Electronic Supplementary Material for *CrystEngComm*

-Supporting Information-

Pyridoxycalix[4]arene palladium(II) complexes as tectons for self-inclusion polymers

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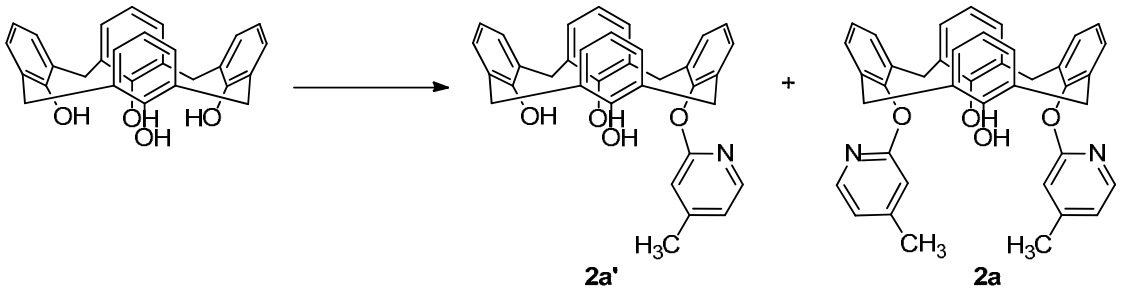
Syntheses of Ligands

26,27,28-trihydroxy-25-(2-(4-methylpyridoxy))-calix[4]arene (**2a'**) and *syn-distal*-26,28-dihydroxy-25,27-bis-(2-(4-methylpyridoxy))-calix[4]arene (**2a**):

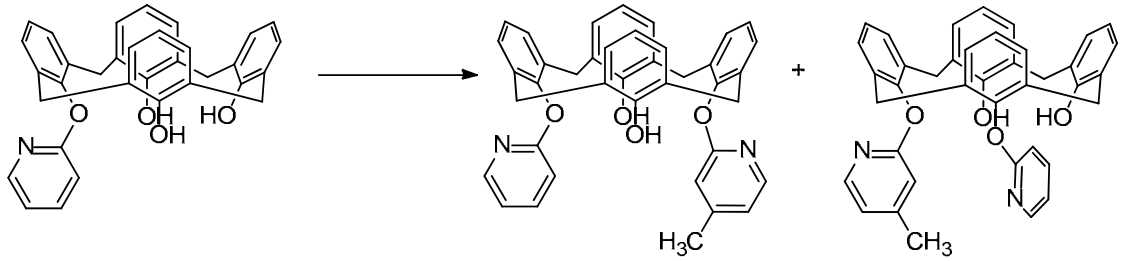


2a' **2a**

Tetrahydroxycalix[4]arene[1] (305 mg, 0.71 mmol) and Na_2CO_3 (1.470 g , 14.0 mmol) are suspended in 2-bromo-4-methylpyridine[2] (6.820 g, 39.88 mmol) and heated to 160 °C for three days. After cooling the reaction mixture to room temperature, dichloromethane (10 mL) was added and the mixture filtered through Celite 535 and washed three times with dichloromethane (5 mL). Dichloromethane was removed by rotary evaporation and excess bromopyridine (5.310g, 31.05 mmol) was recovered by Kugelrohr-distillation (110–120 °C, 0.35 mbar). The remained residue was dried in vacuo (30 min, 160 °C, 0.35 mbar) to give 428 mg of a deep purple solid. TLC (SiO_2, petroleum ether/ethyl acetate 5:2): R_f = 0.66, 0.45 (**2a'**), 0.34 (**2a**), 0.24. Separation by flash-chromatography and subsequent drying in vacuo (100-110 °C, 0.35 mbar) gave: First fraction (R_f = 0.45): 85 mg (23%) of **2a'** as colorless solid with mp. 242 °C. ^{1}H NMR (400.1 MHz, $CDCl_3$): δ = 2.43 ppm (s, 3H, -CH_3), 3.43 (d, J = 13.5 Hz, 2H, Ar-CH_2-Ar), 3.52 (d, J = 13.6 Hz, 2H, Ar-CH_2-Ar), 4.09 (d, J = 13.6 Hz, 2H, Ar-CH_2-Ar), 4.30 (d, J = 14.0 Hz, 2H, Ar-CH_2-

Ar), 6.66-6.73 (m, 3H, ArH), 6.91 (s, 1H, Py-3-H, 6.97-7.05 (m, 8H, ArH, Py-5-H), 7.15 (d, 2H, *J* = 8.0 Hz, ArH), 8.14 (s, 1H, Py-6-H), 8.95 (s, br, 2H, Ar-O*H*), 9.55 (s, br, 1H, Ar-O*H*). ^{13}C NMR (100.6 MHz, $CDCl_3$): δ = 21.34 ppm (q, -*C*H$_3$), 31.98 (t, Ar-*C*H$_2$-Ar), 32.05 (t, Ar-*C*H$_2$-Ar), 110.46 (d, Py-C-3), 120.79 (d, Py-C-5), 121.14, 122.16, 127.34, 128.35, 128.48, 128.79, 129.05, 129.54, 134.66, 146.47 (d, Py-C-6), 147.71(s, Ar*C*-O), 149.35 (s, Ar*C*-O), 150.98 (s, Ar*C*-O), 152.98 (s, Ar*C*-O), 163.20 (s, Py-C-2). IR (KBr): $\tilde{\nu}$ = 3331 cm^{-1} (br, s), 3022 (m), 2931 (m), 1607 (s), 1562 (m), 1466 (s), 1446 (s), 1395 (s), 1286 (m), 1263 (m), 1243 (m), 1184 (m), 1151 (m), 1091 (w), 946 (s), 911 (w), 818 (s), 786 (m), 753 (s). UV/Vis (CH_3CN): $\lambda_{max.}$ (lg ε) = 272 nm (4.2), 194 (5.3)**.** MS (FAB): *m/z* (%): 663.3 (7), 538.2 (6) [M+Na$^+$], 516.2 (100) [M+H$^+$]. Elemental analysis calcd. for $C_{34}H_{29}NO_4 \cdot ½H_2O$ (524.62 g/mol): C 77.84, H 5.76, N 2.67. Found: C 77.95, H 5.64, N 2.61. Second fraction (R_f = 0.34): 120 mg (28%) of **2a** as colorless solid with mp. 273–278 °C. ^{1}H NMR (400.1 MHz, $CDCl_3$): δ = 2.44 ppm (s, 6H, -C*H*$_3$), 3.37 (d, *J* = 14.0 Hz, 4H, Ar´-C*H*$_2$-Ar), 4.03 (d, *J* = 14.1 Hz, 4H, Ar´-C*H*$_2$-Ar), 6.71 (t, *J* = 7.2 Hz, 2H, ArH), 6.86 (t, *J* = 6.5 Hz, 2H, ArH), 6.94-6.95 (m, 6H, Py-5-H, ArH), 7.04 (d, *J* = 6.5 Hz, 6H, ArH), 8.20 (d, *J* = 5.0 Hz, 2H, Py-6-H). ^{13}C NMR (100.6 MHz, $CDCl_3$): δ = 20.56 ppm (q, -*C*H$_3$), 31.07 (t, Ar-*C*H$_2$-Ar), 109.94 (d, Py-C-3), 118.77 (d, Py-C-5), 119.29 (d, Ar*C*-H), 125.76 (d, ArC), 127.53 (s, Py-C-4), 127.88, 128.42 (both d, both Ar*C*), 132.39 (s, Ar*C*-CH$_2$Ar), 144.92 (d, Py-C-6), 145.86 (s, Ar*C*-OH), 152.01 (s, Ar*C*-OPy), 161.97 (s, Py-C-2). IR (KBr): $\tilde{\nu}$ = 3480 cm^{-1} (s, br), 3022 (m) 2931 (m), 1752 (s), 1605 (m), 1464 (s), 1396 (s), 1287 (m), 1264 (m), 1187 (m), 1153 (s), 1086 (m), 990 (m), 946 (w), 907 (w), 821 (m), 786 (m), 773 (m), 753 (m), 612 (w). UV/Vis (CH_3CN): $\lambda_{max.}$ = 280 nm. MS (FAB): *m/z* (%): 663.3 (7) [M + 57$^+$], 629.3 (50) [M + Na$^+$], 607.3 [M + H$^+$] (100), 516.2 (9) [M$^+$-Py]. Elemental analysis calcd. for $C_{40}H_{34}N_2O_4$ (606.72 g/mol): C 79.19, H 5.65, N 4.62. Found: C 78.97, H 5.69, N 4.62.

syn-distal-26,28-Dihydroxy-25-(2-pyridoxy)-27-(2-(4-methylpyridoxy))-calix[4]arene (**3a**) and *rac-syn-proxi*-27,28-Dihydroxy-25-(2-pyridoxy)-26-(2-(4-methylpyridoxy))-calix[4]arene (**3a'**):



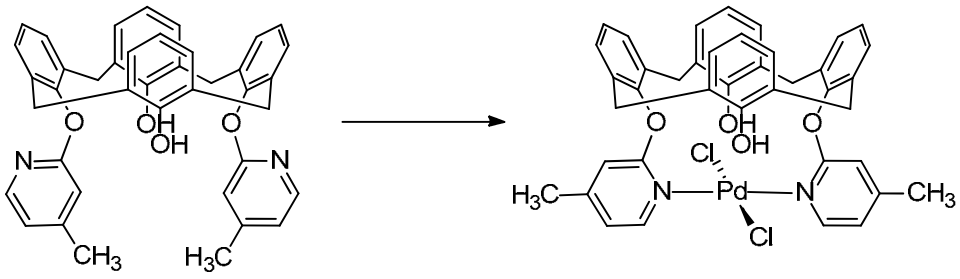
Monopyridoxycalixarene[3] **1a'** (512 mg, 1.02 mmol) and sodium carbonate (2.13 mg, 20.14 mmol) are suspended in 2-bromo-4-methylpyridine in a screw-capped vessel, flushed with argon and heated for three days at 160°C. After cooling the reaction mixture to room temperature, inorganic salts were filtered off and washed with dichloromethane. Dichloromethane was removed at the rotary evaporator and 2-bromo-4-methylpyridine was recovered by distillation in vacuo (100°C, 0.85 mbar). The brown residue was separated by flash-chromatography (SiO_2, petroleum ether/ethyl acetate 3:1 to 1:1), recrystallized from dichloromethane/methanol and dried in vacuo (1 h, 100-110°C): First fraction (R_f = 0.29 in PE/EA 3:1): 135 mg (22 %) of **3a** as a colourless solid with mp. 244 °C. ^{1}H NMR (400.1 MHz, $CDCl_3$): δ = 2.44 ppm (s, 3H, -C*H*$_3$), 3.36 (d, *J* = 13.9 Hz, 4H, ArC*H*$_2$Ar), 4.04 (dd, ^3J = 13.6, Hz, ^4J = 3.8 Hz, 4H, ArC*H*$_2$Ar), 6.71 (t, *J* = 7.5 Hz, 2H, ArH), 6.83-6.87 (m, 3H, ArH, Py-5-H), 6.94 (d, ^3J = 7.3 Hz, ^4J = 1.5 Hz, 6H, ArH, Ar-O*H*), 7.02 (s, 1H, Py-3-H), 7.04 (d, *J* = 6.3 Hz, 5H, ArH, Py-5'-H), 7.19 (d, *J* = 8.1 Hz, 1H, Py-3'-H), 7.77 („t", ^3J =7.8 Hz ,^4J = 1.9 Hz, 1H, Py-4'-H), 8.11 (d, *J* = 5.1 Hz, 1H, Py-6-H), 8.25 (dd, ^3J = 5.1 Hz, ^4J = 1.3, 1H, Py-6'-H). ^{13}C NMR (100.6 MHz, $CDCl_3$): δ = 21.30 ppm (q, -*C*H$_3$), 32.13 (t, Ar-*C*H$_2$-Ar), 32.16 (t, Ar*C*H$_2$Ar), 110.71 (d, Py-C-3'), 110.91 (d, Py-C-3), 118.66 (d, Py-C-5'), 119.61 (d, Ar*C*-H), 120.13 (d, Py-C-5), 126.47 (d, Ar*C*-H), 126.52 (d, Ar*C*-H), 128.51 (s, Ar'*C*-CH$_2$-Ar), 128.56 (s, Ar'*C*-CH$_2$-Ar), 128.89 (d, Ar*C*-H), 128. 93 (d, Ar*C*-H), 129.20 (d, Ar*C*-H), 129.24 (d, Ar*C*-H), 133.58 (s, Ar*C*-CH$_2$-Ar'), 139.84 (d, Py-C-4'), 147.14 (d, Py-C-6), 147.58 (s, Ar*C*-OH), 148.21 (d, Py-C-6'), 151.54 (s, Py-C-4), 153.09 (s, Ar*C*-OPy), 163.68 (s, Py-C-2'), 163.87 (s, Py-C-2). IR (KBr): $\tilde{\nu}$ = 3468 cm^{-1} (br, s), 3021 (w), 2931 (m), 1606 (m), 1588 (m), 1570 (m),

1466 (s), 1427 (s), 1396 (m), 1286 (m), 1265 (m), 1236 (m), 1207 (w), 1187 (m), 1149 (m), 1085 (m), 989 (w), 947 (m), 909 (w), 872 (w), 823 (w), 775 (w), 754 (m), 608 (w), 517 (w), 471 (w), 411 (w). UV/Vis (CH_3CN): $\lambda_{max.}$ (lg ε) = 270 nm (3.6), 210 (4.3). MS (FAB): *m/z* (%): 593.4 (100) [M + H^+], 615.4 (42) [M + Na^+]. Elemental analysis calcd. for $C_{39}H_{32}N_2O_4 \cdot ½H_2O$ (601.69 g/mol): C 77.85 , H 5.53, N 4.66. Found: C 77.48, H 5.26, N 4.46. Second fraction (R_f = 0.24 in PE/EA 3:1): 202 mg (33 %) of *rac*-**3a'** as a colorless solid with mp. 234 °C. ^{1}H NMR (400.1 MHz, $CDCl_3$): δ = 2.25 ppm (s, 3H, -C*H*$_3$), 3.31 (d, *J* = 13.1 Hz, 1H, Ar-C*H*$_2$-Ar), 3.47 (d, *J* = 14.2 Hz, 1H, Ar-C*H*$_2$-Ar), 3.50 (d, *J* = 14.4 Hz, 1H, Ar-C*H*$_2$-Ar), 3.61 (d, *J* = 13.6 Hz, 1H, Ar-C*H*$_2$-Ar), 3.82 (d, *J* = 13.2 Hz, 1H, Ar-C*H*$_2$-Ar), 3.98 (d, *J* = 14.4 Hz, 1H, Ar-C*H*$_2$-Ar), 4.00 (d, *J* = 13.1 Hz, 1H, Ar-C*H*$_2$-Ar), 4.26 (d, *J* = 13.6 Hz, 1H, Ar-C*H*$_2$-Ar), 6.34 („br“ s, 1H, Py-3-H), 6.55 (d, *J* = 8.3 Hz, 1H, Py-3'-H), 6.62 (t, *J* = 7.6 Hz, 1H, ArH), 6.67 (t, *J* = 7.5 Hz, 1H, ArH), 6.73 (d, *J* = 4.8 Hz, 1H, Py-5-H), 6.82-6.88 (m, 2H, ArH), 6.91 („t“, *J* = 6.1 Hz, 1H, Py-5'-H), 7.01-7.08 (m, 4H, ArH), 7.16-7.21 (m, 4H, ArH), 7.54 („t“, ^3J = 7.8 Hz, ^4J = 2 Hz, 1H, Py-4'-H), 8.01 (d, J = 10.6 Hz, 1H, Py-6-H), 8.17 („d“, ^3J = 9.9 Hz, ^4J = 2.8 Hz, 1H, Py-6'-H). ^{13}C NMR (100.6 MHz, $CDCl_3$): δ = 21.17 ppm (q, -*C*H$_3$), 31.45 (t, Ar-*C*H$_2$-Ar), 31.94 (t, Ar-*C*H$_2$-Ar), 33.20 (t, Ar-*C*H$_2$-Ar), 33.16 (t, Ar-*C*H$_2$-Ar), 110.64 (d, Py-C-3'), 111.02 (d, Py-C-3), 118.03 (d, Py-C-5'), 119.53 (d, Py-C-5), 120.81 (d, Ar*C*-H), 120.99 (d, Ar*C*-H), 126.46 (d, Ar*C*-H), 128.42, 128.66, 128.72, 128.76, 128. 83, 128.88, 129.04, 129.25, 129.40, 129.46, 129.51, 134.23 (s, Ar*C*-CH$_2$-Ar), 134.33 (s, Ar*C*-CH$_2$-Ar), 135.31 (s, Ar*C*-CH$_2$-Ar), 135.36 (s, Ar*C*-CH$_2$-Ar), 139.20 (d, Py-C-4'), 146.69 (d, Py-C-6), 147.69 (d, Py-C-6'), 148.17 (s, Ar*C*-OH), 148.39 (s, Ar*C*-OH), 151.57, 151.63 (both s, Py-C-4, Ar*C*-O-Py), 163.65, 163.77 (both s, Py-C-2', Py-C-2). IR (KBr): $\tilde{\nu}$ = 3365 cm^{-1} (br, s), 3022 (w), 2928 (w), 2859 (w), 1601 (m), 1570 (m), 1466 (m), 1428 (m), 1398 (m), 1366 (w), 1287 (m), 1266 (m), 1246 (m), 1188 (m), 1151 (m), 1089 (w), 990 (w), 946 (w), 913 (w), 875 (w), 822 (w), 805 (w), 778 (m), 758 (m), 604 (w), 562 (w), 519 (w), 450 (w). UV/Vis (CH_3CN): $\lambda_{max.}$ (lg ε) = 270 nm (4.1), 213 (4.7). MS (FAB): *m/z* (%): 593.4 (100) [M + H^+], 615.4 (17) [M + Na^+]. Elemental analysis calcd. for $C_{39}H_{32}N_2O_4 \cdot ½H_2O$ (601.69 g/mol): C 77.85, H 5.53, N 4.66. Found: C 77.49, H 5.26, N 4.46

Electronic Supplementary Material for *CrystEngComm*

Syntheses of Palladium Complexes

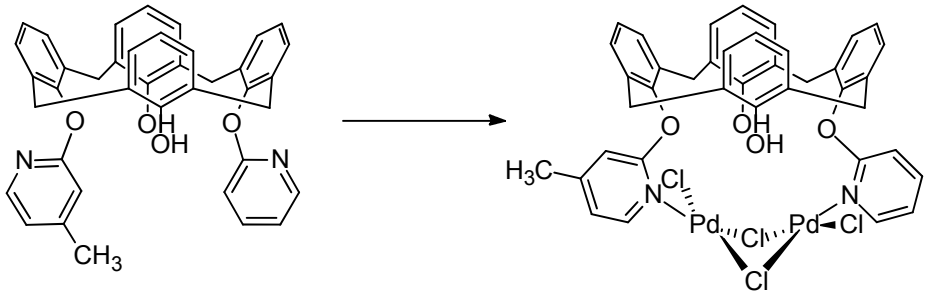
(*syn-distal*-26,28-dihydroxy-25,27-bis-(2-(4-methylpyridoxy)-calix[4]arene)-palladium(II) chloride (**2b**):



2a **2b**

Calixarene **2a (**92 mg, 0.15 mmol) and palladium(II) chloride (28 mg, 0.16 mmol) are suspended in a mixture of dichloromethane (20 mL) and methanol (5 mL) and refluxed 16–18 h. After cooling the reaction mixture to room temperature the yellow solution was filtered and solvents were removed in vacuo to yield 118 mg (quantitative) of **2b** a**s** bright yellow solid with mp. >310 °C. Single-crystals suitable for X ray diffraction were grown by slow diffusion of methanol into a saturated solution of **2b** in dichloromethane. ^{1}H NMR (400.1 MHz, CD_2Cl_2): δ = 2.33 ppm (s, 6H, -C*H*$_3$), 3.39 (d, *J* = 14.0 Hz, 4H, Ar´-C*H*$_2$-Ar), 3.92 (d, *J* = 13.5 Hz, 4H, Ar´-C*H*$_2$-Ar), 6.50 (s, 2H), 6.64 (t, *J* = 7.5 Hz, 2H, Ar-4-H), 6.96 (d, *J* = 6.0 Hz, 2H Py-5-H), 7.06 (d, *J* = 6.0 Hz; Ar´-4-H; „t“, Ar-3/5-H; 6H),7.19 (d, *J* = 7.5 Hz, 4H, Ar´-3/5-H), 8.43 (s, 2H, Ar-O*H*), 8.55 (d, *J* = 6.0 Hz, 2H, Py-6-H). ^{13}C NMR (100.6 MHz, CD_2Cl_2): δ = 21.45 ppm (q, -*C*H$_3$), 33.18 (t, Ar-*C*H$_2$-Ar), 110.65 (d, Py-C-3), 119.59 (d, Ar-C-4), 121.05 (d, Py-C-5), 126.92 (d, Ar´-C-4), 127.96 (s, Ar-C-2/4), 128.56 (d, Ar-C-3/5), 131.06 (d, Ar-C-3/5), 133.06 (s, Ar´-C-2/4), 147.71 (s, Ar´*C*-O-Py), 151.27 (d, Py-C-6), 154.38 (s, Ar*C*-OH), 155.16 (s, Py-C-4), 163.97 (s, Py-C-2). IR (KBr): $\tilde{\nu}$ = 3470 cm^{-1} (s), 3054 (m) 2951 (m), 1625 (s), 1585 (w), 1563 (m) 1488 (m), 1476 (s), 1435 (s), 1307 (s), 1250 (m), 1191 (s), 1175 (s), 1159 (m), 1085 (m), 1033 (m), 1013 (w), 962 (m), 909 (w), 847 (w), 819 (w), 801 (m), 773 (m), 754 (m), 737 (m), 649 (w), 612 (w). UV/Vis (CH_3CN): $\lambda_{max.}$ (lg ε) = 280 nm (4.2). Elemental analysis calcd. for $C_{40}H_{34}N_2O_4PdCl_2 \cdot ¼CH_2Cl_2$ (805.28 g/mol): C 60.03, H 4.32, N 3.48. Found: C 60.00, H 4.25, N 3.41.

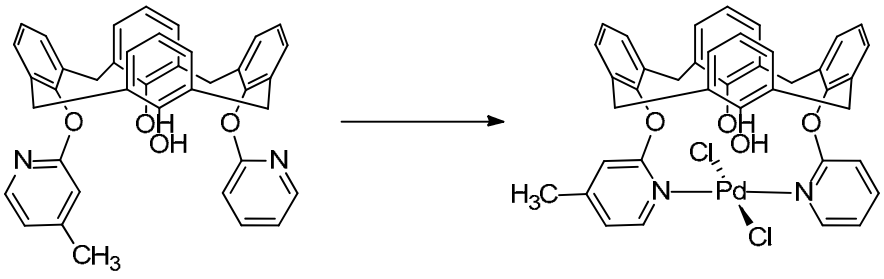
(syn-distal-26,28-dihydroxy-25-(2-pyridoxy)-27-(2-(4-methylpyridoxy))-calix[4]arene)-bis(μ-chloro)-dichlorodipalladium(II) (**3c**):



3a **3c**

Calixarene **3a** (56 mg, 90 μmol) and palladium(II) chloride (17 mg, 90 μmol) were suspended in a mixture of dichloromethane (10 mL) and methanol (2.5 mL) and refluxed for 18 h. After cooling the reaction mixture to room temperature the orange solution was filtered to remove insoluble materials and solvents were removed in vacuo to yield 35 mg of an orange solid. Single-crystals suitable for X ray diffraction were obtained by diffusion of methanol into a saturated solution of **3c** in dichloromethane.

(syn-distal-26,28-Dihydroxy-25-(2-pyridoxy)-27-(2-(4-methylpyridoxy))-calix[4]aren)-palladium(II) chloride (**3b**):



3a **3b**

A solution of palladium(II) chloride (21 mg, 0.118mmol) in dry acetonitrile (15 mL) was stirred under argon in a screw-capped vessel for 2 h at 60 °C. A solution of calixarene **3a** (70 mg, 0.118 mmol) in acetonitrile (10 mL) was added to the mixture and the resulting suspension was vigorously stirred for 24 hours at 60 °C. Subsequently, the suspension was filtered and the precipitate was washed three times with 5 mL of acetonitrile and three times with 20 mL of diethyl ether to yield a yellow solid (44 mg, 49 %). Orange

single-crystals suitable for X ray diffraction were obtained by diffusion of diethyl ether into solution of **3b** in dichloromethane. ^{1}H NMR (400.1 MHz, $CDCl_3$) δ = 2.30 ppm (s, 3H, -C*H*$_3$), 3.35 und 3.37 (2 d, J = 13.6 und 13.4 Hz, 4H, Ar-C*H*$_2$-Ar), 3.96 und 3.99 (2 d, J = 12.6 und 12.9 Hz, 4H, Ar-C*H*$_2$-Ar), 6.45 (s, 1H, Py-3'-H), 6.51 (d, J = 8.4 Hz, 1H, Py-3-H), 6.63 (t, J = 7.6 Hz, 2H, ArH), 6.84 (t, J = 6.8 Hz, 1H, Py-5-H), 6.89 (d, J = 6.0 Hz, 1H, Py-5'-H) , 6.94-6.99 (m, 2H, ArH), 7.03-7.05 (d, J = 7.6 Hz, 4H, ArH), 7.09-7.15 (m, 4H, ArH), 7.46 (t, J = 7.6 Hz, 1H, Py-4-H), 8.41 (s, 2H, OH), 8.58 (d, J = 5.8 Hz, 1H, Py-6'-H), 8.67 (d, J = 5.8 Hz, 1H, Py-6-H). ^{13}C NMR (100.6 MHz, $CDCl_3$) δ = 21.40 ppm (q, -*C*H$_3$), 33.15 (t, Ar-*C*H$_2$-Ar), 110.15 (d, Py-C-3), 110.36 (d, Py-C-3'), 119.11 (d, Py-C-5), 119.27 (d, Ar*C*-H), 120.76 (d, Py-C-5'), 127.13 (d, Ar*C*-H), 127.17 (d, Ar*C*-H), 127.69 (s), 128.23 (d, Ar*C*-H), 130.87 (d, Ar*C*-H), 130.88 (d, Ar*C*-H), 132.73 (s), 132.82 (s), 141.50 (d, Py-C-4), 147.33 (s), 147.40 (s), 151.23 (d, Py-C-6'), 152.13 (d, Py-C-6), 154.08 (s), 154.38 (s), 164.02 (s), 164.16 (s). IR (KBr): $\tilde{\nu}$ = 3474 (m) cm^{-1}, 2920 (m), 2854 (w), 2142 (s), 1509 (s), 1449 (s), 1413 (s), 1357 (m), 1295 (w), 1245 (w), 1205 (w), 1106 (w), 805 (vw), 759 (vw). UV/Vis (*n*-hexane): $\lambda_{max.}$ (lg ε) = 277 nm (4.44), 234 (4.73). MS (FAB): *m/z* (%): 735.9 (12) [M - Cl + H$^+$], 697.9 (10) [M - 2Cl + H$^+$], 593 (8) [M - 2Cl - Pd + H$^+$]. Elemental analysis calcd. for $C_{39}H_{32}Cl_2N_2O_4Pd \cdot ½CH_2Cl_2$ (812.47 g/mol): C 58.39, H 4.09, N 3.45. Found: C 58.49, H 3.79, N 3.41.

[1] C. D. Gutsche, J. A. Levine, *J. Am. Chem. Soc.,* 1982, **104**, 2652.

[2] H. M. Reyes-Rivera, R. O. Hutchins, D. R. Dalton, *J. Heterocyclic Chem.*, 1995, **32**, 665.

[3] G. Dyker, M. Mastalerz, K. Merz, *Eur. J. Org. Chem.*, 2003, 4355-4362

Electronic Supplementary Material for *CrystEngComm*
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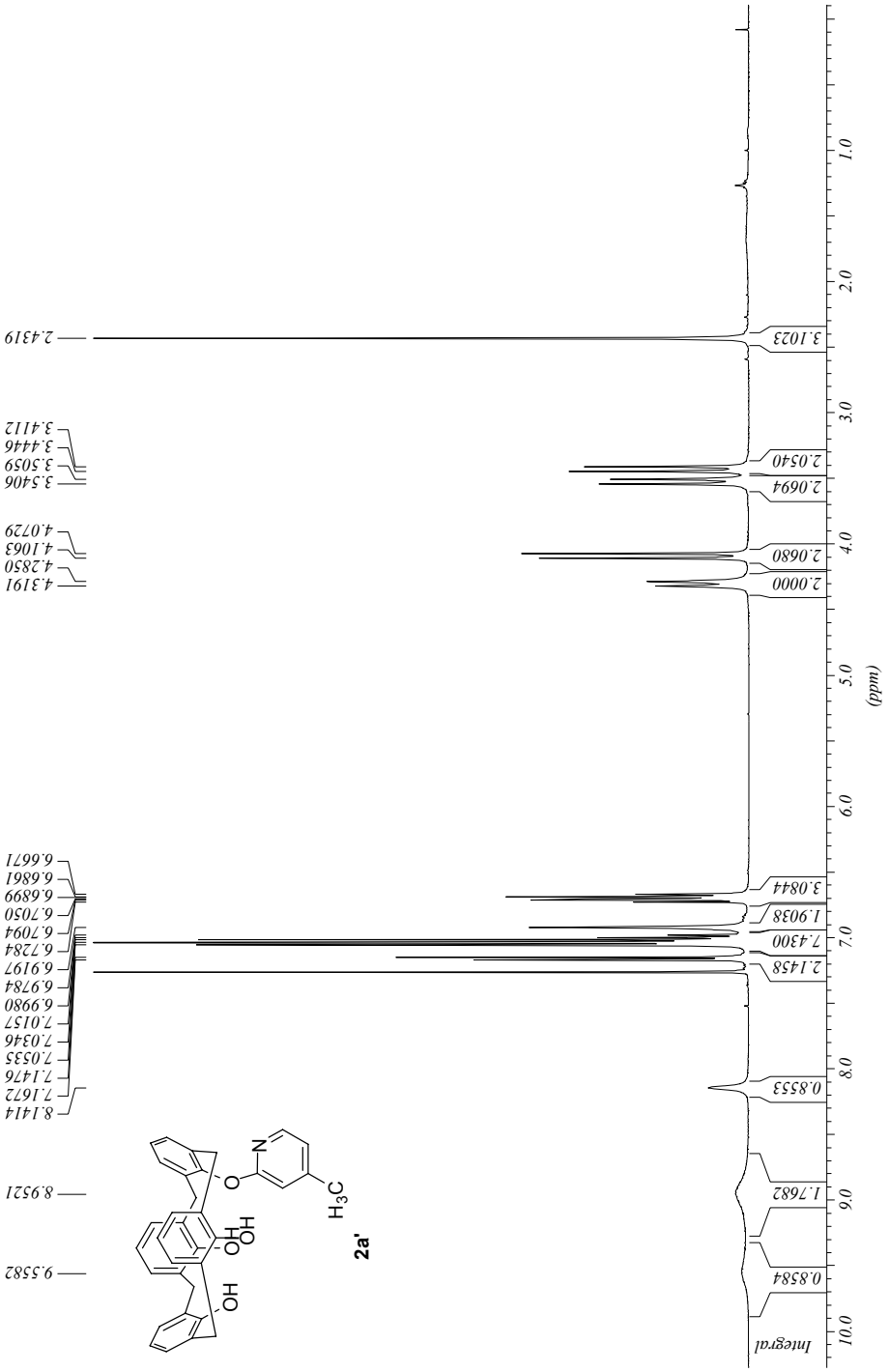
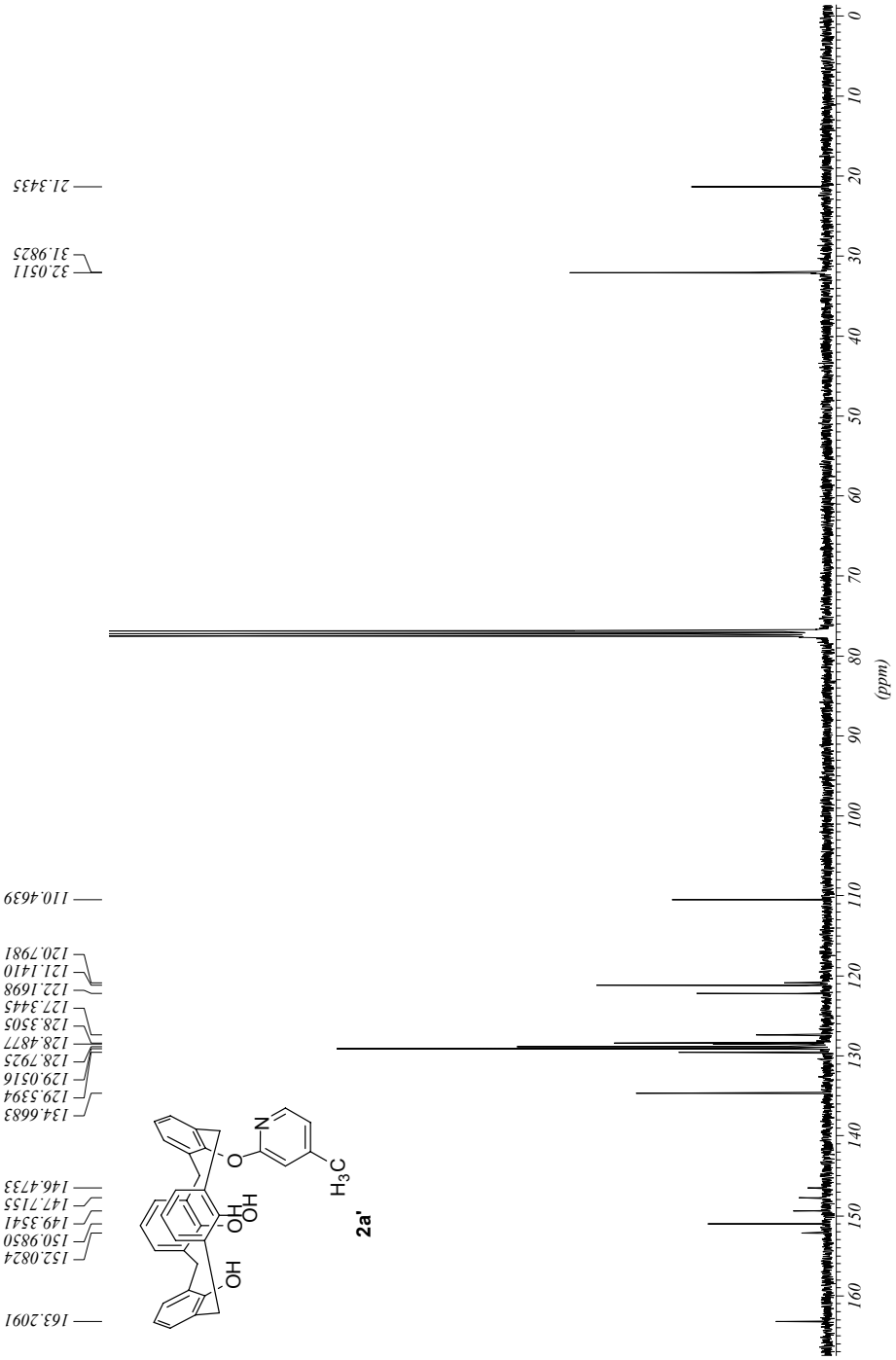
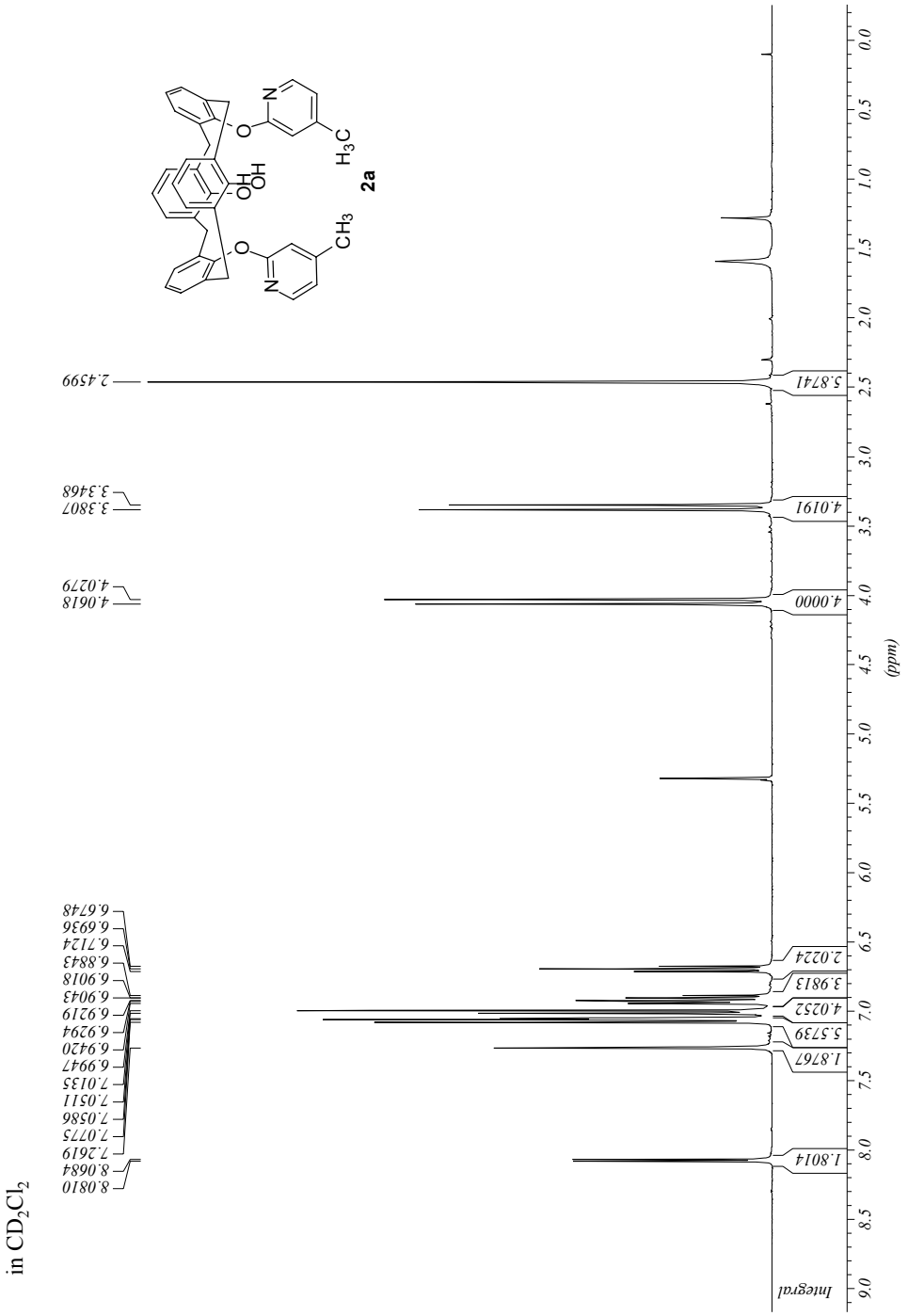
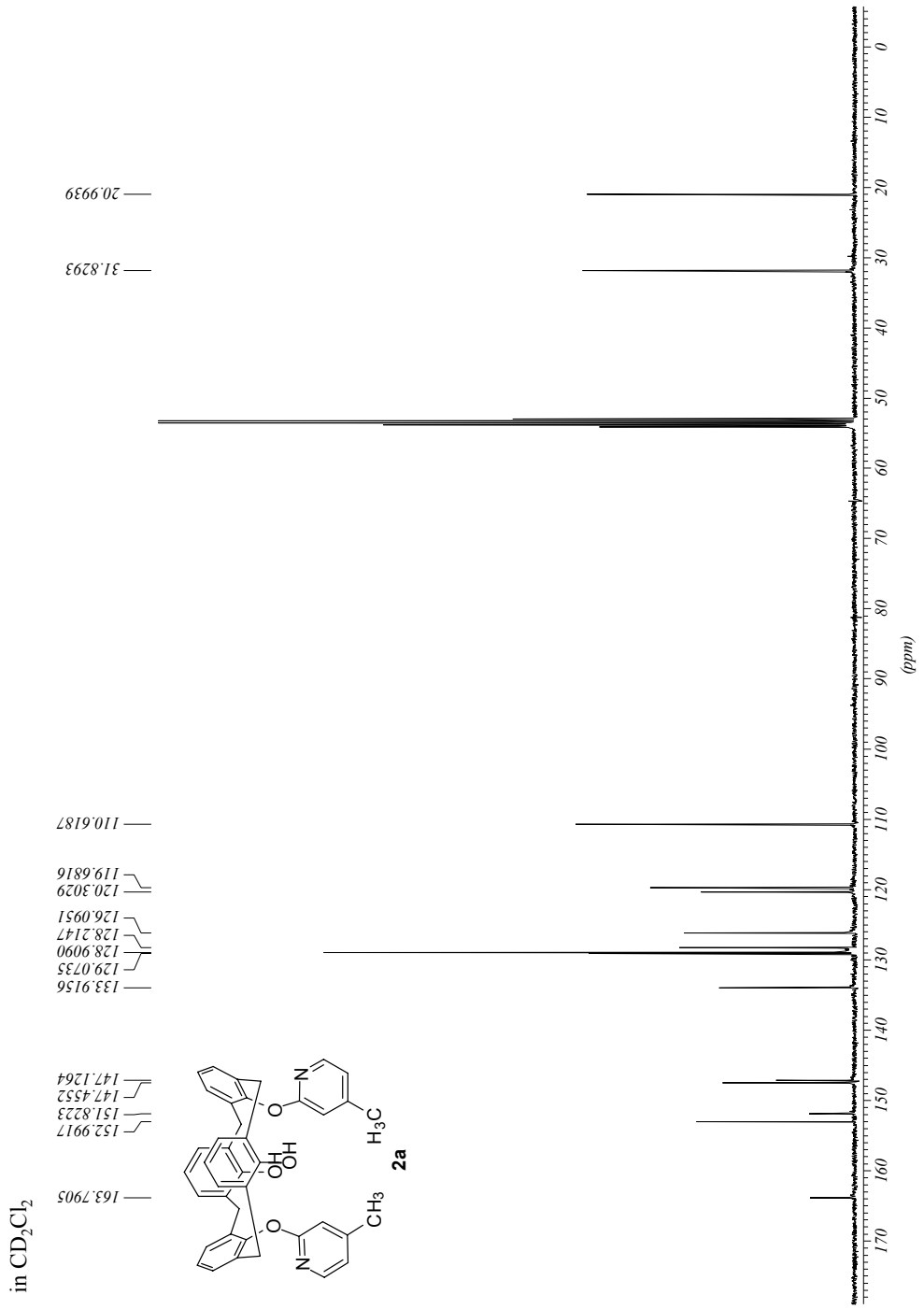
Selected NMR Spectra (400 MHz, $CDCl_3$ unless otherwise stated, 303K)





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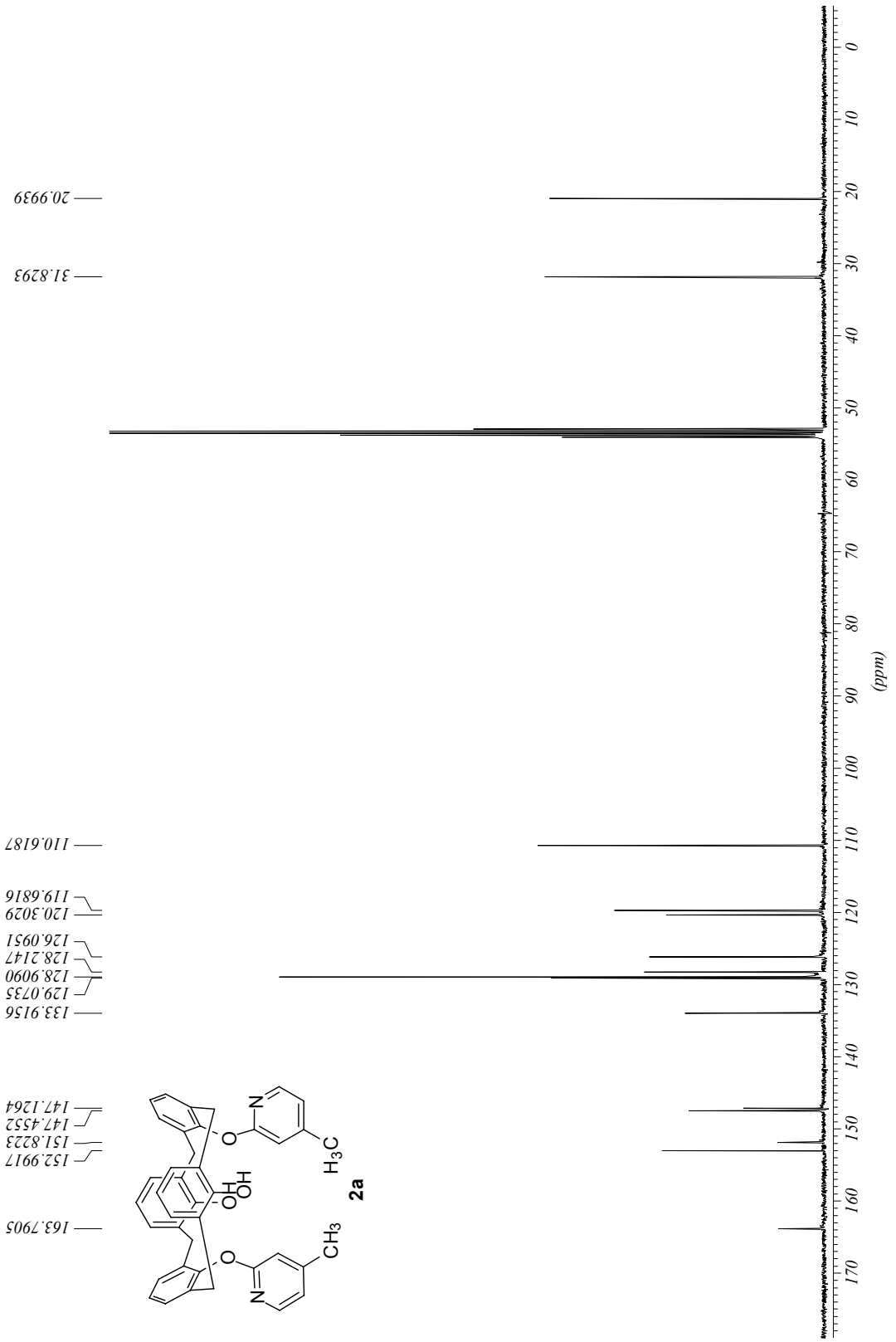
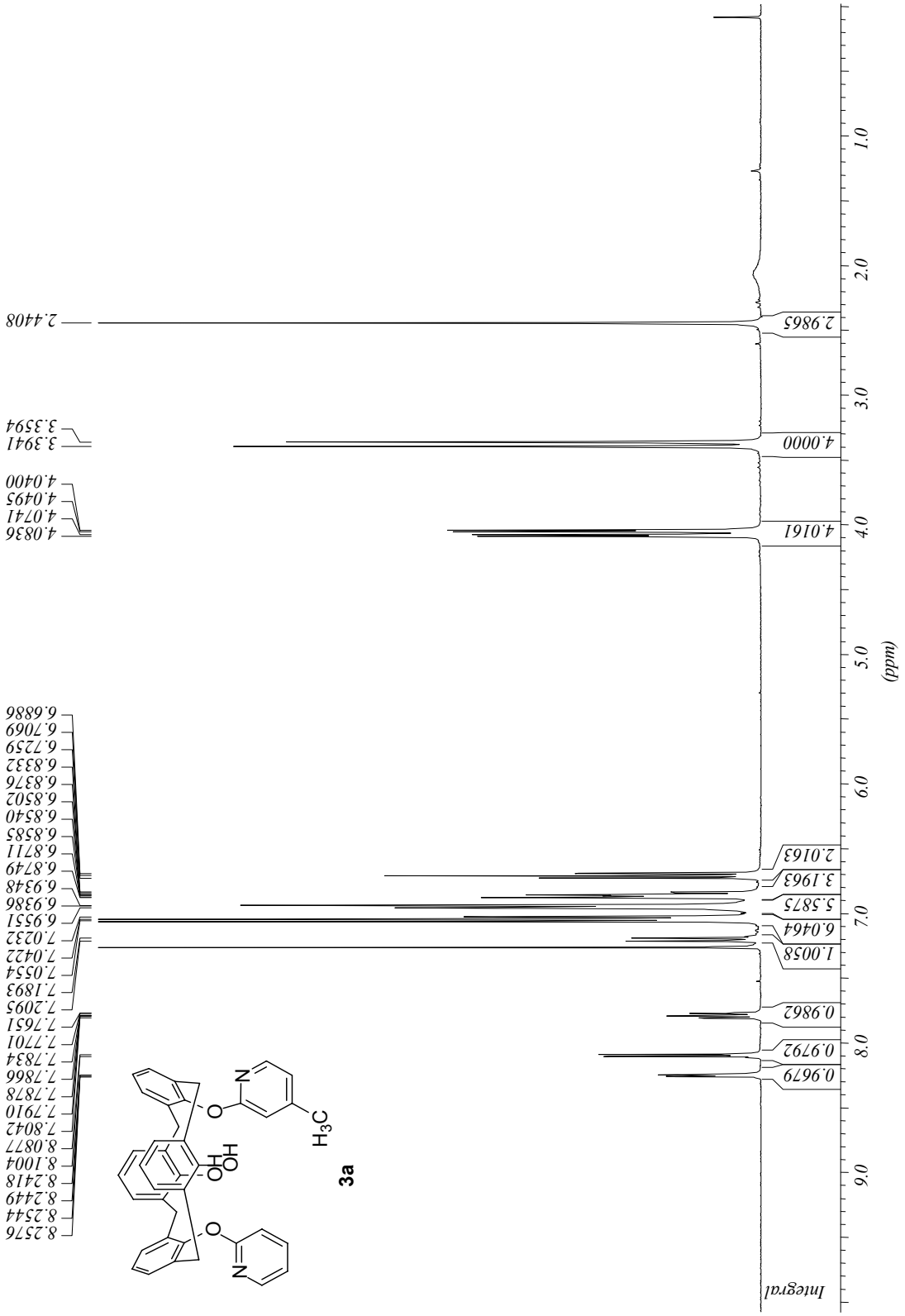
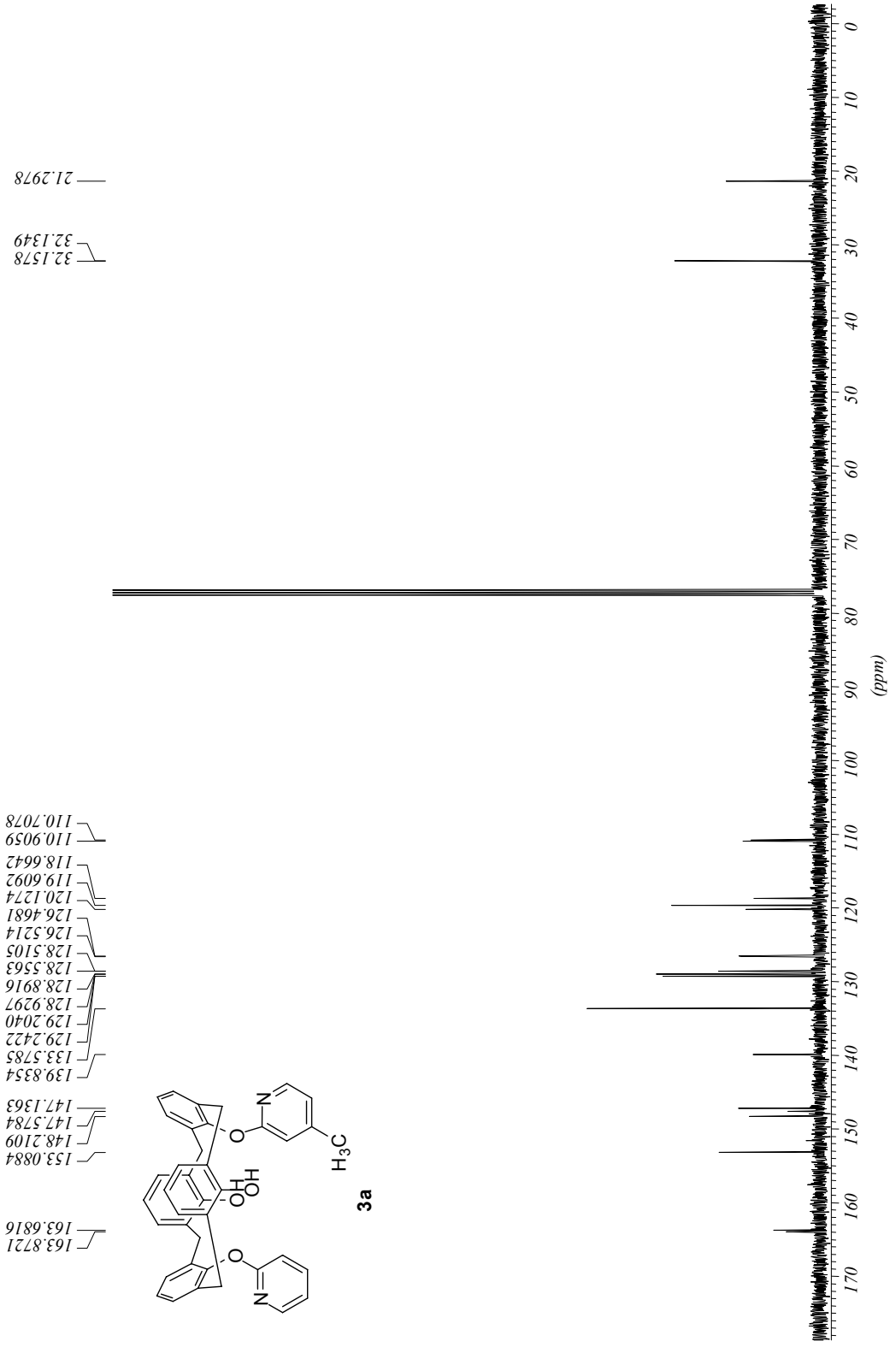
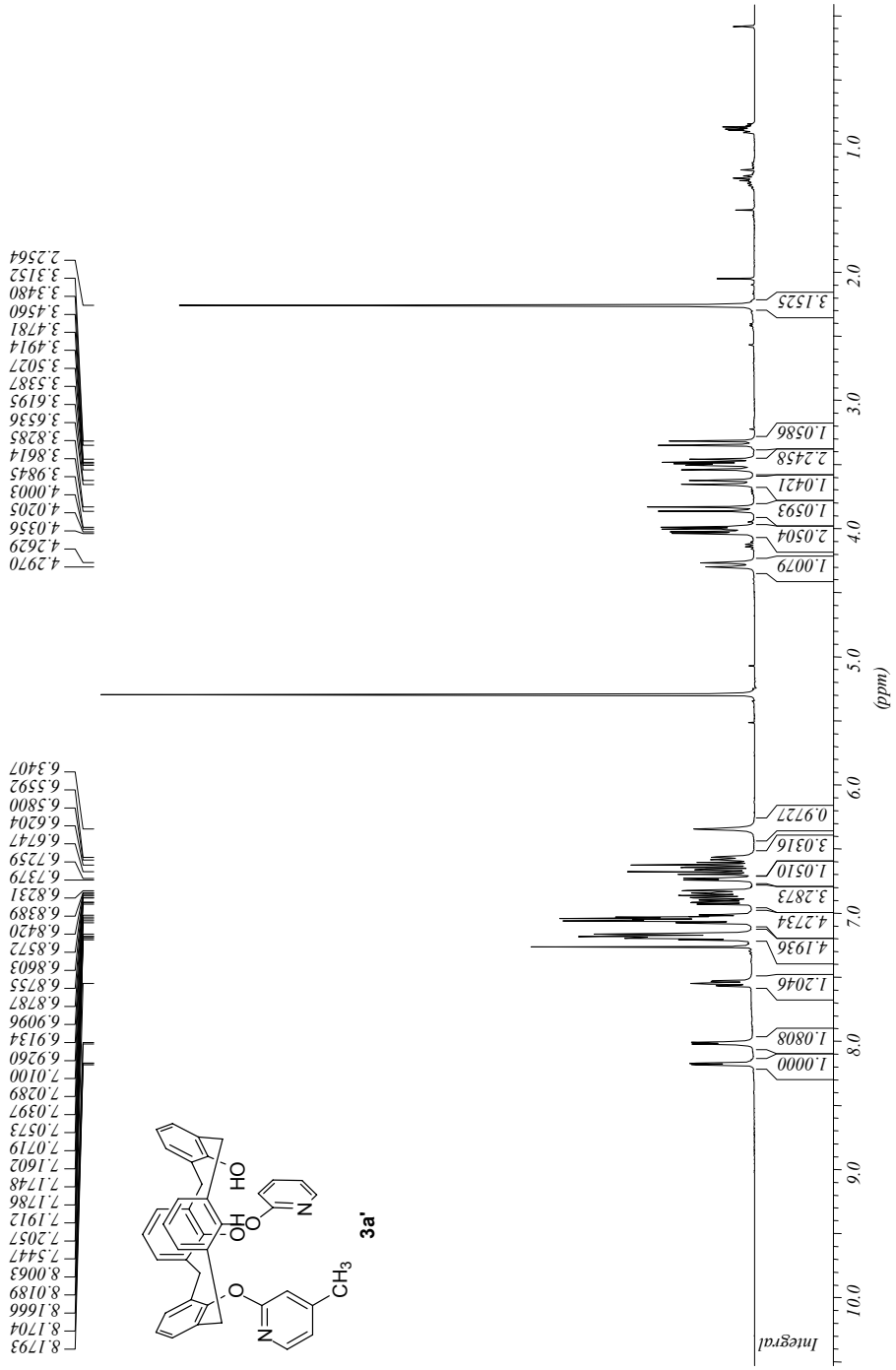
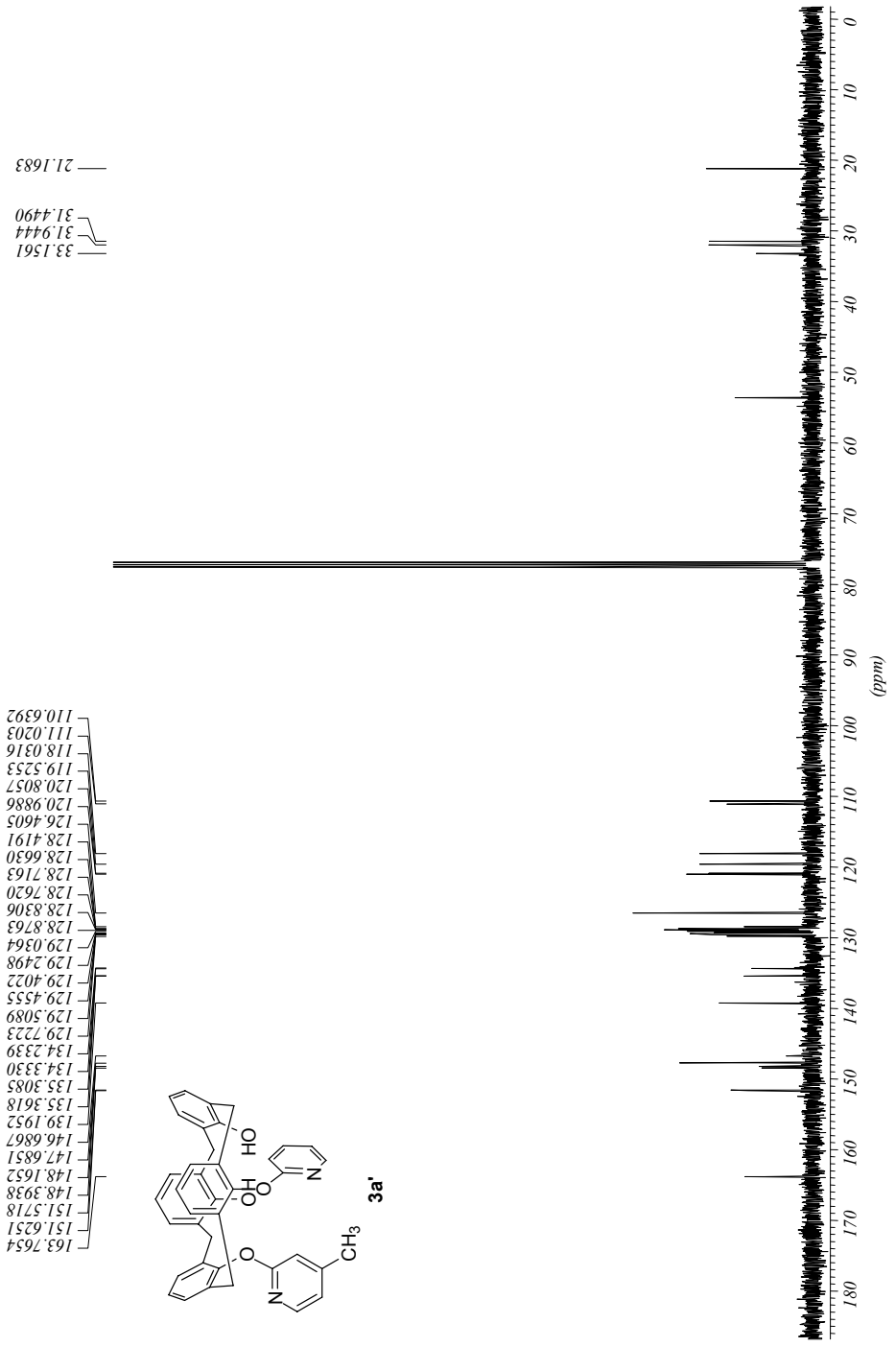
in CD_2Cl_2
2a
(ppm)


20.9939
31.8293
110.6187
119.6816
120.3029
126.0951
128.2147
128.9090
129.0735
133.9156
147.1264
147.4552
151.8223
152.9917
163.7905
(ppm)
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
N
O
H3C
OH
OH
CH3
2a






3a'
integral
(ppm)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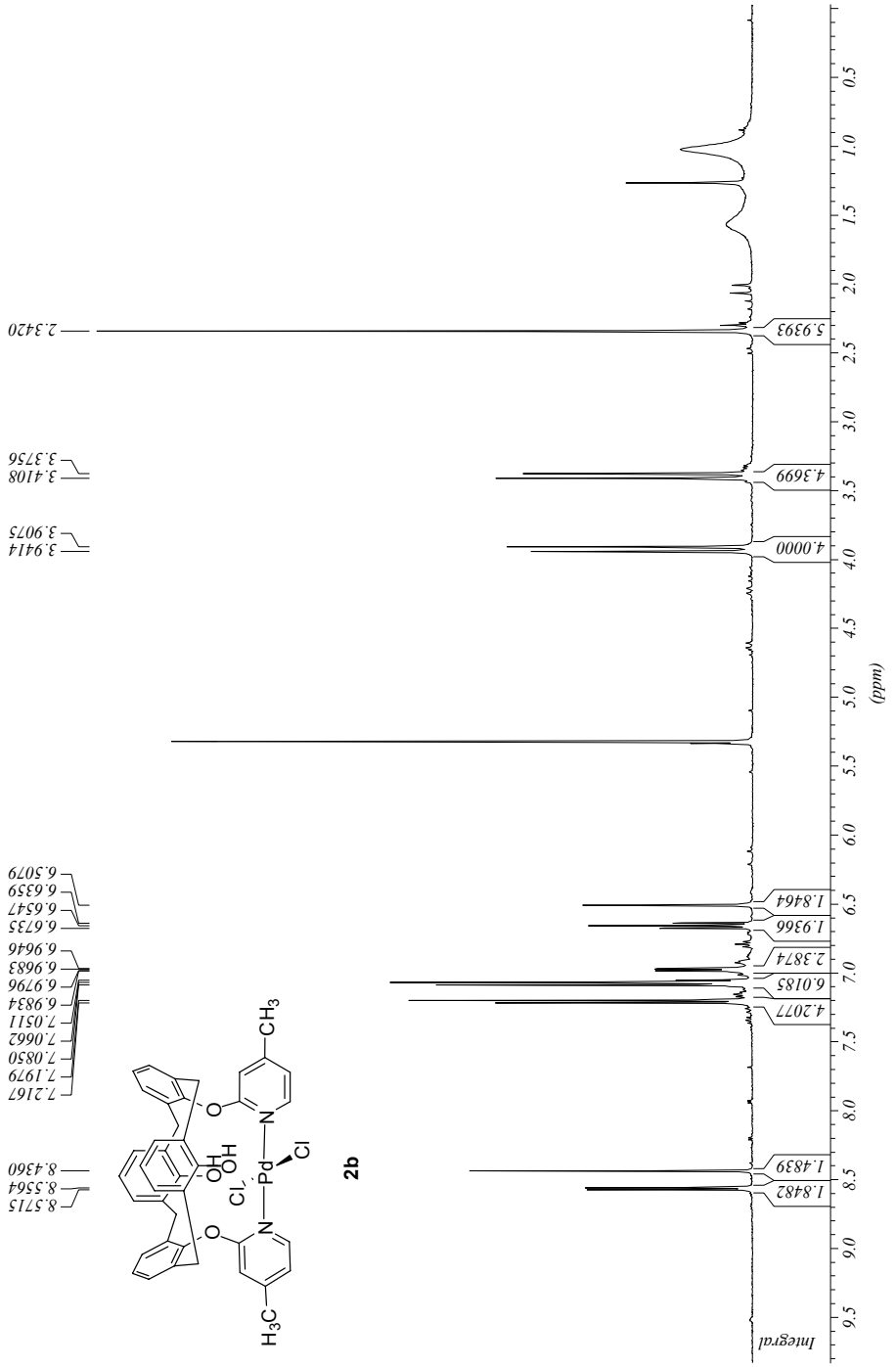
31.4490
31.9444
33.1561
110.6392
111.0203
118.0316
119.5253
120.8057
120.9886
126.4605
128.4191
128.6630
128.7163
128.7620
128.8306
128.8763
129.0364
129.2498
129.4022
129.4555
129.5089
129.7223
134.2339
134.3330
135.3085
135.3618
139.1952
146.6867
147.6851
148.1652
148.3938
151.5718
151.6251
163.7654
OH
O
N
O
N
CH3
3a'
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
(ppm)


2b
Integral
(ppm)
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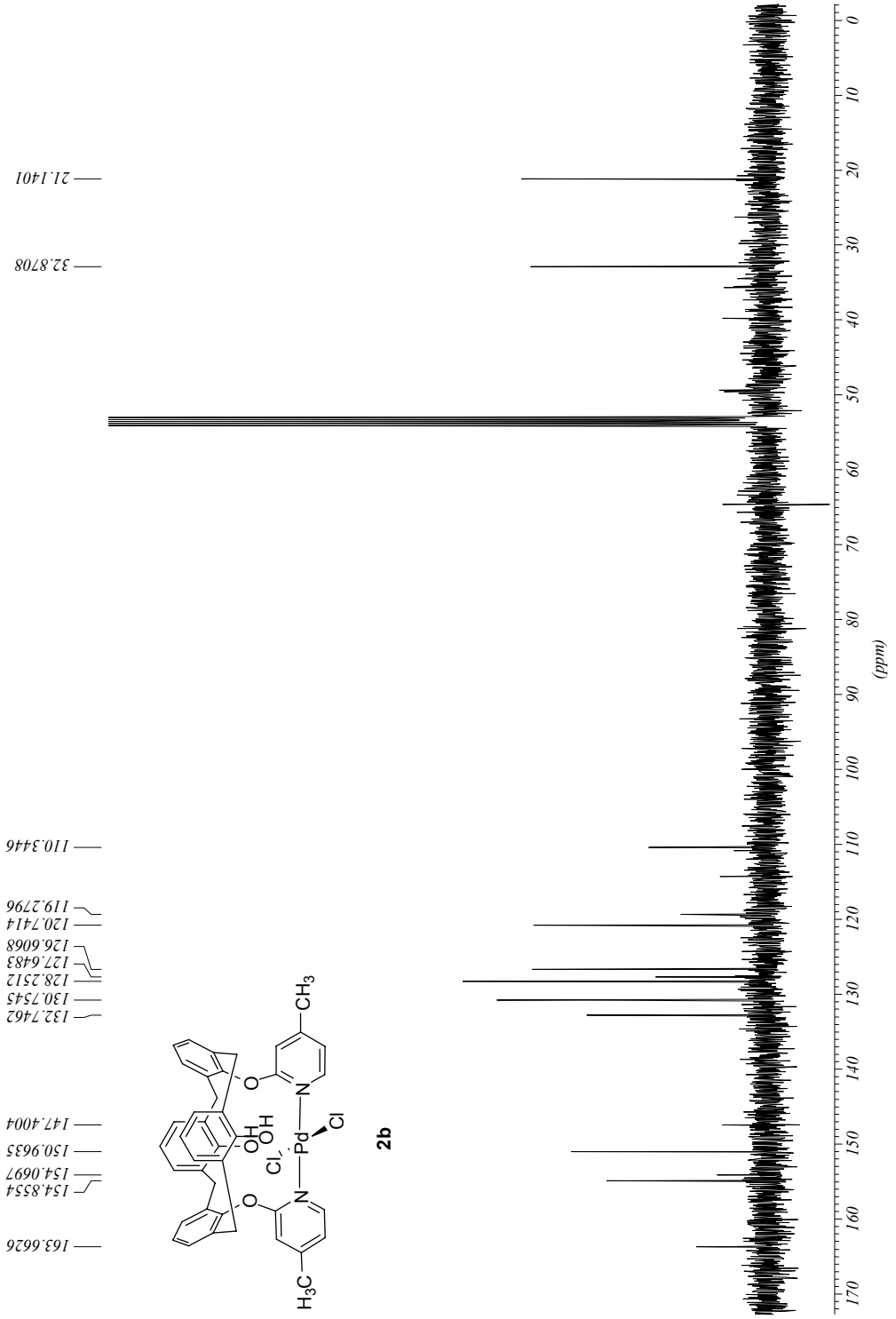
1.8839
8.4360
8.5564
8.5715
4.2077
6.0185
2.3874
1.9366
1.8464
7.2167
7.1979
7.0850
7.0662
7.0511
6.9834
6.9796
6.9683
6.9646
6.6735
6.6547
6.6359
6.5079
4.0000
3.9414
3.9075
4.3699
3.4108
3.3756
5.9393
2.3420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32.8708
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119.2796
120.7414
126.6068
127.6483
128.2512
130.7545
132.7462
147.4004
150.9635
154.0697
154.8554
163.6626
2b
(ppm)