

Ruthenium-Catalyzed Double-Fold C–H Tertiary Alkoxy carbonylation of Arenes Using Di-*tert*-butyldicarbonate

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Supporting Information

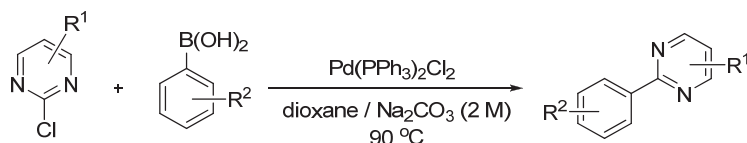
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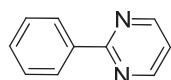
1. General Information

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. ^1H , ^{13}C and ^{19}F NMR 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), dimethyl sulfoxide ($\delta = 2.50$ ppm) or TMS ($\delta = 0.00$ ppm) for ^1H NMR, chloroform ($\delta = 77.16$ ppm) or dimethyl sulfoxide ($\delta = 39.52$ ppm) for ^{13}C NMR, and C_6F_6 ($\delta = -164.9$ ppm) for ^{19}F NMR. Mass spectra and high resolution mass spectra (HRMS) were recorded with an Agilent 5975N using an Electron impact (EI) or Electrospray ionization (ESI) techniques. Elemental analyses were carried out on an Elementar Vario EL elemental analyzer. Silica gel plate GF254 were used for thin layer chromatography (TLC) and silica gel H or 300-400 mesh were used for flash column chromatography. Yields refer to chromatographically and spectroscopically pure compounds, unless otherwise indicated.

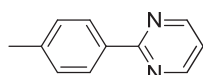
2. Synthesis and Characterization for *tert*-Butoxycarbonylation Substrates



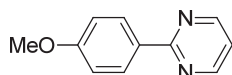
General procedure for preparation of pyrimidine substrates: To a round-bottom flask was added 2-chloropyrimidine (3.0 mmol), arylboronic acid (1.2 equiv.), Pd(PPh₃)₂Cl₂ (2 mol%) and Na₂CO₃ (2 M, 10 mL) in dioxane (10 mL). The reaction mixture was heated at 90 °C until the 2-chloropyrimidine was consumed completely (monitored by TLC). The heterogeneous aqueous was concentrated under reduced pressure and the residue was diluted with EtOAc (15 mL), washed by H₂O (20 mL), brine (20 mL). The organic layer was dried over Na₂SO₄, concentrated and purified by column chromatography on silica gel (eluent: PE / EtOAc = 10:1 to 3:1) to afford the coupling products.



2-Phenylpyrimidine (1a)¹: Following the general procedure with 2-chloropyrimidine (343.5 mg, 3.0 mmol), phenylboronic acid (439.2 mg, 3.6 mmol), Pd(PPh₃)₂Cl₂ (42.1 mg, 0.06 mmol), Na₂CO₃ (2 M, 10 mL) and dioxane (10 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 20/1) afforded **1a** (446.0 mg, 95%) as a white solid. M.p. 36-37 °C. IR (KBr, cm⁻¹): 3065, 3038, 1566, 1555, 1418, 745, 691. ¹H NMR (CDCl₃, 500 MHz): δ 8.81 (d, *J* = 5.0 Hz, 2H), 8.47-8.42 (m, 2H), 7.52-7.48 (m, 3H), 7.19 (t, *J* = 5.0 Hz, 1H); ¹³C NMR (CDCl₃, 125 MHz): δ 164.9, 157.4, 137.7, 130.9, 128.7, 128.3, 119.2. EI-MS *m/z*: 156 (100) [M⁺], 103 (84), 76 (25).

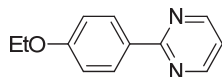


2-*p*-Tolylpyrimidine (1b)¹: Following the general procedure with 2-chloropyrimidine (343.5 mg, 3.0 mmol), *p*-tolylboronic acid (489.6 mg, 3.6 mmol), Pd(PPh₃)₂Cl₂ (42.1 mg, 0.06 mmol), Na₂CO₃ (2 M, 10 mL) and dioxane (10 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 20/1) afforded **1b** (459.0 mg, 90%) as a white solid. M.p. 83-85 °C. IR (KBr, cm⁻¹): 3035, 2918, 1564, 1416, 1179, 841, 786, 730. ¹H NMR (CDCl₃, 500 MHz): δ 8.78 (d, *J* = 5.0 Hz, 2H), 8.33 (d, *J* = 8.0 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 7.14 (t, *J* = 5.0 Hz, 1H), 2.42 (s, 3H); ¹³C NMR (CDCl₃, 125 MHz): δ 165.0, 157.3, 141.2, 135.0, 129.5, 128.2, 118.9, 21.6. EI-MS *m/z*: 170 (100) [M⁺], 169 (65), 117 (59), 89 (24).

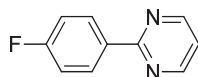


2-(4-Methoxyphenyl)pyrimidine (1c)¹: Following the general procedure with 2-chloropyrimidine (343.5 mg, 3.0 mmol), 4-methoxyphenylboronic acid (547.2 mg, 3.6 mmol), Pd(PPh₃)₂Cl₂ (42.1 mg, 0.06 mmol), Na₂CO₃ (2 M, 10 mL) and dioxane (10 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 20/1) afforded **1c** (541.3 mg, 97%) as a white solid. M.p. 65-66 °C. IR (KBr, cm⁻¹): 3004, 2964, 1604,

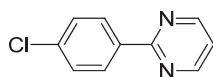
1565, 1415, 1254, 1028, 855, 812, 797, 592. ¹H NMR (CDCl₃, 500 MHz): δ 8.75 (d, *J* = 4.5 Hz, 2H), 8.39 (dd, *J* = 7.0, 2.0 Hz, 2H), 7.11 (t, *J* = 5.0 Hz, 1H), 7.02-6.98 (m, 2H), 3.87 (s, 3H); ¹³C NMR (CDCl₃, 125 MHz): δ 164.7, 162.0, 157.3, 130.4, 129.9, 118.5, 114.1, 55.5. EI-MS *m/z*: 186 (100) [M⁺], 171 (27), 143 (31), 133 (49), 90 (24).



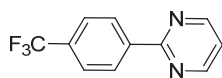
2-(4-Ethoxyphenyl)pyrimidine (1d)¹: Following the general procedure with 2-chloropyrimidine (343.5 mg, 3.0 mmol), 4-ethoxyphenylboronic acid (597.6 mg, 3.6 mmol), Pd(PPh₃)₂Cl₂ (42.1 mg, 0.06 mmol), Na₂CO₃ (2 M, 10 mL) and dioxane (10 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 20/1) afforded **1d** (558.0 mg, 93%) as a white solid. M.p. 120-121 °C. IR (KBr, cm⁻¹): 3441, 3046, 2972, 1606, 1569, 1420, 1244, 854, 797, 641. ¹H NMR (500 MHz, CDCl₃): δ 8.74 (d, *J* = 5.0 Hz, 2H), 8.34 (dd, *J* = 7.0, 2.0 Hz, 2H), 7.10 (t, *J* = 5 Hz, 1H), 6.99-6.97 (m, 2H), 4.10 (q, *J* = 7.0 Hz, 2H), 1.44 (t, *J* = 7.0 Hz, 3H); ¹³C NMR (CDCl₃, 125 MHz): δ 164.5, 161.5, 157.2, 129.9, 118.4, 114.6, 63.7, 14.9. EI-MS *m/z*: 200 (59) [M⁺], 172 (100), 119 (80).



2-(4-Fluorophenyl)pyrimidine (1e)¹: Following the general procedure with 2-chloropyrimidine (343.5 mg, 3.0 mmol), 4-fluorophenylboronic acid (504.0 mg, 3.6 mmol), Pd(PPh₃)₂Cl₂ (42.1 mg, 0.06 mmol), Na₂CO₃ (2 M, 10 mL) and dioxane (10 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 20/1) afforded **1e** (469.8 mg, 90%) as a white solid. M.p. 54-56 °C. IR (KBr, cm⁻¹): 3441, 3047, 1603, 1564, 1418, 1216, 795. ¹H NMR (CDCl₃, 500 MHz): δ 8.78 (d, *J* = 5.0 Hz, 2H), 8.45 (dd, *J* = 8.5, 5.5 Hz, 2H), 7.19-7.14 (m, 3H); ¹⁹F NMR (CDCl₃, 470 MHz): -110.3 (m, Ar-F); ¹³C NMR (CDCl₃, 125 MHz): δ 165.7, 163.7 (d, ¹*J*_{C-F} = 250 Hz), 163.8, 157.3, 133.8 (d, ⁴*J*_{C-F} = 2.5 Hz), 130.3 (d, ³*J*_{C-F} = 7.5 Hz), 119.0, 115.7, 115.5 (d, ²*J*_{C-F} = 21.25 Hz). EI-MS *m/z*: 174 (100) [M⁺], 121 (77), 94 (16).

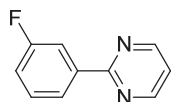


2-(4-Chloro-phenyl)pyrimidine (1f)¹: Following the general procedure with 2-chloropyrimidine (343.5 mg, 3.0 mmol), 4-chlorophenylboronic acid (561.6 mg, 3.6 mmol), Pd(PPh₃)₂Cl₂ (42.1 mg, 0.06 mmol), Na₂CO₃ (2 M, 10 mL) and dioxane (10 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 20/1) afforded **1f** (461.7 mg, 81%) as a white solid. M.p. 103-105 °C. IR (KBr, cm⁻¹): 3071, 1566, 1415, 1085, 1011, 848, 792, 774, 642. ¹H NMR (CDCl₃, 500 MHz): δ 8.79 (d, *J* = 4.5 Hz, 2H), 8.39 (dd, *J* = 7.0, 2.0 Hz, 2H), 7.47-7.44 (m, 2H), 7.19 (t, *J* = 5.0 Hz, 1H); ¹³C NMR (CDCl₃, 125 MHz): δ 163.9, 157.4, 137.2, 136.2, 129.6, 129.0, 119.4. EI-MS *m/z*: 192 (30) [M⁺ (³⁷Cl)], 190 (93) [M⁺ (³⁵Cl)], 139 (33), 137 (100), 102 (43).

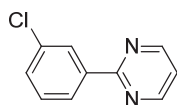


2-(4-(Trifluoromethyl)phenyl)pyrimidine (1g)¹: Following the general procedure with 2-chloropyrimidine (343.5 mg, 3.0 mmol), 4-(trifluoromethyl)phenylboronic acid (684.0 mg, 3.6 mmol), Pd(PPh₃)₂Cl₂ (42.1 mg, 0.06 mmol), Na₂CO₃ (2 M, 10 mL) and dioxane (10 mL). After

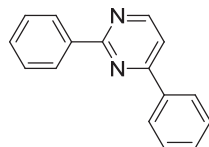
reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 20/1) afforded **1g** (564.5 mg, 84%) as a white solid. M.p. 107-108 °C; IR (KBr, cm^{-1}): 3046, 2928, 1559, 1425, 1327, 1168, 1151, 1106, 1064, 1014, 804, 793. ^1H NMR (CDCl_3 , 500 MHz): δ 8.83 (d, $J = 4.5$ Hz, 2H), 8.56 (d, $J = 8.5$ Hz, 2H), 7.74 (d, $J = 8.5$ Hz, 2H), 7.24 (t, $J = 4.5$ Hz, 1H); ^{19}F NMR (CDCl_3 , 470 MHz): -62.7 (s, Ar-CF₃); ^{13}C NMR (CDCl_3 , 125 MHz): δ 163.5, 157.5, 140.9, 132.5 (q, $^2J_{\text{C-F}} = 32.5$ Hz), 128.6, 125.6 (q, $^3J_{\text{C-F}} = 3.75$ Hz), 124.3 (q, $^1J_{\text{C-F}} = 271.25$ Hz), 120.0. EI-MS m/z : 224 (100) [M^+], 171 (83), 155 (37), 121 (37).



2-(3-Fluorophenyl)pyrimidine (1h)¹: Following the general procedure with 2-chloropyrimidine (343.5 mg, 3.0 mmol), 3-fluorophenylboronic acid (504.0 mg, 3.6 mmol), Pd(PPh₃)₂Cl₂ (42.1 mg, 0.06 mmol), Na₂CO₃ (2 M, 10 mL) and dioxane (10 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 20/1) afforded **1h** (506.3 mg, 97%) as a white solid. M.p. 43-44 °C. IR (KBr, cm^{-1}): 3076, 1613, 1591, 1579, 1488, 1456, 1323, 818, 753. ^1H NMR (CDCl_3 , 500 MHz): δ 8.81 (d, $J = 5.0$ Hz, 2H), 8.24 (dt, $J = 7.5, 1.0$ Hz, 1H), 8.15 (dq, $J = 10.5, 1.5$ Hz, 1H), 7.47-7.43 (m, 1H), 7.21 (t, $J = 5.0$ Hz, 1H), 7.20-7.16 (m, 1H); ^{19}F NMR (CDCl_3 , 470 MHz): -113.1 (m, Ar-F); ^{13}C NMR (CDCl_3 , 125 MHz): δ 164.3, 163.7, 162.4 (d, $^1J_{\text{C-F}} = 242.8$ Hz), 157.4, 140.1, 130.2 (d, $^3J_{\text{C-F}} = 7.5$ Hz), 123.9 (d, $^4J_{\text{C-F}} = 2.6$ Hz), 119.7, 117.8 (d, $^2J_{\text{C-F}} = 21.25$ Hz), 115.2 (d, $^2J_{\text{C-F}} = 23.75$ Hz). EI-MS ($\text{C}_{10}\text{H}_7\text{FN}_2$) m/z (%): 174 (100) [M^+], 121 (75).

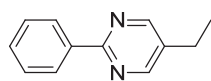


2-(3-Chlorophenyl)pyrimidine (1i)¹: Following the general procedure with 2-chloropyrimidine (343.5 mg, 3.0 mmol), 3-chlorophenylboronic acid (561.6 mg, 3.6 mmol), Pd(PPh₃)₂Cl₂ (42.1 mg, 0.06 mmol), Na₂CO₃ (2 M, 10 mL) and dioxane (10 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 20/1) afforded **1i** (461.7 mg, 81%) as a white solid. M.p. 52-54 °C. IR (KBr, cm^{-1}): 3068, 3030, 2954, 2854, 1565, 1549, 1419, 1406, 778. ^1H NMR (CDCl_3 , 500 MHz): δ 8.81 (d, $J = 5.0$ Hz, 2H), 8.45 (d, $J = 2.0$ Hz, 1H), 7.34-7.32 (m, 1H), 7.46-7.40 (m, 2H), 7.21 (t, $J = 5.0$ Hz, 1H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 163.4, 157.3, 139.3, 134.8, 130.7, 129.8, 128.3, 126.2, 119.5. EI-MS m/z (%): 192 (35) [M^+ (^{37}Cl)], 190 (100) [M^+ (^{35}Cl)], 139 (26), 137 (81), 102 (41).

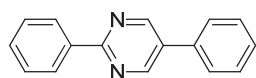


2,4-Diphenylpyrimidine (1j)¹: Following the general procedure with 2,4-dichloropyrimidine (447.0 mg, 3.0 mmol), phenylboronic acid (879.4 mg, 7.2 mmol), Pd(PPh₃)₂Cl₂ (42.1 mg, 0.06 mmol), Na₂CO₃ (2 M, 10 mL) and dioxane (10 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 20/1) afforded **1j** (584.6 mg, 81%) as a white solid. M.p. 70-72 °C. IR (KBr, cm^{-1}): 3032, 1561, 1542, 1423, 1379, 747, 688, 625. ^1H NMR (CDCl_3 , 500 MHz): δ 8.84 (d, $J = 5.5$ Hz, 1H), 8.62-8.59 (m, 2H), 8.25-8.23 (m, 2H), 7.60

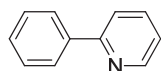
(d, $J = 5.0$ Hz, 1H), 7.56-7.52 (m, 6H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 164.7, 164.0, 158.0, 138.0, 137.1, 131.1, 130.8, 129.1, 128.7, 128.4, 127.3, 114.6. EI-MS m/z : 232 (100) [M^+], 129 (43), 102 (73).



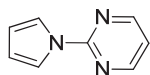
5-Ethyl-2-phenylpyrimidine (1k)¹: Following the general procedure with 2-chloro-5-ethylpyrimidine (427.5 mg, 3.0 mmol), phenylboronic acid (439.2 mg, 3.6 mmol), $\text{Pd}(\text{PPh}_3)_2\text{Cl}_2$ (42.1 mg, 0.06 mmol), Na_2CO_3 (2 M, 10 mL) and dioxane (10 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 20/1) afforded **1k** (518.8 mg, 94%) as a colorless oil. IR (KBr, cm^{-1}): 3063, 3029, 2968, 2932, 2874, 1586, 1544, 1430, 747, 694. ^1H NMR (CDCl_3 , 500 MHz): δ 8.65 (s, 2H), 8.42-8.40 (m, 2H), 7.50-7.46 (m, 3H), 2.68 (q, $J = 7.5$ Hz, 2H), 1.30 (t, $J = 7.5$ Hz, 3H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 162.6, 156.8, 137.5, 134.3, 130.5, 128.7, 128.0, 23.5, 15.1. EI-MS m/z : 184 (100) [M^+], 169 (74), 157 (18), 103 (61).



2,5-Diphenylpyrimidine (1l)²: Following the general procedure with 2,4-dichloropyrimidine (447.0 mg, 3.0 mmol), phenylboronic acid (439.2 mg, 3.6 mmol), $\text{Pd}(\text{PPh}_3)_2\text{Cl}_2$ (42.1 mg, 0.06 mmol), Na_2CO_3 (2 M, 10 mL) and dioxane (10 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 20/1) afforded **1l** (552 mg, 79%) as a white solid. M.p. 182-184 °C. IR (KBr, cm^{-1}): 3028, 1567, 1548, 1429, 694, 631. ^1H NMR (CDCl_3 , 500 MHz): δ 9.03 (s, 2H), 8.51-8.48 (m, 2H), 7.66-7.63 (m, 2H), 7.56-7.45 (m, 6H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 163.6, 155.4, 137.4, 134.7, 131.8, 130.9, 129.6, 128.9, 128.8, 128.3, 126.9. LC-MS (ESI) m/z : 233 [M^+H].

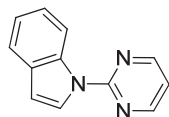


2-Phenylpyridine (1m)³: Following the general procedure with 2-bromopyridine (474.0 mg, 3.0 mmol), phenylboronic acid (439.2 mg, 3.6 mmol), $\text{Pd}(\text{PPh}_3)_2\text{Cl}_2$ (42.1 mg, 0.06 mmol), Na_2CO_3 (2 M, 10 mL) and dioxane (10 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 20/1) afforded **1m** (423.0 mg, 91%) as a colorless liquid. IR (KBr, cm^{-1}): 3060, 2961, 2853, 1651, 1523, 750, 710. ^1H NMR (CDCl_3 , 500 MHz): δ 8.73 (d, $J = 4.5$ Hz, 1H), 8.02 (d, $J = 8.0$ Hz, 2H), 7.81-7.75 (m, 2H), 7.70 (t, $J = 7.5$ Hz, 2H), 7.46-7.43 (m, 1H), 7.28-7.25 (m, 1H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 157.4, 149.5, 139.2, 137.1, 129.2, 128.9, 127.0, 122.2, 120.8. EI-MS m/z (%): 155 (100) [M^+], 128 (27), 102 (13).

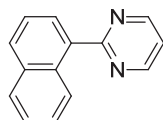


2-(1H-Pyrrol-1-yl)pyrimidine (1o)¹: NaH (60% dispersion in mineral oil, 440 mg, 11.0 mmol) was added in portions at 0 °C to a stirred solution of pyrrole (0.34 g, 5.0 mmol) in DMF (5 mL). After stirring for 30 min at 0 °C, 2-chloropyrimidine (0.69 g, 6.0 mmol) was added and the mixture was stirred at 130 °C for 24 h. Then, the reaction mixture was cooled to ambient temperature, poured into H_2O (25 mL) and extracted with EtOAc (2×30 mL). The combined organic phase was dried over Na_2SO_4 . After filtration and evaporation of the solvents under

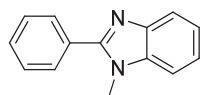
reduced pressure, the crude product was purified by column chromatography on silica gel (petroleum ether/EtOAc = 4/1) to yield **1o** (0.46 g, 64%) as a colorless solid. M.p. 88-91°C. IR (KBr, cm^{-1}): 3146, 2924, 1573, 1482, 1441, 1076, 1058, 1023, 927, 852, 804, 736. ^1H NMR (CDCl_3 , 500 MHz): δ 8.61 (d, $J = 5.0$ Hz, 2H), 7.79 (t, $J = 1.0$ Hz, 2H), 7.04 (t, $J = 5.0$ Hz, 1H), 6.35 (dd, $J = 2.0$ Hz, 1.0 Hz, 2H). ^{13}C NMR (CDCl_3 , 125 MHz): δ 158.4, 156.2, 119.1, 117.2, 112.1. LC-MS (ESI) m/z : 146 [M^+H].



1-(Pyrimidin-2-yl)-1H-indole (1p)¹: NaH (60% dispersion in mineral oil, 440 mg, 11.0 mmol) was added in portions at 0 °C to a stirred solution of indole (1.17 g, 10.0 mmol) in DMF (10 mL). After stirring for 30 min at 0 °C, 2-chloropyrimidine (1.37 g, 12.0 mmol) was added and the mixture was stirred at 130 °C for 24 h. Then, the reaction mixture was cooled to ambient temperature, poured into H_2O (50 mL) and extracted with EtOAc (4×30 mL). The combined organic phase was dried over Na_2SO_4 . After filtration and evaporation of the solvents under reduced pressure, the crude product was purified by column chromatography on silica gel (petroleum ether/EtOAc = 4/1) to yield **1p** (1.80 g, 92%) as a colorless solid. M.p. 66-68 °C. IR (KBr, cm^{-1}): 3138, 3108, 1575, 1525, 1455, 1309, 1204, 1080, 970, 778, 750, 733. ^1H NMR (500 MHz, CDCl_3): δ 8.83 (d, $J = 8.5$ Hz, 1H), 8.70 (d, $J = 4.5$ Hz, 2H), 8.29 (d, $J = 3.5$ Hz, 1H), 7.64 (d, $J = 8.0$ Hz, 1H), 7.38-7.35 (m, 1H), 7.27-7.24 (m, 1H), 7.05-7.02 (m, 1H), 6.72 (d, $J = 3.5$ Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3): δ 158.1, 157.8, 135.4, 131.4, 125.9, 123.7, 122.2, 120.9, 116.4, 116.1, 107.0. LC-MS (ESI) m/z : 196 [M^+H].



2-(Naphthalen-1-yl)pyrimidine (1q)¹: Following the general procedure with 2-chloropyrimidine (343.5 mg, 3.0 mmol), naphthalen-1-ylboronic acid (619.2 mg, 3.6 mmol), $\text{Pd}(\text{PPh}_3)_2\text{Cl}_2$ (42.1 mg, 0.06 mmol), Na_2CO_3 (2 M, 10 mL) and dioxane (10 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 20/1) afforded **1q** (531.5 mg, 86%) as a colorless oil. IR (KBr, cm^{-1}): 3044, 2966, 2925, 1567, 1554, 1419, 1390, 1254, 791, 774; ^1H NMR (CDCl_3 , 500 MHz): δ 8.95 (d, $J = 5.0$ Hz, 2H), 8.62 (d, $J = 8.0$ Hz, 1H), 8.07 (dd, $J = 7.5$, 1.0 Hz, 1H), 7.98 (d, $J = 8.0$ Hz, 1H), 7.92 (d, $J = 7.5$ Hz, 1H), 7.61-7.50 (m, 3H), 7.31 (t, $J = 5.0$ Hz, 1H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 167.2, 157.3, 135.7, 134.2, 131.0, 130.7, 129.5, 128.6, 127.0, 126.0, 125.7, 125.3, 118.9. EI-MS m/z : 206 (65) [M^+], 205 (100), 153 (19), 126 (14).

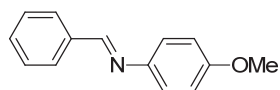


1-Methyl-2-phenyl-1H-benzo[d]imidazole (1r)⁴: NaH (60% dispersion in mineral oil, 440 mg, 11.0 mmol) was added in portions at 0 °C to a stirred solution of 2-phenyl-1H-benzo[d]imidazole (0.97 g, 5.0 mmol) in DMF (5 mL). After stirring for 30 min at 0 °C, iodomethane (0.85 g, 6.0 mmol) was added and the mixture was stirred at room temperature for 2 h. Then, the reaction mixture was poured into H_2O (25 mL) and extracted with EtOAc (2×30 mL). The combined organic phase was dried over Na_2SO_4 . After filtration and evaporation of the solvents under

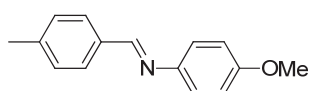
reduced pressure, the crude product was purified by column chromatography on silica gel (petroleum ether/EtOAc = 2/1) to yield **1r** (0.93 g, 89%) as a yellow solid. M.p. 90-92°C. IR (KBr, cm^{-1}): 3442, 2925, 1467, 1437, 1379, 753, 700. ^1H NMR (CDCl_3 , 500 MHz): δ 7.87-7.85 (m, 1H), 7.80-7.78 (m, 2H), 7.57-7.53 (m, 3H), 7.43-7.41 (m, 1H), 7.35-7.32 (m, 2H), 3.88 (s, 3H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 153.7, 142.9, 136.5, 130.2, 129.7, 129.4, 128.7, 122.8, 122.4, 119.8, 109.6, 31.7. LC-MS (ESI) m/z : 209 [M^+H].



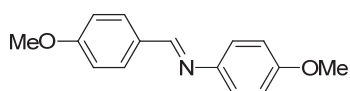
General Procedure for preparation of imines: A solution of aryl amines (7.5 mmol) and substituted benzaldehydes (5.0 mmol) in CH_2Cl_2 (20 mL) was added MgSO_4 (2.0 g), the reaction mixture was stirred at room temperature overnight. The reaction mixture was then filtrated and purified by column chromatography to give pure substituted imines (**3a-3k**).



(E)-N-Benzylidene-4-methoxyaniline (3a)⁵: Following the general procedure with 4-methoxyaniline (0.92 g, 7.5 mmol), benzaldehyde (0.53g, 5.0 mmol), MgSO_4 (2.0 g) and CH_2Cl_2 (20 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether) afforded **3a** (886.2 mg, 84%) as a white solid. M.p. 67-68 °C. IR (KBr, cm^{-1}): 2954, 1622, 1505, 1247, 1030, 834, 753, 687. ^1H NMR (CDCl_3 , 500 MHz): δ 8.51 (s, 1H), 7.93-7.91 (m, 2H), 7.50-7.48 (m, 3H), 7.28 (d, $J = 9.0$ Hz, 2H), 6.97 (d, $J = 9.0$ Hz, 2H), 3.86 (s, 3H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 158.4, 158.3, 144.8, 136.4, 131.0, 128.7, 128.6, 122.2, 114.4, 55.5. EI-MS m/z (%): 211 (89) [M^+], 196 (100), 167 (21).

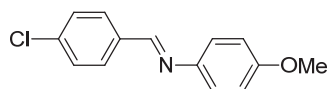


(E)-4-Methoxy-N-(4-methylbenzylidene)aniline (3b)⁵: Following the general procedure with 4-methoxyaniline (0.92 g, 7.5 mmol), 4-methylbenzaldehyde (0.60g, 5.0 mmol), MgSO_4 (2.0 g) and CH_2Cl_2 (20 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether) afforded **3b** (870.1 mg, 77%) as a white solid. M.p. 85-86 °C. IR (KBr, cm^{-1}): 2911, 1623, 1502, 1240, 1031, 836, 816. ^1H NMR (CDCl_3 , 500 MHz): δ 8.47 (s, 1H), 7.81 (d, $J = 8.0$ Hz, 2H), 7.29 (d, $J = 8.0$ Hz, 2H), 7.26 (d, $J = 9.0$ Hz, 2H), 6.96 (d, $J = 9.0$ Hz, 2H), 3.86 (s, 3H), 2.44 (s, 3H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 158.4, 158.1, 145.0, 141.5, 133.8, 129.5, 128.6, 122.1, 114.3, 55.5, 21.6. EI-MS m/z (%): 225 (100) [M^+], 210 (92), 167 (11).

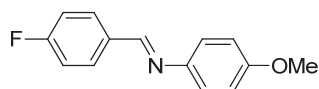


(E)-4-Methoxy-N-(4-methoxybenzylidene)aniline (3c)⁶: Following the general procedure with 4-methoxyaniline (0.92 g, 7.5 mmol), 4-methoxybenzaldehyde (0.68g, 5.0 mmol), MgSO_4 (2.0 g)

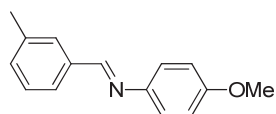
and CH₂Cl₂ (20 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether) afforded **3c** (980.1 mg, 81%) as a white solid. M.p. 142-143 °C. IR (KBr, cm⁻¹): 2959, 1621, 1509, 1249, 1028, 839, 742. ¹H NMR (CDCl₃, 500 MHz): δ 8.43 (s, 1H), 7.87 (d, *J* = 8.5 Hz, 2H), 7.24 (d, *J* = 9.0 Hz, 2H), 7.00 (d, *J* = 9.0 Hz, 2H), 6.95 (d, *J* = 9.0 Hz, 2H), 3.89 (s, 3H), 3.85 (s, 3H); ¹³C NMR (CDCl₃, 125 MHz): δ 162.0, 158.0, 157.9, 130.3, 122.0, 114.3, 114.1, 55.5, 55.4. EI-MS *m/z* (%): 241 (77) [M⁺], 229 (83), 214 (99), 185 (22), 144 (14).



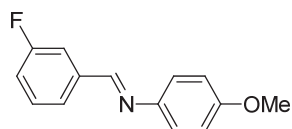
(E)-N-(4-Chlorobenzylidene)-4-methoxyaniline (3d)⁵: Following the general procedure with 4-methoxyaniline (0.92 g, 7.5 mmol), 4-chlorobenzaldehyde (0.70g, 5.0 mmol), MgSO₄ (2.0 g) and CH₂Cl₂ (20 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether) afforded **3d** (1131.6 mg, 92%) as a yellow solid. M.p. 122-124 °C. IR (KBr, cm⁻¹): 2961, 1620, 1505, 1254, 1029, 838, 821. ¹H NMR (CDCl₃, 500 MHz): δ 8.46 (s, 1H), 7.85 (d, *J* = 8.5 Hz, 2H), 7.45 (d, *J* = 9.0 Hz, 2H), 7.26 (d, *J* = 9.0 Hz, 2H), 6.96 (d, *J* = 9.0 Hz, 2H), 3.85 (s, 3H); ¹³C NMR (CDCl₃, 125 MHz): δ 158.5, 156.7, 144.4, 136.9, 134.9, 129.7, 129.0, 122.2, 114.4, 55.5. EI-MS *m/z*: 247 (31) [M⁺ (³⁷Cl)], 245 (100) [M⁺ (³⁵Cl)], 230 (96), 167 (15).



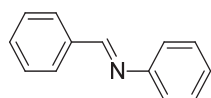
(E)-N-(4-fluorobenzylidene)-4-methoxyaniline (3e)⁷: Following the general procedure with 4-methoxyaniline (0.92 g, 7.5 mmol), 4-fluorobenzaldehyde (0.62g, 5.0 mmol), MgSO₄ (2.0 g) and CH₂Cl₂ (20 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether) afforded **3e** (874.0 mg, 76%) as a white solid. M.p. 96- 97 °C. IR (KBr, cm⁻¹): 2966, 1623, 1506, 1252, 1029, 844, 748. ¹H NMR (CDCl₃, 500 MHz): δ 8.46 (s, 1H), 7.92-7.89 (m, 2H), 7.26-7.24 (m, 2H), 7.19-7.15 (m, 2H), 6.97-6.95 (m, 2H), 3.85 (s, 3H); ¹⁹F NMR (CDCl₃, 470 MHz): -108.6 (m, Ar-F); ¹³C NMR (CDCl₃, 125 MHz): δ 164.5 (d, ¹*J*_{C-F} = 250.0 Hz), 158.3, 156.8, 144.6, 132.8 (d, ⁴*J*_{C-F} = 2.8 Hz), 130.5 (d, ³*J*_{C-F} = 8.8 Hz), 122.1, 115.8 (d, ²*J*_{C-F} = 21.8 Hz), 114.4, 55.5. EI-MS *m/z* (%): 229 (87) [M⁺], 214 (100), 185 (22), 144 (6).



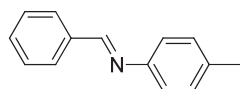
(E)-4-Methoxy-N-(3-methylbenzylidene)aniline (3f)⁸: Following the general procedure with 4-methoxyaniline (0.92 g, 7.5 mmol), 3-methylbenzaldehyde (0.60 g, 5.0 mmol), MgSO₄ (2.0 g) and CH₂Cl₂ (20 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether) afforded **3f** (858.8 mg, 76%) as a white solid. M.p. 39-41 °C. IR (KBr, cm⁻¹): 2952, 1624, 1504, 1245, 1035, 831, 788. ¹H NMR (CDCl₃, 500 MHz): δ 8.48 (s, 1H), 7.78 (s, 1H), 7.68 (d, *J* = 7.5 Hz, 1H), 7.38 (t, *J* = 7.5 Hz, 1H), 7.31 (d, *J* = 7.5 Hz, 1H), 7.28-7.25 (m, 2H), 6.96 (d, *J* = 9.0 Hz, 2H), 3.86 (s, 3H), 2.45 (s, 3H); ¹³C NMR (CDCl₃, 125 MHz): δ 158.7, 158.2, 144.9, 138.5, 136.3, 131.9, 128.7, 128.6, 126.2, 122.2, 114.4, 55.5, 21.3. EI-MS *m/z* (%): 225 (100) [M⁺], 210 (32), 167 (9).



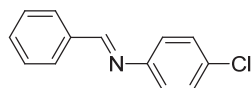
(E)-N-(3-Fluorobenzylidene)-4-methoxyaniline (3g)⁵: Following the general procedure with 4-methoxyaniline (0.92 g, 7.5 mmol), 3-fluorobenzaldehyde (0.62g, 5.0 mmol), MgSO₄ (2.0 g) and CH₂Cl₂ (20 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether) afforded **3g** (713.0 mg, 62%) as a colorless oil. IR (KBr, cm⁻¹): 2961, 1621, 1504, 1249, 1028, 837, 779, 682. ¹H NMR (CDCl₃, 500 MHz): δ 8.48 (d, *J* = 1.0 Hz, 1H), 7.69-7.67 (m, 1H), 7.64 (d, *J* = 8.5 Hz, 1H), 7.47-7.42 (m, 1H), 7.28-7.27 (m, 2H), 7.20-7.16 (m, 1H), 6.97-6.96 (m, 2H), 3.86 (s, 3H); ¹⁹F NMR (CDCl₃, 470 MHz): -112.6 (m, Ar-F); ¹³C NMR (CDCl₃, 125 MHz): δ 163.1 (d, ¹*J*_{C-F} = 245.1 Hz), 158.6, 156.6 (d, ⁴*J*_{C-F} = 3.1 Hz), 144.2, 138.8 (d, ³*J*_{C-F} = 7.3 Hz), 130.2 (d, ³*J*_{C-F} = 8.1 Hz), 124.7 (d, ⁴*J*_{C-F} = 2.6 Hz), 122.3, 117.9 (d, ²*J*_{C-F} = 21.6 Hz), 114.5 (d, ²*J*_{C-F} = 21.3 Hz), 114.4, 55.5. EI-MS *m/z* (%): 229 (90) [M⁺], 214 (100), 185 (23).



(E)-N-Benzylideneaniline (3h)⁶: Following the general procedure with aniline (0.70 g, 7.5 mmol), benzaldehyde (0.53 g, 5.0 mmol), MgSO₄ (2.0 g) and CH₂Cl₂ (20 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether) afforded **1h** (734.4 mg, 81%) as a white solid. M.p. 54-55 °C. IR (KBr, cm⁻¹): 2888, 1626, 1590, 1483, 1192, 762, 693. ¹H NMR (CDCl₃, 500 MHz): δ 8.50 (s, 1H), 7.96-7.94 (m, 2H), 7.53-7.50 (m, 3H), 7.46-7.42 (m, 2H), 7.28-7.25 (m, 3H); ¹³C NMR (CDCl₃, 125 MHz): δ 160.4, 152.0, 136.2, 131.4, 129.1, 128.8, 128.7, 125.9, 120.9. EI-MS *m/z* (%): 181 (100) [M⁺], 152 (4), 104 (10), 77 (34).

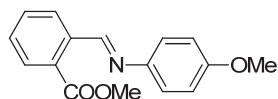


(E)-N-benzylidene-4-methylaniline (3i)⁹: Following the general procedure with *p*-toluidine (0.80 g, 7.5 mmol), benzaldehyde (0.53 g, 5.0 mmol), MgSO₄ (2.0 g) and CH₂Cl₂ (20 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether) afforded **3i** (895.5 mg, 92%) as a white solid. M.p. 33-35 °C. IR (KBr, cm⁻¹): 3024, 2919, 2873, 1627, 1504, 1191, 814, 691, 536. ¹H NMR (CDCl₃, 500 MHz): δ 8.51 (s, 1H), 7.95-7.93 (m, 2H), 7.52-7.49 (m, 3H), 7.24 (d, *J* = 8.5 Hz, 2H), 7.19 (d, *J* = 8.5 Hz, 2H), 2.41 (s, 3H); ¹³C NMR (CDCl₃, 125 MHz): δ 159.6, 149.4, 136.3, 135.8, 131.2, 129.8, 128.8, 128.7, 120.8, 21.0. EI-MS *m/z* (%): 195 (100) [M⁺], 180 (4), 118 (8), 91 (24), 65 (10).



(E)-N-benzylidene-4-chloroaniline (3j)⁶: Following the general procedure with 4-chloroaniline (0.96 g, 7.5 mmol), benzaldehyde (0.53 g, 5.0 mmol), MgSO₄ (2.0 g) and CH₂Cl₂ (20 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether) afforded **3j** (777.6 mg, 78%) as a yellow solid. M.p. 61-62 °C. IR (KBr, cm⁻¹): 2873, 1625, 1483, 1190, 1088, 831, 820, 756, 689. ¹H NMR (CDCl₃, 500 MHz): δ 8.46 (s, 1H), 7.93 (dd, *J* = 7.5, 1.5 Hz,

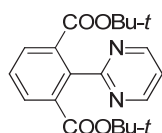
2H), 7.52-7.49 (m, 3H), 7.39-7.37 (m, 2H), 7.20-7.17 (m, 2H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 160.7, 150.4, 135.9, 131.6, 131.5, 129.2, 128.9, 128.8, 122.2. EI-MS m/z : 217 (36) [M^+ (^{37}Cl)], 215 (100) [M^+ (^{35}Cl)], 138 (10), 111 (26), 77 (16).



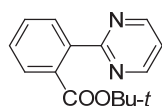
(E)-Methyl 2-(((4-methoxyphenyl)imino)methyl)benzoate (3k)¹⁰: Following the general procedure with 4-methoxyaniline (0.92 g, 7.5 mmol), methyl 2-formylbenzoate (0.82 g, 5.0 mmol), MgSO_4 (2.0 g) and CH_2Cl_2 (20 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether) afforded **3k** (511.1 mg, 38%) as a yellow solid. M.p. 59-60 °C. IR (KBr, cm^{-1}): 3411, 2952, 1713, 1500, 1253, 1120, 841, 761, 706. ^1H NMR (CDCl_3 , 500 MHz): δ 9.26 (s, 1H), 8.27 (dd, $J = 8.0, 1.0$ Hz, 1H), 7.99 (dd, $J = 8.0, 1.0$ Hz, 1H), 7.63 (td, $J = 7.5, 1.0$ Hz, 1H), 7.52 (dd, $J = 7.5, 1.0$ Hz, 1H), 7.34-7.31 (m, 2H), 6.97-6.94 (m, 2H), 3.96 (s, 3H), 3.85 (s, 3H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 167.4, 158.5, 157.6, 144.8, 137.4, 132.3, 130.3, 130.0, 128.3, 122.6, 114.3, 55.5, 52.4. EI-MS m/z (%): 269 (28) [M^+], 254 (100), 238 (13), 166 (15), 105 (14).

3. Synthesis and Characterization for *tert*-Butoxycarbonylation Products

General Procedure for *tert*-Butoxycarbonylation: To a 15 mL flask was added substrates (0.5 mmol), $[\text{RuCl}_2(p\text{-cymene})]_2$ (7.7 mg, 0.0125 mmol), 1-AdCOOH (27.0 mg, 0.15 mmol), K_2CO_3 (172.5 mg, 1.25 mmol), Boc_2O (272.5 mg, 1.25 mmol) and toluene (1.25 mL). The reaction mixture was stirred at 120 °C under N_2 atmosphere. Upon completion, the reaction was purified by column chromatography to give the esterification product.

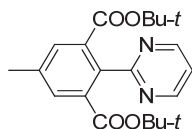


Di-*tert*-butyl 2-(pyrimidin-2-yl)isophthalate (2a): Following the general procedure with **1a** (78.0 mg, 0.5 mmol), $[\text{RuCl}_2(p\text{-cymene})]_2$ (7.7 mg, 0.0125 mmol), 1-AdCOOH (27.0 mg, 0.15 mmol), K_2CO_3 (172.5 mg, 1.25 mmol), Boc_2O (272.5 mg, 1.25 mmol) and toluene (1.25 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10/1) afforded **2a** (147.7 mg, 83%) as a gray white solid. M.p. 158-159 °C. IR (KBr, cm^{-1}): 2977, 1712, 1557, 1409, 1321, 1141, 854, 775. ^1H NMR (CDCl_3 , 500 MHz): δ 8.81 (d, $J = 5.0$ Hz, 2H), 7.99 (d, $J = 8.0$ Hz, 2H), 7.54 (t, $J = 8.0$ Hz, 1H), 7.32 (t, $J = 5.0$ Hz, 1H), 1.30 (s, 18H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 167.4, 166.1, 156.3, 139.1, 133.7, 132.4, 128.4, 119.1, 81.5, 27.7. EI-MS m/z (%): 356 (14) [M^+], 300 (38), 245 (79), 227 (95), 156 (100). Anal. Calcd. For $\text{C}_{20}\text{H}_{24}\text{N}_2\text{O}_4$: C, 67.40; H, 6.79; N, 7.86. Found: C, 67.37; H, 6.68; N, 7.85.

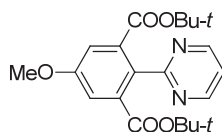


***tert*-Butyl 2-(pyrimidin-2-yl)benzoate (2a')**: IR (KBr, cm^{-1}): 2975, 1717, 1562, 1416, 1299, 1123,

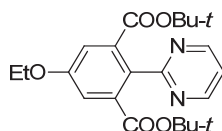
754. ¹H NMR (CDCl₃, 500 MHz): δ 8.85 (d, *J* = 5.0 Hz, 2H), 7.92 (d, *J* = 7.5 Hz, 1H), 7.76 (d, *J* = 7.5 Hz, 1H), 7.58 (td, *J* = 7.5, 1.0 Hz, 1H), 7.52 (td, *J* = 7.5, 1.0 Hz, 1H), 7.30 (t, *J* = 5.0 Hz, 1H), 1.44 (s, 9H); ¹³C NMR (CDCl₃, 125 MHz): δ 168.0, 166.3, 156.8, 138.0, 134.3, 130.4, 129.9, 129.4, 129.1, 119.0, 81.3, 27.8. LC-MS (ESI) *m/z*: 257 [M⁺H]. HRMS: *m/z* calcd for C₁₅H₁₆N₂O₂ [M+H]⁺ 257.1290, Found: 257.1278.



Di-tert-butyl 5-methyl-2-(pyrimidin-2-yl)isophthalate (2b): Following the general procedure with **1b** (85.0 mg, 0.5 mmol), [RuCl₂(*p*-cymene)]₂ (7.7 mg, 0.0125 mmol), 1-AdCOOH (27.0 mg, 0.15 mmol), K₂CO₃ (172.5 mg, 1.25 mmol), Boc₂O (272.5 mg, 1.25 mmol) and toluene (1.25 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10/1) afforded **2b** (175.8 mg, 95%) as a gray white solid. M.p. 157-158 °C. IR (KBr, cm⁻¹): 2984, 1710, 1561, 1410, 1338, 1266, 1155, 846. ¹H NMR (CDCl₃, 500 MHz): δ 8.81 (d, *J* = 5.0 Hz, 2H), 7.78 (s, 2H), 7.30 (t, *J* = 5.0 Hz, 1H), 2.47 (s, 3H), 1.30 (s, 18H); ¹³C NMR (CDCl₃, 125 MHz): δ 167.4, 166.4, 156.3, 138.6, 136.3, 133.6, 132.8, 118.9, 81.4, 27.7, 21.0. LC-MS (ESI) *m/z*: 371 [M⁺H]. HRMS: *m/z* calcd for C₂₁H₂₆N₂O₄ [M⁺H] 371.1971, Found: 371.1963.

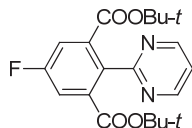


Di-tert-butyl 5-methoxy-2-(pyrimidin-2-yl)isophthalate (2c): Following the general procedure with **1c** (93.0 mg, 0.5 mmol), [RuCl₂(*p*-cymene)]₂ (7.7 mg, 0.0125 mmol), 1-AdCOOH (27.0 mg, 0.15 mmol), K₂CO₃ (172.5 mg, 1.25 mmol), Boc₂O (272.5 mg, 1.25 mmol) and toluene (1.25 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10/1) afforded **2c** (158.3 mg, 82%) as a gray white solid. M.p. 179-180 °C. IR (KBr, cm⁻¹): 2980, 1709, 1567, 1408, 1347, 1268, 1158, 1062, 846. ¹H NMR (CDCl₃, 500 MHz): δ 8.78 (d, *J* = 5.0 Hz, 2H), 7.45 (s, 2H), 7.27 (t, *J* = 5.0 Hz, 1H), 3.89 (s, 3H), 1.27 (s, 18H); ¹³C NMR (CDCl₃, 125 MHz): δ 167.1, 166.1, 159.2, 156.3, 135.2, 131.5, 118.9, 117.6, 81.6, 55.8, 27.7. EI-MS *m/z* (%): 386 (22) [M⁺], 286 (22), 257 (25), 186 (100), 83 (20). HRMS: *m/z* calcd for C₂₁H₂₆N₂O₅ [M⁺] 386.1842, Found: 386.1844.

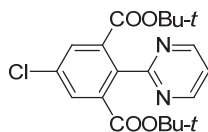


Di-tert-butyl 5-ethoxy-2-(pyrimidin-2-yl)isophthalate (2d): Following the general procedure with **1d** (100.0 mg, 0.5 mmol), [RuCl₂(*p*-cymene)]₂ (7.7 mg, 0.0125 mmol), 1-AdCOOH (27.0 mg, 0.15 mmol), K₂CO₃ (172.5 mg, 1.25 mmol), Boc₂O (272.5 mg, 1.25 mmol) and toluene (1.25 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10/1) afforded **2d** (182.0 mg, 91%) as a gray white solid. M.p. 103-104 °C. IR (KBr, cm⁻¹): 2977, 1724, 1564, 1410, 1341, 1258, 1158, 837. ¹H NMR (CDCl₃, 500 MHz): δ 8.78

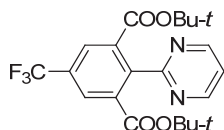
(d, $J = 5.0$ Hz, 2H), 7.46 (s, 2H), 7.29 (t, $J = 5.0$ Hz, 1H), 4.16 (q, $J = 6.0$ Hz, 2H), 1.46 (t, $J = 6.0$ Hz, 3H), 1.29 (s, 18H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 167.2, 166.1, 158.5, 156.3, 135.2, 131.4, 118.8, 118.1, 81.6, 64.1, 27.7, 14.6. LC-MS (ESI) m/z : 401 [M^+H]. HRMS: m/z calcd for $\text{C}_{22}\text{H}_{28}\text{N}_2\text{O}_5$ [M^+H] 401.2076, Found: 401.2070.



Di-tert-butyl 5-fluoro-2-(pyrimidin-2-yl)isophthalate (2e): Following the general procedure with **1e** (87.0 mg, 0.5 mmol), $[\text{RuCl}_2(p\text{-cymene})]_2$ (7.7 mg, 0.0125 mmol), 1-AdCOOH (27.0 mg, 0.15 mmol), K_2CO_3 (172.5 mg, 1.25 mmol), Boc_2O (272.5 mg, 1.25 mmol) and toluene (1.25 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10/1) afforded **2e** (179.5 mg, 96%) as a gray white solid. M.p. 116-117 °C. IR (KBr, cm^{-1}): 2986, 1715, 1561, 1411, 1344, 1258, 1157, 976, 842. ^1H NMR (CDCl_3 , 500 MHz): δ 8.80 (dd, $J = 5.0, 1.0$ Hz, 2H), 7.68 (dd, $J = 8.5, 1.5$ Hz, 2H), 7.33 (td, $J = 5.0, 1.0$ Hz, 1H), 1.32 (s, 18H); ^{19}F NMR (CDCl_3 , 470 MHz): -111.4 (m, Ar-F); ^{13}C NMR (CDCl_3 , 125 MHz): δ 166.5, 164.8 (d, $^4J_{\text{C-F}} = 2.5$ Hz), 161.7 (d, $^1J_{\text{C-F}} = 250.0$ Hz), 156.4, 135.9 (d, $^3J_{\text{C-F}} = 7.5$ Hz), 135.4 (d, $^4J_{\text{C-F}} = 2.5$ Hz), 119.4 (d, $^2J_{\text{C-F}} = 22.5$ Hz), 119.2, 82.2, 27.6. LC-MS (ESI) m/z : 375 [M^+H]. HRMS: m/z calcd for $\text{C}_{20}\text{H}_{23}\text{FN}_2\text{O}_4$ [M^+H] 375.1720, Found: 375.1713.

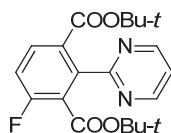


Di-tert-butyl 5-chloro-2-(pyrimidin-2-yl)isophthalate (2f): Following the general procedure with **1f** (95.3 mg, 0.5 mmol), $[\text{RuCl}_2(p\text{-cymene})]_2$ (7.7 mg, 0.0125 mmol), 1-AdCOOH (27.0 mg, 0.15 mmol), K_2CO_3 (172.5 mg, 1.25 mmol), Boc_2O (272.5 mg, 1.25 mmol) and toluene (1.25 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10/1) afforded **2f** (175.7 mg, 90%) as a gray white solid. M.p. 149-152 °C. IR (KBr, cm^{-1}): 2983, 1713, 1567, 1406, 1254, 1150, 891. ^1H NMR (CDCl_3 , 500 MHz): δ 8.78 (d, $J = 5.0$ Hz, 2H), 7.91 (s, 2H), 7.30 (t, $J = 5.0$ Hz, 1H), 1.28 (s, 18H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 166.4, 164.9, 156.4, 137.4, 135.3, 134.5, 132.1, 119.3, 82.3, 27.6. EI-MS m/z (%): 392 (0.49) [M^+ (^{37}Cl)], 390 (0.68) [M^+ (^{35}Cl)], 317 (9), 290 (17), 261 (51), 190 (100). HRMS: m/z calcd for $\text{C}_{20}\text{H}_{23}\text{ClN}_2\text{O}_4$ [M^+] 390.1346, Found: 390.1350.

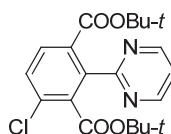


Di-tert-butyl 2-(pyrimidin-2-yl)-5-(trifluoromethyl)isophthalate (2g): Following the general procedure with **1g** (112.0 mg, 0.5 mmol), $[\text{RuCl}_2(p\text{-cymene})]_2$ (7.7 mg, 0.0125 mmol), 1-AdCOOH (27.0 mg, 0.15 mmol), K_2CO_3 (172.5 mg, 1.25 mmol), Boc_2O (272.5 mg, 1.25 mmol) and toluene (1.25 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10/1) afforded **2g** (152.6 mg, 72%) as a gray white solid. M.p. 143-144 °C. IR (KBr, cm^{-1}): 2982, 1726, 1563, 1370, 1275, 1162. ^1H NMR (CDCl_3 , 500 MHz): δ

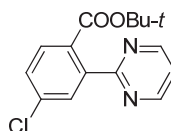
8.83 (d, $J = 5.0$ Hz, 2H), 8.22 (d, $J = 0.5$ Hz, 2H), 7.37 (t, $J = 5.0$ Hz, 1H), 1.33 (s, 18H); ^{19}F NMR (CDCl_3 , 470 MHz): -62.8 (s, Ar- CF_3); ^{13}C NMR (CDCl_3 , 125 MHz): δ 166.2, 164.8, 156.5, 142.0, 134.7, 130.9 (q, $^2J_{\text{C-F}} = 32.5$ Hz), 129.1 (q, $^3J_{\text{C-F}} = 3.3$ Hz), 123.1 (q, $^1J_{\text{C-F}} = 271.2$ Hz), 119.5, 82.5, 27.6. LC-MS (ESI) m/z : 425 [M^+H]. HRMS: m/z calcd for $\text{C}_{21}\text{H}_{23}\text{F}_3\text{N}_2\text{O}_4$ [M^+H] 425.1688, Found: 425.1681.



Di-tert-butyl 4-fluoro-2-(pyrimidin-2-yl)isophthalate (2h): Following the general procedure with **1h** (87.0 mg, 0.5 mmol), $[\text{RuCl}_2(p\text{-cymene})]_2$ (7.7 mg, 0.0125 mmol), 1-AdCOOH (27.0 mg, 0.15 mmol), K_2CO_3 (172.5 mg, 1.25 mmol), Boc_2O (272.5 mg, 1.25 mmol) and toluene (1.25 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10/1) afforded **2h** (132.7 mg, 71%) as a gray white solid. M.p. 119-120 °C. IR (KBr, cm^{-1}): 2984, 1724, 1562, 1449, 1397, 1318, 1249, 1160, 1113, 848. ^1H NMR (CDCl_3 , 500 MHz): δ 8.82 (d, $J = 5.0$ Hz, 2H), 7.94 (dd, $J = 8.5, 5.5$ Hz, 1H), 7.33 (t, $J = 5.0$ Hz, 1H), 7.24 (t, $J = 9.0$ Hz, 1H), 1.40 (s, 9H), 1.30 (s, 9H); ^{19}F NMR (CDCl_3 , 470 MHz): -110.4 (m, Ar-F); ^{13}C NMR (CDCl_3 , 125 MHz): δ 166.5 (d, $^3J_{\text{C-F}} = 7.5$ Hz), 163.0, 161.0 (d, $^1J_{\text{C-F}} = 250.0$ Hz), 156.5, 139.9 (d, $^4J_{\text{C-F}} = 3.7$ Hz), 133.0 (d, $^3J_{\text{C-F}} = 9.3$ Hz), 129.6 (d, $^4J_{\text{C-F}} = 3.7$ Hz), 124.2 (d, $^2J_{\text{C-F}} = 17.6$ Hz), 119.5, 116.4 (d, $^2J_{\text{C-F}} = 22.3$ Hz), 82.7, 81.6, 27.8, 27.7. LC-MS (ESI) m/z : 375 [M^+H]. HRMS: m/z calcd for $\text{C}_{20}\text{H}_{23}\text{FN}_2\text{O}_4$ [M^+H] 375.1720, Found: 375.1711.

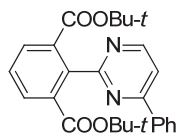


Di-tert-butyl 4-chloro-2-(pyrimidin-2-yl)isophthalate (2i): Following the general procedure with **1i** (95.0 mg, 0.5 mmol), $[\text{RuCl}_2(p\text{-cymene})]_2$ (7.7 mg, 0.0125 mmol), 1-AdCOOH (27.0 mg, 0.15 mmol), K_2CO_3 (172.5 mg, 1.25 mmol), Boc_2O (272.5 mg, 1.25 mmol) and toluene (1.25 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10/1) afforded **2i'** (8.7 mg, 6%) as colorless oil and **2i** (83.8 mg, 43%) as a gray white solid. M.p. 93-94 °C. IR (KBr, cm^{-1}): 2979, 1712, 1563, 1394, 1313, 1252, 1131, 848. ^1H NMR (CDCl_3 , 500 MHz): δ 8.79 (d, $J = 5.0$ Hz, 2H), 7.82 (d, $J = 8.0$ Hz, 1H), 7.52 (d, $J = 8.0$ Hz, 1H), 7.30 (t, $J = 5.0$ Hz, 1H), 1.40 (s, 9H), 1.28 (s, 9H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 165.5, 165.4, 164.5, 156.6, 138.6, 135.2, 134.1, 132.2, 131.2, 130.0, 119.5, 82.9, 81.8, 27.8, 27.6. LC-MS (ESI) m/z : 391 [M^+H]. HRMS: m/z calcd for $\text{C}_{20}\text{H}_{23}\text{ClN}_2\text{O}_4$ [M^+H] 391.1425, Found: 391.1418.

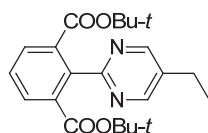


tert-Butyl 4-chloro-2-(pyrimidin-2-yl)benzoate (2i'): IR (KBr, cm^{-1}): 2925, 1720, 1560, 1424, 1301, 1173, 1123, 822. ^1H NMR (CDCl_3 , 500 MHz): δ 8.84 (d, $J = 5.0$ Hz, 2H), 7.92 (d, $J = 2.0$ Hz, 1H), 7.69 (d, $J = 8.0$ Hz, 1H), 7.49 (dd, $J = 8.5, 2.0$ Hz, 1H), 7.30 (t, $J = 5.0$ Hz, 1H), 1.42 (s, 9H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 167.1, 165.2, 156.9, 139.7, 136.5, 132.6, 130.6, 130.0, 129.4,

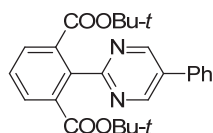
119.4, 81.6, 27.8. LC-MS (ESI) m/z : 291 [M^+H]. HRMS: m/z calcd for $C_{15}H_{15}ClN_2O_2$ [M^+H] 291.0900, Found: 291.0890.



Di-tert-butyl 2-(4-phenylpyrimidin-2-yl)isophthalate (2j): Following the general procedure with **1j** (166.0 mg, 0.5 mmol), $[RuCl_2(p\text{-cymene})]_2$ (7.7 mg, 0.0125 mmol), 1-AdCOOH (27.0 mg, 0.15 mmol), K_2CO_3 (172.5 mg, 1.25 mmol), Boc_2O (272.5 mg, 1.25 mmol) and toluene (1.25 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10/1) afforded **2j** (179.3 mg, 83%) as a gray white solid. M.p. 152-153 °C. IR (KBr, cm^{-1}): 2979, 1711, 1568, 1425, 1369, 1285, 1138, 859, 774. 1H NMR ($CDCl_3$, 500 MHz): δ 8.83 (d, $J = 5.0$ Hz, 1H), 8.13-8.11 (m, 2H), 7.99 (d, $J = 7.5$ Hz, 2H), 7.73 (d, $J = 5.0$ Hz, 1H), 7.54 (d, $J = 8.0$ Hz, 1H), 7.49-7.46 (m, 3H), 1.22 (s, 18H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 167.3, 166.3, 163.7, 156.7, 139.2, 136.3, 133.8, 132.4, 131.0, 128.9, 128.4, 127.3, 114.9, 81.5, 27.7. EI-MS m/z (%): 432 (9) [M^+], 332 (39), 276 (29), 232 (100), 129 (27). HRMS: m/z calcd for $C_{26}H_{28}N_2O_4$ [M^+] 432.2049, Found: 432.2050.

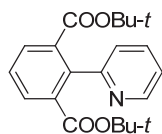


Di-tert-butyl 2-(5-ethylpyrimidin-2-yl)isophthalate (2k): Following the general procedure with **1k** (92.0 mg, 0.5 mmol), $[RuCl_2(p\text{-cymene})]_2$ (7.7 mg, 0.0125 mmol), 1-AdCOOH (27.0 mg, 0.15 mmol), K_2CO_3 (172.5 mg, 1.25 mmol), Boc_2O (272.5 mg, 1.25 mmol) and toluene (1.25 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10/1) afforded **2k** (165.1 mg, 86%) as a gray white solid. M.p. 146-147 °C. IR (KBr, cm^{-1}): 2978, 1719, 1319, 1286, 1140, 768. 1H NMR ($CDCl_3$, 500 MHz): δ 8.66 (s, 2H), 7.97 (d, $J = 7.5$ Hz, 2H), 7.53 (t, $J = 7.5$ Hz, 1H), 2.76 (q, $J = 8.0$ Hz, 2H), 1.37 (t, $J = 8.0$ Hz, 3H), 1.30 (s, 18H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 166.2, 164.7, 155.8, 138.8, 134.2, 133.8, 132.3, 128.3, 81.4, 27.7, 23.5, 15.1. LC-MS (ESI) m/z : 385 [M^+H]. HRMS: m/z calcd for $C_{22}H_{28}N_2O_4$ [$M+H$] $^+$ 385.2127, Found: 385.2120.

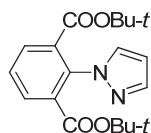


Di-tert-butyl 2-(5-phenylpyrimidin-2-yl)isophthalate (2l): Following the general procedure with **1l** (116.0 mg, 0.5 mmol), $[RuCl_2(p\text{-cymene})]_2$ (7.7 mg, 0.0125 mmol), 1-AdCOOH (27.0 mg, 0.15 mmol), K_2CO_3 (172.5 mg, 1.25 mmol), Boc_2O (272.5 mg, 1.25 mmol) and toluene (1.25 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10/1) afforded **2l** (140.4 mg, 65%) as a gray white solid. M.p. 184-185 °C. IR (KBr, cm^{-1}): 2977, 1717, 1420, 1264, 1140, 762. 1H NMR ($CDCl_3$, 500 MHz): δ 9.03 (s, 2H), 8.02 (d, $J = 8.0$ Hz, 2H), 7.69-7.67 (m, 2H), 7.59-7.50 (m, 4H), 1.32 (s, 18H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 166.1, 165.9, 154.3, 138.7, 134.4, 133.8, 132.5, 132.0, 129.5, 128.9, 128.5, 127.0, 81.7, 27.7. LC-MS (ESI) m/z : 433 [M^+H]. HRMS: m/z calcd for $C_{25}H_{28}N_2O_4$ [M^+H] 433.2127, Found:

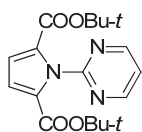
433.2118.



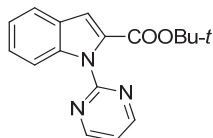
Di-tert-butyl 2-(pyridin-2-yl)isophthalate (2m): Following the general procedure with **1m** (77.5 mg, 0.5 mmol), $[\text{RuCl}_2(p\text{-cymene})]_2$ (7.7 mg, 0.0125 mmol), 1-AdCOOH (27.0 mg, 0.15 mmol), K_2CO_3 (172.5 mg, 1.25 mmol), Boc_2O (272.5 mg, 1.25 mmol) and toluene (1.25 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10/1) afforded **2m** (116.4 mg, 82%) as a gray white solid. M.p. 111-112 °C. IR (KBr, cm^{-1}): 2979, 1719, 1367, 1289, 1140, 855, 773. ^1H NMR (CDCl_3 , 500 MHz): δ 8.65 (d, $J = 4.5$ Hz, 1H), 7.90 (d, $J = 7.5$ Hz, 2H), 7.73 (td, $J = 7.5, 1.5$ Hz, 1H), 7.50 (t, $J = 7.5$ Hz, 1H), 7.35-7.28 (m, 2H), 1.24 (s, 18H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 166.9, 158.6, 148.6, 139.5, 135.4, 134.3, 131.8, 127.9, 124.2, 121.9, 81.5, 27.5. EI-MS m/z (%): 355 (12) $[\text{M}^+]$, 282 (30), 226 (99), 199 (100), 155 (86). Anal. Calcd. For $\text{C}_{21}\text{H}_{25}\text{NO}_4$: C, 70.96; H, 7.09; N, 3.94. Found: C, 71.05; H, 7.10; N, 3.71.



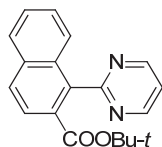
Di-tert-butyl 2-(1H-pyrazol-1-yl)isophthalate (2n): Following the general procedure with **1n** (72.0 mg, 0.5 mmol), $[\text{RuCl}_2(p\text{-cymene})]_2$ (7.7 mg, 0.0125 mmol), 1-AdCOOH (27.0 mg, 0.15 mmol), K_2CO_3 (172.5 mg, 1.25 mmol), Boc_2O (272.5 mg, 1.25 mmol) and toluene (1.25 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10/1) afforded **2n** (156.5 mg, 91%) as a gray white solid. M.p. 78-79 °C. IR (KBr, cm^{-1}): 2980, 1721, 1368, 1294, 1144, 852, 773, 754. ^1H NMR (CDCl_3 , 500 MHz): δ 7.87 (d, $J = 8.0$ Hz, 2H), 7.72 (d, $J = 1.5$ Hz, 1H), 7.60 (d, $J = 2.0$ Hz, 1H), 7.54 (t, $J = 7.5$ Hz, 1H), 6.47 (t, $J = 2.0$ Hz, 1H), 1.35 (s, 18H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 165.2, 140.1, 137.0, 132.6, 132.3, 132.0, 128.5, 106.4, 82.4, 27.6. EI-MS m/z (%): 344 (5) $[\text{M}^+]$, 233 (27), 215 (73), 188 (86), 144 (100). Anal. Calcd. For $\text{C}_{19}\text{H}_{24}\text{N}_2\text{O}_4$: C, 66.26; H, 7.02; N, 8.13. Found: C, 66.12; H, 6.81; N, 8.26.



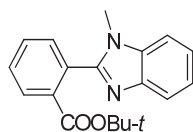
Di-tert-butyl 1-(pyrimidin-2-yl)-1H-pyrrole-2,5-dicarboxylate (2o): Following the general procedure with **1o** (71.5 mg, 0.5 mmol), $[\text{RuCl}_2(p\text{-cymene})]_2$ (7.7 mg, 0.0125 mmol), 1-AdCOOH (27.0 mg, 0.15 mmol), K_2CO_3 (172.5 mg, 1.25 mmol), Boc_2O (272.5 mg, 1.25 mmol) and toluene (1.25 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10/1) afforded **2o** (148.4 mg, 86%) as a gray white solid. M.p. 155-156 °C. IR (KBr, cm^{-1}): 2982, 1719, 1572, 1427, 1264, 1145, 975, 833. ^1H NMR (CDCl_3 , 500 MHz): δ 8.86 (d, $J = 5.0$ Hz, 2H), 7.43 (t, $J = 5.0$ Hz, 1H), 6.94 (s, 2H), 1.35 (s, 18H). ^{13}C NMR (CDCl_3 , 125 MHz): δ 159.1, 158.8, 158.1, 129.7, 120.6, 116.3, 81.3, 28.0. EI-MS m/z (%): 345 (54) $[\text{M}^+]$, 289 (27), 233 (45), 189 (20), 145 (100). Anal. Calcd. For $\text{C}_{18}\text{H}_{23}\text{N}_3\text{O}_4$: C, 62.59; H, 6.71; N, 12.17. Found: C, 62.49; H, 6.64; N, 12.12.



tert-Butyl 1-(pyrimidin-2-yl)-1H-indole-2-carboxylate (2p): Following the general procedure with **1p** (97.5 mg, 0.5 mmol), [RuCl₂(*p*-cymene)]₂ (7.7 mg, 0.0125 mmol), 1-AdCOOH (27.0 mg, 0.15 mmol), K₂CO₃ (172.5 mg, 1.25 mmol), Boc₂O (272.5 mg, 1.25 mmol) and toluene (1.25 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10/1) afforded **2p** (67.9 mg, 46%) as a gray white solid. M.p. 94-95 °C. IR (KBr, cm⁻¹): 2981, 1714, 1566, 1427, 1348, 1159, 847, 753. ¹H NMR (500 MHz, CDCl₃): δ 8.82 (d, *J* = 5.0 Hz, 2H), 8.14 (dd, *J* = 8.5, 1.0 Hz, 1H), 7.70 (dt, *J* = 8.0, 1.0 Hz, 1H), 7.39 (td, *J* = 8.0, 1.0 Hz, 1H), 7.30 (d, *J* = 0.5 Hz, 1H), 7.26 (td, *J* = 7.5, 1.5 Hz, 1H), 7.23 (t, *J* = 5.0 Hz, 1H), 1.50 (s, 9H). ¹³C NMR (125 MHz, CDCl₃): δ 161.2, 158.1, 157.8, 138.3, 132.0, 127.7, 125.9, 122.4, 122.2, 117.9, 113.5, 113.2, 81.6, 28.0. EI-MS *m/z* (%): 295 (19) [M⁺], 239 (15), 195 (100), 168 (5), 142 (9). HRMS: *m/z* calcd for C₁₇H₁₇N₃O₂ [M⁺] 295.1321, Found: 295.1323.

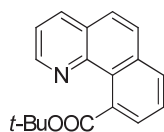


tert-Butyl 1-(pyrimidin-2-yl)-2-naphthoate (2q): Following the general procedure with **1q** (103.0 mg, 0.5 mmol), [RuCl₂(*p*-cymene)]₂ (7.7 mg, 0.0125 mmol), 1-AdCOOH (27.0 mg, 0.15 mmol), K₂CO₃ (172.5 mg, 1.25 mmol), Boc₂O (272.5 mg, 1.25 mmol) and toluene (1.25 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10/1) afforded **2q** (127.0 mg, 83%) as a gray white solid. M.p. 164-166 °C. IR (KBr, cm⁻¹): 2980, 1699, 1556, 1373, 1345, 1303, 1140, 813, 770. ¹H NMR (CDCl₃, 500 MHz): δ 8.94 (d, *J* = 5.0 Hz, 2H), 8.02 (d, *J* = 8.5 Hz, 1H), 7.96 (d, *J* = 8.0 Hz, 1H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.55-7.52 (m, 1H), 7.45-7.39 (m, 3H), 1.33 (s, 9H); ¹³C NMR (CDCl₃, 125 MHz): δ 167.6, 166.4, 156.9, 138.0, 134.9, 131.3, 129.4, 129.0, 128.0, 127.5, 127.0, 126.4, 125.8, 119.3, 81.3, 27.8. EI-MS *m/z* (%): 306 (22) [M⁺], 233 (25), 205 (100), 152 (17), 57 (25). HRMS: *m/z* calcd for C₁₉H₁₈N₂O₂ [M⁺] 306.1368, Found: 306.1372.

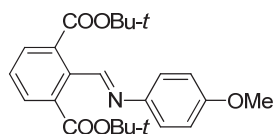


tert-Butyl 2-(1-methyl-1H-benzodimidazol-2-yl)benzoate (2r): Following the general procedure with **1r** (104.0 mg, 0.5 mmol), [RuCl₂(*p*-cymene)]₂ (7.7 mg, 0.0125 mmol), 1-AdCOOH (27.0 mg, 0.15 mmol), K₂CO₃ (172.5 mg, 1.25 mmol), Boc₂O (272.5 mg, 1.25 mmol) and toluene (1.25 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10/1) afforded **2r** (69.3 mg, 45%) as a gray white solid. M.p. 117-118 °C. IR (KBr, cm⁻¹): 2975, 1707, 1467, 1305, 1126, 847, 770, 754. ¹H NMR (CDCl₃, 500 MHz): δ 8.11-8.09 (m, 1H), 7.83 (dd, *J* = 6.5, 1.5 Hz, 1H), 7.67-7.60 (m, 2H), 7.54 (dd, *J* = 7.0, 2.0 Hz, 1H), 7.40-7.31 (m, 3H), 3.59 (s, 3H), 1.16 (s, 9H); ¹³C NMR (CDCl₃, 125 MHz): δ 165.5, 153.7, 135.5, 133.3, 131.6, 131.2, 130.7, 130.5, 129.9, 122.6, 122.1, 119.8, 109.2, 81.5, 30.4, 27.5. EI-MS *m/z* (%): 308 (28) [M⁺], 235 (16), 207 (100), 195 (10), 122 (11). Anal. Calcd. For

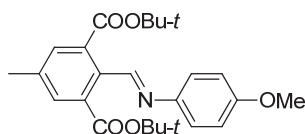
C₁₉H₂₀N₂O₂: C, 74.00; H, 6.54; N, 9.08. Found: C, 73.84; H, 6.45; N, 8.81.



tert-Butyl benzo[h]quinoline-10-carboxylate (2s): Following the general procedure with **1s** (89.5 mg, 0.5 mmol), [RuCl₂(*p*-cymene)]₂ (7.7 mg, 0.0125 mmol), 1-AdCOOH (27.0 mg, 0.15 mmol), K₂CO₃ (172.5 mg, 1.25 mmol), Boc₂O (272.5 mg, 1.25 mmol) and toluene (1.25 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10/1) afforded **2s** (69.8 mg, 50%) as a gray white solid. M.p. 132-133 °C. IR (KBr, cm⁻¹): 2970, 1712, 1301, 1148, 1111, 838, 752. ¹H NMR (CDCl₃, 500 MHz): δ 8.93 (dd, *J* = 4.5, 2.0 Hz, 1H), 8.18 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.95 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.83 (d, *J* = 9.0 Hz, 1H), 7.73-7.70 (m, 2H), 7.76 (dd, *J* = 7.0, 1.5 Hz, 1H), 7.54 (dd, *J* = 8.0, 4.5 Hz, 1H), 1.77 (s, 9H); ¹³C NMR (CDCl₃, 125 MHz): δ 171.0, 147.3, 145.3, 135.4, 134.1, 134.0, 128.8, 127.8, 127.4, 127.3, 126.8, 126.1, 125.9, 121.9, 81.4, 28.3. EI-MS *m/z* (%): 279 (26) [M⁺], 229 (41), 214 (100), 194 (60), 179 (93). HRMS: *m/z* calcd for C₁₈H₁₇NO₂ [M⁺] 279.1259, Found: 279.1256.

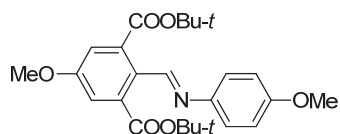


(E)-Di-tert-butyl 2-(((4-methoxyphenyl)imino)methyl)isophthalate (4a): Following the general procedure with **3a** (105.5 mg, 0.5 mmol), [RuCl₂(*p*-cymene)]₂ (7.7 mg, 0.0125 mmol), 1-AdCOOH (27.0 mg, 0.15 mmol), K₂CO₃ (172.5 mg, 1.25 mmol), Boc₂O (272.5 mg, 1.25 mmol) and toluene (1.25 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10/1) afforded **4a** (199.3 mg, 97%) as a gray white solid. M.p. 103-105 °C. IR (KBr, cm⁻¹): 2977, 1701, 1504, 1248, 1143, 1033, 834, 743. ¹H NMR (*d*₆-DMSO, 500 MHz): δ 8.98 (s, 1H), 7.90 (d, *J* = 8.0 Hz, 2H), 7.64 (t, *J* = 8.0 Hz, 1H), 7.27 (d, *J* = 9.0 Hz, 2H), 7.00 (d, *J* = 9.0 Hz, 2H), 3.78 (s, 3H), 1.42 (s, 18H); ¹³C NMR (*d*₆-DMSO, 125 MHz): δ 166.3, 158.5, 158.1, 144.2, 136.9, 134.1, 132.3, 129.8, 122.8, 114.8, 82.2, 55.7, 28.1. EI-MS *m/z* (%): 411 (12) [M⁺], 355 (13), 299 (100), 193 (58), 177 (57). Anal. Calcd. For C₂₄H₂₉NO₅: C, 70.05; H, 7.10; N, 3.40. Found: C, 70.02; H, 7.09; N, 3.39.

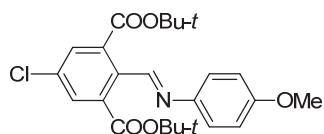


(E)-Di-tert-butyl 2-(((4-methoxyphenyl)imino)methyl)-5-methylisophthalate (4b): Following the general procedure with **3b** (112.5 mg, 0.5 mmol), [RuCl₂(*p*-cymene)]₂ (7.7 mg, 0.0125 mmol), 1-AdCOOH (27.0 mg, 0.15 mmol), K₂CO₃ (172.5 mg, 1.25 mmol), Boc₂O (272.5 mg, 1.25 mmol) and toluene (1.25 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10/1) afforded **4b** (191.3 mg, 90%) as a gray white solid. M.p. 110-111 °C. IR (KBr, cm⁻¹): 2979, 1708, 1628, 1503, 1272, 1158, 1032, 846, 827, 752. ¹H NMR (CDCl₃, 500 MHz): δ 9.03 (s, 1H), 7.72 (s, 2H), 7.29 (d, *J* = 9.0 Hz, 2H), 6.93 (d, *J* = 9.0 Hz, 2H), 3.84 (s, 3H), 2.45 (s, 3H), 1.49 (s, 18H); ¹³C NMR (CDCl₃, 125 MHz): δ 166.5, 158.8, 158.1, 144.8, 138.9, 135.0, 134.0, 132.7, 122.4, 114.2, 82.0, 55.4, 28.1, 21.0. EI-MS *m/z* (%): 425 (15)

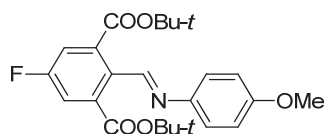
[M⁺], 369 (15), 313 (100), 296 (20), 225 (15). Anal. Calcd. For C₂₅H₃₁NO₅: C, 70.57; H, 7.34; N, 3.16. Found: C, 70.67; H, 7.30; N, 3.16.



(E)-Di-tert-butyl 5-methoxy-2-(((4-methoxyphenyl)imino)methyl)isophthalate (4c): Following the general procedure with **3c** (120.5 mg, 0.5 mmol), [RuCl₂(*p*-cymene)]₂ (7.7 mg, 0.0125 mmol), 1-AdCOOH (27.0 mg, 0.15 mmol), K₂CO₃ (172.5 mg, 1.25 mmol), Boc₂O (272.5 mg, 1.25 mmol) and toluene (1.25 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10/1) afforded **4c** (211.7 mg, 96%) as a gray white solid. M.p. 111-112 °C. IR (KBr, cm⁻¹): 2978, 1713, 1604, 1505, 1342, 1108, 847, 835. ¹H NMR (CDCl₃, 500 MHz): δ 8.99 (s, 1H), 7.41 (s, 2H), 7.29-7.27 (m, 2H), 6.95-6.92 (m, 2H), 3.91 (s, 3H), 3.85 (s, 3H), 1.49 (s, 18H); ¹³C NMR (CDCl₃, 125 MHz): δ 166.2, 159.5, 158.3, 158.1, 135.6, 129.7, 122.3, 117.5, 114.2, 82.2, 55.7, 55.4, 28.1, 28.0. EI-MS *m/z* (%): 441 (25) [M⁺], 385 (12), 329 (100), 241 (21), 207 (18). HRMS: *m/z* calcd for C₂₅H₃₁NO₆ [M⁺] 441.2151, Found: 441.2154.

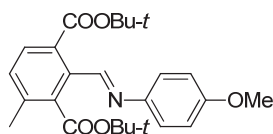


(E)-Di-tert-butyl 5-chloro-2-(((4-methoxyphenyl)imino)methyl)isophthalate (4d): Following the general procedure with **3d** (122.8 mg, 0.5 mmol), [RuCl₂(*p*-cymene)]₂ (7.7 mg, 0.0125 mmol), 1-AdCOOH (27.0 mg, 0.15 mmol), K₂CO₃ (172.5 mg, 1.25 mmol), Boc₂O (272.5 mg, 1.25 mmol) and toluene (1.25 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10/1) afforded **4d** (204.9 mg, 92%) as a gray white solid. M.p. 100-101 °C. IR (KBr, cm⁻¹): 2979, 1711, 1503, 1242, 1158, 900, 825. ¹H NMR (CDCl₃, 500 MHz): δ 9.01 (s, 1H), 7.89 (s, 2H), 7.29 (d, *J* = 9.0 Hz, 2H), 6.94 (d, *J* = 9.0 Hz, 2H), 3.85 (s, 3H), 1.50 (s, 18H); ¹³C NMR (CDCl₃, 125 MHz): δ 165.0, 158.4, 157.7, 136.3, 135.5, 134.7, 132.1, 122.4, 114.2, 82.8, 55.4, 28.0. EI-MS *m/z*: 447 (6) [M⁺ (³⁷Cl)], 445 (10) [M⁺ (³⁵Cl)], 389 (11), 333 (100), 316 (24). HRMS: *m/z* calcd for C₂₄H₂₈ClNO₅ [M⁺] 445.1651, Found: 445.1652.

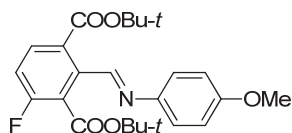


(E)-Di-tert-butyl 5-fluoro-2-(((4-methoxyphenyl)imino)methyl)isophthalate (4e): Following the general procedure with **3e** (114.5 mg, 0.5 mmol), [RuCl₂(*p*-cymene)]₂ (7.7 mg, 0.0125 mmol), 1-AdCOOH (27.0 mg, 0.15 mmol), K₂CO₃ (172.5 mg, 1.25 mmol), Boc₂O (272.5 mg, 1.25 mmol) and toluene (1.25 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10/1) afforded **4e** (205.9 mg, 96%) as a gray white solid. M.p. 132-133 °C. IR (KBr, cm⁻¹): 2978, 1705, 1505, 1249, 1151, 832, 753. ¹H NMR (CDCl₃, 500 MHz): δ 9.02 (s, 1H), 7.63 (d, *J* = 8.5 Hz, 2H), 7.30 (d, *J* = 8.5 Hz, 2H), 6.95 (d, *J* = 9.0 Hz, 2H), 3.85 (s, 3H), 1.50 (s, 18H); ¹⁹F NMR (CDCl₃, 470 MHz): -110.9 (m, Ar-F); ¹³C NMR (CDCl₃, 125 MHz): δ 165.0 (d, ⁴J_{C-F} = 2.1 Hz), 161.8 (d, ¹J_{C-F} = 250.0 Hz), 158.3, 158.0, 144.4, 136.2 (d, ³J_{C-F} = 7.1 Hz), 134.1 (d, ⁴J_{C-F} = 2.8 Hz), 122.4, 119.3 (d, ²J_{C-F} = 23.2 Hz), 114.8, 82.7, 55.4, 28.0. EI-MS *m/z*

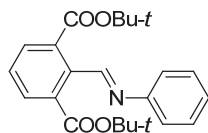
(%): 429 (12) [M⁺], 373 (14), 317 (100), 300 (17), 195 (8). Anal. Calcd. For C₂₄H₂₈FNO₅: C, 67.12; H, 6.57; N, 3.26. Found: C, 67.04; H, 6.53; N, 3.31.



(E)-Di-tert-butyl 2-(((4-methoxyphenyl)imino)methyl)-4-methylisophthalate (4f): Following the general procedure with **3f** (112.5 mg, 0.5 mmol), [RuCl₂(*p*-cymene)]₂ (7.7 mg, 0.0125 mmol), 1-AdCOOH (27.0 mg, 0.15 mmol), K₂CO₃ (172.5 mg, 1.25 mmol), Boc₂O (272.5 mg, 1.25 mmol) and toluene (1.25 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10/1) afforded **4f** (74.4 mg, 35%) as a gray white solid. M.p. 95-96 °C. IR (KBr, cm⁻¹): 2975, 1729, 1701, 1503, 1244, 1150, 831. ¹H NMR (CDCl₃, 500 MHz): δ 8.97 (s, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.30 (d, *J* = 9.0 Hz, 1H), 7.26-7.24 (m, 2H), 6.94-6.92 (m, 2H), 3.84 (s, 3H), 2.46 (s, 3H), 1.50 (s, 9H), 1.48 (s, 9H); ¹³C NMR (CDCl₃, 125 MHz): δ 167.8, 165.6, 158.3, 158.2, 144.6, 139.6, 135.7, 135.2, 131.2, 130.6, 130.2, 122.4, 114.2, 82.3, 81.9, 55.4, 28.3, 28.1, 19.9. EI-MS *m/z* (%): 425 (5) [M⁺], 369 (20), 313 (100), 296 (17). Anal. Calcd. For C₂₅H₃₁NO₅: C, 70.57; H, 7.34; N, 3.29. Found: C, 70.23; H, 6.98; N, 3.40.

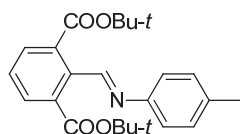


(E)-Di-tert-butyl 4-fluoro-2-(((4-methoxyphenyl)imino)methyl)isophthalate (4g): Following the general procedure with **3g** (114.5 mg, 0.5 mmol), [RuCl₂(*p*-cymene)]₂ (7.7 mg, 0.0125 mmol), 1-AdCOOH (27.0 mg, 0.15 mmol), K₂CO₃ (172.5 mg, 1.25 mmol), Boc₂O (272.5 mg, 1.25 mmol) and toluene (1.25 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10/1) afforded **4g** (190.9 mg, 89%) as a gray white solid. M.p. 94-95 °C. IR (KBr, cm⁻¹): 2982, 1732, 1704, 1504, 1246, 1160, 851, 833. ¹H NMR (CDCl₃, 500 MHz): δ 8.99 (s, 1H), 7.98 (dd, *J* = 8.5, 5.5 Hz, 1H), 7.28-7.24 (m, 2H), 7.19 (t, *J* = 8.5 Hz, 1H), 6.95-6.92 (m, 2H), 3.85 (s, 3H), 1.52 (s, 9H), 1.51 (s, 9H); ¹⁹F NMR (CDCl₃, 470 MHz): -109.7 (m, Ar-F); ¹³C NMR (CDCl₃, 125 MHz): δ 164.6, 163.7, 161.5 (¹*J*_{C-F} = 254.9 Hz), 158.5, 156.5, 144.2, 138.1 (d, ⁴*J*_{C-F} = 3.8 Hz), 133.1 (d, ³*J*_{C-F} = 9.3 Hz), 128.7 (d, ⁴*J*_{C-F} = 3.3 Hz), 124.5 (d, ²*J*_{C-F} = 18.2 Hz), 122.4, 116.6 (d, ²*J*_{C-F} = 22.2 Hz), 114.2, 83.1, 82.4, 55.4, 28.1. EI-MS *m/z* (%): 429 (7) [M⁺], 373 (12), 317 (100), 300 (13), 122 (15). HRMS: *m/z* calcd for C₂₄H₂₈FNO₅ [M⁺] 429.1952, Found: 429.1950.

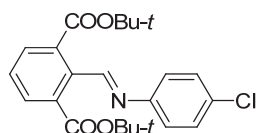


(E)-Di-tert-butyl 2-((phenylimino)methyl)isophthalate (4h): Following the general procedure with **3h** (90.5 mg, 0.5 mmol), [RuCl₂(*p*-cymene)]₂ (7.7 mg, 0.0125 mmol), 1-AdCOOH (27.0 mg, 0.15 mmol), K₂CO₃ (172.5 mg, 1.25 mmol), Boc₂O (272.5 mg, 1.25 mmol) and toluene (1.25 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10/1) afforded **4h** (154.3 mg, 81%) as a gray white solid. M.p. 77-79 °C. IR (KBr, cm⁻¹): 2976, 1717, 1369, 1271, 1148, 847, 754. ¹H NMR (CDCl₃, 500 MHz): δ 9.09 (s, 1H), 7.97

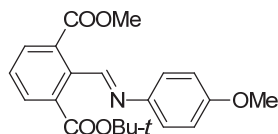
(d, $J = 8.0$ Hz, 2H), 7.51 (t, $J = 7.5$ Hz, 1H), 7.43-7.40 (m, 2H), 7.34-7.32 (m, 2H), 7.27-7.23 (m, 1H), 1.51 (s, 18H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 166.0, 161.5, 151.6, 138.1, 133.9, 132.4, 129.0, 128.7, 125.9, 121.0, 82.2, 28.1. EI-MS m/z (%): 381 (1) [M^+], 233 (36), 193 (99), 177 (97), 57 (100). HRMS: m/z calcd for $\text{C}_{23}\text{H}_{27}\text{NO}_4$ [M^+] 381.1940, Found: 381.1939.



(E)-Di-tert-butyl 2-((p-tolylimino)methyl)isophthalate (4i): Following the general procedure with **3i** (97.5 mg, 0.5 mmol), $[\text{RuCl}_2(p\text{-cymene})]_2$ (7.7 mg, 0.0125 mmol), 1-AdCOOH (27.0 mg, 0.15 mmol), K_2CO_3 (172.5 mg, 1.25 mmol), Boc_2O (272.5 mg, 1.25 mmol) and toluene (1.25 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10/1) afforded **4i** (160.0 mg, 81%) as a gray white solid. M.p. 106-107 °C. IR (KBr, cm^{-1}): 2976, 2931, 1721, 1369, 1271, 1170, 848, 744. ^1H NMR (d_6 -DMSO, 500 MHz): δ 9.08 (s, 1H), 7.95 (d, $J = 8.0$ Hz, 2H), 7.50 (t, $J = 8.0$ Hz, 1H), 7.23-7.20 (m, 4H), 2.39 (s, 3H), 1.50 (s, 18H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 166.1, 160.5, 135.7, 134.0, 133.4, 132.3, 129.7, 129.6, 128.6, 121.0, 82.1, 28.1, 21.0. EI-MS m/z (%): 395 (1) [M^+], 339 (18), 283 (100), 266 (18), 195 (12). Anal. Calcd. For $\text{C}_{24}\text{H}_{29}\text{NO}_4$: C, 72.89; H, 7.39; N, 3.54. Found: C, 72.65; H, 7.31; N, 3.36.



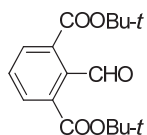
(E)-Di-tert-butyl 2-(((4-chlorophenyl)imino)methyl)isophthalate (4j): Following the general procedure with **3j** (107.8 mg, 0.5 mmol), $[\text{RuCl}_2(p\text{-cymene})]_2$ (7.7 mg, 0.0125 mmol), 1-AdCOOH (27.0 mg, 0.15 mmol), K_2CO_3 (172.5 mg, 1.25 mmol), Boc_2O (272.5 mg, 1.25 mmol) and toluene (1.25 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 10/1) afforded **4j** (151.7 mg, 73%) as a gray white solid. M.p. 138-139 °C. IR (KBr, cm^{-1}): 2976, 1718, 1272, 1149, 830. ^1H NMR (d_6 -DMSO, 500 MHz): δ 9.06 (s, 1H), 7.98 (d, $J = 8.0$ Hz, 2H), 7.52 (t, $J = 8.0$ Hz, 1H), 7.38 (d, $J = 8.5$ Hz, 2H), 7.26 (d, $J = 9.0$ Hz, 2H), 1.51 (s, 18H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 165.9, 162.2, 150.3, 138.1, 133.8, 132.5, 131.4, 129.1, 128.8, 122.3, 82.2, 28.1. EI-MS m/z : 417 (2) [M^+ (^{37}Cl)], 415 (6) [M^+ (^{35}Cl)], 359 (9), 303 (100), 286 (23). HRMS: m/z calcd for $\text{C}_{23}\text{H}_{26}\text{ClNO}_4$ [M^+] 415.1550, Found: 415.1552.



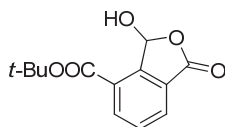
(E)-1-tert-Butyl 3-methyl 2-(((4-methoxyphenyl)imino)methyl)isophthalate (4k): Following the general procedure with **3k** (134.5 mg, 0.5 mmol), $[\text{RuCl}_2(p\text{-cymene})]_2$ (7.7 mg, 0.0125 mmol), 1-AdCOOH (27.0 mg, 0.15 mmol), K_2CO_3 (172.5 mg, 1.25 mmol), Boc_2O (272.5 mg, 1.25 mmol) and toluene (1.25 mL). After reaction was over, purification by column chromatography on silica gel (petroleum ether/EtOAc = 5/1) afforded **4k** (131.4 mg, 81%) as a yellow solid. M.p. 97-98 °C. IR (KBr, cm^{-1}): 2971, 1723, 1504, 1305, 1251, 1144, 1033, 976, 835, 748. ^1H NMR (CDCl_3 , 500 MHz): δ 9.12 (s, 1H), 8.00 (d, $J = 8.0$ Hz, 2H), 7.52 (t, $J = 7.5$ Hz, 1H), 7.31 (d, $J = 8.5$ Hz, 2H), 6.96-6.93 (m, 2H), 3.87 (s, 3H), 3.85 (s, 3H), 1.52 (s, 9H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 167.6,

165.9, 158.7, 158.3, 138.4, 134.0, 133.0, 132.4, 131.8, 128.7, 122.3, 114.3, 82.2, 55.4, 52.5, 28.1. EI-MS m/z (%): 369 (9) [M^+], 313 (86), 298 (100), 282 (49), 254 (60). HRMS: m/z calcd for $C_{21}H_{24}NO_5$ [M^+H] 370.1654, Found: 370.1647.

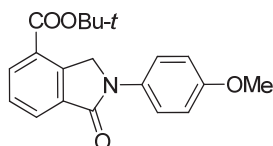
4. Further Transformation of 4a



Di-tert-butyl 2-formylisophthalate (5): A solution of **4a** (205.5 mg, 0.5mmol) in 2.5 mL THF was added 1M HCl (2.5 ml) slowly at 0 °C. 30 min later, the reaction mixture was extracted with EtOAc (2×15 mL). The organic layer was dried over anhydrous sodium sulfate and concentrated to get crude product, which was purified by column chromatography on silica gel (petroleum ether/EtOAc = 20/1) to give **5** (150.2 mg, 98%) as a colorless oil. IR (KBr, cm^{-1}): 2979, 2934, 1917, 1369, 1301, 1147, 847.9, 751.9. 1H NMR ($CDCl_3$, 500 MHz): δ 10.68 (s, 1H), 8.05 (d, J = 8.0 Hz, 2H), 7.53 (t, J = 8.0 Hz, 1H), 1.58 (s, 18H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 194.4, 164.8, 142.4, 133.4, 131.6, 129.3, 83.2, 28.0. ESI-MS m/z (%): 307 [M^+H]. HRMS (ESI): m/z calcd for $C_{17}H_{23}O_5$ [M^+H] 307.1545, Found: 307.1554.



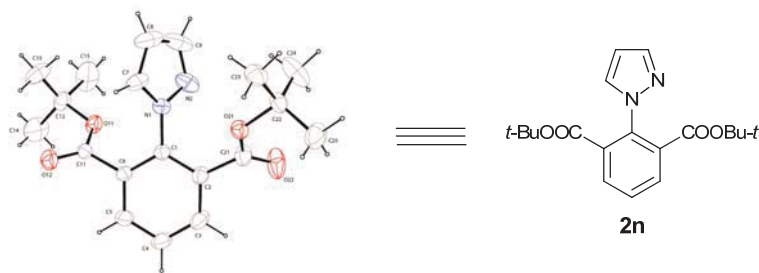
tert-Butyl 3-hydroxy-1-oxo-1,3-dihydroisobenzofuran-4-carboxylate (6): A solution of **4a** (205.5 mg, 0.5mmol) in 2.5 mL THF was added 1M HCl (2.5 mL) slowly at 25 °C. 3 h later, the reaction mixture was extracted with EtOAc (2×15 mL). The organic layer was dried over anhydrous sodium sulphate and concentrated to get crude product, which was purified by column chromatography on silica gel (petroleum ether/EtOAc = 5/1) to give **6** (107.5 mg, 86%) as a white solid. M.p. 134-135 °C. IR (KBr, cm^{-1}): 3391, 2985, 174, 1328, 1145, 1098, 887, 804, 749. 1H NMR ($CDCl_3$, 500 MHz): δ 8.24 (dd, J = 7.5, 1.0 Hz, 1H), 8.06 (dd, J = 7.5, 1.0 Hz, 1H), 7.70 (t, J = 7.0 Hz, 1H), 6.96 (d, J = 1.0 Hz, 1H), 4.68 (d, J = 1.0 Hz, 1H), 1.65 (s, 9H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 167.9, 164.2, 147.5, 135.7, 131.0, 129.3, 128.3, 127.6, 97.3, 83.5, 28.1. MS m/z (%): 250 (2) [M^+], 195 (36), 177 (100), 150 (24). Anal. Calcd. For $C_{13}H_{14}O_5$: C, 62.39; H, 5.64. Found: C, 62.10; H, 5.50.



tert-Butyl 2-(4-methoxyphenyl)-1-oxoisindoline-4-carboxylate (7): A solution of **4a** (205.5 mg, 0.5 mmol) and $ZnCl_2$ (68.0 mg, 0.5 mmol) in 5 mL MeOH was added $NaBH_3CN$ slowly at 25 °C. After stirring for 3 h, the reaction mixture was extracted with EtOAc (2×15 mL). The organic layer was dried over anhydrous sodium sulphate and concentrated to get crude product, which was

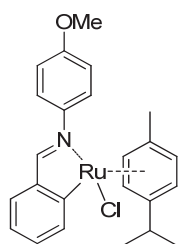
purified by column chromatography on silica gel (petroleum ether/EtOAc = 5/1) to give **7** (161.1 mg, 95%) as a white solid. M.p. 153-154 °C. IR (KBr, cm^{-1}): 2991, 2973, 1715, 1681, 1512, 1252, 1156, 822, 744. ^1H NMR (CDCl_3 , 500 MHz): δ 8.20 (dd, $J = 8.0, 1.0$ Hz, 1H), 8.10 (dd, $J = 7.5, 1.0$ Hz, 1H), 7.83-7.79 (m, 2H), 7.60 (t, $J = 7.5$ Hz, 1H), 7.00-6.98 (m, 2H), 5.14 (s, 2H), 3.85 (s, 3H), 1.67 (s, 9H); ^{13}C NMR (CDCl_3 , 125 MHz): δ 166.2, 164.5, 156.7, 141.6, 134.5, 133.2, 132.4, 128.5, 127.9, 126.9, 121.3, 114.3, 82.2, 55.5, 52.7, 28.3. EI-MS m/z (%): 339 (36) [M^+], 283 (72), 267 (36), 57 (100). HRMS: m/z calcd for $\text{C}_{20}\text{H}_{21}\text{NO}_4$ [M^+] 339.1471, Found: 339.1474.

5. X-Ray crystal structure for compound **2n**



Crystallographic data for **2n**: $\text{C}_{19}\text{H}_{24}\text{N}_2\text{O}_4$, $M = 344.40$, orthorhombic, P21 21 21 (No. 19), $a = 8.088(5)$ Å, $b = 12.766(5)$ Å, $c = 19.413(5)$ Å, $V = 2004.4(16)$ Å³, $Z = 4$, Crystal size: $0.24 \times 0.22 \times 0.17$ mm, $T = 295$ K, $\rho_{\text{calcd}} = 1.141$ g·cm⁻³, $R_1 = 0.0427$ ($I > 4\sigma(I)$), $wR_2 = 0.1248$ (all data), GOF = 1.022, reflections collected/unique: 4532 / 3254 ($R_{\text{int}} = 0.0277$), Data: 3254, restraints: 0, parameters: 227. CCDC 995322 contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

6. Synthesis and Characterization for **8**



$[\text{RuCl}_2(p\text{-cymene})]_2$ (61.2 mg, 0.1 mmol), **3a** (42.2 mg, 0.2 mmol), KOAc (40 mg, 0.4 mmol) and methanol (5 mL) were introduced in a dried Schlenk tube under argon, equipped with magnetic stirring bar and the mixture was stirred at ambient temperature for 20 h. The solvent was then evaporated under vacuum and the given crude was purified by column chromatography on silica gel (petroleum ether/EtOAc = 3/1) to give complex **8** (161.1 mg, 95%) as a red solid. M.p. 201-202 °C. IR (KBr, cm^{-1}): 2968, 1603, 1583, 1201, 1037, 833. ^1H NMR (CDCl_3 , 500 MHz): δ 8.17 (d, $J = 7.0$ Hz, 1H), 8.06 (s, 1H), 7.71 (dt, $J = 10.0, 2.5$ Hz, 2H), 7.51 (dd, $J = 7.5, 1.0$ Hz, 1H), 7.16 (td, $J = 7.5, 1.5$ Hz, 1H), 6.99 (td, $J = 7.5, 1.5$ Hz, 1H), 6.92 (dt, $J = 9.0, 2.0$ Hz, 2H), 5.46 (dd, $J = 6.0, 0.5$ Hz, 1H), 5.21 (d, $J = 6.0$ Hz, 1H), 4.87 (dd, $J = 6.0, 0.5$ Hz, 1H), 4.83 (d, $J = 5.5$ Hz, 1H), 3.87 (s, 3H), 2.39-2.34 (m, 1H), 2.05 (s, 3H), 0.97 (d, $J = 7.0$ Hz, 1H), 0.84 (d, $J =$

7.0 Hz, 1H). ^{13}C NMR (CDCl_3 , 125 MHz): δ 188.8, 171.2, 158.8, 148.4, 146.0, 139.1, 130.1, 129.5, 123.4, 122.5, 122.4, 113.7, 102.1, 100.4, 92.4, 89.3, 82.9, 82.5, 55.5, 30.8, 22.9, 21.5, 18.8. EI-MS m/z (%): 210 (100) $[\text{M-RuCl-}p\text{-cymene}]^+$, 196 (37), 167 (22), 119 (42). HRMS: m/z calcd for $\text{C}_{24}\text{H}_{26}\text{NO}^{102}\text{Ru} [\text{M-Cl}]^+$ 446.1058, Found: 446.1062.

References:

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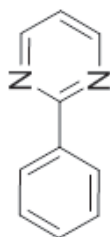
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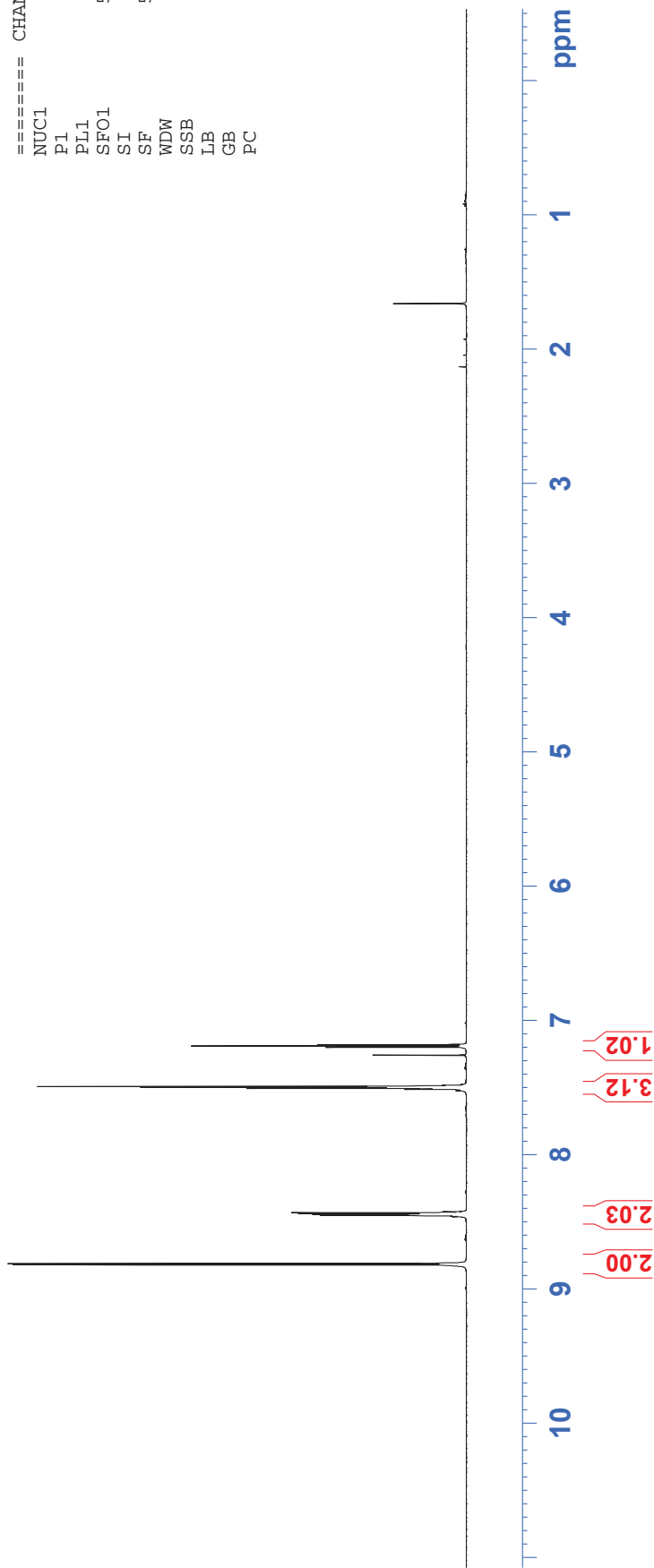
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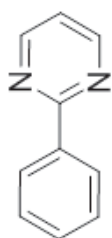
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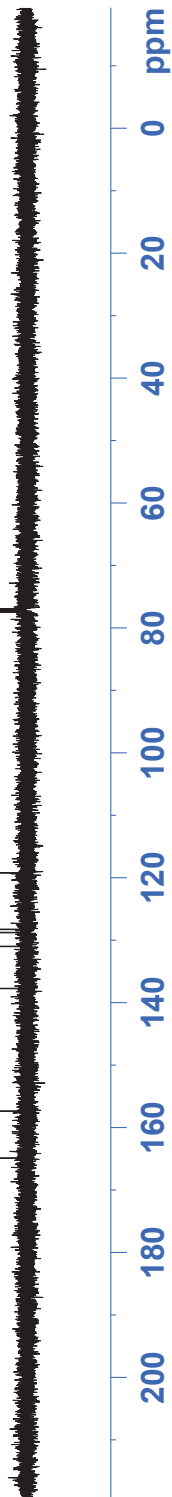
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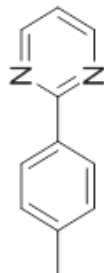
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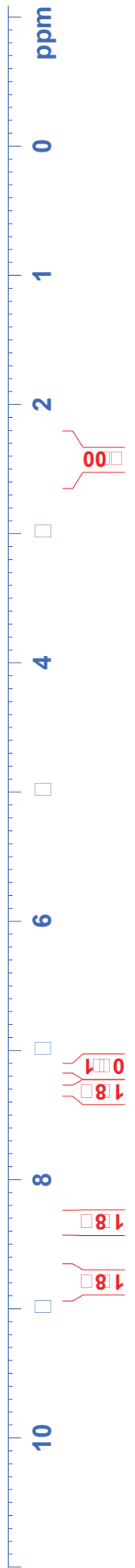
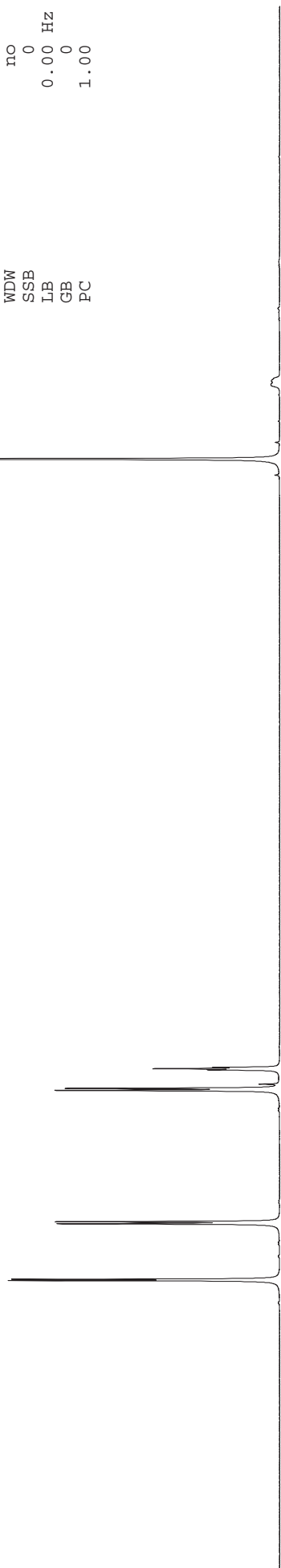
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7.308
7.292
7.149
7.139
7.130
8.779
8.770
8.340
8.324



1b

2.420



SBR-SM-2-0
C13CPD CDCl3

```

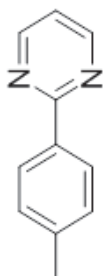
NAME      XB20081013
EXPNO     2
PROCNO    1
Date_     20081013
Time      13.31
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         480
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         203.2
DW         16.650 usec
DE         6.00 usec
TE         297.2 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

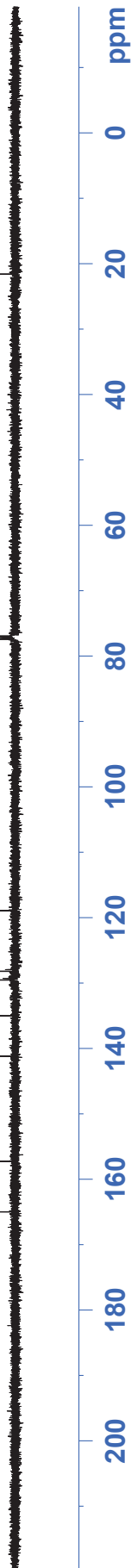
===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        2.00 dB
PL12       16.50 dB
PL13       16.50 dB
SFO2       500.1320005 MHz
SI         32768
SF         125.7577762 MHz
WDW        no
SSB        0
LB         0.00 Hz
GB         0
PC         1.40
  
```

21.59

164.94
157.30
141.16
134.99
129.50
128.20
118.90



1b



SBR-0-3
 PROTON CDCl3

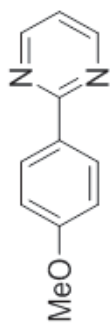
```

NAME      XB20081022
EXPNO     2
PROCNO    1
Date_     20081022
Time_     10.22
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH       10330.578 Hz
FIDRES    0.157632 Hz
AQ        3.1720407 sec
RG        228.1
DE        48.400 usec
TE        6.00 usec
TE        295.1 K
D1        1.00000000 sec
TD0       1
  
```

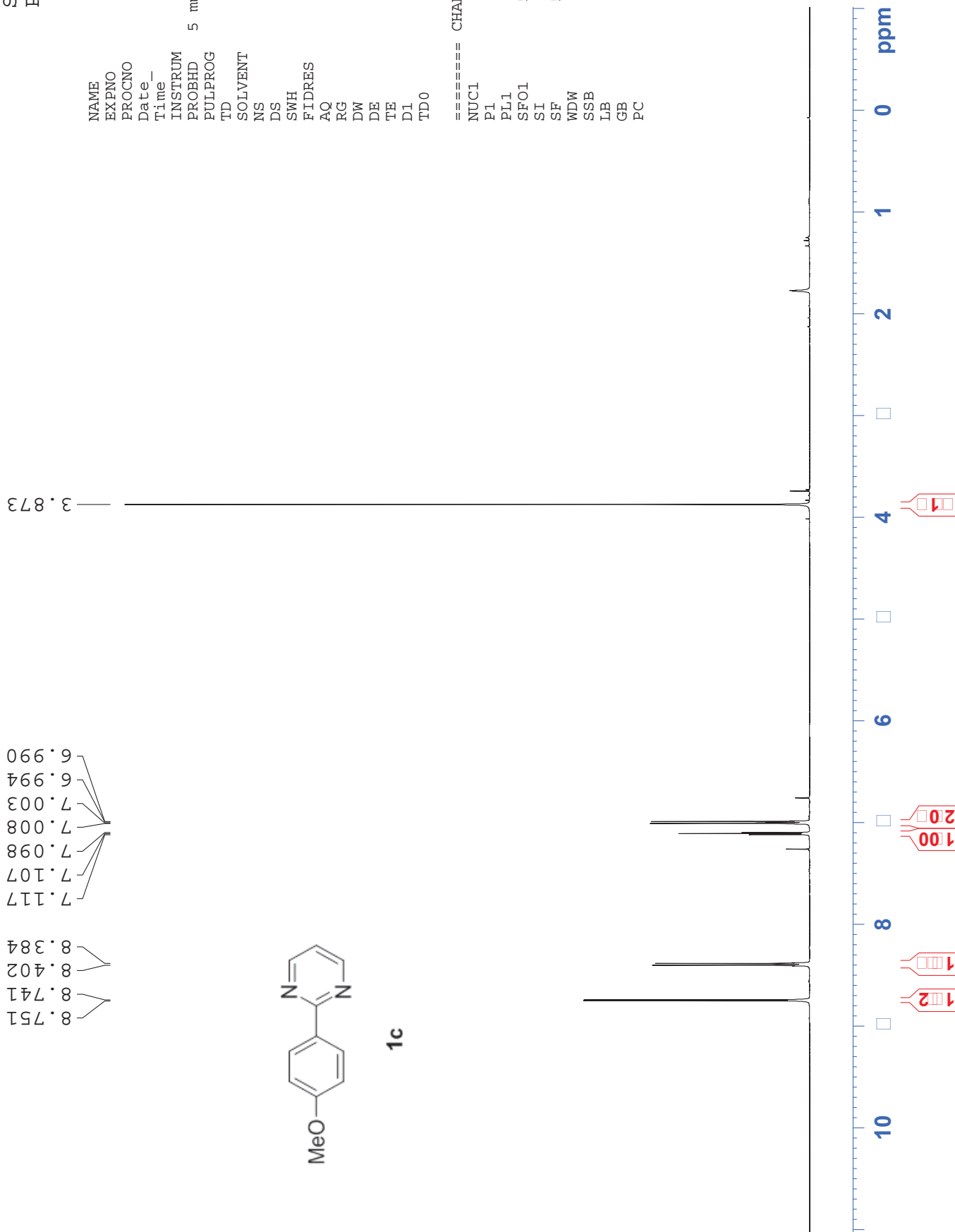
```

===== CHANNEL f1 =====
NUC1      1H
P1        14.50 usec
PL1       2.00 dB
SF01      500.1330885 MHz
SI        32768
SF        500.1300133 MHz
WDW       no
SSB       0
LB        0.00 Hz
GB        0
PC        1.00
  
```

8.751
 8.741
 8.402
 8.384
 7.117
 7.107
 7.098
 7.008
 7.003
 6.994
 6.990



1c



SBR-0-3
C13CPD CDCl3

```

NAME      XB20081022
EXPNO     3
PROCNO    1
Date_     20081022
Time      11.16
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         101.6
DW         16.650 usec
DE         6.00 usec
TE         570.1 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        2.00 dB
PL12       16.50 dB
PL13       16.50 dB
SFO2       500.1320005 MHz
SI         32768
SF         125.7577745 MHz
WDW        no
SSB        0
LB         0.00 Hz
GB         0
PC         1.40
  
```

55.49

114.06

118.47

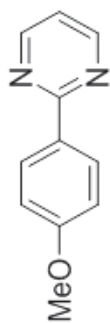
129.89

130.38

157.28

162.04

164.65



1c



HXH-3-133
 PROTON CDC13

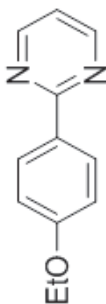
NAME XB20120924
 EXPNO 15
 PROCNO 1
 Date_ 20120924
 Time_ 11.05
 INSTRUM spect
 PROBHD 5 mm PATXO 19F
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 8
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1720407 sec
 RG 128
 DW 48.400 usec
 DE 6.00 usec
 TE 295.9 K
 D1 1.0000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 13.72 usec
 PL1 1.00 dB
 SF01 500.1330885 MHz
 SI 32768
 SF 500.1300129 MHz
 WDW hc
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

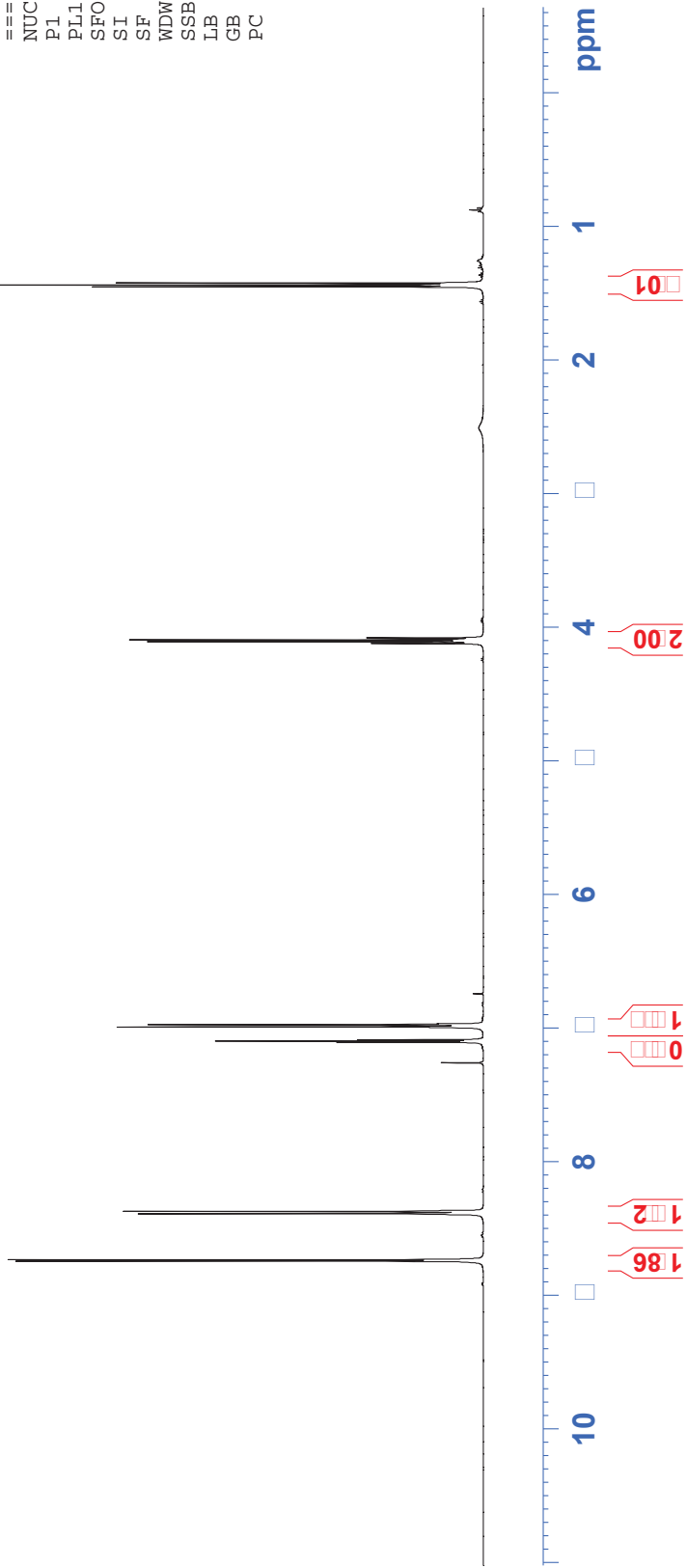
1.450
 1.436
 1.422

4.121
 4.107
 4.093
 4.079

8.744
 8.735
 8.390
 8.386
 8.376
 8.372
 7.107
 7.097
 7.088
 6.997
 6.992
 6.987
 6.978
 6.974



1d



HXH-3-133
C13CPD CDCl3

```

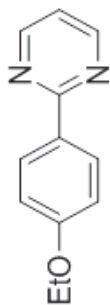
NAME       XB20120926
EXPNO      7
PROCNO     1
Date_      20120926
Time_      14.31
INSTRUM    spect
PROBHD     5 mm PATXO 19F
PULPROG    zgpg30
TD          65536
SOLVENT    CDCl3
NS          256
DS          4
SWH         30030.029 Hz
FIDRES     0.458222 Hz
AQ          1.0912410 sec
RG          128
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
  
```

```

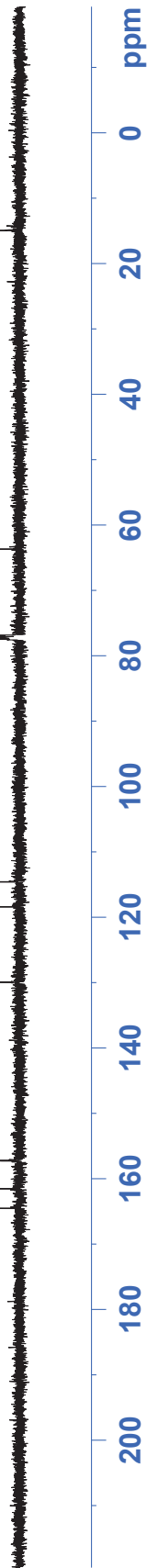
===== CHANNEL f1 =====
NUC1       13C
P1         9.50 usec
PL1        -0.50 dB
SFO1       125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        1.00 dB
PL12       16.31 dB
PL13       16.50 dB
SFO2       500.1320005 MHz
SI         32768
SF         125.7577761 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```

164.52
161.53
157.23
129.93
118.39
114.57
63.67
14.89



1d



SBR-0-6
 PROTON CDCl3

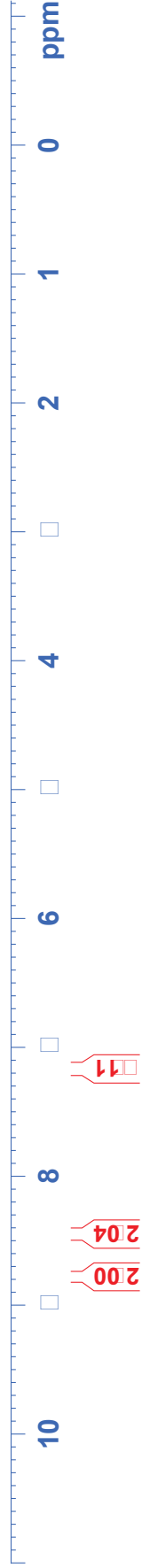
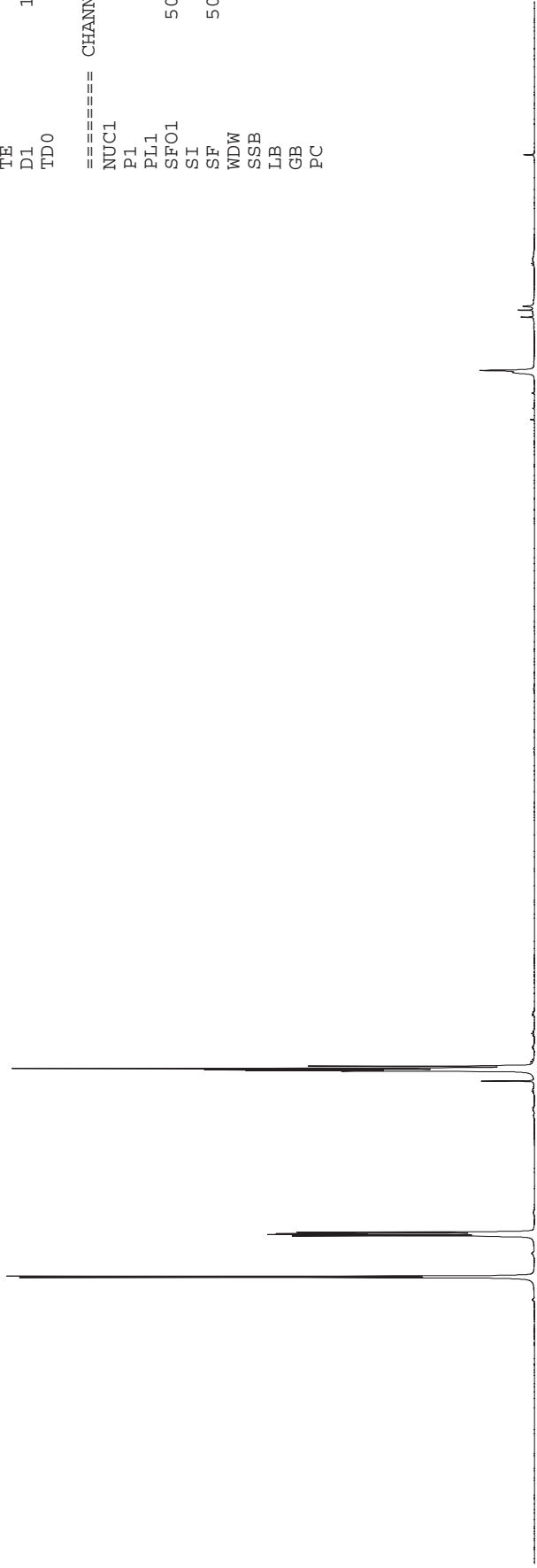
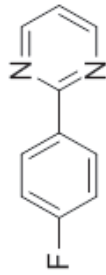
```

NAME      XB20081024
EXPNO     12
PROCNO    1
Date_     20081024
Time      9.45
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        10330.578 Hz
FIDRES     0.157632 Hz
AQ         3.1720407 sec
RG         256
DW         48.400 usec
DE         6.00 usec
TE         293.9 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         14.50 usec
PL1        2.00 dB
SFO1       500.1330885 MHz
SI         32768
SF         500.1300130 MHz
WDW        no
SSB        0
LB         0.00 Hz
GB         0
PC         1.00
  
```

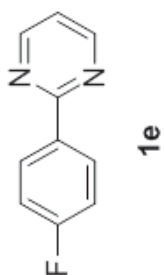
7.144
 7.162
 7.173
 7.179
 7.182
 7.182
 7.179
 7.173
 7.162
 7.144

8.784
 8.774
 8.461
 8.450
 8.443
 8.432



SBR-0-6
19Fdeft CDCI3

-110.234
-110.245
-110.250
-110.257
-110.263
-110.270
-110.277
-110.281
-110.293



NAME XB20081024
EXPNO 13
PROCNO 1
Date_ 20081024
Time_ 9.47
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg
TD 131072
SOLVENT CDCI3
NS 16
DS 4
SWH 100000.000 Hz
FIDRES 0.762939 Hz
AQ 0.6554150 sec
RG 322.5
DW 5.000 usec
DE 6.00 usec
TE 293.8 K
D1 1.00000000 sec
TD0 1
===== CHANNEL f1 =====
NUC1 19F
P1 19.30 usec
PL1 4.00 dB
SFO1 470.5453180 MHz
SI 65536
SF 470.5923770 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

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

SBR-0-6
C13CPD CDCl3

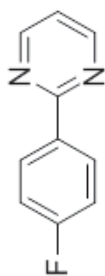
```

NAME          XB20081024
EXPNO         14
PROCNO        1
Date_         20081024
Time_         9.55
INSTRUM       spect
PROBHD        5 mm PATXO 19F
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            128
DS            4
SWH           30030.029 Hz
FIDRES        0.458222 Hz
AQ            1.0912410 sec
RG            101.6
DW            16.650 usec
DE            6.00 usec
TE            295.1 K
D1            2.0000000 sec
d11           0.0300000 sec
DELTA        1.89999998 sec
TD0           1

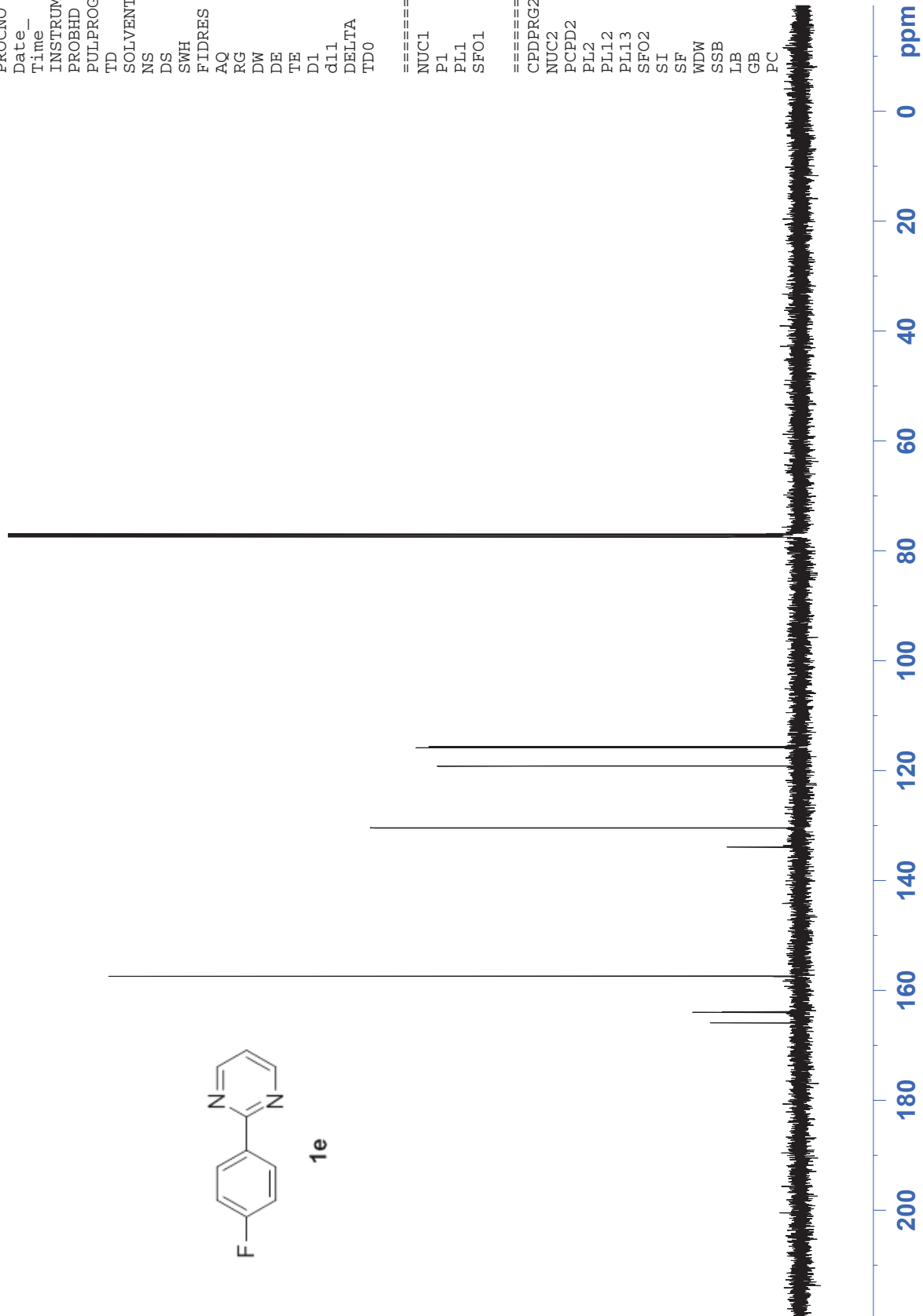
===== CHANNEL f1 =====
NUC1          13C
P1            9.50 usec
PL1          -0.50 dB
SFO1         125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2          1H
PCPD2        80.00 usec
PL2           2.00 dB
PL12         16.50 dB
PL13         16.50 dB
SFO2         500.1320005 MHz
SI           32768
SF           125.7577748 MHz
WDW           EM
SSB           0
LB           1.00 Hz
GB           0
PC           1.40
  
```

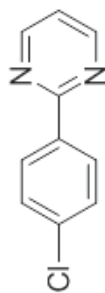
165.85
163.95
163.85
157.38
133.88
133.86
130.42
130.35
119.12
115.77
115.60



1e



7.183
7.193
7.203
7.448
7.462
7.465
7.465
8.378
8.382
8.392
8.395
8.785
8.785
8.795

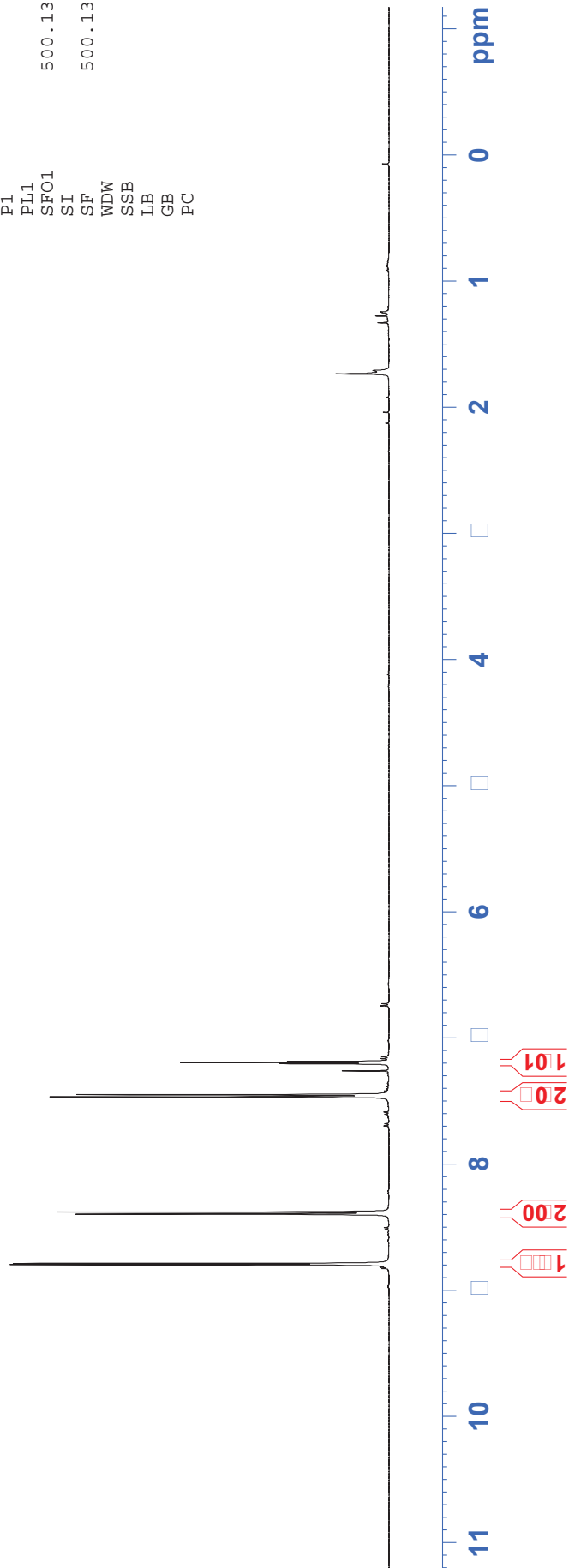


1f

SBR-0-5
PROTON CDCl3

NAME XB20081029
EXPNO 21
PROCNO 1
Date_ 20081029
Time_ 15.51
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 256
DW 48.400 usec
DE 6.00 usec
TE 293.8 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 2.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300133 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



SBR-0-5
C13CPD CDCl3

```

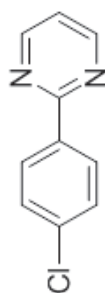
NAME      XB20081029
EXPNO     24
PROCNO    1
Date_     20081029
Time_     17.17
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         127
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         161.3
DE         16.650 usec
TE         6.00 usec
TE         295.5 K
D1         2.00000000 sec
d11        0.03000000 sec
DELTA     1.89999998 sec
TD0        1
  
```

```

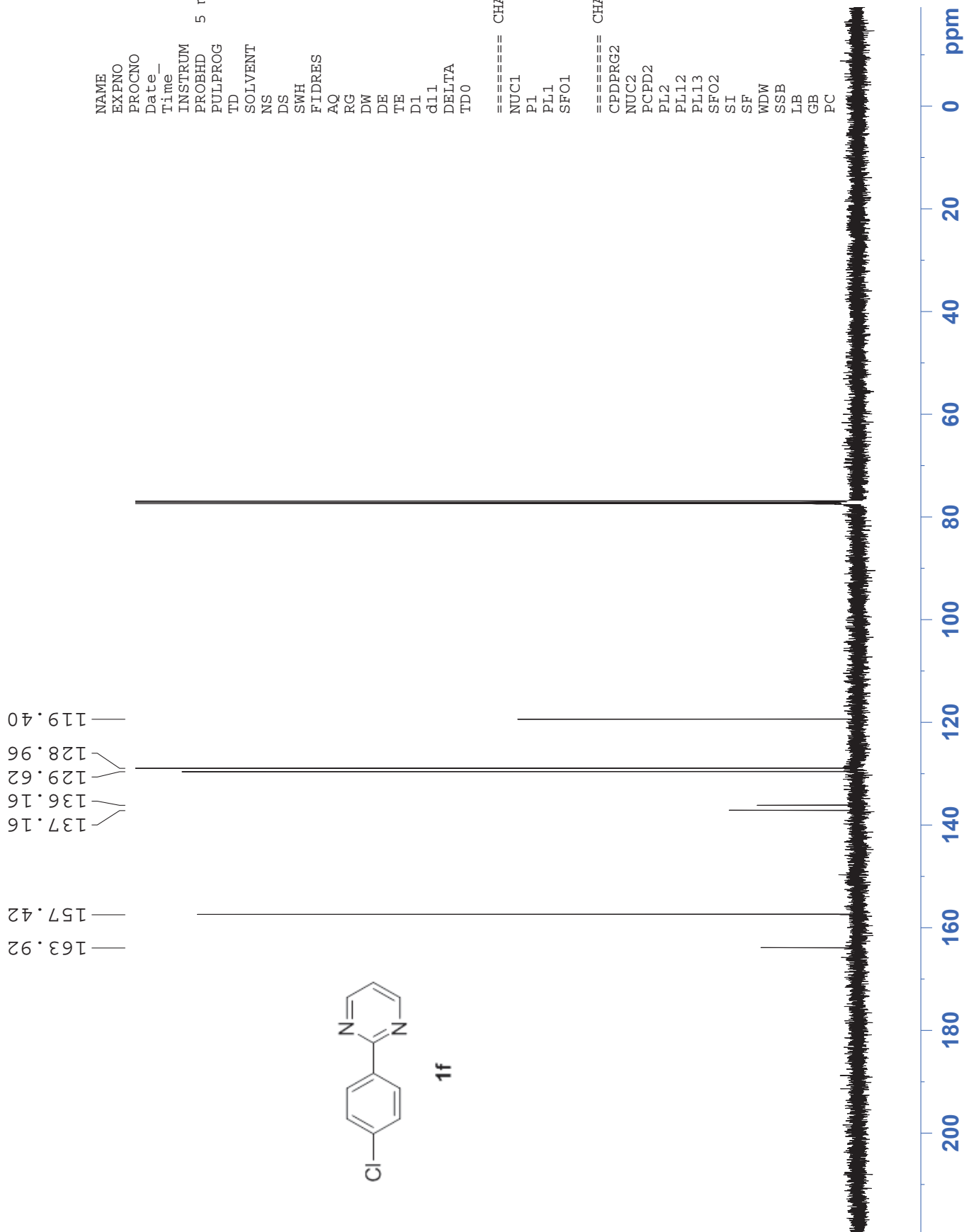
===== CHANNEL f1 =====
NUC1       13C
P1         9.50 usec
PL1        -0.50 dB
SFO1       125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        2.00 dB
PL12       16.50 dB
PL13       16.50 dB
SFO2       500.1320005 MHz
SI         32768
SF         125.7577745 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```

163.92
157.42
137.16
136.16
129.62
128.96
119.40



1f

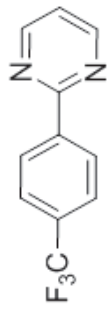


ZXJ-0-7
 PROTON CDCl3

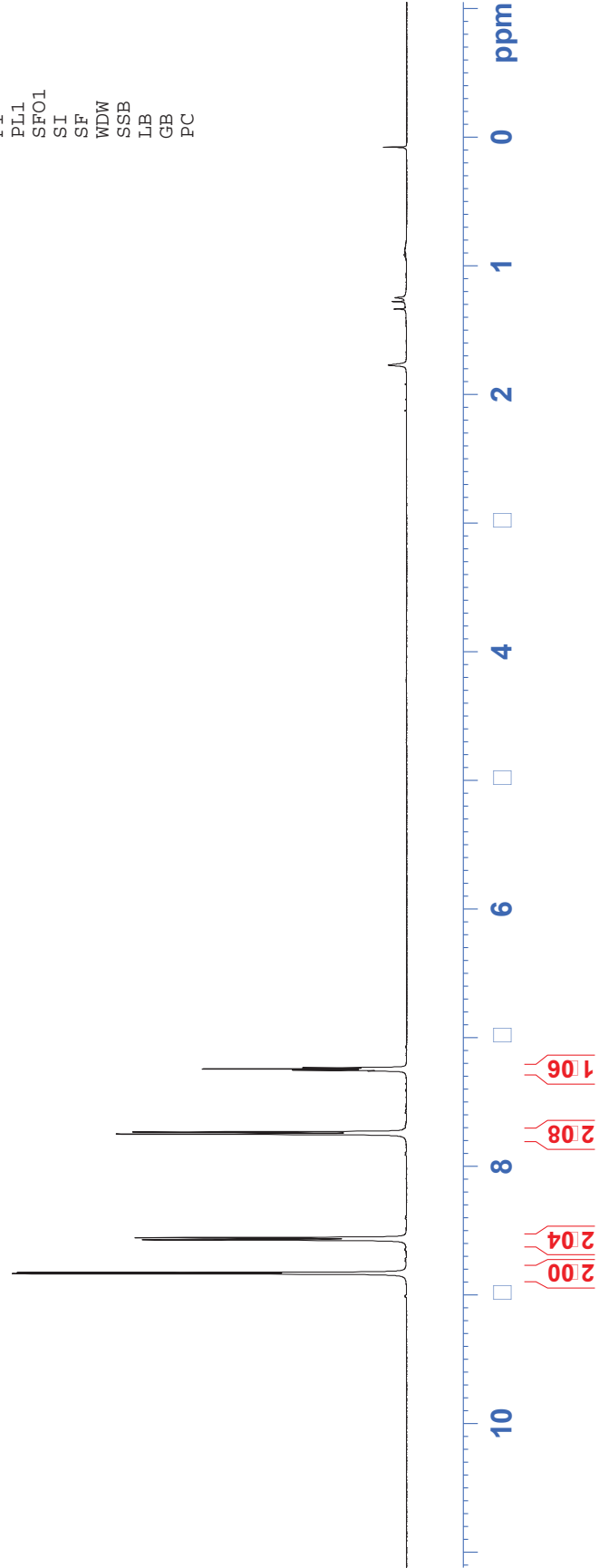
NAME XB20090109
 EXPNO 51
 PROCNO 1
 Date_ 20090109
 Time_ 11.20
 INSTRUM spect
 PROBHD 5 mm PATXO 19F
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1720407 sec
 RG 181
 DW 48.400 usec
 DE 6.00 usec
 TE 293.3 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 15.66 usec
 PL1 2.00 dB
 SFO1 500.1330885 MHz
 SI 32768
 SF 500.1300130 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

8.836
 8.826
 8.572
 8.556
 7.750
 7.734
 7.253
 7.243
 7.234

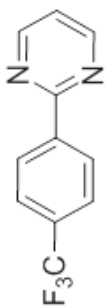


1g



ZXJ-0-7
19Fdeft CDCI3

-62.719



1g

NAME XB20090109
EXPNO 52
PROCNO 1
Date_ 20090109
Time_ 11.22
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg
TD 131072
SOLVENT CDCI3
NS 16
DS 4
SWH 100000.000 Hz
FIDRES 0.762939 Hz
AQ 0.6554150 sec
RG 203.2
DW 5.000 usec
DE 6.00 usec
TE 293.2 K
D1 1.00000000 sec
TD0 1

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

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

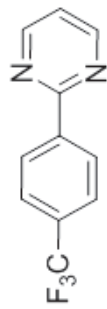
ZXJ-0-7
C13CPD CDCl3

NAME XB20090109
EXPNO 55
PROCNO 1
Date_ 20090109
Time 13.48
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 295.0 K
D1 2.0000000 sec
d11 0.0300000 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 2.00 dB
PL12 16.50 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

163.39
157.39
140.82
132.71
132.45
132.20
131.94
128.45
125.56
125.53
125.51
125.48
125.21
123.05
120.89
119.82



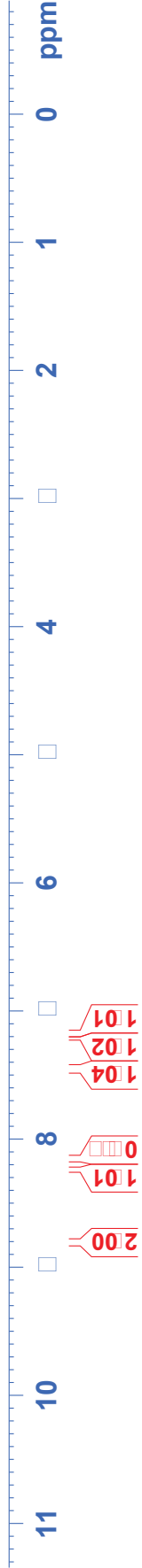
ZXJ-1-373
 PROTON CDCl3

```

NAME      XB20091013
EXPNO     2
PROCNO    1
Date_     20091013
Time      11.42
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         181
DW         48.400 usec
DE         6.00 usec
TE         294.5 K
D1         1.00000000 sec
TD0        1

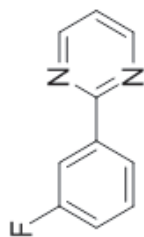
===== CHANNEL f1 =====
NUC1       1H
P1         15.98 usec
PL1        2.00 dB
SFO1       500.1330885 MHz
SI         32768
SF         500.1300129 MHz
WDW        no
SSB        0
LB         0.00 Hz
GB         0
PC         1.00
  
```

8.245
8.234
8.232
8.229
8.167
8.164
8.162
8.159
8.147
8.144
8.142
8.139
7.474
7.462
7.458
7.446
7.442
7.430
7.220
7.211
7.206
7.201
7.199
7.197
7.194
7.191
7.182
7.180
7.177
7.175
7.166
7.164
7.160
7.159



ZXJ-1-373
19Fdeft CDCI3

-113.077
-113.088
-113.095
-113.109
-113.117
-113.129



1h

NAME XB20091013
EXPNO 1
PROCNO 1
Date_ 20091013
Time_ 11.39
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg
TD 131072
SOLVENT CDCI3
NS 16
DS 4
SWH 100000.000 Hz
FIDRES 0.762939 Hz
AQ 0.6554150 sec
RG 322.5
DW 5.000 usec
DE 6.00 usec
TE 294.6 K
D1 1.00000000 sec
TD0 1

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

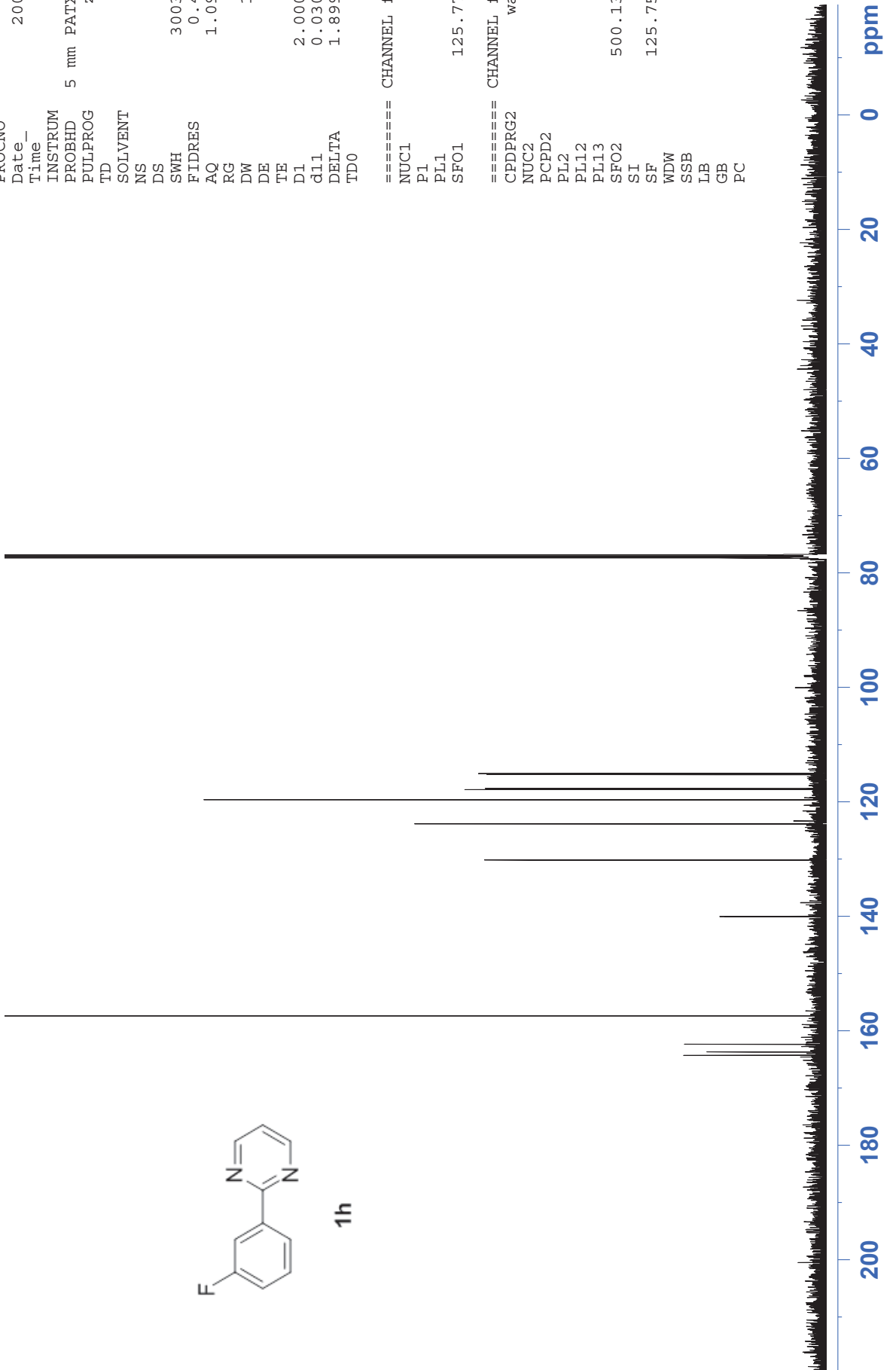
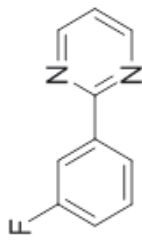
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 ppm

ZXJ-1-370
C13CPD CDCl3

```

NAME      XB20091013
EXPNO     6
PROCNO    1
Date_     20091013
Time      15.45
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         143.7
DW         16.650 usec
DE         6.00 usec
TE         296.4 K
D1         2.0000000 sec
d11        0.0300000 sec
DELTA     1.89999998 sec
TDO        1
===== CHANNEL f1 =====
NUC1       13C
P1         9.50 usec
PL1        -0.50 dB
SFO1       125.7703643 MHz
===== CHANNEL f2 =====
CPDPRG2    waitz16
NUC2       1H
PCPD2      80.00 usec
PL2        2.00 dB
PL12       16.50 dB
PL13       16.50 dB
SFO2       500.1320005 MHz
SI         32768
SF         125.7577745 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```

164.32
163.73
163.71
162.37
157.42
140.11
140.04
130.23
130.17
123.88
123.86
119.66
117.86
117.69
115.26
115.07

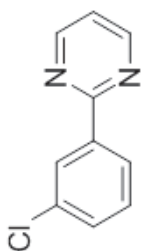


HXH-4-33
 PROTON CDC13

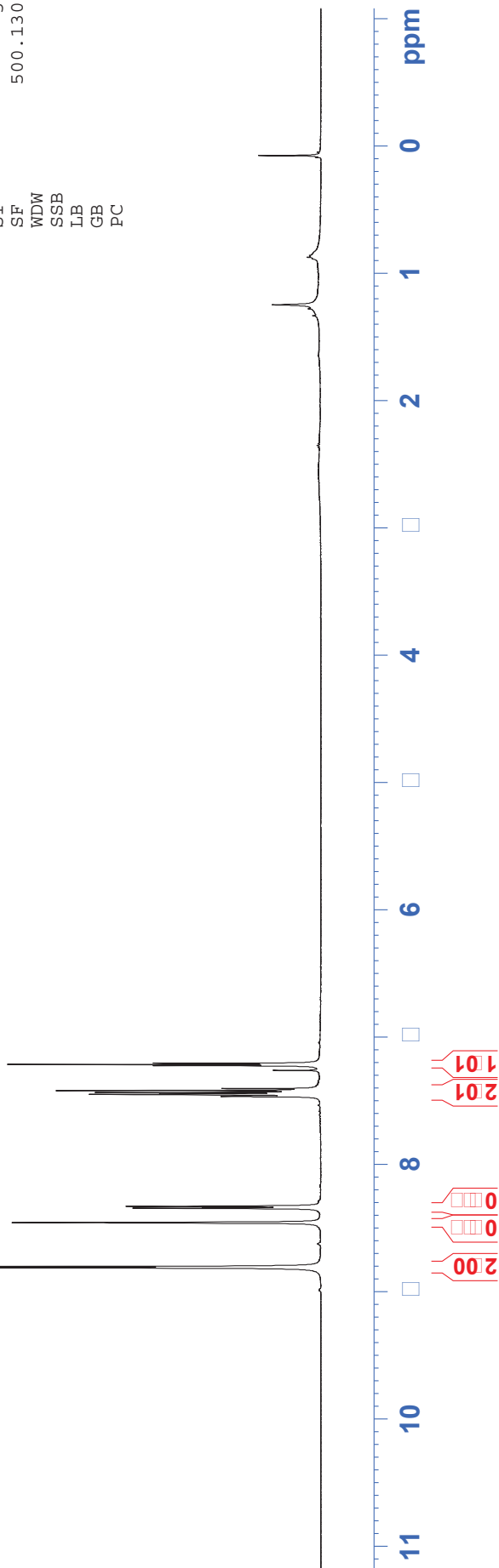
NAME XB20121112
 EXPNO 6
 PROCNO 1
 Date 20121112
 Time 10.28
 INSTRUM spect
 PROBHD 5 mm PATXO 19F
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 8
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1720407 sec
 RG 161.3
 DW 48.400 usec
 DE 6.00 usec
 TE 296.4 K
 D1 1.0000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 13.72 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

8.811
 8.801
 8.456
 8.452
 8.345
 8.342
 8.339
 8.330
 8.327
 7.467
 7.464
 7.460
 7.451
 7.448
 7.445
 7.434
 7.418
 7.403
 7.223
 7.213
 7.204



1i



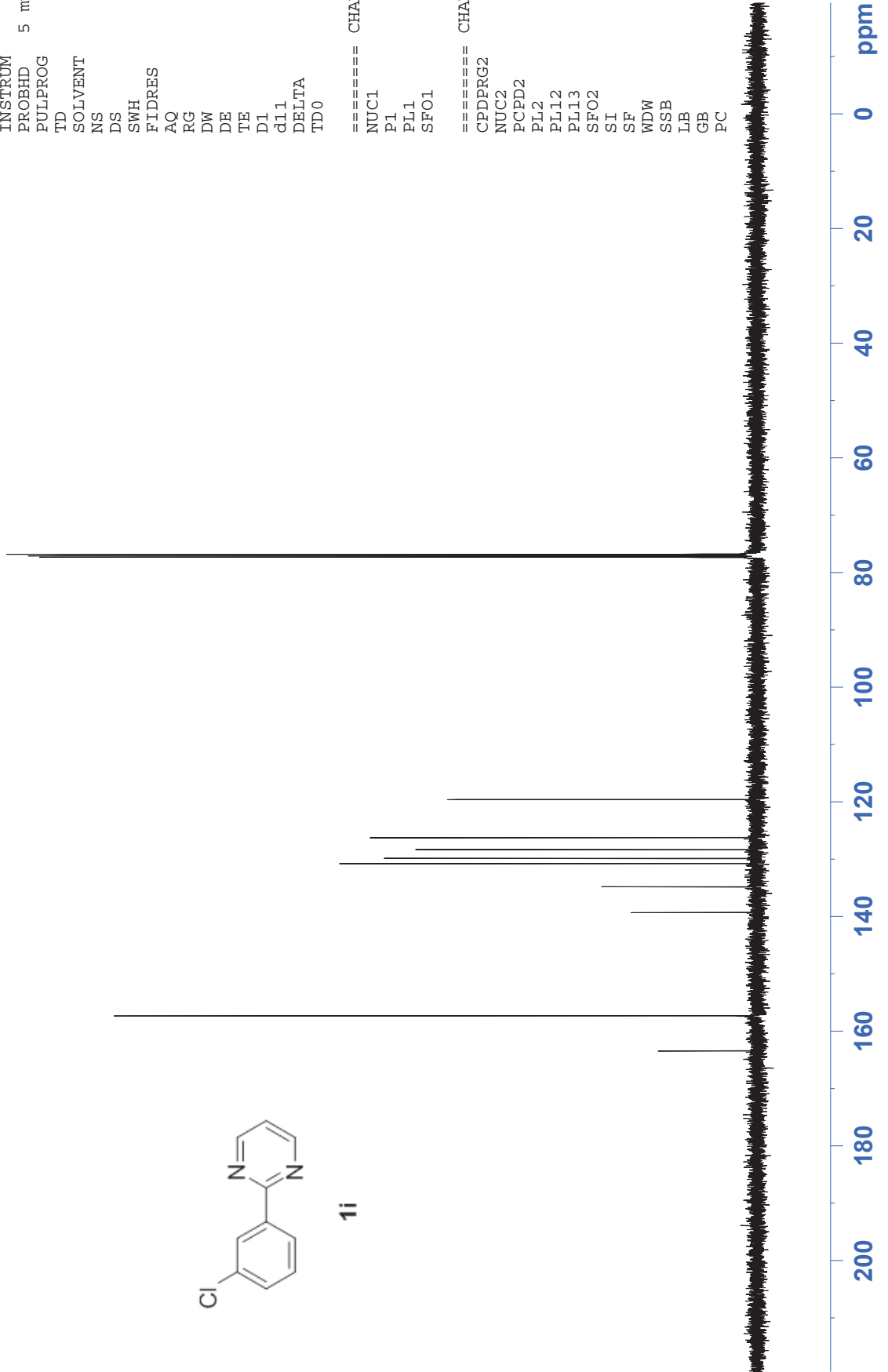
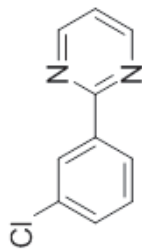
HXH-4-33
 C13CPD CDCl₃:

```

NAME      XB20121112
EXPNO    7
PROCNO   1
Date_    20121112
Time     10.36
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         90.5
DW         16.650 usec
DE         6.00 usec
TE         297.5 K
D1         2.00000000 sec
d11        0.03000000 sec
DELTA     1.89999998 sec
TD0        1
===== CHANNEL f1 =====
NUC1      13C
P1         9.50 usec
PL1        -0.50 dB
SFO1      125.7703643 MHz
===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2     80.00 usec
PL2        1.00 dB
PL12      16.31 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
  
```

139.31
 134.80
 130.77
 129.86
 128.32
 126.24
 119.59

163.45
 157.32



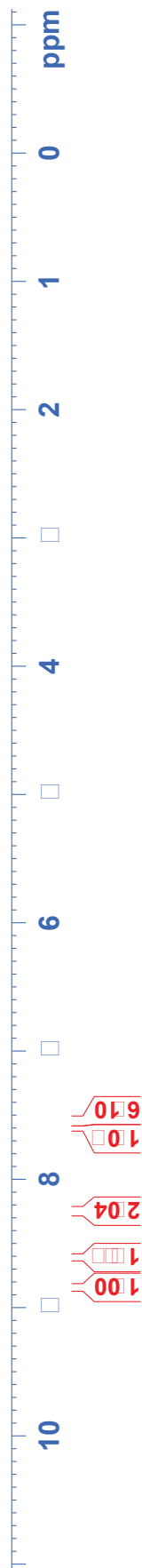
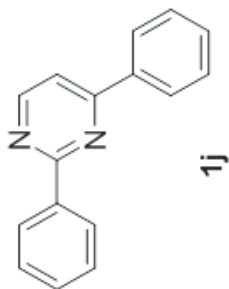
ZXJ-0-26
 PROTON CDC13

```

NAME      XB20090104
EXPNO     23
PROCNO    1
Date_     20090104
Time      10.28
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zg30
TD         65536
SOLVENT   CDC13
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         293.4 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         15.66 usec
PL1        2.00 dB
SFO1       500.1330885 MHz
SI         32768
SF         500.1300132 MHz
WDW        no
SSB        0
LB         0.00 Hz
GB         0
PC         1.00
  
```

8.604
8.603
8.599
8.596
8.250
8.248
8.245
8.243
8.241
8.237
8.234
8.230
7.608
7.603
7.598
7.593
7.571
7.567
7.560
7.556
7.552
7.549
7.543
7.539
7.533
7.529
7.527
7.521
7.519
7.516



ZXJ-0-26
C13CPD CDC13

```

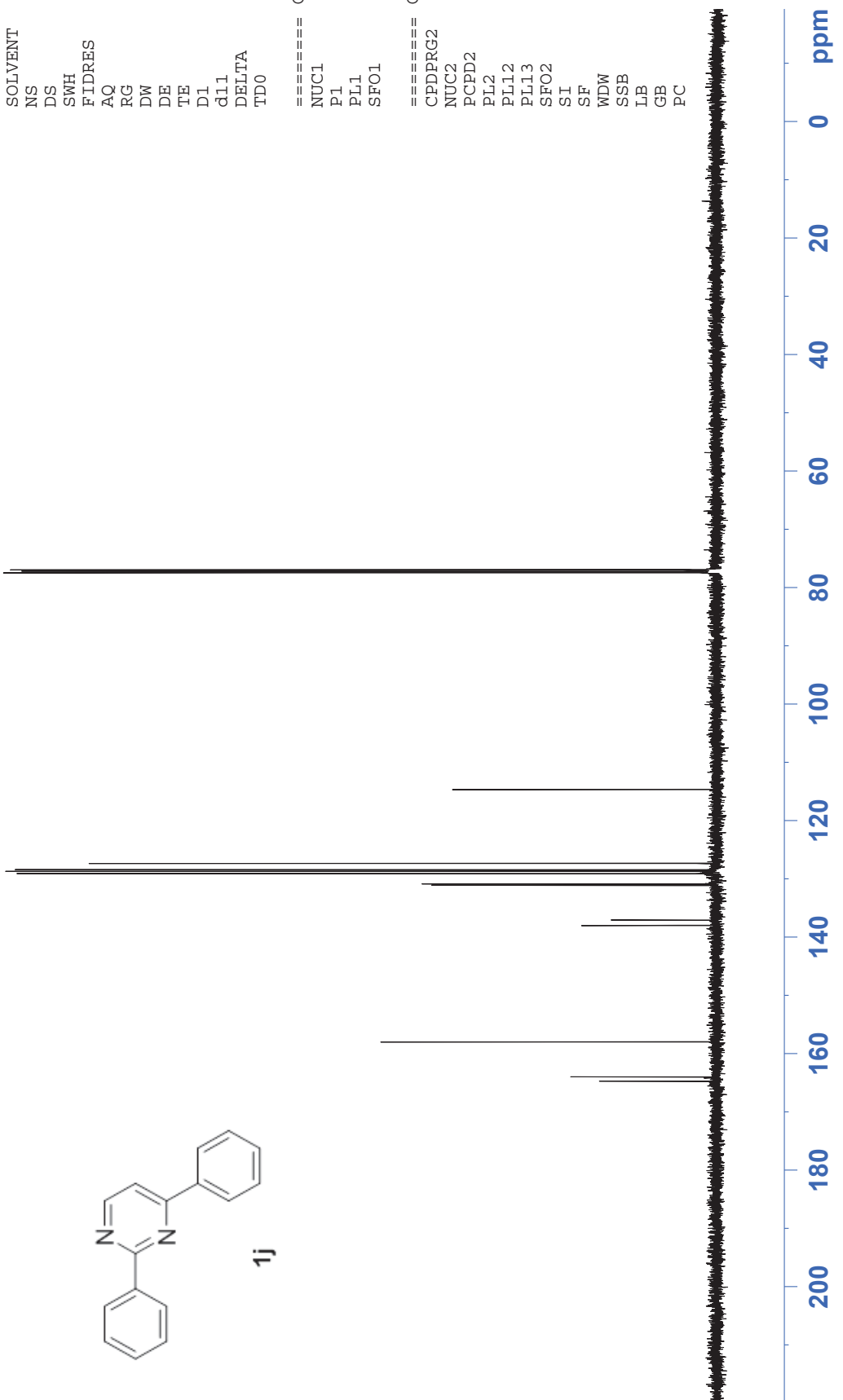
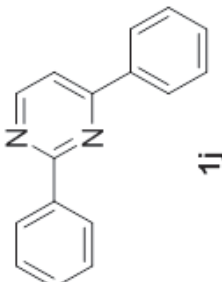
NAME      XB20090104
EXPNO     25
PROCNO    1
Date_     20090104
Time_     13.42
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDC13
NS         128
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         203.2
DW         16.650 usec
DE         6.00 usec
TE         294.8 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       2.00 dB
PL12     16.50 dB
PL13     16.50 dB
SFO2     500.1320005 MHz
SI        32768
SF        125.7577783 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```

164.69
163.97
157.97
137.97
137.06
131.09
130.84
129.06
128.67
128.40
127.32
114.64



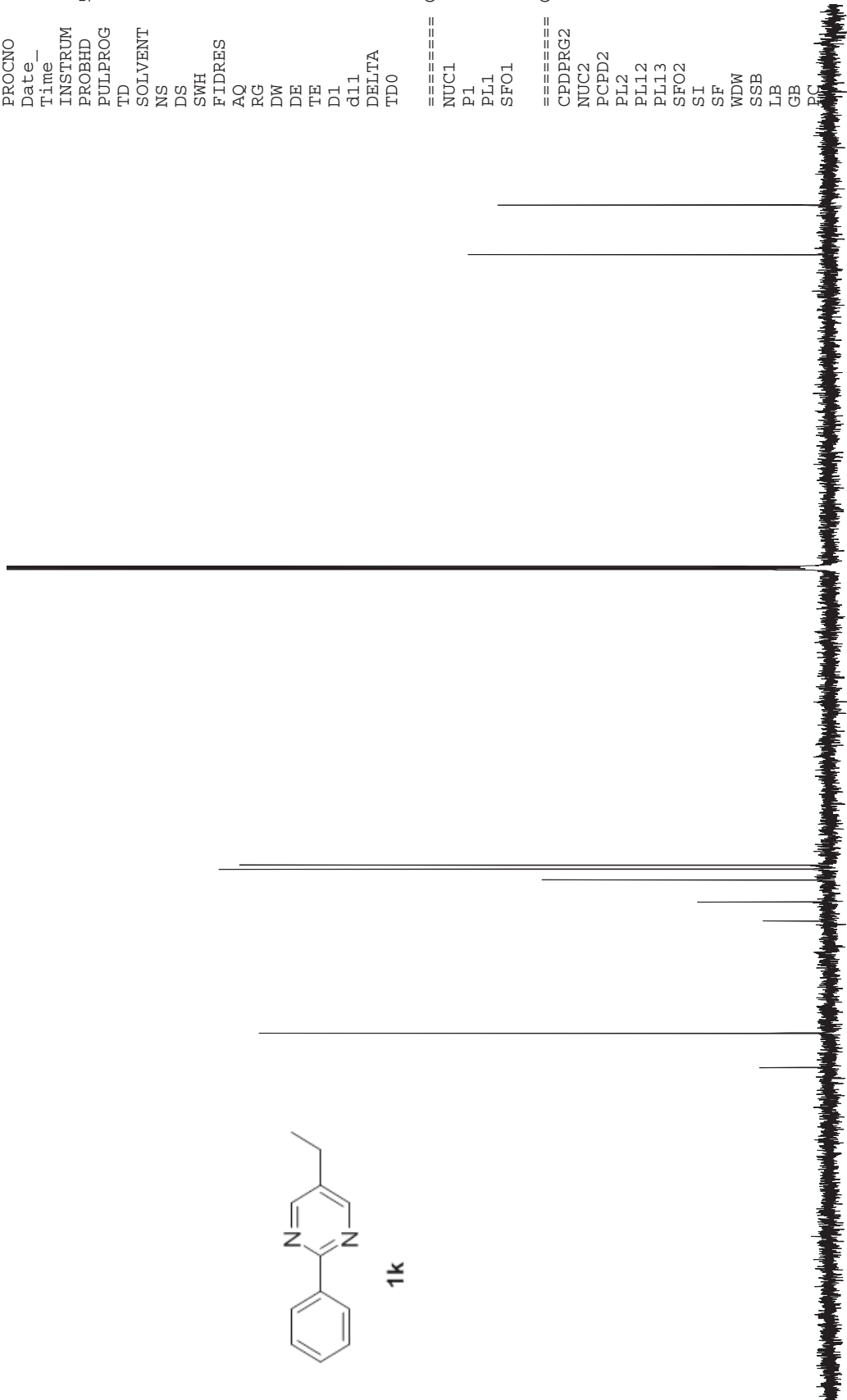
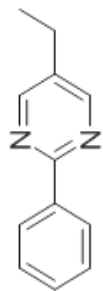
WH-1-48
 C13CPD CDCL3

NAME xb20121025
 EXPNO 15
 PROCNO 1
 Date_ 20121025
 Time_ 19.41
 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 297.6 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.89999998 sec
 TDO 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 16.31 dB
 PL13 16.50 dB
 SFO2 500.1320005 MHz
 SI 32768
 SF 125.7577742 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.40

15.08
 23.54

128.04
 128.72
 130.57
 134.36
 137.58
 156.80
 162.68



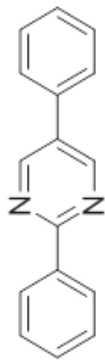
200 180 160 140 120 100 80 60 40 20 0 ppm

ZXJ-0-27
 PROTON CDCl3

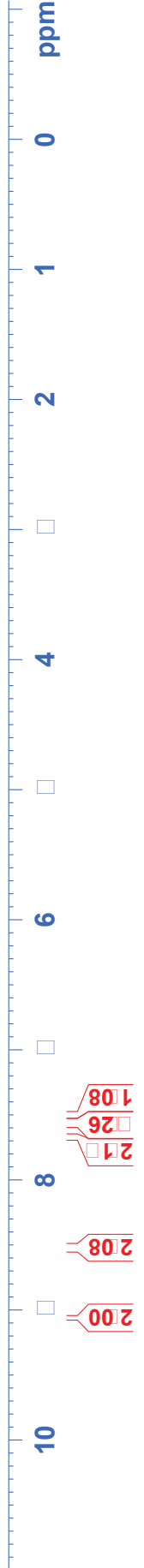
NAME XB20090218
 EXPNO 1
 PROCNO 1
 Date_ 20090218
 Time_ 10.29
 INSTRUM spect
 PROBHD 5 mm PATXO 19F
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1720407 sec
 RG 322.5
 DW 48.400 usec
 DE 6.00 usec
 TE 293.7 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 15.66 usec
 PL1 2.00 dB
 SFO1 500.1330885 MHz
 SI 32768
 SF 500.1300000 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

9.058
 8.528
 8.522
 8.519
 8.512
 8.508
 7.677
 7.674
 7.670
 7.660
 7.654
 7.580
 7.577
 7.566
 7.554
 7.550
 7.543
 7.540
 7.534
 7.531
 7.514
 7.512
 7.510
 7.501
 7.497
 7.493
 7.485
 7.482
 7.480



11



ZXJ-0-27
C13CPD CDCl3

```

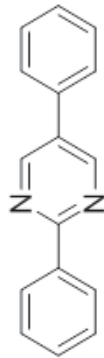
NAME      XB20090218
EXPNO     2
PROCNO    1
Date_     20090218
Time_     16.31
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         512
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         161.3
DE         16.650 usec
TE         6.00 usec
TE         294.9 K
D1         2.00000000 sec
d11        0.03000000 sec
DELTA     1.89999998 sec
TD0        1
  
```

```

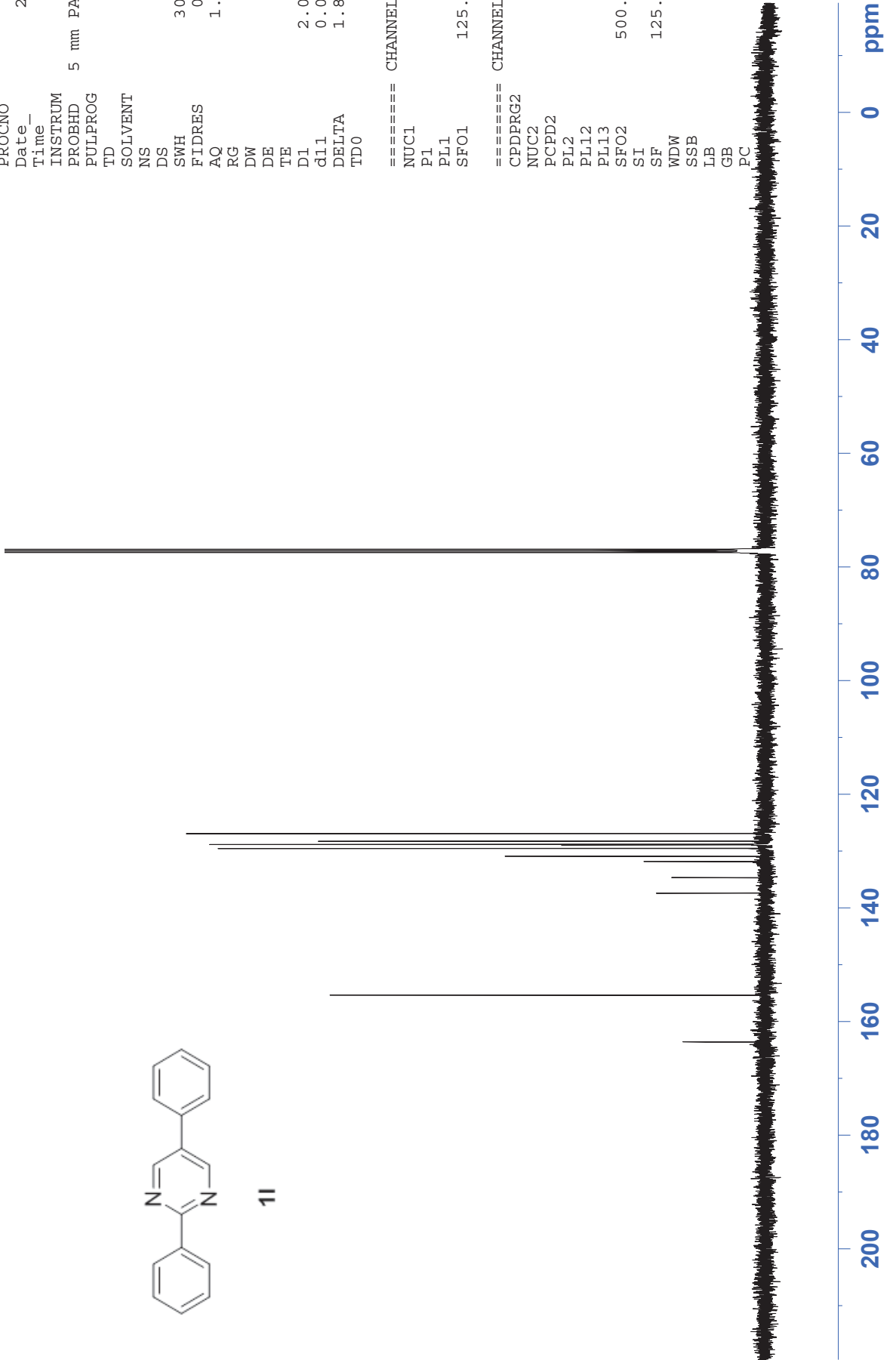
===== CHANNEL f1 =====
NUC1      13C
P1        9.50 usec
PL1       -0.50 dB
SFO1     125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       2.00 dB
PL12     16.50 dB
PL13     16.50 dB
SFO2     500.1320005 MHz
SI        32768
SF        125.7577737 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```

126.93
128.25
128.82
128.91
128.95
129.55
130.91
131.83
134.68
137.43
155.37
163.60



11



HXH-H+C
C13CPD CDCl3

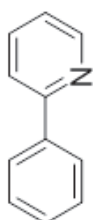
```

NAME          XB20120927
EXPNO         4
PROCNO        1
Date_         20120927
Time_         11.31
INSTRUM       spect
PROBHD        5 mm PATXO 19F
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            128
DS            4
SWH           30030.029 Hz
FIDRES        0.458222 Hz
AQ            1.0912410 sec
RG            228.1
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

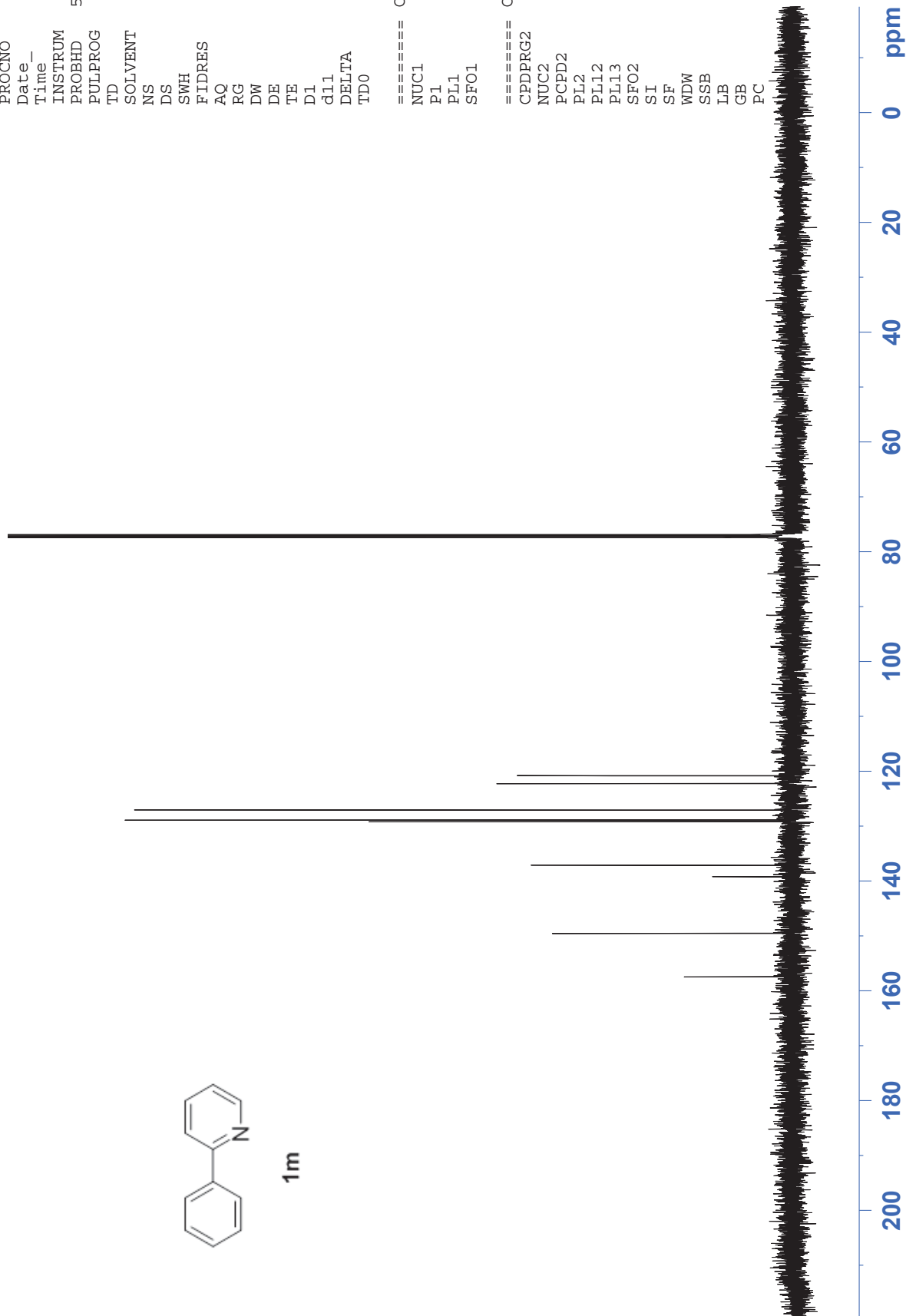
===== CHANNEL f1 =====
NUC1          13C
P1            9.50 usec
PL1           -0.50 dB
SFO1          125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           1.00 dB
PL12          16.31 dB
PL13          16.50 dB
SFO2          500.1320005 MHz
SI            32768
SF            125.7577746 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```

157.48
149.57
139.24
137.15
129.21
128.92
127.09
122.29
120.84



1m

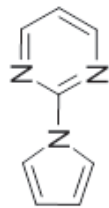


XSG-FT
PROTON CDCL3

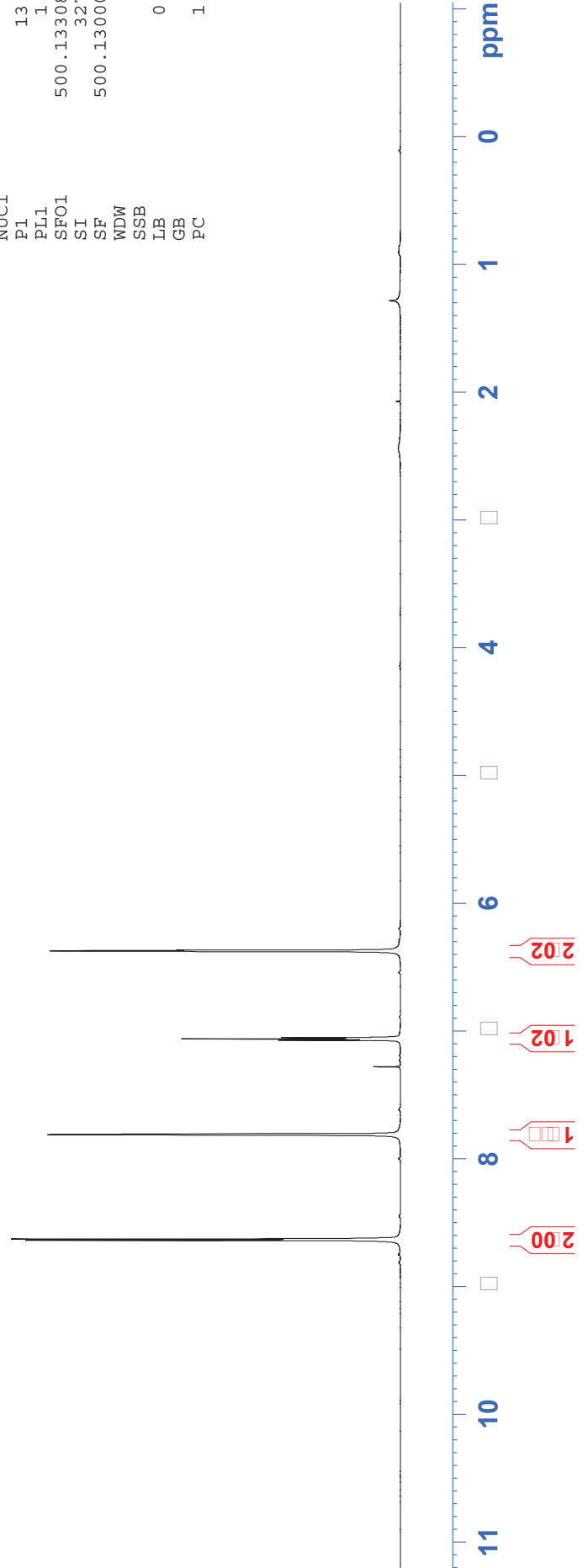
NAME XB20120223
 EXPNO 7
 PROCNO 1
 Date_ 20120223
 Time_ 17.42
 INSTRUM spect
 PROBHD 5 mm PATXO 19F
 PULPROG zg30
 TD 65536
 SOLVENT CDCL3
 NS 8
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1720407 sec
 RG 203.2
 DW 48.400 usec
 DE 6.00 usec
 TE 293.8 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 13.65 usec
 PL1 1.00 dB
 SFO1 500.1330885 MHz
 SI 32768
 SF 500.1300027 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

8.639
 8.629
 7.814
 7.811
 7.810
 7.072
 7.062
 7.057
 7.052
 6.373
 6.372
 6.370
 6.367



1o



XSG-FT C
C13CPD CDCl3

```

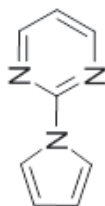
NAME          xb20120224
EXPNO         5
PROCNO        1
Date_         20120224
Time_         10.29
INSTRUM       spect
PROBHD        5 mm PATXO 19F
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            128
DS            4
SWH           30030.029 Hz
FIDRES        0.458222 Hz
AQ            1.0912410 sec
RG            161.3
DW            16.650 usec
DE            6.00 usec
TE            295.2 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           2.00 dB
PL12         16.77 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
  
```

119.07
117.15
112.04

158.37
156.21



1o

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

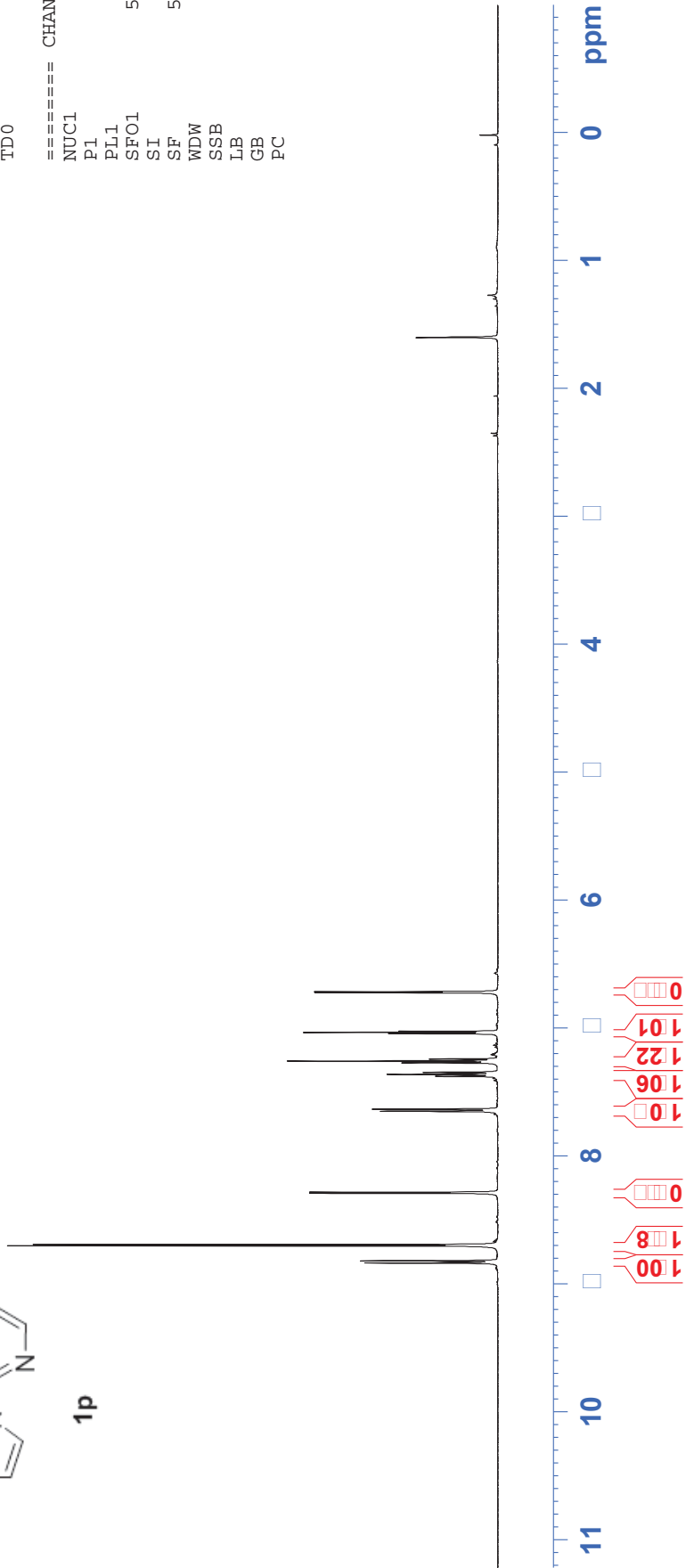
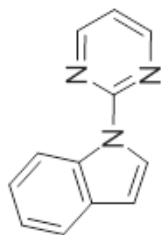
314
 PROTON CDCl3

```

NAME      XB20110402
EXPNO     11
PROCNO    1
Date_     20110402
Time      16.49
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         8
DS         2
SWH       10330.578 Hz
FIDRES    0.157632 Hz
AQ         3.1720407 sec
RG         181
DW         48.400 usec
DE         6.00 usec
TE         293.7 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1      1H
P1        15.60 usec
PL1       2.00 dB
SFO1     500.1330885 MHz
SI        32768
SF        500.1300129 MHz
WDW       no
SSB       0
LB        0.00 Hz
GB        0
PC        1.00
  
```

8.838
 8.821
 8.703
 8.693
 8.292
 8.284
 7.651
 7.636
 7.635
 7.378
 7.364
 7.362
 7.347
 7.273
 7.271
 7.260
 7.258
 7.243
 7.046
 7.044
 7.037
 7.035
 7.027
 7.025
 6.724
 6.717



XSG-1-314
C13CPD CDCl3

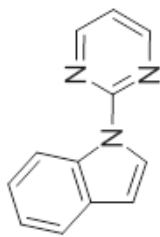
```

NAME          XB20120221
EXPNO         4
PROCNO        1
Date_         20120221
Time_         17.50
INSTRUM       spect
PROBHD        5 mm PATXO 19F
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            128
DS            4
SWH           30030.029 Hz
FIDRES        0.458222 Hz
AQ            1.0912410 sec
RG            114
DW            16.650 usec
DE            6.00 usec
TE            295.4 K
D1            2.0000000 sec
d11           0.0300000 sec
DELTA         1.89999998 sec
TD0           1

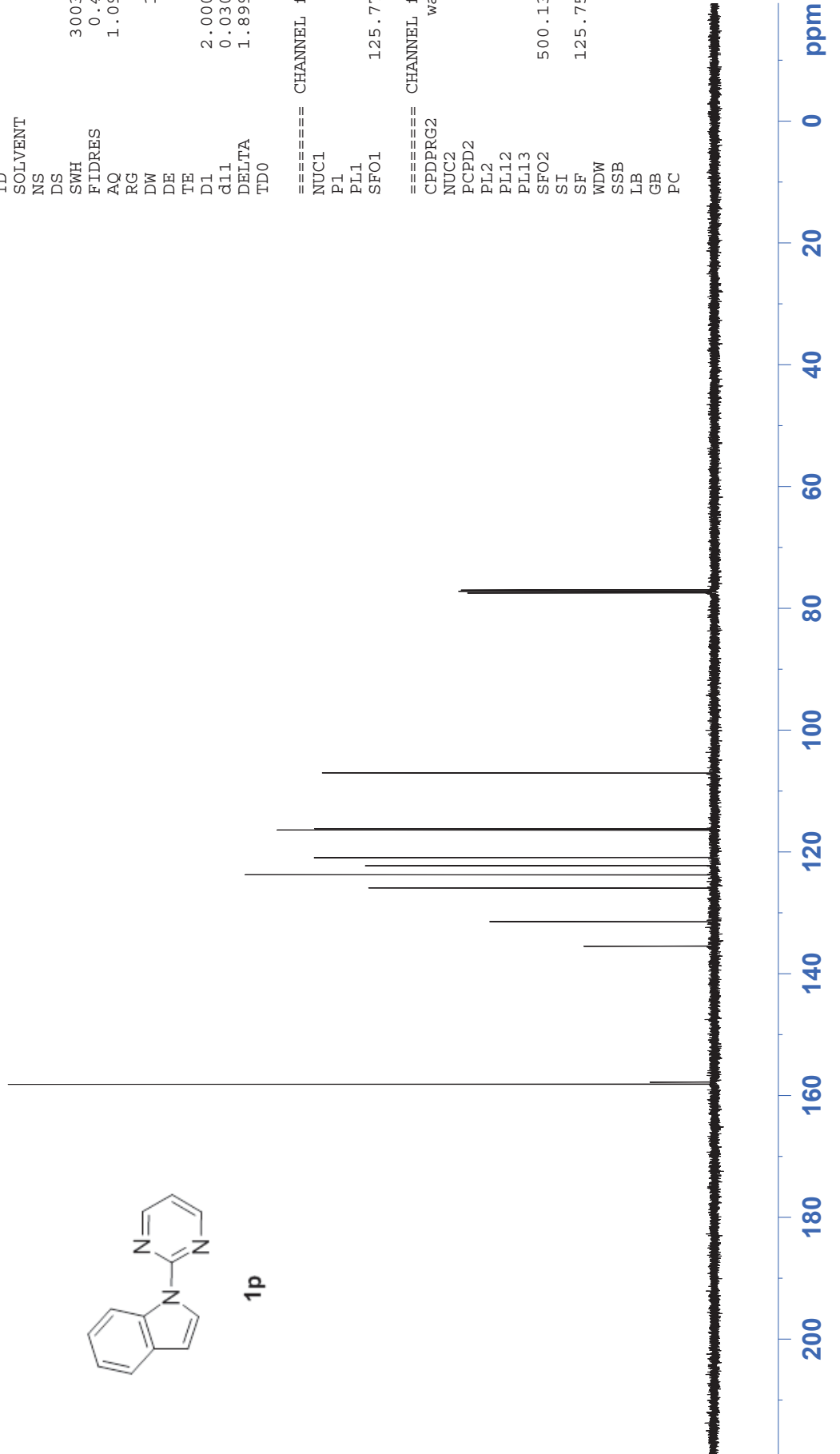
===== CHANNEL f1 =====
NUC1          13C
P1            9.50 usec
PL1           -0.50 dB
SFO1         125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2       waitz16
NUC2          1H
PCPD2         80.00 usec
PL2           2.00 dB
PL12          16.77 dB
PL13          16.50 dB
SFO2         500.1320005 MHz
SI            32768
SF            125.7577883 MHz
WDW           no
SSB           0
LB            0.00 Hz
GB            0
PC            1.40
    
```

158.11
157.77
135.43
131.39
125.88
123.71
122.20
120.89
116.37
116.14
106.99



1p

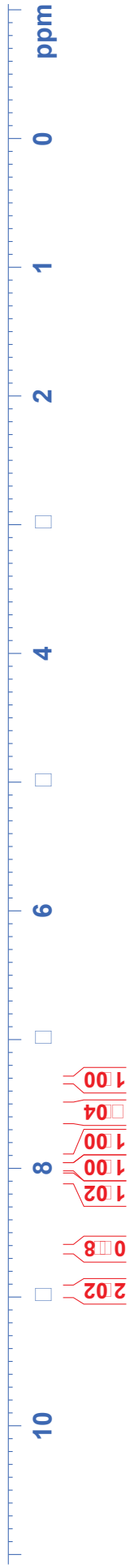
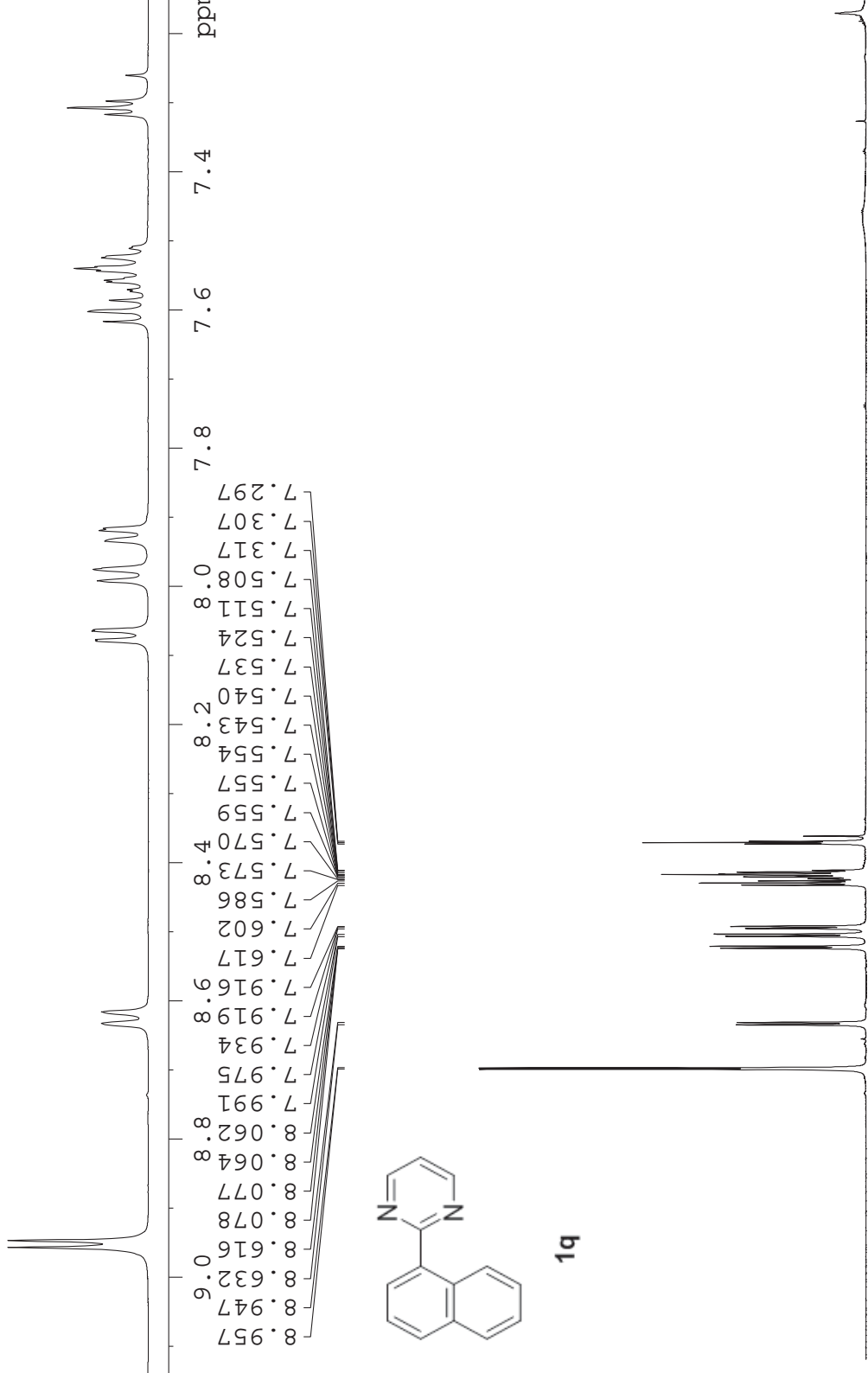


WH-1-46
 PROTON CDC13

7.307
 7.317
 7.508
 7.511
 7.524
 7.537
 7.540
 7.543
 7.554
 7.557
 7.559
 7.570
 7.573
 7.586
 7.602
 7.617
 7.916
 7.919
 7.934
 7.975
 7.991
 8.062
 8.064
 8.077
 8.078
 8.616
 8.632
 8.947
 8.957

NAME xb20121025
 EXPNO 6
 PROCNO 1
 Date_ 20121025
 Time_ 18.16
 INSTRUM spect
 PROBHD 5 mm PATXO 19F
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 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 296.1 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 13.72 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-1-46
C13CPD CDCl3

```

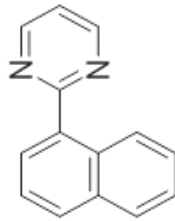
NAME          xb20121025
EXPNO         14
PROCNO        1
Date_         20121025
Time_         19.28
INSTRUM       spect
PROBHD        5 mm PATXO 19F
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            129
DS            4
SWH           30030.029 Hz
FIDRES        0.458222 Hz
AQ            1.0912410 sec
RG            143.7
DE            16.650 usec
TE            297.5 K
D1            2.0000000 sec
d11           0.0300000 sec
DELTA         1.89999998 sec
TD0           1
  
```

```

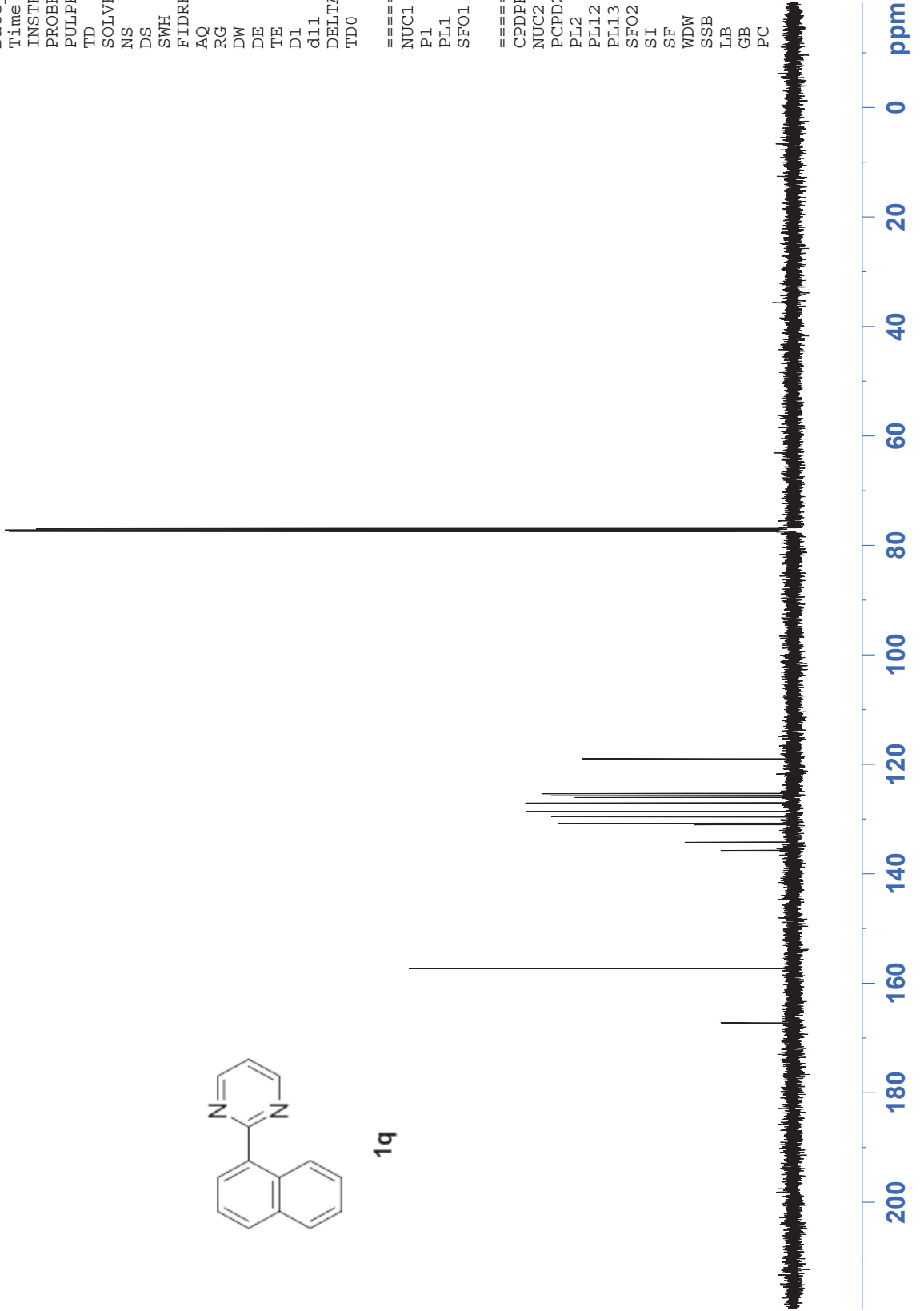
===== CHANNEL f1 =====
NUC1          13C
P1            9.50 usec
PL1           -0.50 dB
SFO1         125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2          1H
PCPD2        80.00 usec
PL2           1.00 dB
PL12         16.31 dB
PL13         16.50 dB
SFO2         500.1320005 MHz
SI           32768
SF           125.7577766 MHz
WDW           EM
SSB           0
LB           1.00 Hz
GB           0
PC           1.40
  
```

167.25
157.31
135.72
134.21
131.03
130.78
129.58
128.63
127.05
126.05
125.72
125.32
118.99



1q

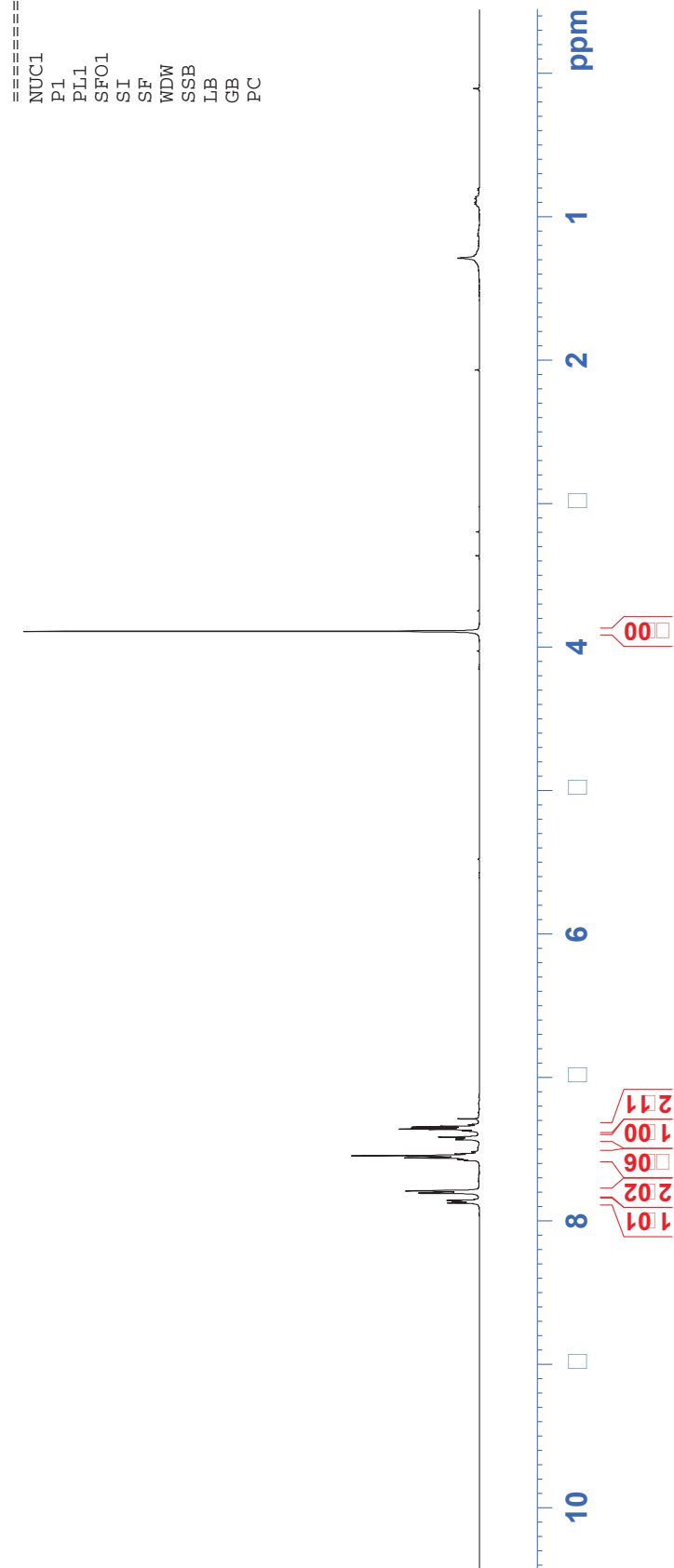
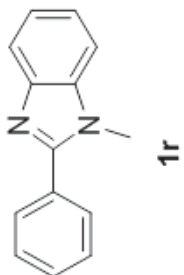


HXH-5-BM
PROTON CDCl3

```

NAME          XB20130417
EXPNO         7
PROCNO        1
Date_         20130417
Time_         11.35
INSTRUM       spect
PROBHD        5 mm PATXO 19F
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            8
DS            2
SWH           10330.578 Hz
FIDRES        0.157632 Hz
AQ            3.1720407 sec
RG            181
DW            48.400 usec
DE            6.00 usec
TE            296.9 K
D1            1.00000000 sec
TD0           1

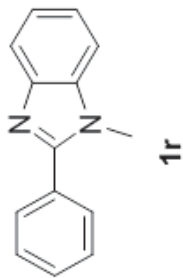
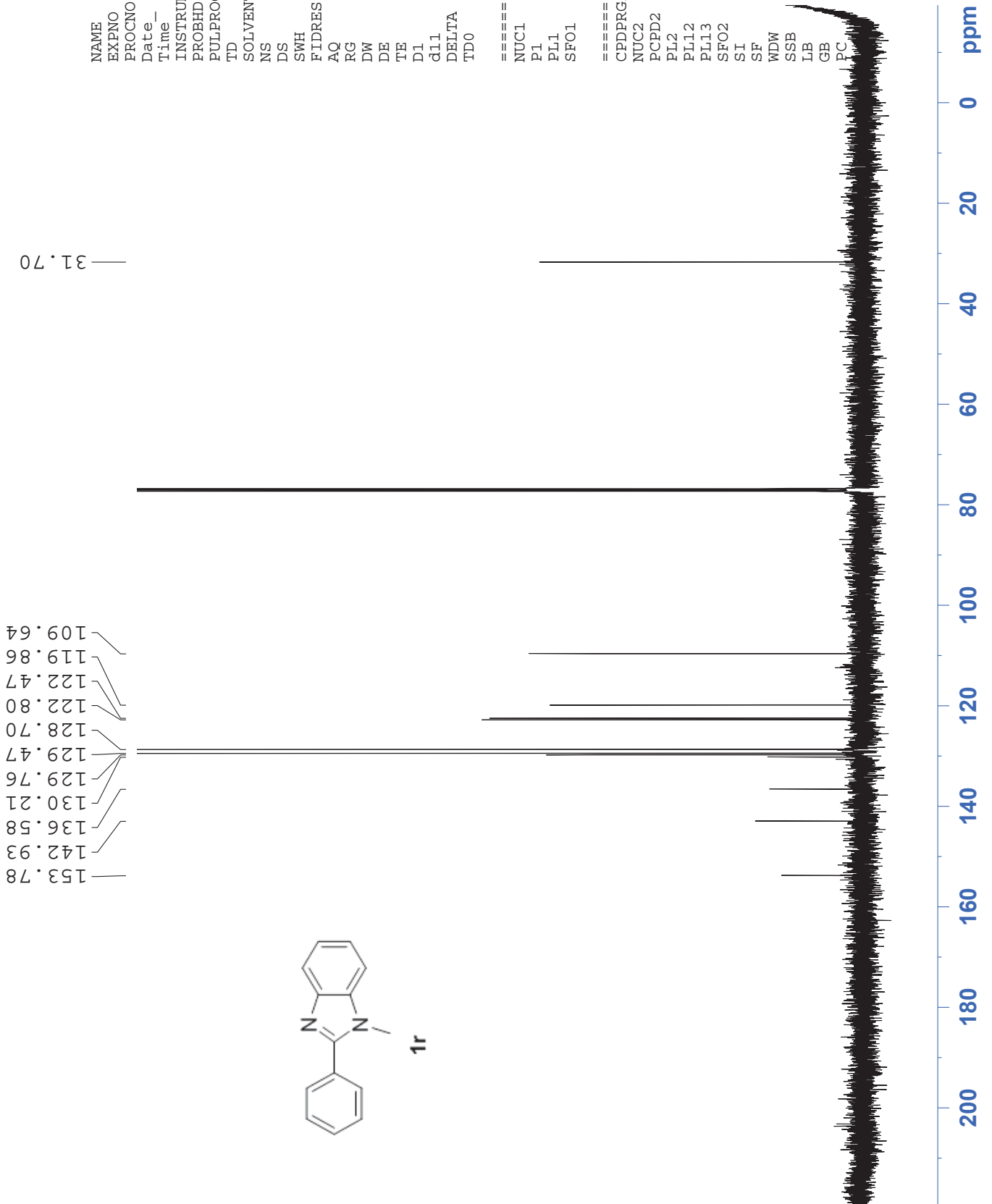
===== CHANNEL f1 =====
NUC1          1H
P1            13.72 usec
PL1           1.00 dB
SFO1          500.1330885 MHz
SI            32768
SF            500.1300000 MHz
WDW           no
SSB           0
LB            0.00 Hz
GB            0
PC            1.00
  
```



HXH-5-BM
 C13CPD CDCl₃:

NAME XB20130417
 EXPNO 8
 PROCNO 1
 Date_ 20130417
 Time_ 11.44
 INSTRUM spect
 PROBHD 5 mm PATXO 19F
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl₃
 NS 128
 DS 4
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0912410 sec
 RG 128
 DW 16.650 usec
 DE 6.00 usec
 TE 298.0 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.8999999 sec
 TDO 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 16.31 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



HXH-5-30-1
C13CPD CDCl3

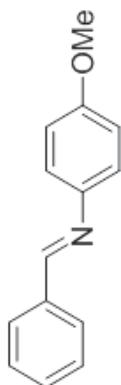
```

NAME          XB20130318
EXPNO         7
PROCNO        1
Date_         20130318
Time_         11.10
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            296.8 K
d1            2.0000000 sec
d11           0.0300000 sec
DELTA         1.89999998 sec
TD0           1

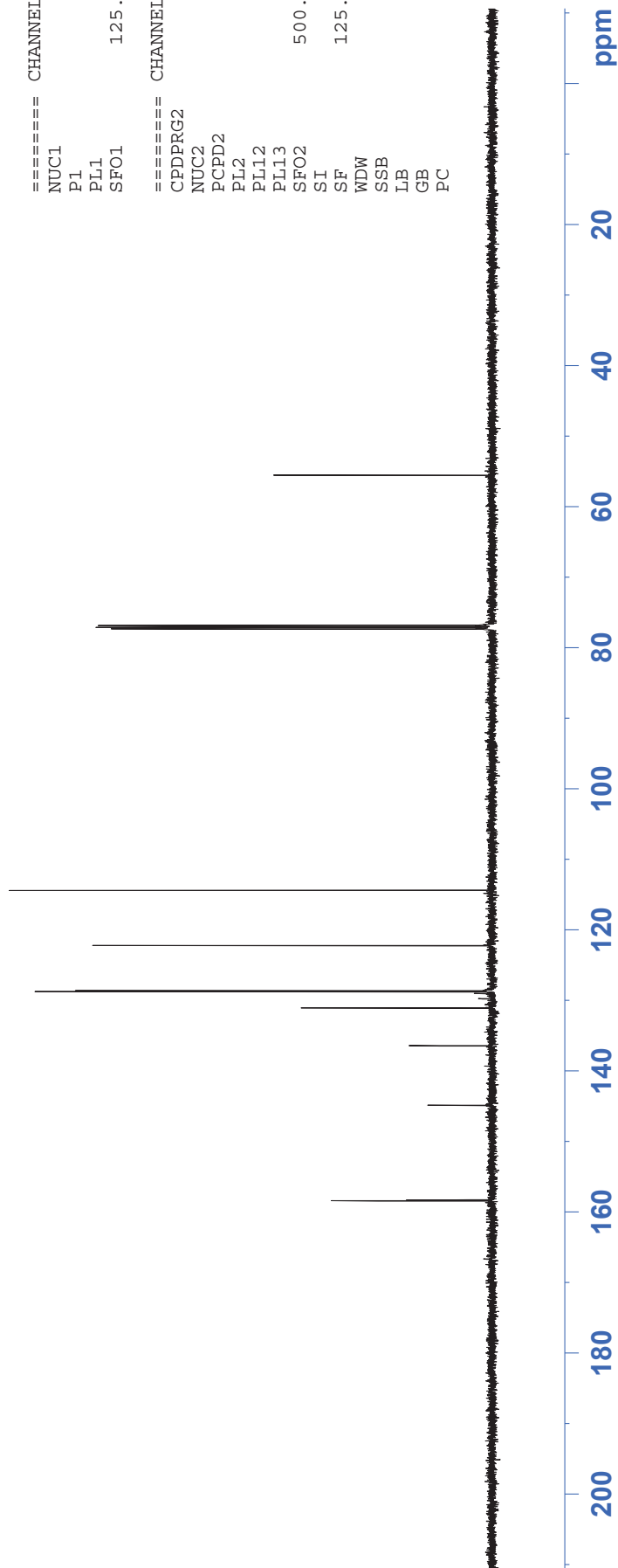
===== CHANNEL f1 =====
NUC1          13C
P1            9.50 usec
PL1           -0.50 dB
SF01          125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           1.00 dB
PL12          16.31 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
  
```

158.44
158.32
144.88
136.44
131.08
128.76
128.63
122.23
114.41
55.52



3a

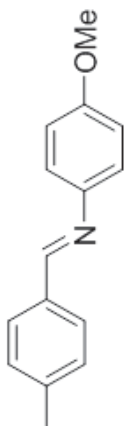


HXH-5-35-1
 PROTON CDCl3

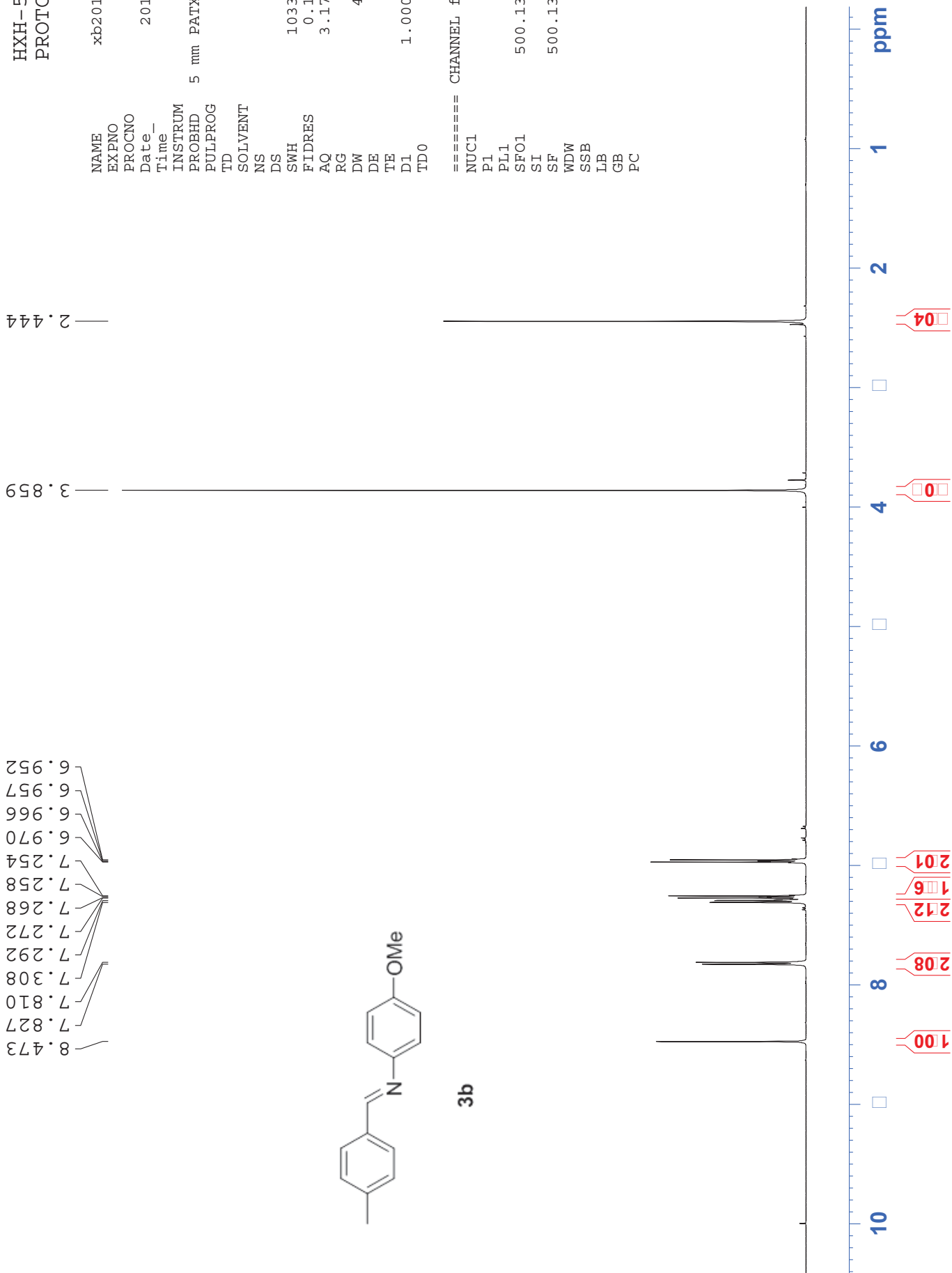
NAME xb20130322
 EXPNO 22
 PROCNO 1
 Date_ 20130322
 Time 14.00
 INSTRUM spect
 PROBHD 5 mm PATXO 19F
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1720407 sec
 RG 143.7
 DW 48.400 usec
 DE 6.00 usec
 TE 296.2 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 13.72 usec
 PL1 1.00 dB
 SFO1 500.1330885 MHz
 SI 32768
 SF 500.1300000 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

8.473
 7.827
 7.810
 7.308
 7.292
 7.272
 7.268
 7.258
 7.254
 6.970
 6.966
 6.957
 6.952



3.859
 2.444



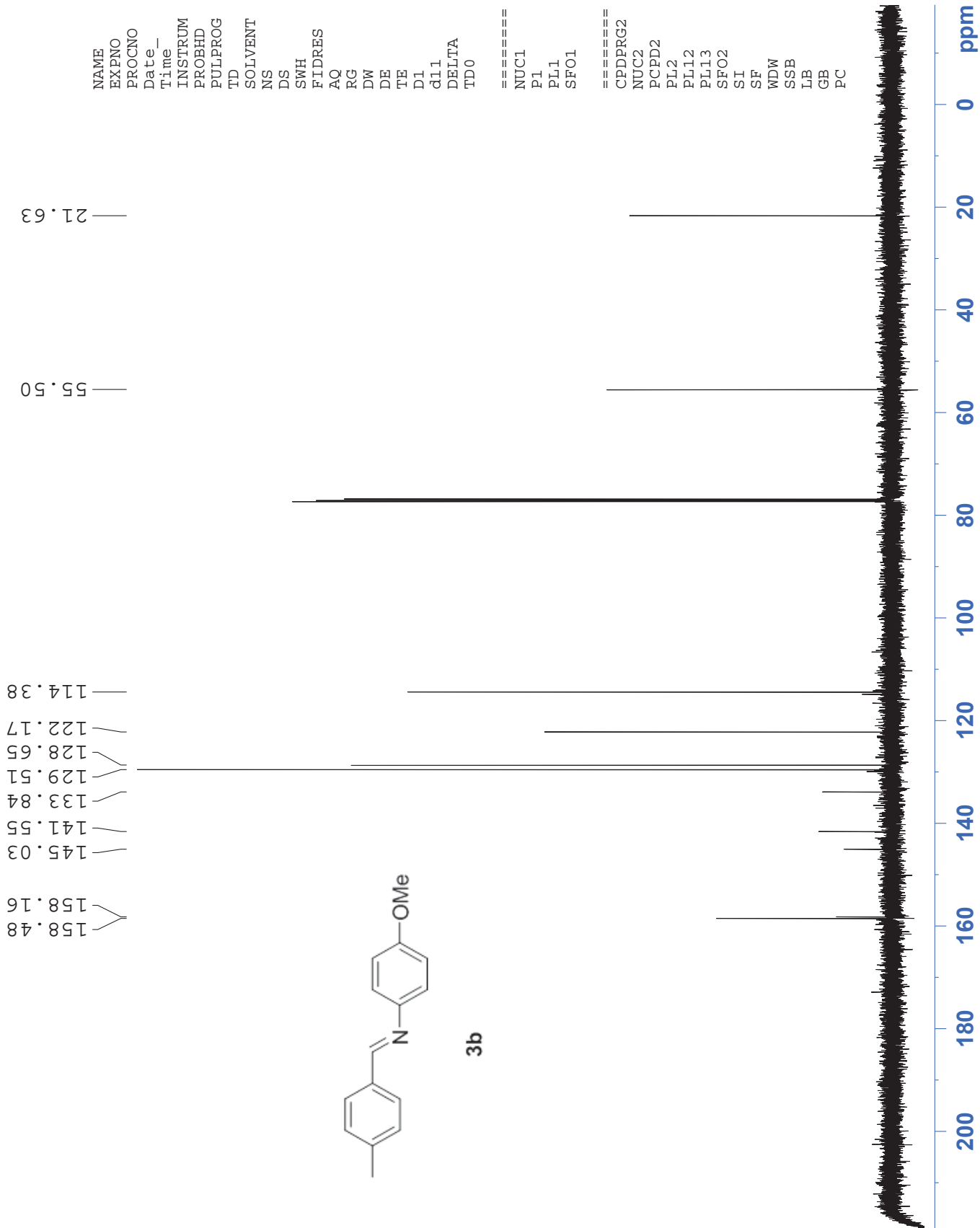
HXH-5-35-1
 C13CPD CDCl3

```

NAME      xb20130322
EXPNO     26
PROCNO    1
Date_     20130322
Time      21.23
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         120
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         228.1
DE         16.650 usec
TE         297.2 K
d1         2.00000000 sec
d11        0.03000000 sec
DELTA     1.89999998 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         9.50 usec
PL1        -0.50 dB
SFO1       125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2        1H
PCPD2      80.00 usec
PL2         1.00 dB
PL12       16.31 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
  
```



HXH-5-33-2
 PROTON CDCl3

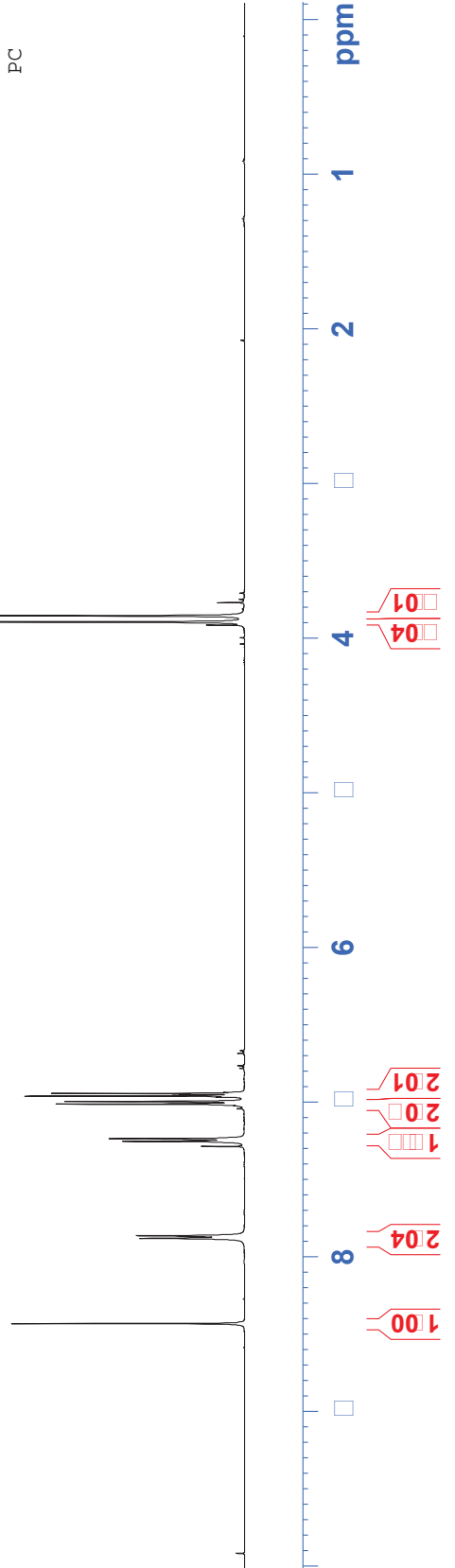
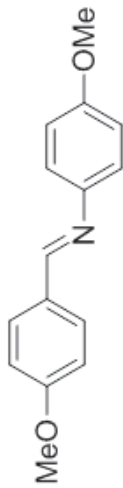
```

NAME      XB20130321
EXPNO     6
PROCNO    1
Date_     20130321
Time      7.20
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        10330.578 Hz
FIDRES     0.157632 Hz
AQ         3.1720407 sec
RG         181
DW         48.400 usec
DE         6.00 usec
TE         295.8 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         13.72 usec
PL1        1.00 dB
SFO1       500.1330885 MHz
SI         32768
SF         500.1300000 MHz
WDW        no
SSB        0
LB         0.00 Hz
GB         0
PC         1.00
  
```

3.894
 3.854

8.431
 7.880
 7.863
 7.253
 7.236
 7.012
 6.995
 6.960
 6.956
 6.947
 6.942



HXH-5-33-2
 C13CPD CDCl3

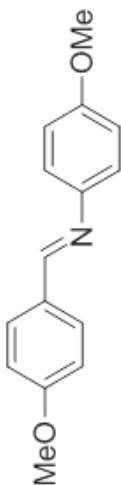
```

NAME      XB20130321
EXPNO     7
PROCNO    1
Date_     20130321
Time      7.28
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         128
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         101.6
DW         16.650 usec
DE         6.00 usec
TE         296.9 K
D1         2.00000000 sec
d11        0.03000000 sec
DELTA     1.89999998 sec
TD0        1
===== CHANNEL f1 =====
NUC1      13C
P1        9.50 usec
PL1       -0.50 dB
SFO1     125.7703643 MHz
===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2        1.00 dB
PL12     16.31 dB
PL13     16.50 dB
SFO2     500.1320005 MHz
SI        32768
SF        125.7577890 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
  
```

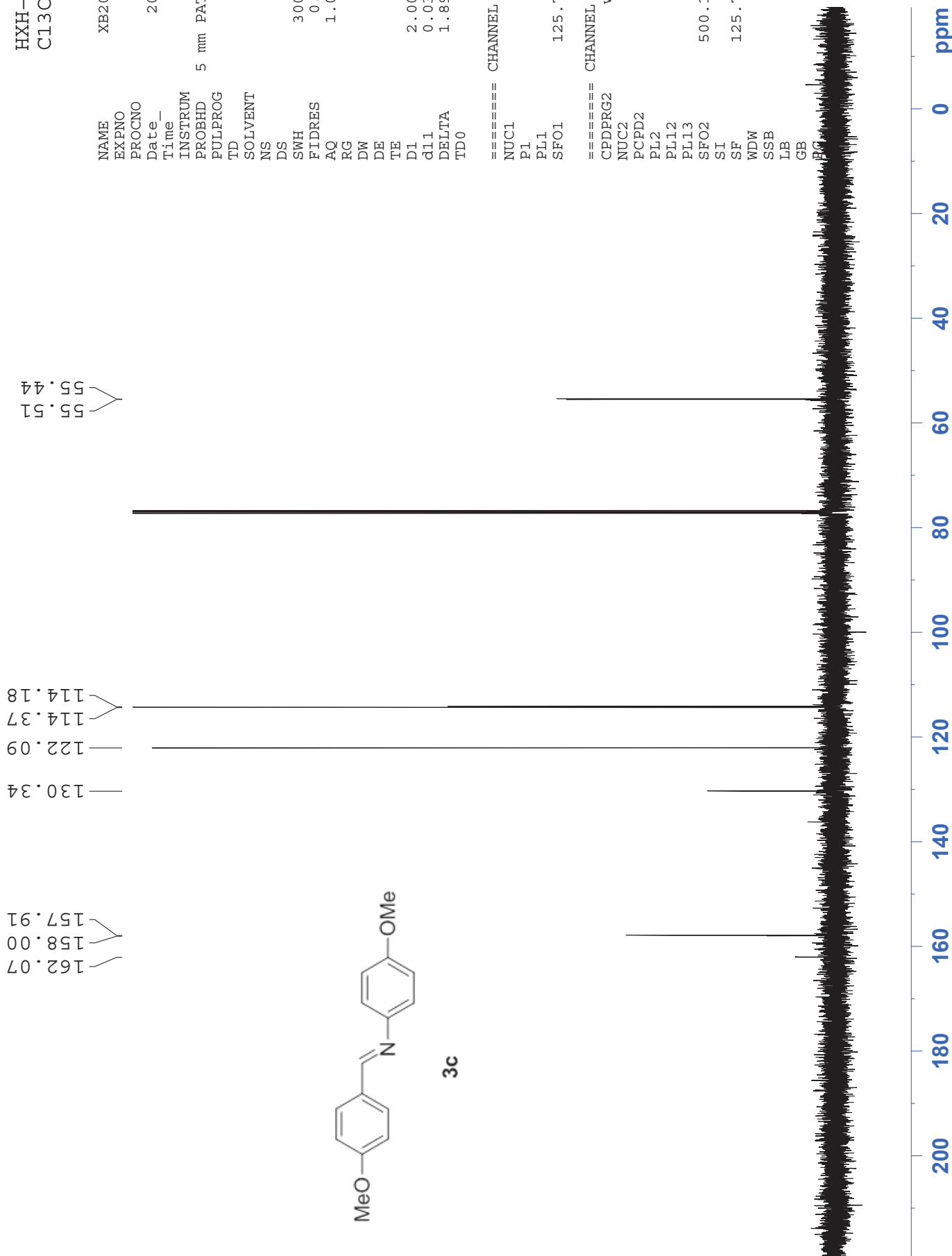
55.51
 55.44

114.18
 114.37
 122.09
 130.34

162.07
 158.00
 157.91



3c



HXH-5-35-2
 PROTON CDCl₃

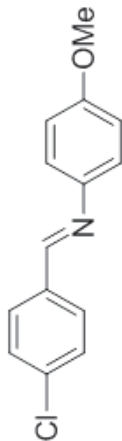
```

NAME      XB20130323
EXPNO    2
PROCNO   1
Date_    20130323
Time     22.08
INSTRUM  spect
PROBHD   5 mm PATXO 19F
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        16
DS        2
SWH      10330.578 Hz
FIDRES   0.157632 Hz
AQ       3.1720407 sec
RG       161.3
DW       48.400 usec
DE       6.00 usec
TE       295.6 K
D1       1.00000000 sec
TD0      1
  
```

```

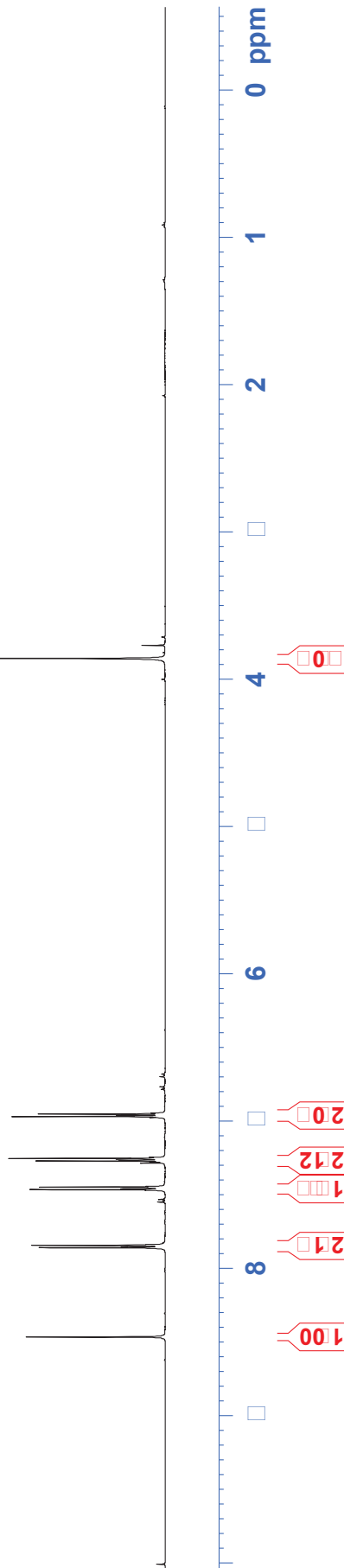
===== CHANNEL f1 =====
NUC1    1H
P1      13.72 usec
PL1     1.00 dB
SF01    500.1330885 MHz
SI      32768
SF      500.1300000 MHz
WDW     no
SSB     0
LB      0.00 Hz
GB      0
PC      1.00
  
```

8.464
 7.858
 7.842
 7.467
 7.450
 7.273
 7.268
 7.259
 7.255
 6.971
 6.966
 6.957
 6.953



3d

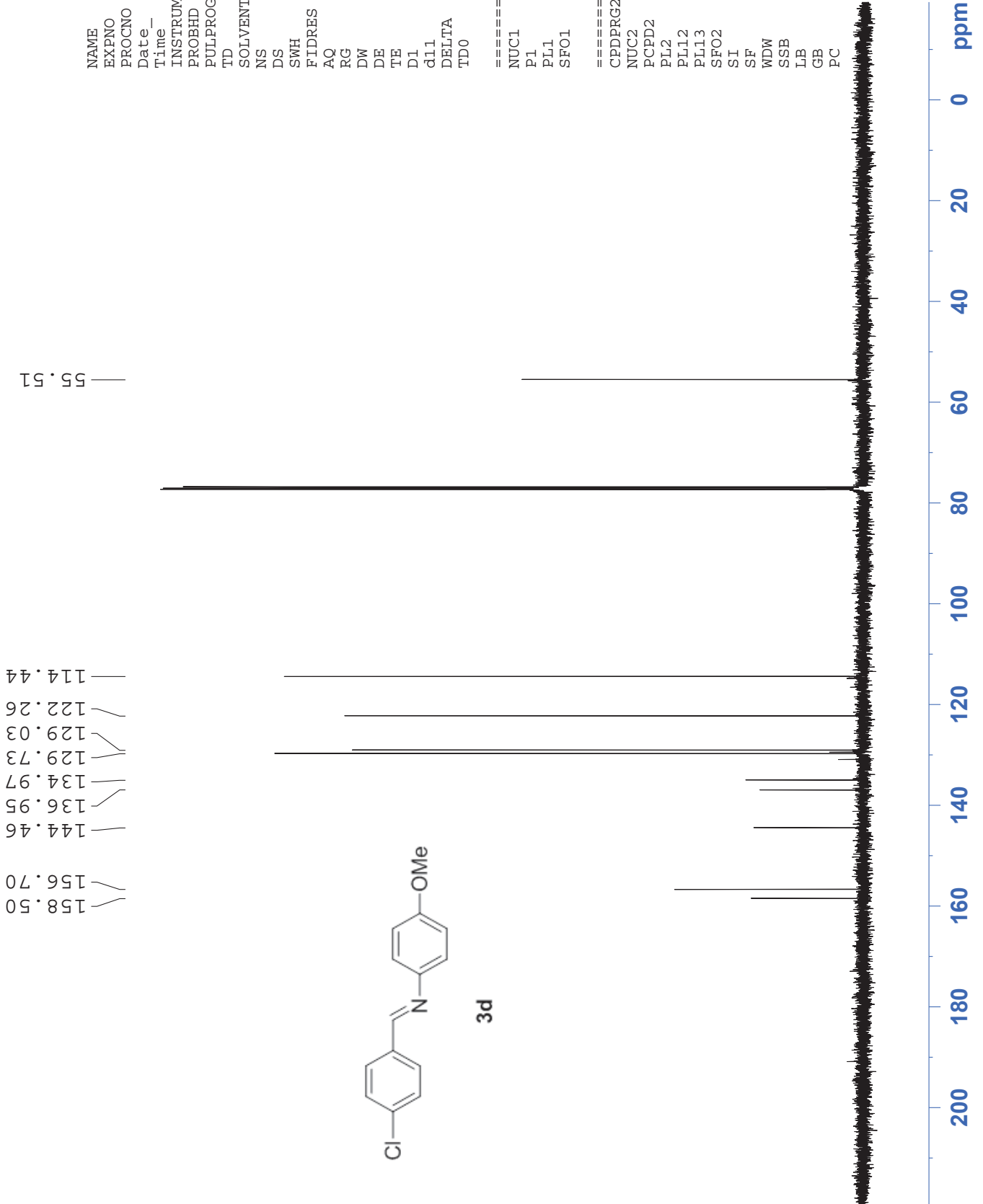
3.860



HXH-5-35-2
C13CPD CDC13

```

NAME          XB20130323
EXPNO         3
PROCNO        1
Date_         20130323
Time_         22.17
INSTRUM       spect
PROBHD        5 mm PAXO 19F
PULPROG       zgpg30
TD            65536
SOLVENT       CDC13
NS            128
DS            4
SWH           30030.029 Hz
FIDRES        0.458222 Hz
AQ            1.0912410 sec
RG            203.2
DW            16.650 usec
DE            6.00 usec
TE            296.9 K
D1            2.0000000 sec
d11           0.0300000 sec
DELTA         1.89999998 sec
TDO           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         16.31 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
  
```



HXH-5-30-3
 PROTON CDCl3

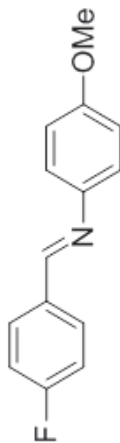
```

NAME      XB20130319
EXPNO     1
PROCNO    1
Date_     20130319
Time      17.02
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         8
DS         2
SWH        10330.578 Hz
FIDRES     0.157632 Hz
AQ         3.1720407 sec
RG         161.3
DW         48.400 usec
DE         6.00 usec
TE         295.7 K
D1         1.00000000 sec
TD0        1
  
```

```

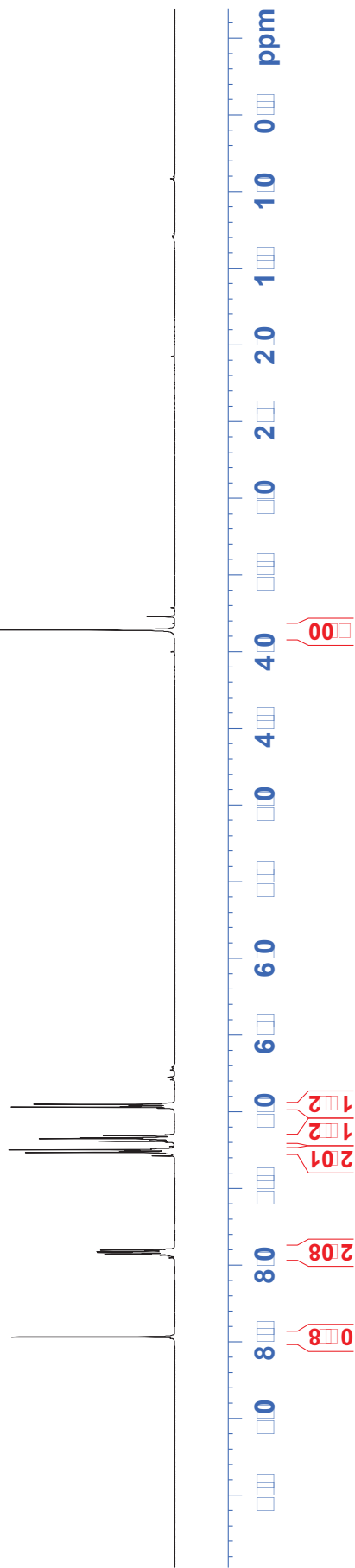
===== CHANNEL f1 =====
NUC1      1H
P1        13.72 usec
PL1       1.00 dB
SFO1      500.1330885 MHz
SI        32768
SF        500.1300000 MHz
WDW       no
SSB       0
LB        0.00 Hz
GB        0
PC        1.00
  
```

8.466
 7.928
 7.917
 7.910
 7.899
 7.264
 7.259
 7.250
 7.246
 7.191
 7.173
 7.156
 6.970
 6.966
 6.957
 6.953



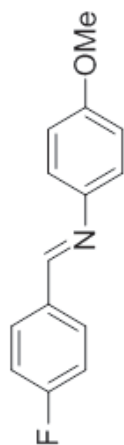
3e

3.859



HXH-5-30-3
19Fdeft CDCI3 D:\\ deng 13

-108.655



3e

```
NAME      XB20130319
EXPNO     2
PROCNO    1
Date_     20130319
Time      17.04
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zg
TD         131072
SOLVENT   CDCI3
NS         8
DS         4
SWH       10000.000 Hz
FIDRES    0.762939 Hz
AQ         0.6554150 sec
RG         322.5
DW         5.000 usec
DE         6.00 usec
TE         295.7 K
D1         1.00000000 sec
TD0        1

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

ppm

-180

-160

-140

-120

-100

-80

-60

-40

-20

0

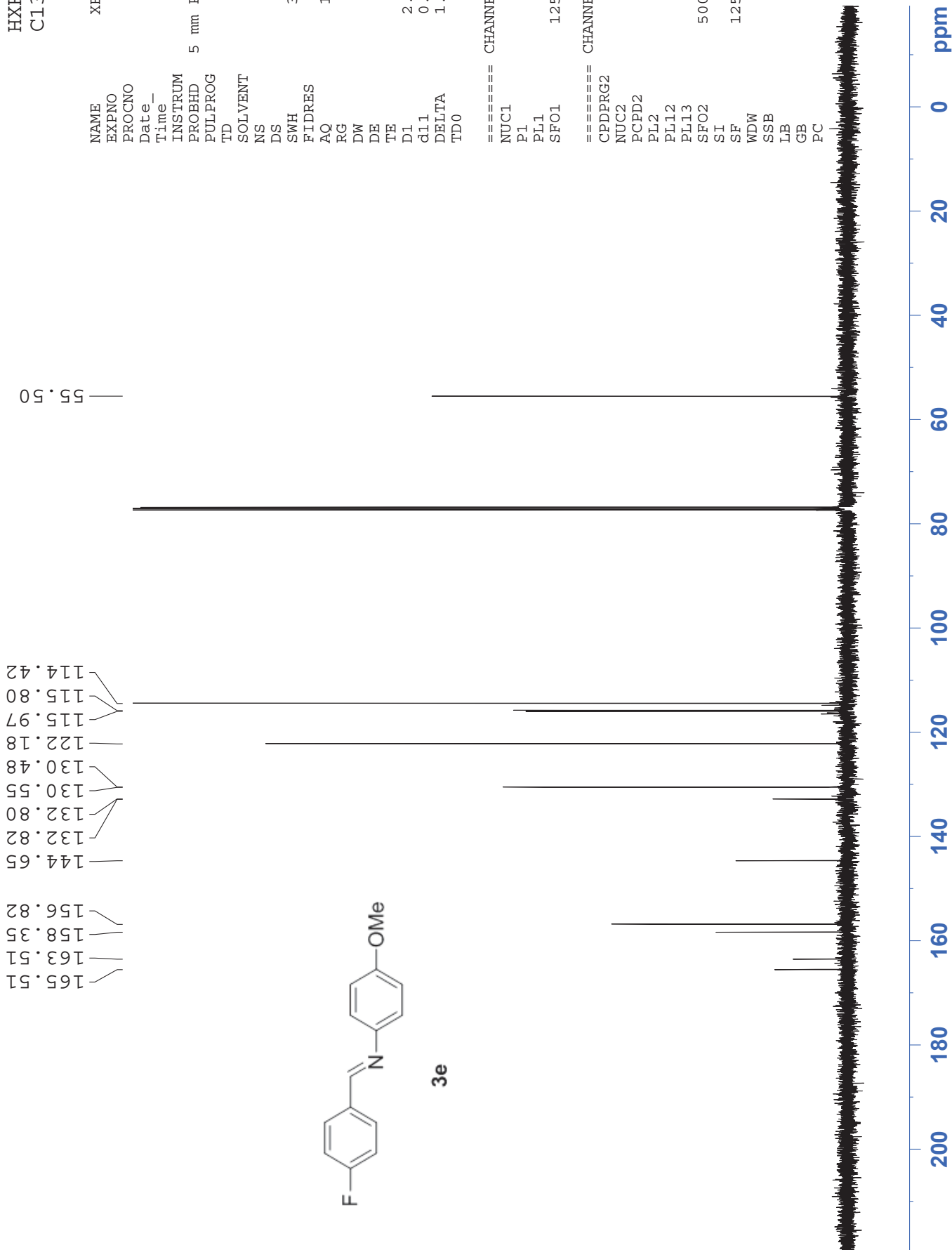
HXH-5-30-3
 C13CPD CDCl3

```

NAME      XB20130319
EXPNO     3
PROCNO    1
Date_     20130319
Time      17.12
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         119
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         296.9 K
D1         2.00000000 sec
d11        0.03000000 sec
DELTA     1.89999998 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         9.50 usec
PL1        -0.50 dB
SFO1       125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2        1H
PCPD2       80.00 usec
PL2         1.00 dB
PL12        16.31 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
  
```



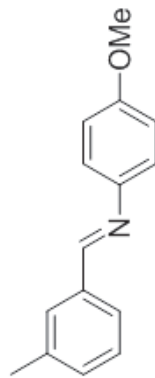
HXH-3-ME
PROTON CDCl3

NAME XB20130403
 EXPNO 17
 PROCNO 1
 Date_ 20130403
 Time_ 14.03
 INSTRUM spect
 PROBHD 5 mm PATXO 19F
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1720407 sec
 RG 143.7
 DW 48.400 usec
 DE 6.00 usec
 TE 295.8 K
 D1 1.00000000 sec
 TDO 1

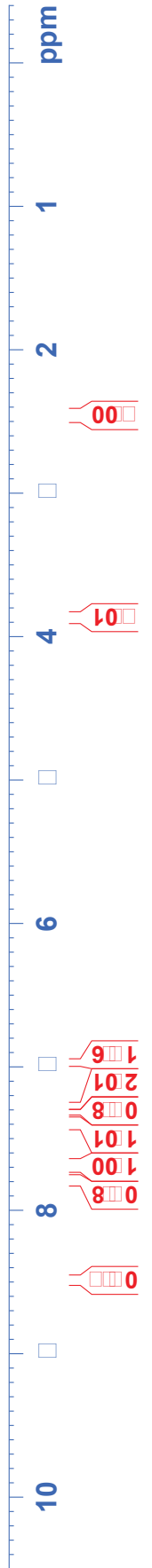
==== CHANNEL f1 =====
 NUC1 1H
 P1 13.72 usec
 PL1 1.00 dB
 SFO1 500.1330885 MHz
 SI 32768
 SF 500.1300000 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

8.484
7.788
7.690
7.674
7.401
7.386
7.370
7.319
7.305
7.305
7.286
7.279
7.275
7.266
7.261
7.255
6.977
6.973
6.959

3.863
2.455



3f



HXH-3-ME
 C13CPD CDC13

```

NAME XB20130403
EXPNO 18
PROCNO 1
Date_ 20130403
Time_ 14.12
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 1625.5
DE 16.650 usec
TE 297.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
  
```

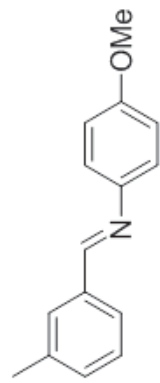
```

===== CHANNEL f1 =====
NUC1 13C
P1 9.150 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.31 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
  
```

158.74
 158.26
 144.99
 138.51
 136.39
 131.96
 128.77
 128.64
 126.26
 122.20
 114.40

55.51
 21.34

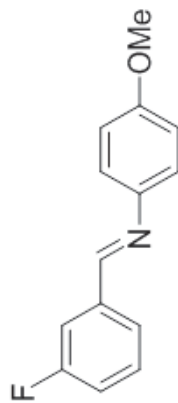


3f



HXH-3-F
19Fdefc CDCl3 D:\\ deng 21

-112.635
-112.654
-112.667
-112.685



3g

NAME XB20130409
EXPNO 2
PROCNO 1
Date_ 20130409
Time_ 13.10
INSTRUM spect
PROBHD 5 mm PAXO 19F
PULPROG zg
TD 131072
SOLVENT CDCl3
NS 8
DS 4
SWH 100000.000 Hz
FIDRES 0.762939 Hz
AQ 0.6554150 sec
RG 322.5
DW 5.000 usec
DE 6.00 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1

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



HXH-3-F
C13CPD CDCl3

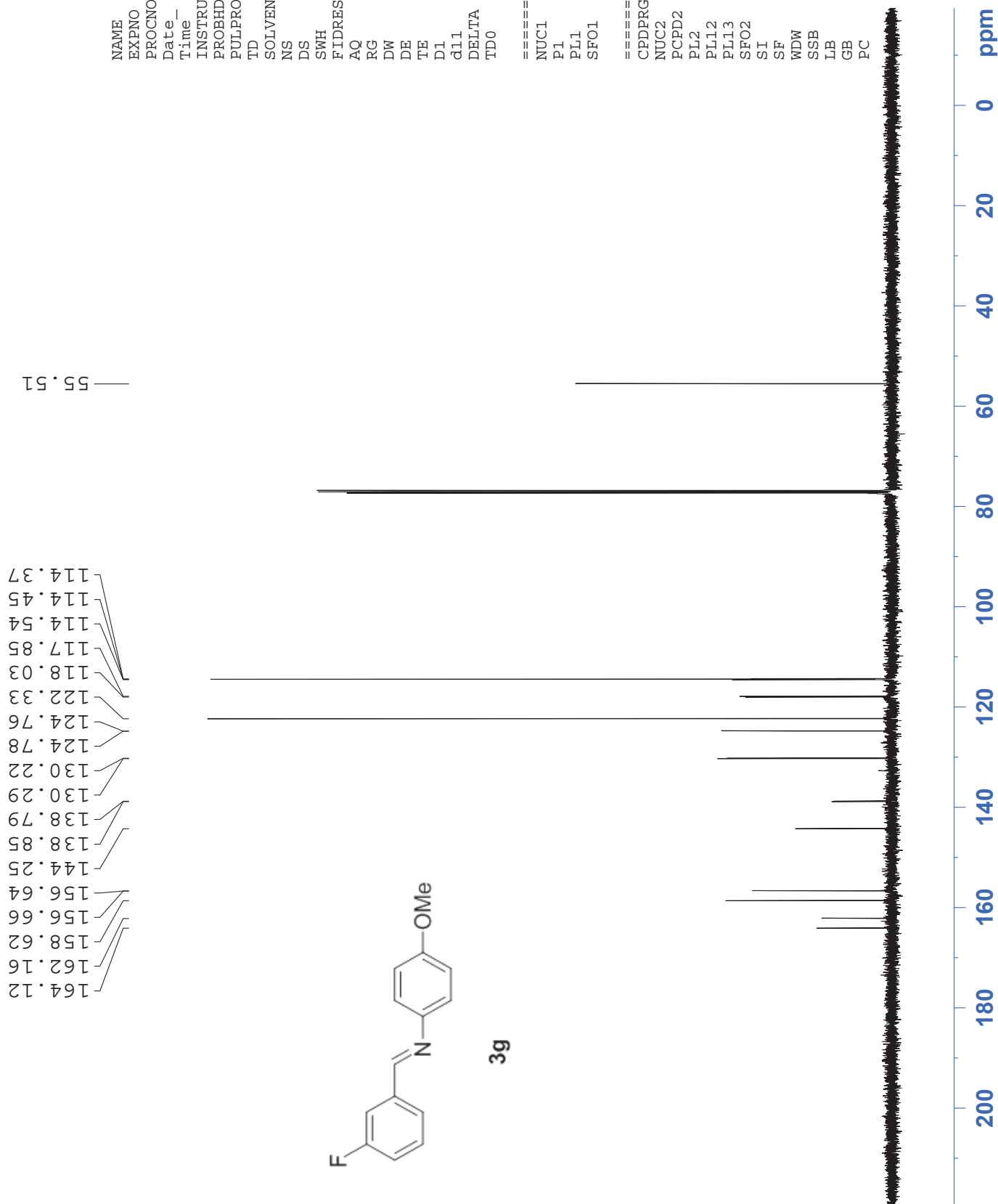
```

NAME      XB20130409
EXPNO     3
PROCNO    1
Date_     20130409
Time_     13.19
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         1625.5
DE         16.650 usec
TE         6.00 usec
TE         297.3 K
D1         2.0000000 sec
d11        0.0300000 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       16.31 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
  
```



HXH-5-33-1
 PROTON CDCl3

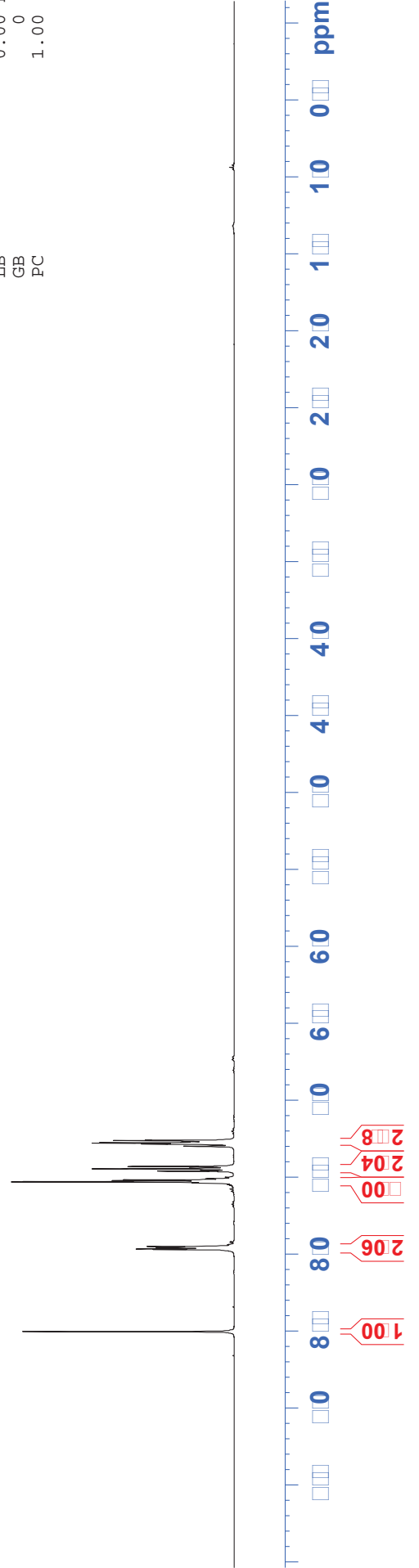
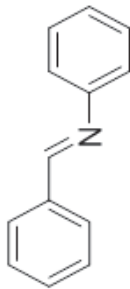
```

NAME      XB20130321
EXPNO     4
PROCNO    1
Date_     20130321
Time_     7.05
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         143.7
DW         48.400 usec
DE         6.00 usec
TE         295.6 K
D1         1.00000000 sec
TD0        1
  
```

```

===== CHANNEL f1 =====
NUC1      1H
P1         13.72 usec
PL1        1.00 dB
SF01      500.1330885 MHz
SI         32768
SF         500.1300000 MHz
WDW        no
SSB         0
LB         0.00 Hz
GB         0
PC         1.00
  
```

7.957
7.955
7.949
7.539
7.535
7.530
7.526
7.520
7.516
7.510
7.508
7.463
7.459
7.455
7.444
7.443
7.431
7.428
7.424
7.286
7.283
7.281
7.280
7.277
7.275
7.271
7.268
7.266
7.260
7.258



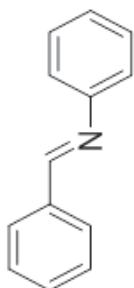
HXH-5-33-1
C13CPD CDCl3

```

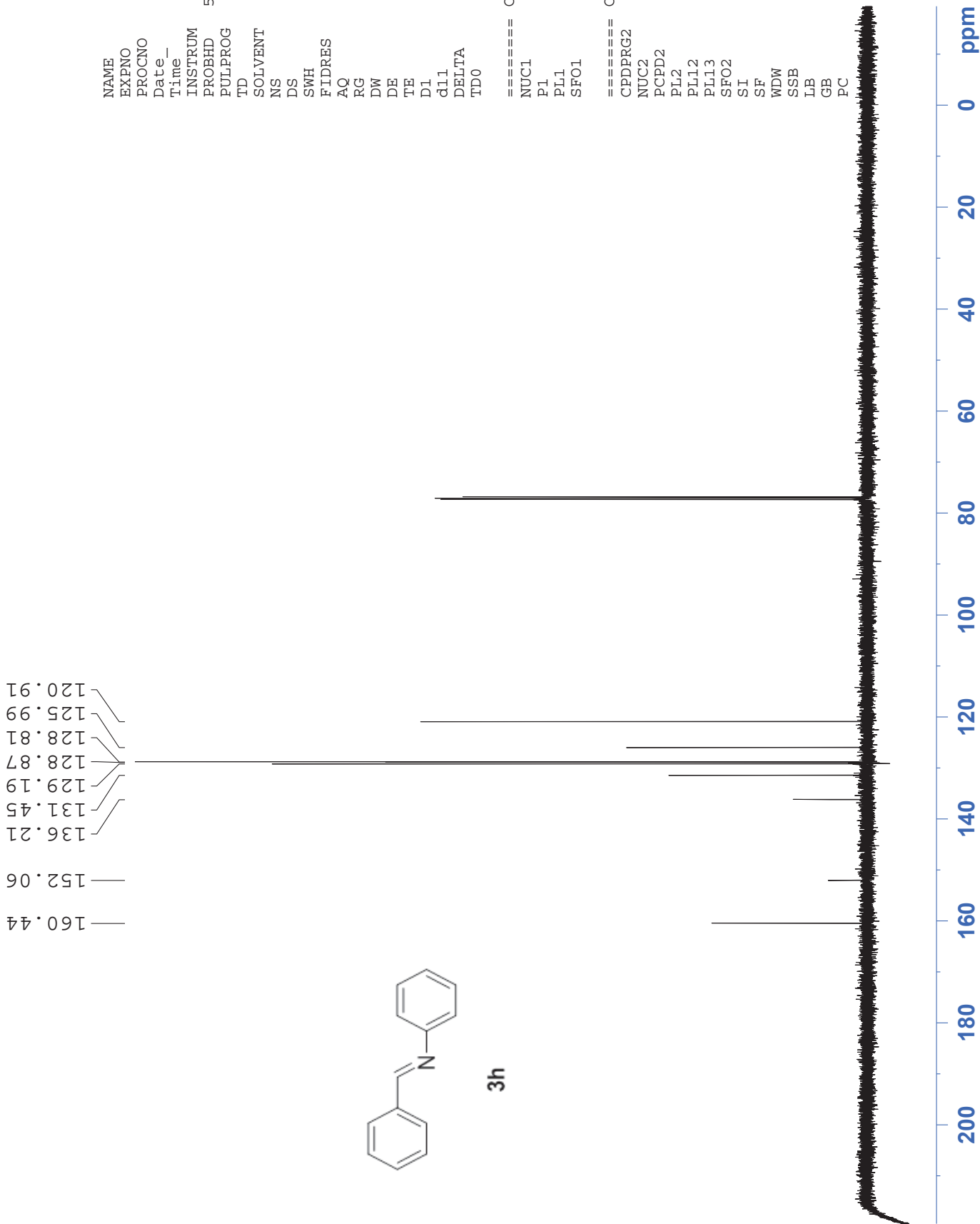
NAME      XB20130321
EXPNO     5
PROCNO    1
Date_     20130321
Time_     7.14
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         128
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         228.1
DW         16.650 usec
DE         6.00 usec
TE         296.8 K
D1         2.0000000 sec
d11        0.0300000 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      16.31 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
  
```

120.91
125.99
128.81
128.87
129.19
131.45
136.21
152.06
160.44



3h



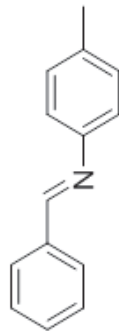
7.186
7.189
7.198
7.202
7.238
7.254
7.286
7.498
7.500
7.505
7.506
7.508
7.513
7.518
7.525
7.936
7.938
7.940
7.943
7.950
7.955
8.511

2.418

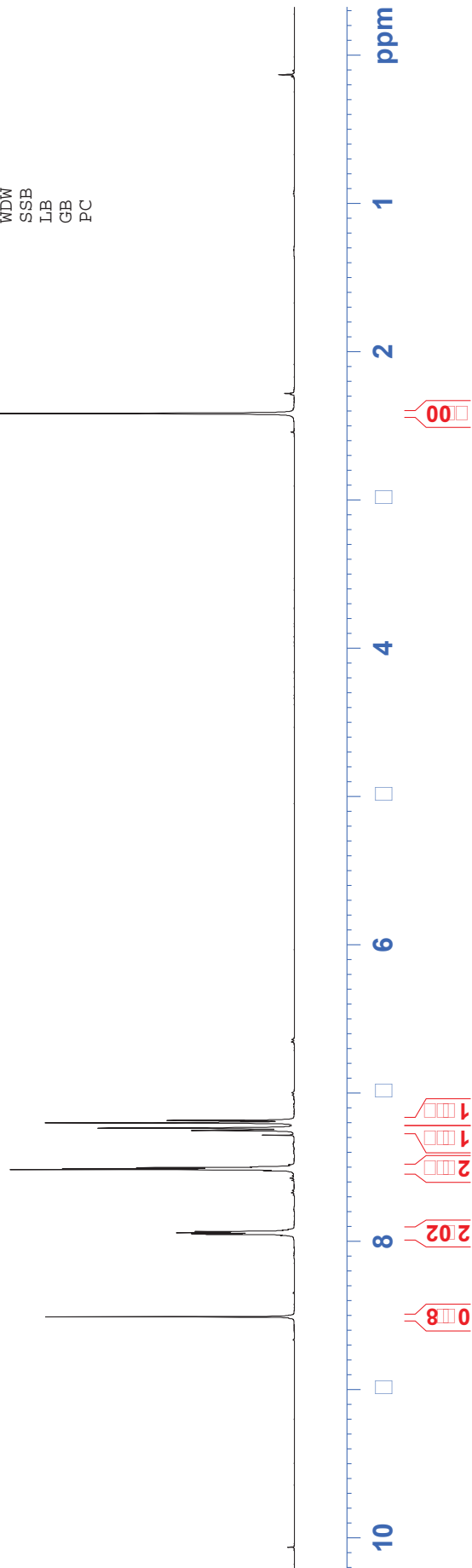
HXH-PH-ME
PROTON CDCl3

NAME XB20130409
EXPNO 15
PROCNO 1
Date_ 20130409
Time_ 14.36
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 143.7
DW 48.400 usec
DE 6.00 usec
TE 296.3 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.72 usec
PL1 1.00 dB
SFO1 500.1330885 MHz
SI 32768
SF 500.1300000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



3i



HXH-PH-ME
C13CPD CDC13

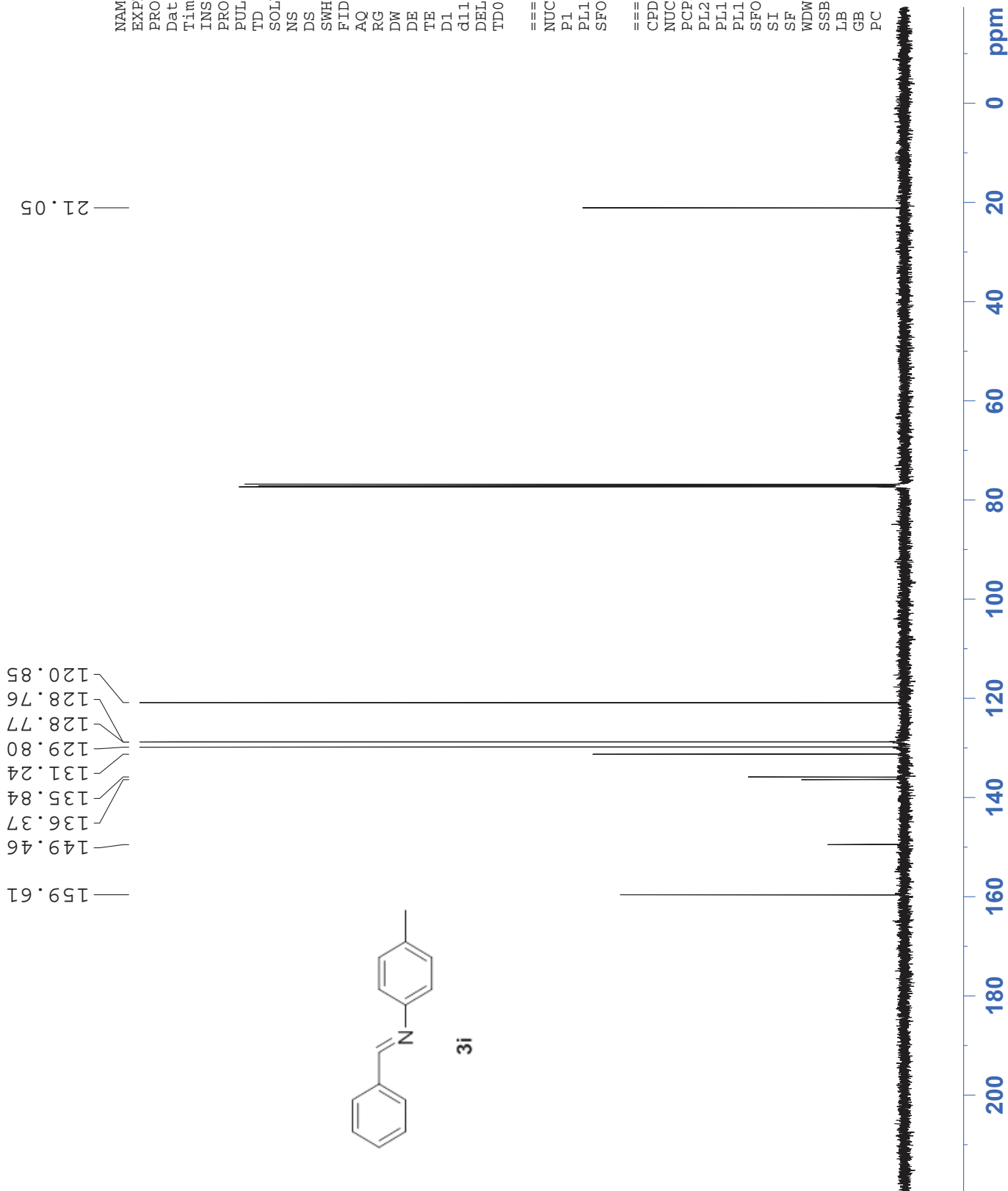
```

NAME      XB20130409
EXPNO     6
PROCNO    1
Date_     20130409
Time      13.35
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDC13
NS         176
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         287.4
DW         16.650 usec
DE         6.00 usec
TE         297.4 K
D1         2.00000000 sec
d11        0.03000000 sec
DELTA     1.89999998 sec
TD0        1
  
```

```

===== CHANNEL f1 =====
NUC1      13C
P1        9.50 usec
PL1       -0.50 dB
SFO1     125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2     80.00 usec
PL2        1.00 dB
PL12     16.31 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
  
```

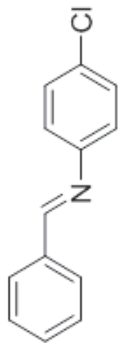


HXH-PH-CL
 PROTON CDCl3

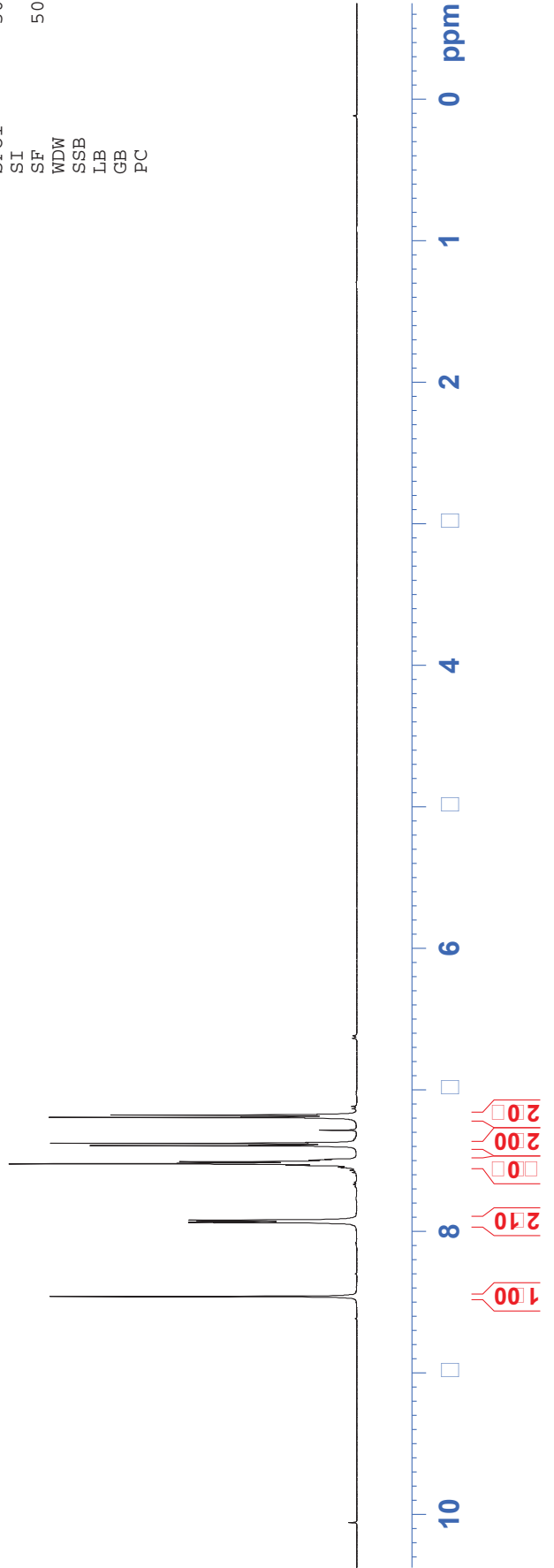
NAME XB20130409
 EXPNO 7
 PROCNO 1
 Date_ 20130409
 Time 13.40
 INSTRUM spect
 PROBHD 5 mm PATXO 19F
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1720407 sec
 RG 181
 DW 48.400 usec
 DE 6.00 usec
 TE 296.3 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.72 usec
 PL1 1.00 dB
 SFO1 500.1330885 MHz
 SI 32768
 SF 500.1300000 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

8.461
 7.939
 7.936
 7.925
 7.921
 7.923
 7.508
 7.396
 7.392
 7.382
 7.378
 7.201
 7.196
 7.192
 7.182
 7.178



3j



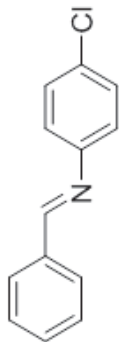
HXH-PH-CL
C13CPD CDC13

NAME XB20130409
 EXPNO 8
 PROCNO 1
 Date_ 20130409
 Time_ 13.49
 INSTRUM spect
 PROBHD 5 mm PATXO 19F
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 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 297.4 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

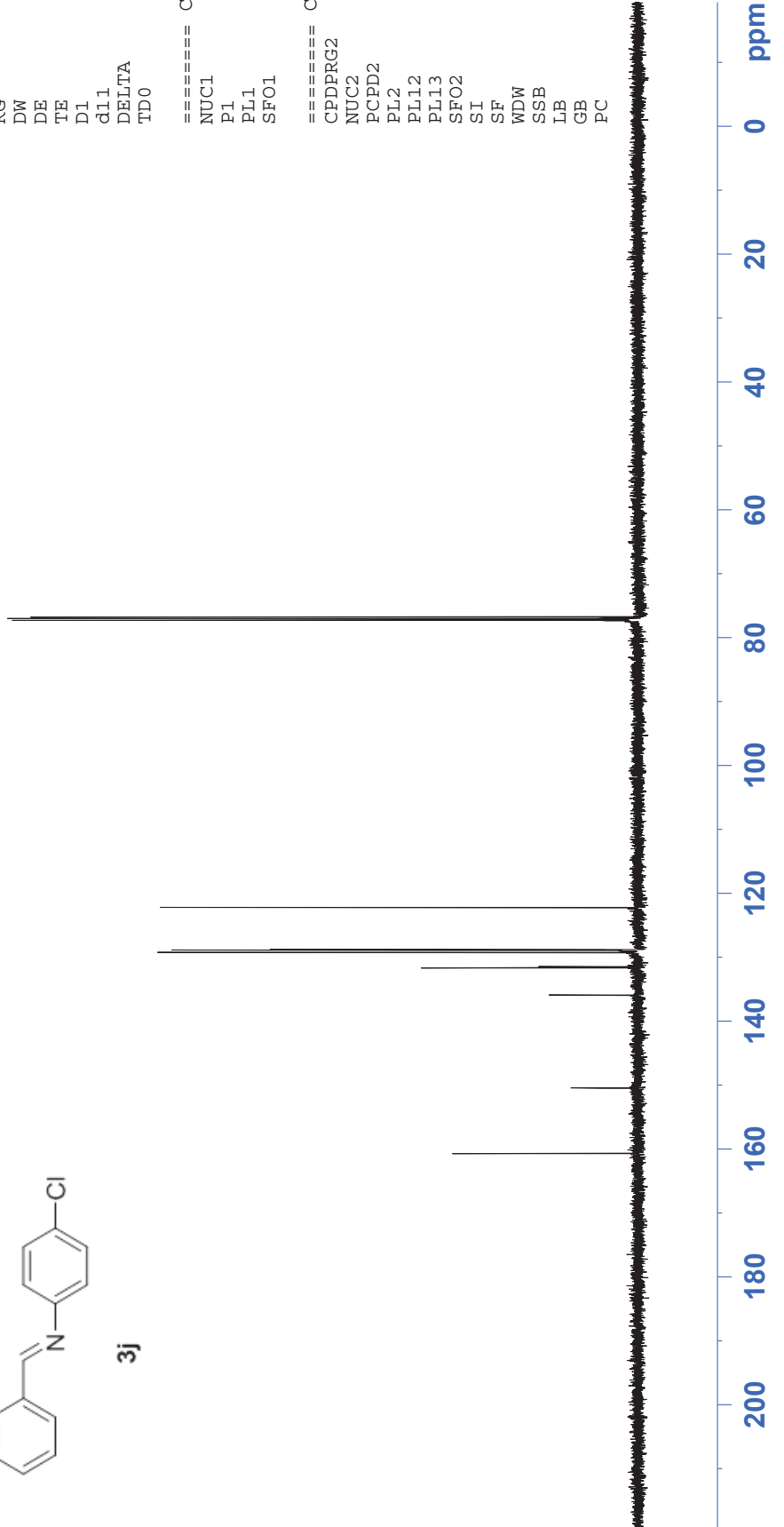
===== CHANNEL f1 =====
 NUC1 13C
 P1 9.50 usec
 PL1 -0.50 dB
 SFO1 125.7703643 MHz

 ===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 1.00 dB
 PL12 16.31 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

160.74
 150.49
 135.94
 131.67
 131.50
 129.26
 128.92
 128.85
 122.23



3j

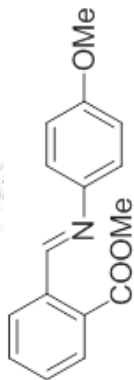


HXH-7-74
 PROTON CDCl3

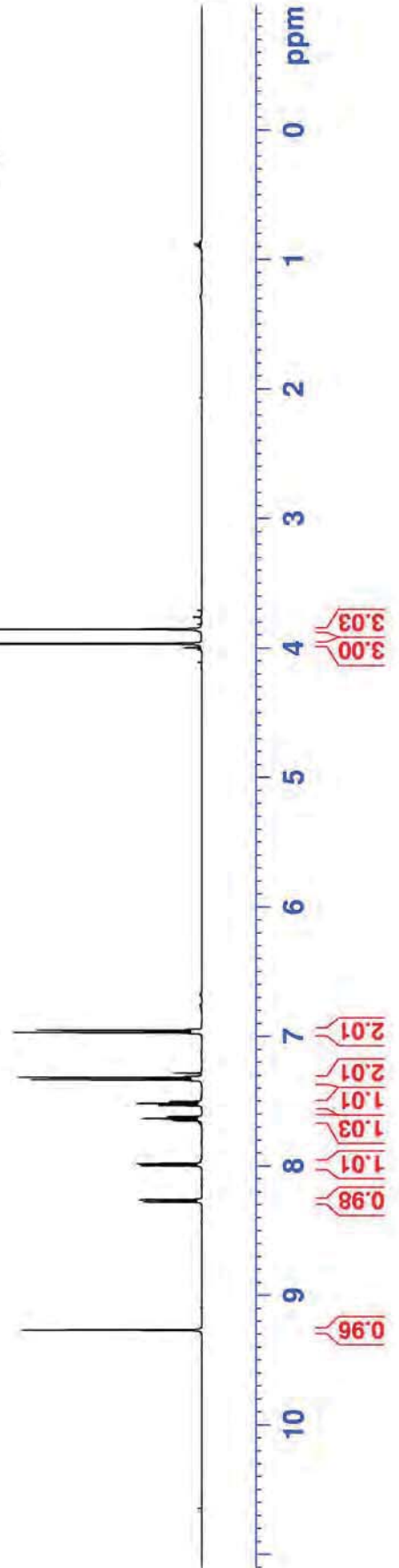
NAME	XB20140624
EXPNO	1
PROCNO	1
Date_	20140624
Time	9.04
INSTRUM	spect
PROBHD	5 mm PATXO 19F
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1720407 sec
RG	128
DW	48.400 usec
DE	6.00 usec
TE	296.0 K
D1	1.00000000 sec
TD0	1

===== CHANNEL f1 =====	
NUC1	1H
P1	14.14 usec
PL1	1.00 dB
SFO1	500.1330885 MHz
SI	32768
SF	500.1300000 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

8.281
8.279
8.265
8.264
8.002
8.000
7.986
7.984
7.653
7.652
7.639
7.638
7.623
7.537
7.534
7.521
7.519
7.506
7.504
7.343
7.337
7.332
7.323
7.319
7.312
6.979
6.972
6.968
6.959
6.955
6.948
3.969
3.857



3k



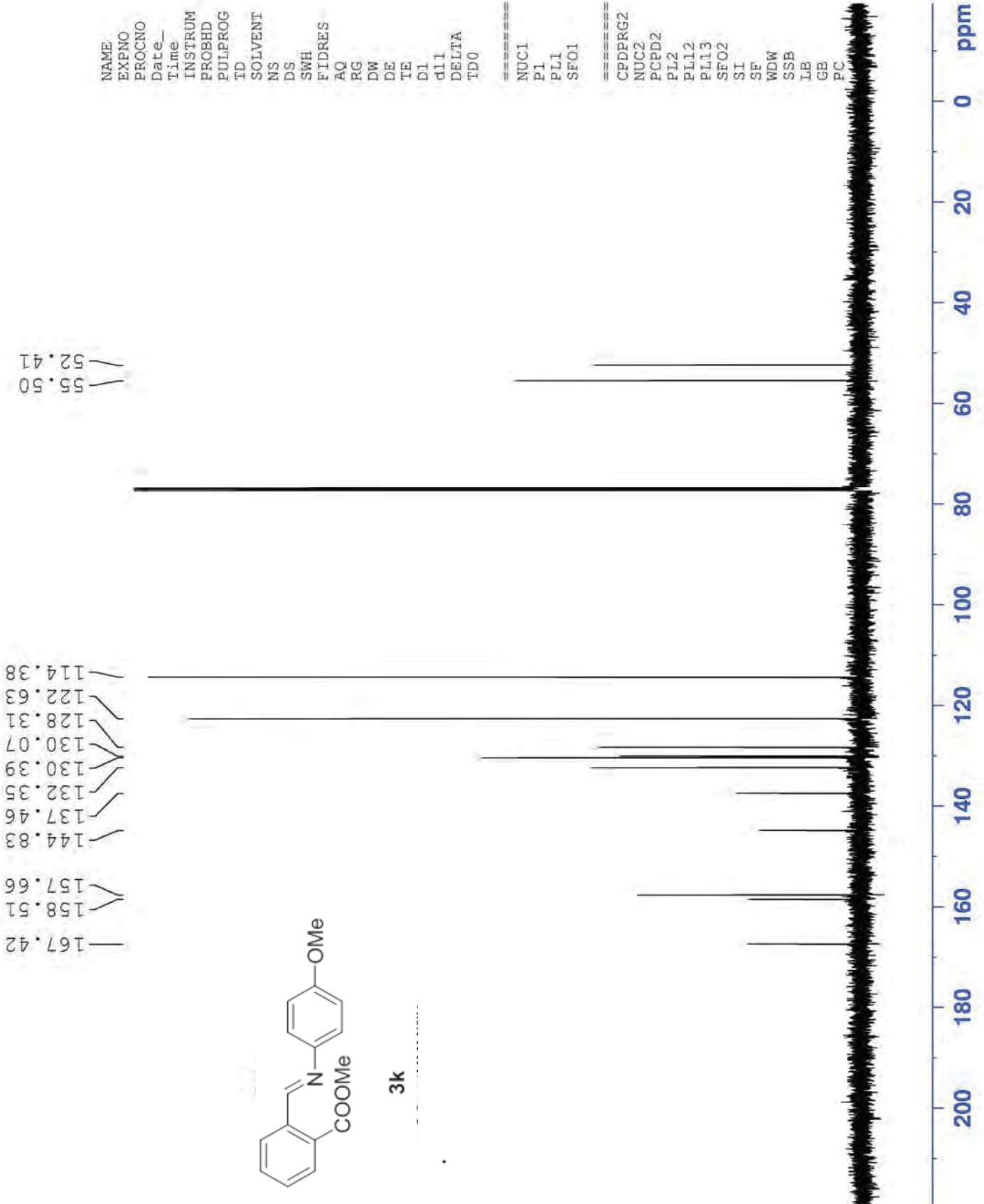
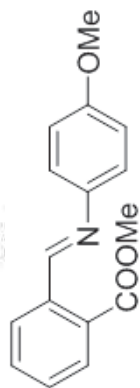
HXH-7-74
C13CPD CDC13

NAME XB20140624
EXPNO 3
PROCNO 1
Date_ 20140624
Time 9.10
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 63
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 296.7 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

167.42
158.51
157.66
144.83
137.46
132.35
130.39
130.07
128.31
122.63
114.38
55.50
52.41

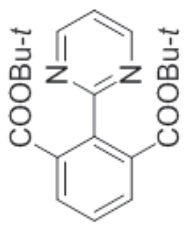


HXH-5-67-2
 PROTON CDC13

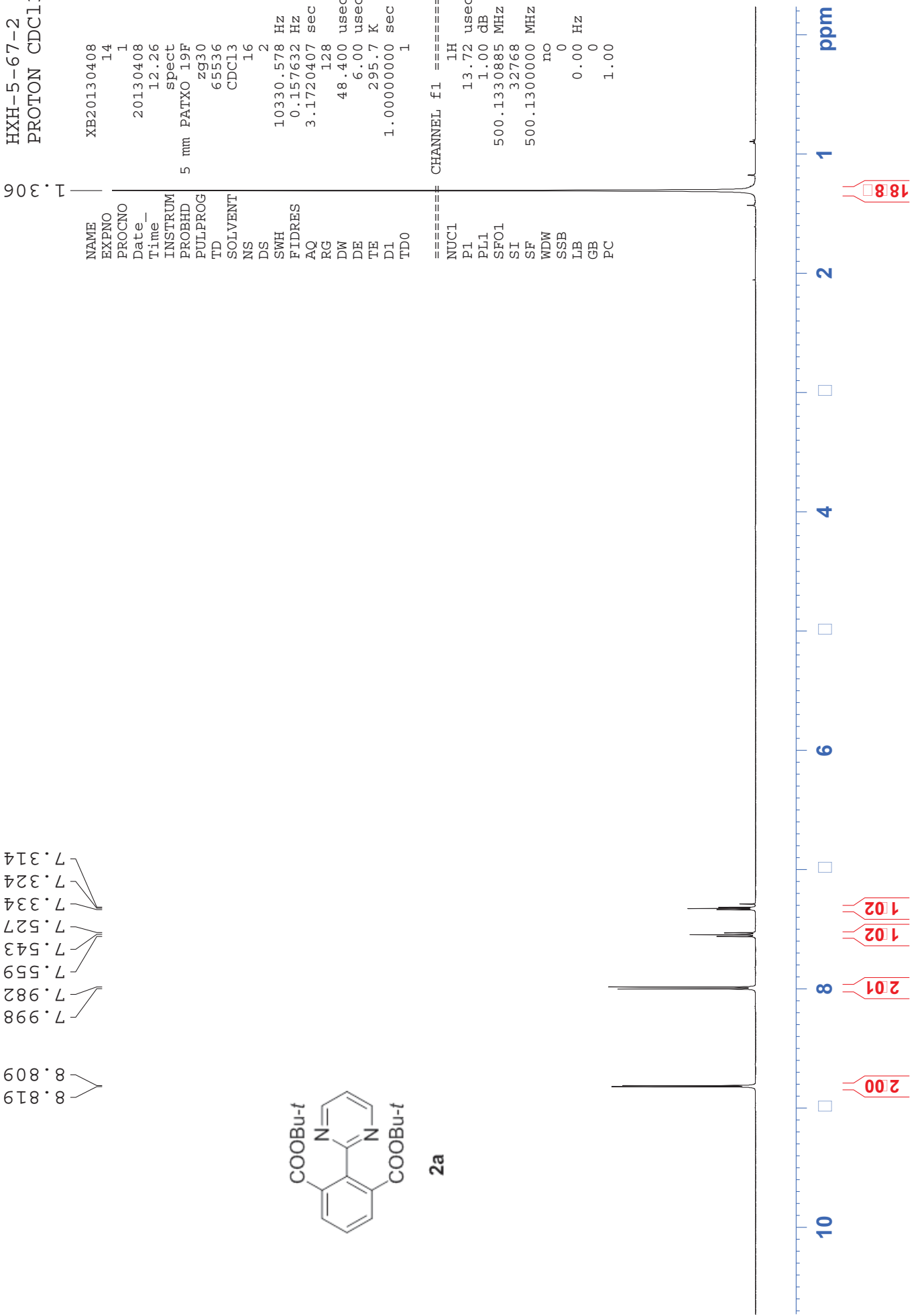
NAME XB20130408
 EXPNO 14
 PROCNO 1
 Date_ 20130408
 Time_ 12.26
 INSTRUM spect
 PROBHD 5 mm PATXO 19F
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1720407 sec
 RG 128
 DW 48.400 usec
 DE 6.00 usec
 TE 295.7 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.72 usec
 PL1 1.00 dB
 SFO1 500.1330885 MHz
 SI 32768
 SF 500.1300000 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

8.819
 8.809
 7.998
 7.982
 7.559
 7.543
 7.527
 7.334
 7.324
 7.314



2a



HXH-5-67-2
 C13CPD CDCl3

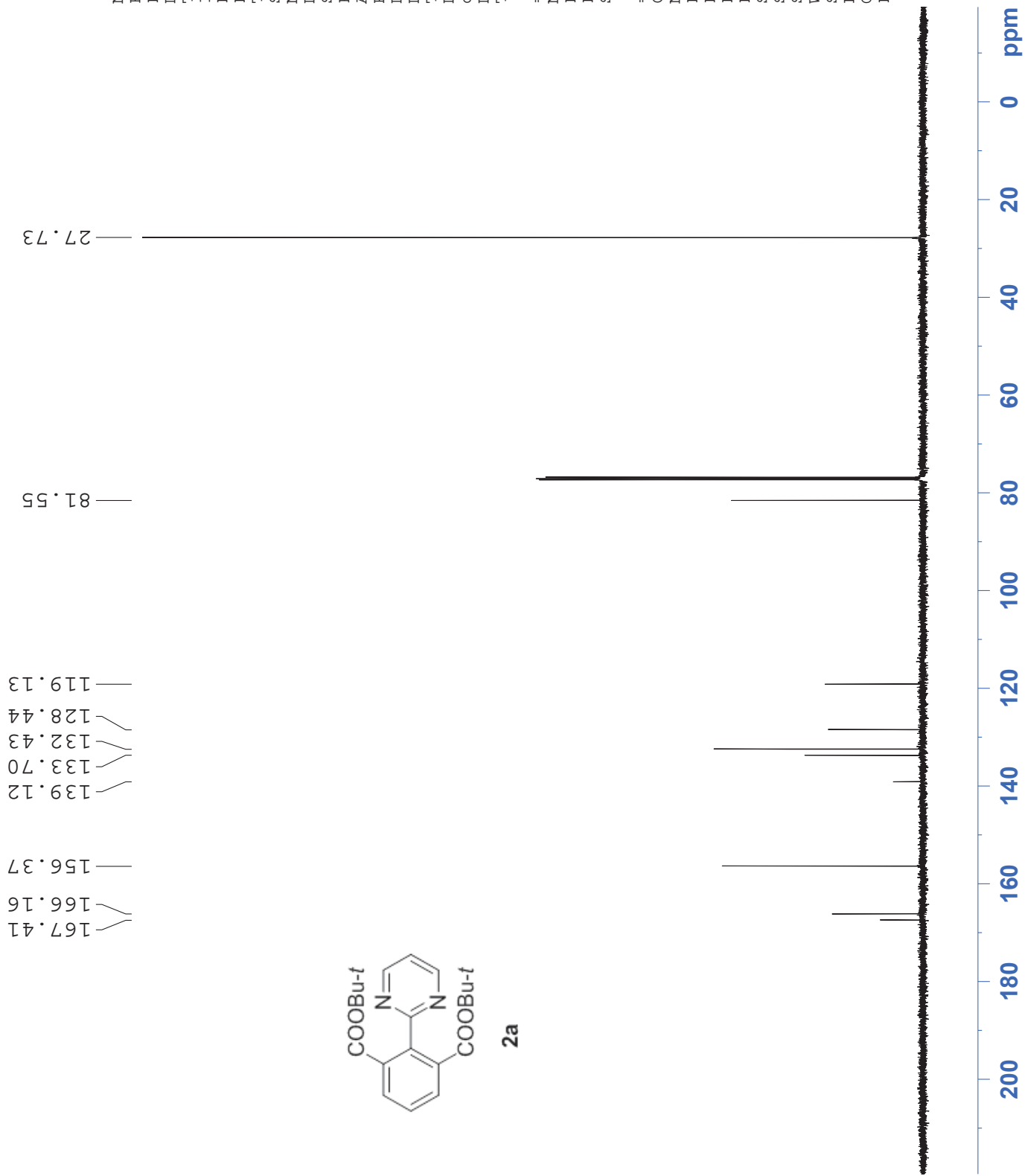
```

NAME      XB20130408
EXPNO     15
PROCNO    1
Date_     20130408
Time_     12.34
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         296.9 K
D1         2.0000000 sec
d11        0.0300000 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     16.31 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
  
```



HXH-MONO
C13CPD CDC13

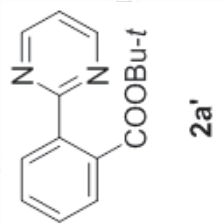
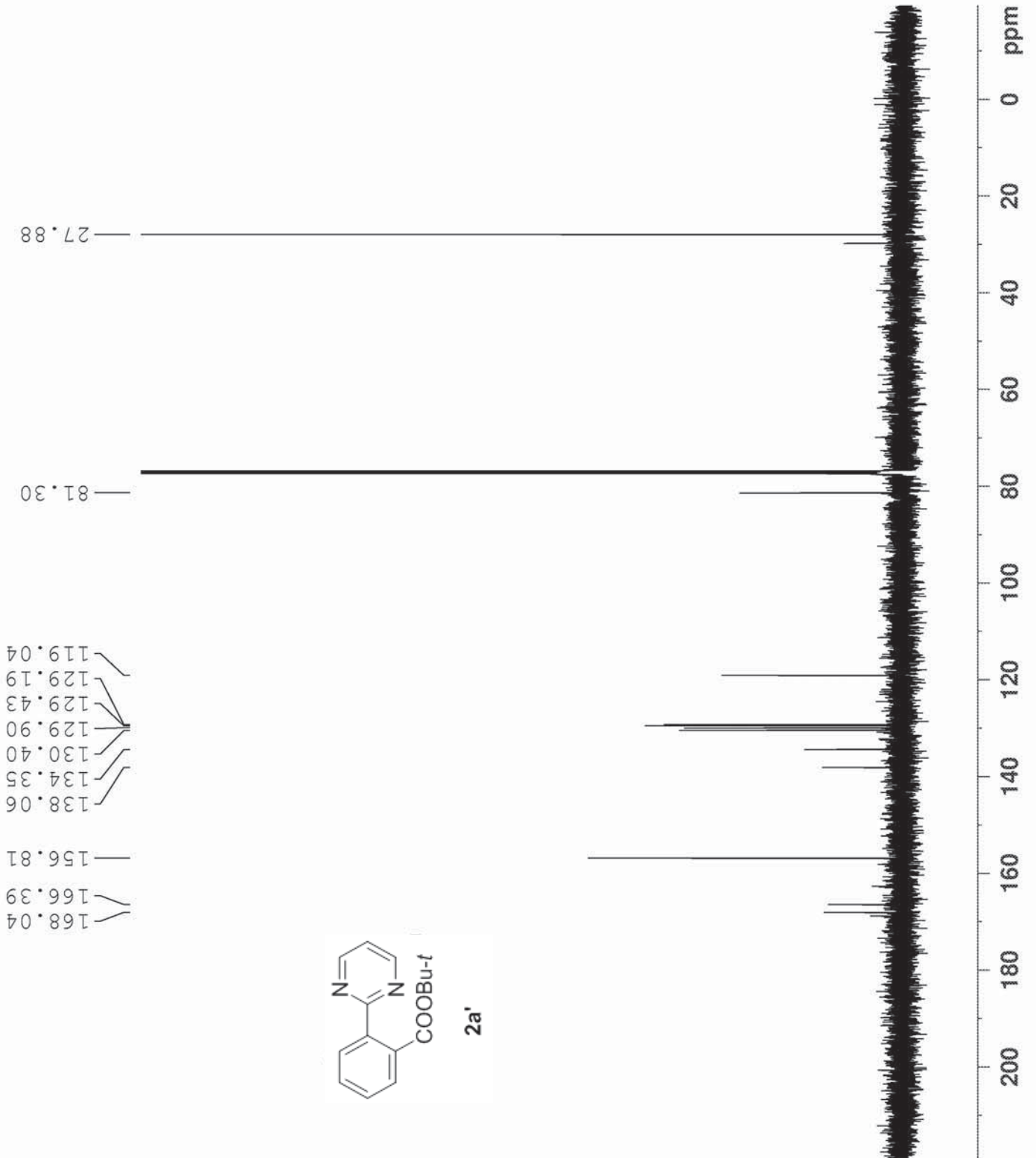
```

NAME      XB20140430
EXPNO     8
PROCNO    1
Date_     20140430
Time      9.46
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDC13
NS         191
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         297.2 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

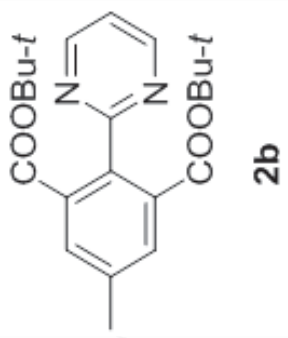
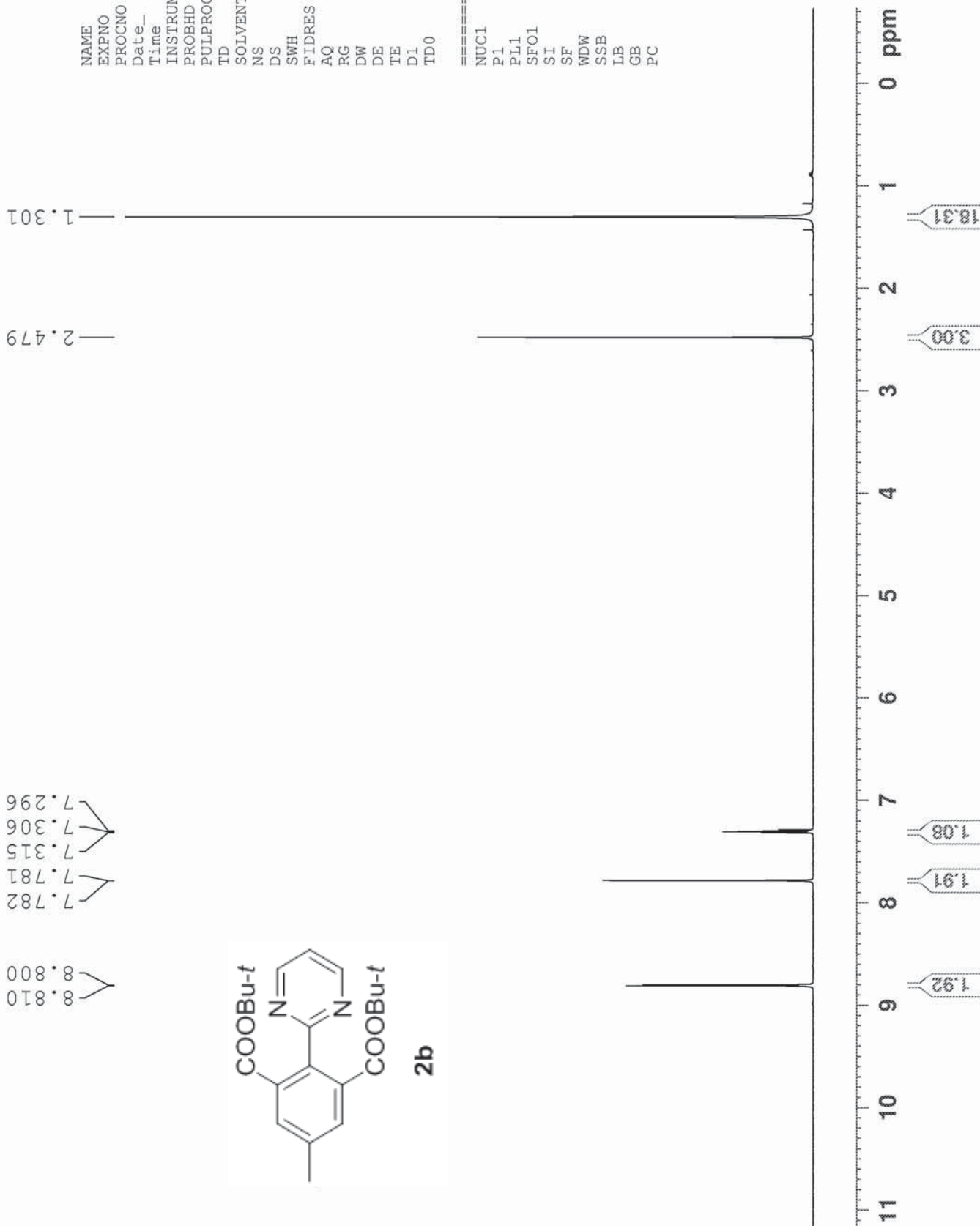
===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       1.00 dB
PL12     16.05 dB
PL13     16.50 dB
SFO2     500.1320005 MHz
SI        32768
SF        125.7577890 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```



HXH-155-1
 PROTON CDCl3

NAME XE20140414
 EXPNO 16
 PROCNO 1
 Date_ 20140414
 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 143.7
 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
 SF01 500.1330885 MHz
 SI 32768
 SF 500.1300000 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

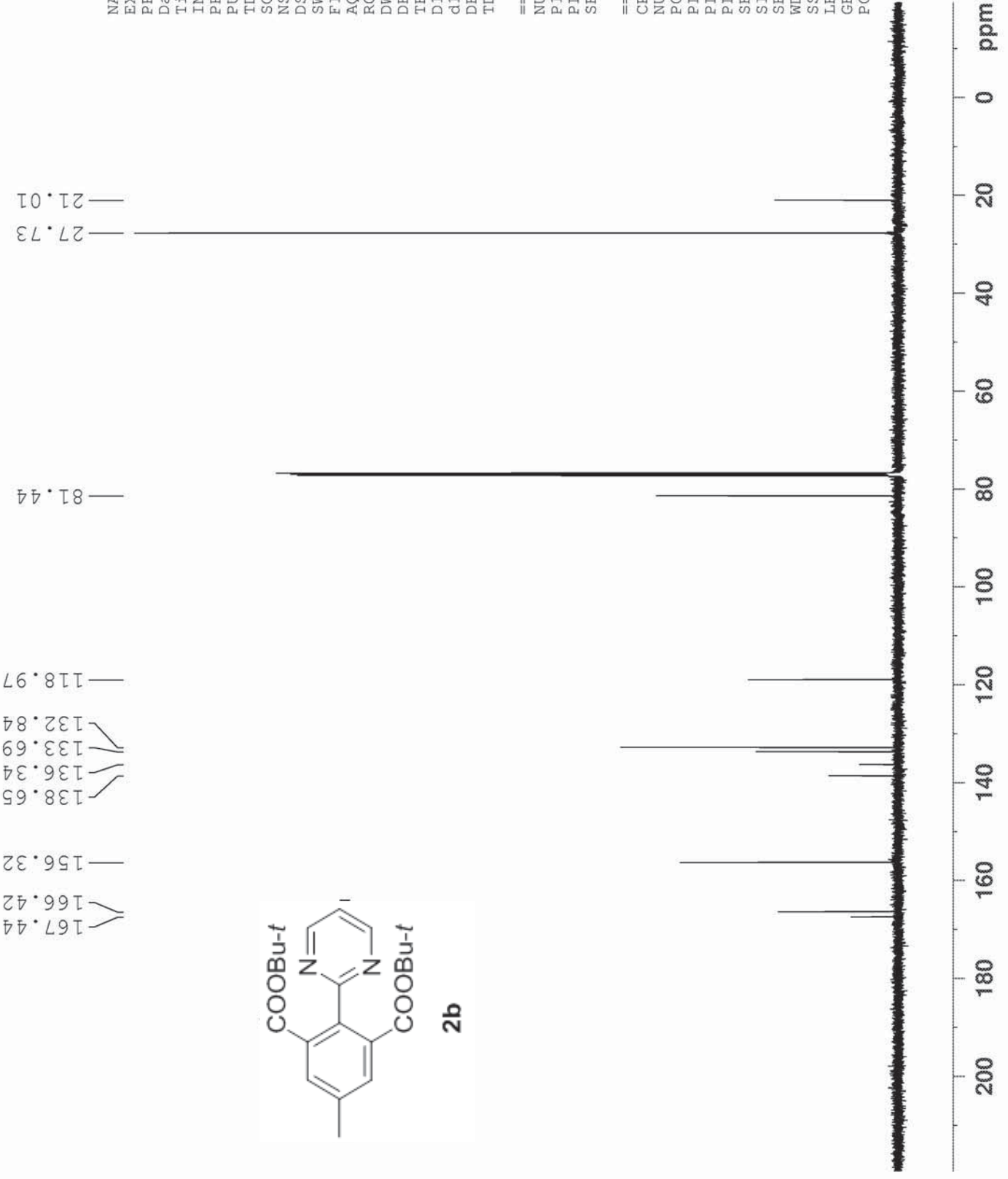


HXH-155-1
C13CPD CDC13

NAME XB20140414
 EXPNO 34
 PROCNO 1
 Date_ 20140415
 Time 2.26
 INSTRUM spect
 PROBD 5 mm PATXO 19F
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 256
 DS 4
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0912410 sec
 RG 143.7
 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



HXM-5-134
 PROTON CDCl3

NAME XB20130524
 EXPNO 6
 PROCNO 1
 Date_ 20130524
 Time_ 9.40
 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 295.8 K
 D1 1.00000000 sec
 TDO 1

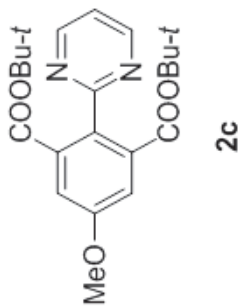
==== CHANNEL f1 =====
 NUC1 1H
 P1 14.14 usec
 PL1 1.00 dB
 SFO1 500.1330885 MHz
 SI 32768
 SF 500.1300129 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1.270

3.896

7.456
 7.288
 7.278
 7.268

8.770
 8.780



10 9 8 7 6 5 4 3 2 1 0 ppm

18.18

3.00

1.01

1.93

1.97

HXM-5-134
C13CPD CDC13

```

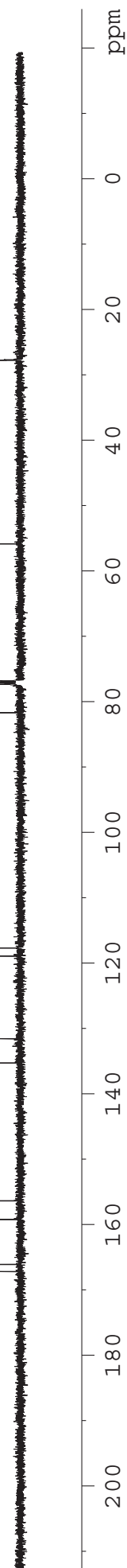
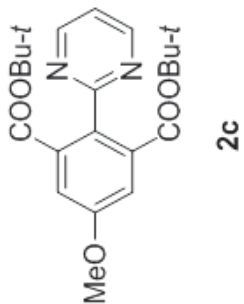
NAME       XB20130524
EXPNO      7
PROCNO     1
Date_      20130524
Time       9.50
INSTRUM    spect
PROBHD     5 mm PATXO 19F
PULPROG    zgpg30
TD          65536
SOLVENT    CDC13
NS          128
DS          4
SWH         30030.029 Hz
FIDRES     0.458222 Hz
AQ          1.0912410 sec
RG          362
DW          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
  
```

27.70 —
55.81 —
81.69 —
117.67 —
118.89 —
131.53 —
135.28 —
156.33 —
159.21 —
166.12 —
167.17 —



HXH-151-1
 PROTON CDC13

NAME XB20140414
 EXPNO 8
 PROCNO 1
 Date_ 20140414
 Time 10.44
 INSTRUM spect
 PROBHD 5 mm PATXO 19F
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1720407 sec
 RG 128
 DW 48.400 usec
 DE 6.00 usec
 TE 295.9 K
 D1 1.00000000 sec
 TD0 1

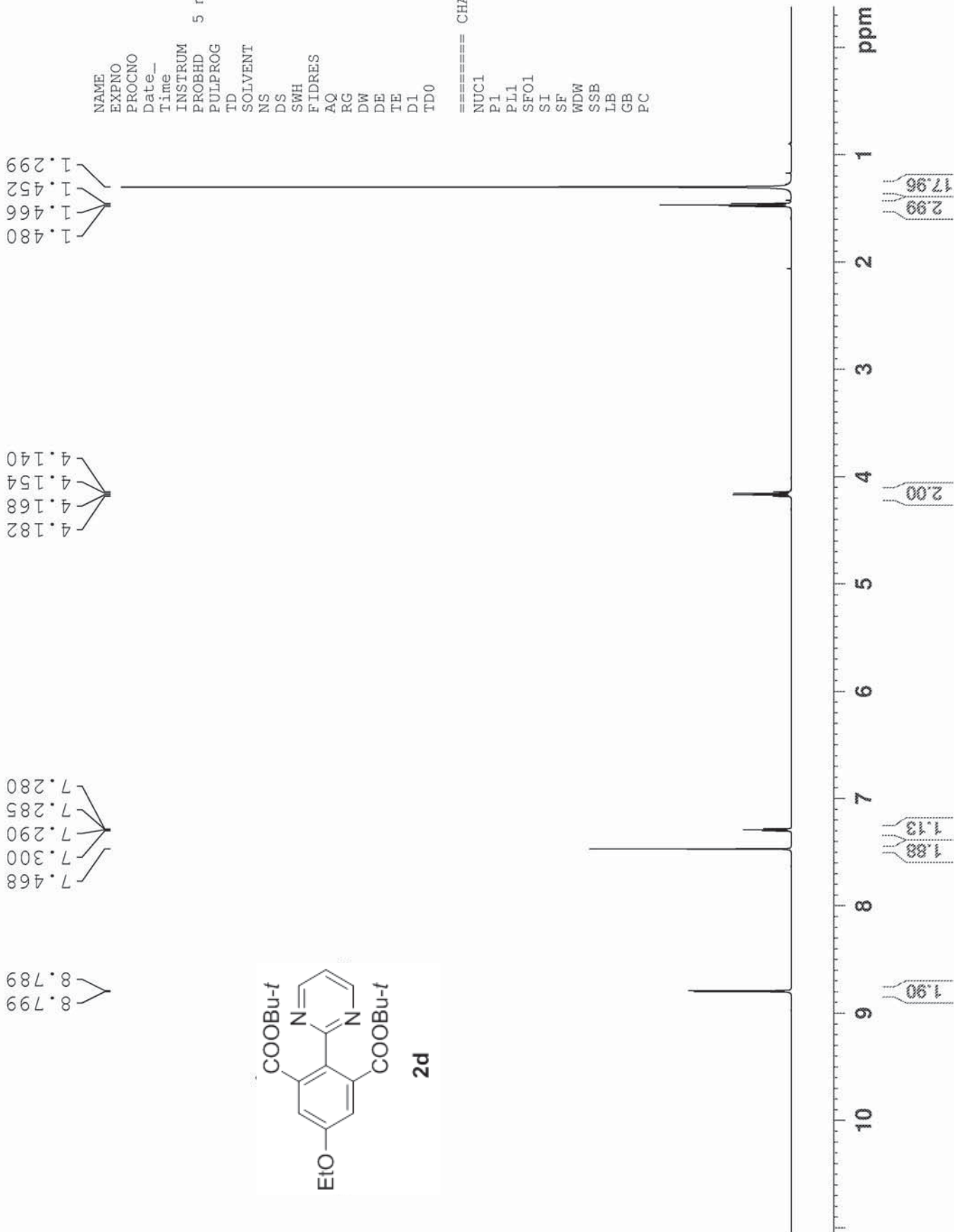
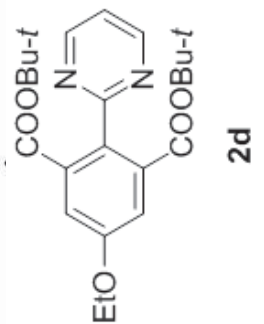
==== CHANNEL f1 =====
 NUC1 1H
 P1 14.14 usec
 PL1 1.00 dB
 SFO1 500.1330885 MHz
 SI 32768
 SF 500.1300000 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1.480
 1.466
 1.452
 1.299

4.182
 4.168
 4.154
 4.140

7.468
 7.300
 7.290
 7.285
 7.280

8.789
 8.799

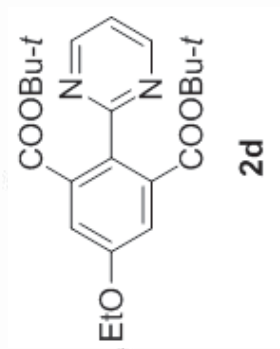
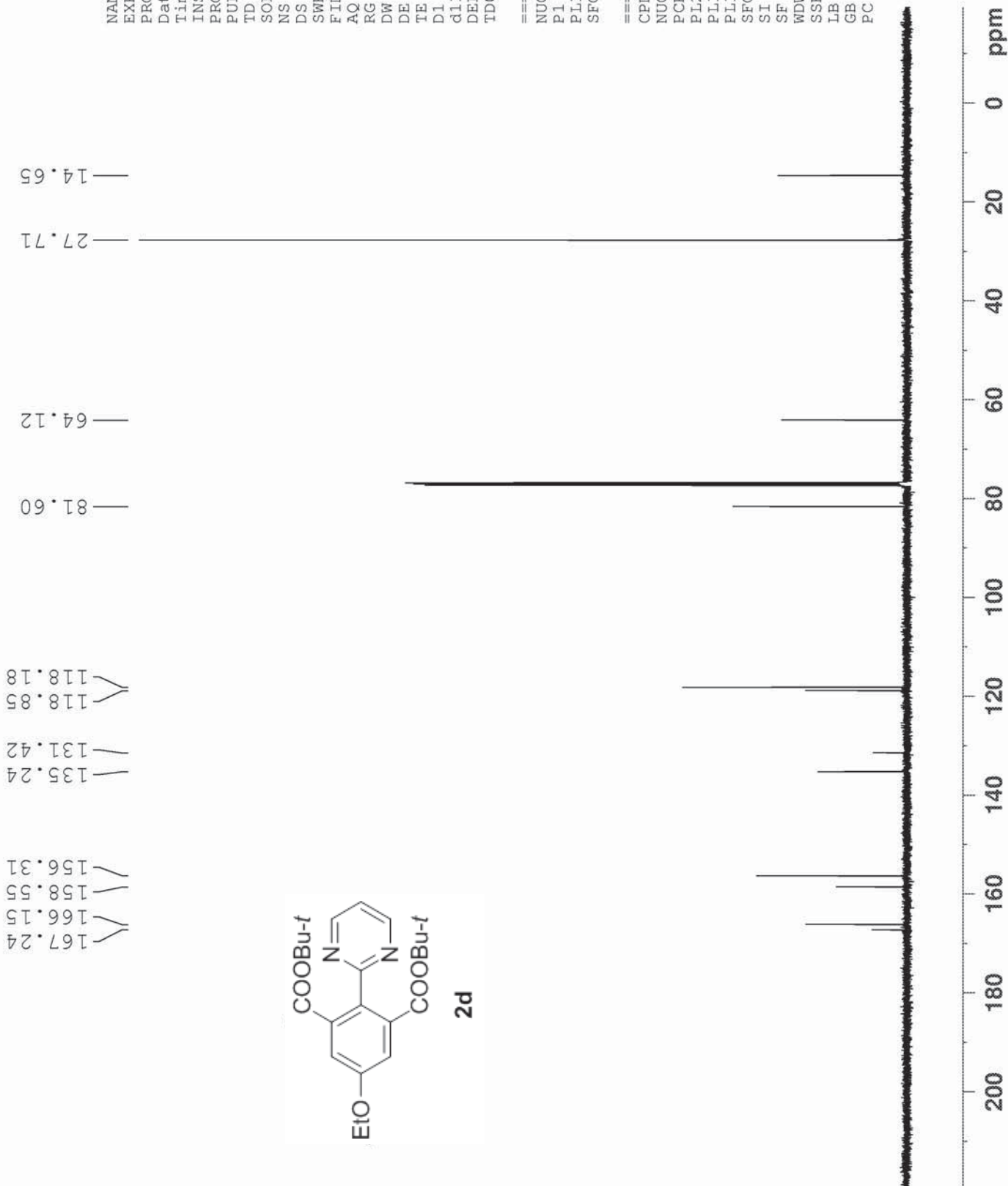


HXH-151-1
 C13CPD CDC13

NAME XB20140414
 EXPNO 32
 PROCNO 1
 Date_ 20140415
 Time 1.35
 INSTRUM spect
 PROBD 5 mm PATXO 19F
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 256
 DS 4
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0912410 sec
 RG 143.7
 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

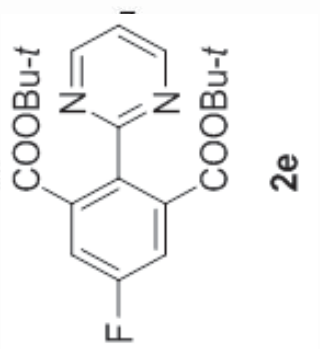
==== CHANNEL f1 =====
 NUC1 13C
 P1 9.50 usec
 PL1 -0.50 dB
 SFO1 125.7703643 MHz

==== 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



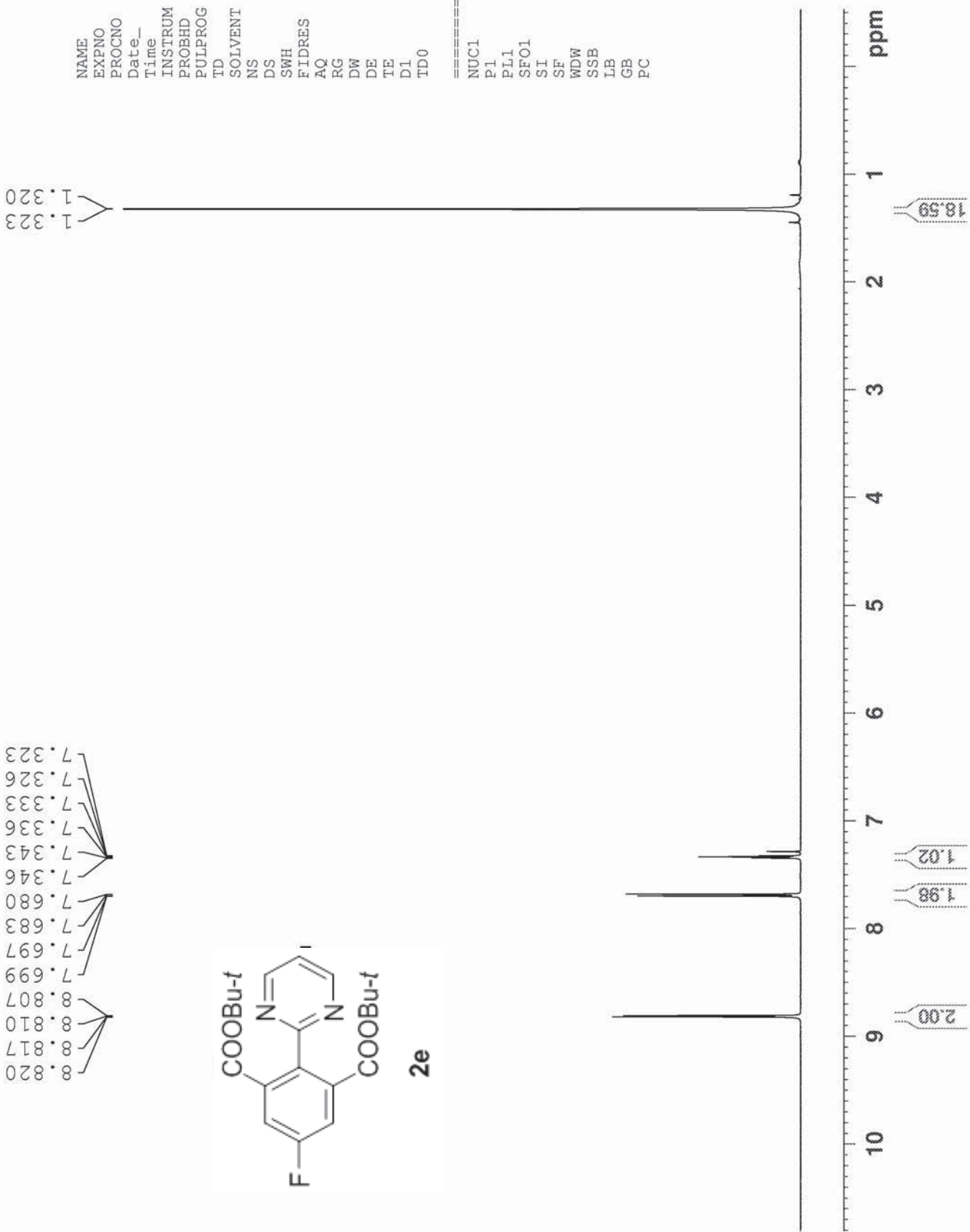
HXH-151-5
 PROTON CDCl3

7.323
 7.326
 7.333
 7.336
 7.343
 7.346
 7.680
 7.683
 7.697
 7.699
 8.007
 8.010
 8.017
 8.020



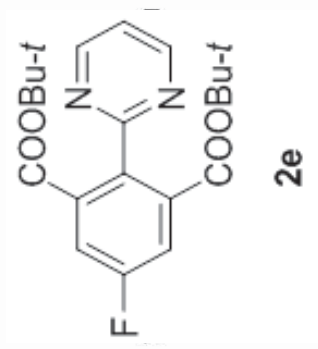
NAME XE20140414
 EXPNO 13
 PROCNO 1
 Date_ 20140414
 Time 11.05
 INSTRUM spect
 PROBHD 5 mm PATXO 19F
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1720407 sec
 RG 161.3
 DW 48.400 usec
 DE 6.00 usec
 TE 296.0 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 14.14 usec
 PL1 1.00 dB
 SFO1 500.1330885 MHz
 SI 32768
 SF 500.1300000 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



1111.465
1111.483
1111.501

HXH-151-5
19Fdeft CDC13 D:\\ deng 49



```

NAME          XB20140414
EXPNO         14
PROCNO        1
Date_         20140414
Time_         11.07
INSTRUM       spect
PROBHD        5 mm PATXO 19F
PULPROG       zg
TD            131072
SOLVENT       CDC13
NS            16
DS            4
SWH           100000.000 Hz
FIDRES        0.762939 Hz
AQ            0.6554150 sec
RG            322.5
DW            5.000 usec
DE            6.00 usec
TE            295.9 K
D1            1.00000000 sec
TD0           1

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



HXH-151-5
C13CPD CDCl3

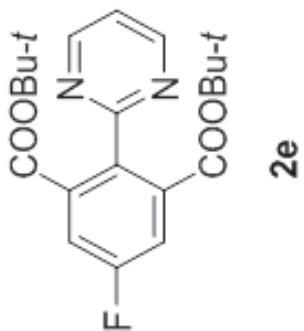
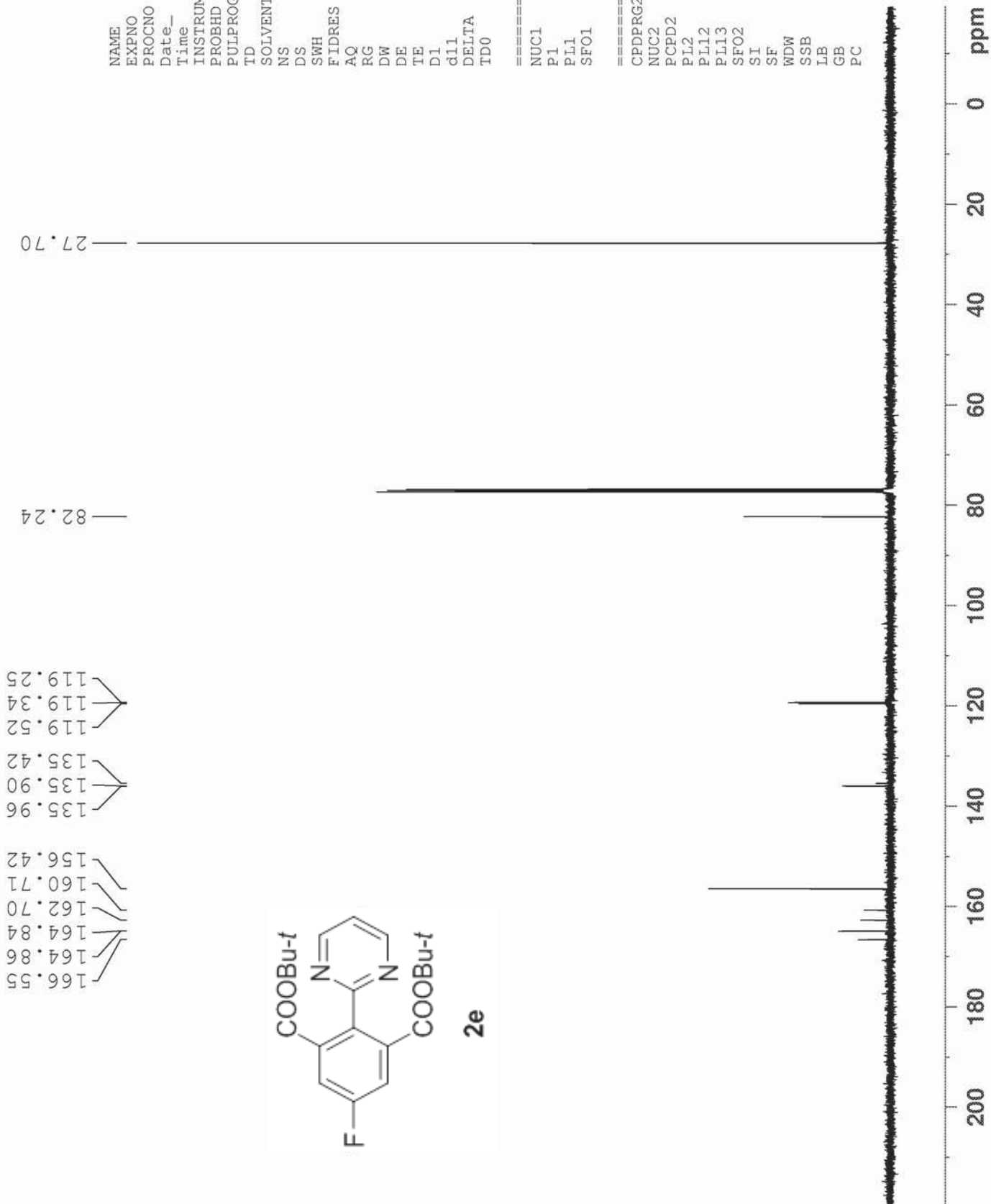
```

NAME      XB20140414
EXPNO     27
PROCNO    1
Date_     20140415
Time      0.35
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         143.7
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
  
```



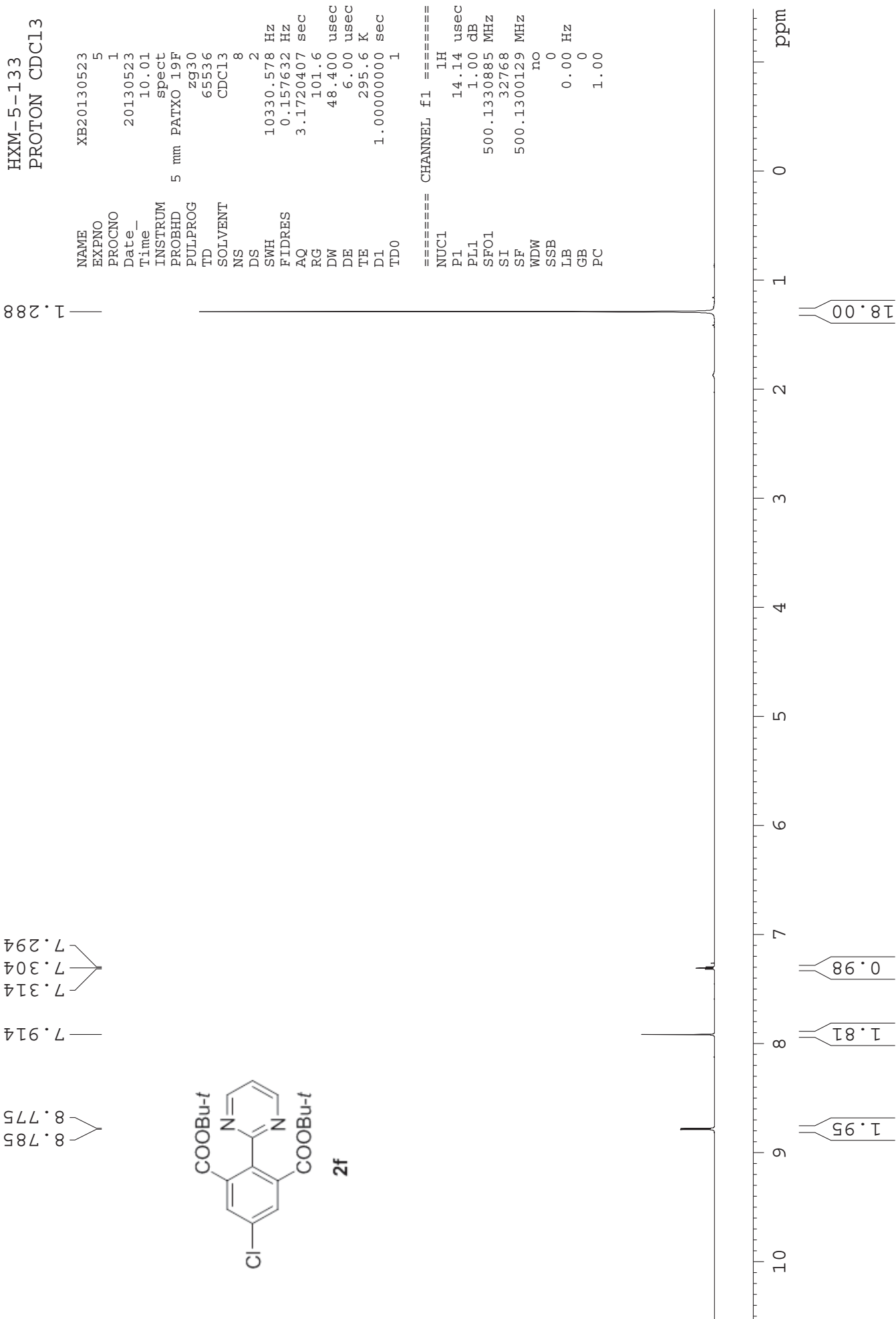
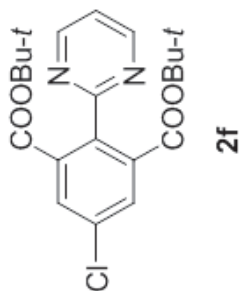
HXM-5-133
 PROTON CDCl3

NAME XB20130523
 EXPNO 5
 PROCNO 1
 Date_ 20130523
 Time 10.01
 INSTRUM spect
 PROBHD 5 mm PATXO 19F
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1720407 sec
 RG 101.6
 DW 48.400 usec
 DE 6.00 usec
 TE 295.6 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 14.14 usec
 PL1 1.00 dB
 SF01 500.1330885 MHz
 SI 32768
 SF 500.1300129 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1.2888

8.785
 8.775
 7.914
 7.314
 7.304
 7.294



HXM-5-133
C13CPD CDC13

```

NAME      XB20130523
EXPNO     21
PROCNO    1
Date_     20130523
Time      17.15
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDC13
NS         128
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         512
DW         16.650 usec
DE         6.00 usec
TE         296.8 K
D1         2.00000000 sec
d11        0.03000000 sec
DELTA     1.89999998 sec
TD0        1
  
```

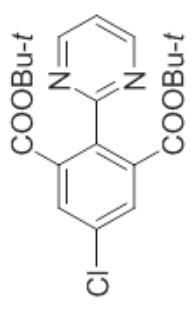
```

===== CHANNEL f1 =====
NUC1      13C
P1        9.50 usec
PL1       -0.50 dB
SFO1     125.7703643 MHz
  
```

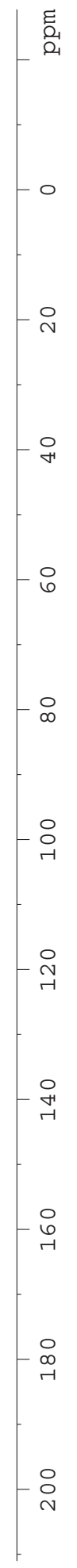
```

===== 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        0.20
  
```

27.69 —
82.31 —
119.34 —
132.14 —
134.59 —
135.35 —
137.42 —
156.45 —
164.90 —
166.40 —



2f

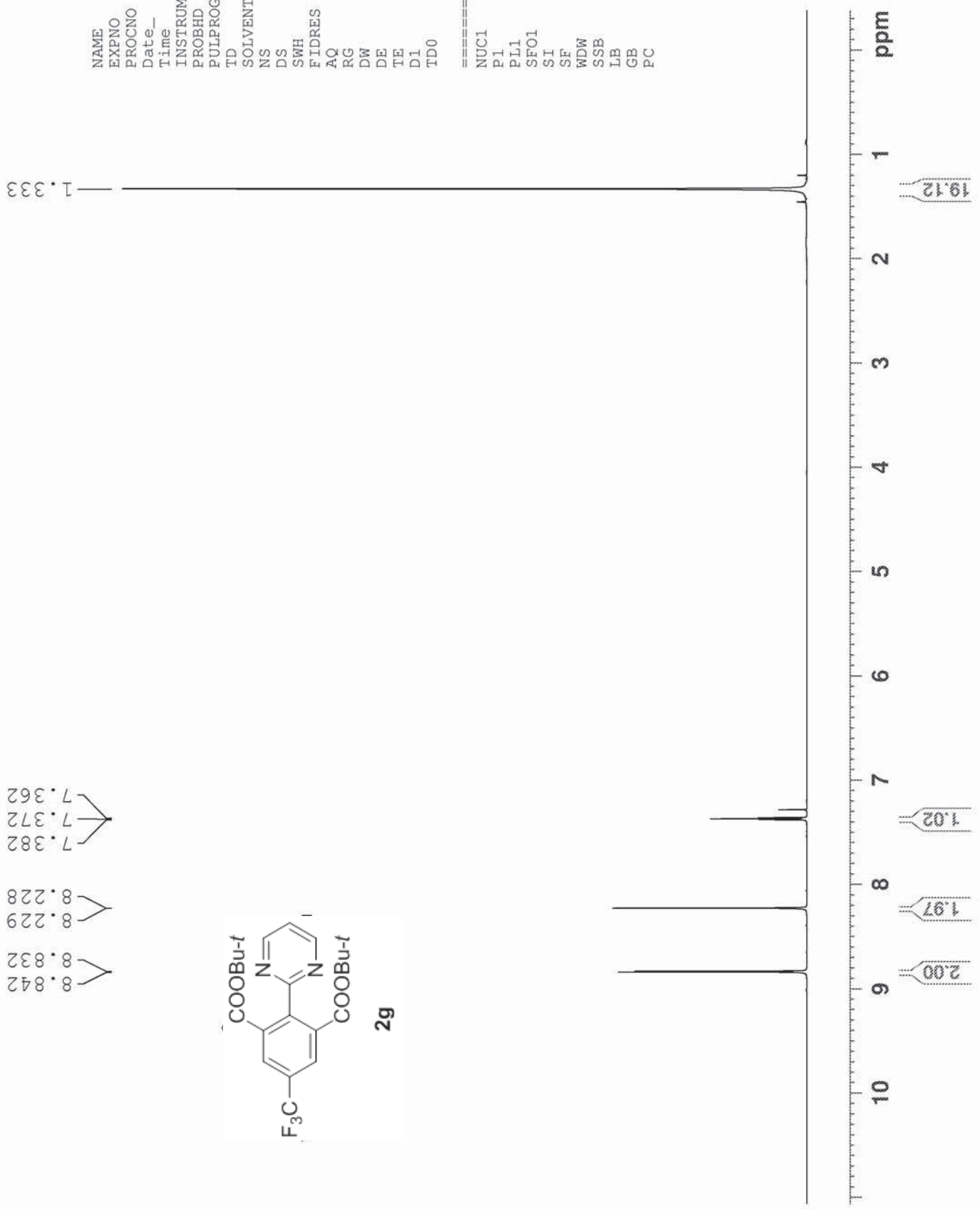
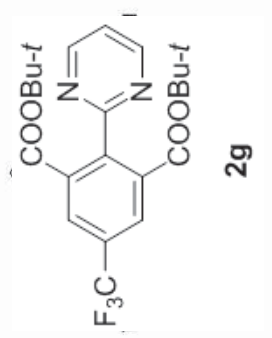


HXH-151-2
 PROTON CDC13

NAME XB20140414
 EXPNO 9
 PROCNO 1
 Date_ 20140414
 Time 10.50
 INSTRUM spect
 PROBD 5 mm PATXO 19F
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1720407 sec
 RG 143.7
 DW 48.400 usec
 DE 6.00 usec
 TE 295.9 K
 D1 1.00000000 sec
 TD0 1

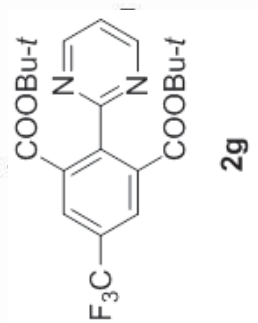
==== CHANNEL f1 =====
 NUC1 1H
 P1 14.14 usec
 PL1 1.00 dB
 SFO1 500.1330885 MHz
 SI 32768
 SF 500.1300000 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

8.842
 8.832
 8.229
 8.228
 7.382
 7.372
 7.362



HXH-151-2
19Fdeflt CDC13 D:\\ deng 47

62.869



```
NAME XB20140414
EXPNO 10
PROCNO 1
Date_ 20140414
Time 10.52
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg
TD 131072
SOLVENT CDC13
NS 16
DS 4
SWH 100000.000 Hz
FIDRES 0.762939 Hz
AQ 0.6554150 sec
RG 256
DW 5.000 usec
DE 6.00 usec
TE 295.9 K
D1 1.00000000 sec
TD0 1

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

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

HXH-151-2
C13CPD CDC13

```

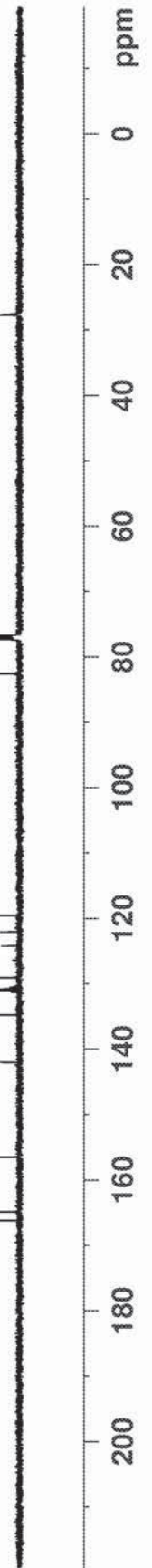
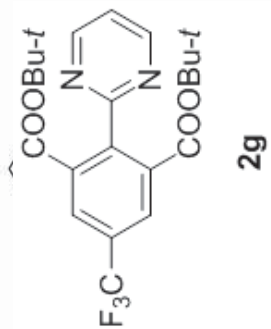
NAME      XB20140414
EXPNO     25
PROCNO    1
Date_     20140415
Time      0.13
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDC13
NS         512
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         143.7
DW         16.650 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
WDM       EM
SSB       0
LB        1.00 Hz
GB        0
PC        0.20
  
```

166.21
164.87
156.51
142.02
134.78
131.35
131.08
130.81
130.54
129.13
129.05
126.43
124.26
122.09
119.92
119.57
82.58
27.69

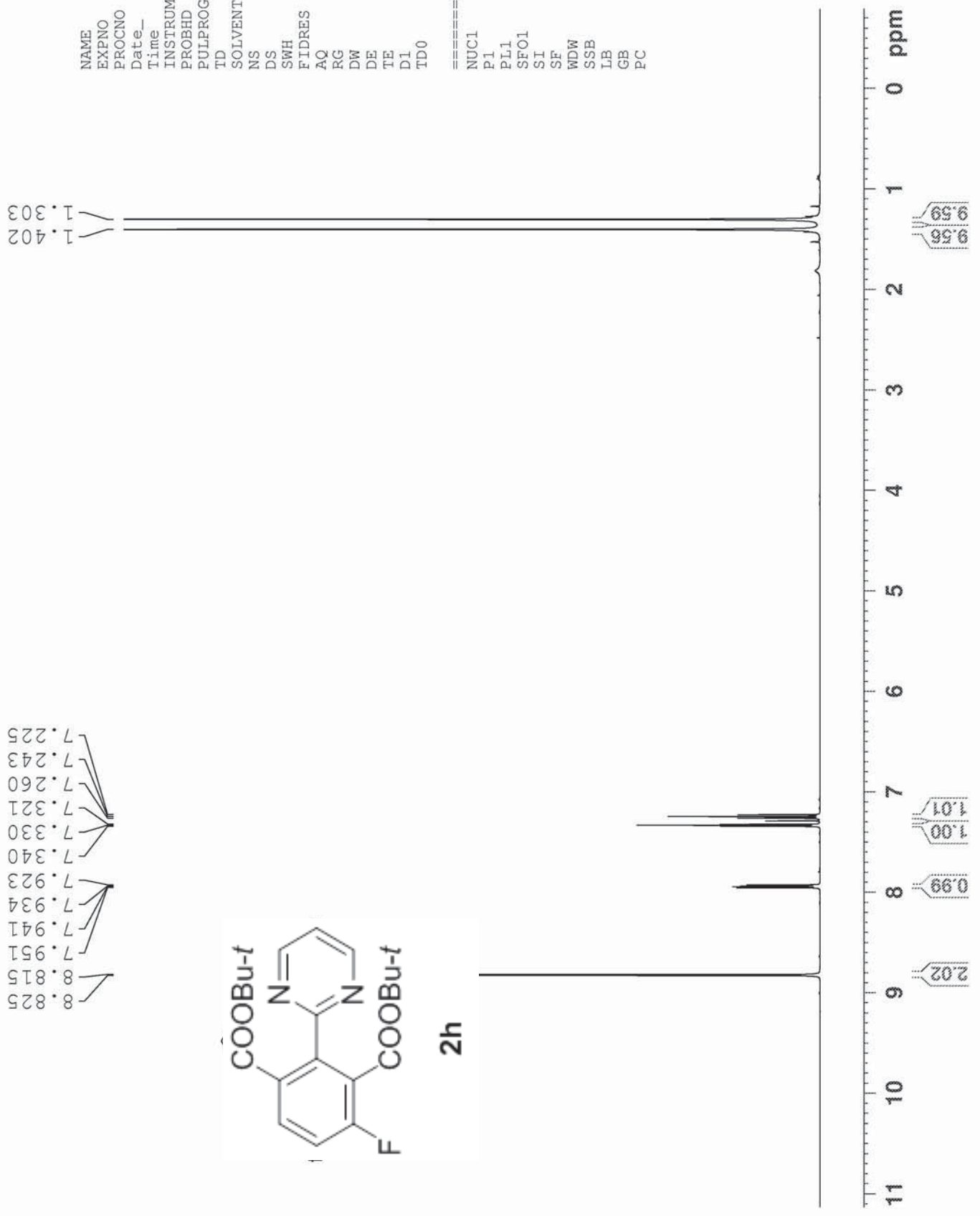
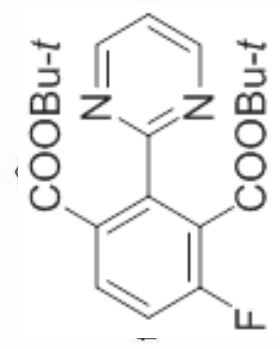


HXH-155-3
 PROTON CDCl3

NAME XB20140414
 EXPNO 17
 PROCNO 1
 Date_ 20140414
 Time 11.24
 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 143.7
 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 500.1300000 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

8.825
 8.815
 7.951
 7.941
 7.934
 7.923
 7.340
 7.330
 7.330
 7.321
 7.260
 7.243
 7.225



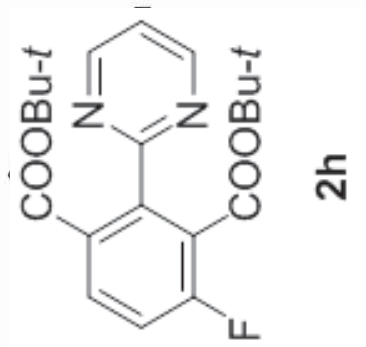
HXH-155-3
 19Fdeflt CDC13 D:\\ deng 52

110.400
 110.412
 110.419
 110.429

```

NAME          XB20140414
EXPNO         18
PROCNO        1
Date_         20140414
Time          11.26
INSTRUM       spect
PROBHD        5 mm PATXO 19F
PULPROG       zg
TD            131072
SOLVENT       CDC13
NS            16
DS            4
SWH           100000.000 Hz
FIDRES        0.762939 Hz
AQ            0.6554150 sec
RG            322.5
DW            5.000 usec
DE            6.00 usec
TE            295.9 K
D1            1.00000000 sec
TD0           1

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

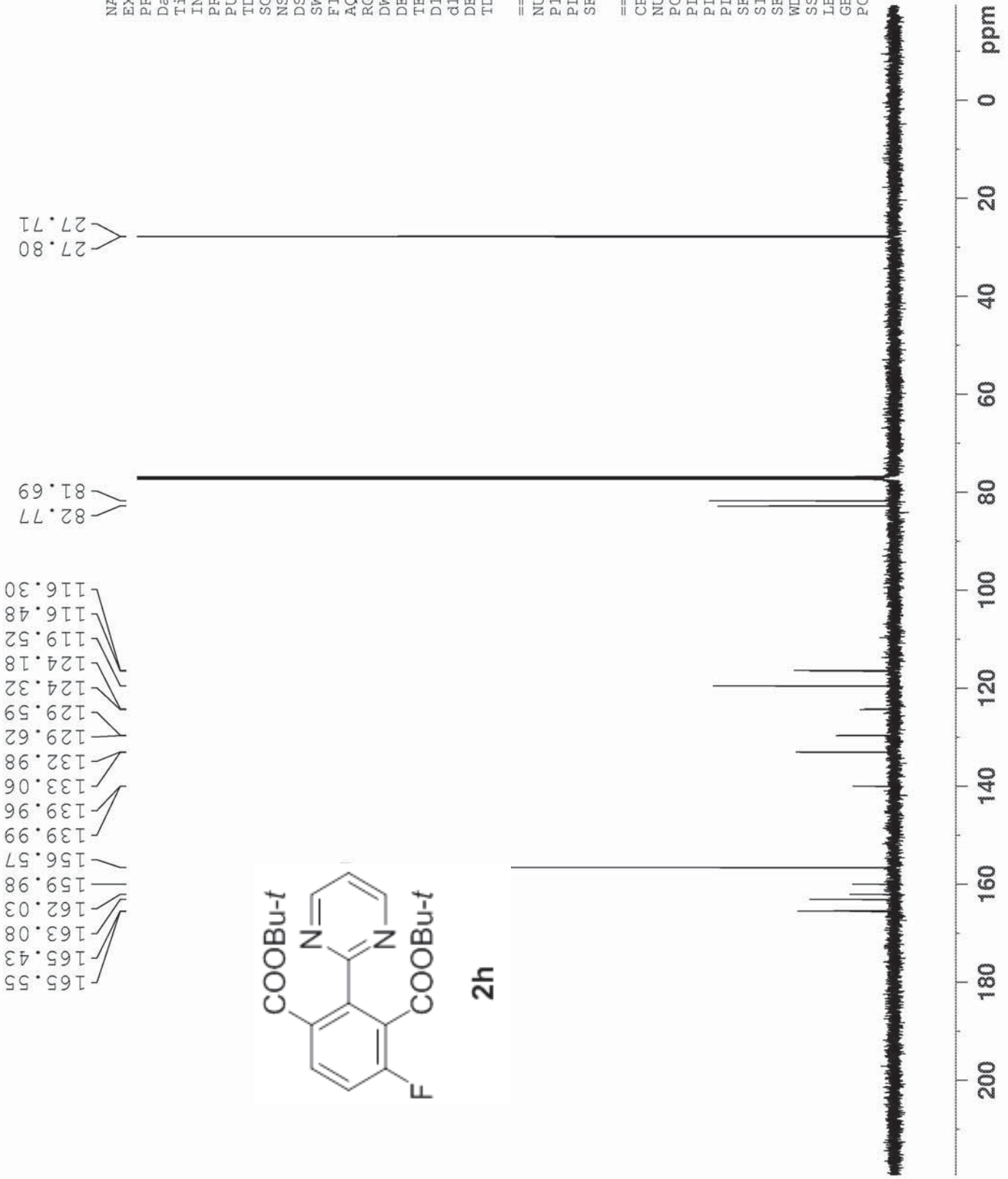


HXH-155-3
C13CPD CDC13

NAME XB20140414
 EXPNO 35
 PROCNO 1
 Date_ 20140415
 Time 2.45
 INSTRUM spect
 PROBD 5 mm PATXO 19F
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 256
 DS 4
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0912410 sec
 RG 143.7
 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

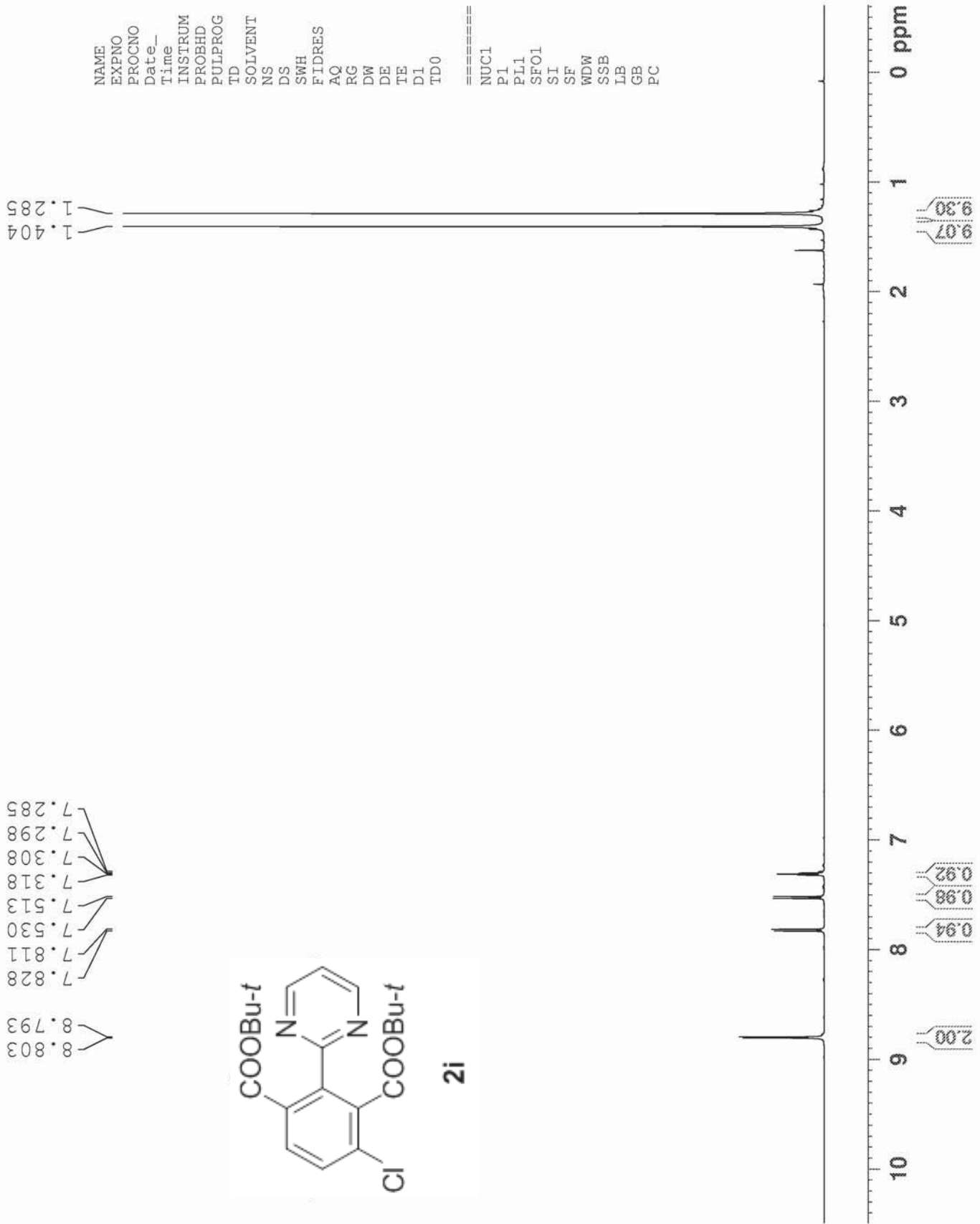
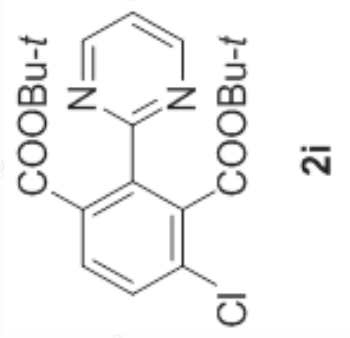


HXH-156-2
 PROTON CDC13

NAME XB20140417
 EXPNO 10
 PROCNO 1
 Date_ 20140417
 Time 12.06
 INSTRUM spect
 PROBD 5 mm PATXO 19F
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 8
 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 295.8 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 14.14 usec
 PL1 1.00 dB
 SF01 500.1330885 MHz
 SI 32768
 SF 500.1300000 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

8.803
 8.793
 7.828
 7.811
 7.811
 7.530
 7.513
 7.318
 7.308
 7.298
 7.285



HXH-156-2
C13CPD CDC13

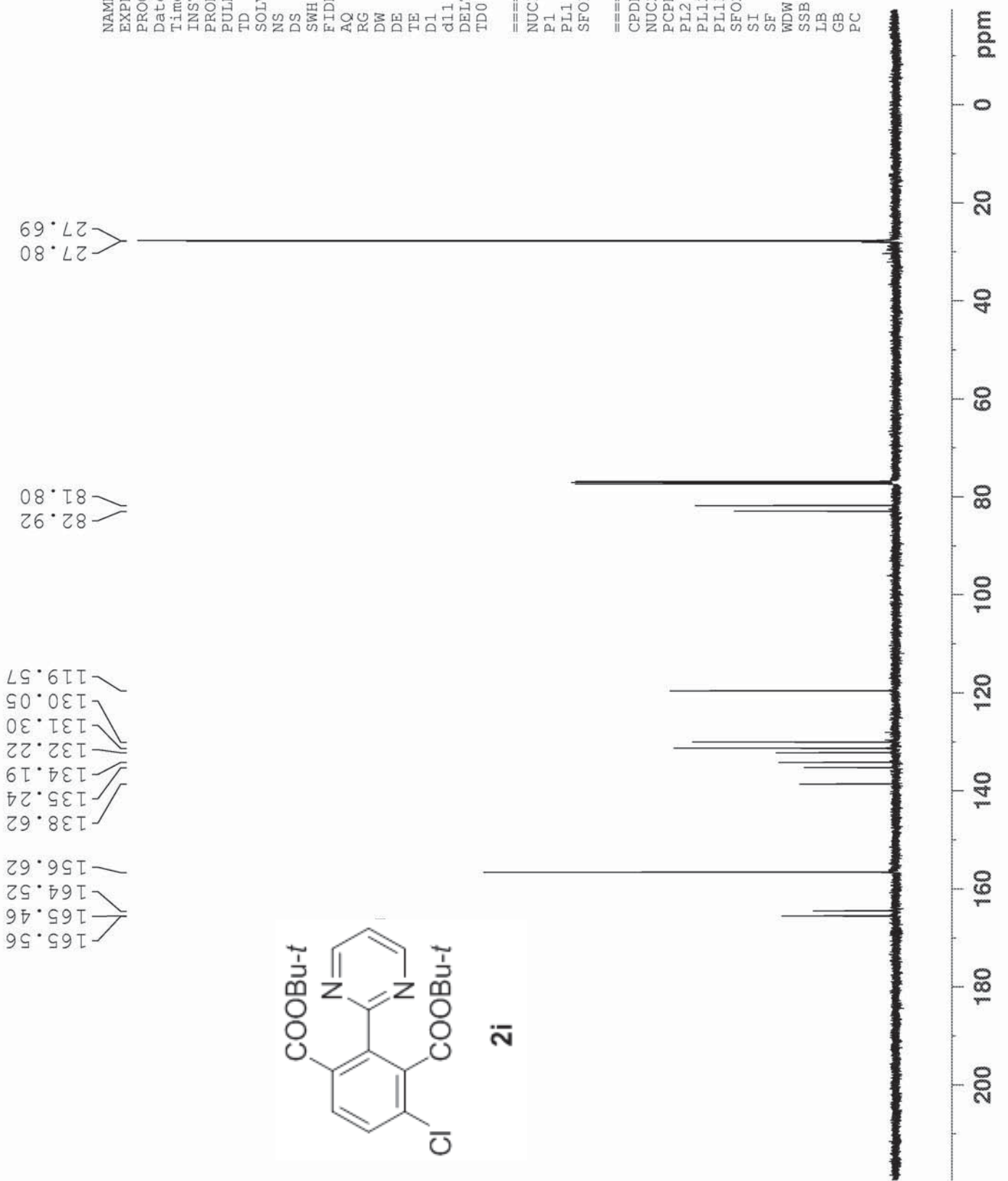
```

NAME      XB20140417
EXPNO     12
PROCNO    1
Date_     20140417
Time      12.16
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDC13
NS         128
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         143.7
DE         16.650 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
  
```

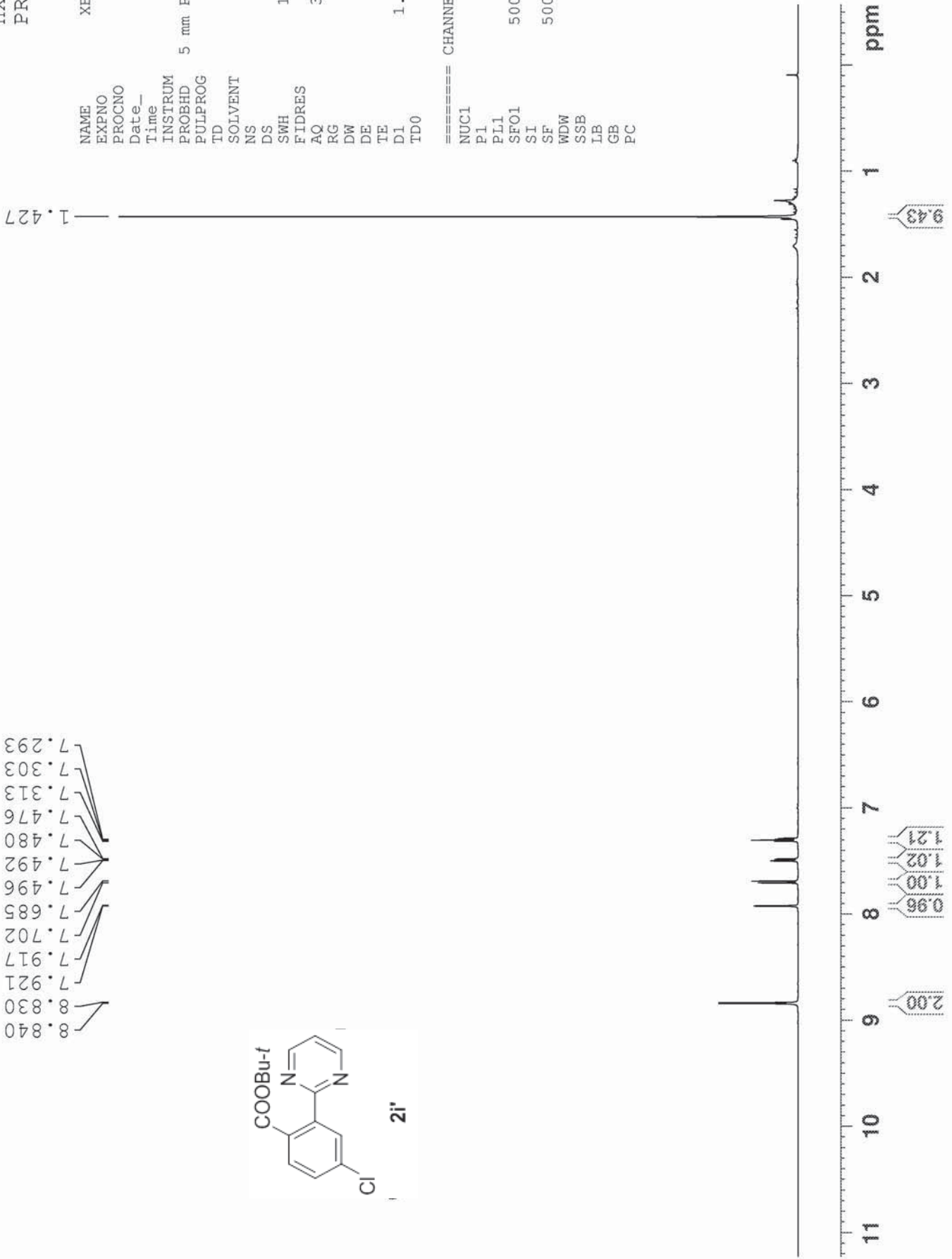
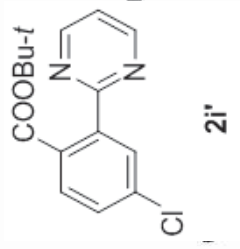


HXH-156-1
 PROTON CDCl3

NAME XB20140416
 EXPNO 5
 PROCNO 1
 Date_ 20140416
 Time 10.40
 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 295.9 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 14.14 usec
 PL1 1.00 dB
 SF01 500.1330885 MHz
 SI 32768
 SF 500.1300000 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

8.840
 8.830
 7.921
 7.917
 7.702
 7.685
 7.496
 7.492
 7.480
 7.476
 7.313
 7.303
 7.293



HXH-156-1
C13CPD CDC13

```

NAME       XB20140416
EXPNO      12
PROCNO     1
Date_      20140416
Time       11.27
INSTRUM    spect
PROBHD     5 mm PATXO 19F
PULPROG    zgpg30
TD          65536
SOLVENT    CDC13
NS          128
DS          4
SWH         30030.029 Hz
FIDRES     0.458222 Hz
AQ          1.0912410 sec
RG          143.7
DW          16.650 usec
DE          6.00 usec
TE          297.2 K
D1          2.0000000 sec
d11         0.0300000 sec
DELTA      1.89999998 sec
TD0        1
  
```

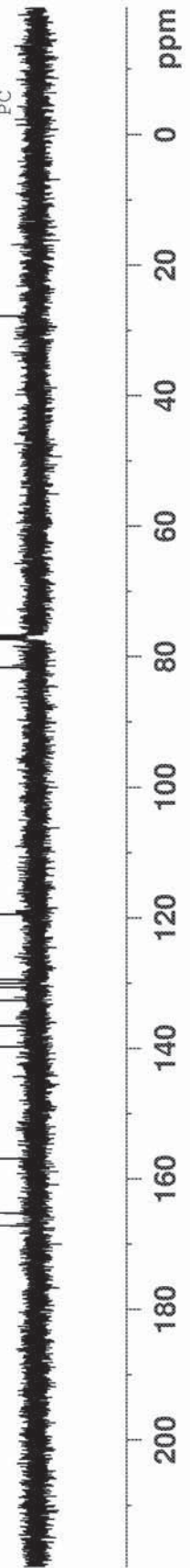
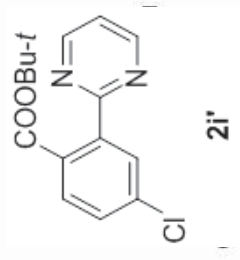
```

===== 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
  
```

119.45
129.42
130.05
130.63
132.66
136.50
139.74
156.93
165.24
167.15

81.69
27.84

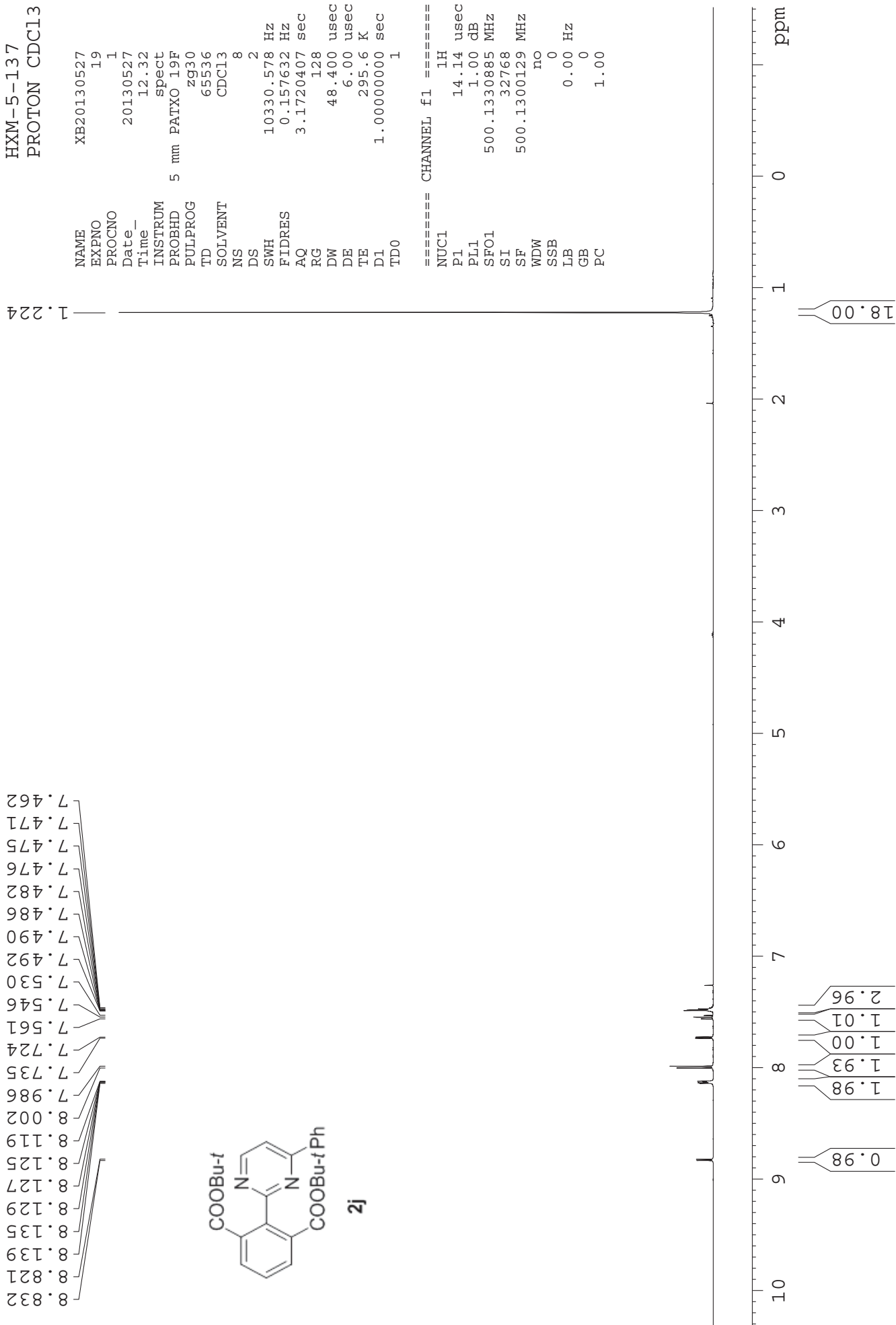
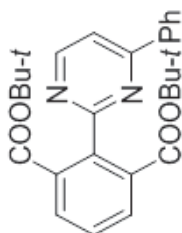


HXM-5-137
 PROTON CDCl3

NAME XB20130527
 EXPNO 19
 PROCNO 1
 Date_ 20130527
 Time_ 12.32
 INSTRUM spect
 PROBHD 5 mm PATXO 19F
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1720407 sec
 RG 128
 DW 48.400 usec
 DE 6.00 usec
 TE 295.6 K
 D1 1.00000000 sec
 TDO 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

8.832
 8.821
 8.139
 8.135
 8.129
 8.127
 8.125
 8.119
 8.002
 7.986
 7.735
 7.724
 7.561
 7.546
 7.530
 7.492
 7.490
 7.486
 7.482
 7.476
 7.475
 7.471
 7.462



HXM-5-137
C13CPD CDC13

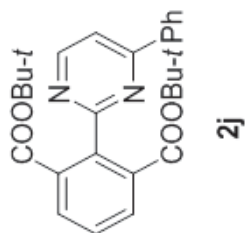
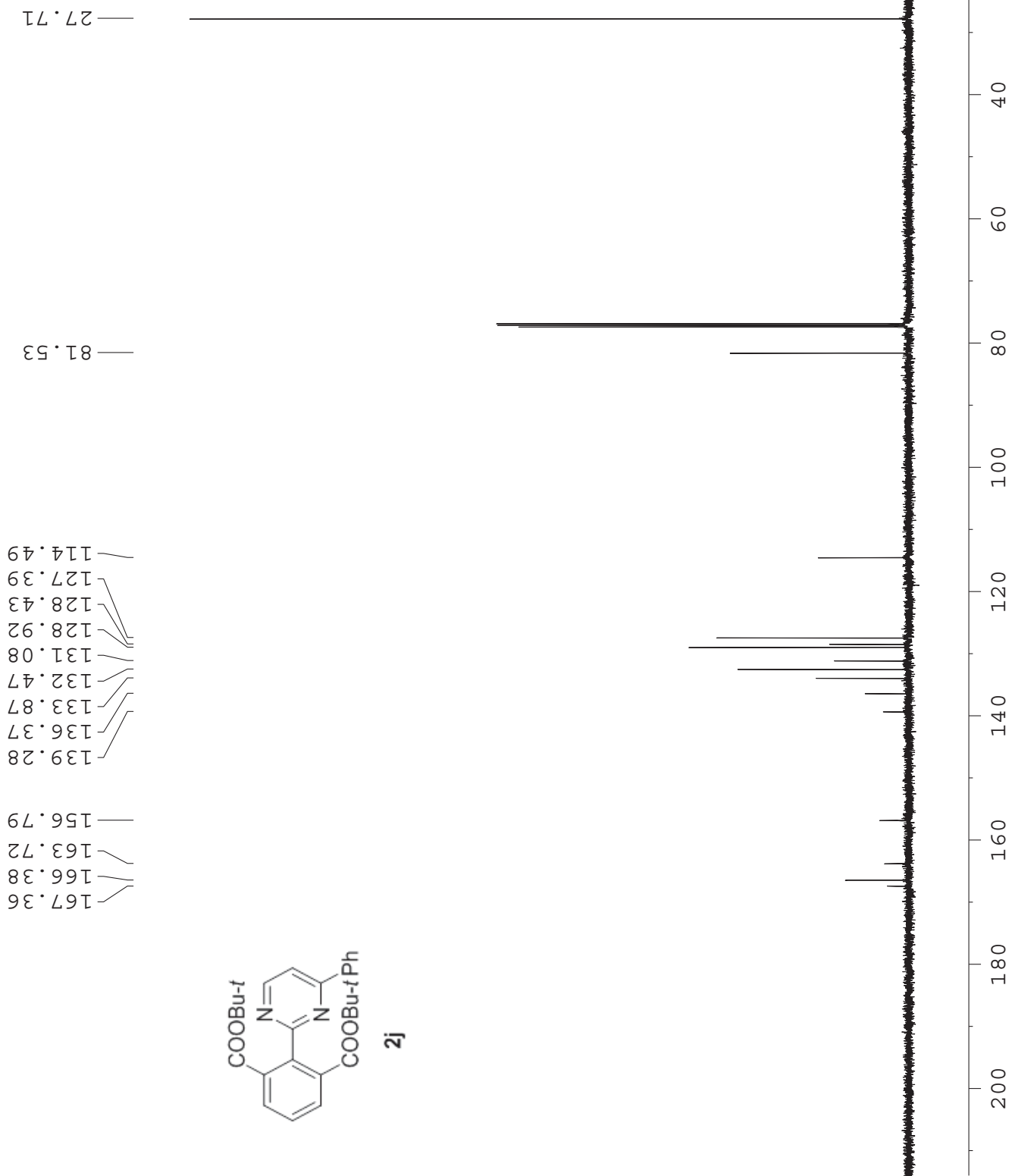
```

NAME          XB20130527
EXPNO         20
PROCNO        1
Date_         20130527
Time          12.41
INSTRUM       spect
PROBHD        5 mm PATXO 19F
PULPROG       zgpg30
TD            65536
SOLVENT       CDC13
NS            128
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            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
  
```



HXH-151-3
 PROTON CDC13

NAME XB20140414
 EXPNO 11
 PROCNO 1
 Date_ 20140414
 Time 10.58
 INSTRUM spect
 PROBHD 5 mm PATXO 19F
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1720407 sec
 RG 143.7
 DW 48.400 usec
 DE 6.00 usec
 TE 295.9 K
 D1 1.00000000 sec
 TD0 1

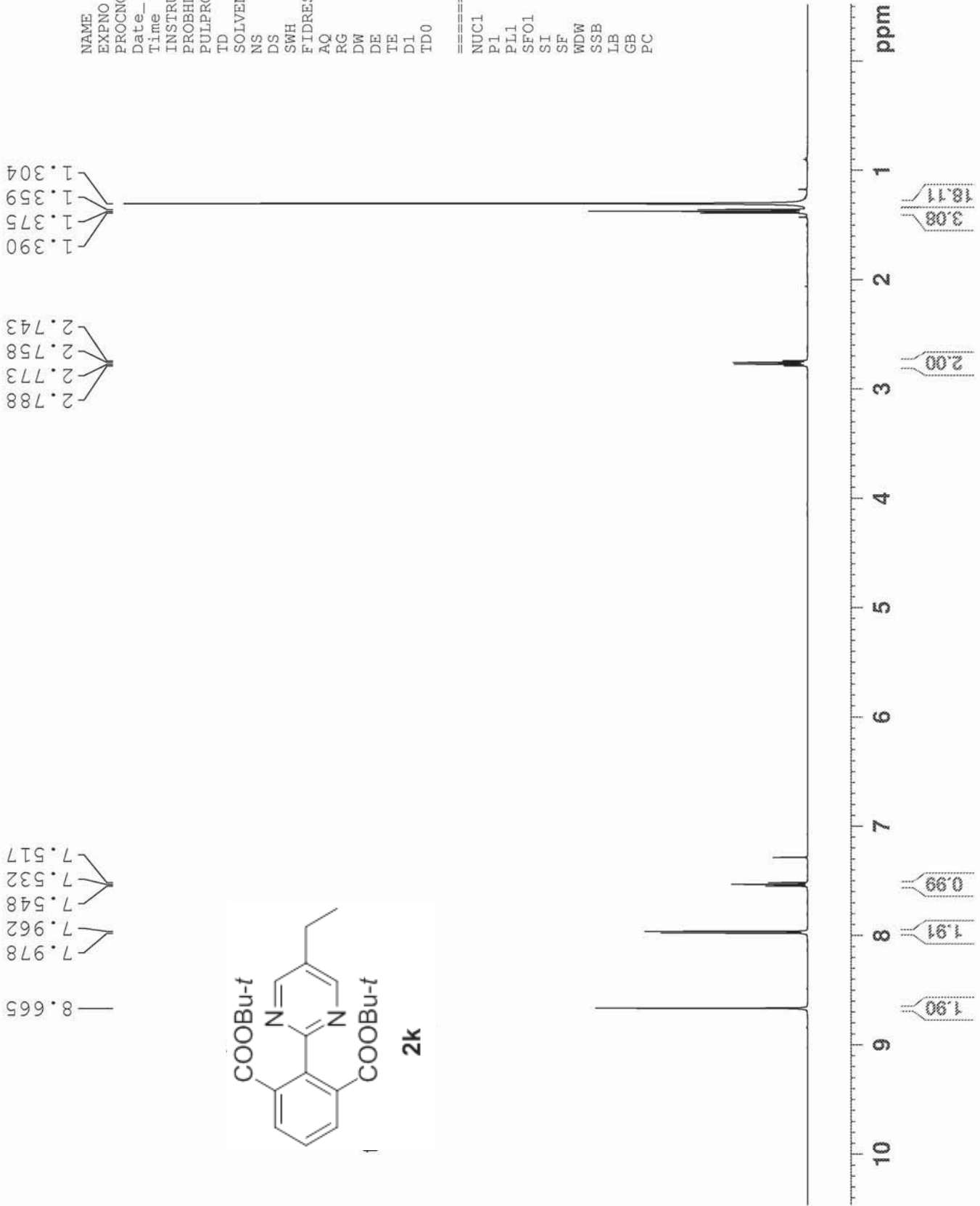
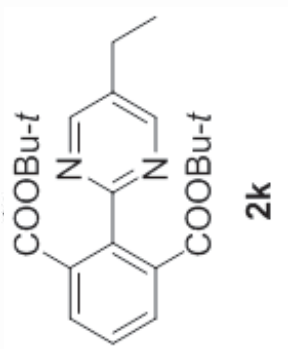
==== CHANNEL f1 =====
 NUC1 1H
 P1 14.14 usec
 PL1 1.00 dB
 SFO1 500.1330885 MHz
 SI 32768
 SF 500.1300000 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1.390
 1.375
 1.359
 1.304

2.788
 2.773
 2.758
 2.743

8.665

7.978
 7.962
 7.548
 7.532
 7.517

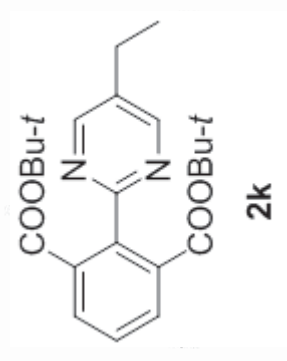
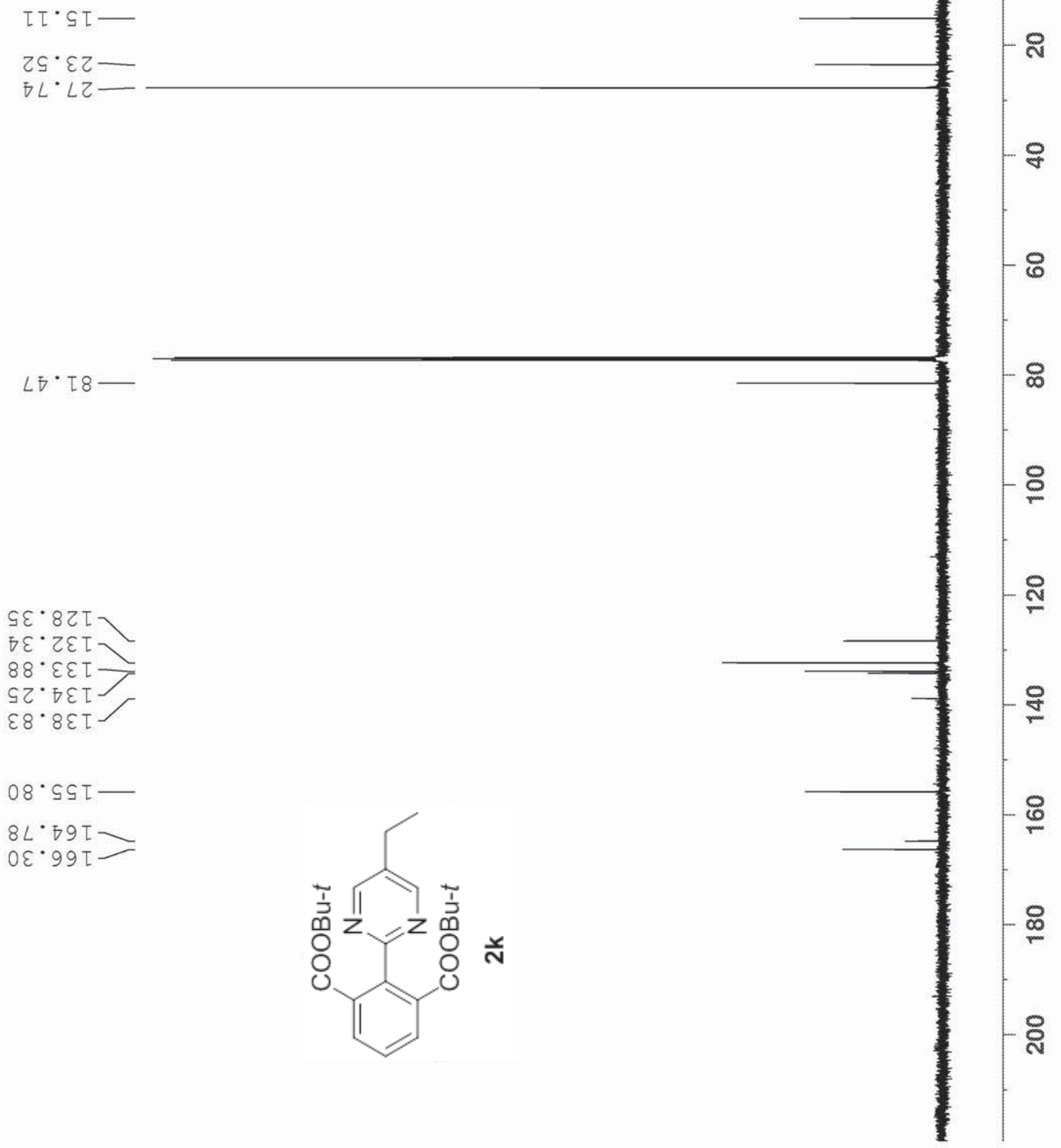


HXH-151-3
C13CPD CDC13

NAME XB20140414
 EXPNO 29
 PROCNO 1
 Date_ 20140415
 Time 0.56
 INSTRUM spect
 PROBD 5 mm PATXO 19F
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 256
 DS 4
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0912410 sec
 RG 143.7
 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
 SF01 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
 SF02 500.1320005 MHz
 SI 32768
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

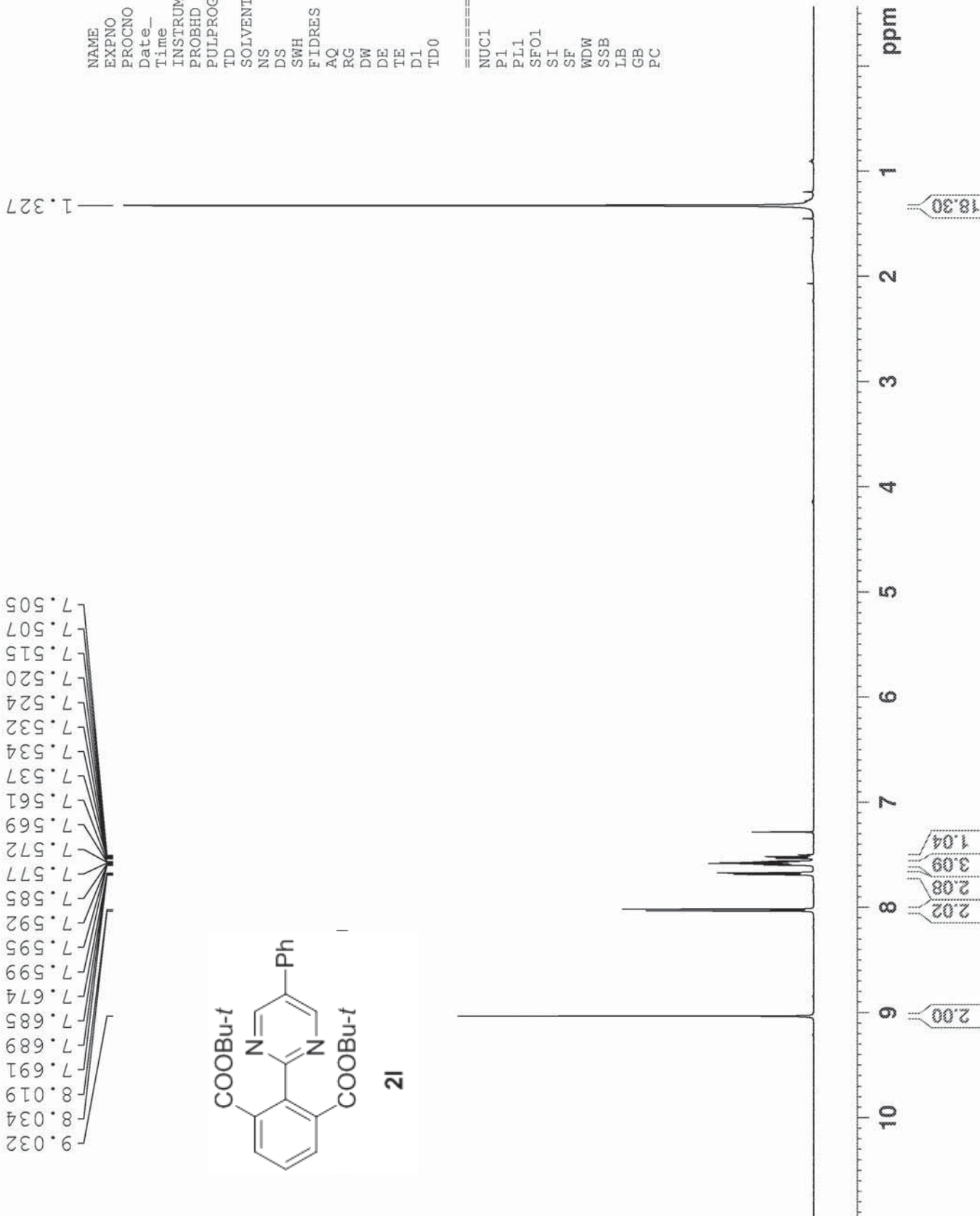
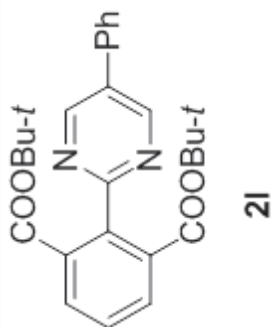


HXH-151-4
 PROTON CDC13

NAME XB20140414
 EXPNO 15
 PROCNO 1
 Date_ 20140414
 Time 11.13
 INSTRUM spect
 PROBHD 5 mm PATXO 19F
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 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 295.9 K
 D1 1.00000000 sec
 TD0 1

=====
 CHANNEL f1 =====
 NUC1 1H
 P1 14.14 usec
 PL1 1.00 dB
 SF01 500.1330885 MHz
 SI 32768
 SF 500.1300000 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

9.032
 8.034
 8.019
 7.691
 7.689
 7.685
 7.674
 7.599
 7.595
 7.592
 7.585
 7.577
 7.572
 7.569
 7.561
 7.537
 7.534
 7.532
 7.524
 7.520
 7.515
 7.507
 7.505

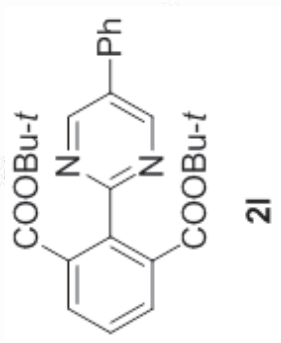
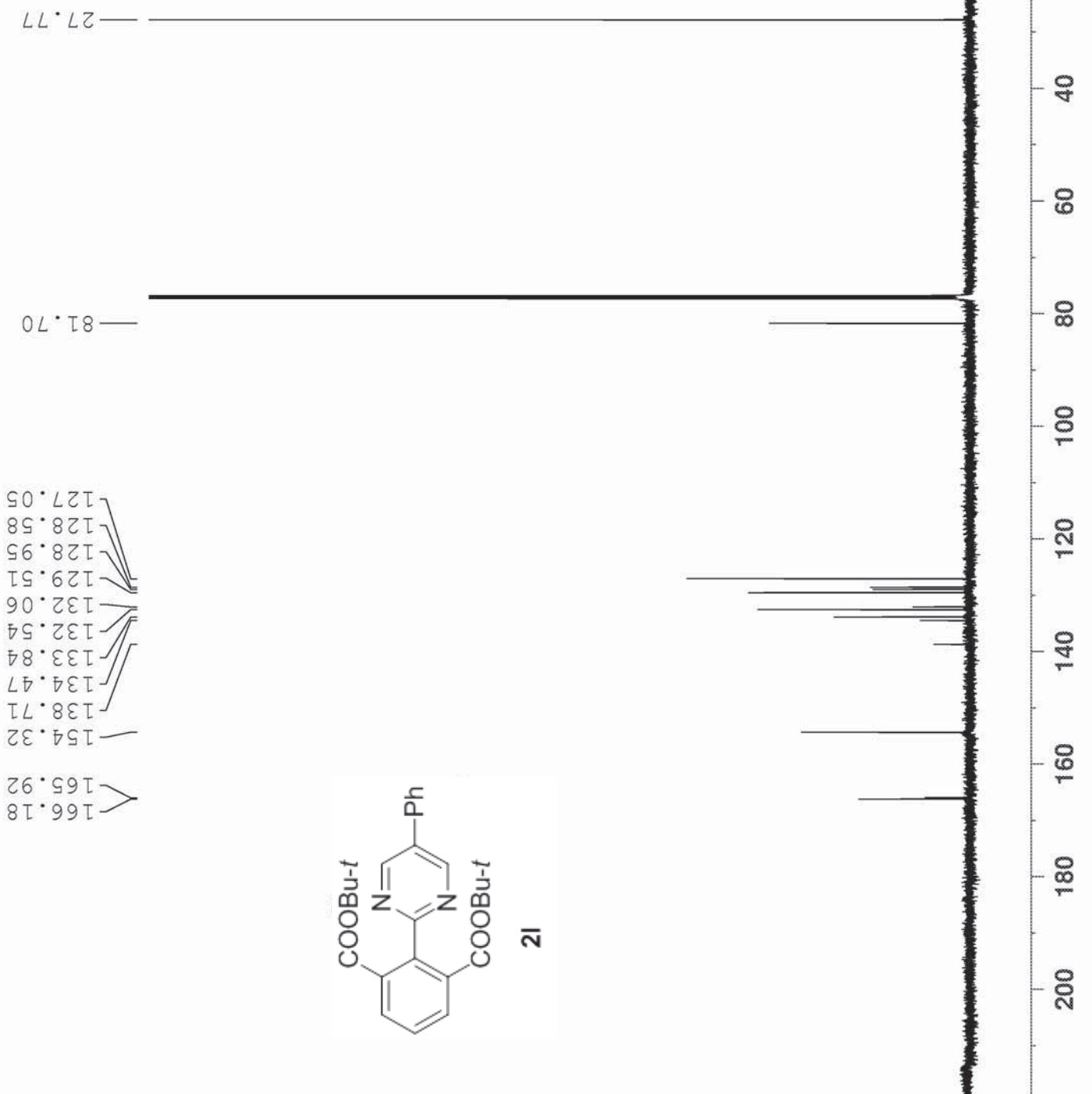


HXH-151-4
 C13CPD CDC13

NAME XB20140414
 EXPNO 33
 PROCNO 1
 Date_ 20140415
 Time 2.07
 INSTRUM spect
 PROBHD 5 mm PATXO 19F
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 512
 DS 4
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0912410 sec
 RG 143.7
 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

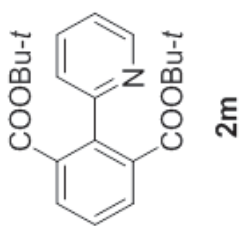
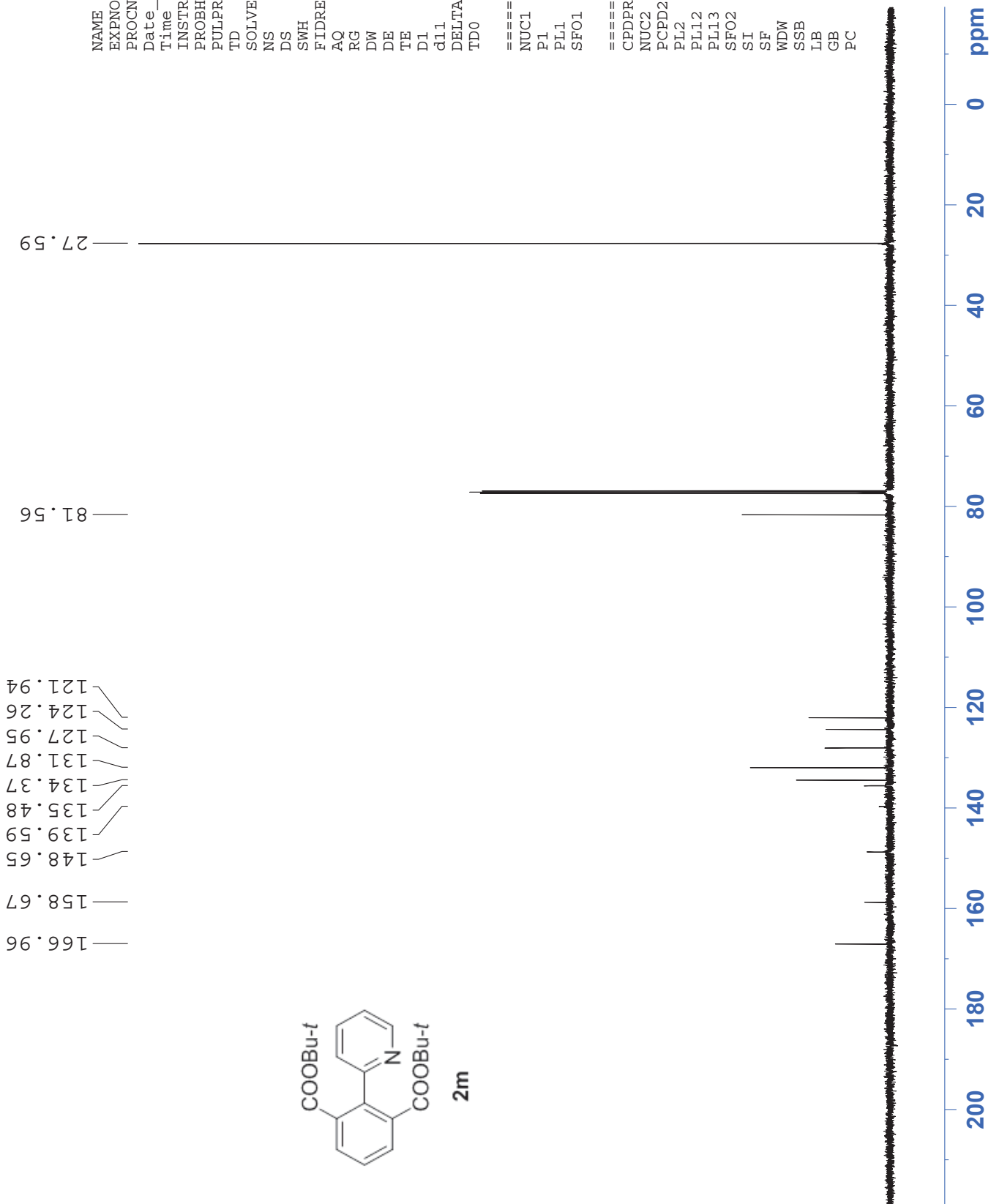
==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 1.00 dB
 PL12 16.05 dB
 PL13 16.50 dB
 SFO2 500.1320005 MHz
 SI 32768
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



HXH-5-72-2
C13CPD CDCl3

```

NAME      XB20130409
EXPNO     10
PROCNO    1
Date_     20130409
Time_     14.03
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         128
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         322.5
DW         16.650 usec
DE         6.00 usec
TE         297.4 K
D1         2.0000000 sec
d11        0.0300000 sec
DELTA     1.89999998 sec
TDO        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      16.31 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
  
```



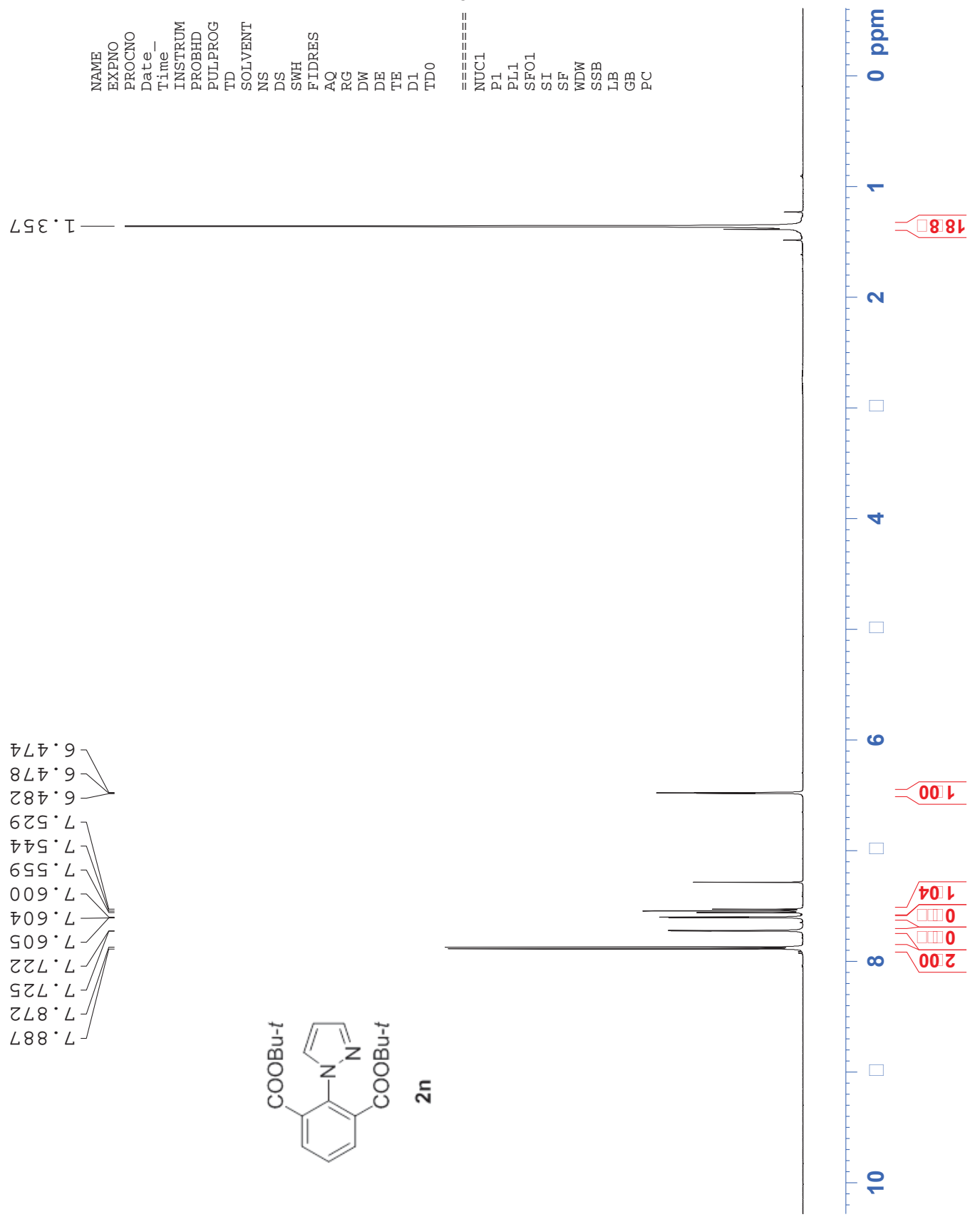
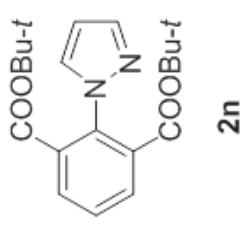
HXH-5-72-3
 PROTON CDCl₃

```

NAME      XB20130410
EXPNO    2
PROCNO    1
Date_     20130410
Time_     13.18
INSTRUM   spect
PROBHD    5 mm PAXO 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        13.72 usec
PL1       1.00 dB
SFO1      500.1330885 MHz
SI        32768
SF        500.1300000 MHz
WDW       no
SSB       0
LB        0.00 Hz
GB        0
PC        1.00
  
```

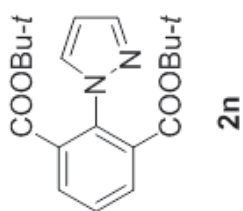
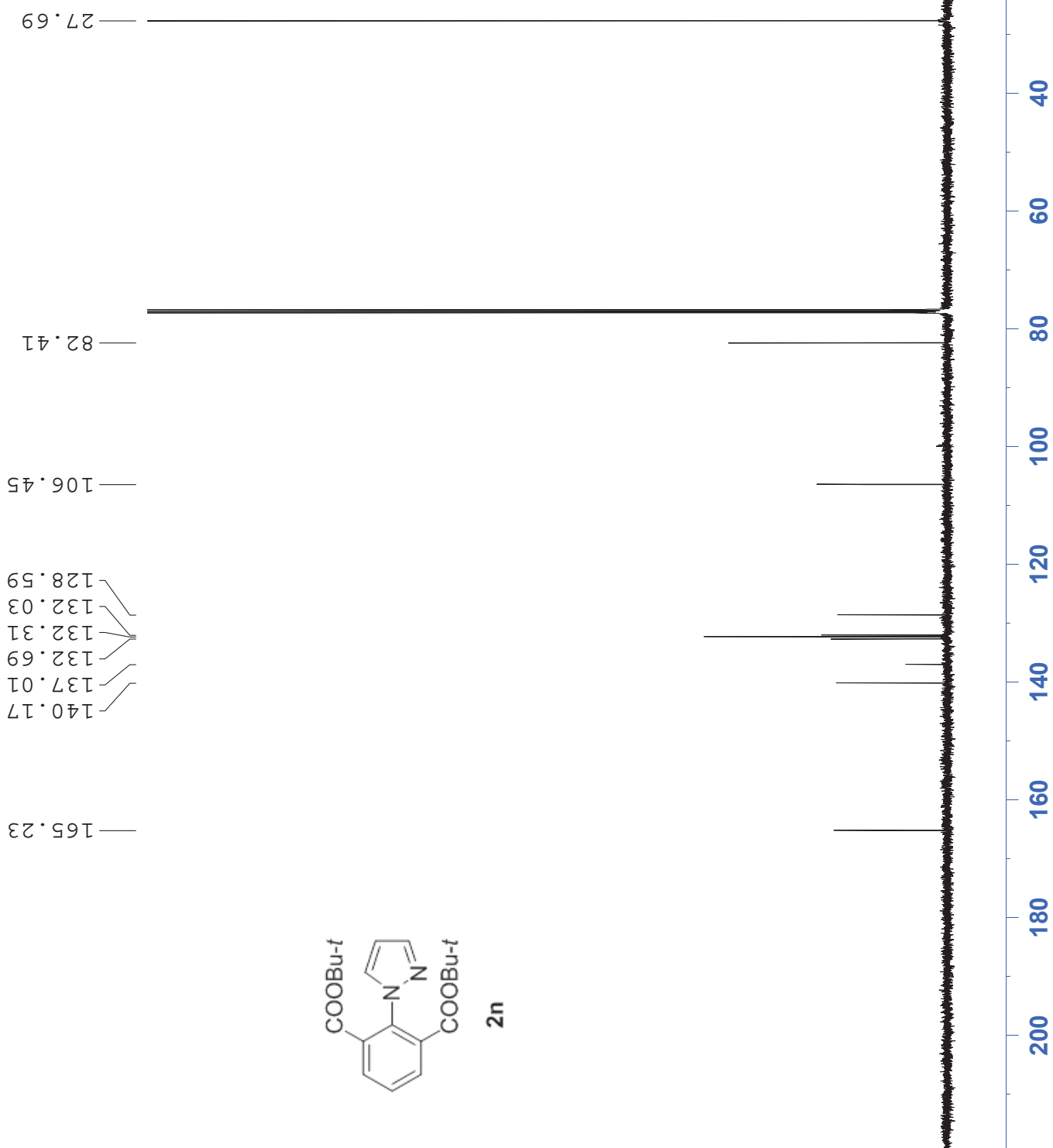
7.887
 7.872
 7.872
 7.725
 7.722
 7.605
 7.604
 7.600
 7.559
 7.544
 7.529
 6.482
 6.478
 6.474



HXH-5-72-3
C13CPD CDCl3

```

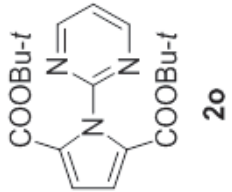
NAME      XB20130410
EXPNO     22
PROCNO    1
Date_     20130410
Time_     20.59
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         512
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ          1.0912410 sec
RG          128
DW          16.650 usec
DE          6.00 usec
TE          297.8 K
D1          2.00000000 sec
d11         0.03000000 sec
DELTA      1.89999998 sec
TDO        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        16.31 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
  
```



HXH-5-73
 PROTON CDCl3

8.861
 8.852
 7.448
 7.438
 7.428
 6.949

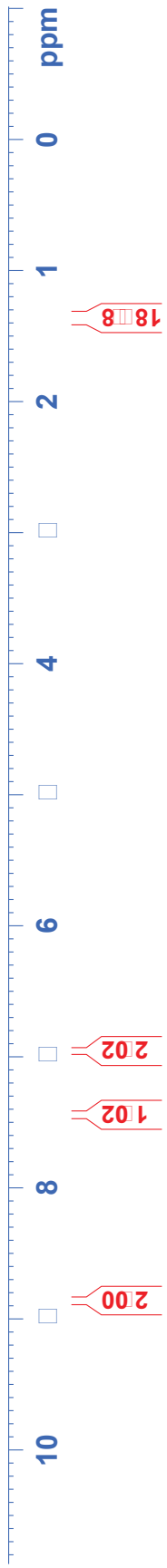
1.360



```

NAME      XB20130410
EXPNO     3
PROCNO    1
Date_     20130410
Time_     13.23
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        10330.578 Hz
FIDRES     0.157632 Hz
AQ         3.1720407 sec
RG         128
DW         48.400 usec
DE         6.00 usec
TE         295.8 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         13.72 usec
PL1        1.00 dB
SF01       500.1330885 MHz
SI         32768
SF         500.1300000 MHz
WDW        no
SSB        0
LB         0.00 Hz
GB         0
PC         1.00
  
```



HXH-5-73
 C13CPD CDCl3

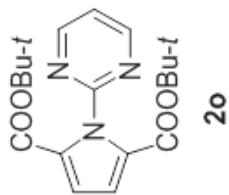
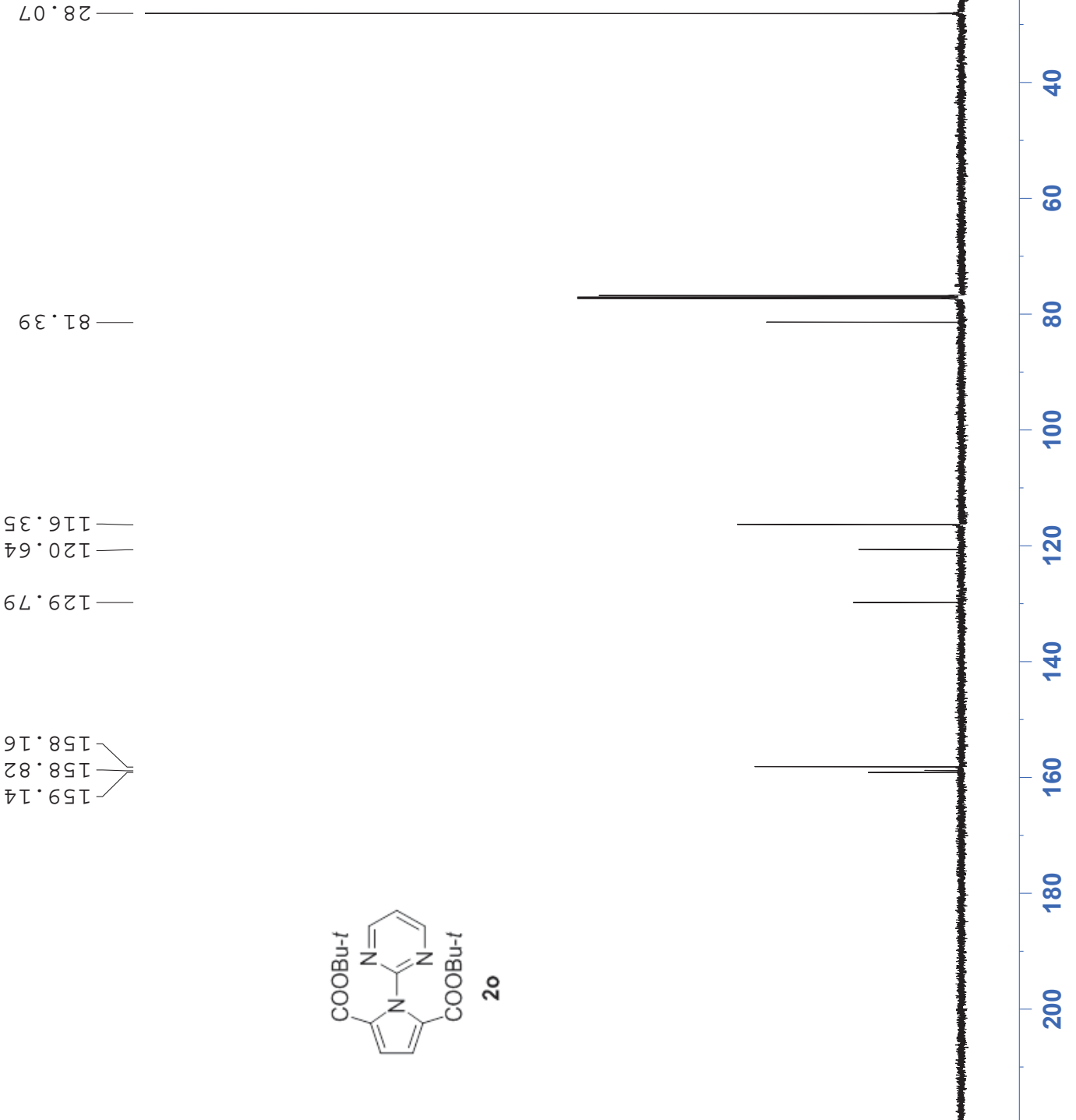
```

NAME      XB20130410
EXPNO     5
PROCNO    1
Date_     20130410
Time_     13.33
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         128
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         181
DE         16.650 usec
TE         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      16.31 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
  
```



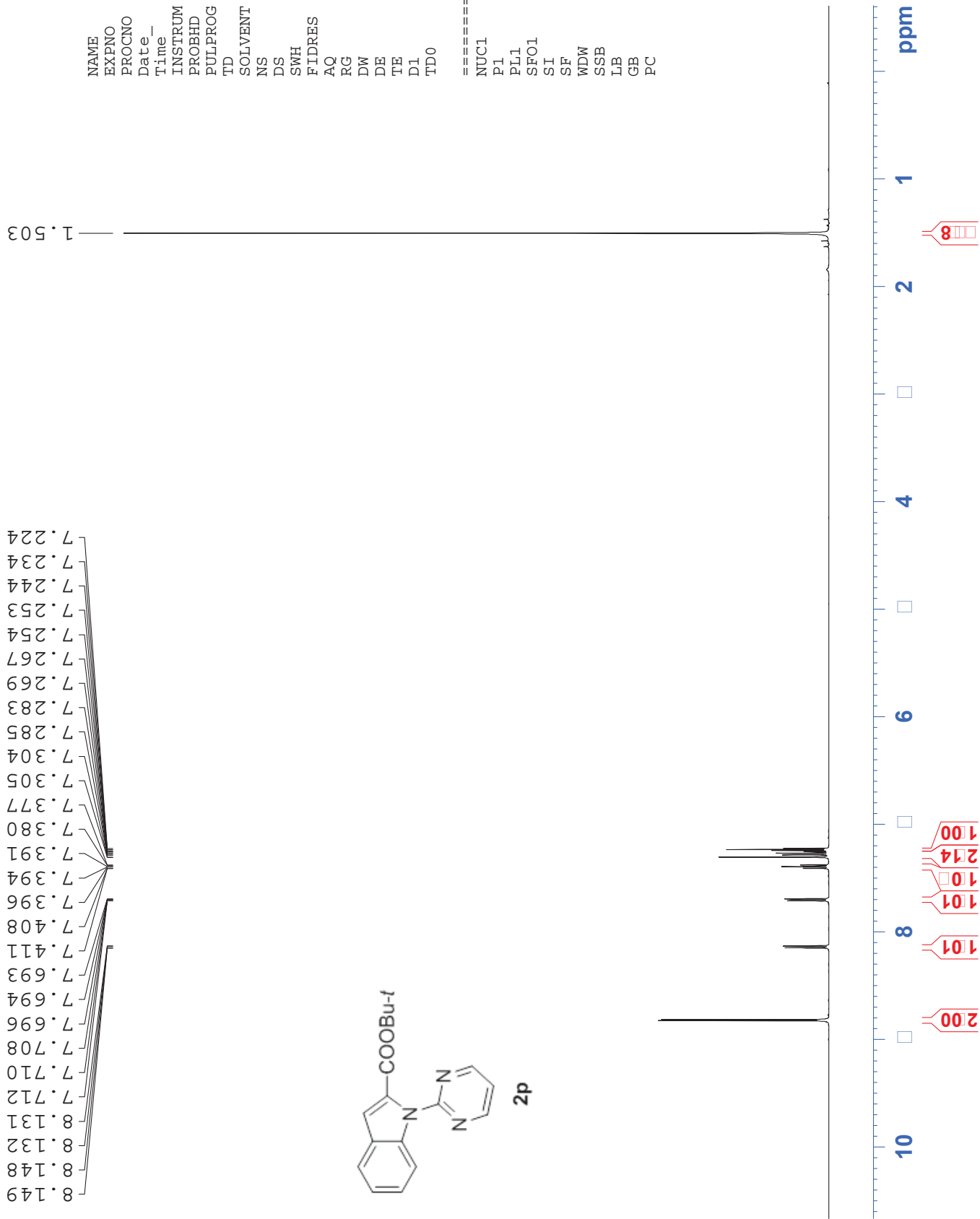
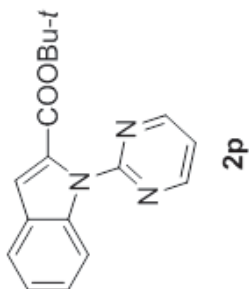
HXH-5-75
 PROTON CDCl3

```

NAME      XB20130417
EXPNO     9
PROCNO    1
Date_     20130417
Time      11.49
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         8
DS         2
SWH        10330.578 Hz
FIDRES     0.157632 Hz
AQ         3.1720407 sec
RG         181
DW         48.400 usec
DE         6.00 usec
TE         297.0 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         13.72 usec
PL1        1.00 dB
SFO1       500.1330885 MHz
SI         32768
SF         500.1300000 MHz
WDW        no
SSB        0
LB         0.00 Hz
GB         0
PC         1.00
  
```

8.149
 8.148
 8.132
 8.131
 7.712
 7.710
 7.708
 7.696
 7.694
 7.693
 7.411
 7.408
 7.396
 7.394
 7.391
 7.380
 7.377
 7.305
 7.304
 7.285
 7.283
 7.269
 7.267
 7.254
 7.253
 7.244
 7.234
 7.224



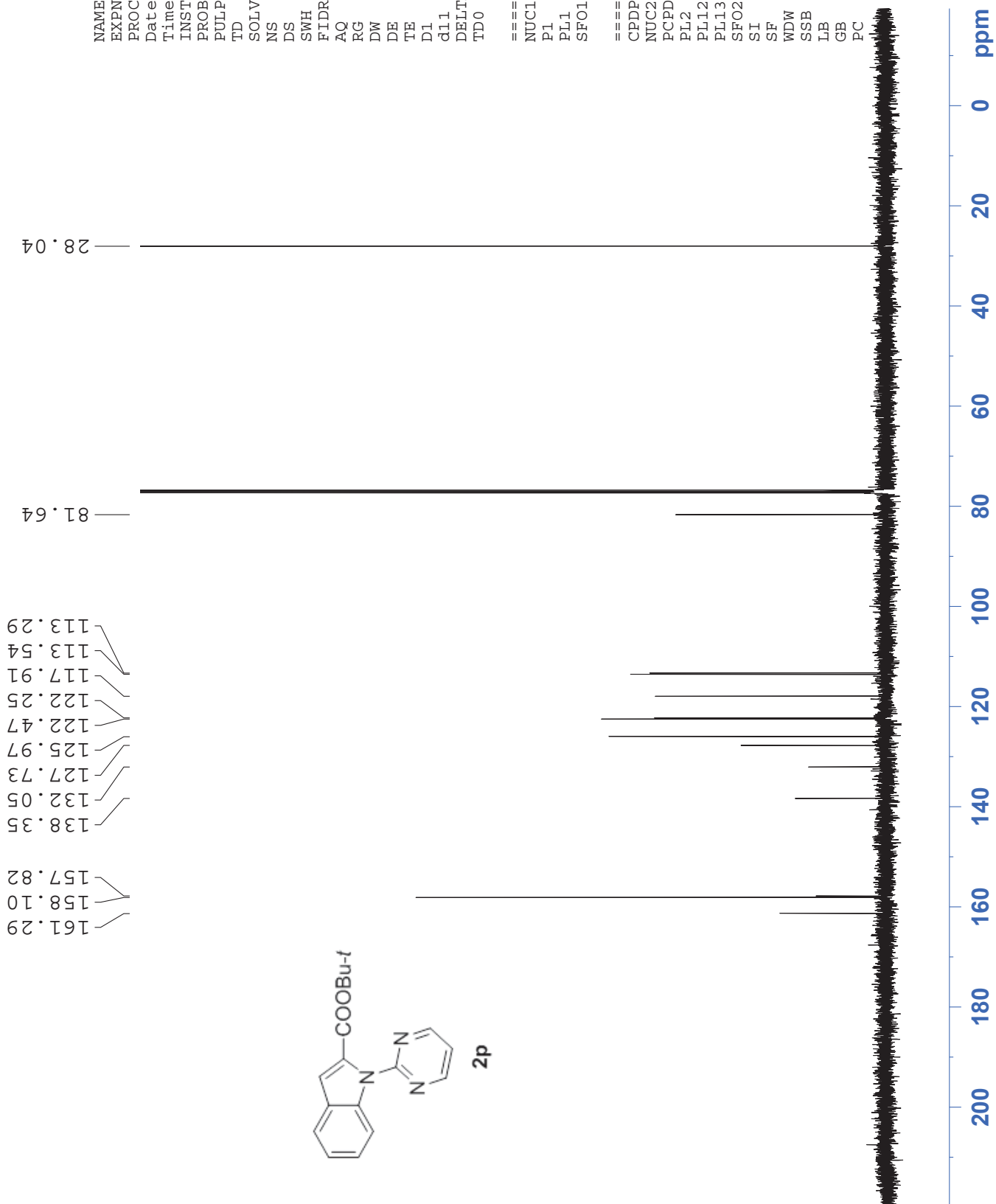
HXH-5-75
C13CPD CDCl3

```

NAME          XB20130417
EXPNO         10
PROCNO        1
Date_         20130417
Time_        11.58
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            128
DW            16.650 usec
DE            6.00 usec
TE            298.0 K
D1            2.0000000 sec
d11           0.0300000 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          16.31 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
  
```



HXM-5-138
C13CPD CDCl3

```

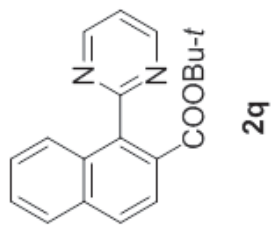
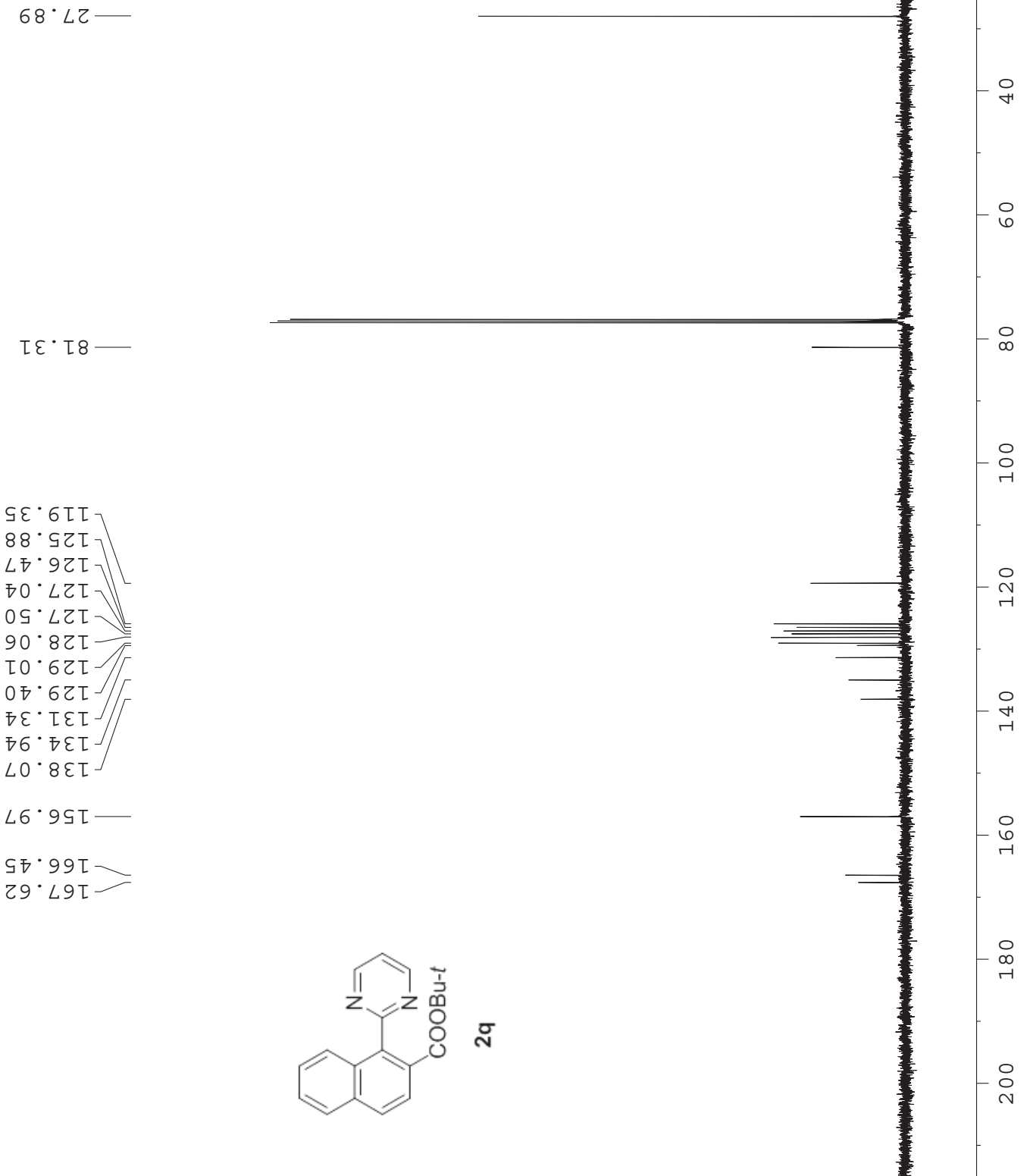
NAME      XB20130527
EXPNO     31
PROCNO    1
Date_     20130527
Time_     17.22
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         128
DS         4
SWH       30030.029 Hz
FIDRES    0.458222 Hz
AQ         1.0912410 sec
RG         456.1
DE         16.650 usec
TE         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
  
```

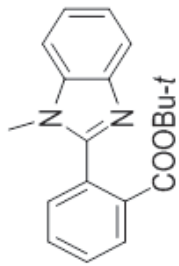


HXH-5-72-1
 PROTON CDCl3

7.833
7.823
7.820
7.670
7.667
7.655
7.652
7.641
7.638
7.634
7.623
7.620
7.608
7.605
7.562
7.559
7.548
7.547
7.545
7.409
7.406
7.396
7.391
7.371
7.368
7.356
7.354
7.345
7.342
7.338
7.330
7.327
7.316
7.313
3.597

NAME XB20130410
 EXPNO 1
 PROCNO 1
 Date_ 20130410
 Time_ 13.12
 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 228.1
 DW 48.400 usec
 DE 6.00 usec
 TE 295.8 K
 D1 1.00000000 sec
 TD0 1

2r



==== CHANNEL f1 =====
 NUC1 1H
 P1 13.72 usec
 PL1 1.00 dB
 SF01 500.1330885 MHz
 SI 32768
 SF 500.1300000 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



HXH-5-72-1
C13CPD CDC13

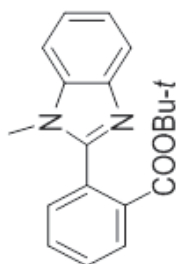
```

NAME      XB20130410
EXPNO     21
PROCNO    1
Date_     20130410
Time      20.26
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         90.5
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

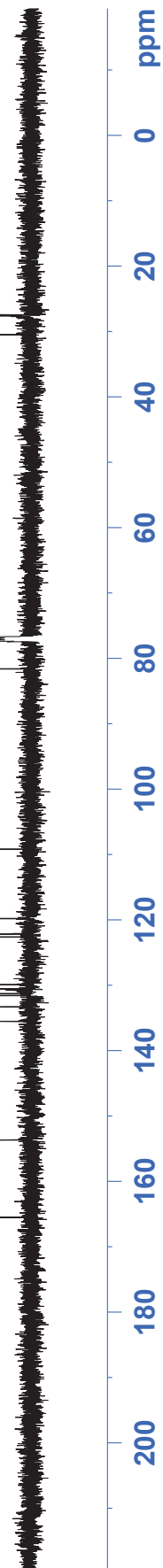
===== CHANNEL f1 =====
NUC1      13C
P1         9.50 usec
PL1        -0.50 dB
SFO1      125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2     80.00 usec
PL2        1.00 dB
PL12      16.31 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
  
```

165.54
153.72
135.54
133.33
131.63
131.28
130.77
130.58
129.92
122.65
122.18
119.80
109.19
81.59
30.48
27.59



2r



HXH-5-68
C13CPD CDC13

```

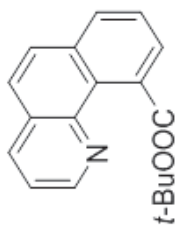
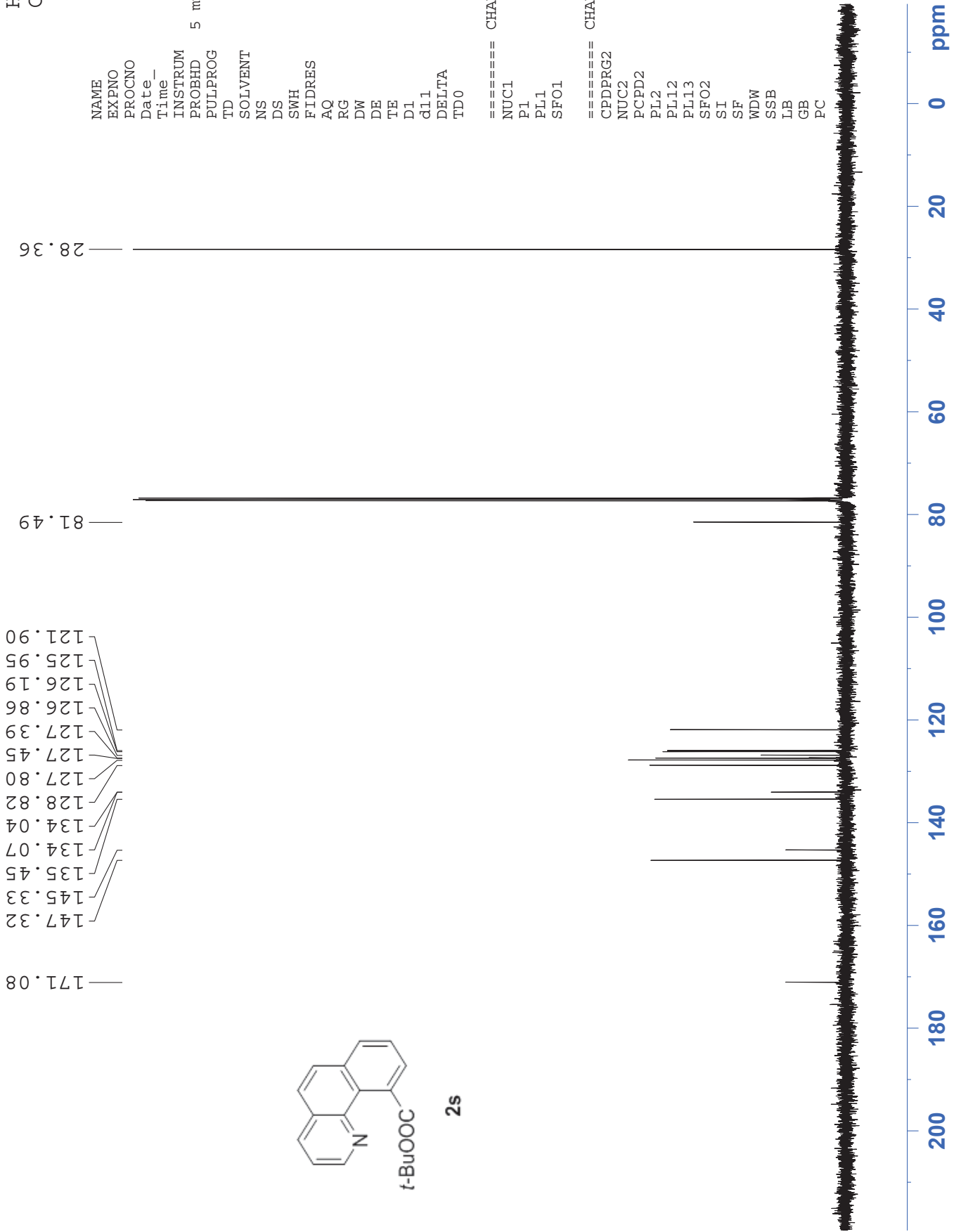
NAME      XB20130412
EXPNO     19
PROCNO    1
Date_     20130412
Time_     18.11
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDC13
NS         128
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         203.2
DE         16.650 usec
TE         6.00 usec
TE         297.2 K
D1         2.00000000 sec
d11        0.03000000 sec
DELTA     1.89999998 sec
TD0        1
  
```

```

===== CHANNEL f1 =====
NUC1      13C
P1        9.50 usec
PL1       -0.50 dB
SFO1     125.7703643 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2     80.00 usec
PL2       1.00 dB
PL12     16.31 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
  
```

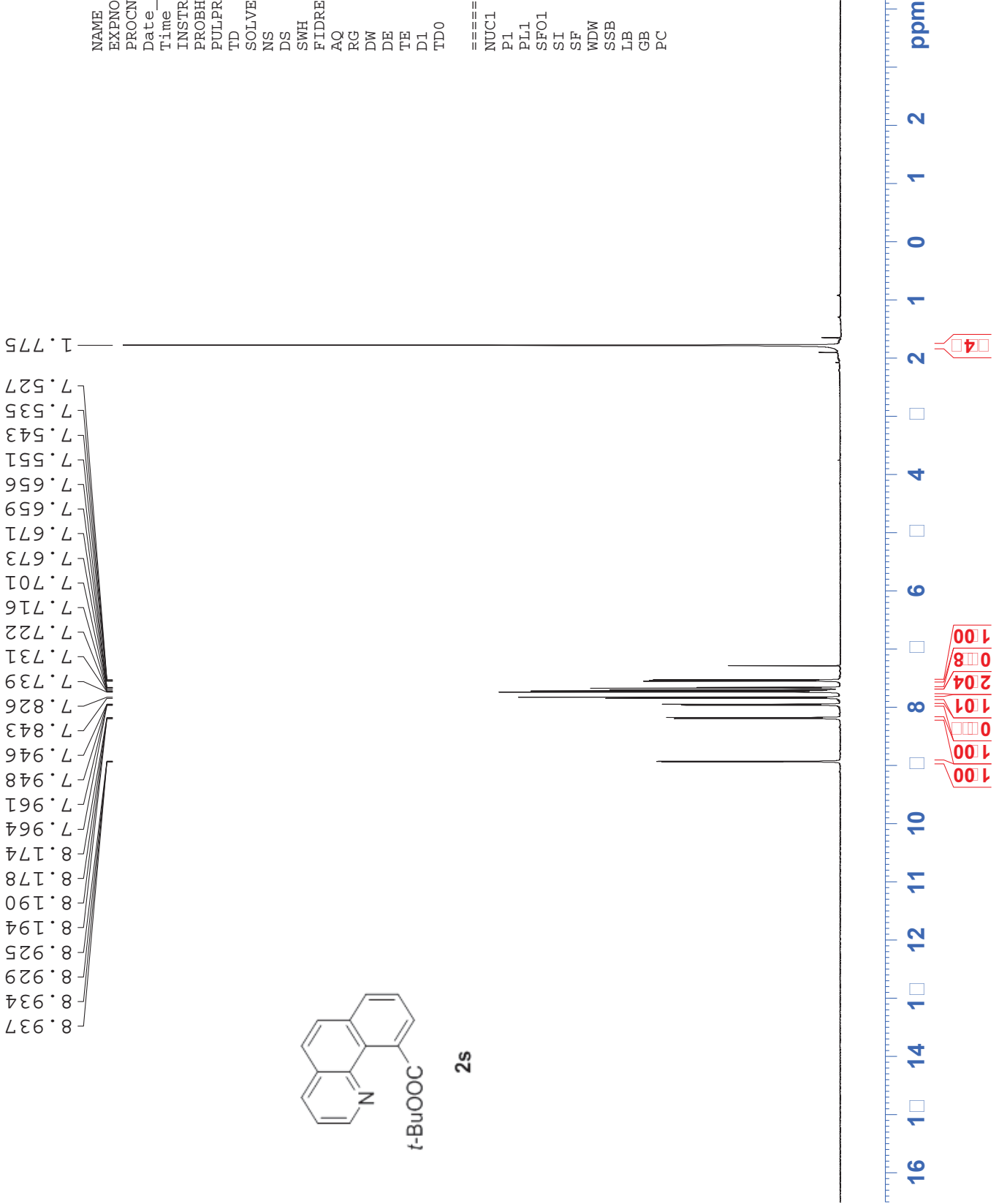


2s

HXH-5-68
 PROTON CDCl3

NAME XB20130412
 EXPNO 18
 PROCNO 1
 Date_ 20130412
 Time_ 18.02
 INSTRUM spect
 PROBHD 5 mm PATXO 19F
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1720407 sec
 RG 203.2
 DW 48.400 usec
 DE 6.00 usec
 TE 295.9 K
 D1 1.00000000 sec
 TD0 1

=====
 CHANNEL f1 =====
 NUC1 1H
 P1 13.72 usec
 PL1 1.00 dB
 SFO1 500.1330885 MHz
 SI 32768
 SF 500.1300000 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



HXH-5-32-1
 PROTON DMSO

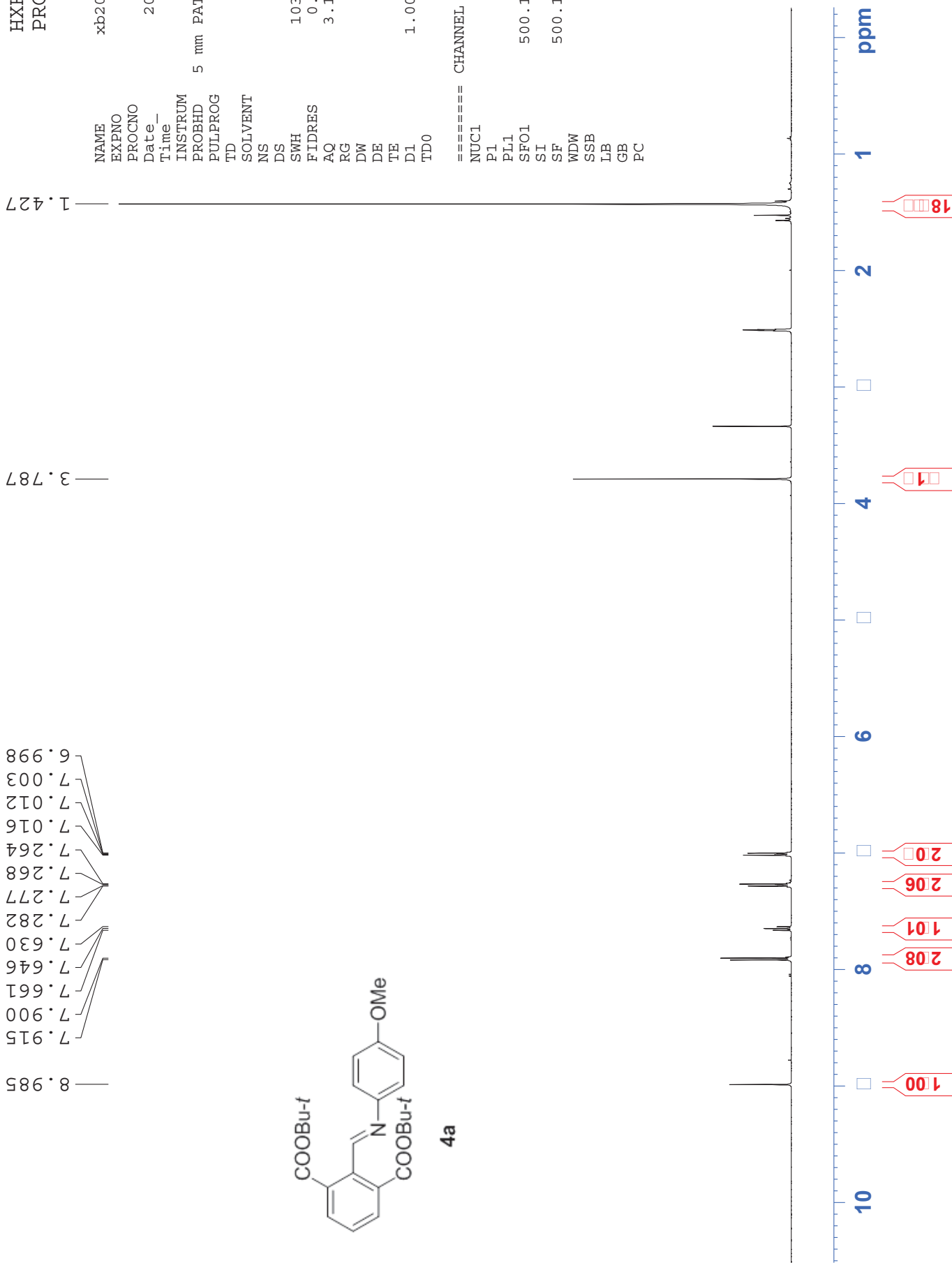
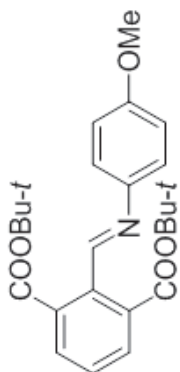
NAME xb20130322
 EXPNO 12
 PROCNO 1
 Date_ 20130322
 Time_ 13.03
 INSTRUM spect
 PROBHD 5 mm PATXO 19F
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 8
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1720407 sec
 RG 228.1
 DW 48.400 usec
 DE 6.00 usec
 TE 296.5 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 13.72 usec
 PL1 1.00 dB
 SFO1 500.1330885 MHz
 SI 32768
 SF 500.1300000 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1.427

3.787

8.985
 7.915
 7.900
 7.661
 7.646
 7.630
 7.282
 7.277
 7.268
 7.264
 7.016
 7.012
 7.003
 6.998



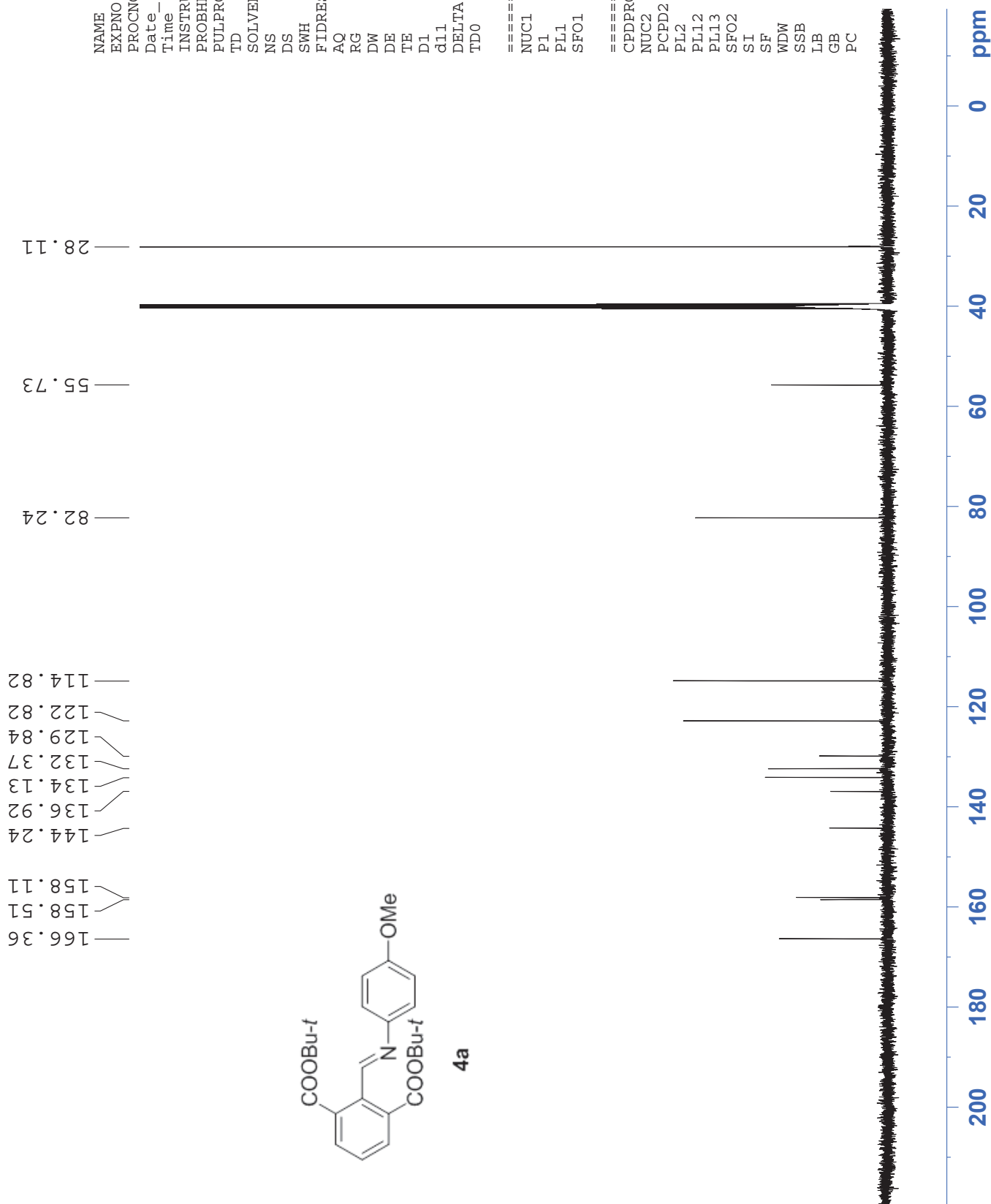
HXH-5-32-1
 C13CPD DMSC

```

NAME          xb20130322
EXPNO         24
PROCNO        1
Date_         20130322
Time_         21.09
INSTRUM       spect
PROBHD        5 mm PATXO 19F
PULPROG       zgpg30
TD            65536
SOLVENT       DMSO
NS            512
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            297.3 K
D1            2.0000000 sec
d11           0.0300000 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         16.31 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
  
```



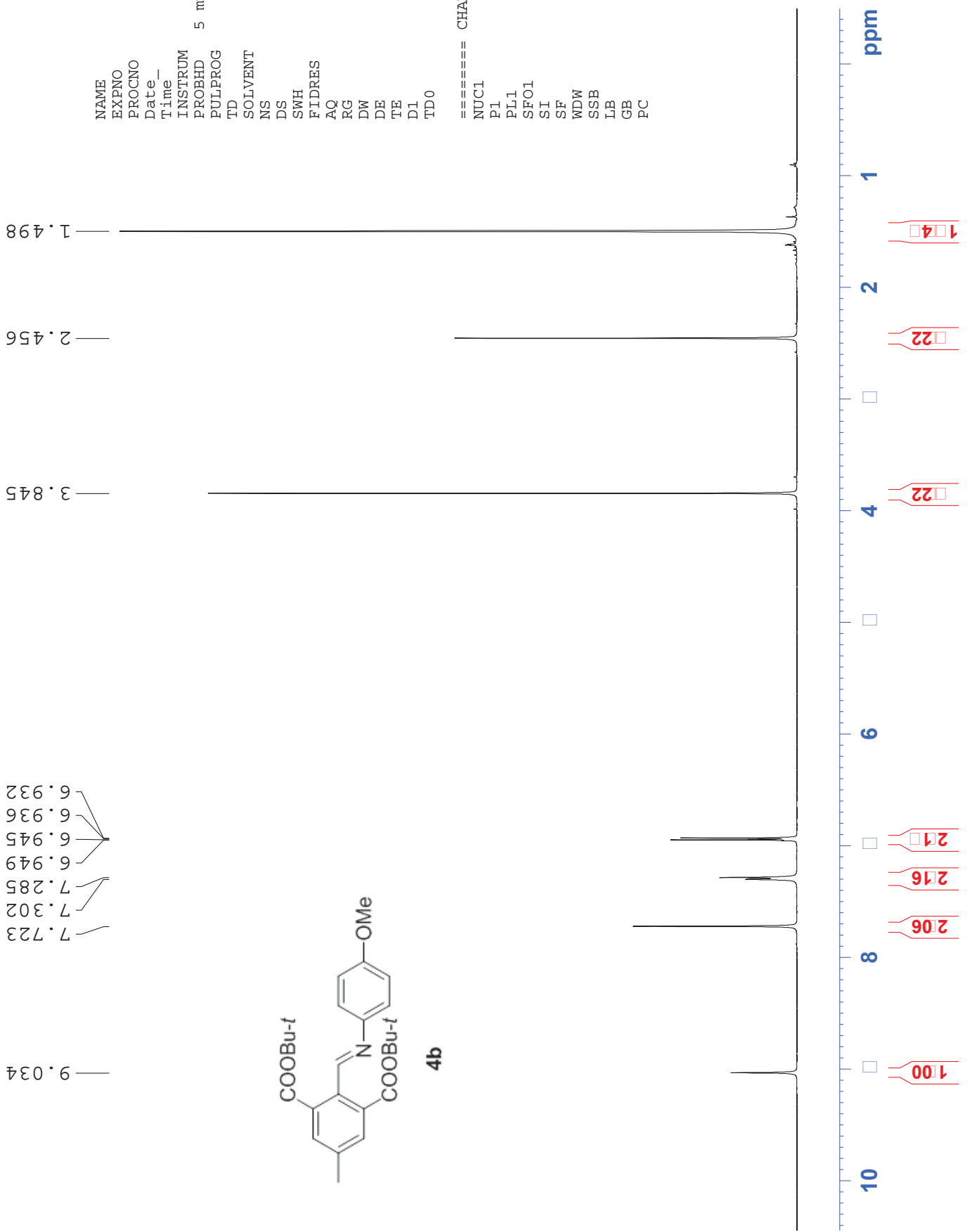
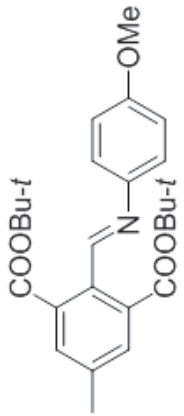
HXH-5-40-1
 PROTON CDCl3

```

NAME      xb20130325
EXPNO     7
PROCNO    1
Date_     20130325
Time_     9.37
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         8
DS         2
SWH        10330.578 Hz
FIDRES     0.157632 Hz
AQ         3.1720407 sec
RG         90.5
DW         48.400 usec
DE         6.00 usec
TE         295.9 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         13.72 usec
PL1        1.00 dB
SFO1       500.1330885 MHz
SI         32768
SF         500.1300000 MHz
WDW        no
SSB        0
LB         0.00 Hz
GB         0
PC         1.00
  
```

9.034
 7.723
 7.302
 7.285
 6.949
 6.945
 6.936
 6.932



HXH-5-40-1
 C13CPD CDCl3

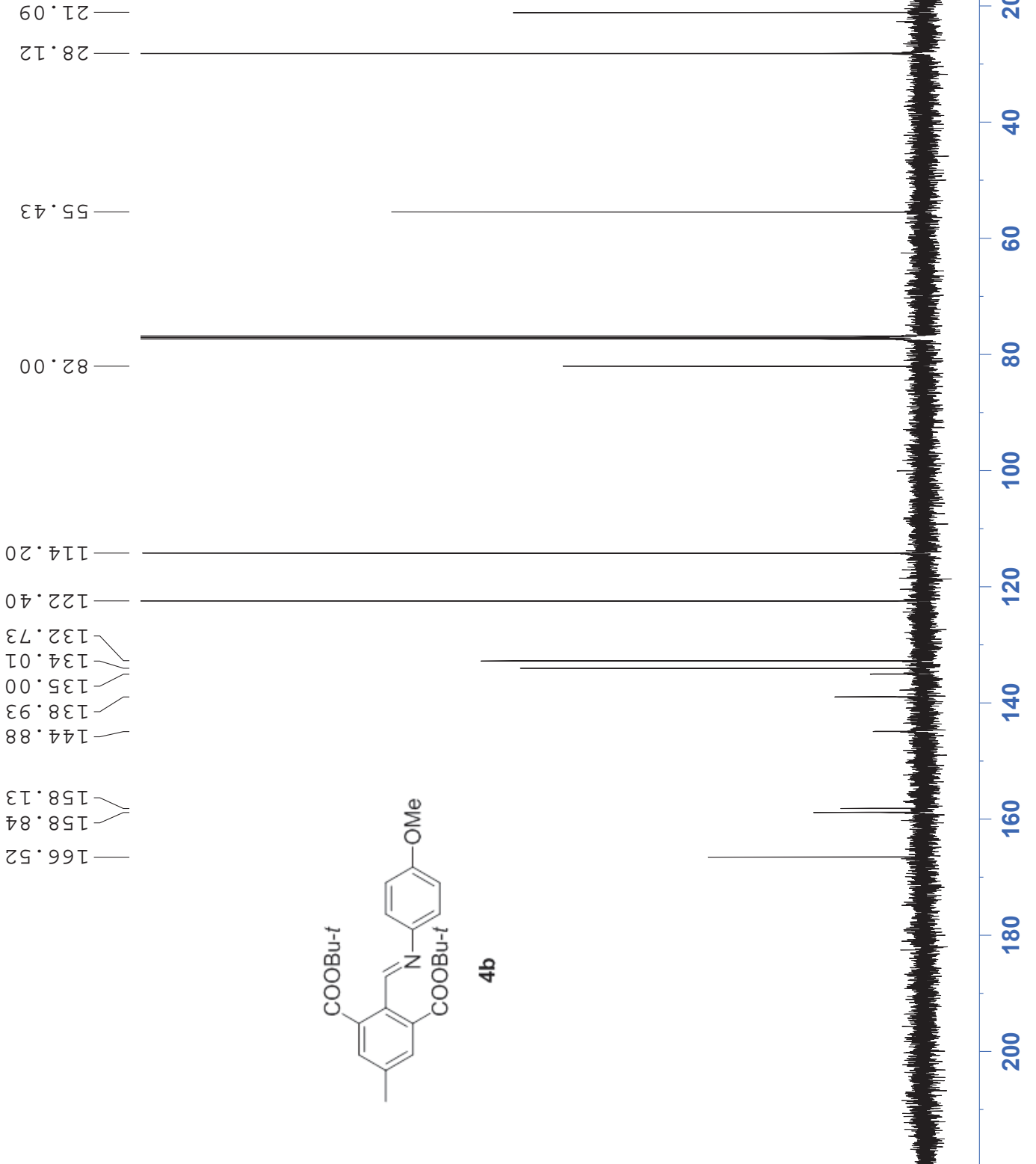
```

NAME      xb20130325
EXPNO     9
PROCNO    1
Date_     20130325
Time_     9.46
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         128
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         2580.3
DW         16.650 usec
DE         6.00 usec
TE         296.9 K
D1         2.00000000 sec
d11        0.03000000 sec
DELTA     1.89999998 sec
TD0        1
  
```

```

===== CHANNEL f1 =====
NUC1      13C
P1        9.50 usec
PL1       -0.50 dB
SFO1     125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       1.00 dB
PL12     16.31 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
  
```



HXH-36-1
C13CPD CDCl3

```

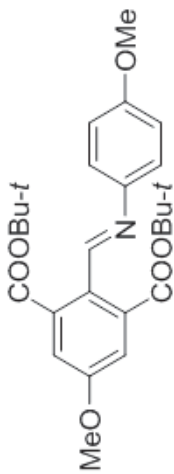
NAME      XB20130323
EXPNO     6
PROCNO    1
Date_     20130323
Time_     23.41
INSTRUM   spect
PROBHD    5 mm PAXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         512
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         90.5
DW         16.650 usec
DE         6.00 usec
TE         297.4 K
D1         2.0000000 sec
d11        0.0300000 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       16.31 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
  
```

166.24
159.52
158.31
158.14
135.66
129.70
122.39
117.56
114.20
82.28
55.79
55.44
28.10
28.01



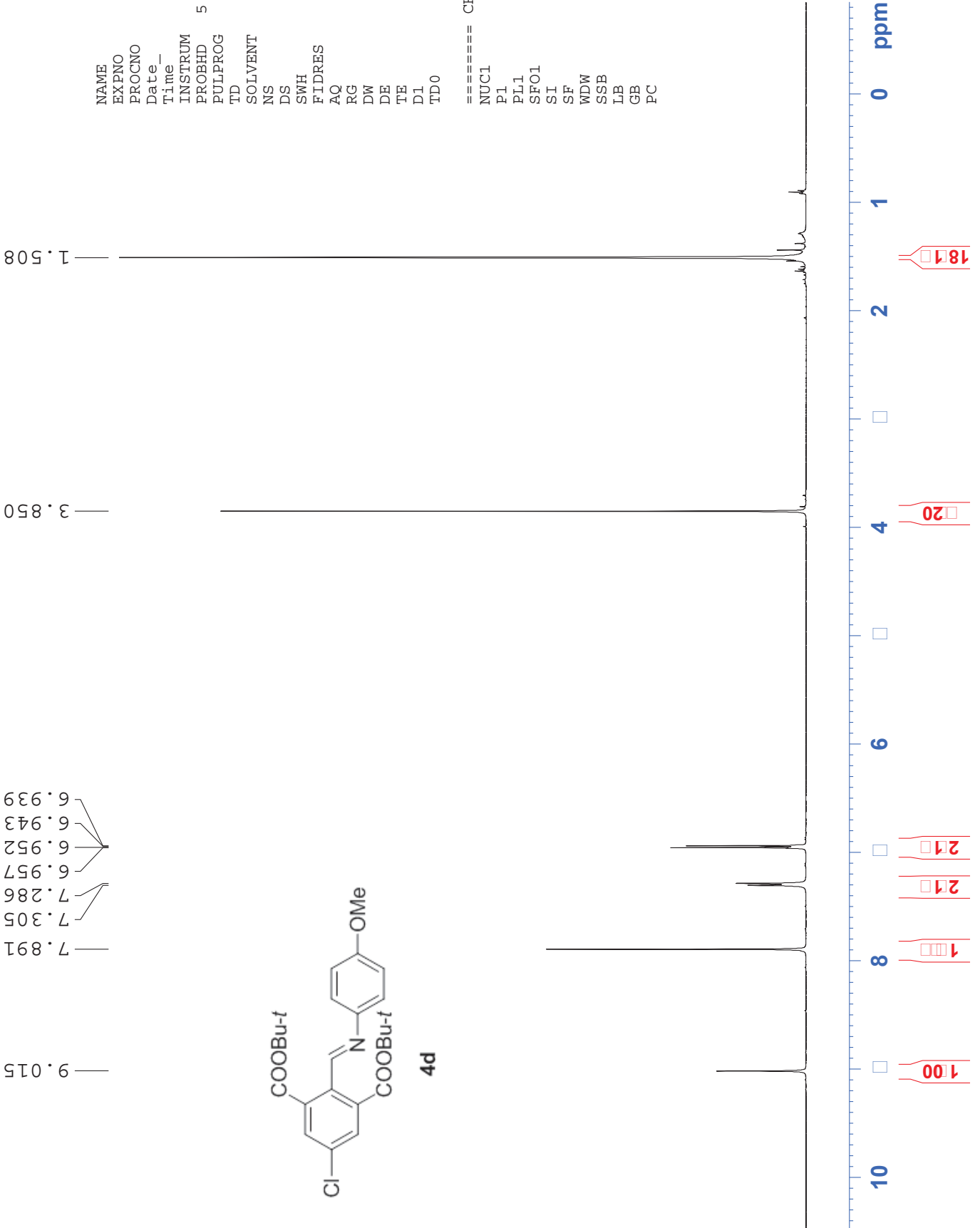
4c



HXH-5-40-2
 PROTON CDCl3

NAME xb20130325
 EXPNO 10
 PROCNO 1
 Date_ 20130325
 Time_ 9.52
 INSTRUM spect
 PROBHD 5 mm PATXO 19F
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1720407 sec
 RG 114
 DW 48.400 usec
 DE 6.00 usec
 TE 295.9 K
 D1 1.00000000 sec
 TD0 1

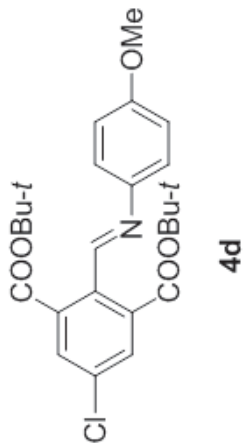
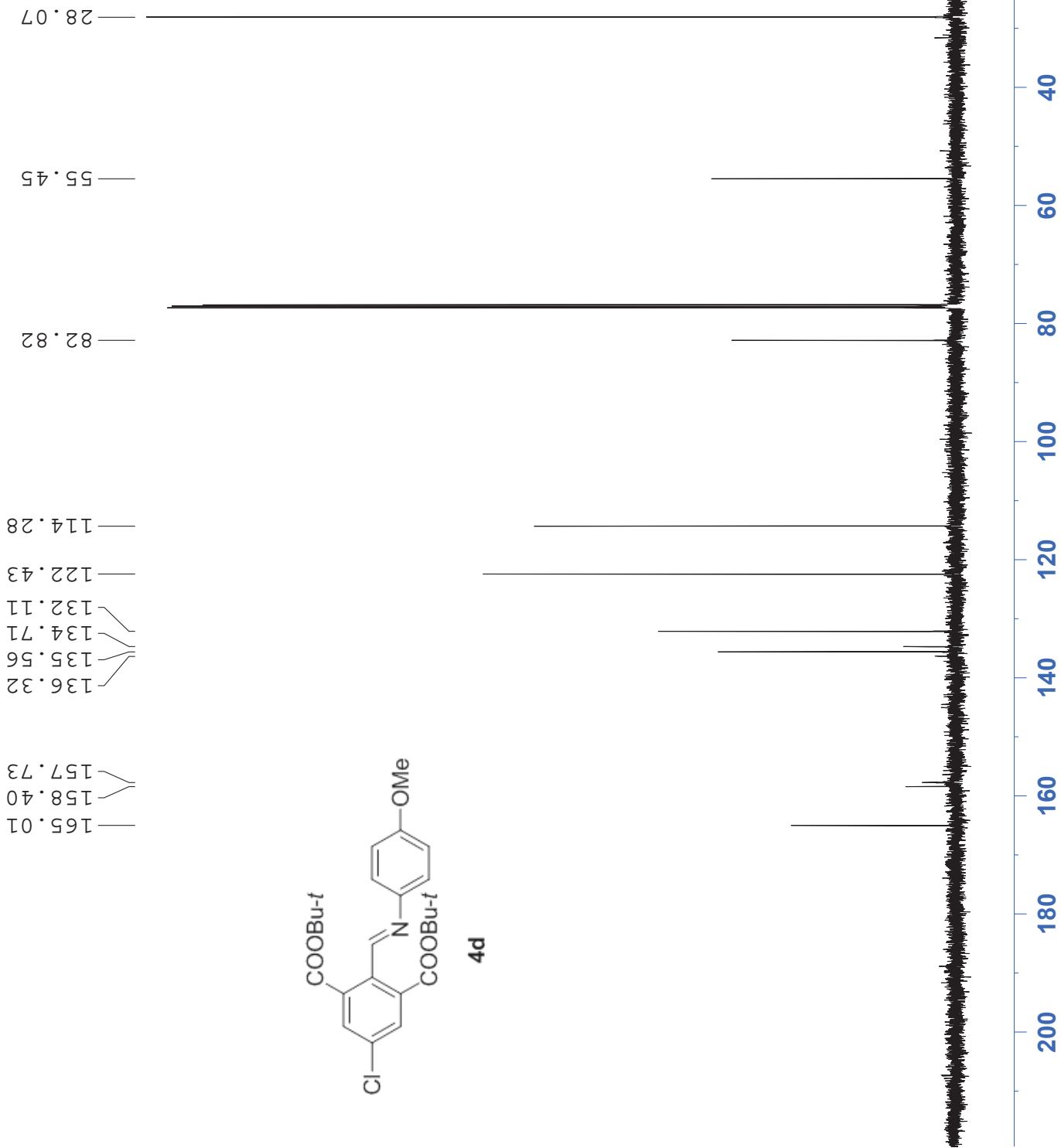
==== CHANNEL f1 =====
 NUC1 1H
 P1 13.72 usec
 PL1 1.00 dB
 SF01 500.1330885 MHz
 SI 32768
 SF 500.1300000 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



HXH-5-40-2
C13CPD CDC13

```

NAME          xb20130325
EXPNO         11
PROCNO        1
Date_         20130325
Time_         10.00
INSTRUM       spect
PROBHD        5 mm PATXO 19F
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            128
DS            4
SWH           30030.029 Hz
FIDRES        0.458222 Hz
AQ            1.0912410 sec
RG            181
DE            16.650 usec
TE            6.00 usec
TE           297.0 K
D1            2.0000000 sec
d11           0.0300000 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          16.31 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
  
```

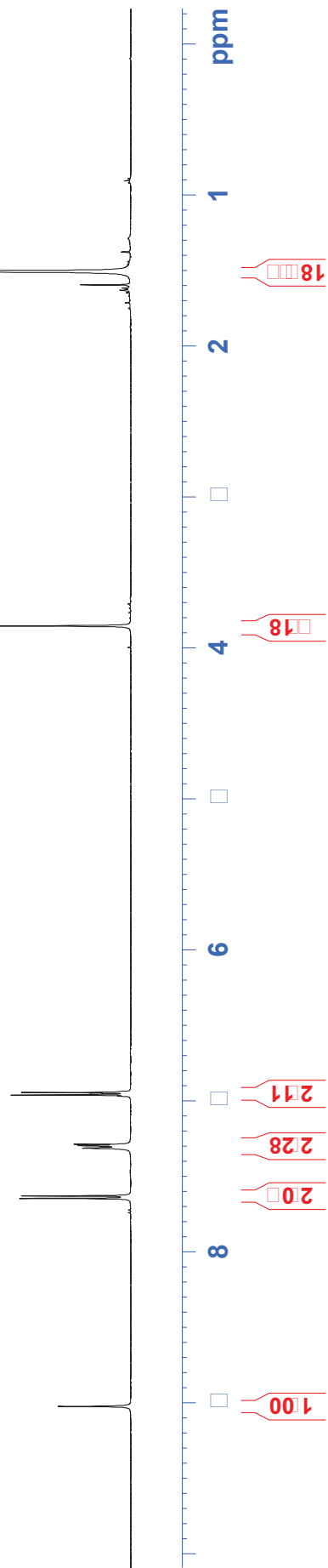
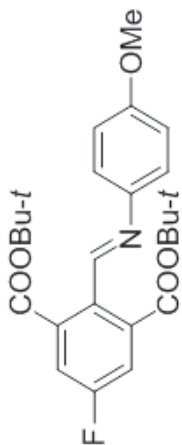


HXH-5-32-2
 PROTON CDCl3

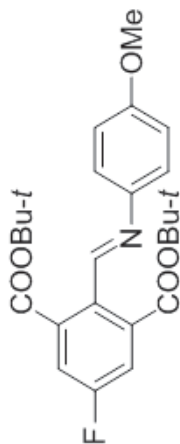
NAME xb20130322
 EXPNO 14
 PROCNO 1
 Date_ 20130322
 Time_ 13.14
 INSTRUM spect
 PROBHD 5 mm PATXO 19F
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1720407 sec
 RG 203.2
 DW 48.400 usec
 DE 6.00 usec
 TE 296.1 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 13.72 usec
 PL1 1.00 dB
 SFO1 500.1330885 MHz
 SI 32768
 SF 500.1300000 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

9.022
 7.644
 7.628
 7.311
 7.294
 7.286
 6.960
 6.956
 6.947
 6.942
 3.855
 1.506



-110.951



4e

```

NAME          xb20130322
EXPNO         15
PROCNO        1
Date_         20130322
Time          13.15
INSTRUM       spect
PROBHD        5 mm PATXO 19F
PULPROG       zg
TD             131072
SOLVENT       CDC13
NS             8
DS             4
SWH           100000.000 Hz
FIDRES        0.762939 Hz
AQ            0.6554150 sec
RG            287.4
DW            5.000 usec
DE            6.00 usec
TE            296.1 K
D1            1.00000000 sec
TD0           1

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

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



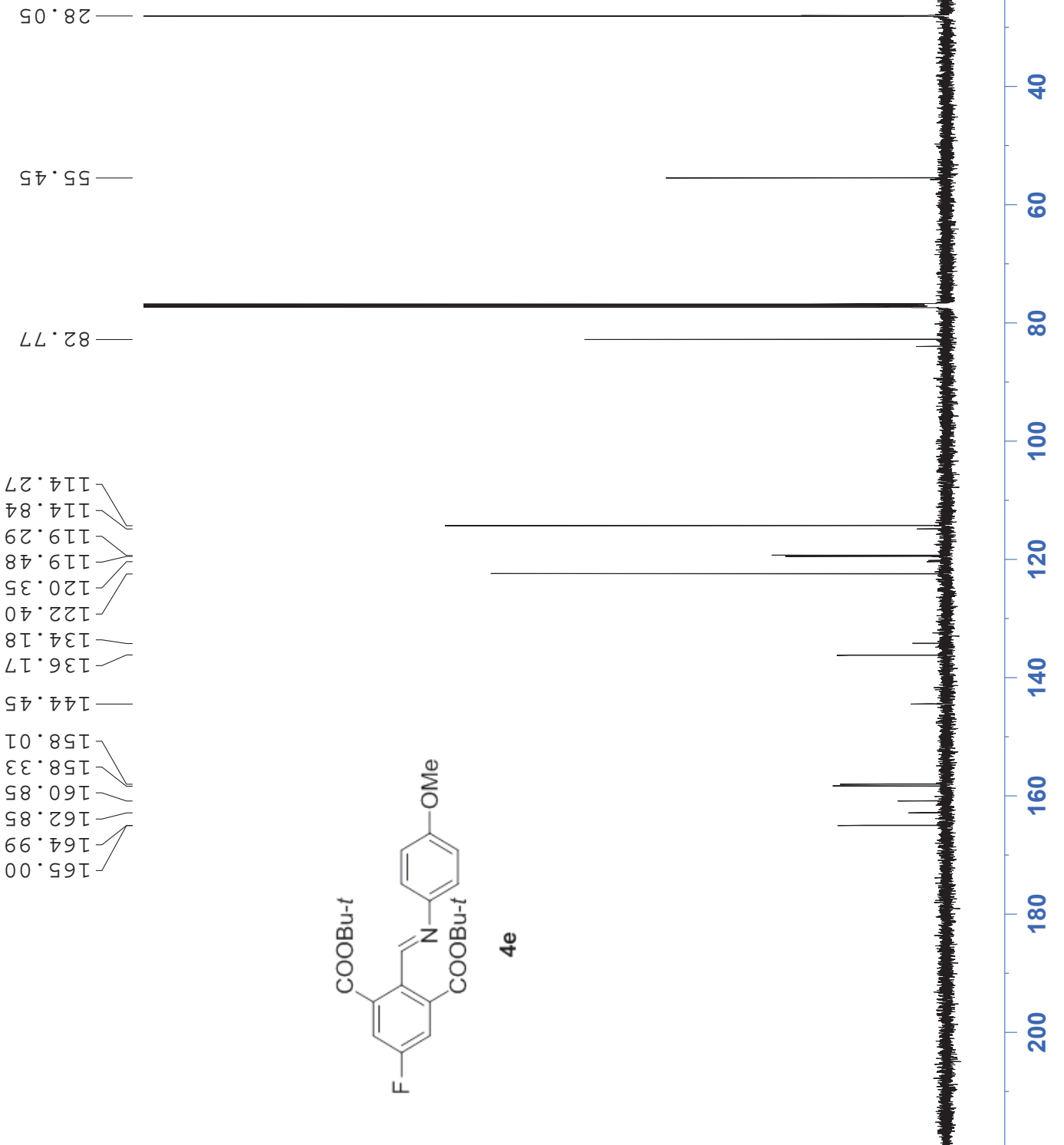
HXH-5-32-2
 C13CPD CDCl₃:

```

NAME      XB20130323
EXPNO     5
PROCNO    1
Date_     20130323
Time_     23.09
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         161.3
DE         16.650 usec
TE         6.00 usec
TE         297.3 K
D1         2.0000000 sec
d11        0.0300000 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       16.31 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
  
```



HXM-5-112
 PROTON CDCl3

```

NAME      XB20130419
EXPNO     1
PROCNO    1
Date_     20130419
Time      11.39
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         295.5 K
D1         1.00000000 sec
TD0        1

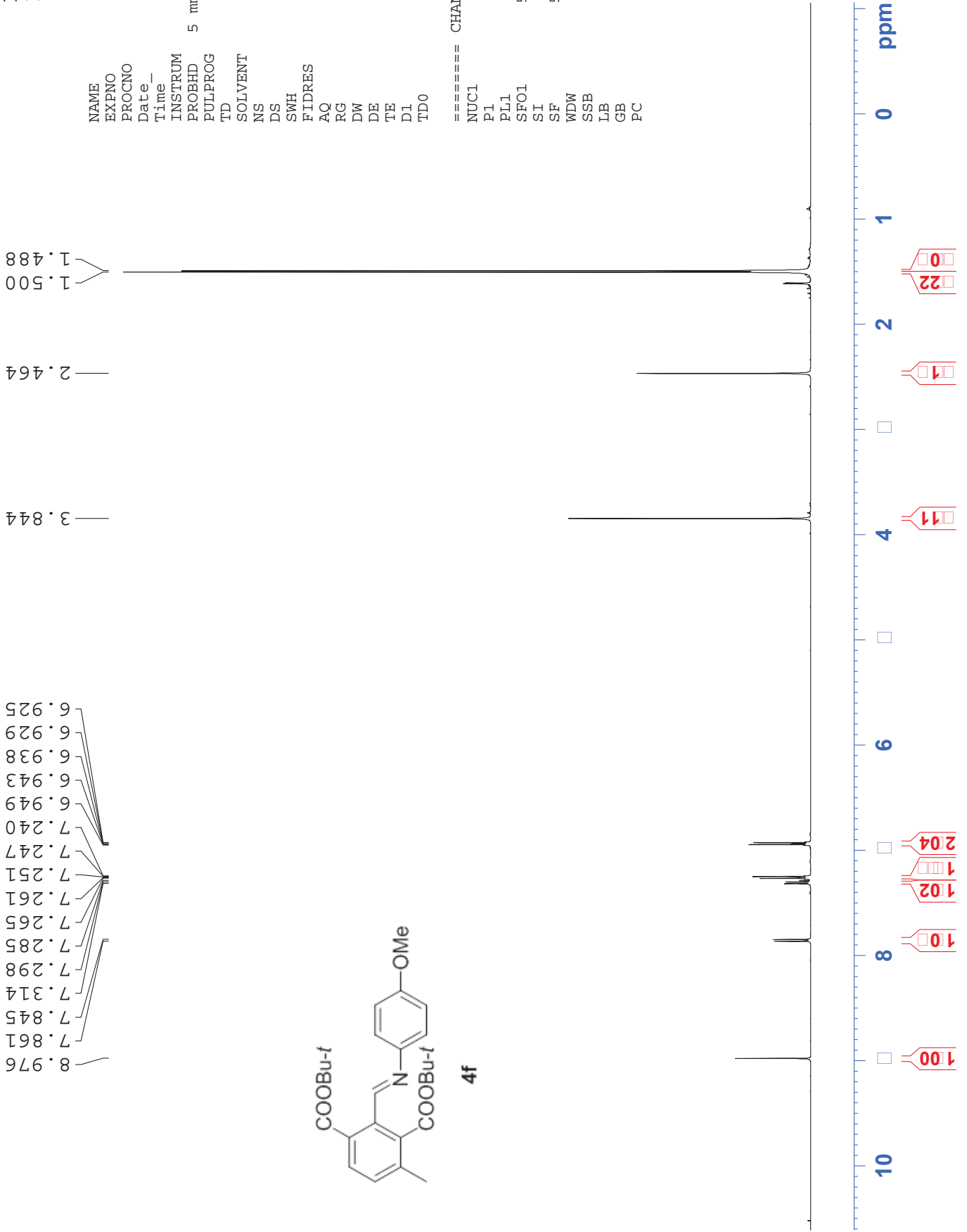
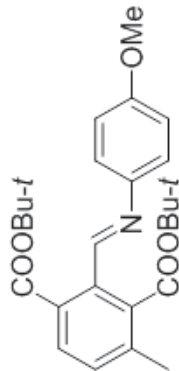
===== CHANNEL f1 =====
NUC1       1H
P1         13.72 usec
PL1        1.00 dB
SFO1       500.1330885 MHz
SI         32768
SF         500.1300000 MHz
WDW        no
SSB        0
LB         0.00 Hz
GB         0
PC         1.00
  
```

1.500
 1.488

2.464

3.844

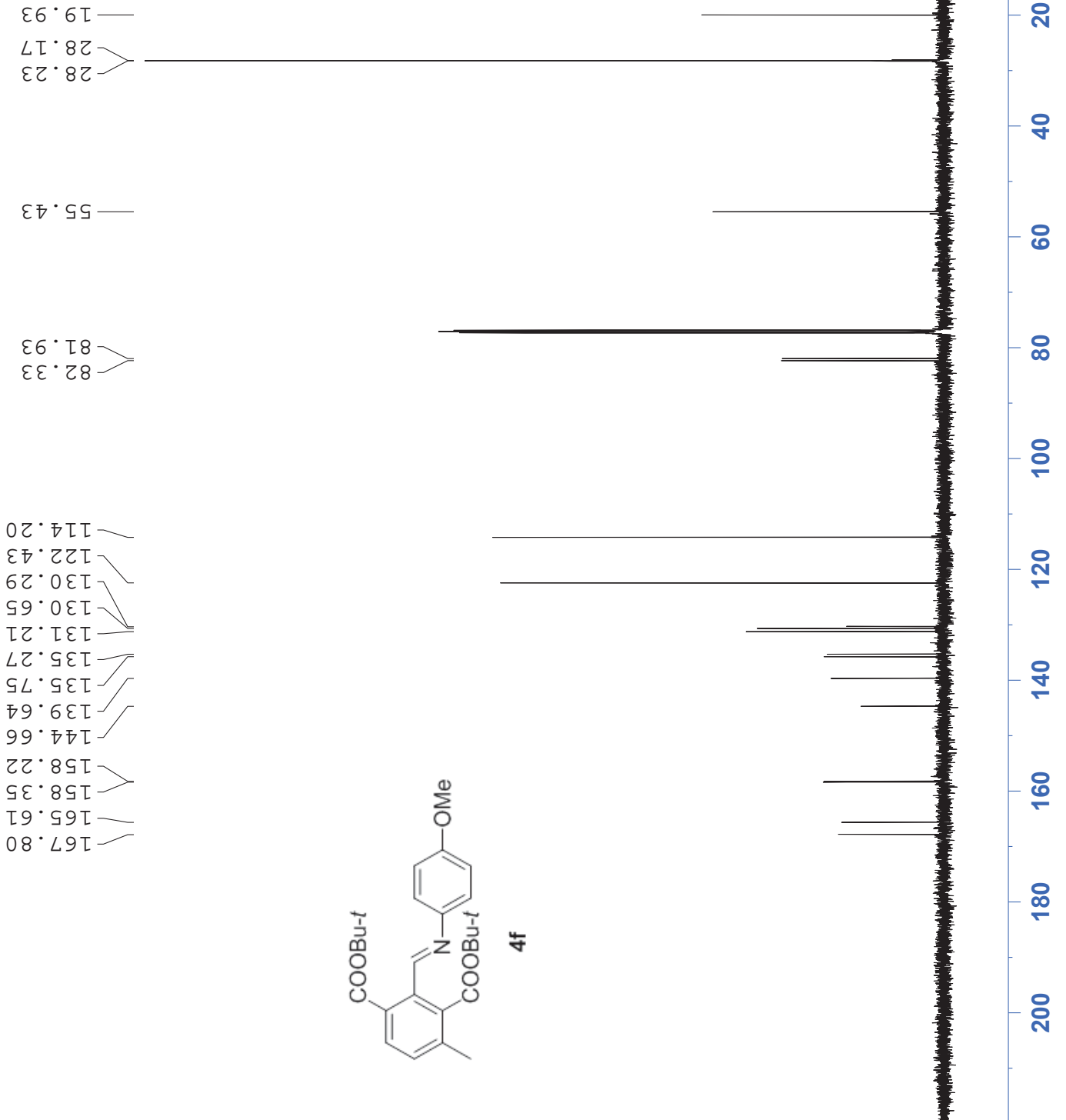
8.976
 7.861
 7.845
 7.314
 7.298
 7.285
 7.265
 7.261
 7.251
 7.247
 7.240
 6.949
 6.943
 6.938
 6.929
 6.925



HXM-5-112
C13CPD CDC13

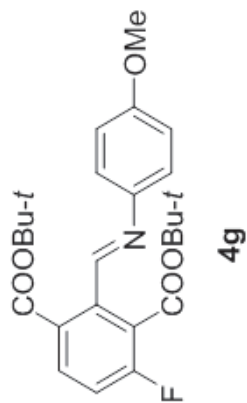
```

NAME      XB20130419
EXPNO     17
PROCNO    1
Date_     20130419
Time      14.54
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDC13
NS         128
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         128
DW         16.650 usec
DE         6.00 usec
TE         296.7 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   waitz16
NUC2       1H
PCPD2     80.00 usec
PL2        1.00 dB
PL12       16.31 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
  
```



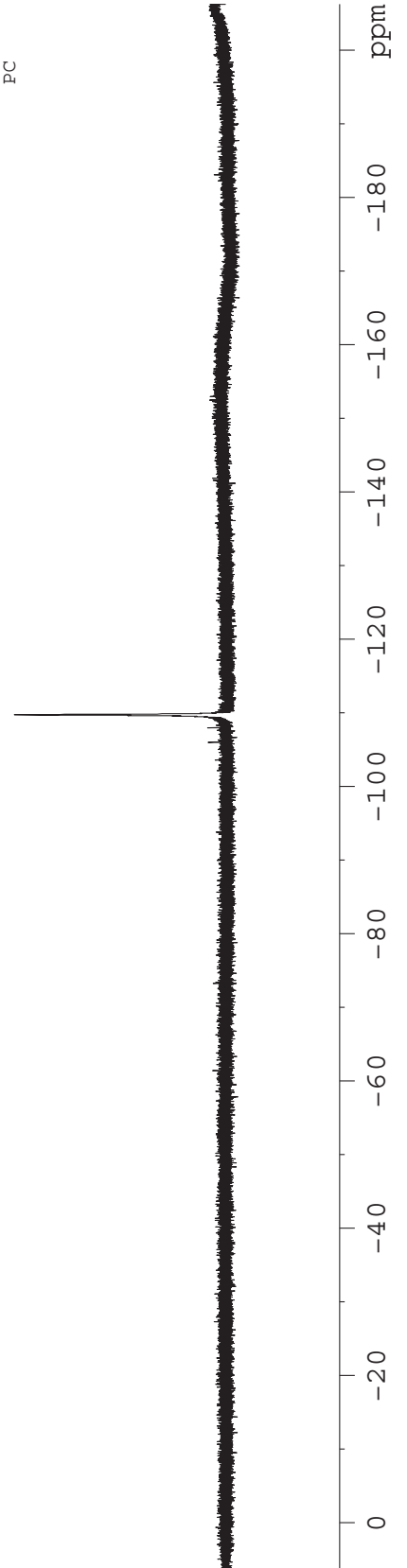
— -109.716

HXH-3-F
19Fdeflt CDC13 D:\\ deng 47



```
NAME          XB20130417
EXPNO         1
PROCNO        1
Date_         20130417
Time_         11.03
INSTRUM       spect
PROBHD        5 mm PATXO 19F
PULPROG       zg
TD            131072
SOLVENT       CDC13
NS            8
DS            4
SWH           100000.000 Hz
FIDRES        0.762939 Hz
AQ            0.6554150 sec
RG            287.4
DW            5.000 usec
DE            6.00 usec
TE            297.1 K
D1            1.00000000 sec
TD0           1

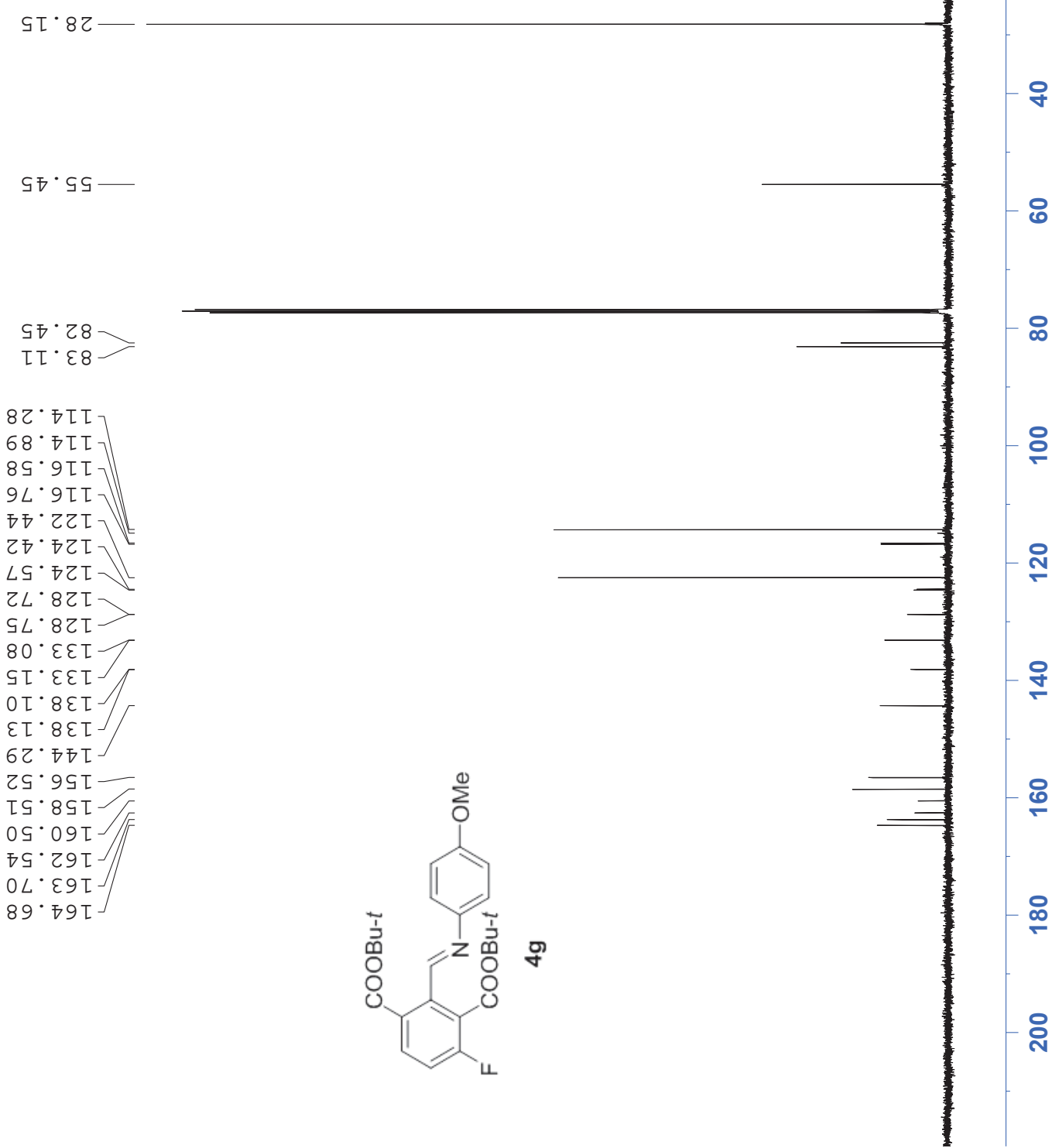
===== CHANNEL f1 =====
NUC1          19F
P1            19.30 usec
PL1           4.00 dB
SFO1          470.5453180 MHz
SI            65536
SF            470.5923770 MHz
WDW           no
SSB           0
LB            0.00 Hz
GB            0
PC            1.00
```



HXH-5-67-1
C13CPD CDC13

```

NAME          XB20130408
EXPNO         23
PROCNO        1
Date_         20130409
Time_         11.11
INSTRUM       spect
PROBHD        5 mm PATXO 19F
PULPROG       zgpg30
TD            65536
SOLVENT       CDC13
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           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        16.31 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
  
```

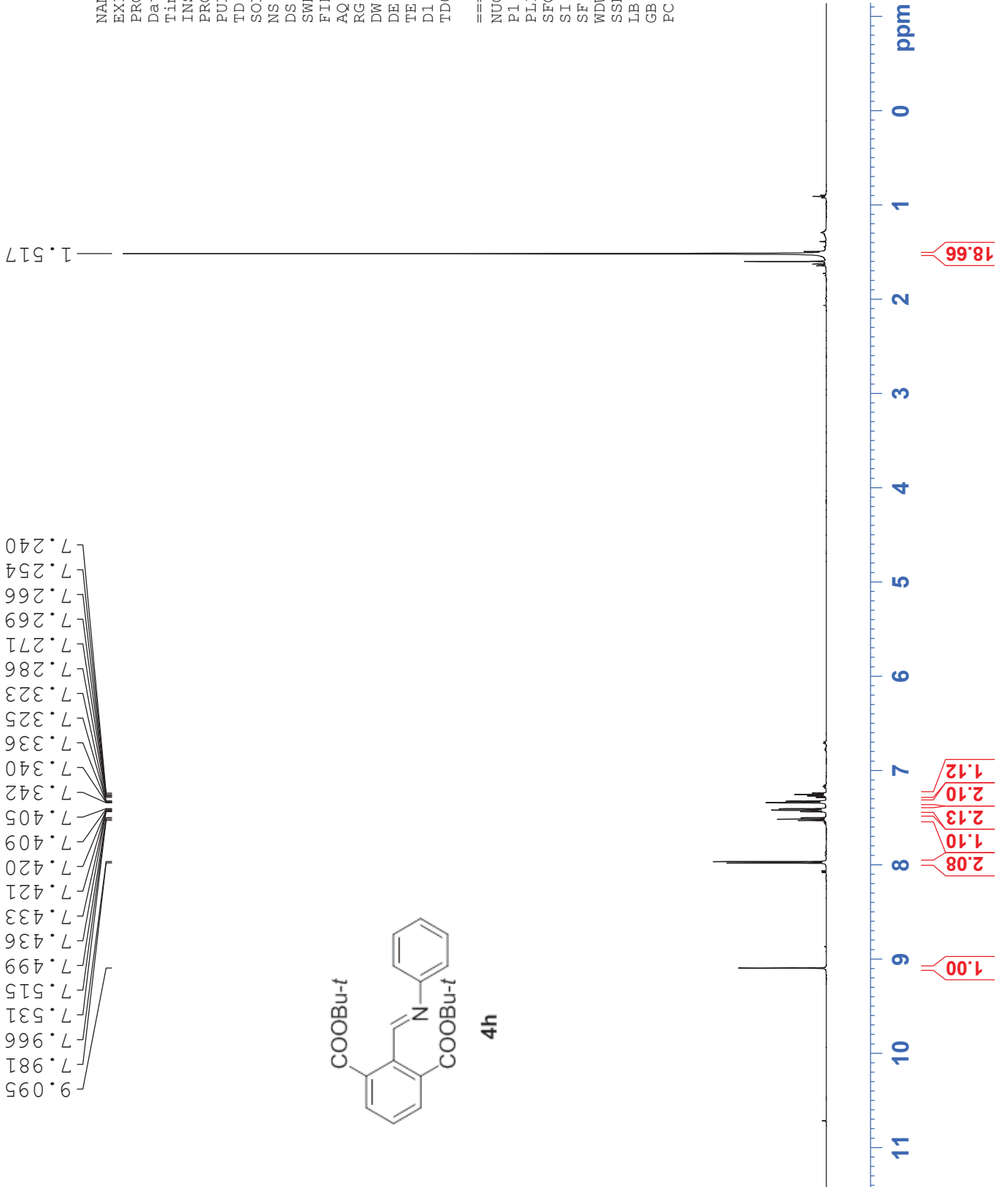
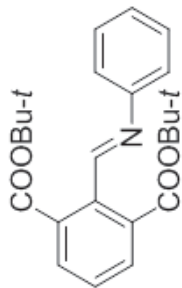


HXM-5-114
 PROTON CDC13

NAME XB20130424
 EXPNO 1
 PROCNO 1
 Date 20130424
 Time_ 11.05
 INSTRUM spect
 PROBHD 5 mm PATXO 19F
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 8
 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 295.5 K
 D1 1.00000000 sec
 TD0 1

=====
 CHANNEL f1 =====
 NUC1 1H
 P1 13.72 usec
 PL1 1.00 dB
 SF01 500.1330885 MHz
 SI 32768
 SF 500.1300000 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

9.095
 7.981
 7.966
 7.931
 7.915
 7.499
 7.436
 7.433
 7.421
 7.420
 7.409
 7.405
 7.342
 7.340
 7.336
 7.325
 7.323
 7.286
 7.271
 7.269
 7.266
 7.254
 7.240



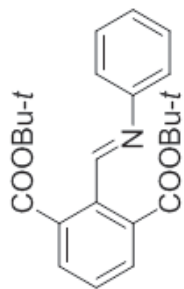
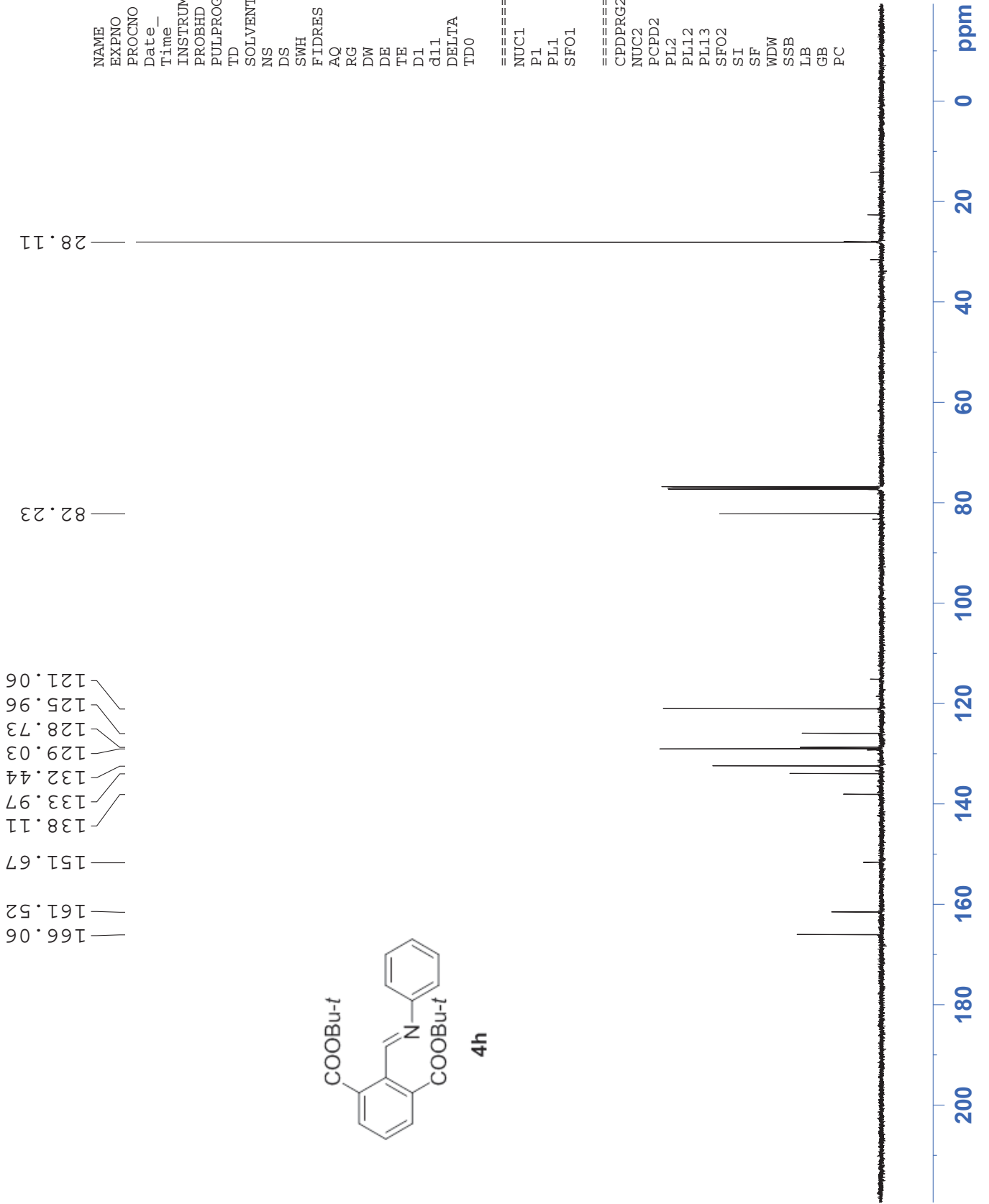
HXM-5-114
C13CPD CDCl3

```

NAME      XB20130424
EXPNO     2
PROCNO    1
Date_     20130424
Time_     11.13
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         128
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         203.2
DW         16.650 usec
DE         6.00 usec
TE         296.7 K
D1         2.0000000 sec
d11        0.0300000 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       16.31 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
    
```



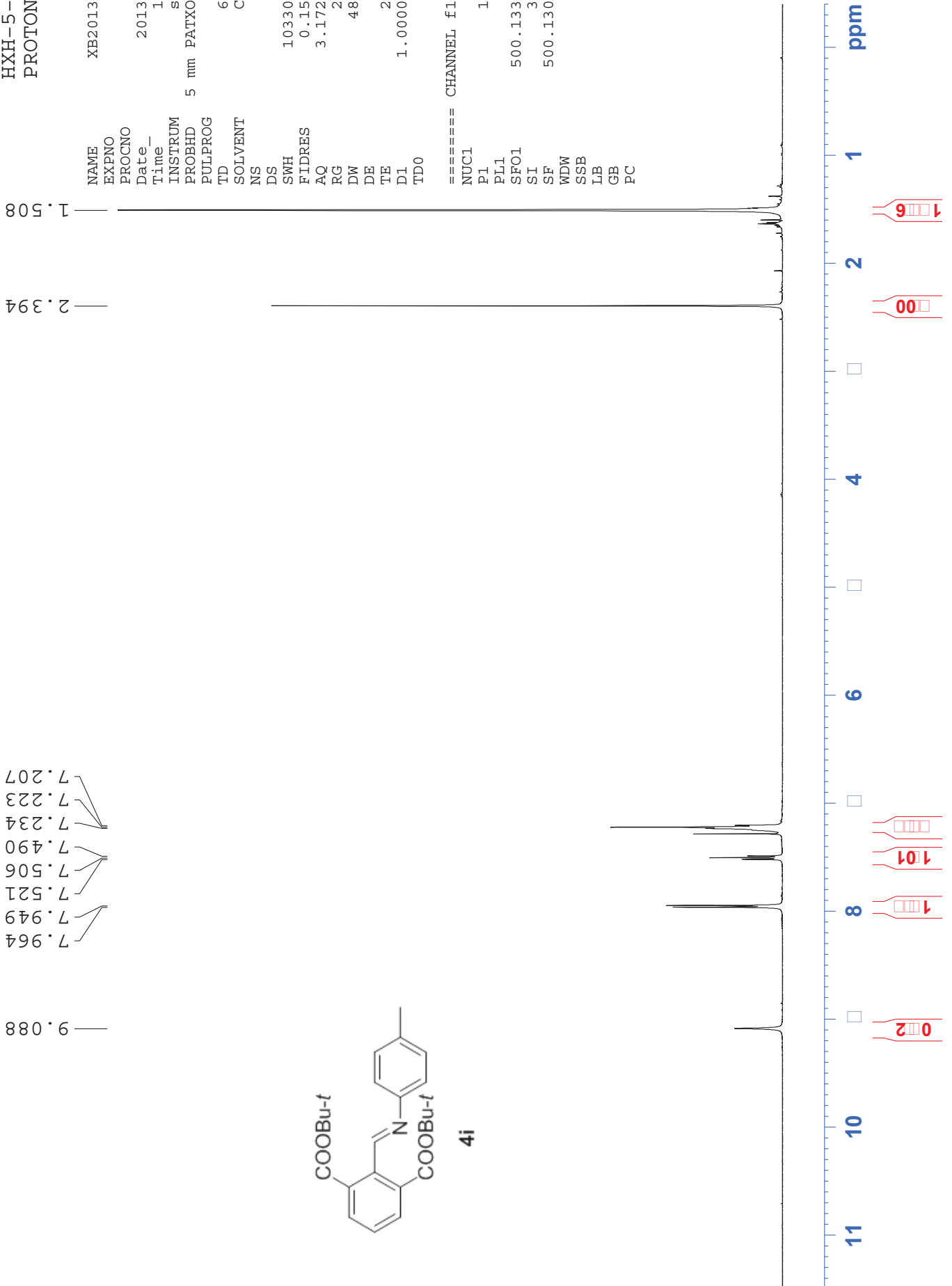
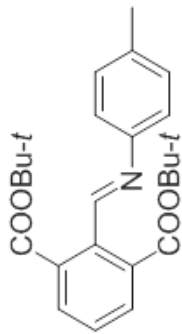
HXH-5-64-1
 PROTON CDCl3

```

NAME      XB20130408
EXPNO     16
PROCNO    1
Date_     20130408
Time_     12.40
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         295.9 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         13.72 usec
PL1        1.00 dB
SFO1       500.1330885 MHz
SI         32768
SF         500.1300000 MHz
WDW        no
SSB        0
LB         0.00 Hz
GB         0
PC         1.00
  
```

7.207
 7.223
 7.234
 7.490
 7.506
 7.521
 7.949
 7.964
 9.088



HXH-5-64-1
C13CPD CDCl3

```

NAME      XB20130408
EXPNO     20
PROCNO    1
Date_     20130409
Time      7.45
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
  
```

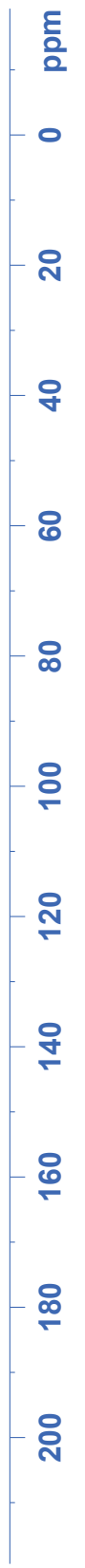
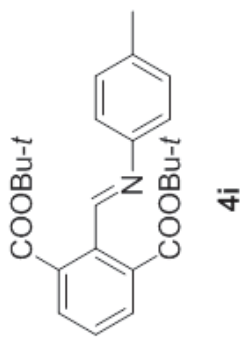
```

===== 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      16.31 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
  
```

166.13
160.51
135.76
134.00
133.42
132.38
129.76
129.64
128.65
121.01
82.17
28.12
28.04
21.06

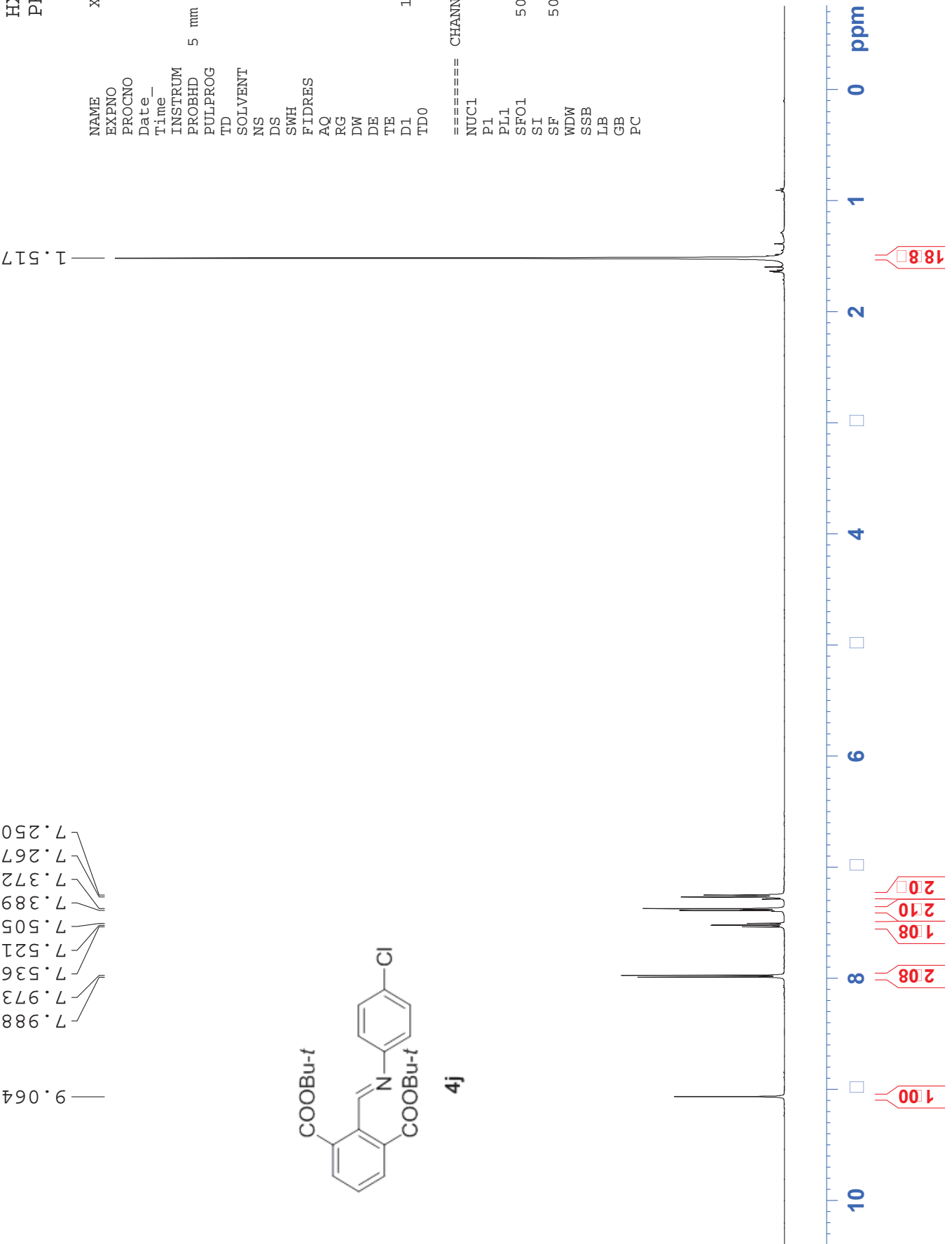
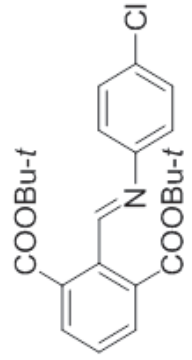


HXH-5-64-2
 PROTON CDCl3

NAME XB20130408
 EXPNO 17
 PROCNO 1
 Date 20130408
 Time 12.46
 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 114
 DW 48.400 usec
 DE 6.00 usec
 TE 295.8 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 13.72 usec
 PL1 1.00 dB
 SFO1 500.1330885 MHz
 SI 32768
 SF 500.1300000 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

7.988
 7.973
 7.536
 7.521
 7.505
 7.389
 7.372
 7.267
 7.250
 9.064



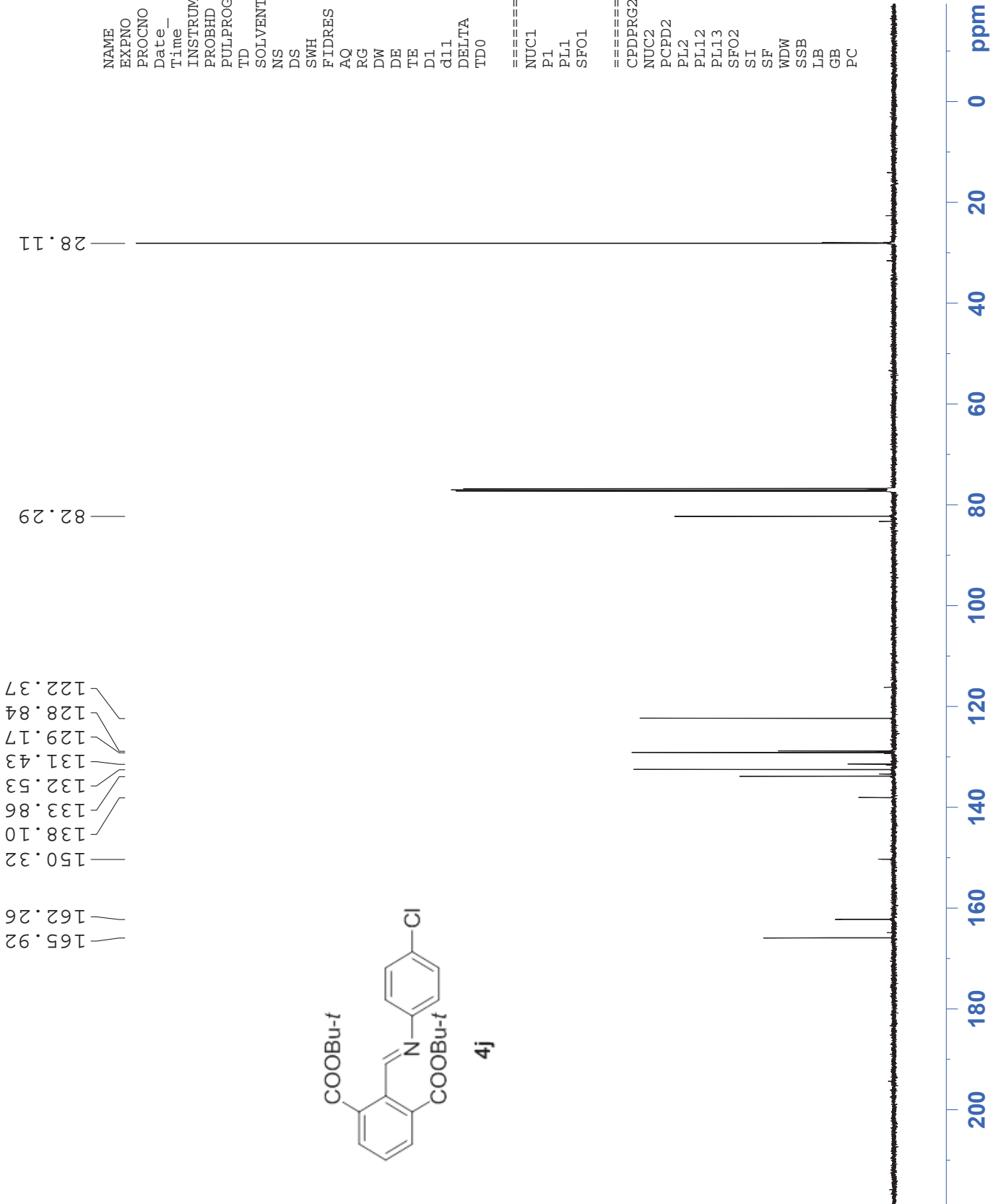
HXH-5-64-2
 C13CPD CDCl3

```

NAME      XB20130408
EXPNO     21
PROCNO    1
Date_     20130409
Time_     8.18
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          2580.3
DE          16.650 usec
TE          297.7 K
D1          2.0000000 sec
d11         0.0300000 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        16.31 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
  
```



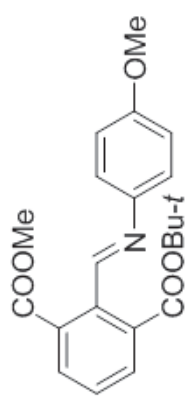
HXH-7-75
 PROTON CDCl3

NAME XB20140624
 EXPNO 4
 PROCNO 1
 Date_ 20140624
 Time 9.17
 INSTRUM spect
 PROBHD 5 mm PAXO 19F
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1720407 sec
 RG 128
 DW 48.400 usec
 DE 6.00 usec
 TE 296.1 K
 D1 1.00000000 sec
 TD0 1

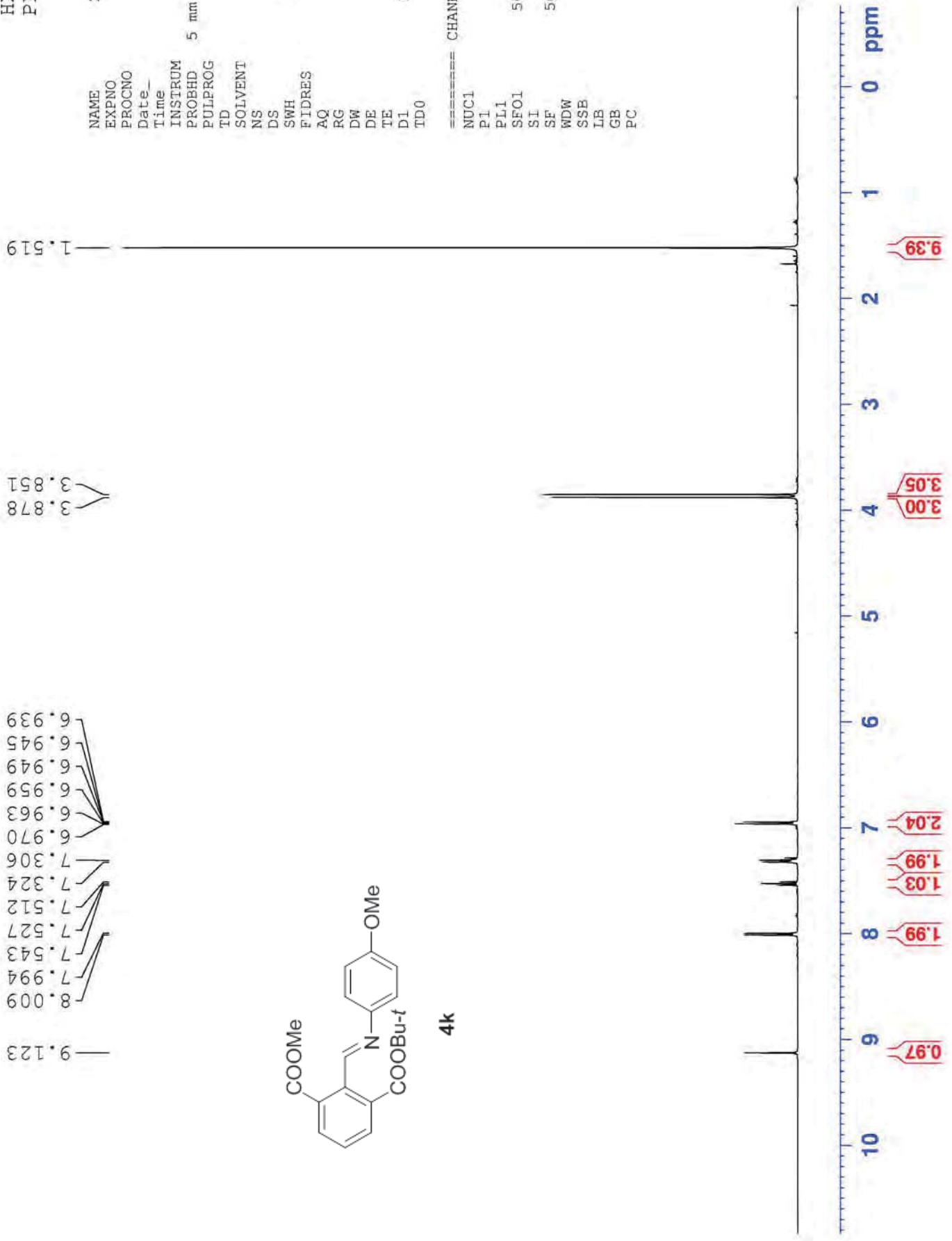
==== CHANNEL f1 ====
 NUC1 1H
 P1 14.14 usec
 PL1 1.00 dB
 SF01 500.1330885 MHz
 SI 32768
 SF 500.1300000 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

3.878
 3.851

9.123
 8.009
 7.994
 7.543
 7.527
 7.512
 7.324
 7.306
 6.970
 6.963
 6.959
 6.949
 6.945
 6.939



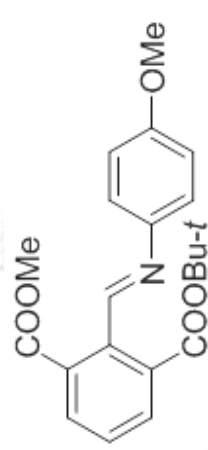
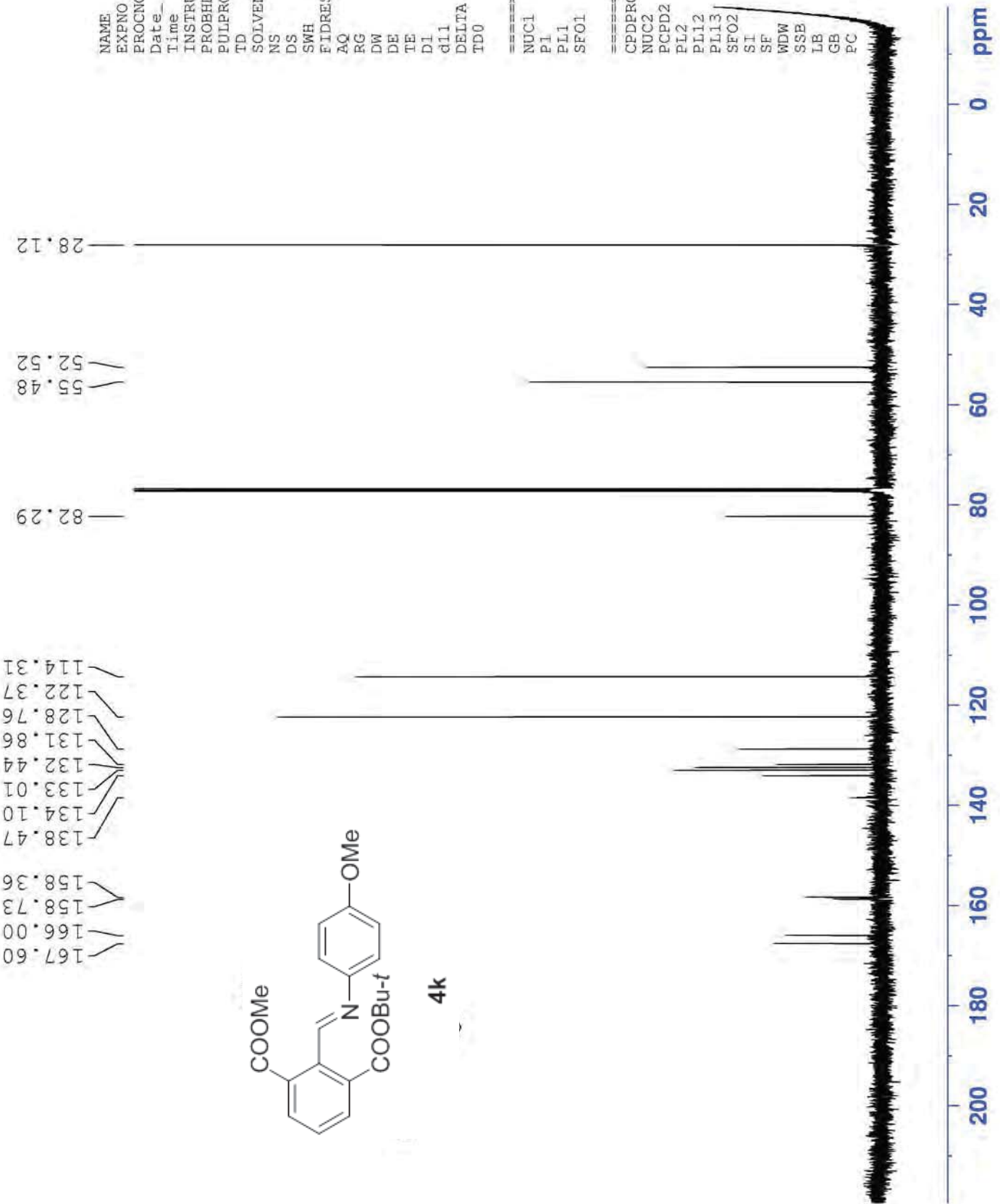
4k



HXH-7-75
C13CPD CDC13

NAME XB20140624
 EXPNO 5
 PROCNO 1
 Date_ 20140624
 Time 9.20
 INSTRUM spect
 PROBHD 5 mm PATXO 19F
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 168
 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 296.7 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



4k

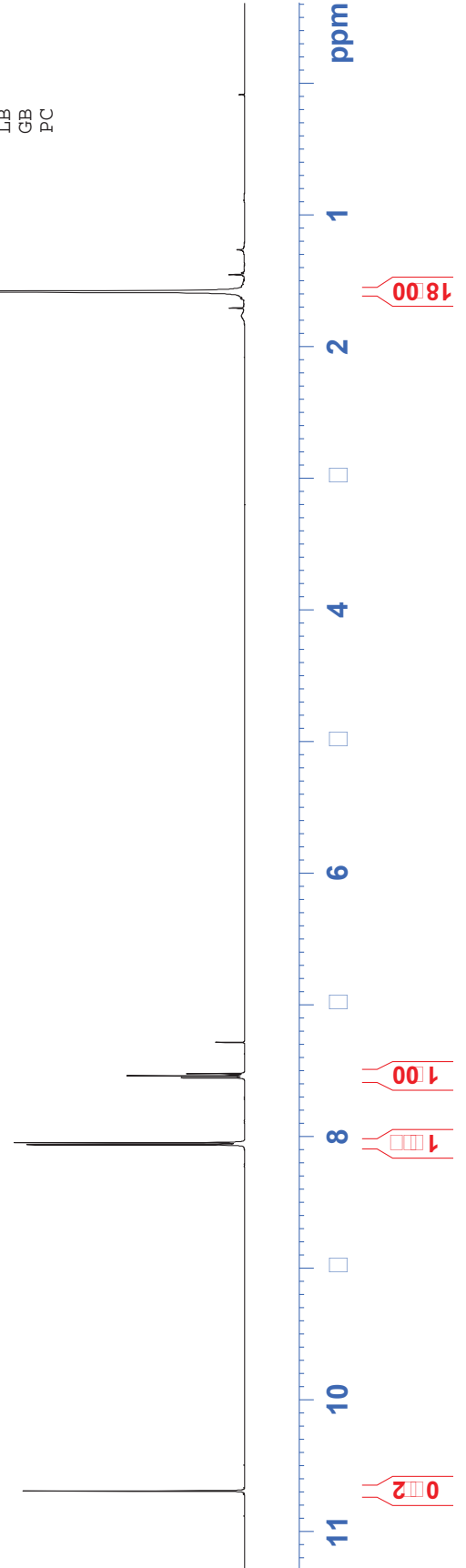
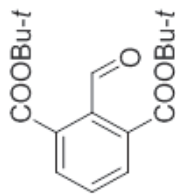
HXM-5-111
 PROTON CDC13

```

NAME      XB20130417
EXPNO     2
PROCNO    1
Date_     20130417
Time_     11.09
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zg30
TD         65536
SOLVENT   CDC13
NS         8
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         297.0 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         13.72 usec
PL1        1.00 dB
SF01       500.1330885 MHz
SI         32768
SF         500.1300000 MHz
WDW        nc
SSB        0
LB         0.00 Hz
GB         0
PC         1.00
  
```

10.689
 8.063
 8.047
 7.554
 7.538
 7.523
 1.581



HXM-5-111
C13CPD CDCl3

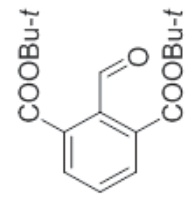
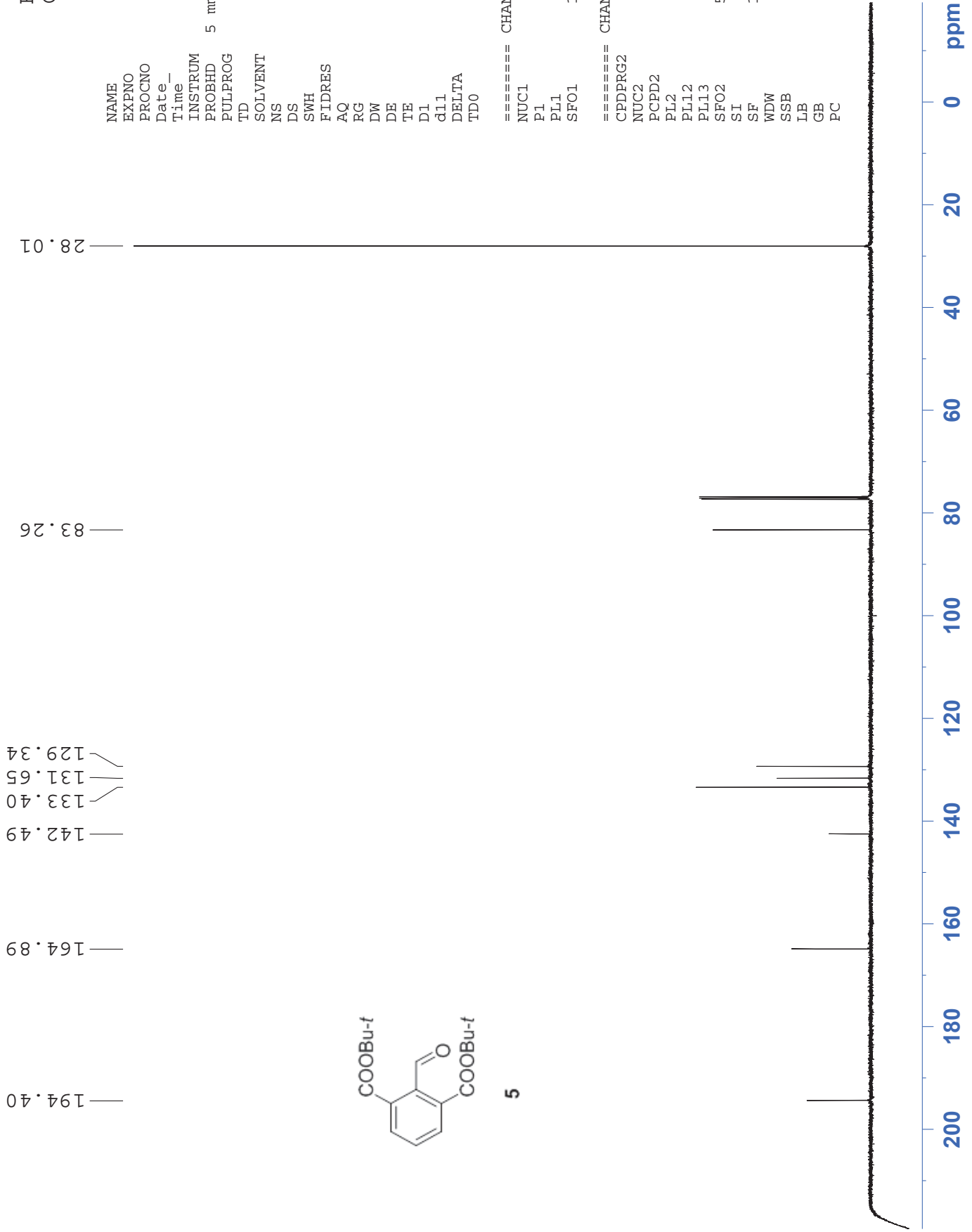
```

NAME      XB20130417
EXPNO     4
PROCNO    1
Date_     20130417
Time_     11.19
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         128
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         128
DW         16.650 usec
DE         6.00 usec
TE         297.9 K
D1         2.0000000 sec
d11        0.0300000 sec
DELTA      1.89999998 sec
TDO        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      16.31 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
  
```

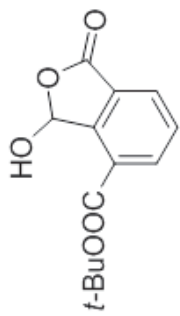
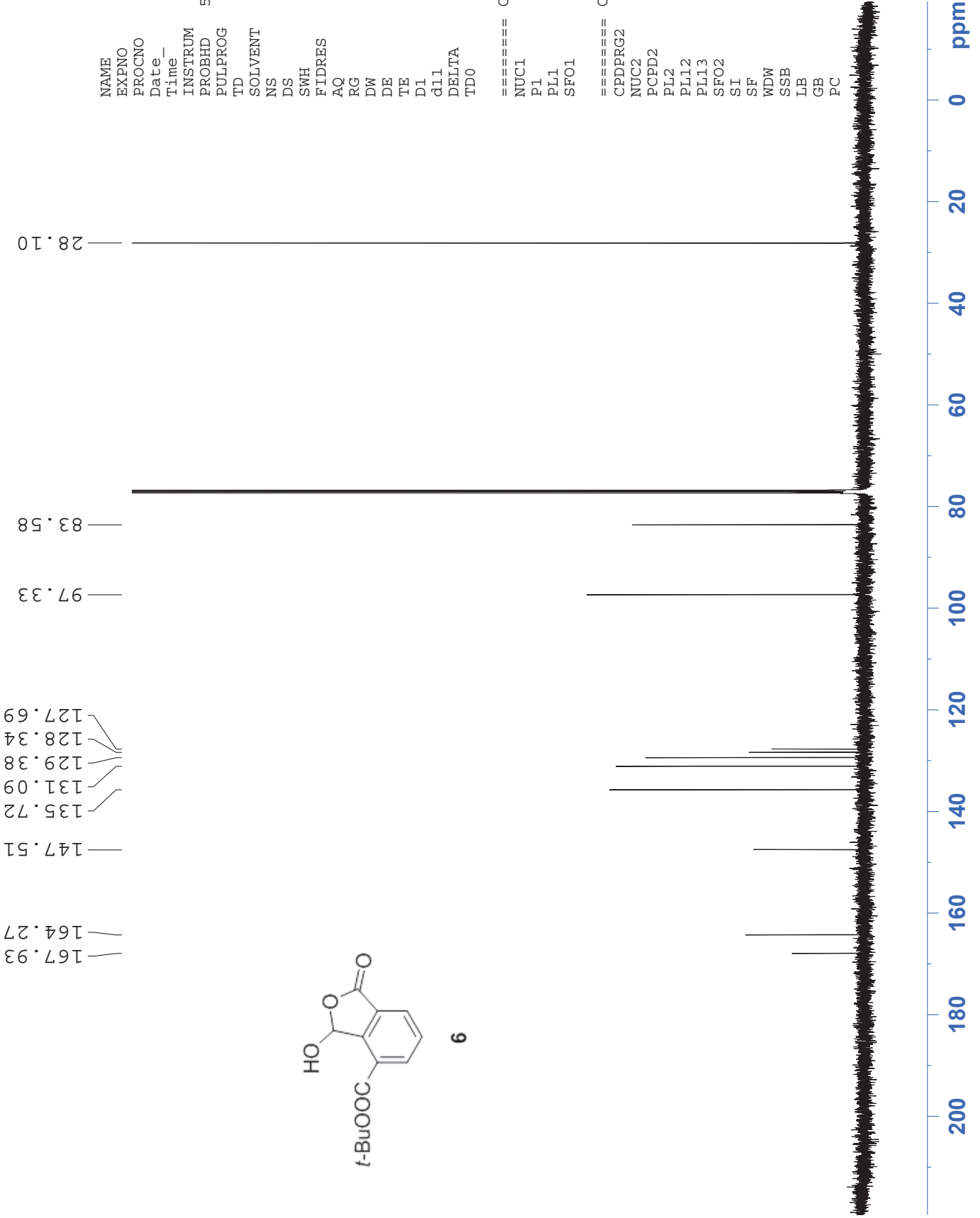


HXH-37
C13CPD CDCl3

```

NAME      XB20130323
EXPNO     7
PROCNO    1
Date_     20130324
Time      0.13
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         512
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         90.5
DW         16.650 usec
DE         6.00 usec
TE         297.4 K
D1         2.0000000 sec
d11        0.0300000 sec
DELTA     1.89999998 sec
TDO        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     16.31 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
  
```

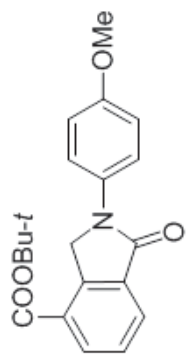
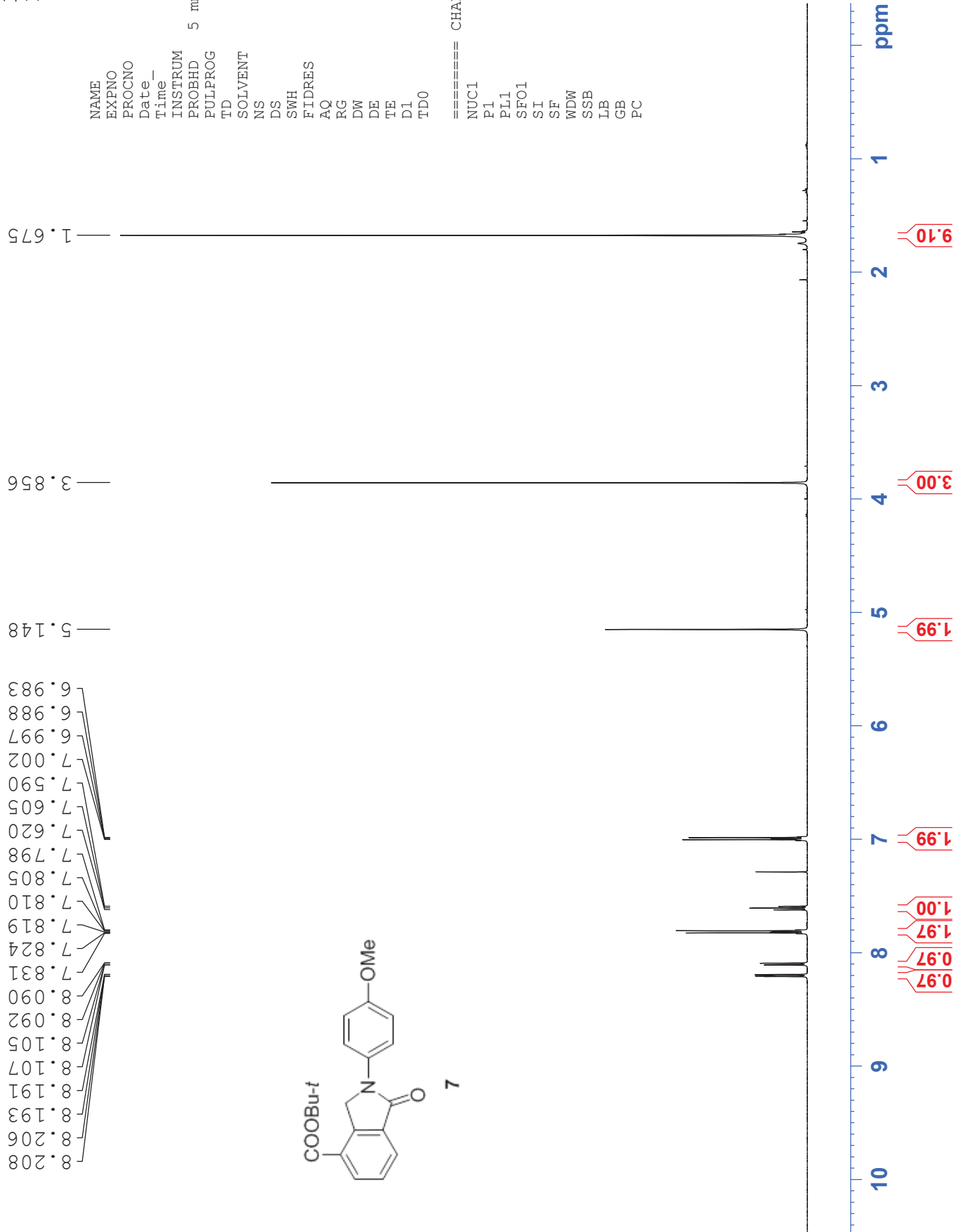


HXH-6-64-1
 PROTON CDC13

```

NAME          xb20130705
EXPNO         2
PROCNO        1
Date_         20130705
Time_         13.17
INSTRUM       spect
PROBHD        5 mm PATXO 19F
PULPROG       zg30
TD            65536
SOLVENT       CDC13
NS            8
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            500.1300000 MHz
WDW           no
SSB           0
LB            0.00 Hz
GB            0
PC            1.00
  
```



HXH-6-64-1
C13CPD CDCl3

```

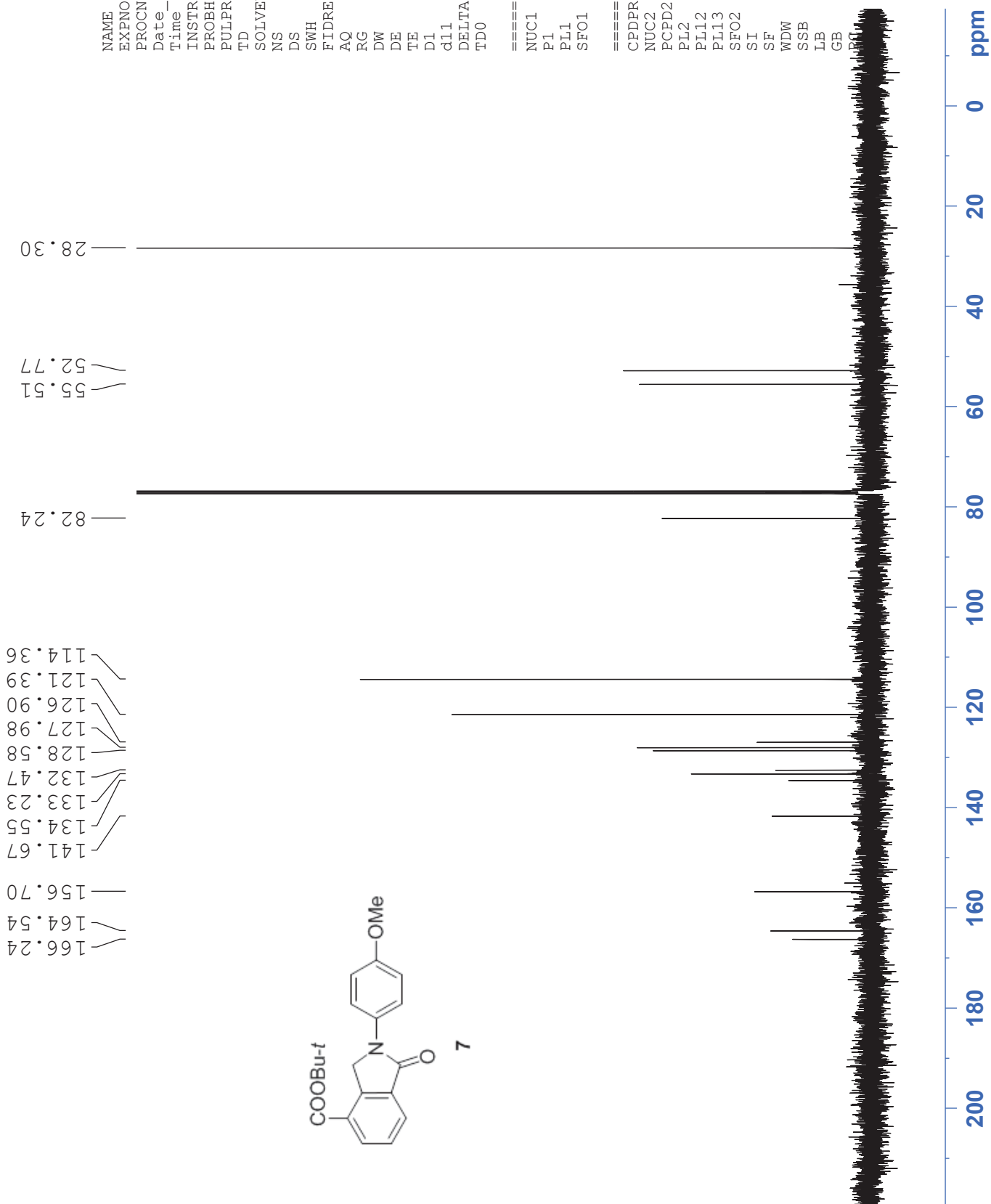
NAME          xb20130705
EXPNO         4
PROCNO        1
Date_         20130705
Time_         13.28
INSTRUM       spect
PROBHD        5 mm PATXO 19F
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            128
DS            4
SWH           30030.029 Hz
FIDRES        0.458222 Hz
AQ            1.0912410 sec
RG            143.7
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
SF01         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
  
```

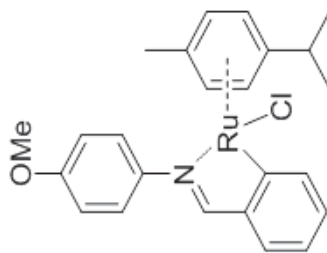


HXH
 PROTON CDC13

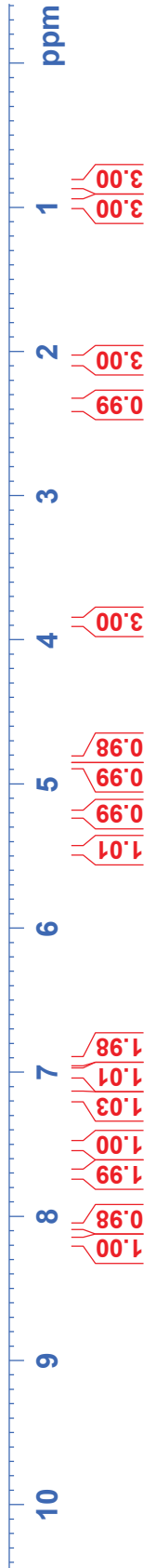
XB20131009
 EXPNO 1
 PROCNO 1
 Date 20131009
 Time 14.10
 INSTRUM spect
 PROBHD 5 mm PATXO 19F
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1720407 sec
 RG 181
 DW 48.400 usec
 DE 6.00 usec
 TE 296.7 K
 D1 1.00000000 sec
 TD0 1

=====
 CHANNEL f1 =====
 NUC1 1H
 P1 14.14 usec
 PL1 1.00 dB
 SF01 500.1330885 MHz
 SI 32768
 SF 500.1300129 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

8.176
 8.161
 8.064
 7.718
 7.714
 7.705
 7.701
 7.515
 7.513
 7.500
 7.498
 7.182
 7.180
 7.168
 7.165
 7.153
 7.150
 7.014
 7.012
 7.000
 6.998
 6.985
 6.983
 6.939
 6.932
 6.928
 6.919
 6.915
 5.463
 5.461
 5.451
 5.449
 5.215
 5.203
 4.873
 4.871
 4.861
 4.859
 4.838
 4.826
 3.871
 2.386
 2.372
 2.358
 2.2057
 0.978
 0.964
 0.845
 0.831



8



HXH
C13CPD CDCl3

```

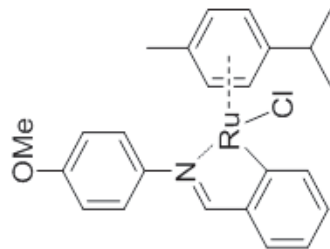
NAME      XB20131010
EXPNO     1
PROCNO    1
Date_     20131010
Time_     9.24
INSTRUM   spect
PROBHD    5 mm PATXO 19F
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         256
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         128
DE         16.650 usec
TE         6.00 usec
TE         298.4 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
  
```

188.81
171.20
158.84
148.44
146.05
139.18
130.14
129.56
123.41
122.46
113.79
102.11
100.48
92.44
89.37
82.98
82.51
55.58
30.84
22.90
21.50
18.80



8

ppm