

Supporting Information

Sonogashira Cross-Coupling Reactions of 3,5-Dibromo-2,6-dichloropyridine

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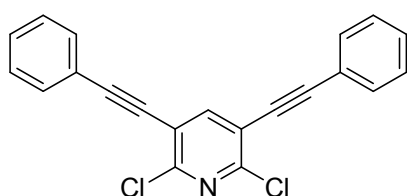
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General procedure and analytical data for 4a-g

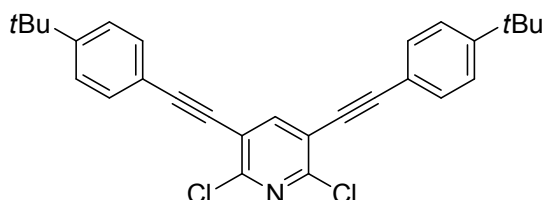
An oven-dried and argon-flushed pressure tube was charged with 3,5-dibromo-2,6-dichloropyridine **3** (0.33 mmol), Pd(dba)₂ (2.0 mol%) and HP(tBu)₃BF₄ (2.0 mol%), followed by anhydrous THF (3.0 mL). The suspension was degassed by bubbling argon through the solution for 10 min. Afterwards, the appropriate alkyne (1.3 mmol) and Et₃N (1.3 mmol) were added. The tube was sealed with a Teflon valve and the reaction mixture was stirred at room temperature for 20 h. The cooled reaction mixture was diluted with water and extracted with DCM. The combined organic layers were dried (Na₂SO₄), filtered and the filtrate was concentrated in vacuo. The residue was purified by column chromatography.

2,6-Dichloro-3,5-bis(phenylethynyl)pyridine (4a)



Starting with 3,5-dibromo-2,6-dichloropyridine **3** (100 mg, 0.327 mmol), Pd(dba)₂ (3.8 mg, 2.0 mol%), HP(tBu)₃BF₄ (1.9 mg, 2.0 mol%), ethynylbenzene (0.075 mL, 0.687 mmol), Et₃N (0.182 mL, 1.308 mmol) and THF (3.0 mL), **4a** was isolated as a colorless solid (58 mg, 66%); mp = 130-132 °C. ¹H NMR (300 MHz, CDCl₃): δ = 7.35-7.40 (m, 6H, CH), 7.52-7.58 (m, 4H, CH), 7.96 (s, 1H, CH). ¹³C NMR (75 MHz, CDCl₃): δ = 82.7 (C_{alkyne}), 98.8 (C_{alkyne}), 119.2 (C), 121.8 (C), 128.5 (CH), 129.4 (CH), 131.8 (CH), 144.7 (CH), 149.5 (C). IR (ATR, cm⁻¹): $\tilde{\nu}$ = 3048 (w), 2215 (m), 1572 (w), 1487 (m), 1397 (w), 1386 (m), 1276 (w), 1229 (w), 1156 (m), 1106 (m), 1002 (w), 925 (m), 832 (w), 779 (m), 751 (s), 734 (w), 681 (s), 527 (m), 458 (m), 383 (w). GC-MS (EI, 70 eV): m/z (%): 348 (M⁺, 26), 347 (100), 311 (3), 278 (3), 277 (15), 275 (10), 251 (3), 249 (4), 248 (6), 224 (5), 207 (4), 175 (7), 173 (8), 160 (2), 150 (3), 125 (7), 124 (4), 112 (3), 99 (3), 75 (2), 44 (2), 43 (2). HRMS (EI, 70 eV): calcd. for C₂₁H₁₁Cl₂N (M⁺): 347.02631, found 347.02588 and calcd. for C₂₁H₁₁Cl³⁷ClN (M⁺): 349.02336, found 349.02364.

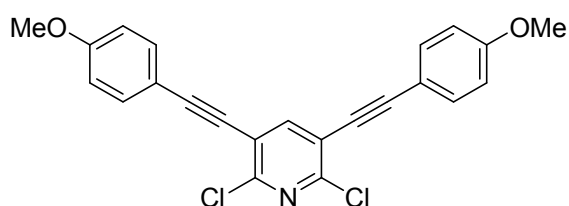
2,6-Dichloro-3,5-bis((4-tert-butylphenyl)ethynyl)pyridine (4b)



Starting with 3,5-dibromo-2,6-dichloropyridine **3** (100 mg, 0.327 mmol), Pd(dba)₂ (3.8 mg, 2.0 mol%), HP(tBu)₃BF₄ (1.9 mg, 2.0 mol%), 1-tert-butyl-4-ethynylbenzene (0.123 mL, 0.687 mmol), Et₃N (0.182 mL, 1.308 mmol) and THF (3.0 mL), **4b** was isolated as a yellow solid (87 mg, 58%); mp = 191-193 °C. ¹H NMR (400 MHz, CDCl₃): δ = 1.32 (s, 18H, CH₃ tBu), 7.38-7.41 (s, 4H, CH), 7.48-7.51 (s, 4H, CH), 7.96 (s, 1H, CH). ¹³C NMR (100 MHz, CDCl₃): δ = 31.1 (CH₃ tBu), 34.9 (C_{tBu}), 82.2 (C_{alkyne}), 98.4 (C_{alkyne}), 118.8 (C), 119.4 (C), 125.5 (CH), 131.6 (CH), 144.6 (CH), 149.2 (C), 152.9 (C). IR (ATR, cm⁻¹): $\tilde{\nu}$ = 2960 (m), 2867 (w), 2216 (w), 1909 (w), 1606 (w), 1503

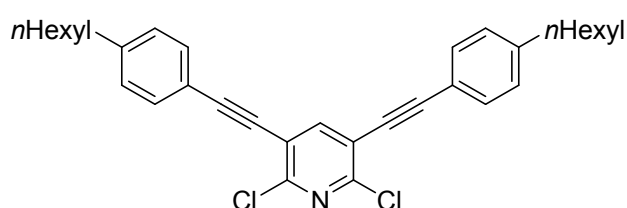
(m), 1461 (w), 1396 (w), 1383 (m), 1268 (m), 1162 (m), 1100 (m), 905 (m), 831 (s), 733 (w), 622 (w), 562 (m), 490 (w), 471 (m). GC-MS (EI, 70 eV): m/z (%): 460 (M^+ , 22), 459 (67), 449 (5), 448 (14), 447 (20), 446 (73), 445 (34), 444 (100), 418 (4), 416 (7), 405 (2), 402 (4), 400 (3), 388 (5), 362 (3), 360 (3), 341 (3), 314 (6), 301 (7), 289 (3), 215 (30), 201 (13), 187 (26), 151 (4), 57 (8), 41 (18). HRMS (EI, 70 eV): calcd. for $C_{29}H_{27}Cl_2N$ (M^+): 459.15151, found 459.15132 and calcd. for $C_{29}H_{27}Cl^{37}ClN$ (M^+): 461.14856, found 416.149000.

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



Starting with 3,5-dibromo-2,6-dichloropyridine **3** (100 mg, 0.327 mmol), $Pd(dba)_2$ (3.8 mg, 2.0 mol%), $HP(tBu)_3BF_4$ (1.9 mg, 2.0 mol%), 1-ethynyl-4-methoxybenzene (0.089 mL, 0.687 mmol), Et_3N (0.182 mL, 1.308 mmol) and THF (3.0 mL), **4c** was isolated as a colorless solid (95 mg, 71%); mp = 150-152 °C. 1H NMR (400 MHz, $CDCl_3$): δ = 3.82 (s, 6H, MeO), 6.89-6.90 (m, 4H, CH), 7.46-7.50 (m, 4H, CH), 7.89 (s, 1H, CH). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 55.3 (MeO), 81.8 (C_{alkyne}), 98.3 (C_{alkyne}), 113.9 (C), 114.2 (CH), 119.5 (C), 133.4 (CH), 144.2 (CH), 148.7 (C), 160.5 (C). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3048 (w), 2936 (w), 2836 (w), 2209 (s), 1604 (m), 1566 (m), 1506 (s), 1416 (m), 1394 (s), 1384 (m), 1299 (m), 1246 (s), 1184 (m), 1107 (m), 1030 (m), 991 (w), 913 (w), 825 (s), 742 (m), 666 (m), 530 (m), 495 (w), 473 (m), 407 (m). GC-MS (EI, 70 eV): m/z (%): 408 (M^+ , 26), 407 (100), 394 (14), 392 (20), 364 (5), 349 (4), 323 (3), 321 (5), 251 (11), 249 (3), 225 (3), 224 (3), 204 (5), 203 (10), 198 (2), 183 (4), 182 (6), 160 (6), 136 (2), 125 (4), 112 (3), 99 (3), 39 (3). HRMS (EI, 70 eV): calcd. for $C_{23}H_{15}Cl_2NO_2$ (M^+): 407.04744, found 407.04728 and calcd. for $C_{23}H_{15}Cl^{37}ClNO_2$ (M^+): 409.04449, found 409.04479.

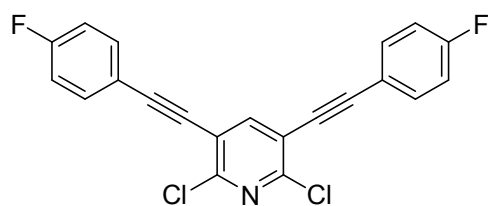
2,6-Dichloro-3,5-bis((4-*n*-hexylphenyl)ethynyl)pyridine (**4d**)



Starting with 3,5-dibromo-2,6-dichloropyridine **3** (100 mg, 0.327 mmol), $Pd(dba)_2$ (3.8 mg, 2.0 mol%), $HP(tBu)_3BF_4$ (1.9 mg, 2.0 mol%), 1-ethynyl-4-*n*-hexylbenzene (0.144 mL, 0.687 mmol), Et_3N (0.182 mL, 1.308 mmol) and THF (3.0 mL), **4d** was isolated as an orange solid (128 mg, 76%); mp = 57-59 °C. 1H NMR (400 MHz, $CDCl_3$): δ = 0.96 (t, $^3J_{H-H}$ = 7.1 Hz, 6H, CH), 1.33-1.43 (m, 12H, CH_2), 1.64-1.72 (m, 4H, CH_2), 2.69 (brt, $^3J_{H-H}$ = 7.5 Hz, 4H, CH_2), 7.24-7.26 (m, 4H, CH_2), 7.52-7.55 (m, 4H, CH), 8.01 (s, 1H, CH). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 14.0 (CH_3), 22.5 (CH_2), 28.9 (CH_2), 31.1 (CH_2), 31.6 (CH_2), 35.9 (CH_2), 82.2 (C_{alkyne}), 98.4 (C_{alkyne}), 118.9 (C), 119.4 (C), 128.6 (CH), 131.7 (CH), 144.4 (CH), 144.8 (C), 149.1 (C). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2956 (w), 2921 (m), 2852 (m), 2213 (m), 1911 (w), 1506 (m), 1467 (m), 1411 (m),

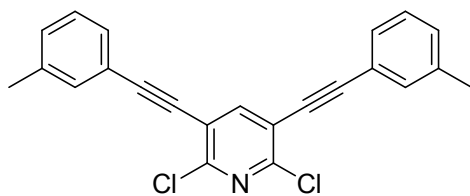
1394 (w), 1381 (m), 1279 (w), 1157 (m), 1108 (s), 989 (w), 909 (m), 841 (m), 825 (s), 724 (m), 672 (m), 647 (m), 634 (w), 580 (w), 541 (m), 533 (m), 419 (m). MS (EI, 70 eV): m/z (%): 517 (M^+ , 64), 516 (32), 515 (100), 446 (29), 445 (13), 444 (46), 375 (11), 374 (12), 373 (14), 329 (3), 314 (2), 303 (2), 301 (4), 288 (2), 187 (2), 121 (3), 83 (2), 69 (5), 60 (3), 57 (3), 44 (5), 43 (10), 40 (2). HRMS (EI, 70 eV): calcd. for $C_{33}H_{35}Cl_2N$ (M^+): 515.21411, found 515.21315 and calcd. for $C_{33}H_{35}Cl^{37}ClN$ (M^+): 517.21116, found 517.21138. Anal. calcd. for $C_{33}H_{35}Cl_2N$ (516.54): C, 76.73; H, 6.83; N, 2.71. Found: C, 76.69; H, 6.820; N, 2.690.

2,6-Dichloro-3,5-bis((4-fluorophenyl)ethynyl) pyridine (**4e**)



Starting with 3,5-dibromo-2,6-dichloropyridine **3** (100 mg, 0.327 mmol), $Pd(dba)_2$ (3.8 mg, 2.0 mol%), $HP(tBu)_3BF_4$ (1.9 mg, 2.0 mol%), 1-ethynyl-4-fluorobenzene (0.079 mL, 0.687 mmol), Et_3N (0.182 mL, 1.308 mmol) and THF (3.0 mL), **4e** was isolated as a orange solid (68 mg, 54%); mp = 168-170 °C. 1H NMR (400 MHz, $CDCl_3$): δ = 6.98-7.04 (m, 4H, CH), 7.45-7.50 (m, 4H, CH), 7.89 (s, 1H, CH). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 82.4 (C_{alkyne}), 97.1 (C_{alkyne}), 116.0 (d, $^2J_{C-F}$ = 22.2 Hz, CH), 117.9 (d, $^4J_{C-F}$ = 3.5 Hz, C), 119.1 (C), 133.8 (d, $^3J_{C-F}$ = 9.0 Hz, CH), 144.6 (CH), 149.5 (C), 162.9 (d, $^1J_{C-F}$ = 253.9 Hz, CF). ^{19}F NMR (282.4 MHz, $CDCl_3$): δ = -108.1 (F). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3040 (w), 2216 (w), 1890 (w), 1599 (m), 1499 (m), 1384 (m), 1279 (w), 1219 (m), 1154 (m), 1108 (m), 1014 (w), 935 (m), 846 (m), 830 (s), 746 (m), 734 (m), 668 (w), 601 (w), 527 (m), 460 (w), 428 (m), 400 (w). MS (EI, 70 eV): m/z (%): 384 (M^+ , 18), 383 (100), 314 (3), 313 (14), 312 (4), 311 (6), 286 (4), 192 (2), 169 (2), 147 (8), 144 (3), 143 (4), 57 (2), 43 (2), 36 (3). HRMS (EI, 70 eV): calcd. for $C_{21}H_9Cl_2F_2N$ (M^+): 383.00746, found 383.00728 and calcd. for $C_{21}H_9Cl^{37}ClFN$ (M^+): 385.00451, found 385.00463 and calcd. for $C_{21}H_9^{37}Cl_2F_2N$ (M^+): 387.00156, found 387.00217. Anal. calcd. for $C_{21}H_9Cl_2F_2N$ (384.21): C, 65.65; H, 2.36; N, 3.65. Found: C, 65.38; H, 2.331; N, 3.648.

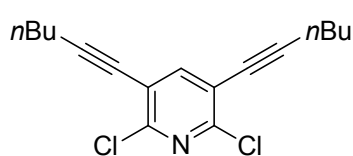
2,6-Dichloro-3,5-bis(*m*-tolylethynyl)pyridine (**4f**)



Starting with 3,5-dibromo-2,6-dichloropyridine **3** (100 mg, 0.327 mmol), $Pd(dba)_2$ (3.8 mg, 2.0 mol%), $HP(tBu)_3BF_4$ (1.9 mg, 2.0 mol%), 1-ethynyl-3-methylbenzene (0.088 mL, 0.687 mmol), Et_3N (0.182 mL, 1.308 mmol) and THF (3.0 mL), **4f** was isolated as a colorless solid (91 mg, 74%); mp = 104-106 °C. 1H NMR (400 MHz, $CDCl_3$): δ = 2.36 (s, 6H, CH_3), 7.19-7.22 (m, 2H, CH), 7.24-7.28 (m, 2H, CH), 7.35-7.38 (m, 4H, CH), 7.94 (s, 1H, CH). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 21.2 (CH_3), 82.4 (C_{alkyne}), 98.4 (C_{alkyne}), 119.3 (C), 121.7 (C), 128.4 (CH), 128.9 (CH), 130.4 (CH), 132.3 (CH), 138.3 (C), 144.7 (CH), 149.4 (C). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2913 (w), 2215 (m), 1599 (w), 1579 (m), 1513 (w), 1481 (m), 1393 (w), 1383 (m), 1277 (w), 1231 (w),

1199 (m), 1149 (m), 1108 (m), 1043 (w), 910 (m), 882 (m), 792 (m), 784 (s), 732 (m), 686 (s), 618 (w), 524 (w), 458 (m), 448 (m). GC-MS (EI, 70 eV): m/z (%): 376 (M^+ , 25), 375 (100), 305 (2), 304 (5), 303 (4), 302 (6), 301 (6), 290 (2), 289 (4), 288 (9), 277 (3), 276 (4), 275 (2), 274 (2), 263 (2), 189 (3), 188 (3), 187 (2), 151 (6), 139 (5), 138 (3). HRMS (EI, 70 eV): calcd. for $C_{23}H_{15}Cl_2N$ (M^+): 375.05761, found 375.05751 and calcd. for $C_{23}H_{15}Cl^{37}ClN$ (M^+): 377.05466, found 377.05504. Anal. calcd. for $C_{23}H_{15}Cl_2N$ (376.28): C, 73.42; H, 4.02; N, 3.72. Found: C, 73.64; H, 4.125; N, 3.814.

2,6-Dichloro-3,5-di(hex-1-ynyl)pyridine (**4g**)

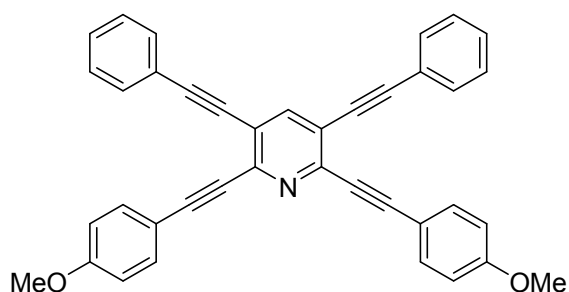


Starting with 3,5-dibromo-2,6-dichloropyridine **3** (100 mg, 0.327 mmol), $Pd(dba)_2$ (3.8 mg, 2.0 mol%), $HP(tBu)_3BF_4$ (1.9 mg, 2.0 mol%), *n*-hex-1-yne (0.077 mL, 0.687 mmol), Et_3N (0.182 mL, 1.308 mmol) and THF (3.0 mL), **4g** was isolated as a colorless oil (42 mg, 42%). 1H NMR (400 MHz, $CDCl_3$): δ = 0.92 (t, $^3J_{H-H}$ = 7.3 Hz, 6H, CH_3), 1.42-1.61 (m, 4H, CH), 2.44 (t, $^3J_{H-H}$ = 7.3 Hz, 4H, CH_2), 7.69 (s, 1H, C). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 13.6 (CH_3), 19.4 (CH_2), 22.0 (CH_2), 30.3 (CH_2), 74.5 (C_{alkyne}), 100.1 (C_{alkyne}), 119.7 (C), 145.3 (CH), 148.9 (C). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2958 (w), 2932 (w), 2871 (w), 2235 (m), 1714 (m), 1464 (w), 1382 (s), 1227 (m), 1119 (m), 1092 (m), 915 (m), 737 (m), 646 (m), 483 (w). GC-MS (EI, 70 eV): m/z (%): 308 (M^+ , 21), 307 (100), 294 (25), 292 (41), 274 (14), 272 (46), 270 (11), 266 (34), 265 (10), 264 (43), 258 (14), 257 (10), 256 (37), 250 (6), 244 (20), 242 (9), 238 (10), 236 (24), 230 (16), 228 (14), 221 (14), 220 (14), 216 (16), 215 (11), 214 (20), 208 (17), 206 (11), 204 (11), 202 (20), 200 (27), 192 (19), 188 (20), 186 (16), 178 (19), 165 (23), 151 (43), 125 (13), 99 (13), 81 (17), 75 (15), 63 (13), 43 (30), 41 (55), 39 (18), 29 (13). HRMS (EI, 70 eV): calcd. for $C_{17}H_{19}Cl_2N$ (M^+): 307.08891, found 307.08884 and calcd. for $C_{17}H_{19}Cl^{37}ClN$ (M^+): 309.08596, found 309.08616.

General procedure and analytical data for 5a-e

An oven-dried and argon-flushed pressure tube was charged with the appropriate 2,6-dichloro-3,5-dialkynyl-substituted pyridines **4** (0.2 mmol), PdCl₂(CH₃CN)₂ (5.0 mol%), XPhos (10.0 mol%) and CuI (5.0 mol%) followed by anhydrous 1,4-dioxane (2.6 mL). The suspension was degassed by bubbling argon through the solution for 10 min. Afterwards, the appropriate alkyne (0.74 mmol) and HN(*i*Pr)₂ (0.65 mL) were added. The tube was sealed with a Teflon valve and the reaction mixture was stirred at 80 °C for 20 h. The cooled reaction mixture was diluted with water and extracted with DCM. The combined organic layers were dried (Na₂SO₄), filtered and the filtrate was concentrated in vacuo. The residue was purified by column chromatography.

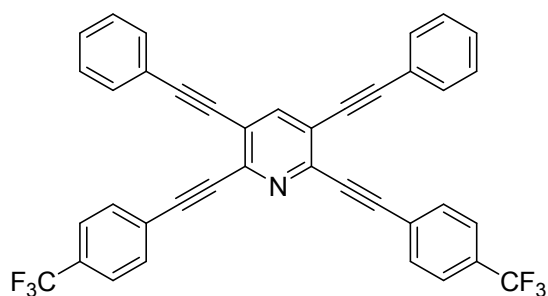
2,6-Bis((4-methoxyphenyl)ethynyl)-3,5-bis(phenylethynyl)pyridine (5a)



Starting with 2,6-dichloro-3,5-bis(phenylethynyl)pyridine **4a** (65 mg, 0.186 mmol), PdCl₂(CH₃CN)₂ (2.4 mg, 5.0 mol%), XPhos (8.9 mg, 10.0 mol%), 1-ethynyl-4-methoxy-benzene (0.096 mL, 0.744 mmol), CuI (1.8 mg, 5.0 mol%), HN(*i*Pr)₂ (0.65 mL, 4.625 mmol) and 1,4-dioxane

(2.6 mL), **5a** was isolated as a yellow solid (93 mg, 93%); mp = 206-208 °C. ¹H NMR (300 MHz, CDCl₃): δ = 3.81 (s, 6H, MeO), 6.83-6.88 (m, 4H, CH), 7.34-7.39 (m, 6H, CH), 7.54-7.59 (m, 8H, CH), 7.93 (s, 1H, CH). ¹³C NMR (75 MHz, CDCl₃): δ = 55.3 (MeO), 85.6 (C_{alkyne}), 86.9 (C_{alkyne}), 95.6 (C_{alkyne}), 97.2 (C_{alkyne}), 114.1 (CH), 114.1 (C), 120.7 (C), 122.6 (C), 128.5 (CH), 129.0 (CH), 131.7 (CH), 133.5 (CH), 141.0 (CH), 143.9 (C), 160.5 (C). IR (ATR, cm⁻¹): ν̃ = 3048 (w), 2928 (w), 2836 (w), 2541 (w), 2201 (m), 1601 (m), 1565 (m), 1508 (m), 1485 (m), 1441 (m), 1409 (m), 1295 (m), 1247 (s), 1170 (m), 1153 (m), 1135 (m), 1105 (m), 1069 (m), 1022 (m), 918 (m), 900 (m), 835 (s), 815 (m), 798 (m), 752 (s), 689 (s), 675 (m), 642 (w), 531 (s), 472 (w), 432 (w), 414 (w). MS (EI, 70 eV): m/z (%): 540 (M⁺, 39), 539 (100), 524 (4), 4453 (4), 452 (7), 451 (5), 450 (5), 449 (2), 270 (3), 226 (5), 225 (6), 207 (2), 66 (5), 65 (3), 57 (2), 44 (8), 39 (2). HRMS (ESI, 70 eV): calcd. for C₃₉H₂₆NO₂ ([M+H]⁺): 540.19581, found 540.19558.

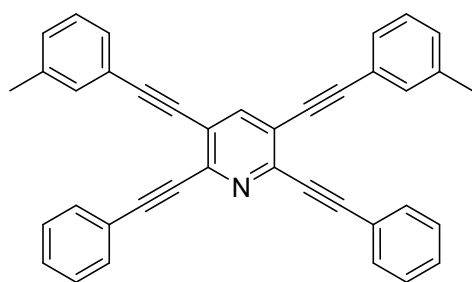
2,6-Bis((4-(trifluoromethyl)phenyl)ethynyl)-3,5-bis(phenylethynyl)pyridine (5b)



Starting with 2,6-dichloro-3,5-bis(phenylethynyl)pyridine **4a** (65 mg, 0.186 mmol), PdCl₂(CH₃CN)₂ (2.4 mg, 5.0 mol%), XPhos (8.9 mg, 10.0 mol%), 1-ethynyl-4-(trifluoromethyl)benzene (0.122 mL, 0.744 mmol), CuI (1.8 mg, 5.0 mol%), HN(*i*Pr)₂ (0.65 mL, 4.625 mmol) and 1,4-dioxane (2.6 mL), **5a**

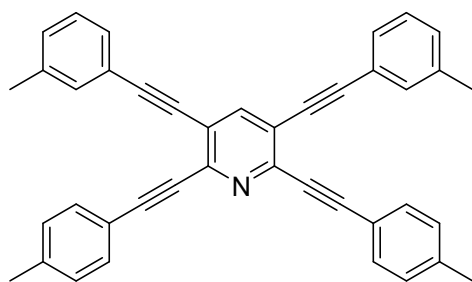
was isolated as a yellow solid (104 mg, 91%); mp = 205-207 °C. ¹H NMR (300 MHz, CDCl₃): δ = 7.34-7.41 (m, 6H, CH), 7.53-7.61 (m, 8H, CH), 7.69-7.71 (m, 4H, CH), 8.01 (s, 1H, CH). ¹³C NMR (75 MHz, CDCl₃): δ = 85.0 (C_{alkyne}), 89.3 (C_{alkyne}), 93.2 (C_{alkyne}), 98.4 (C_{alkyne}), 122.2 (C), 122.4 (C), 124.0 (q, ¹J_{C-F} = 272.4 Hz, CF₃), 125.4 (q, ³J_{C-F} = 3.9 Hz, CH), 125.8 (C), 128.7 (CH), 129.5 (CH), 131.0 (q, ²J_{C-F} = 33.2 Hz, C), 131.7 (CH), 132.4 (CH), 141.3 (CH), 143.0 (C). ¹⁹F NMR (282.4 MHz, CDCl₃): δ = -62.5 (CF₃). IR (ATR, cm⁻¹): ν̃ = 3055 (w), 2928 (w), 2204 (m), 1610 (m), 1515 (w), 1487 (s), 1319 (s), 1223 (w), 1161 (s), 1117 (s), 1103 (s), 1064 (s), 1014 (m), 913 (m), 837 (m), 755 (m), 735 (m), 687 (m), 594 (m), 549 (w), 526 (m), 390 (w). MS (EI, 70 eV): m/z (%): 616 (M⁺, 51), 615 (100), 614 (12), 546 (3), 544 (3), 294 (4), 145 (2), 114 (11), 101 (3), 99 (3), 91 (3), 86 (6), 85 (4), 83 (4), 81 (3), 73 (12), 71 (4), 70 (4), 66 (11), 65 (6), 64 (3), 60 (12), 56 (9), 55 (7), 44 (20), 43 (15), 42 (9), 41 (9), 40 (4), 39 (6). HRMS (EI, 70 eV): calcd. for C₃₉H₁₉F₆N (M⁺): 615.14162, found 615.14346. Anal. calcd. for C₃₉H₁₉F₆N (615.57): C, 76.10; H, 3.11; N, 2.28. Found: C, 76.06; H, 2.908; N, 2.071.

2,6-Bis(phenylethynyl)-3,5-bis(*m*-tolylethynyl)pyridine (5c).



Starting with 2,6-dichloro-3,5-bis(*m*-tolylethynyl)-pyridine **4f** (70 mg, 0.186 mmol), PdCl₂(CH₃CN)₂ (2.4 mg, 5.0 mol%), XPhos (8.9 mg, 10.0 mol%), ethynylbenzene (0.065 mL, 0.744 mmol), CuI (1.8 mg, 5.0 mol%), HN(*i*Pr)₂ (0.65 mL, 4.625 mmol) and 1,4-dioxane (2.6 mL), **5c** was isolated as an orange solid (85 mg, 90%); mp = 136-138 °C. ¹H NMR (300 MHz, CDCl₃): δ = 2.32 (s, 6H, CH₃), 7.17-7.27 (m, 4H, CH), 7.32-7.41 (m, 10H, CH), 7.63-7.67 (m, 4H, CH), 7.94 (s, 1H, CH). ¹³C NMR (75 MHz, CDCl₃): δ = 21.1 (CH₃), 85.2 (C_{alkyne}), 87.7 (C_{alkyne}), 95.0 (C_{alkyne}), 98.0 (C_{alkyne}), 121.6 (C), 122.1 (C), 122.2 (C), 128.4 (CH), 128.7 (CH), 129.3 (CH), 130.0 (CH), 132.2 (CH), 132.4 (CH), 138.2 (C), 140.8 (CH), 143.4 (C). IR (ATR, cm⁻¹): ν̃ = 3035 (w), 2917 (w), 2856 (w), 2204 (m), 1596 (m), 1579 (w), 1489 (m), 1442 (m), 1414 (m), 1223 (m), 1153 (m), 1126 (w), 1024 (w), 997 (w), 912 (m), 874 (w), 782 (m), 767 (s), 754 (s), 685 (s), 620 (w), 553 (w), 531 (m), 487 (m), 466 (w), 444 (w). MS (EI, 70 eV): m/z (%): 508 (M⁺, 52), 507 (100), 506 (15), 505 (5), 492 (3), 491 (3), 490 (3), 240 (2), 239 (2), 238 (1), 237 (1). HRMS (ESI, 70 eV): calcd. for C₃₉H₂₆N ([M+H]⁺): 508.20598, found 508.20651.

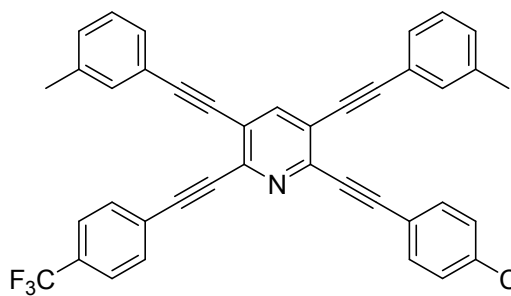
2,6-Bis(*p*-tolylethynyl)-3,5-bis(*m*-tolylethynyl)pyridine (**5d**)



Starting with 2,6-dichloro-3,5-bis(*m*-tolylethynyl) pyridine **4f** (70 mg, 0.186 mmol), PdCl₂(CH₃CN)₂ (2.4 mg, 5.0 mol%), XPhos (8.9 mg, 10.0 mol%), 1-ethynyl-4-methylbenzene (0.121 mL, 0.744 mmol), CuI (1.8 mg, 5.0 mol%), HN(*i*Pr)₂ (0.65 mL, 4.625 mmol) and 1,4-dioxane (2.6 mL), **5d** was isolated as a yellow solid (87 mg, 87%); mp = 210-212 °C.

¹H NMR (300 MHz, CDCl₃): δ = 2.33 (s, 6H, CH₃), 2.37 (s, 6H, CH₃), 7.14-7.28 (m, 8H, CH), 7.36-7.41 (m, 4H, CH), 7.52-7.55 (m, 4H, CH), 7.93 (s, 1H, CH). ¹³C NMR (75 MHz, CDCl₃): δ = 21.2 (CH₃), 21.6 (CH₃), 85.3 (C_{alkyne}), 87.3 (C_{alkyne}), 95.4 (C_{alkyne}), 97.7 (C_{alkyne}), 119.1 (C), 121.3 (C), 122.3 (C), 128.4 (CH), 128.7 (CH), 129.2 (CH), 130.0 (CH), 132.1 (CH), 132.4 (CH), 138.2 (C), 139.7 (C), 140.8 (CH), 143.7 (C). IR (ATR, cm⁻¹): $\tilde{\nu}$ = 3031 (w), 2945 (m), 2915 (w), 2853 (w), 2210 (m), 1597 (w), 1574 (w), 1509 (m), 1481 (m), 1409 (m), 1277 (w), 1220 (w), 1192 (w), 1177 (w), 1150 (w), 1121 (w), 1041 (m), 1019 (w), 916 (m), 904 (m), 871 (w), 839 (w), 807 (m), 792 (s), 775 (s), 705 (w), 685 (s), 673 (w), 646 (w), 528 (s), 489 (m), 462 (w), 446 (s), 401 (w). MS (EI, 70 eV): m/z (%): 536 (M⁺,43), 535 (100), 534 (9), 533 (2), 520 (4), 518 (3), 503 (2), 428 (1), 268 (2), 260 (2), 254 (2), 252 (3), 44 (2). HRMS (ESI, 70 eV): calcd. for C₄₁H₃₀N ([M+H]⁺): 536.23748, found 536.23728.

2,6-Bis((4-(trifluoromethyl)phenyl)ethynyl)-3,5-bis(*m*-tolylethynyl)pyridine (**5e**)



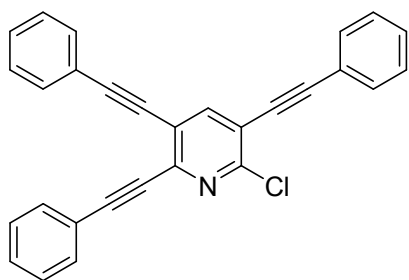
Starting with 2,6-dichloro-3,5-bis(*m*-tolylethynyl) pyridine **4f** (70 mg, 0.186 mmol), PdCl₂(CH₃CN)₂ (2.4 mg, 5.0 mol%), XPhos (8.9 mg, 10.0 mol%), 1-ethynyl-4-(trifluoromethyl)benzene (0.121 mL, 0.744 mmol), CuI (1.8 mg, 5.0 mol%), HN(*i*Pr)₂ (0.65 mL, 4.625 mmol) and 1,4-dioxane (2.6 mL), **5e** was isolated as a yellow solid (103 mg, 86%); mp = 178-180 °C. ¹H NMR (300 MHz, CDCl₃): δ = 2.31 (s, 6H, CH₃), 7.19-7.27 (m, 4H, CH), 7.32-7.35 (m, 4H, CH), 7.56-7.58 (m, 4H, CH), 7.68-7.71 (m, 4H, CH), 7.95 (s, 1H, CH). ¹³C NMR (75 MHz, CDCl₃): δ = 21.1 (CH₃), 84.8 (C_{alkyne}), 89.5 (C_{alkyne}), 93.0 (C_{alkyne}), 98.7 (C_{alkyne}), 122.0 (C), 122.4 (C), 123.8 (q, ¹J_{C-F} = 272.3 Hz, CF₃), 125.3 (q, ³J_{C-F} = 3.8 Hz, CH), 125.8 (C), 128.5 (CH), 128.7 (CH), 130.3 (CH), 130.9 (q, ²J_{C-F} = 33.7 Hz, C), 132.3 (CH), 132.4 (CH), 138.3 (C), 141.0 (CH), 142.8 (C). ¹⁹F NMR (282.4 MHz, CDCl₃): δ = -62.5 (CF₃). IR (ATR, cm⁻¹): $\tilde{\nu}$ = 3037 (w), 2921 (w), 2863 (w), 2204 (m), 1612 (m), 1516 (w), 1482 (m), 1405 (m), 1380 (w), 1320 (s), 1156 (m), 1117 (s), 1104 (m), 1065 (s), 1015 (m), 917 (w), 834 (m), 782 (m), 769 (m), 719 (m), 834 (m), 782 (m), 769 (m), 686 (m), 594 (m), 521 (w), 440 (w), 386 (w). MS (EI, 70 eV): m/z (%): 644 (M⁺,44), 643 (100), 642 (10), 641 (3), 628 (3), 624 (4), 558 (2), 308 (3), 307 (3), 279 (2), 244 (2), 237 (3), 139 (2), 44 (5). HRMS (ESI,

70 eV): calcd. for $C_{41}H_{24}F_6N$ ($[M+H]^+$): 644.18075, found 644.18053. Anal. calcd. for $C_{41}H_{23}F_6N$ (643.62): C, 76.51; H, 3.60; N, 2.18. Found: C, 76.33; H, 3.466; N, 1.940.

General procedure and analytical data for 6a-e

An oven-dried and argon-flushed pressure tube was charged with 3,5-dibromo-2,6-dichloropyridine **3** (0.33 mmol), $Pd(dba)_2$ (3.0 mol%) and $HP(tBu)_3BF_4$ (3.0 mol%), followed by anhydrous THF (3.0 mL). The suspension was degassed by bubbling argon through the solution for 10 min. Afterwards, the appropriate alkyne (1.3 mmol) and Et_3N (1.3 mmol) were added. The tube was sealed with a Teflon valve and stirred at room temperature 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.

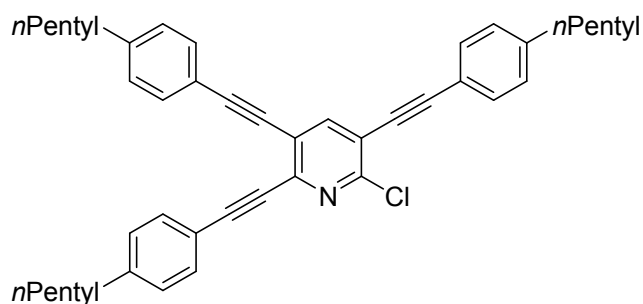
2-Chloro-3,5,6-tris(phenylethynyl)pyridine (6a)



Starting with 3,5-dibromo-2,6-dichloropyridine **3** (100 mg, 0.327 mmol), $Pd(dba)_2$ (5.6 mg, 3.0 mol%), $HP(tBu)_3BF_4$ (2.9 mg, 3.0 mol%), ethynylbenzene (0.143 mL, 1.308 mmol), Et_3N (0.182 mL, 1.308 mmol) and THF (3.0 mL), **6a** was isolated as a yellow solid (79 mg, 58%); mp = 140-142 °C. 1H NMR (400 MHz, $CDCl_3$): δ = 7.32-7.39 (m, 9H, CH), 7.54-7.62 (m, 6H, CH), 7.96 (s,

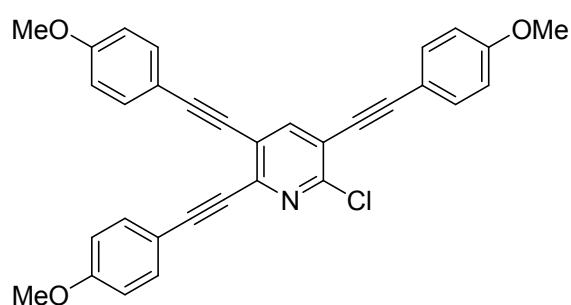
1H, CH). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 83.8 (C_{alkyne}), 84.3 (C_{alkyne}), 87.1 (C_{alkyne}), 96.2 (C_{alkyne}), 97.2 (C_{alkyne}), 98.5 (C_{alkyne}), 119.2 (C), 121.6 (C), 121.8 (C), 122.0 (C), 122.2 (C), 128.5 (CH), 128.5 (CH), 128.5 (CH), 129.2 (CH), 129.4 (CH), 129.6 (CH), 131.7 (CH), 131.8 (CH), 132.2 (CH), 142.8 (C), 143.0 (CH), 150.5 (C). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3044 (w), 2212 (m), 1595 (w), 1507 (w), 1491 (m), 1417 (m), 1386 (m), 1333 (w), 1153 (m), 1122 (m), 1067 (w), 1012 (w), 909 (w), 858 (w), 750 (s), 681 (s), 594 (m), 528 (m), 431 (m). GC-MS (EI, 70 eV): m/z (%): 414 (M^+ , 36), 413 (100), 412 (9), 377 (14), 376 (20), 375 (15), 373 (11), 350 (10), 338 (5), 281 (5), 250 (7), 249 (5), 224 (5), 207 (9), 189 (21), 188 (8), 175 (9), 174 (6), 161 (8), 156 (4), 150 (5), 136 (6), 133 (5), 117 (3), 112 (4), 100 (4), 87 (4), 76 (4), 75 (7), 39 (3). HRMS (EI, 70 eV): calcd. for $C_{29}H_{16}ClN$ (M^+): 413.09658, found 413.09657.

2-Chloro-3,5,6-tris((4-*n*-pentylphenyl)ethynyl)pyridine (**6b**)



Starting with 3,5-dibromo-2,6-dichloropyridine **3** (100 mg, 0.327 mmol), Pd(dba)₂ (5.6 mg, 3.0 mol%), HP(tBu)₃BF₄ (2.6 mg, 3.0 mol%), 1-ethynyl-4-*n*-pentylbenzene (0.254 mL, 1.308 mmol), Et₃N (0.182 mL, 1.308 mmol) and THF (3.0 mL), **6b** was isolated as an orange solid (98 mg, 48%); mp = 86-88 °C. ¹H NMR (400 MHz, CDCl₃): δ = 0.88 (t, ³J_{H-H} = 6.5 Hz, 3H, CH₃), 0.89 (t, ³J_{H-H} = 6.9 Hz, 3H, CH₃), 0.89 (t, ³J_{H-H} = 6.6 Hz, 3H, CH₃), 1.28-1.36 (m, 12H, CH₂), 1.57-1.64 (m, 12H, CH₂), 2.59-2.64 (m, 6H, CH₂), 7.15-7.19 (m, 6H, CH), 7.46-7.54 (m, 6H, CH), 7.91 (s, 1H, CH). ¹³C NMR (100 MHz, CDCl₃): δ = 13.9 (CH₃), 13.9 (CH₃), 13.9 (CH₃), 22.4 (CH₂), 22.4 (CH₂), 22.4 (CH₂), 30.8 (CH₂), 30.8 (CH₂), 30.8 (CH₂), 31.4 (CH₂), 31.4 (CH₂), 31.4 (CH₂), 35.9 (CH₂), 35.9 (CH₂), 83.4 (C_{alkyne}), 83.9 (C_{alkyne}), 86.9 (C_{alkyne}), 96.6 (C_{alkyne}), 97.4 (C_{alkyne}), 98.8 (C_{alkyne}), 119.0 (C), 119.2 (C), 119.2 (C), 119.4 (C), 121.6 (C), 128.5 (CH), 128.6 (CH), 128.6 (CH), 131.1 (CH), 131.7 (CH), 132.2 (CH), 142.7 (C), 142.8 (CH), 144.5 (C), 144.7 (C), 144.9 (C), 150.1 (C). IR (ATR, cm⁻¹): $\tilde{\nu}$ = 3031 (w), 2954 (m), 2925 (s), 2855 (m), 2215 (m), 1903 (w), 1688 (w), 1605 (w), 1509 (m), 1416 (m), 1387 (s), 1334 (m), 1223 (m), 1153 (m), 1122 (s), 1010 (w), 906 (m), 835 (m), 812 (s), 752 (m), 729 (m), 548 (s), 529 (s). MS (EI, 70 eV): m/z (%): 624 (M⁺, 46), 623 (100), 569 (2), 568 (6), 566 (12), 510 (14), 496 (1), 466 (2), 454 (4), 453 (7), 452 (2), 440 (1), 329 (3), 312 (2), 246 (7), 227 (3), 73 (14), 60 (19), 44 (31), 43 (7), 41 (4). HRMS (EI, 70 eV): calcd. for C₄₄H₄₆ClN (M⁺): 623.33133, found 623.33093 and calcd. for C₄₄H₄₆³⁷ClN (M⁺): 625.32838, found 625.33064.

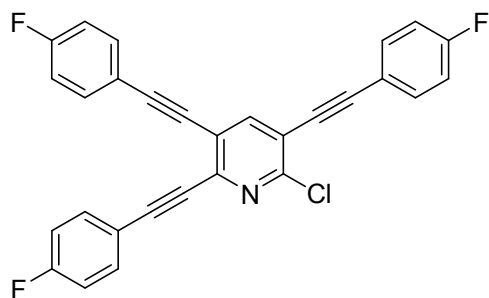
2-Chloro-3,5,6-tris((4-methoxyphenyl)ethynyl)pyridine (**6c**)



Starting with 3,5-dibromo-2,6-dichloropyridine **3** (100 mg, 0.327 mmol), Pd(dba)₂ (5.6 mg, 3.0 mol%), HP(tBu)₃BF₄ (2.9 mg, 3.0 mol%), 1-ethynyl-4-methoxybenzene (0.169 mL, 1.308 mmol), Et₃N (0.182 mL, 1.308 mmol) and THF (3.0 mL), **6c** was isolated as an orange solid (108 mg, 66%); mp = 148-150 °C. ¹H NMR (400 MHz, CDCl₃): δ = 3.79 (s, 3H, MeO), 3.80 (s, 3H, MeO), 3.80 (s, 3H, MeO), 6.84-6.89 (m, 6H, CH), 7.46-7.55 (m, 6H, CH), 7.87 (s, 1H, CH). ¹³C NMR (100 MHz, CDCl₃): δ = 55.3 (MeO), 55.3 (MeO), 55.3 (MeO), 83.0 (C_{alkyne}), 83.5 (C_{alkyne}), 86.6 (C_{alkyne}), 96.4 (C_{alkyne}), 97.2 (C_{alkyne}), 98.6 (C_{alkyne}), 113.9 (C), 114.1 (C), 114.1 (C), 114.1 (CH), 114.2 (CH), 114.2 (CH), 114.4 (C), 119.1 (C), 121.5 (C), 133.2 (CH), 133.4 (CH), 133.8 (CH), 142.5 (CH), 149.8 (C), 160.3 (C), 160.4 (C), 160.6 (C). IR (ATR, cm⁻¹): $\tilde{\nu}$ = 2998 (w), 2932 (w), 2836 (w), 2196 (m), 1601 (m), 1562 (m), 1506 (s),

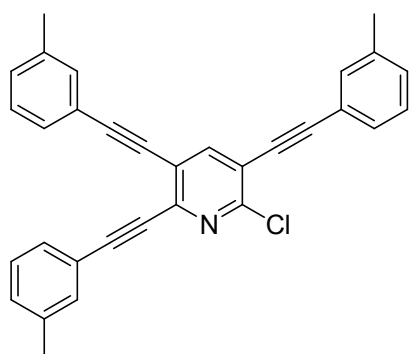
1385 (m), 1294 (m), 1245 (s), 1172 (m), 1149 (m), 1122 (m), 1106 (m), 1031 (m), 918 (w), 905 (w), 827 (s), 779 (m), 752 (m), 705 (m), 661 (w), 564 (m), 530 (m), 489 (m), 427 (w), 387 (w). MS (EI, 70 eV): m/z (%): 504 (M^+ , 29), 503 (100), 490 (4), 489 (3), 488 (8), 473 (2), 460 (3), 445 (2), 338 (3), 329 (2), 252 (3), 230 (2), 187 (2), 176 (2), 169 (3), 44 (2). HRMS (EI, 70 eV): calcd. for $C_{32}H_{22}ClNO_3$ (M^+): 503.12827, found 503.12902.

2-Chloro-3,5,6-tris((4-fluorophenyl)ethynyl)pyridine (**6d**)



Starting with 3,5-dibromo-2,6-dichloropyridine **3** (100 mg, 0.327 mmol), $Pd(dba)_2$ (5.6 mg, 3.0 mol%), $HP(tBu)_3BF_4$ (2.9 mg, 3.0 mol%), ethynylbenzene (0.149 mL, 1.308 mmol), Et_3N (0.182 mL, 1.308 mmol) and THF (3.0 mL), **6d** was isolated as a yellow solid (78 mg, 51%); mp = 184-186 °C. 1H NMR (300 MHz, $CDCl_3$): δ = 7.01-7.10 (m, 6H, CH), 7.48-7.57 (m, 6H, CH), 7.91 (s, 1H, CH). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 83.5 (C_{alkyne}), 84.0 (C_{alkyne}), 86.8 (C_{alkyne}), 95.1 (C_{alkyne}), 96.1 (C_{alkyne}), 97.6 (C_{alkyne}), 115.9 (d, $^2J_{C-F}$ = 22.0 Hz, CH), 116.09 (d, $^2J_{C-F}$ = 22.4 Hz, CH), 116.1 (d, $^2J_{C-F}$ = 22.4 Hz, CH), 117.8 (d, $^4J_{C-F}$ = 3.8 Hz, C), 118.0 (d, $^4J_{C-F}$ = 3.8 Hz, C), 118.3 (d, $^4J_{C-F}$ = 3.8 Hz, C), 133.6 (d, $^3J_{C-F}$ = 8.3 Hz, CH), 133.8 (d, $^3J_{C-F}$ = 8.3 Hz, CH), 134.2 (d, $^3J_{C-F}$ = 8.4 Hz, CH), 142.6 (C), 142.9 (CH), 150.5 (C), 163.0 (d, $^1J_{C-F}$ = 251.4 Hz, CF), 163.3 (d, $^1J_{C-F}$ = 251.2 Hz, CF), 163.5 (d, $^1J_{C-F}$ = 251.2 Hz, CF). ^{19}F NMR (282.4 MHz, $CDCl_3$): δ = -108.7 (F). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2219 (m), 1600 (m), 1566 (w), 1507 (s), 1419 (m), 1388 (m), 1337 (w), 1282 (w), 1228 (s), 1153 (m), 1126 (m), 1090 (m), 1011 (w), 915 (w), 828 (s), 797 (m), 753 (w), 712 (w), 608 (m), 528 (m), 455 (w), 405 (w), 387 (w). GC-MS (EI, 70 eV): m/z (%): 468 (M^+ , 36), 467 (100), 466 (11), 431 (15), 430 (11), 429 (16), 411 (7), 404 (4), 286 (5), 234 (7), 233 (3), 215 (6), 192 (4), 178 (4), 144 (5), 143 (4). HRMS (EI, 70 eV): calcd. for $C_{29}H_{13}ClF_3N$ (M^+): 467.06831, found 467.06865. Anal. calcd. for $C_{29}H_{13}ClF_3N$ (467.87): C, 74.45; H, 2.80; N, 2.99. Found: C, 74.45; H, 2.603; N, 2.683.

2-Chloro-3,5,6-tris(*m*-tolylethynyl)pyridine (**6e**)



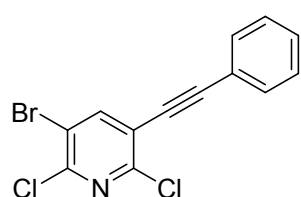
Starting with 3,5-dibromo-2,6-dichloropyridine **3** (100 mg, 0.327 mmol), $Pd(dba)_2$ (5.6 mg, 3.0 mol%), $HP(tBu)_3BF_4$ (2.9 mg, 3.0 mol%), 1-ethynyl-3-methylbenzene (0.169 mL, 1.308 mmol), Et_3N (0.182 mL, 1.308 mmol) and THF (3.0 mL), **6e** was isolated as an orange solid (83 mg, 56%); mp = 126-128 °C. 1H NMR (400 MHz, $CDCl_3$): δ = 2.31 (brs, 3H, CH_3), 2.33 (brs, 3H, CH_3), 2.36 (brs, 3H, CH_3), 7.18-7.28 (m, 6H, CH), 7.36-7.45 (m, 6H, CH), 7.92 (s, 1H, CH). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 21.1 (CH_3), 21.2 (CH_3), 21.2 (CH_3), 83.6 (C_{alkyne}), 84.2

(C_{alkyne}), 87.0 (C_{alkyne}), 96.6 (C_{alkyne}), 97.5 (C_{alkyne}), 98.7 (C_{alkyne}), 119.2 (C), 121.7 (C), 121.7 (C), 121.8 (C), 122.1 (C), 128.3 (CH), 128.4 (CH), 128.4 (CH), 128.6 (CH), 128.8 (CH), 128.9 (CH), 129.3 (CH), 130.1 (CH), 130.2 (CH), 130.5 (CH), 132.3 (CH), 132.9 (CH), 138.1 (C), 138.2 (C), 138.2 (C), 142.8 (C), 124.9 (CH), 150.3 (C). IR (ATR, cm⁻¹): $\tilde{\nu}$ = 2918 (w), 2211 (m), 1598 (w), 1578 (w), 1503 (m), 1402 (w), 1380 (m), 1337 (w), 1199 (m), 1118 (m), 1033 (m), 917 (m), 902 (m), 875 (m), 779 (s), 682 (s), 602 (w), 505 (w), 476 (m), 439 (m), 406 (w). MS (EI, 70 eV): m/z (%): 456 (M⁺, 41), 455 (100), 454 (11), 440 (5), 404 (5), 402 (4), 388 (4), 228 (2), 220 (2), 202 (3), 201 (5), 200 (2), 195 (2), 194 (2), 188 (2), 187 (2), 139 (1). HRMS (EI, 70 eV): calcd. for C₃₂H₂₂ClN (M⁺): 455.14353, found 455.14260 and calcd. for C₃₂H₂₂³⁷ClN (M⁺): 457.14058, found 457.14178.

General procedure and analytical data for 7a-e

An oven-dried and argon-flushed pressure tube was charged with 3,5-dibromo-2,6-dichloropyridine **3** (0.33 mmol), PdCl₂(CH₃CN)₂ (3.0 mol%), tBuXPhos (6.0 mol%) and CuI (5.0 mol%) followed by anhydrous 1,4-dioxane (3.0 mL). The suspension was degassed by bubbling argon through the solution for 10 min. Afterwards, the appropriate alkyne (0.4 mmol) and HN(*i*Pr)₂ (1.3 mmol) were added. The tube was sealed with a Teflon valve and the reaction mixture was stirred at 80 °C for 20 h. The cooled reaction mixture was diluted with water and extracted with DCM. The combined organic layers were dried (Na₂SO₄), filtered and the filtrate was concentrated in vacuo. The residue was purified by column chromatography.

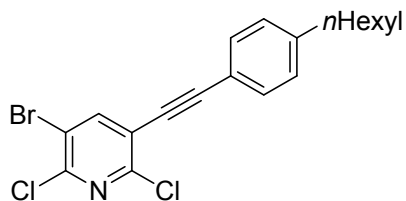
3-Bromo-2,6-dichloro-5-(phenylethynyl)pyridine (7a)



Starting with 3,5-dibromo-2,6-dichloropyridine **3** (100 mg, 0.327 mmol), PdCl₂(CH₃CN)₂ (2.5 mg, 3.0 mol%), tBuXPhos (8.3 mg, 6.0 mol%), CuI (3.1 mg, 5.0 mol%), ethynylbenzene (0.047 mL, 0.425 mmol), HN(*i*Pr)₂ (0.183 mL, 1.308 mmol) and 1,4-dioxane (3.0 mL), **7a** was isolated as a slightly yellow solid (53 mg, 50%); mp = 130-132 °C. ¹H NMR (400 MHz, CDCl₃): δ = 7.34-7.40 (m, 3H, CH), 7.53-7.56 (m, 2H, CH), 8.05 (s, 1H, CH). ¹³C NMR (100 MHz, CDCl₃): δ = 82.2 (C_{alkyne}), 98.8 (C_{alkyne}), 118.1 (C), 120.7 (C), 121.5 (C), 128.6 (CH), 129.7 (CH), 131.8 (CH), 145.6 (CH), 148.3 (C), 149.6 (C). IR (ATR, cm⁻¹): $\tilde{\nu}$ = 3056 (w), 2217 (m), 1508 (w), 1488 (m), 1441 (w), 1393 (m), 1340 (m), 1270 (m), 1127 (m), 1156 (m), 1102 (s), 1084 (s), 907 (m), 833 (w), 784 (m), 752 (s), 686 (s), 673 (m), 683 (w), 589 (w), 529 (m), 512 (m), 439 (418 (w), 385 (w). GC-MS (EI, 70 eV): m/z (%): 327 (M⁺, 100), 326 (10), 325 (61), 213 (10), 212 (5), 211 (32), 210 (3), 176 (14), 175 (11), 160 (5), 150 (10), 149 (6), 135 (2), 133 (3), 123 (4), 111 (3), 110 (3), 98 (5), 92 (5), 77 (3), 75 (11), 74 (6), 51 (4), 50 (3). HRMS (EI, 70 eV): calcd. for C₁₃H₆BrCl₂N (M⁺): 324.90552, found 324.90549 and

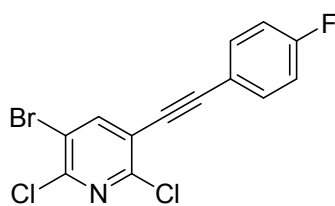
calcd. for $C_{13}H_6^{81}BrCl_2N$ (M^+): 326.90347, found 326.90308 and calcd. for $C_{13}H_6^{81}BrCl^{37}ClN$ (M^+): 328.90052, found 328.90066 and calcd. for $C_{13}H_6^{81}Br^{37}Cl_2N$ (M^+): 330.89757, found 330.89823. Anal. calcd. for $C_{13}H_6BrCl_2N$ (327.00): C, 47.75; H, 1.85; N, 4.28. Found: C, 47.81; H, 1.874; N, 4.001.

3-Bromo-2,6-dichloro-5-((4-*n*-hexylphenyl)ethynyl)pyridine (**7b**)



Starting with 3,5-dibromo-2,6-dichloropyridine **3** (100 mg, 0.327 mmol), $PdCl_2(CH_3CN)_2$ (2.5 mg, 3.0 mol%), *t*BuXPhos (8.3 mg, 6.0 mol%), CuI (3.1 mg, 5.0 mol%), 1-ethynyl-4-*n*-hexylbenzene (0.088 mL, 0.425 mmol), $HN(iPr)_2$ (0.183 mL, 1.308 mmol) and 1,4-dioxane (3.0 mL), **7b** was isolated as a slightly yellow solid (56 mg, 43%); mp = 50-52 °C. 1H NMR (400 MHz, $CDCl_3$): δ = 0.86 (t, $^3J_{H-H}$ = 6.6 Hz, 3H, CH_3), 1.23 -1.35 (m, 6H, CH), 1.56-1.63 (m, 2H, CH), 2.61 (t, $^3J_{H-H}$ = 7.3 Hz, 2H, CH_2), 7.16-7.18 (m, 2H, CH), 7.43-7.46 (m, 2H, CH), 8.02 (s, 1H, CH). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 14.1 (CH_3), 22.6 (CH_2), 28.9 (CH_2), 31.2 (CH_2), 31.7 (CH_2), 36.1 (CH_2), 81.2 (C_{alkyne}), 99.4 (C_{alkyne}), 118.1 (C), 118.7 (C), 121.0 (C), 128.7 (CH), 131.8 (CH), 145.2 (C), 145.5 (CH), 148.1 (C), 149.6 (C). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3050 (w), 2955 (w), 2922 (m), 2853 (m), 2209 (s), 1807 (w), 1604 (w), 1394 (s), 1341 (m), 1272 (w), 1224 (w), 1157 (s), 1117 (w), 1084 (s), 1018 (w), 820 (m), 723 (m), 668 (m), 625 (m), 588 (m), 551 (s), 511 (m), 440 (w), 423 (w). GC-MS (EI, 70 eV): m/z (%): 411 (M^+ , 55), 410 (9), 409 (42), 353 (3), 342 (44), 341 (15), 340 (100), 339 (9), 338 (50), 332 (4), 268 (4), 224 (22), 188 (18), 175 (2), 173 (5), 102 (2), 41 (13), 32 (4). HRMS (ESI, 70 eV): calcd. for $C_{19}H_{19}BrCl_2N$ ($[M+H]^+$): 410.00724, found 410.00654. Anal. calcd. for $C_{19}H_{18}BrCl_2N$ (411.16): C, 55.50; H, 4.41; N, 3.41. Found: C, 55.66; H, 4.217; N, 3.228.

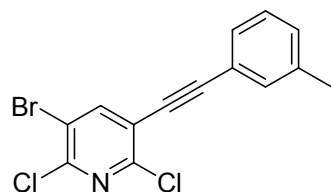
3-Bromo-2,6-dichloro-5-((4-fluorophenyl)ethynyl)pyridine (**7c**)



Starting with 3,5-dibromo-2,6-dichloropyridine **3** (100 mg, 0.327 mmol), $PdCl_2(CH_3CN)_2$ (2.5 mg, 3.0 mol%), *t*BuXPhos (8.3 mg, 6.0 mol%), CuI (3.1 mg, 5.0 mol%), 1-ethynyl-4-fluoro-benzene (51 mg, 0.425 mmol), $HN(iPr)_2$ (0.183 mL, 1.308 mmol) and 1,4-dioxane (3.0 mL), **7c** was isolated as a slightly yellow solid (52 mg, 46%); mp = 122-124 °C. 1H NMR (300 MHz, $CDCl_3$): δ = 7.04-7.10 (m, 2H, CH), 7.50-7.55 (m, 2H, CH), 8.03 (s, 1H, CH). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 82.0 (C_{alkyne}), 97.7 (C_{alkyne}), 116.0 (d, $^2J_{C-F}$ = 23.4 Hz, CH), 117.7 (d, $^4J_{C-F}$ = 3.4 Hz, C), 118.1 (C), 120.5 (C), 133.9 (d, $^3J_{C-F}$ = 8.4 Hz, CH), 145.5 (CH), 148.4 (C), 149.6 (C), 163.3 (d, $^1J_{C-F}$ = 255.4 Hz, CF). ^{19}F NMR (282.4 MHz, $CDCl_3$): δ = -107.8 (F). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3046 (w), 2922 (w), 2215 (m), 1902 (w), 1656 (w), 1596 (m), 1504 (s), 1393 (m), 1340 (m), 1228 (m), 1154 (s), 1095 (w), 1083 (s), 1012 (w), 907 (m), 838 (s), 816 (w), 755 (m), 666 (m), 606 (w), 587 (m), 532 (m), 510 (w), 426 (m), 398 (w). GC-MS (EI, 70 eV): m/z (%): 345 (M^+ , 100), 344 (13), 343 (54), 307 (3), 229 (32), 227 (4), 194 (12), 173 (5), 168

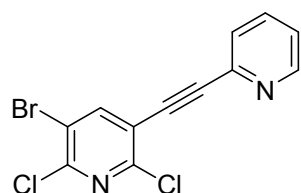
(15), 167 (5), 148 (4), 143 (4), 142 (4), 133 (3), 132 (3), 123 (5), 114 (2), 103 (4), 101 (9), 99 (7), 86 (4), 84 (5), 75 (3), 57 (2), 44 (4). HRMS (ESI, 70 eV): calcd. for C₁₃H₆BrCl₂FN ([M+H]⁺): 343.90392, found 343.90372.

3-Bromo-2,6-dichloro-5-(*m*-tolylethynyl)pyridine (7d)



Starting with 3,5-dibromo-2,6-dichloropyridine **3** (100 mg, 0.327 mmol), PdCl₂(CH₃CN)₂ (2.5 mg, 3.0 mol%), *t*BuXPhos (8.3 mg, 6.0 mol%), CuI (3.1 mg, 5.0 mol%), 1-ethynyl-3-methyl-benzene (0.054 mL, 0.425 mmol), HN(*i*Pr)₂ (0.183 mL, 1.308 mmol) and 1,4-dioxane (3.0 mL), **7d** was isolated as a slightly yellow solid (68 mg, 61%); mp = 106-108 °C. ¹H NMR (400 MHz, CDCl₃): δ = 2.35 (s, 3H, CH₃), 7.19-7.28 (m, 2H, CH), 7.34-7.37 (m, 2H, CH), 8.03 (s, 1H, CH). ¹³C NMR (100 MHz, CDCl₃): δ = 21.2 (CH₃), 81.9 (C_{alkyne}), 99.1 (C_{alkyne}), 118.0 (C), 120.7 (C), 121.3 (C), 128.4 (CH), 128.9 (CH), 130.6 (CH), 132.4 (CH), 138.3 (C), 145.5 (CH), 148.2 (C), 149.6 (C). IR (ATR, cm⁻¹): $\tilde{\nu}$ = 2918 (w), 2206 (m), 1971 (w), 1593 (w), 1484 (m), 1390 (m), 1338 (m), 1276 (w), 1228 (m), 1162 (m), 1145 (m), 1109 (w), 1084 (s), 1038 (w), 996 (w), 939 (w), 896 (m), 868 (m), 792 (s), 722 (m), 688 (m), 673 (w), 642 (w), 628 (m), 591 (m), 508 (w), 439 (m). GC-MS (EI, 70 eV): m/z (%): 341 (M⁺, 100), 340 (16), 339 (62), 338 (5), 306 (3), 226 (7), 225 (9), 224 (20), 199 (3), 190 (13), 189 (11), 188 (15), 174 (4), 171 (3), 164 (8), 163 (8), 139 (4), 115 (3), 112 (7), 110 (3), 99 (3), 94 (4), 81 (8), 74 (3), 63 (4), 39 (4). HRMS (ESI, 70 eV): calcd. for C₁₄H₉BrCl₂N ([M+H]⁺): 339.92899, found 339.92872.

3-Bromo-2,6-dichloro-5-(pyridin-2-ylethynyl)pyridine (7e)



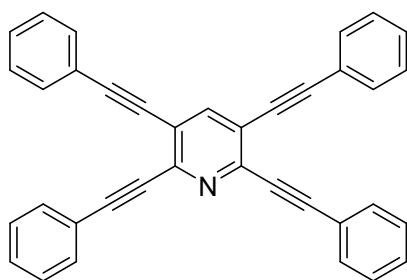
Starting with 3,5-dibromo-2,6-dichloropyridine **3** (100 mg, 0.327 mmol), PdCl₂(CH₃CN)₂ (2.5 mg, 3.0 mol%), *t*BuXPhos (8.3 mg, 6.0 mol%), CuI (3.1 mg, 5.0 mol%), 2-ethynylpyridine (0.048 mL, 0.425 mmol), HN(*i*Pr)₂ (0.183 mL, 1.308 mmol) and 1,4-dioxane (3.0 mL), **7e** was isolated as a slightly yellow solid (44 mg, 41%); mp = 130-132 °C. ¹H NMR (400 MHz, CDCl₃): δ = 7.31 (ddd, ³J_{H-H} = 7.8 Hz, ⁴J_{H-H} = 4.3 Hz, ⁵J_{H-H} = 1.3 Hz, 1H, CH), 7.56-7.58 (m 1H, CH), 7.72 (ddd, ³J_{H-H} = 8.2 Hz, ³J_{H-H} = 7.8 Hz, ⁴J_{H-H} = 1.7 Hz, 1H, CH), 8.11 (s, 1H, CH), 8.64 (ddd, ³J_{H-H} = 5.1 Hz, ⁴J_{H-H} = 1.9 Hz, ⁵J_{H-H} = 0.9 Hz, 1H, CH). ¹³C NMR (100 MHz, CDCl₃): δ = 81.5 (C_{alkyne}), 97.1 (C_{alkyne}), 118.2 (C), 119.7 (C), 123.9 (CH), 127.8 (CH), 136.4 (CH), 141.9 (C), 146.2 (CH), 149.3 (C), 150.0 (C), 150.3 (CH). IR (ATR, cm⁻¹): $\tilde{\nu}$ = 2920 (w), 1580 (m), 1562 (m), 1504 (w), 1462 (s), 1391 (s), 1340 (m), 1287 (m), 1227 (m), 1152 (m), 1094 (s), 1043 (w), 991 (m), 903 (m), 887 (w), 805 (w), 795 (s), 772 (s), 735 (m), 678 (m), 631 (m), 528 (m), 504 (w), 438 (m), 400 (w). GC-MS (EI, 70 eV): m/z (%): 328 (M⁺, 100), 327 (9), 326 (61), 294 (3), 293 (26), 291 (20), 249 (11), 247 (17), 212 (12), 186 (9), 185 (6), 178 (2), 177 (16), 151 (4), 150 (4), 124 (5), 123

(5), 112 (2), 111 (3), 110 (3), 108 (2), 99 (6), 98 (6), 86 (3), 85 (3), 78 (6), 74 (4), 62 (4), 51 (7), 50 (3). HRMS (ESI, 70 eV): calcd. for $C_{12}H_6BrCl_2N_2$ ($[M+H]^+$): 326.90859, found 326.90864.

General procedure and analytical data for 8a-g

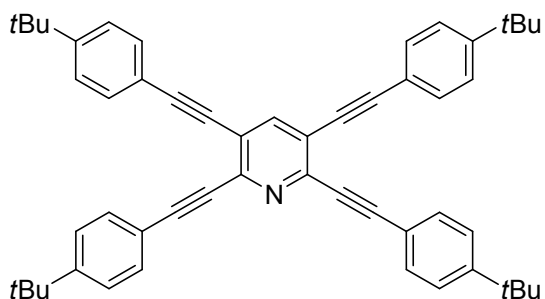
An oven-dried and argon-flushed pressure tube was charged with 3,5-dibromo-2,6-dichloropyridine **3** (0.33 mmol), $PdCl_2(CH_3CN)_2$ (5.0 mol%), XPhos (10.0 mol%) and CuI (5 mol%), followed by anhydrous 1,4-dioxane (4.0 mL). The suspension was degassed by bubbling argon through the solution for 10 min. Afterwards, the appropriate alkyne (1.3 mmol) and $HN(iPr)_2$ (1.0 mL) were added. The tube was sealed with a Teflon valve and the reaction mixture was stirred at 80 °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-Tetrakis(phenylethynyl)pyridine (**8a**)



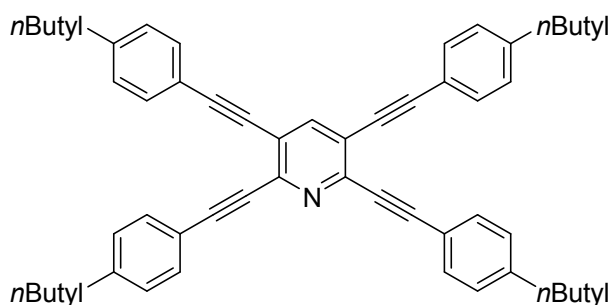
Starting with 3,5-dibromo-2,6-dichloropyridine **3** (100 mg, 0.327 mmol), $PdCl_2(CH_3CN)_2$ (4.2 mg, 5.0 mol%), XPhos (15.6 mg, 10.0 mol%), ethynylbenzene (0.337 mL, 2.616 mmol), CuI (3.1 mg, 5.0 mol%), $HN(iPr)_2$ (1.0 mL, 7.115 mmol) and 1,4-dioxane (4.0 mL), **8a** was isolated as a yellow solid (151 mg, 96%); mp = 169-171 °C. 1H NMR (400 MHz, $CDCl_3$): δ = 7.30-7.41 (m, 12H, CH), 7.55-7.66 (m, 8H, CH), 7.97 (s, 1H, CH). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 85.4 (C_{alkyne}), 87.6 (C_{alkyne}), 95.0 (C_{alkyne}), 97.6 (C_{alkyne}), 121.4 (C), 122.1 (C), 122.4 (c), 128.4 (CH), 128.5 (CH), 129.1 (CH), 129.3 (CH), 131.7 (CH), 132.1 (CH), 141.6 (CH), 143.5 (C). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3077 (w), 2955 (w), 2922 (w), 2850 (w), 2203 (m), 1596 (m), 1568 (m), 1489 (m), 1440 (m), 1413 (m), 1291 (w), 1134 (w), 1066 (w), 1024 (w), 997 (w), 908 (m), 744 (s), 679 (s), 614 (w), 528 (s), 463 (w), 446 (w), 416 (w). MS (EI, 70 eV): m/z (%): 480 (M^+ , 42), 479 (100), 478 (21), 477 (8), 476 (10), 475 (4), 450 (2), 401 (3), 239 (5), 238 (7), 237 (3), 224 (5), 200 (2), 175 (2), 129 (6), 101 (3), 97 (3), 85 (4), 84 (4), 83 (4), 73 (19), 71 (6), 60 (23), 57 (10), 56 (4), 55 (9), 44 (14), 43 (15), 41 (9), 40 (4). HRMS (EI, 70 eV): calcd. for $C_{37}H_{21}N$ (M^+): 479.16685, found 479.16645.

2,3,5,6-Tetrakis((4-*tert*-butylphenyl)ethynyl)pyridine (**8b**)



Starting with 3,5-dibromo-2,6-dichloropyridine **3** (100 mg, 0.327 mmol), PdCl₂(CH₃CN)₂ (4.2 mg, 5.0 mol%), XPhos (15.6 mg, 10.0 mol%), 1-*tert*-butyl-4-ethynylbenzene (0.535 mL, 2.616 mmol), CuI (3.1 mg, 5.0 mol%), HN(*i*Pr)₂ (1.0 mL, 7.115 mmol) and 1,4-dioxane (4.0 mL), **8b** was isolated as an orange solid (216 mg, 94%); mp = 125-127 °C. ¹H NMR (400 MHz, CDCl₃): δ = 1.32 (s, 18H, CH₃ *t*Bu), 1.33 (s, 18H, CH₃ *t*Bu), 7.36-7.40 (m, 8H, CH), 7.50-7.59 (m, 8H, CH), 7.95 (s, 1H, CH). ¹³C NMR (100 MHz, CDCl₃): δ = 31.1 (CH₃ *t*Bu), 34.9 (C_{*t*Bu}), 85.1 (C_{alkyne}), 87.4 (C_{alkyne}), 95.2 (C_{alkyne}), 97.7 (C_{alkyne}), 119.2 (C), 119.5 (C), 121.4 (C), 125.4 (CH), 125.5 (CH), 131.5 (CH), 132.0 (CH), 141.1 (CH), 143.5 (C), 152.5 (C), 152.7 (C). IR (ATR, cm⁻¹): $\tilde{\nu}$ = 2959 (s), 2903 (w), 2865 (w), 2204 (m), 1604 (w), 1504 (m), 1461 (m), 1416 (m), 1362 (m), 1262 (s), 1201 (w), 1161 (w), 1103 (s), 1016 (s), 911 (w), 830 (s), 799 (s), 770 (m), 736 (w), 697 (w), 559 (s), 392 (m). MS (EI, 70 eV): m/z (%): 704 (M⁺, 60), 703 (100), 688 (11), 632 (5), 600 (2), 560 (3), 352 (5), 337 (7), 207 (8), 145 (3), 123 (2), 116 (2), 115 (3), 114 (23), 98 (7), 97 (6), 86 (16), 85 (5), 84 (4), 83 (7), 73 (6), 66 (19), 65 (10), 57 (17), 56 (16), 55 (14), 45 (22), 44 (68), 43 (30), 42 (18), 41 (17), 39 (10). HRMS (ESI, 70 eV): calcd. for C₅₃H₅₄N ([M+H]⁺): 704.42508, found 704.42416.

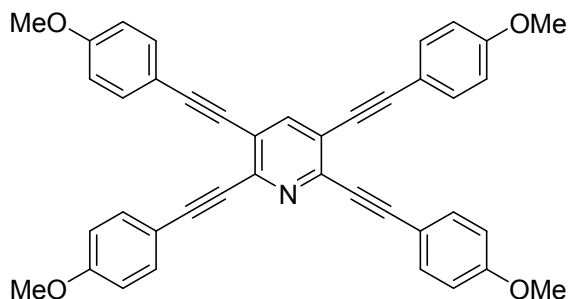
2,3,5,6-Tetrakis((4-*n*-butylphenyl)ethynyl)pyridine (**8c**)



Starting with 3,5-dibromo-2,6-dichloro-pyridine **3** (100 mg, 0.327 mmol), PdCl₂(CH₃CN)₂ (4.2 mg, 5.0 mol%), XPhos (15.6 mg, 10.0 mol%), 1-*n*-butyl-4-ethynylbenzene (0.460 mL, 2.616 mmol), CuI (3.1 mg, 5.0 mol%), HN(*i*Pr)₂ (1.0 mL, 7.115 mmol) and 1,4-dioxane (4.0 mL), **8c** was isolated as a yellow solid (221 mg, 96%); mp = 116-118 °C. ¹H NMR (300 MHz, CDCl₃): δ = 0.91 (t, ³J_{H-H} = 7.8 Hz, 6H, CH₃), 0.921 (t, ³J_{H-H} = 7.5 Hz, 6H, CH₃), 1.29-1.41 (m, 8H, CH₂), 1.54-1.65 (m, 8H, CH₂), 2.59-2.65 (m, 8H, CH₂), 7.14-7.19 (m, 8H, CH), 7.47-7.56 (m, 8H, CH), 7.93 (s, 1H, CH). ¹³C NMR (75 MHz, CDCl₃): δ = 13.9 (CH₃), 13.9 (CH₃), 22.3 (CH₂), 22.3 (CH₂), 33.3 (CH₂), 33.3 (CH₂), 35.6 (CH₂), 35.7 (CH₂), 85.1 (C_{alkyne}), 85.4 (C_{alkyne}), 95.3 (C_{alkyne}), 97.7 (C_{alkyne}), 119.3 (C), 119.7 (C), 121.4 (C), 128.5 (CH), 128.6 (CH), 131.6 (CH), 132.6 (CH), 140.9 (CH), 143.4 (C), 144.3 (C), 144.6 (C). IR (ATR, cm⁻¹): $\tilde{\nu}$ = 3030 (w), 2954 (m), 2925 (s), 2856 (s), 2204 (m), 1686 (w), 1605 (m), 1509 (s), 1465 (w), 1412 (m), 1377 (w), 1156 (w), 1132 (w), 1070 (w), 912 (m), 821 (s), 770 (s), 728 (m), 668 (w), 595 (w), 541 (m), 455 (w). MS (EI, 70 eV): m/z (%): 704 (M⁺, 53), 703 (100), 660 (2), 618 (13), 546 (3), 352 (3), 281 (2), 267 (7), 207 (4), 105 (2), 97 (2), 91 (3), 83 (3), 77 (2), 73 (4), 69 (5), 60 (3), 57 (6), 55 (5), 45 (4), 44

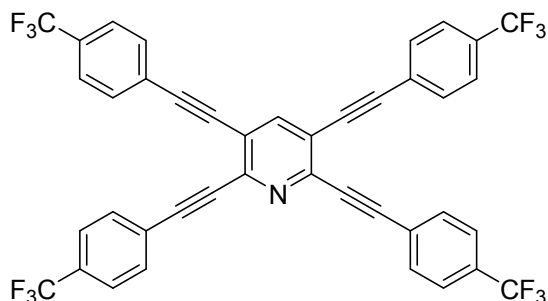
(98), 43 (9), 41 (6), 36 (10). HRMS (ESI, 70 eV): calcd. for $C_{53}H_{54}N$ ($[M+H]^+$): 704.42508, found 704.42452 and calcd. for $C_{53}H_{54}NNa$ ($[M+Na]^+$): 726,40702, found 726.40633.

2,3,5,6-Tetrakis((4-methoxyphenyl)ethynyl)pyridine (**8d**)



Starting with 3,5-dibromo-2,6-dichloropyridine **3** (100 mg, 0.327 mmol), $PdCl_2(CH_3CN)_2$ (4.2 mg, 5.0 mol%), XPhos (15.6 mg, 10.0 mol%), 1-ethynyl-4-methoxybenzene (0.340 mL, 2.616 mmol), CuI (3.1 mg, 5.0 mol%), $HN(iPr)_2$ (1.0 mL, 7.115 mmol) and 1,4-dioxane (4.0 mL), **8d** was isolated as a yellow solid (185 mg, 94%); mp = 211-213 °C. 1H NMR (400 MHz, $CDCl_3$): δ = 3.80 (s, 6H, MeO), 3.81 (s, 6H, MeO), 6.84-6.89 (m, 8H, CH), 7.47-7.51 (m, 8H, CH), 7.86 (s, 1H, CH). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 55.3 (MeO), 55.3 (MeO), 84.6 (C_{alkyne}), 87.0 (C_{alkyne}), 95.1 (C_{alkyne}), 97.5 (C_{alkyne}), 114.1 (CH), 114.1 (CH), 114.3 (C), 114.6 (C), 121.1 (C), 132.2 (CH), 133.8 (CH), 140.5 (CH), 143.2 (C), 160.2 (C), 160.4 (C). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3048 (w), 2955 (w), 2932 (w), 2540 (w), 2201 (m), 1603 (s), 1566 (m), 1508 (s), 1455 (m), 1439 (m), 1409 (m), 1292 (m), 1246 (m), 1172 (m), 1155 (m), 1132 (m), 1105 (m), 1022 (m), 923 (w), 899 (w), 826 (s), 786 (w), 767 (w), 663 (w), 642 (w), 609 (m), 532 (m), 415 (w). MS (EI, 70 eV): m/z (%): 600 (M^+ , 40), 599 (90), 584 (5), 498 (3), 300 (5), 281 (4), 274 (3), 273 (4), 213 (4), 207 (7), 172 (2), 135 (16), 129 (21), 115 (13), 112 (6), 111 (5), 110 (4), 109 (3), 105 (4), 101 (16), 97 (10), 93 (9), 87 (17), 85 (19), 84 (20), 83 (17), 73 (78), 71 (24), 70 (15), 69 (26), 67 (11), 61 (14), 60 (100), 57 (40), 56 (19), 55 (44), 54 (6), 45 (22), 44 (97), 43 (83), 42 (18), 41 (54), 40 (33), 39 (20). HRMS (EI, 70 eV): calcd. for $C_{41}H_{29}NO_4$ (M^+): 599.20911, found 599.20875. Anal. calcd. for $C_{41}H_{29}NO_4$ (599.67): C, 82.12; H, 4.87; N, 2.34. Found: C, 82.41; H, 5.124; N, 2.368.

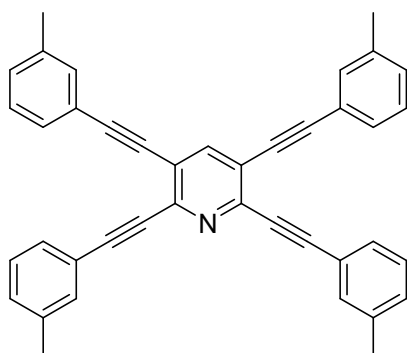
2,3,5,6-Tetrakis((4-(trifluoromethyl)phenyl)ethynyl)pyridine (**8e**)



Starting with 3,5-dibromo-2,6-dichloropyridine **3** (100 mg, 0.327 mmol), $PdCl_2(CH_3CN)_2$ (4.2 mg, 5.0 mol%), XPhos (15.6 mg, 10.0 mol%), 1-ethynyl-4-(trifluoromethyl)-benzene (0.426 mL, 2.616 mmol), CuI (3.1 mg, 5.0 mol%), $HN(iPr)_2$ (1.0 mL, 7.115 mmol) and 1,4-dioxane (4.0 mL), **8e** was isolated as a yellow solid (228 mg, 93%); mp = 202-204 °C. 1H NMR (300 MHz, $CDCl_3$): δ = 7.61-7.70 (m, 16H, CH), 8.04 (s, 1H, CH). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 86.9 (C_{alkyne}), 88.9 (C_{alkyne}), 93.7 (C_{alkyne}), 96.6 (C_{alkyne}), 121.5 (C), 124.3 (q, $^1J_{C-F}$ = 273.1 Hz, CF_3), 124.3 (q, $^1J_{C-F}$ = 273.1 Hz, CF_3), 125.6 (q, $^3J_{C-F}$ = 4.8 Hz, CH), 125.7 (q, $^3J_{C-F}$ = 4.9 Hz, CH), 125.8 (C), 125.8 (C), 131.1 (q, $^2J_{C-F}$ = 32.8 vHz, C), 131.3 (q, $^2J_{C-F}$

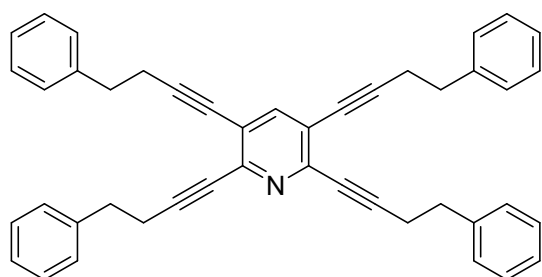
= 32.8 Hz, C), 131.9 (CH), 132.3 (CH), 141.7 (CH), 143.6 (C). ^{19}F NMR (282.4 MHz, CDCl_3): δ = -62.6 (CF_3), -62.6 (CF_3). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 2211 (w), 1923 (w), 1613 (m), 1514 (m), 1416 (m), 1320 (s), 1162 (m), 1120 (m), 1102 (s), 1064 (s), 1015 (m), 913 (w), 835 (s), 770 (w), 755 (m), 687 (m), 592 (m), 524 (m), 483 (w). MS (EI, 70 eV): m/z (%): 752 (M^+ , 39), 751 (100), 750 (8), 733 (3), 732 (6), 683 (2), 682 (5), 681 (3), 613 (2), 362 (3), 341 (39; 281 (1), 93 (5), 73 (7), 71 (3), 69 (3), 60 (9), 44 (12), 40 (5). HRMS (EI, 70 eV): calcd. for $\text{C}_{41}\text{H}_{17}\text{F}_{12}\text{N}$ (M^+): 751.11639, found 751.11596. Anal. calcd. for $\text{C}_{41}\text{H}_{17}\text{F}_{12}\text{N}$ (751.56): C, 65.52; H, 2.28; N, 1.86. Found: C, 65.42; H, 2.189; N, 1.825.

2,3,5,6-Tetrakis(*m*-tolylethynyl)pyridine (**8f**)



Starting with 3,5-dibromo-2,6-dichloropyridine **3** (100 mg, 0.327 mmol), $\text{PdCl}_2(\text{CH}_3\text{CN})_2$ (4.2 mg, 5.0 mol%), XPhos (15.6 mg, 10.0 mol%), 1-ethynyl-3-methylbenzene (0.337 mL, 2.616 mmol), CuI (3.1 mg, 5.0 mol%), $\text{HN}(i\text{Pr})_2$ (1.0 mL, 7.115 mmol) and 1,4-dioxane (4.0 mL), **8f** was isolated as a yellow solid (159 mg, 91%); mp = 160-162 °C. ^1H NMR (400 MHz, CDCl_3): δ = 2.22 (s, 6H, CH_3), 2.24 (s, 6H, CH_3), 7.09-7.18 (m, 8H, CH), 7.29-7.39 (m, 8H, CH), 7.83 (s, 1H, CH). ^{13}C NMR (100 MHz, CDCl_3): δ = 21.1 (CH_3), 21.1 (CH_3), 85.3 (C_{alkyne}), 87.5 (C_{alkyne}), 95.3 (C_{alkyne}), 97.8 (C_{alkyne}), 121.5 (C), 122.0 (C), 122.3 (C), 128.3 (CH), 128.3 (CH), 128.8 (CH), 129.2 (CH), 130.0 (CH), 130.2 (CH), 132.3 (CH), 132.8 (CH), 138.0 (C), 138.1 (C), 140.7 (CH), 143.6 (C). IR (ATR, cm^{-1}): $\tilde{\nu}$ = 3025 (w), 2947 (w), 2917 (w), 2856 (w), 2201 (m), 1599 (m), 1578 (m), 1483 (m), 1415 (m), 1377 (w), 1223 (w), 1189 (w), 1122 (w), 1091 (w), 1036 (w), 906 (m), 873 (m), 777 (s), 683 (s), 520 (w), 489 (m), 456 (m), 437 (m), 387 (w). MS (EI, 70 eV): m/z (%): 536 (M^+ , 41), 535 (100), 534 (7), 533 (2), 520 (4), 505 (2), 252 (4), 244 (2), 73 (2), 60 (4), 44 (6), 43 (4). HRMS (EI, 70 eV): calcd. for $\text{C}_{41}\text{H}_{29}\text{N}$ (M^+): 535.22945, found 535.23043. Anal. calcd. for $\text{C}_{41}\text{H}_{29}\text{N}$ (535.68): C, 91.93; H, 5.46; N, 2.61. Found: C, 91.53; H, 5.374; N, 2.471.

2,3,5,6-Tetrakis(4-phenylbut-1-ynyl)pyridine (**8g**)

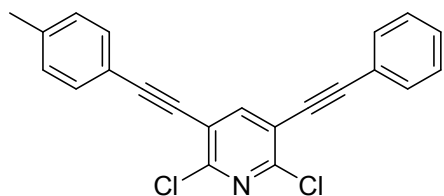


Starting with 3,5-dibromo-2,6-dichloropyridine **3** (100 mg, 0.327 mmol), $\text{PdCl}_2(\text{CH}_3\text{CN})_2$ (4.2 mg, 5.0 mol%), XPhos (15.6 mg, 10.0 mol%), but-3-ynylbenzene (0.370 mL, 2.616 mmol), CuI (3.1 mg, 5.0 mol%), $\text{HN}(i\text{Pr})_2$ (1.0 mL, 7.115 mmol) and 1,4-dioxane (4.0 mL), **8g** was isolated as a yellow solid (122 mg, 63%); mp = 104-106 °C. ^1H NMR (400 MHz, CDCl_3): δ = 2.71-2.76 (m, 8H, CH_2), 2.89-2.97 (m, 8H, CH_2), 7.19-7.33 (m, 20 H, CH), 7.57 (s, 1H, CH). ^{13}C NMR (100 MHz, CDCl_3): δ = 21.8 (CH_2), 21.8

(CH₂), 34.7 (CH₂), 34.8 (CH₂), 77.5 (C_{alkyne}), 79.7 (C_{alkyne}), 95.0 (C_{alkyne}), 97.5 (C_{alkyne}), 121.1 (C), 126.3 (CH), 126.4 (CH), 128.3 (CH), 128.3 (CH), 128.4 (CH), 128.4 (CH), 140.3 (C), 140.4 (C), 141.7 (CH), 143.2 (C). IR (ATR, cm⁻¹): $\tilde{\nu}$ = 3083 (w), 3023 (w), 2924 (w), 2855 (w), 2230 (m), 1717 (m), 1601 (m), 1494 (m), 1450 (m), 1413 (s), 1336 (w), 1250 (w), 1200 (w), 1074 (m), 1029 (m), 906 (m), 770 (m), 747 (m), 696 (s), 579 (w), 511 (m), 486 (w), 464 (w). MS (EI, 70 eV): m/z (%): 592 (M⁺, 21), 591 (68), 590 (100), 500 (17), 499 (6), 498 (7), 408 (16), 407 (6), 406 (7), 392 (7), 368 (4), 316 (5), 315 (5), 302 (3), 147 (4), 121 (14), 117 (3), 104 (4), 92 (4), 91 (29), 87 (3), 86 (2), 65 (3), 45 (3), 44 (8), 43 (5). HRMS (EI, 70 eV): calcd. for C₄₅H₃₇N (M⁺): 591.29205, found 591.29003.

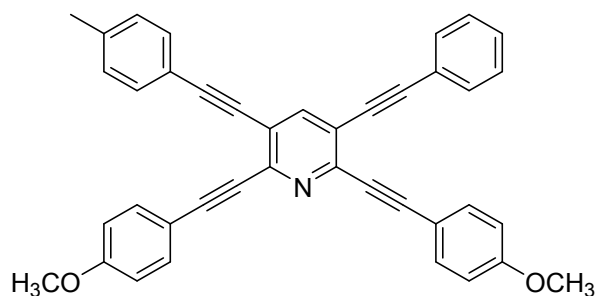
Synthesis of compounds 9 and 10

2,6-dichloro-3-(phenylethynyl)-5-(*p*-tolylethynyl)pyridine (9)



Starting with 3-bromo-2,6-dichloro-5-(phenylethynyl)-pyridine **7a** (100 mg, 0.306 mmol), Pd(dba)₂ (3.5 mg, 2 mol%), HP(tBu)₃BF₄ (1.8 mg, 2.0 mol%), 4-Methylphenylacetylen (0.0427 mL, 0.337 mmol), Et₃N (0.170 ml, 1.224 mmol) and THF (3 mL), **9a** was obtained as a yellow solid (85 mg, 77%); m.p = 132-133 °C. ¹H NMR (300 MHz, CDCl₃): δ = 2.39 (s, 3H, CH₃), 7.19 (d, ³J = 8.1 Hz, 2H, CH), 7.36-7.42 (m, 3H, CH), 7.46 (d, ³J = 8.1 Hz, 2H, CH), 7.54-7.61 (m, 2H, CH), 7.96 (s, 1H, CH). ¹³C NMR (75 MHz, CDCl₃): δ = 21.8 (CH₃), 82.4 (C_{alkyne}), 82.9 (C_{alkyne}), 98.2 (C_{alkyne}), 98.7 (C_{alkyne}), 118.9 (C), 119.3 (C), 119.6 (C), 122.0 (C), 128.7 (CH), 129.4 (CH), 129.6 (CH), 131.9 (CH), 131.9 (CH), 140.0 (C), 144.7 (CH), 149.4 (C), 149.5 (C). IR (ATR, cm⁻¹): $\tilde{\nu}$ = 2956 (w), 2920 (w), 2854 (w), 2208 (m), 1572 (w), 1502 (m), 1487 (m), 1443 (m), 1392 (m), 1382 (s), 1275 (m), 1227 (m), 1155 (m), 1107 (s), 1066 (m), 1003 (m), 987 (m), 910 (s), 810 (s), 789 (m), 752 (vs), 732 (s), 683 (s), 677 (s), 640 (s), 613 (s), 561 (m), 528 (vs). GC-MS (EI, 70 eV): m/z (%): 365 (11), 364 (15), 363 (66), 362 (25), 361 (M⁺, 100), 290 (19), 289 (11), 288 (23), 263 (8), 181 (16), 145 (8), 139 (9), 131 (15). HRMS (EI, 70 eV): calcd. for C₂₂H₁₃NCl₂ (M⁺): 361.04196, found 361.04161; calcd. for C₂₂H₁₃NCl³⁷Cl (M⁺): 363.03901, found 363.03870; calcd. for C₂₂H₁₃N³⁷Cl₂ (M⁺): 365.03606, found 365.03696.

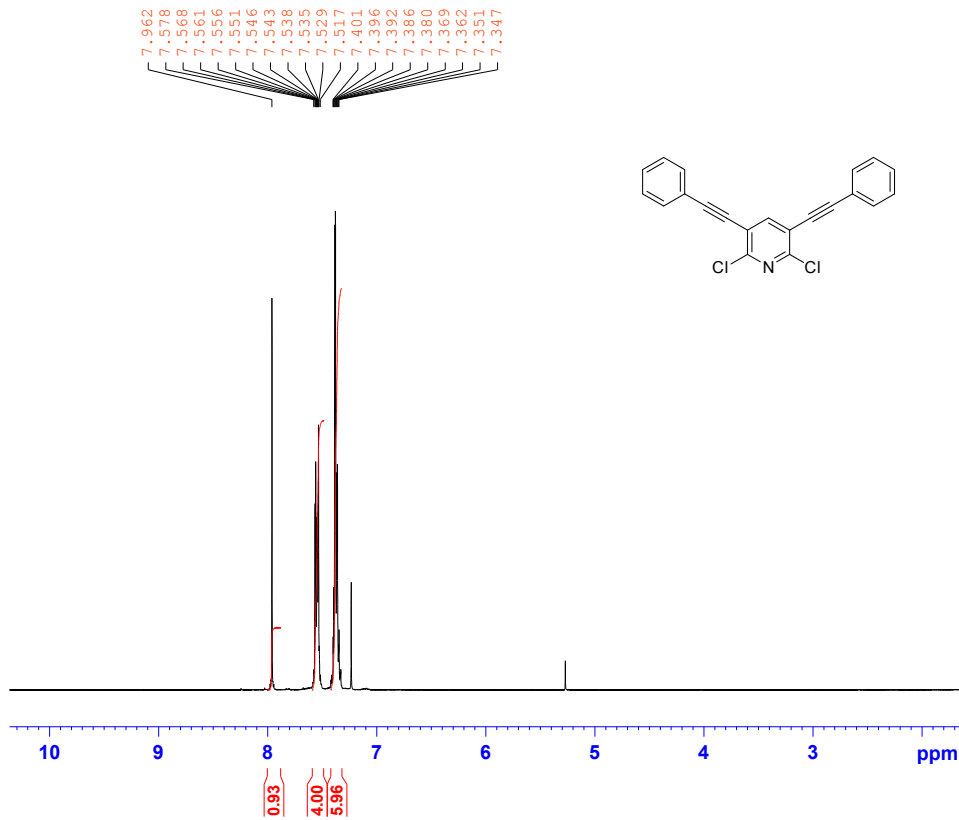
2,6-bis((4-methoxyphenyl)ethynyl)-3-(phenylethynyl)-5-(*p*-tolylethynyl)pyridine (10)



Starting with 2,6-dichloro-3-(phenylethynyl)-5-(*p*-tolylethynyl)pyridine **9a** (100 mg, 0.276 mmol), PdCl₂(CH₃CN)₂ (3.6 mg, 5.0 mol%), X-Phos (13.2 mg, 10 mol%), CuI (2.6 mg, 5 mol%), 4-Methoxyphenylacetylen (0.132 mL, 1.021 mmol), (*i*PrO)₂NH (0.126 ml, 0.897 mmol) and dioxane (3 mL), **10a** was obtained as an orange solid (151 mg, 99%); m.p. = 188-189 °C. ¹H NMR (300 MHz, CDCl₃): δ = 2.39 (s, 3H, CH₃), 3.83 (s, 3H, OCH₃), 3.83 (s, 3H, OCH₃), 6.88 (d, ³J = 8.9 Hz, 2H, CH), 6.88 (d, ³J = 8.9 Hz, 2H, CH), 7.18 (d, ³J = 7.9 Hz, 2H, CH), 7.35-7.41 (m, 3H, CH), 7.48 (d, ³J = 8.1 Hz, 2H, CH), 7.56-7.61 (m, 2H, CH), 7.58 (d, ³J = 8.8 Hz, 2H, CH), 7.59 (d, ³J = 8.8 Hz, 2H, CH), 7.93 (s, 1H, CH). ¹³C NMR (75 MHz, CDCl₃): δ = 21.7 (CH₃), 55.4 (OCH₃), 55.4 (OCH₃), 85.2 (C_{alkyne}), 85.8 (C_{alkyne}), 87.0 (C_{alkyne}), 87.1 (C_{alkyne}), 95.8 (C_{alkyne}), 95.8 (C_{alkyne}), 97.4 (C_{alkyne}), 97.8 (C_{alkyne}), 114.3 (CH), 114.3 (C), 114.4 (C), 119.6 (C), 120.9 (C), 121.1 (C), 122.7 (C), 128.6 (CH), 129.2 (CH), 129.4 (CH), 131.8 (CH), 131.8 (CH), 134.0 (CH), 139.5 (CH), 141.1 (CH), 143.7 (C), 143.8 (C), 160.7 (C). IR (ATR, cm⁻¹): $\tilde{\nu}$ = 2957 (w), 2934 (w), 2200 (w), 1725 (w), 1603 (m), 1566 (w), 1508 (s), 1456 (m), 1440 (m), 1410 (m), 1290 (m), 1246 (s), 1174 (m), 1157 (s), 1105 (m), 1030 (s), 924 (m), 820 (vs), 802 (s), 752 (vs), 689 (s), 577 (m), 528 (vs). GC-MS (ESI, 70 eV): m/z (%): 554 (18), 553 (M⁺, 49), 276 (5), 207 (9), 84 (5), 57 (5), 44 (51), 43 (9), 40 (100). HRMS (ESI, 70 eV): calcd. for C₄₀H₂₇NO₂ (M+H⁺): 554.21146, found 554.21119.

1H- and 13C-NMR Spectra of compounds 4a-g

Reimann/ SRE- SP- 44
AulH CDCl3 /opt/topspin 1206 46



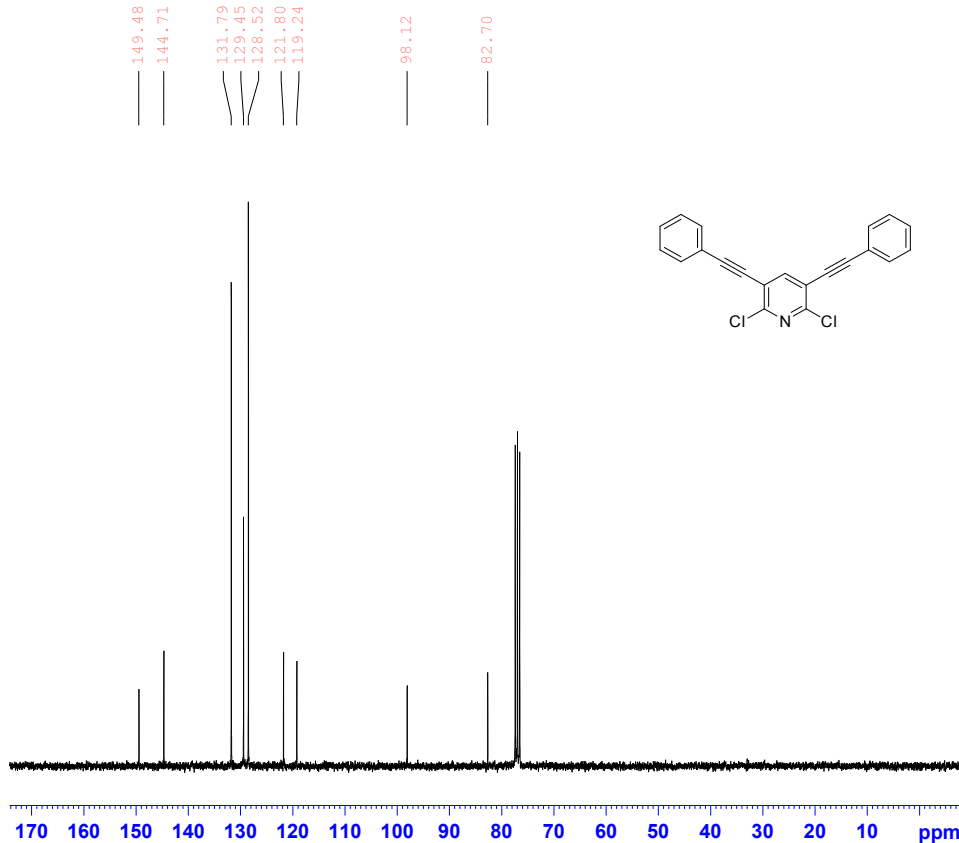
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TE 296.0 K
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TD0 1

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F2 - Processing parameters
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Reimann/ SRE- SP- 44
Aul3C CDCl3 /opt/topspin 1206 46



Current Data Parameters
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EXPNO 11
PROCNO 1

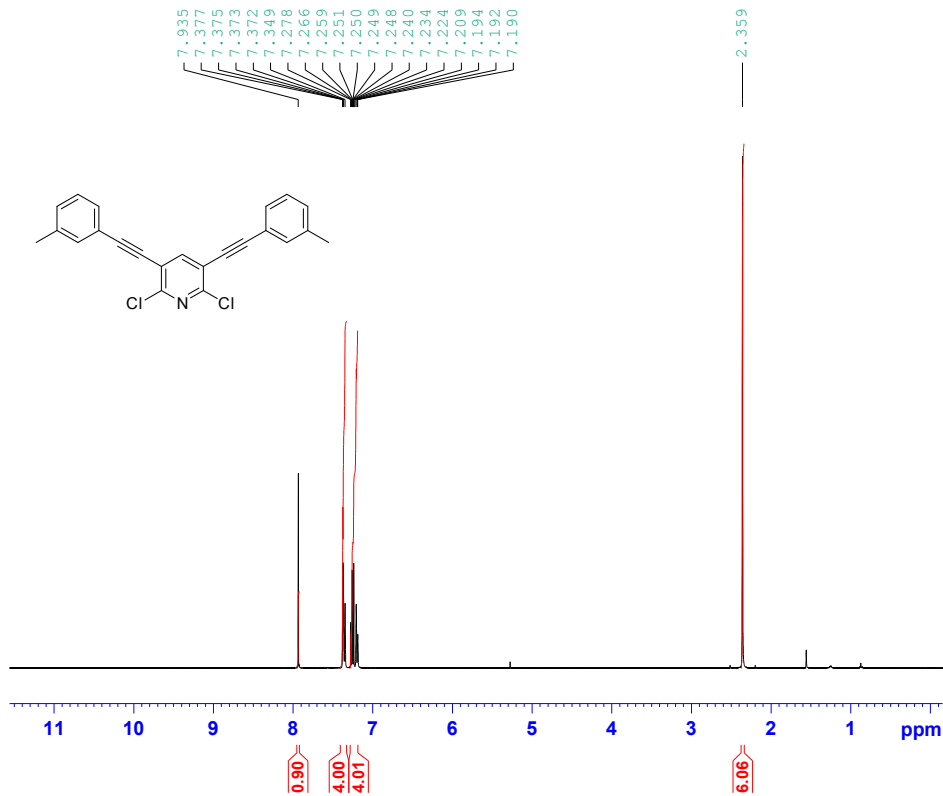
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DS 4
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FIDRES 0.643831 Hz
AQ 0.7766516 sec
RG 32768
DW 23.700 usec
DE 6.00 usec
TE 296.5 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.89999998 sec
TD0 1

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P1 9.60 usec
PL1 -1.10 dB
SFO1 75.4771825 MHz

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

F2 - Processing parameters
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Reimann/ SRE 838
 Au1H CDCl3 /opt/topspin 1206 7



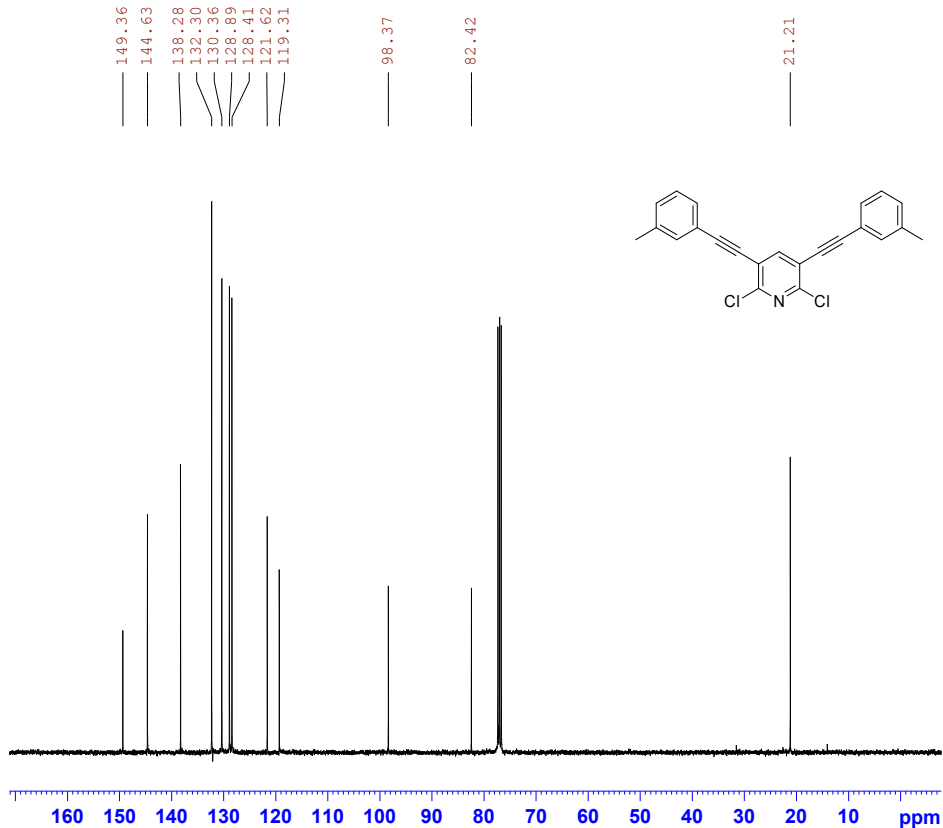
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 TD 32768
 SOLVENT CDCl3
 NS 32
 DS 4
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447731 sec
 RG 181
 DW 62.400 usec
 DE 6.00 usec
 TE 297.0 K
 D1 1.50000000 sec
 TD0 1

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 P1 12.20 usec
 PL1 -1.00 dB
 SFO1 400.1324000 MHz

F2 - Processing parameters
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 SF 400.1300294 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
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Reimann/ SRE 838
 Au13C CDCl3 /opt/topspin 1206 7



Current Data Parameters
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 EXPNO 11
 PROCNO 1

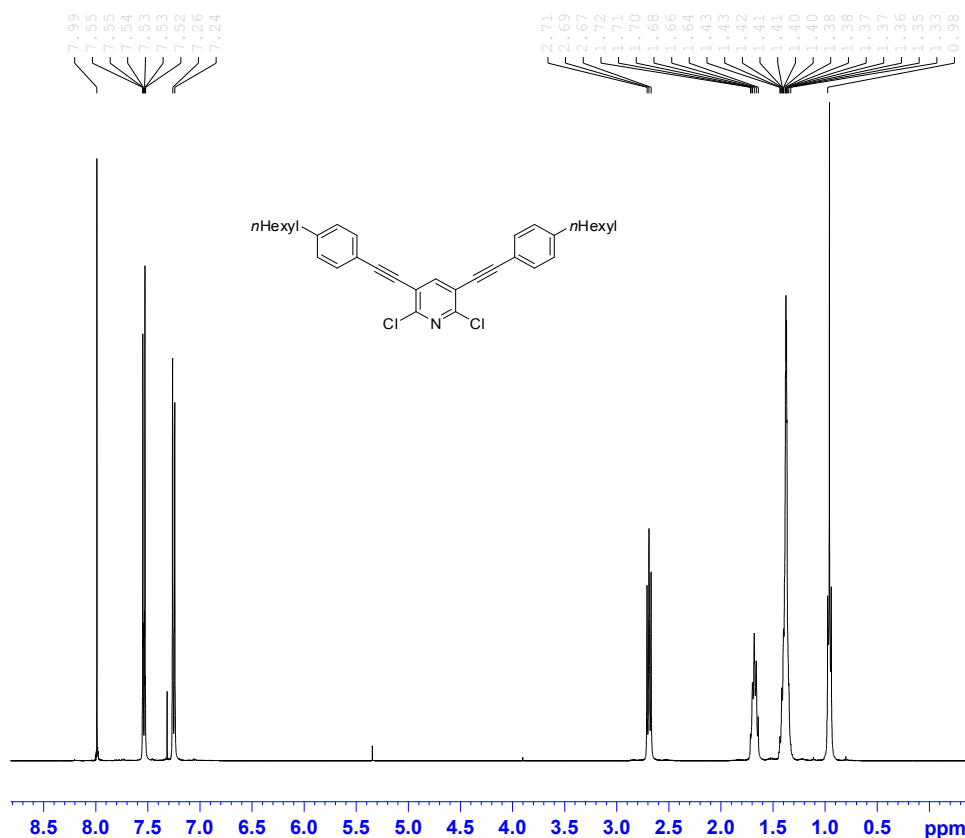
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 NS 1000
 DS 4
 SWH 29940.119 Hz
 FIDRES 0.456850 Hz
 AQ 1.0945013 sec
 RG 13004
 DW 16.700 usec
 DE 6.00 usec
 TE 297.0 K
 D1 1.70000005 sec
 d11 0.03000000 sec
 DELTA 1.60000002 sec
 TD0 1

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 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
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Reimann/ SRE 836
Au1H CDC13 /opt/topspin 1206 8



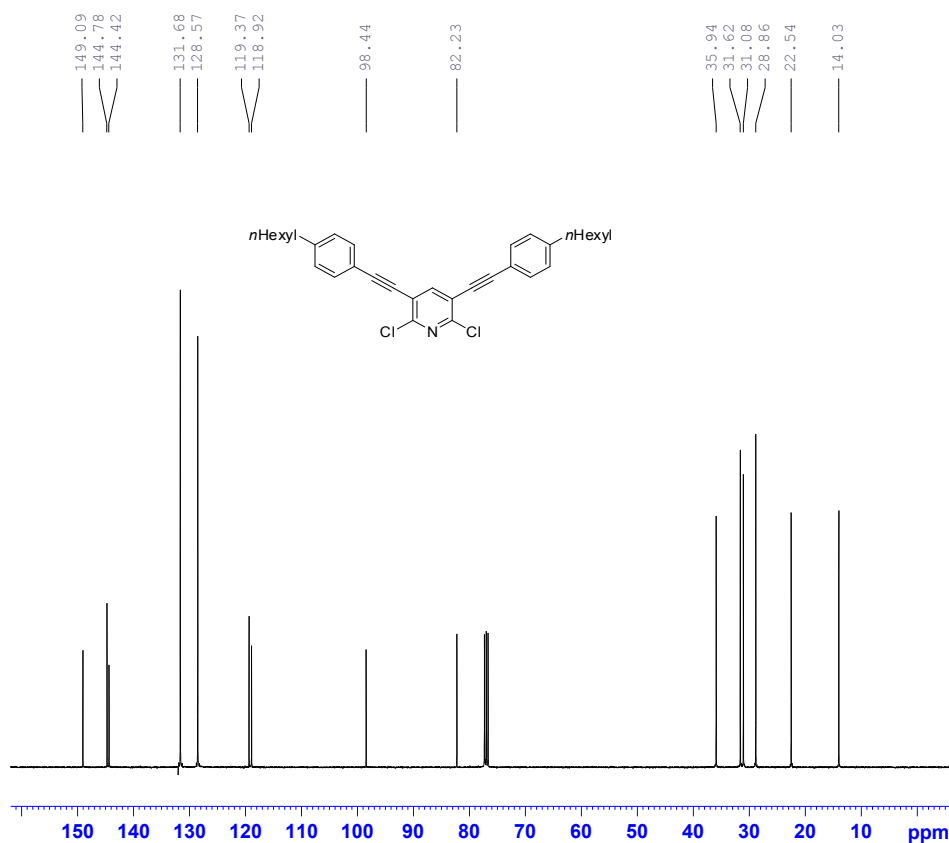
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SOLVENT CDC13
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DS 4
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 45.3
DW 62.400 usec
DE 6.00 usec
TE 297.0 K
D1 1.50000000 sec
TD0 1

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

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
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PC 1.00

Reimann/ SRE 836
Au13C CDC13 /opt/topspin 1206 8



Current Data Parameters
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EXPNO 11
PROCNO 1

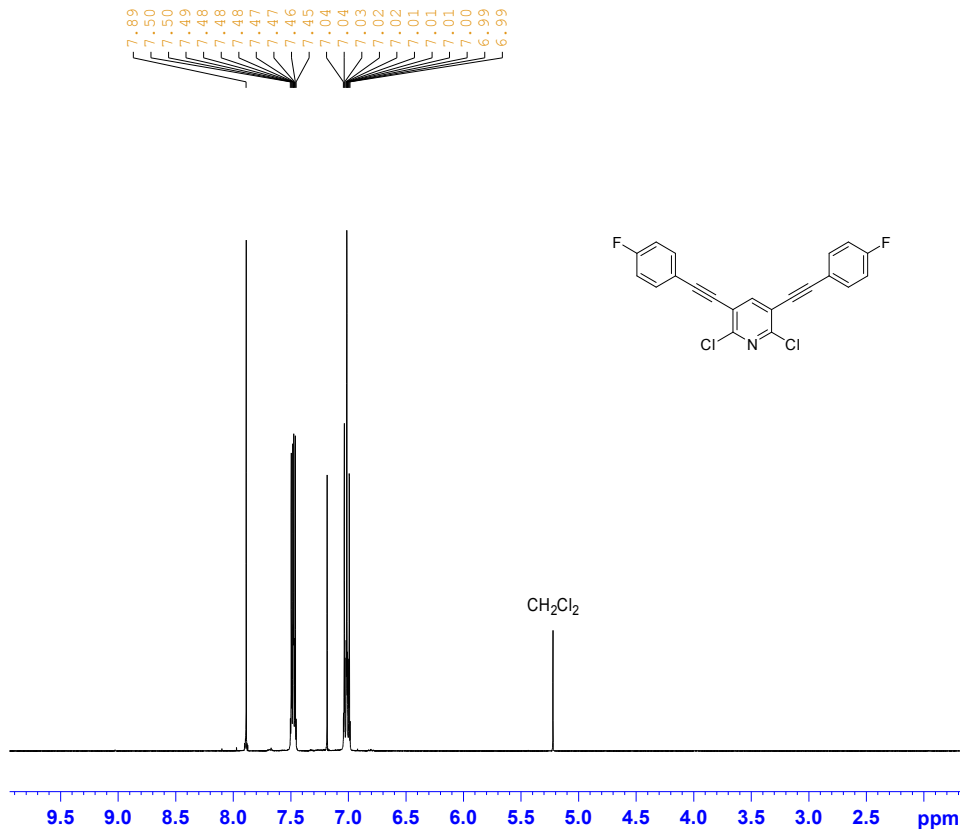
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NS 1000
DS 4
SWH 29940.119 Hz
FIDRES 0.456850 Hz
AQ 1.0945013 sec
RG 9195.2
DW 16.700 usec
DE 6.00 usec
TE 297.0 K
D1 1.70000005 sec
d11 0.03000000 sec
DELTA 1.60000002 sec
TD0 1

==== 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
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SSB 0
LB 1.00 Hz
GB 0
PC 1.00

Reimann/ SRE 843
 Au1H CDC13 /opt/topspin 1207 5



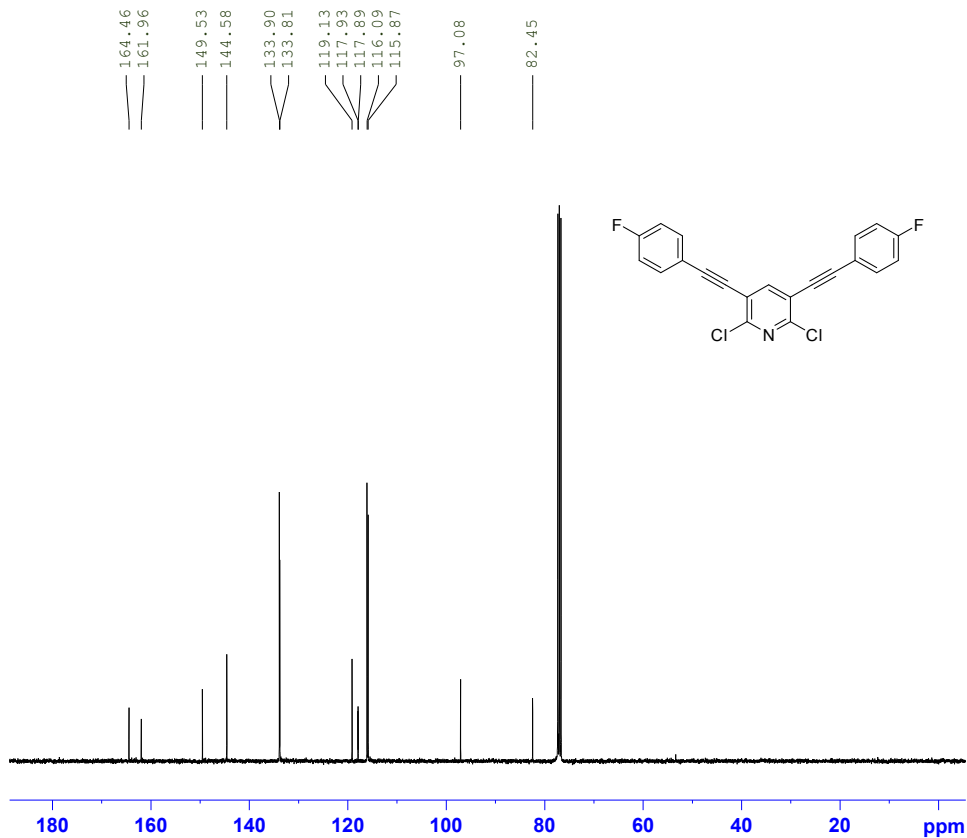
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 SOLVENT CDC13
 NS 32
 DS 4
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447731 sec
 RG 512
 DW 62.400 usec
 DE 6.00 usec
 TE 297.0 K
 D1 1.50000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.10 usec
 PL1 -1.00 dB
 SFO1 400.1324000 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300513 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

Reimann/ SRE 843
 Au13C CDC13 /opt/topspin 1207 5



Current Data Parameters
 NAME SRE 843 13C
 EXPNO 11
 PROCNO 1

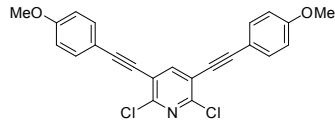
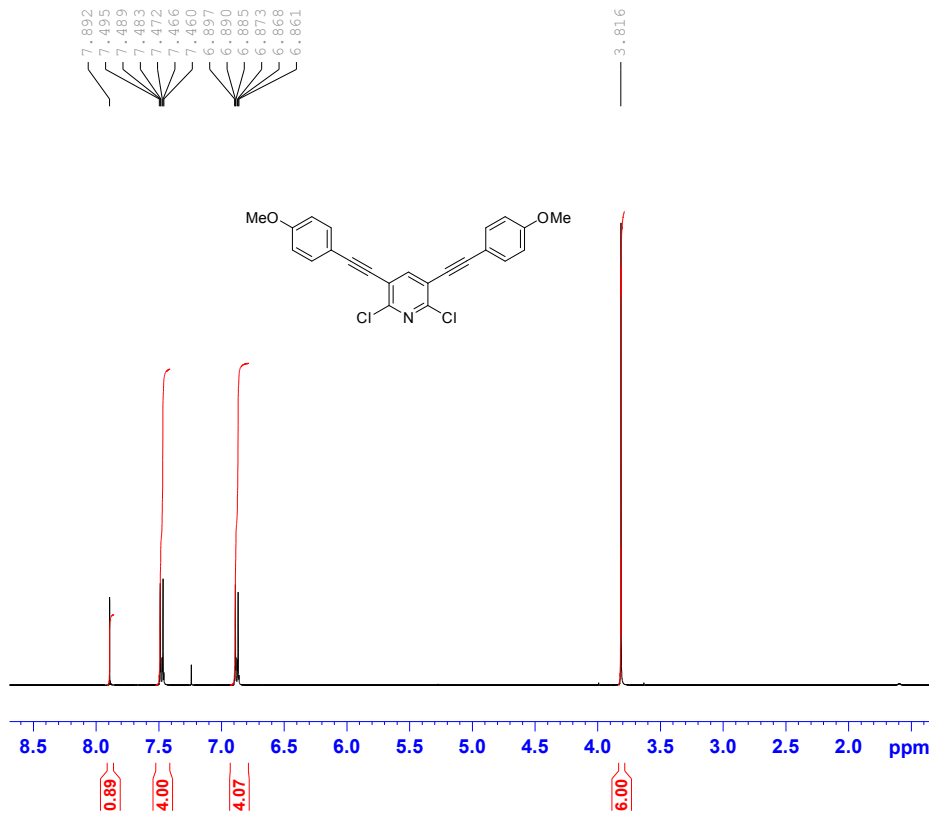
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 FIDRES 0.456850 Hz
 AQ 1.0945013 sec
 RG 20642.5
 DW 16.700 usec
 DE 6.00 usec
 TE 297.0 K
 D1 1.70000005 sec
 d11 0.03000000 sec
 DELTA 1.60000002 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 -0.50 dB
 SFO1 100.6260690 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -2.00 dB
 PL12 17.00 dB
 PL13 19.00 dB
 SFO2 400.1318000 MHz

F2 - Processing parameters
 SI 32768
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Reimann/ SRE 837
 AulH CDCl3 /opt/topspin 1206 4



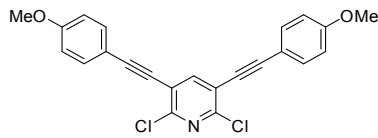
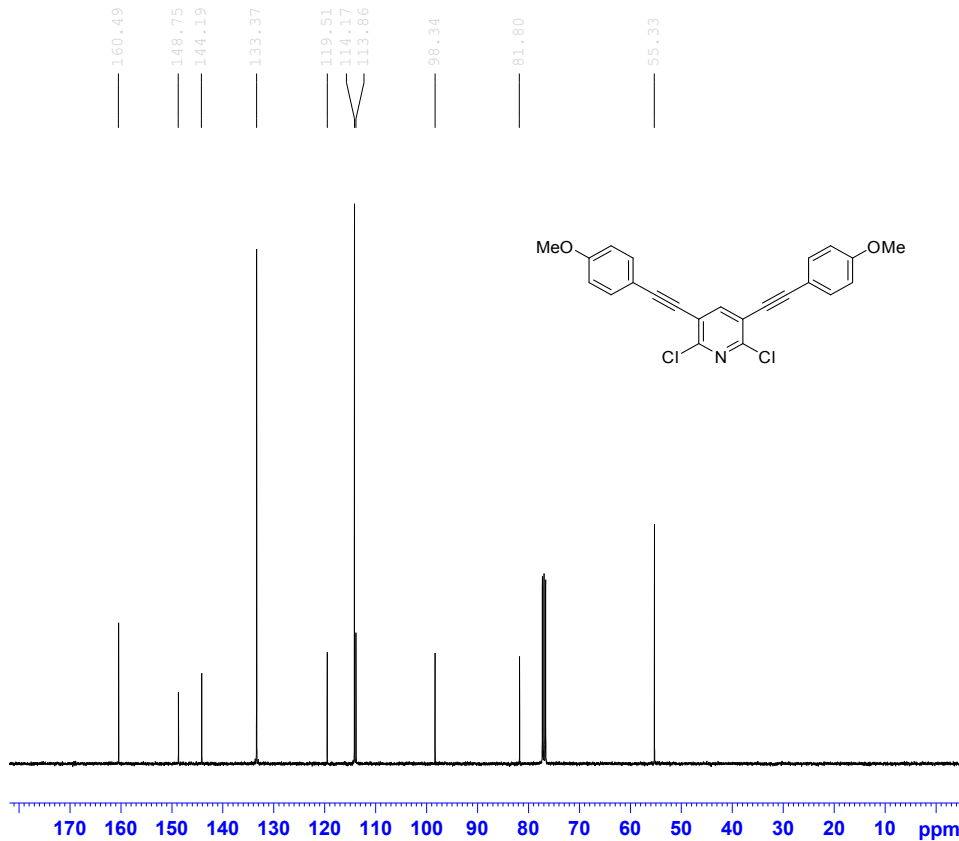
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 PROCNO 1

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 TD 32768
 SOLVENT CDCl3
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 DS 4
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447731 sec
 RG 161.3
 DW 62.400 usec
 DE 6.00 usec
 TE 297.0 K
 D1 1.50000000 sec
 TDO 1

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

F2 - Processing parameters
 SI 32768
 SF 400.1300291 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 FC 1.00

Reimann/ SRE 837
 Au13C CDCl3 /opt/topspin 1206 4



Current Data Parameters
 NAME SRE 837 13C
 EXPNO 11
 PROCNO 1

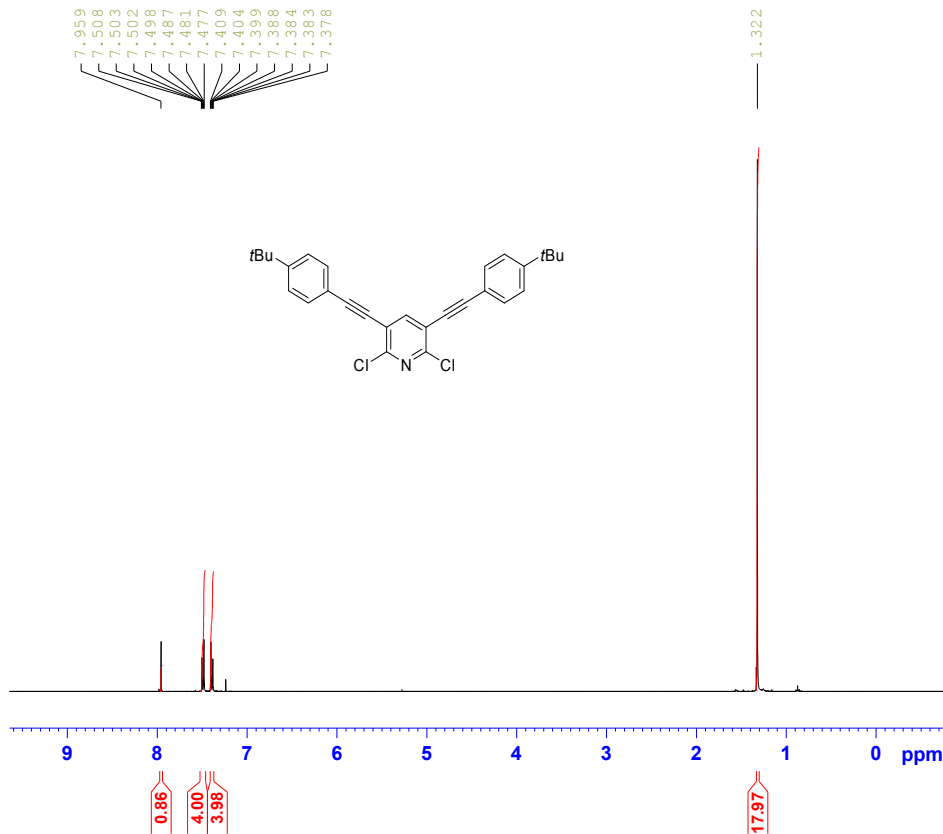
F2 - Acquisition Parameters
 Date_ 20120628
 Time 17.07
 INSTRUM AV400
 PROBHD 5 mm QNP 1H/29
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 500
 DS 4
 SWH 29940.119 Hz
 FIDRES 0.456850 Hz
 AQ 1.0945013 sec
 RG 10321.3
 DW 16.700 usec
 DE 6.00 usec
 TE 297.0 K
 D1 1.70000005 sec
 d11 0.03000000 sec
 DELTA 1.60000002 sec
 TDO 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 100.6127774 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

Reimann/ SRE 841
 AulH CDC13 /opt/topspin 1206 12



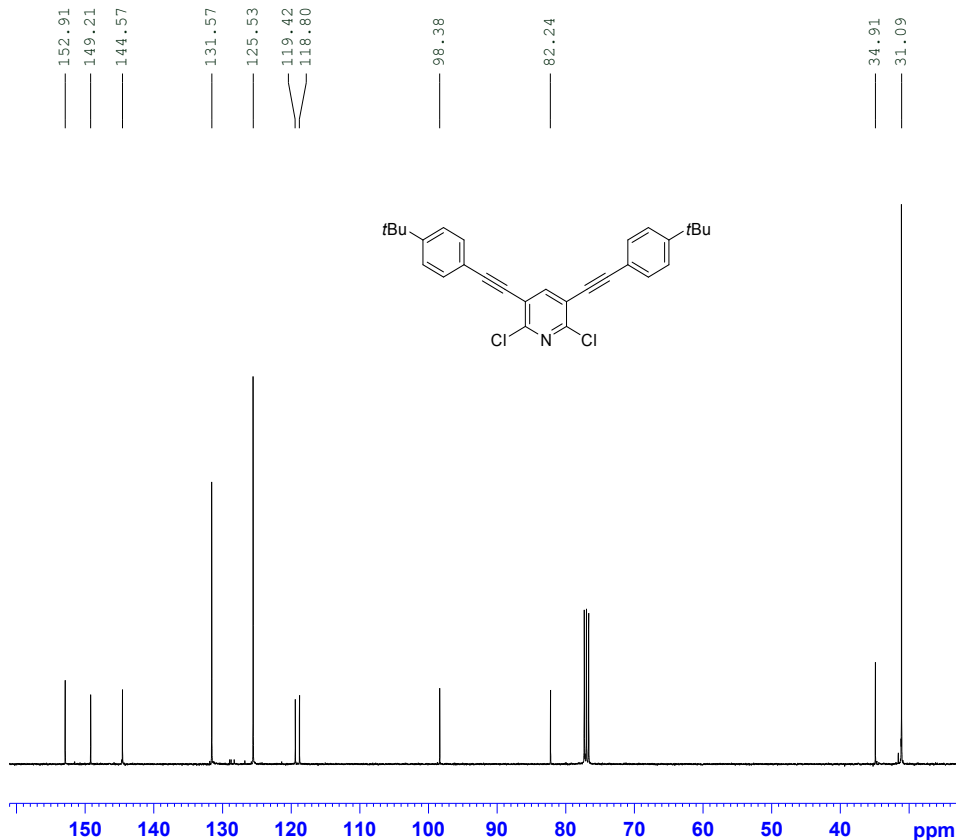
Current Data Parameters
 NAME SRE 841 1H
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120629
 Time 1.59
 INSTRUM AV400
 PROBHD 5 mm QNP 1H/29
 PULPROG zg30
 TD 32768
 SOLVENT CDC13
 NS 32
 DS 4
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447731 sec
 RG 101.6
 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 400.1300298 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

Reimann/ SRE 841
 Aul3C CDC13 /opt/topspin 1206 12



Current Data Parameters
 NAME SRE 841 13C
 EXPNO 11
 PROCNO 1

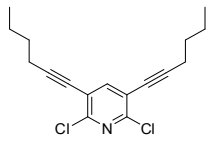
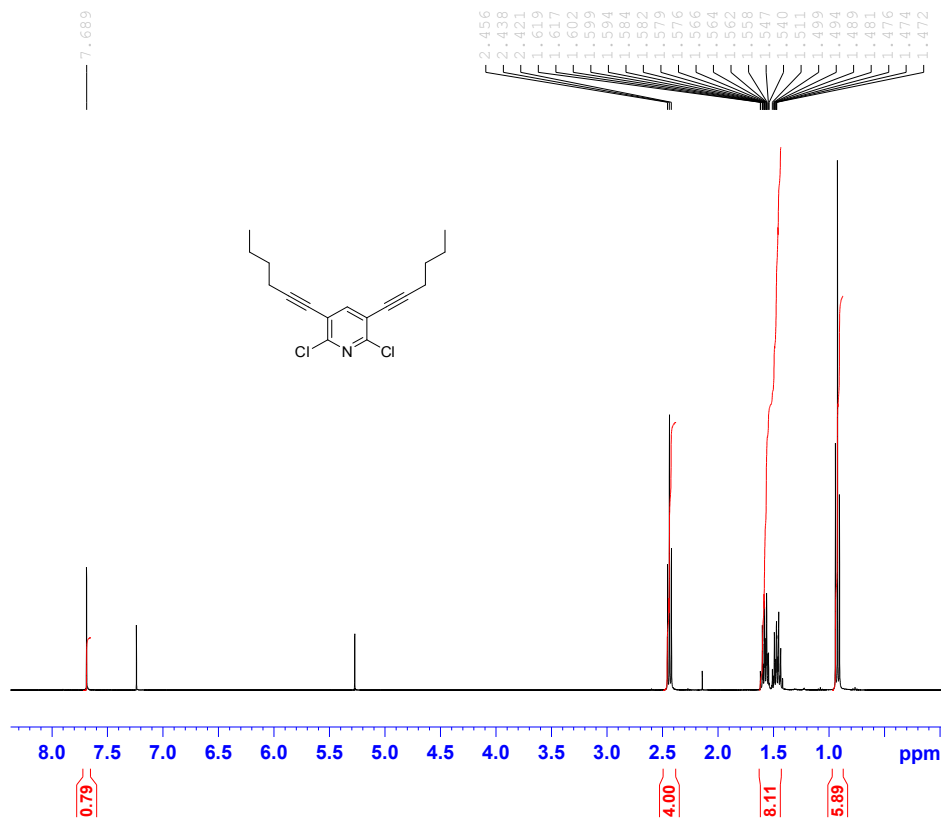
F2 - Acquisition Parameters
 Date_ 20120629
 Time 2.48
 INSTRUM AV400
 PROBHD 5 mm QNP 1H/29
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 1000
 DS 4
 SWH 29940.119 Hz
 FIDRES 0.456850 Hz
 AQ 1.0945013 sec
 RG 13004
 DW 16.700 usec
 DE 6.00 usec
 TE 297.0 K
 D1 1.70000005 sec
 d11 0.03000000 sec
 DELTA 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
 P2 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 100.6127773 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

Reimann/ SRE 842
AulH CDC13 /opt/topspin 1206 11



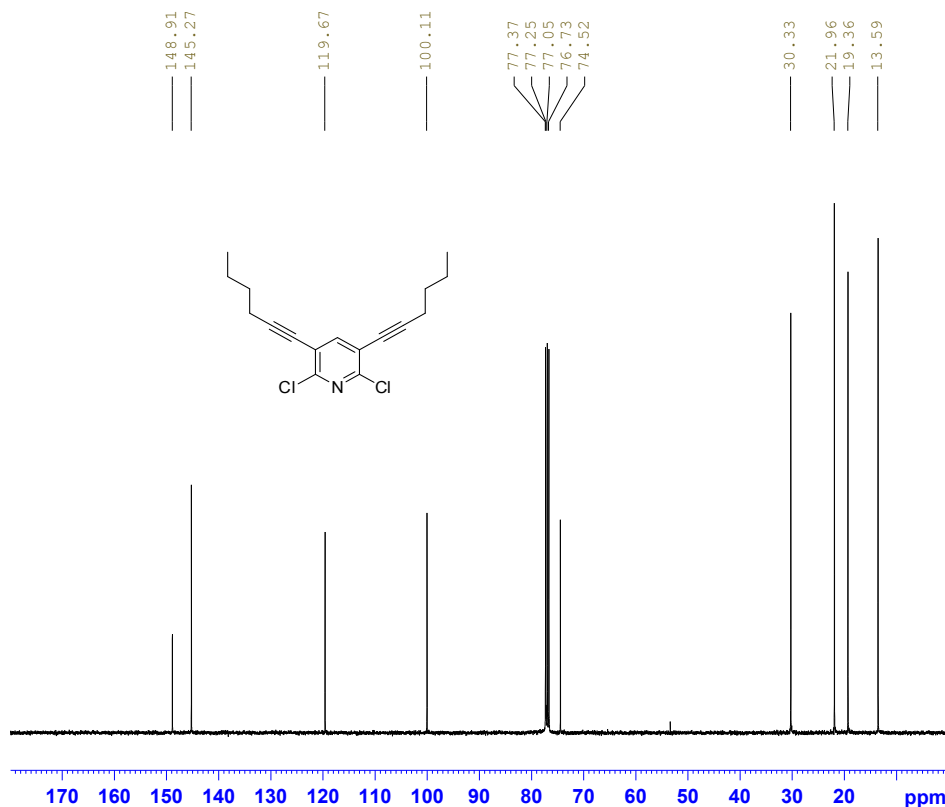
Current Data Parameters
NAME SRE 842 1H
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120629
Time 0.08
INSTRUM AV400
PROBHD 5 mm QNP 1H/29
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 32
DS 4
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 161.3
DW 62.400 usec
DE 6.00 usec
TE 297.0 K
D1 1.5000000 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 400.1300299 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

Reimann/ SRE 842
Aul3C CDCl3 /opt/topspin 1206 11



Current Data Parameters
NAME SRE 842 13 C
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120629
Time_ 1.44
INSTRUM AV400
PROBHD 5 mm QNP 1H/29
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2000
DS 4
SWH 29940.119 Hz
FIDRES 0.456850 Hz
AQ 1.0945013 sec
RG 13004
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

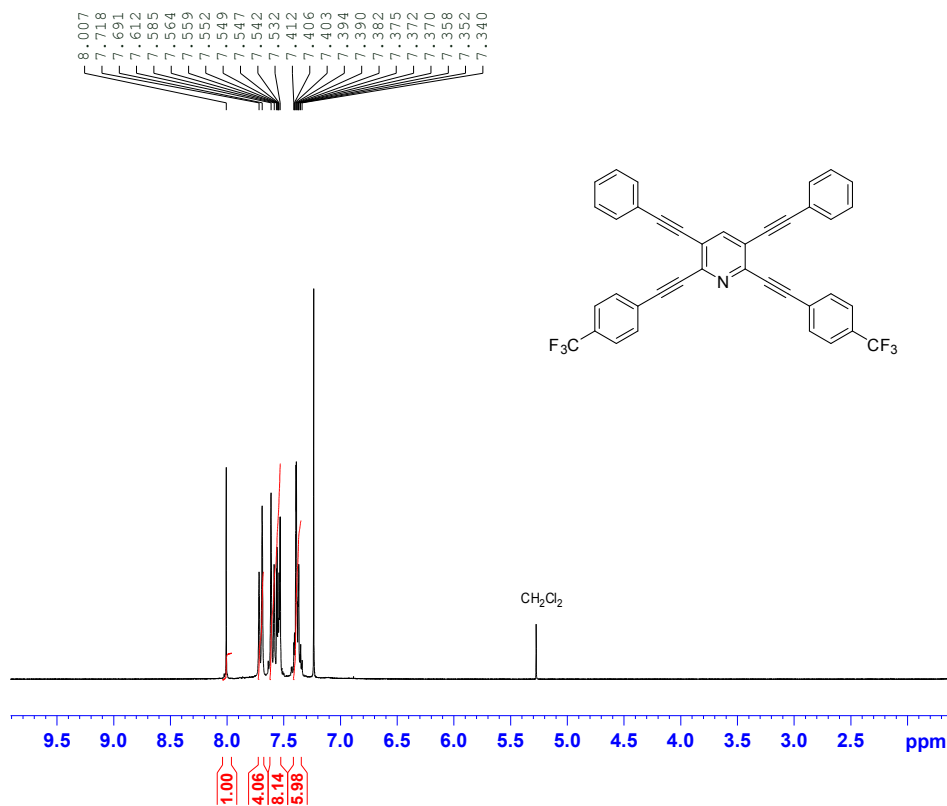
===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 100.6260690 MHz

===== 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 100.6127737 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

¹H- and ¹³C-NMR Spectra of compounds 5a-e

Reimann/ SRE 882
AulH CDCl3 /opt/topspin 1208 47



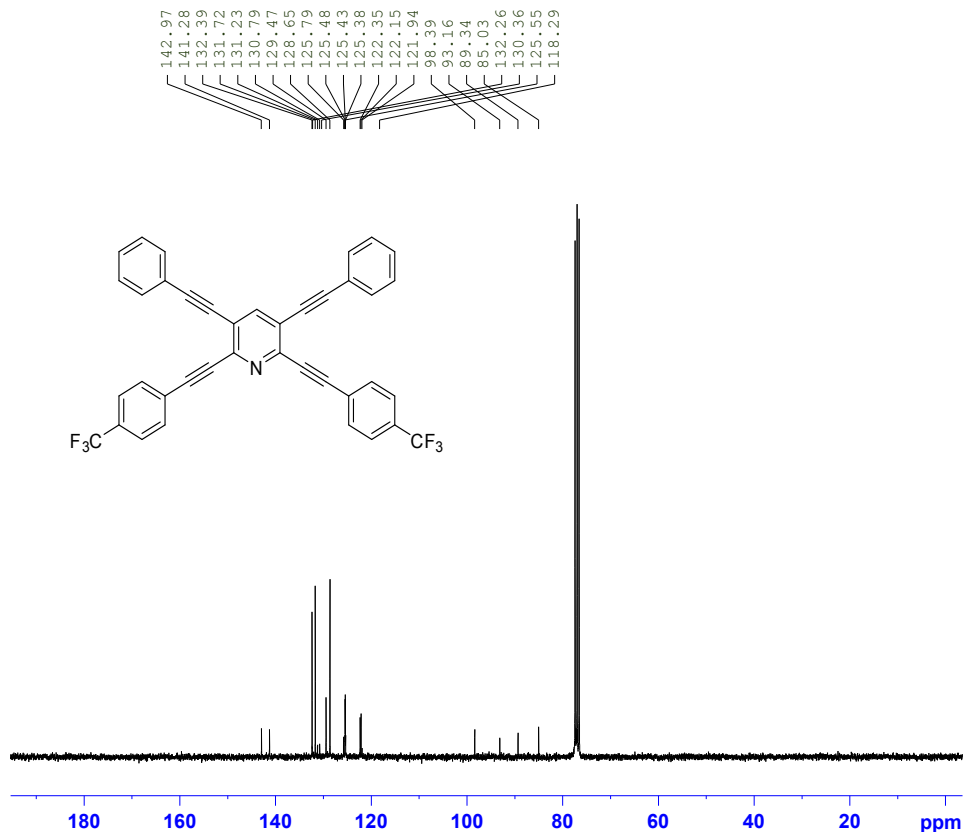
Current Data Parameters
NAME SRE 882 1H
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120811
Time_ 9.33
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 512
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
SF01 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300222 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

Reimann/ SRE 882
Aul13C CDCl3 /opt/topspin 1208 47



Current Data Parameters
NAME SRE 882 13C
EXPNO 11
PROCNO 1

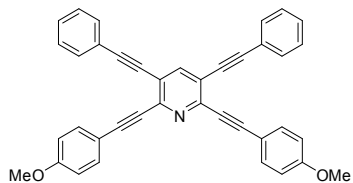
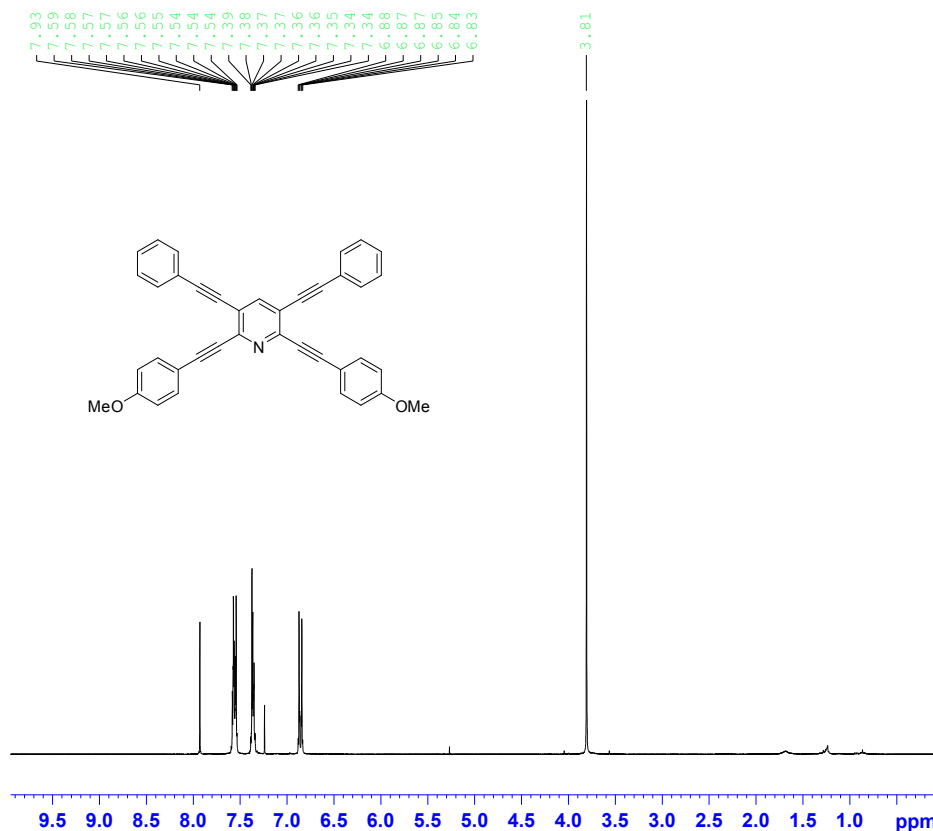
F2 - Acquisition Parameters
Date_ 20120811
Time_ 11.09
INSTRUM AV300
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 2000
DS 4
SWH 21097.047 Hz
FIDRES 0.648331 Hz
AQ 0.7766516 sec
RG 32768
DW 23.700 usec
DE 6.00 usec
TE 296.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.60 usec
PL1 -1.10 dB
SF01 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
SF02 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

Reimann/ SRE 883
AulH CDCl3 /opt/topspin 1208 48



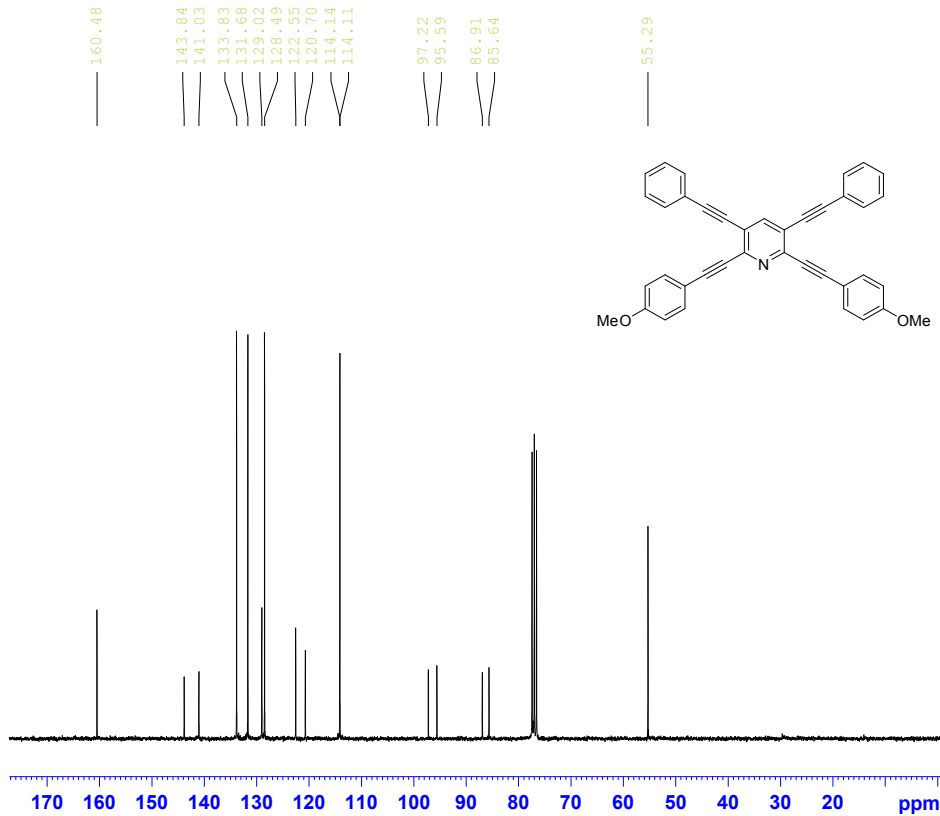
Current Data Parameters
NAME SRE 883 1H
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120811
Time_ 11.34
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 143.7
DW 81.000 usec
DE 6.00 usec
TE 295.9 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.00 usec
PL1 0.00 dB
SF01 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

Reimann/ SRE 883
Aul3C CDCl3 /opt/topspin 1208 48



Current Data Parameters
NAME SRE 883 13C
EXPNO 11
PROCNO 1

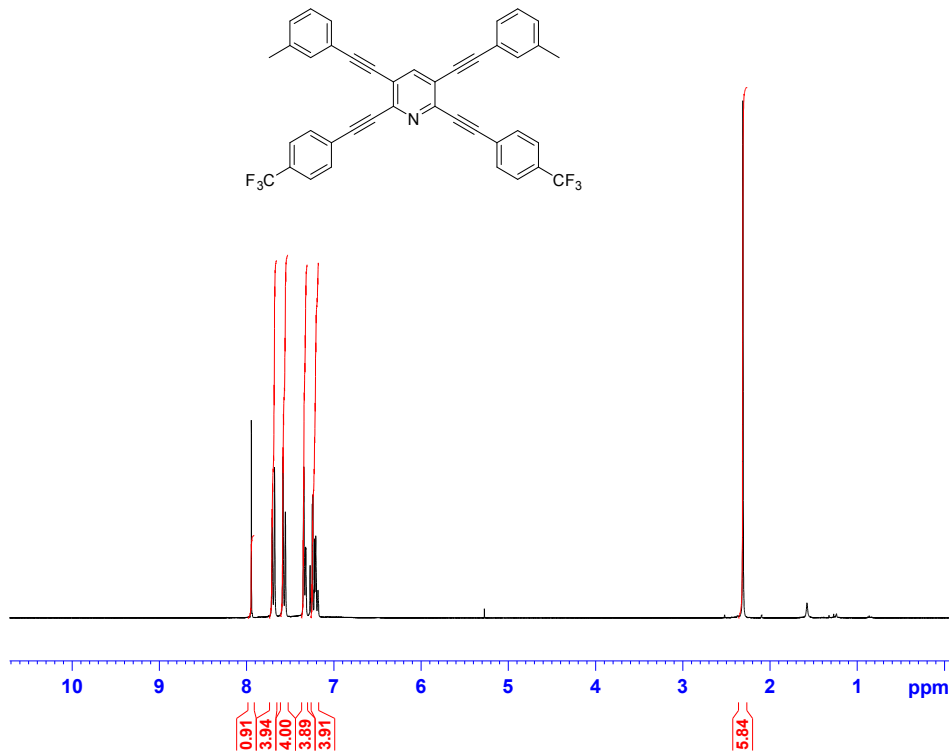
F2 - Acquisition Parameters
Date_ 20120811
Time_ 13.10
INSTRUM AV300
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 2000
DS 4
SWH 21097.047 Hz
FIDRES 0.643831 Hz
AQ 0.7766516 sec
RG 32768
DW 23.700 usec
DE 6.00 usec
TE 296.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 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 75.4677565 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Reimann/ SRE 887
AulH CDCl3 /opt/topspin 1208 50



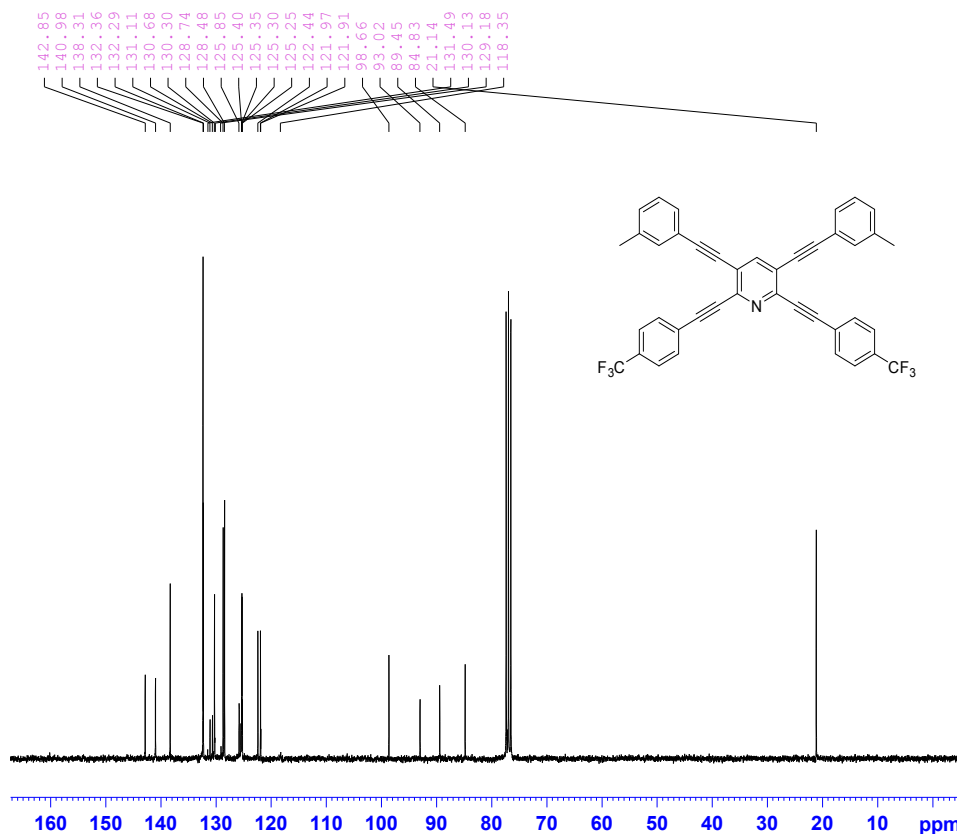
Current Data Parameters
NAME SRE 887 1H
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120811
Time_ 14.33
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
TDO 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 887
 Aul3C CDC13 /opt/topspin 1208 50



Current Data Parameters
 NAME SRE 887 13C
 EXPNO 11
 PROCNO 1

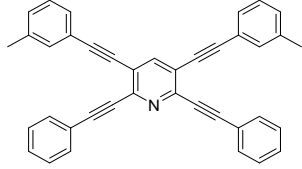
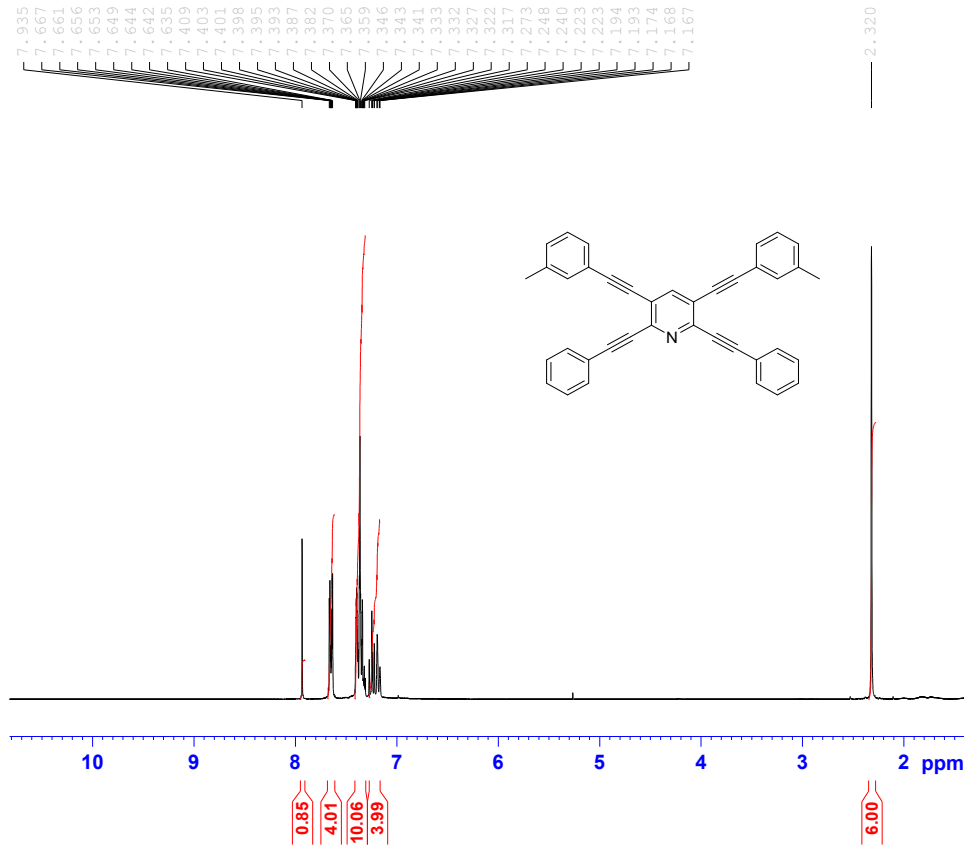
F2 - Acquisition Parameters
 Date_ 20120811
 Time_ 16.09
 INSTRUM AV300
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 32768
 SOLVENT CDC13
 NS 2000
 DS 4
 SWH 21097.047 Hz
 FIDRES 0.643831 Hz
 AQ 0.7766516 sec
 RG 32768
 DW 23.700 usec
 DE 6.00 usec
 TE 296.5 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 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 75.4677557 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Reimann/ SRE 888
 Au1H CDC13 /opt/topspin 1208 51



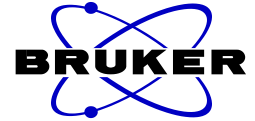
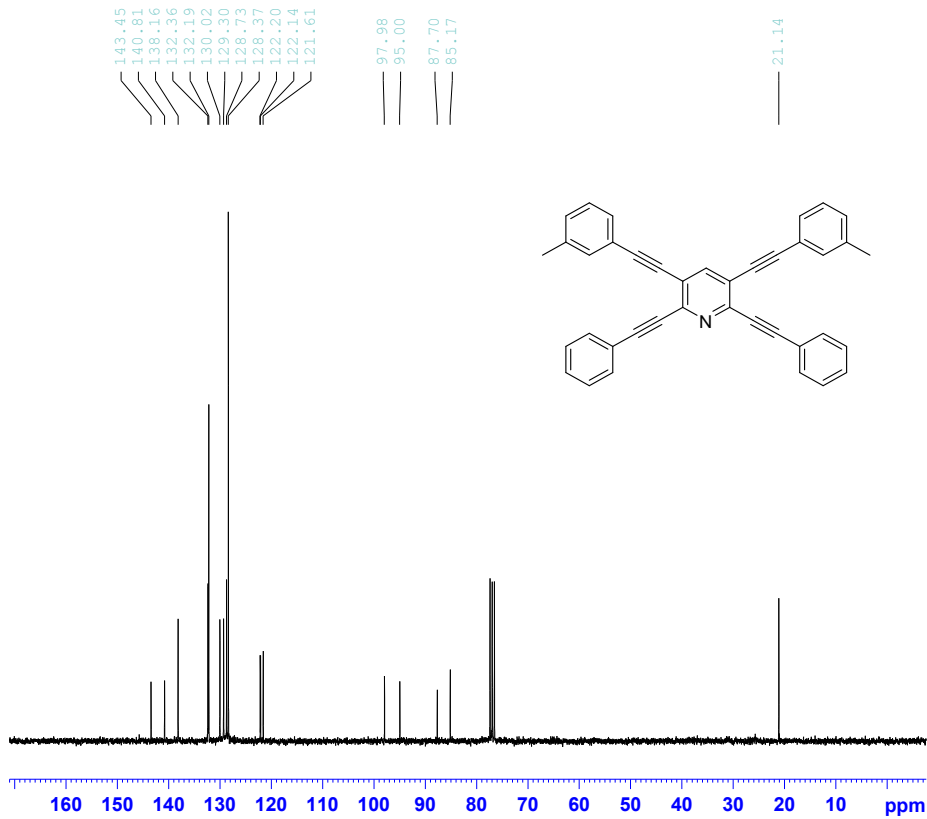
Current Data Parameters
 NAME SRE 888 1H
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120811
 Time 16.33
 INSTRUM AV300
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT CDC13
 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 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 300.1300216 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

Reimann/ SRE 888
 Au13C CDC13 /opt/topspin 1208 51



Current Data Parameters
 NAME SRE 888 13C
 EXPNO 11
 PROCNO 1

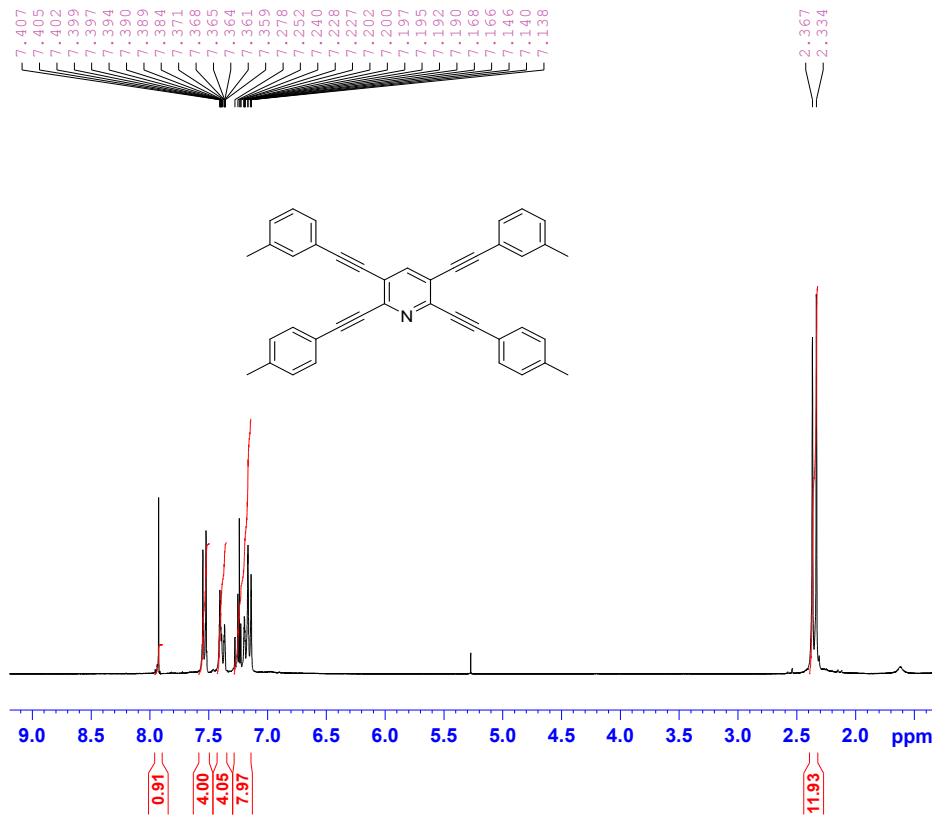
F2 - Acquisition Parameters
 Date_ 20120811
 Time 16.47
 INSTRUM AV300
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 32768
 SOLVENT CDC13
 NS 256
 DS 4
 SWH 21097.047 Hz
 FIDRES 0.643831 Hz
 AQ 0.7766516 sec
 RG 32768
 DW 23.700 usec
 DE 6.00 usec
 TE 296.5 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 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
 FL13 21.00 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677586 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Reimann/ SRE 889
 Au1H CDC13 /opt/topspin 1208 52



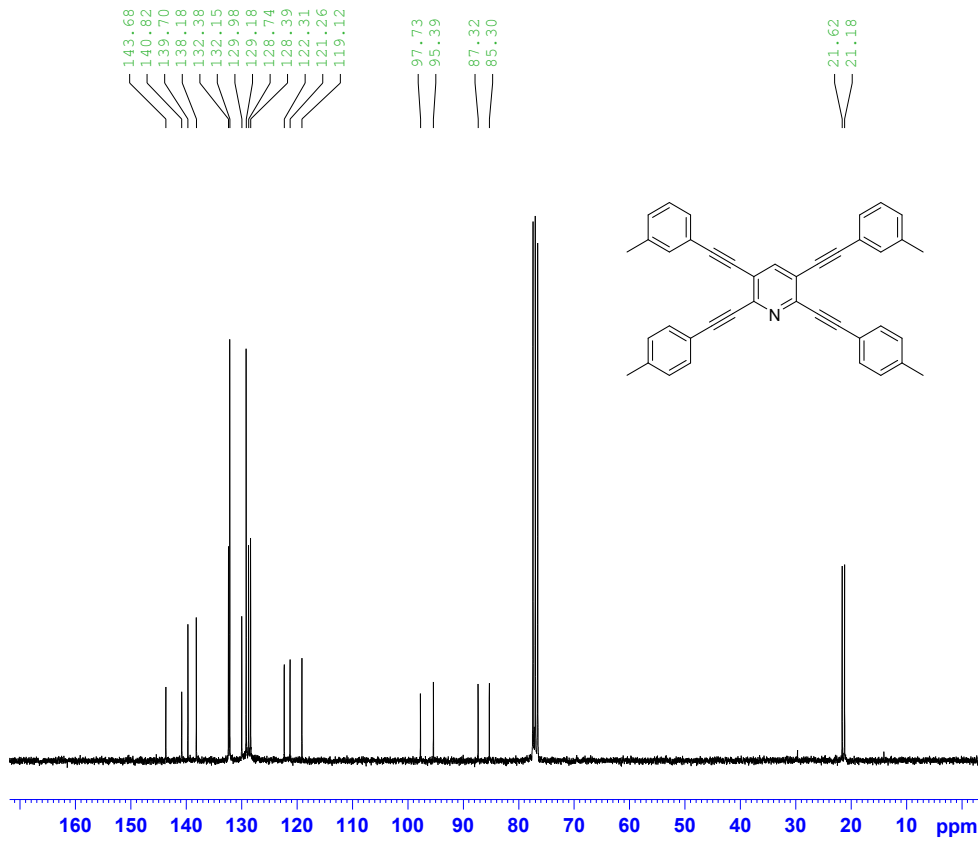
Current Data Parameters
 NAME SRE 889 1H
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120811
 Time 17.06
 INSTRUM AV300
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT CDC13
 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 295.9 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 300.1300216 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

Reimann/ SRE 889
Aul3C CDCl3 /opt/topspin 1208 52



Current Data Parameters
NAME SRE 889 13C
EXPNO 11
PROCNO 1

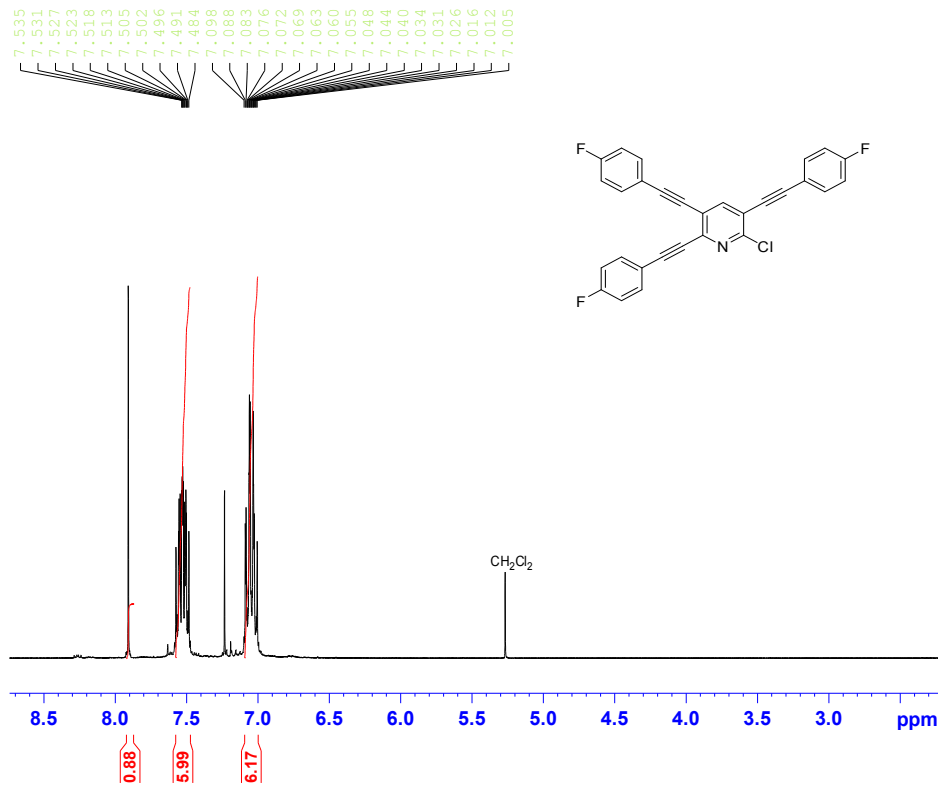
F2 - Acquisition Parameters
Date_ 20120811
Time_ 18.41
INSTRUM AV300
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 2000
DS 4
SWH 21097.047 Hz
FIDRES 0.643831 Hz
AQ 0.7766516 sec
RG 32768
DW 23.700 usec
DE 6.00 usec
TE 296.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.899999998 sec
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 75.4677556 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Reimann/ SRE 849
AulH CDCl3 /opt/topspin 1207 31



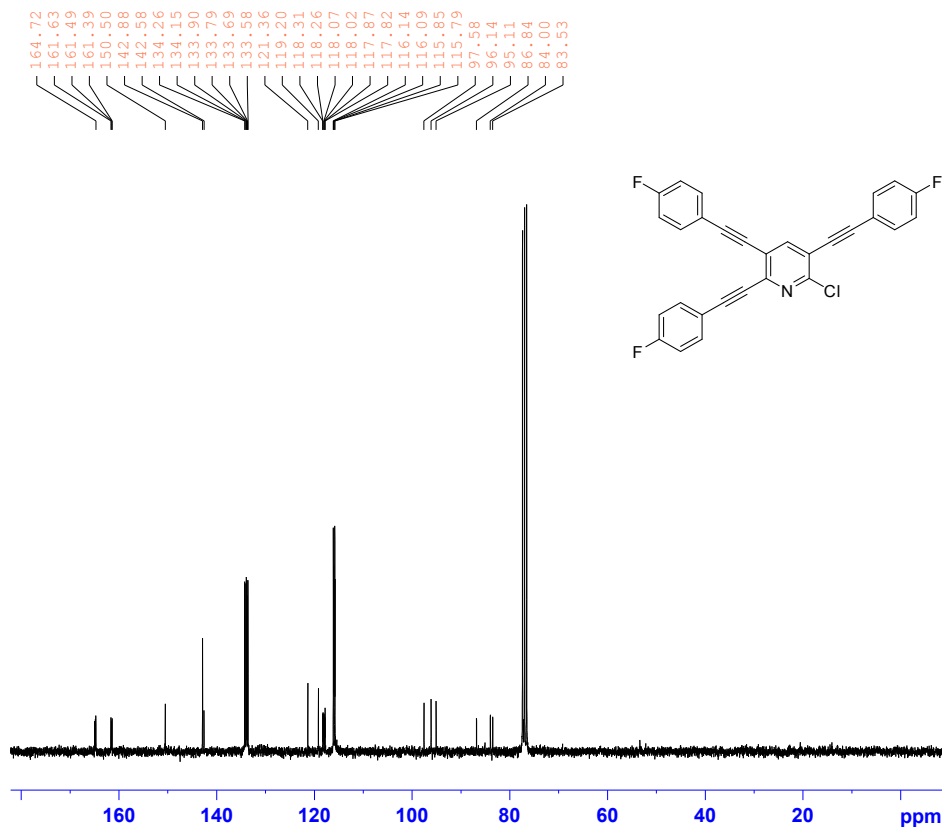
Current Data Parameters
NAME SRE 849 1H
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120705
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 296.1 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 300.1300232 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

Reimann/ SRE 849
Aul3C CDCl3 /opt/topspin 1207 31



Current Data Parameters
NAME SRE 849 13C
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120705
Time 6.16
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 2.0000000 sec
d11 0.0300000 sec
DELTA 1.89999998 sec
TD0 1

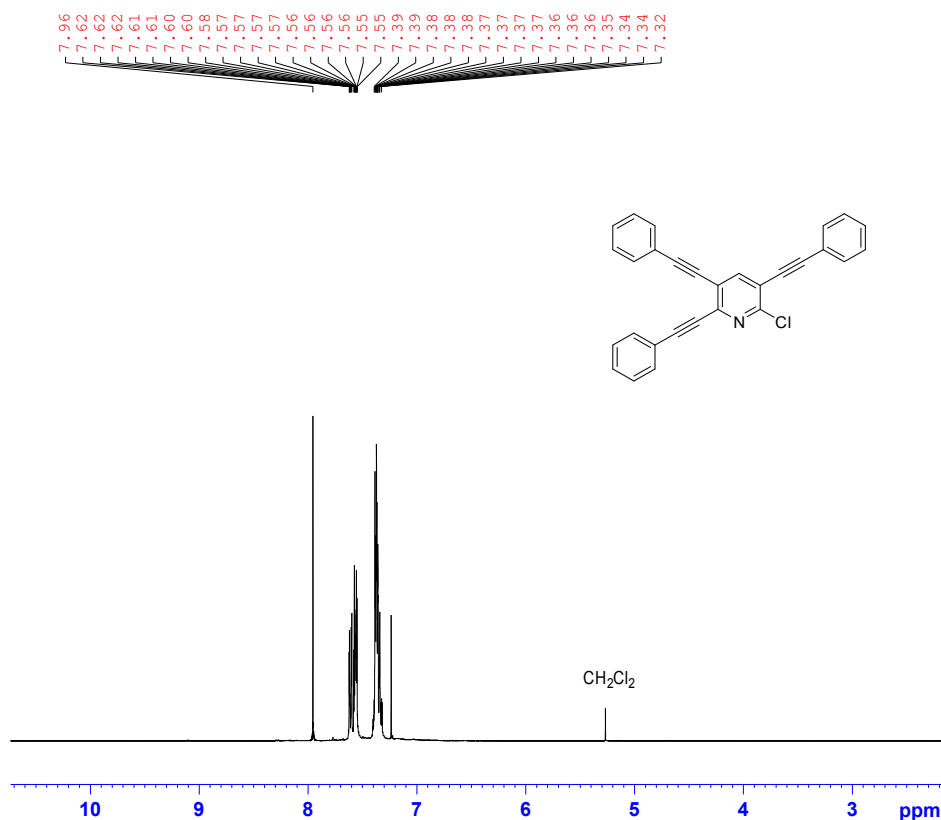
===== CHANNEL f1 =====
NUC1 13C
P1 9.60 usec
PL1 -1.10 dB
SFO1 75.4771825 MHz

===== 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 75.4677546 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹H- and ¹³C-NMR Spectra of compounds 6a-e

Reimann/ SRE 839
Aul1H CDCl3 /opt/topspin 1206 5

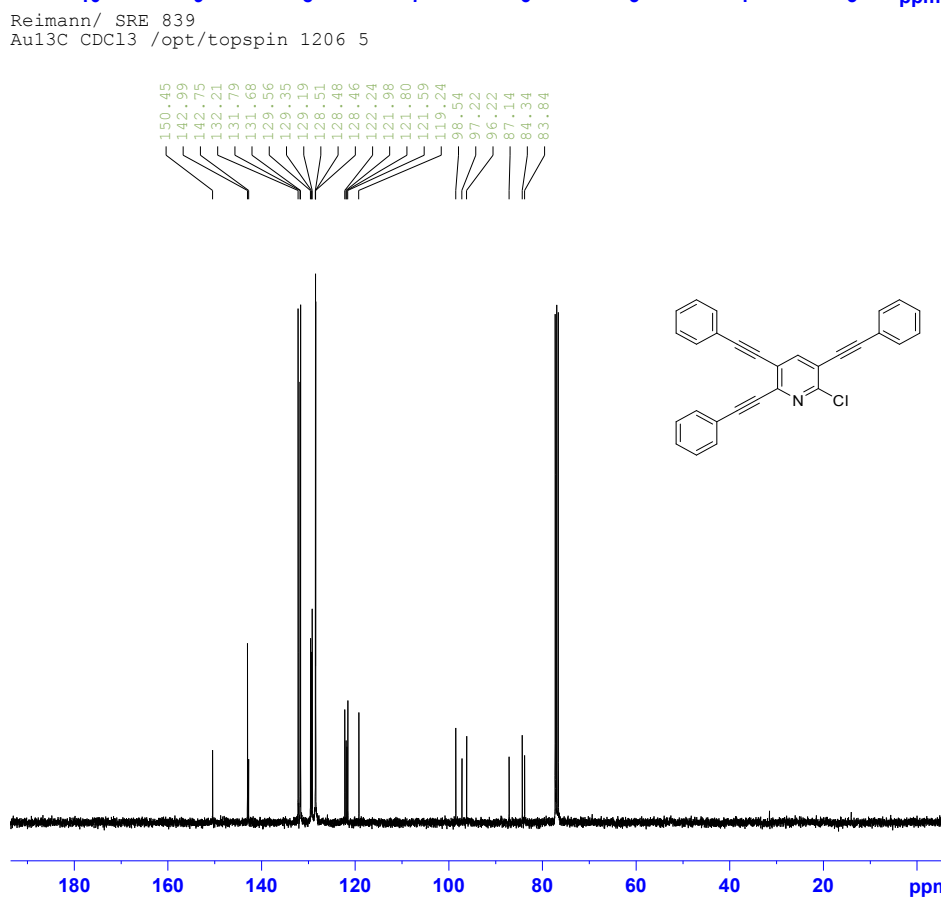


Current Data Parameters
NAME SRE 839 1H
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120628
Time 17.22
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 203.2
DW 62.400 usec
DE 6.00 usec
TE 297.0 K
D1 1.5000000 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 400.1300309 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



Current Data Parameters
NAME SRE 839 13C
EXPNO 11
PROCNO 1

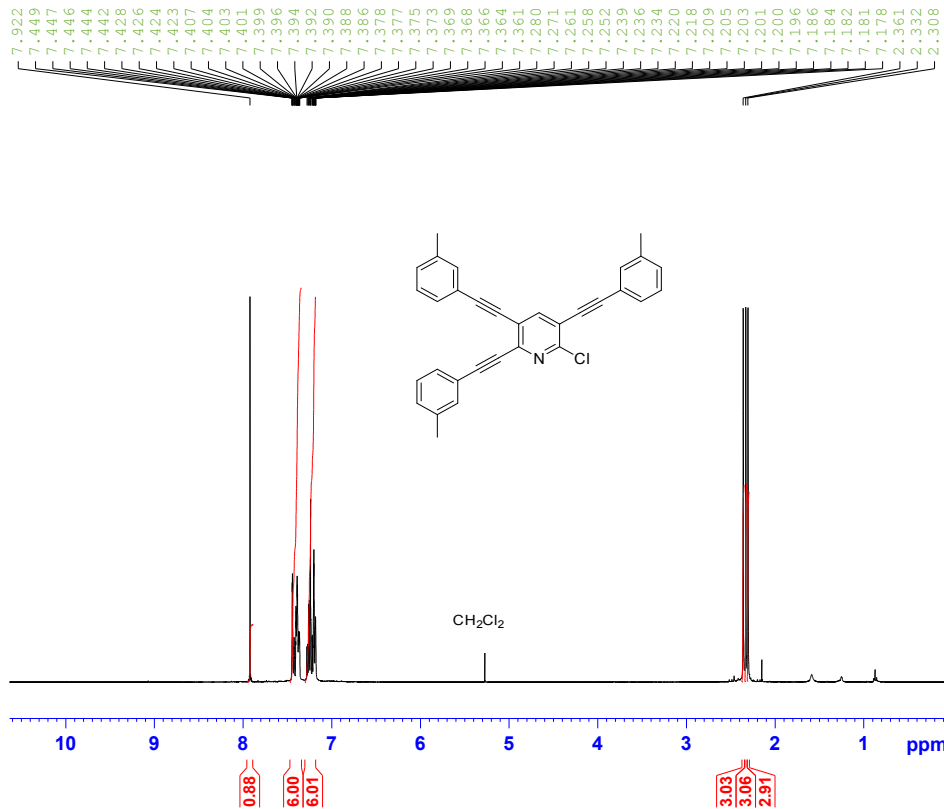
F2 - Acquisition Parameters
Date_ 20120628
Time 17.47
INSTRUM AV400
PROBHD 5 mm QNP 1H/29
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 500
DS 4
SWH 29940.119 Hz
FIDRES 0.456850 Hz
AQ 1.0945013 sec
RG 9195.2
DW 16.700 usec
DE 6.00 usec
TE 297.0 K
D1 1.70000005 sec
d11 0.03000000 sec
DELTA 1.60000002 sec
TD0 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 100.6127799 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

Reimann/ SRE 848
 Au1H CDCl3 /opt/topspin 1207 2



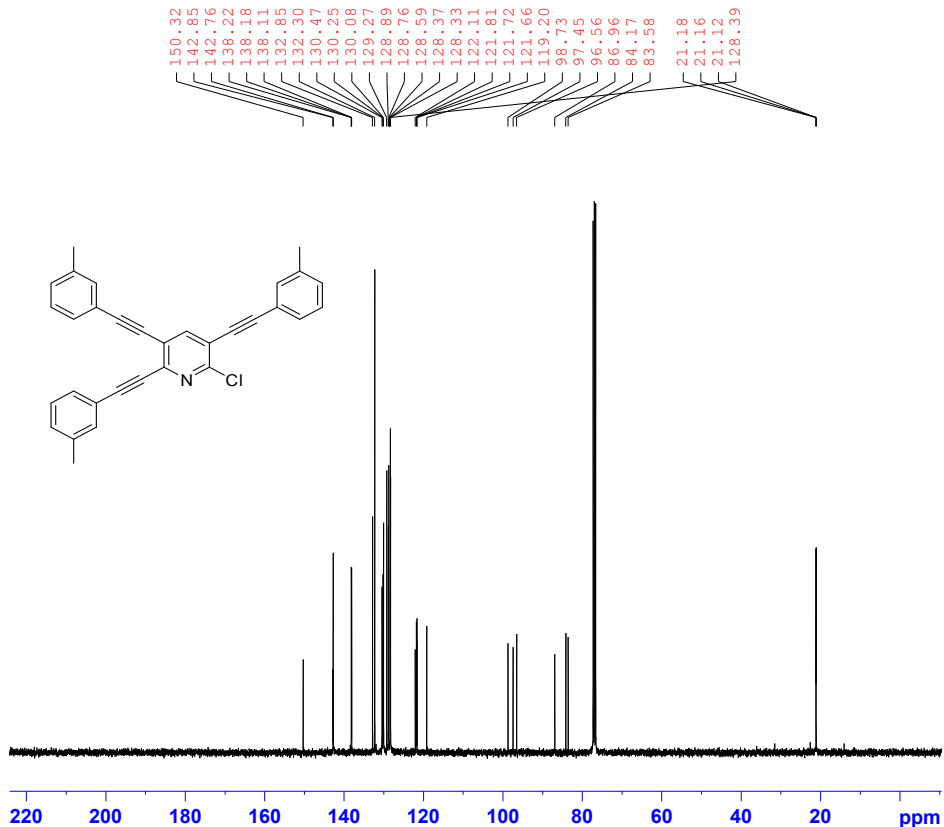
Current Data Parameters
 NAME SRE 848 1H
 EXNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120704
 Time 16.08
 INSTRUM AV400
 PROBHD 5 mm QNP 1H/29
 FULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 32
 DS 4
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447731 sec
 RG 143.7
 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 400.1300298 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

Reimann/ SRE 848
 Au13C CDCl3 /opt/topspin 1207 2



Current Data Parameters
 NAME SRE 848 13C
 EXFNO 11
 PROCNO 1

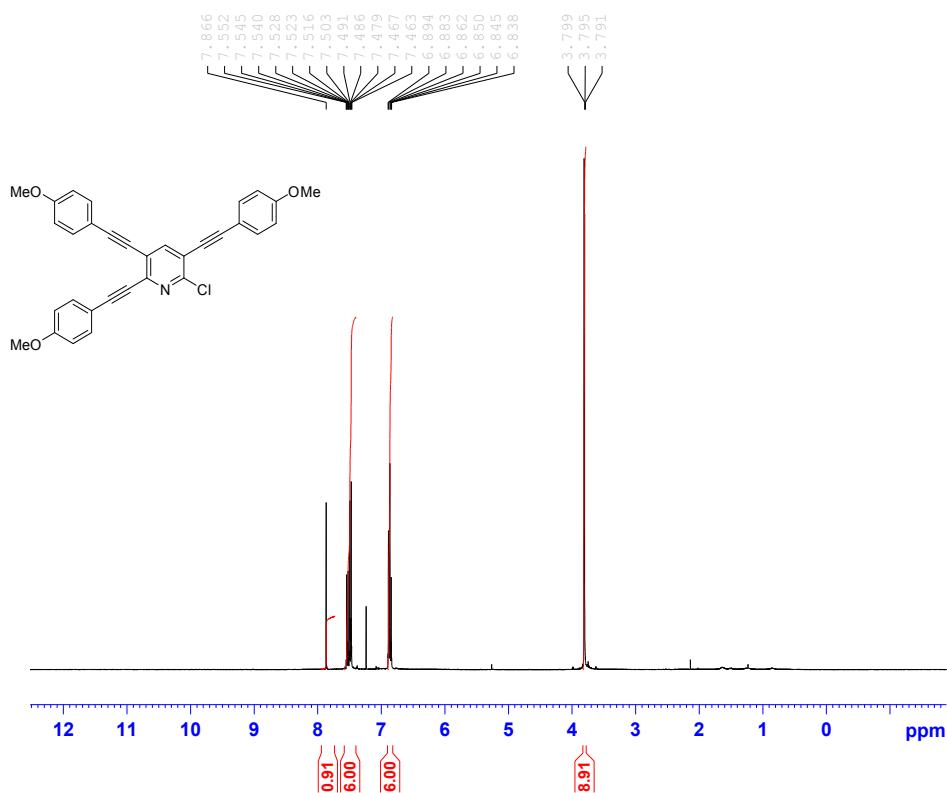
F2 - Acquisition Parameters
 Date_ 20120704
 Time 16.57
 INSTRUM AV400
 PROBHD 5 mm QNP 1H/29
 FULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1000
 DS 4
 SWH 29940.119 Hz
 FIDRES 0.456850 Hz
 AQ 1.0945013 sec
 RG 11585.2
 DW 16.700 usec
 DE 6.00 usec
 TE 297.0 K
 D1 1.70000005 sec
 d11 0.03000000 sec
 DELTA 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 100.6127800 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

Reimann/ SRE 850
 Au1H CDC13 /opt/topspin 1207 3



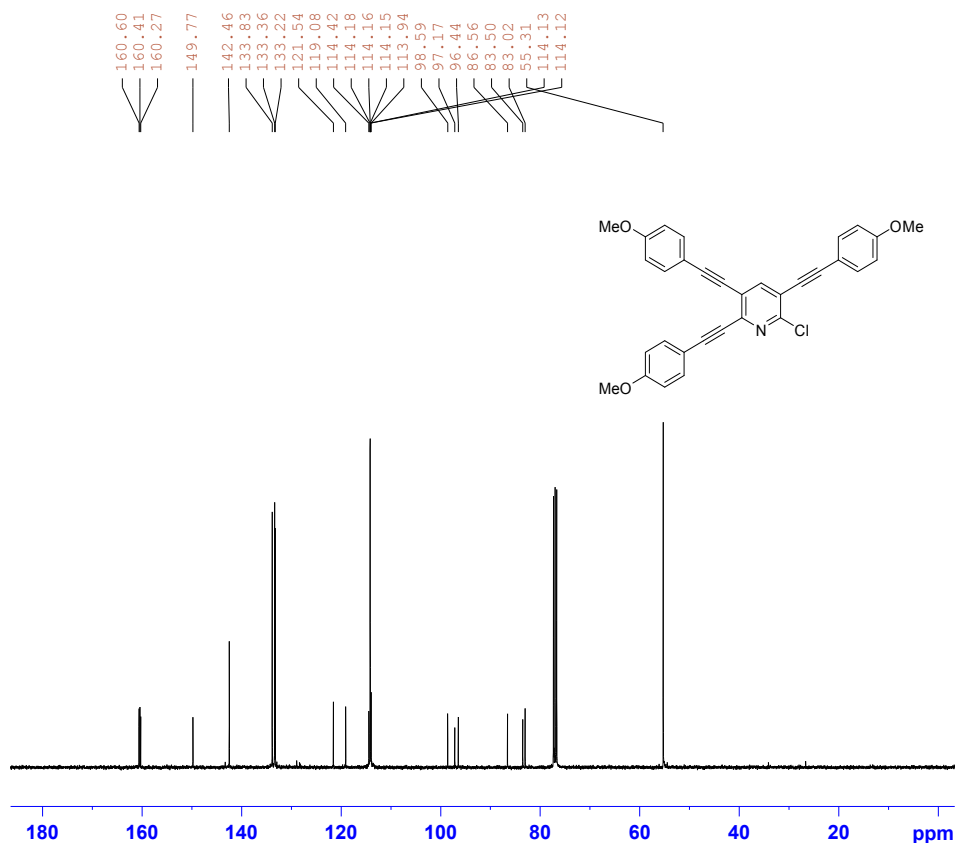
Current Data Parameters
 NAME SRE 850 1H
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120704
 Time 17.12
 INSTRUM AV400
 PROBHD 5 mm QNP 1H/29
 PULPROG zg30
 TD 32768
 SOLVENT CDC13
 NS 32
 DS 4
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447731 sec
 RG 143.7
 DW 62.400 usec
 DE 6.00 usec
 TE 297.0 K
 D1 1.5000000 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 400.1300300 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

Reimann/ SRE 850
 Au13C CDC13 /opt/topspin 1207 3



Current Data Parameters
 NAME SRE 850 13C
 EXPNO 11
 PROCNO 1

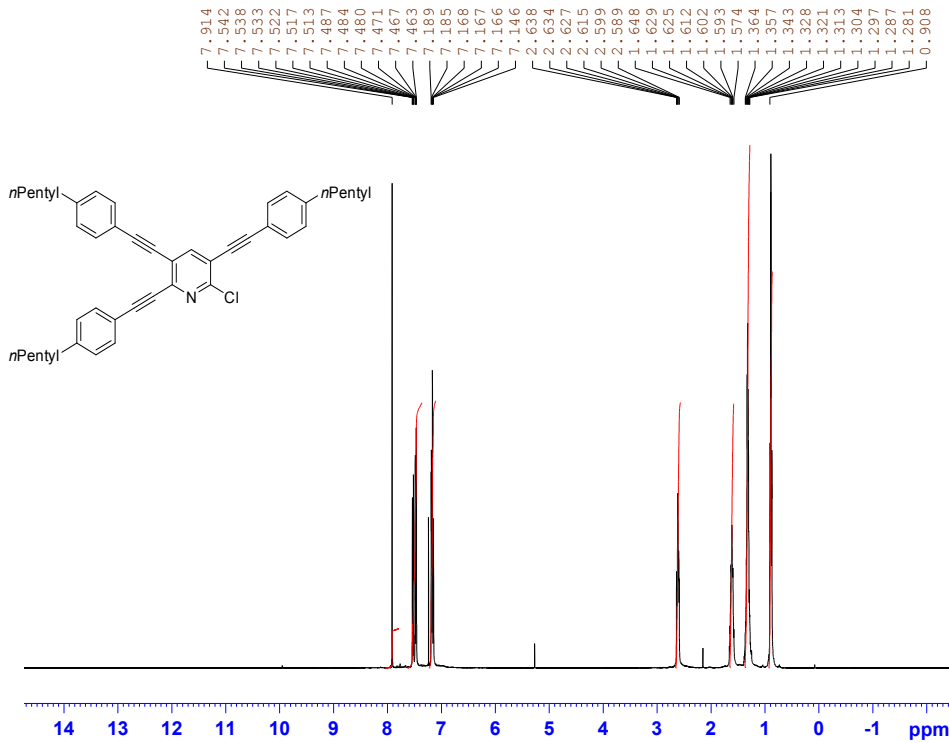
F2 - Acquisition Parameters
 Date_ 20120704
 Time 18.00
 INSTRUM AV400
 PROBHD 5 mm QNP 1H/29
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 1000
 DS 4
 SWH 29940.119 Hz
 FIDRES 0.456850 Hz
 AQ 1.0945013 sec
 RG 13004
 DW 16.700 usec
 DE 6.00 usec
 TE 297.0 K
 D1 1.70000005 sec
 d11 0.03000000 sec
 DELTA 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 100.6127783 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

Reimann/ SRE 847
AulH CDC13 /opt/topspin 1207 5



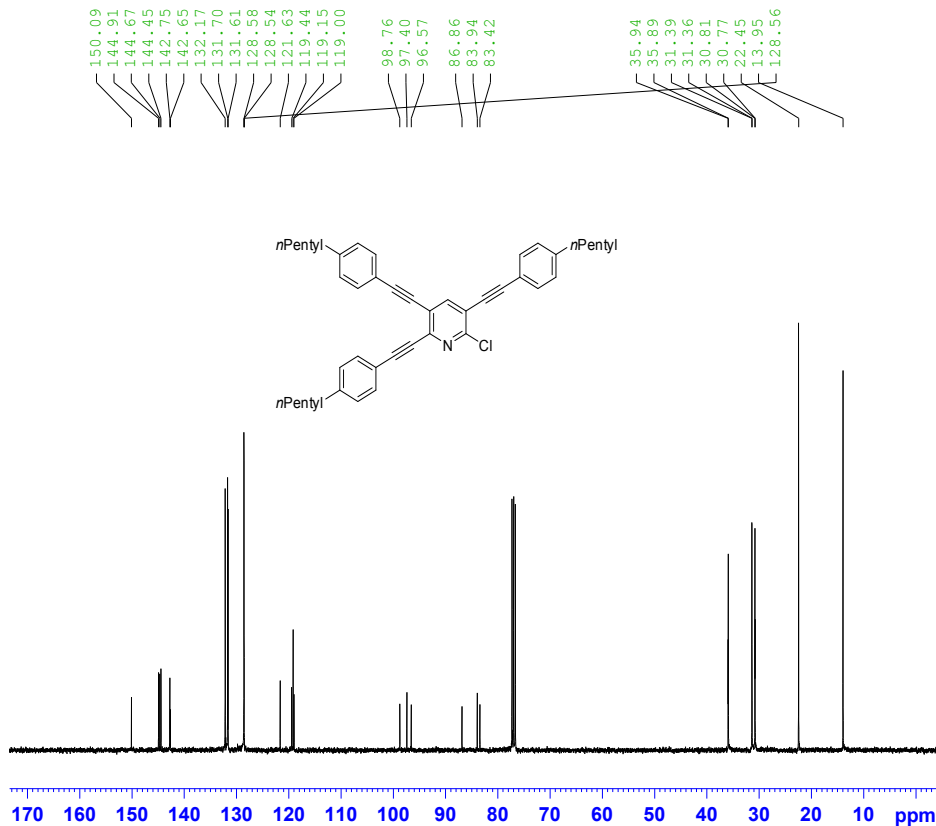
Current Data Parameters
NAME SRE 847 1H
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120704
Time 19.19
INSTRUM AV400
PROBHD 5 mm QNP 1H/29
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 32
DS 4
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 71.8
DW 62.400 usec
DE 6.00 usec
TE 297.0 K
D1 1.5000000 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 400.1300302 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

Reimann/ SRE 847
Aul13C CDC13 /opt/topspin 1207 5



Current Data Parameters
NAME SRE 847 13C
EXPNO 11
PROCNO 1

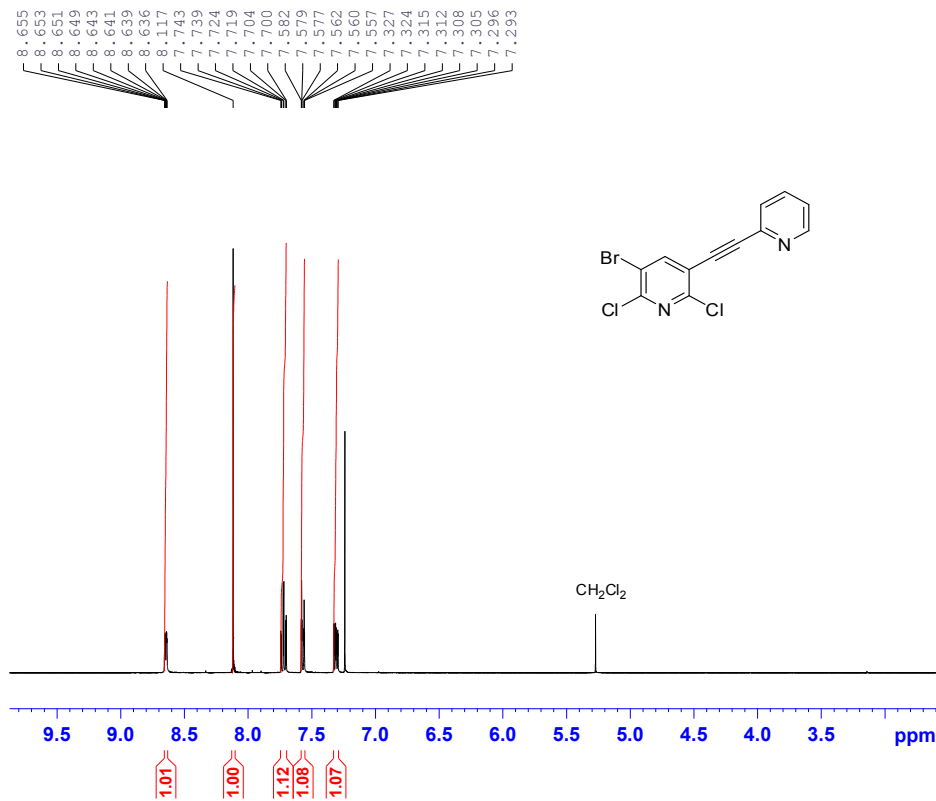
F2 - Acquisition Parameters
Date_ 20120704
Time 19.43
INSTRUM AV400
PROBHD 5 mm QNP 1H/29
PULPROG zgpg30
TD 85536
SOLVENT CDC13
NS 500
DS 4
SWH 29940.119 Hz
FIDRES 0.456850 Hz
AQ 1.0945013 sec
RG 13004
DW 16.700 usec
DE 6.00 usec
TE 297.0 K
D1 1.7000005 sec
d11 0.0300000 sec
DELTA 1.6000002 sec
TD0 1

===== 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 100.6127813 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

Reimann/ SRE 844
AulH CDC13 /opt/topspin 1207 1



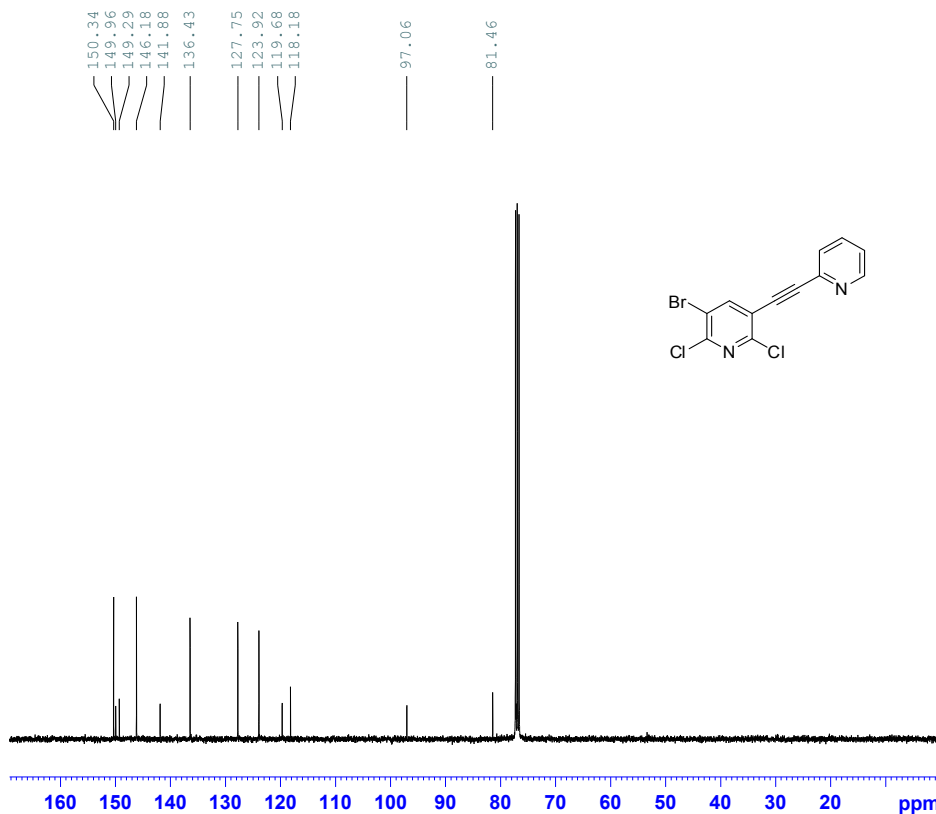
Current Data Parameters
NAME SRE 844 1H
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120704
Time 15.05
INSTRUM AV400
PROBHD 5 mm QNP 1H/29
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 32
DS 4
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 512
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 400.1300294 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

Reimann/ SRE 844
Aul13C CDC13 /opt/topspin 1207 1



Current Data Parameters
NAME SRE 840 13C
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120704
Time 15.53
INSTRUM AV400
PROBHD 5 mm QNP 1H/29
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1000
DS 4
SWH 29940.119 Hz
FIDRES 0.456850 Hz
AQ 1.0945013 sec
RG 13004
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

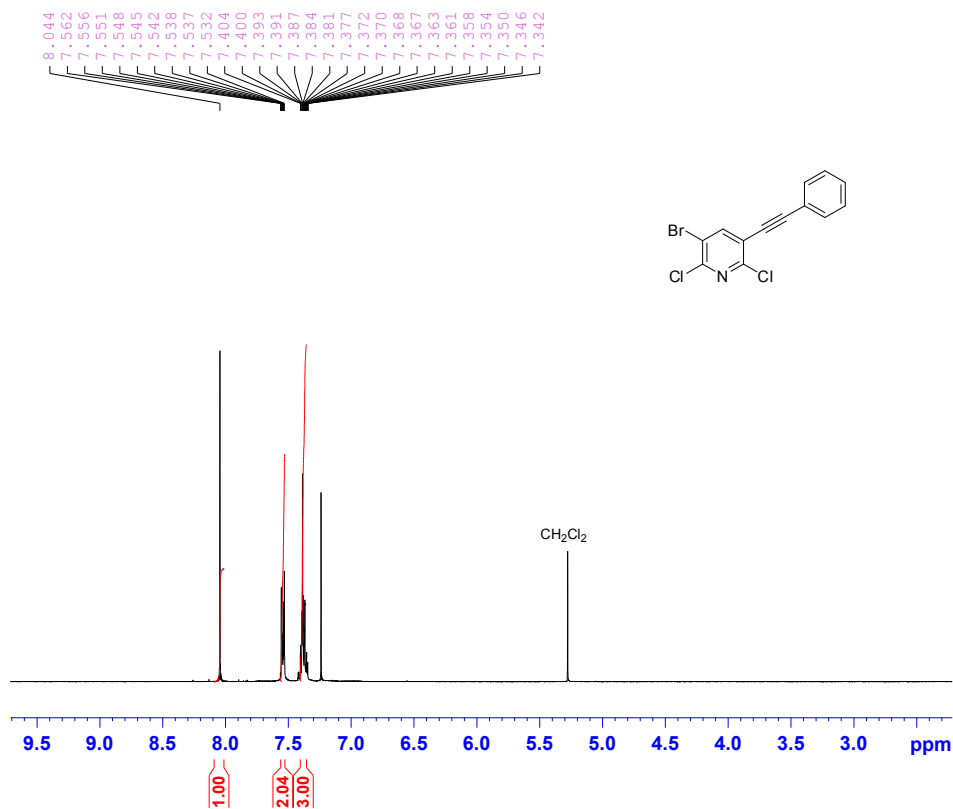
===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 100.6260690 MHz

===== 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 100.6127759 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

¹H- and ¹³C-NMR Spectra of Compounds 7a-e

Reimann/ SRE 840
AulH CDCl3 /opt/topspin 1206 6



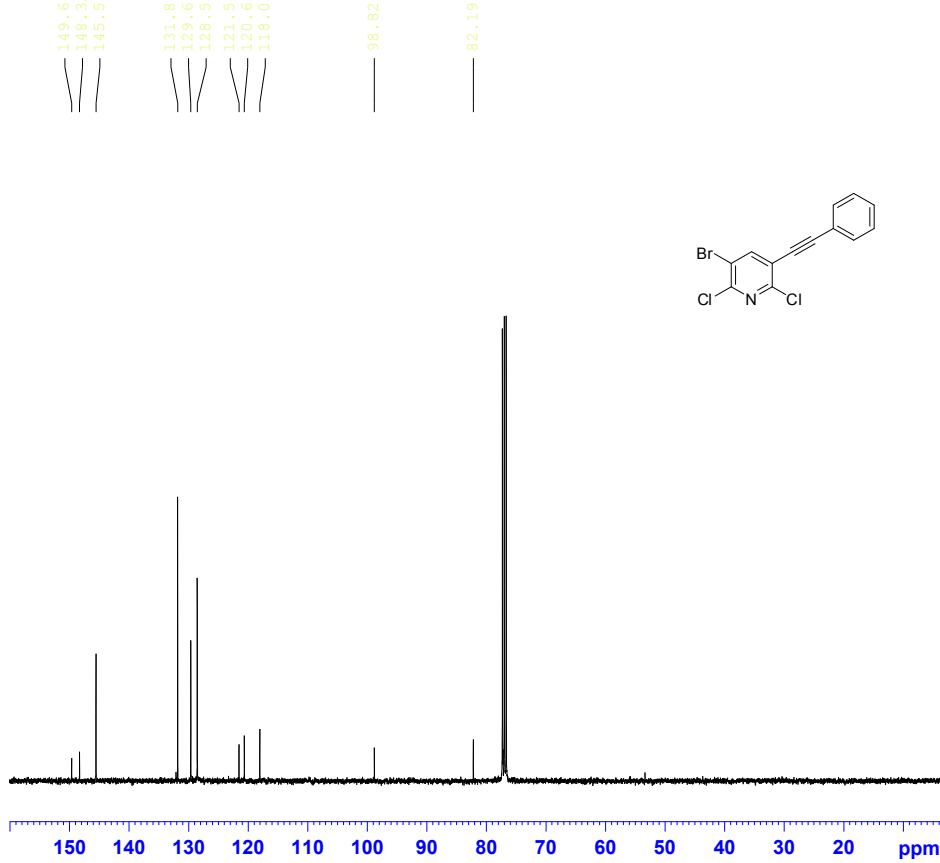
Current Data Parameters
NAME SRE 840 1H
EXNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120628
Time 18.02
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 512
DW 62.400 usec
DE 6.00 usec
TE 297.0 K
D1 1.50000000 sec
TDO 1

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

F2 - Processing parameters
SI 32768
SF 400.1300297 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

Reimann/ SRE 840
 Au13C CDCl3 /opt/topspin 1206 6



Current Data Parameters
 NAME SRE 840 13C
 EXPNO 11
 PROCNO 1

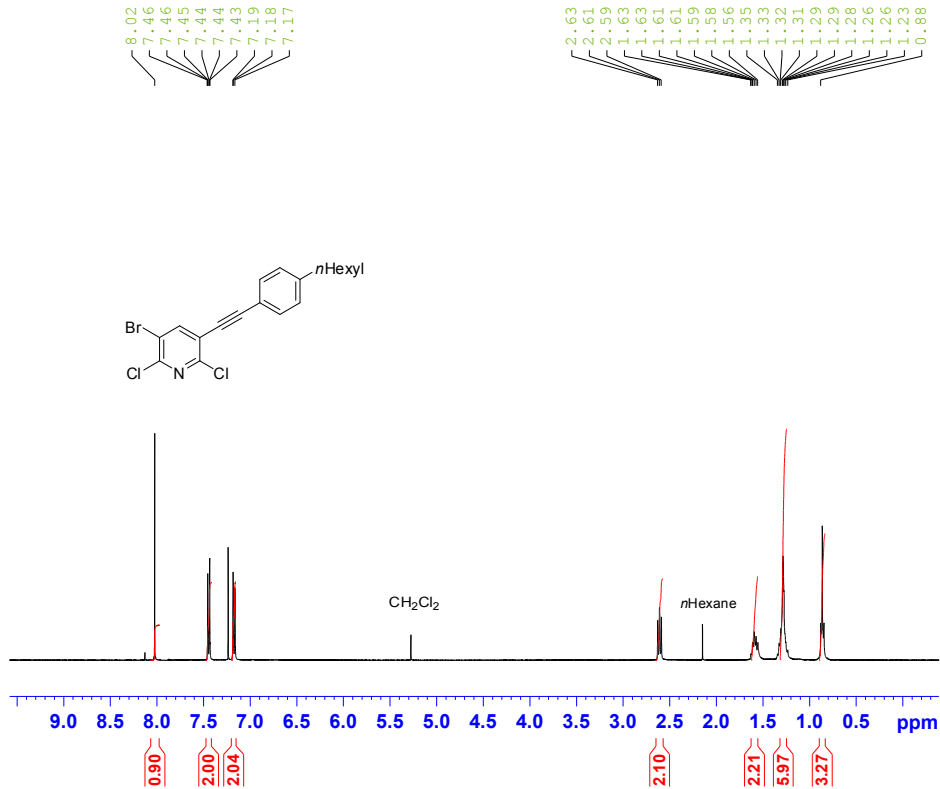
F2 - Acquisition Parameters
 Date_ 20120628
 Time_ 18.51
 INSTRUM AV400
 PROBHD 5 mm QNP 1H/29
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1000
 DS 4
 SWH 29940.119 Hz
 FIDRES 0.456850 Hz
 AQ 1.0945013 sec
 RG 13004
 DW 16.700 usec
 DE 6.00 usec
 TE 297.0 K
 D1 1.70000005 sec
 d11 0.03000000 sec
 DELTA 1.60000002 sec
 TDO 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 100.6127756 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 FC 1.00

Reimann/ SRE 851
 Au1H CDCl3 /opt/topspin 1207 4



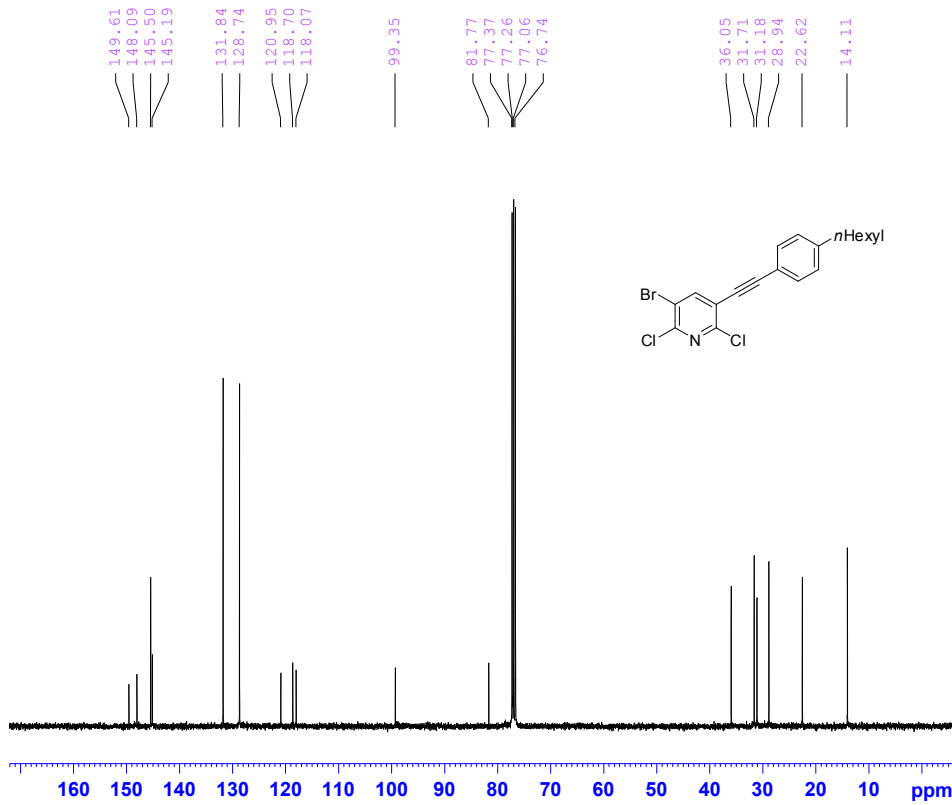
Current Data Parameters
 NAME SRE 851 1H
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120704
 Time_ 18.15
 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 256
 DW 62.400 usec
 DE 6.00 usec
 TE 297.0 K
 D1 1.50000000 sec
 TDO 1

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

F2 - Processing parameters
 SI 32768
 SF 400.1300300 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

Reimann/ SRE 851
 Aul3C CDC13 /opt/topspin 1207 4



Current Data Parameters
 NAME SRE 851 13C
 EXPNO 11
 PROCNO 1

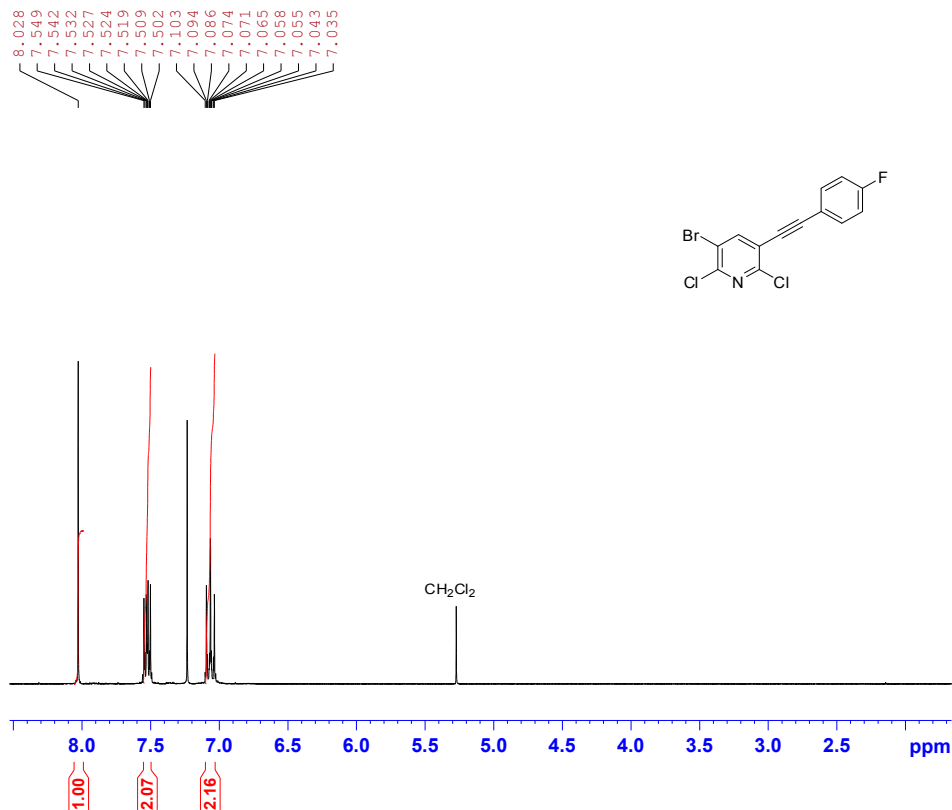
F2 - Acquisition Parameters
 Date_ 20120704
 Time 19.04
 INSTRUM AV400
 PROBHD 5 mm QNP 1H/29
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 1000
 DS 4
 SWH 29940.119 Hz
 FIDRES 0.456850 Hz
 AQ 1.0945013 sec
 RG 13004
 DW 16.700 usec
 DE 6.00 usec
 TE 297.0 K
 D1 1.70000005 sec
 d11 0.03000000 sec
 DELTA 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
 EPCD2 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 100.6127757 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

Reimann, SRE 853
 Aul1H CDC13 /opt/topspin 1207 22



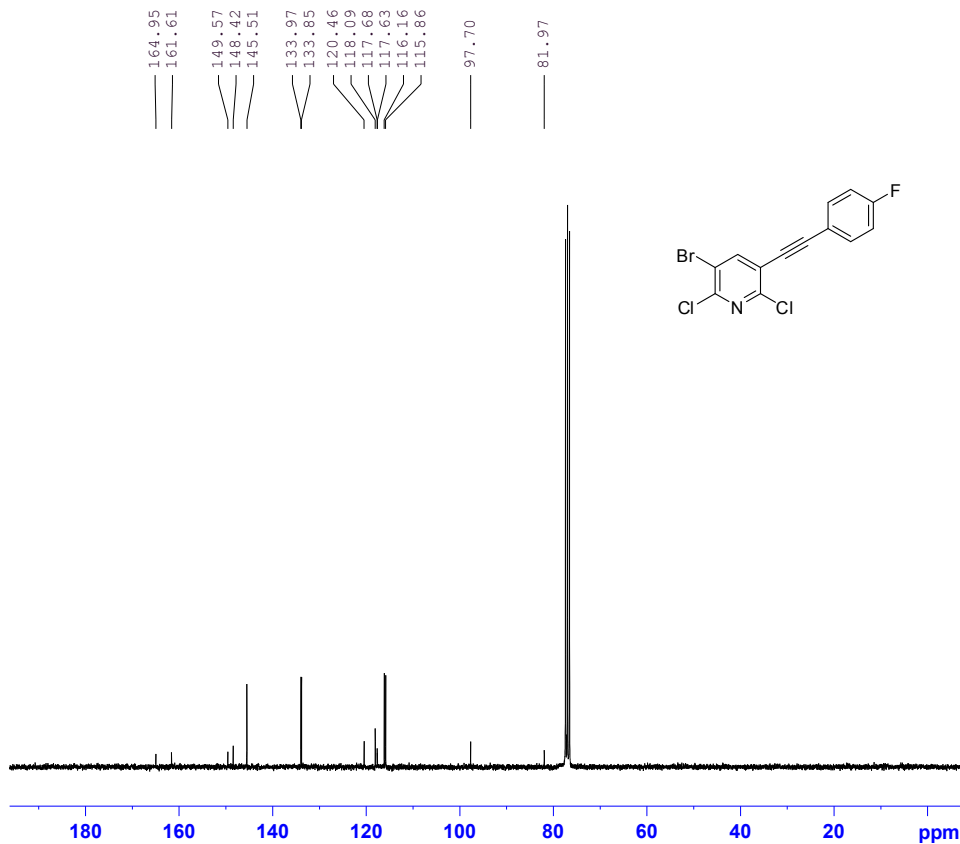
Current Data Parameters
 NAME SRE 853 1H
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120713
 Time 3.31
 INSTRUM AV300
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT CDC13
 NS 32
 DS 4
 SWH 6172.839 Hz
 FIDRES 0.188380 Hz
 AQ 2.6542580 sec
 RG 724.1
 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 300.1300233 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

Reimann / SRE 853
 Au13C CDC13 /opt/topspin 1207 52



Current Data Parameters
 NAME SRE 853 3000 13C
 EXPNO 10
 PROCNO 1

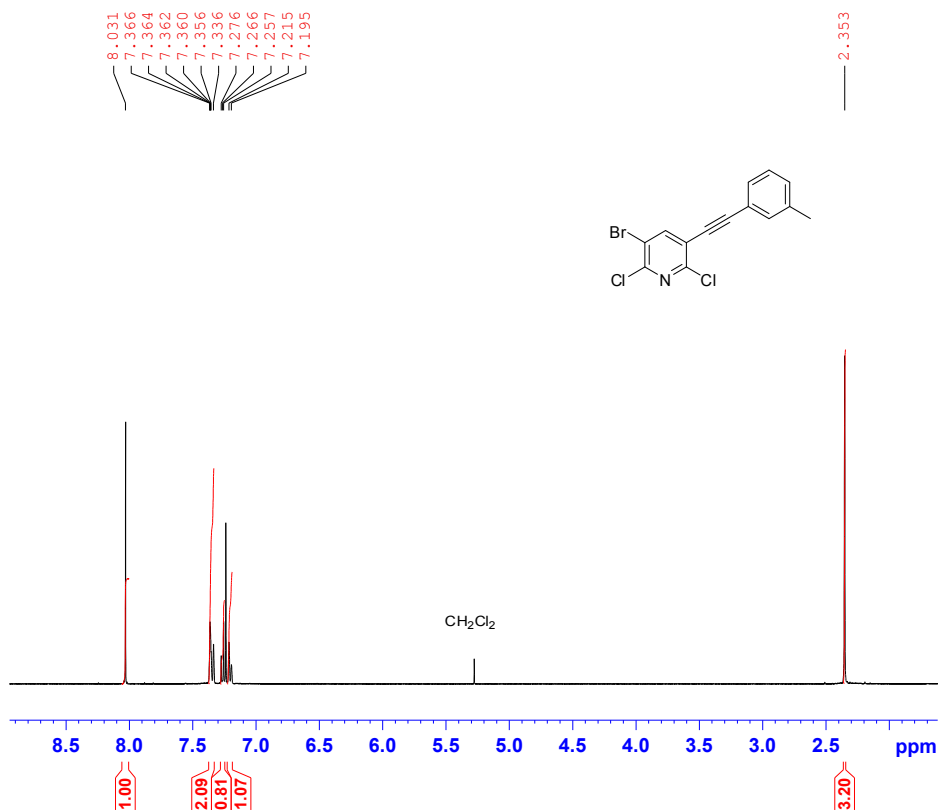
F2 - Acquisition Parameters
 Date_ 20120715
 Time 1.27
 INSTRUM AV300
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 32768
 SOLVENT CDC13
 NS 3000
 DS 4
 SWH 21097.047 Hz
 FIDRES 0.643831 Hz
 AQ 0.7766516 sec
 RG 32768
 DW 23.700 usec
 DE 6.00 usec
 TE 296.1 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 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 75.4677537 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Reimann, SRE 854
 Au1H CDC13 /opt/topspin 1207 12



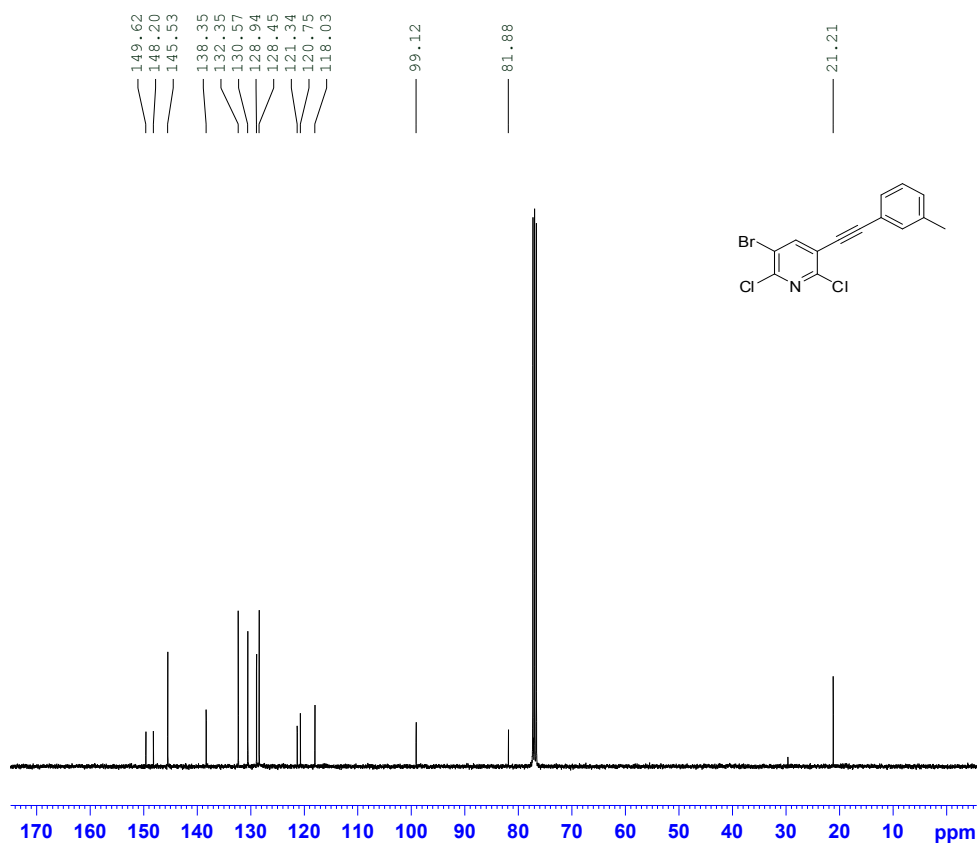
Current Data Parameters
 NAME SRE 854 1H
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120713
 Time 22.53
 INSTRUM AV400
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT CDC13
 NS 32
 DS 4
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447731 sec
 RG 512
 DW 62.400 usec
 DE 6.00 usec
 TE 297.0 K
 D1 1.50000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.10 usec
 PL1 -1.00 dB
 SFO1 400.1324000 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300297 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

Reimann, SRE 854
Aul3C CDCl3 /opt/topspin 1207 12



Current Data Parameters
NAME SRE 854 13C
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date 20120714
Time 0.29
INSTRUM AV400
PROBHD 5 mm PABBO BE-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2000
DS 4
SWH 29940.119 Hz
FIDRES 0.456850 Hz
AQ 1.0945013 sec
RG 18390.4
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

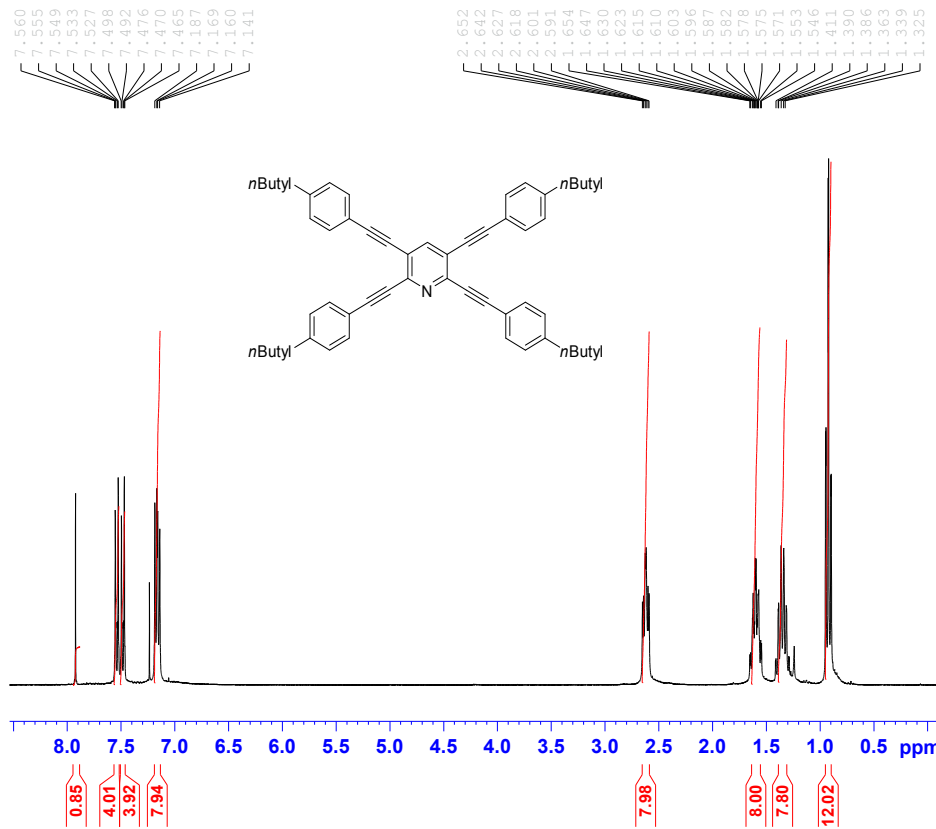
===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
SFO1 100.6260690 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
FCFD2 100.00 usec
PL2 -2.00 dB
PL12 17.00 dB
PL13 19.00 dB
SFO2 400.1318000 MHz

F2 - Processing parameters
SI 32768
SF 100.6127753 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

¹H- and ¹³C-NMR Spectra of Compounds 8a-g

Reimann/ SRE 884
AulH CDC13 /opt/topspin 1208 49



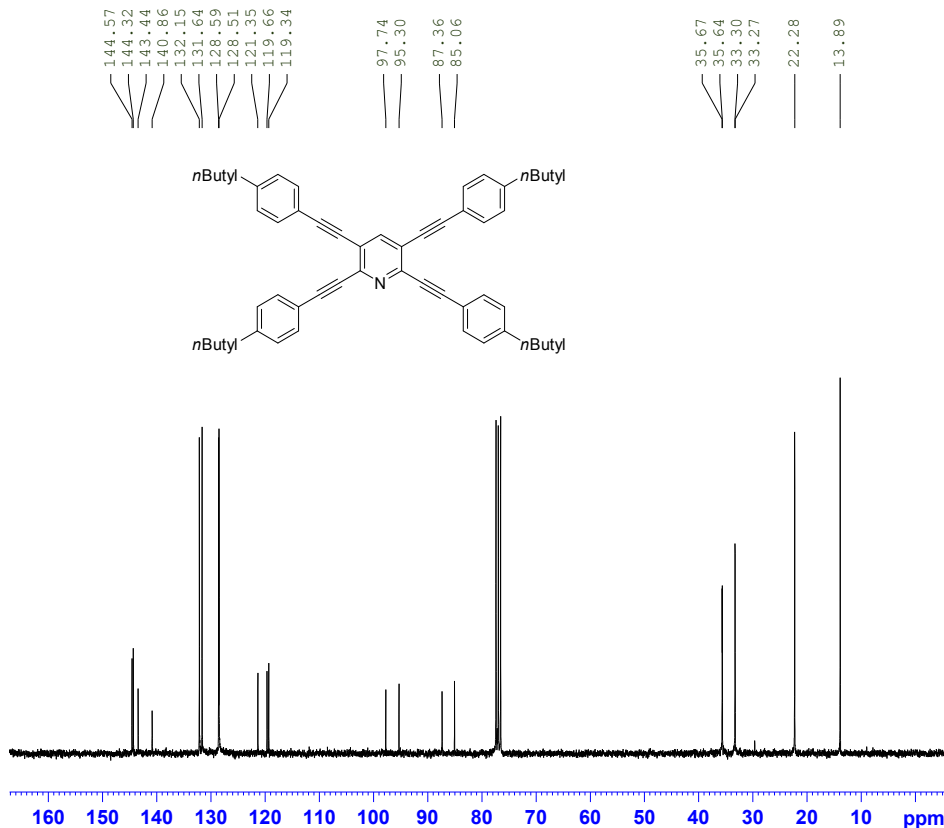
Current Data Parameters
NAME SRE 884 1H
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120811
Time 13.28
INSTRUM AV300
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDC13
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 296.0 K
D1 1.00000000 sec
TDO 1

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

F2 - Processing parameters
SI 32768
SF 300.1300223 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

Reimann/ SRE 884
Aul13C CDC13 /opt/topspin 1208 49



Current Data Parameters
NAME SRE 884 13C
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120811
Time 14.16
INSTRUM AV300
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDC13
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 296.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1

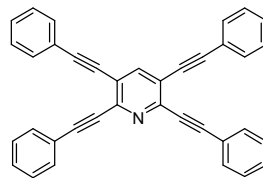
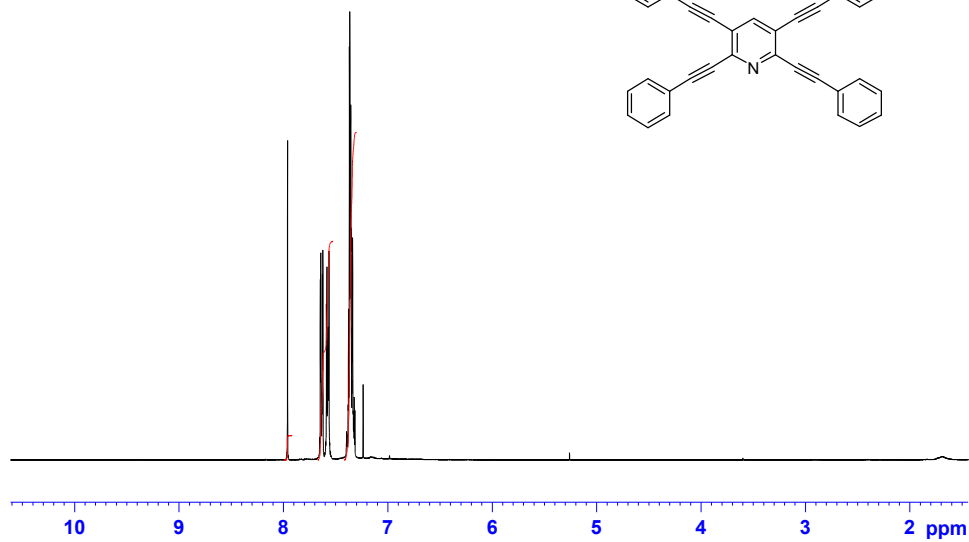
===== CHANNEL f1 =====
NUC1 13C
P1 9.60 usec
PL1 -1.10 dB
SFO1 75.4771825 MHz

===== 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 857
AulH CDCl3 /opt/topspin 1207 8

7.967
7.652
7.638
7.632
7.601
7.595
7.579
7.575
7.565
7.559
7.555
7.549
7.407
7.400
7.396
7.392
7.389
7.382
7.378
7.376
7.352
7.346
7.343
7.339
7.335
7.328
7.324
7.321
7.317
7.300



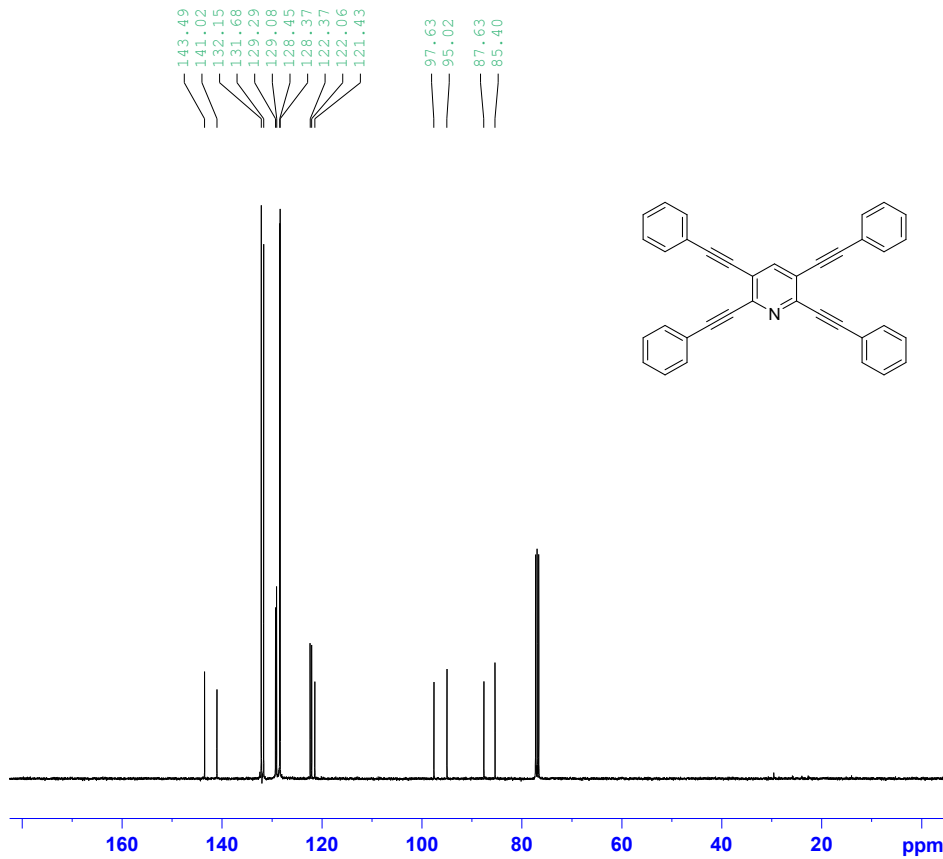
Current Data Parameters
NAME SRE 857 1H
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120712
Time 19.50
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 4
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 114
DW 62.400 usec
DE 6.00 usec
TE 297.0 K
D1 1.50000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.10 usec
PL1 -1.00 dB
SFO1 400.1324000 MHz

F2 - Processing parameters
SI 32768
SF 400.1300302 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

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Aul3C CDC13 /opt/topspin 1207 8



Current Data Parameters
NAME SRE 857 13C
EXPNO 11
PROCNO 1

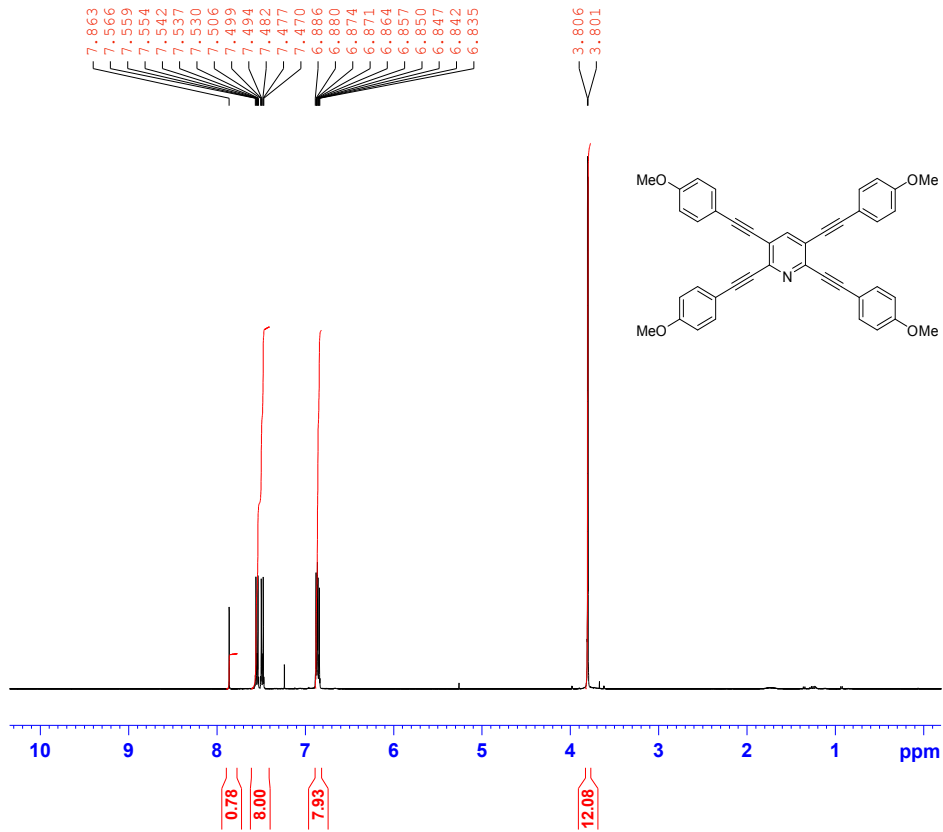
F2 - Acquisition Parameters
Date_ 20120712
Time_ 19.47
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1000
DS 4
SWH 29940.119 Hz
FIDRES 0.456850 Hz
AQ 1.0945013 sec
RG 32768
DW 16.700 usec
DE 6.00 usec
TE 297.0 K
D1 1.70000005 sec
d11 0.03000000 sec
DELTA 1.60000002 sec
TDO 1

==== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
SFO1 100.6260690 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -2.00 dB
PL12 17.00 dB
PL13 19.00 dB
SFO2 400.1318000 MHz

F2 - Processing parameters
SI 32768
SF 100.6127850 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

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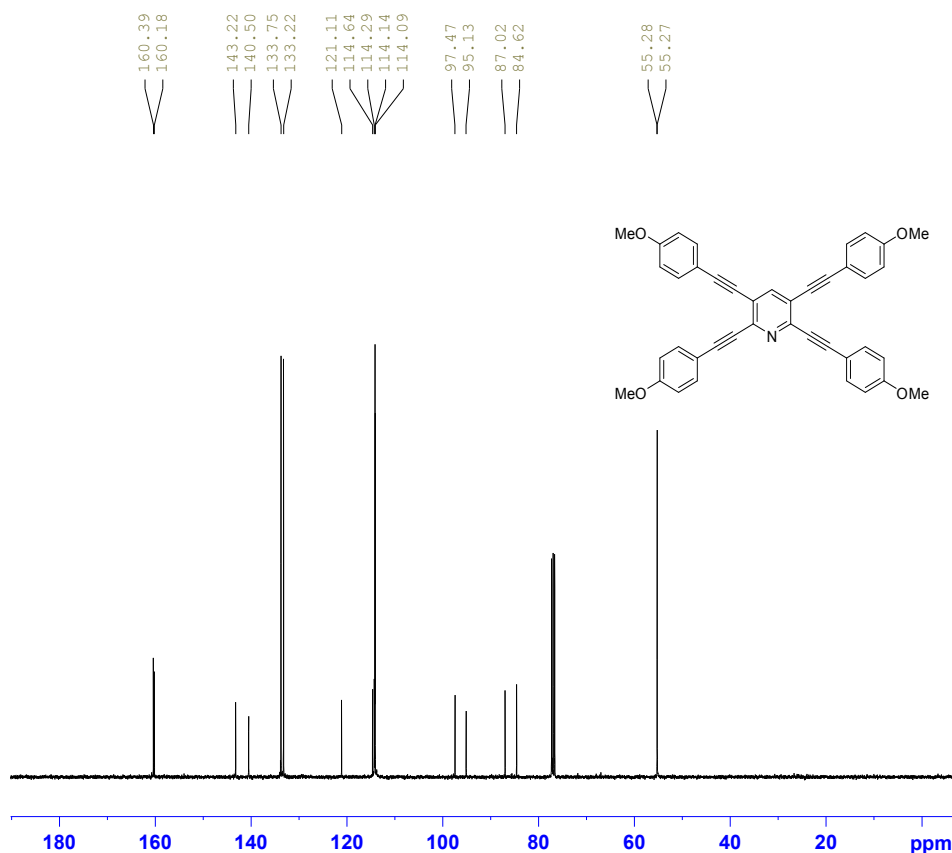
Current Data Parameters
NAME SRE 858 1H
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120712
Time_ 22.01
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 32
DS 4
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 128
DW 62.400 usec
DE 6.00 usec
TE 297.0 K
D1 1.50000000 sec
TDO 1

==== CHANNEL f1 =====
NUC1 1H
P1 11.10 usec
PL1 -1.00 dB
SFO1 400.1324000 MHz

F2 - Processing parameters
SI 32768
SF 400.1300304 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

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 Au13C CDC13 /opt/topspin 1207 9



Current Data Parameters
 NAME SRE 858 13 C
 EXPNO 11
 PROCNO 1

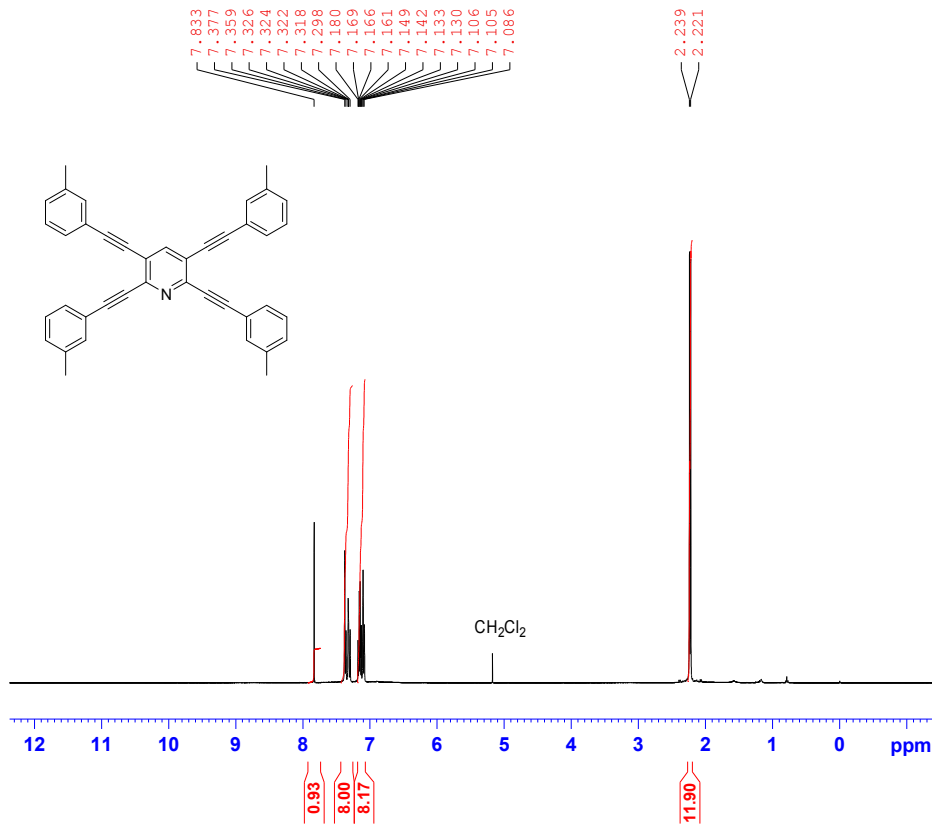
F2 - Acquisition Parameters
 Date_ 20120712
 Time 21.58
 INSTRUM AV400
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1000
 DS 4
 SWH 29940.119 Hz
 FIDRES 0.456850 Hz
 AQ 1.0945013 sec
 RG 32768
 DW 16.700 usec
 DE 6.00 usec
 TE 297.0 K
 D1 1.70000005 sec
 d11 0.03000000 sec
 DELTA 1.60000002 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 -0.50 dB
 SFO1 100.6260690 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -2.00 dB
 PL12 17.00 dB
 PL13 19.00 dB
 SFO2 400.1318000 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127798 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

Reimann, SRE 862
Aul1H CDC13 /opt/topspin 1207 11



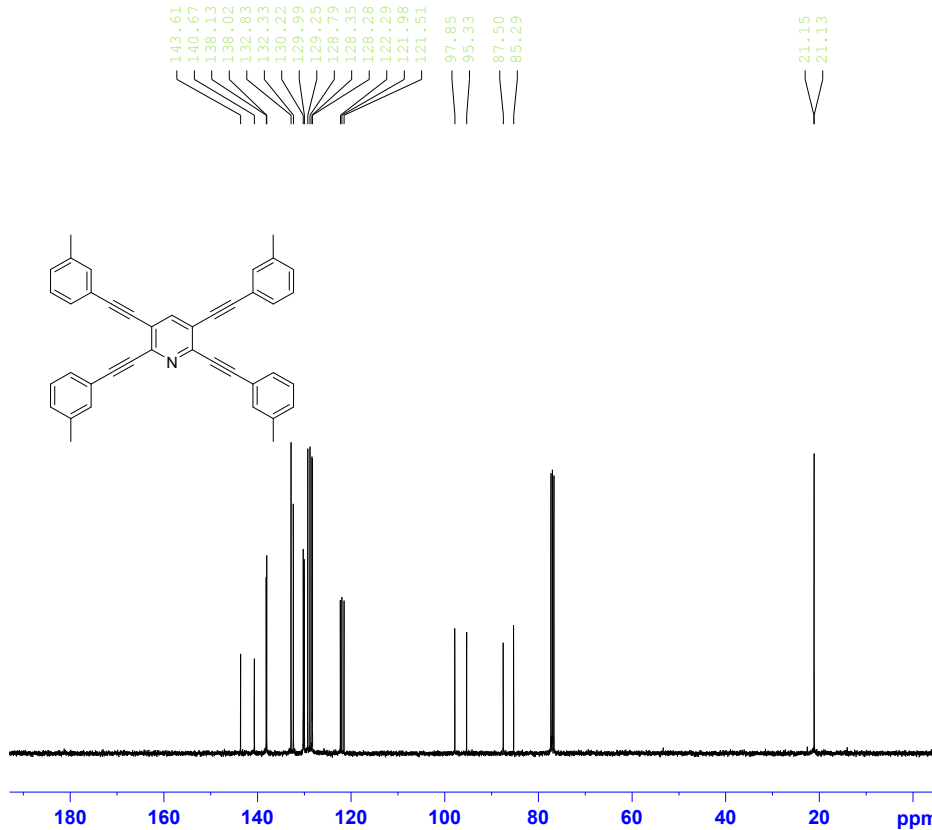
Current Data Parameters
NAME SRE 862 1H
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120712
Time 22.43
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 32
DS 4
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 101.6
DW 62.400 usec
DE 6.00 usec
TE 297.0 K
D1 1.5000000 sec
TDO 1

==== CHANNEL f1 =====
NUC1 1H
P1 11.10 usec
PL1 -1.00 dB
SFO1 400.1324000 MHz

F2 - Processing parameters
SI 32768
SF 400.1300661 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

Reimann, SRE 862
Aul13C CDC13 /opt/topspin 1207 11



Current Data Parameters
NAME SRE 862 13C
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120712
Time 22.40
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 500
DS 4
SWH 29940.119 Hz
FIDRES 0.456850 Hz
AQ 1.0945013 sec
RG 32768
DW 16.700 usec
DE 6.00 usec
TE 297.0 K
D1 1.7000000 sec
d11 0.0300000 sec
DELTA 1.6000000 sec
TDO 1

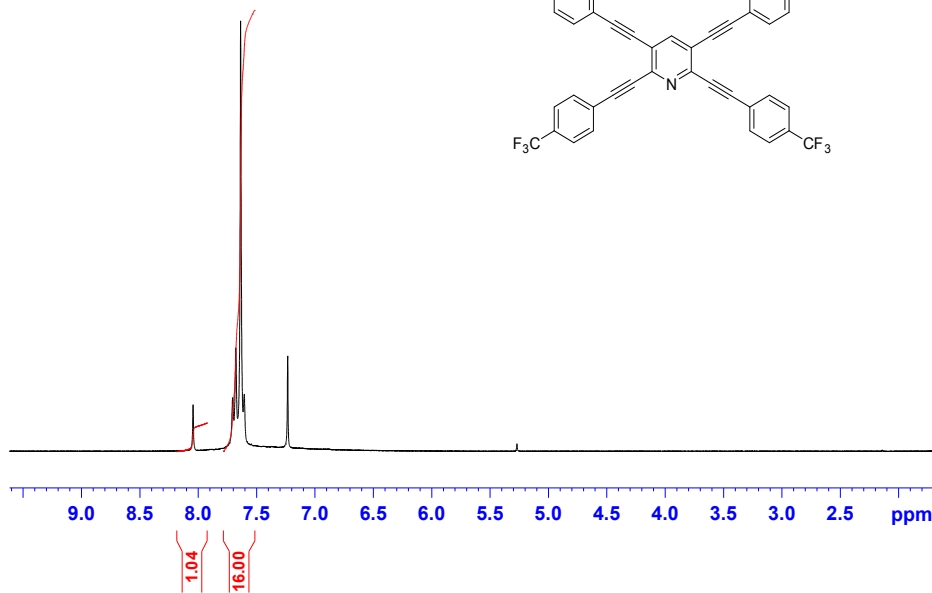
==== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
SFO1 100.6260690 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -2.00 dB
PL12 17.00 dB
PL13 19.00 dB
SFO2 400.1318000 MHz

F2 - Processing parameters
SI 32768
SF 100.6127817 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

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AulH CDCl3 /opt/topspin 1207 23

8.043
7.705
7.678
7.636
7.605



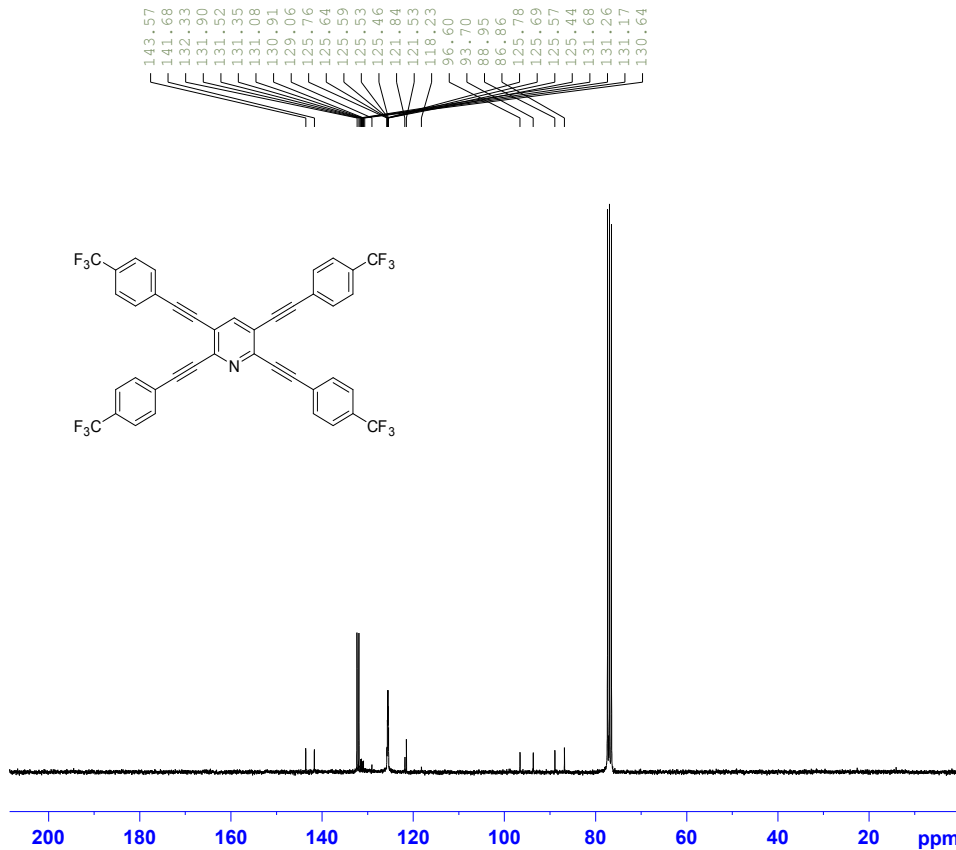
Current Data Parameters
NAME SRE 859 1H
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120713
Time 4.44
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 1.0000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 11.00 usec
PL1 0.00 dB
SF01 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300235 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

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 Aul3C CDCl3 /opt/topspin 1207 53



Current Data Parameters
 NAME SRE 859 13C 8000
 EXPNO 10
 PROCNO 1

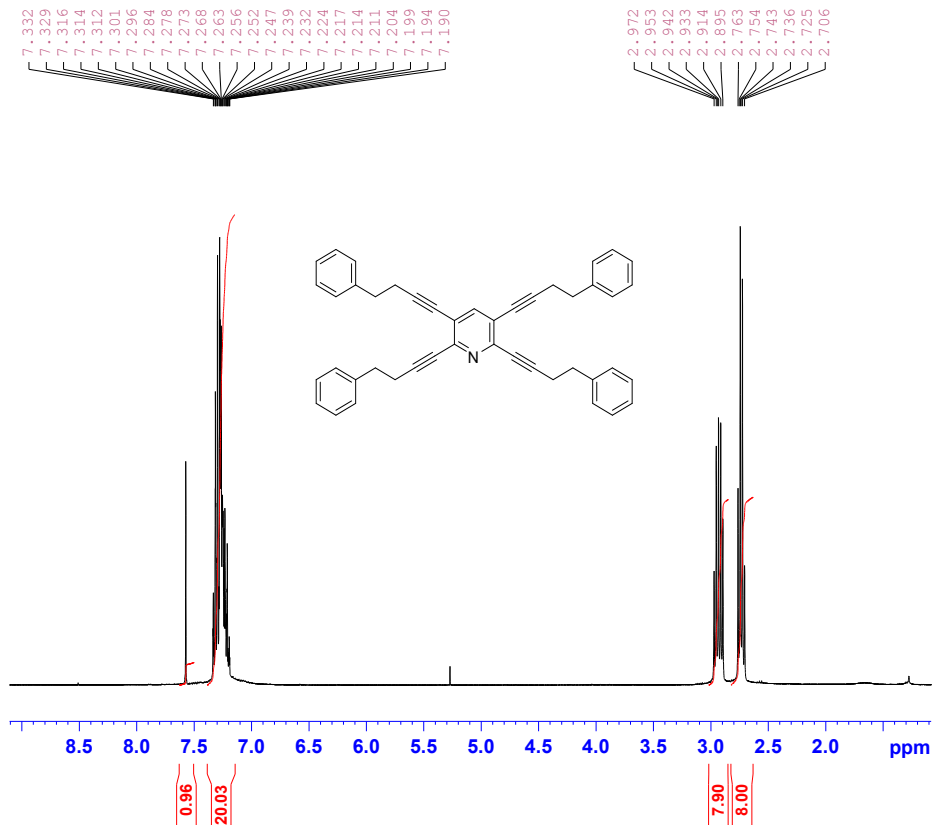
F2 - Acquisition Parameters
 Date_ 20120715
 Time 8.02
 INSTRUM AV300
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 8000
 DS 4
 SWH 21097.047 Hz
 FIDRES 0.643831 Hz
 AQ 0.7766516 sec
 RG 32768
 DW 23.700 usec
 DE 6.00 usec
 TE 295.9 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.60 dB
 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 873
 AulH CDCl3 /opt/topspin 1208 13



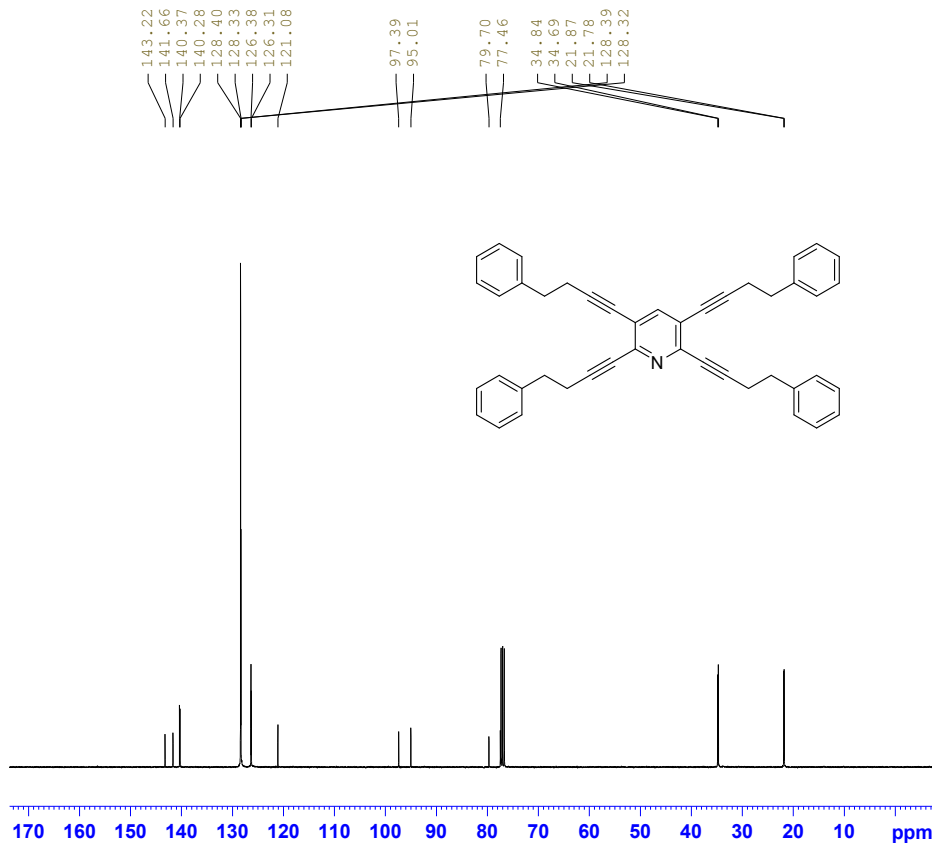
Current Data Parameters
 NAME SRE 873 1H
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120802
 Time 13.02
 INSTRUM AV400
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 32
 DS 4
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447731 sec
 RG 90.5
 DW 62.400 usec
 DE 6.00 usec
 TE 297.0 K
 D1 1.5000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.10 usec
 PL1 -1.00 dB
 SFO1 400.1324000 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300299 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

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Aul13C CDCl3 /opt/topspin 1208 13



Current Data Parameters
NAME SRE 873 13 C
EXPNO 11
PROCNO 1

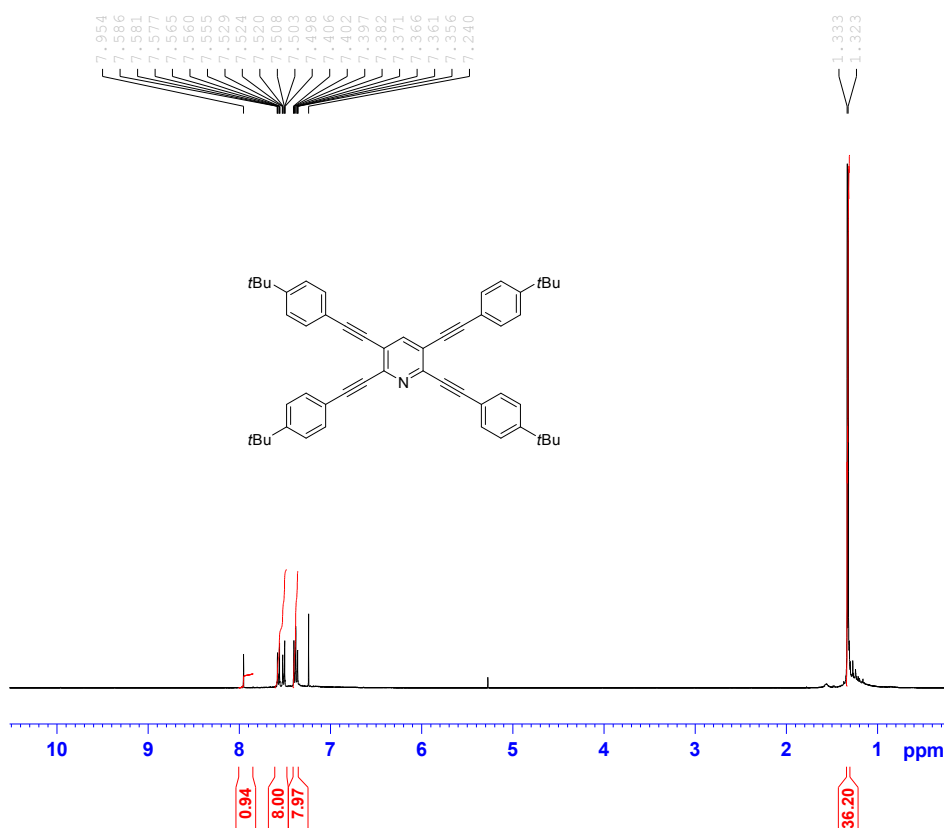
F2 - Acquisition Parameters
Date_ 20120802
Time 13.51
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT cdcl3
NS 1000
DS 4
SWH 29940.119 Hz
FIDRES 0.456850 Hz
AQ 1.0945013 sec
RG 32768
DW 16.700 usec
DE 6.00 usec
TE 297.0 K
D1 1.7000005 sec
d11 0.0300000 sec
DELTA 1.6000002 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
SFO1 100.6260690 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -2.00 dB
PL12 17.00 dB
PL13 19.00 dB
SFO2 400.1318000 MHz

F2 - Processing parameters
SI 32768
SF 100.6127827 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

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AulH CDCl3 /opt/topspin 1208 17



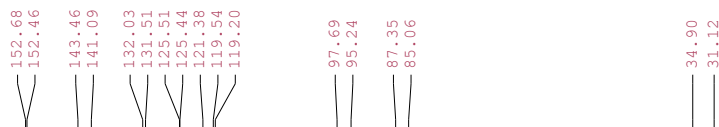
Current Data Parameters
NAME SRE 872 1H
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120802
Time 19.48
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 4
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 181
DW 62.400 usec
DE 6.00 usec
TE 297.0 K
D1 1.5000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.10 usec
PL1 -1.00 dB
SFO1 400.1324000 MHz

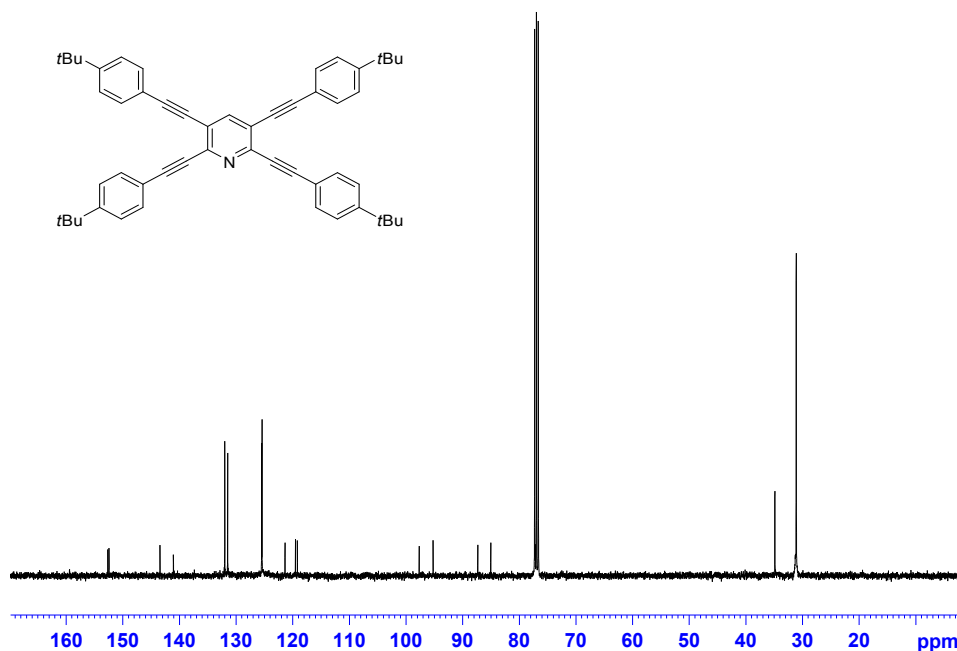
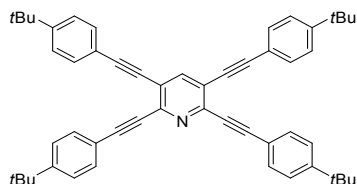
F2 - Processing parameters
SI 32768
SF 400.1300293 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

Reimann, SRE 872
 Au13C CDC13 /opt/topspin 1208 17



Current Data Parameters
 NAME SRE 872 13C
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120802
 Time 20.38
 INSTRUM AV400
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 1000
 DS 4
 SWH 29940.119 Hz
 FIDRES 0.456850 Hz
 AQ 1.0945013 sec
 RG 32768
 DW 16.700 usec
 DE 6.00 usec
 TE 297.0 K
 D1 1.70000005 sec
 d11 0.03000000 sec
 DELTA 1.60000002 sec
 TDO 1



===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 -0.50 dB
 SFO1 100.6260690 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -2.00 dB
 PL12 17.00 dB
 PL13 19.00 dB
 SFO2 400.1318000 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127766 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

Parameter	Value
1 Solvent	CDC13
2 Temperature	298.2
3 Pulse Sequence	zg30
4 Number of Scans	16
5 Receiver Gain	51
6 Relaxation Delay	1.0000
7 Pulse Width	10.0000
8 Acquisition Time	5.2954
9 Acquisition Date	2016-12-21T09:14:00
10 Modification Date	2016-12-21T09:14:28
11 Spectrometer Frequency	300.13
12 Spectral Width	6188.1
13 Lowest Frequency	-1246.8
14 Nucleus	1H
15 Acquired Size	32768
16 Spectral Size	32768

