Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Synthesis of Tetraarylpyridines by Chemo-Selective Suzuki-Miyaura Reactions of 3,5-Dibromo-2,6-dichloropyridine

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General Information

All reactions were carried out in oven-dried pressure tubes under argon atmosphere. Solvents for reactions were dried and distilled by standard methods or purchased in extra dry quality. Solvents for liquid chromatography and extraction were always distilled prior to use (heptane, ethyl acetate, dichloromethane). All chemicals, if not otherwise stated, including, ligands, boronic acids and bases, were purchased from commercial sources and used without further purification.

^{1}H-NMR Spectroscopy: Bruker AV 300 (300 MHz) and Bruker AV 400 (400 MHz). All NMR spectra presented in this work were recorded in $CDCl_3$ solution. All chemical shifts are given in ppm. All coupling constants are indicated as *J*. References: TMS or residual $CHCl_3$ were taken as internal standard. Peak characterization: s = singlet, brs = broad singlet, d = doublet, brd = broad doublet, t = triplet, dd = doublet of doublet, q = quartet, m = multiplet.

^{13}C-NMR Spectroscopy: Bruker AV 300 (75 MHz) and Bruker AV 400 (100 MHz). All NMR spectra presented in this work were recorded in $CDCl_3$ solution. All chemical shifts are given in ppm. All coupling constants are indicated as *J*. References: TMS or residual $CHCl_3$ were taken as internal standard. Peak characterization: d = doublet, t = triplet, q = quartet. DEPT method was used for determining the presence of primary, secondary, tertiary and quaternary carbon atoms.

^{19}F-NMR Spectroscopy: Bruker AV 300 (282 MHz).

Mass Spectrometry (MS): Finnigan MAT 95 XP (electron ionization EI, 70 eV); 6890 N/5973 (Agilent), 6210 Time-of-Flight LC/MS (Agilent).

Gas Chromatography MS (GCMS): Agilent HP-5890 with an Agilent HP-5973 Mass Selective Detector (EI) and HP-5 capillary column using helium carrier gas. Only the measurements with an average deviation from the theoretical mass of ± 2 mDa were accounted as correct.

High resolution MS (HRMS (ESI)): Agilent 1969A TOF. Only the measurements with an average deviation from the theoretical mass of ± 2 mDa were accounted as correct.

Infrared Spectroscopy (IR): Nicolet 550 FT-IR spectrometer with ATR sampling technique for solids as well as liquids. Signal characterization: w = weak, m = medium, s = strong.

X-ray Crystallography: Data were collected on a Bruker Kappa APEX II Duo diffractometer. The structure was solved by direct methods and refined by full-matrix least-squares procedures on F2 with the SHELXTL software package (Sheldrick, G. M. *Acta Crystallogr.* **2008**, *A64*, 112.). XP (Bruker AXS) was used for graphical representation.
CCDC 986651-986652 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Elemental Analysis (EA): C/H/N/S - Microanalysator TruSpec CHNS (Leco).

Melting point determination (mp): Micro-Hot-Stage Galen^{TM} III Cambridge Instruments. The melting points have not been corrected.

Thin layer chromatography (TLC): Merck Silica 60 F254 on aluminum tin foil from Macherey-Nagel. Detection with UV light at 254 nm and/or 366 nm without dipping reagent.

Column Chromatography: Separation on Fluka silica gel 60 (0.063-0.200 mm, 70-320 mesh). Eluents were distilled before use.

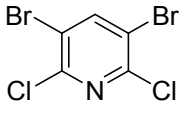
General Procedures and Experimental Data

General Procedure for the synthesis of starting material 3.

To a stirred solution of HOAc (200 mL/0.1 mol of **1**; 100%) and 2,6-diaminopyridine **1** (10.9 g, 0.1 mol) was added bromine (11.4 mL, 0.22 mol) at 10 °C. The temperature was allowed to warm to 20 °C and the reaction mixture was stirred for additional 20 h. Na_2SO_3 was added to the solution (20 mL, 0.1 M) and subsequently Na_2CO_3 (0.1 M) until a neutral ph-value was reached. The latter was extracted with EtOAc (8 × 50 mL). The combined organic layers were dried (Na_2SO_4), filtered and the filtrate was concentrated in vacuo. 2,6-Diamino-3,5-dibromopyridine **2** was obtained as a brownish solid and used for the second step without further purification.

To a stirred solution of HCl and 2,6-diamino-3,5-dibromopyridine **2** (15 g, 0.056 mol) was added $NaNO_2$ (9.3 g, 0.14 mol) at room temperature. The solution was stirred for 20 h. Subsequently, water was added (300 mL) and the latter was extracted with EtOAc (3 × 50 mL). The combined organic layers were dried (Na_2SO_4), filtered and the filtrate was concentrated in vacuo. 2,6-Dichloro-3,5-dibromopyridine **3** was obtained as colorless solid (6.5 g, 38% over two steps) after purification by flash chromatography (*n*-hexane/EtOAc).

3,5-Dibromo-2,6-dichloropyridine (3).

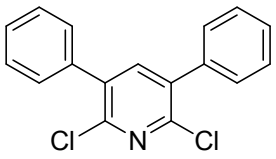


Compound **38** was isolated as a colorless solid; mp = 87-88 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.13 (s, 1H, CH). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 118.9 (C-Br), 146.5 (CH), 148.5 (C-Cl). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3081 (w), 3028 (w), 1516 (m), 1371 (s), 1324 (m), 1297 (m), 1222 (w), 1165 (s), 1053 (m), 1037 (s), 921 (m), 845 (w), 712 (m), 667 (m), 622 (w), 588 (m), 496 (m), 462 (m). GC-MS (EI, 70 eV): m/z (%): 305 (M^+, 100), 303 (39), 272 (10), 270 (15), 268 (7), 228 (7), 226 (14), 224 (9), 191 (7), 189 (6), 164 (4), 153 (6), 147 (10), 145 (16), 112 (5), 110 (14), 86 (5), 84 (16), 75 (26), 74 (9), 49 (11). HRMS (EI, 70 eV): calcd. for $C_5HBr_2Cl_2N$ (M^+): 302.78473, found 302.784924 and calcd. for $C_5HBr^{81}BrCl_2N$ (M^+): 304.78268, found 304.782710 and calcd. for $C_5H^{81}Br_2Cl_2N$ (M^+): 306.78064, found 306.780338 and calcd. for $C_5H^{81}Br_2Cl^{37}ClN$ (M^+): 308.77769, found 308.777837. Anal. calcd. for $C_5HBr_2Cl_2N$ (305.78): C, 19.64; H, 0.33; N, 4.659. Found: C, 19.80; H, 0.3439; N, 4.658.

General procedure for the synthesis of 2,6-dichloro-3,5-diaryl-substituted pyridines 4a-f

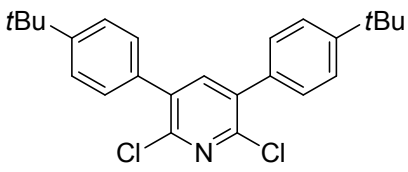
An oven-dried and argon-flushed pressure tube was charged with 3,5-dibromo-2,6-dichloropyridine **3** (0.33 mmol), $PdCl_2(PPh_3)_2$ (5.0 mol%), boronic acid (0.8 mmol) and K_3PO_4 (0.98 mmol), followed by anhydrous toluene (4.0 mL). The tube was sealed with a Teflon valve and the reaction mixture was stirred at 100 °C for 20 h. The cooled reaction mixture was diluted with water and extracted with DCM. The combined organic layers were dried (Na_2SO_4), filtered and the filtrate was concentrated in vacuo. The residue was purified by column chromatography.

2,6-Dichloro-3,5-diphenylpyridine (4a)



Starting with 3,5-dibromo-2,6-dichloropyridine **3** (100 mg, 0.327 mmol), $PdCl_2(PPh_3)_2$ (11.5 mg, 5.0 mol%), phenylboronic acid (95.7 mg, 0.785 mmol), K_3PO_4 (208 mg, 0.981 mmol) and toluene (4.0 mL), **4a** was isolated as a colorless oil (73 mg, 74%); mp = 128-129 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.41-7.49 (m, 10H, CH), 7.67 (s, 1H, CH). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 128.5 (CH), 128.6 (CH), 129.2 (CH), 135.8 (C), 136.0 (C), 142.7 (CH), 146.8 (C-Cl). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3057 (w), 2921 (w), 2027 (w), 1959 (w), 1577 (m), 1530 (w), 1445 (m), 1384 (s), 1223 (w), 1120 (m), 1029 (m), 1006 (w), 870 (w), 765 (m), 700 (s), 671 (m), 650 (w), 598 (w), 523 (w), 464 (w), 377 (w). GC-MS (EI, 70 eV): m/z (%): 303 (M^+, 20), 299 (100), 264 (3), 229 (11), 228 (18), 227 (23), 203 (4), 202 (16), 201 (9), 176 (2), 150 (3), 132 (2), 126 (2), 114 (8), 101 (7), 100 (6), 88 (4), 77 (4), 75 (3), 51 (4). HRMS (EI, 70 eV): calcd. for $C_{17}H_{11}Cl_2N$ (M^+): 299.02631, found 299.02605 and calcd. for $C_{17}H_{11}Cl^{37}ClN$ (M^+): 301.02336, found 301.02348 and calcd. for $C_{17}H_{11}{}^{37}Cl_2N$ (M^+): 303.02041, found 303.02057.

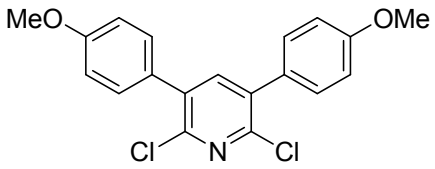
2,6-Dichloro-3,5-bis(4-*tert*-butylphenyl)pyridine (4b)



Starting with 3,5-dibromo-2,6-dichloropyridine **3** (100 mg, 0.327 mmol), $PdCl_2(PPh_3)_2$ (11.5 mg, 5.0 mol%), 4-*tert*-butylphenyl)boronic acid (139.7 mg, 0.785 mmol), K_3PO_4 (208 mg, 0.981 mmol) and toluene (4.0 mL), **4b** was isolated as a colorless solid (78 mg, 58%); mp = 146-148 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 1.29 (s, 18H, $CH_{3\ tBu}$), 7.33-7.42 (m, 4H, CH), 7.62 (s, 1H, CH). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 31.3 ($CH_{3\ tBu}$), 34.7 (C), 125.4 (CH), 128.9 (CH), 133.1 (C), 135.7 (C), 142.9 (CH), 146.5 (C), 151.8 (C). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3035 (w), 2972 (m), 2947 (m), 2836 (m), 1609 (w), 1575 (w), 1530 (m), 1460 (m), 1379 (s), 1363 (m), 1267 (m), 1222 (w), 1202 (m), 1134 (s), 1123 (s), 1105 (s), 1018 (w), 1002 (m), 925 (m), 908 (w), 875 (m), 832 (s), 755

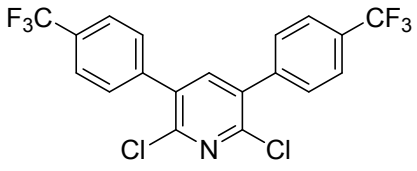
(w), 730 (w), 669 (m), 641 (w), 621 (s), 598 (m), 572 (s), 534 (m), 511 (m), 471 (w). GC-MS (EI, 70 eV): m/z (%): 412 (M^+, 10), 411 (36), 400 (14), 399 (18), 398 (65), 397 (26), 396 (100), 368 (4), 353 (2), 310 (3), 282 (3), 268 (3), 267 (3), 240 (4), 227 (3), 190 (9), 162 (13), 127 (3), 57 (10), 41 (7). HRMS (EI, 70 eV): calcd. for $C_{25}H_{27}Cl_2N$ (M^+): 411.15151, found 411.15136 and calcd. for $C_{25}H_{27}Cl^{37}ClN$ (M^+): 413.14856, found 413.14895.

2,6-Dichloro-3,5-bis(4-methoxyphenyl)pyridine (4c)



Starting with 3,5-dibromo-2,6-dichloropyridine **3** (100 mg, 0.327 mmol), $PdCl_2(PPh_3)_2$ (11.5 mg, 5.0 mol%), 4-methoxyphenylboronic acid (119.3 mg, 0.785 mmol), K_3PO_4 (208 mg, 0.981 mmol) and toluene (4.0 mL), **4c** was isolated as a colorless solid (71 mg, 60%); mp = 84-86 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 3.84 (s, 6H, MeO), 6.94-6.99 (m, 4H, CH), 7.37-7.42 (m, 4H, CH), 7.62 (s, 1H, CH). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 55.3 (MeO), 113.9 (CH), 128.3 (C), 130.5 (CH), 135.5 (C), 142.5 (CH), 146.3 (C-Cl), 159.8 (C). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3063 (w), 2954 (w), 2907 (w), 2892 (w), 2829 (m), 1607 (s), 1577 (m), 1526 (m), 1511 (s), 1452 (m), 1418 (m), 1384 (s), 1304 (m), 1289 (s), 1244 (s), 1177 (s), 1109 (s), 1031 (s), 1018 (m), 995 (s), 911 (w), 875 (m), 824 (s), 785 (m), 732 (w), 679 (m), 590 (m), 541 (m), 526 (m), 497 (w), 448 (w), 414 (w). GC-MS (EI, 70 eV): m/z (%): 360 (M^+, 22), 359 (100), 344 (11), 318 (5), 316 (8), 309 (2), 303 (2), 273 (3), 246 (4), 238 (3), 230 (3), 214 (4), 203 (6), 202 (4), 179 (6), 176 (4), 94 (2). HRMS (EI, 70 eV): calcd. for $C_{19}H_{15}Cl_2NO_2$ (M^+): 359.04744, found 359.04731 and calcd. for $C_{19}H_{15}Cl^{37}ClNO_2$ (M^+): 361.04449, found 361.04454 and calcd. for $C_{19}H_{15}{}^{37}Cl_2NO_2$ (M^+): 363.04154, found 363.04216. Anal. calcd. for $C_{19}H_{15}Cl_2NO_2$ (360.23): C, 63.35; H, 4.20; N, 3.89. Found: C, 63.31; H, 4.133; N, 3.961.

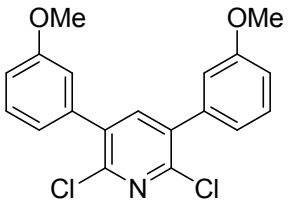
2,6-Dichloro-3,5-bis(4-(trifluoromethyl)phenyl)pyridine (4d)



Starting with 3,5-dibromo-2,6-dichloropyridine **3** (100 mg, 0.327 mmol), $PdCl_2(PPh_3)_2$ (11.5 mg, 5.0 mol%), 4-(trifluoromethyl)phenylboronic acid (149.1 mg, 0.785 mmol), K_3PO_4 (208 mg, 0.981 mmol) and toluene (4.0 mL), **4d** was isolated as a colorless solid (97 mg, 68%); mp = 35-36 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.58-7.61 (m, 4H, CH), 7.67 (s, 1H, CH), 7.72-7.75 (m, 4H, CH). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 123.8 (q, $^1J_{C\text{-}F}$ = 272.9 Hz, CF_3), 125.6 (q, $^3J_{C\text{-}F}$ = 3.8 Hz, CH), 129.7 (CH), 131.1 (q, $^2J_{C\text{-}F}$ = 32.8 Hz, C), 134.8 (C), 139.3 (C), 142.3 (CH), 147.6 (C). ^{19}F NMR (282.4 MHz, $CDCl_3$): δ = -62.4 (CF_3). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 1619 (w), 1581 (w), 1413 (w), 1388 (m), 1317 (s), 1164 (m), 1107 (s), 1065 (s), 1018 (m), 1003 (m), 957 (m), 908 (m), 838 (m), 715 (m), 699 (m), 679 (m), 621 (w), 603 (w), 523 (w), 410 (w). GC-MS (EI, 70 eV): m/z (%): 436 (M^+, 22), 435 (100), 416 (9), 380 (6), 365 (6), 344 (8), 338 (12), 295 (12), 294 (4), 276 (7), 227 (7), 200

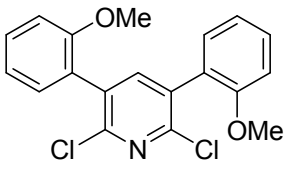
(2), 169 (2), 69 (3). HRMS (EI, 70 eV): calcd. for $C_{19}H_9Cl_2F_6N$ (M^+): 435.00108, found 435.00096 and calcd. for $C_{19}H_9Cl^{37}ClF_6N$ (M^+): 436.99813, found 436.99778 and calcd. for $C_{19}H_9{}^{37}Cl_2F_6N$ (M^+): 438.99518, found 438.99558. Anal. calcd. for $C_{19}H_9Cl_2F_6N$ (436.18): C, 52.32; H, 2.08; N, 3.21. Found: C, 52.22; H, 1.998; N, 3.288.

2,6-Dichloro-3,5-bis(3-methoxyphenyl)pyridine (4e)



Starting with 3,5-dibromo-2,6-dichloropyridine **3** (100 mg, 0.327 mmol), $PdCl_2(PPh_3)_2$ (11.5 mg, 5.0 mol%), 3-methoxyphenyl-boronic acid (119.3 mg, 0.785 mmol), K_3PO_4 (208 mg, 0.981 mmol) and toluene (4.0 mL), **4e** was isolated as a colorless oil (81 mg, 69%). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 3.83 (s, 6H, MeO), 6.94-7.05 (m, 6H, CH), 7.36 (m, 2H, CH), 7.67 (s, 1H, CH). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 55.4 (MeO), 114.1 (CH), 115.0 (CH), 121.6 (CH), 129.6 (CH), 135.7 (C), 137.2 (C), 142.6 (CH), 146.8 (C-Cl), 159.5 (C). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3001 (w), 2937 (w), 2835 (w), 1579 (s), 1529 (w), 1489 (m), 1450 (m), 1427 (m), 1378 (s), 1319 (w), 1288 (s), 1268 (m), 1210 (s), 1178 (m), 1117 (s), 1082 (w), 1041 (s), 1020 (s), 926 (m), 858 (m), 836 (m), 779 (s), 731 (w), 698 (s), 649 (m), 568 (w), 528 (m), 468 (m). GC-MS (EI, 70 eV): m/z (%): 360 (M^+, 22), 359 (100), 318 (4), 316 (6), 273 (3), 230 (3), 215 (3), 214 (6), 203 (4), 202 (4), 201 (3). HRMS (ESI, 70 eV): calcd. for $C_{19}H_{16}Cl_2NO_2$ ($[M+H]^+$): 360.05486, found 360.05526.

2,6-Dichloro-3,5-bis(2-methoxyphenyl)pyridine (4f)

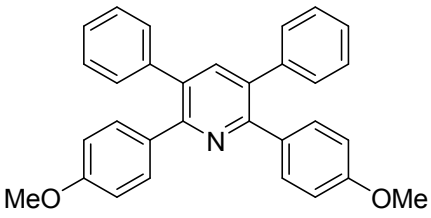


Starting with 3,5-dibromo-2,6-dichloropyridine **3** (100 mg, 0.327 mmol), $PdCl_2(PPh_3)_2$ (11.5 mg, 5.0 mol%), 2-methoxyphenyl-boronic acid (119.3 mg, 0.785 mmol), K_3PO_4 (208 mg, 0.981 mmol) and toluene (4.0 mL), **4f** was isolated as a colorless solid (59 mg, 50%); mp = 157-159 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 3.80 (s, 6H, MeO), 6.96-7.04 (m, 4H, CH), 7.23 (brdd, $^3J_{H-H}$ = 7.8 Hz, $^4J_{H-H}$ = 1.8 Hz, 2H, CH), 7.90 (ddd, $^3J_{H-H}$ = 8.3 Hz, $^3J_{H-H}$ = 7.1 Hz, $^4J_{H-H}$ = 1.8 Hz 2H, CH), 7.60 (s, 1H,CH). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 55.5 (MeO), 111.1 (CH), 120.5 (CH), 125.3 (C), 130.2 (CH), 130.9 (CH), 132.5 (C), 144.1 (CH), 148.1 (C), 156.6 (C). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2996 (w), 2967 (w), 2936 (w), 2835 (w), 1601 (w), 1580 (m), 1492 (m), 1434 (m), 1383 (m), 1276 (w), 1250 (m), 1236 (w), 1181 (m), 1162 (w), 1123 (m), 1023 (m), 999 (m), 917 (m), 873 (m), 785 (m), 760 (s), 691 (m), 604 (m), 575 (w), 532 (w), 514 (m), 491 (m), 437 (w). GC-MS (EI, 70 eV): m/z (%): 360 (M^+, 22), 359 (100), 326 (17), 325 (10), 324 (49), 311 (11), 309 (32), 293 (14), 274 (46), 273 (20), 272 (11), 206 (18), 259 (76), 244 (4), 243 (6), 230 (9), 214 (8), 202 (6), 180 (7), 176 (5), 175 (4), 162 (4), 130 (8), 88 (4). HRMS (EI, 70 eV): calcd. for $C_{19}H_{15}Cl_2NO_2$ (M^+): 359.04744, found 359.04757 and calcd. for $C_{19}H_{15}Cl^{37}ClNO_2$ (M^+): 361.04449, found 361.04474 and calcd. for $C_{19}H_{15}{}^{37}Cl_2NO_2$ (M^+): 363.04154, found 363.04168.

General procedure for the synthesis of 2,3,5,6-tetraaryl-substituted pyridines 5a-d

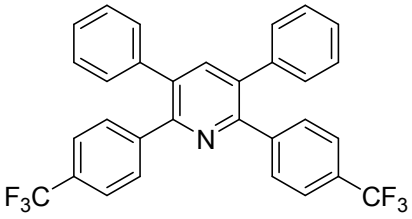
An oven-dried and argon-flushed pressure tube was charged with the appropriate 2,6-dichloro-3,5-diaryl-substituted pyridines **4** (0.3 mmol), $Pd(dba)_2$ (2.5 mol%), *n*$BuPAd_2$ (5.0 mol%), boronic acid (1.2 mmol) and K_3PO_4 (1.2 mmol) followed by anhydrous toluene (5.0 mL). The tube was sealed with a Teflon valve and the reaction mixture was stirred at 100 °C for 20 h. The cooled reaction mixture was diluted with water and extracted with DCM. The combined organic layers were dried (Na_2SO_4), filtered and the filtrate was concentrated in vacuo. The residue was purified by column chromatography.

2,6-Bis(4-methoxyphenyl)-3,5-diphenylpyridine (5a)



Starting with 2,6-dichloro-3,5-diphenylpyridine 5**a** (128 mg, 0.29 mmol), $Pd(dba)_2$ (4.2 mg, 2.5 mol%), *n*$BuPAd_2$ (5.2 mg, 5.0 mol%), 4-methoxyphenylboronic acid (175 mg, 1.15 mmol), K_3PO_4 (245 mg, 1.15 mmol) and toluene (5.0 mL), **5a** was isolated as a colorless solid (102 mg, 79%); mp = 204-206 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 3.66 (s, 6H, MeO), 6.65-6.69 (m, 4H, CH), 7.14-7.20 (m, 10H, CH), 7.34-7.38 (m, 4H, CH), 7.60 (s, 1H, CH). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 55.2 (MeO), 113.1 (CH), 127.0 (CH), 128.3 (CH), 129.4 (CH), 131.4 (CH), 132.5 (C), 133.3 (C), 140.1 (C), 141.2 (CH), 154.6 (C), 159.3 (C). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3054 (w), 3030 (w), 2951 (w), 2929 (w), 2834 (w), 1604 (s), 1577 (m), 1506 (s), 1446 (s), 1421 (s), 1386 (m), 1299 (m), 1246 (s), 1172 (s), 1108 (w), 1074 (w), 1030 (m), 1005 (w), 911 (w), 878 (w), 837 (s), 792 (m), 769 (s), 756 (m), 733 (w), 699 (s), 641 (m), 619 (w), 559 (m), 538 (m), 524 (w), 417 (w). GC-MS (EI, 70 eV): m/z (%): 444 (M^+, 21), 443 (72), 442 (100), 400 (3), 399 (9), 398 (9), 355 (9), 341 (3), 328 (2), 292 (2), 281 (2), 207 (3), 184 (5), 183 (6), 177 (9), 170 (4), 169 (5). HRMS (ESI, 70 eV): calcd. for $C_{31}H_{26}NO_2$ ($[M+H]^+$): 444.19581, found 444.19624. Anal. calcd. for $C_{31}H_{25}NO_2$ (443.54): C, 83.95; H,5.68; N, 3.16. Found: C, 84.08; H, 5.728; N, 2.953.

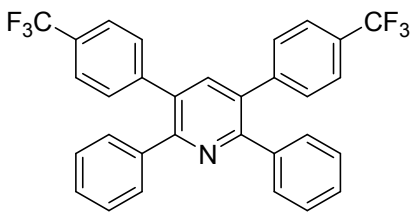
2,6-Bis(4-(trifluoromethyl)phenyl)-3,5-diphenyl-pyridine (5b)



Starting with 2,6-dichloro-3,5-diphenylpyridine **4a** (87.1 mg, 0.29 mmol), $Pd(dba)_2$ (4.2 mg, 2.5 mol%), *n*$BuPAd_2$ (5.2 mg, 5.0 mol%), 4-(trifluoromethyl)-phenylboronic acid (218 mg, 1.15 mmol), K_3PO_4 (245 mg, 1.15 mmol) and toluene (5.0 mL), **5b** was isolated as a colorless solid (111 mg, 74%); mp = 186-188 °C.

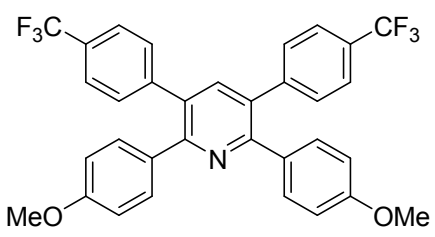
^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.26 (m, 10H, CH), 7.51-7.54 (m, 4H, CH), 7.61-7.64 (m, 4H, CH), 7.85 (s, 1H, CH). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 124.2 (q, $^{1}J_{C\text{-}F}$ = 272.8 Hz, CF_3), 124.9 (q, $^{3}J_{C\text{-}F}$ = 3.8 Hz, CH), 127.8 (CH), 128.7 (CH), 129.5 (CH), 129.9 (q, $^{2}J_{C\text{-}F}$ = 32.4 Hz, C), 130.4 (CH), 135.3 (C), 138.7 (C), 141.5 (CH), 143.2 (C), 154.0 (C). ^{19}F NMR (282.4 MHz, $CDCl_3$): δ = -62.1 (CF_3). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3059 (w), 1617 (w), 1577 (w), 1529 (w), 1448 (w), 1422 (w), 1406 (w), 1385 (w), 1320 (s), 1161 (m), 1108 (s), 1065 (s), 1015 (m), 956 (w), 938 (w), 913 (w), 878 (w), 850 (m), 795 (m), 782 (m), 700 (s), 646 (w), 627 (w), 591 (w), 551 (w), 528 (w), 490 (w), 449 (w), 410 (w). GC-MS (EI, 70 eV): m/z (%): 519 (M^+, 65), 518 (100), 500 (4), 448 (2), 372 (3), 303 (3), 276 (4), 250 (2), 214 (2), 190 (4). HRMS (EI, 70 eV): calcd. for $C_{31}H_{18}F_6N$ (M^+): 518.13380, found 518.13376.

2,6-Diphenyl-3,5-bis(4-(trifluoromethyl)phenyl)pyridine (5c)



Starting with 2,6-dichloro-3,5-bis(4-(trifluoromethyl)-phenyl)pyridine **4d** (125 mg, 0.29 mmol), $Pd(dba)_2$ (4.2 mg, 2.5 mol%), *n*BuPAd$_2$ (5.2 mg, 5.0 mol%), phenylboronic acid (140 mg, 1.15 mmol), K_3PO_4 (245 mg, 1.15 mmol) and toluene (5.0 mL), **5c** was isolated as a colorless solid (112 mg, 75%); mp = 188-189 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.26-7.32 (m, 6H, CH), 7.40 (brd, $^{3}J_{H\text{-}H}$ = 8.3 Hz, 4H, CH), 7.46-7.49 (m, 4H, CH), 7.57 (brd, $^{3}J_{H\text{-}H}$ = 8.5 Hz, 4H, CH), 7.76 (s, 1H, CH). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 124.1 (q, $^{1}J_{C\text{-}F}$ = 272.1 Hz, CF_3), 125.4 (q, $^{3}J_{C\text{-}F}$ = 3.6 Hz, CH), 128.1 (CH), 128.4 (CH), 129.5 (q, $^{2}J_{C\text{-}F}$ = 32.5 Hz, C), 129.8 (CH), 130.1 (CH), 133.0 (C), 139.1 (C), 140.9 (CH), 143.2 (C), 156.1 (C). ^{19}F NMR (282.4 MHz, $CDCl_3$): δ = -62.1 (CF_3). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2963 (w), 2838 (w), 1605 (m), 1579 (m), 1501 (w), 1460 (w), 1431 (m), 1402 (w), 1319 (s), 1249 (s), 1172 (s), 1123 (s), 1108 (s), 1065 (s), 1034 (m), 1017 (m), 1002 (m), 912 (w), 881 (w), 839 (s), 789 (w), 734 (m), 698 (w), 658 (m), 595 (m), 542 (w), 483 (w), 408 (w). GC-MS (EI, 70 eV): m/z (%): 519 (M^+, 57), 518 (100), 500 (4), 450 (2), 420 (5), 371 (3), 249 (5), 190 (4), 176 (2). HRMS (EI, 70 eV): calcd. for $C_{31}H_{18}F_6N$ (M^+): 518.13380, found 518.13387.

2,6-Bis(4-methoxyphenyl)-3,5-bis(4-(trifluoromethyl)phenyl)pyridine (5d)



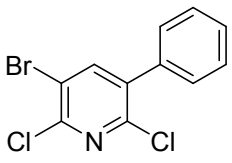
Starting with 2,6-dichloro-3,5-bis(4-(trifluoromethyl)-phenyl)pyridine **4d** (125 mg, 0.29 mmol), $Pd(dba)_2$ (4.2 mg, 2.5 mol%), *n*BuPAd$_2$ (5.2 mg, 5.0 mol%), 4-methoxyphenylboronic acid (175 mg, 1.15 mmol), K_3PO_4 (245 mg, 1.15 mmol) and toluene (5.0 mL), **5d** was isolated as a colorless solid (96 mg, 58%); mp = 259-260 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 3.79 (s, 6H, MeO), 6.78-6.80 (m, 4H, CH),

7.37-7.41 (m, 8H, CH), 7.55-7.58 (m, 4H, CH), 7.67 (s, 1H, CH). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 55.2 (MeO), 113.5 (CH), 124.1 (q, $^1J_{C-F}$ = 272.1 Hz, CF_3), 125.5 (q, $^3J_{C-F}$ = 3.7 Hz, CH), 129.4 (q, $^2J_{C-F}$ = 32.5 Hz, C), 129.8 (CH), 131.5 (CH), 132.1 (C), 141.1 (CH), 143.5 (C), 143.6 (C), 155.5 (C), 159.8 (C). ^{19}F NMR (282.4 MHz, $CDCl_3$): δ = -62.1 (CF_3). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2963 (w), 2838 (w), 1605 (m), 1579 (m), 1511 (m), 1431 (m), 1402 (m), 1385 (m), 1318 (s), 1303 (s), 1172 (s), 1108 (s), 1065 (s), 1034 (m), 1017 (m), 1002 (w), 932 (w), 912 (w), 881 (w), 839 (s), 789 (m), 734 (m), 595 (m), 542 (m), 521 (w), 483 (w), 408 (w), 396 (w). GC-MS (EI, 70 eV): m/z (%): 580 (M^+, 20), 579 (78), 578 (100), 560 (4), 535 (8), 534 (8), 520 (3), 492 (4), 491 (6), 422 (2), 290 (4), 248 (2), 233 (3), 192 (3), 177 (5). HRMS (ESI, 70 eV): calcd. for $C_{33}H_{24}F_6NO_2$ ($(M+H)^+$): 580.17028, found 580.17022. Anal. calcd. for $C_{33}H_{23}F_6NO_2$ (579.53): C, 68.39; H, 4.00; N, 2.42. Found: C, 68.15; H, 3.740; N, 2.742.

General procedure for the synthesis of 3-bromo-2,6-dichloro-5-aryl-substituted pyridines 6a-f

An oven-dried and argon-flushed pressure tube was charged with 3,5-dibromo-2,6-dichloropyridine **3** (0.33 mmol), $Pd(PPh_3)_4$ (5.0 mol%), boronic acid (0.4 mmol) and K_3PO_4 (0.98 mmol), followed by anhydrous toluene (4.0 mL). The tube was sealed with a Teflon valve and the reaction mixture was stirred at 100 °C for 20 h. The cooled reaction mixture was diluted with water and extracted with DCM. The combined organic layers were dried (Na_2SO_4), filtered and the filtrate was concentrated in vacuo. The residue was purified by column chromatography.

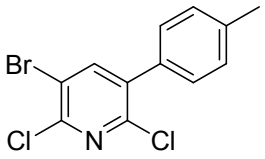
3-Bromo-2,6-dichloro-5-phenylpyridine (6a)



Starting with 3,5-dibromo-2,6-dichloropyridine **3** (100 mg, 0.327 mmol), $Pd(PPh_3)_4$ (18.9 mg, 5.0 mol%), phenylboronic acid (47.8 mg, 0.392 mmol), K_3PO_4 (208 mg, 0.981 mmol) and toluene (4.0 mL), **6a** was isolated as a colorless oil (56 mg, 57%). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.39-7.48 (m, 5H, CH), 7.90 (s, 1H, CH). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 118.6 (C-Br), 128.6 (CH), 129.0 (CH), 129.1 (CH), 135.1 (C), 137.0 (C), 144.6 (CH), 147.0 (C), 148.2 (C). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3054 (w), 2923 (w), 1809 (w), 1603 (w), 1562 (w), 1513 (m), 1446 (m), 1387 (s), 1336 (m), 1221 (m), 1171 (m), 1115 (m), 1076 (w), 1037 (w), 1013 (m), 908 (m), 859 (m), 764 (s), 734 (w), 695 (s), 578 (s), 543 (m), 459 (w), 403 (w). GC-MS (EI, 70 eV): m/z (%): 303 (M^+, 100), 301 (66), 268 (3), 266 (2), 189 (13), 188 (6), 187 (38), 186 (5), 152 (13), 151 (14), 136 (3), 126 (6), 125 (6), 112 (2), 111 (2), 100 (3), 99 (4), 77 (3), 75 (5), 74 (4), 63 (4), 62 (3), 51 (4). HRMS (EI, 70 eV): calcd. for $C_{11}H_6BrCl_2N$ (M^+): 300.90552, found 300.90537 and calcd. for $C_{11}H_6{}^{81}BrCl_2N$ (M^+): 302.90347, found 300.90302 and calcd. for $C_{11}H_6{}^{81}BrCl^{37}ClN$ (M^+): 304.90052,

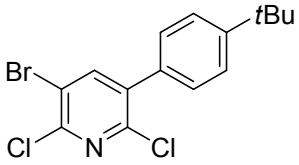
found 304.90072. Anal. calcd. for $C_{11}H_6BrCl_2N$ (302.98): C, 43.61; H, 2.00; N, 4.62. Found: C, 44.01; H, 1.715; N, 4.499.

3-Bromo-2,6-dichloro-5-*p*-tolylpyridine (6b)



Starting with 3,5-dibromo-2,6-dichloropyridine **3** (100 mg, 0.327 mmol), $Pd(PPh_3)_4$ (18.9 mg, 5.0 mol%), *p*-tolylboronic acid (53.4 mg, 0.392 mmol), K_3PO_4 (208 mg, 0.981 mmol) and toluene (4.0 mL), **6b** was isolated as a colorless solid (41 mg, 49%); mp = 124-126 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 2.34 (s, 3H, CH_3), 7.18-7.26 (m, 4H, CH), 7.82 (s, 1H, CH). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 21.3 (CH_3), 118.5 (C-Br), 128.9 (CH), 129.2 (CH), 132.1 (C), 137.0 (C), 139.1 (C), 144.6 (CH), 146.9 (C), 147.6 (C). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3050 (w), 3034 (w), 2916 (w), 2851 (w), 2729 (w), 1658 (m), 1513 (m), 1389 (m), 1380 (m), 1334 (m), 1222 (m), 1197 (w), 1028 (w), 1010 (m), 965 (w), 861 (m), 819 (s), 734 (m), 671 (m), 633 (m), 571 (s), 521 (m), 502 (m), 460 (m), 408 (w). GC-MS (EI, 70 eV): m/z (%): 317 (M^+, 100), 316 (13), 315 (59), 281 (3), 280 (3), 246 (3), 202 (18), 201 (13), 200 (53), 173 (4), 166 (13), 165 (11), 164 (23), 151 (3), 139 (11), 138 (6), 115 (5), 100 (12), 99 (4), 87 (5), 83 (5), 69 (4), 63 (5), 62 (3). HRMS (EI, 70 eV): calcd. for $C_{12}H_8BrCl_2N$ (M^+): 314.92117, found 314.92182 and calcd. for $C_{12}H_8{}^{81}BrCl_2N$ (M^+): 316.91912, found 316.91927 and calcd. for $C_{12}H_8{}^{81}BrCl^{37}ClN$ (M^+): 318.91617, found 318.91658. Anal. calcd. for $C_{12}H_8BrCl_2N$ (317.00): C, 45.47; H, 2.54; N, 4.42. Found: C, 45.55; H, 2.482; N, 4.316.

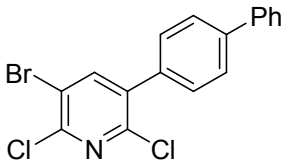
3-Bromo-2,6-dichloro-5-(4-*tert*-butylphenyl)pyridine (6c)



Starting with 3,5-dibromo-2,6-dichloropyridine **3** (100 mg, 0.327 mmol), $Pd(PPh_3)_4$ (18.9 mg, 5.0 mol%), 4-*tert*-butylphenyl-boronic acid (69.8 mg, 0.392 mmol), K_3PO_4 (208 mg, 0.981 mmol) and toluene (4.0 mL), **6c** was isolated as a colorless solid (61 mg, 52%); mp = 85-87 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 1.34 (s, 9H, $CH_{3\ tBu}$), 7.33-7.37 (m, 2H, CH), 7.45-7.48 (m, 2H, CH), 7.89 (s, 1H, CH). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 31.2 ($CH_{3\ tBu}$), 34.7 (C), 118.6 (C-Br), 125.6 (CH), 128.8 (CH), 132.1 (C), 137.0 (C), 144.7 (CH), 147.0 (C), 147.9 (C), 152.3 (C). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3044 (w), 2958 (m), 2900 (w), 2865 (w), 1610 (m), 1513 (m), 1459 (w), 1381 (s), 1363 (m), 1332 (m), 1308 (w), 1220 (m), 1166 (m), 1122 (s), 1104 (s), 1027 (s), 1009 (s), 918 (m), 862 (m), 839 (s), 828 (s), 750 (w), 737 (w), 670 (s), 650 (w), 629 (w), 611 (s), 587 (s), 536 (m), 522 (w), 460 (w), 420 (w). GC-MS (EI, 70 eV): m/z (%): 359 (M^+, 22), 357 (13), 348 (6), 347 (7), 346 (47), 345 (16), 344 (100), 343 (10), 342 (61), 318 (7), 316 (15), 314 (9), 228 (4), 227 (7), 200 (5), 191 (4), 190 (4), 187 (5), 177 (5), 176 (2), 164 (5), 159 (4), 158 (7), 157 (5), 115 (2). HRMS (EI, 70 eV): calcd. for $C_{15}H_{14}BrCl_2N$ (M^+): 356.96812, found 356.96798 and calcd. for $C_{15}H_{14}{}^{81}BrCl_2N$ (M^+): 358.96607, found 358.96581 and calcd. for $C_{15}H_{14}{}^{81}BrCl^{37}ClN$ (M^+):

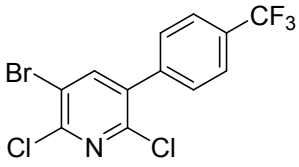
360.96312, found 360.96390. Anal. calcd. for $C_{15}H_{14}BrCl_2N$ (359.09): C, 50.17; H, 3.93; N, 3.90. Found: C, 50.14; H, 3.700; N, 3.944.

3-Bromo-2,6-dichloro-5-(biphenyl-4-yl)pyridine (6d)



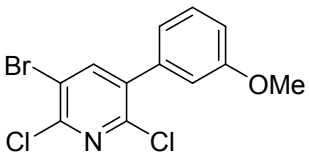
Starting with 3,5-dibromo-2,6-dichloropyridine **3** (100 mg, 0.327 mmol), $Pd(PPh_3)_4$ (18.9 mg, 5.0 mol%), biphenyl-4-ylboronic acid (77.7 mg, 0.392 mmol), K_3PO_4 (208 mg, 0.981 mmol) and toluene (4.0 mL), **6d** was isolated as a colorless solid (79 mg, 64%); mp = 93-95 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.35.7.52 (m, 5H, CH), 7.60-7.70 (m, 4H, CH), 7.94 (s, 1H, CH). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 118.7 (C-Br), 127.1 (C), 127.3 (CH), 127.9 (CH), 128.9 (CH), 129.6 (CH), 133.8 (C), 136.7 (C), 140.0 (C), 142.0 (C), 144.6 (CH), 147.0 (C), 148.2 (C). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3077 (w), 3051 (w), 2920 (w), 2733 (w), 1597 (w), 1578 (w), 1486 (w), 1389 (s), 1334 (m), 1226 (m), 1172 (m), 1111 (s), 1072 (w), 1029 (m), 1007 (s),908 (m), 838 (s), 765 (s), 736 (m), 698 (s), 652 (s), 642 (m), 584 (s), 512 (m), 391 (w). GC-MS (EI, 70 eV): m/z (%): 379 (M^+, 100), 378 (12), 377 (63), 265 (3), 264 (2), 263 (10), 262 (2), 261 (3), 228 (8), 227 (21), 226 (5), 225 (4), 200 (6), 176 (3), 151 (3), 132 (3), 114 (4), 100 (5), 99 (3), 88 (3), 75 (3), 51 (2). HRMS (EI, 70 eV): calcd. for $C_{17}H_{10}BrCl_2N$ (M^+): 376.93682, found 376.93644 and calcd. for $C_{17}H_{10}BrCl^{37}ClN$ (M^+): 378.93387, found 378.93428 and calcd. for $C_{17}H_{10}{}^{81}Br^{37}Cl_2N$ (M^+): 382.92887, found 382.92995. Anal. calcd. for $C_{17}H_{10}BrCl_2N$ (379.08): C, 53.86; H, 2.660; N, 3.69. Found: C, 54.05; H, 2.357; N, 3.507.

3-Bromo-2,6-dichloro-5-(4-(trifluoromethyl)phenyl)pyridine (6e)



Starting with 3,5-dibromo-2,6-dichloropyridine **3** (100 mg, 0.327 mmol), $Pd(PPh_3)_4$ (18.9 mg, 5.0 mol%), 4-(trifluoromethyl)-boronic acid (74.5 mg, 0.392 mmol), K_3PO_4 (208 mg, 0.981 mmol) and toluene (4.0 mL), **6e** was isolated as a colorless oil (69 mg, 57%). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.53-7.56 (m, 2H, CH), 7.71-7.75 (m, 2H, CH), 7.90 (s, 1H, CH). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 118.9 (C-Br), 123.8 (q, $^1J_{C\text{-}F}$ = 272.4 Hz, CF_3), 125.6 (q, $^3J_{C\text{-}F}$ = 3.7 Hz, CH), 129.6 (CH), 131.2 (q, $^2J_{C\text{-}F}$ = 32.8 Hz, C), 135.6 (C), 138.6 (C), 144.5 (CH), 146.8 (C), 149.2 (C). ^{19}F NMR (282.4 MHz, $CDCl_3$) δ = -62.4 (CF_3). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3053 (w), 1619 (w), 1573 (w), 1514 (w), 1390 (m), 1319 (s), 1252 (m), 1221 (m), 1165 (m), 1108 (s), 1024 (s), 1012 (s), 915 (m), 841 (m), 700 (m), 666 (m), 610 (m), 579 (m), 541 (m), 503 (w), 469 (w), 420 (w), 382 (m). GC-MS (EI, 70 eV): m/z (%): 371 (M^+, 100), 370 (9), 369 (61), 352 (5), 300 (2), 257 (11), 256 (6), 255 (35), 254 (6), 236 (4), 221 (5), 220 (7), 205 (4), 200 (7), 193 (3), 169 (3), 151 (5), 124 (2), 99 (3), 75 (4), 74 (3), 69 (4), 62 (2). HRMS (EI, 70 eV): calcd. for $C_{12}H_5BrCl_2F_3N$ (M^+): 368.89290, found 368.89284 and calcd. for $C_{12}H_5{}^{81}BrCl_2F_3N$ (M^+): 370.89086, found 370.89053 and calcd. for $C_{12}H_5{}^{81}BrCl^{37}ClF_3N$ (M^+): 372.88791, found 372.88781.

3-Bromo-2,6-dichloro-5-(3-methoxyphenyl)pyridine (6f)

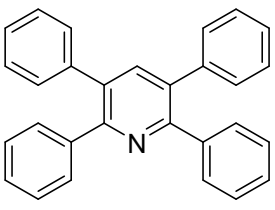


Starting with 3,5-dibromo-2,6-dichloropyridine **3** (100 mg, 0.327 mmol), $Pd(PPh_3)_4$ (18.9 mg, 5.0 mol%), 3-methoxyphenyl-boronic acid (59.6 mg, 0.392 mmol), K_3PO_4 (208 mg, 0.981 mmol) and toluene (4.0 mL), **6f** was isolated as a colorless solid (61 mg, 56%); mp = 81-82 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 3.83 (s, 3H, MeO), 6.92-6.98 (m, 3H, CH), 7.36 (dd, $^3J_{H-H}$ = 8.1 Hz, $^3J_{H-H}$ = 8.0 Hz, 1H, CH), 7.89 (s, 1H, CH). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 55.4 (MeO), 114.5 (CH), 115.9 (CH), 118.6 (C-Br), 121.4 (CH), 129.7 (CH), 136.3 (C), 136.9 (C), 144.6 (CH), 146.9 (C), 148.3 (C), 159.5 (C). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3043 (w), 2917 (w), 2834 (w), 1944 (w), 1588 (m), 1514 (w), 1461 (m), 1425 (m), 1379 (m), 1265 (m), 1226 (m), 1214 (m), 1165 (s), 1124 (m), 1022 (s), 902 (s), 792 (s), 698 (m), 657 (m), 626 (w), 553 (w), 458 (w). GC-MS (EI, 70 eV): m/z (%): 333 (M^+, 100), 332 (8), 331 (61), 305 (4), 303 (10), 301 (6), 292 (6), 290 (12), 288 (7), 283 (2), 268 (4), 255 (4), 253 (4), 217 (4), 175 (3), 174 (16), 173 (3), 151 (5), 148 (2), 147 (2), 139 (6), 138 (6), 87 (3), 75 (3), 63 (4). HRMS (EI, 70 eV): calcd. for $C_{12}H_8BrCl_2NO$ (M^+): 330.91608, found 330.91615 and calcd. for $C_{12}H_8{}^{81}BrCl_2NO$ (M^+): 332.91404, found 332.91380 and calcd. for $C_{12}H_8{}^{81}BrCl^{37}ClNO$ (M^+): 334.91109, found 334.91121 and calcd. for $C_{12}H_8{}^{81}Br^{37}Cl_2N\,O$ (M^+): 336.90814, found 336.90877.

General procedure for the synthesis of 2,3,5,6-tetraaryl-substituted pyridines 7a-f

An oven-dried and argon-flushed pressure tube was charged with 3,5-dibromo-2,6-dichloropyridine **3** (0.25 mmol), $PdCl_2(MeCN)_2$, SPhos, boronic acid (1.75 mmol) and K_3PO_4 (1.88 mmol), followed by anhydrous toluene (4.0 mL). The tube was sealed with a Teflon valve and the reaction mixture was stirred at 100 °C for 20 h. The cooled reaction mixture was diluted with water and extracted with DCM. The combined organic layers were dried (Na_2SO_4), filtered and the filtrate was concentrated in vacuo. The residue was purified by column chromatography.

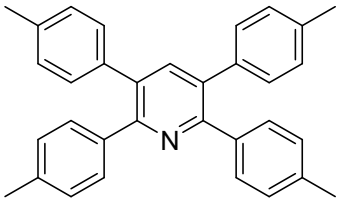
2,3,5,6-Tetraphenylpyridine (7a)



Starting with 3,5-dibromo-2,6-dichloropyridine **3** (75.7 mg, 0.25 mmol), $PdCl_2(MeCN)_2$ (0.8 mg, 1.25 mol%), SPhos (5.1 mg, 5.0 mol%), phenylboronic acid (213 mg, 1.75 mmol), K_3PO_4 (398 mg, 1.88 mmol) and toluene (4.0 mL), **7a** was isolated as a colorless solid (92 mg, 96%); mp = 244-246 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.22-7.30 (m, 16H, CH), 7.47-7.51 (m, 4H, CH), 7.77 (s, 1H, CH). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 127.5 (CH), 128.0 (CH), 128.1 (CH), 128.6 (CH), 129.8 (CH), 130.4 (CH), 134.6 (C), 139.8 (C), 139.9 (C), 141.5 (CH), 155.5 (C). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3080 (w), 3054

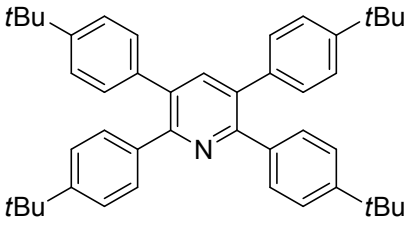
(w), 3023 (w), 2927 (w), 2857 (w), 1444 (m), 1416 (s), 1386 (m), 1179 (w), 1072 (w), 1017 (w), 908 (m), 854 (w), 779 (m), 757 (s), 732 (m), 690 (s), 537 (m), 528 (m), 499 (m), 409 (w), 390 (w). GC-MS (EI, 70 eV): m/z (%): 384 (M^+, 16), 383 (66), 382 (100), 306 (3), 305 (3), 304 (10), 303 (7), 302 (6), 276 (8), 190 (7), 189 (5), 188 (3), 183 (13), 77 (4). HRMS (ESI, 70 eV): calcd. for $C_{29}H_{22}N$ ($[M+H]^+$): 384.17468, found 384.17447. Anal. calcd. for $C_{29}H_{21}N$ (383.48): C, 90.83; H, 5.52; N, 3.65. Found: C, 90.50; H, 5.329; N, 3.431.

2,3,5,6-Tetra-*p*-tolylpyridine (7b)



Starting with 3,5-dibromo-2,6-dichloropyridine **3** (75.7 mg, 0.25 mmol), $PdCl_2(MeCN)_2$ (0.8 mg, 1.25 mol%), SPhos (5.1 mg, 5.0 mol%), *p*-tolylboronic acid (238 mg, 1.75 mmol), K_3PO_4 (398 mg, 1.88 mmol) and toluene (4.0 mL), **7b** was isolated as a colorless solid (99 mg, 91%); mp = 284-286 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 2.33 (s, 6H, CH_3), 2.34 (s, 6H, CH_3), 7.03-7.17 (m, 12H, CH), 7.38-7.41 (m, 4H, CH), 7.70 (s, 1H, CH). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 21.4 (CH_3), 21.5 (CH_3), 128.7 (CH), 129.3 (CH), 129.3 (CH), 130.3 (CH), 134.1 (C), 137.0 (C), 137.2 (C), 137.2 (C), 137.7 (C), 141.2 (CH), 155.0 (C). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3119 (w), 3021 (w), 2859 (w), 1607 (w), 1568 (w), 1496 (m), 1426 (s), 1380 (w), 1308 (w), 1181 (m), 1112 (m), 1089 (w), 1014 (w), 1004 (m), 926 (w), 880 (w), 818 (s), 781 (m), 728 (m), 718 (w), 681 (w), 645 (w), 621 (m), 556 (m), 530 (m), 516 (m), 462 (m), 433 (w), 408 (m), 382 (w). GC-MS (EI, 70 eV): m/z (%): 440 (M^+, 18), 439 (72), 438 (100), 331 (4), 315 (2), 220 (3), 211 (2), 207 (3), 204 (8), 197 (7), 196 (6), 182 (4). HRMS (ESI, 70 eV): calcd. for $C_{33}H_{30}N$ ($[M+H]^+$): 440.23728, found 440.23695. Anal. calcd. for $C_{33}H_{29}N$ (439.59): C, 90.83; H, 5.52. Found: C, 90.61; H, 5.950.

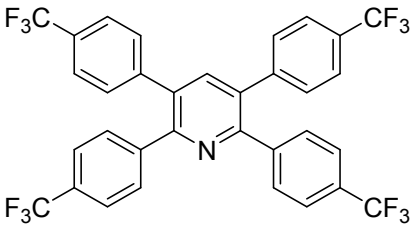
2,3,5,6-Tetrakis(4-*tert*butylphenyl)pyridine (7c)



Starting with 3,5-dibromo-2,6-dichloropyridine **3** (75.7 mg, 0.25 mmol), $PdCl_2(MeCN)_2$ (0.8 mg, 1.25 mol%), SPhos (5.1 mg, 5.0 mol%), 4-*tert*butylphenylboronic acid (312 mg, 1.75 mmol), K_3PO_4 (398 mg, 1.88 mmol) and toluene (4.0 mL), **7c** was isolated as a colorless solid (147 mg, 97%); mp = 314-316 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 1.30 (s, 18H, $CH_{3\ tBu}$), 1.33 (s, 18H, $CH_{3\ tBu}$), 7.18-7.33 (m, 12H, CH), 7.43-7.47 (m, 12H, CH), 7.75 (s, 1H, CH). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 31.5 ($CH_{3\ tBu}$), 31.6 ($CH_{3\ tBu}$), 34.8 (C_{tBu}), 34.8 (C_{tBu}), 124.9 (CH), 125.4 (CH), 129.4 (CH), 130.0 (CH), 134.0 (C), 137.0 (C), 137.1 (C), 141.7 (CH), 150.3 (C), 150.8 (C), 154.9 (C). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3030 (w), 2962 (s), 2902 (m), 2865 (m), 1609 (w), 1584 (w), 1512 (m), 1474 (m), 1460 (m), 1430 (m), 1391 (m), 1361 (m), 1268 (m), 1204 (m), 1203 (m), 1118 (s), 1015 (m), 1003 (m), 927 (w), 835 (s), 794 (m), 756 (w), 667 (w), 629 (m), 580 (m),

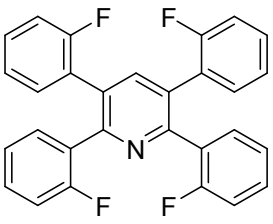
563 (m), 508 (w), 411 (w). GC-MS (EI, 70 eV): m/z (%): 608 (M^+, 38), 607 (100), 606 (88), 592 (9), 591 (6), 590 (9), 576 (5), 495 (11), 494 (17), 464 (2), 289 (7), 169 (2), 165 (2), 151 (3), 145 (3), 139 (3), 125 (6), 123 (5), 111 (9), 109 (7), 105 (3), 97 (13), 95 (10), 83 (12), 81 (9), 71 (14), 69 (13), 57 (25), 55 (14), 44 (12), 43 (12), 41 (19). HRMS (ESI, 70 eV): calcd. for $C_{45}H_{54}N$ ($[M+H]^+$): 608.42508, found 608.42535.

2,3,5,6-Tetrakis(4-(trifluoromethyl)phenyl)pyridine (7d)



Starting with 3,5-dibromo-2,6-dichloropyridine **3** (75.7 mg, 0.25 mmol), $PdCl_2(MeCN)_2$ (0.8 mg, 1.25 mol%), SPhos (5.1 mg, 5.0 mol%), 4-(trifluoromethyl)phenylboronic acid (332 mg, 1.75 mmol), K_3PO_4 (398 mg, 1.88 mmol) and toluene (4.0 mL), **7d** was isolated as a colorless solid (158 mg, 97%); mp = 253-254 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.39-7.42 (m, 4H, CH), 7.54-7.64 (m, 12H, CH), 7.83 (s, 1H, CH). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 124.2 (q, $^1J_{C\text{-}F}$ = 271.8 Hz, CF_3), 124.3 (q, $^1J_{C\text{-}F}$ = 271.7 Hz, CF_3), 125.4 (q, $^3J_{C\text{-}F}$ = 3.6 Hz, CH), 126.0 (q, $^3J_{C\text{-}F}$ = 3.8 Hz, CH), 130.0 (CH), 130.6 (CH), 130.6 (q, $^2J_{C\text{-}F}$ = 32.0 Hz, C), 130.6 (q, $^2J_{C\text{-}F}$ = 32.2 Hz, C), 134.2 (C), 141.6 (C), 142.4 (C), 142.6 (CH), 155.0 (C). ^{19}F NMR (282.4 MHz, $CDCl_3$): δ = -62.2 (CF_3), -62.2 (CF_3). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2937 (w), 1617 (m), 1572 (w), 1439 (m), 1406 (m), 1322 (s), 1164 (s), 1104 (s), 1061 (s), 1014 (s), 934 (w), 843 (s), 795 (m), 714 (m), 697 (w), 630 (m), 500 (w), 470 (m), 413 (m), 402 (w). GC-MS (EI, 70 eV): m/z (%): 655 (M^+, 51), 654 (100), 652 (6), 636 (7), 468 (5), 281 (2), 248 (3), 224 (3), 181 (3), 169 (3), 119 (4), 69 (13), 44 (12), 43 (10). HRMS (ESI, 70 eV): calcd. for $C_{33}H_{18}F_{12}N$ ($[M+H]^+$): 656.12421, found 656.12529. Anal. calcd. for $C_{33}H_{17}F_{12}N$ (655.48): C, 60.47; H, 2.61. Found: C, 60.24 H, 2.555.

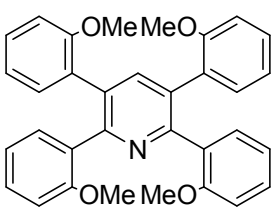
2,3,5,6-Tetra(2-fluorophenyl)pyridine (7e)



Starting with 3,5-dibromo-2,6-dichloropyridine **3** (75.7 mg, 0.25 mmol), $PdCl_2(MeCN)_2$ (0.8 mg, 1.25 mol%), SPhos (5.1 mg, 5.0 mol%), 2-fluorophenylboronic acid (244.9 mg, 1.75 mmol), K_3PO_4 (398 mg, 1.88 mmol) and toluene (4.0 mL), **7e** was isolated as a colorless solid (113 mg, 99%); mp = 223-224 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 6.76-6.85 (m, 2H, CH), 6.90-7.03 (m, 4H, CH), 7.02-7.22 (m, 8H, CH), 7.45-7.51 (m, 2H, CH), 7.78 (t, $^5J_{C\text{-}F}$ = 1.0 Hz, 1H, CH). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 115.6 (d, $^2J_{C\text{-}F}$ = 15.0 Hz, CH), 115.9 (d, $^2J_{C\text{-}F}$ = 15.0 Hz, CH), 124.2 (d, $^4J_{C\text{-}F}$ = 3.6 Hz, CH), 124.3 (d, $^4J_{C\text{-}F}$ = 3.6 Hz, CH), 126.5 (d, $^2J_{C\text{-}F}$ = 15.0 Hz, C) 128.1 (d, $^2J_{C\text{-}F}$ = 15.0 Hz, C), 130.0 (d, $^3J_{C\text{-}F}$ = 8.0 Hz, CH), 130.4 (d, $^3J_{C\text{-}F}$ = 8.0 Hz, CH), 131.0 (C), 131.7 (d, $^3J_{C\text{-}F}$ = 3.0 Hz, CH), 132.2 (d, $^3J_{C\text{-}F}$ = 3.0 Hz, CH), 141.2 (CH), 153.1 (C), 159.8 (d, $^1J_{C\text{-}F}$ = 247.6 Hz, CF), 159.8 (d, $^1J_{C\text{-}F}$ = 249.0 Hz, CF). ^{19}F NMR (282.4 MHz, $CDCl_3$): δ = -115.0 (d, $J_{F\text{-}F}$ = 2.0 Hz, F), -115.3 (d, $J_{F\text{-}F}$ = 2.0 Hz,

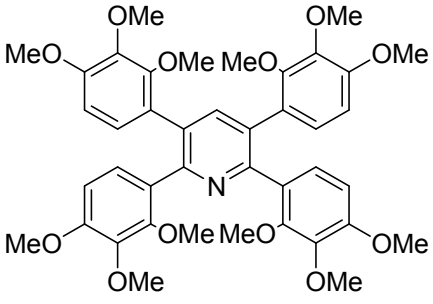
F). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3059 (w), 1494 (w), 1489 (w), 1449 (m), 1422 (m), 1230 (m), 1103 (w), 817 (m), 749 (s), 710 (w), 664 (m), 570 (w). GC-MS (EI, 70 eV): m/z (%): 455 (M^+, 77), 454 (100), 437 (10), 436 (29), 414 (3), 394 (3), 358 (2), 337 (5), 312 (5), 292 (2), 238 (2), 214 (5), 197 (4), 121 (4). HRMS (EI, 70 eV): calcd. for $C_{29}H_{16}NF_4$ ($[M\text{-}H^+]^-$): 454.12071, found 454.12134, calcd. for $C_{29}H_{17}NF_4$ (M^-) 455.12804, found 455.12916. Anal. calcd. for $C_{29}H_{17}NF_4$ (455.45): C, 76.48; H, 3.76; N, 3.08. Found: C, 75.83; H, 3.64; N, 2.82.

2,3,5,6-Tetrakis(2-methoxyphenyl)pyridine (7f)



Starting with 3,5-dibromo-2,6-dichloropyridine **3** (75.7 mg, 0.25 mmol), $PdCl_2(MeCN)_2$ (2.6 mg, 4.0 mol%), SPhos (8.2 mg, 8.0 mol%), 2-methoxyphenylboronic acid (266 mg, 1.75 mmol), K_3PO_4 (398 mg, 1.88 mmol) and toluene (4.0 mL), **7f** was isolated as a colorless solid (108 mg, 86%); mp = 228-230 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 3.36 (s, 6H, MeO), 3.58 (s, 6H, MeO), 6.65 (d, $^3J_{H\text{-}H}$ = 8.3 Hz, 2H, CH), 6.68-7.23 (m, 12H, CH), 7.51 (dd, $^3J_{H\text{-}H}$ = 7.7 Hz, $^4J_{H\text{-}H}$ = 1.8 Hz, 2H, CH), 7.80 (s, 1H, CH). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 54.9 (MeO), 55.2 (MeO), 110.6 (CH), 110.6 (CH), 120.1 (CH), 120.5 (CH), 128.5 (CH), 129.1 (CH), 129.5 (C), 130.4 (C), 131.4 (CH), 132.3 (CH), 141.3 (CH), 154.3 (C), 156.5 (C), 156.6 (C). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2997 (w), 2956 (w), 2832 (m), 1599 (m), 1580 (m), 1494 (m), 1459 (m), 1434 (m), 1416 (m), 1386 (w), 1253 (m), 1180 (m), 1161 (w), 1118 (w), 1079 (m), 1023 (s), 919 (m), 805 (m), 795 (w), 754 (s), 670 (m), 643 (w), 585 (w), 500 (m), 432 (w), 385 (w). GC-MS (EI, 70 eV): m/z (%): 504 (M^+, 16), 503 (48), 502 (35), 488 (7), 474 (15), 473 (34), 472 (100), 458 (7), 442 (9), 398 (29), 397 (12), 396 (40), 350 (4), 252 (7), 244 (5), 199 (7), 191 (6), 183 (10), 176 (6). HRMS (EI, 70 eV): calcd. for $C_{33}H_{29}NO_4$ (M^+): 503.20911, found 503.20812. Anal. calcd. for $C_{33}H_{29}NO_4$ (503.59): C, 78.71; H, 5.80; N, 2.78. Found: C, 78.55; H, 5.560; N, 2.734.

2,3,5,6-Tetrakis(2,3,4-trimethoxyphenyl)pyridine (7g)



Starting with 3,5-dibromo-2,6-dichloropyridine **3** (75.7 mg, 0.25 mmol), $PdCl_2(MeCN)_2$ (2.6 mg, 4.0 mol%), SPhos (8.2 mg, 8.0 mol%), 2,3,4-trimethoxyphenylboronic acid (371 mg, 1.75 mmol), K_3PO_4 (398 mg, 1.88 mmol) and toluene (4.0 mL), **7g** was isolated as a colorless solid (89 mg, 48%); mp = 190-192 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 3.62 (brs, 6H, MeO), 3.68 (brs, 6H, MeO), 3.76 (s, 6H, MeO), 3.80 (s, 6H, MeO), 3.80 (s, 6H, MeO), 3.83 (s, 6H, MeO), 6.46 (d, $^3J_{H\text{-}H}$ = 8.7 Hz, 2H, CH), 6.60 (d, $^3J_{H\text{-}H}$ = 8.7 Hz, 2H, CH), 6.72 (d, $^3J_{H\text{-}H}$ = 8.7 Hz, 2H, CH), 7.06 (d, $^3J_{H\text{-}H}$ = 8.4 Hz, 2H, CH), 7.81 (brs, 1H, CH). ^{13}C NMR (75 MHz, $CDCl_3$): δ =

56.1 (MeO), 56.2 (MeO), 60.8 (MeO), 60.9 (MeO), 70.0 (MeO), 61.1 (MeO), 106.6 (CH), 107.1 (CH), 125.8 (CH), 126.0 (CH), 126.3 (C), 128.6 (C), 131.7 (C), 141.4 (CH), 142.0 (C), 142.2 (C), 151.7 (C), 151.7 (C), 153.1 (C), 153.6 (C), 153.8 (C). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2932 (w), 2837 (w), 1598 (m), 1498 (m), 1459 (s), 1407 (s), 1374 (m), 1289 (s), 1232 (m), 1201 (m), 1170 (m), 1084 (s), 1006 (s), 920 (w), 800 (s), 699 (m), 609 (m), 436 (m). GC-MS (EI, 70 eV): m/z (%): 744 (M^+, 19), 743 (46), 742 (11), 730 (8), 729 (32), 728 (78), 714 (13), 713 (40), 712 (100), 696 (10), 682 (14), 666 (7), 576 (21), 356 (13), 325 (3), 281 (6), 267 (4), 207 (13), 105 (11), 84 (7), 77 (6), 69 (9), 57 (8), 44 (41), 43 (14), 41 (6). HRMS (ESI, 70 eV): calcd. for $C_{41}H_{46}NO_{12}$ ($[M+H]^+$): 744.30145, found 744.30009. Anal. calcd. for $C_{41}H_{45}NO_{12}$ (743.80): C, 66.21; H, 6.10; N, 1.88. Found: C, 66.27; H, 6.329; N, 1.708.

NMR – Spectra

Reimann/ SRE 595
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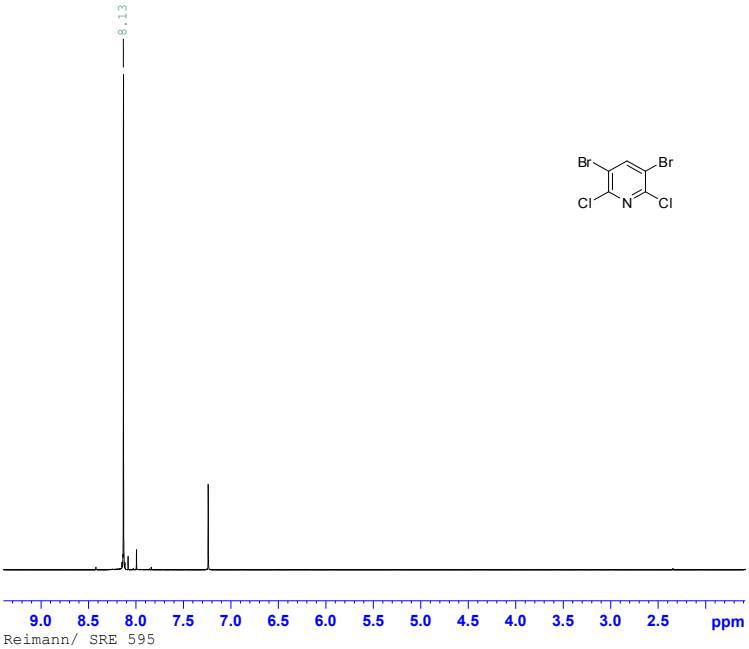


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Reimann/ SRE 595
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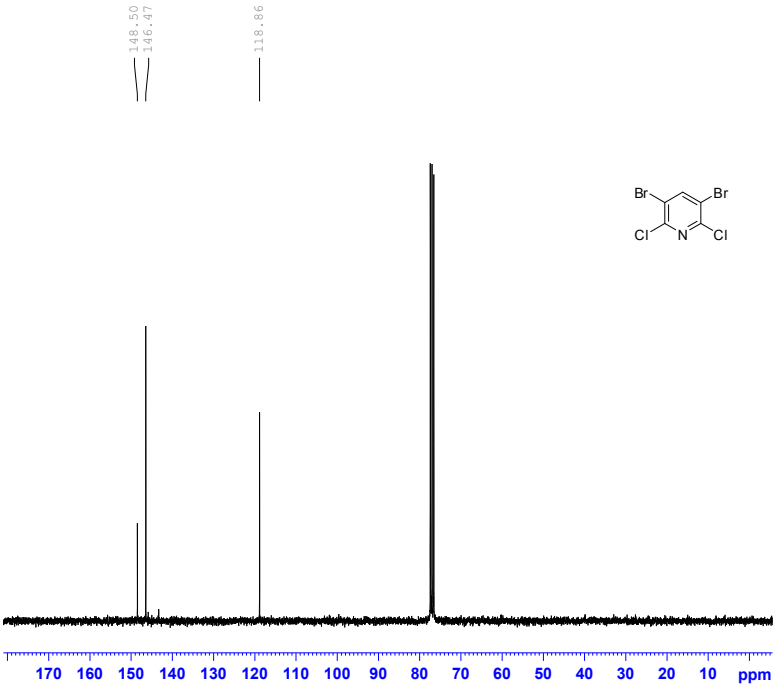


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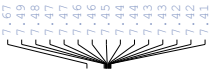
RG                32768
DW               23.700 usec
DE                6.00 usec
TE               296.6 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1

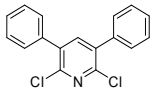
======== CHANNEL f1 ========
NUC1                13C
P1                9.60 usec
PL1               -1.10 dB
SFO1         75.4771825 MHz

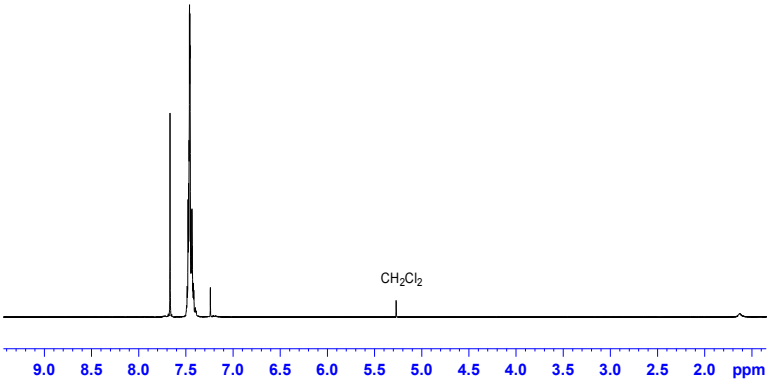
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2            100.00 usec
PL2                0.00 dB
PL12              19.00 dB
PL13              21.00 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                32768
SF          75.4677535 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

S.Reimann, SRE-814
Au1H CDCl3 /opt/topspin 1206 29







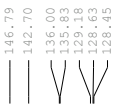

```
Current Data Parameters
NAME          SRE 814 1H
EXPNO                 10
PROCNO                 1

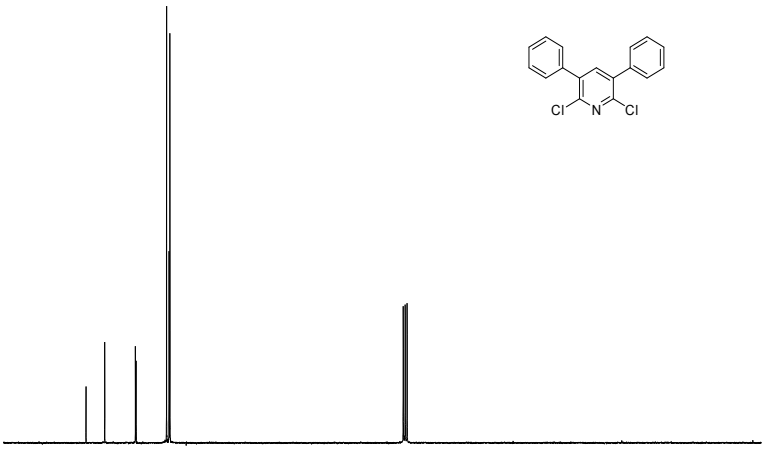
F2 - Acquisition Parameters
Date_           20120617
Time               0.23
INSTRUM           AV300
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   32
DS                    4
SWH            6172.839 Hz
FIDRES         0.188380 Hz
AQ             2.6542580 sec
RG                161.3
DW               81.000 usec
DE                6.00 usec
TE               295.6 K
D1            1.00000000 sec
TD0                    1

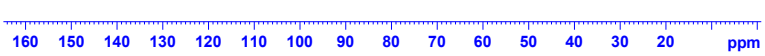
======== CHANNEL f1 ========
NUC1                  1H
P1                11.00 usec
PL1                0.00 dB
SFO1         300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF           300.1300218 MHz
WDW                   EM
SSB                    0
LB                 0.10 Hz
GB                     0
PC                  1.00
```

S.Reimann, SRE-814
Au13C CDCl3 /opt/topspin 1206 29








```
Current Data Parameters
NAME          SRE 814 13C
EXPNO                  11
PROCNO                  1

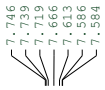
F2 - Acquisition Parameters
Date_           20120617
Time               2.00
INSTRUM           AV300
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                32768
SOLVENT           CDCl3
NS                 2048
DS                    4
SWH           21097.047 Hz
FIDRES         0.643831 Hz
AQ             0.7766516 sec
RG                32768
DW              23.700 usec
DE                6.00 usec
TE               296.0 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                    1

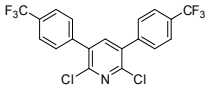
======== CHANNEL f1 ========
NUC1                 13C
P1                9.60 usec
PL1               -1.10 dB
SFO1         75.4771825 MHz

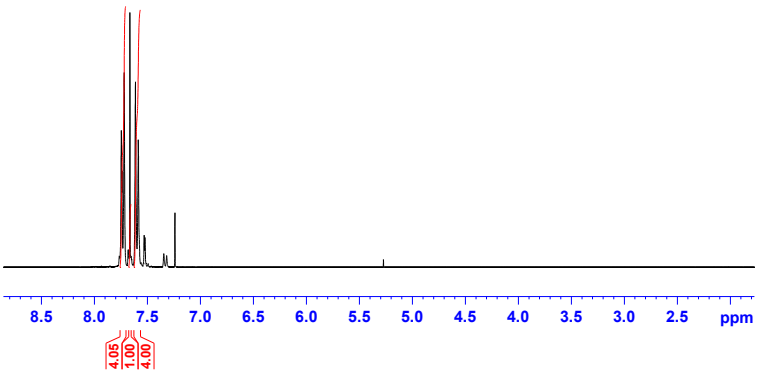
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2           100.00 usec
PL2                0.00 dB
PL12              19.00 dB
PL13              21.00 dB
SFO2         300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF           75.4677573 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                  1.40
```

Reimann/ SRE- SP- 43
Au1H CDCl3 /opt/topspin 1206 44







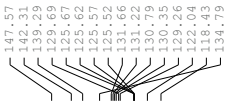

```
Current Data Parameters
NAME                  SP43-1H
EXPNO                      10
PROCNO                      1

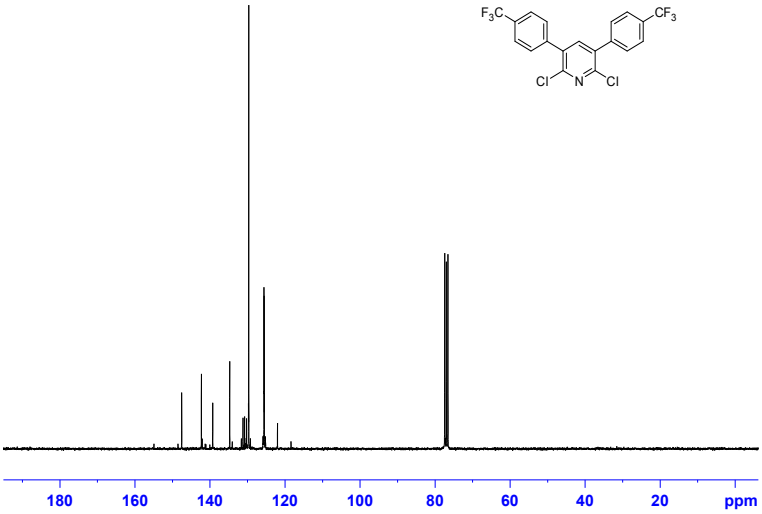
F2 - Acquisition Parameters
Date_               20120623
Time                   13.32
INSTRUM                AV300
PROBHD   5 mm PABBO BB-
PULPROG                zg30
TD                     32768
SOLVENT                CDCl3
NS                        32
DS                         4
SWH                6172.839 Hz
FIDRES                0.188380 Hz
AQ                 2.6542580 sec
RG                     322.5
DW                    81.000 usec
DE                     6.00 usec
TE                    295.9 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                       1H
P1                     11.00 usec
PL1                     0.00 dB
SFO1             300.1318534 MHz

F2 - Processing parameters
SI                     32768
SF               300.1300214 MHz
WDW                       EM
SSB                        0
LB                      0.10 Hz
GB                         0
PC                      1.00
```

Reimann/ SRE- SP- 43
Au13C CDCl3 /opt/topspin 1206 44






```
Current Data Parameters
NAME                 SP43-13C
EXPNO                      11
PROCNO                      1

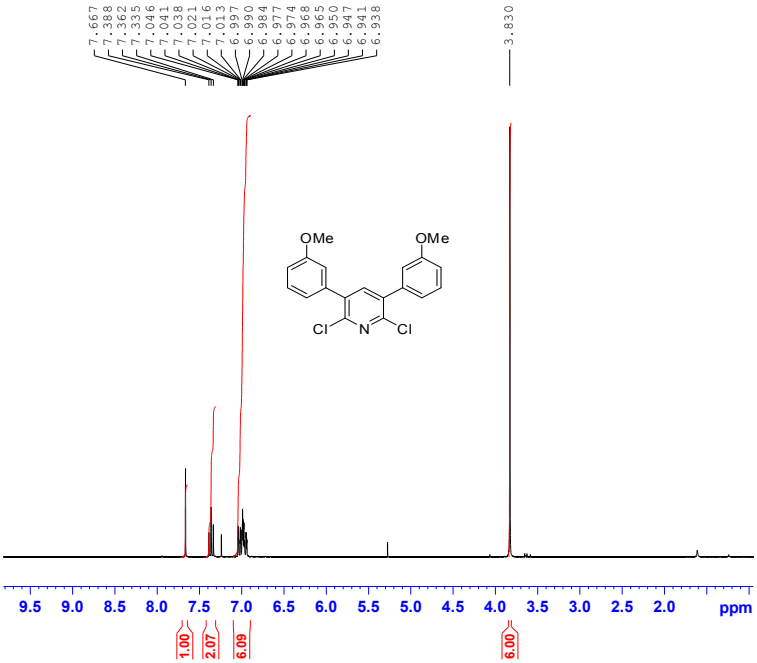
F2 - Acquisition Parameters
Date_               20120623
Time                   15.08
INSTRUM                AV300
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                     32768
SOLVENT                CDCl3
NS                      2000
DS                         4
SWH               21097.047 Hz
FIDRES                0.643831 Hz
AQ                 0.7766516 sec
RG                     32768
DW                    23.700 usec
DE                     6.00 usec
TE                    296.5 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      13C
P1                      9.60 usec
PL1                    -1.10 dB
SFO1             75.4771825 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                 100.00 usec
PL2                     0.00 dB
PL12                   19.00 dB
PL13                   21.00 dB
SFO2             300.1312005 MHz

F2 - Processing parameters
SI                     32768
SF               75.4677530 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```

S.Reimann, SRE-SP-31
Au1H CDCl3 /opt/topspin 1206 26



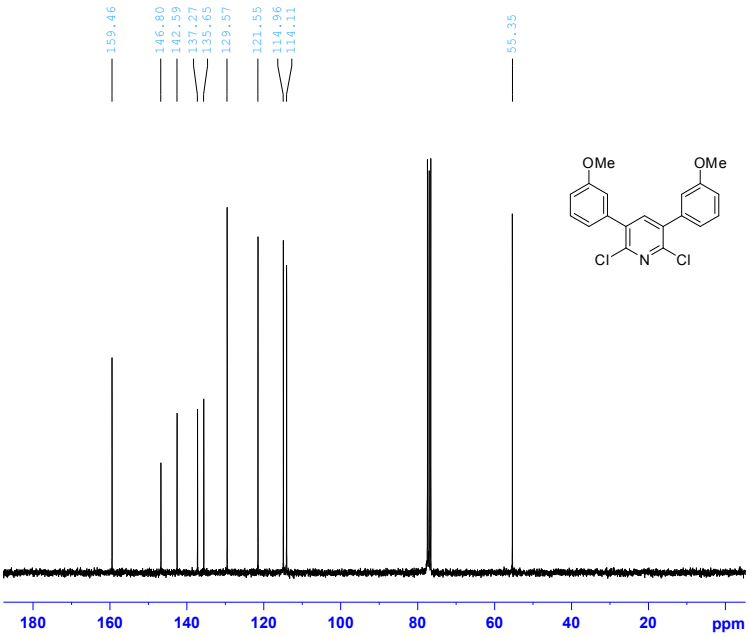

```
Current Data Parameters
NAME                  SP31-1H
EXPNO                      11
PROCNO                      1

F2 - Acquisition Parameters
Date_              20120616
Time                  20.15
INSTRUM                AV300
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                       32
DS                        4
SWH                6172.839 Hz
FIDRES            0.188380 Hz
AQ                2.6542580 sec
RG                    322.5
DW                   81.000 usec
DE                    6.00 usec
TE                   296.0 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                    11.00 usec
PL1                    0.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                    32768
SF              300.1300215 MHz
WDW                      EM
SSB                       0
LB                     0.10 Hz
GB                        0
PC                     1.00
```

S.Reimann, SRE-SP-31
Au13C CDCl3 /opt/topspin 1206 26




```
Current Data Parameters
NAME                SP31-13C
EXPNO                     10
PROCNO                     1

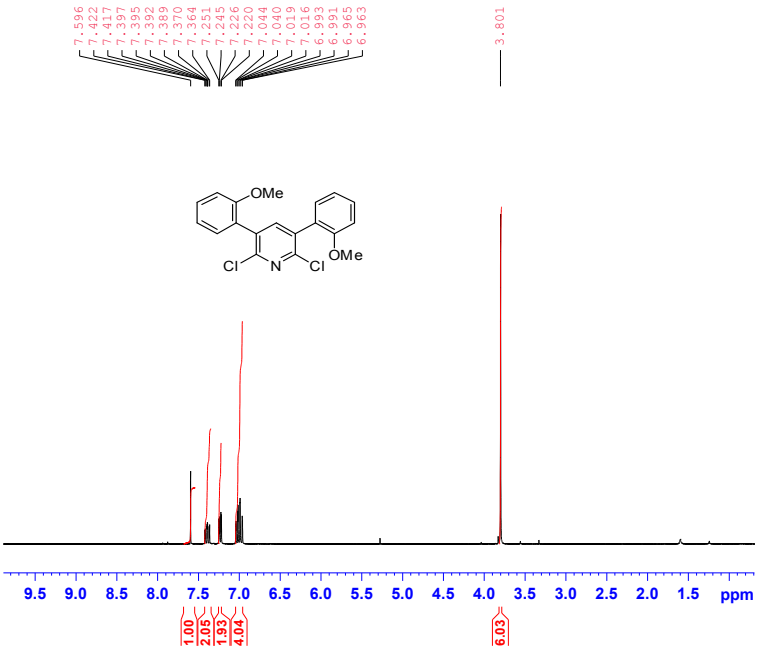
F2 - Acquisition Parameters
Date_              20120616
Time                  20.13
INSTRUM                AV300
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                    32768
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               21097.047 Hz
FIDRES            0.643831 Hz
AQ                0.7766516 sec
RG                    32768
DW                   23.700 usec
DE                    6.00 usec
TE                   296.4 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     13C
P1                    9.60 usec
PL1                  -1.10 dB
SFO1          75.4771825 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                      1H
PCPD2                100.00 usec
PL2                    0.00 dB
PL12                  19.00 dB
PL13                  21.00 dB
SFO2          300.1312005 MHz

F2 - Processing parameters
SI                    32768
SF              75.4677552 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

S.Reimann, SRE-820
Au1H CDCl3 /opt/topspin 1206 28



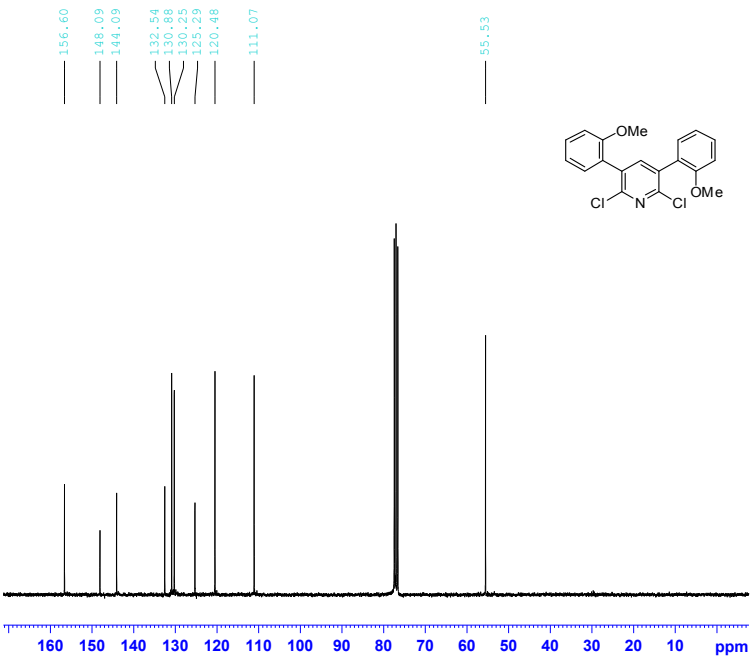
Current Data Parameters
NAME SRE 820 1H
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120616
Time_ 21.39
INSTRUM AV300
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 4
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 322.5
DW 81.000 usec
DE 6.00 usec
TE 295.8 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300213 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

S.Reimann, SRE-820
Au13C CDCl3 /opt/topspin 1206 28



Current Data Parameters
NAME SRE 82013C
EXPNO 11
PROCNO 1

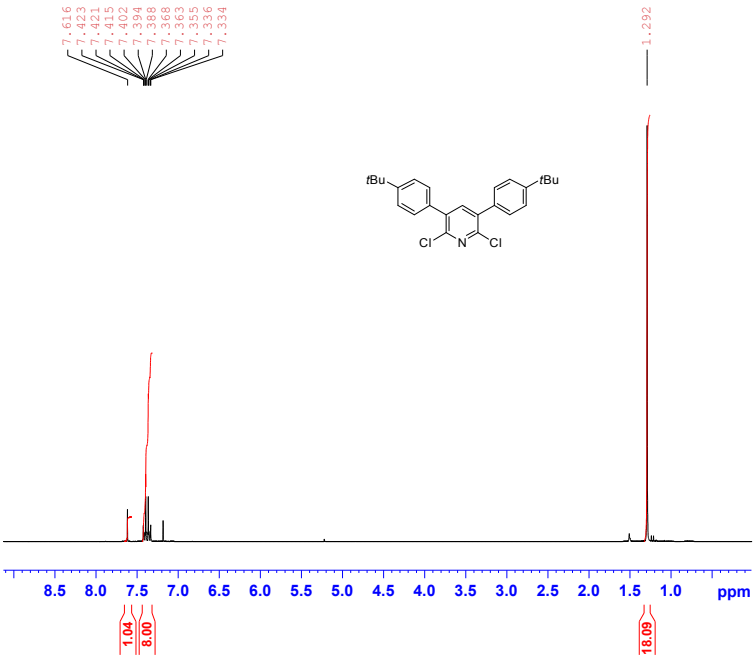
F2 - Acquisition Parameters
Date_ 20120617
Time_ 0.05
INSTRUM AV300
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 3072
DS 4
SWH 21097.047 Hz
FIDRES 0.643831 Hz
AQ 0.7766516 sec
RG 32768
DW 23.700 usec
DE 6.00 usec
TE 296.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -1.10 dB
SFO1 75.4771825 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 19.00 dB
PL13 21.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677544 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Reimann/ SRE 831
Au1H CDCl3 /opt/topspin 1206 45



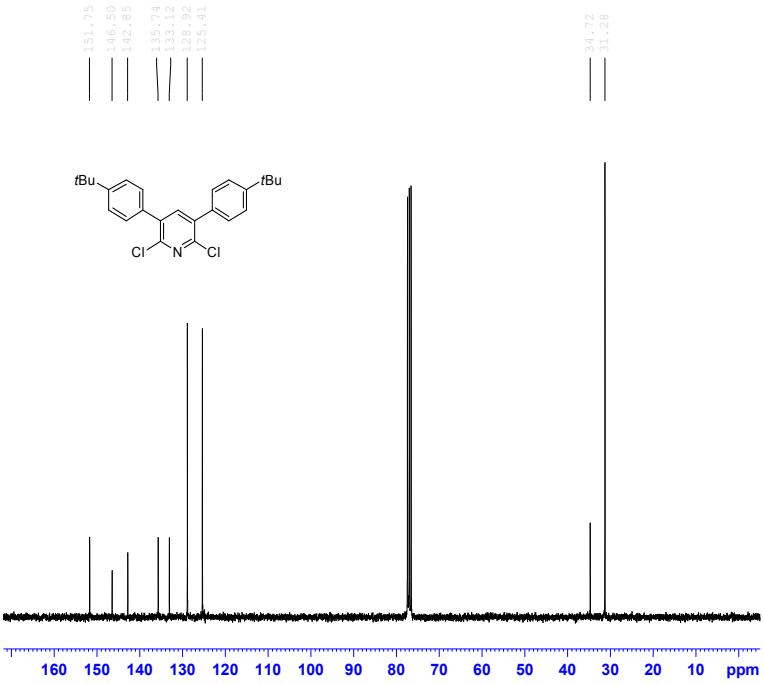

```
Current Data Parameters
NAME            SRE 831 1H
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_            20120623
Time                15.33
INSTRUM            AV300
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     4
SWH             6172.839 Hz
FIDRES             0.188380 Hz
AQ              2.6542580 sec
RG                 322.5
DW                81.000 usec
DE                 6.00 usec
TE                296.0 K
D1              1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 11.00 usec
PL1                 0.00 dB
SFO1          300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF            300.1300388 MHz
WDW                   EM
SSB                    0
LB                  0.10 Hz
GB                     0
PC                  1.00
```

Reimann/ SRE 831
Au13C CDCl3 /opt/topspin 1206 45




```
Current Data Parameters
NAME          SRE 831 13C
EXPNO                  11
PROCNO                  1

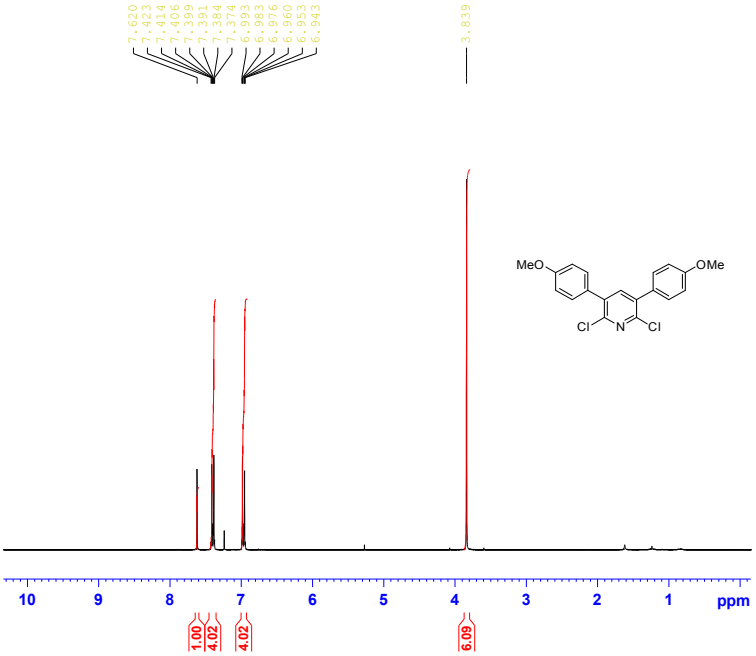
F2 - Acquisition Parameters
Date_            20120623
Time                16.21
INSTRUM            AV300
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  1000
DS                     4
SWH            21097.047 Hz
FIDRES             0.643831 Hz
AQ              0.7766516 sec
RG                 32768
DW                23.700 usec
DE                 6.00 usec
TE                296.5 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                  9.60 usec
PL1                -1.10 dB
SFO1          75.4771825 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2             100.00 usec
PL2                 0.00 dB
PL12               19.00 dB
PL13               21.00 dB
SFO2          300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF            75.4677529 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

S.Reimann, SRE-815
Au1H CDCl3 /opt/topspin 1206 33



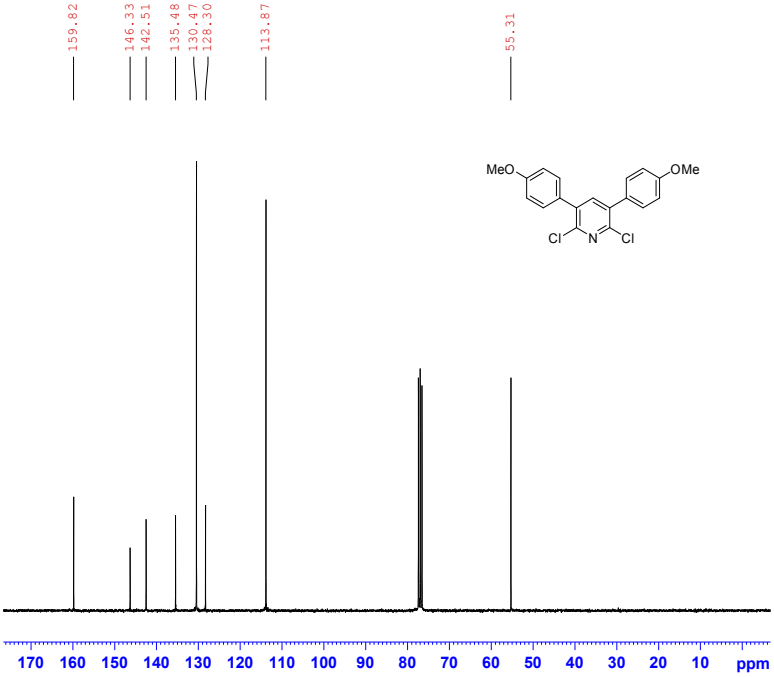
Current Data Parameters
NAME SRE 815 1H
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120617
Time 9.04
INSTRUM AV300
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 4
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 181
DW 81.000 usec
DE 6.00 usec
TE 295.5 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300220 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

S.Reimann, SRE-815
Au13C CDCl3 /opt/topspin 1206 33



Current Data Parameters
NAME SRE 815 13C
EXPNO 11
PROCNO 1

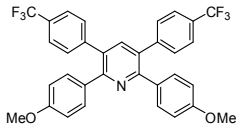
F2 - Acquisition Parameters
Date_ 20120617
Time 10.42
INSTRUM AV300
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 2048
DS 4
SWH 21097.047 Hz
FIDRES 0.643831 Hz
AQ 0.7766516 sec
RG 32768
DW 23.700 usec
DE 6.00 usec
TE 296.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

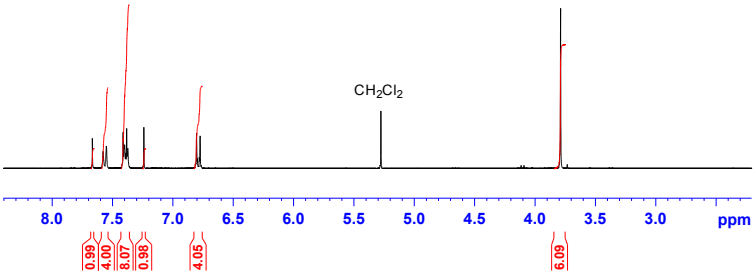
======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -1.10 dB
SFO1 75.4771825 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 19.00 dB
PL13 21.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677564 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Reimann/ SRE- SP 48
Au1H CDCl3 /opt/topspin 1206 56





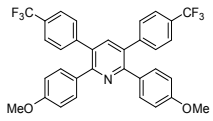

```
Current Data Parameters
NAME                  SP48-1H
EXPNO                      10
PROCNO                      1

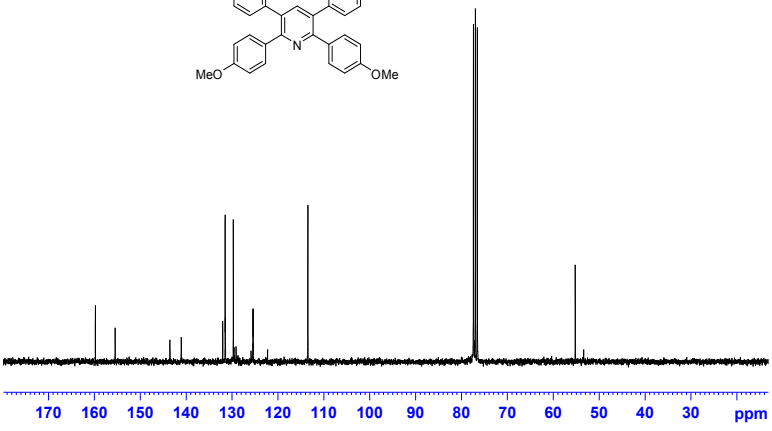
F2 - Acquisition Parameters
Date_               20120630
Time                   14.57
INSTRUM                AV300
PROBHD   5 mm PABBO BB-
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                        32
DS                         4
SWH                 6172.839 Hz
FIDRES              0.188380 Hz
AQ                  2.6542580 sec
RG                      322.5
DW                   81.000 usec
DE                    6.00 usec
TE                    296.3 K
D1                  1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                    11.00 usec
PL1                    0.00 dB
SFO1             300.1318534 MHz

F2 - Processing parameters
SI                         32768
SF                300.1300214 MHz
WDW                           EM
SSB                            0
LB                          0.10 Hz
GB                             0
PC                          1.00
```

Reimann/ SRE- SP 48
Au13C CDCl3 /opt/topspin 1206 56






```
Current Data Parameters
NAME                  SP48-13C
EXPNO                      11
PROCNO                      1

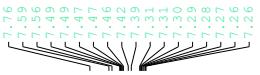
F2 - Acquisition Parameters
Date_               20120630
Time                   15.46
INSTRUM                AV300
PROBHD   5 mm PABBO BB-
PULPROG               zgpg30
TD                     32768
SOLVENT                CDCl3
NS                      1000
DS                         4
SWH                21097.047 Hz
FIDRES              0.643831 Hz
AQ                  0.7766516 sec
RG                      32768
DW                   23.700 usec
DE                    6.00 usec
TE                    296.8 K
D1                  2.00000000 sec
d11                 0.03000000 sec
DELTA               1.89999998 sec
TD0                         1

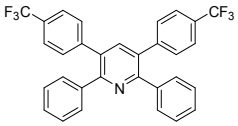
======== CHANNEL f1 ========
NUC1                      13C
P1                     9.60 usec
PL1                   -1.10 dB
SFO1             75.4771825 MHz

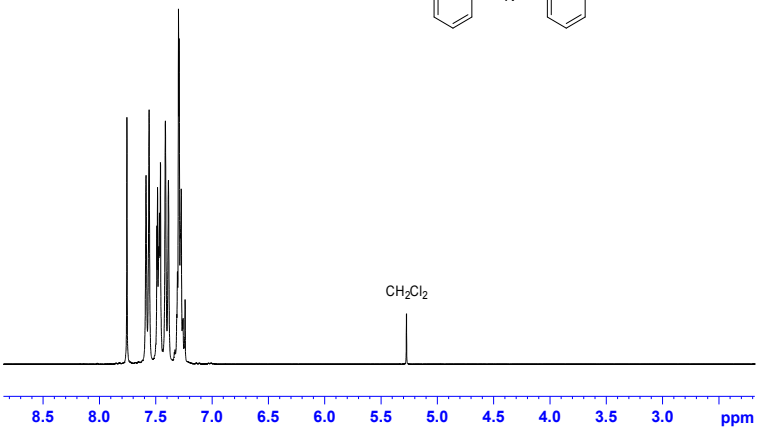
======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                100.00 usec
PL2                    0.00 dB
PL12                  19.00 dB
PL13                  21.00 dB
SFO2             300.1312005 MHz

F2 - Processing parameters
SI                         32768
SF                75.4677528 MHz
WDW                           EM
SSB                            0
LB                          1.00 Hz
GB                             0
PC                          1.40
```

Reimann/ SRE- SP 47
Au1H CDCl3 /opt/topspin 1206 54







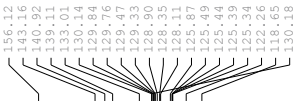

```
Current Data Parameters
NAME                  SP47-1H
EXPNO                      10
PROCNO                      1

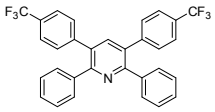
F2 - Acquisition Parameters
Date_              20120630
Time_                 13.17
INSTRUM               AV300
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                       32
DS                        4
SWH                6172.839 Hz
FIDRES             0.188380 Hz
AQ                 2.6542580 sec
RG                      128
DW                   81.000 usec
DE                    6.00 usec
TE                   296.2 K
D1                1.00000000 sec
TD0                         1

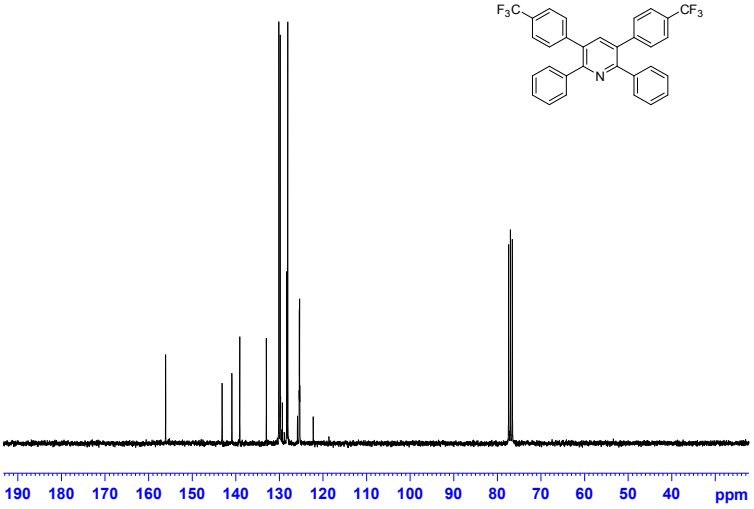
======== CHANNEL f1 ========
NUC1                       1H
P1                      11.00 usec
PL1                      0.00 dB
SFO1            300.1318534 MHz

F2 - Processing parameters
SI                        32768
SF                300.1300213 MHz
WDW                          EM
SSB                           0
LB                         0.10 Hz
GB                            0
PC                         1.00
```

Reimann/ SRE- SP 47
Au13C CDCl3 /opt/topspin 1206 54








```
Current Data Parameters
NAME                 SP47-13C
EXPNO                      11
PROCNO                      1

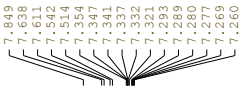
F2 - Acquisition Parameters
Date_              20120630
Time_                 13.42
INSTRUM               AV300
PROBHD    5 mm PABBO BB-
PULPROG            zgpg30
TD                    32768
SOLVENT               CDCl3
NS                      500
DS                        4
SWH               21097.047 Hz
FIDRES             0.643831 Hz
AQ                 0.7766516 sec
RG                    32768
DW                   23.700 usec
DE                    6.00 usec
TE                   296.7 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                         1

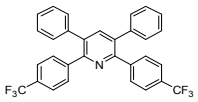
======== CHANNEL f1 ========
NUC1                      13C
P1                       9.60 usec
PL1                     -1.10 dB
SFO1            75.4771825 MHz

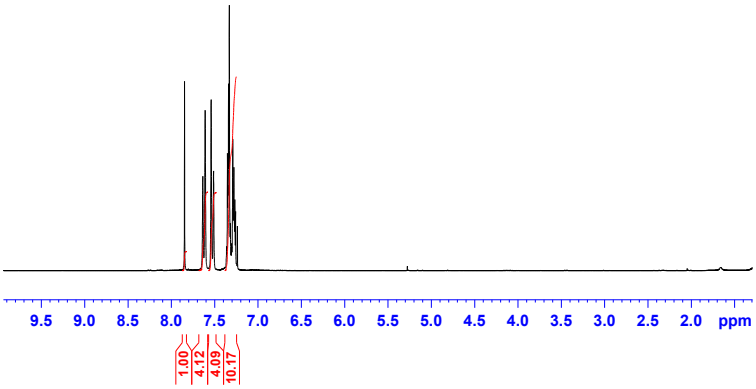
======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  100.00 usec
PL2                      0.00 dB
PL12                    19.00 dB
PL13                    21.00 dB
SFO2            300.1312005 MHz

F2 - Processing parameters
SI                        32768
SF                75.4677547 MHz
WDW                          EM
SSB                           0
LB                         1.00 Hz
GB                            0
PC                         1.40
```

Reimann/ SRE- SP 50
Au1H CDCl3 /opt/topspin 1206 55







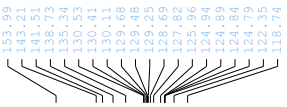

```
Current Data Parameters
NAME                  SP50
EXPNO                   10
PROCNO                   1

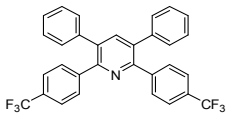
F2 - Acquisition Parameters
Date_              20120630
Time_                 14.06
INSTRUM              AV300
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                      32
DS                       4
SWH               6172.839 Hz
FIDRES            0.188380 Hz
AQ                2.6542580 sec
RG                     114
DW                  81.000 usec
DE                   6.00 usec
TE                  296.2 K
D1             1.00000000 sec
TD0                      1

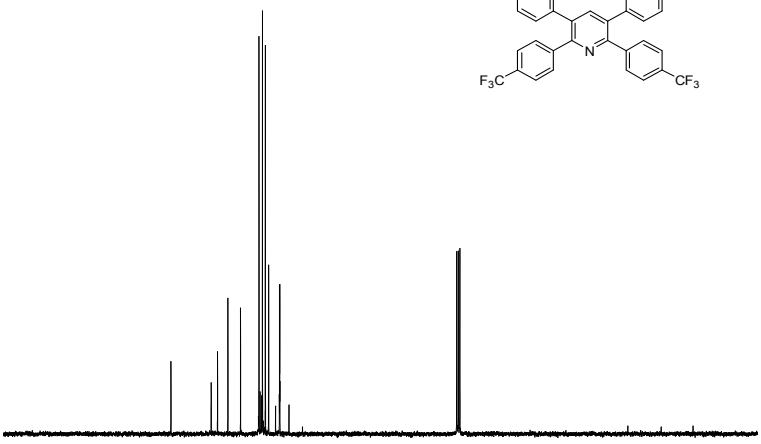
======== CHANNEL f1 ========
NUC1                   1H
P1                  11.00 usec
PL1                  0.00 dB
SFO1         300.1318534 MHz

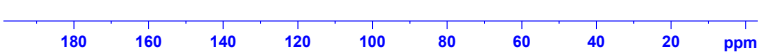
F2 - Processing parameters
SI                   32768
SF            300.1300216 MHz
WDW                     EM
SSB                      0
LB                    0.10 Hz
GB                       0
PC                    1.00
```

Reimann/ SRE- SP 50
Au13C CDCl3 /opt/topspin 1206 55










```
Current Data Parameters
NAME             SP50-13C
EXPNO                  11
PROCNO                  1

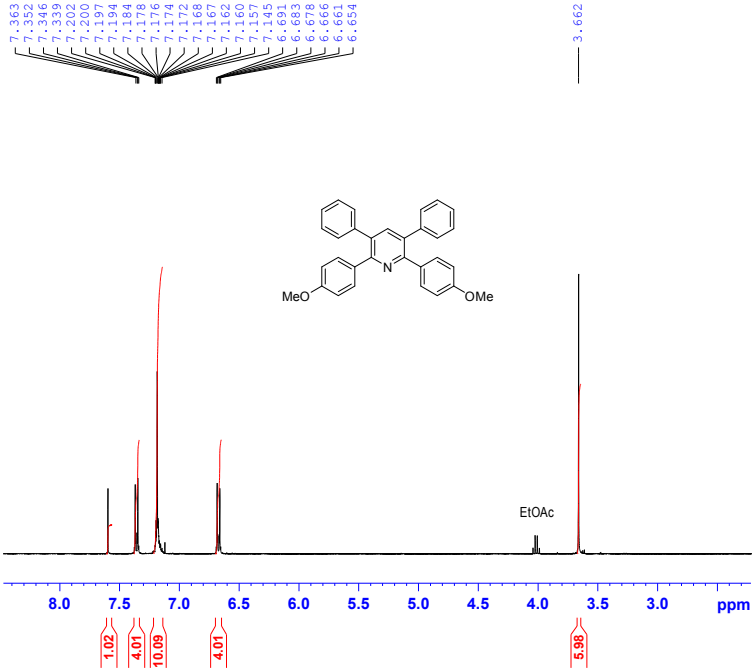
F2 - Acquisition Parameters
Date_              20120630
Time_                 14.31
INSTRUM              AV300
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   32768
SOLVENT              CDCl3
NS                     500
DS                       4
SWH              21097.047 Hz
FIDRES            0.643831 Hz
AQ                0.7766516 sec
RG                   32768
DW                  23.700 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                   9.60 usec
PL1                 -1.10 dB
SFO1          75.4771825 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                   1H
PCPD2              100.00 usec
PL2                  0.00 dB
PL12                19.00 dB
PL13                21.00 dB
SFO2         300.1312005 MHz

F2 - Processing parameters
SI                   32768
SF            75.4677544 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

Reimann/ SRE - SP- 51
Au1H CDCl3 /opt/topspin 1206 10



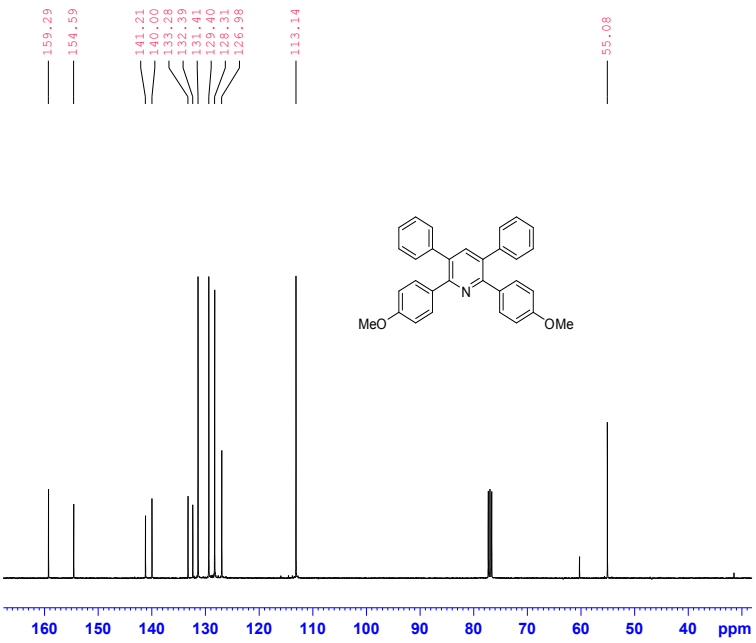
Current Data Parameters
NAME SRE SP 51 1H
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120628
Time 23.04
INSTRUM AV400
PROBHD 5 mm QNP 1H/29
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 4
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 57
DW 62.400 usec
DE 6.00 usec
TE 297.0 K
D1 1.50000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 12.20 usec
PL1 -1.00 dB
SFO1 400.1324000 MHz

F2 - Processing parameters
SI 32768
SF 400.1300772 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

Reimann/ SRE - SP- 51
Au13C CDCl3 /opt/topspin 1206 10



Current Data Parameters
NAME SRE SP 51 13C
EXPNO 11
PROCNO 1

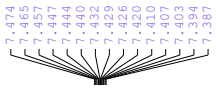
F2 - Acquisition Parameters
Date_ 20120628
Time 23.53
INSTRUM AV400
PROBHD 5 mm QNP 1H/29
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1000
DS 4
SWH 29940.119 Hz
FIDRES 0.456850 Hz
AQ 1.0945013 sec
RG 10321.3
DW 16.700 usec
DE 6.00 usec
TE 297.0 K
D1 1.70000005 sec
d11 0.03000000 sec
DELTA 1.60000002 sec
TD0 1

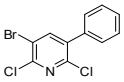
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 100.6260690 MHz

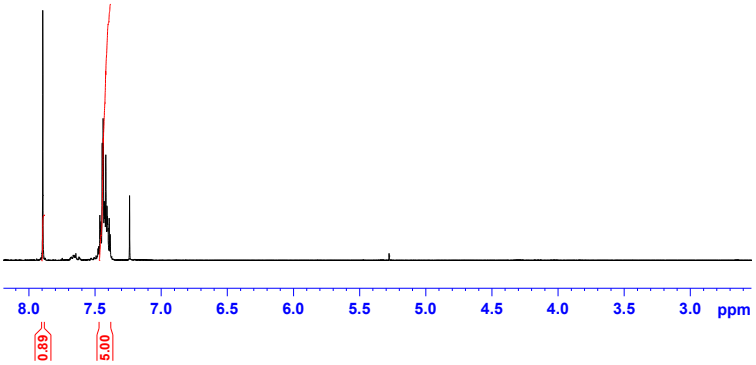
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -1.00 dB
PL12 19.00 dB
PL13 21.00 dB
SFO2 400.1318000 MHz

F2 - Processing parameters
SI 32768
SF 100.6127874 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

S.Reimann, SRE-821
Au1H CDCl3 /opt/topspin 1206 31







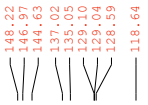

```
Current Data Parameters
NAME                 SRE821-1H
EXPNO                       10
PROCNO                       1

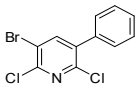
F2 - Acquisition Parameters
Date_               20120617
Time                    5.13
INSTRUM                AV300
PROBHD   5 mm PABBO BB-
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                        32
DS                         4
SWH                6172.839 Hz
FIDRES             0.188380 Hz
AQ                 2.6542580 sec
RG                     322.5
DW                    81.000 usec
DE                     6.00 usec
TE                    295.5 K
D1                 1.00000000 sec
TD0                         1

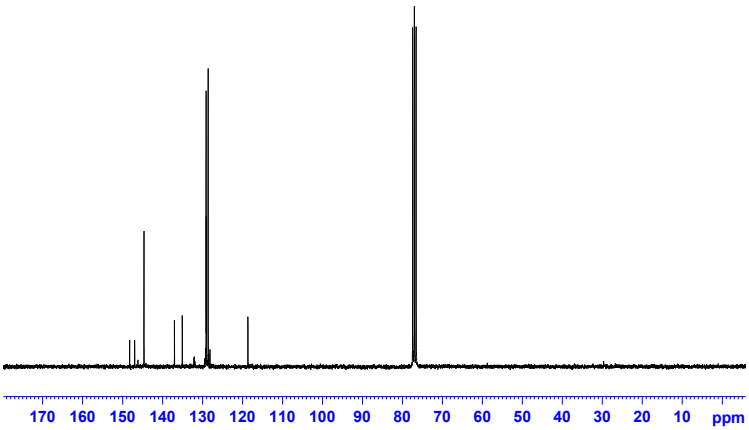
======== CHANNEL f1 ========
NUC1                       1H
P1                      11.00 usec
PL1                      0.00 dB
SFO1            300.1318534 MHz

F2 - Processing parameters
SI                         32768
SF                 300.1300214 MHz
WDW                           EM
SSB                            0
LB                          0.10 Hz
GB                             0
PC                          1.00
```

S.Reimann, SRE-821
Au13C CDCl3 /opt/topspin 1206 31








```
Current Data Parameters
NAME                 SRE821-13C
EXPNO                       11
PROCNO                       1

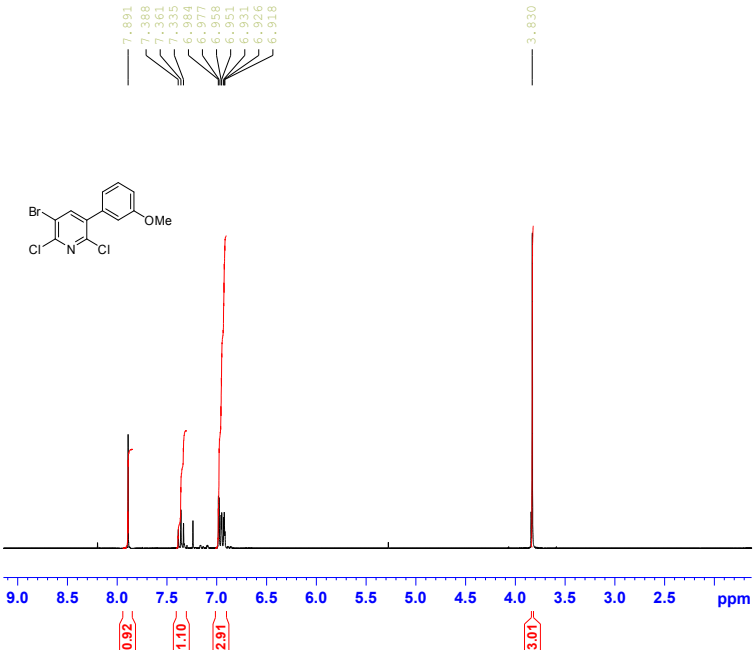
F2 - Acquisition Parameters
Date_               20120617
Time                    6.52
INSTRUM                AV300
PROBHD   5 mm PABBO BB-
PULPROG              zgpg30
TD                     32768
SOLVENT                CDCl3
NS                      2048
DS                         4
SWH               21097.047 Hz
FIDRES             0.643831 Hz
AQ                 0.7766516 sec
RG                     32768
DW                    23.700 usec
DE                     6.00 usec
TE                    296.0 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      13C
P1                       9.60 usec
PL1                     -1.10 dB
SFO1            75.4771825 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  100.00 usec
PL2                      0.00 dB
PL12                    19.00 dB
PL13                    21.00 dB
SFO2            300.1312005 MHz

F2 - Processing parameters
SI                         32768
SF                 75.4677541 MHz
WDW                           EM
SSB                            0
LB                          1.00 Hz
GB                             0
PC                          1.40
```

S.Reimann,SRE-823
Au1H CDCl3 /opt/topspin 1206 32



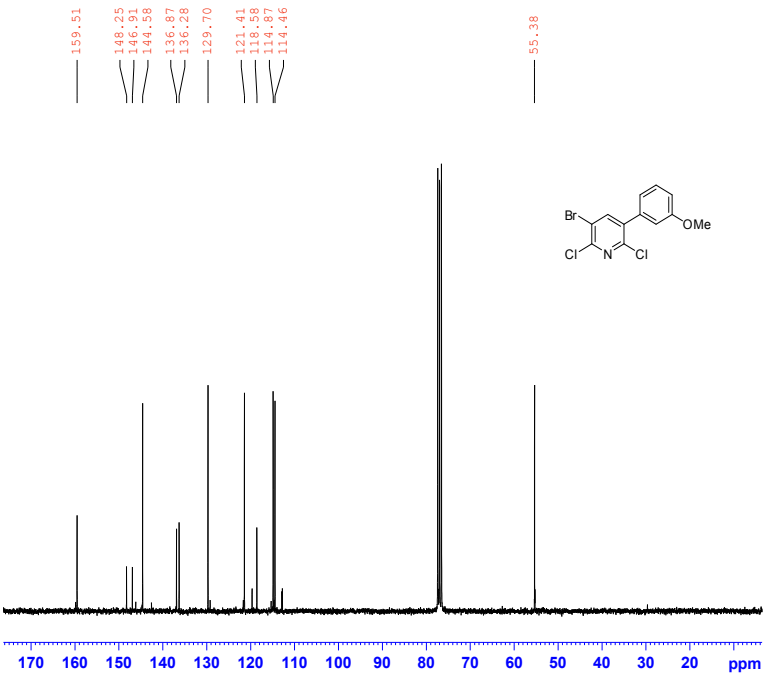

```
Current Data Parameters
NAME            SRE823-1H
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_           20120617
Time                7.09
INSTRUM           AV300
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     4
SWH             6172.839 Hz
FIDRES          0.188380 Hz
AQ              2.6542580 sec
RG                 322.5
DW                81.000 usec
DE                 6.00 usec
TE                295.6 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 11.00 usec
PL1                 0.00 dB
SFO1         300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF           300.1300214 MHz
WDW                   EM
SSB                    0
LB                  0.10 Hz
GB                     0
PC                  1.00
```

S.Reimann,SRE-823
Au13C CDCl3 /opt/topspin 1206 32




```
Current Data Parameters
NAME          SRE823-13C
EXPNO                  11
PROCNO                  1

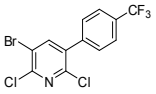
F2 - Acquisition Parameters
Date_           20120617
Time                8.47
INSTRUM           AV300
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  2048
DS                     4
SWH            21097.047 Hz
FIDRES          0.643831 Hz
AQ              0.7766516 sec
RG                 32768
DW                23.700 usec
DE                 6.00 usec
TE                296.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1

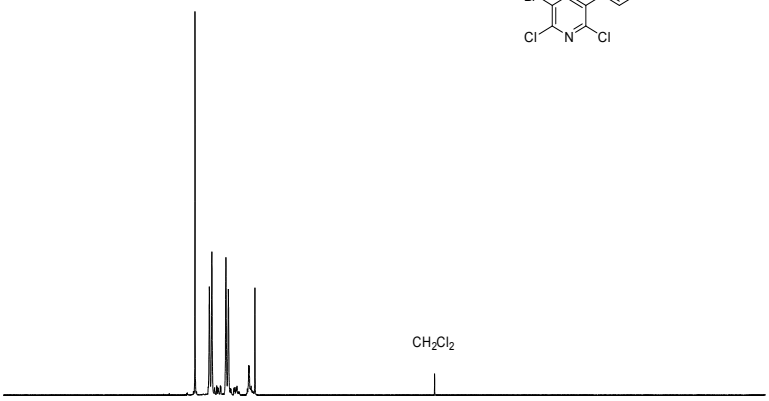
======== CHANNEL f1 ========
NUC1                  13C
P1                 9.60 usec
PL1                -1.10 dB
SFO1         75.4771825 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             100.00 usec
PL2                 0.00 dB
PL12               19.00 dB
PL13               21.00 dB
SFO2         300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF           75.4677545 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Reimann/ SRE- SP- 39
Au1H CDCl3 /opt/topspin 1206 43





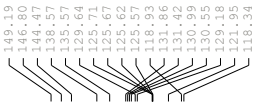

```
Current Data Parameters
NAME              SP39-1H
EXPNO                  10
PROCNO                  1

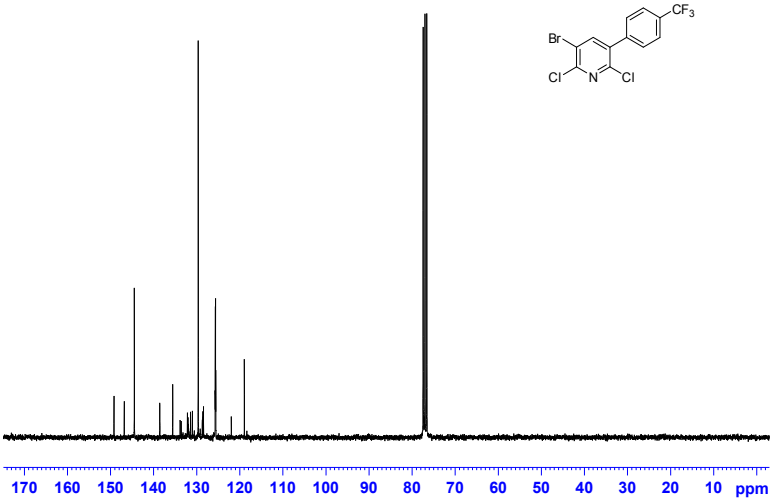
F2 - Acquisition Parameters
Date_            20120623
Time                12.19
INSTRUM             AV300
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    32
DS                     4
SWH             6172.839 Hz
FIDRES          0.188380 Hz
AQ              2.6542580 sec
RG                 456.1
DW                81.000 usec
DE                 6.00 usec
TE                295.8 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.00 usec
PL1                0.00 dB
SFO1         300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF           300.1300214 MHz
WDW                   EM
SSB                    0
LB                  0.10 Hz
GB                     0
PC                  1.00
```

Reimann/ SRE-SP-39
Au13C CDCl3 /opt/topspin 1206 54






```
Current Data Parameters
NAME            SP39-13C-2
EXPNO                  10
PROCNO                  1

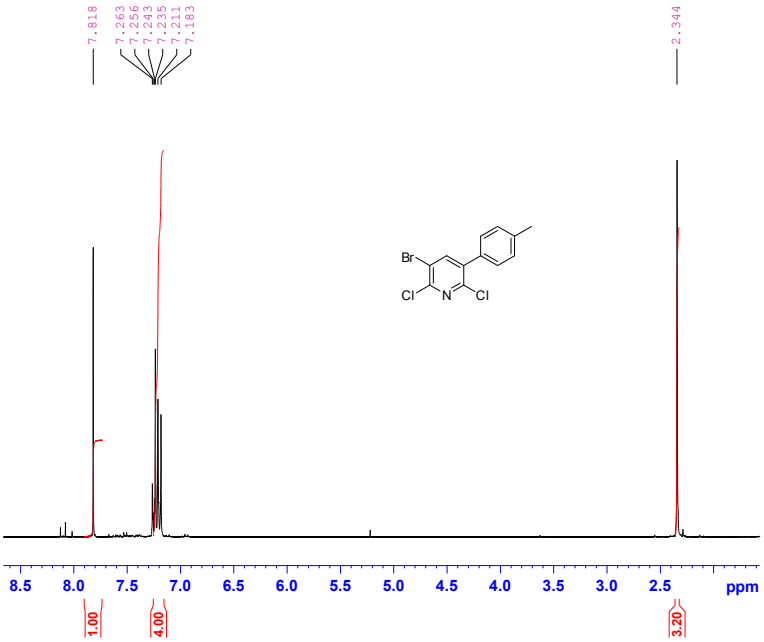
F2 - Acquisition Parameters
Date_            20120626
Time                13.55
INSTRUM             AV300
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  2000
DS                     4
SWH            21097.047 Hz
FIDRES          0.643831 Hz
AQ              0.7766516 sec
RG                 32768
DW                23.700 usec
DE                 6.00 usec
TE                296.6 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.60 usec
PL1               -1.10 dB
SFO1         75.4771825 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2            100.00 usec
PL2                0.00 dB
PL12              19.00 dB
PL13              21.00 dB
SFO2         300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF           75.4677533 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

S.Reimann, SRE-822
Au1H CDCl3 /opt/topspin 1206 34



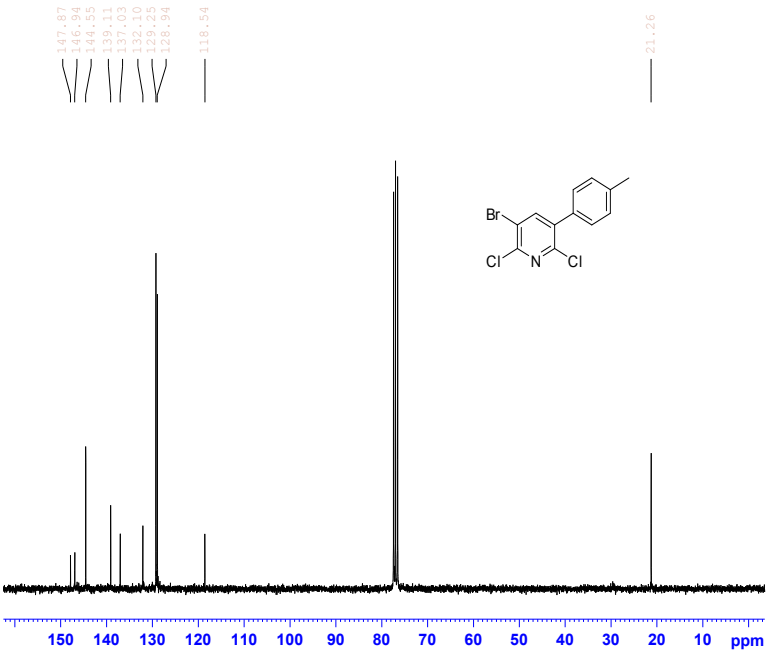

```
Current Data Parameters
NAME          SRE 822 1H
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120617
Time              10.59
INSTRUM           AV300
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD                32768
SOLVENT           CDCl3
NS                   32
DS                    4
SWH            6172.839 Hz
FIDRES         0.188380 Hz
AQ             2.6542580 sec
RG                322.5
DW               81.000 usec
DE                6.00 usec
TE               295.5 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.00 usec
PL1                0.00 dB
SFO1         300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF           300.1300388 MHz
WDW                   EM
SSB                    0
LB                  0.10 Hz
GB                     0
PC                  1.00
```

S.Reimann, SRE-822
Au13C CDCl3 /opt/topspin 1206 34




```
Current Data Parameters
NAME        SRE 822 13C
EXPNO                11
PROCNO                1

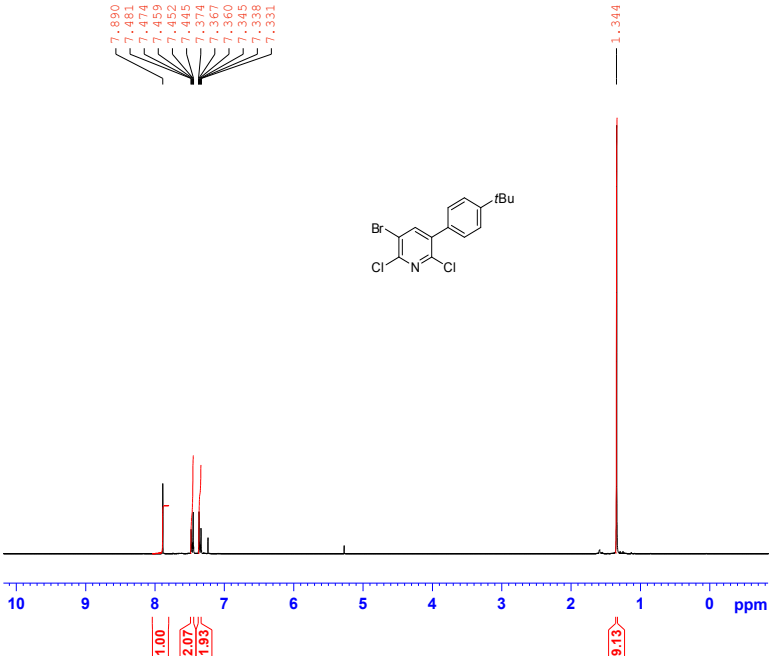
F2 - Acquisition Parameters
Date_           20120617
Time              11.48
INSTRUM           AV300
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD                32768
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           21097.047 Hz
FIDRES         0.643831 Hz
AQ             0.7766516 sec
RG                32768
DW               23.700 usec
DE                6.00 usec
TE               296.1 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                9.60 usec
PL1              -1.10 dB
SFO1         75.4771825 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2            100.00 usec
PL2                0.00 dB
PL12              19.00 dB
PL13              21.00 dB
SFO2         300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF           75.4677567 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Reimann/ SRE 832
Au1H CDCl3 /opt/topspin 1206 41



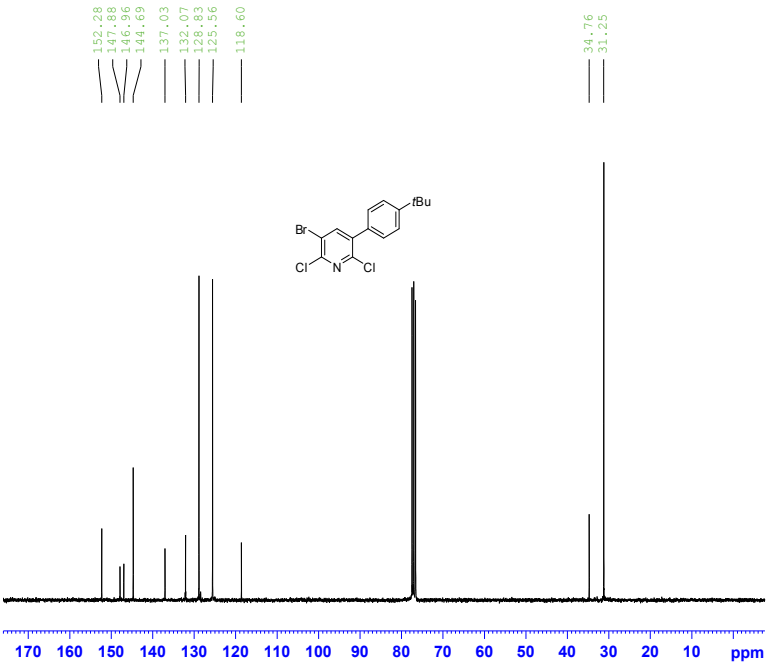

```
Current Data Parameters
NAME          SRE 832 1H
EXPNO                10
PROCNO                1

F2 - Acquisition Parameters
Date_          20120623
Time               8.26
INSTRUM          AV300
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD               32768
SOLVENT          CDCl3
NS                  32
DS                   4
SWH           6172.839 Hz
FIDRES        0.188380 Hz
AQ            2.6542580 sec
RG                203.2
DW               81.000 usec
DE                6.00 usec
TE               295.7 K
D1            1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                1H
P1                11.00 usec
PL1                0.00 dB
SFO1        300.1318534 MHz

F2 - Processing parameters
SI               32768
SF          300.1300221 MHz
WDW                 EM
SSB                  0
LB                0.10 Hz
GB                   0
PC                1.00
```

Reimann/ SRE 832
Au13C CDCl3 /opt/topspin 1206 41




```
Current Data Parameters
NAME         SRE 832 13C
EXPNO                11
PROCNO                1

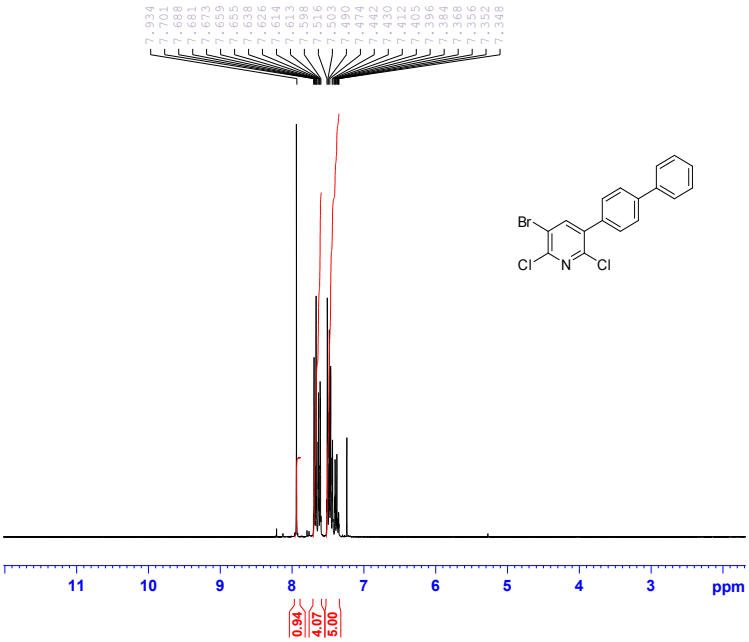
F2 - Acquisition Parameters
Date_          20120623
Time              10.01
INSTRUM          AV300
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD               32768
SOLVENT          CDCl3
NS                2000
DS                   4
SWH          21097.047 Hz
FIDRES        0.643831 Hz
AQ            0.7766516 sec
RG                32768
DW               23.700 usec
DE                6.00 usec
TE               296.2 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1                9.60 usec
PL1               -1.10 dB
SFO1         75.4771825 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2           100.00 usec
PL2                0.00 dB
PL12              19.00 dB
PL13              21.00 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
SI               32768
SF          75.4677527 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```

Reimann/ SRE- SP- 40
Au1H CDCl3 /opt/topspin 1206 48



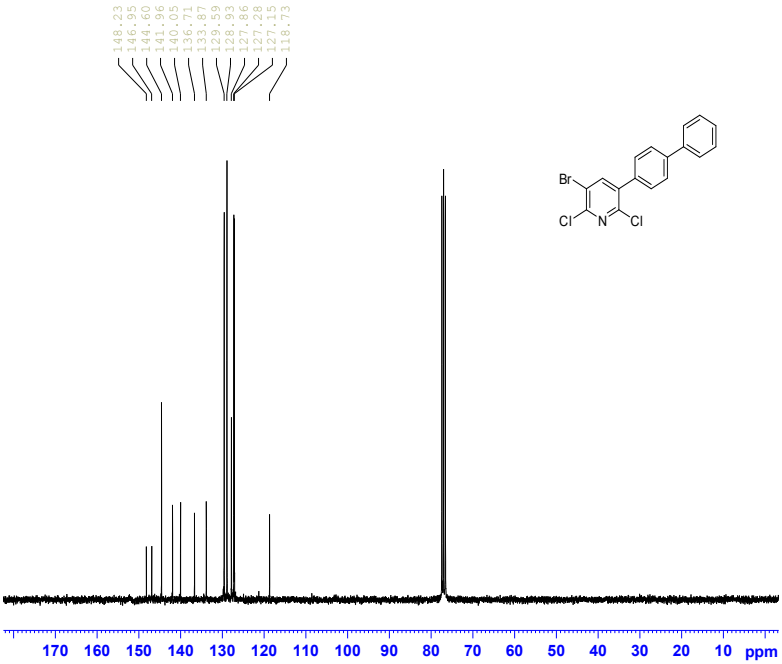
Current Data Parameters
NAME SRE SP-40 1H
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120623
Time 18.33
INSTRUM AV300
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 4
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 322.5
DW 81.000 usec
DE 6.00 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300220 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

Reimann/ SRE- SP- 40
Au13C CDCl3 /opt/topspin 1206 48



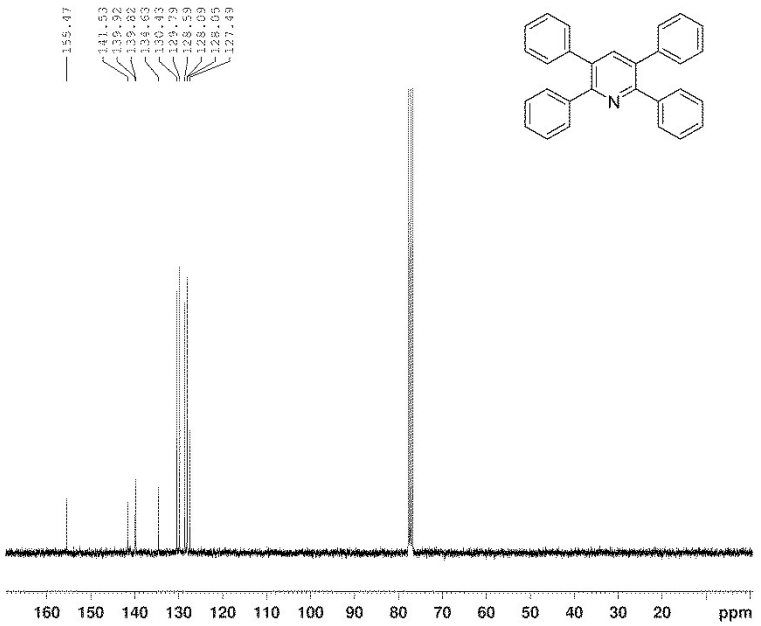
Current Data Parameters
NAME SRE SP 40 13 C
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120623
Time 19.22
INSTRUM AV300
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1000
DS 4
SWH 21097.047 Hz
FIDRES 0.643831 Hz
AQ 0.7766516 sec
RG 32768
DW 23.700 usec
DE 6.00 usec
TE 296.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -1.10 dB
SFO1 75.4771825 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 19.00 dB
PL13 21.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677534 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



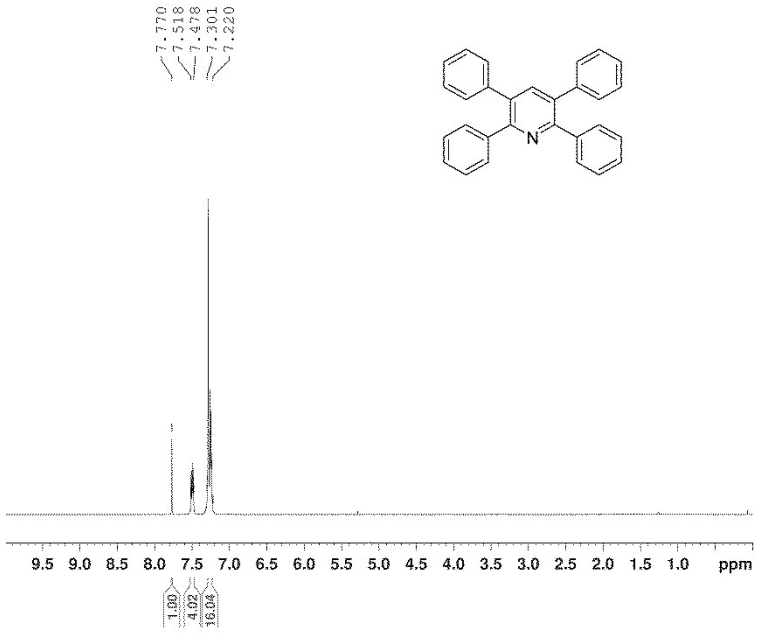

```
Current Data Parameters
NAME                 141022.u304
EXPNO                        12
PROCNO                        1

F2 - Acquisition Parameters
Date_               20141023
Time                     7.45
INSTRUM                  spect
PROBHD     5 mm PABBO BB-
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                         840
DS                           4
SWH                  18028.846 Hz
FIDRES                0.275098 Hz
AQ                    1.8175918 sec
RG                        2050
DW                      27.733 usec
DE                      10.00 usec
TE                      298.2 K
D1                   2.00000000 sec
D11                  0.03000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                        13C
P1                        10.00 usec
PL1                       -0.50 dB
PL1W                 33.23691986 W
SFO1                 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                        1H
PCPD2                     72.00 usec
PL2          0 dB
PL12                      17.00 dB
PL13                      17.00 dB
PL2W                 11.25325108 W
PL12W                 0.22453187 W
PL13W                 0.22453187 W
SFO2                 300.1312005 MHz

F2 - Processing parameters
SI                        32768
SF                   75.4677330 MHz
WDW                          EM
SSB          0
LB                        1.00 Hz
GB           0
PC                        1.40
```

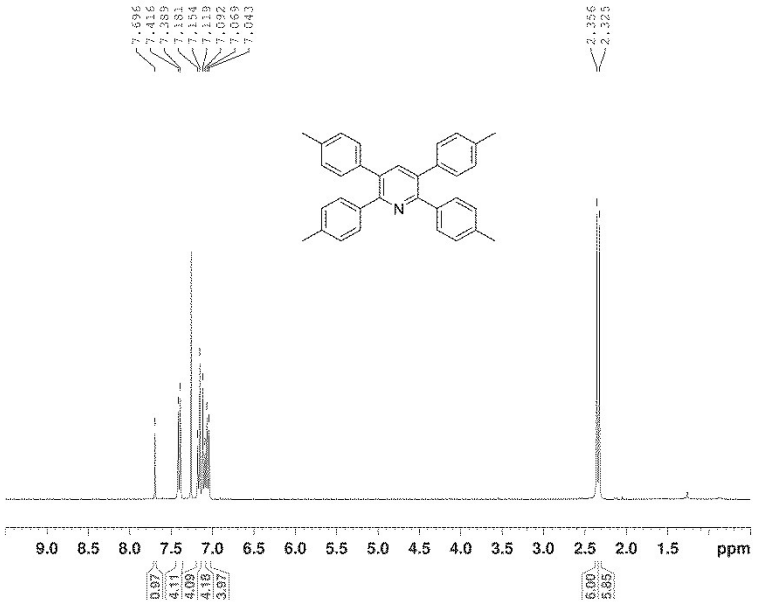



```
Current Data Parameters
NAME                 141022.u304
EXPNO                        10
PROCNO                        1

F2 - Acquisition Parameters
Date_               20141022
Time                     8.29
INSTRUM                  spect
PROBHD     5 mm PABBO BB-
PULPROG                  zg30
TD                       65536
SOLVENT                  CDCl3
NS                          16
DS                           2
SWH                  6188.119 Hz
FIDRES                0.094423 Hz
AQ                    5.2953587 sec
RG                         161
DW                      80.800 usec
DE                      10.00 usec
TE                      298.2 K
D1                   1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                        1H
P1                        10.00 usec
PL1          0 dB
PL1W                 11.25325108 W
SFO1                 300.1318534 MHz

F2 - Processing parameters
SI                        32768
SF                   300.1300098 MHz
WDW                          EM
SSB          0
LB                        0.30 Hz
GB           0
PC                        1.00
```

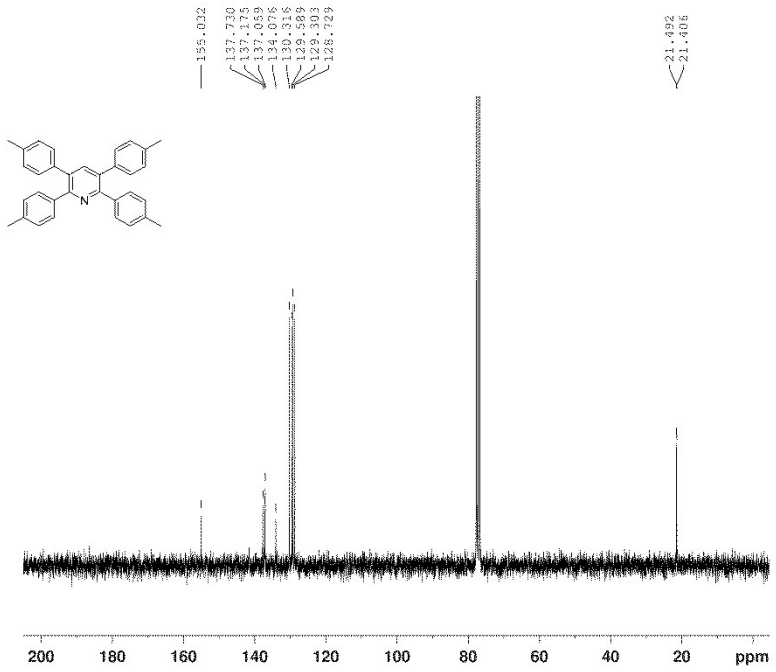



```
Current Data Parameters
NAME          141127.u321
EXPNO              10
PROCNO              1

F2 - Acquisition Parameters
Date_          20141127
Time              13.07
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD               65536
SOLVENT           CDCl3
NS                  16
DS                   2
SWH            6188.119 Hz
FIDRES         0.094423 Hz
AQ             5.2953587 sec
RG                 362
DW              80.800 usec
DE              10.00 usec
TE              296.2 K
D1           1.00000000 sec
TD0                 1

======== CHANNEL f1 ========
NUC1               1H
P1              10.00 usec
PL1       0 dB
PLW        11.25325108 W
SFO1      300.1318534 MHz

F2 - Processing parameters
SI                32768
SF          300.1300060 MHz
WDW                 EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



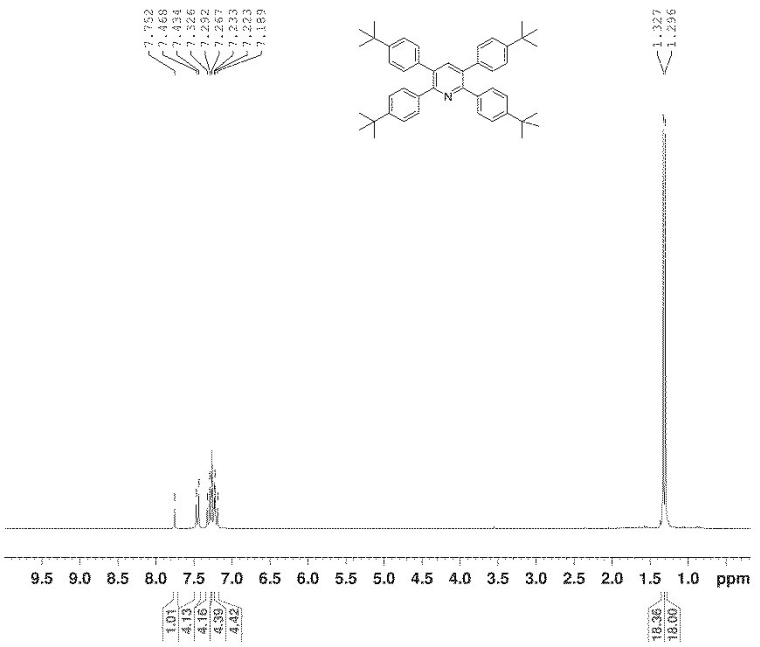

```
Current Data Parameters
NAME          141128.210
EXPNO              10
PROCNO              1

F2 - Acquisition Parameters
Date_          20141128
Time              13.08
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD               65536
SOLVENT           CDCl3
NS                 768
DS                   4
SWH           15000.000 Hz
FIDRES         0.228882 Hz
AQ             2.1845834 sec
RG                2050
DW              33.333 usec
DE              10.00 usec
TE              299.3 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                 1

======== CHANNEL f1 ========
NUC1               13C
P1              10.00 usec
PL1             -1.00 dB
SFO1         62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2               1H
PCPD2           70.00 usec
PL12            15.00 dB
PL13            15.00 dB
PL2             -2.50 dB
SFO2        250.1310005 MHz

F2 - Processing parameters
SI                32768
SF           62.8952237 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



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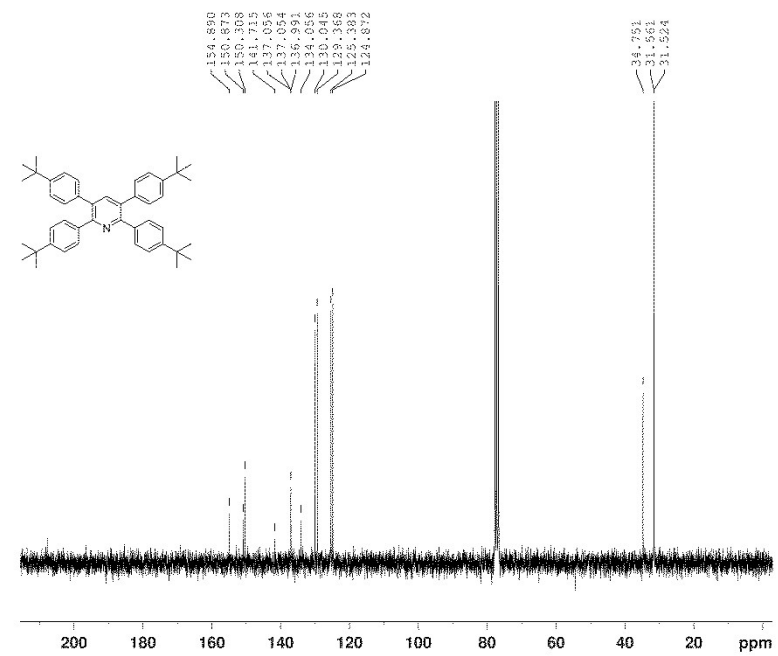
```
Current Data Parameters
NAME                 141024.238
EXPNO                        10
PROCNO                        1

F2 - Acquisition Parameters
Date_               20141025
Time                    12.30
INSTRUM                 spect
PROBHD    5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 5165.289 Hz
FIDRES              0.078816 Hz
AQ                  6.3439350 sec
RG                        845
DW                     96.800 usec
DE                     10.00 usec
TE                     297.2 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     10.00 usec
PL1                    -2.50 dB
SFO1              250.1315447 MHz

F2 - Processing parameters
SI                        32768
SF                250.1300005 MHz
WDW                          EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      1.00
```



BRUKER

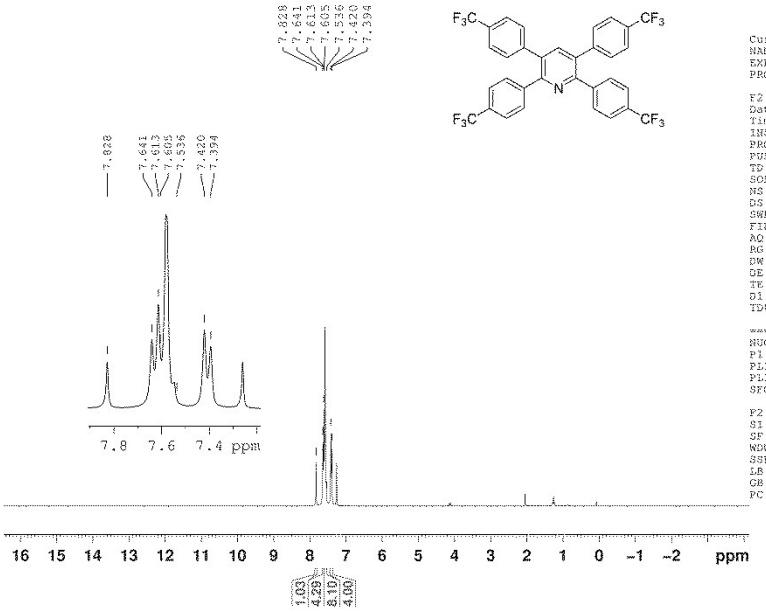
```
Current Data Parameters
NAME                 141024.238
EXPNO                        11
PROCNO                        1

F2 - Acquisition Parameters
Date_               20141025
Time                    13.44
INSTRUM                 spect
PROBHD    5 mm PABBO BB-
PULPROG                 zgpg30
TD                     65536
SOLVENT                CDCl3
NS                      1024
DS                         4
SWH                15000.000 Hz
FIDRES              0.228882 Hz
AQ                  2.1845834 sec
RG                       2050
DW                     33.333 usec
DE                     10.00 usec
TE                     298.1 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                     10.00 usec
PL1                    -1.00 dB
SFO1              62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                  70.00 usec
PL12                   15.00 dB
PL13                   15.00 dB
PL2                    -2.50 dB
SFO2              250.1310005 MHz

F2 - Processing parameters
SI                        32768
SF                62.8952239 MHz
WDW                          EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
```

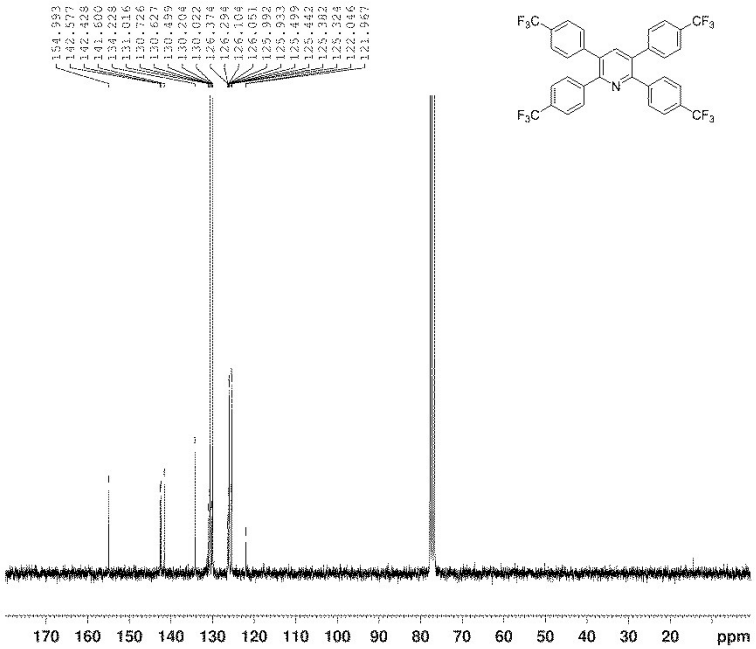



```
Current Data Parameters
NAME          141127.u322
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_              20141127
Time                 13.13
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              6188.119 Hz
FIDRES           0.094423 Hz
AQ               5.2953587 sec
RG                    256
DW                 80.800 usec
DE                 10.00 usec
TE                298.2 K
D1             1.00000000 sec
TD0                     1

========== CHANNEL f1 ==========
NUC1                   1H
P1                 10.00 usec
PL1        0 dB
PLW        11.25325108 W
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                  32768
SF          300.1300058 MHz
WDW                    EM
SSB        0
LB                  0.30 Hz
GB         0
PC                  1.00
```



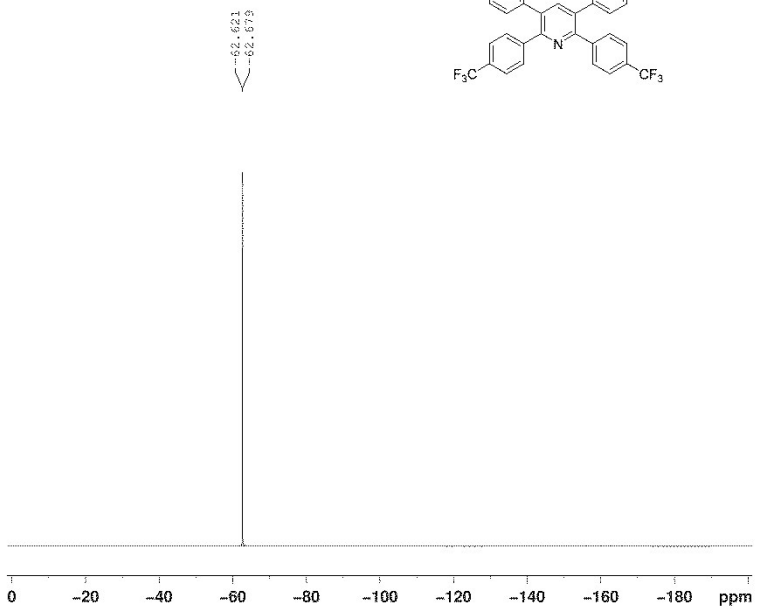

```
Current Data Parameters
NAME          141201.210
EXPNO                  10
PROCNO                  1

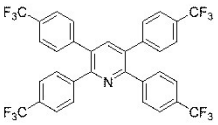
F2 - Acquisition Parameters
Date_              20141202
Time                 2.28
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   3000
DS                      4
SWH             15000.000 Hz
FIDRES           0.228882 Hz
AQ               2.1845834 sec
RG                   2050
DW                 33.333 usec
DE                 10.00 usec
TE                298.1 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                     1

========== CHANNEL f1 ==========
NUC1                  13C
P1                 10.00 usec
PL1                -1.00 dB
SFO1          62.9015280 MHz

========== CHANNEL f2 ==========
CPDPRG2           waltz16
NUC2                   1H
PCPD2              70.00 usec
PL12               15.00 dB
PL13               15.00 dB
PL2                -2.50 dB
SFO2         250.1310005 MHz

F2 - Processing parameters
SI                  32768
SF            62.8952234 MHz
WDW                    EM
SSB        0
LB                  1.00 Hz
GB         0
PC                  1.40
```





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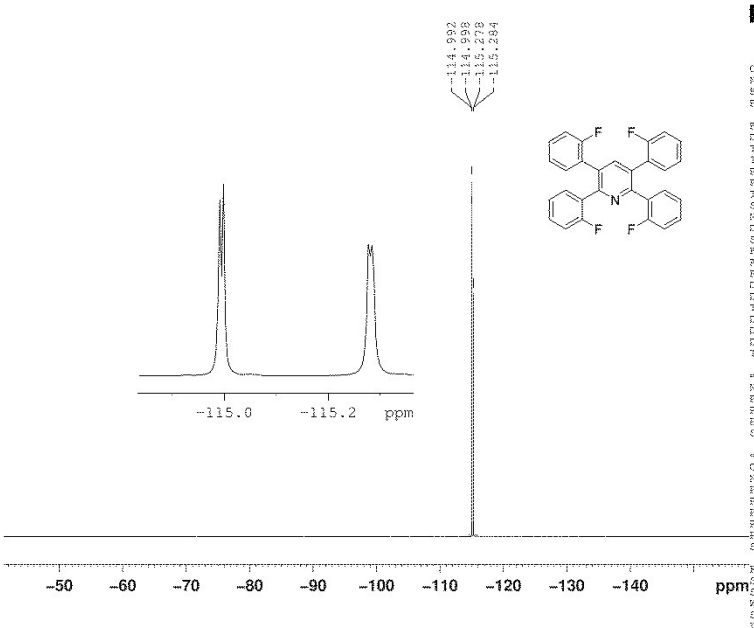
```
Current Data Parameters
NAME          141127.u322
EXPNO                  11
PROCNO                  1

F2 - Acquisition Parameters
Date_              20141127
Time                  13.16
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG           zgfhigqn
TD                  131072
SOLVENT               CDCl3
NS                       64
DS                        4
SWH               66964.289 Hz
FIDRES            0.510897 Hz
AQ                0.9787210 sec
RG                     2050
DW                  7.467 usec
DE                 10.00 usec
TE                  298.2 K
D1               1.00000000 sec
D11              0.03000000 sec
D12              0.00002000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   19F
P1                   10.00 usec
PL1                  -3.00 dB
PL1W          15.53680420 W
SFO1          282.3761148 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                72.00 usec
PL2        0 dB
PL12                 17.00 dB
PL2W          11.25325108 W
PL12W          0.22453187 W
SFO2          300.1312005 MHz

F2 - Processing parameters
SI                    65536
SF            282.4043550 MHz
WDW                      EM
SSB        0
LB                    0.30 Hz
GB         0
PC                    1.00
```



BRUKER

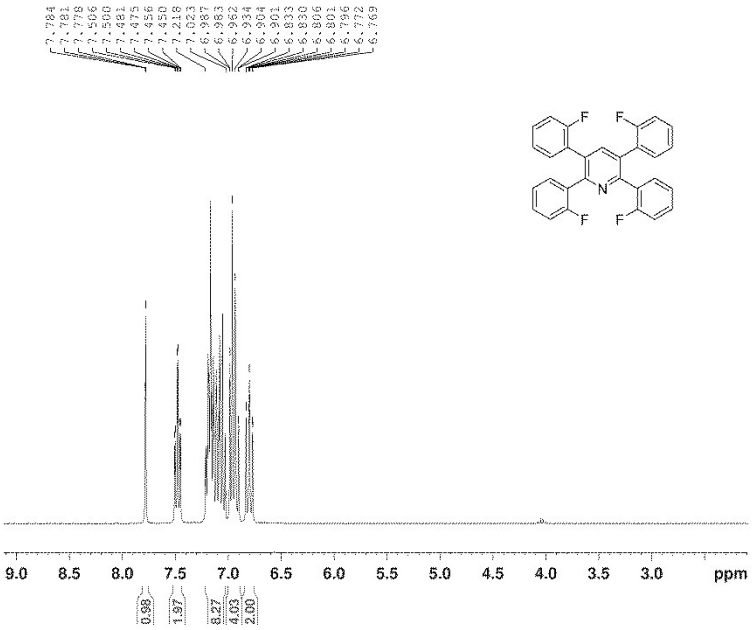
```
Current Data Parameters
NAME          141105.u309
EXPNO                  11
PROCNO                  1

F2 - Acquisition Parameters
Date_              20141105
Time                  10.44
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG           zgfhigqn
TD                  131072
SOLVENT               CDCl3
NS                       64
DS                        4
SWH               66964.289 Hz
FIDRES            0.510897 Hz
AQ                0.9787210 sec
RG                     2050
DW                  7.467 usec
DE                 10.00 usec
TE                  298.2 K
D1               1.00000000 sec
D11              0.03000000 sec
D12              0.00002000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   19F
P1                   10.00 usec
PL1                  -3.00 dB
PL1W          15.53680420 W
SFO1          282.3761148 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                72.00 usec
PL2        0 dB
PL12                 17.00 dB
PL2W          11.25325108 W
PL12W          0.22453187 W
SFO2          300.1312005 MHz

F2 - Processing parameters
SI                    65536
SF            282.4043550 MHz
WDW                      EM
SSB        0
LB                    0.30 Hz
GB         0
PC                    1.00
```

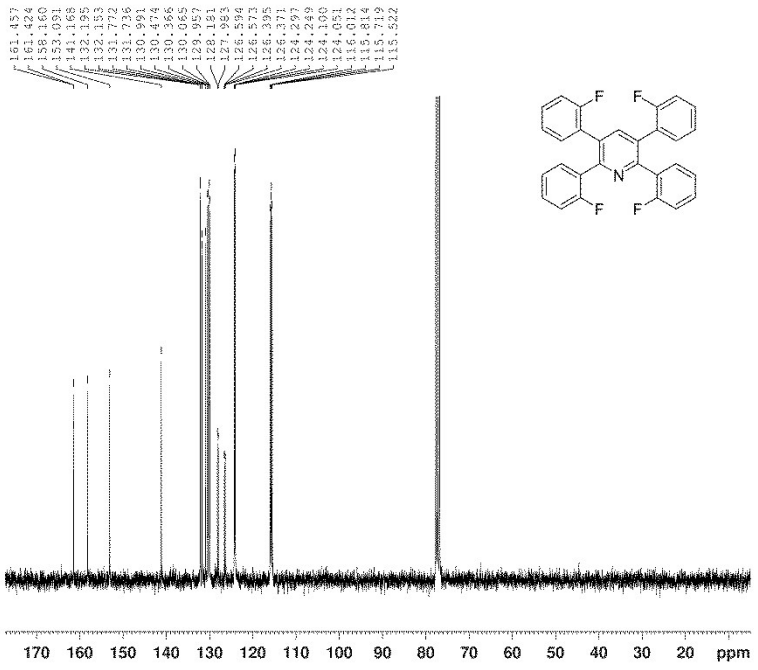



```
Current Data Parameters
NAME          141105.u309
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_          20141105
Time               10.40
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            6188.119 Hz
FIDRES         0.094423 Hz
AQ             5.2953587 sec
RG                   114
DW                80.800 usec
DE                10.00 usec
TE                298.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 10.00 usec
PL1       0 dB
PL1W       11.25325108 W
SFO1       300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF          300.1300337 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



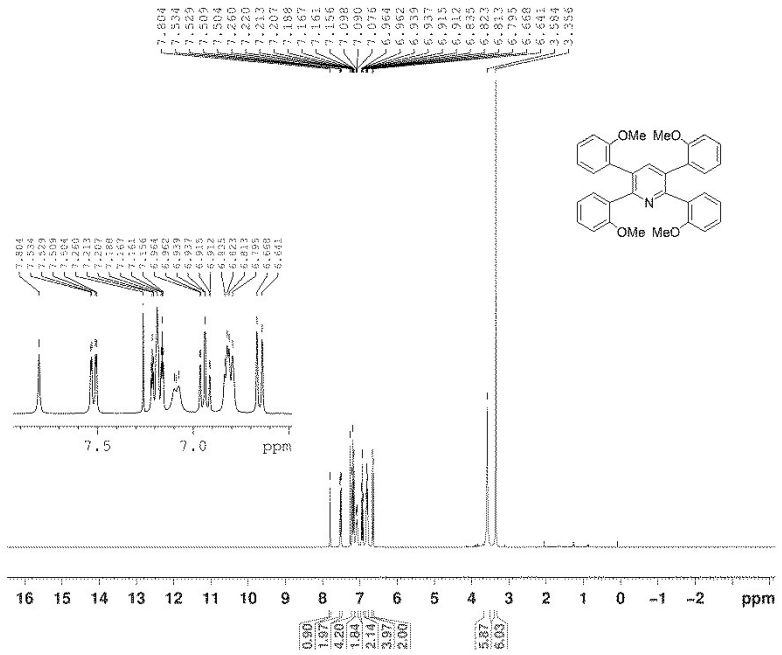

```
Current Data Parameters
NAME          141105.u309
EXPNO                  12
PROCNO                  1

F2 - Acquisition Parameters
Date_          20141105
Time               20.50
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ             1.8175818 sec
RG                  2050
DW                27.733 usec
DE                10.00 usec
TE                298.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 10.00 usec
PL1               -0.50 dB
PL1W       33.25691986 W
SFO1        75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              72.00 usec
PL2       0 dB
PL12              17.00 dB
PL13              17.00 dB
PL2W       11.25325108 W
PL12W       0.22453187 W
PL13W       0.22453187 W
SFO2       300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF          75.4677318 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

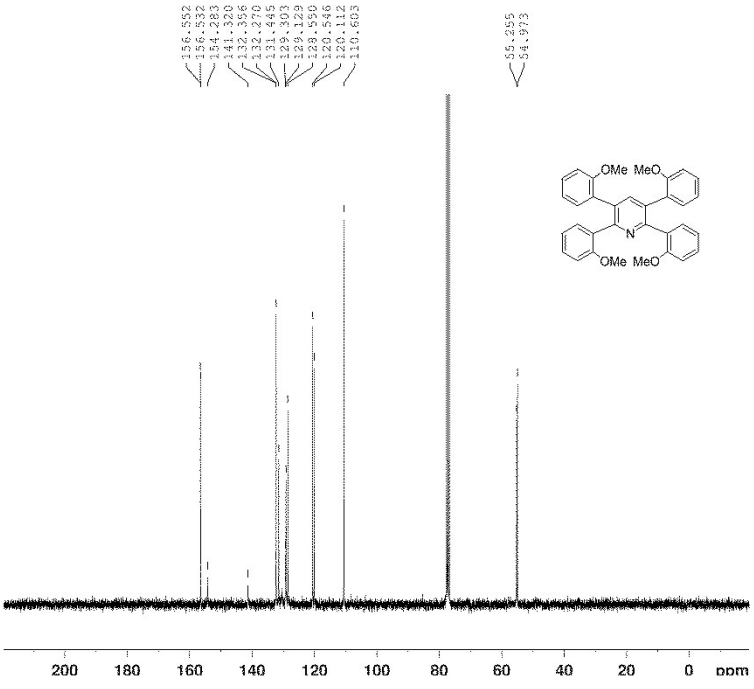



```
Current Data Parameters
NAME          141105.u311
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_              20141105
Time                  10.55
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH              6188.119 Hz
FIDRES           0.094423 Hz
AQ               5.2953587 sec
RG                     114
DW                80.800 usec
DE                10.00 usec
TE                298.2 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  10.00 usec
PL1        0 dB
PL1W       11.25325108 W
SFO1       300.1318534 MHz

F2 - Processing parameters
SI                   32768
SF            300.1300060 MHz
WDW                     EM
SSB        0
LB                   0.30 Hz
GB         0
PC                   1.00
```



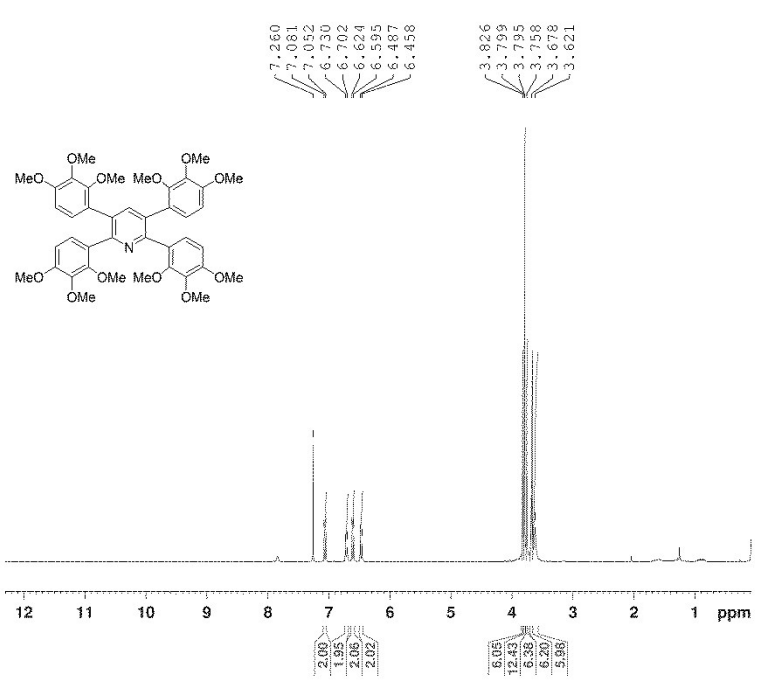

```
Current Data Parameters
NAME          141105.u311
EXPNO                  11
PROCNO                  1

F2 - Acquisition Parameters
Date_              20141105
Time                  23.46
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH             18028.846 Hz
FIDRES           0.275098 Hz
AQ               1.8175818 sec
RG                    2050
DW                27.733 usec
DE                10.00 usec
TE                298.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                  10.00 usec
PL1                 -0.50 dB
PL1W        33.25691986 W
SFO1        75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                   1H
PCPD2               72.00 usec
PL2        0 dB
PL12               17.00 dB
PL13               17.00 dB
PL2W        11.25325108 W
PL12W        0.22453187 W
PL13W        0.22453187 W
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                   32768
SF            75.4677348 MHz
WDW                     EM
SSB        0
LB                   1.00 Hz
GB         0
PC                   1.40
```



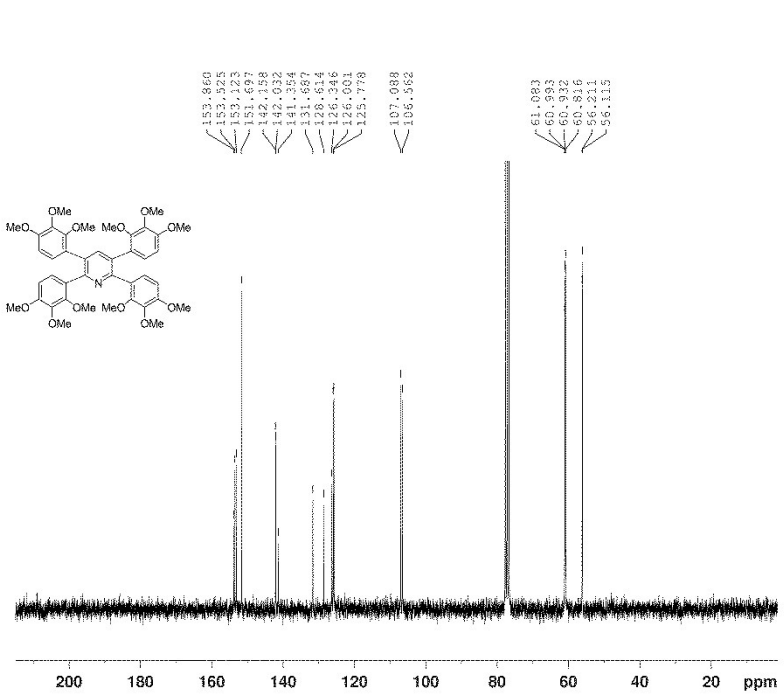
BRUKER

```
Current Data Parameters
NAME          141105.u310
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_          20141105
Time              10.50
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD               65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            6188.119 Hz
FIDRES         0.094423 Hz
AQ             5.2953587 sec
RG                  161
DW               80.805 usec
DE               10.00 usec
TE               298.2 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                10.00 usec
PL1       0 dB
PL1W        11.25325108 W
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                32768
SF          300.1300060 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



BRUKER

```
Current Data Parameters
NAME          141201.202
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_          20141201
Time              11.30
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD               65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           15000.000 Hz
FIDRES         0.228882 Hz
AQ             2.1845834 sec
RG                 2050
DW              33.333 usec
DE               10.00 usec
TE               298.7 K
D1            2.00000000 sec
D11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PL1               -1.00 dB
SFO1         62.9019280 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             70.00 usec
PL12              15.00 dB
PL13              15.00 dB
PL2               -2.50 dB
SFO2        250.1310005 MHz

F2 - Processing parameters
SI                32768
SF          62.8952254 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```