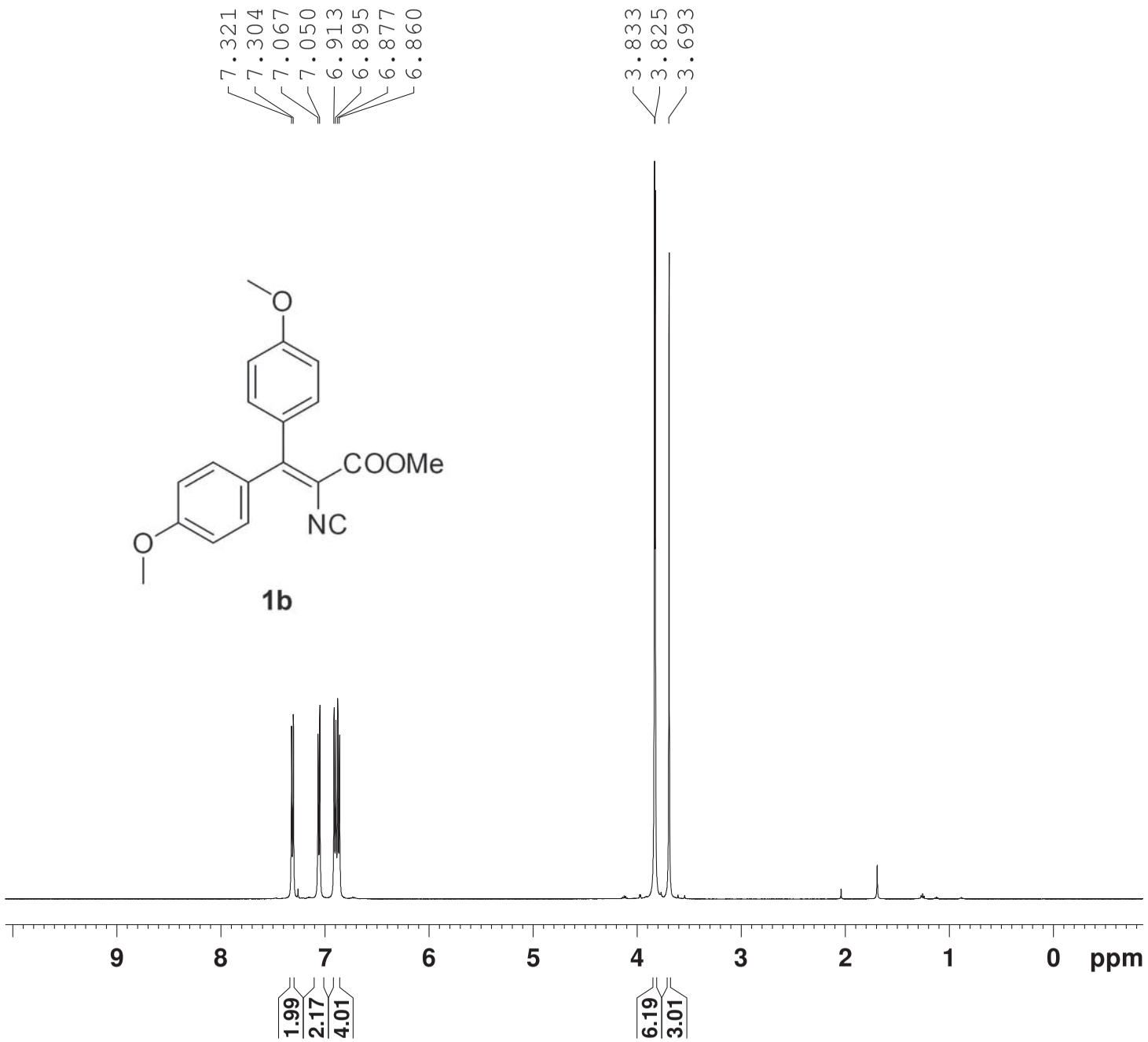

YY-1-90
PROTON CDCl3

| | |
|---|---|
| NAME | XB20140529 |
| EXPNO | 4 |
| PROCNO | 1 |
| Date_ | 20140529 |
| Time | 15.54 |
| 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 | 143.7 |
| 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 |



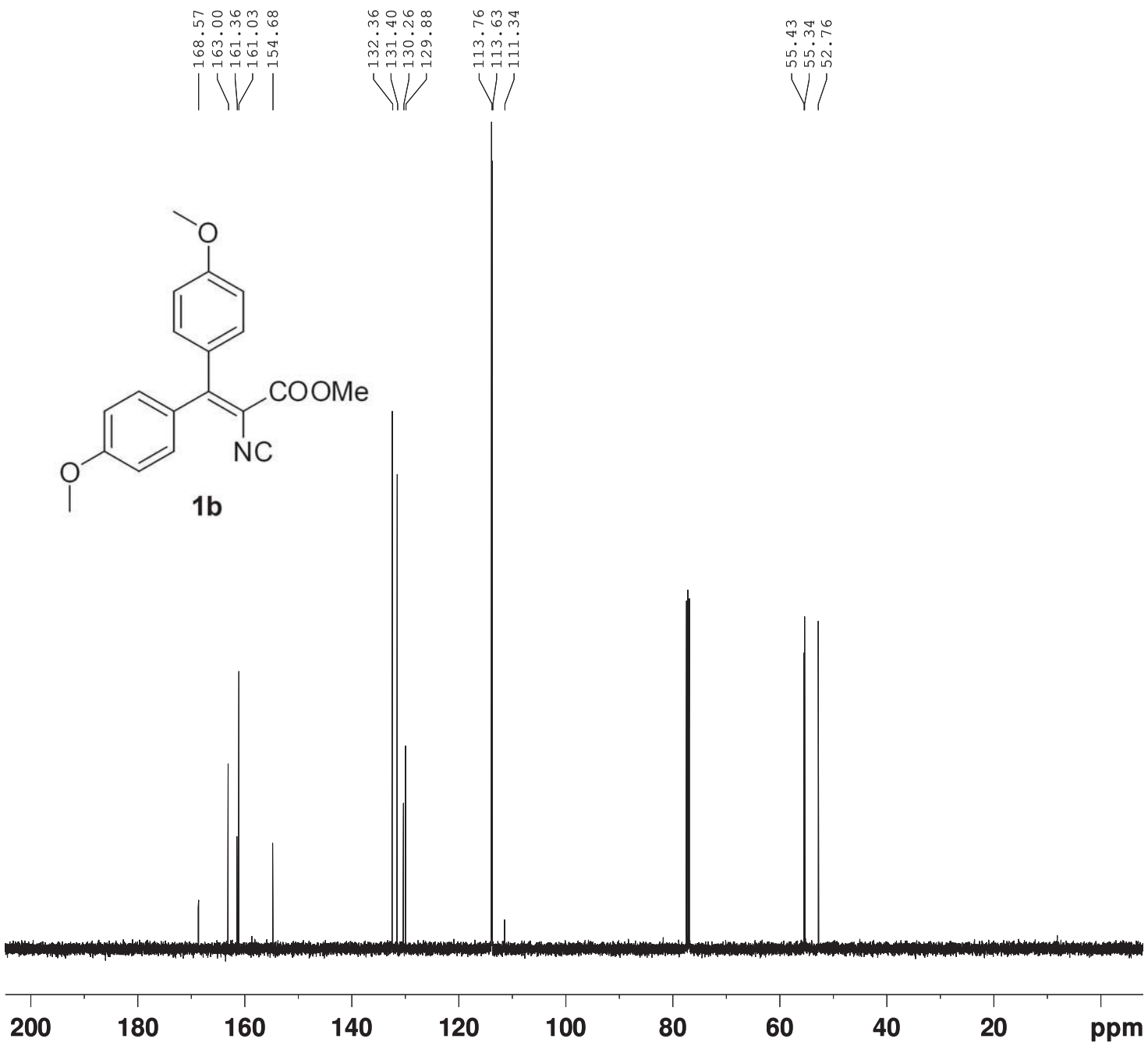

YY-1-90
C13CPD CDCl3

| | |
|---|---|
| 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 |



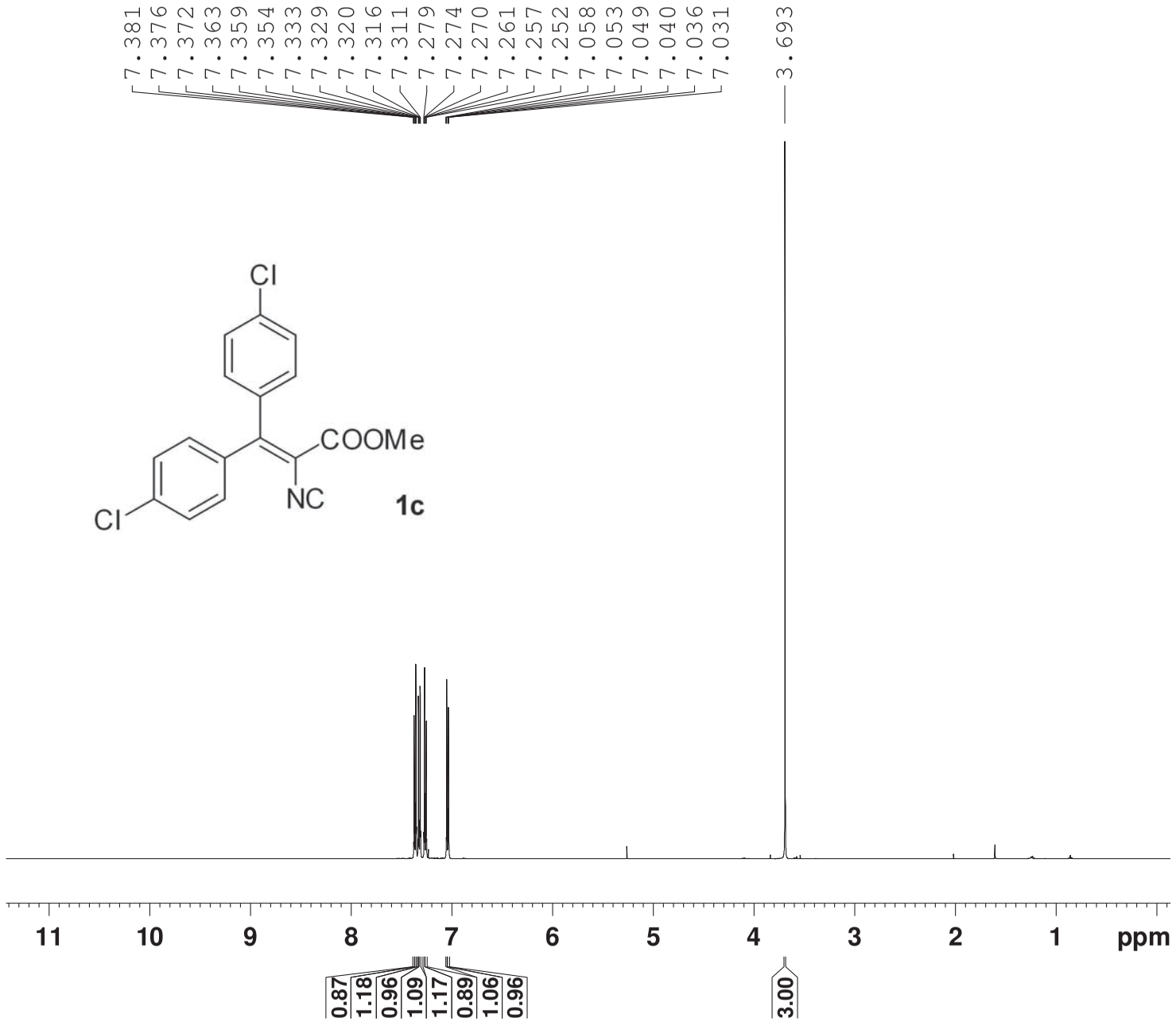

MH-2-42-S
PROTON CDCl3

| | |
|---|---|
| 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 |




MH-2-42-S
C13CPD CDCl3

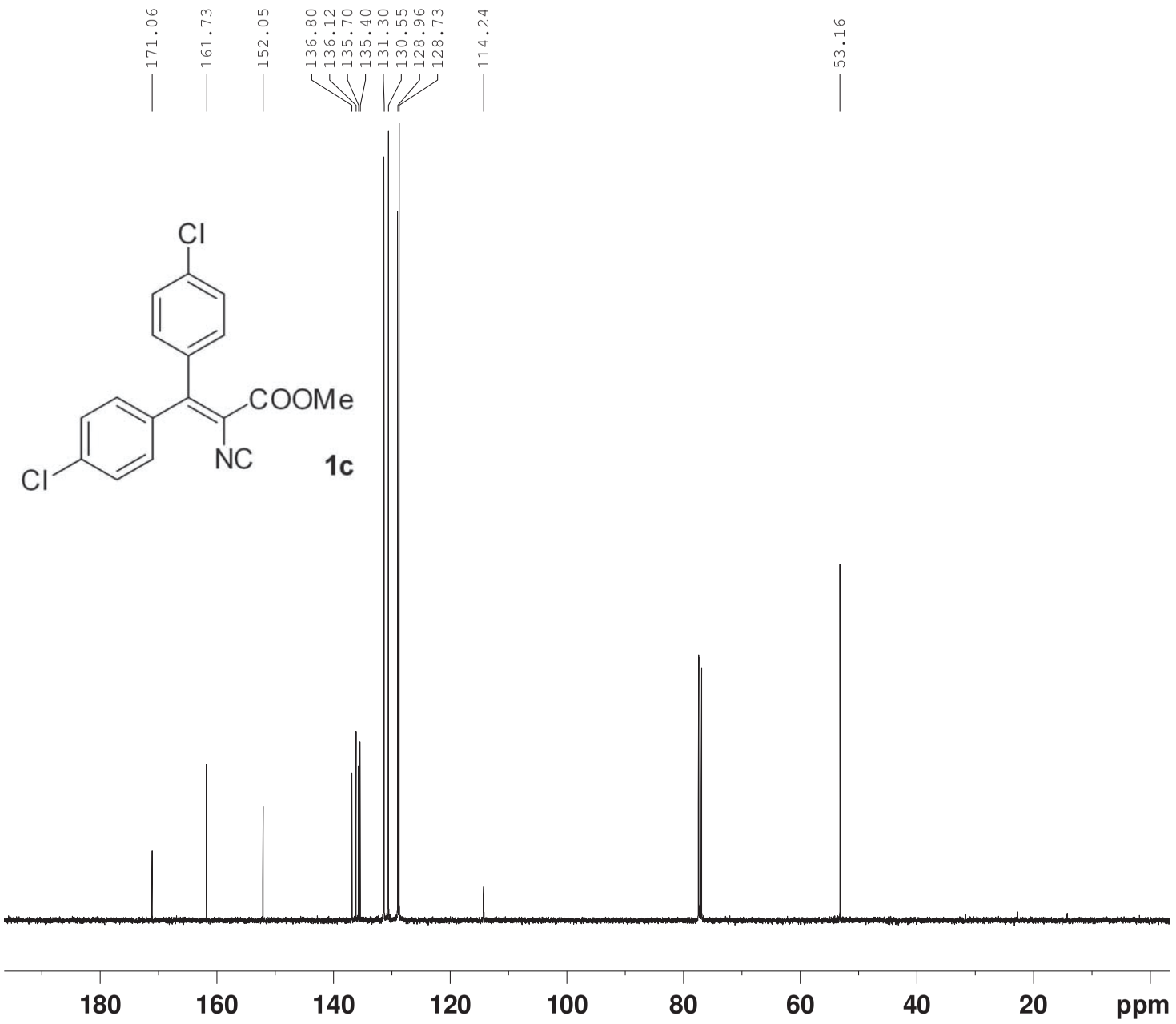
| | |
|---|---|
| NAME | XB20140707 |
| EXPNO | 20 |
| PROCNO | 1 |
| Date_ | 20140707 |
| Time | 15.22 |
| INSTRUM | spect |
| PROBHD | 5 mm PATXO 19F |
| PULPROG | zgpg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 256 |
| DS | 4 |
| SWH | 30030.029 Hz |
| FIDRES | 0.458222 Hz |
| AQ | 1.0912410 sec |
| 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 |




YY-1-98
PROTON CDCl3

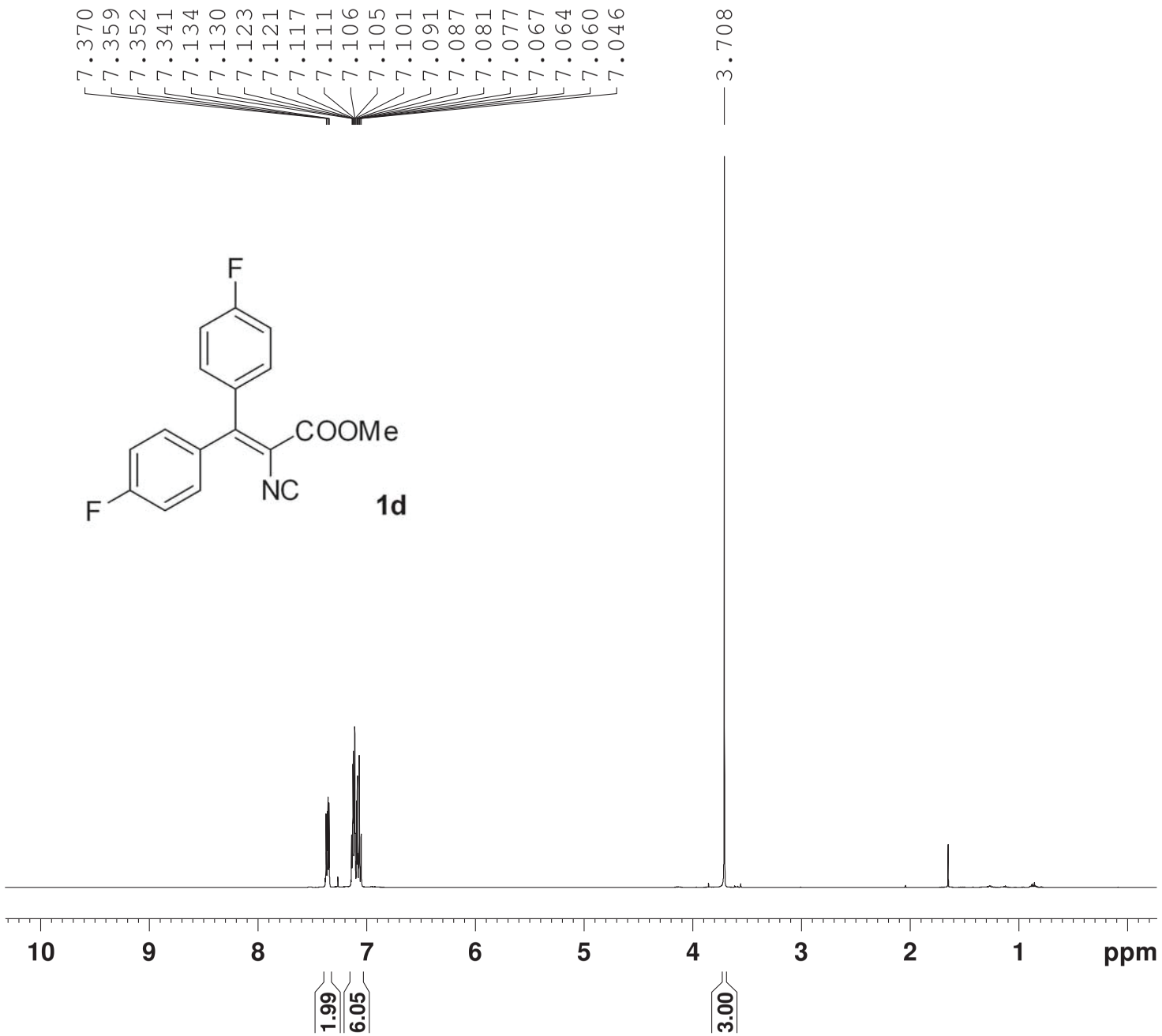
| | |
|---|---|
| NAME | XB20140609-evening |
| EXPNO | 20 |
| PROCNO | 1 |
| Date_ | 20140609 |
| Time | 11.53 |
| INSTRUM | spect |
| PROBHD | 5 mm PATXO 19F |
| PULPROG | zg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 10330.578 Hz |
| FIDRES | 0.157632 Hz |
| AQ | 3.1720407 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 | 500.1300250 MHz |
| WDW | no |
| SSB | 0 |
| LB | 0.00 Hz |
| GB | 0 |
| PC | 1.00 |



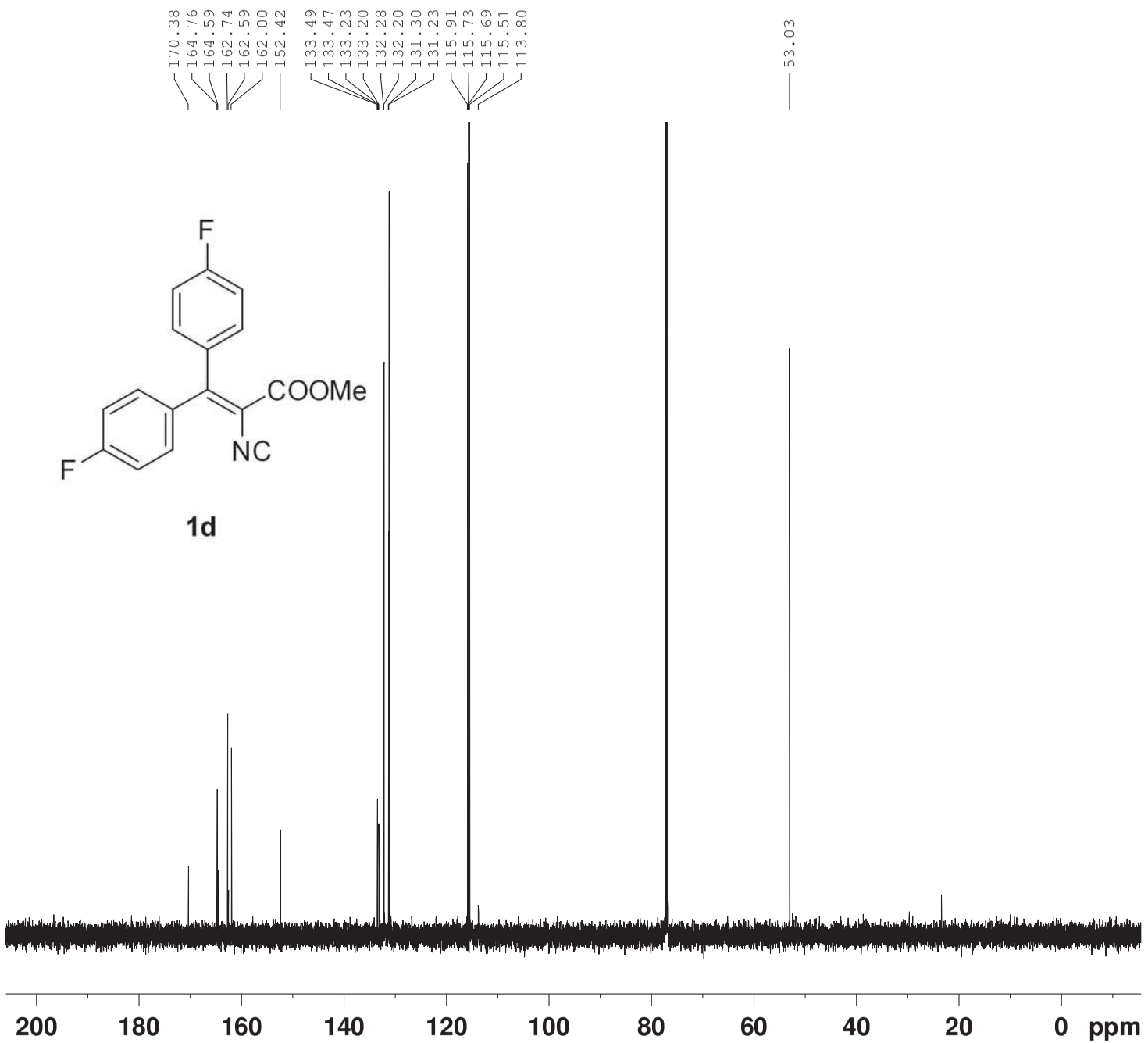

YY-1-98
C13CPD CDCl3

| | |
|---|---|
| NAME | XB20140609-evening |
| 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 |



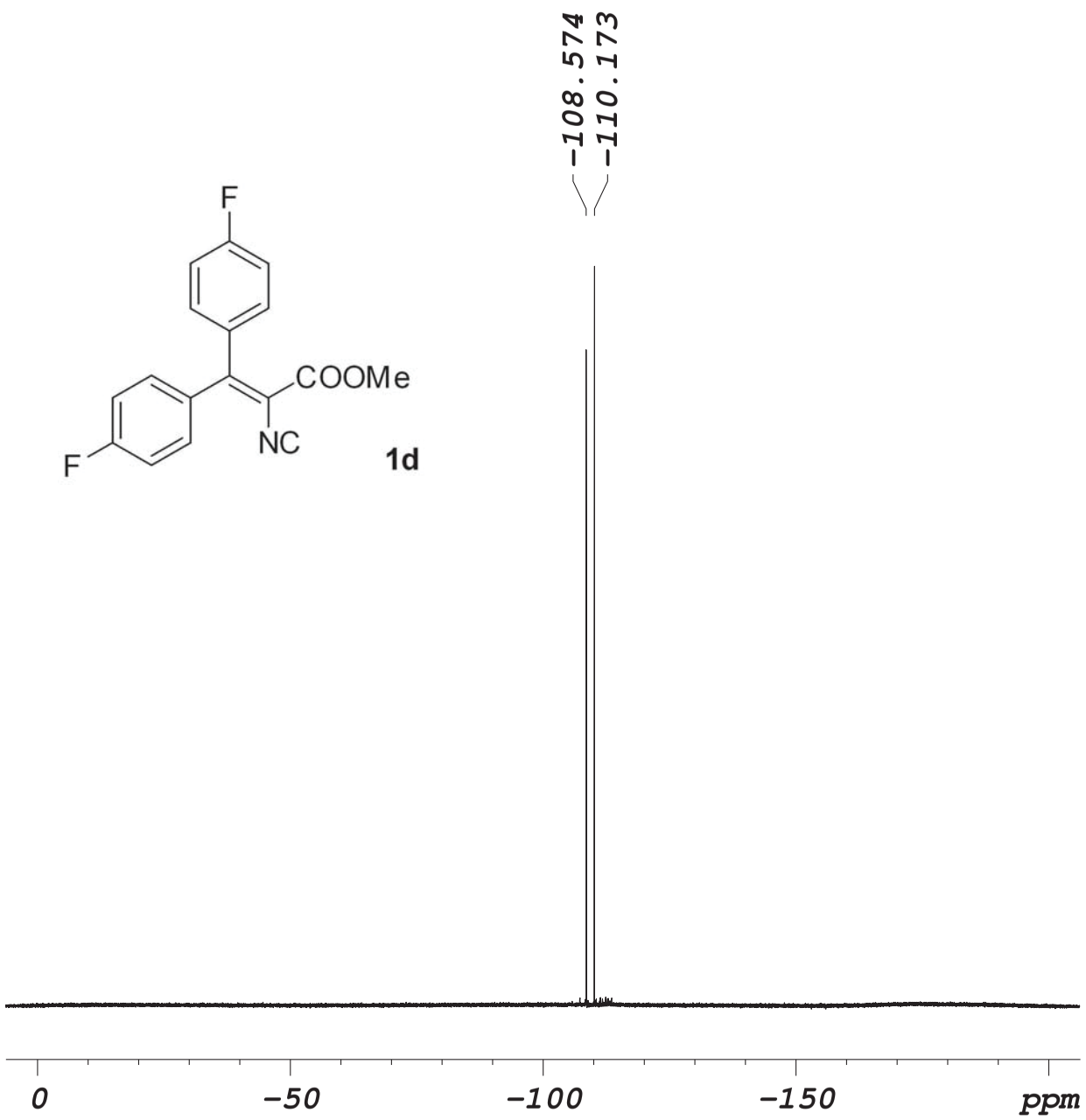

MH-2-44
PROTON CDCl3

| | |
|---|---|
| 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 | 500.1300127 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 |

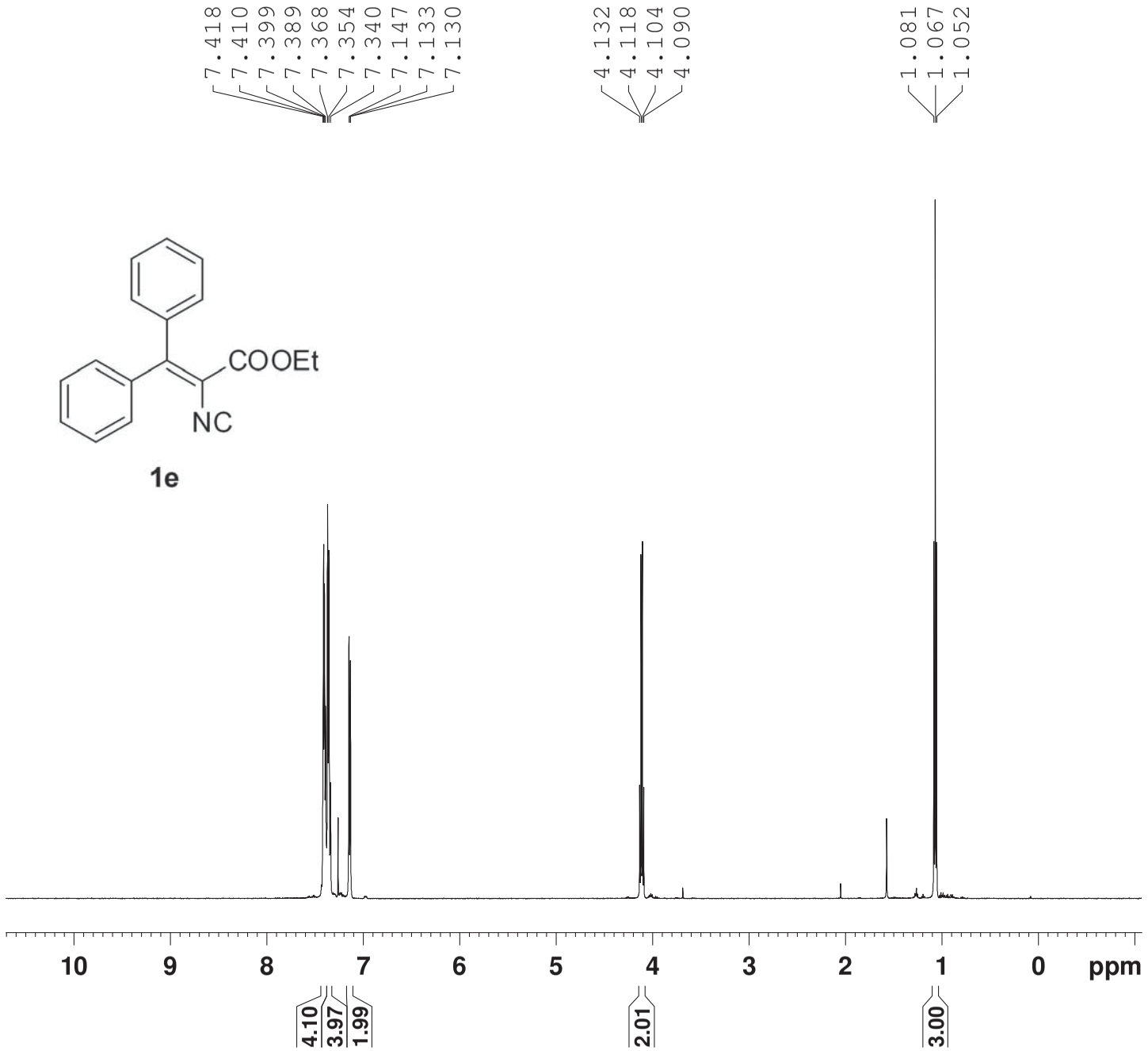



YY-1-94
19Fdeft CDC13 D:\\ deng 46

| | |
|---|---|
| NAME | XB20140627 |
| EXPNO | 18 |
| PROCNO | 1 |
| Date_ | 20140627 |
| Time | 11.05 |
| INSTRUM | spect |
| PROBHD | 5 mm PATXO 19F |
| PULPROG | zg |
| TD | 131072 |
| SOLVENT | CDC13 |
| 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 ========

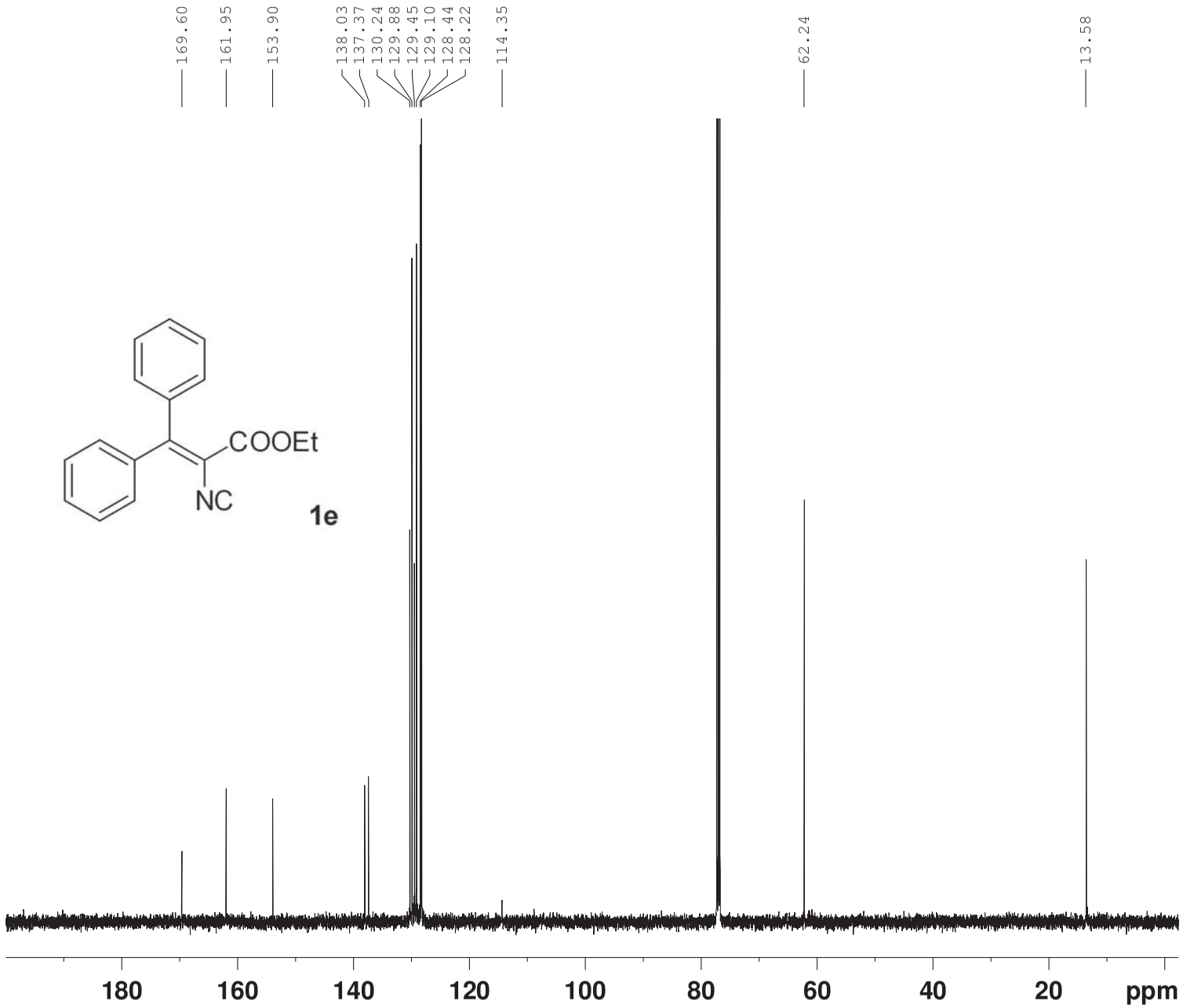
| | |
|---|---|
| NUC1 | 19F |
| P1 | 19.30 usec |
| PL1 | 4.00 dB |
| SFO1 | 470.5453180 MHz |
| SI | 65536 |
| SF | 470.5923770 MHz |




WH-6-29-S
PROTON CDCl3

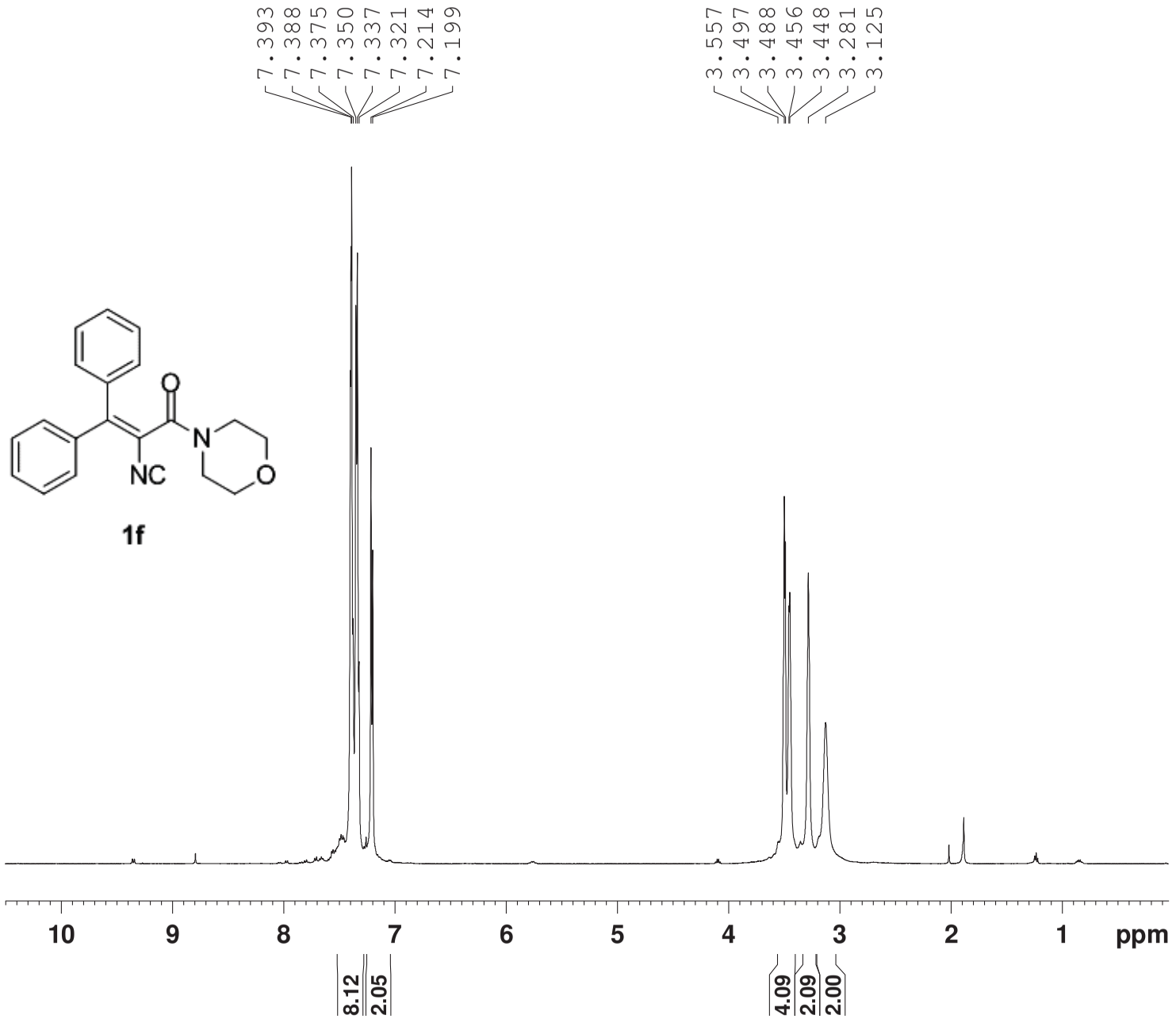
| | |
|---|---|
| NAME | XB20140526 |
| EXPNO | 20 |
| PROCNO | 1 |
| Date_ | 20140526 |
| Time | 17.24 |
| INSTRUM | spect |
| PROBHD | 5 mm PATXO 19F |
| PULPROG | zg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 10330.578 Hz |
| FIDRES | 0.157632 Hz |
| AQ | 3.1720407 sec |
| 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 |



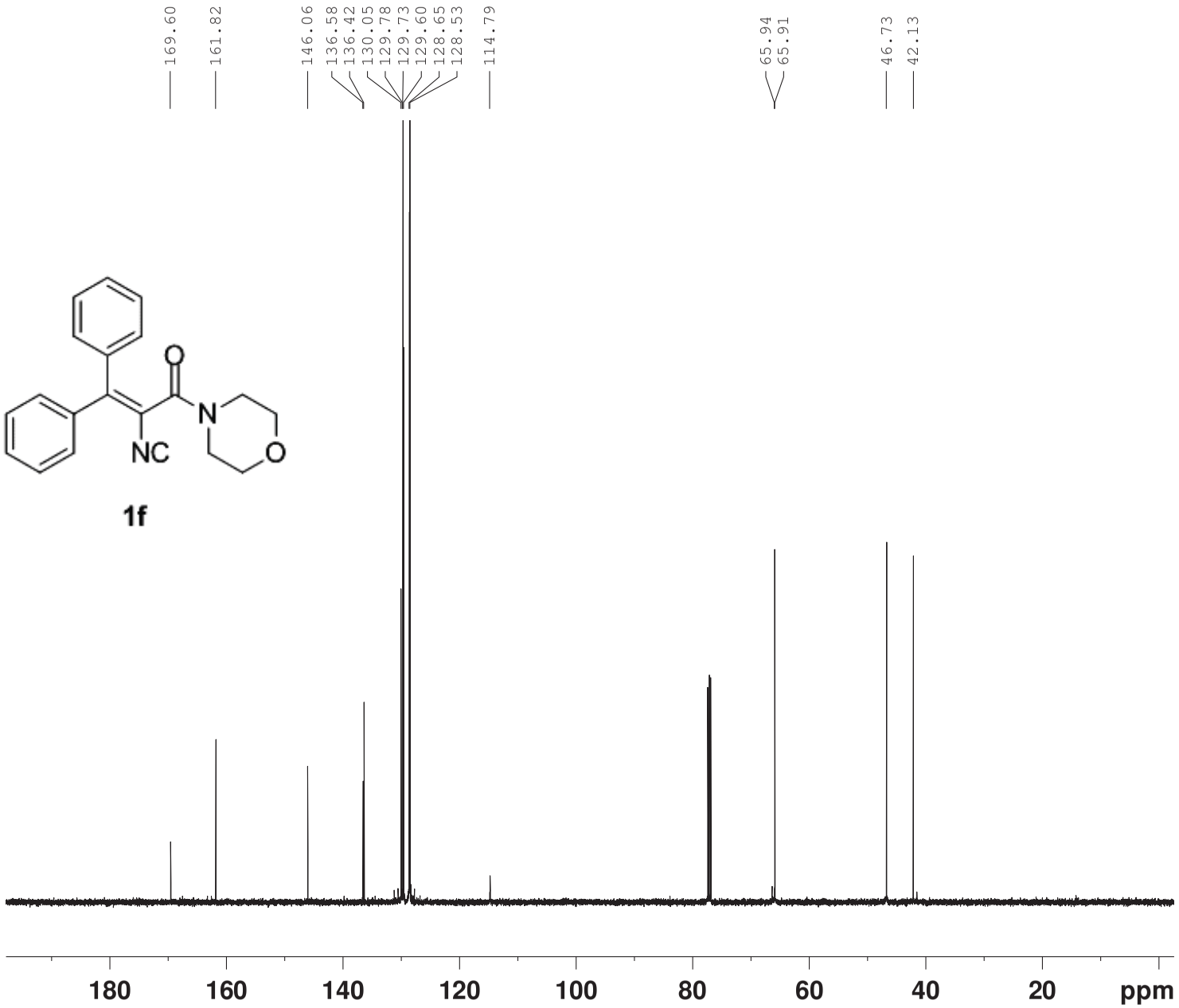

WH-6-29-S
C13CPD CDCl3

| | |
|---|---|
| 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 |



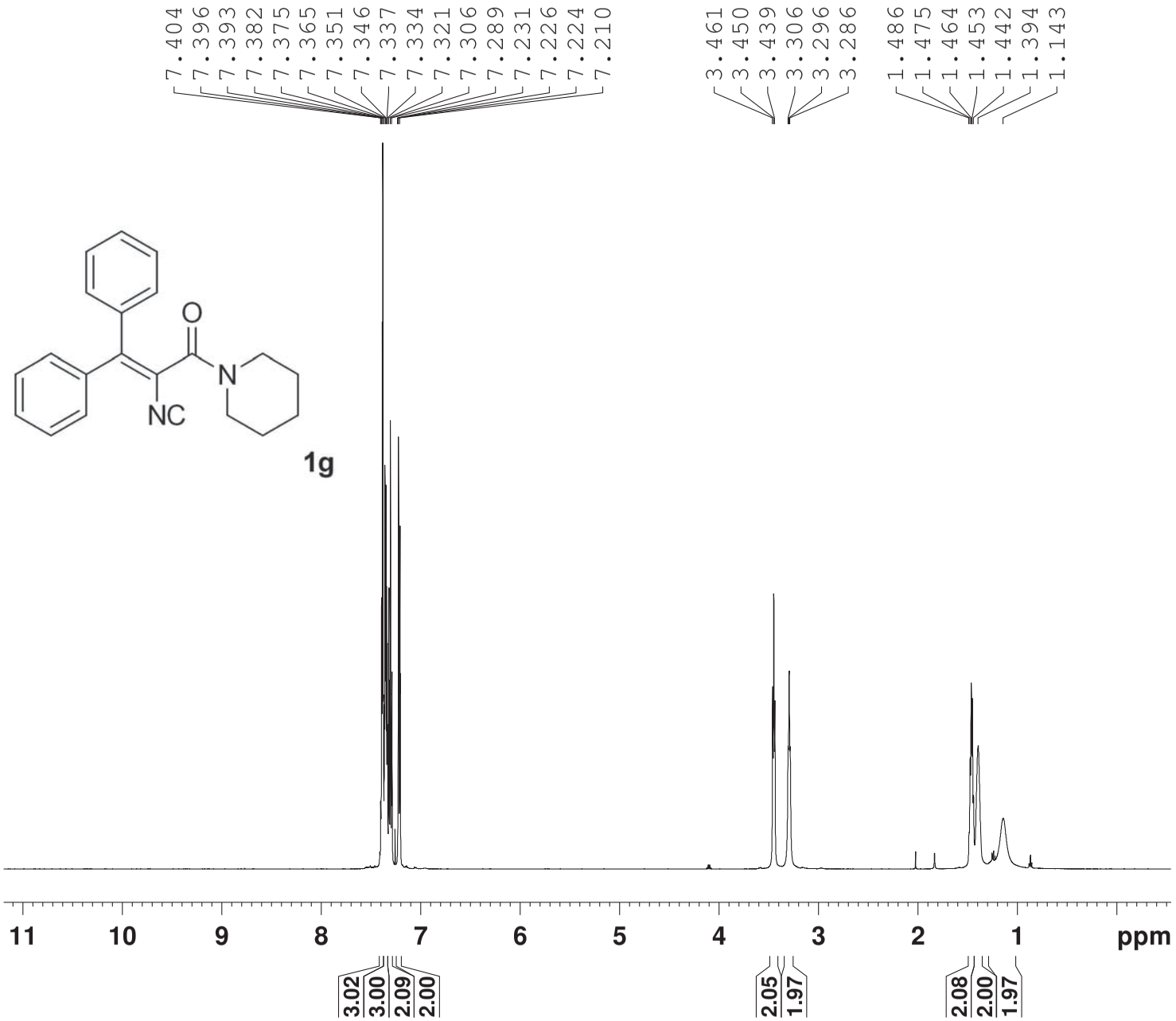

WH-7-5
PROTON CDCl3

| | |
|---|---|
| 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 | 500.1300127 MHz |
| WDW | no |
| SSB | 0 |
| LB | 0.00 Hz |
| GB | 0 |
| PC | 1.00 |



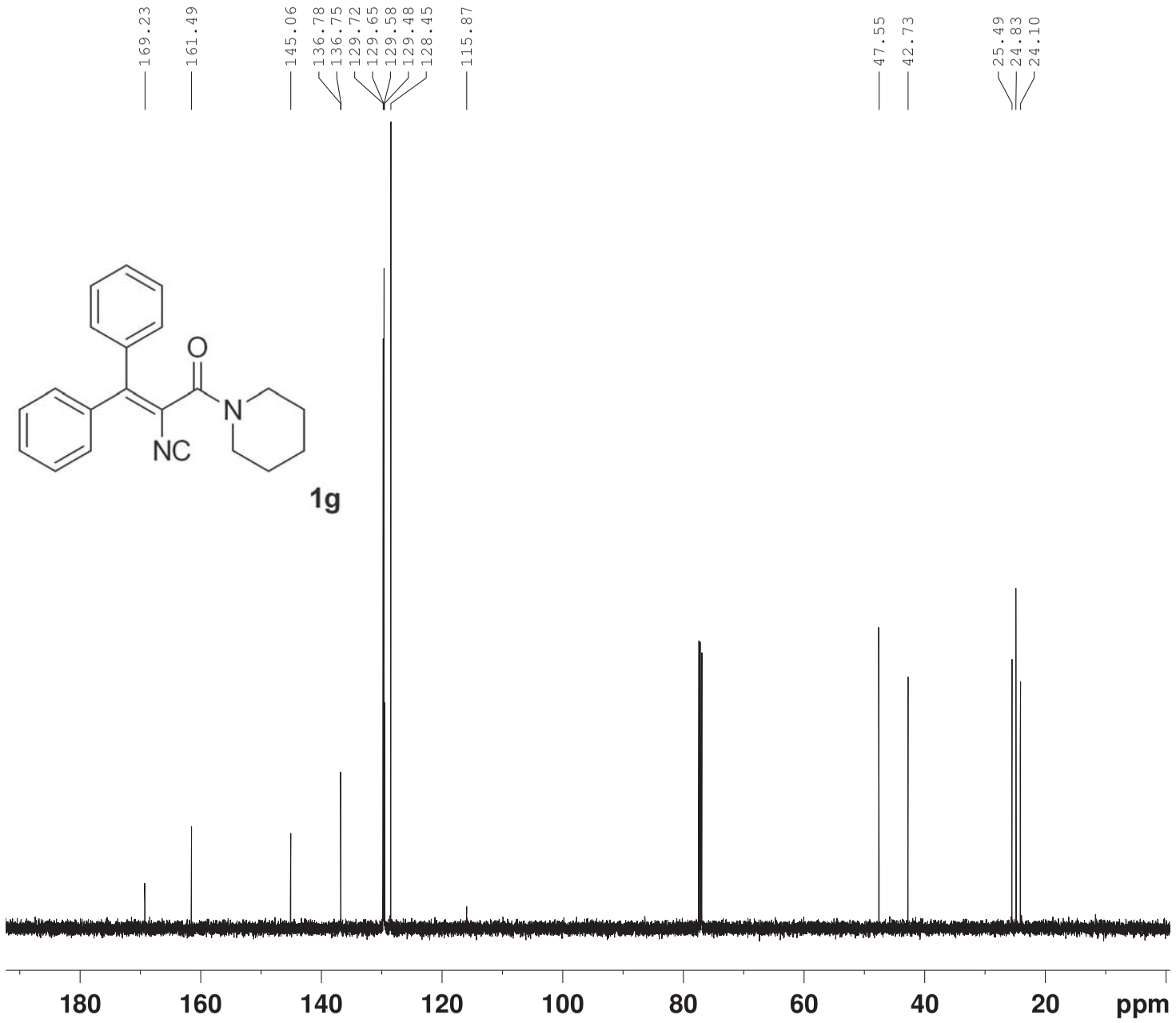

WH-7-5
C13CPD CDCl3

| | |
|---|---|
| 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 |



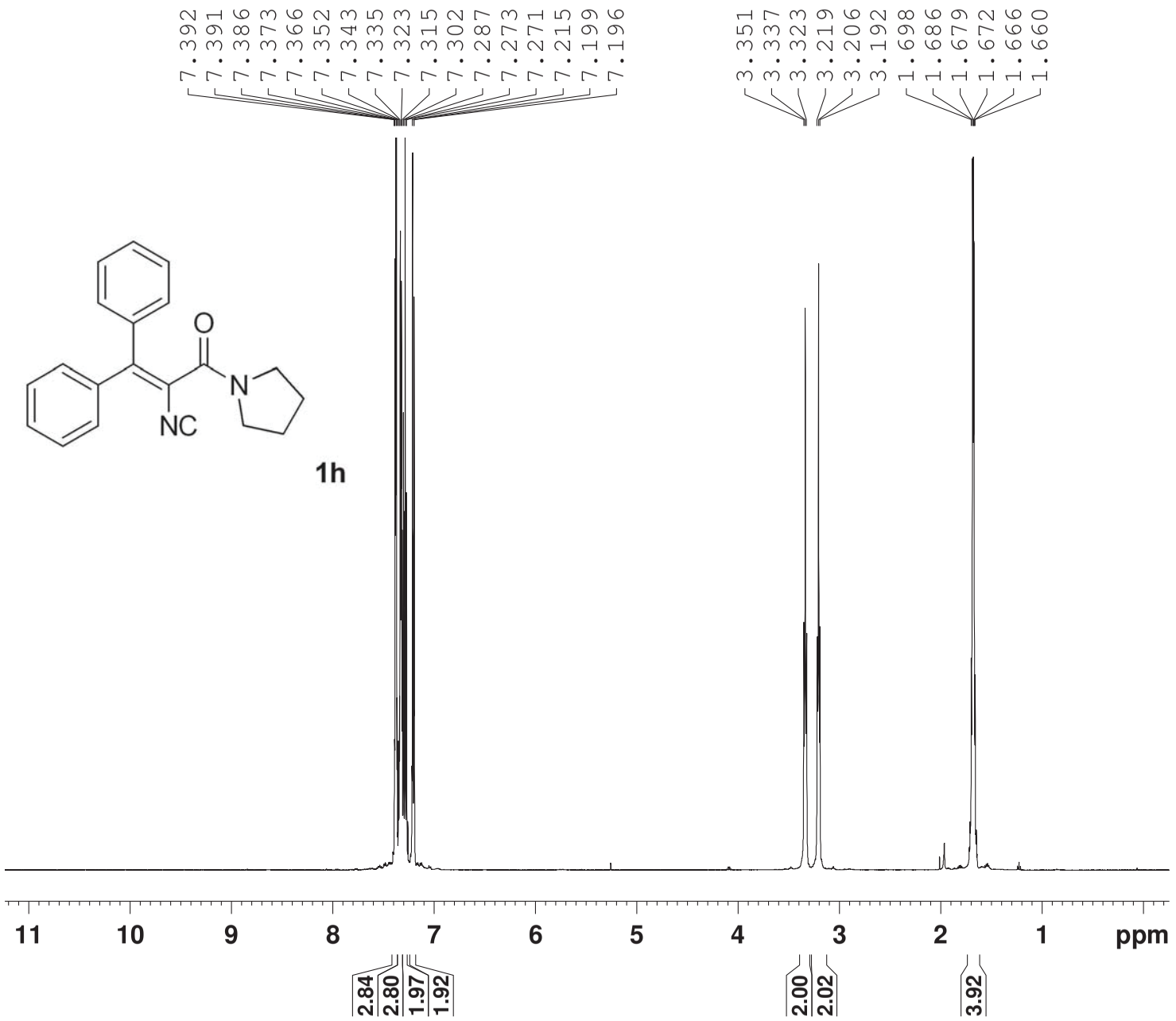

WH-7-7
PROTON CDCl3

| | | |
|---|---|---|
| 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 | |



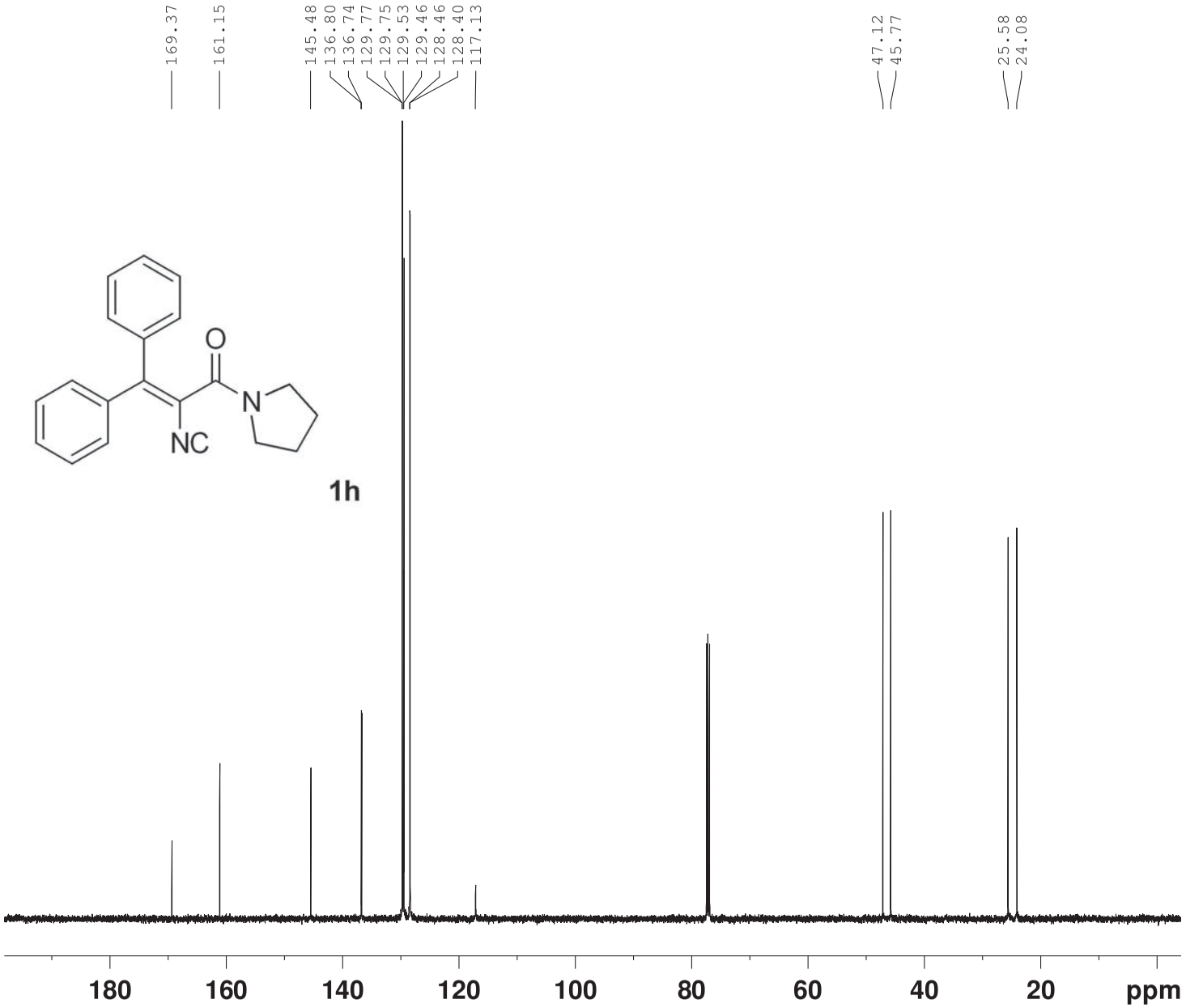

WH-7-7
C13CPD CDCl3

| | |
|---|---|
| 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 |



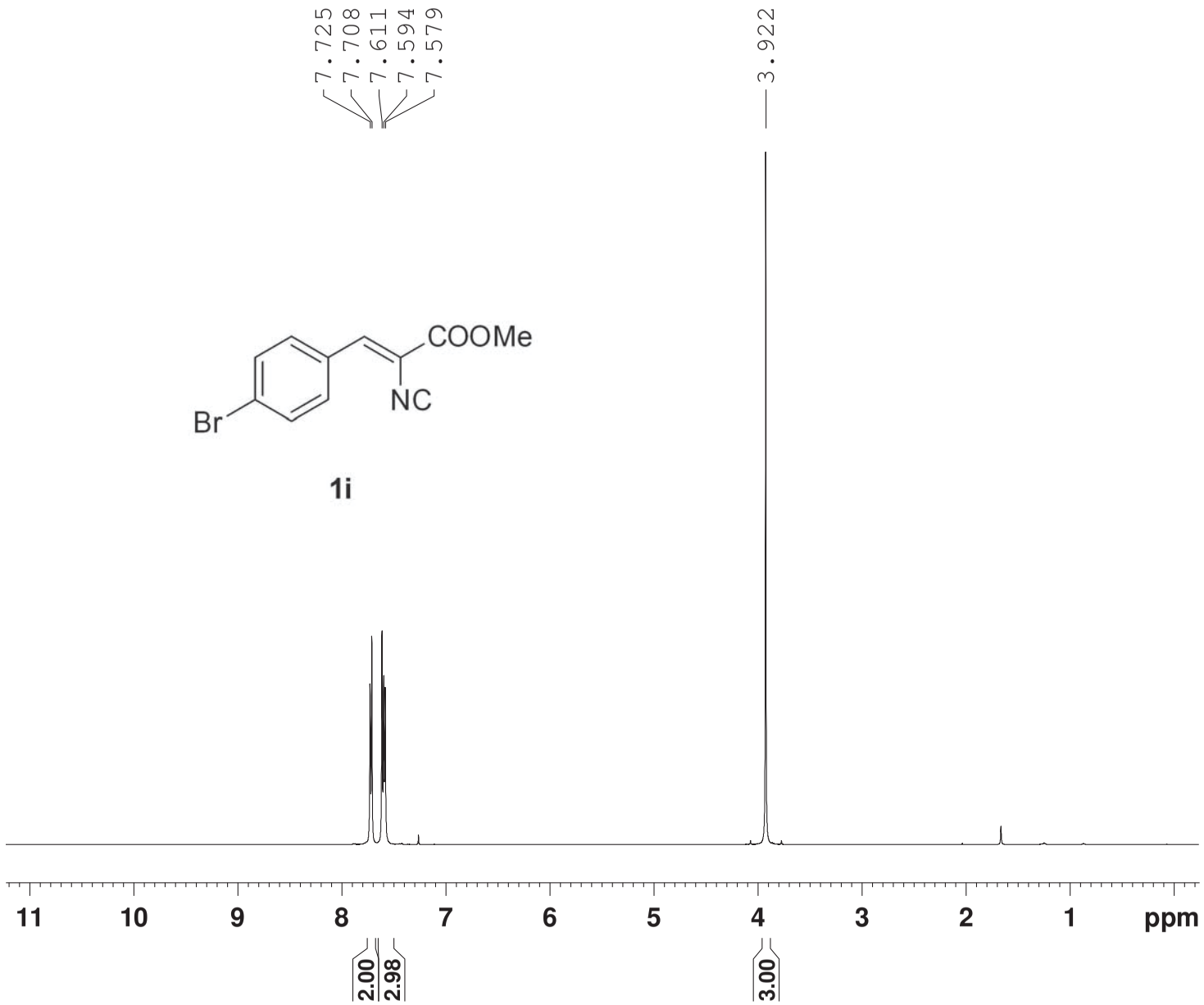

WH-7-23
PROTON CDCl3

| | |
|---|---|
| NAME | XB20140609-evening |
| 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 |



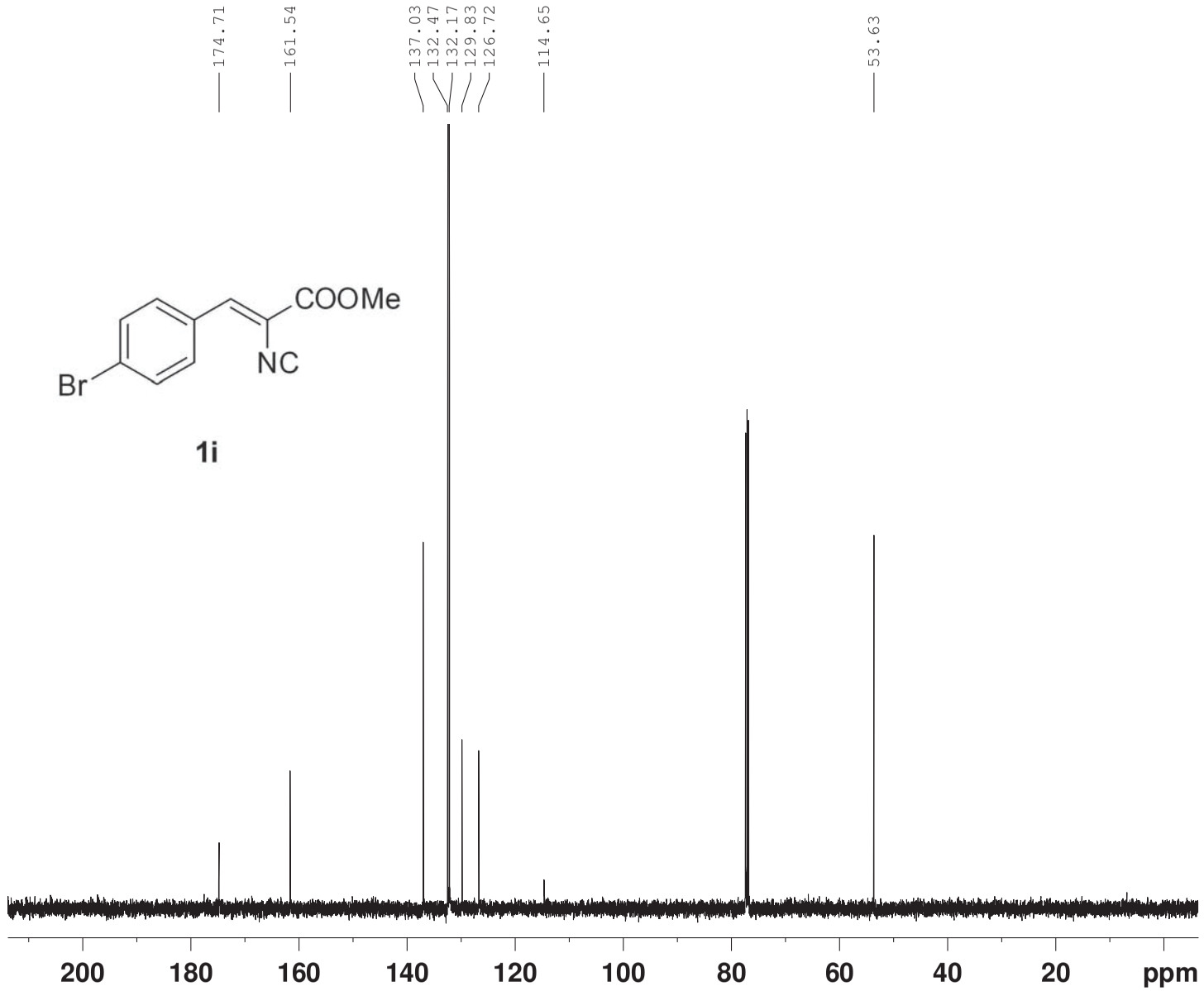

WH-7-23
C13CPD CDCl3

| | |
|---|---|
| NAME | XB20140609-evening |
| 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 |



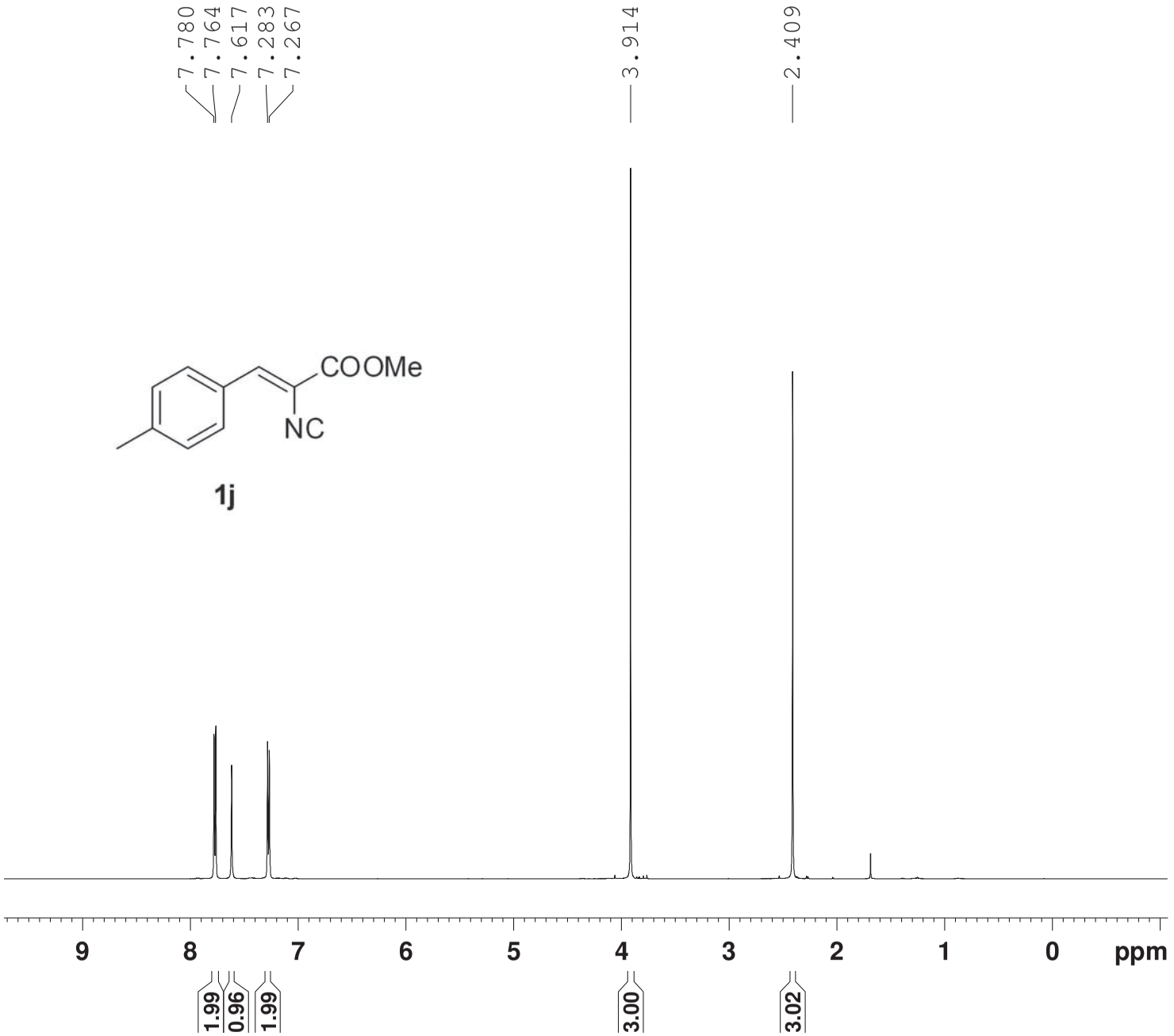

YY-1-100
PROTON CDCl3

| | | |
|---|---|---|
| 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 | |



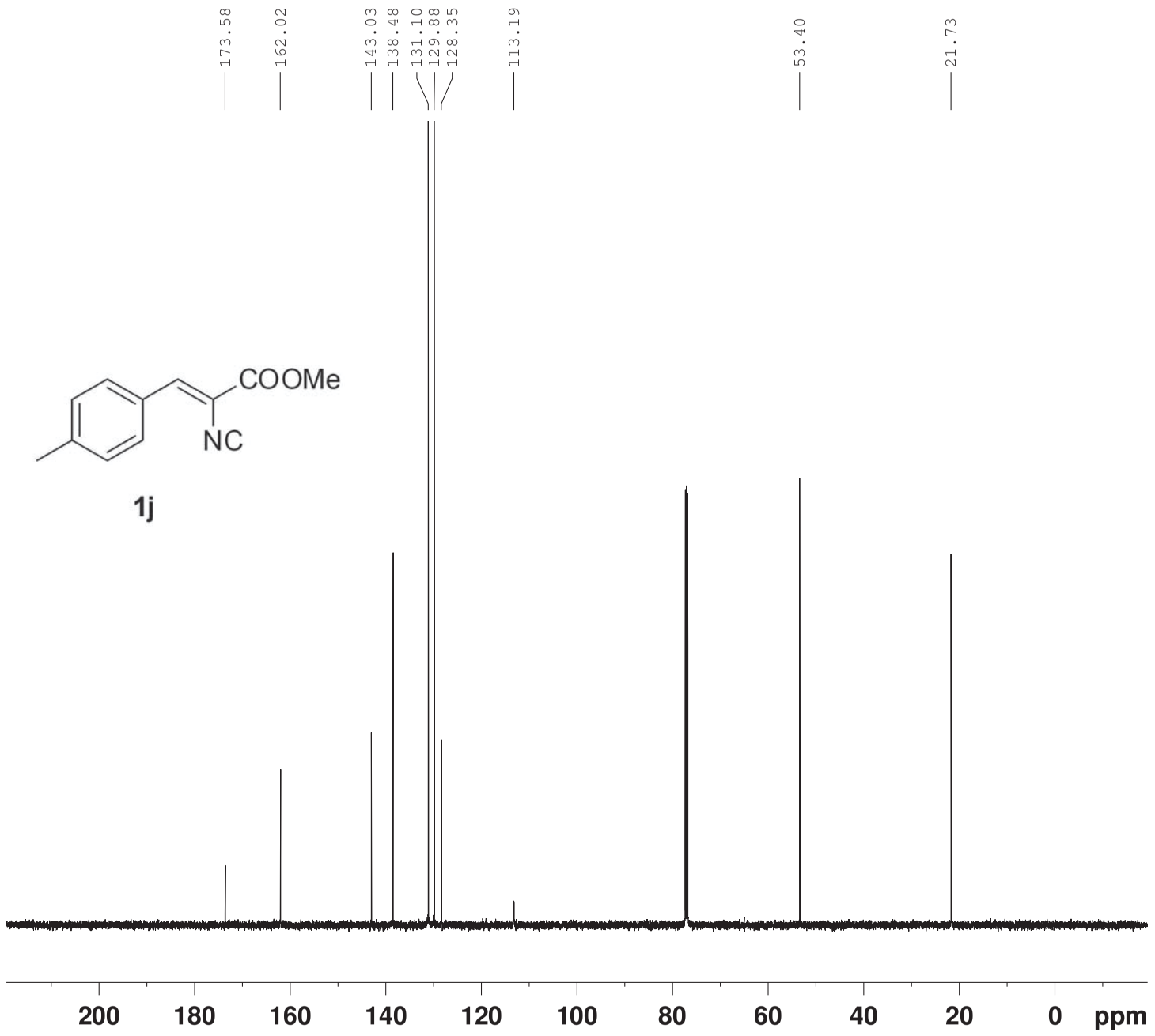

YY-1-100
C13CPD CDCl3

| | |
|---|---|
| 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 |




WH-7-35
PROTON CDCl3

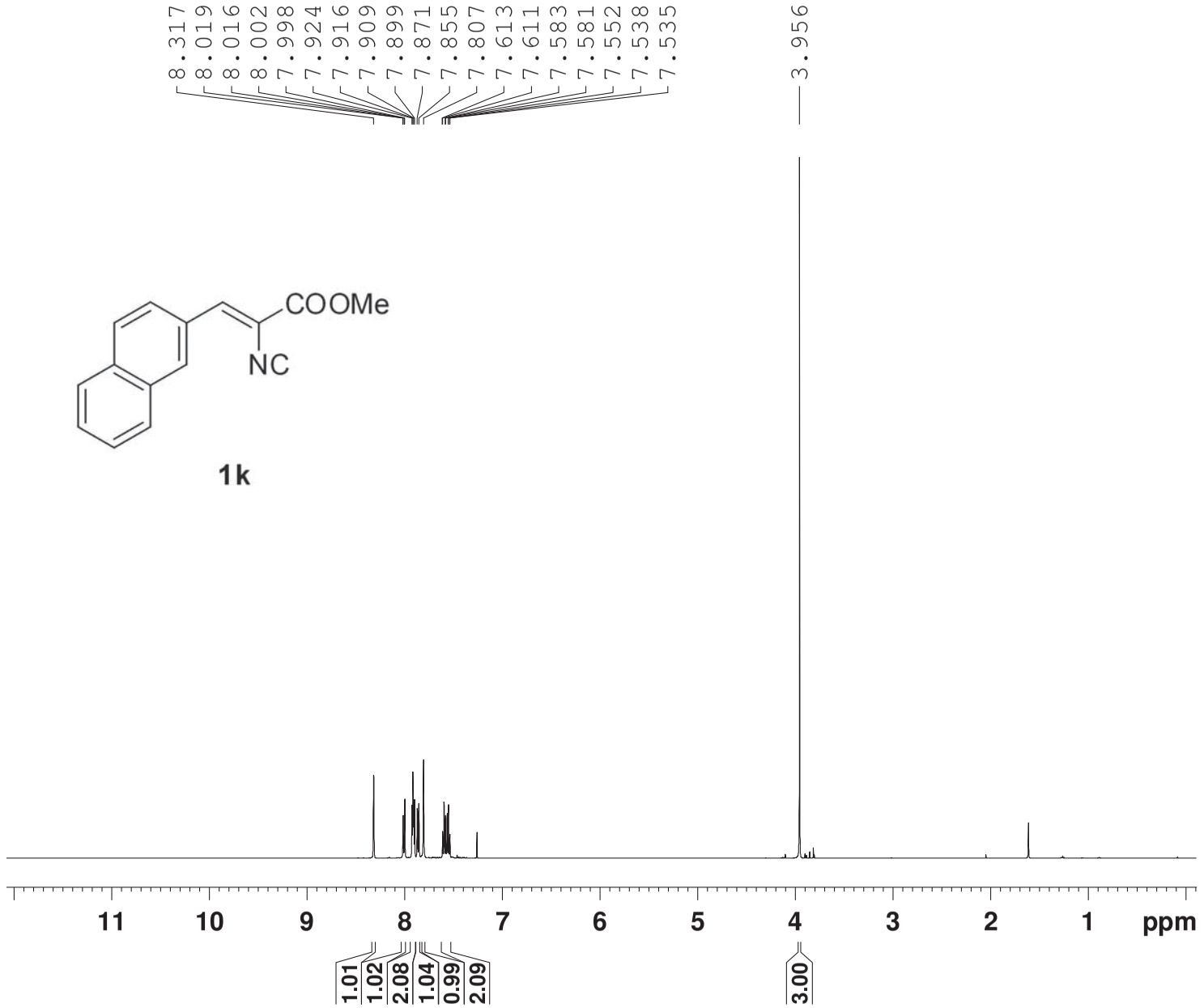
| | |
|---|---|
| NAME | XB20140617 |
| EXPNO | 21 |
| PROCNO | 1 |
| Date_ | 20140617 |
| Time | 19.02 |
| INSTRUM | spect |
| PROBHD | 5 mm PATXO 19F |
| PULPROG | zg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 10330.578 Hz |
| FIDRES | 0.157632 Hz |
| AQ | 3.1720407 sec |
| 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 | 500.1300128 MHz |
| WDW | no |
| SSB | 0 |
| LB | 0.00 Hz |
| GB | 0 |
| PC | 1.00 |




WH-7-35
C13CPD CDCl3

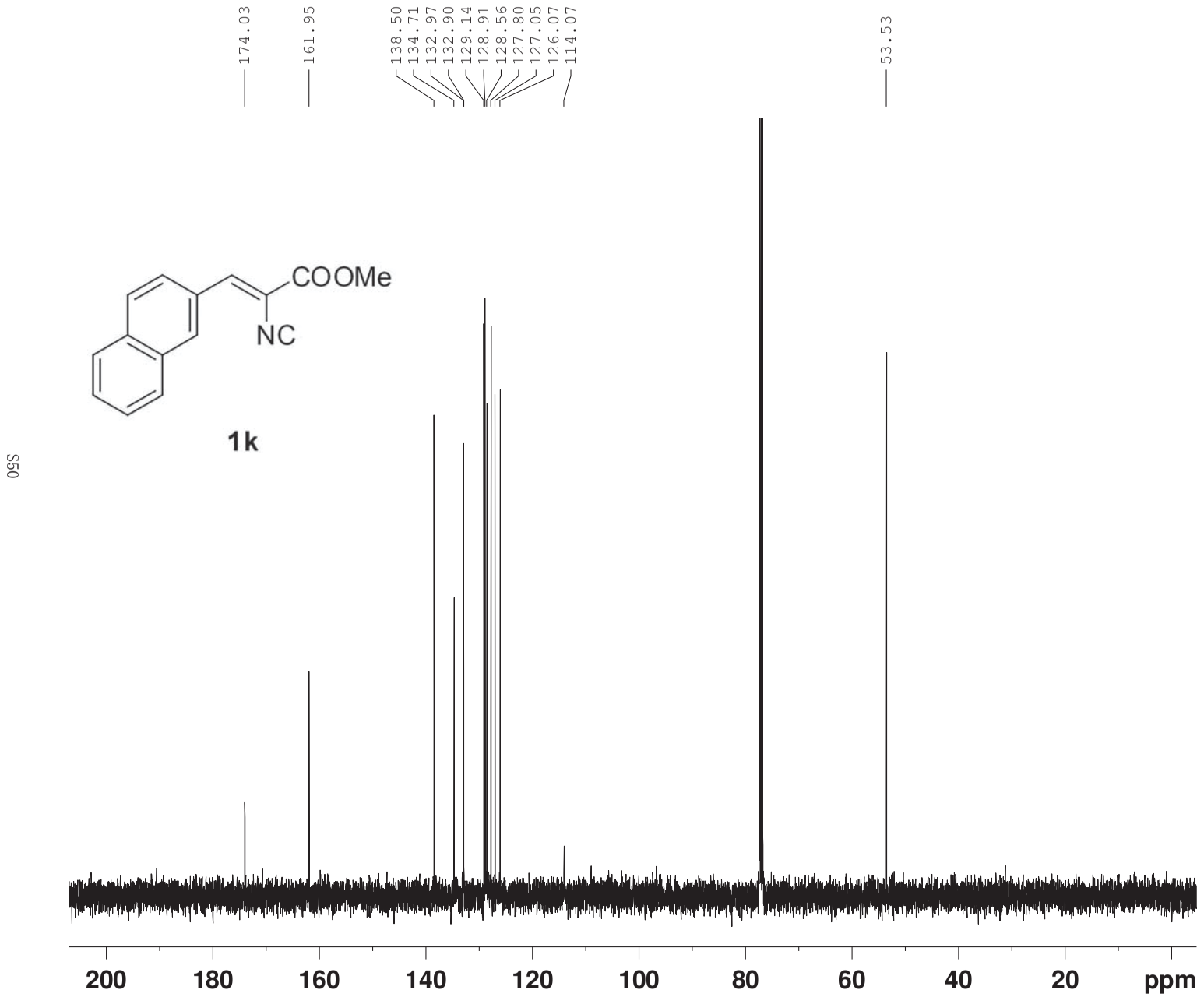
| | |
|---|---|
| NAME | XB20140617 |
| EXPNO | 22 |
| PROCNO | 1 |
| Date_ | 20140617 |
| Time | 19.19 |
| INSTRUM | spect |
| PROBHD | 5 mm PATXO 19F |
| PULPROG | zgpg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 256 |
| DS | 4 |
| SWH | 30030.029 Hz |
| FIDRES | 0.458222 Hz |
| AQ | 1.0912410 sec |
| 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-7-29
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 | |

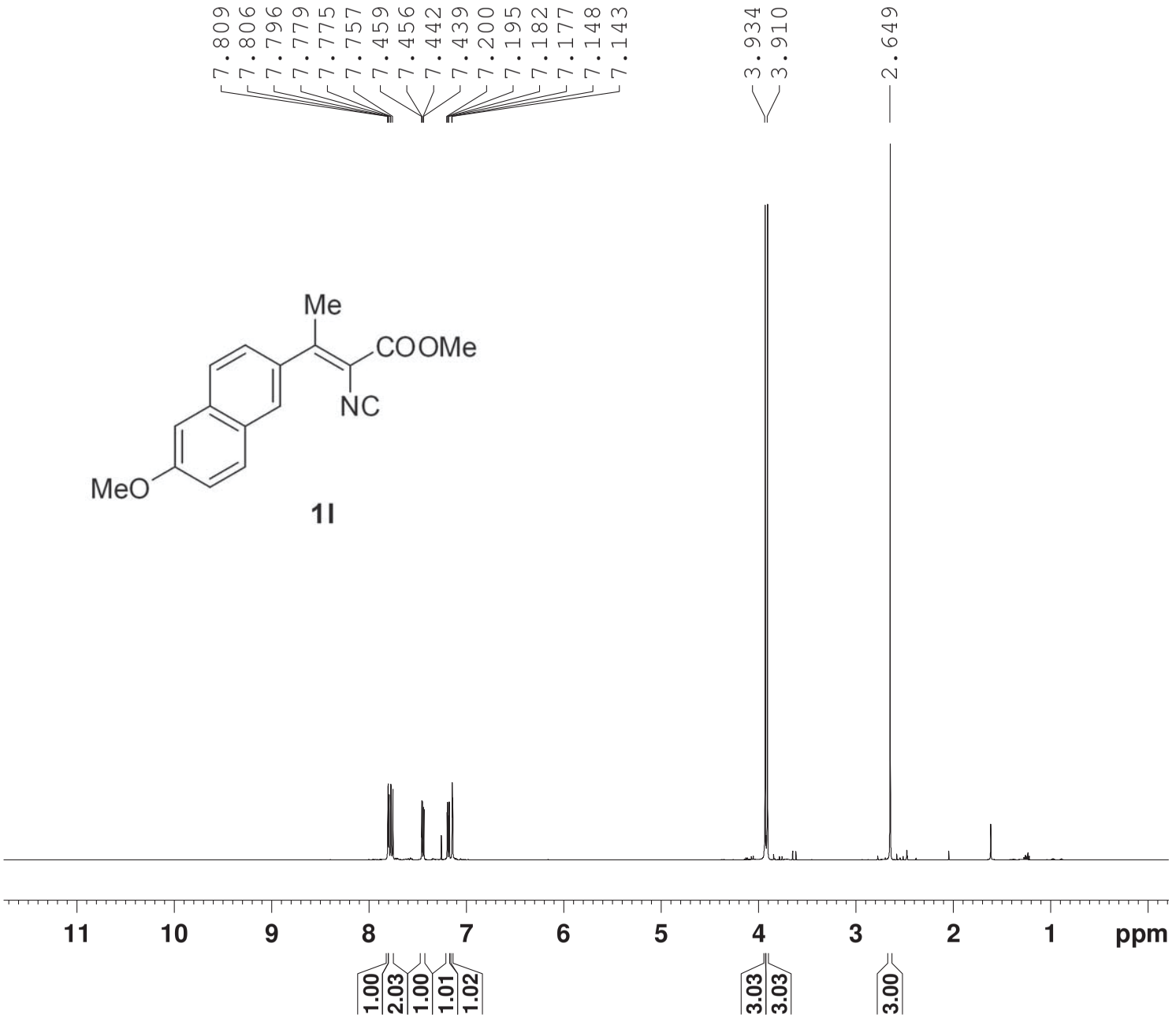
| ======== CHANNEL f1 ======== | | |
|---|---|---|
| NUC1 | 1H | |
| P1 | 14.14 | usec |
| PL1 | 1.00 | dB |
| SFO1 | 500.1330885 | MHz |
| SI | 32768 | |
| SF | 500.1300126 | MHz |
| WDW | no | |
| SSB | 0 | |
| LB | 0.00 | Hz |
| GB | 0 | |
| PC | 1.00 | |




S50

WH-7-29
C13CPD CDCl3

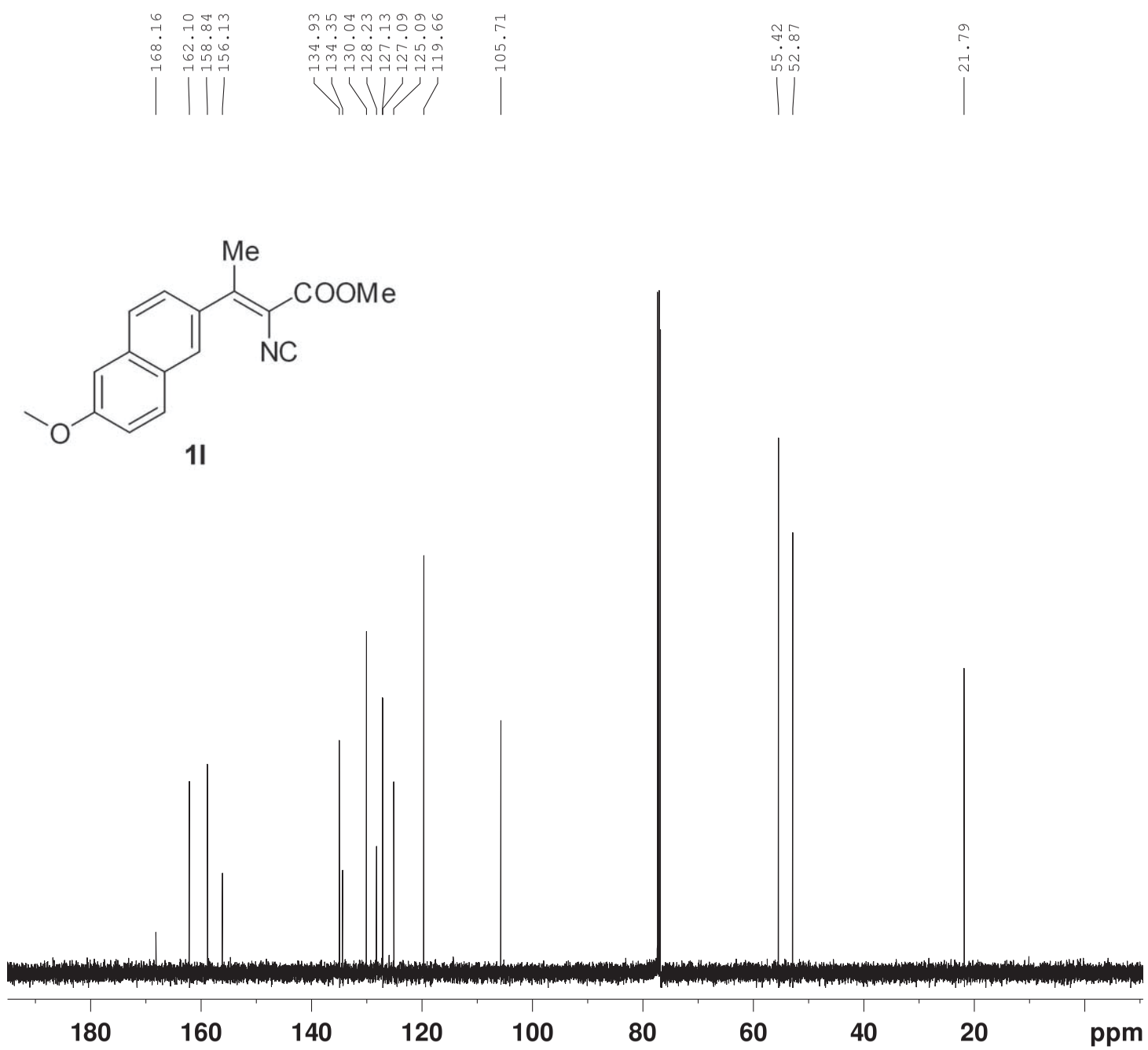
| | | |
|---|---|---|
| NAME | XB20140613 | |
| EXPNO | 7 | |
| PROCNO | 1 | |
| Date_ | 20140613 | |
| Time | 11.42 | |
| INSTRUM | spect | |
| PROBHD | 5 mm PATXO 19F | |
| PULPROG | zgpg30 | |
| TD | 65536 | |
| SOLVENT | CDCl3 | |
| NS | 128 | |
| DS | 4 | |
| SWH | 30030.029 | Hz |
| FIDRES | 0.458222 | 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 | |




MH-2-57
PROTON CDCl3

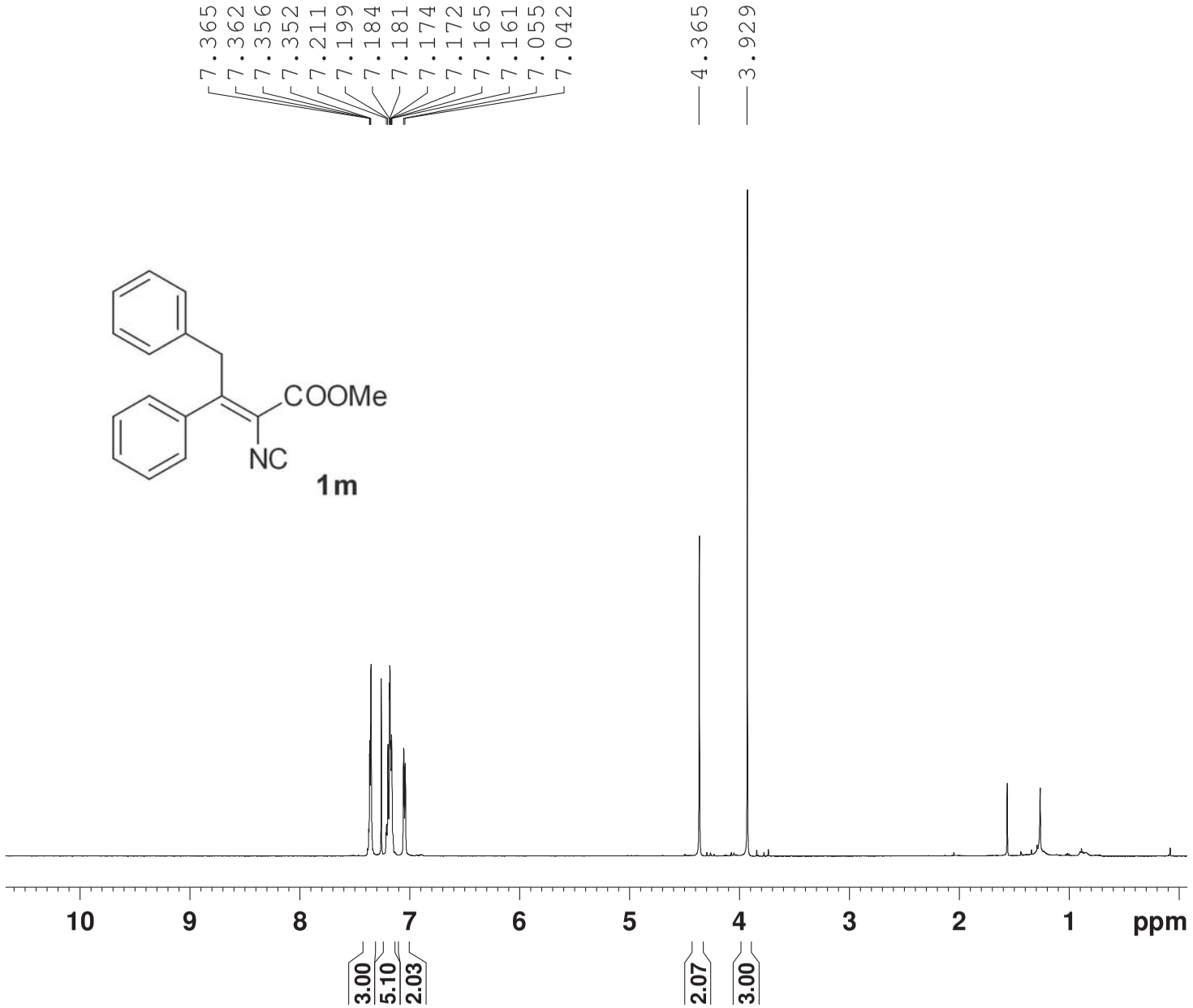
| | |
|---|---|
| NAME | XB20140714 |
| EXPNO | 17 |
| PROCNO | 1 |
| Date_ | 20140714 |
| Time | 12.57 |
| INSTRUM | spect |
| PROBHD | 5 mm PATXO 19F |
| PULPROG | zg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 10330.578 Hz |
| FIDRES | 0.157632 Hz |
| AQ | 3.1720407 sec |
| 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 |



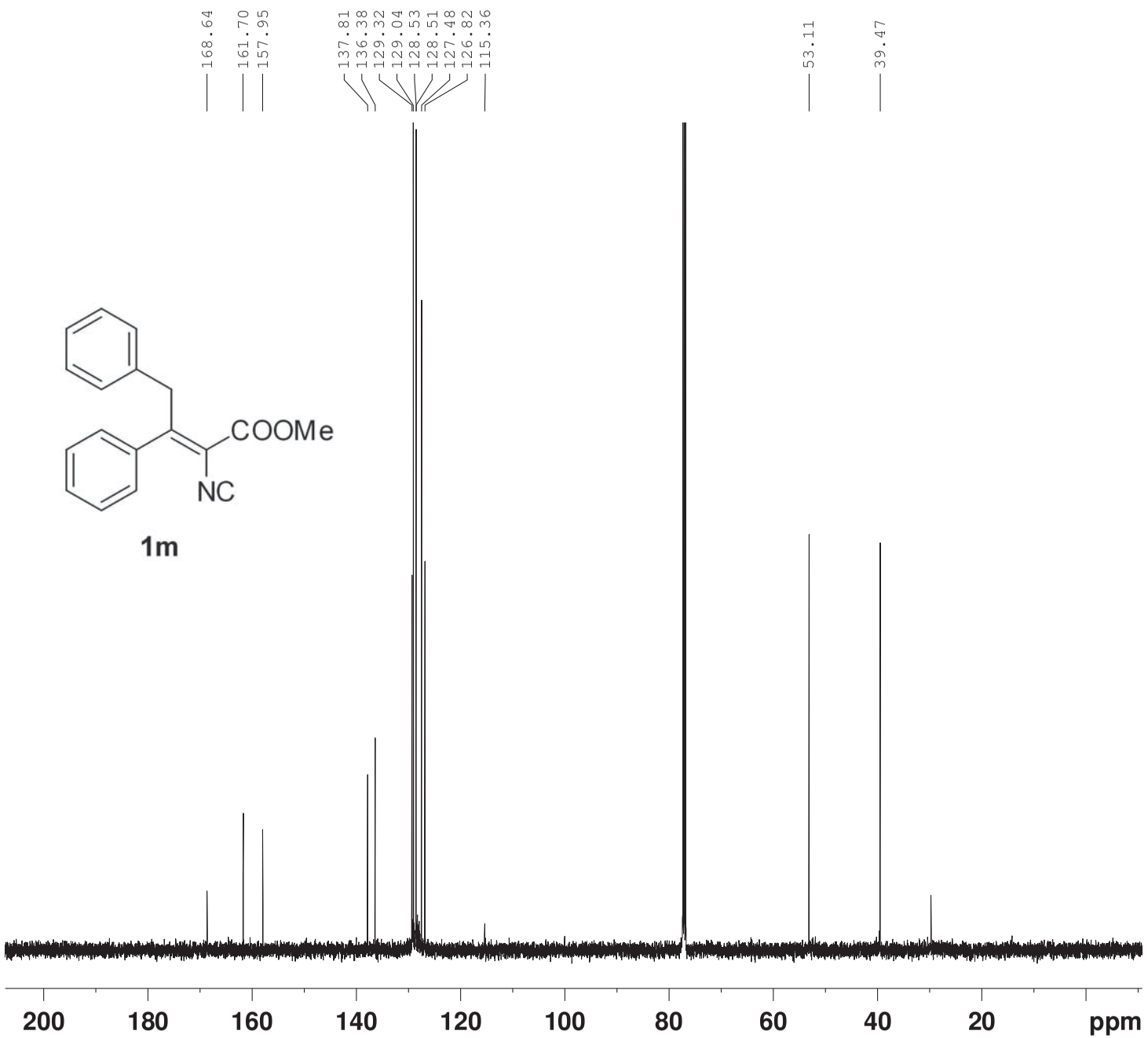

MH-2-57
C13CPD CDCl3

| | |
|---|---|
| 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 | no |
| SSB | 0 |
| LB | 0.00 Hz |
| GB | 0 |
| PC | 1.40 |



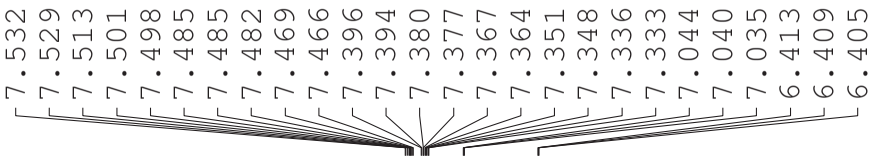

WH-7-40-S
PROTON CDCl3

| | |
|---|---|
| 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 |

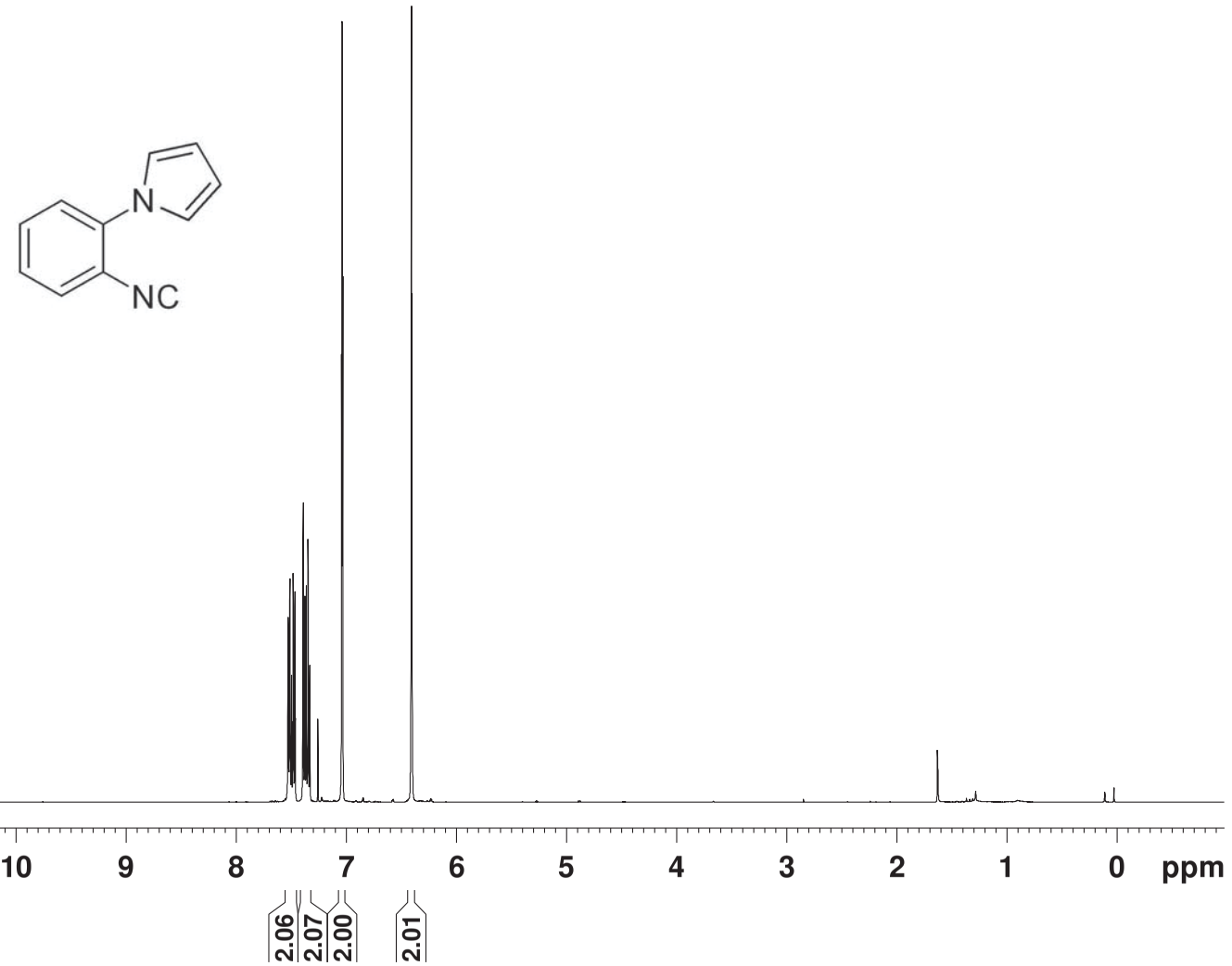



WH-7-40-S
C13CPD CDCl3

| | |
|---|---|
| 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 |

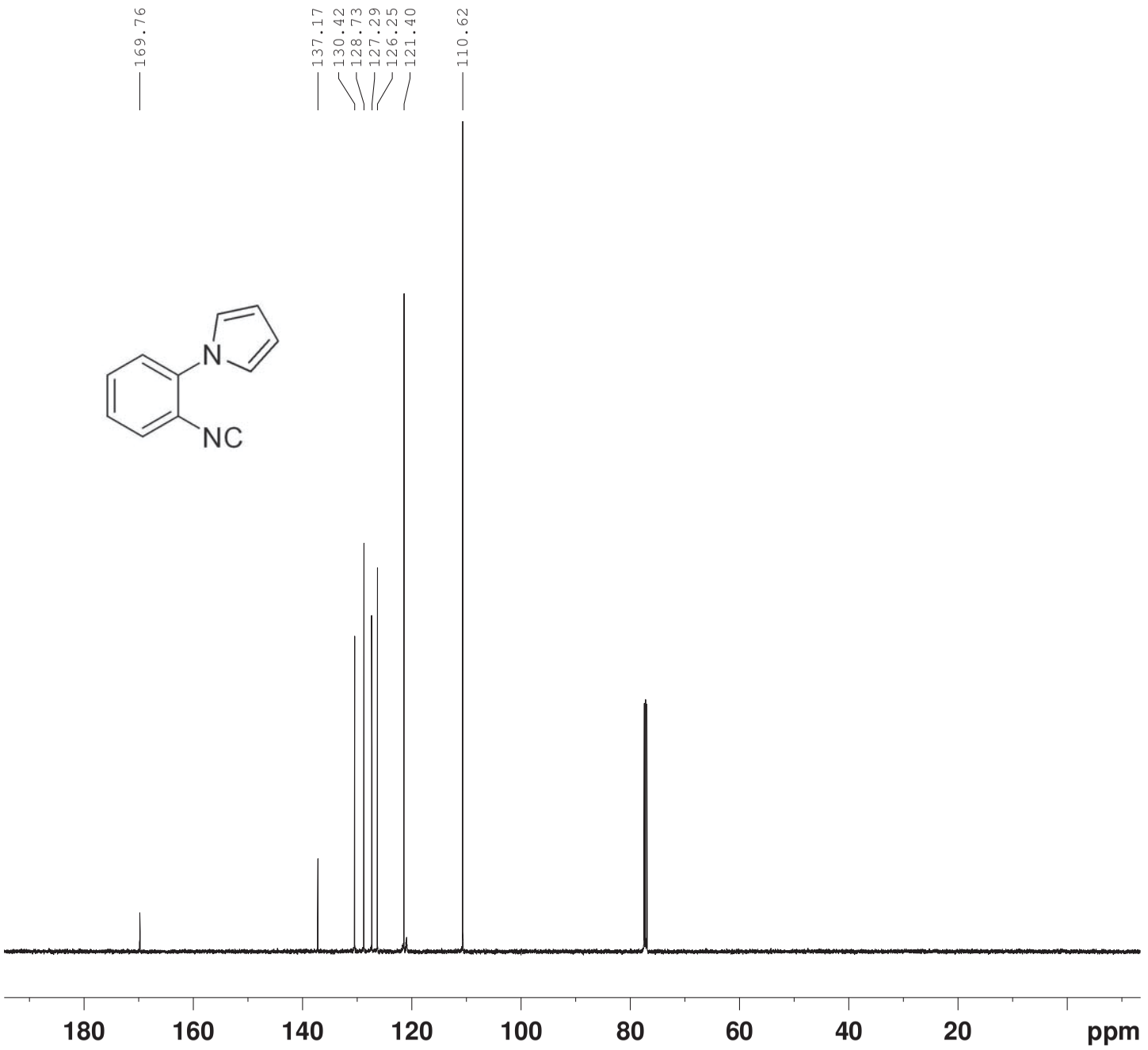



MH-3-123-S
PROTON CDCl3



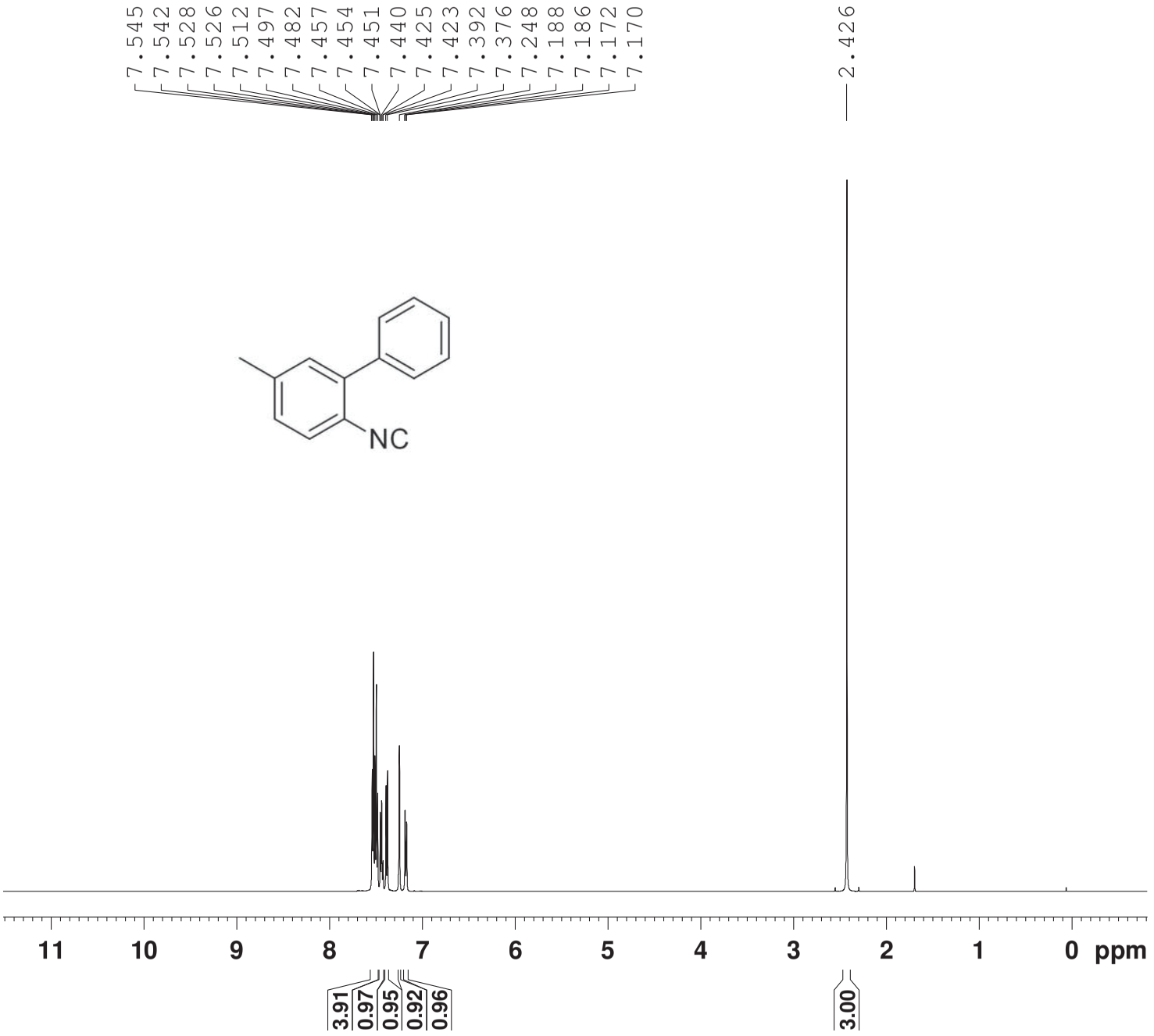

| | |
|---|---|
| NAME | XB20151202 |
| EXPNO | 3 |
| PROCNO | 1 |
| Date_ | 20151202 |
| Time | 11.58 |
| INSTRUM | spect |
| PROBHD | 5 mm PATXO 19F |
| PULPROG | zg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 10330.578 Hz |
| FIDRES | 0.157632 Hz |
| AQ | 3.1720407 sec |
| RG | 90.5 |
| DW | 48.400 usec |
| DE | 6.00 usec |
| TE | 294.3 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 |



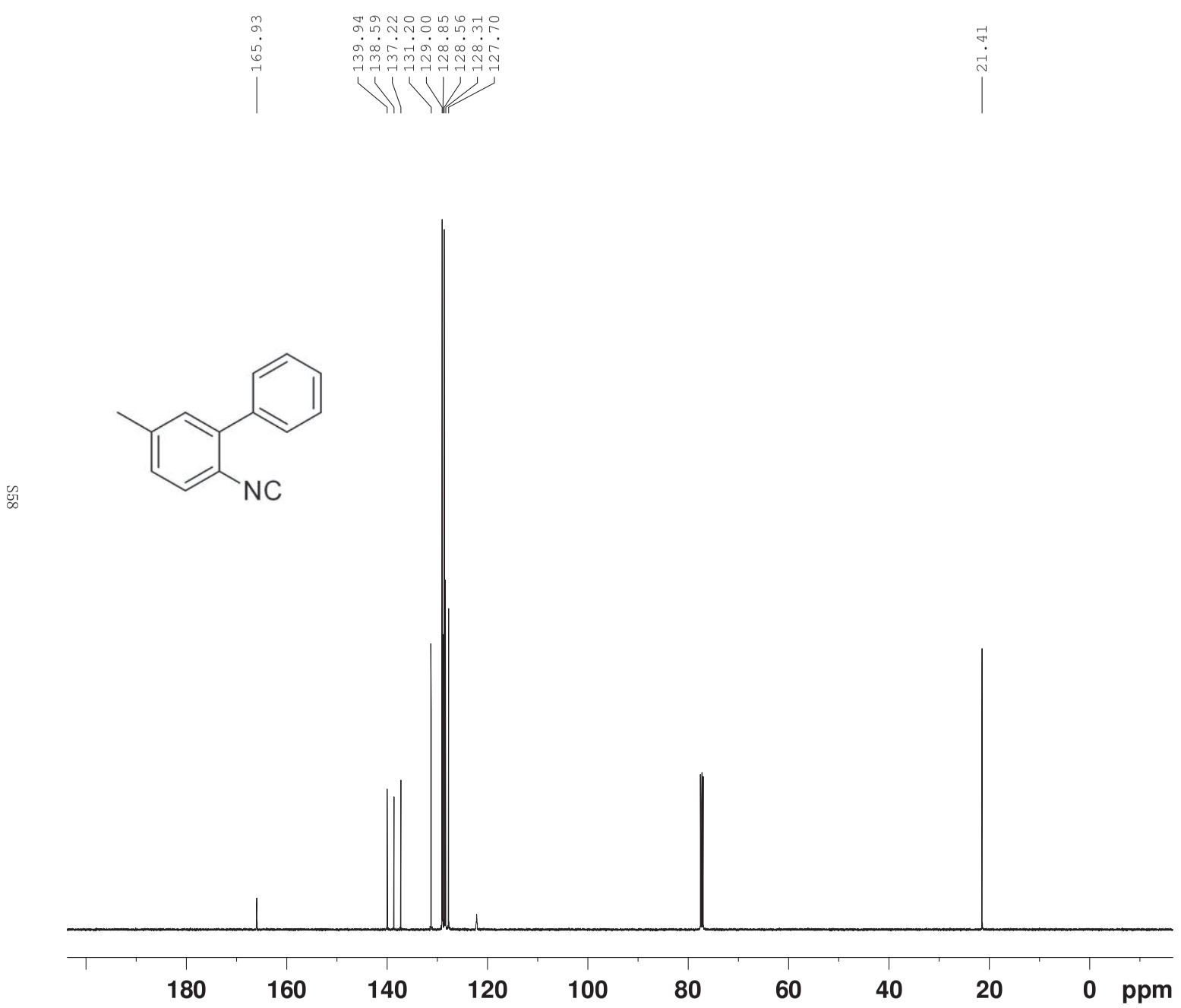

MH-3-123-S
C13CPD CDCl3

| | |
|---|---|
| NAME | XB20151202 |
| EXPNO | 5 |
| PROCNO | 1 |
| Date_ | 20151202 |
| Time | 12.29 |
| 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 | 128 |
| DW | 16.650 usec |
| DE | 6.00 usec |
| TE | 296.1 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 |



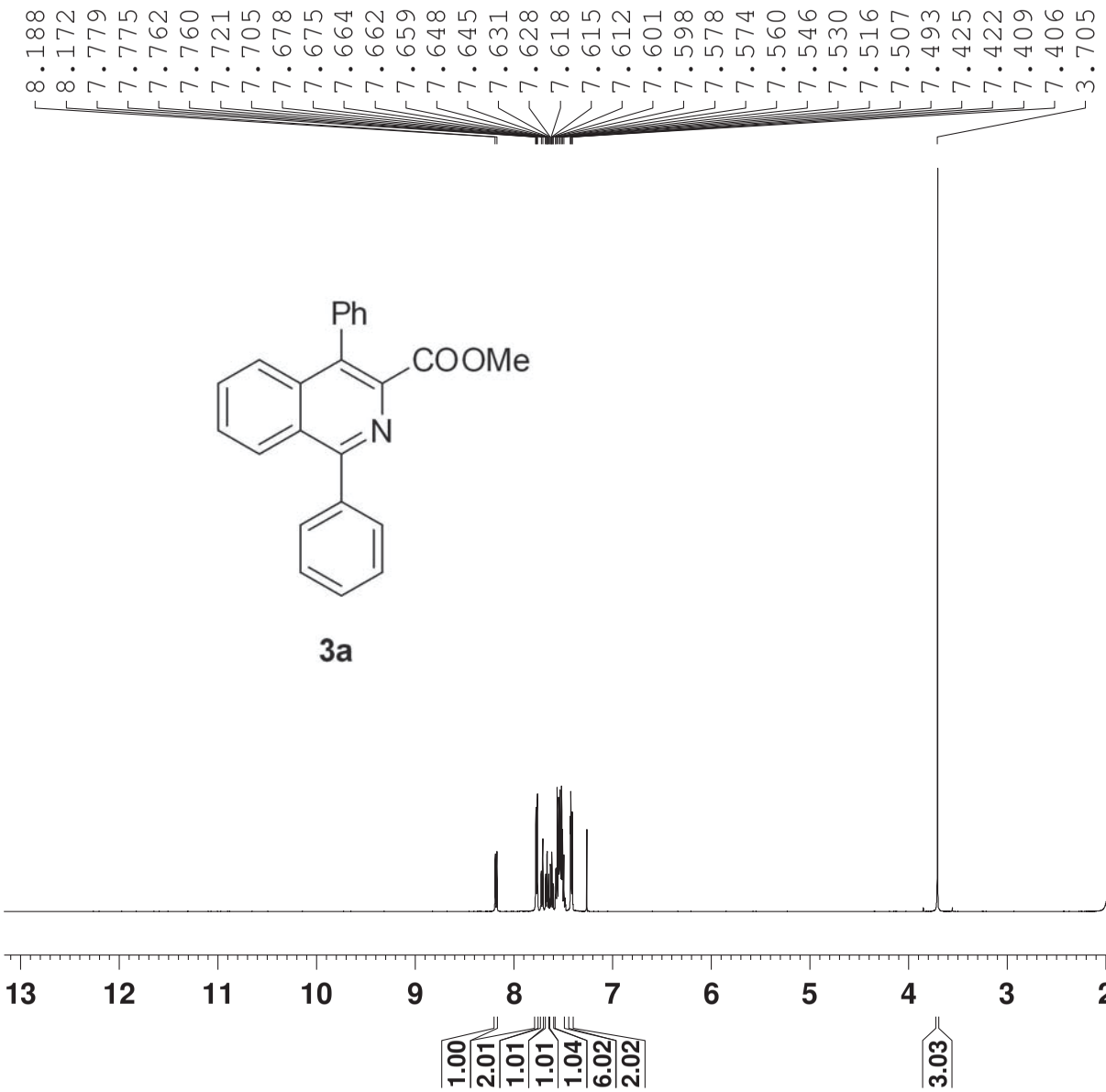

MH-3-124-S
PROTON CDCl3

| | | |
|---|---|---|
| NAME | XB20151202 | |
| EXPNO | 6 | |
| PROCNO | 1 | |
| Date_ | 20151202 | |
| Time | 12.35 | |
| 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 | 45.3 | |
| DW | 48.400 | usec |
| DE | 6.00 | usec |
| TE | 295.1 | 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 | 500.1300129 | MHz |
| WDW | no | |
| SSB | 0 | |
| LB | 0.00 | Hz |
| GB | 0 | |
| PC | 1.00 | |



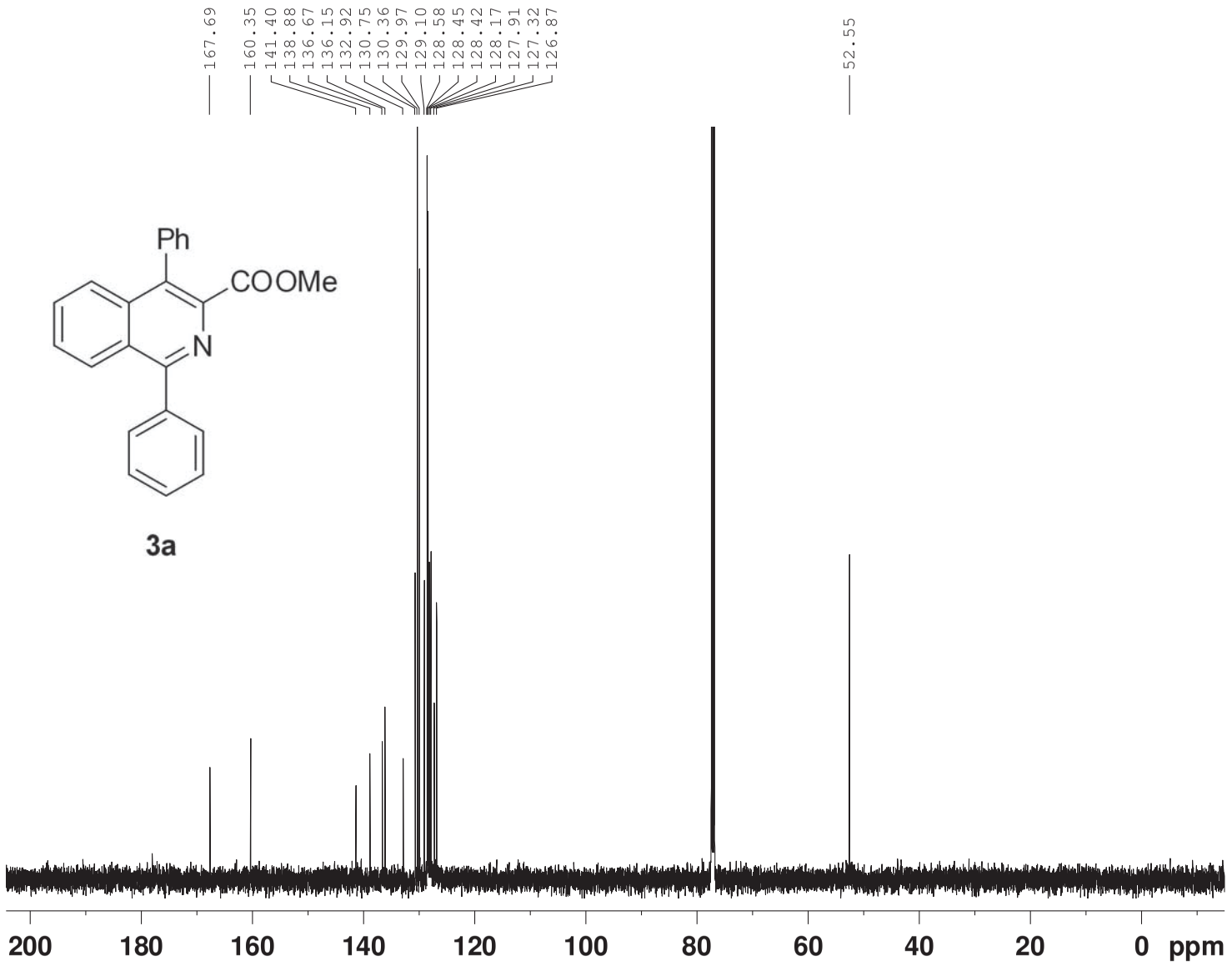

MH-3-124-S
C13CPD CDCl3

| | |
|---|---|
| NAME | XB20151202 |
| EXPNO | 7 |
| PROCNO | 1 |
| Date_ | 20151202 |
| Time | 13.04 |
| 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 | 128 |
| DW | 16.650 usec |
| DE | 6.00 usec |
| TE | 295.9 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 |



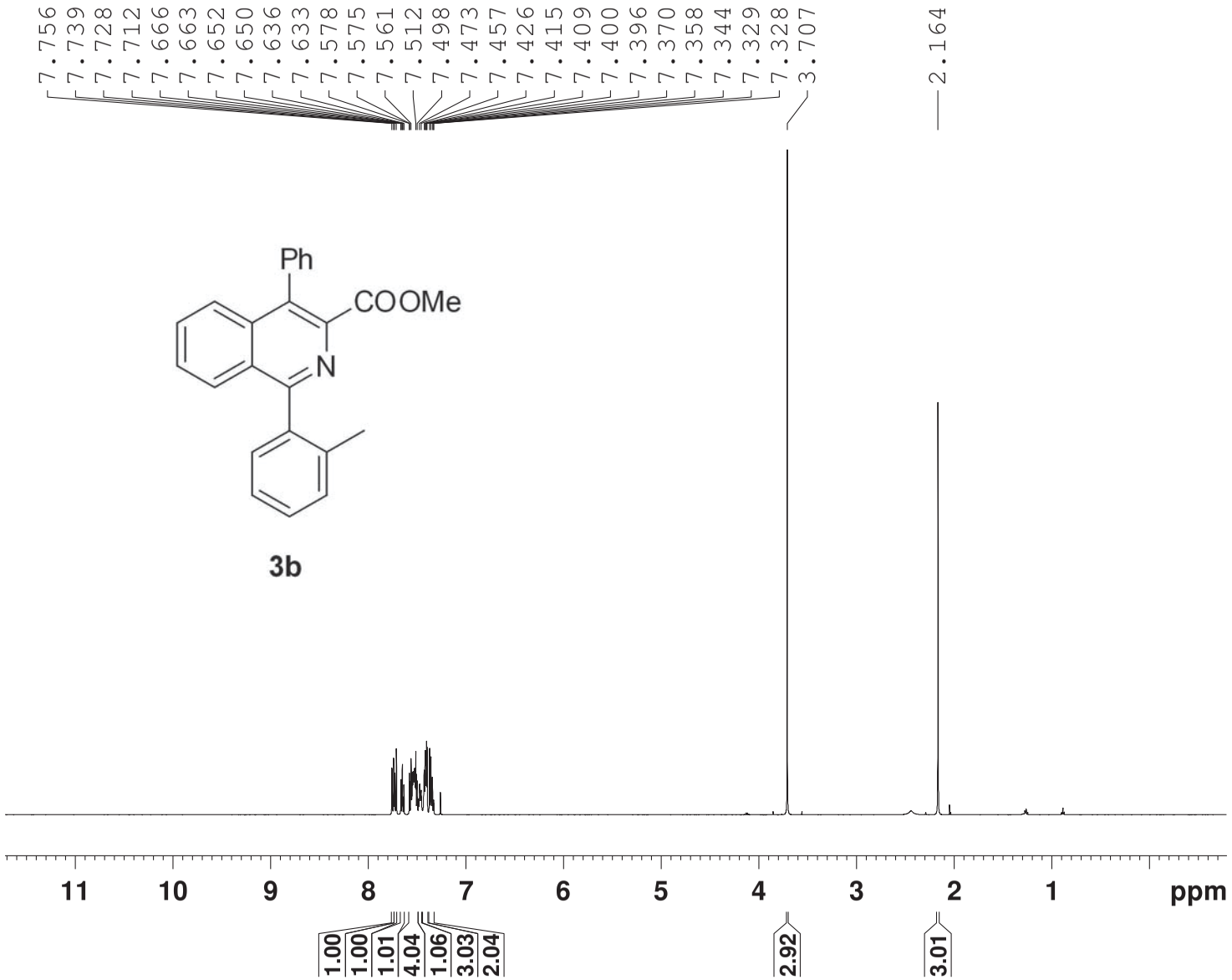

MH-2-64
PROTON CDCl3

| | | |
|---|---|---|
| NAME | XB20140730 | |
| EXPNO | 9 | |
| PROCNO | 1 | |
| Date_ | 20140730 | |
| Time | 15.52 | |
| 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 | 298.1 | 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 | |



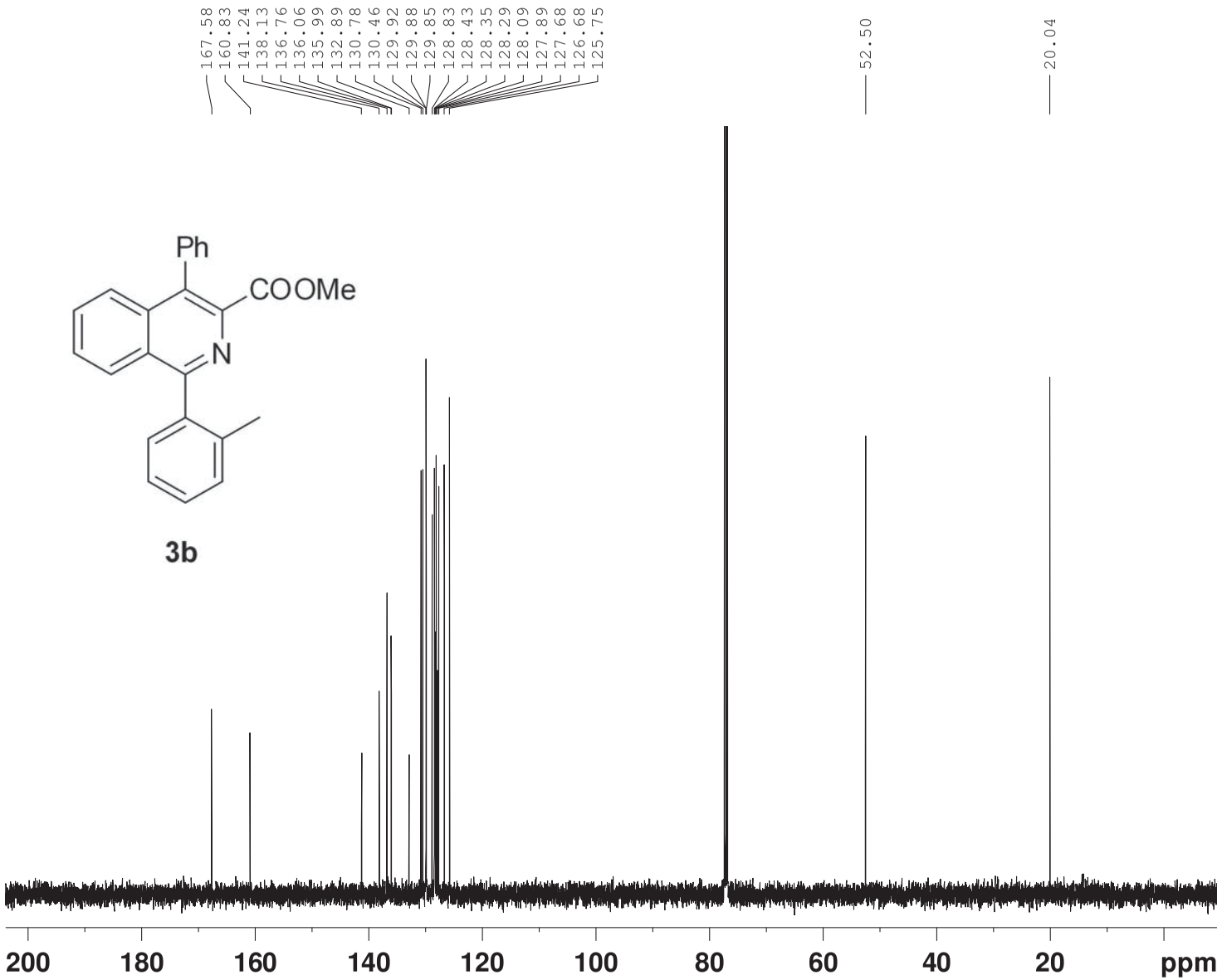

MH-2-64
C13CPD CDCl3

| | | |
|---|---|---|
| NAME | XB20140730 | |
| EXPNO | 10 | |
| PROCNO | 1 | |
| Date_ | 20140730 | |
| Time | 15.49 | |
| INSTRUM | spect | |
| PROBHD | 5 mm PATXO 19F | |
| PULPROG | zgpg30 | |
| TD | 65536 | |
| SOLVENT | CDCl3 | |
| NS | 428 | |
| DS | 4 | |
| SWH | 30030.029 | Hz |
| FIDRES | 0.458222 | Hz |
| AQ | 1.0912410 | sec |
| RG | 456.1 | |
| DW | 16.650 | usec |
| DE | 6.00 | usec |
| TE | 298.9 | 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 | 125.7577735 | MHz |
| WDW | EM | |
| SSB | 0 | |
| LB | 1.00 | Hz |
| GB | 0 | |
| PC | 1.40 | |



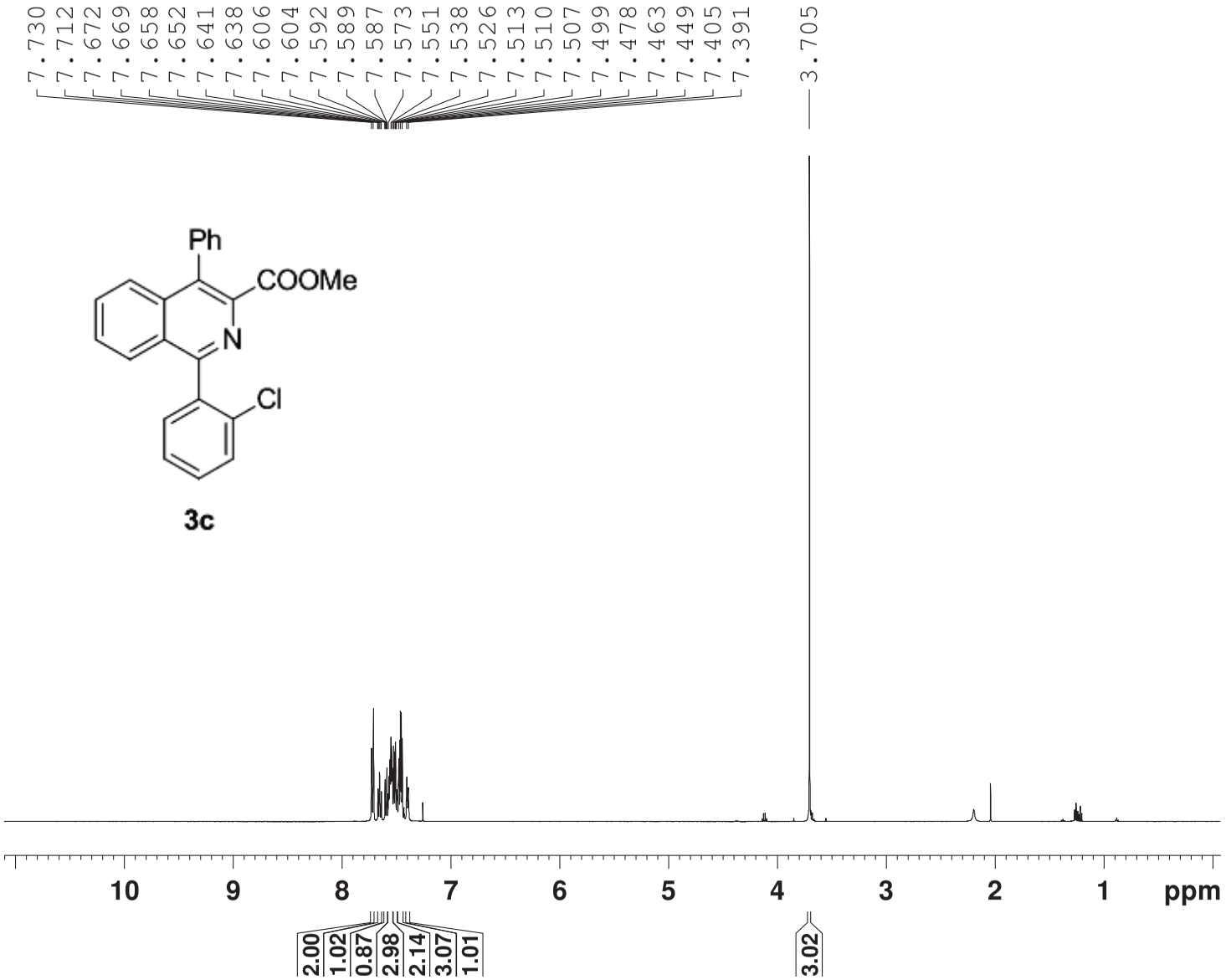

MH-2-4
PROTON CDCl3

| | |
|---|---|
| NAME | XB20140602 |
| EXPNO | 15 |
| PROCNO | 1 |
| Date_ | 20140602 |
| Time | 19.59 |
| 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 |




MH-2-4
C13CPD CDCl3

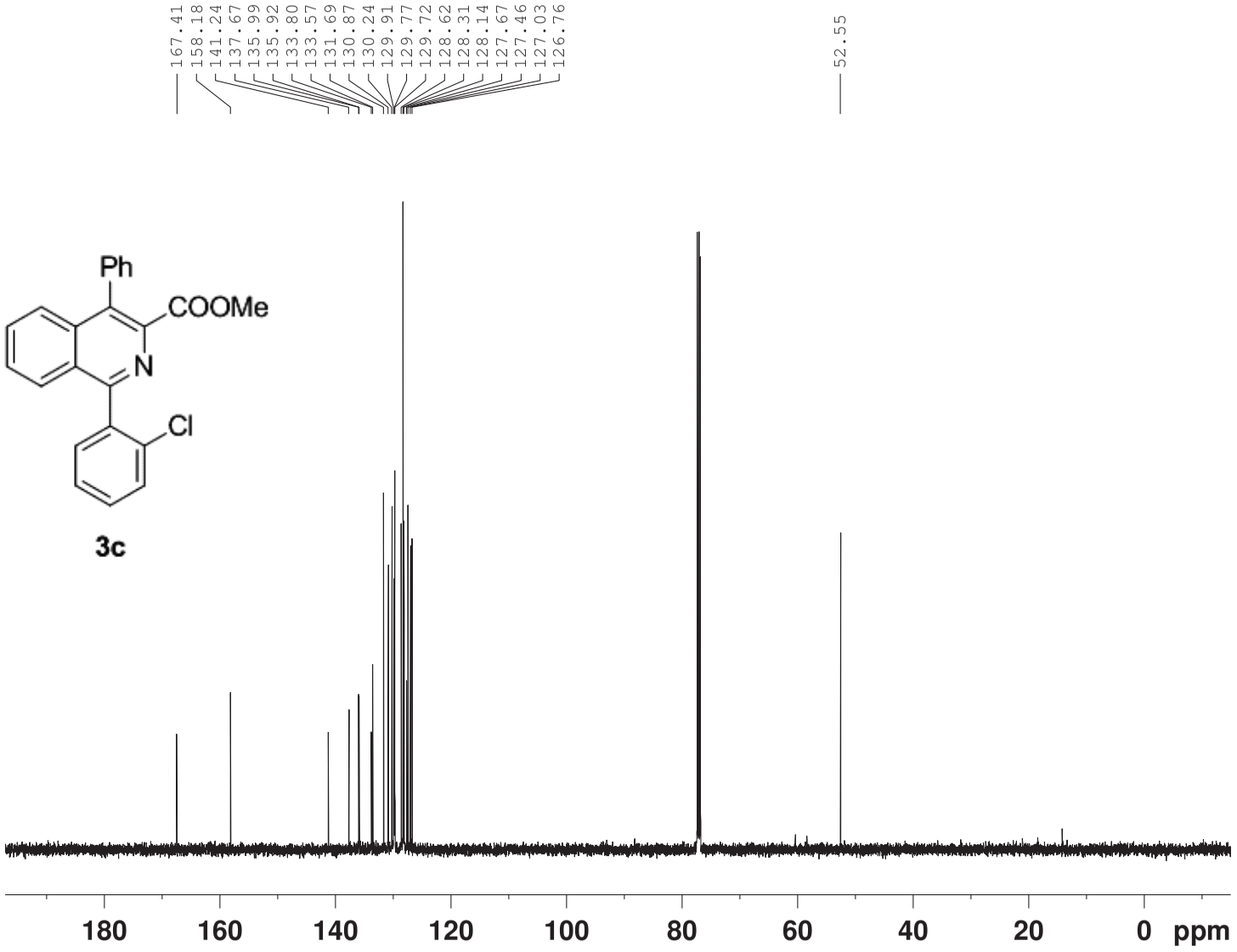
| | |
|---|---|
| NAME | XB20140602 |
| EXPNO | 16 |
| PROCNO | 1 |
| Date_ | 20140602 |
| Time | 20.08 |
| INSTRUM | spect |
| PROBHD | 5 mm PATXO 19F |
| PULPROG | zgpg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 128 |
| DS | 4 |
| SWH | 30030.029 Hz |
| FIDRES | 0.458222 Hz |
| AQ | 1.0912410 sec |
| RG | 406.4 |
| DW | 16.650 usec |
| DE | 6.00 usec |
| TE | 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 |




MH-2-24
PROTON CDCl3

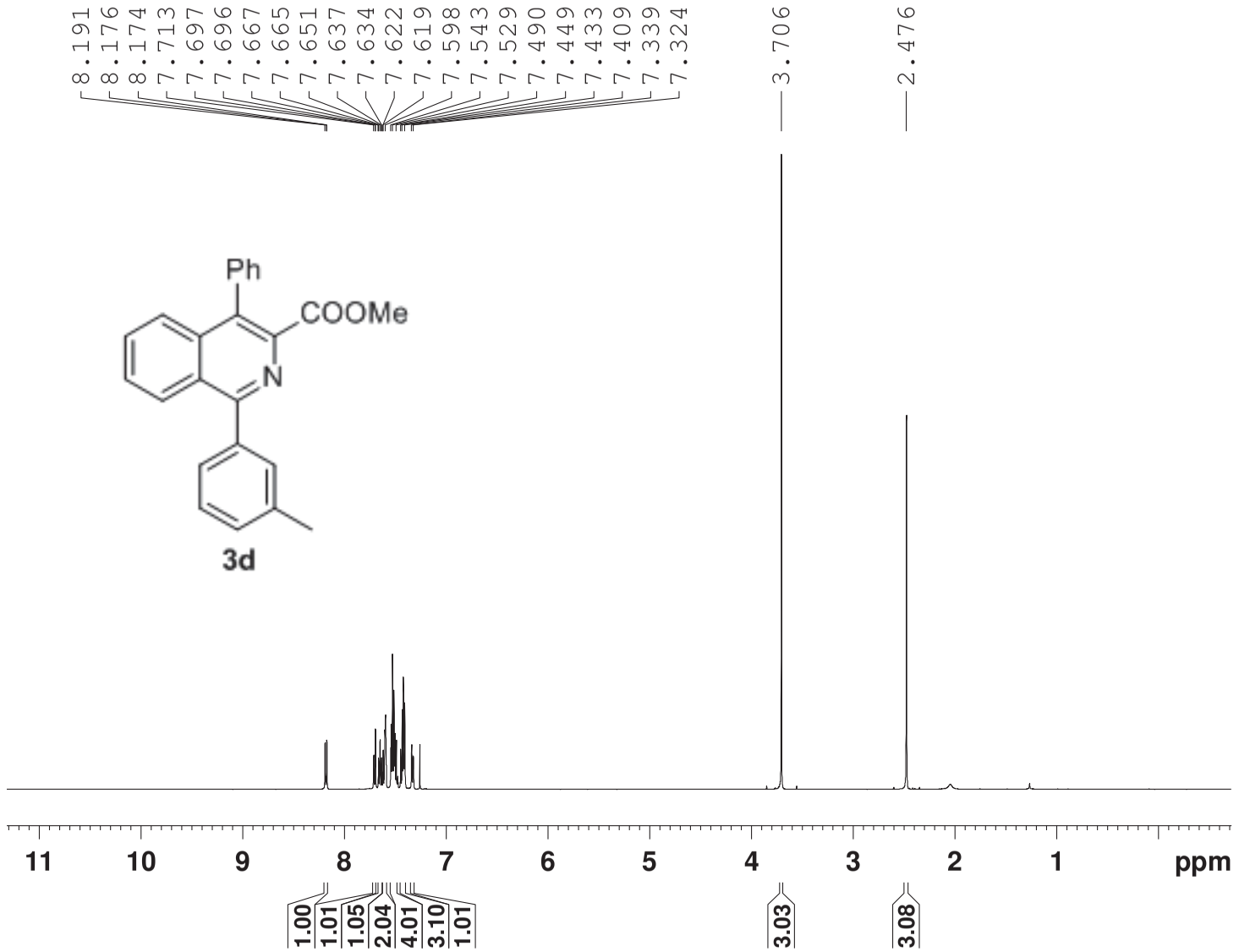
| | | |
|---|---|---|
| NAME | XB20140706 | |
| EXPNO | 19 | |
| PROCNO | 1 | |
| Date_ | 20140706 | |
| Time | 21.51 | |
| INSTRUM | spect | |
| PROBHD | 5 mm PATXO 19F | |
| PULPROG | zg30 | |
| TD | 65536 | |
| SOLVENT | CDCl3 | |
| NS | 16 | |
| DS | 2 | |
| SWH | 10330.578 | Hz |
| FIDRES | 0.157632 | Hz |
| AQ | 3.1720407 | sec |
| RG | 90.5 | |
| 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 | 500.1300128 | MHz |
| WDW | no | |
| SSB | 0 | |
| LB | 0.00 | Hz |
| GB | 0 | |
| PC | 1.00 | |

**3c**



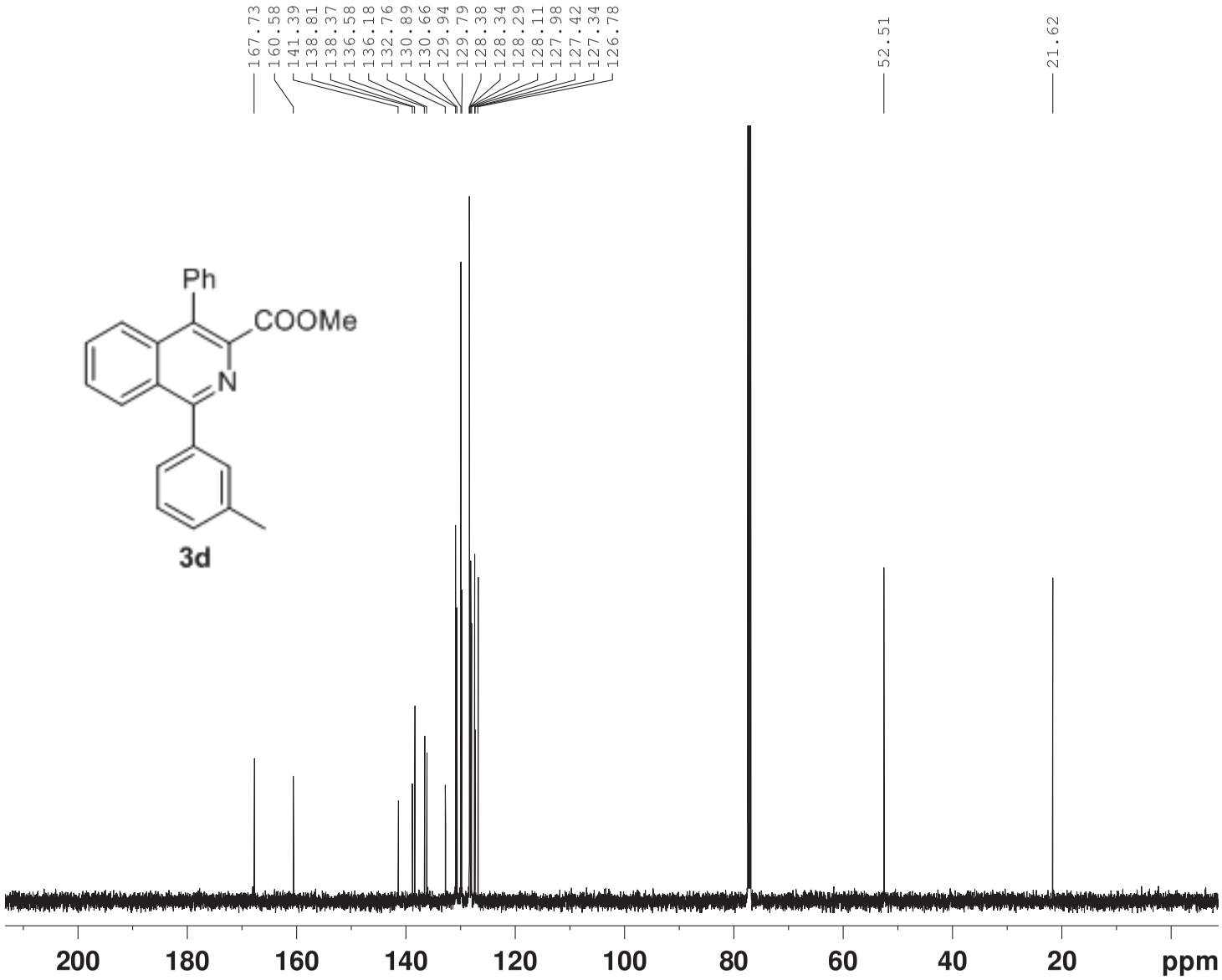

MH-2-24
C13CPD CDCl3

| | | |
|---|---|---|
| NAME | XB20140706 | |
| EXPNO | 20 | |
| PROCNO | 1 | |
| Date_ | 20140706 | |
| Time | 22.07 | |
| 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 | 128 | |
| 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 | |



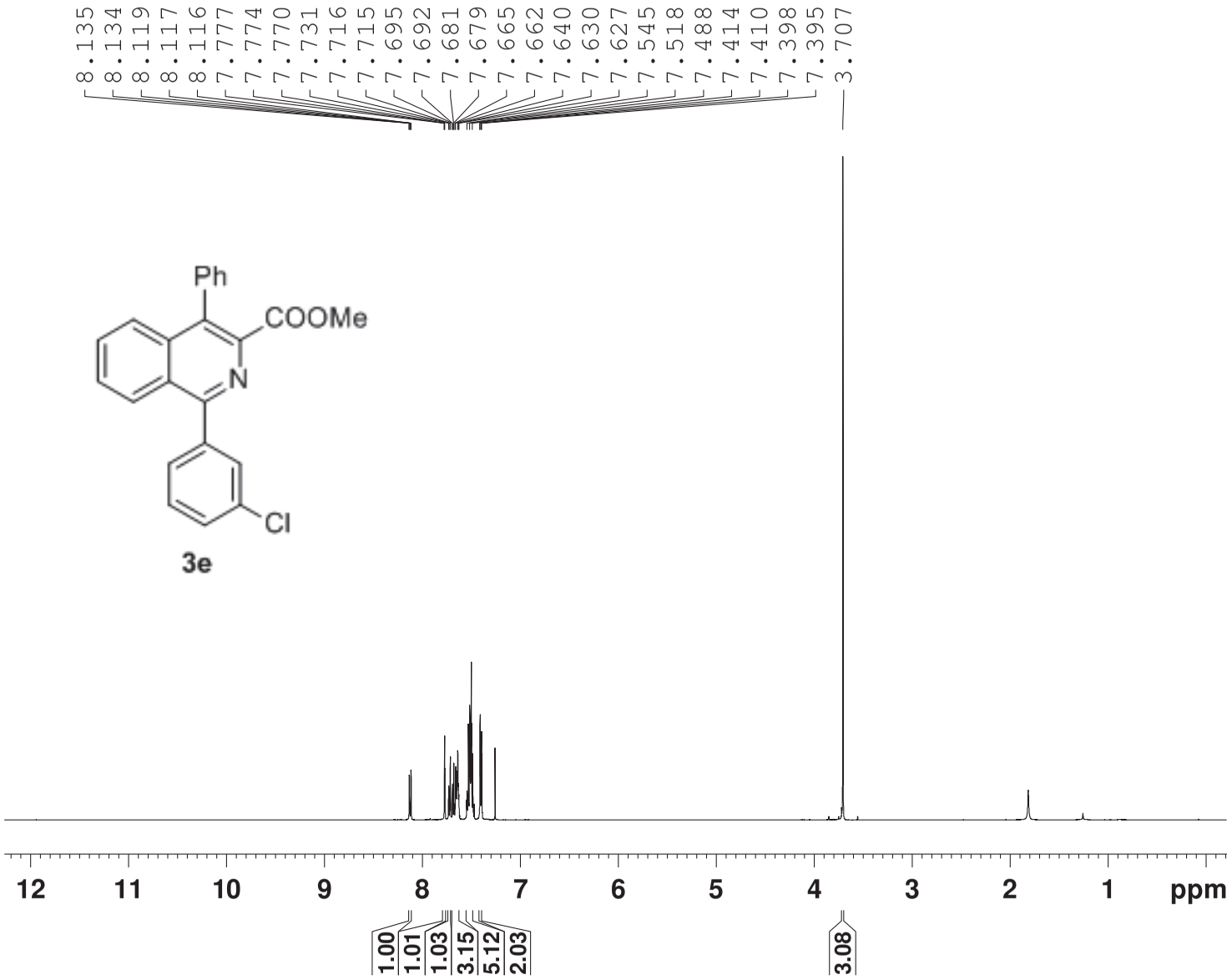

MH-2-67
PROTON CDCl3

| | |
|---|---|
| NAME | XB20140730 |
| EXPNO | 11 |
| PROCNO | 1 |
| Date_ | 20140730 |
| Time | 15.57 |
| 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 | 128 |
| 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 | 500.1300129 MHz |
| WDW | no |
| SSB | 0 |
| LB | 0.00 Hz |
| GB | 0 |
| PC | 1.00 |



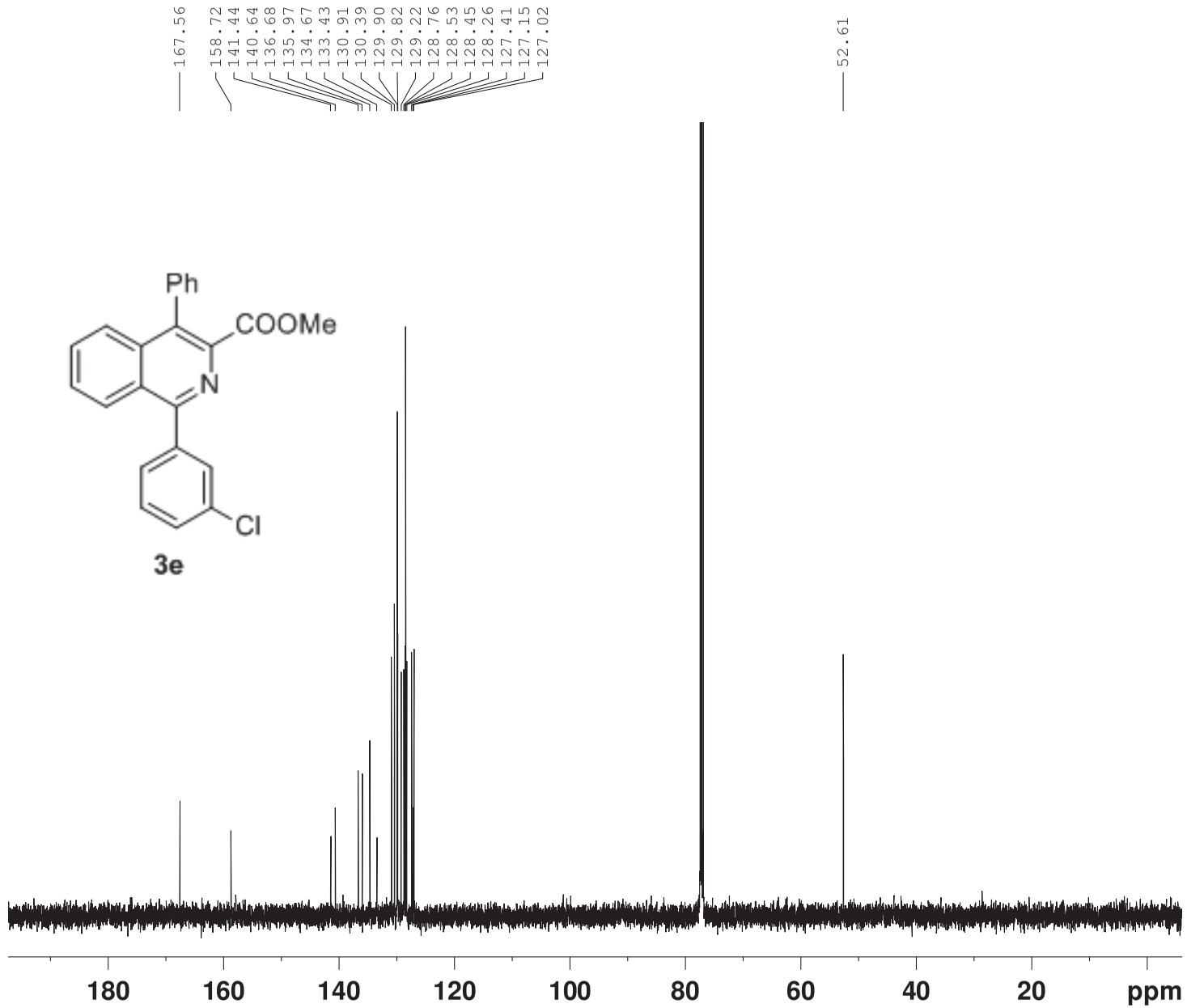

MH-2-67
C13CPD CDCl3

| | |
|---|---|
| NAME | XB20140730 |
| EXPNO | 12 |
| PROCNO | 1 |
| Date_ | 20140730 |
| Time | 21.09 |
| 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 | 1448.2 |
| 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 | 125.7577782 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 1.00 Hz |
| GB | 0 |
| PC | 1.40 |



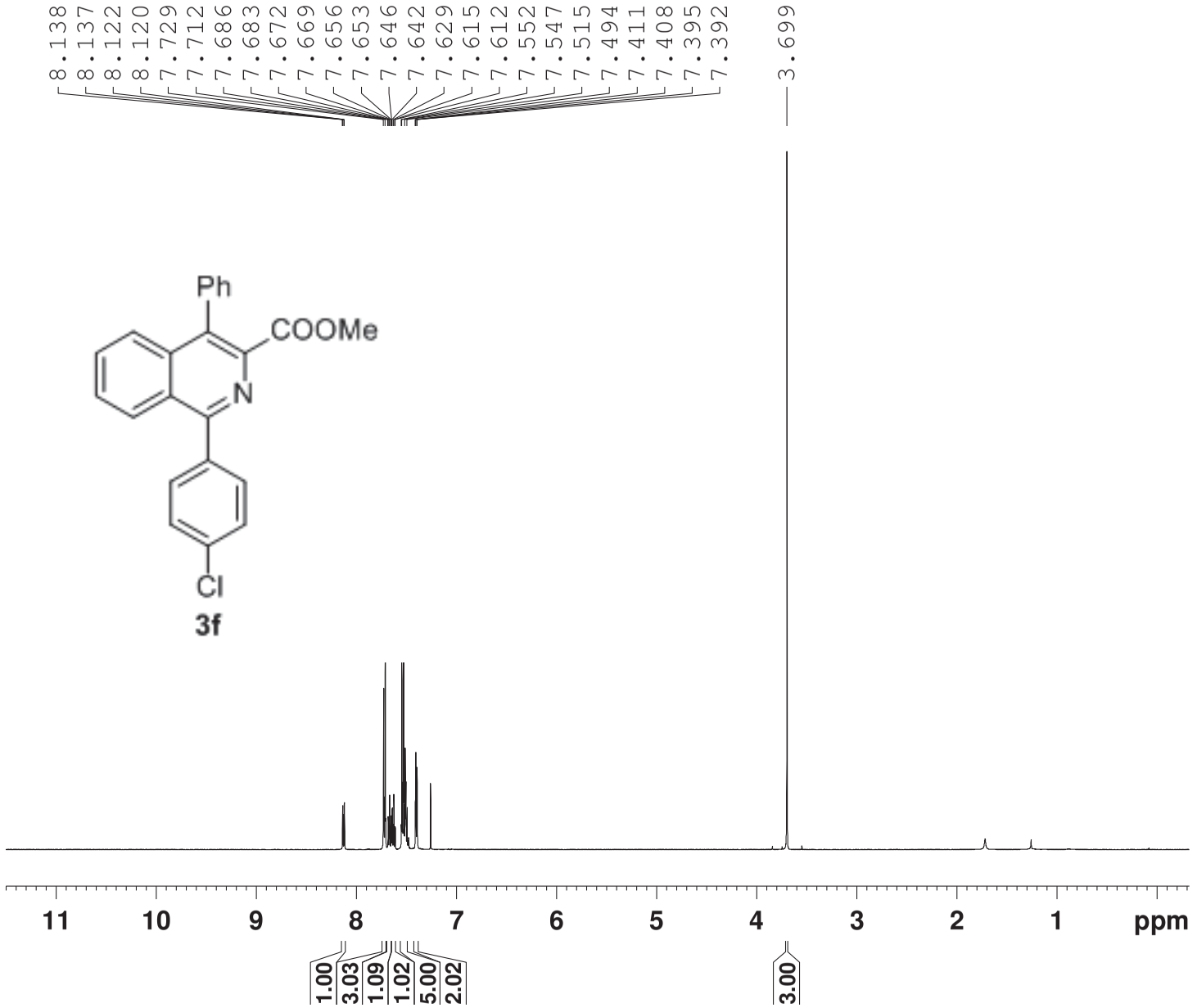

MH-2-68
PROTON CDCl3

| | | |
|---|---|---|
| NAME | XB20140730 | |
| EXPNO | 13 | |
| PROCNO | 1 | |
| Date_ | 20140730 | |
| Time | 21.15 | |
| 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 | 228.1 | |
| 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 | 500.1300128 | MHz |
| WDW | no | |
| SSB | 0 | |
| LB | 0.00 | Hz |
| GB | 0 | |
| PC | 1.00 | |



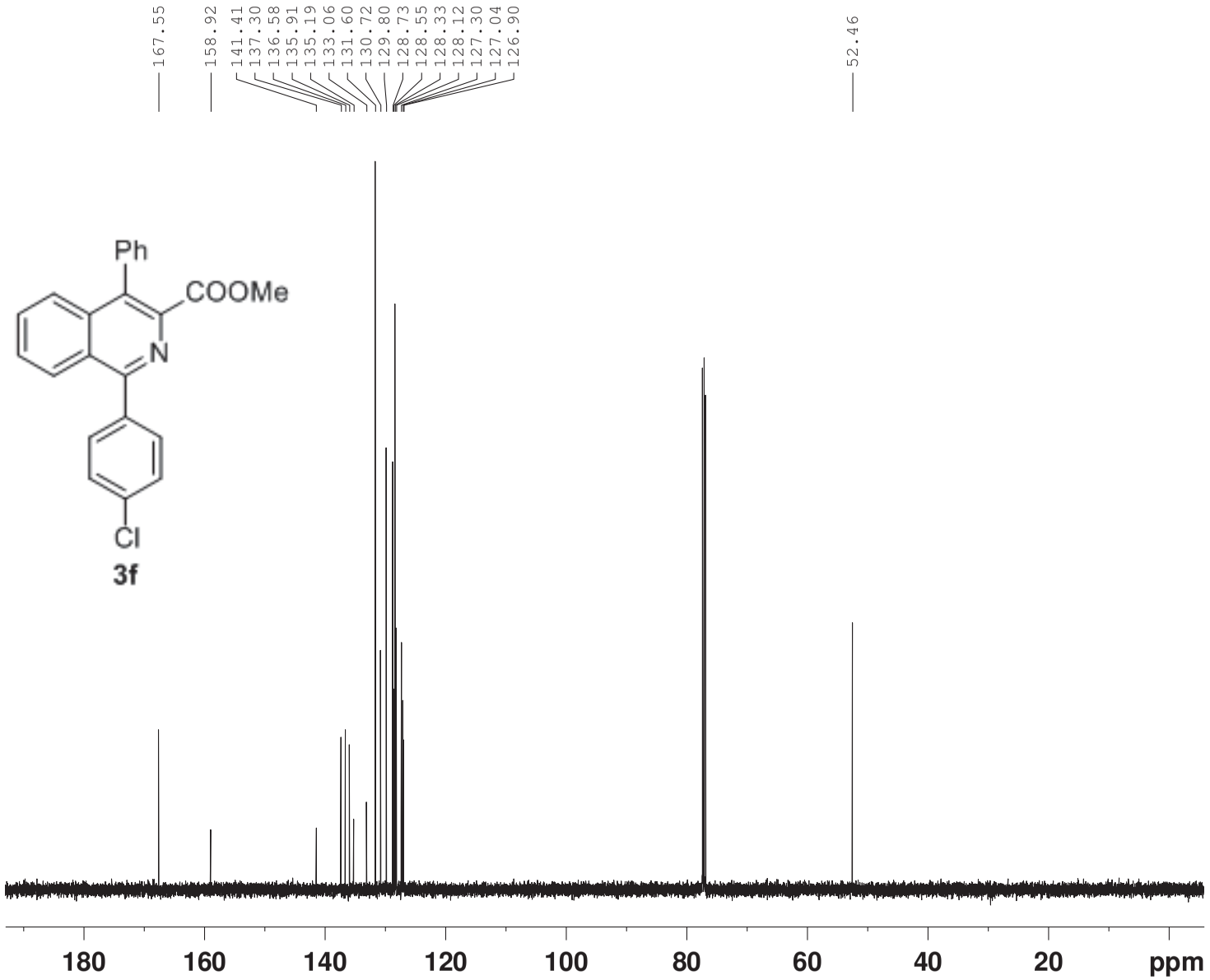

MH-2-68
C13CPD CDCl3

| | |
|---|---|
| NAME | XB20140730 |
| EXPNO | 14 |
| PROCNO | 1 |
| Date_ | 20140730 |
| Time | 21.31 |
| 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 | 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 | 125.7577744 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 1.00 Hz |
| GB | 0 |
| PC | 1.40 |



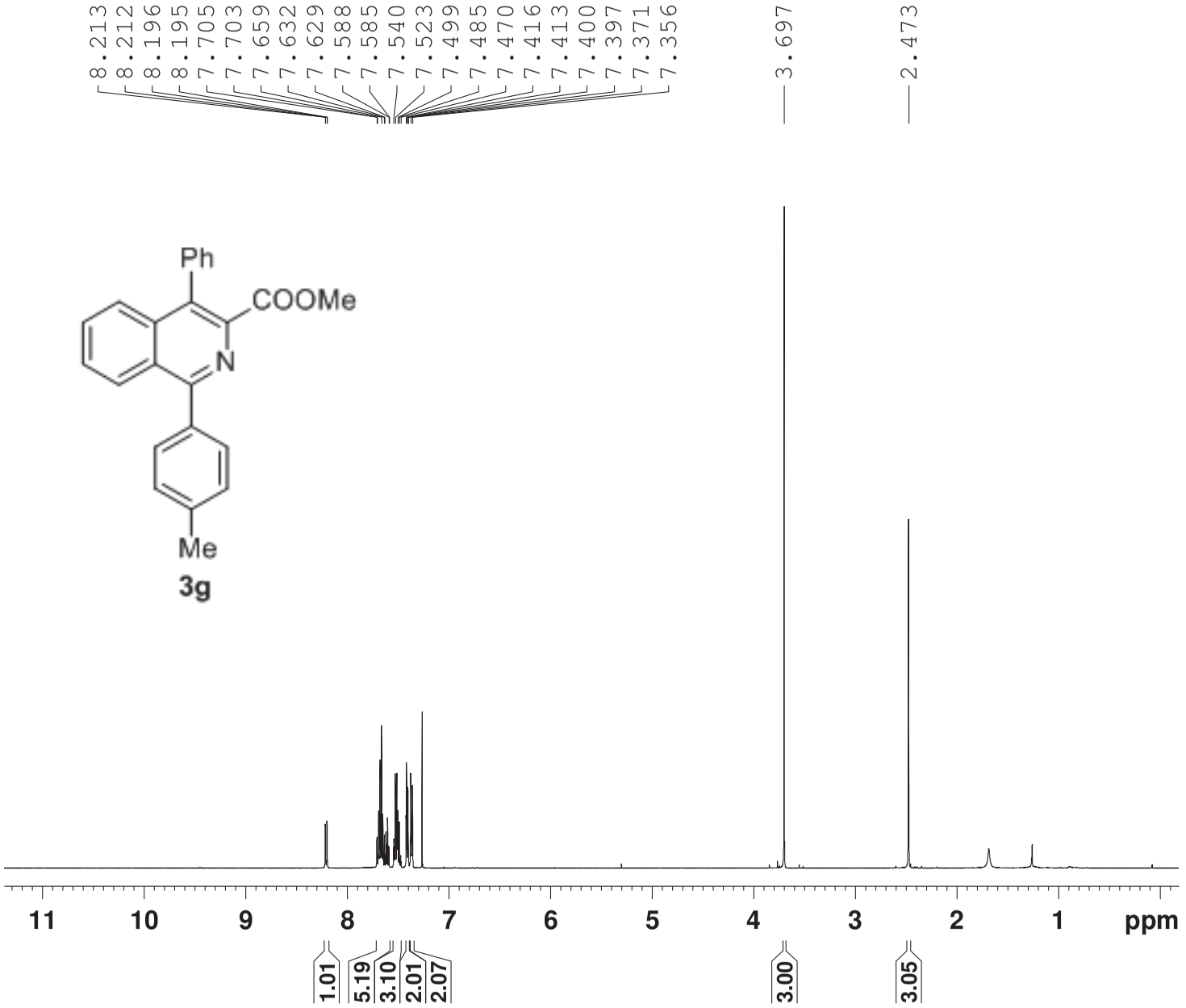

MH-2-28
PROTON CDCl3 D:\\ deng 47

| | |
|---|---|
| NAME | XB20141023 |
| EXPNO | 1 |
| PROCNO | 1 |
| Date_ | 20141023 |
| Time | 11.21 |
| 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 | 296.6 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 |




MH-2-28
C13CPD CDCl3

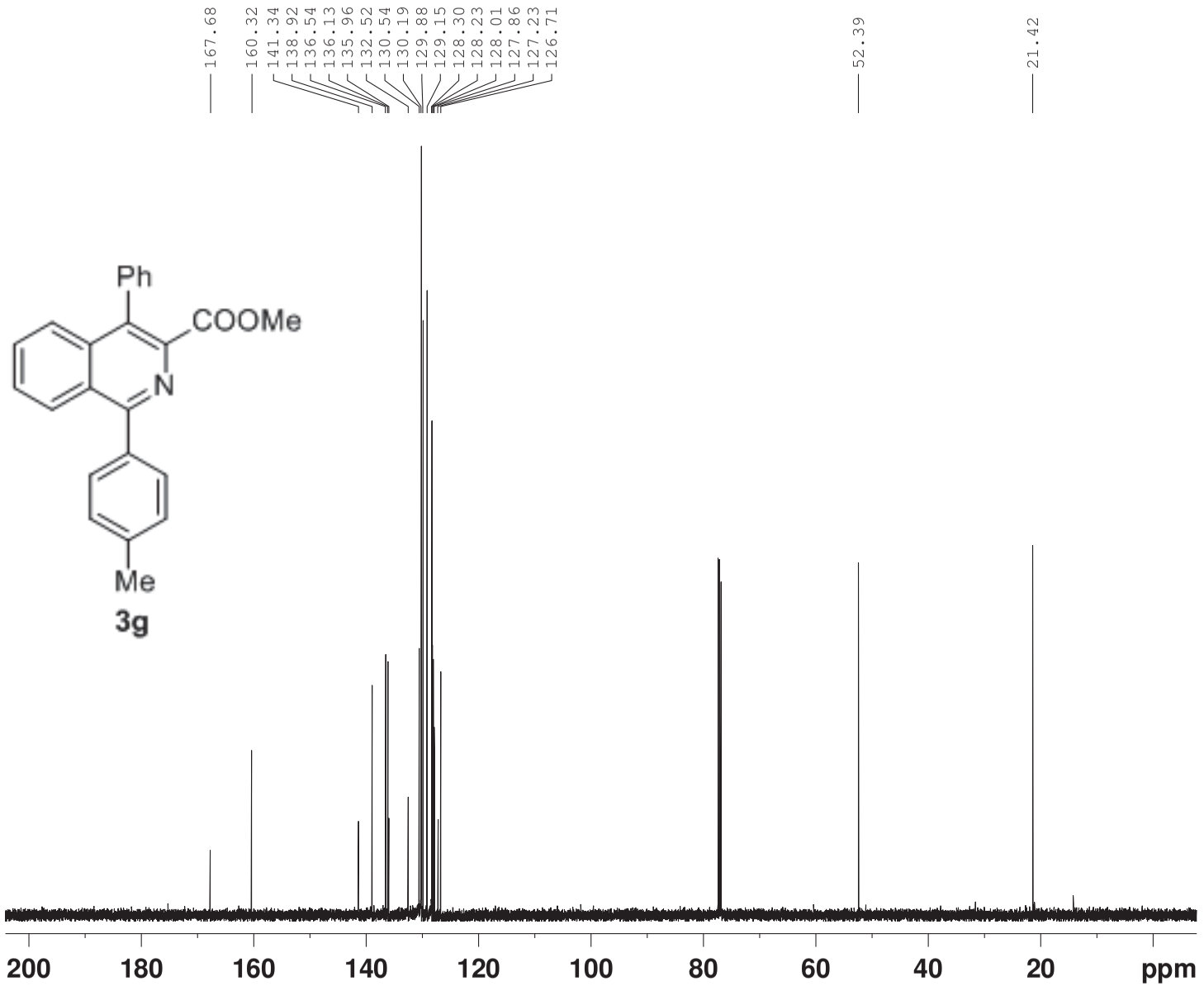
| | | |
|---|---|---|
| NAME | XB20140705 | |
| EXPNO | 20 | |
| PROCNO | 1 | |
| Date_ | 20140705 | |
| Time | 22.53 | |
| INSTRUM | spect | |
| PROBHD | 5 mm PATXO 19F | |
| PULPROG | zgpg30 | |
| TD | 65536 | |
| SOLVENT | CDCl3 | |
| NS | 256 | |
| DS | 4 | |
| SWH | 30030.029 | Hz |
| FIDRES | 0.458222 | Hz |
| AQ | 1.0912410 | sec |
| RG | 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 | no | |
| SSB | 0 | |
| LB | 0.00 | Hz |
| GB | 0 | |
| PC | 1.40 | |




MH-2-31
PROTON CDCl3

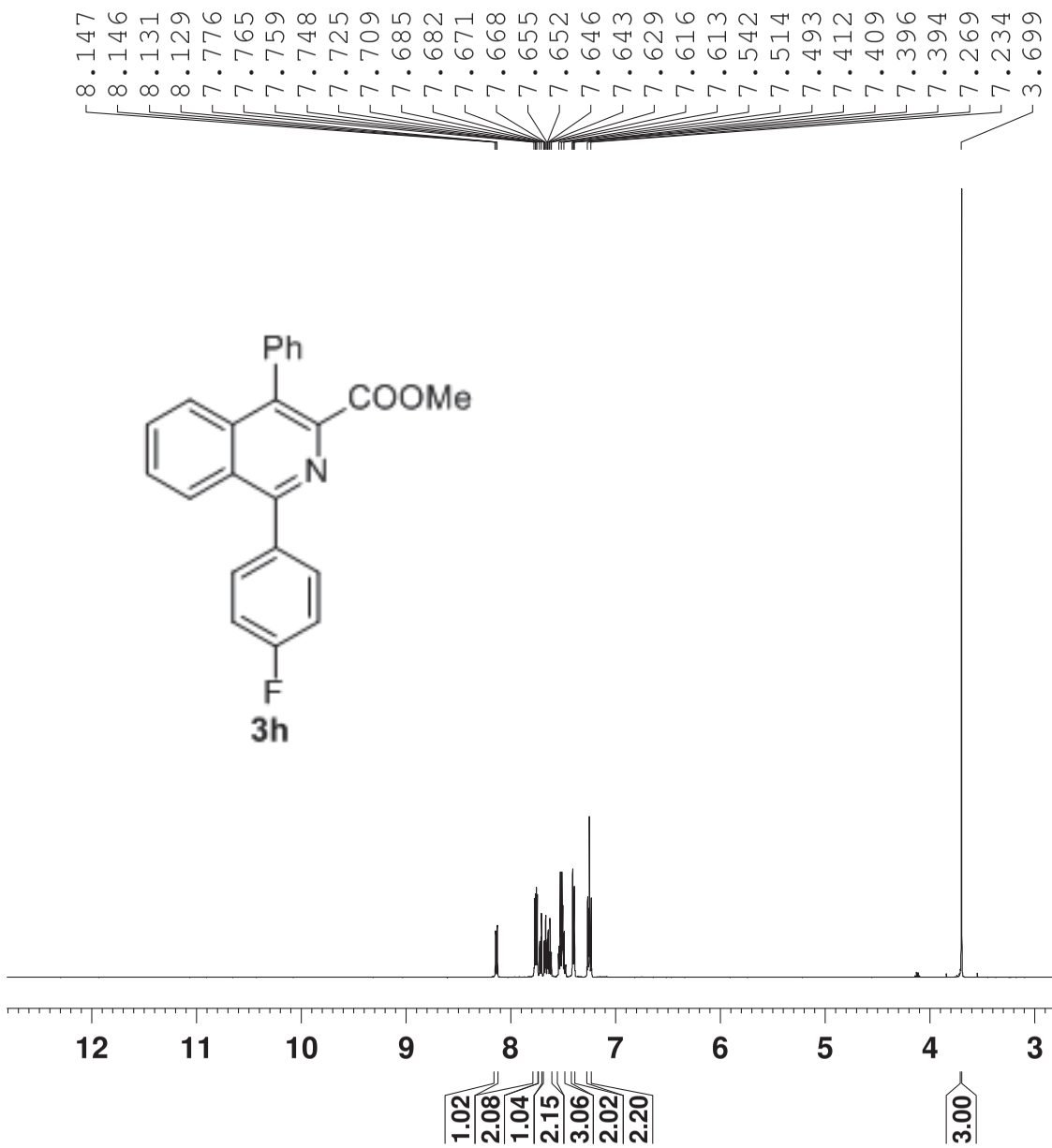
| | |
|---|---|
| NAME | XB20141023 |
| EXPNO | 3 |
| PROCNO | 1 |
| Date_ | 20141023 |
| Time | 11.55 |
| INSTRUM | spect |
| PROBHD | 5 mm PATXO 19F |
| PULPROG | zg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 10330.578 Hz |
| FIDRES | 0.157632 Hz |
| AQ | 3.1720407 sec |
| RG | 362 |
| 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 | 500.1300129 MHz |
| WDW | no |
| SSB | 0 |
| LB | 0.00 Hz |
| GB | 0 |
| PC | 1.00 |




MH-2-31
C13CPD CDCl3

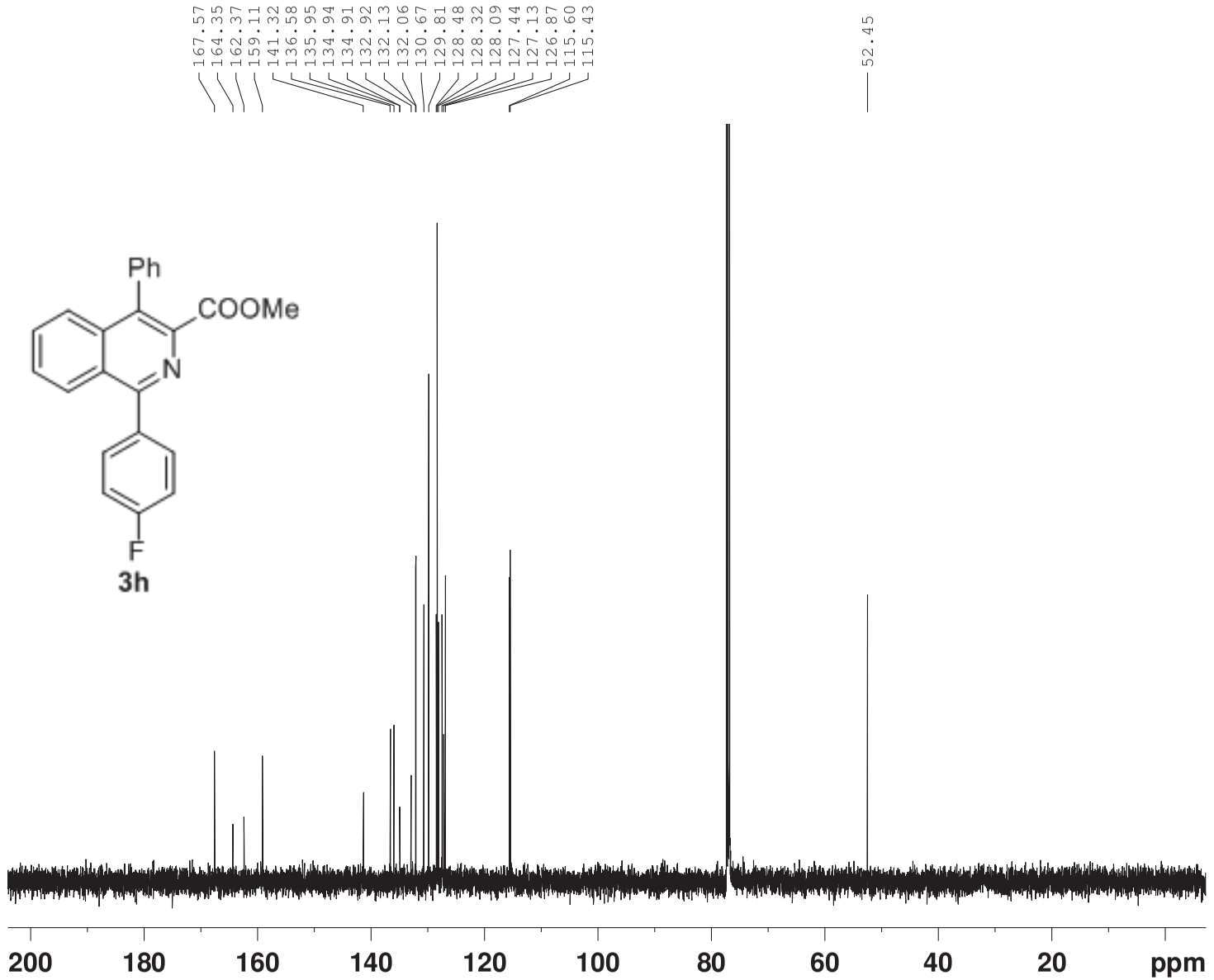
| | |
|---|---|
| NAME | XB20140706 |
| EXPNO | 18 |
| PROCNO | 1 |
| Date_ | 20140706 |
| Time | 21.45 |
| INSTRUM | spect |
| PROBHD | 5 mm PATXO 19F |
| PULPROG | zgpg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 256 |
| DS | 4 |
| SWH | 30030.029 Hz |
| FIDRES | 0.458222 Hz |
| AQ | 1.0912410 sec |
| 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 | no |
| SSB | 0 |
| LB | 0.00 Hz |
| GB | 0 |
| PC | 1.40 |




MH-2-32 AGAIN
PROTON CDCl3

| | |
|---|---|
| NAME | XB20140705 |
| EXPNO | 14 |
| PROCNO | 1 |
| Date_ | 20140705 |
| Time | 23.11 |
| 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 |

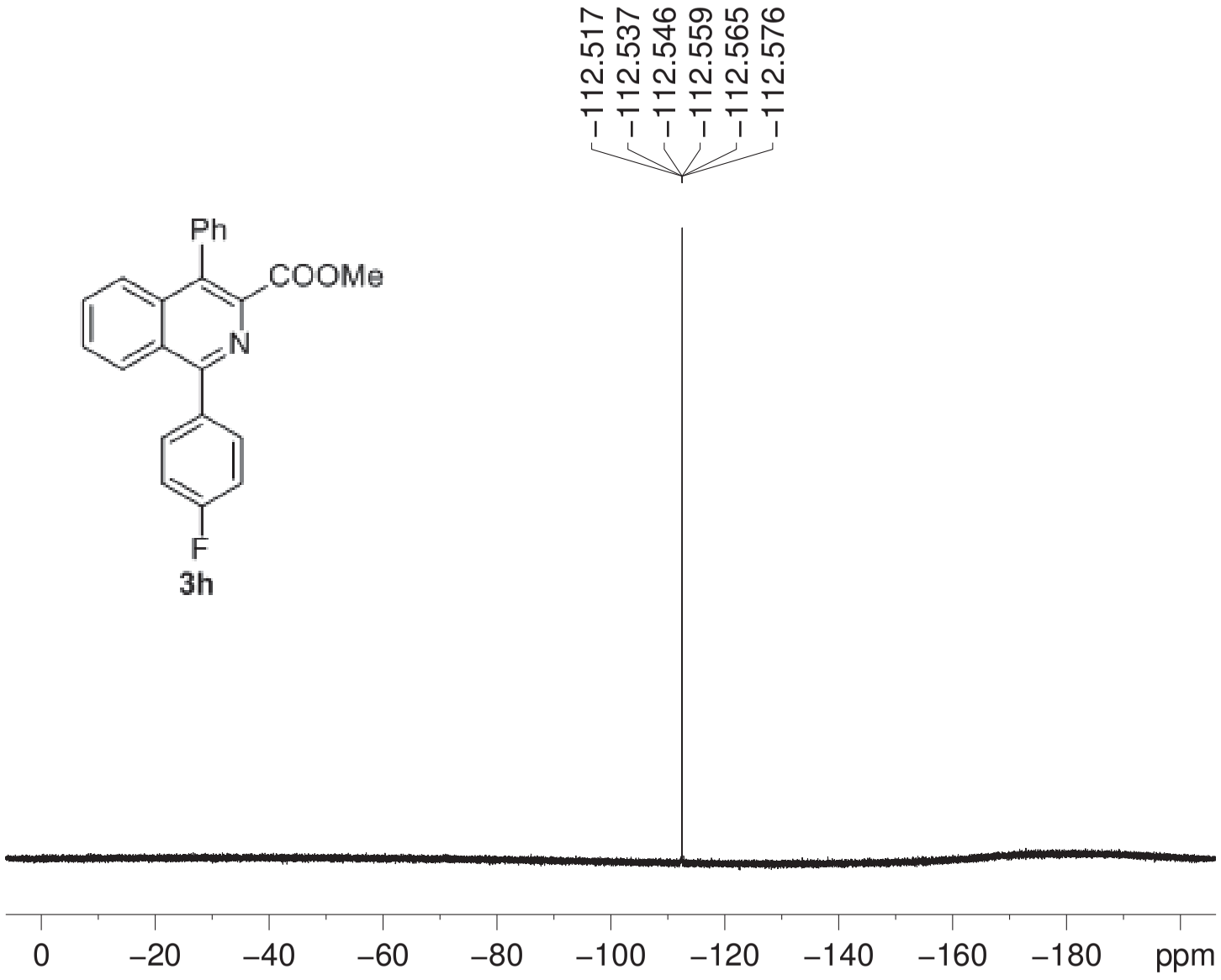
| ======== CHANNEL f1 ======== | |
|---|---|
| NUC1 | 1H |
| P1 | 14.14 usec |
| PL1 | 1.00 dB |
| SFO1 | 500.1330885 MHz |
| SI | 32768 |
| SF | 500.1300129 MHz |
| WDW | no |
| SSB | 0 |
| LB | 0.00 Hz |
| GB | 0 |
| PC | 1.00 |

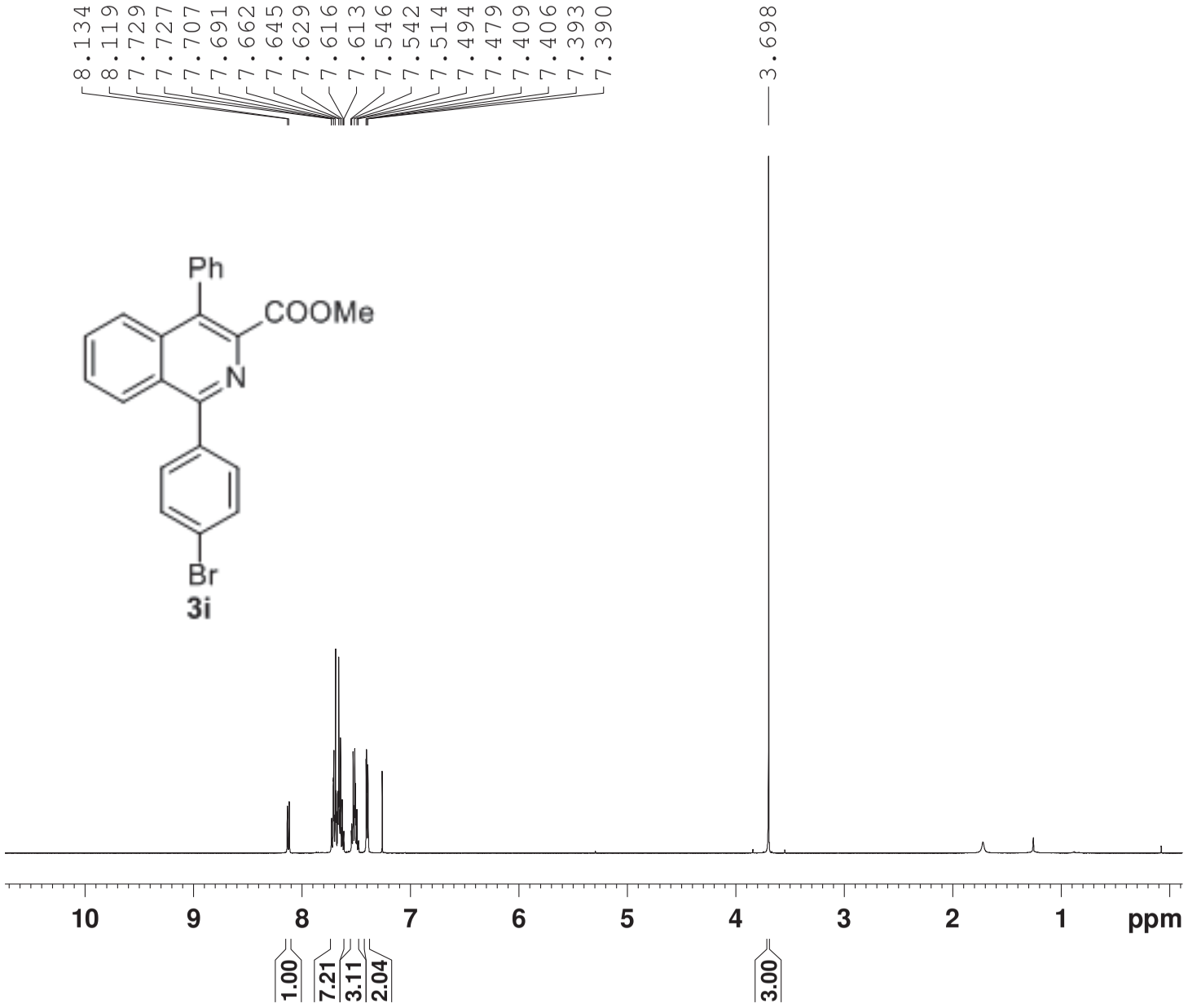



MH-2-32
C13CPD CDCl3

| | |
|---|---|
| NAME | XB20140705 |
| EXPNO | 16 |
| PROCNO | 1 |
| Date_ | 20140705 |
| Time | 22.08 |
| 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 | 128 |
| 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 |

MH-2-32
19Fdeft CDCl3 D:\\ deng 46

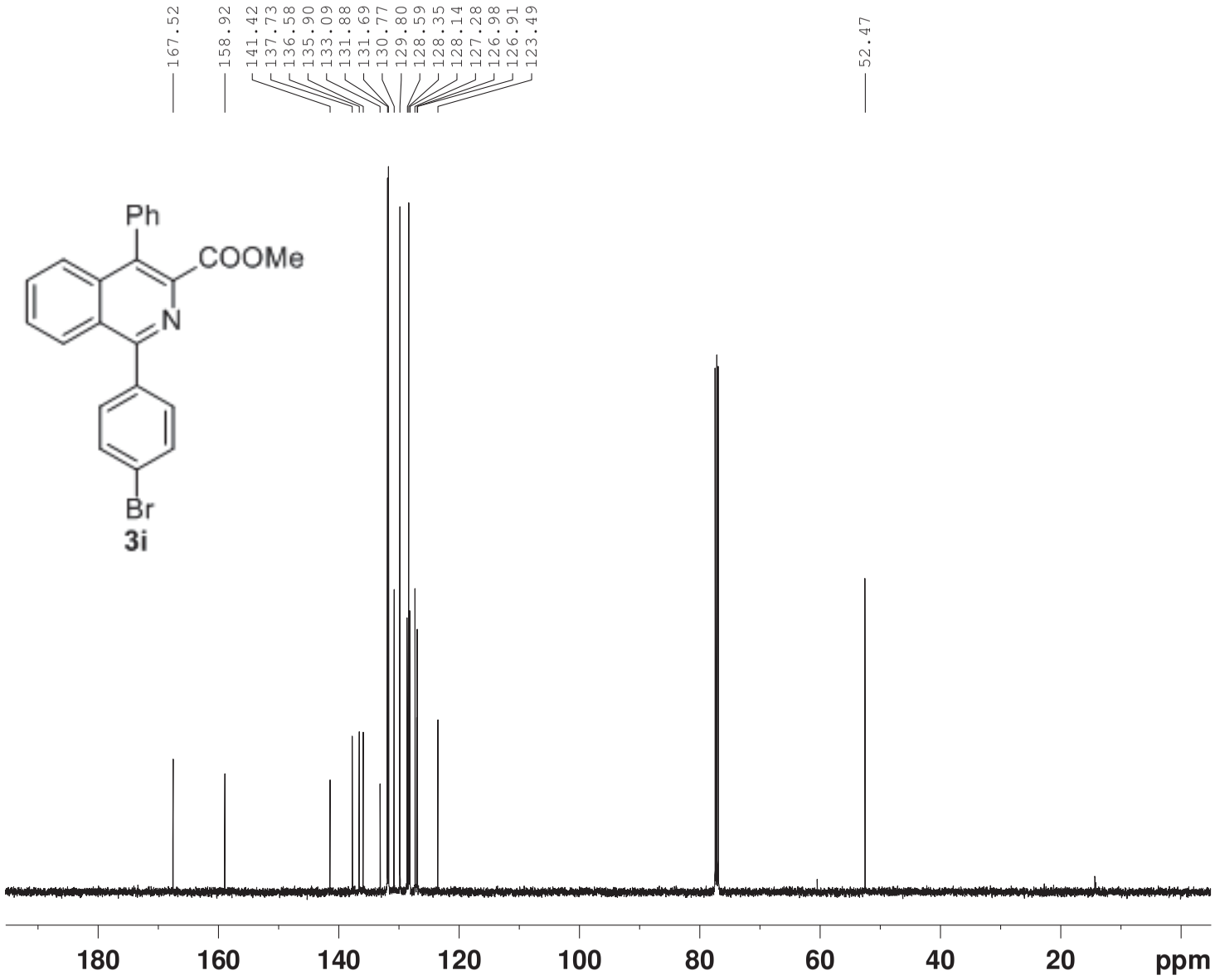





MH-2-34
PROTON CDCl3

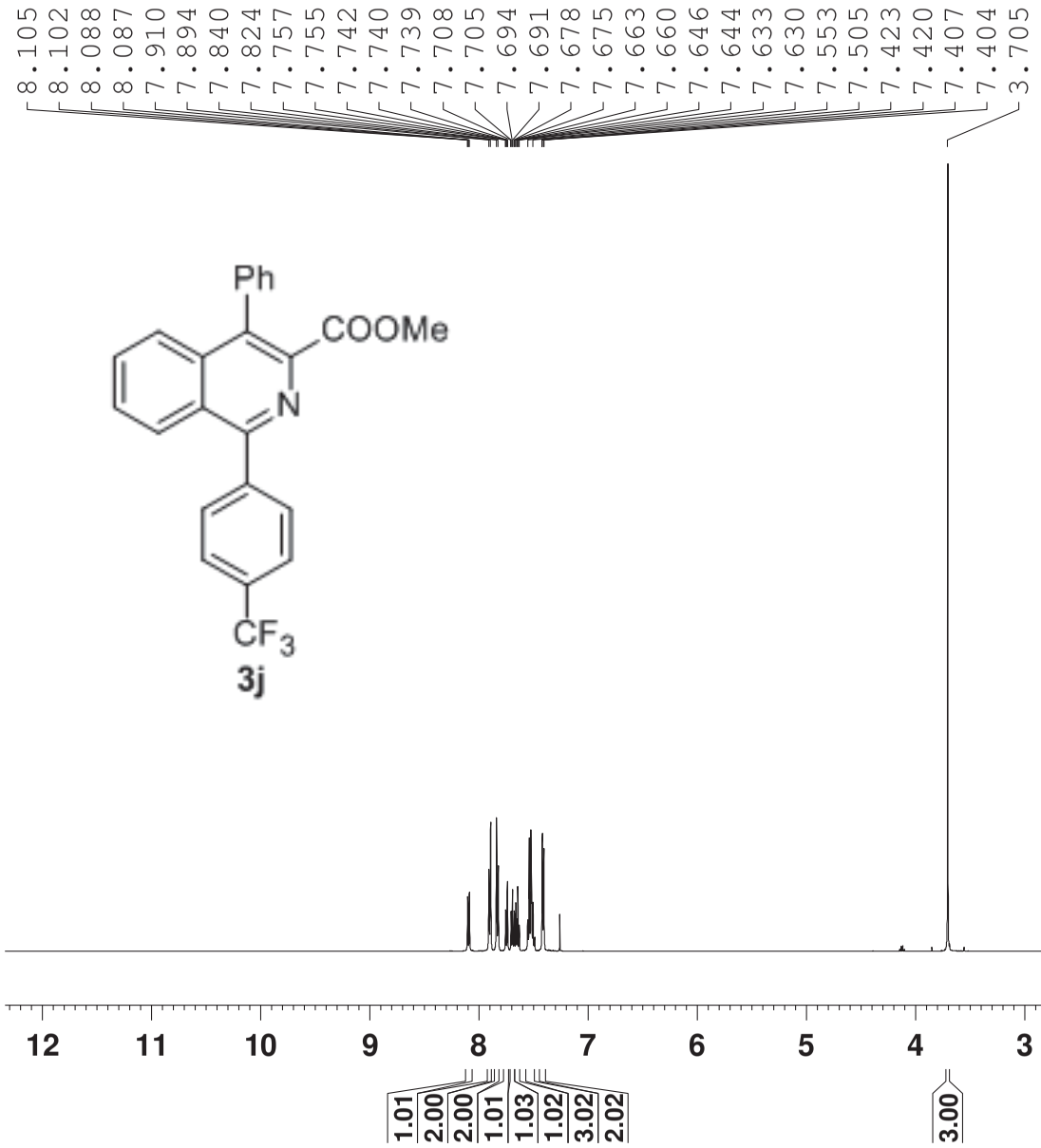
| | |
|---|---|
| NAME | XB20141023 |
| EXPNO | 7 |
| PROCNO | 1 |
| Date_ | 20141023 |
| Time | 12.00 |
| INSTRUM | spect |
| PROBHD | 5 mm PATXO 19F |
| PULPROG | zg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 10330.578 Hz |
| FIDRES | 0.157632 Hz |
| AQ | 3.1720407 sec |
| RG | 287.4 |
| 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 | 500.1300129 MHz |
| WDW | no |
| SSB | 0 |
| LB | 0.00 Hz |
| GB | 0 |
| PC | 1.00 |



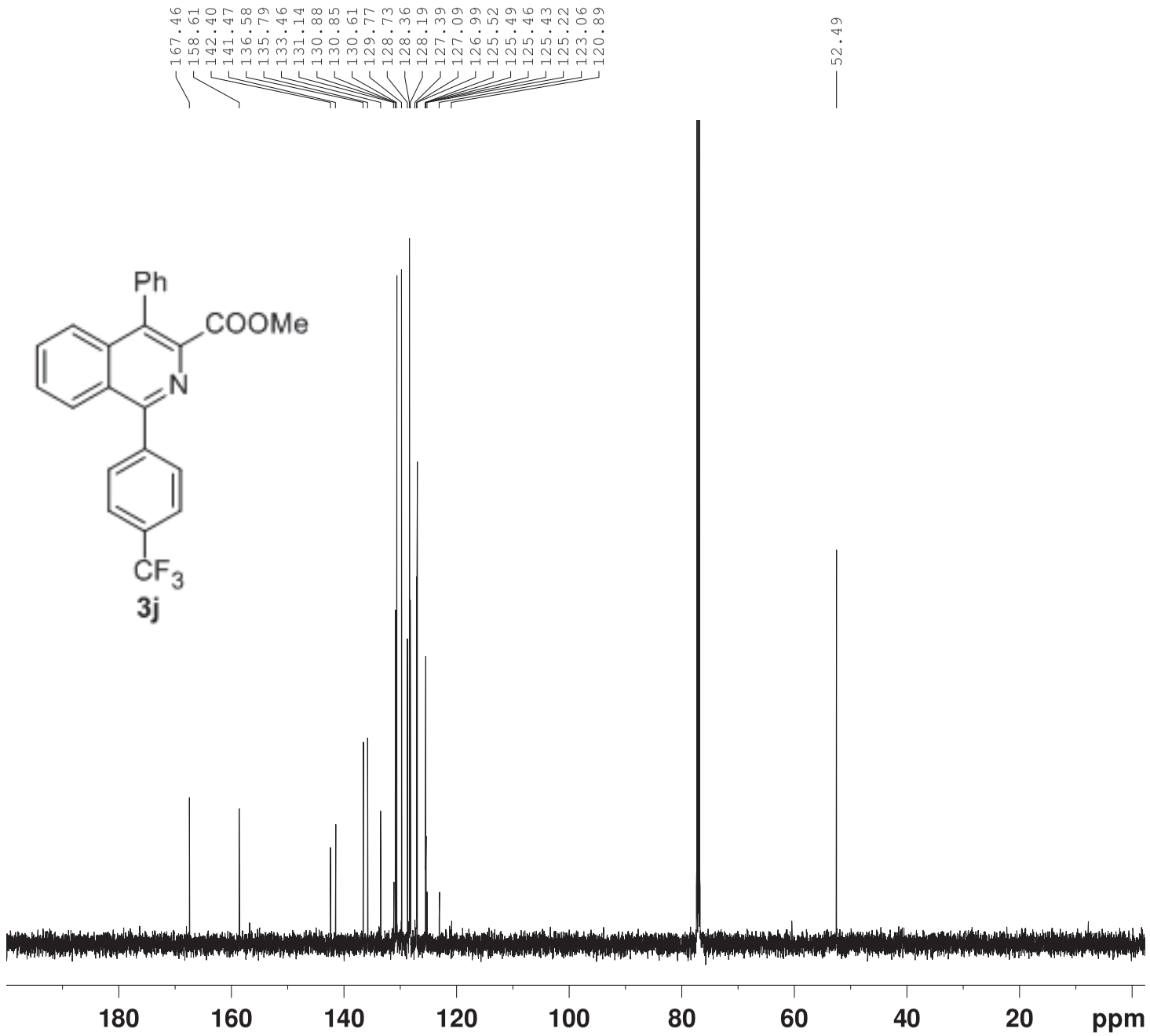

MH-2-34
C13CPD CDCl3

| | | |
|---|---|---|
| NAME | XB20140705 | |
| EXPNO | 18 | |
| PROCNO | 1 | |
| Date_ | 20140705 | |
| Time | 22.34 | |
| 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 | 287.4 | |
| 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 | |




MH-2-35
PROTON CDCl3

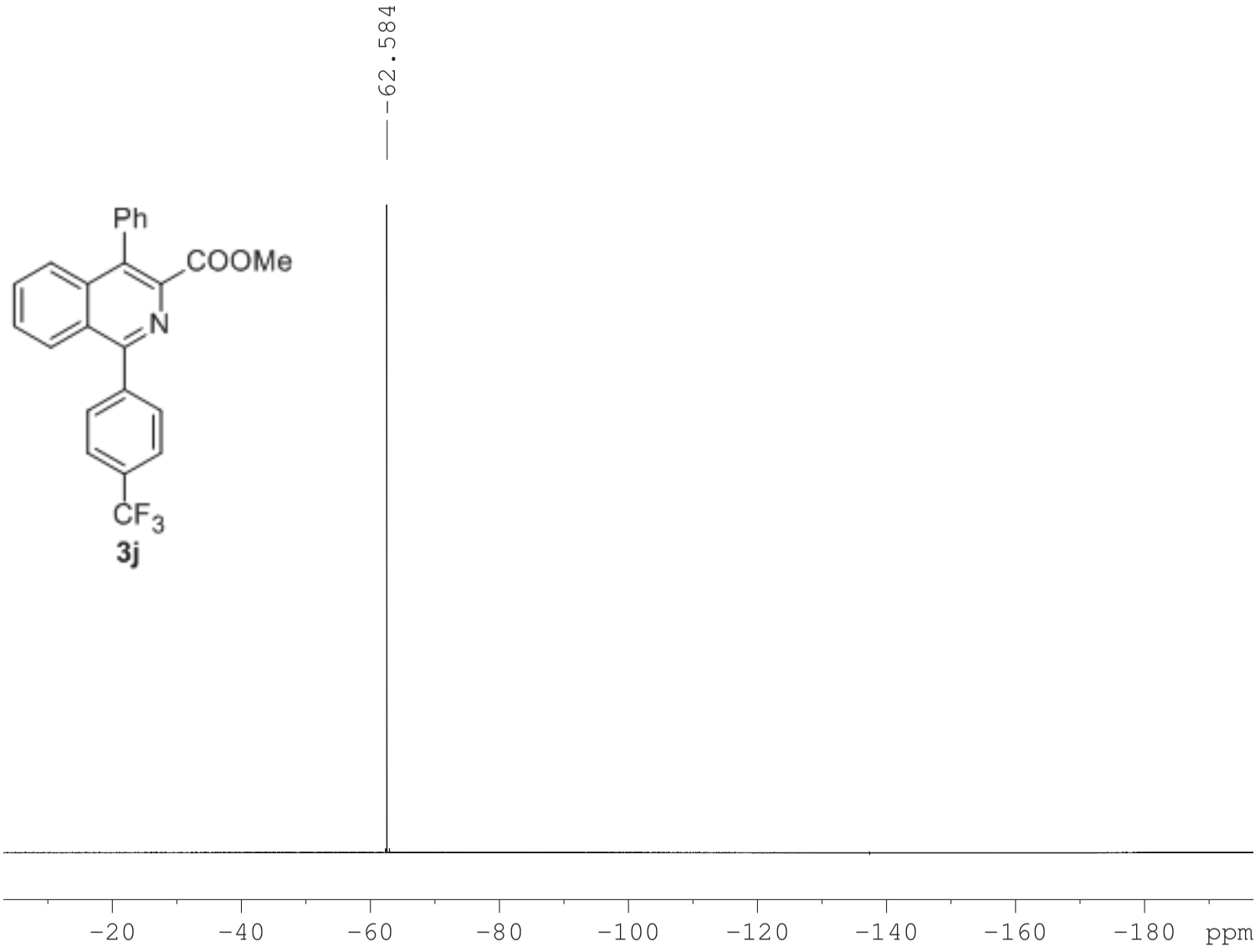
| | | |
|---|---|---|
| NAME | XB20140705 | |
| EXPNO | 11 | |
| PROCNO | 1 | |
| Date_ | 20140705 | |
| Time | 21.29 | |
| INSTRUM | spect | |
| PROBHD | 5 mm PATXO 19F | |
| PULPROG | zg30 | |
| TD | 65536 | |
| SOLVENT | CDCl3 | |
| NS | 16 | |
| DS | 2 | |
| SWH | 10330.578 | Hz |
| FIDRES | 0.157632 | Hz |
| AQ | 3.1720407 | sec |
| RG | 161.3 | |
| 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 | |

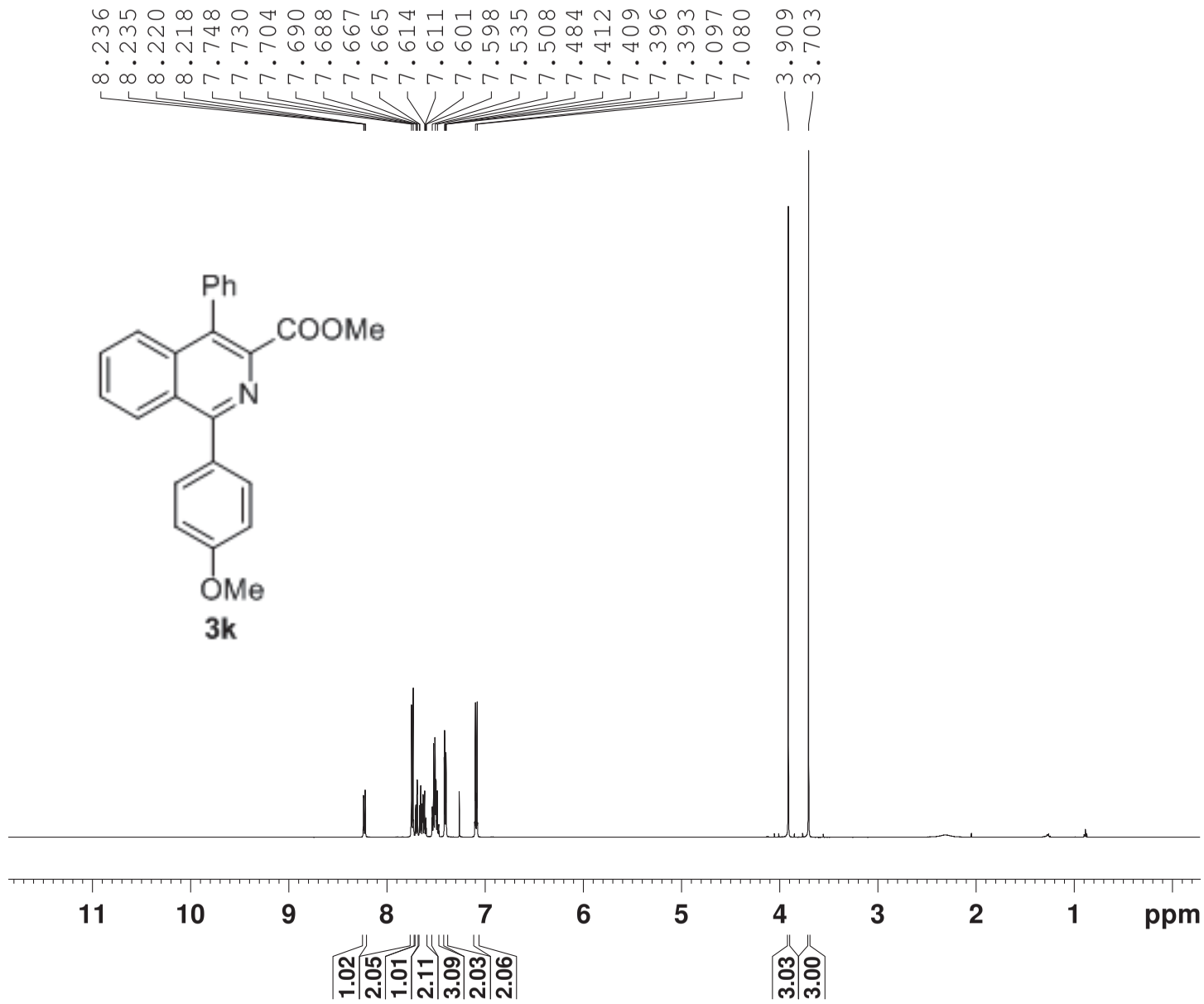



MH-2-35
C13CPD CDCl3

| | | |
|---|---|---|
| NAME | XB20140705 | |
| EXPNO | 13 | |
| PROCNO | 1 | |
| Date_ | 20140705 | |
| Time | 21.46 | |
| 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 | 128 | |
| 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 | 0.20 | |

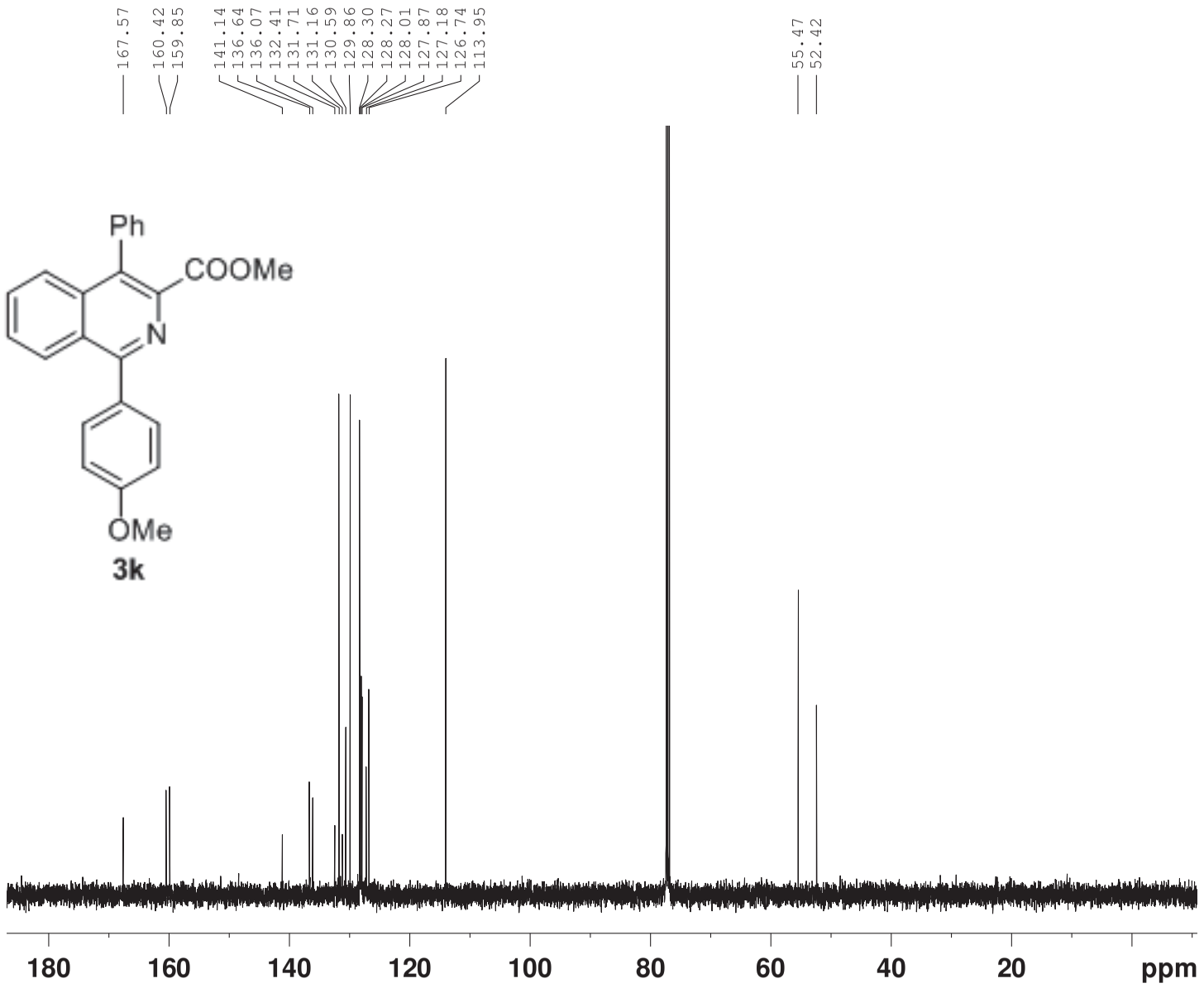
MH-2-35
19Fdeft CDCl3 D:\\ deng 45





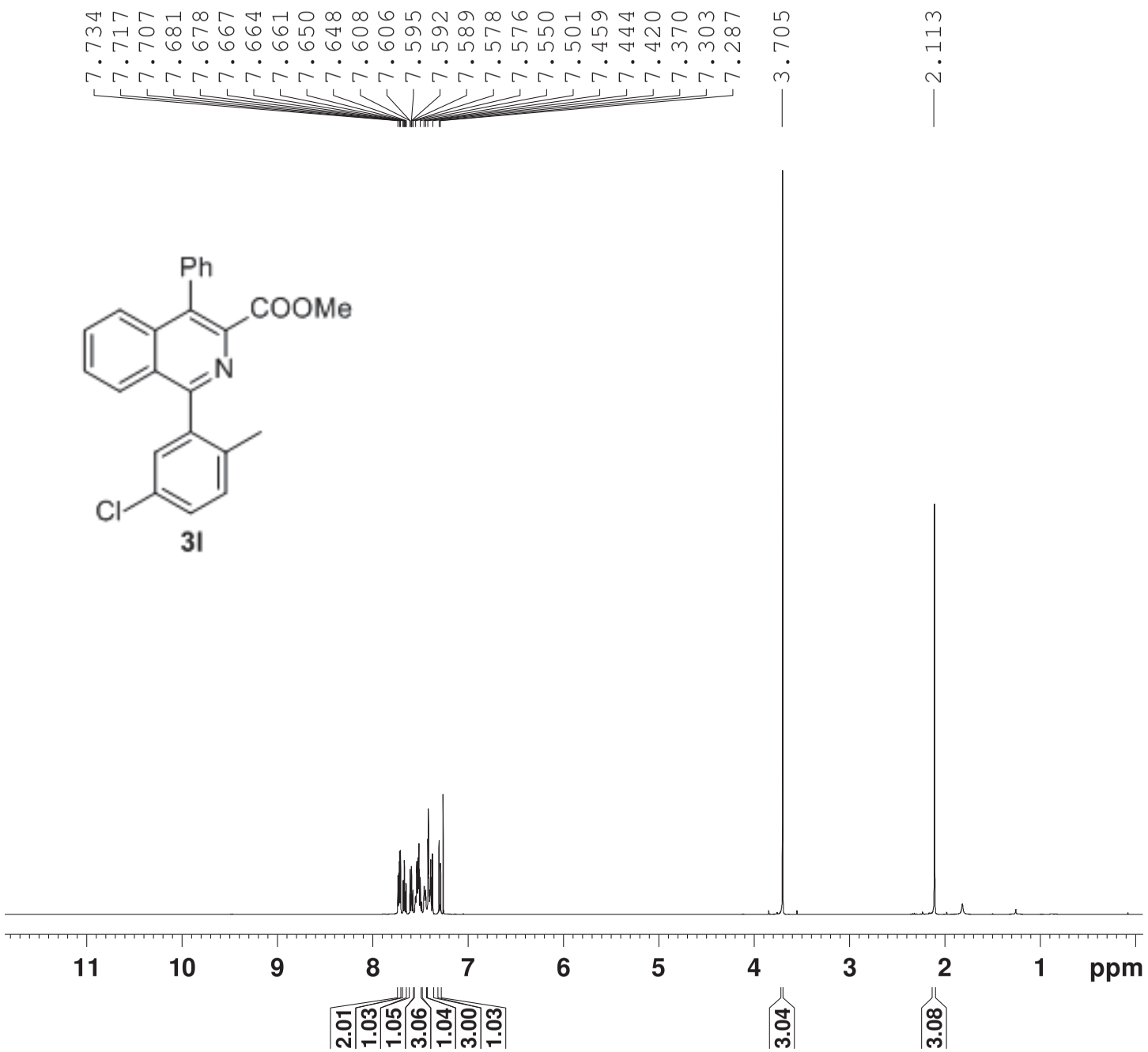

MH-2-2
PROTON CDCl3

| | |
|---|---|
| NAME | XB20140602 |
| EXPNO | 12 |
| PROCNO | 1 |
| Date_ | 20140602 |
| Time | 19.42 |
| 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 | 203.2 |
| 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 |



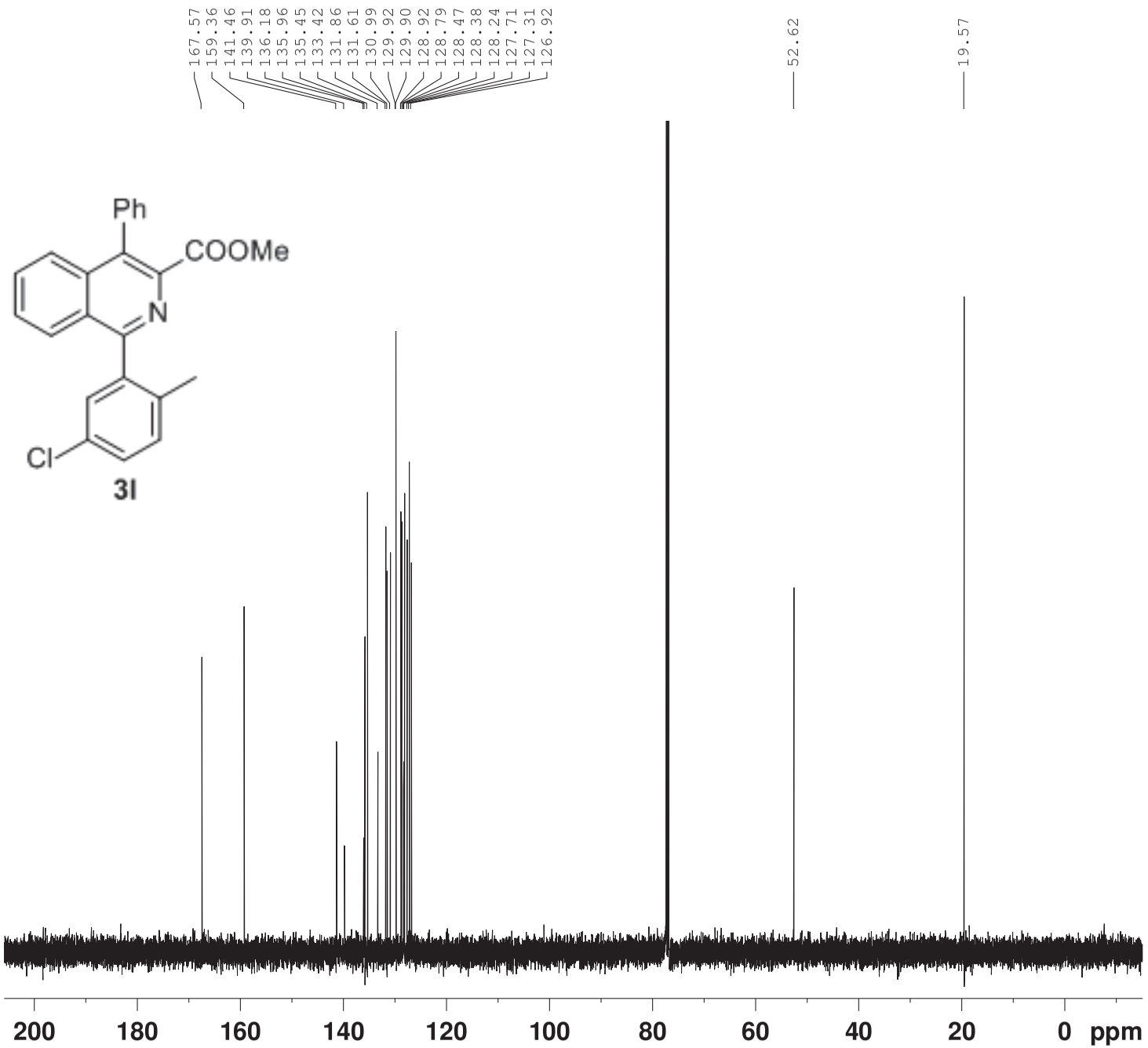

MH-2-2
C13CPD CDCl3

| | |
|---|---|
| NAME | XB20140602 |
| EXPNO | 14 |
| PROCNO | 1 |
| Date_ | 20140602 |
| Time | 19.53 |
| 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 | 297.0 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 |



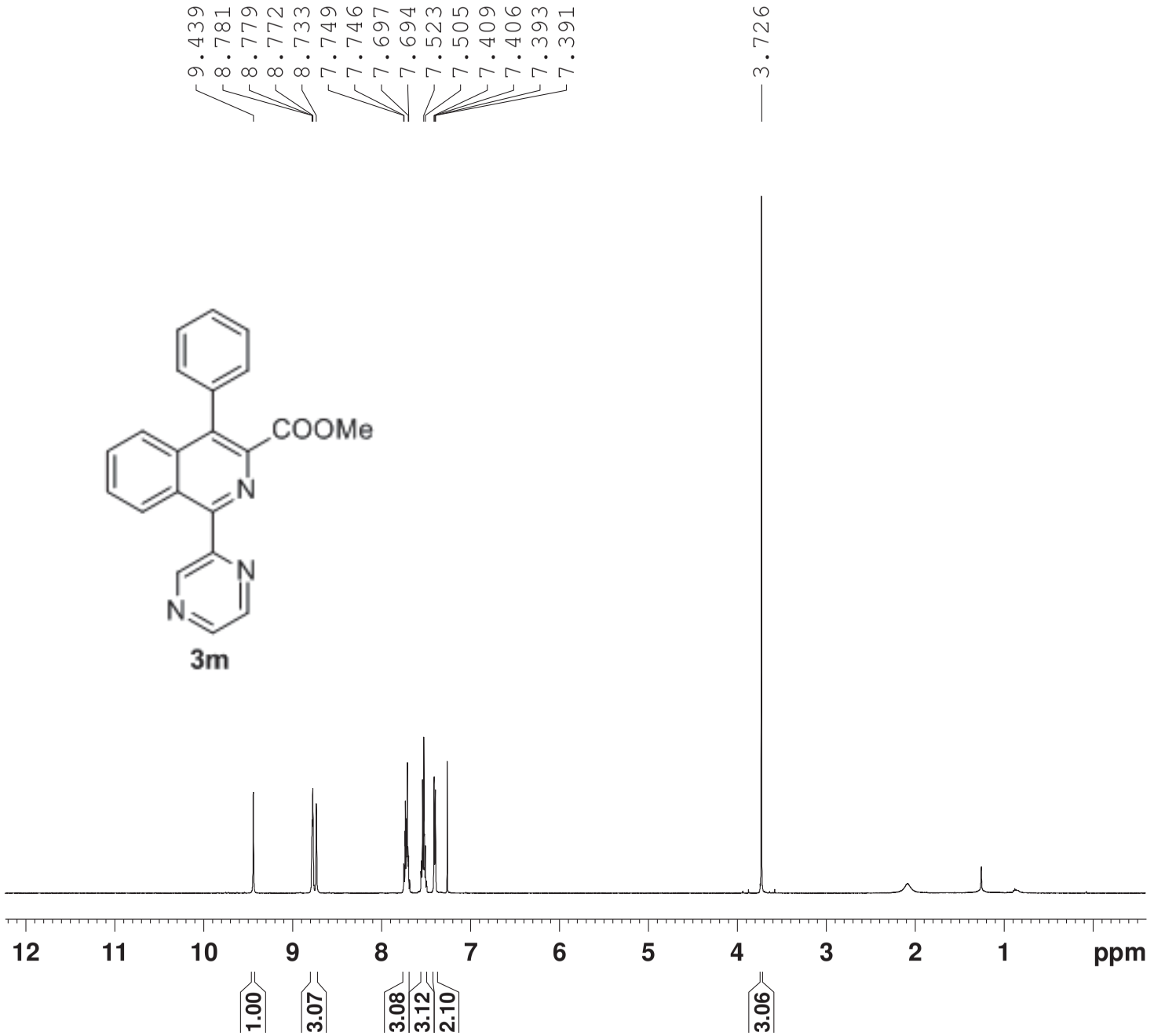

MH-2-6
PROTON CDCl3

| | | |
|---|---|---|
| NAME | XB20140926 | |
| EXPNO | 15 | |
| PROCNO | 1 | |
| Date_ | 20140926 | |
| Time | 15.32 | |
| 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 | 143.7 | |
| DW | 48.400 | usec |
| DE | 6.00 | usec |
| TE | 297.4 | 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 | 500.1300129 | MHz |
| WDW | no | |
| SSB | 0 | |
| LB | 0.00 | Hz |
| GB | 0 | |
| PC | 1.00 | |



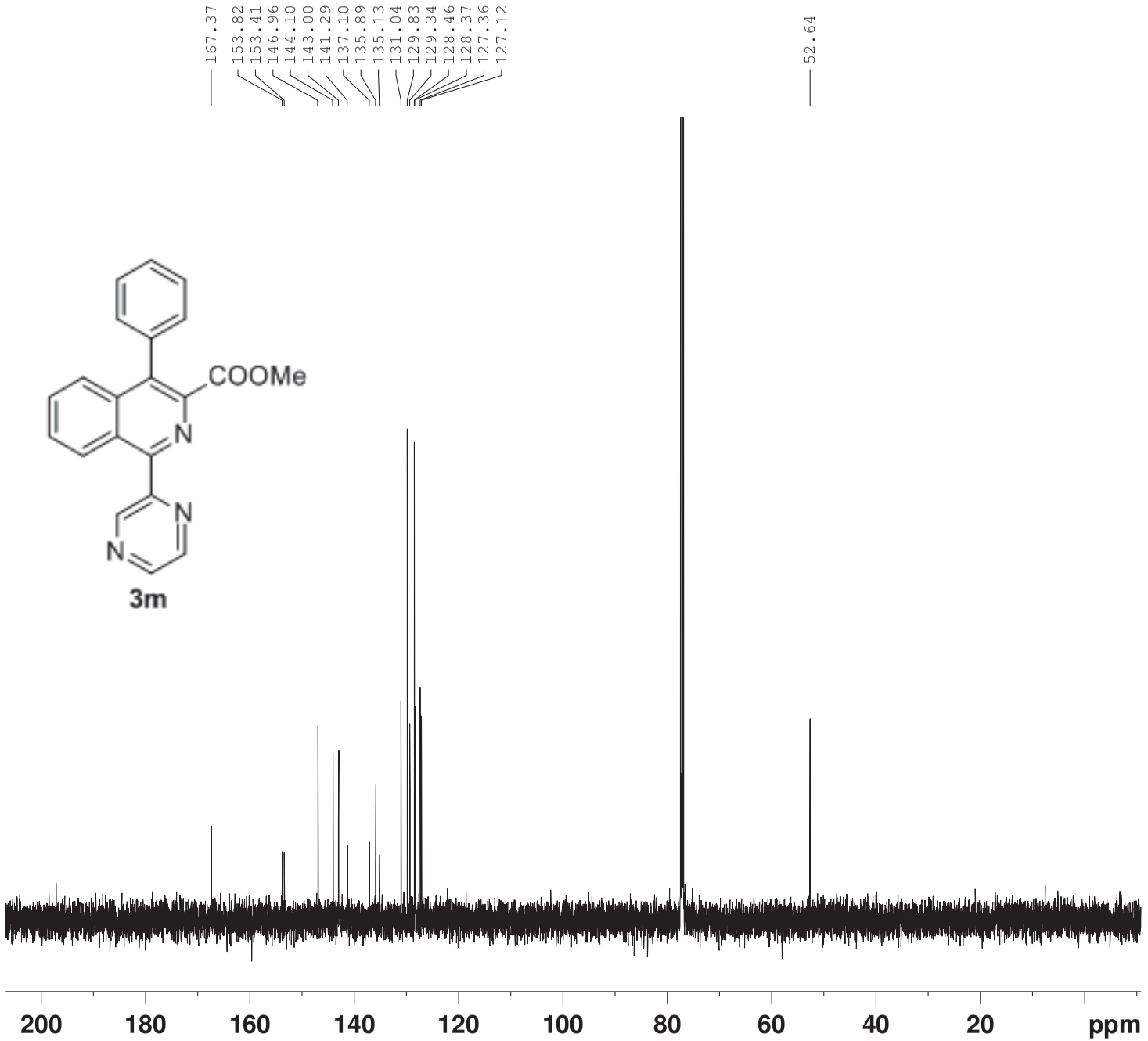

MH-2-6
C13CPD CDCl3

| | |
|---|---|
| NAME | XB20140926 |
| EXPNO | 16 |
| PROCNO | 1 |
| Date_ | 20140926 |
| Time | 15.47 |
| 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 | 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 | no |
| SSB | 0 |
| LB | 0.00 Hz |
| GB | 0 |
| PC | 1.40 |



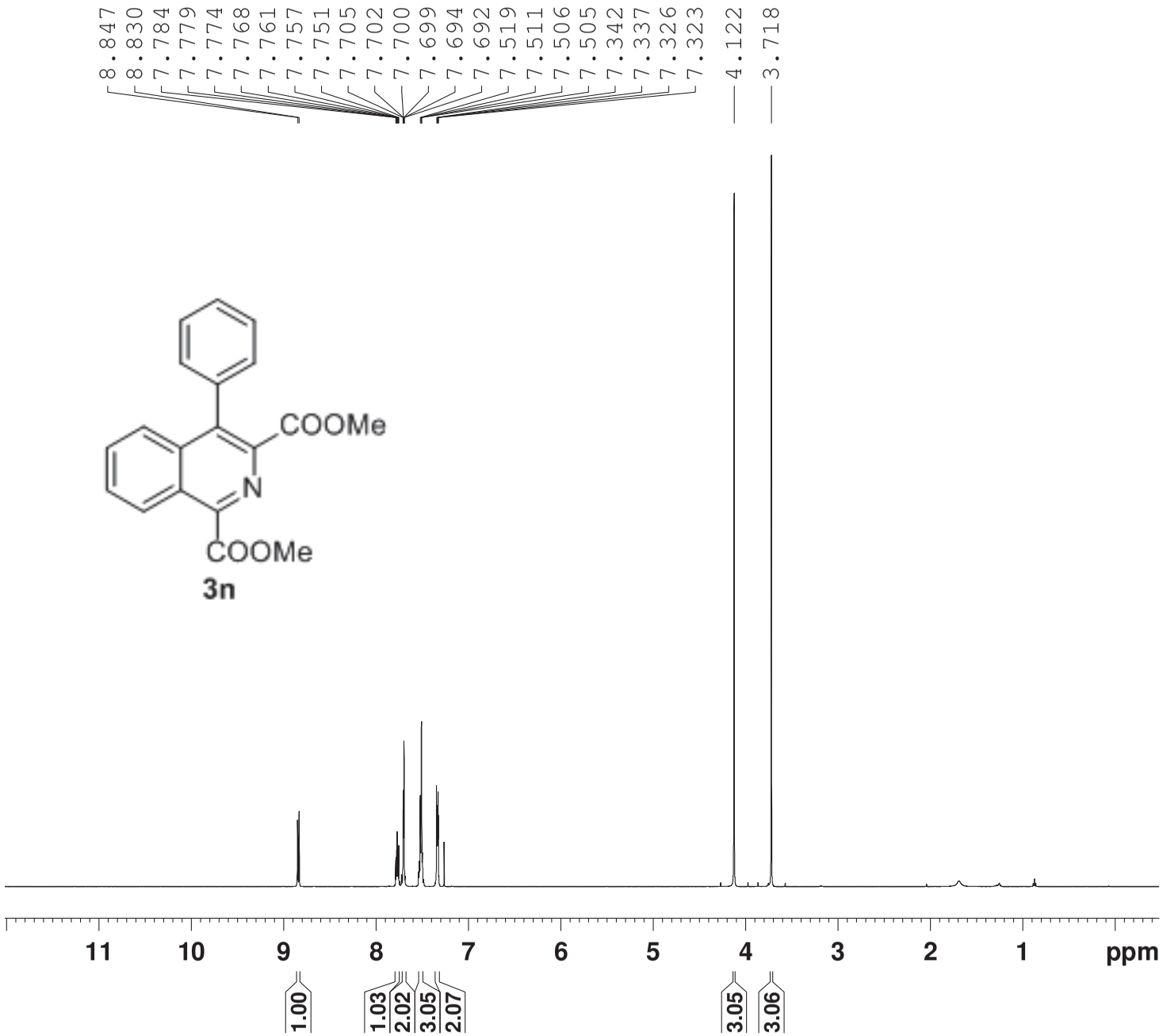

MH-2-78
PROTON CDCl3

| | |
|---|---|
| NAME | MH20140901 |
| EXPNO | 24 |
| PROCNO | 1 |
| Date_ | 20140902 |
| Time | 3.54 |
| 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 | 322.5 |
| DW | 48.400 usec |
| DE | 6.00 usec |
| TE | 298.3 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 |



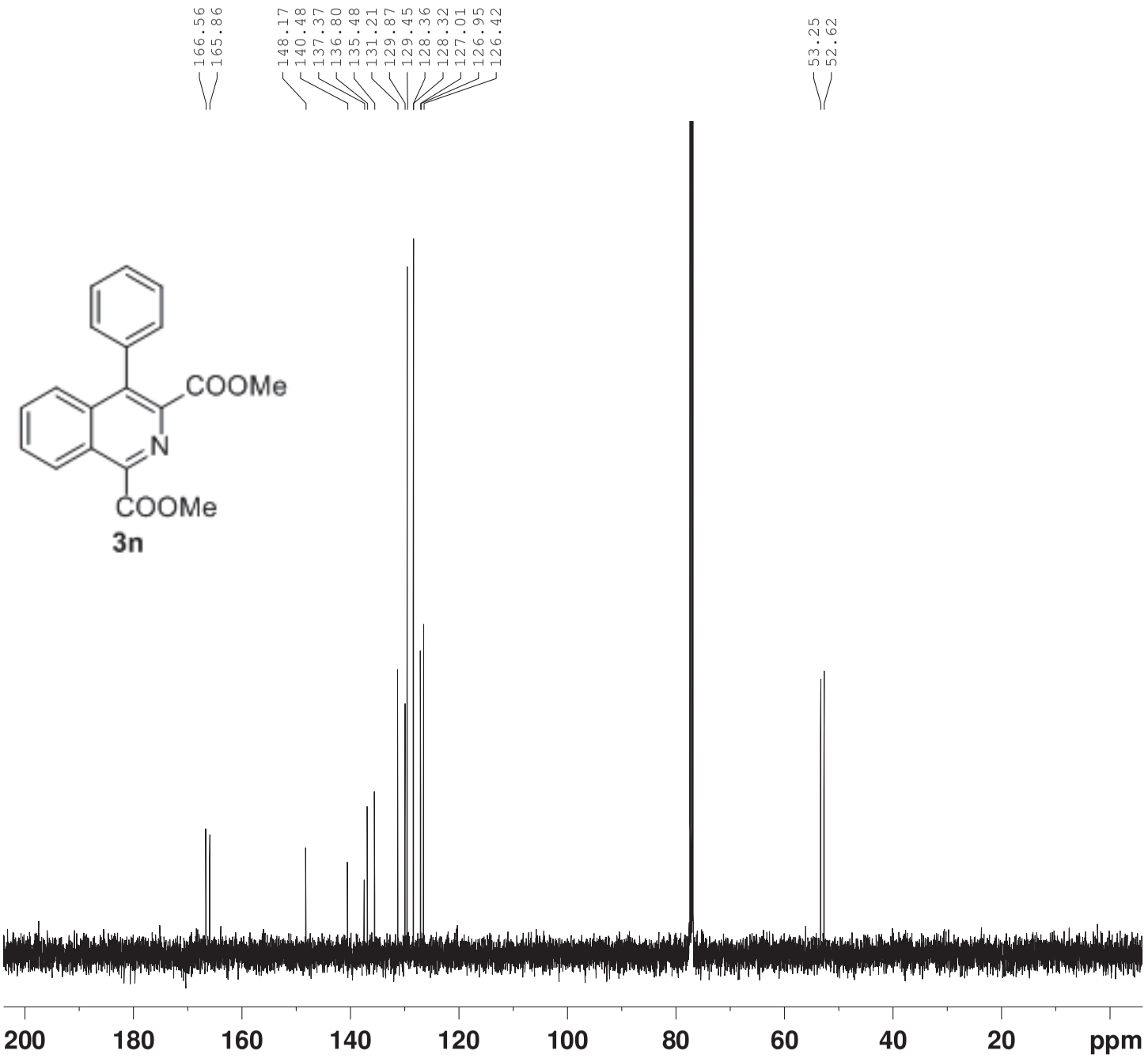

MH-2-78
C13CPD CDCl3

| | |
|---|---|
| NAME | MH20140901 |
| EXPNO | 25 |
| PROCNO | 1 |
| Date_ | 20140902 |
| Time | 4.10 |
| 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 | 912.3 |
| DW | 16.650 usec |
| DE | 6.00 usec |
| TE | 299.5 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 | 125.7577718 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 1.00 Hz |
| GB | 0 |
| PC | 1.40 |



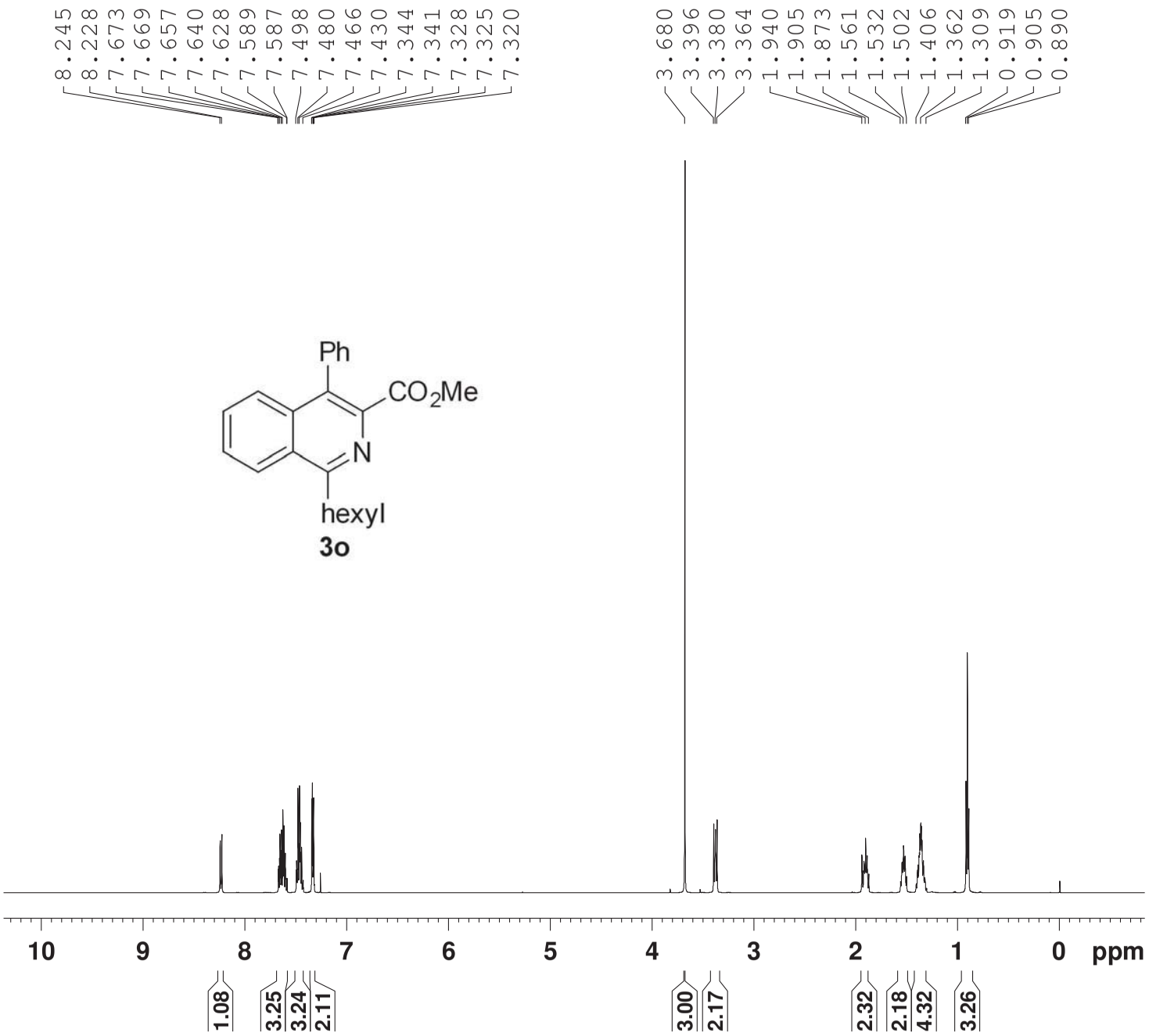

MH-1-124
PROTON CDCl3

| | |
|---|---|
| NAME | XB20140527 |
| EXPNO | 1 |
| PROCNO | 1 |
| Date_ | 20140527 |
| Time | 10.48 |
| 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 | 296.1 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 |




MH-1-124
C13CPD CDCl3

| | |
|---|---|
| NAME | XB20140527 |
| EXPNO | 3 |
| PROCNO | 1 |
| Date_ | 20140527 |
| Time | 10.58 |
| 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 | 161.3 |
| 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 |




MH-3-106
PROTON CDCl3

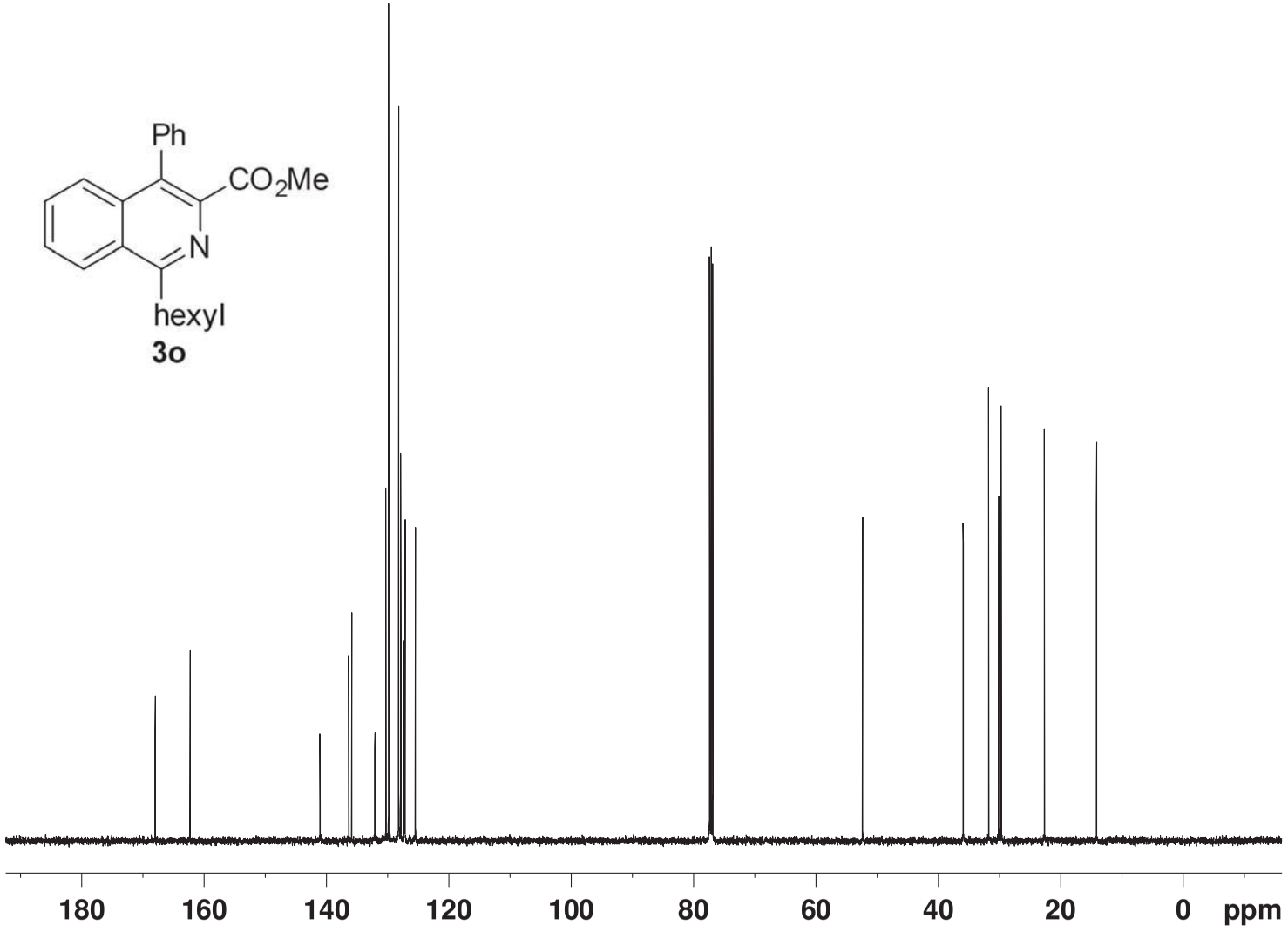
| | |
|---|---|
| NAME | xb20151105 |
| EXPNO | 20 |
| PROCNO | 1 |
| Date_ | 20151105 |
| Time | 21.36 |
| INSTRUM | spect |
| PROBHD | 5 mm PATXO 19F |
| PULPROG | zg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 10330.578 Hz |
| FIDRES | 0.157632 Hz |
| AQ | 3.1720407 sec |
| RG | 57 |
| DW | 48.400 usec |
| DE | 6.00 usec |
| TE | 294.6 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 |

MH-3-106
C13CPD CDCl3

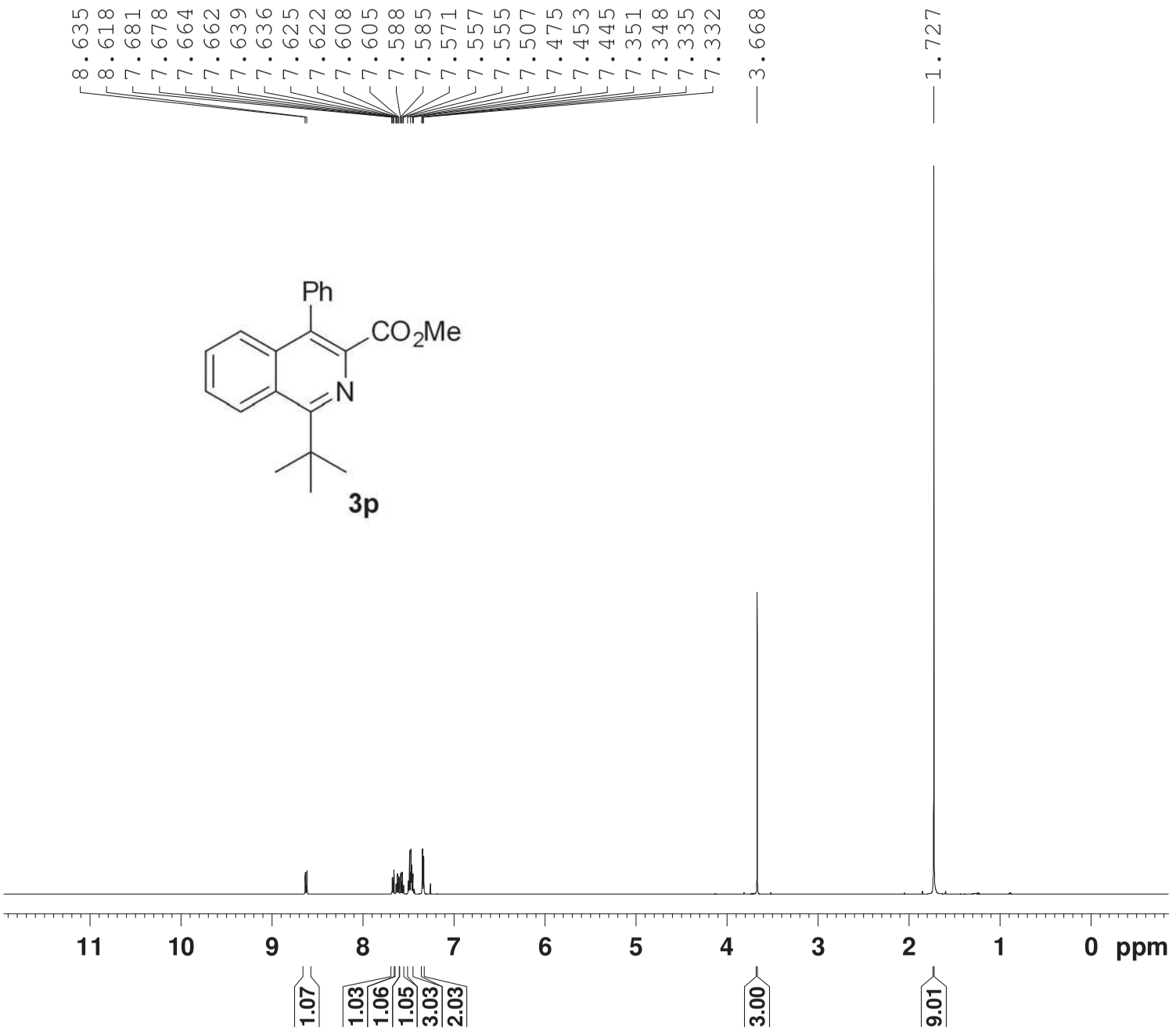
167.98
162.27
141.05
136.35
135.85
132.08
130.29
129.83
128.19
128.16
127.83
127.27
127.14
125.44
52.35
35.91
31.76
30.11
29.70
22.65
14.13




**3o**

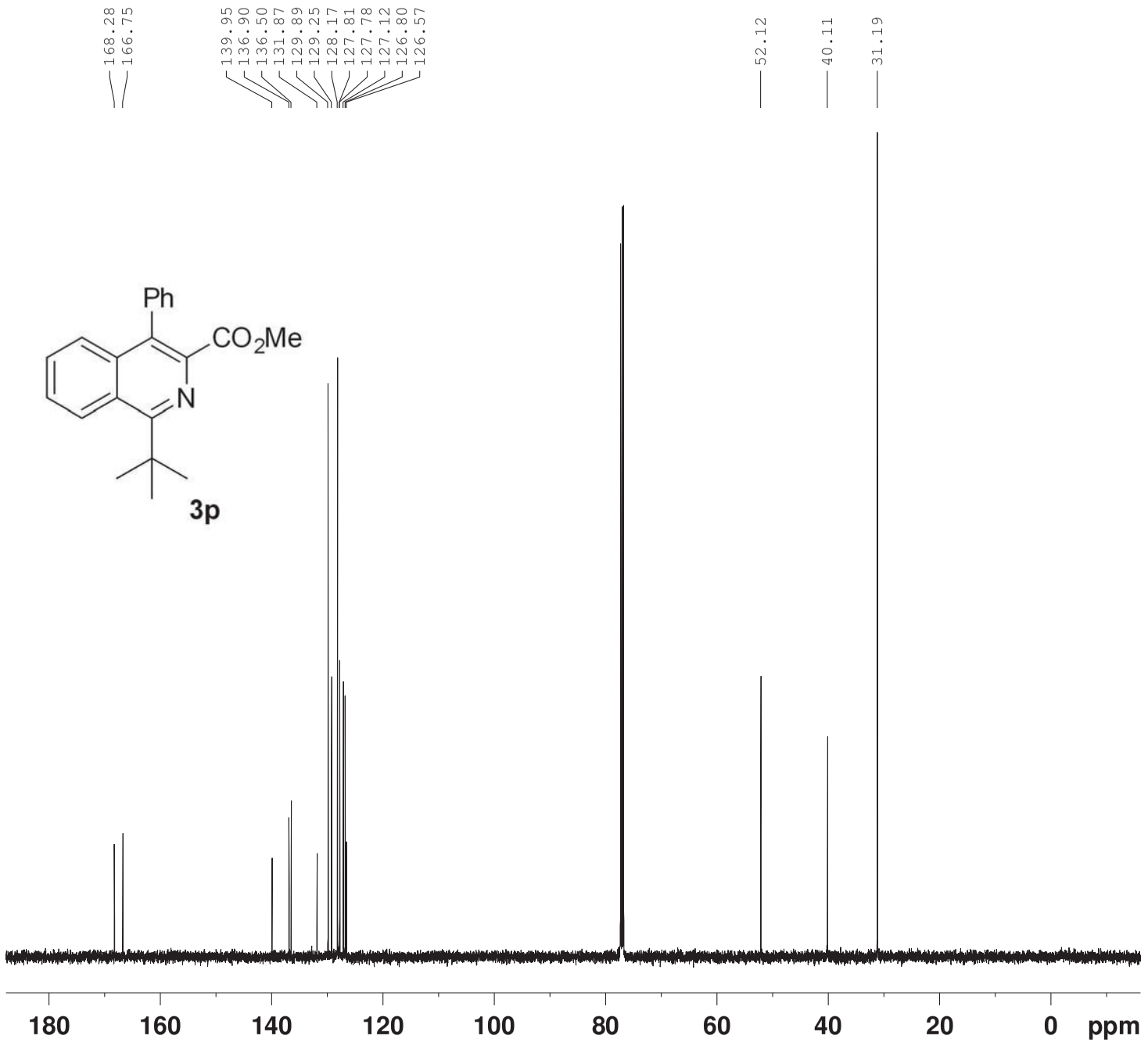



| | |
|---|---|
| NAME | xb20151105 |
| EXPNO | 22 |
| PROCNO | 1 |
| Date_ | 20151105 |
| Time | 21.42 |
| INSTRUM | spect |
| PROBHD | 5 mm PATXO 19F |
| PULPROG | zgpg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 512 |
| DS | 4 |
| SWH | 30030.029 Hz |
| FIDRES | 0.458222 Hz |
| AQ | 1.0912410 sec |
| RG | 128 |
| DW | 16.650 usec |
| DE | 6.00 usec |
| TE | 295.5 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 |



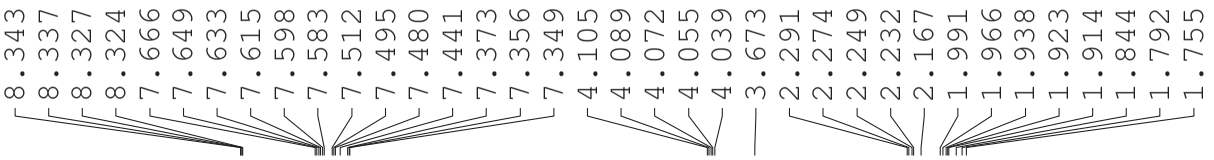

MH-2-14
PROTON CDCl3

| | |
|---|---|
| NAME | XB20140706 |
| EXPNO | 12 |
| PROCNO | 1 |
| Date_ | 20140706 |
| Time | 19.03 |
| 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 | 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 | 500.1300127 MHz |
| WDW | no |
| SSB | 0 |
| LB | 0.00 Hz |
| GB | 0 |
| PC | 1.00 |




MH-2-14
C13CPD CDCl3

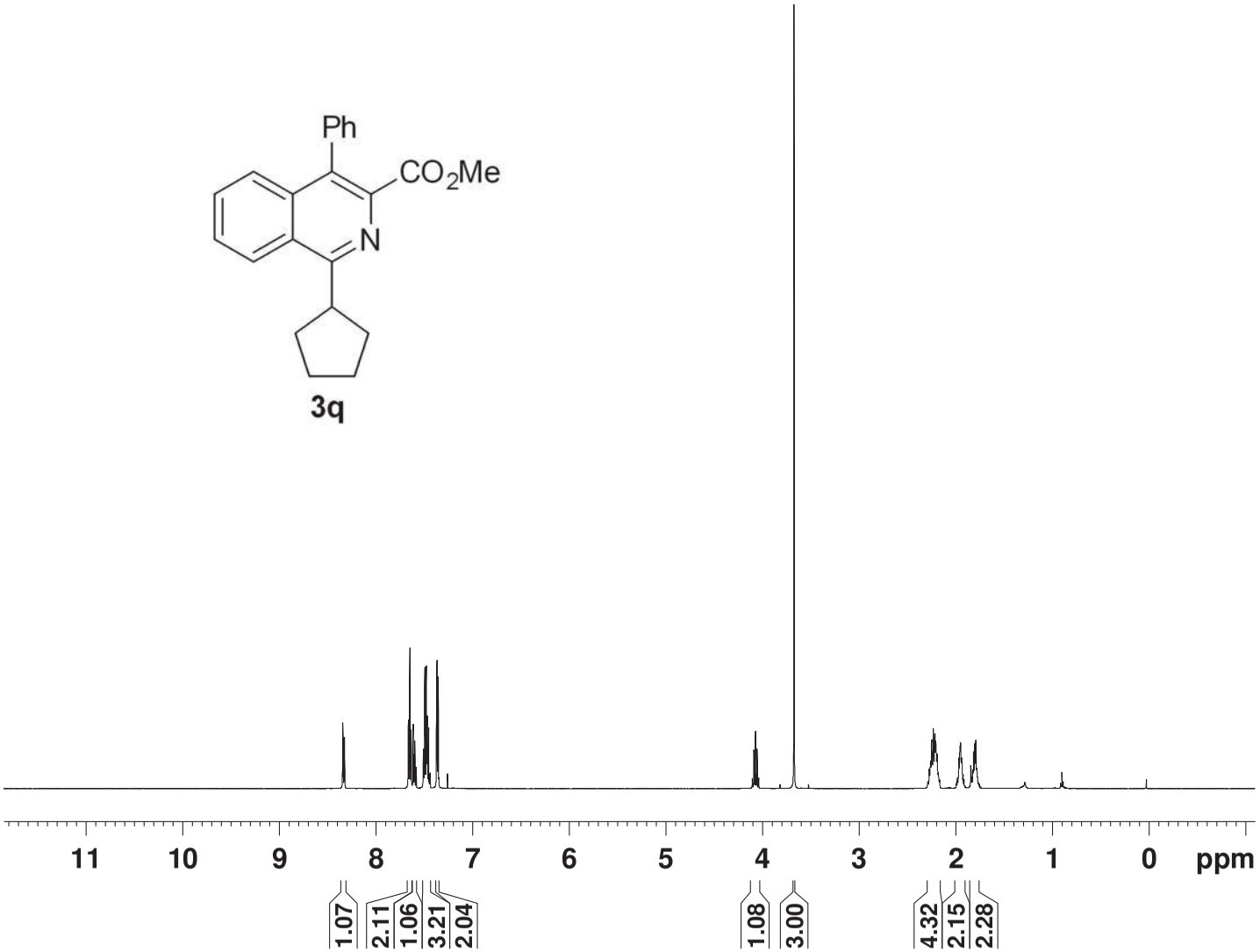
| | | |
|---|---|---|
| NAME | XB20140706 | |
| EXPNO | 13 | |
| PROCNO | 1 | |
| Date_ | 20140706 | |
| Time | 19.18 | |
| INSTRUM | spect | |
| PROBHD | 5 mm PATXO 19F | |
| PULPROG | zgpg30 | |
| TD | 65536 | |
| SOLVENT | CDCl3 | |
| NS | 256 | |
| DS | 4 | |
| SWH | 30030.029 | Hz |
| FIDRES | 0.458222 | Hz |
| AQ | 1.0912410 | sec |
| RG | 128 | |
| 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 | |



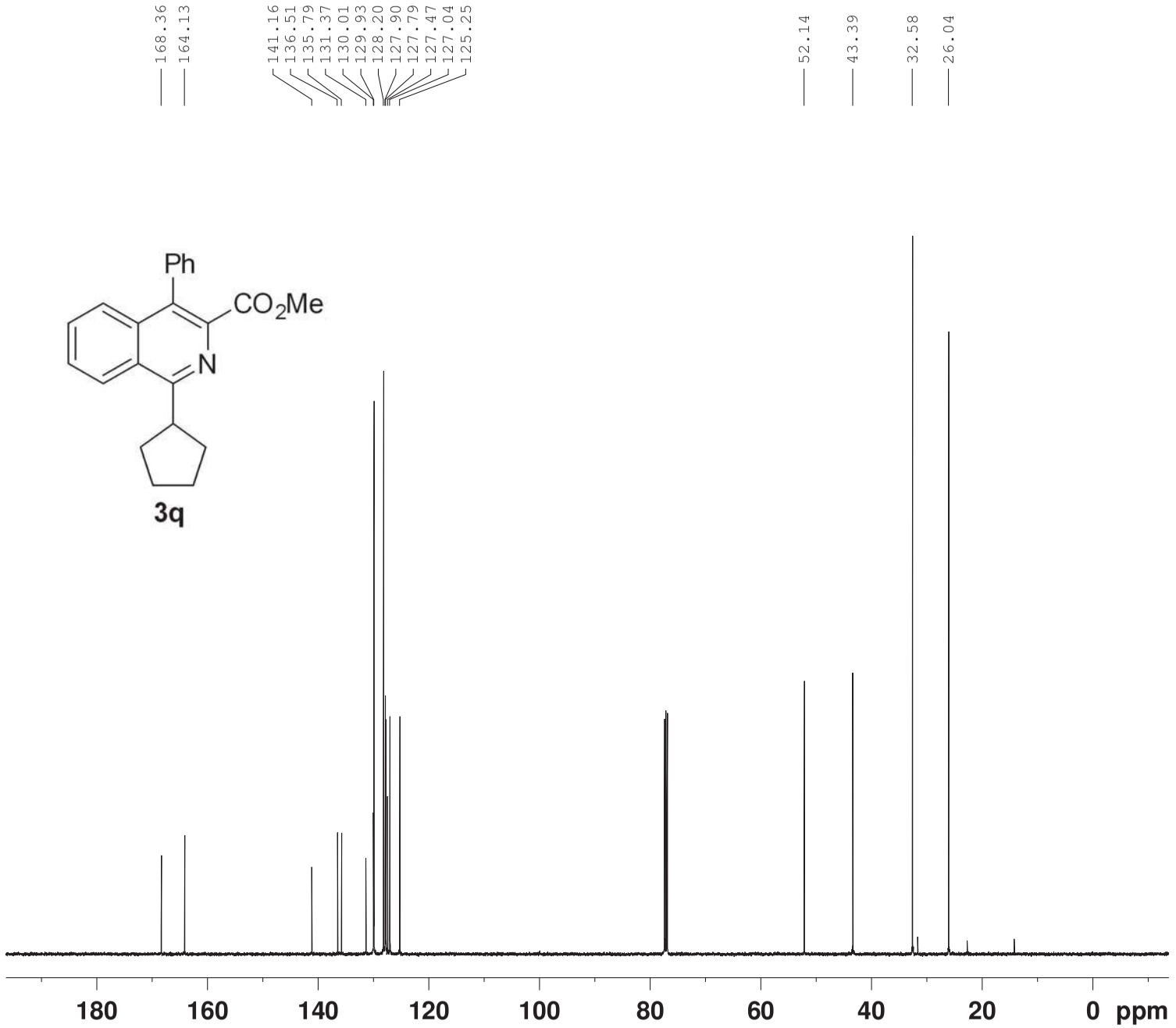

MH-3-111
PROTON CDCl3




3q

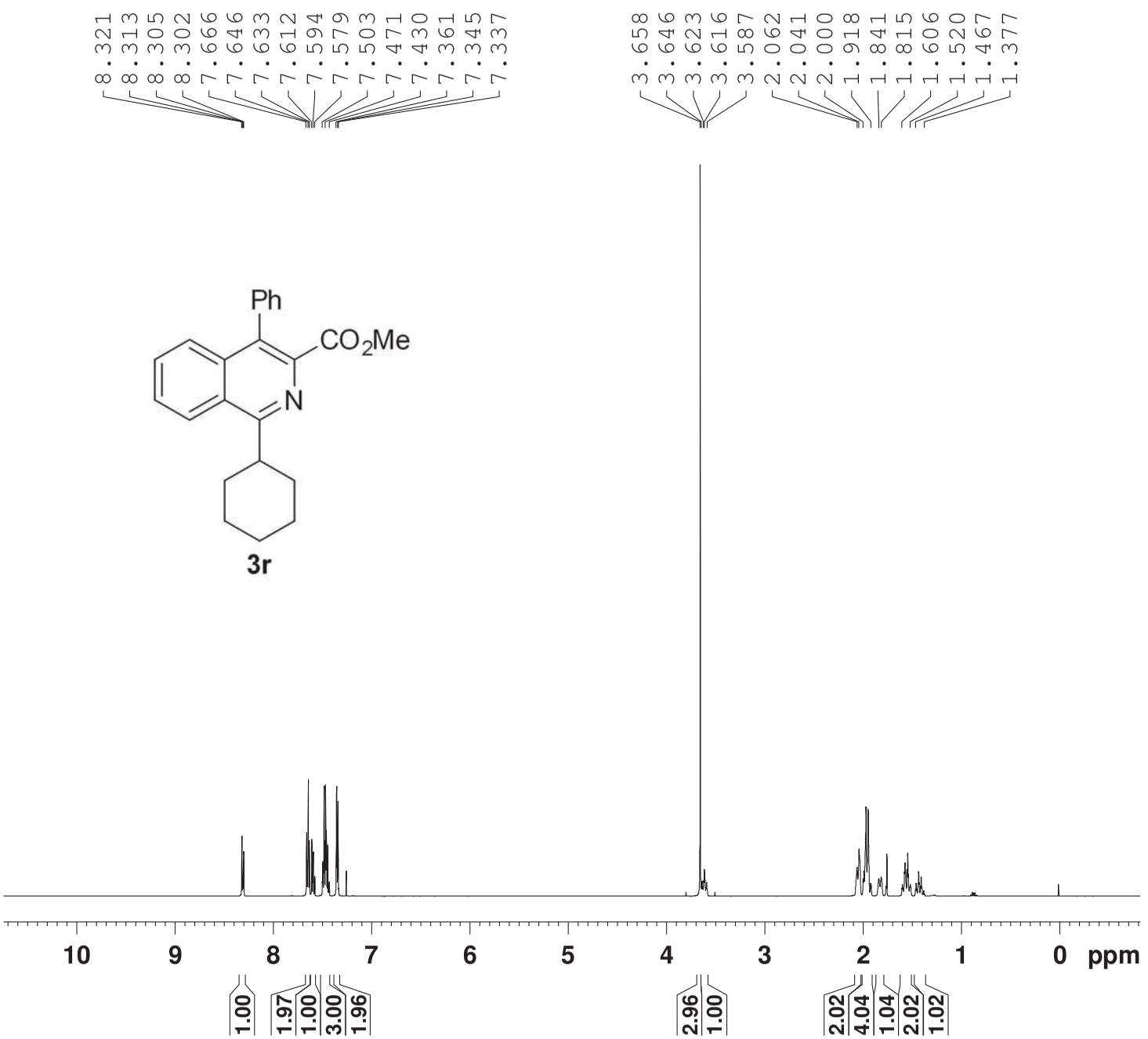



| | | |
|---|---|---|
| NAME | xb20151105 | |
| EXPNO | 23 | |
| PROCNO | 1 | |
| Date_ | 20151105 | |
| Time | 22.13 | |
| INSTRUM | spect | |
| PROBHD | 5 mm PATXO 19F | |
| PULPROG | zg30 | |
| TD | 65536 | |
| SOLVENT | CDCl3 | |
| NS | 16 | |
| DS | 2 | |
| SWH | 10330.578 | Hz |
| FIDRES | 0.157632 | Hz |
| AQ | 3.1720407 | sec |
| RG | 40.3 | |
| 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 | |



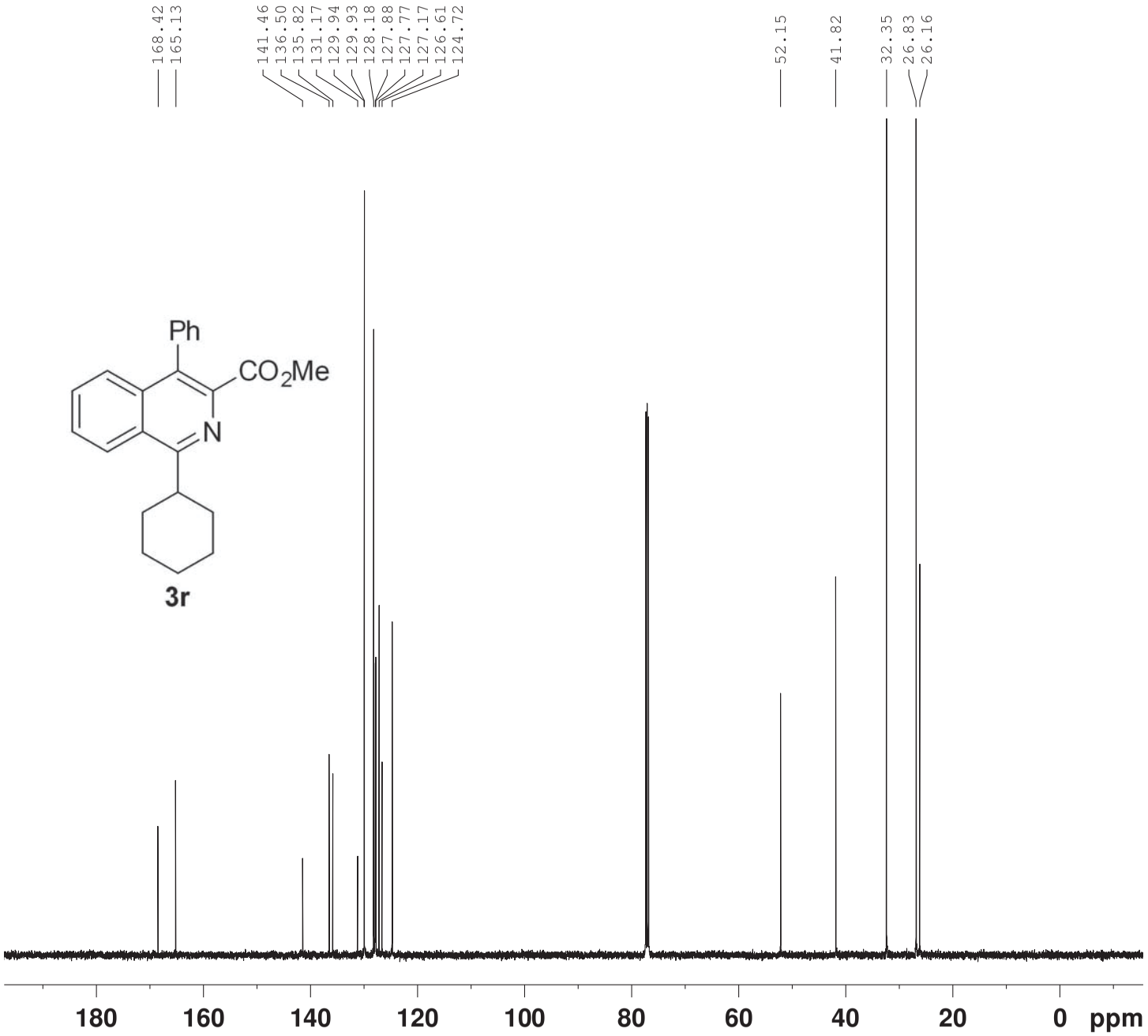

MH-3-111
C13CPD CDCl3

| | |
|---|---|
| NAME | XB20151106 |
| EXPNO | 3 |
| PROCNO | 1 |
| Date_ | 20151106 |
| Time | 9.28 |
| 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 | 406.4 |
| DW | 16.650 usec |
| DE | 6.00 usec |
| TE | 296.2 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 |



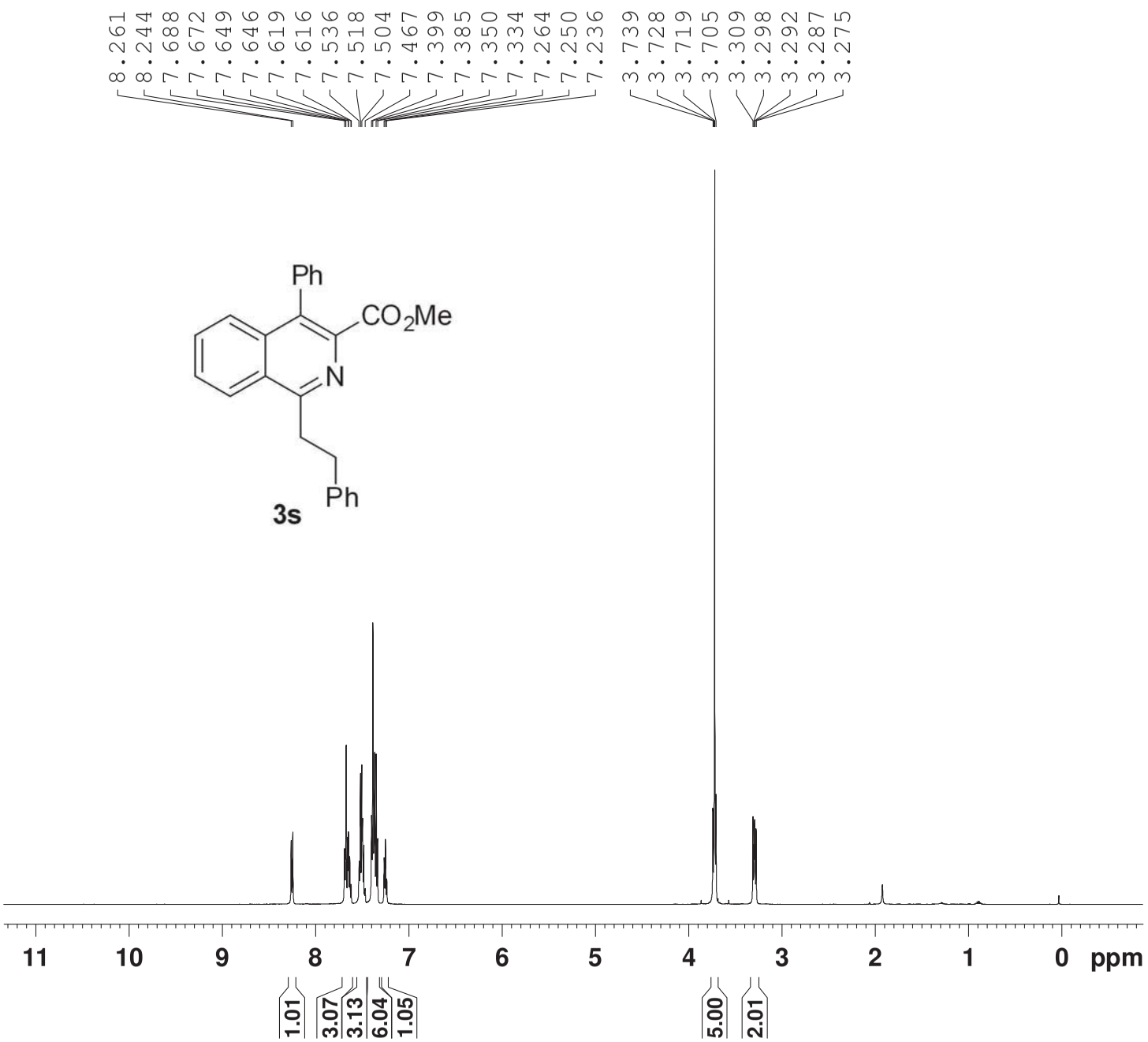

MH-3-117
PROTON CDCl3

| | |
|---|---|
| NAME | XB20151106 |
| EXPNO | 4 |
| PROCNO | 1 |
| Date_ | 20151106 |
| Time | 9.39 |
| 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 | 294.9 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 |




MH-3-117
C13CPD CDCl3

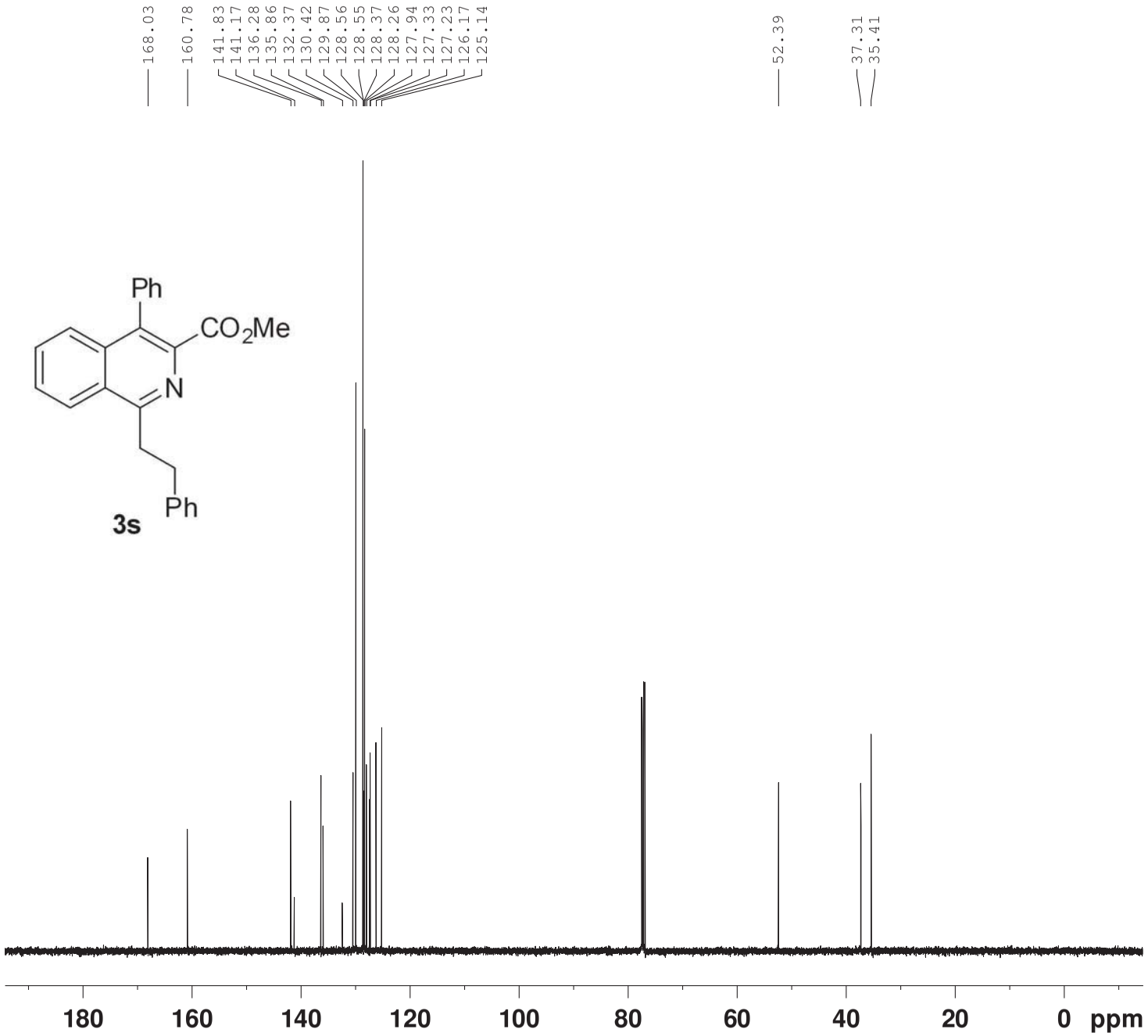
| | |
|---|---|
| NAME | XB20151106 |
| EXPNO | 5 |
| PROCNO | 1 |
| Date_ | 20151106 |
| Time | 10.07 |
| INSTRUM | spect |
| PROBHD | 5 mm PATXO 19F |
| PULPROG | zgpg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 512 |
| DS | 4 |
| SWH | 30030.029 Hz |
| FIDRES | 0.458222 Hz |
| AQ | 1.0912410 sec |
| RG | 362 |
| DW | 16.650 usec |
| DE | 6.00 usec |
| TE | 296.3 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 |



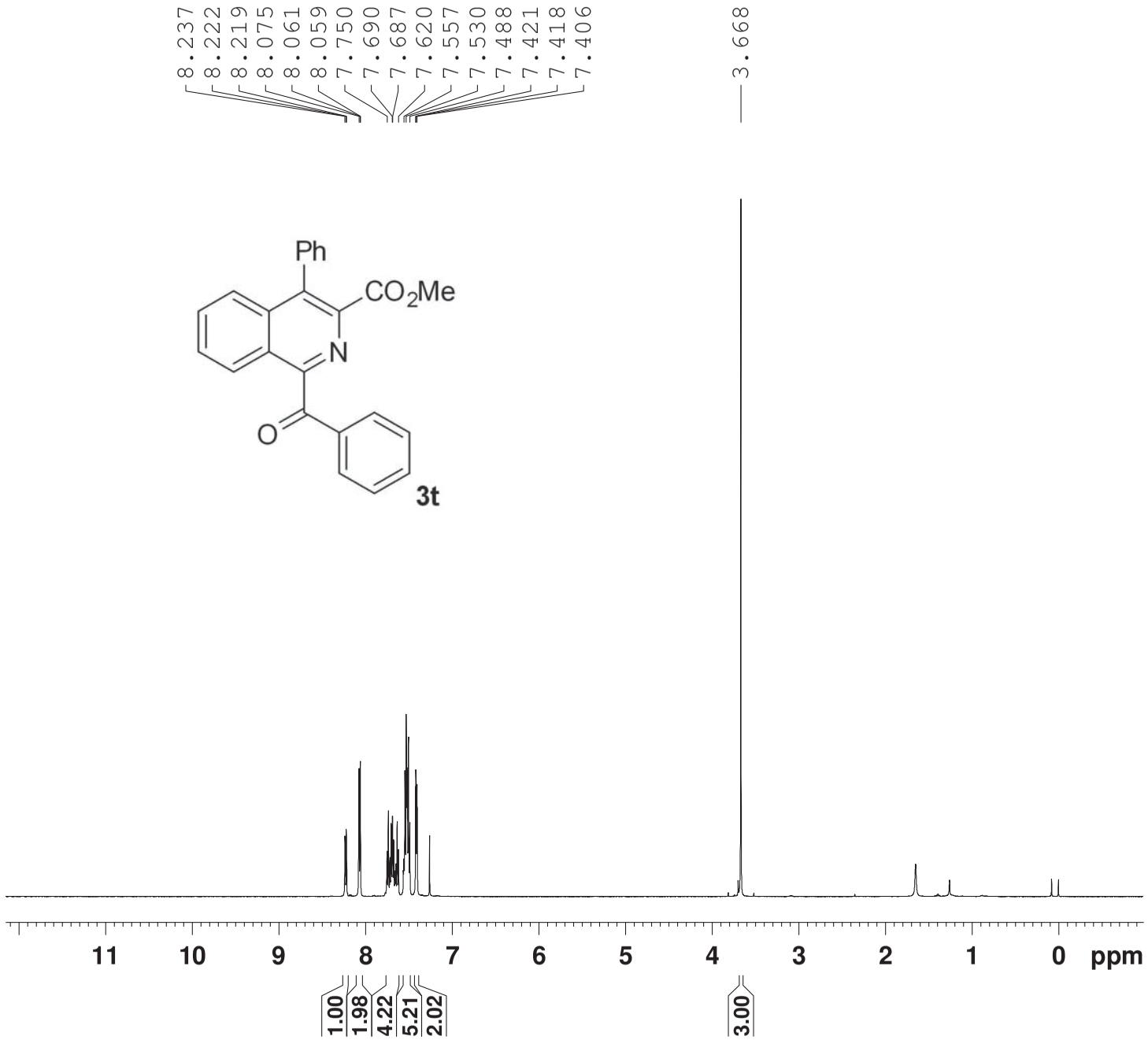

MH-3-122-A
PROTON CDCl3

| | | |
|---|---|---|
| NAME | xb20151124 | |
| EXPNO | 16 | |
| PROCNO | 1 | |
| Date_ | 20151124 | |
| Time | 2.01 | |
| 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 | 295.2 | 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 | 500.1300127 | MHz |
| WDW | no | |
| SSB | 0 | |
| LB | 0.00 | Hz |
| GB | 0 | |
| PC | 1.00 | |

MH-3-122-A
C13CPD CDCl3




| | |
|---|---|
| NAME | xb20151124 |
| EXPNO | 18 |
| PROCNO | 1 |
| Date_ | 20151124 |
| Time | 2.31 |
| 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 | 296.6 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 |

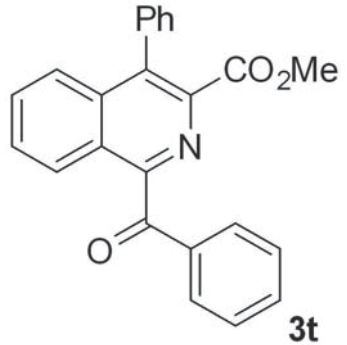



MH-3-54-DOWN
PROTON CDCl3

| | | |
|---|---|---|
| NAME | XB20150519 | |
| EXPNO | 13 | |
| PROCNO | 1 | |
| Date_ | 20150519 | |
| Time | 15.32 | |
| 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 | 161.3 | |
| 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 | |

MH-3-54-DOWN
C13CPD CDCl3

193.92
167.14
155.94
140.56
136.44
136.15
135.52
135.29
134.01
131.29
131.05
129.65
129.33
128.57
128.38
128.36
126.91
126.61
126.28
52.52

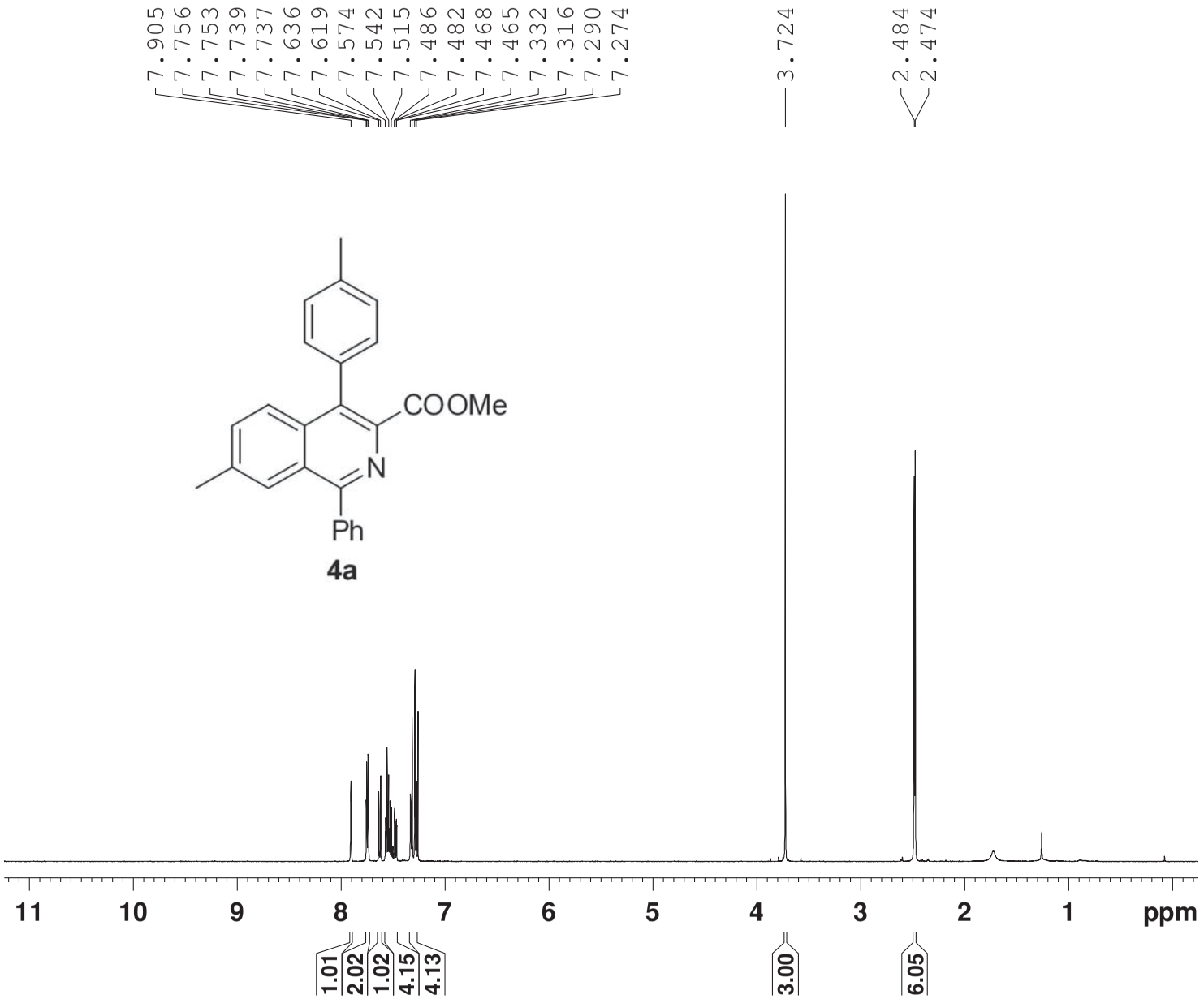



3t

SI00

200 180 160 140 120 100 80 60 40 20 0 ppm

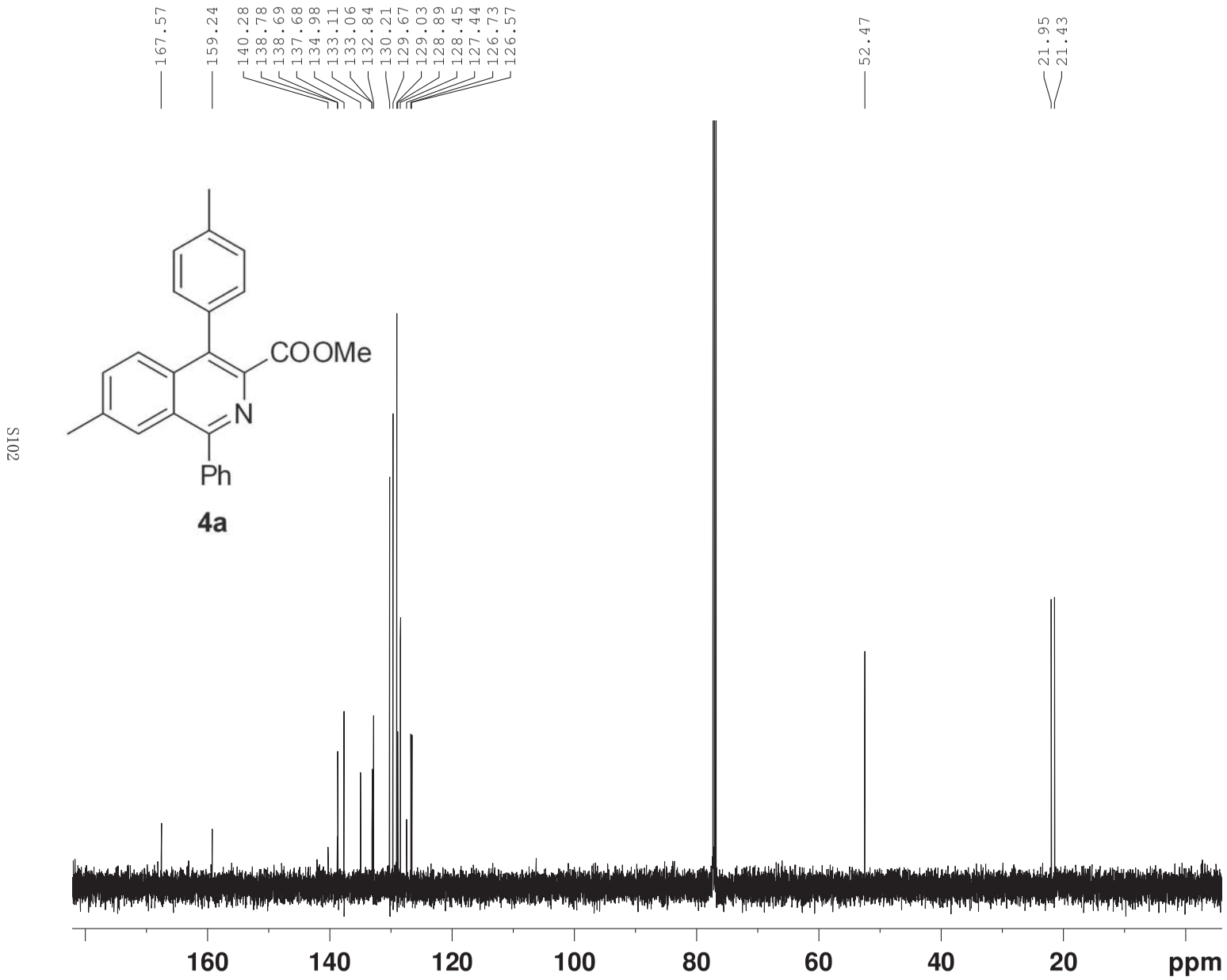
| | |
|---|---|
| NAME | XB20150519 |
| EXPNO | 14 |
| PROCNO | 1 |
| Date_ | 20150519 |
| Time | 15.47 |
| INSTRUM | spect |
| PROBHD | 5 mm PATXO 19F |
| PULPROG | zgpg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 256 |
| DS | 4 |
| SWH | 30030.029 Hz |
| FIDRES | 0.458222 Hz |
| AQ | 1.0912410 sec |
| RG | 181 |
| DW | 16.650 usec |
| DE | 6.00 usec |
| TE | 297.1 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 |




MH-2-39
PROTON CDCl3

| | |
|---|---|
| NAME | XB20141023 |
| EXPNO | 9 |
| PROCNO | 1 |
| Date_ | 20141023 |
| Time | 12.12 |
| 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 | 362 |
| DW | 48.400 usec |
| DE | 6.00 usec |
| TE | 296.7 K |
| D1 | 1.00000000 sec |
| TD0 | 1 |

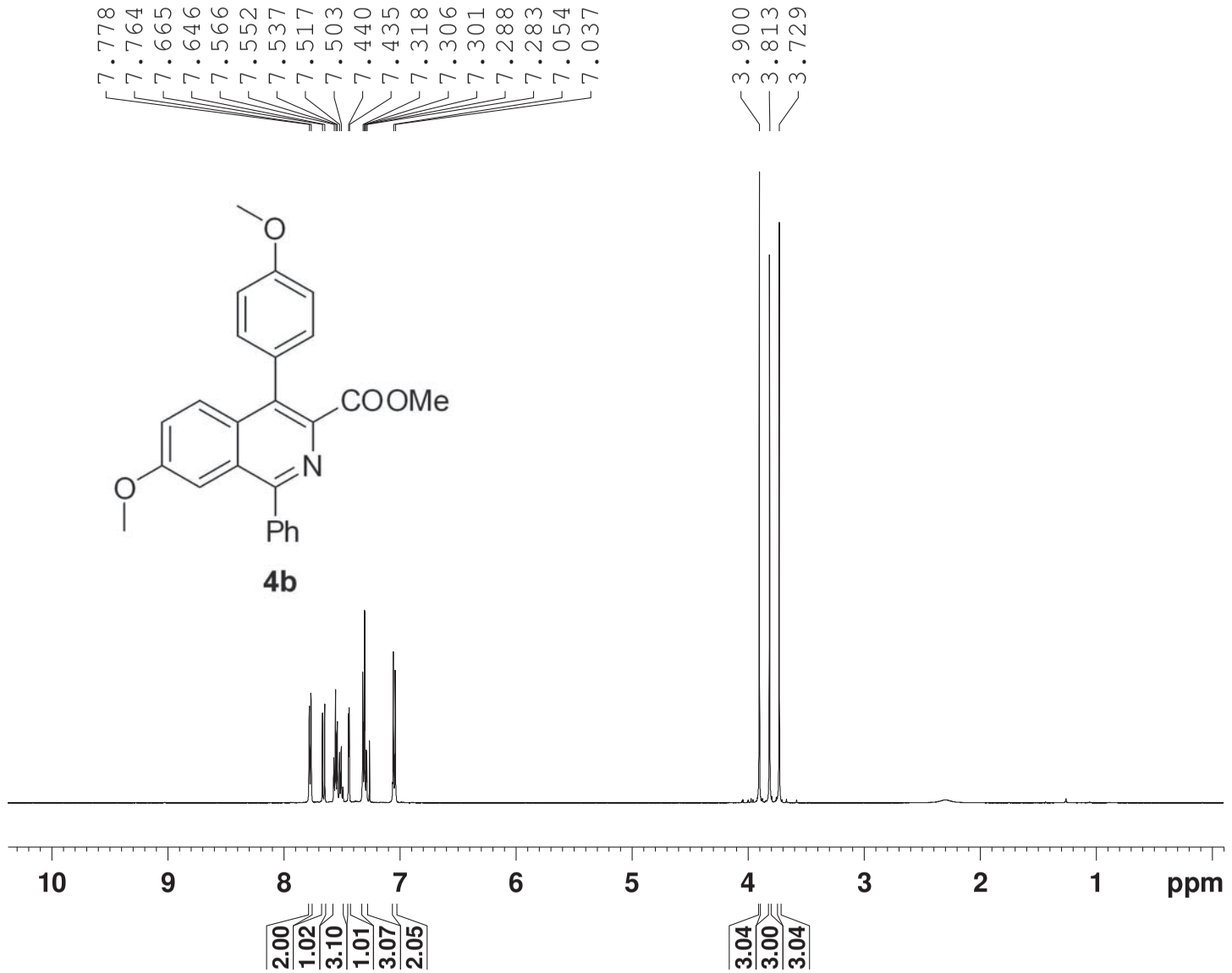
| ======== CHANNEL f1 ======== | |
|---|---|
| NUC1 | 1H |
| P1 | 14.14 usec |
| PL1 | 1.00 dB |
| SFO1 | 500.1330885 MHz |
| SI | 32768 |
| SF | 500.1300129 MHz |
| WDW | no |
| SSB | 0 |
| LB | 0.00 Hz |
| GB | 0 |
| PC | 1.00 |




SI02

MH-2-39
C13CPD CDCl3

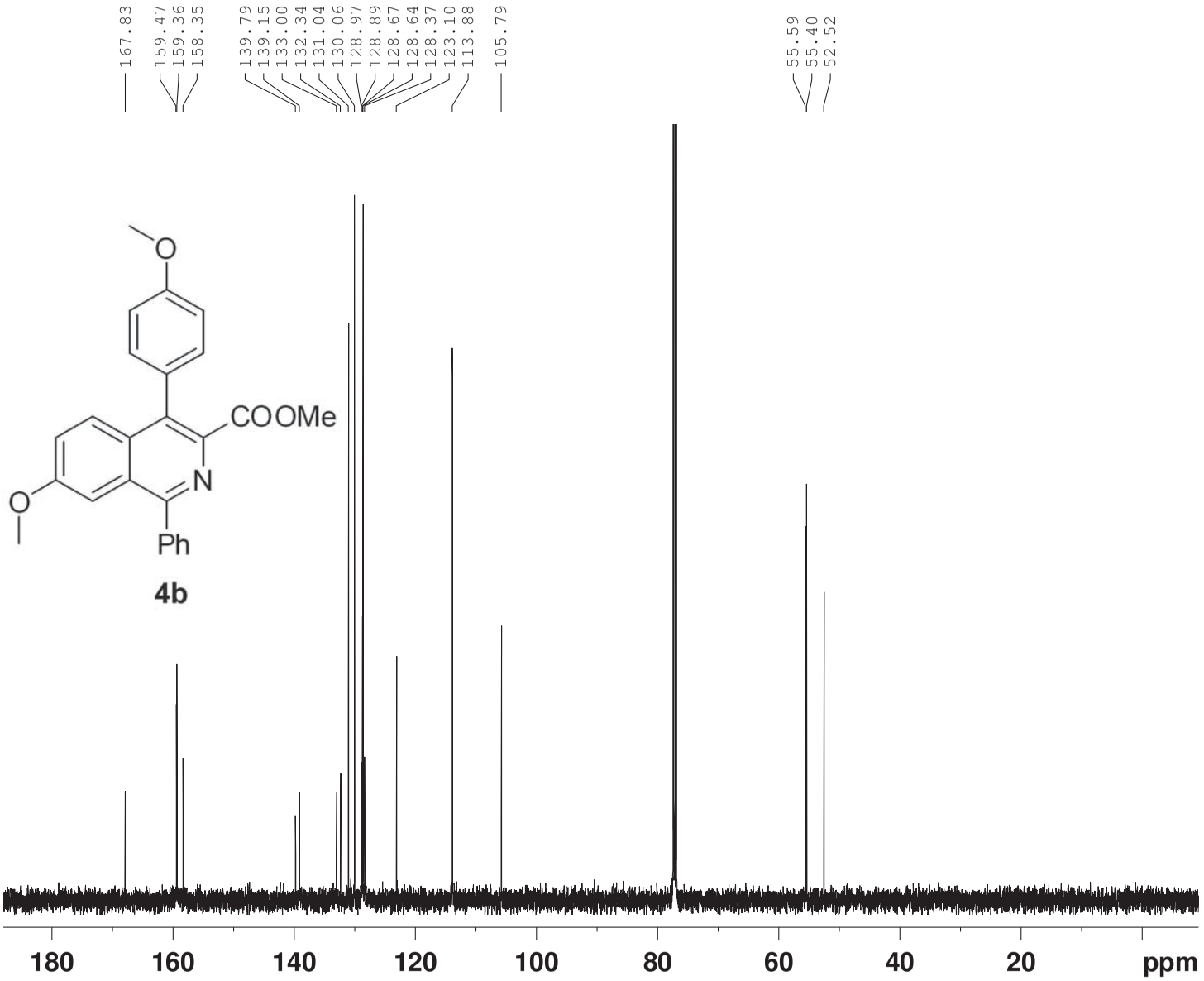
| | |
|---|---|
| NAME | XB20140706 |
| EXPNO | 3 |
| PROCNO | 1 |
| Date_ | 20140706 |
| Time | 17.24 |
| INSTRUM | spect |
| PROBHD | 5 mm PATXO 19F |
| PULPROG | zgpg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 256 |
| DS | 4 |
| SWH | 30030.029 Hz |
| FIDRES | 0.458222 Hz |
| AQ | 1.0912410 sec |
| RG | 128 |
| 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 |




MH-2-42
PROTON CDCl3

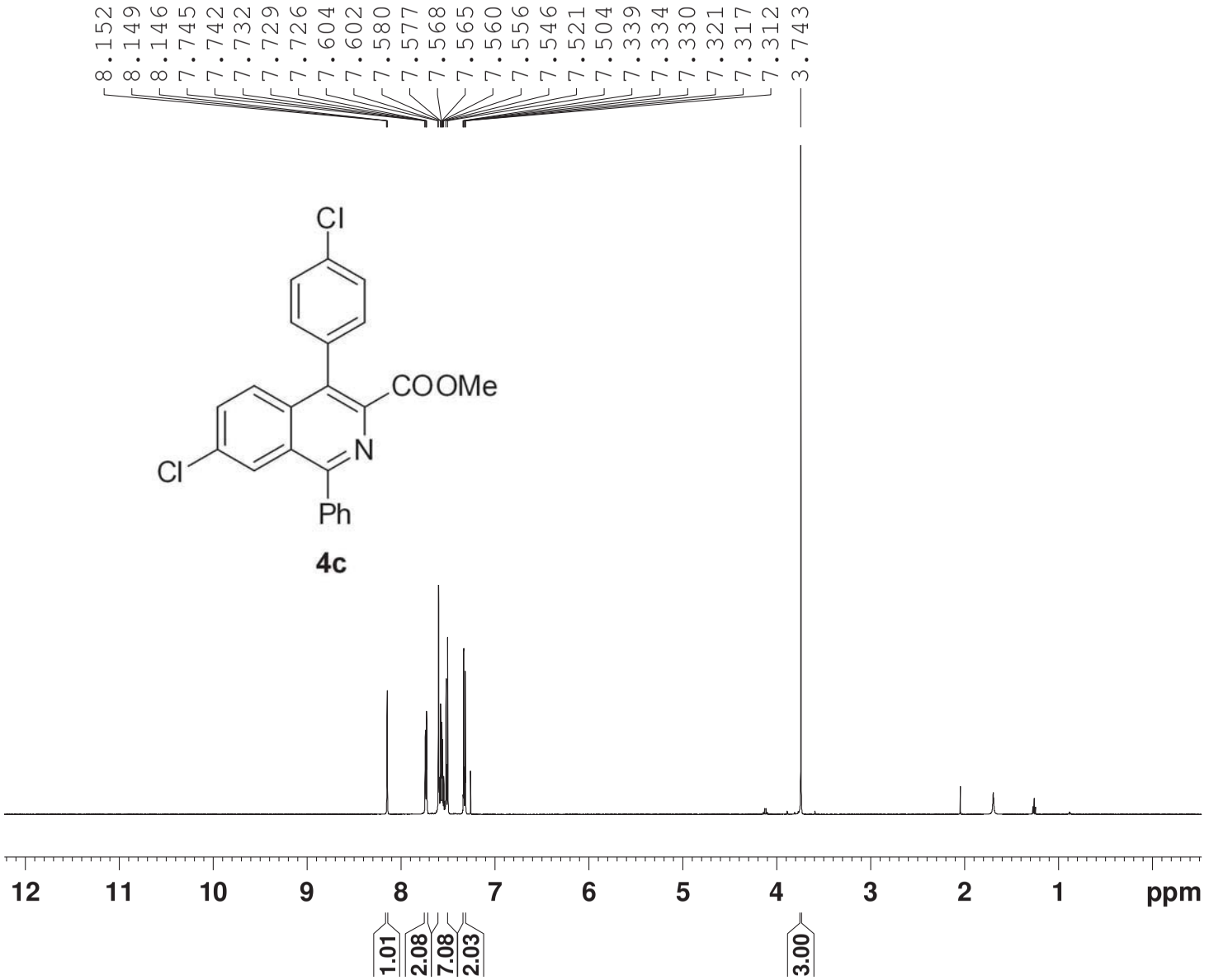
| | |
|---|---|
| NAME | MH20140901 |
| EXPNO | 21 |
| PROCNO | 1 |
| Date_ | 20140902 |
| Time | 3.30 |
| INSTRUM | spect |
| PROBHD | 5 mm PATXO 19F |
| PULPROG | zg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 10330.578 Hz |
| FIDRES | 0.157632 Hz |
| AQ | 3.1720407 sec |
| RG | 181 |
| DW | 48.400 usec |
| DE | 6.00 usec |
| TE | 298.3 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 |



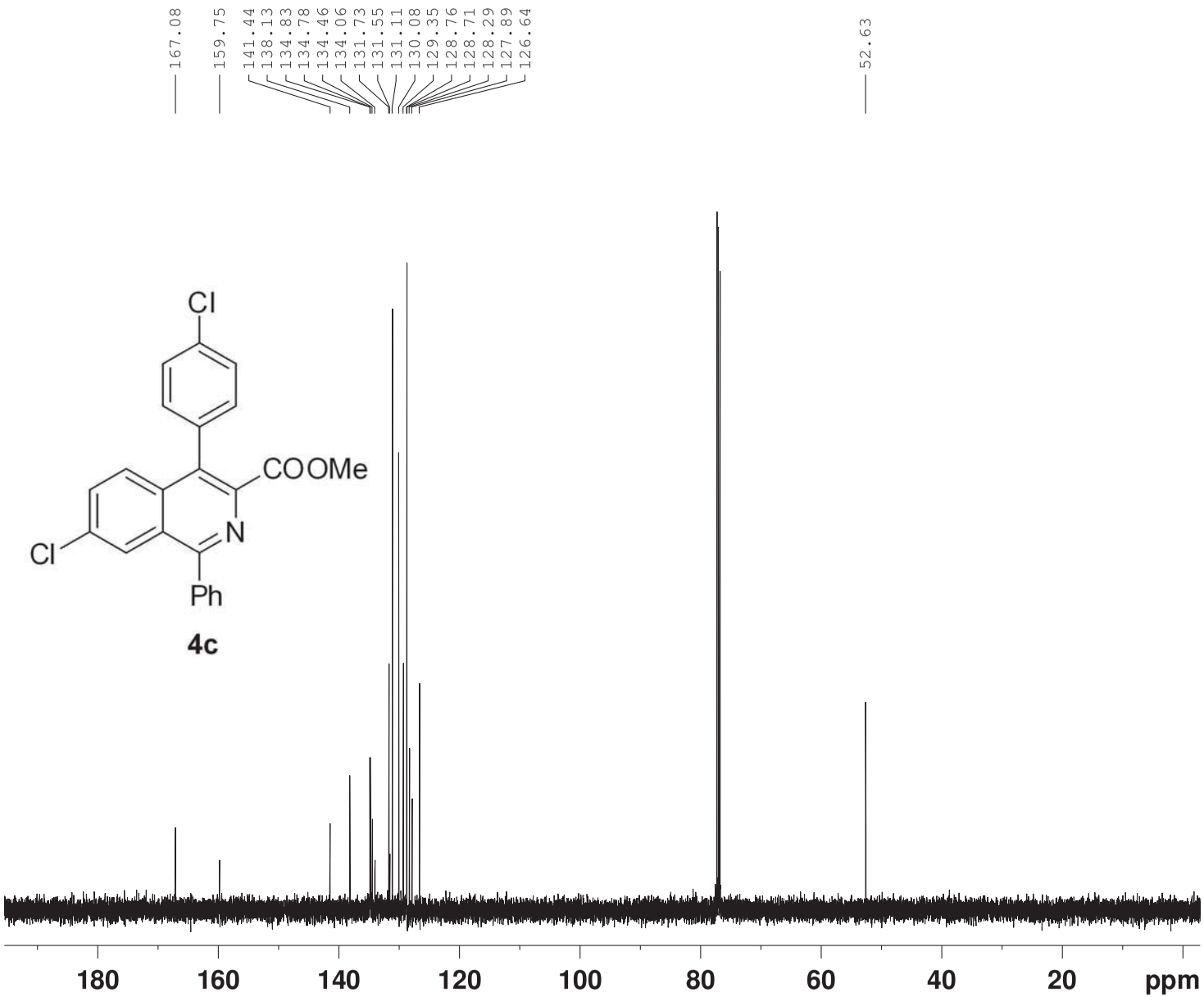

MH-2-42
C13CPD CDCl3

| | |
|---|---|
| NAME | MH20140901 |
| EXPNO | 23 |
| PROCNO | 1 |
| Date_ | 20140902 |
| Time | 3.48 |
| 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 | 912.3 |
| DW | 16.650 usec |
| DE | 6.00 usec |
| TE | 299.5 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 | 125.7577755 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 1.00 Hz |
| GB | 0 |
| PC | 1.40 |



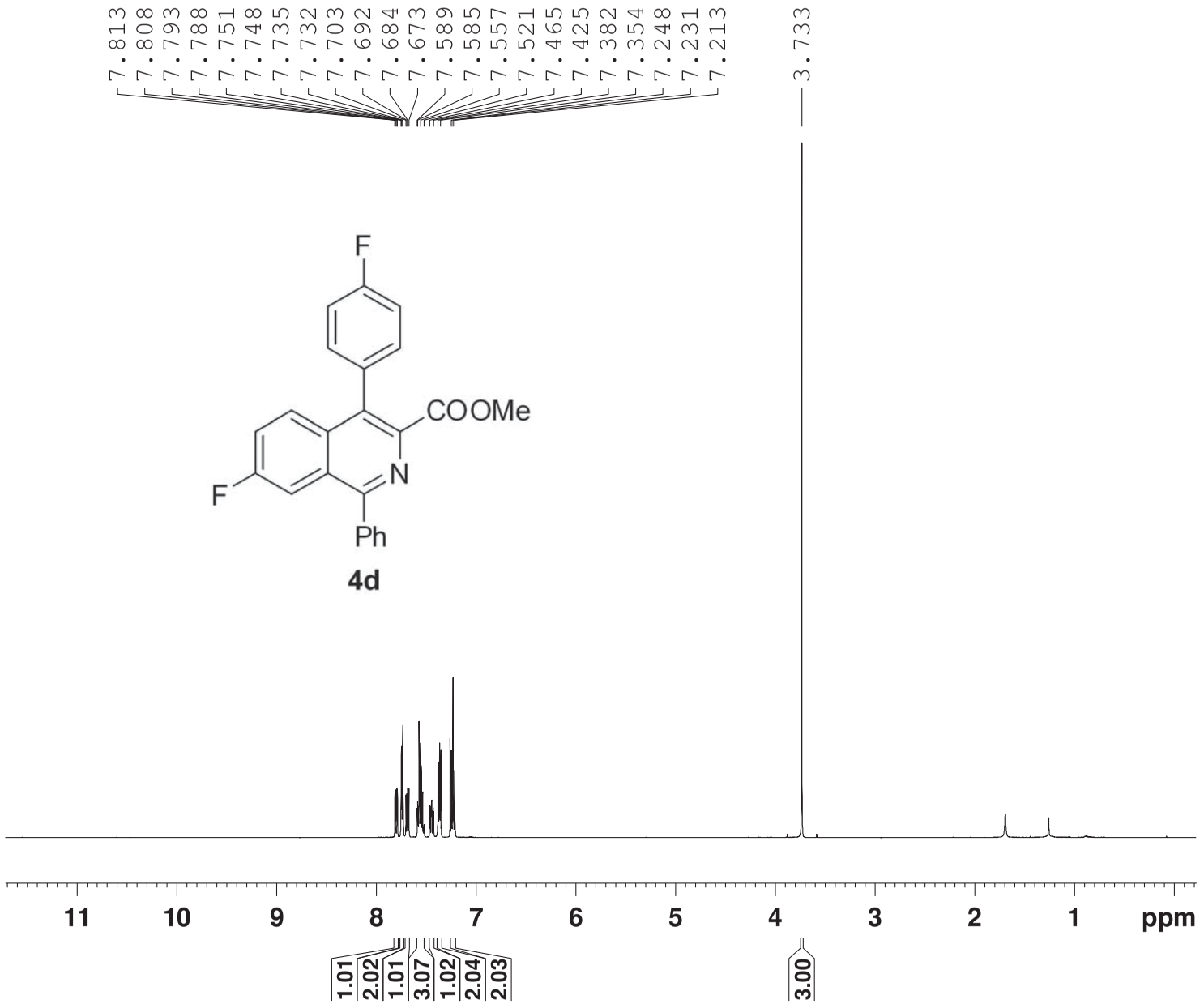

MH-2-16
PROTON CDCl3

| | |
|---|---|
| NAME | XB20140612 |
| EXPNO | 8 |
| PROCNO | 1 |
| Date_ | 20140612 |
| Time | 11.50 |
| 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 | 296.9 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 |




MH-2-16
C13CPD CDCl3

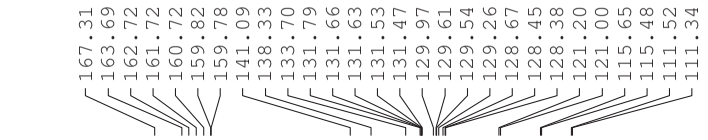
| | | |
|---|---|---|
| NAME | XB20140612 | |
| EXPNO | 9 | |
| PROCNO | 1 | |
| Date_ | 20140612 | |
| Time | 12.05 | |
| INSTRUM | spect | |
| PROBHD | 5 mm PATXO 19F | |
| PULPROG | zgpg30 | |
| TD | 65536 | |
| SOLVENT | CDCl3 | |
| NS | 256 | |
| DS | 4 | |
| SWH | 30030.029 | Hz |
| FIDRES | 0.458222 | Hz |
| AQ | 1.0912410 | sec |
| RG | 114 | |
| DW | 16.650 | usec |
| DE | 6.00 | usec |
| TE | 298.1 | 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 | |



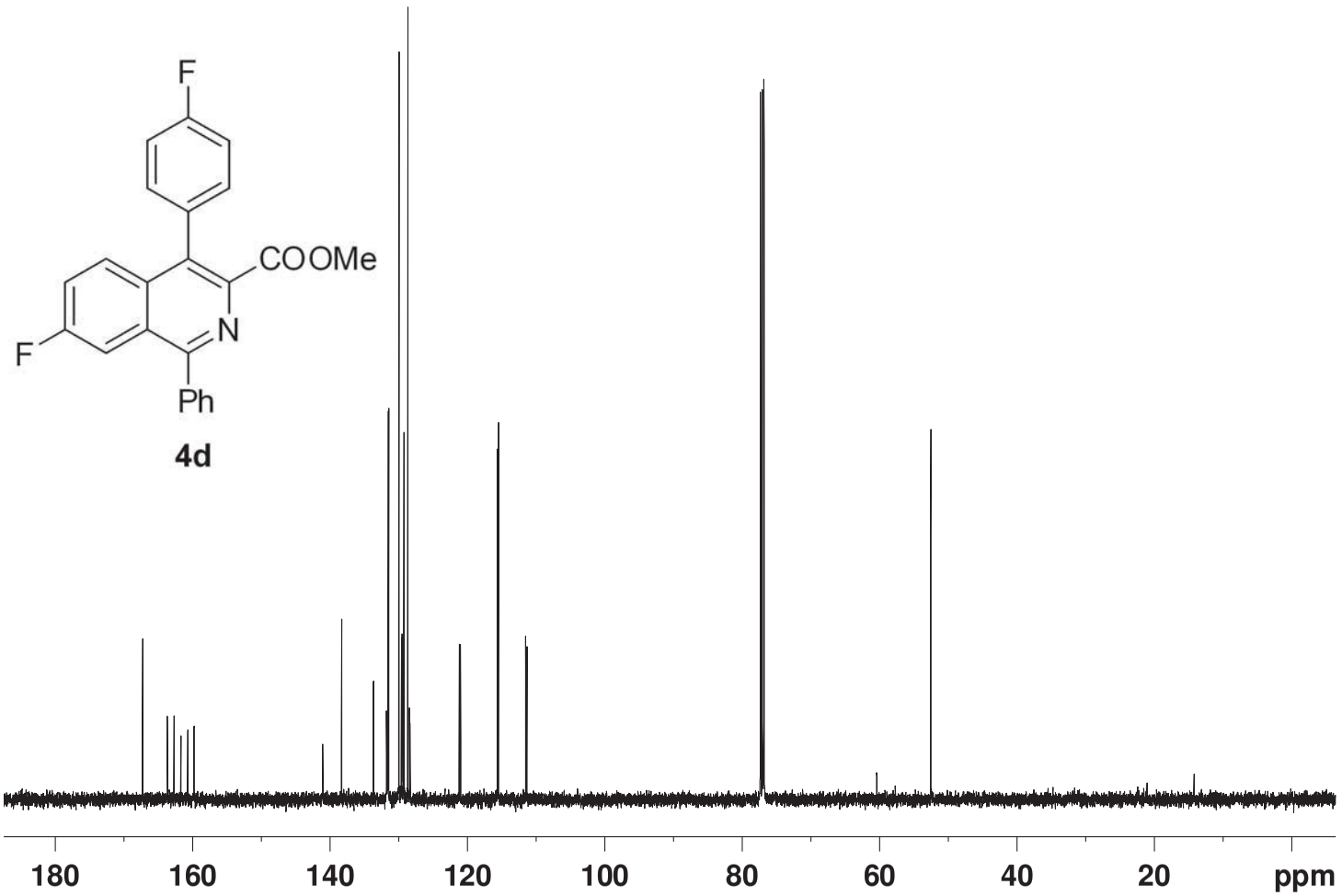

MH-2-45
PROTON CDCl3

| | | |
|---|---|---|
| NAME | XB20141023 | |
| EXPNO | 10 | |
| PROCNO | 1 | |
| Date_ | 20141023 | |
| Time | 12.18 | |
| 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 | 296.8 | K |
| D1 | 1.00000000 | sec |
| TD0 | 1 | |

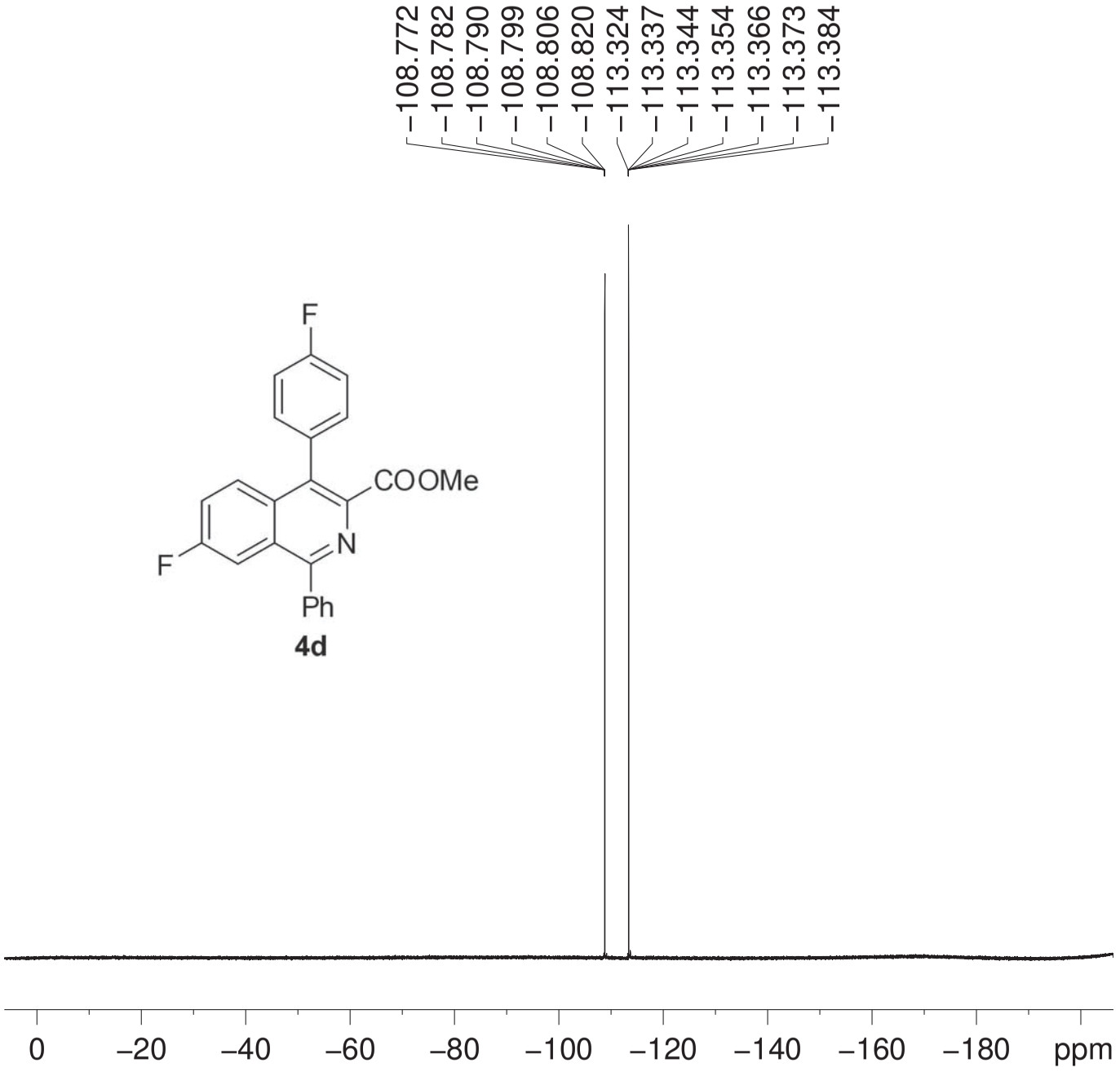
| ======== CHANNEL f1 ======== | | |
|---|---|---|
| NUC1 | 1H | |
| P1 | 14.14 | usec |
| PL1 | 1.00 | dB |
| SFO1 | 500.1330885 | MHz |
| SI | 32768 | |
| SF | 500.1300128 | MHz |
| WDW | no | |
| SSB | 0 | |
| LB | 0.00 | Hz |
| GB | 0 | |
| PC | 1.00 | |




MH-2-45
C13CPD CDCl3




| | |
|---|---|
| NAME | XB20140705 |
| EXPNO | 10 |
| PROCNO | 1 |
| Date_ | 20140705 |
| Time | 21.23 |
| 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 | 322.5 |
| 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 |

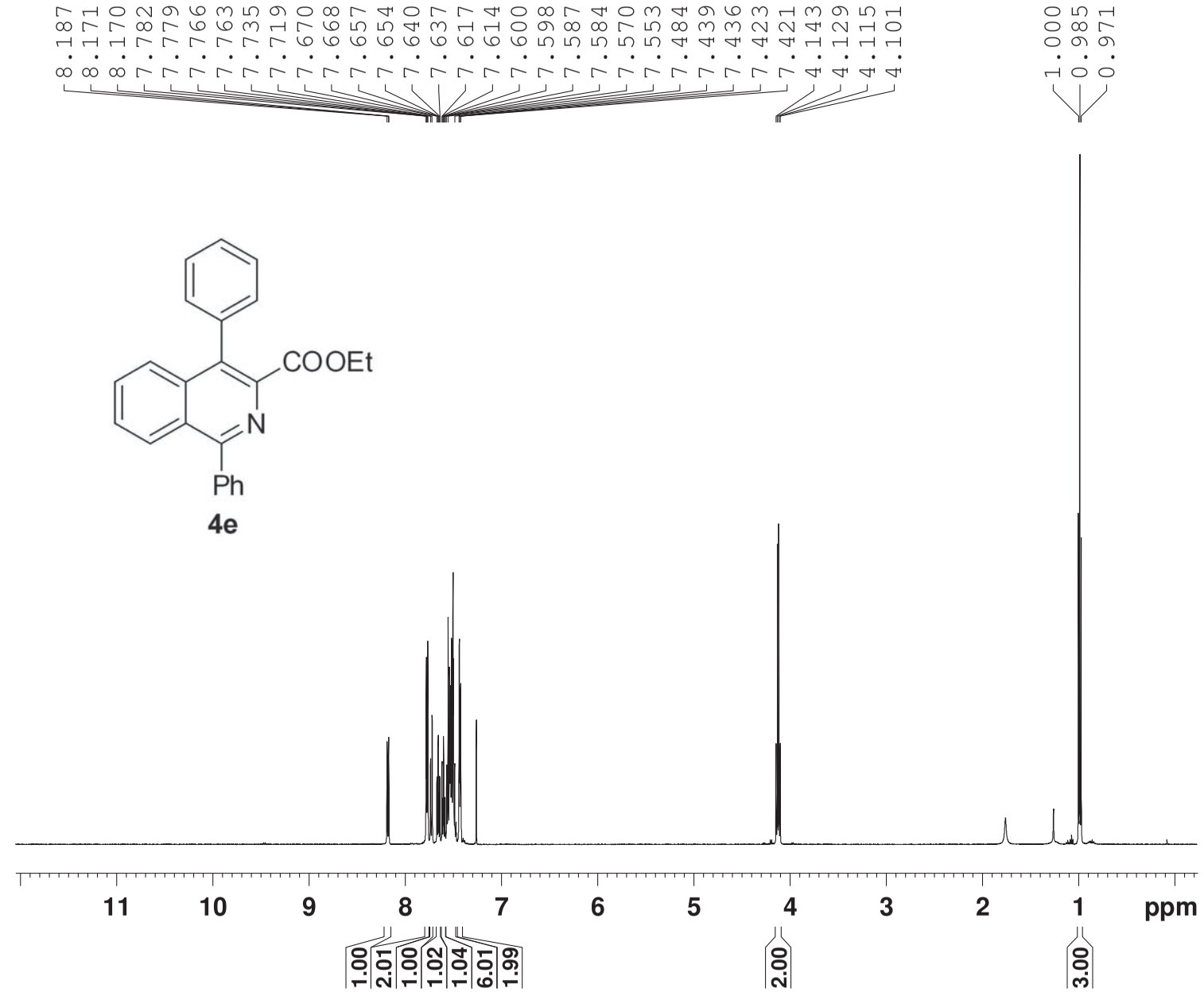



MH−2−45
19Fdeft CDCl3 D:\\ deng 44

| | |
|---|---|
| NAME | XB20140705 |
| EXPNO | 9 |
| PROCNO | 1 |
| Date_ | 20140705 |
| Time | 21.08 |
| 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 | 296.4 K |
| D1 | 1.00000000 sec |
| TD0 | 1 |

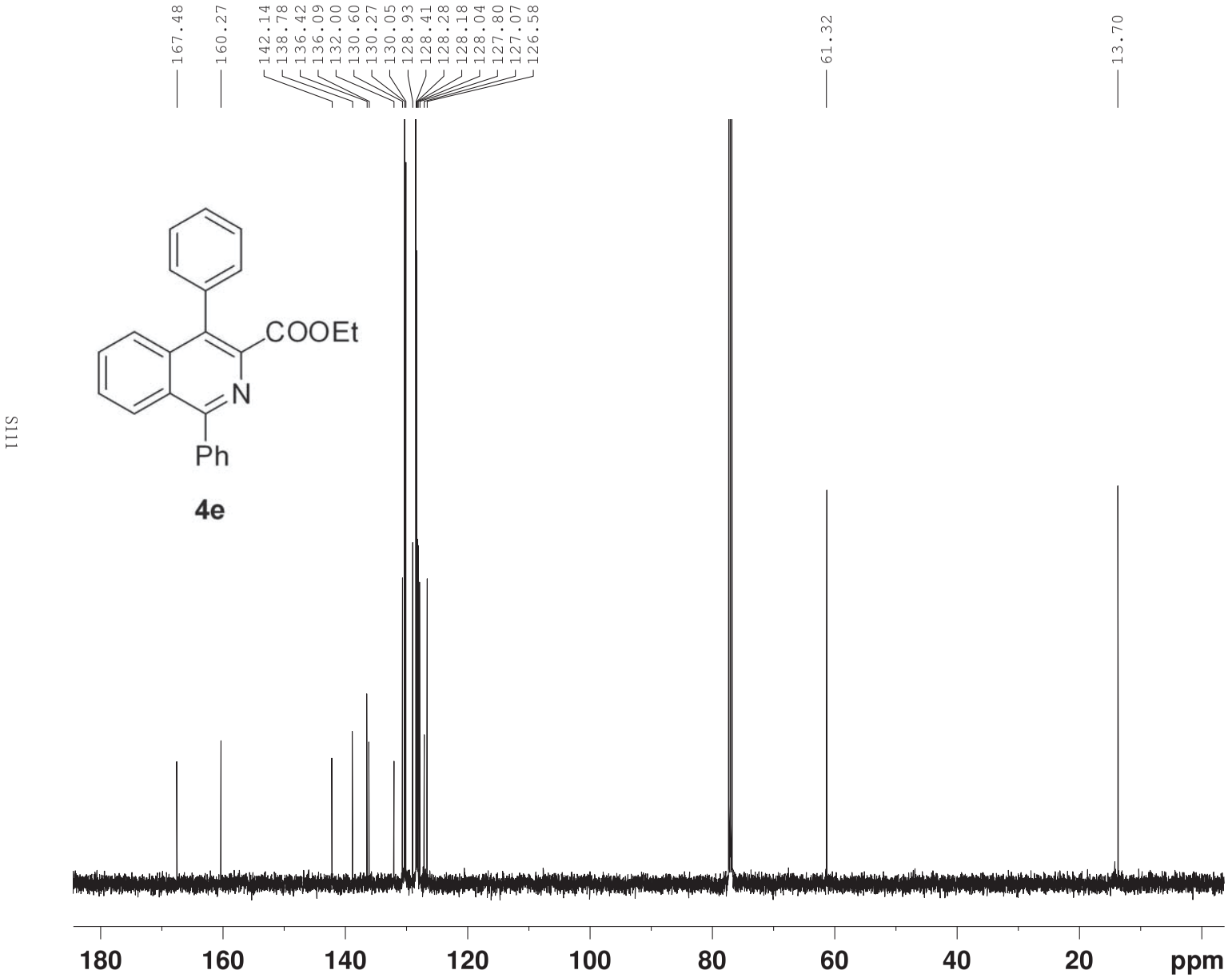
======== CHANNEL f1 ====

| | |
|---|---|
| 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 |



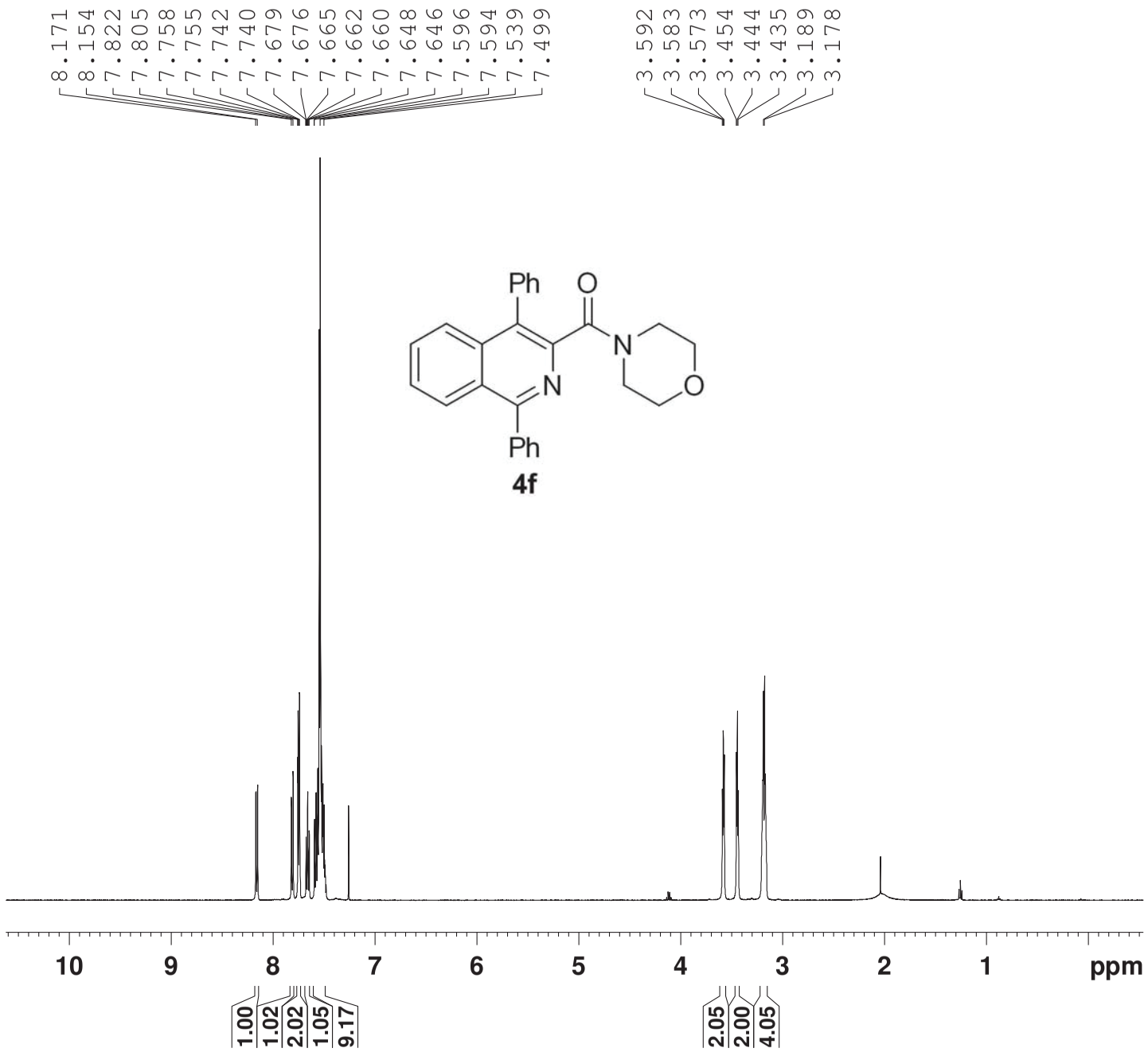

MH-2-36
PROTON CDCl3

| | |
|---|---|
| NAME | XB20141023 |
| EXPNO | 8 |
| PROCNO | 1 |
| Date_ | 20141023 |
| Time | 12.06 |
| 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 | 296.8 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 |




MH-2-36
C13CPD CDCl3

| | | |
|---|---|---|
| NAME | XB20140706 | |
| EXPNO | 9 | |
| PROCNO | 1 | |
| Date_ | 20140706 | |
| Time | 18.36 | |
| 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 | 128 | |
| 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 | |

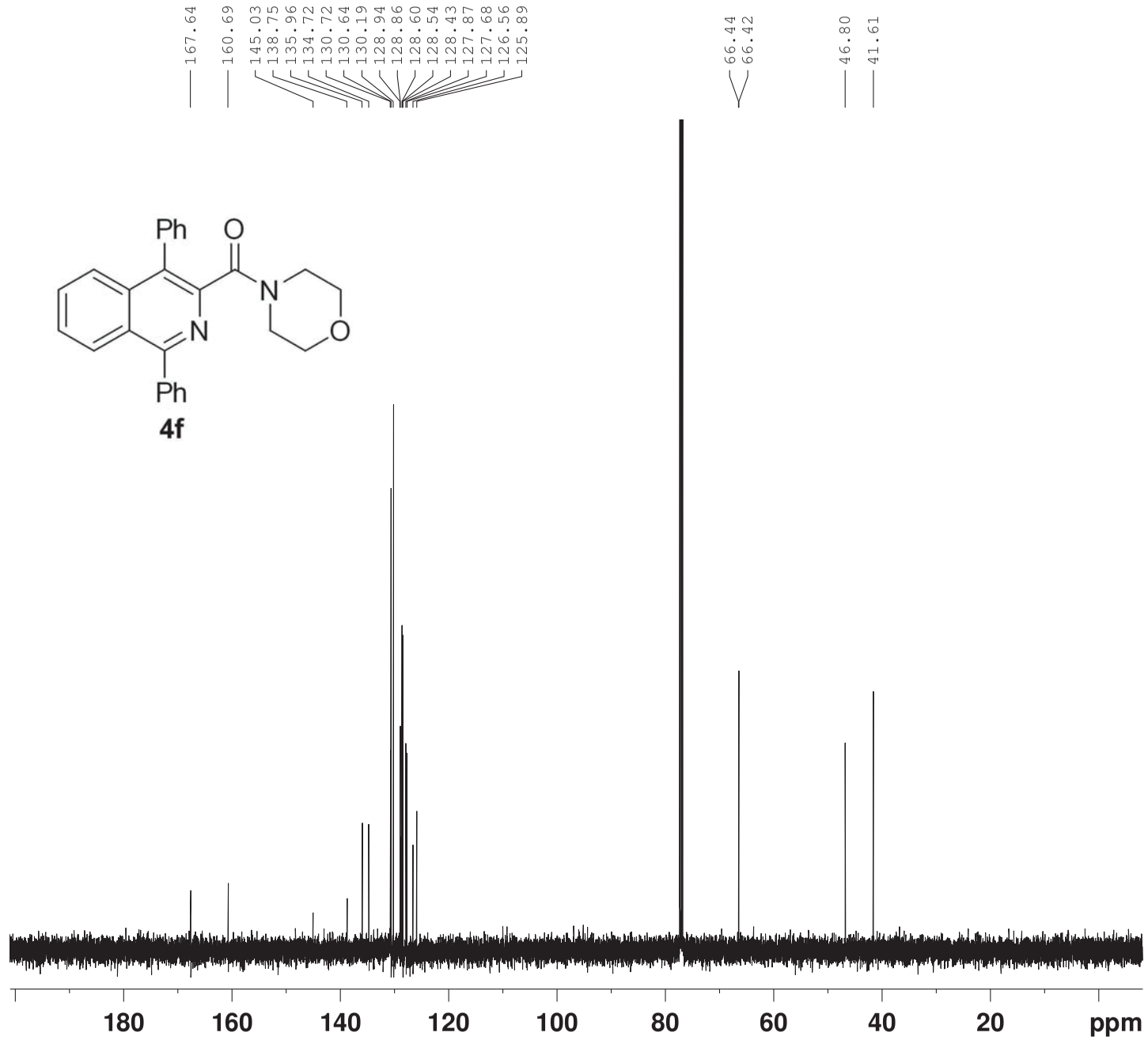



SII2

MH-2-15
PROTON CDCl3

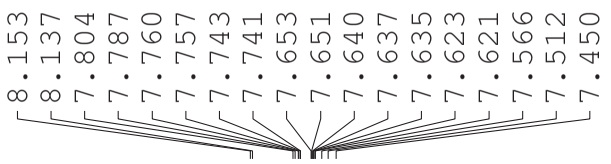
| | |
|---|---|
| NAME | XB20140612 |
| EXPNO | 6 |
| PROCNO | 1 |
| Date_ | 20140612 |
| Time | 11.28 |
| INSTRUM | spect |
| PROBHD | 5 mm PATXO 19F |
| PULPROG | zg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 10330.578 Hz |
| FIDRES | 0.157632 Hz |
| AQ | 3.1720407 sec |
| RG | 203.2 |
| DW | 48.400 usec |
| DE | 6.00 usec |
| TE | 296.8 K |
| D1 | 1.00000000 sec |
| TD0 | 1 |

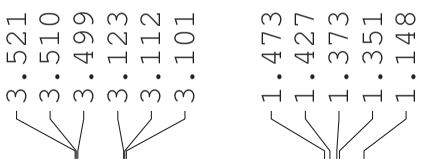
| ======== CHANNEL f1 ======== | |
|---|---|
| NUC1 | 1H |
| P1 | 14.14 usec |
| PL1 | 1.00 dB |
| SFO1 | 500.1330885 MHz |
| SI | 32768 |
| SF | 500.1300127 MHz |
| WDW | no |
| SSB | 0 |
| LB | 0.00 Hz |
| GB | 0 |
| PC | 1.00 |




MH-2-15
C13CPD CDCl3

| | |
|---|---|
| NAME | XB20140612 |
| EXPNO | 7 |
| PROCNO | 1 |
| Date_ | 20140612 |
| Time | 11.44 |
| 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 | 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 |

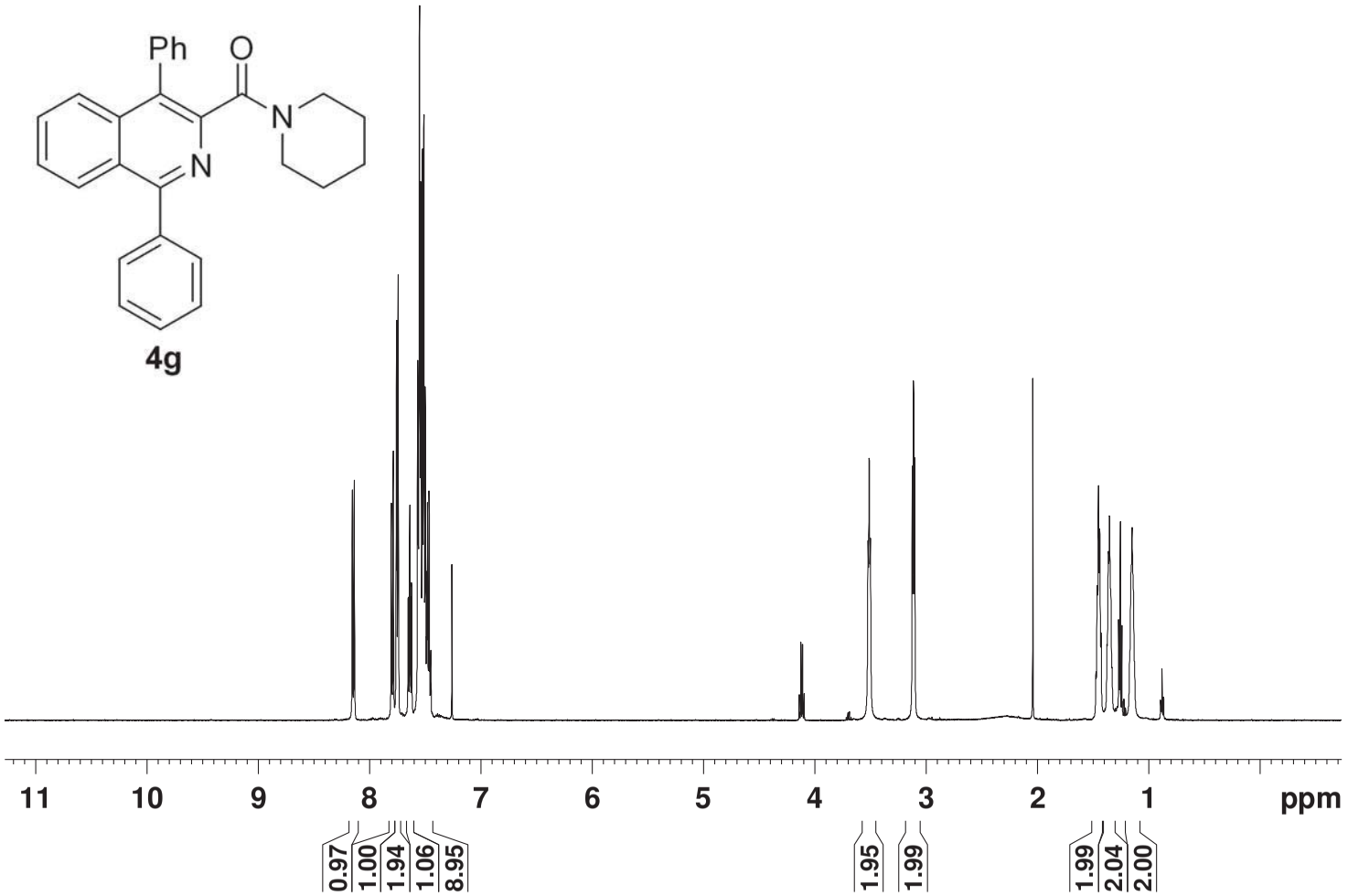



MH-2-46
PROTON CDCl3



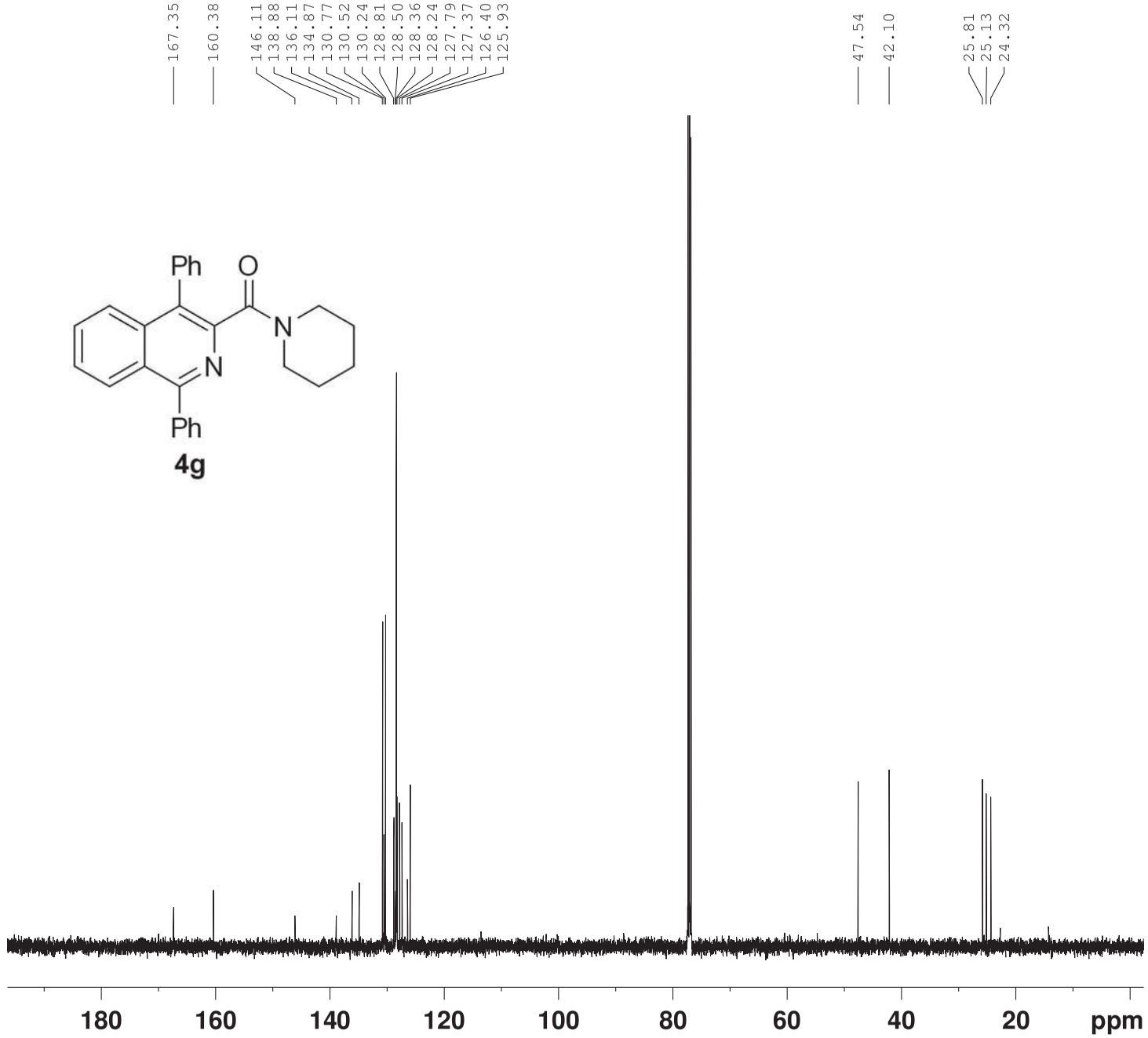

**4g**



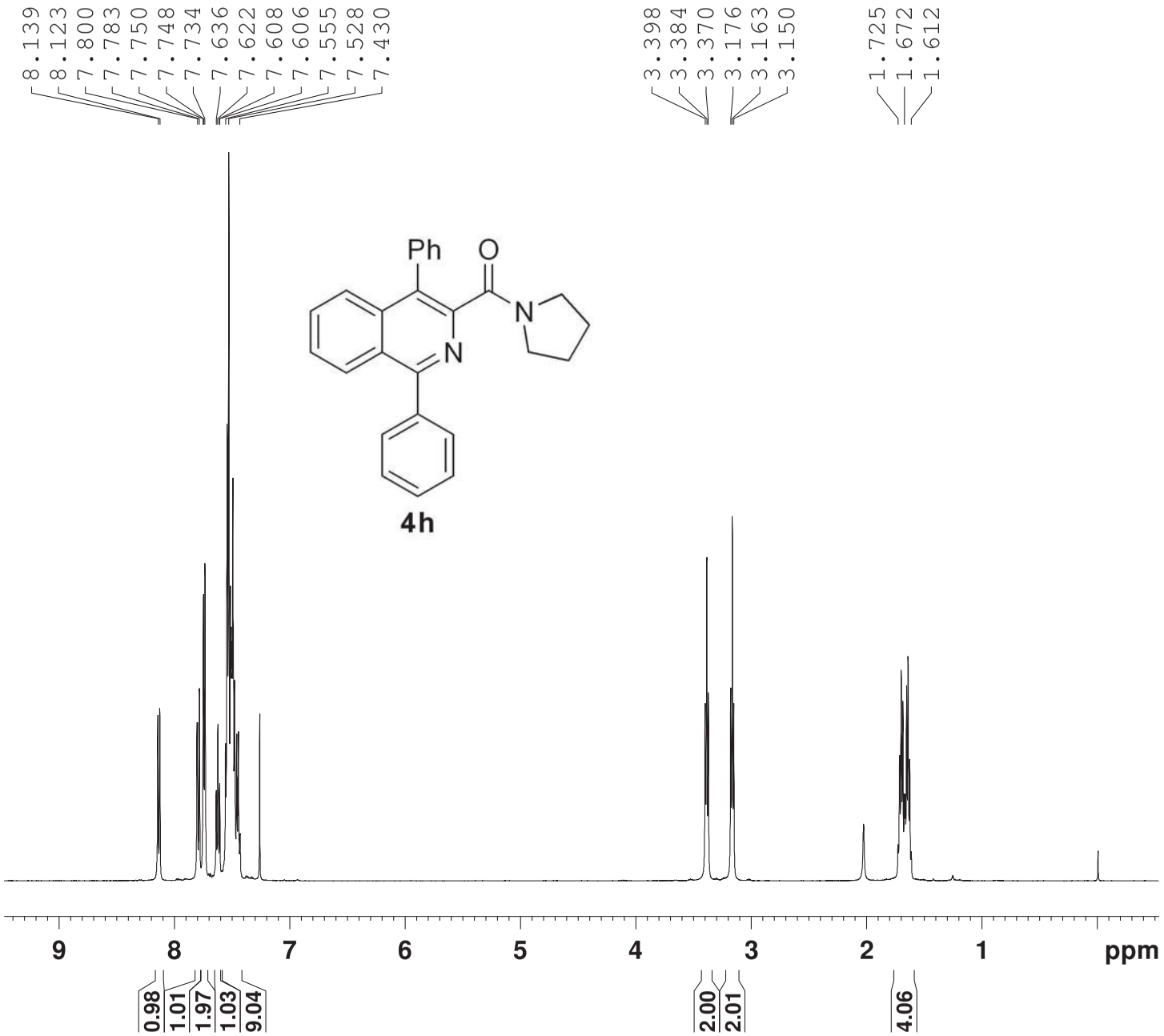

| | | |
|---|---|---|
| NAME | XB20140714 | |
| EXPNO | 10 | |
| PROCNO | 1 | |
| Date_ | 20140714 | |
| Time | 11.52 | |
| INSTRUM | spect | |
| PROBHD | 5 mm PATXO 19F | |
| PULPROG | zg30 | |
| TD | 65536 | |
| SOLVENT | CDCl3 | |
| NS | 16 | |
| DS | 2 | |
| SWH | 10330.578 | Hz |
| FIDRES | 0.157632 | 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 | 500.1300129 | MHz |
| WDW | no | |
| SSB | 0 | |
| LB | 0.00 | Hz |
| GB | 0 | |
| PC | 1.00 | |

MH-2-46
C13CPD CDCl3



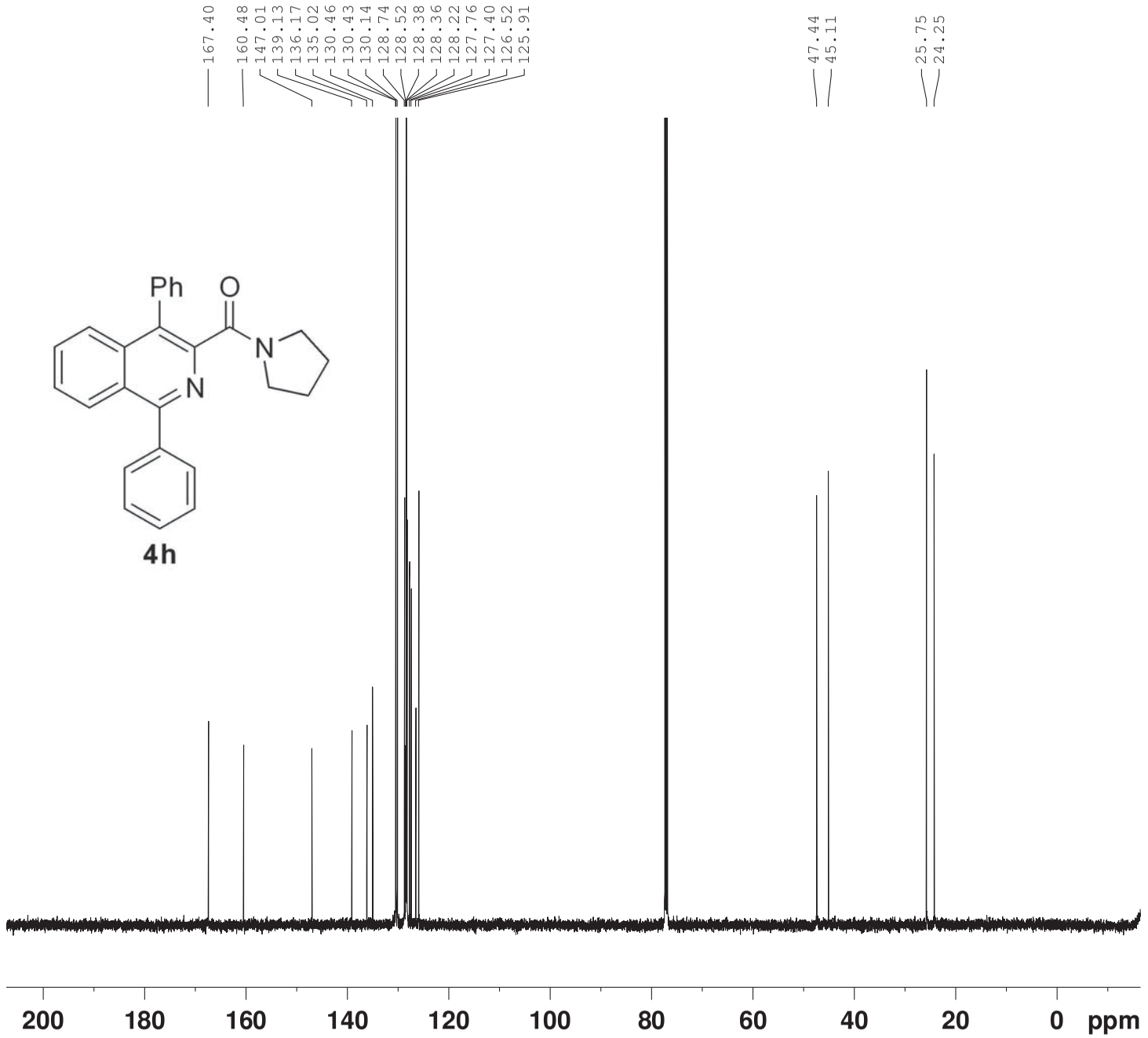

| | |
|---|---|
| NAME | XB20140714 |
| EXPNO | 12 |
| PROCNO | 1 |
| Date_ | 20140714 |
| Time | 12.09 |
| INSTRUM | spect |
| PROBHD | 5 mm PATXO 19F |
| PULPROG | zgpg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 256 |
| DS | 4 |
| SWH | 30030.029 Hz |
| FIDRES | 0.458222 Hz |
| AQ | 1.0912410 sec |
| RG | 101.6 |
| 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 |




MH-2-47
PROTON CDCl3

| | | |
|---|---|---|
| NAME | XB20150831 | |
| EXPNO | 16 | |
| PROCNO | 1 | |
| Date_ | 20150831 | |
| Time | 13.04 | |
| 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 | 295.4 | K |
| D1 | 1.00000000 | sec |
| TD0 | 1 | |

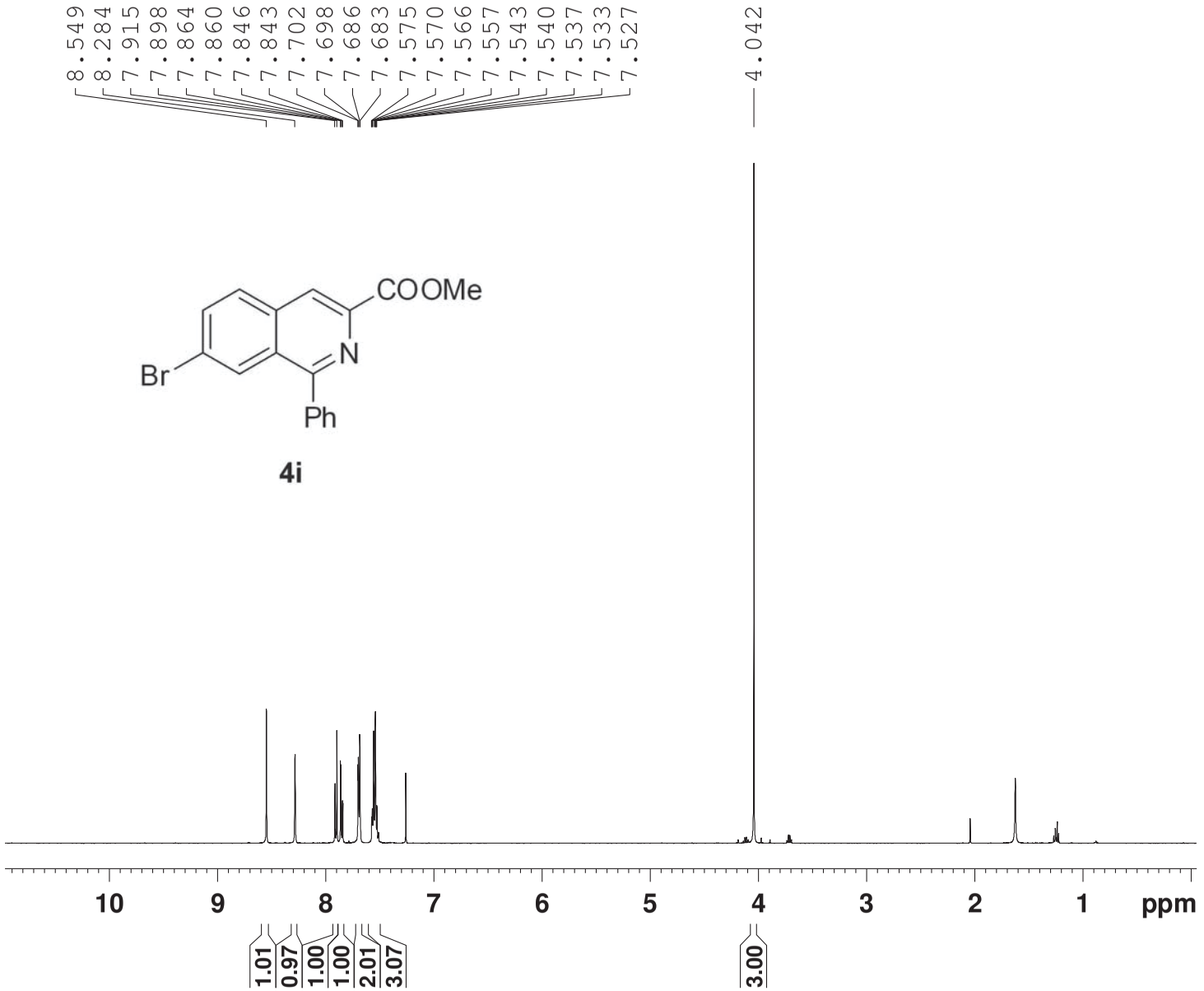
| ======== CHANNEL f1 ======== | | |
|---|---|---|
| NUC1 | 1H | |
| P1 | 14.14 | usec |
| PL1 | 1.00 | dB |
| SFO1 | 500.1330885 | MHz |
| SI | 32768 | |
| SF | 500.1300126 | MHz |
| WDW | no | |
| SSB | 0 | |
| LB | 0.00 | Hz |
| GB | 0 | |
| PC | 1.00 | |




S117

MH-2-47
C13CPD CDCl3

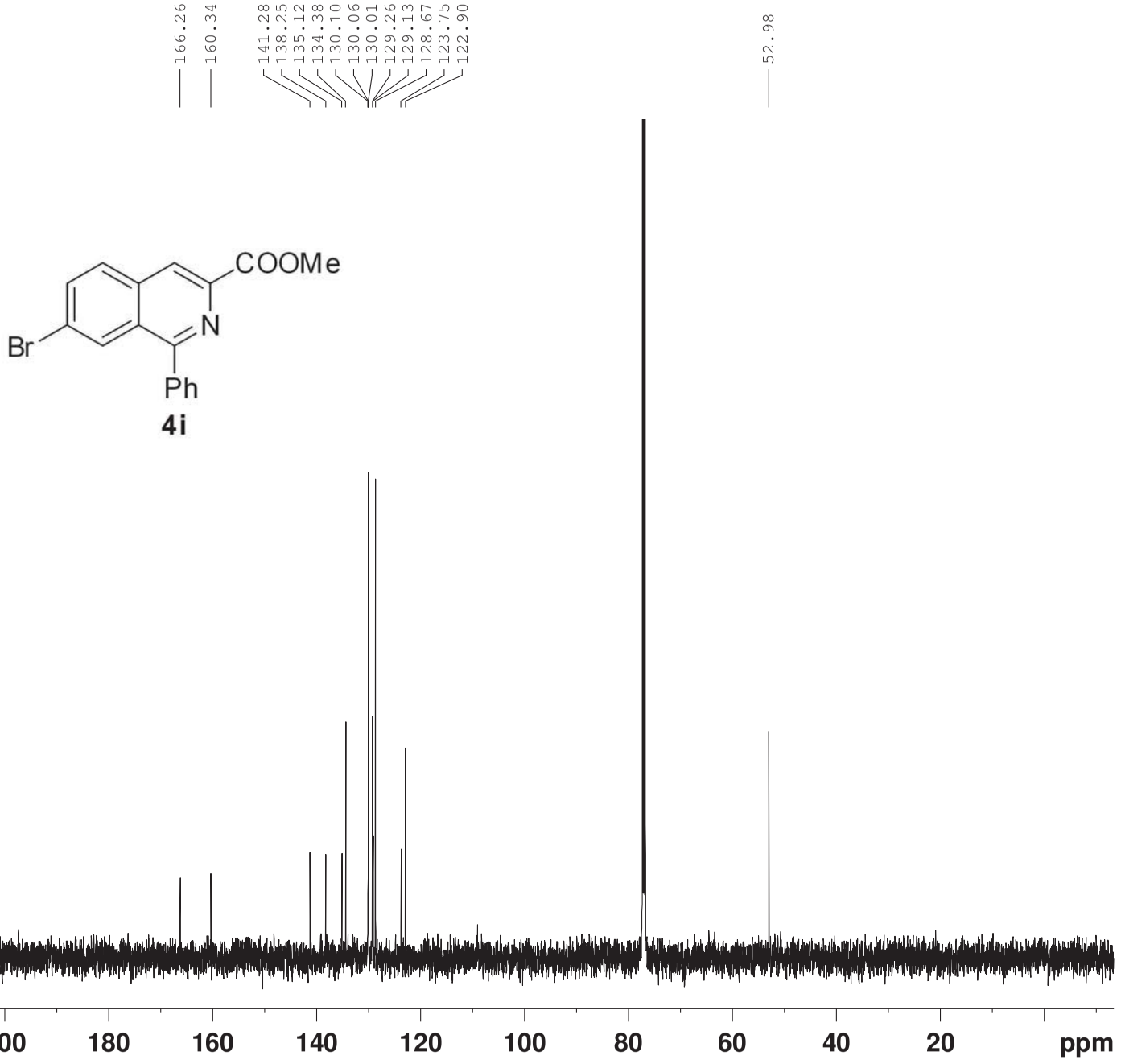
| | |
|---|---|
| NAME | XB20150831-C4 |
| EXPNO | 20 |
| PROCNO | 1 |
| Date_ | 20150901 |
| Time | 0.44 |
| INSTRUM | spect |
| PROBHD | 5 mm PATXO 19F |
| PULPROG | zgpg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 512 |
| DS | 4 |
| SWH | 30030.029 Hz |
| FIDRES | 0.458222 Hz |
| AQ | 1.0912410 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 |



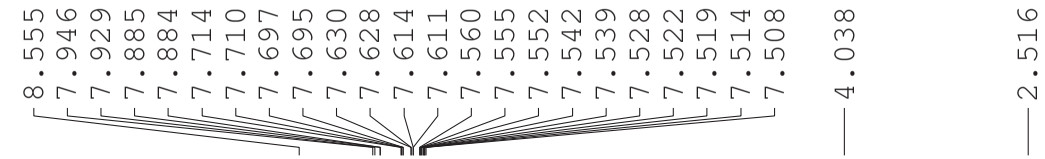

MH-2-51
PROTON CDCl3

| | | |
|---|---|---|
| NAME | XB20140714 | |
| EXPNO | 15 | |
| PROCNO | 1 | |
| Date_ | 20140714 | |
| Time | 12.36 | |
| 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 | 296.9 | 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 | |

MH-2-51
C13CPD CDCl3



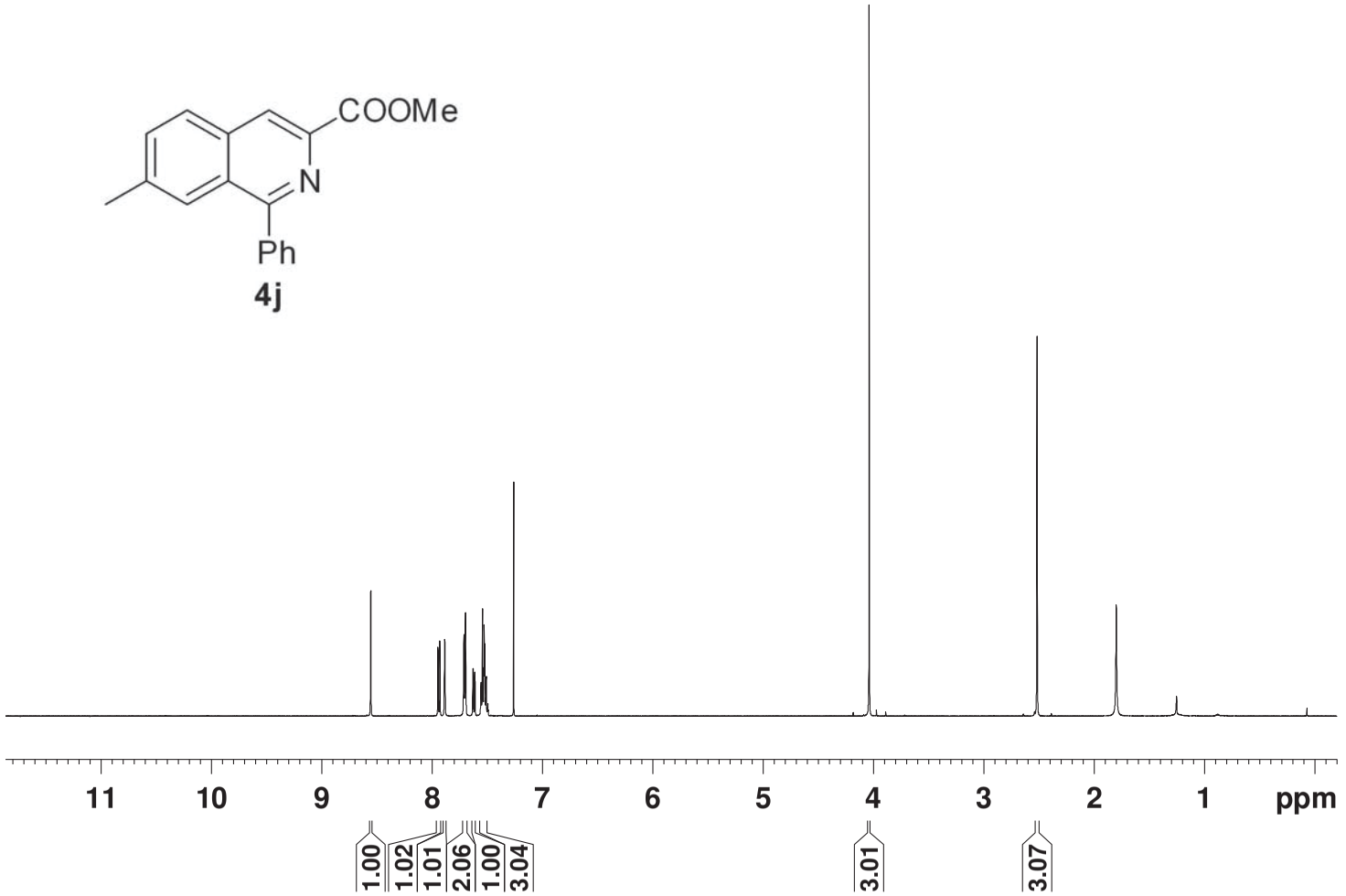

| | |
|---|---|
| NAME | XB20140714 |
| EXPNO | 16 |
| PROCNO | 1 |
| Date_ | 20140714 |
| Time | 12.51 |
| INSTRUM | spect |
| PROBHD | 5 mm PATXO 19F |
| PULPROG | zgpg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 256 |
| DS | 4 |
| SWH | 30030.029 Hz |
| FIDRES | 0.458222 Hz |
| AQ | 1.0912410 sec |
| RG | 90.5 |
| 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 | 2.00 Hz |
| GB | 0 |
| PC | 1.40 |



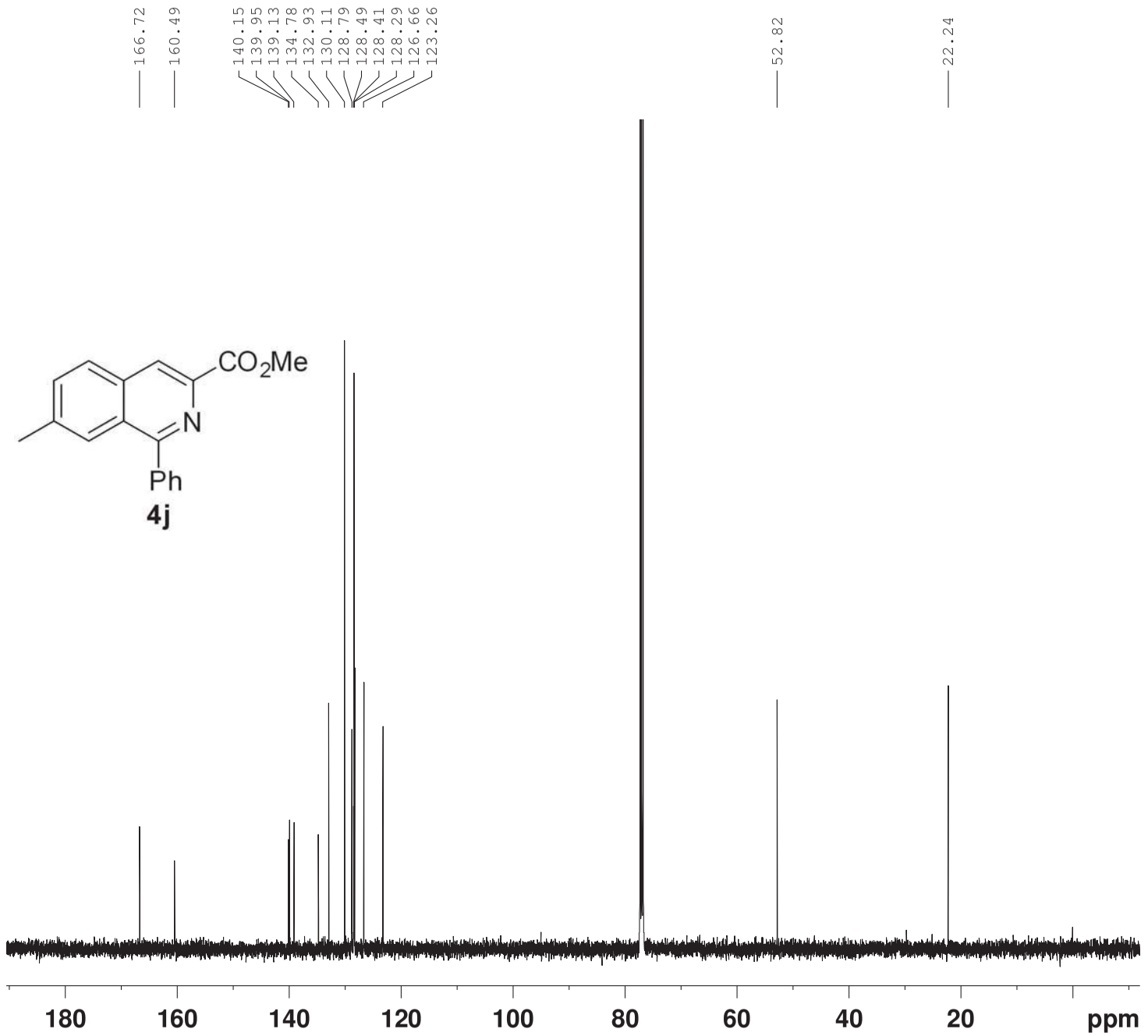

MH-2-62
PROTON CDCl3




**4j**

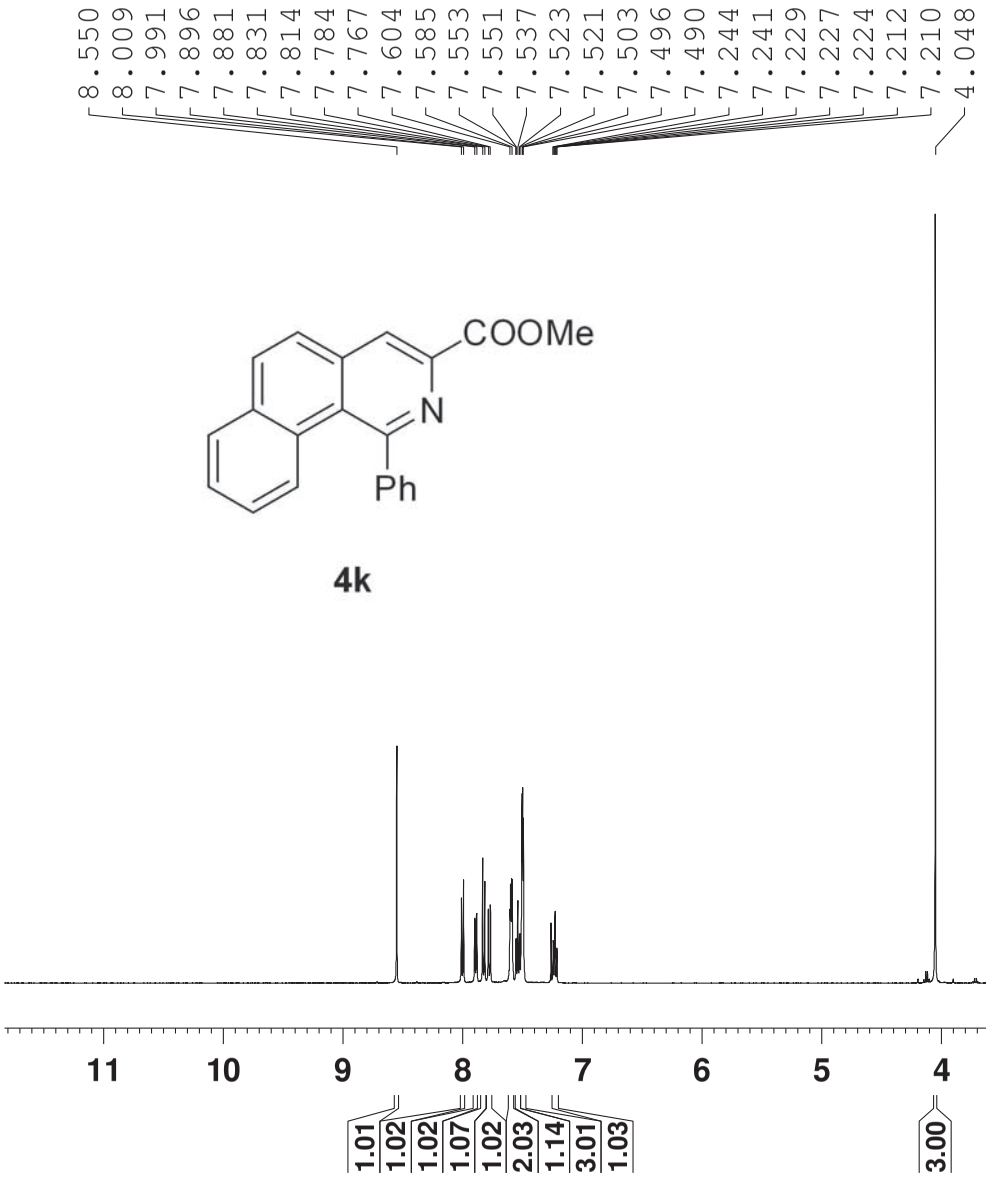



| | |
|---|---|
| NAME | XB20140730 |
| EXPNO | 7 |
| PROCNO | 1 |
| Date_ | 20140730 |
| Time | 15.05 |
| INSTRUM | spect |
| PROBHD | 5 mm PATXO 19F |
| PULPROG | zg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 10330.578 Hz |
| FIDRES | 0.157632 Hz |
| AQ | 3.1720407 sec |
| RG | 406.4 |
| DW | 48.400 usec |
| DE | 6.00 usec |
| TE | 297.5 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 |



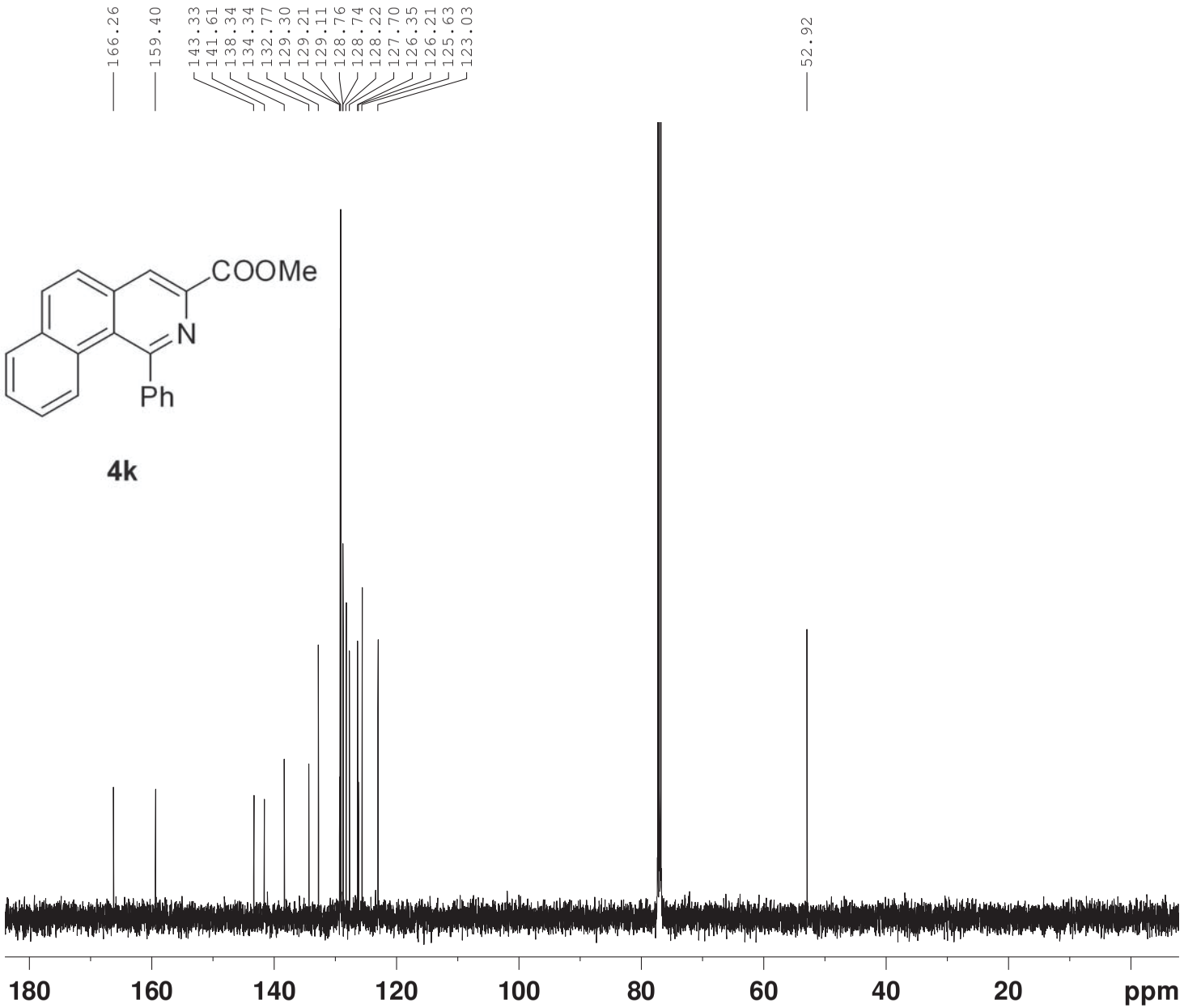

MH-2-62
C13CPD CDCl3

| | |
|---|---|
| NAME | XB20150831-C4 |
| EXPNO | 22 |
| PROCNO | 1 |
| Date_ | 20150901 |
| Time | 2.16 |
| 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 | 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 | 0.20 |



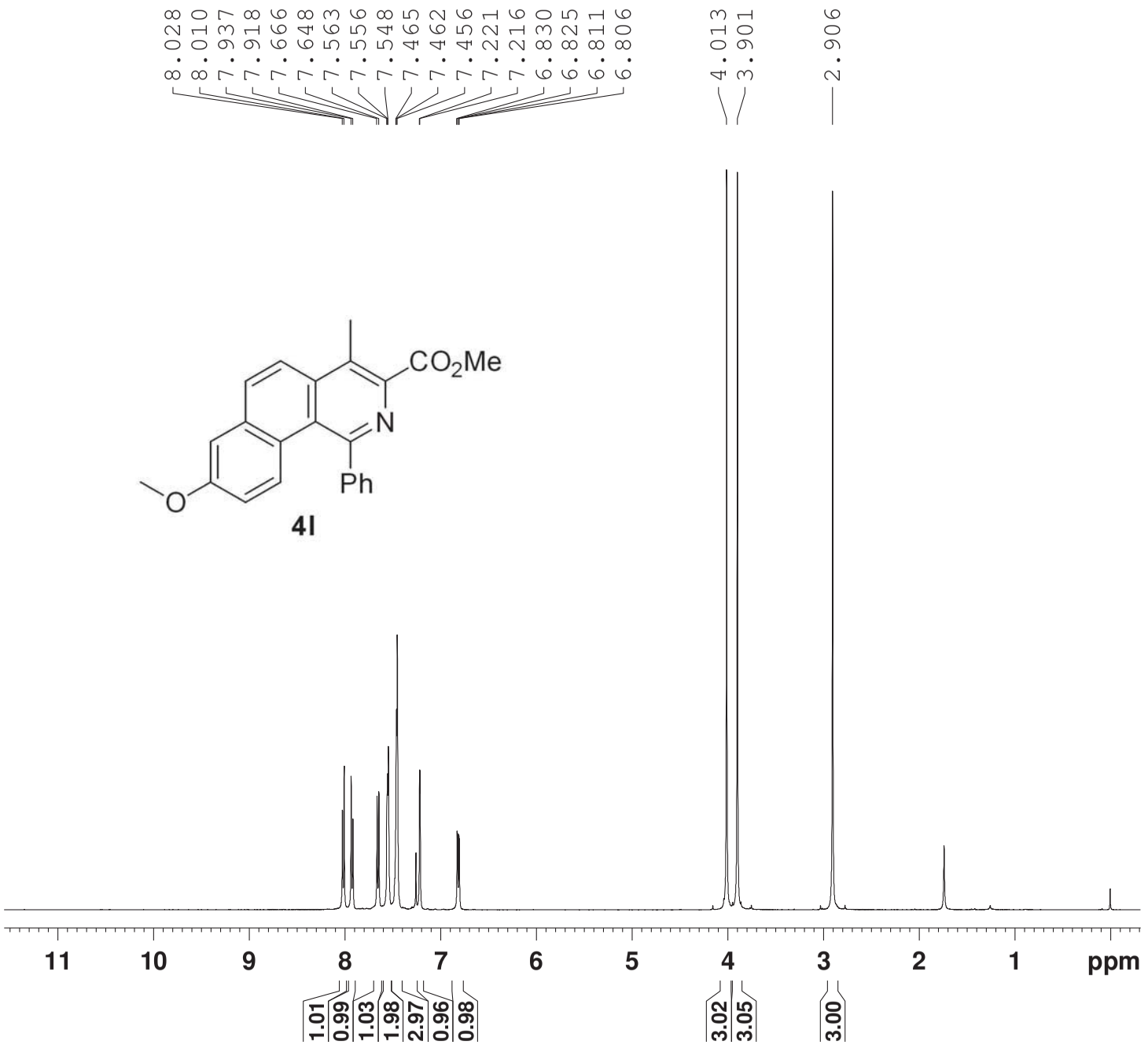

MH-2-50
PROTON CDCl3

| | | |
|---|---|---|
| NAME | XB20140714 | |
| EXPNO | 13 | |
| PROCNO | 1 | |
| Date_ | 20140714 | |
| Time | 12.15 | |
| 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 | 203.2 | |
| 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 | |



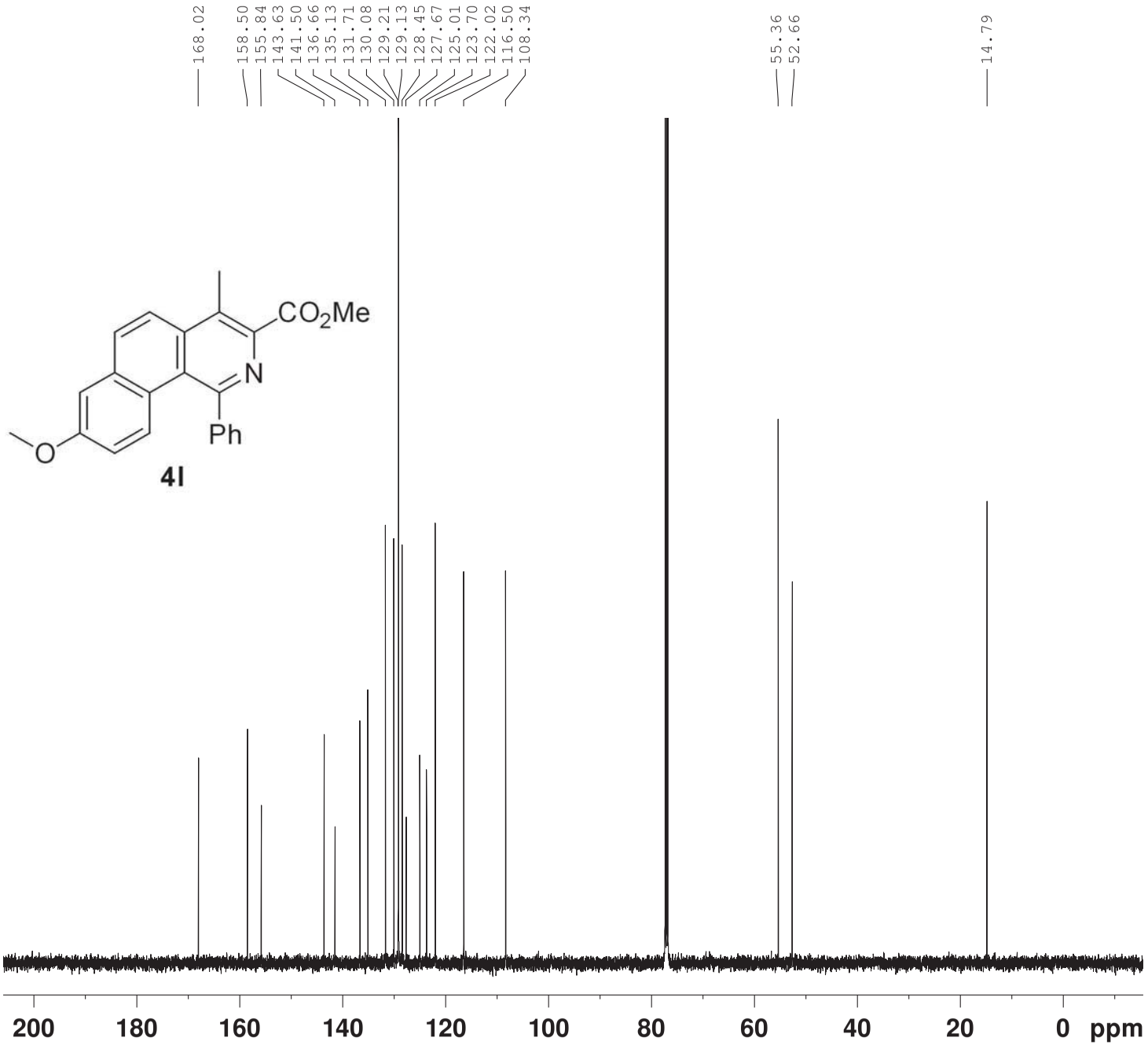

MH-2-50
C13CPD CDCl3

| | |
|---|---|
| NAME | XB20140714 |
| EXPNO | 14 |
| PROCNO | 1 |
| Date_ | 20140714 |
| Time | 12.30 |
| 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 | 128 |
| 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 |



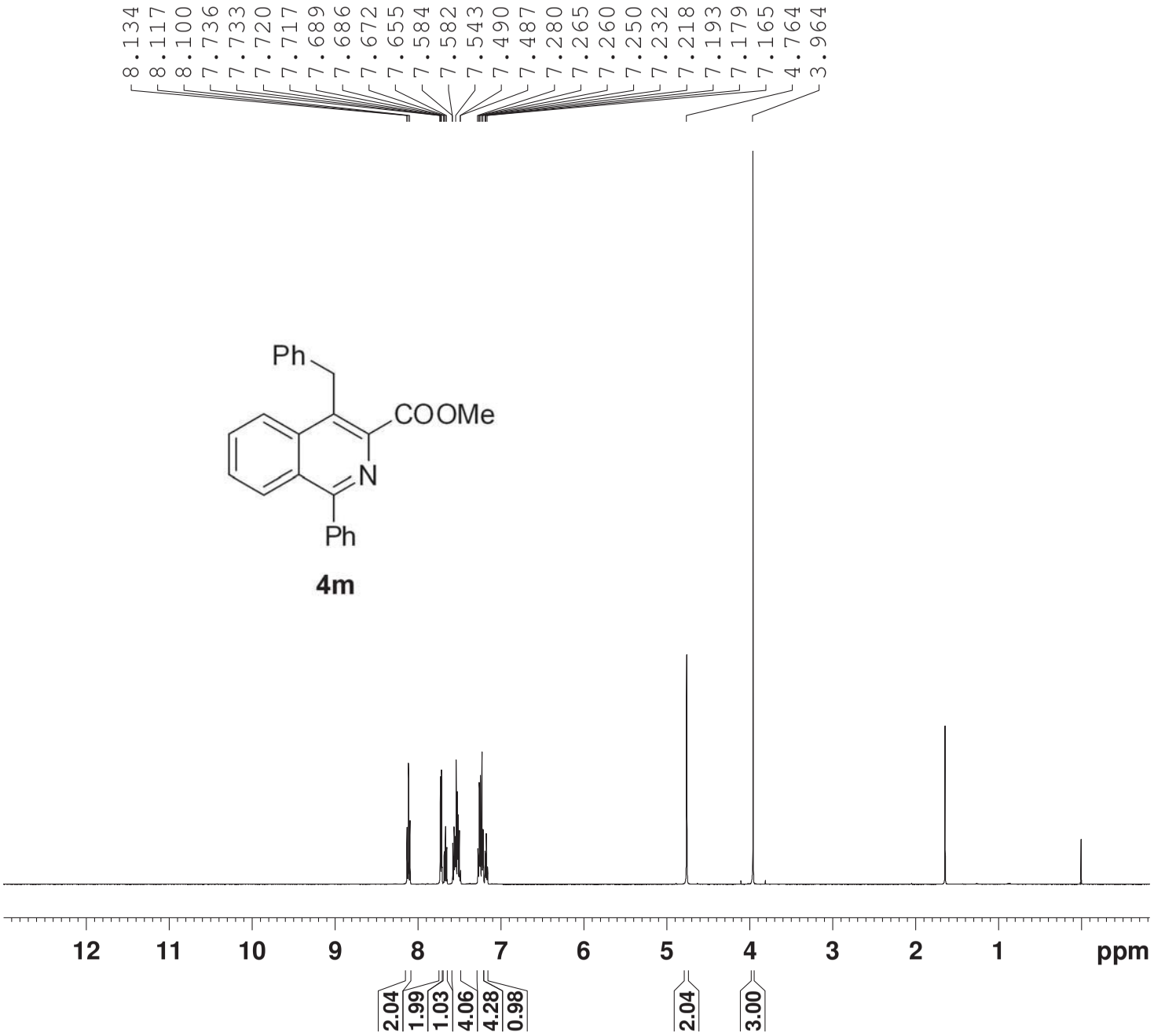

MH-2-59
PROTON CDCl3

| | |
|---|---|
| NAME | XB20150831 |
| EXPNO | 17 |
| PROCNO | 1 |
| Date_ | 20150831 |
| Time | 13.10 |
| 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 | 295.6 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 | 500.1300123 MHz |
| WDW | no |
| SSB | 0 |
| LB | 0.00 Hz |
| GB | 0 |
| PC | 1.00 |



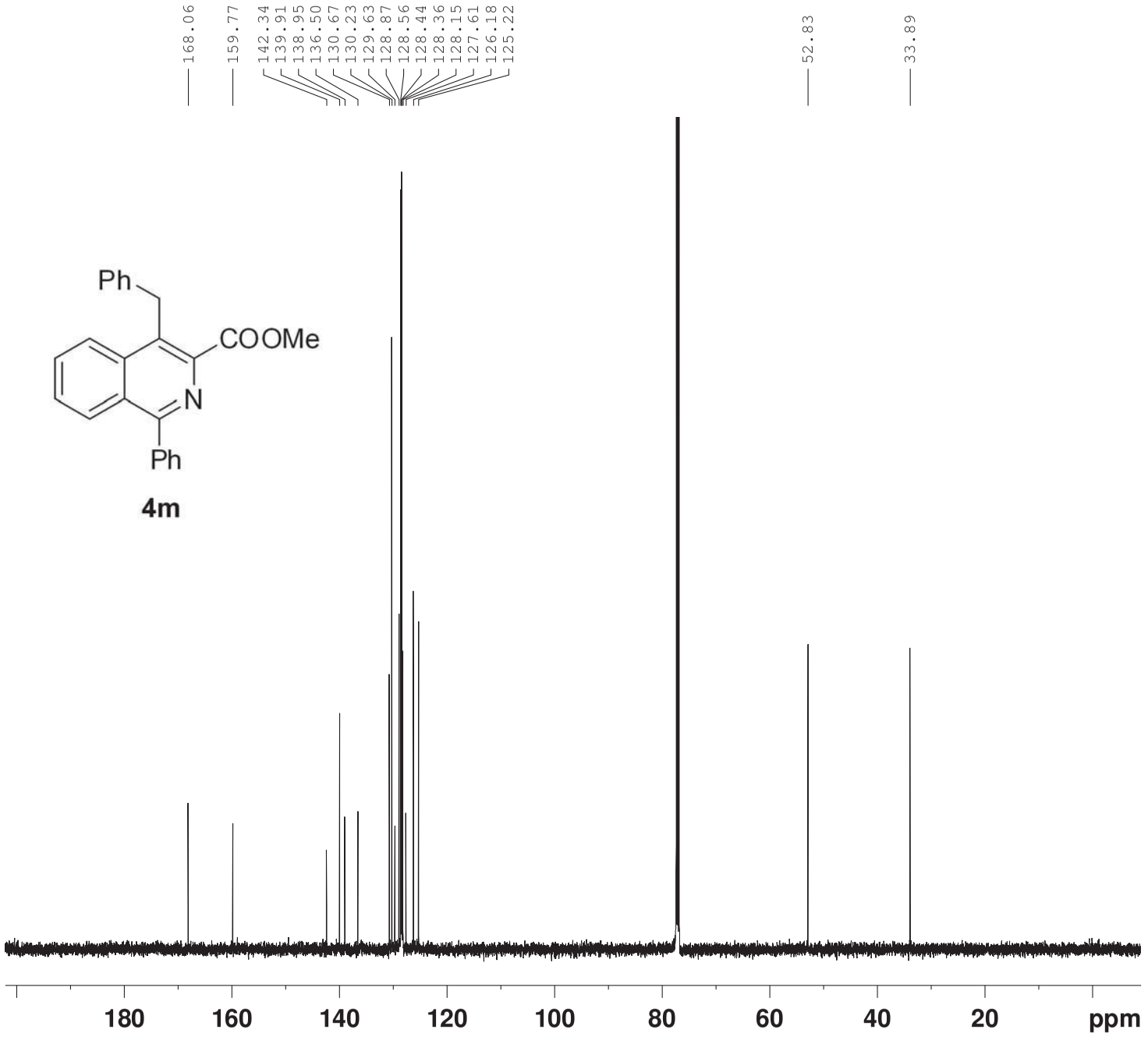

MH-2-59
C13CPD CDCl3

| | |
|---|---|
| NAME | XB20150831-C4 |
| EXPNO | 21 |
| PROCNO | 1 |
| Date_ | 20150901 |
| Time | 1.17 |
| 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 | 456.1 |
| 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 |



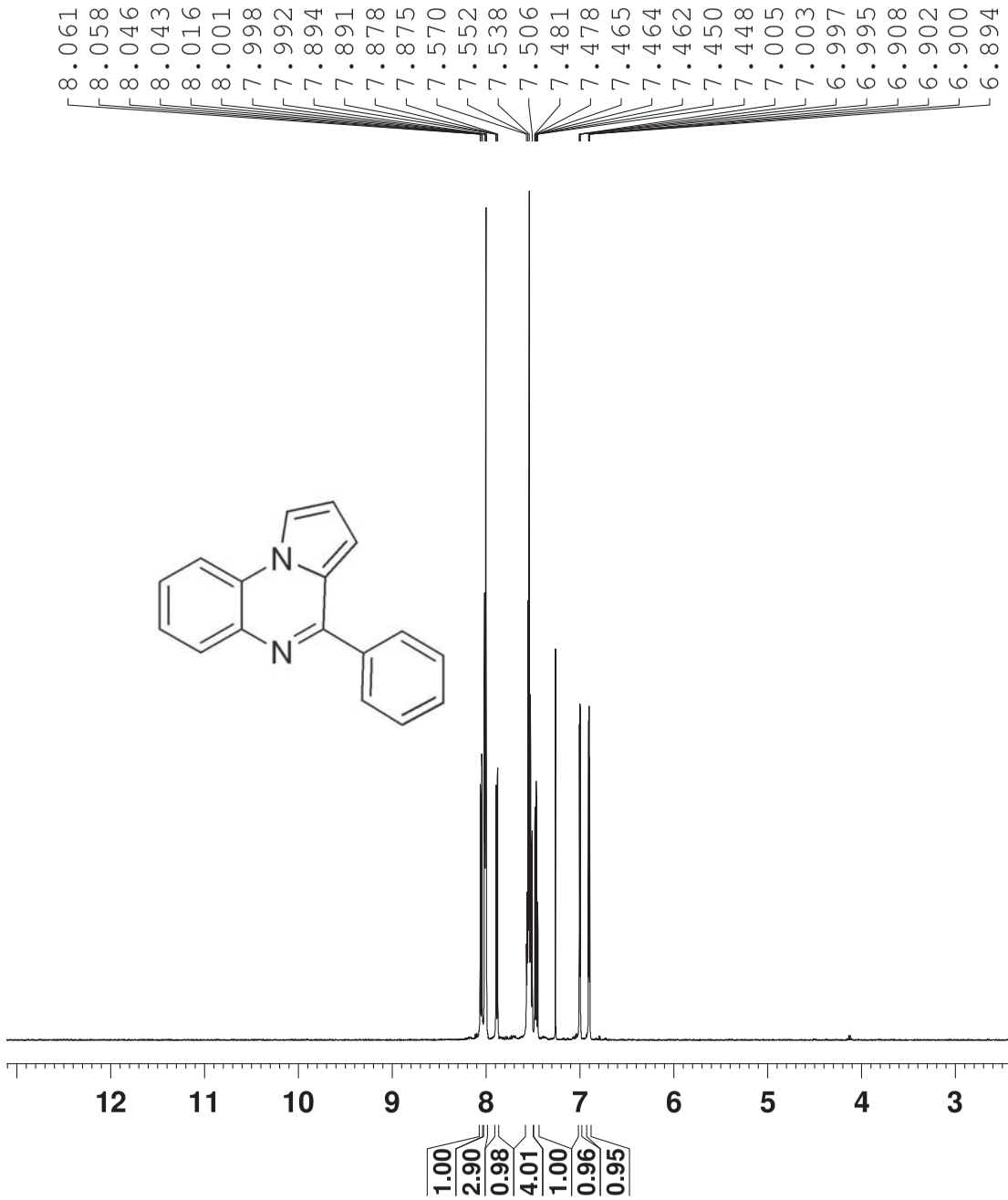

MH-3-97-A
PROTON CDCl3

| | | |
|---|---|---|
| NAME | XB20150928 | |
| EXPNO | 16 | |
| PROCNO | 1 | |
| Date_ | 20150928 | |
| Time | 16.34 | |
| 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 | 181 | |
| DW | 48.400 | usec |
| DE | 6.00 | usec |
| TE | 295.3 | 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 | |




MH-3-97-A
C13CPD CDCl3

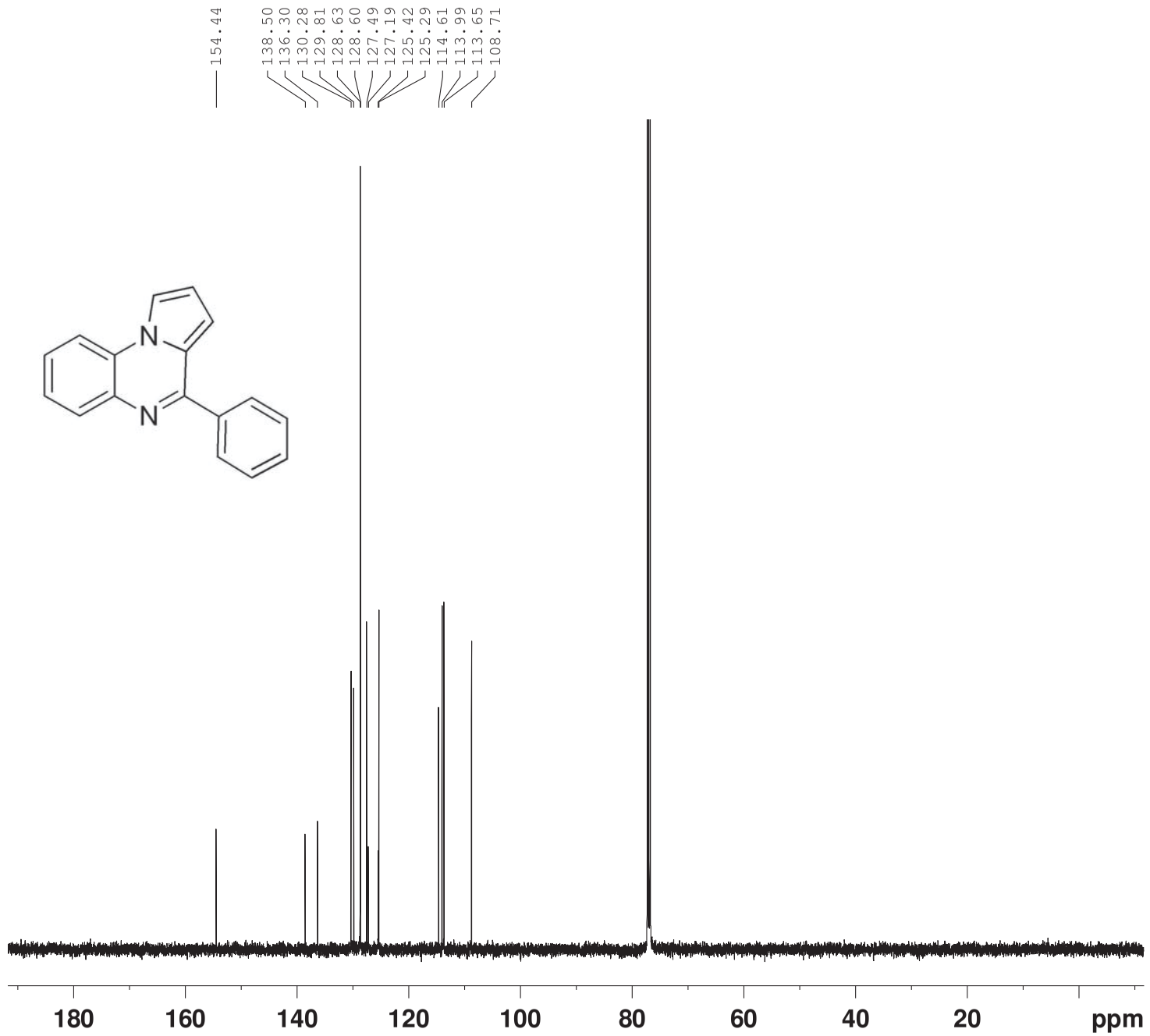
| | |
|---|---|
| NAME | MH20150928-C |
| EXPNO | 22 |
| PROCNO | 1 |
| Date_ | 20150929 |
| Time | 1.21 |
| INSTRUM | spect |
| PROBHD | 5 mm PATXO 19F |
| PULPROG | zgpg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 1024 |
| DS | 4 |
| SWH | 30030.029 Hz |
| FIDRES | 0.458222 Hz |
| AQ | 1.0912410 sec |
| RG | 128 |
| 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 |




MH-3-123
PROTON CDCl3

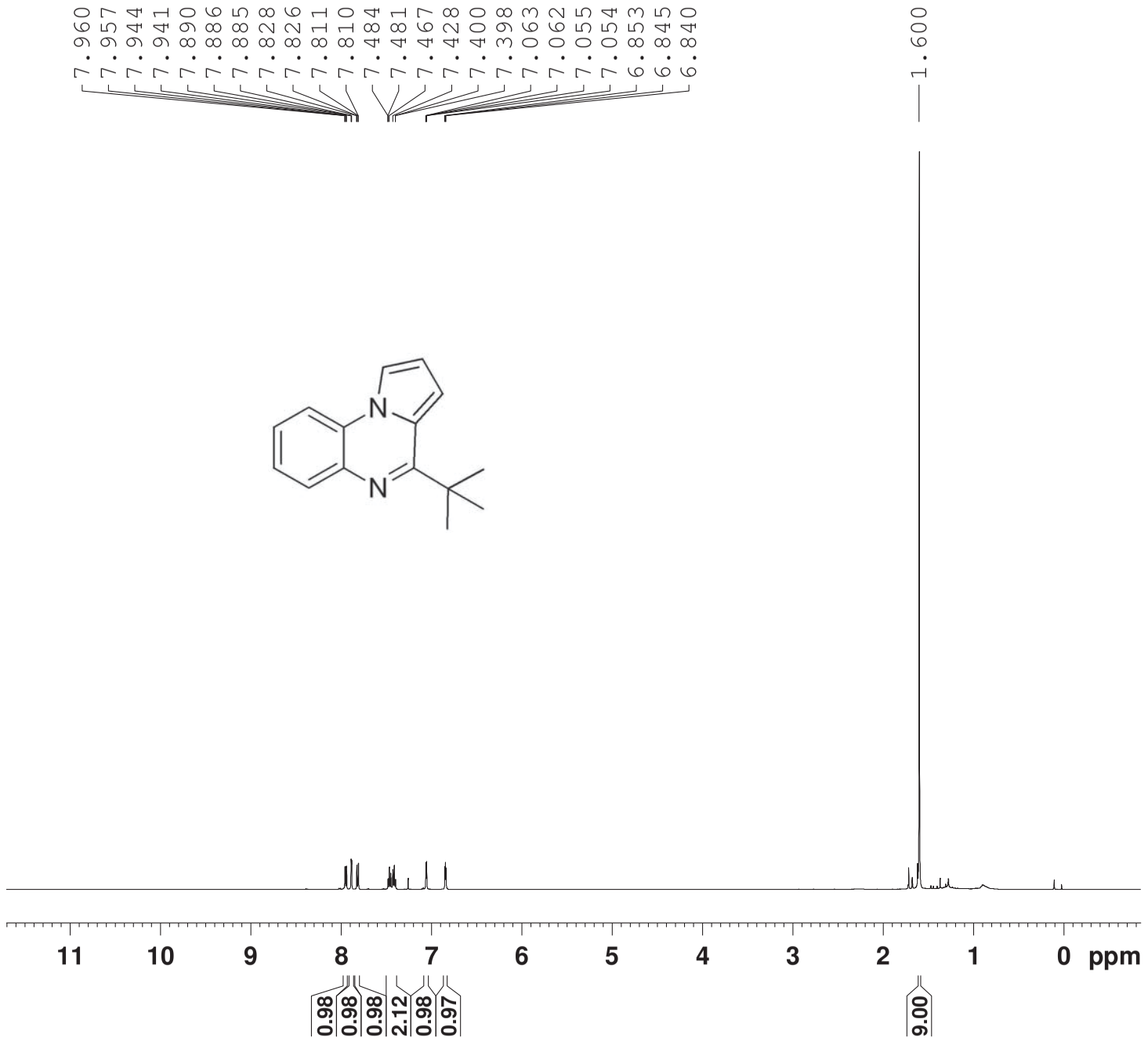
| | | |
|---|---|---|
| NAME | XB20151128 | |
| EXPNO | 1 | |
| PROCNO | 1 | |
| Date_ | 20151128 | |
| Time | 23.11 | |
| INSTRUM | spect | |
| PROBHD | 5 mm PATXO 19F | |
| PULPROG | zg30 | |
| TD | 65536 | |
| SOLVENT | CDCl3 | |
| NS | 16 | |
| DS | 2 | |
| SWH | 10330.578 | Hz |
| FIDRES | 0.157632 | Hz |
| AQ | 3.1720407 | sec |
| RG | 256 | |
| DW | 48.400 | usec |
| DE | 6.00 | usec |
| TE | 295.4 | 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 | 500.1300129 | MHz |
| WDW | no | |
| SSB | 0 | |
| LB | 0.00 | Hz |
| GB | 0 | |
| PC | 1.00 | |




MH-3-123
C13CPD CDCl3

| | |
|---|---|
| NAME | XB20151128 |
| EXPNO | 2 |
| PROCNO | 1 |
| Date_ | 20151129 |
| Time | 0.07 |
| 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 | 297.5 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 |

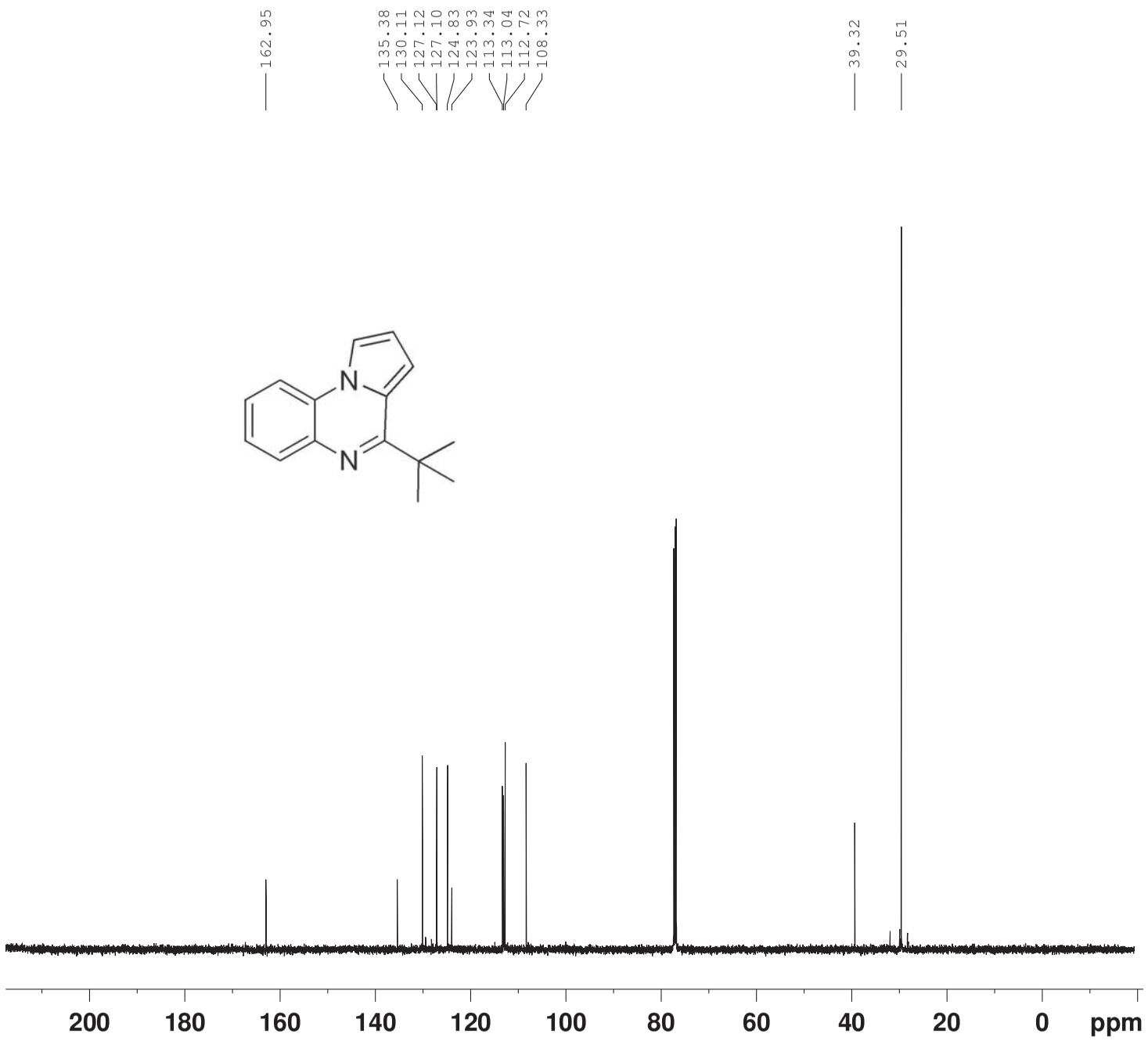



MH-5B
PROTON CDCl3

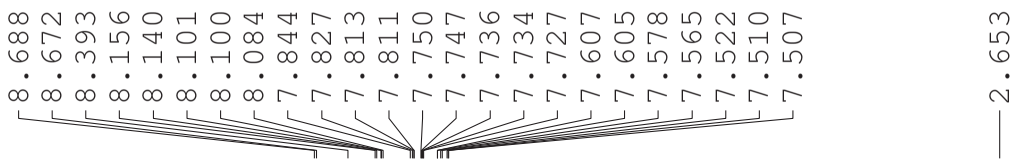
| | |
|---|---|
| NAME | XB20151215 |
| EXPNO | 11 |
| PROCNO | 1 |
| Date_ | 20151215 |
| Time | 15.25 |
| INSTRUM | spect |
| PROBHD | 5 mm PATXO 19F |
| PULPROG | zg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 16 |
| DS | 2 |
| SWH | 10330.578 Hz |
| FIDRES | 0.157632 Hz |
| AQ | 3.1720407 sec |
| RG | 101.6 |
| DW | 48.400 usec |
| DE | 6.00 usec |
| TE | 294.6 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 |

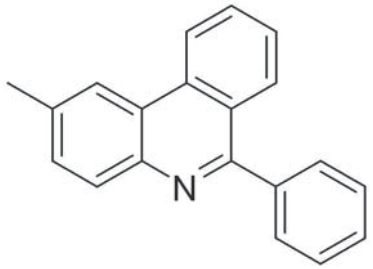
MH-5B
C13CPD CDCl3




| | |
|---|---|
| NAME | XB20151215 |
| EXPNO | 13 |
| PROCNO | 1 |
| Date_ | 20151215 |
| Time | 15.35 |
| 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 | 128 |
| DW | 16.650 usec |
| DE | 6.00 usec |
| TE | 295.3 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 |

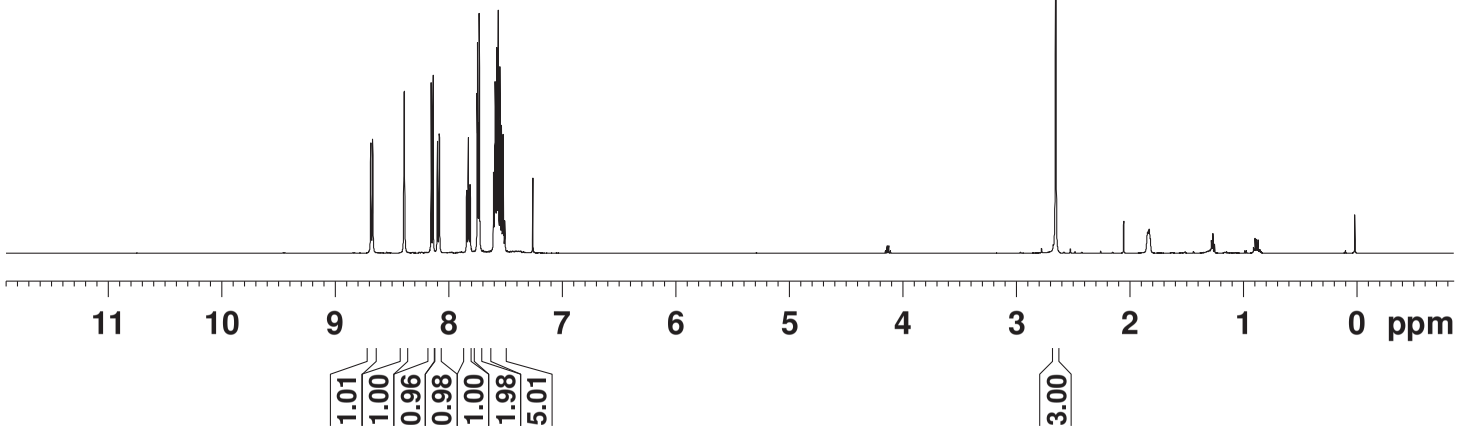


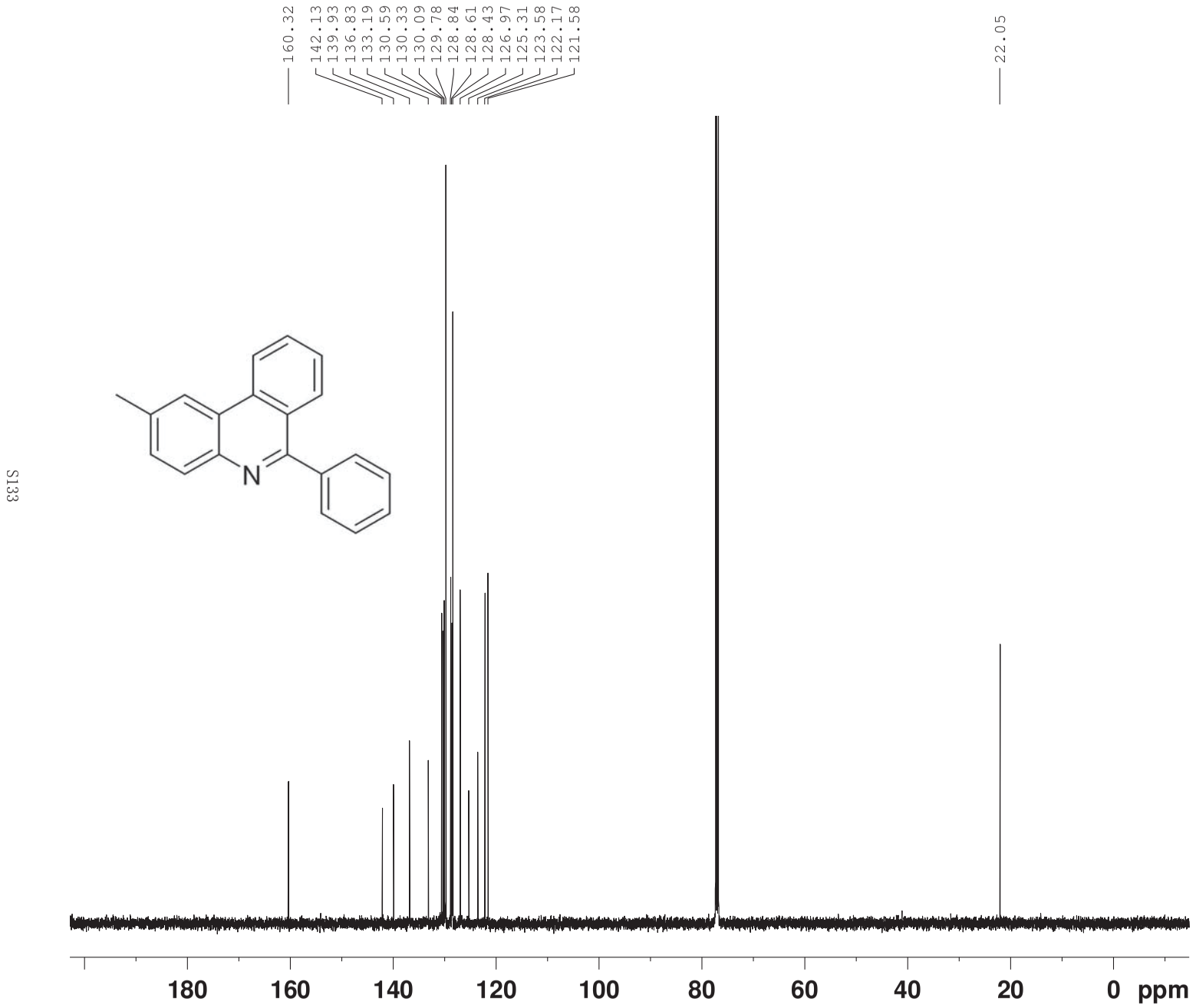

MH-3-124
PROTON CDCl3




| | |
|---|---|
| NAME | xb20151124 |
| EXPNO | 21 |
| PROCNO | 1 |
| Date_ | 20151124 |
| Time | 3.12 |
| 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 | 295.6 K |
| D1 | 1.00000000 sec |
| TD0 | 1 |

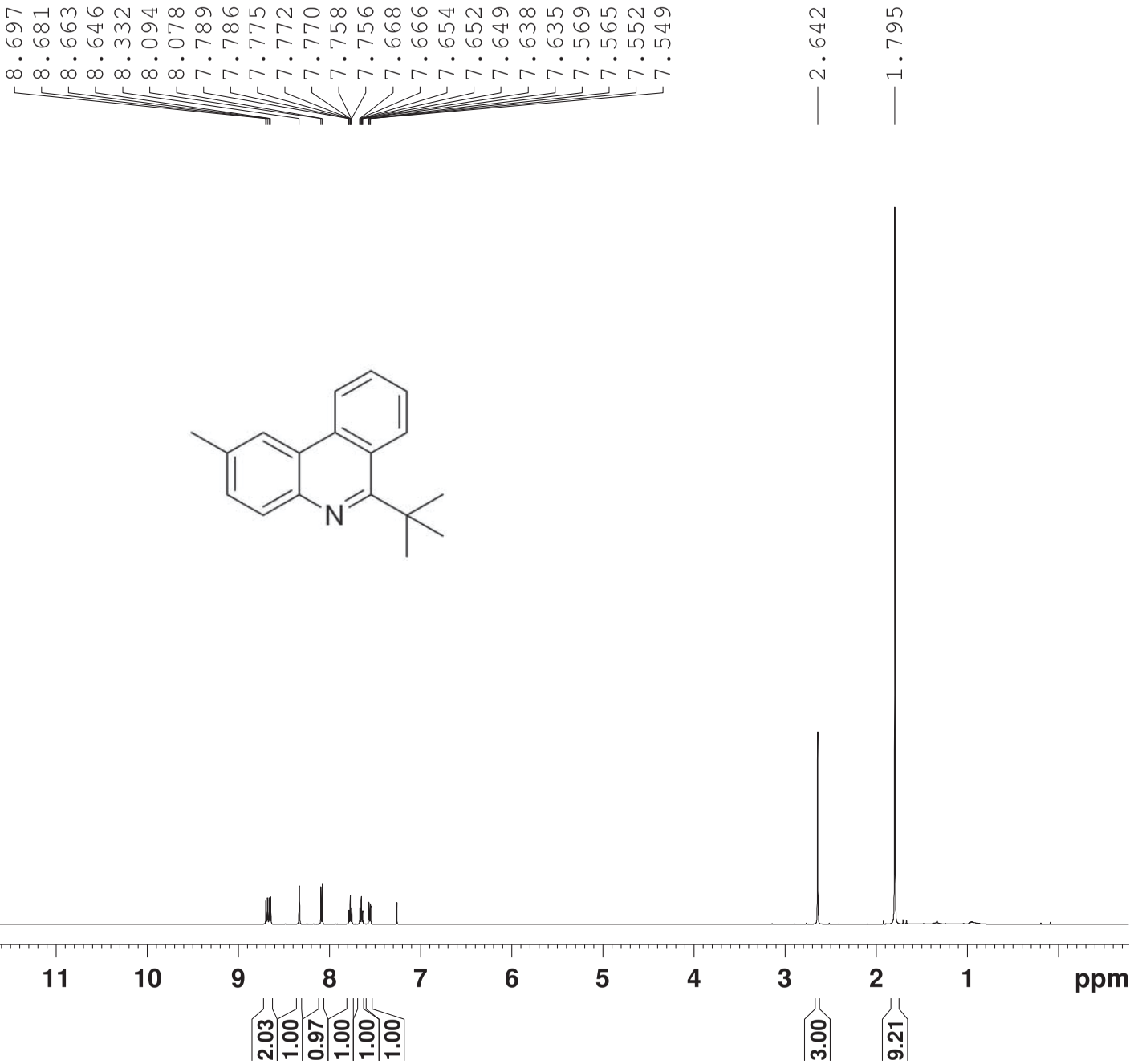
| ======== CHANNEL f1 ======== | |
|---|---|
| NUC1 | 1H |
| P1 | 14.14 usec |
| PL1 | 1.00 dB |
| SFO1 | 500.1330885 MHz |
| SI | 32768 |
| SF | 500.1300126 MHz |
| WDW | no |
| SSB | 0 |
| LB | 0.00 Hz |
| GB | 0 |
| PC | 1.00 |





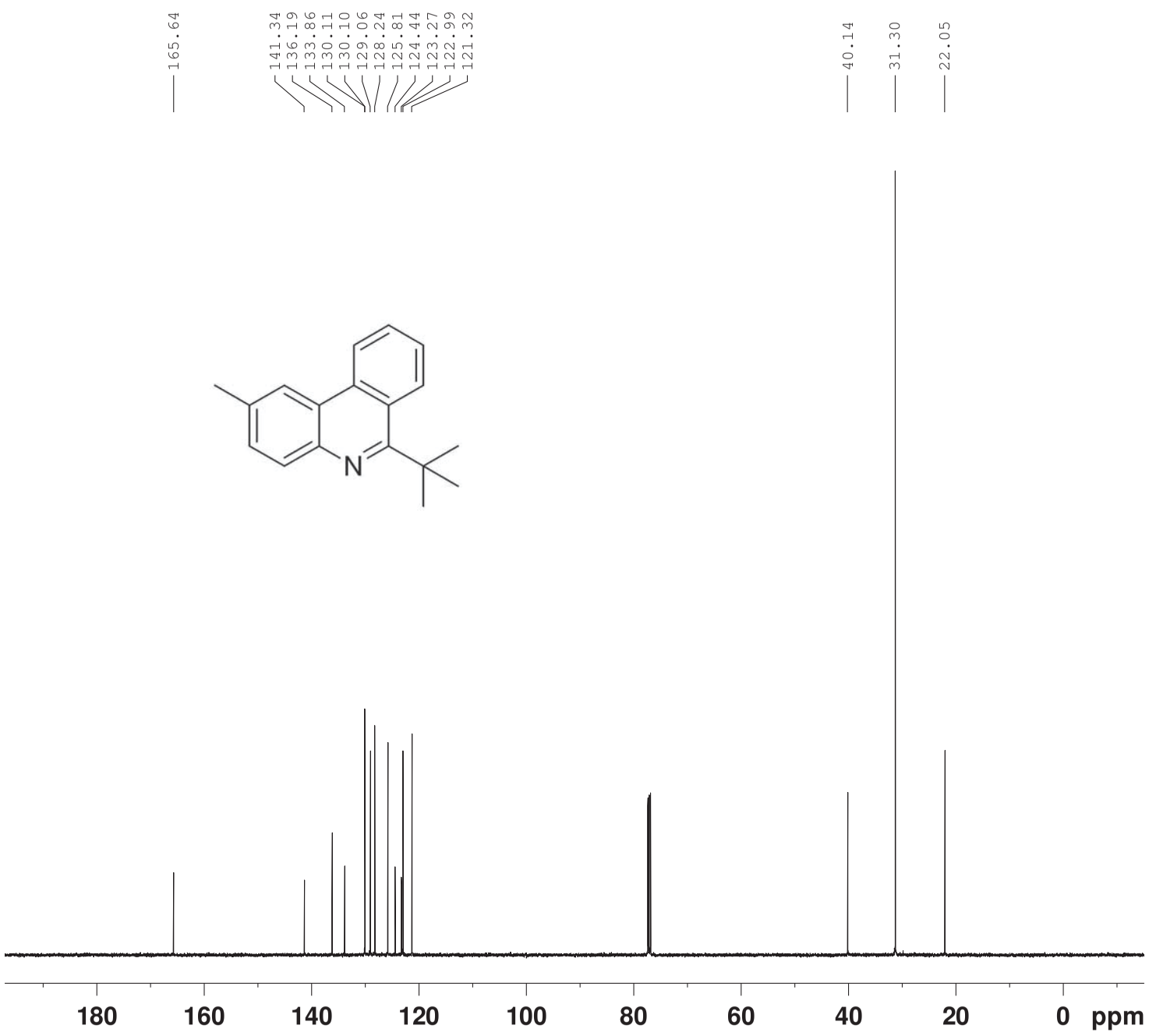

MH-3-124
C13CPD CDCl3

| | |
|---|---|
| NAME | xb20151124 |
| EXPNO | 22 |
| PROCNO | 1 |
| Date_ | 20151124 |
| Time | 3.41 |
| 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 | 296.2 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 |




MH-5d
PROTON CDCl3

| | |
|---|---|
| NAME | XB20151214 |
| EXPNO | 17 |
| PROCNO | 1 |
| Date_ | 20151214 |
| Time | 14.09 |
| 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 | 35.9 |
| DW | 48.400 usec |
| DE | 6.00 usec |
| TE | 294.9 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 |




MH-5d
C13CPD CDCl3

| | |
|---|---|
| NAME | XB20151214 |
| EXPNO | 18 |
| PROCNO | 1 |
| Date_ | 20151214 |
| Time | 14.24 |
| INSTRUM | spect |
| PROBHD | 5 mm PATXO 19F |
| PULPROG | zgpg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 276 |
| 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 | 296.2 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 |