Electronic Supplementary Information

One-Pot Synthesis of 2,4,6-Triarylpyridines from *β*-Nitrostyrenes, Substituted Salicylic Aldehydes and Ammonium Acetate

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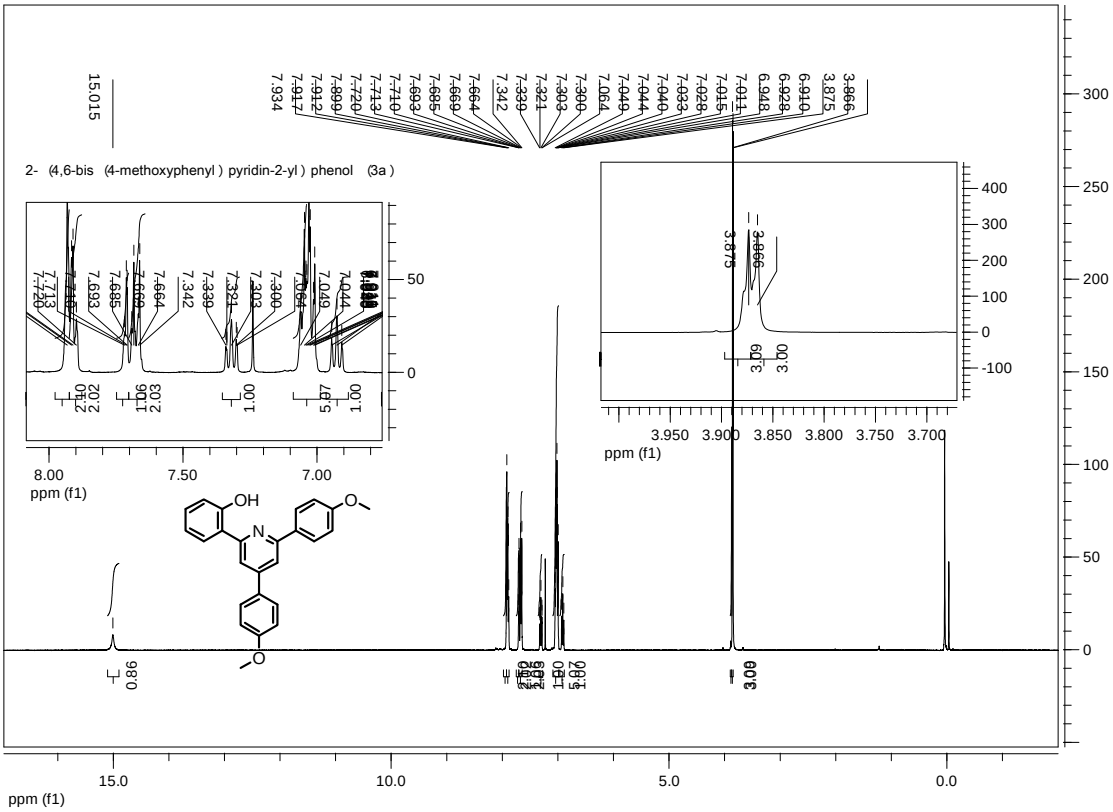
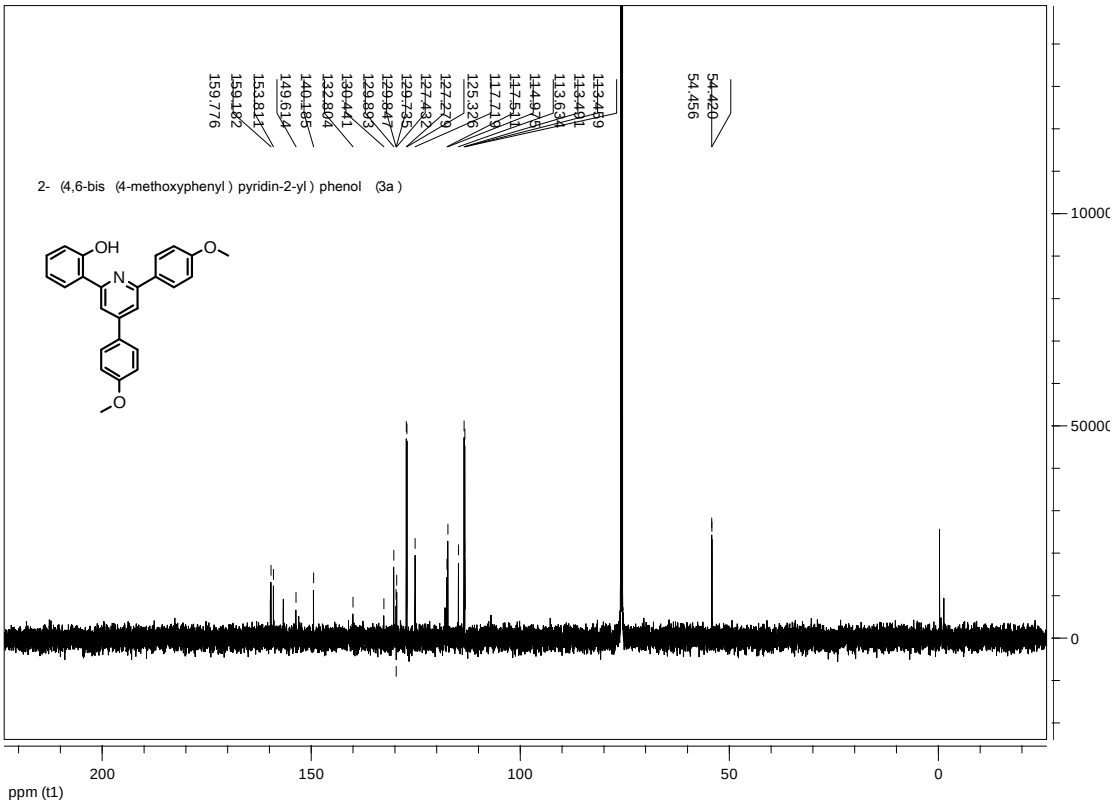
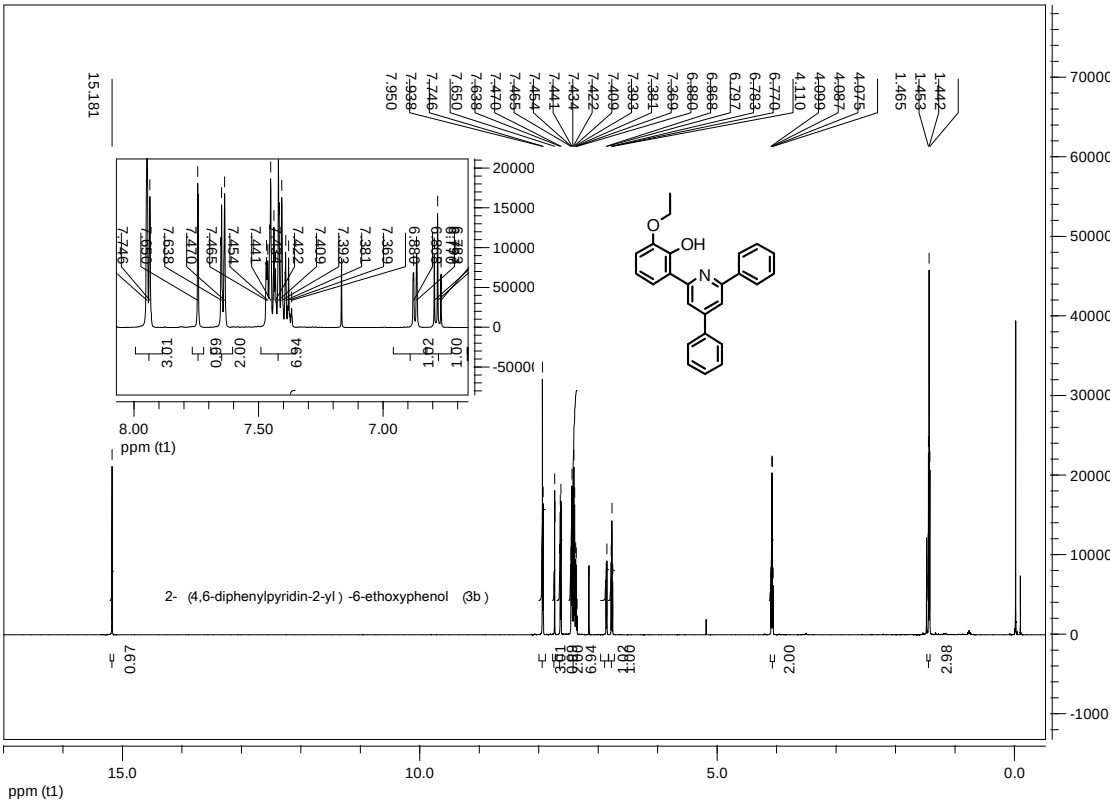
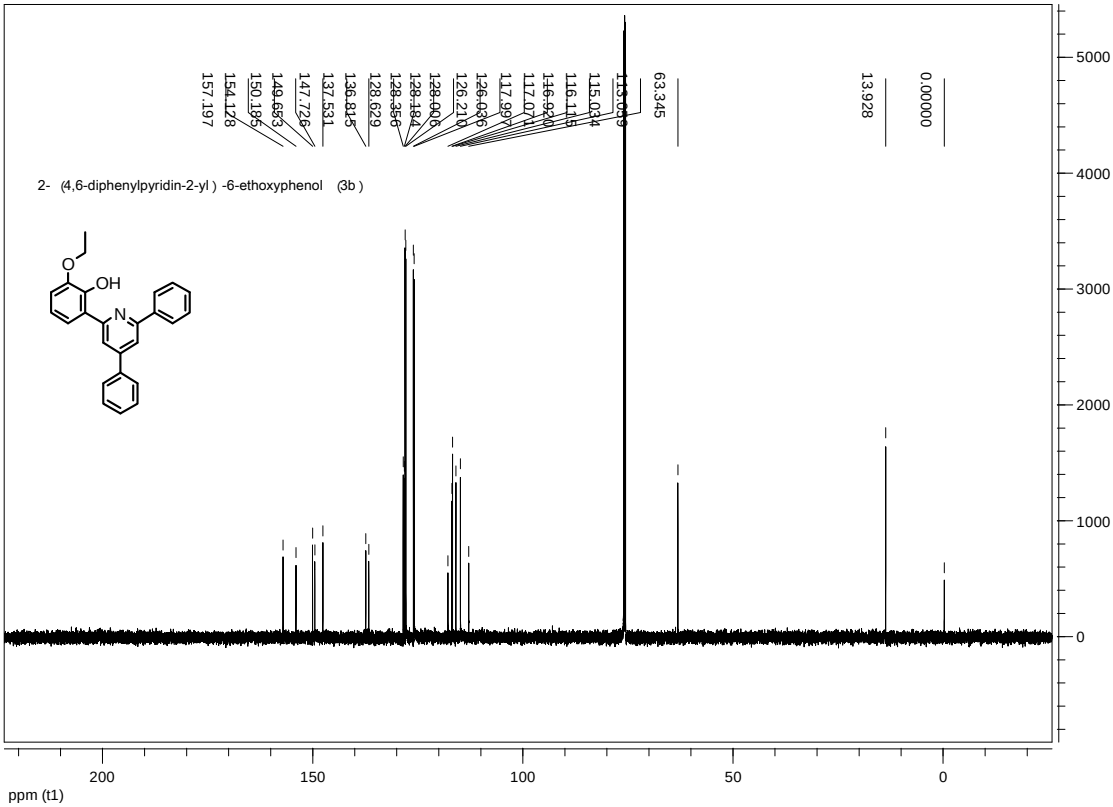




2-(4,6-diphenylpyridin-2-yl)-6-ethoxyphenol (**3b**)





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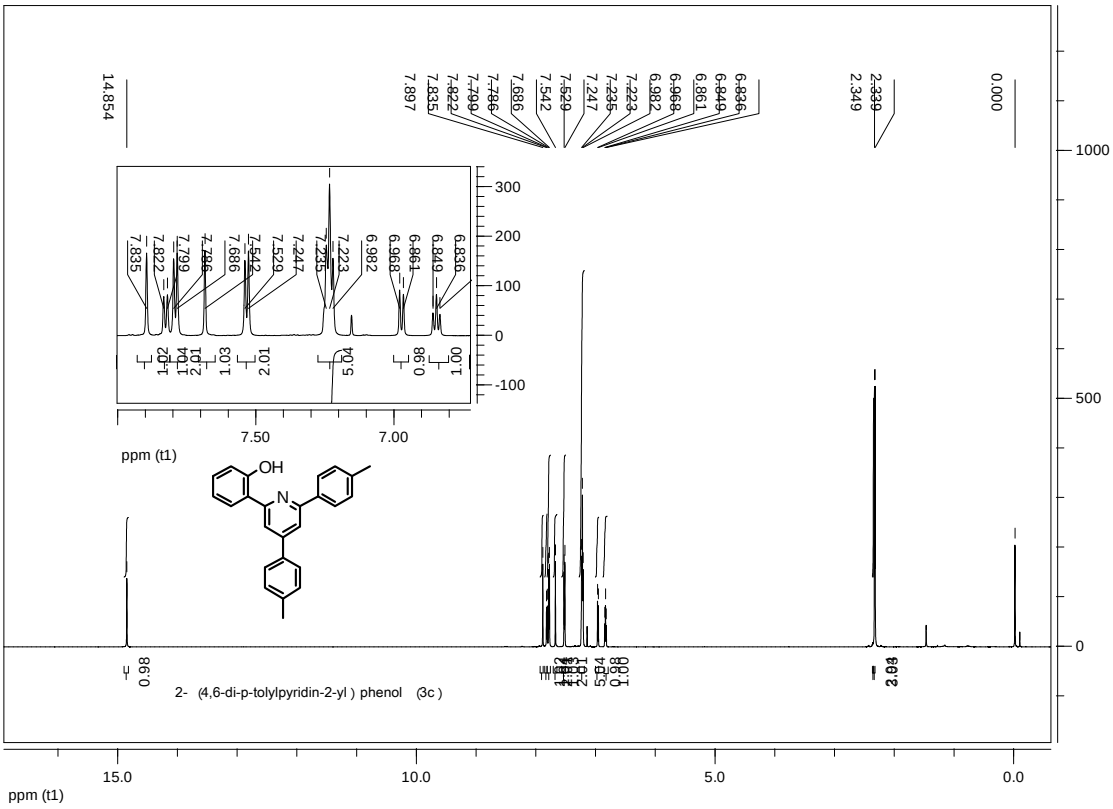

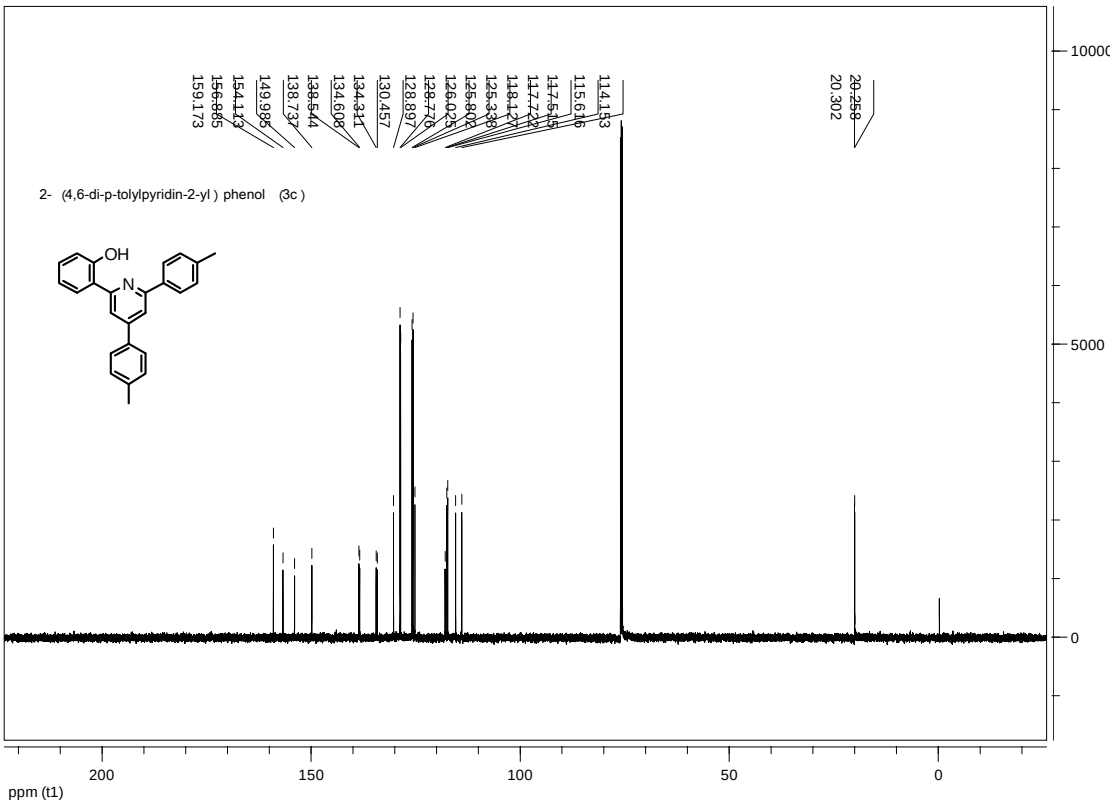

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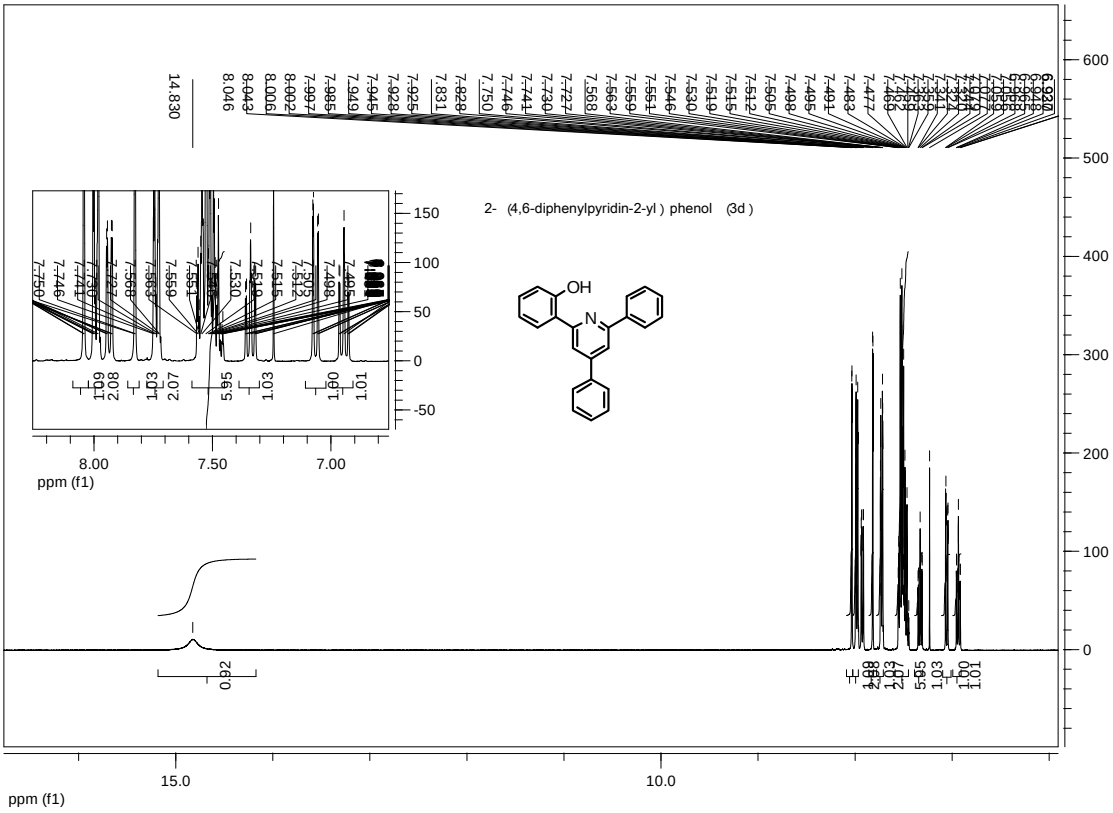
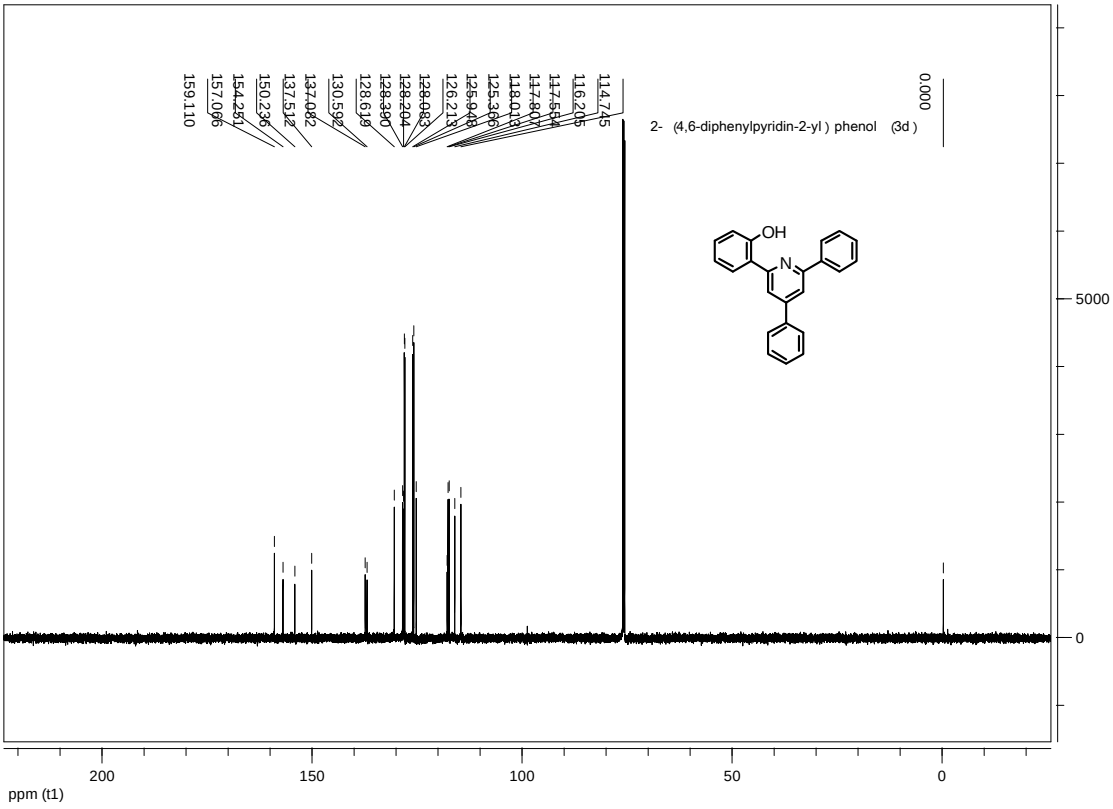
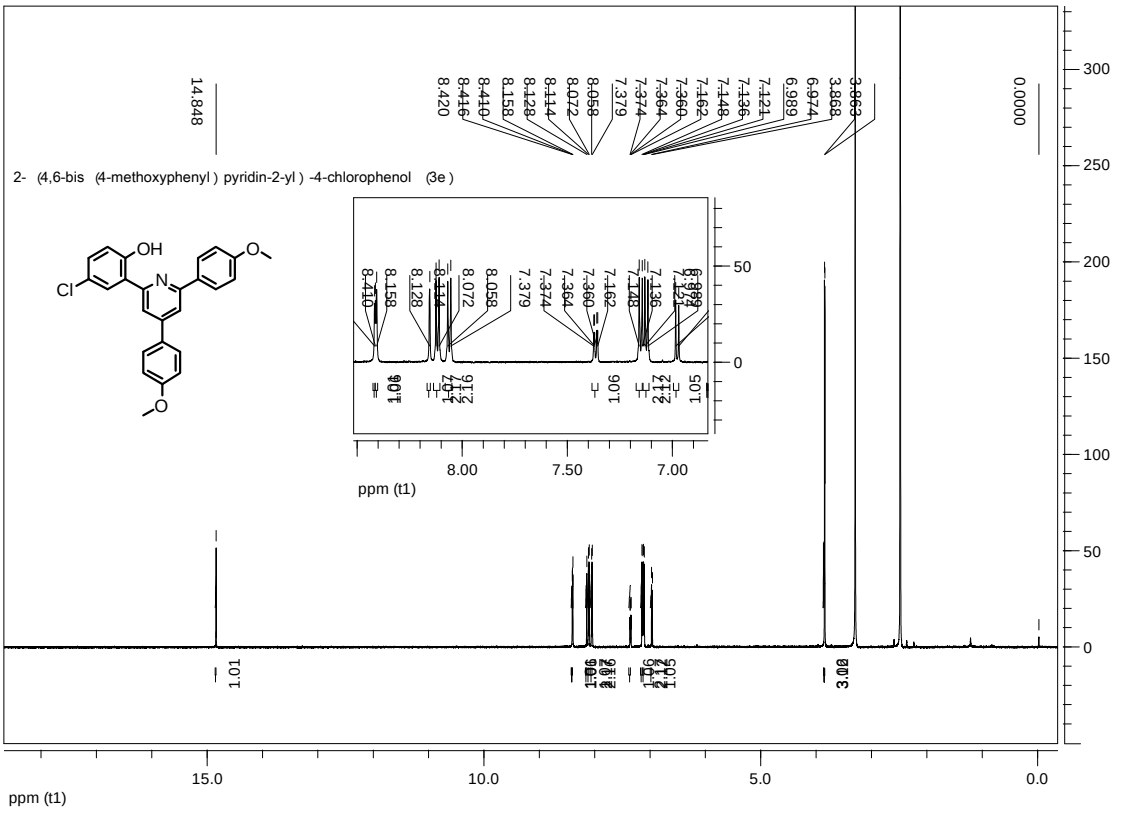
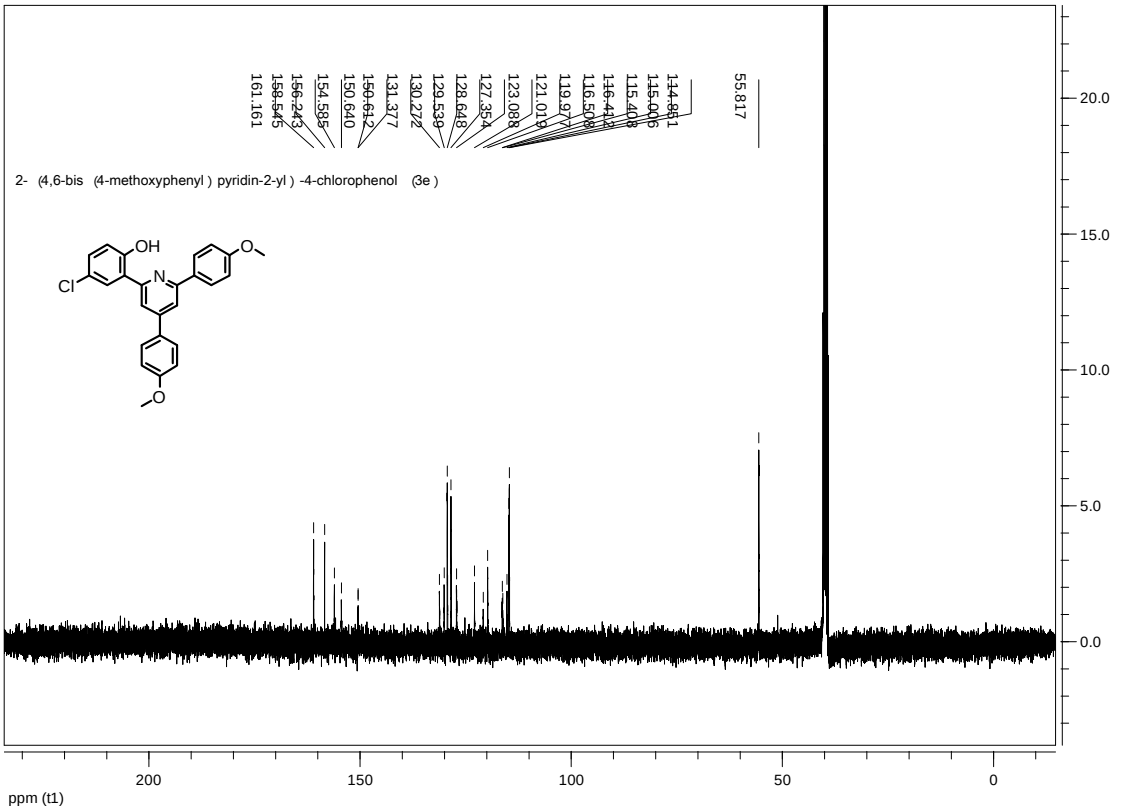


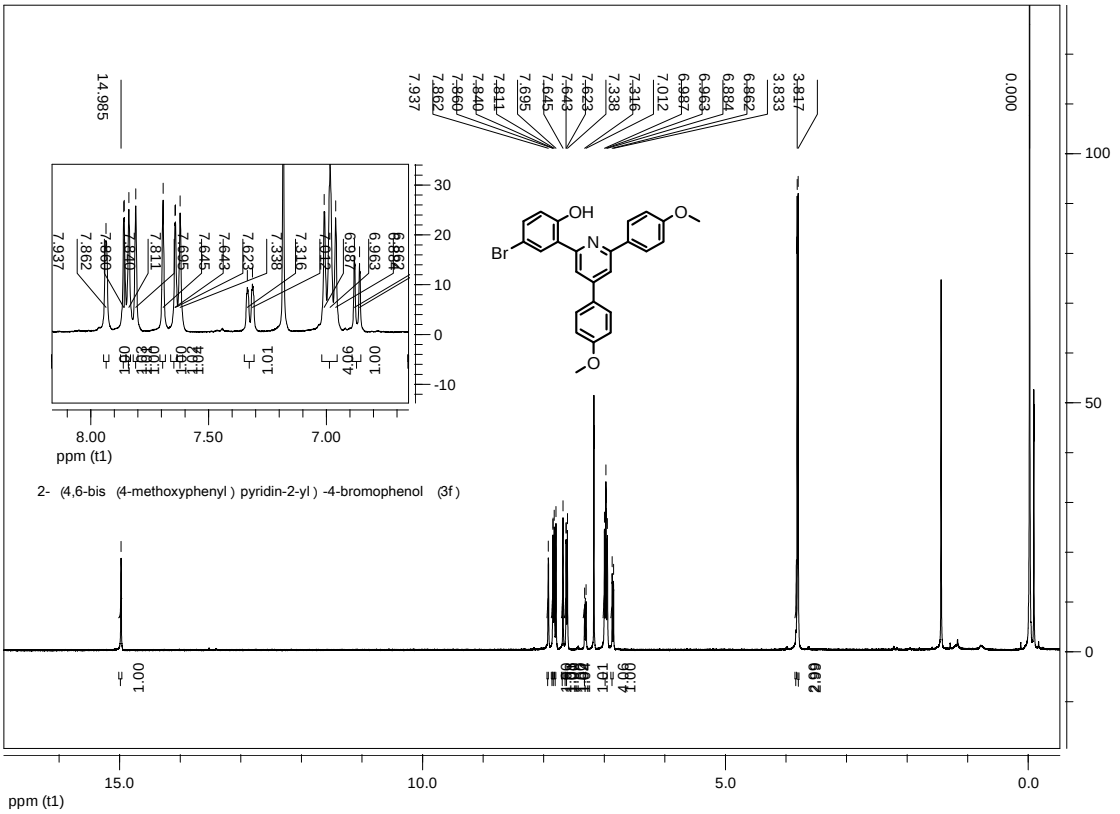


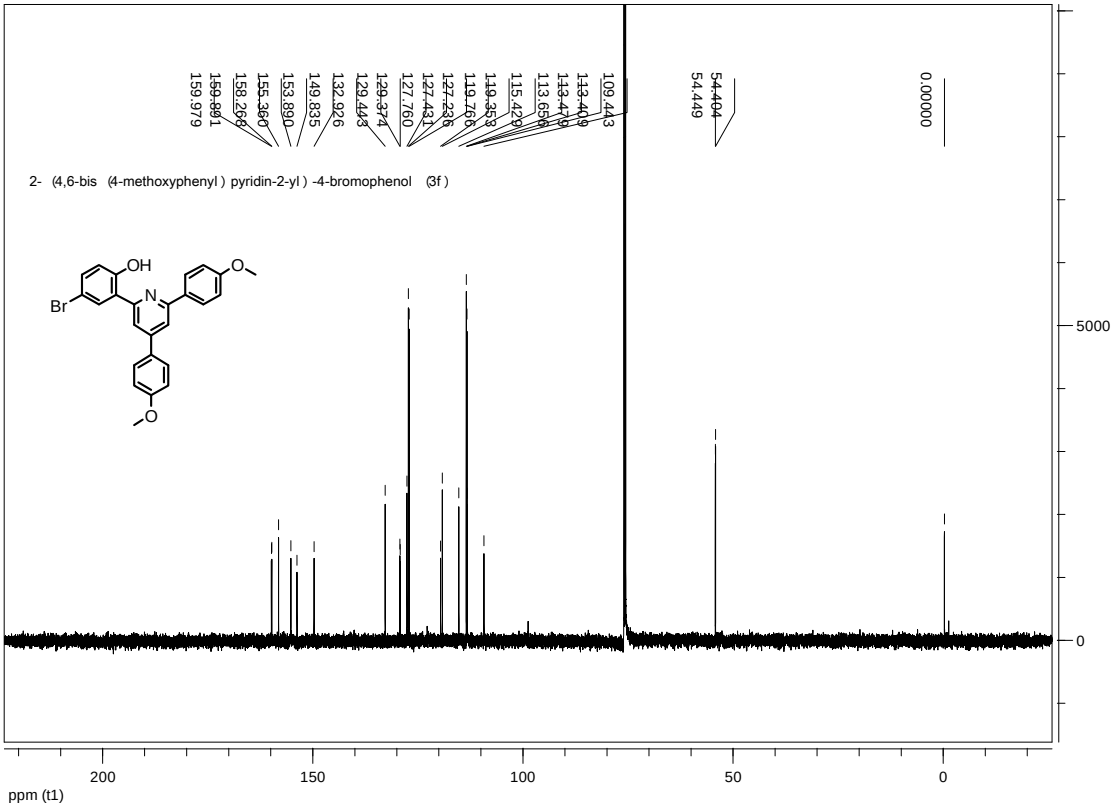
2-(4,6-bis(4-methoxyphenyl)pyridin-2-yl)-4-chlorophenol (**3e**)





2-(4,6-bis(4-methoxyphenyl)pyridin-2-yl)-4-bromophenol (**3f**)





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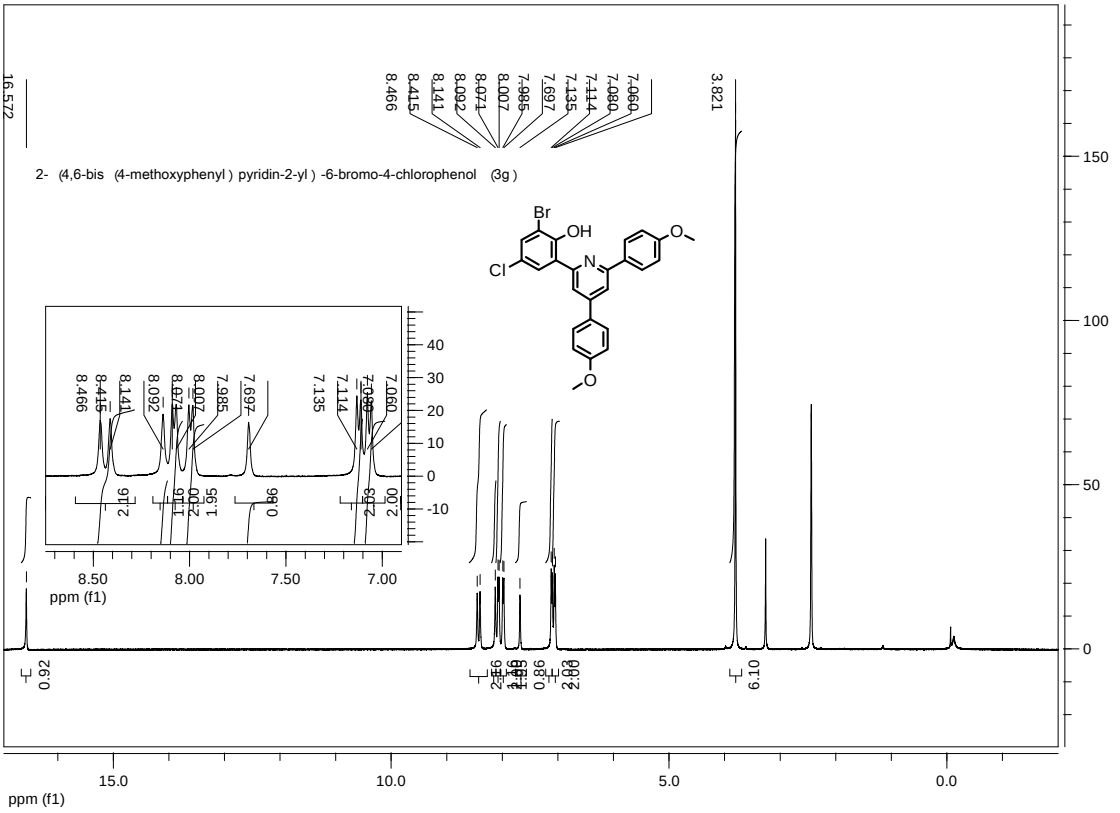

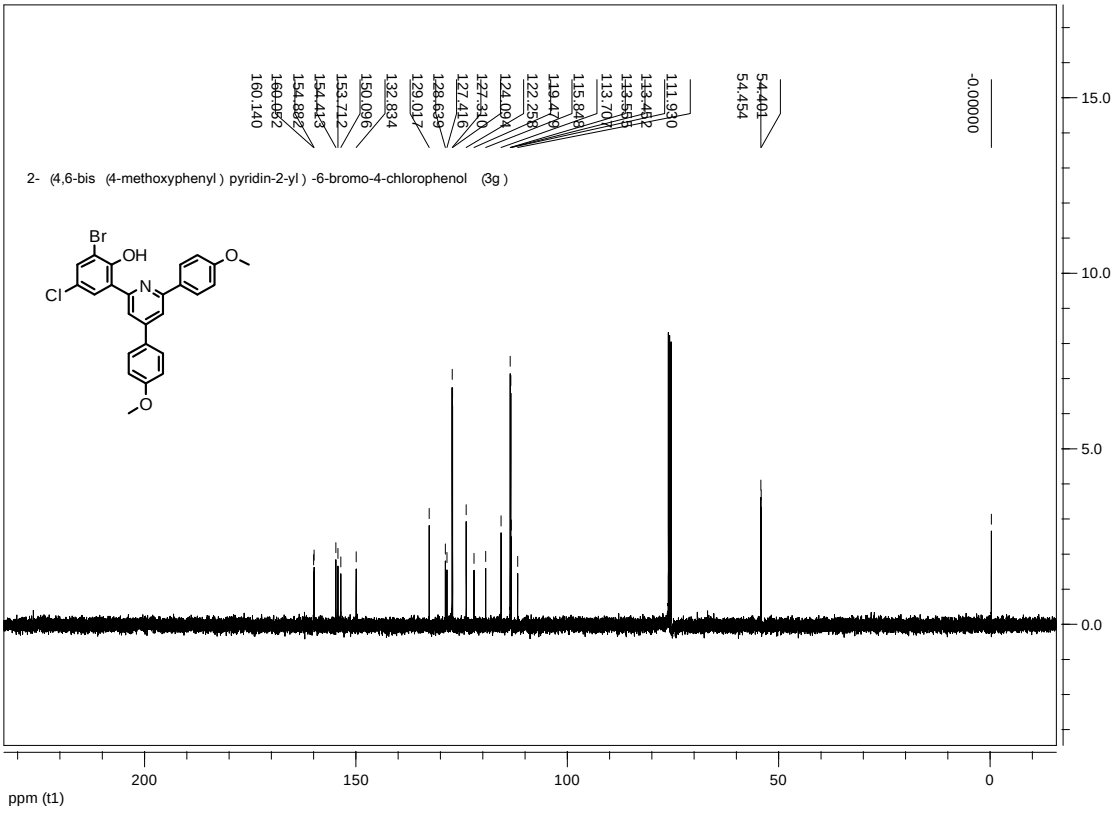

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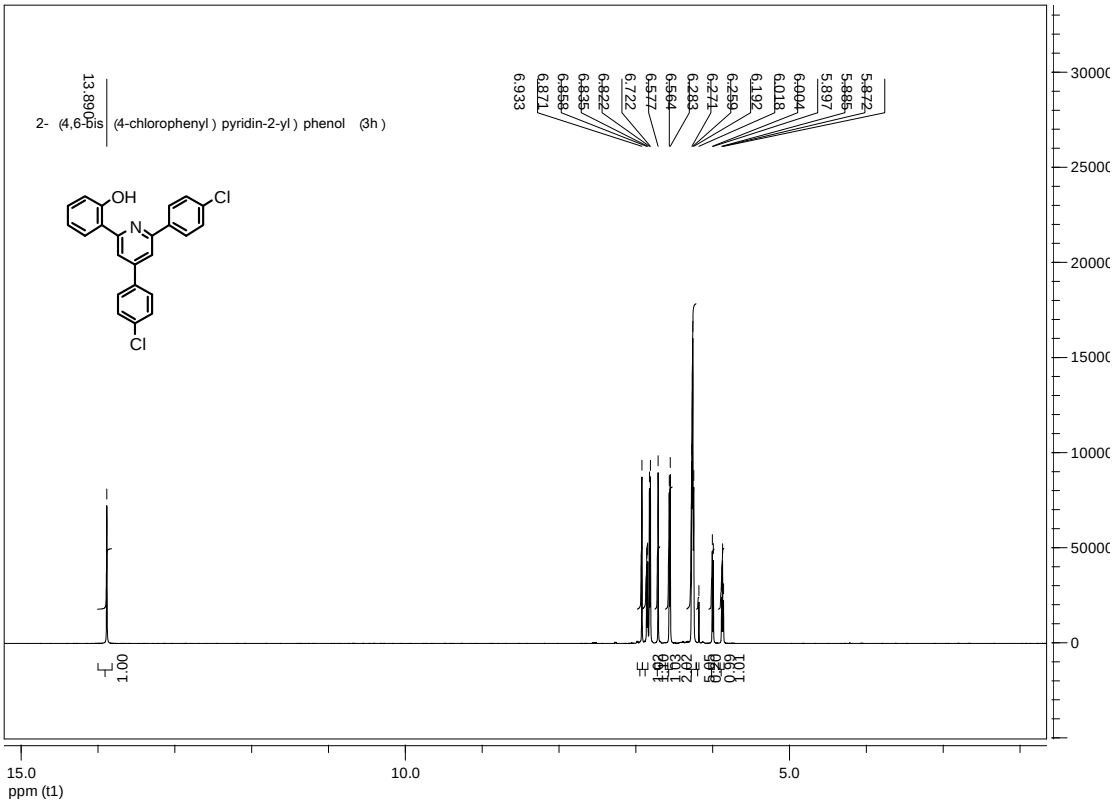

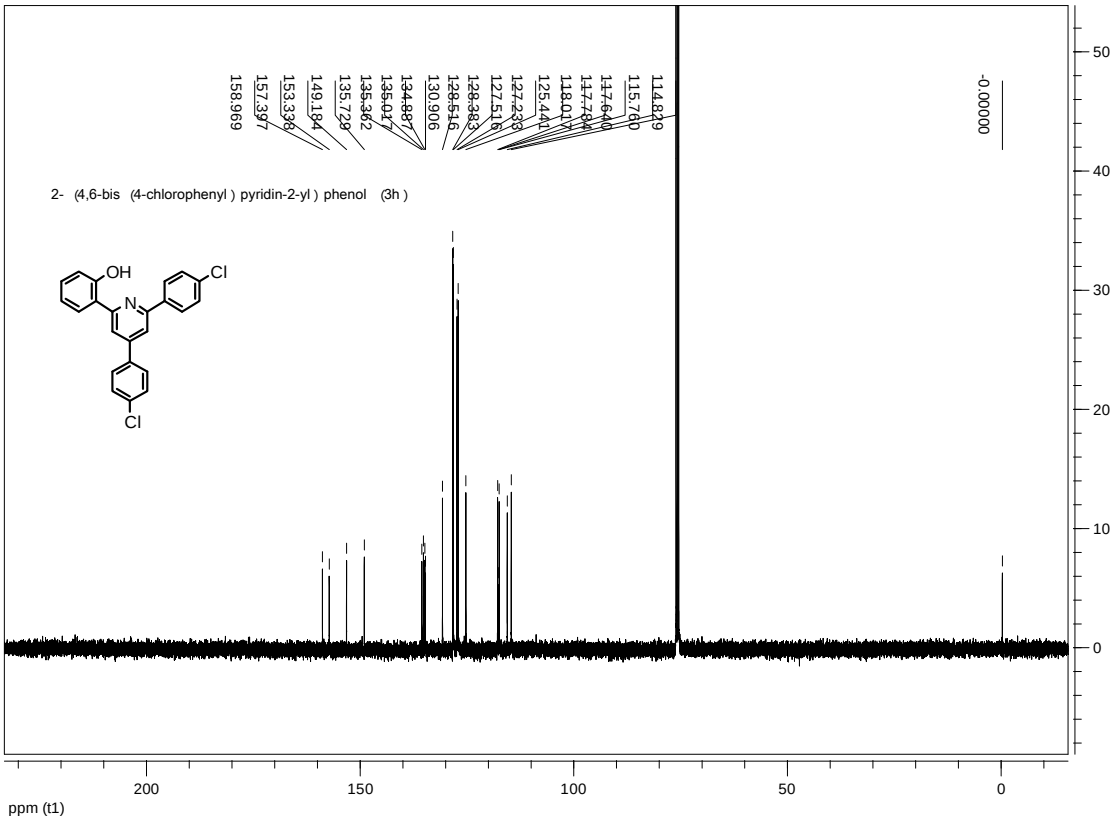

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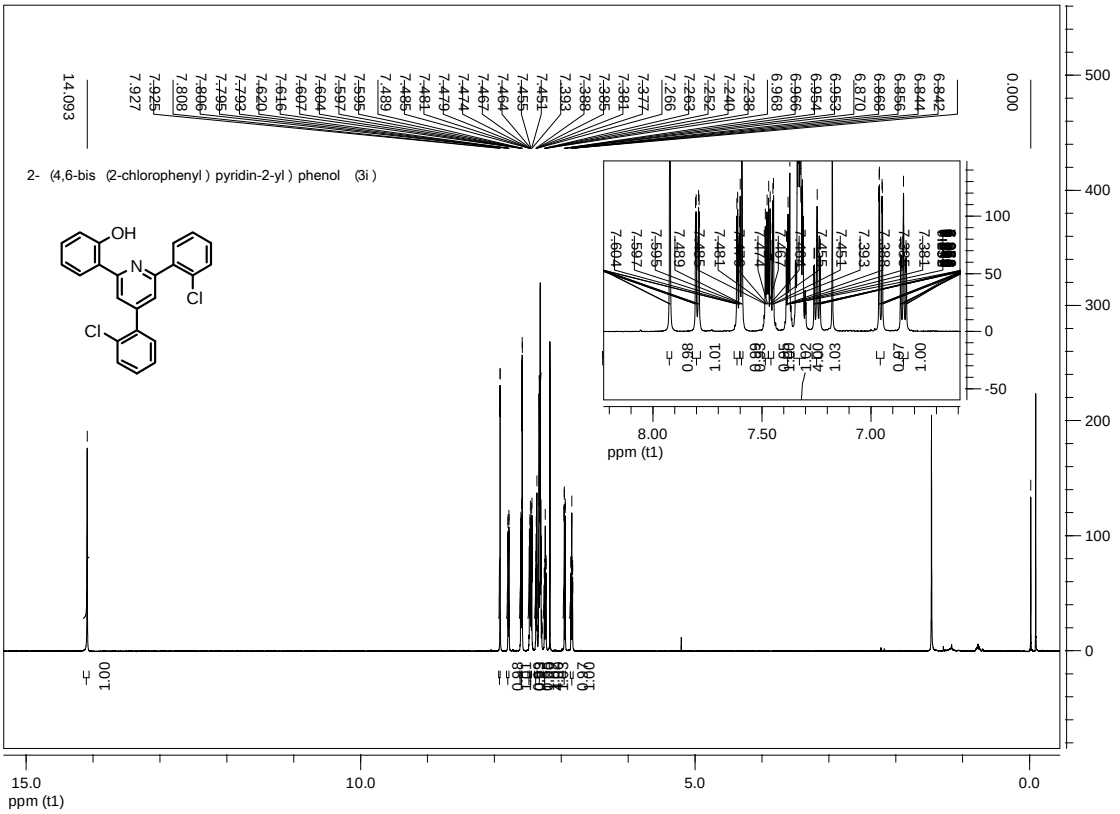

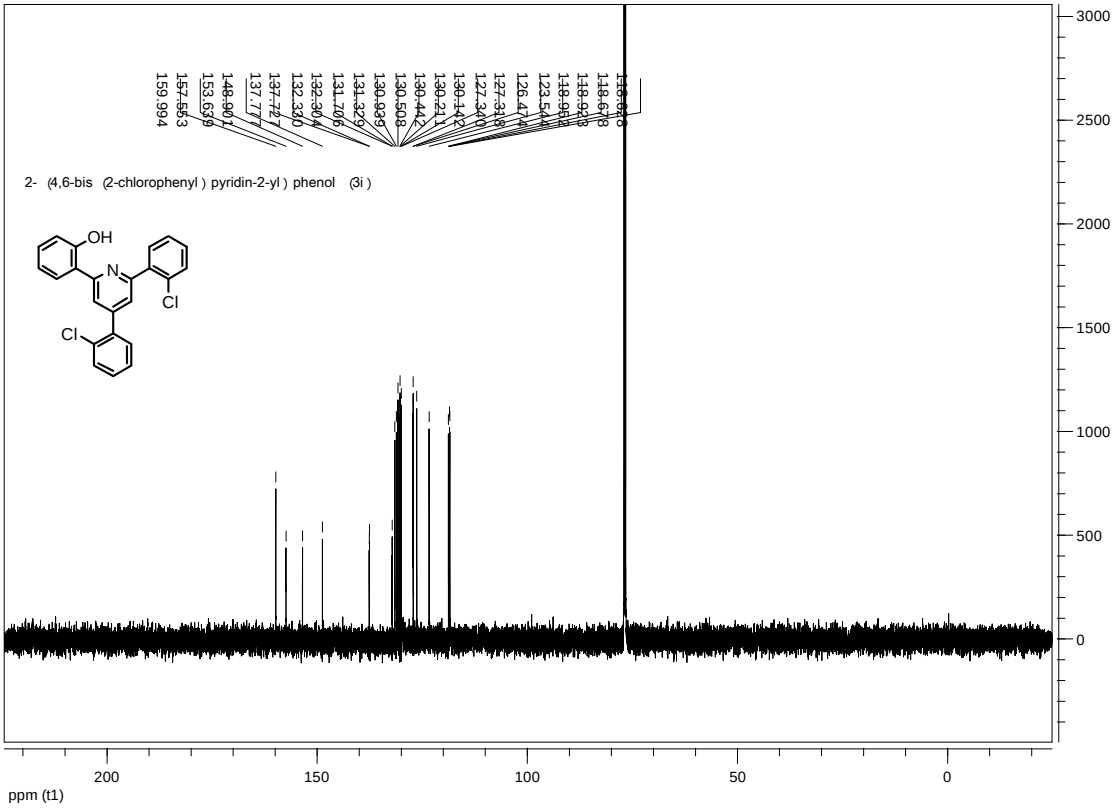

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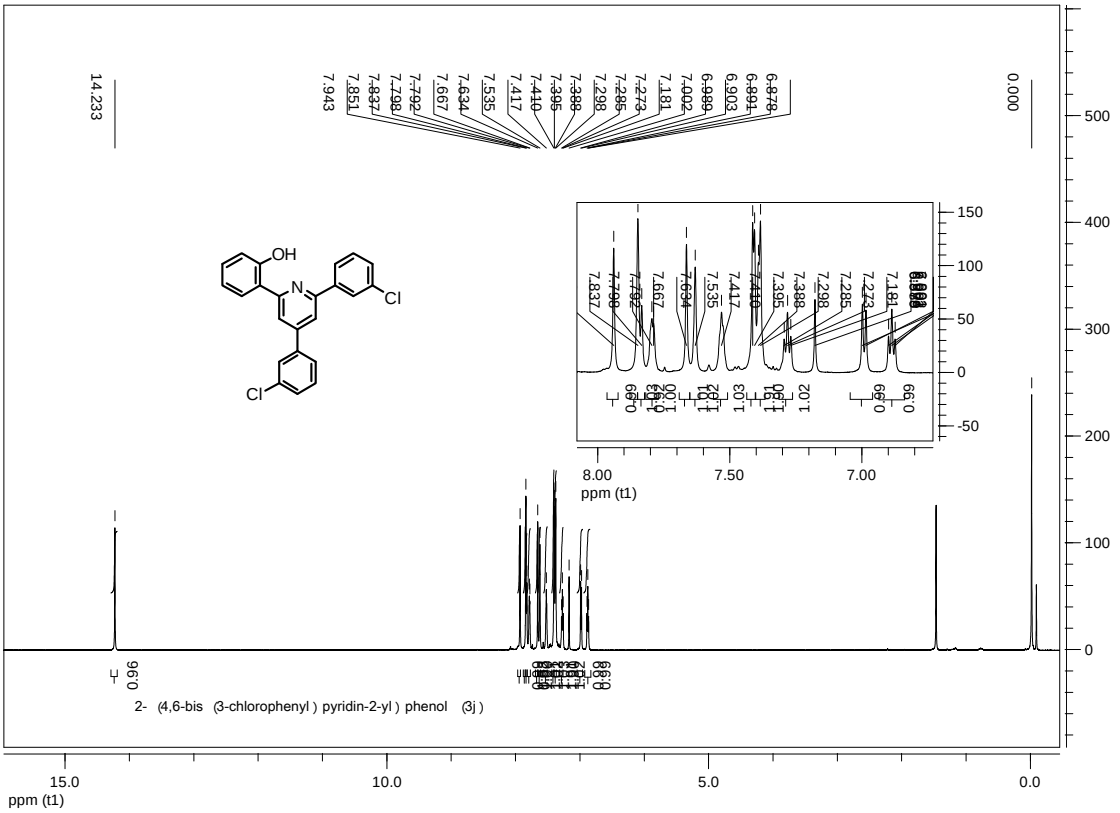

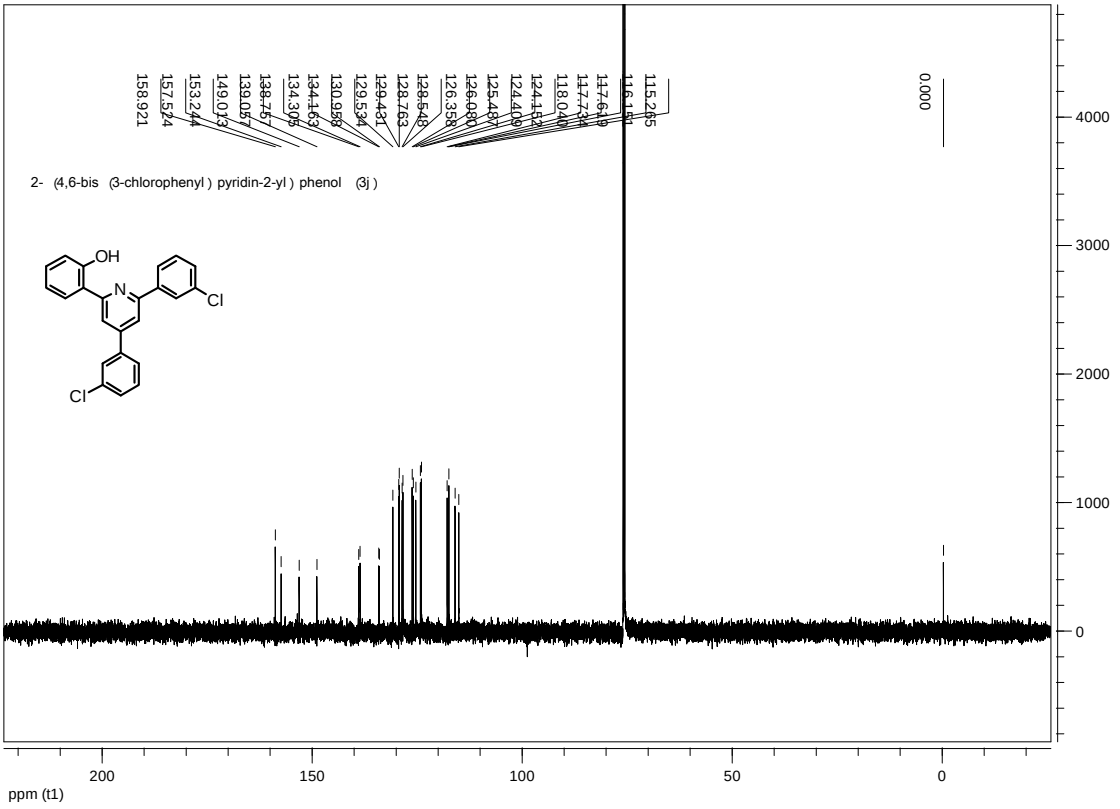

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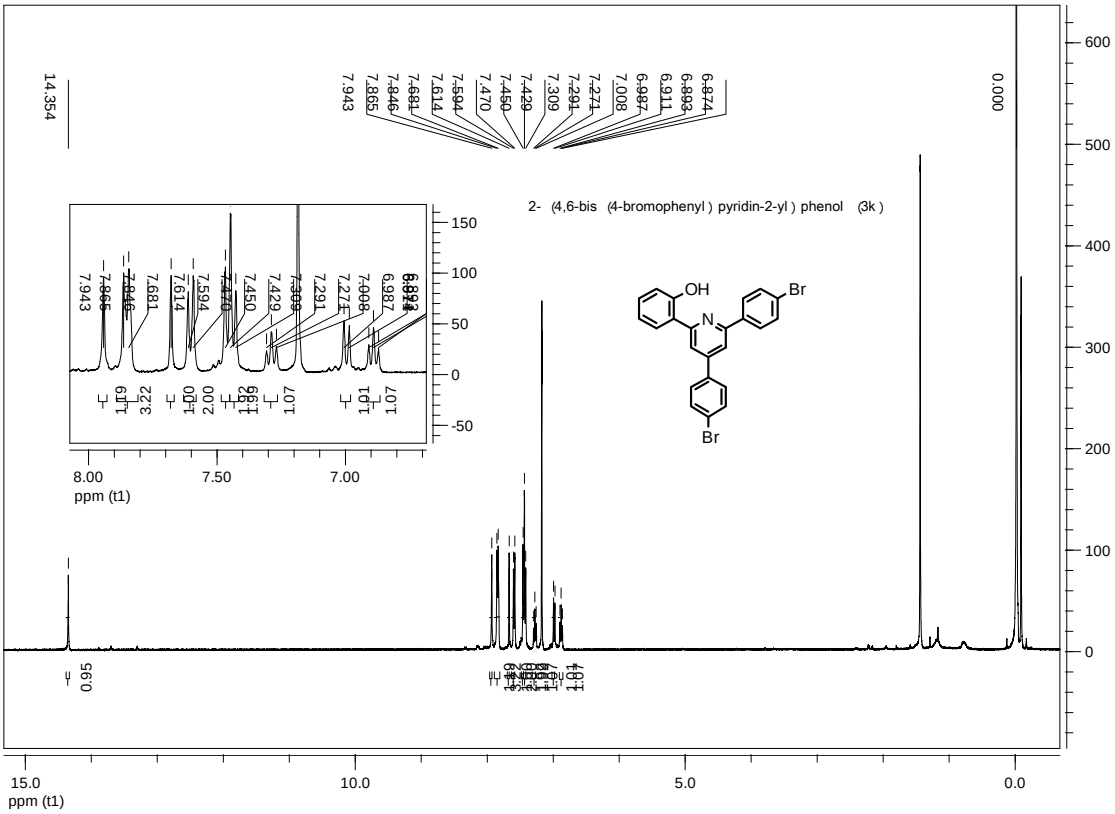
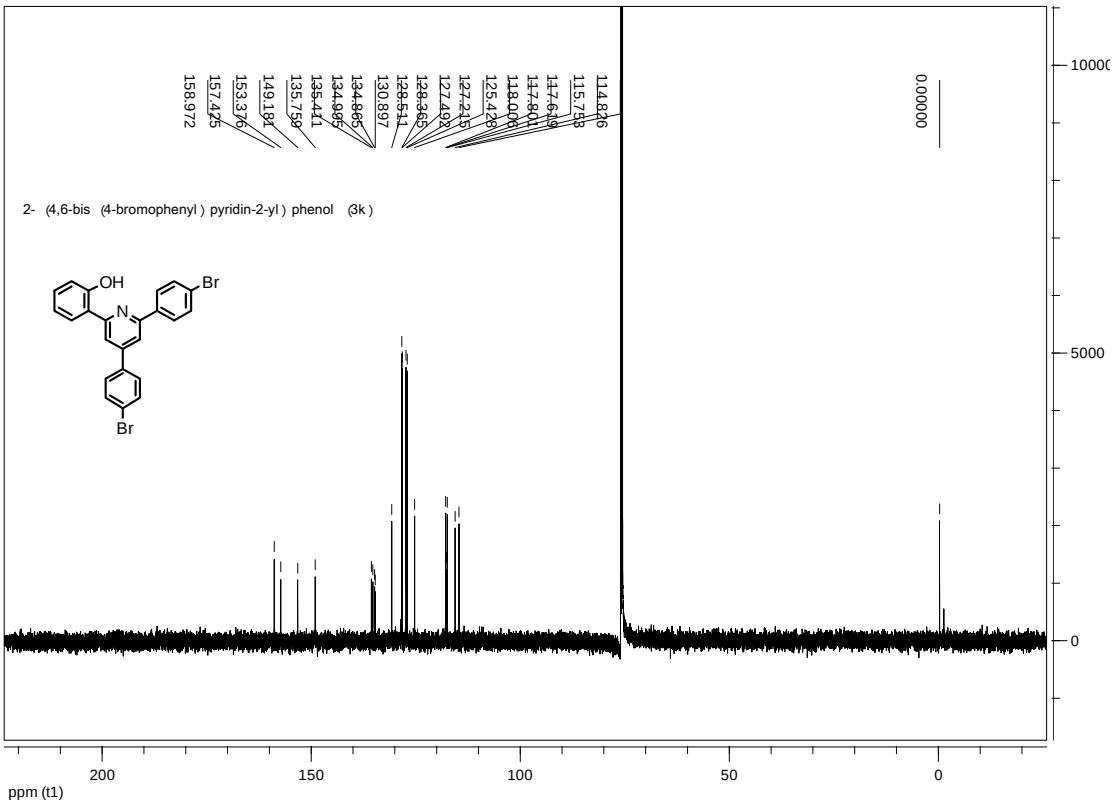
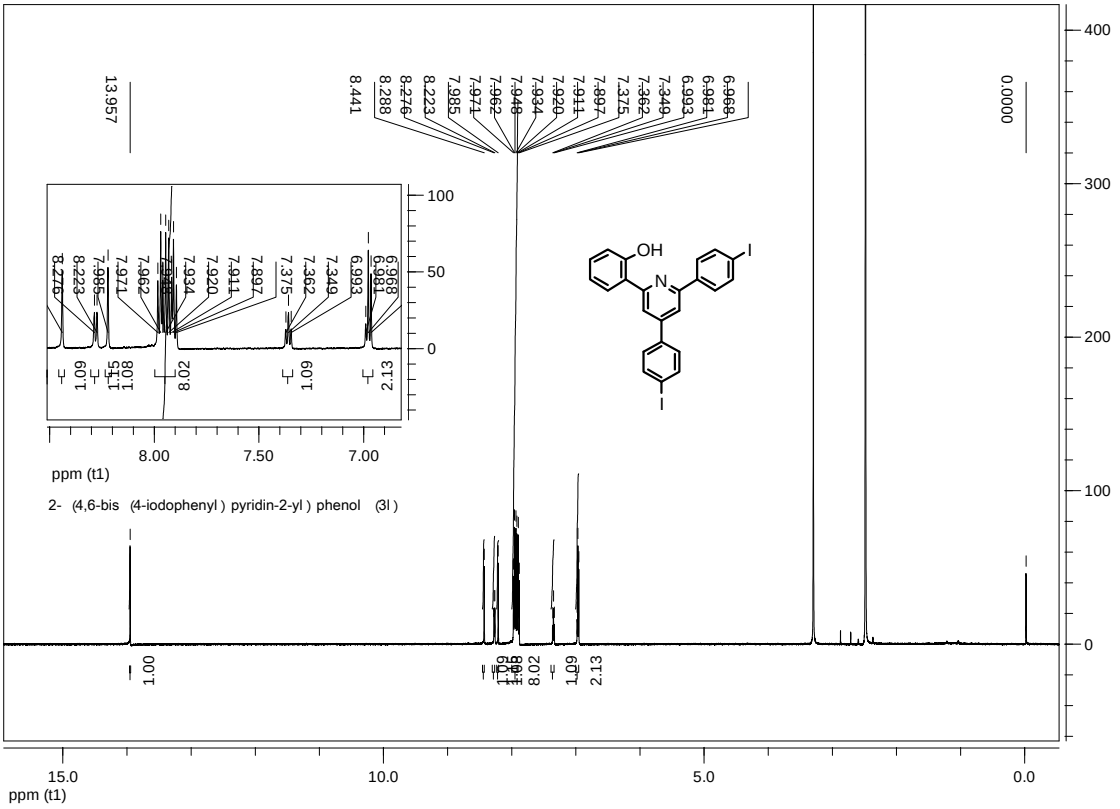
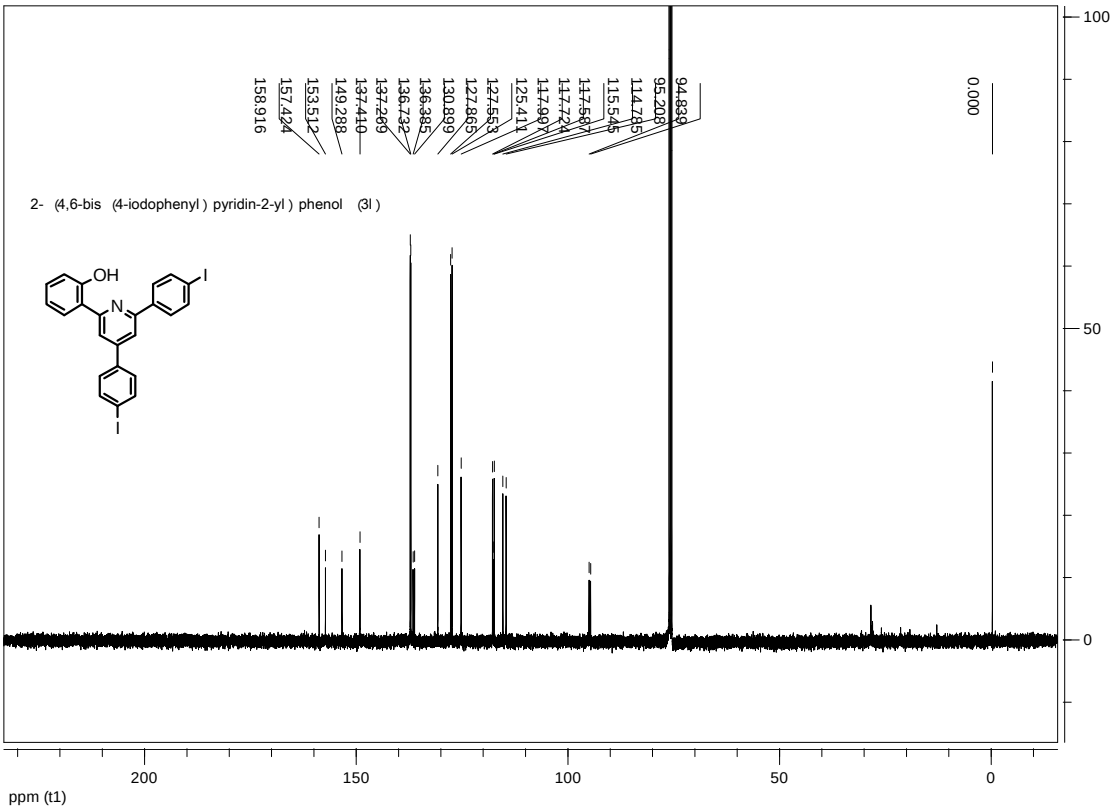


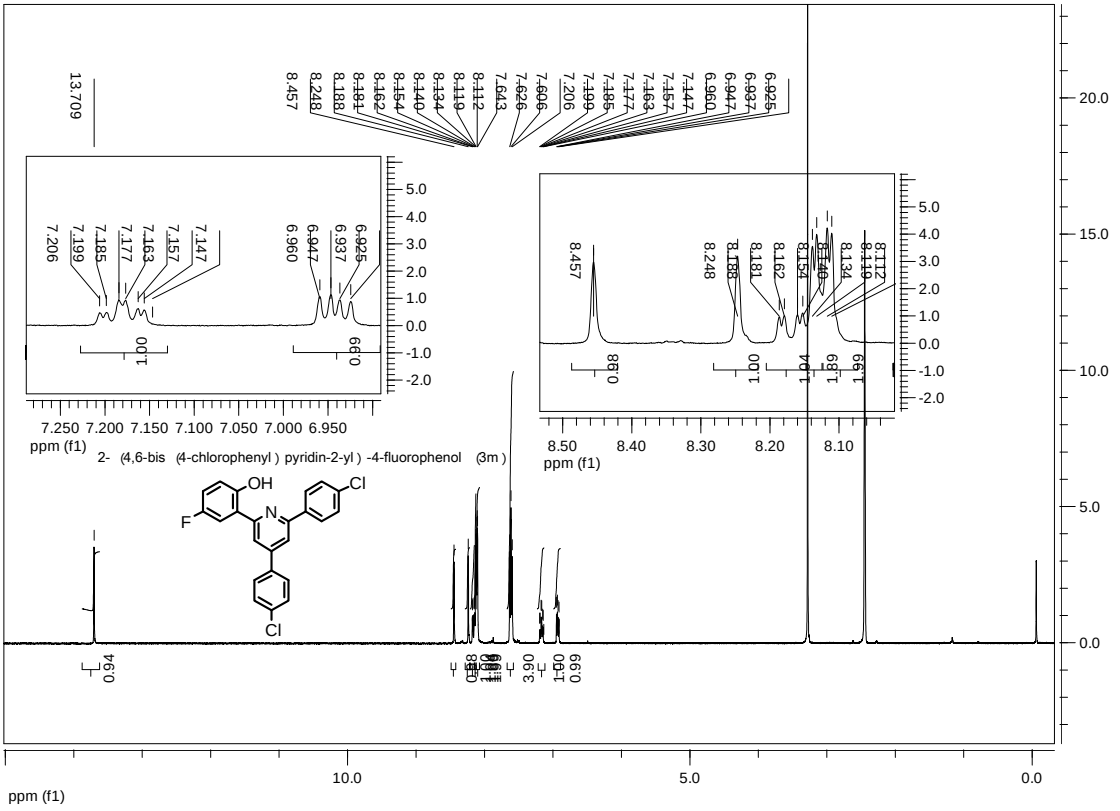


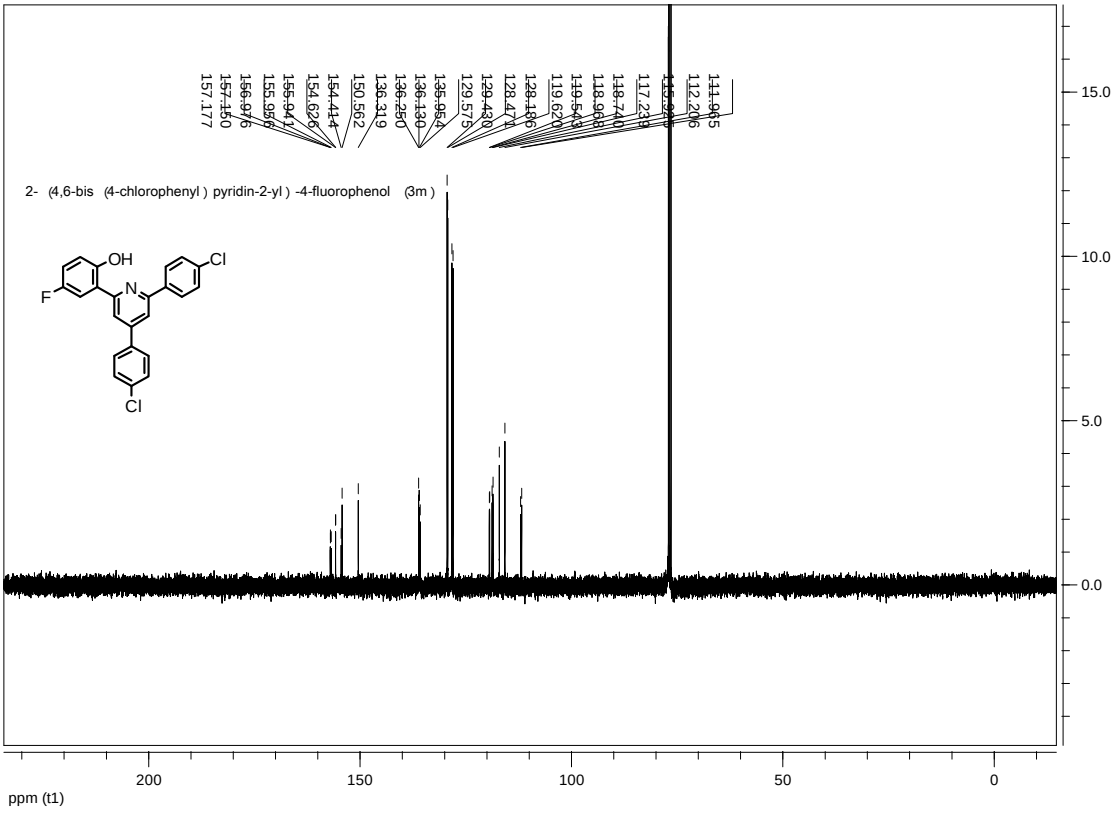
2-(4,6-bis(4-iodophenyl)pyridin-2-yl)phenol (**3l**)



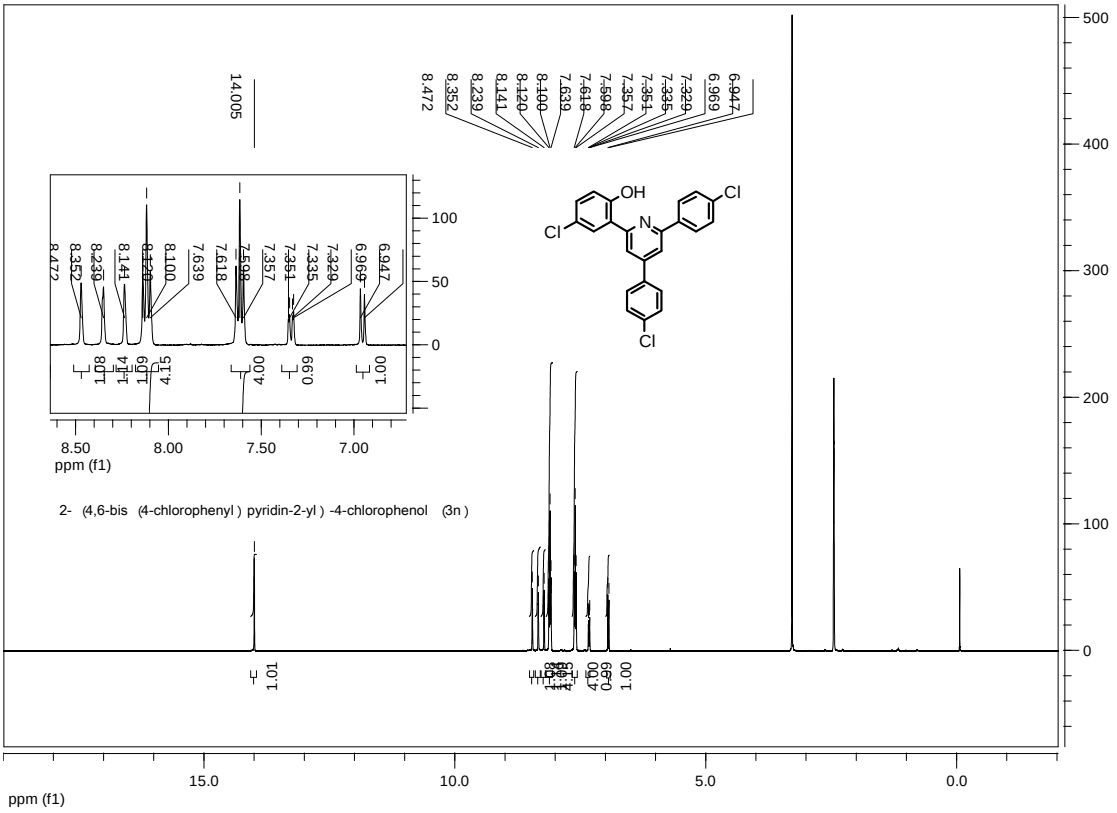


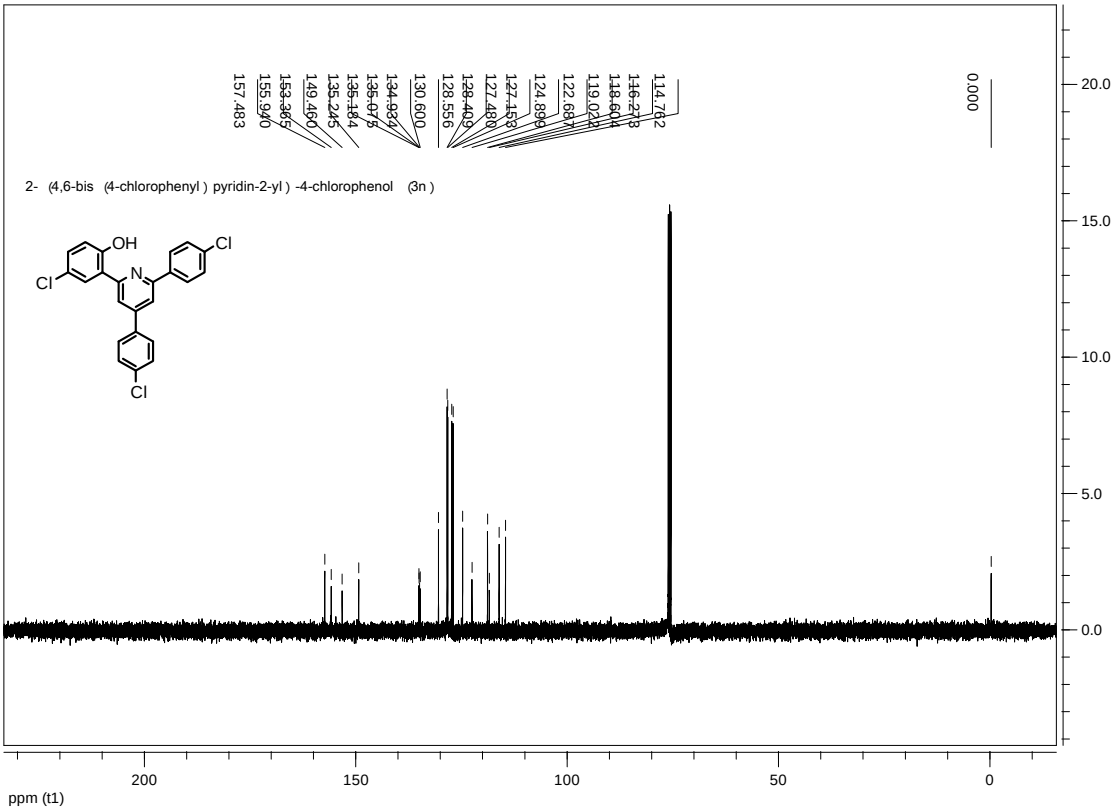
2-(4,6-bis(4-chlorophenyl)pyridin-2-yl)-4-fluorophenol (**3m**)



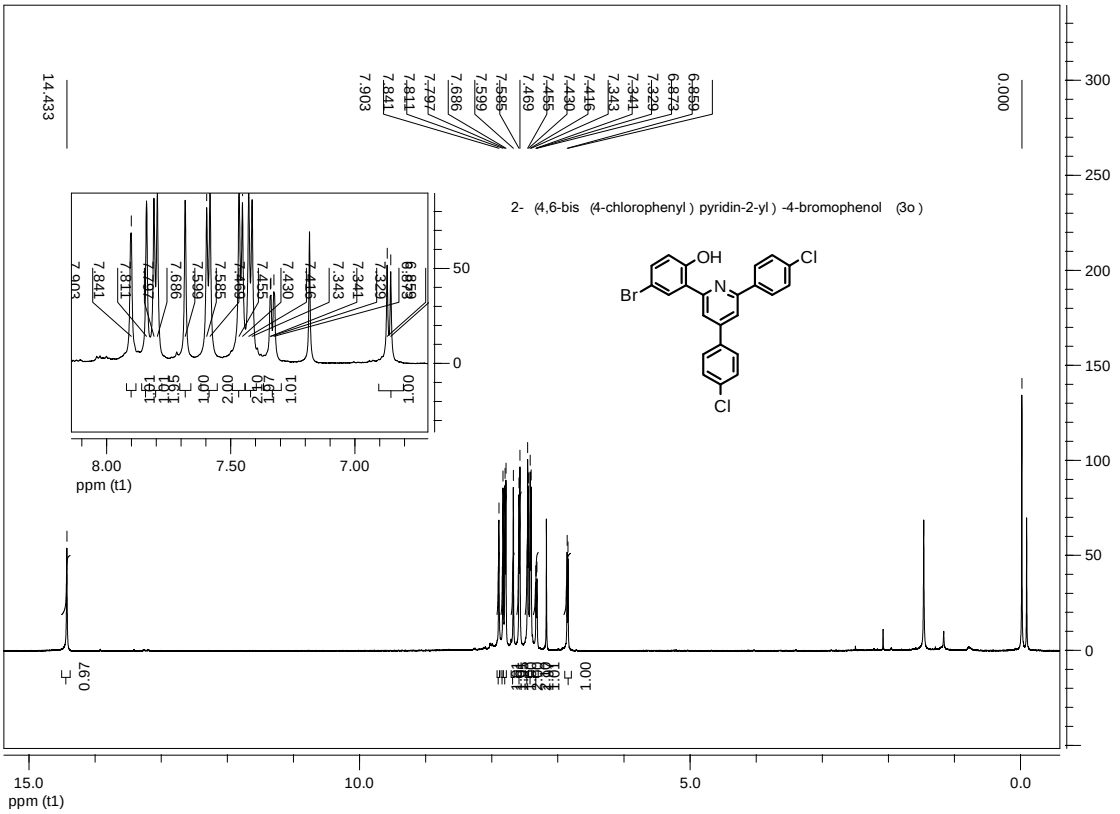


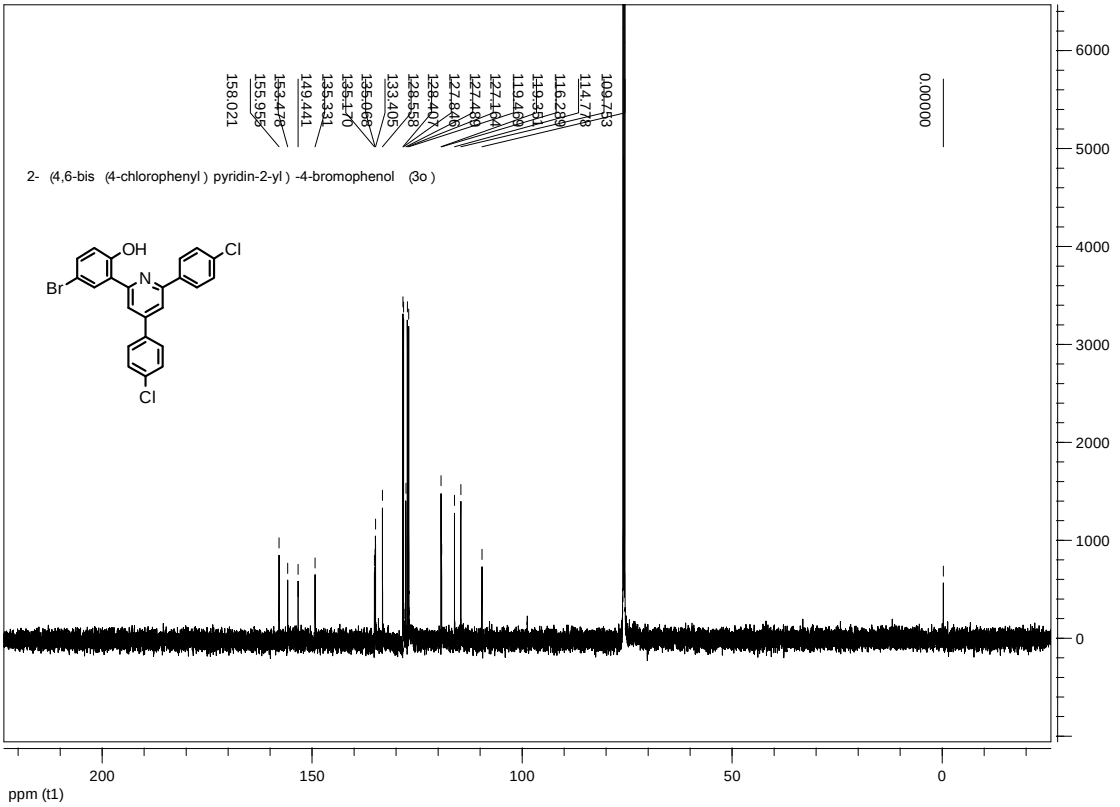
2-(4,6-bis(4-chlorophenyl)pyridin-2-yl)-4-chlorophenol (**3n**)



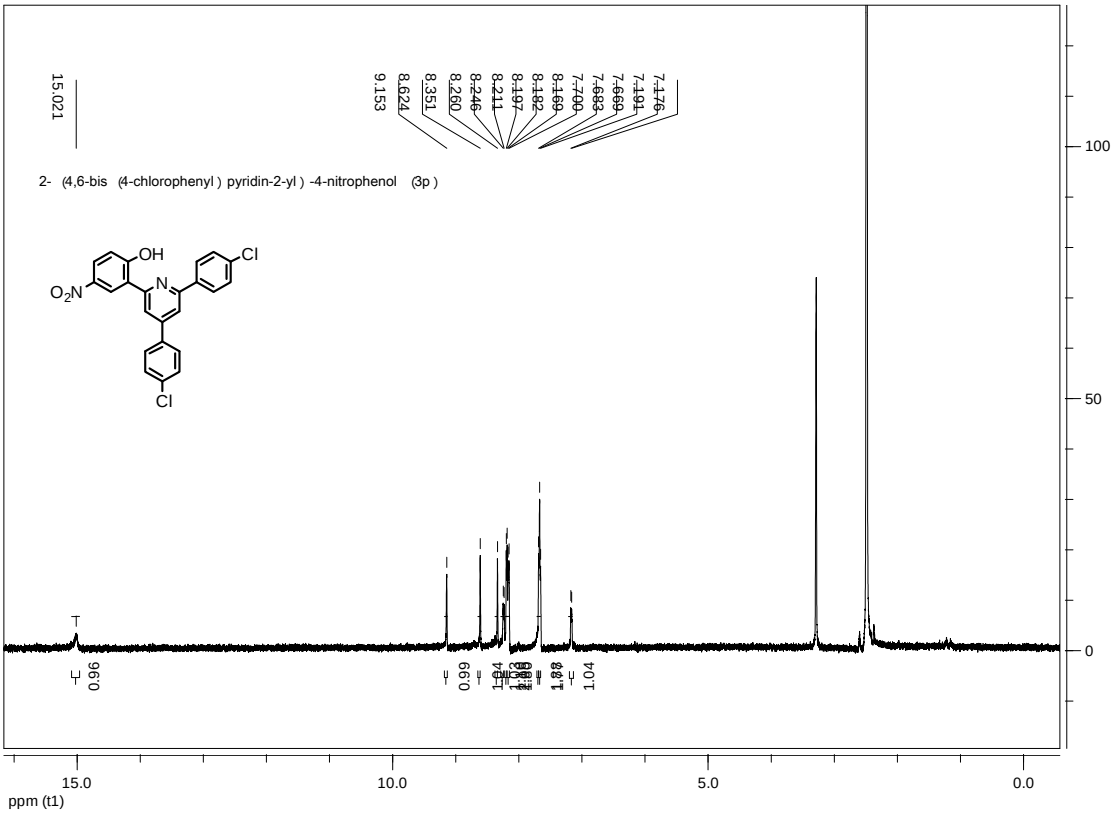


2-(4,6-bis(4-chlorophenyl)pyridin-2-yl)-4-bromophenol (**3o**)

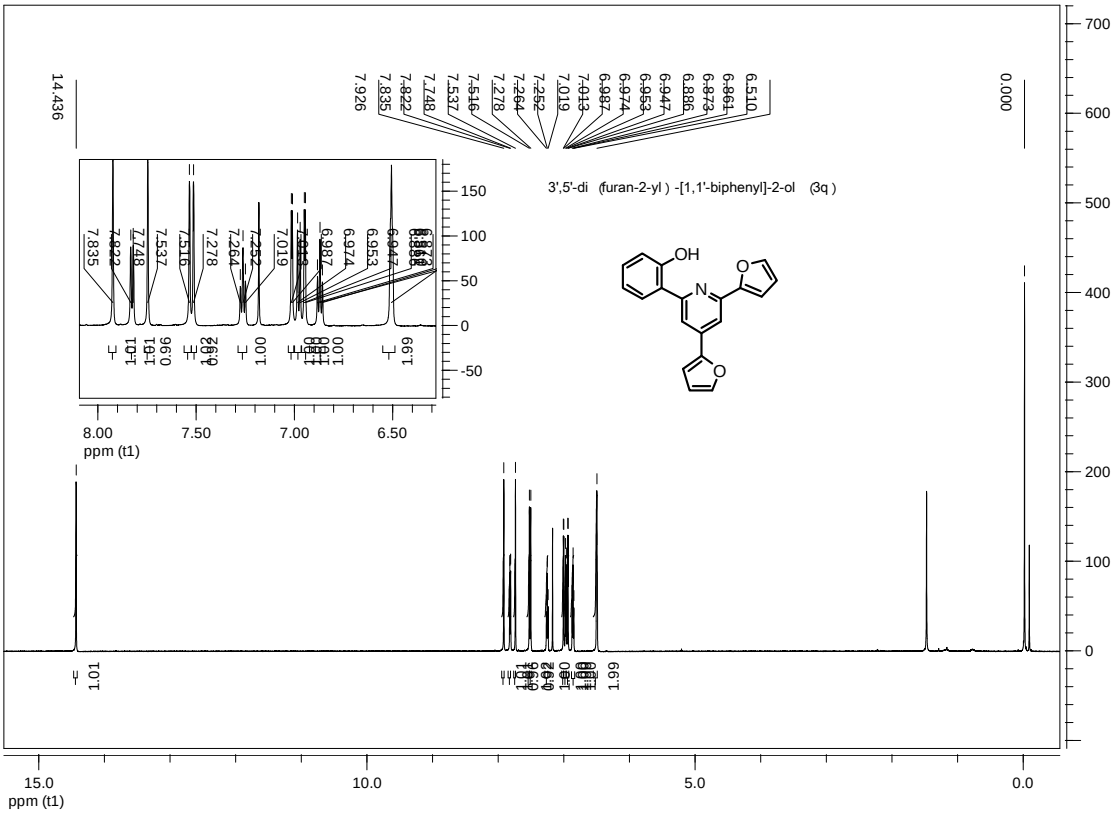


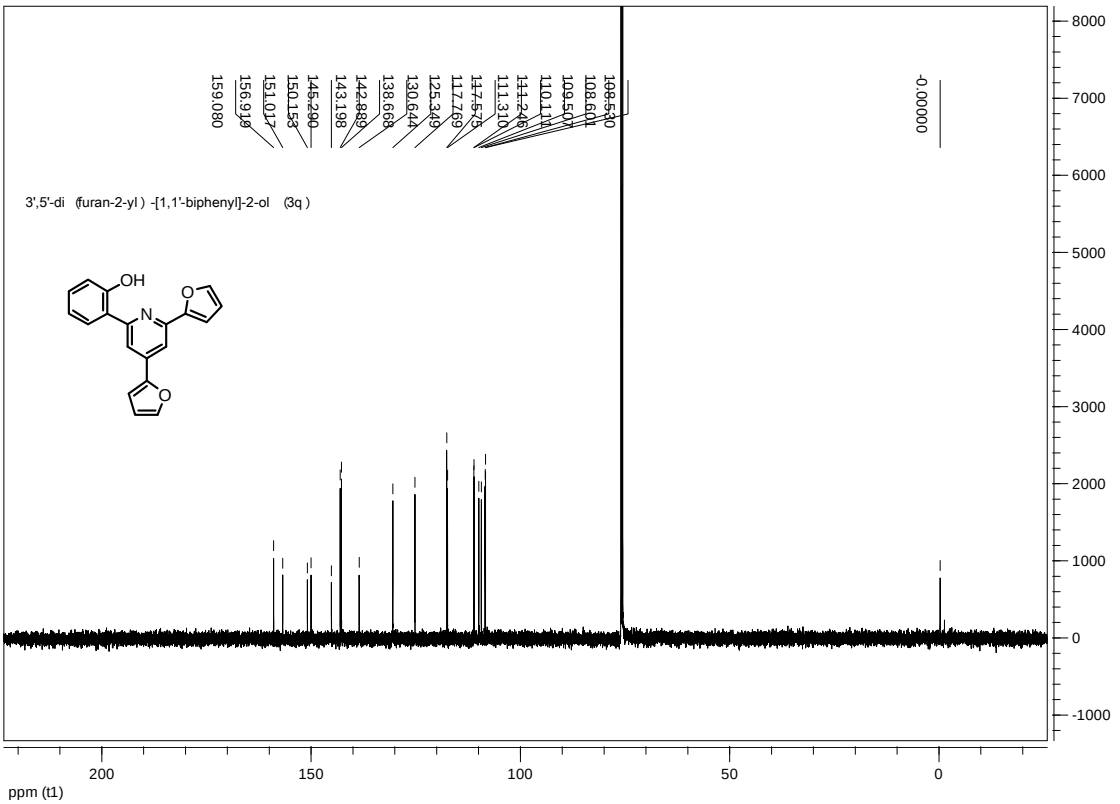


2-(4,6-bis(4-chlorophenyl)pyridin-2-yl)-4-nitrophenol (**3p**)

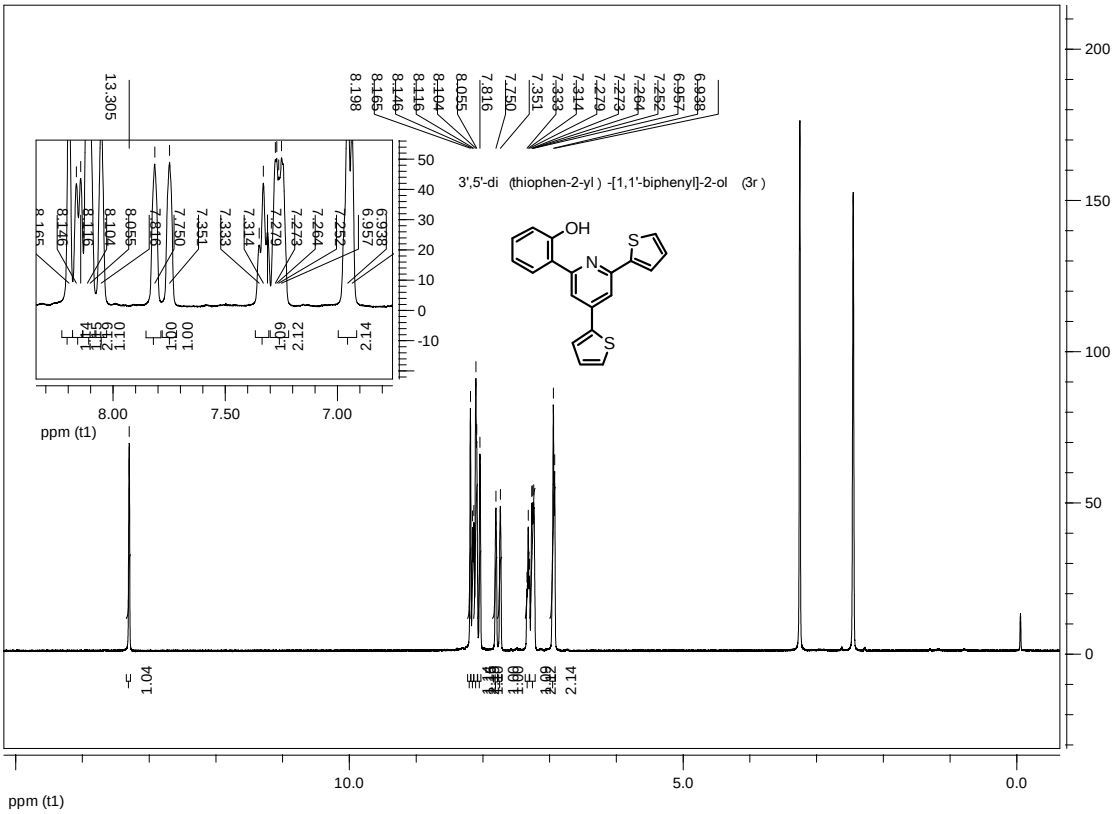


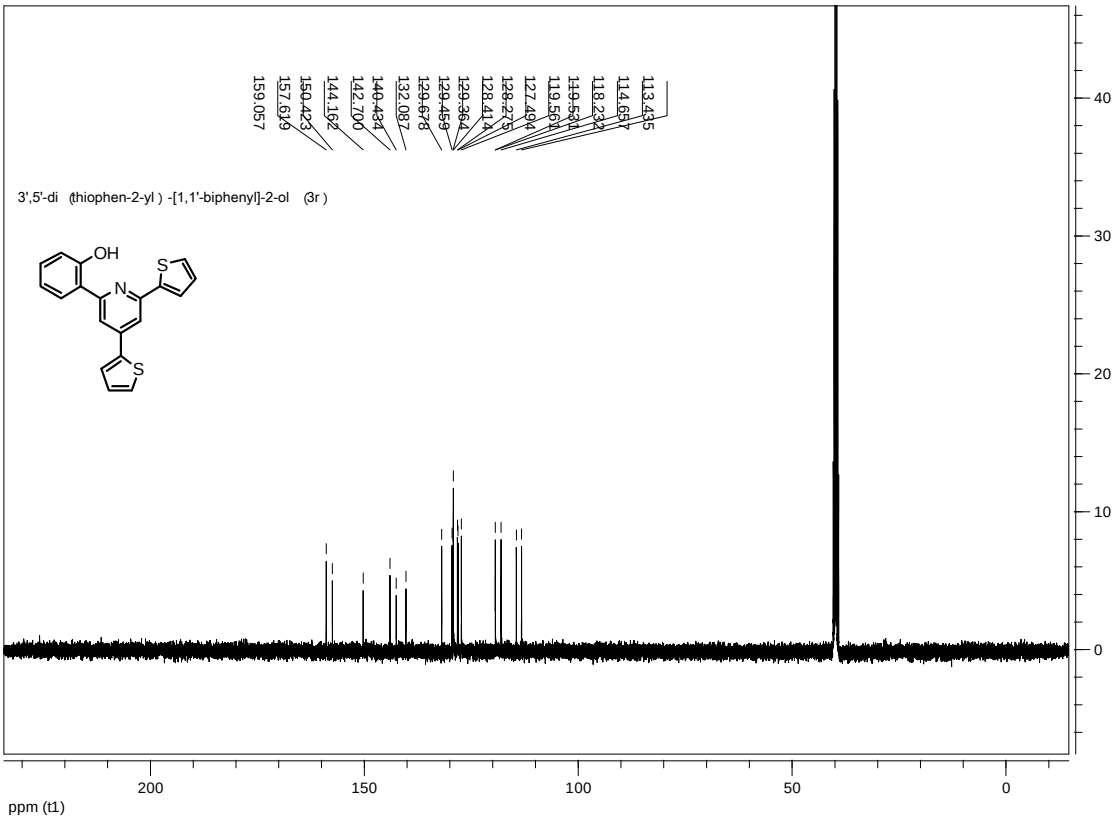
3',5'-di(furan-2-yl)-[1,1'-biphenyl]-2-ol (**3q**)



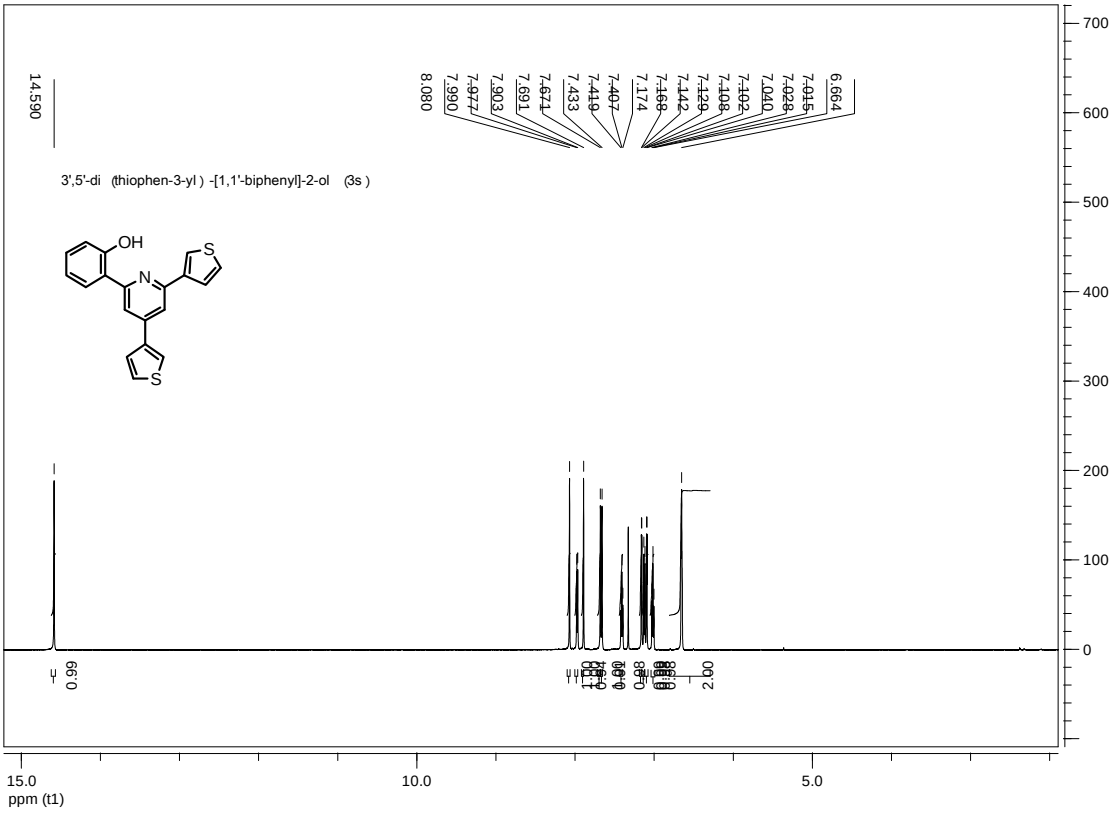


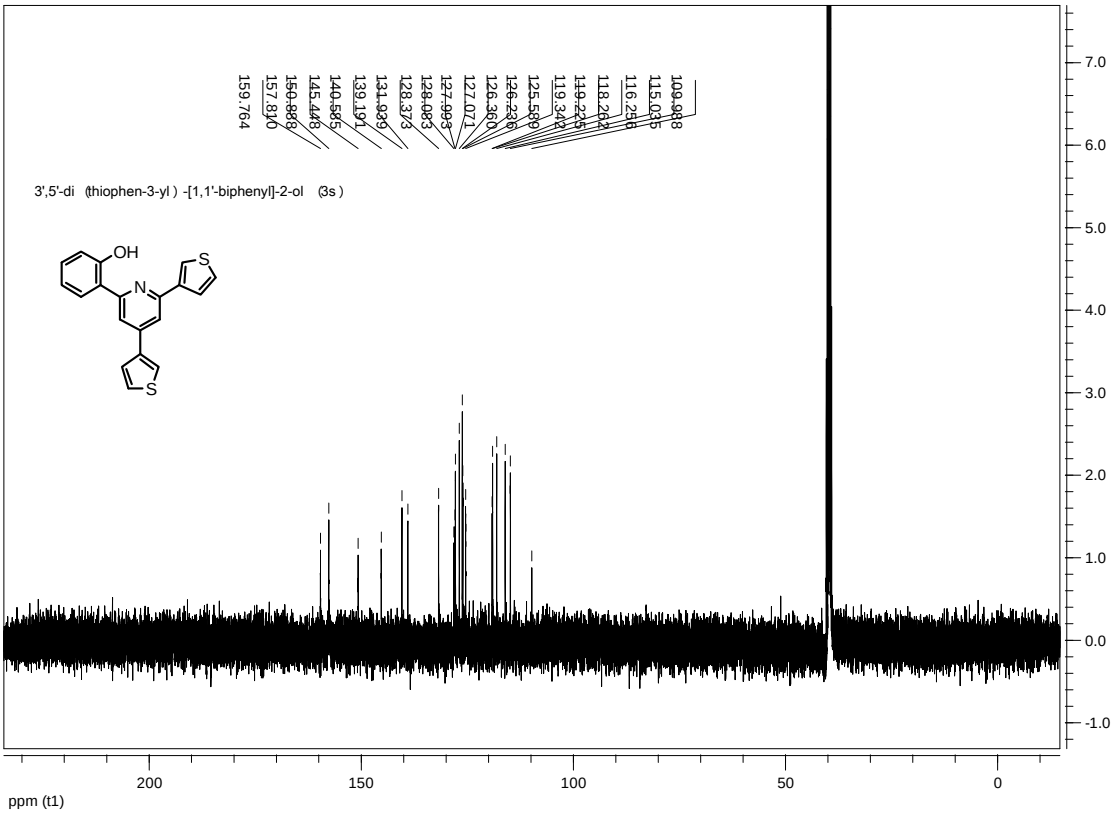
3',5'-di(thiophen-2-yl)-[1,1'-biphenyl]-2-ol (**3r**)



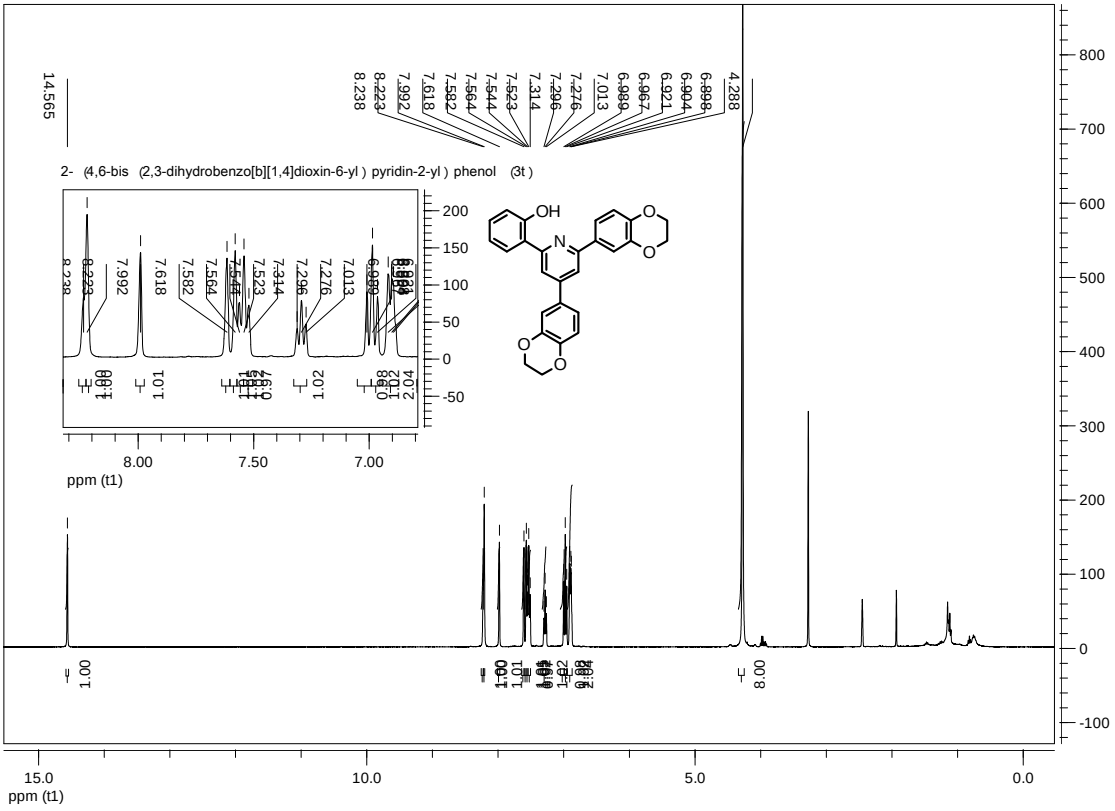


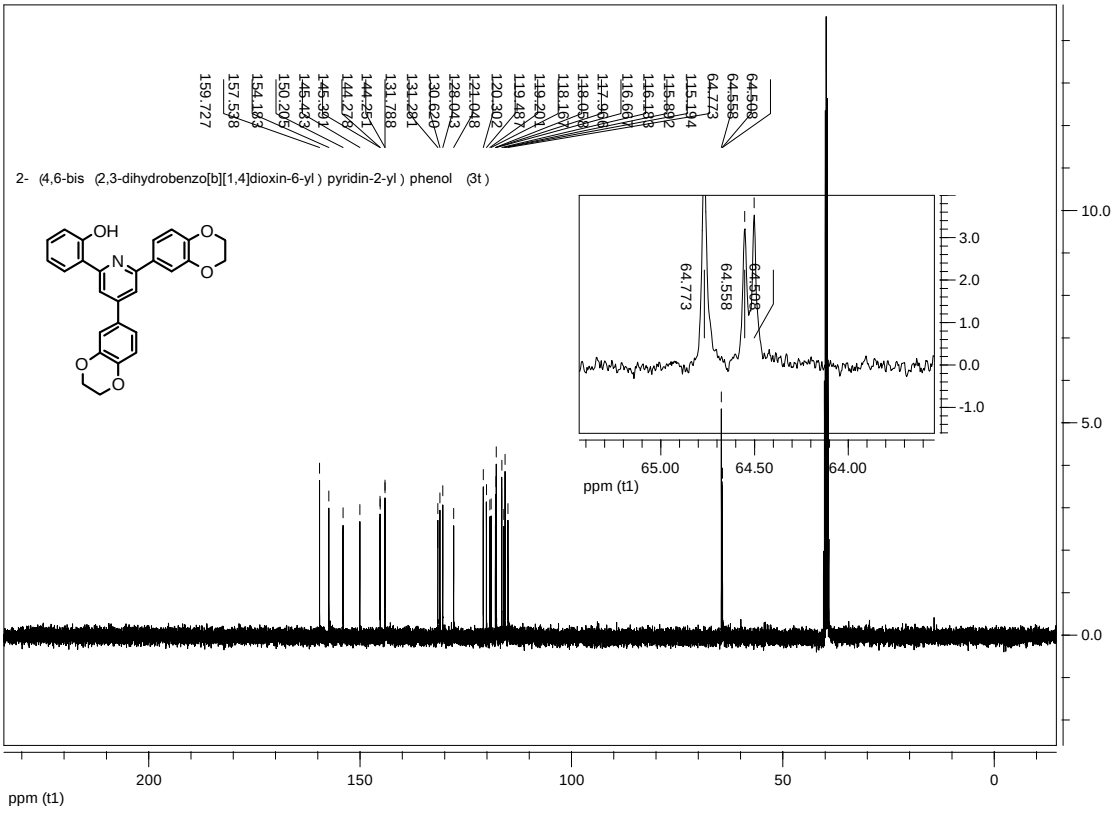
3',5'-di(thiophen-3-yl)-[1,1'-biphenyl]-2-ol (**3s**)



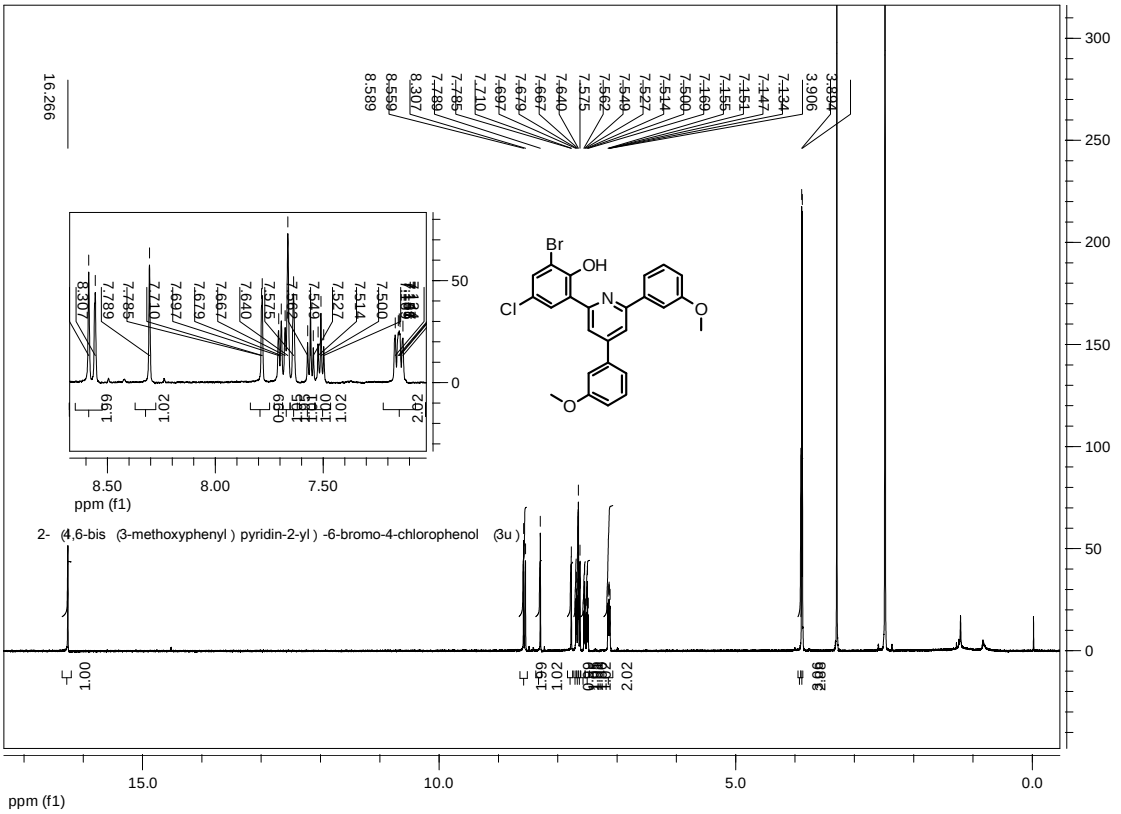


2-(4,6-bis(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)pyridin-2-yl)phenol (**3t**)





2-(4,6-bis(3-methoxyphenyl)pyridin-2-yl)-6-bromo-4-chlorophenol (**3u**)



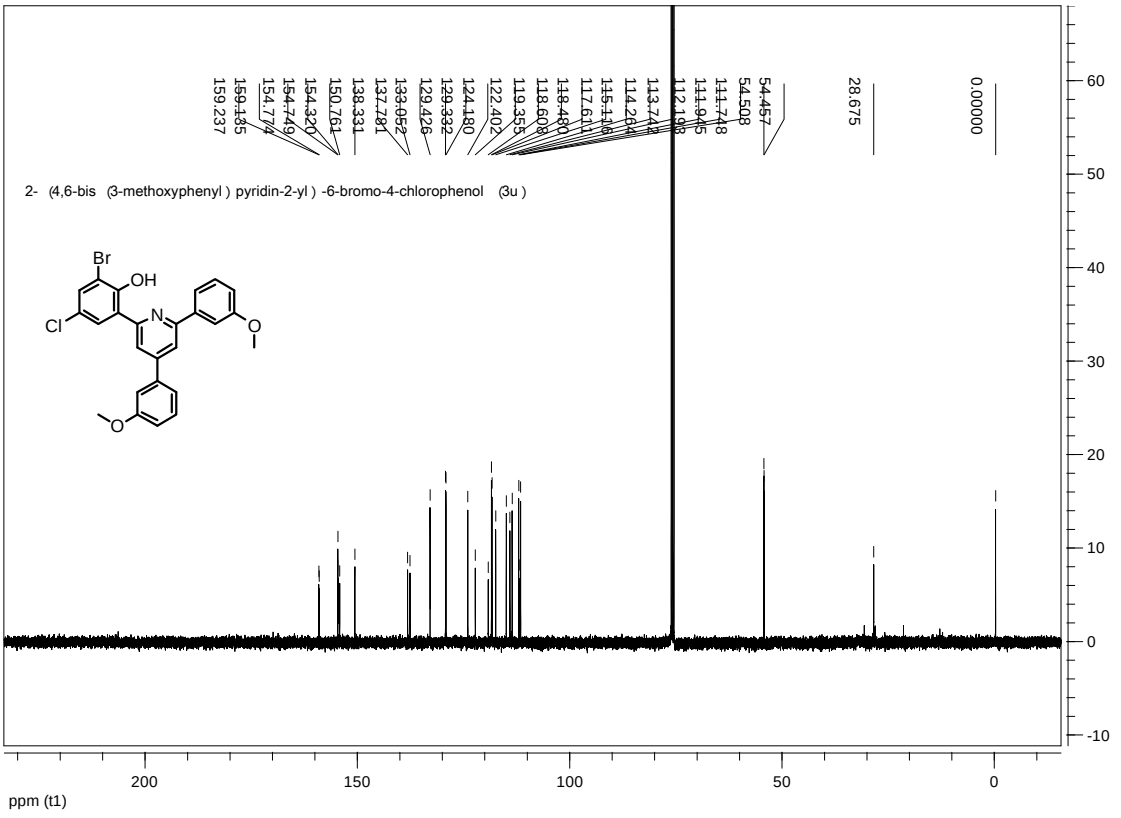


Table S1. Crystal data and structure refinement for **3b**.

Identification code	**3b**
Empirical formula	$C_{25}H_{21}NO_2$
Formula weight	367.43
Temperature	296 K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, C2/c
Unit cell dimensions	a = 21.5950(12) Å alpha = 90 deg.
	b = 11.9233(6) Å beta = 125.106(2) deg.
	c = 18.1759(9) Å gamma = 90 deg.
Volume	3828.7(3) $Å^3$
Z, Calculated density	8, 1.275 Mg/m^3
Absorption coefficient	0.080 mm^{-1}
F(000)	1552
Crystal size	0.35 x 0.33 x 0.3 mm
Theta range for data collection	2.31 to 27.49 deg.
Limiting indices	-26<=h<=28, -12<=k<=15, -23<=l<=19
Reflections collected / unique	9243 / 4389 [R(int) = 0.0207]
Completeness to theta = 27.49	96.4 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4234 / 0 / 255
Goodness-of-fit on F^2	1.038
Final R indices [I>2sigma(I)]	R1 = 0.0453, wR2 = 0.1126
R indices (all data)	R1 = 0.0677, wR2 = 0.1248
Largest diff. peak and hole	0.191 and -0.169 e.A^-3

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **3b**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N(1)	1151(1)	8219(1)	4104(1)	36(1)
O(1)	765(1)	7247(1)	5029(1)	49(1)
O(2)	809(1)	5542(1)	5941(1)	48(1)
C(2)	1781(1)	7244(1)	3566(1)	39(1)
C(6)	1514(1)	6312(1)	4606(1)	36(1)
C(4)	1385(1)	9134(1)	3121(1)	40(1)
C(7)	1153(1)	6343(1)	5051(1)	36(1)
C(1)	1484(1)	7277(1)	4077(1)	35(1)
C(8)	1182(1)	5410(1)	5541(1)	39(1)
C(18)	760(1)	10147(1)	3749(1)	36(1)
C(3)	1733(1)	8173(1)	3079(1)	37(1)
C(5)	1105(1)	9135(1)	3644(1)	36(1)
C(9)	1566(1)	4460(1)	5594(1)	46(1)
C(13)	2706(1)	7572(1)	2828(1)	45(1)
C(11)	1906(1)	5329(1)	4682(1)	44(1)
C(10)	1929(1)	4430(1)	5162(1)	49(1)
C(23)	266(1)	10051(1)	4006(1)	43(1)
C(12)	2050(1)	8161(1)	2537(1)	38(1)
C(19)	936(1)	11219(1)	3622(1)	47(1)
C(22)	-33(1)	10992(1)	4138(1)	48(1)
C(20)	635(1)	12154(1)	3751(1)	53(1)
C(21)	153(1)	12052(1)	4018(1)	49(1)
C(15)	2676(1)	8191(1)	1557(1)	52(1)
C(14)	3018(1)	7599(2)	2343(1)	52(1)
C(17)	1708(1)	8754(2)	1739(1)	52(1)
C(26)	456(1)	4998(2)	6906(1)	61(1)
C(25)	860(1)	4647(2)	6493(1)	55(1)
C(16)	2017(1)	8765(2)	1248(1)	57(1)

Table S3. Bond lengths [A] and angles [deg] for **3b**.

N(1)-C(5)	1.3436(17)
N(1)-C(1)	1.3487(17)
O(1)-C(7)	1.3522(16)
O(2)-C(8)	1.3674(16)
O(2)-C(25)	1.4251(18)
C(2)-C(3)	1.383(2)
C(2)-C(1)	1.4016(18)
C(6)-C(11)	1.4044(19)
C(6)-C(7)	1.4092(18)
C(6)-C(1)	1.4772(19)
C(4)-C(5)	1.3890(18)
C(4)-C(3)	1.396(2)
C(7)-C(8)	1.4043(19)
C(8)-C(9)	1.375(2)
C(18)-C(19)	1.390(2)
C(18)-C(23)	1.3943(19)
C(18)-C(5)	1.4881(18)
C(3)-C(12)	1.4887(17)
C(9)-C(10)	1.396(2)
C(13)-C(14)	1.385(2)
C(13)-C(12)	1.385(2)
C(11)-C(10)	1.365(2)
C(23)-C(22)	1.381(2)
C(12)-C(17)	1.385(2)
C(19)-C(20)	1.377(2)
C(22)-C(21)	1.381(2)
C(20)-C(21)	1.384(2)
C(15)-C(14)	1.368(2)
C(15)-C(16)	1.373(2)
C(17)-C(16)	1.388(2)
C(26)-C(25)	1.501(2)

C(5)-N(1)-C(1)	120.31(11)
C(8)-O(2)-C(25)	117.22(11)
C(3)-C(2)-C(1)	120.45(13)
C(11)-C(6)-C(7)	117.80(12)
C(11)-C(6)-C(1)	120.82(12)
C(7)-C(6)-C(1)	121.38(12)
C(5)-C(4)-C(3)	119.78(13)
O(1)-C(7)-C(8)	116.70(11)

O(1)-C(7)-C(6)	122.88(12)
C(8)-C(7)-C(6)	120.42(12)
N(1)-C(1)-C(2)	120.24(12)
N(1)-C(1)-C(6)	116.77(11)
C(2)-C(1)-C(6)	122.99(12)
O(2)-C(8)-C(9)	124.89(13)
O(2)-C(8)-C(7)	114.96(12)
C(9)-C(8)-C(7)	120.16(13)
C(19)-C(18)-C(23)	117.78(13)
C(19)-C(18)-C(5)	121.32(12)
C(23)-C(18)-C(5)	120.87(12)
C(2)-C(3)-C(4)	117.90(12)
C(2)-C(3)-C(12)	121.40(12)
C(4)-C(3)-C(12)	120.70(13)
N(1)-C(5)-C(4)	121.32(12)
N(1)-C(5)-C(18)	116.29(11)
C(4)-C(5)-C(18)	122.37(12)
C(8)-C(9)-C(10)	119.56(14)
C(14)-C(13)-C(12)	120.73(15)
C(10)-C(11)-C(6)	121.13(13)
C(11)-C(10)-C(9)	120.92(14)
C(22)-C(23)-C(18)	120.97(14)
C(17)-C(12)-C(13)	118.09(13)
C(17)-C(12)-C(3)	121.15(13)
C(13)-C(12)-C(3)	120.75(13)
C(20)-C(19)-C(18)	121.06(14)
C(21)-C(22)-C(23)	120.63(14)
C(19)-C(20)-C(21)	120.78(14)
C(22)-C(21)-C(20)	118.77(14)
C(14)-C(15)-C(16)	119.72(14)
C(15)-C(14)-C(13)	120.50(15)
C(12)-C(17)-C(16)	120.94(15)
O(2)-C(25)-C(26)	108.18(13)
C(15)-C(16)-C(17)	120.00(16)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters (A^2 x 10^3) for **3b**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
N(1)	44(1)	34(1)	41(1)	2(1)	30(1)	2(1)
O(1)	70(1)	39(1)	62(1)	13(1)	53(1)	16(1)
O(2)	66(1)	42(1)	56(1)	11(1)	47(1)	7(1)
C(2)	46(1)	37(1)	41(1)	-2(1)	30(1)	3(1)
C(6)	41(1)	33(1)	38(1)	-1(1)	26(1)	0(1)
C(4)	49(1)	38(1)	41(1)	6(1)	31(1)	4(1)
C(7)	44(1)	32(1)	39(1)	-1(1)	27(1)	2(1)
C(1)	40(1)	34(1)	35(1)	-2(1)	24(1)	-1(1)
C(8)	47(1)	37(1)	40(1)	1(1)	29(1)	0(1)
C(18)	41(1)	36(1)	37(1)	3(1)	25(1)	4(1)
C(3)	40(1)	43(1)	36(1)	-1(1)	26(1)	0(1)
C(5)	40(1)	36(1)	38(1)	2(1)	26(1)	1(1)
C(9)	60(1)	35(1)	49(1)	7(1)	35(1)	5(1)
C(13)	50(1)	50(1)	42(1)	1(1)	30(1)	5(1)
C(11)	55(1)	40(1)	51(1)	3(1)	39(1)	7(1)
C(10)	63(1)	36(1)	59(1)	6(1)	42(1)	13(1)
C(23)	48(1)	38(1)	55(1)	3(1)	37(1)	1(1)
C(12)	43(1)	41(1)	38(1)	-4(1)	28(1)	-3(1)
C(19)	60(1)	41(1)	61(1)	7(1)	46(1)	3(1)
C(22)	52(1)	47(1)	62(1)	3(1)	43(1)	7(1)
C(20)	69(1)	34(1)	70(1)	6(1)	49(1)	3(1)
C(21)	58(1)	40(1)	57(1)	1(1)	38(1)	10(1)
C(15)	62(1)	59(1)	58(1)	-9(1)	49(1)	-9(1)
C(14)	49(1)	60(1)	58(1)	-6(1)	38(1)	4(1)
C(17)	52(1)	66(1)	51(1)	12(1)	37(1)	12(1)
C(26)	71(1)	67(1)	65(1)	16(1)	51(1)	5(1)
C(25)	68(1)	53(1)	62(1)	19(1)	47(1)	8(1)
C(16)	67(1)	70(1)	50(1)	12(1)	43(1)	5(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **3b**.

	x	y	z	U(eq)
H(1)	791	7763	4734	73
H(2)	2018	6580	3554	46
H(4)	1340	9786	2793	48
H(9)	1583	3827	5924	55
H(13)	2945	7146	3367	54
H(11)	2159	5290	4394	53
H(10)	2197	3774	5202	58
H(23)	132	9328	4091	52
H(19)	1269	11308	3444	57
H(22)	-368	10908	4313	58
H(20)	760	12879	3655	64
H(21)	-47	12699	4116	59
H(15)	2892	8207	1227	62
H(14)	3474	7202	2557	62
H(17)	1255	9159	1524	63
H(26A)	706	5659	7286	91
H(26B)	470	4383	7273	91
H(26C)	-71	5180	6429	91
H(25A)	1398	4482	6970	66
H(25B)	624	3962	6127	66
H(16)	1773	9169	698	68

Table S6. Torsion angles [deg] for **3b**.

C(11)-C(6)-C(7)-O(1)	179.52(13)
C(1)-C(6)-C(7)-O(1)	-0.4(2)
C(11)-C(6)-C(7)-C(8)	-0.8(2)
C(1)-C(6)-C(7)-C(8)	179.22(13)
C(5)-N(1)-C(1)-C(2)	-0.2(2)
C(5)-N(1)-C(1)-C(6)	179.63(12)
C(3)-C(2)-C(1)-N(1)	-0.5(2)
C(3)-C(2)-C(1)-C(6)	179.65(13)
C(11)-C(6)-C(1)-N(1)	-174.44(13)
C(7)-C(6)-C(1)-N(1)	5.5(2)
C(11)-C(6)-C(1)-C(2)	5.4(2)
C(7)-C(6)-C(1)-C(2)	-174.63(14)
C(25)-O(2)-C(8)-C(9)	3.6(2)
C(25)-O(2)-C(8)-C(7)	-176.17(14)
O(1)-C(7)-C(8)-O(2)	-0.2(2)
C(6)-C(7)-C(8)-O(2)	-179.87(13)
O(1)-C(7)-C(8)-C(9)	179.99(14)
C(6)-C(7)-C(8)-C(9)	0.3(2)
C(1)-C(2)-C(3)-C(4)	0.5(2)
C(1)-C(2)-C(3)-C(12)	179.57(13)
C(5)-C(4)-C(3)-C(2)	0.3(2)
C(5)-C(4)-C(3)-C(12)	-178.83(13)
C(1)-N(1)-C(5)-C(4)	1.0(2)
C(1)-N(1)-C(5)-C(18)	-177.37(12)
C(3)-C(4)-C(5)-N(1)	-1.0(2)
C(3)-C(4)-C(5)-C(18)	177.23(13)
C(19)-C(18)-C(5)-N(1)	154.41(14)
C(23)-C(18)-C(5)-N(1)	-23.55(19)
C(19)-C(18)-C(5)-C(4)	-23.9(2)
C(23)-C(18)-C(5)-C(4)	158.10(14)
O(2)-C(8)-C(9)-C(10)	-179.51(14)
C(7)-C(8)-C(9)-C(10)	0.3(2)
C(7)-C(6)-C(11)-C(10)	0.7(2)
C(1)-C(6)-C(11)-C(10)	-179.30(15)
C(6)-C(11)-C(10)-C(9)	-0.1(3)
C(8)-C(9)-C(10)-C(11)	-0.4(3)
C(19)-C(18)-C(23)-C(22)	-0.6(2)
C(5)-C(18)-C(23)-C(22)	177.43(14)
C(14)-C(13)-C(12)-C(17)	1.3(2)
C(14)-C(13)-C(12)-C(3)	-177.32(14)

C(2)-C(3)-C(12)-C(17)	146.34(15)
C(4)-C(3)-C(12)-C(17)	-34.6(2)
C(2)-C(3)-C(12)-C(13)	-35.1(2)
C(4)-C(3)-C(12)-C(13)	144.04(15)
C(23)-C(18)-C(19)-C(20)	0.3(2)
C(5)-C(18)-C(19)-C(20)	-177.70(15)
C(18)-C(23)-C(22)-C(21)	0.0(2)
C(18)-C(19)-C(20)-C(21)	0.6(3)
C(23)-C(22)-C(21)-C(20)	0.9(3)
C(19)-C(20)-C(21)-C(22)	-1.2(3)
C(16)-C(15)-C(14)-C(13)	0.0(3)
C(12)-C(13)-C(14)-C(15)	-1.1(3)
C(13)-C(12)-C(17)-C(16)	-0.4(2)
C(3)-C(12)-C(17)-C(16)	178.22(16)
C(8)-O(2)-C(25)-C(26)	176.43(14)
C(14)-C(15)-C(16)-C(17)	0.9(3)
C(12)-C(17)-C(16)-C(15)	-0.7(3)

Symmetry transformations used to generate equivalent atoms:

Table S7. Hydrogen bonds for **3b** [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...N(1)	0.84	1.80	2.5465(14)	147.3

Symmetry transformations used to generate equivalent atoms:

Table S8. Crystal data and structure refinement for **3d**.

Identification code	**3d**
Empirical formula	C_{23} H_{17} N O
Formula weight	323.38
Temperature	296 K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 8.7224(7) A alpha = 90 deg. b = 20.6209(19) A beta = 108.261(3) deg. c = 9.7045(10) A gamma = 90 deg.
Volume	1657.6(3) A^3
Z, Calculated density	4, 1.296 Mg/m^3
Absorption coefficient	0.079 mm^-1
F(000)	680
Crystal size	0.35 x 0.33 x 0.3 mm
Theta range for data collection	1.98 to 27.52 deg.
Limiting indices	-8<=h<=11, -25<=k<=26, -12<=l<=10
Reflections collected / unique	17754 / 3818 [R(int) = 0.0431]
Completeness to theta = 27.52	98.5 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3765 / 0 / 227
Goodness-of-fit on F^2	1.041
Final R indices [I>2sigma(I)]	R1 = 0.0649, wR2 = 0.1946
R indices (all data)	R1 = 0.1070, wR2 = 0.2235
Largest diff. peak and hole	0.708 and -0.331 e.A^-3

Table S9. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **3d**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N(1)	4703(2)	7030(1)	9815(2)	40(1)
C(2)	4792(2)	8183(1)	9889(2)	41(1)
C(4)	6571(3)	7597(1)	8930(2)	41(1)
C(5)	5909(2)	7026(1)	9220(2)	38(1)
C(1)	4129(2)	7598(1)	10133(2)	38(1)
C(3)	6025(2)	8190(1)	9270(2)	38(1)
C(6)	2811(3)	7564(1)	10787(2)	40(1)
O(1)	3010(3)	6402(1)	11086(3)	80(1)
C(18)	6517(2)	6381(1)	8955(2)	39(1)
C(7)	2342(3)	6975(1)	11253(3)	46(1)
C(12)	6755(2)	8811(1)	9006(2)	38(1)
C(19)	8112(3)	6301(1)	8978(2)	45(1)
C(17)	7395(3)	8873(1)	7868(3)	46(1)
C(9)	356(3)	7513(1)	12059(3)	66(1)
C(23)	5527(3)	5833(1)	8735(3)	49(1)
C(20)	8696(3)	5694(1)	8798(3)	52(1)
C(8)	1132(3)	6964(1)	11905(3)	58(1)
C(10)	752(3)	8100(1)	11570(4)	69(1)
C(22)	6124(3)	5229(1)	8544(3)	56(1)
C(13)	6830(3)	9342(1)	9898(3)	50(1)
C(14)	7546(3)	9909(1)	9675(3)	59(1)
C(21)	7709(3)	5159(1)	8590(3)	55(1)
C(11)	1972(3)	8117(1)	10951(3)	59(1)
C(15)	8181(3)	9965(1)	8548(3)	59(1)
C(16)	8094(3)	9448(1)	7645(3)	54(1)

Table S10. Bond lengths [A] and angles [deg] for **3d**.

N(1)-C(1)	1.346(3)
N(1)-C(5)	1.349(2)
C(2)-C(3)	1.387(3)
C(2)-C(1)	1.389(3)
C(4)-C(5)	1.379(3)
C(4)-C(3)	1.388(3)
C(5)-C(18)	1.485(3)
C(1)-C(6)	1.478(3)
C(3)-C(12)	1.487(3)
C(6)-C(11)	1.391(3)
C(6)-C(7)	1.402(3)
O(1)-C(7)	1.349(3)
C(18)-C(19)	1.394(3)
C(18)-C(23)	1.397(3)
C(7)-C(8)	1.390(3)
C(12)-C(13)	1.386(3)
C(12)-C(17)	1.390(3)
C(19)-C(20)	1.383(3)
C(17)-C(16)	1.382(3)
C(9)-C(8)	1.352(4)
C(9)-C(10)	1.382(4)
C(23)-C(22)	1.385(3)
C(20)-C(21)	1.374(3)
C(10)-C(11)	1.377(3)
C(22)-C(21)	1.376(4)
C(13)-C(14)	1.376(3)
C(14)-C(15)	1.377(4)
C(15)-C(16)	1.367(4)

C(1)-N(1)-C(5)	119.94(17)
C(3)-C(2)-C(1)	120.25(18)
C(5)-C(4)-C(3)	120.39(18)
N(1)-C(5)-C(4)	121.02(18)
N(1)-C(5)-C(18)	116.63(17)
C(4)-C(5)-C(18)	122.31(17)
N(1)-C(1)-C(2)	120.74(18)
N(1)-C(1)-C(6)	116.94(17)
C(2)-C(1)-C(6)	122.30(18)
C(2)-C(3)-C(4)	117.63(18)

C(2)-C(3)-C(12)	121.09(18)
C(4)-C(3)-C(12)	121.26(17)
C(11)-C(6)-C(7)	117.15(19)
C(11)-C(6)-C(1)	121.25(19)
C(7)-C(6)-C(1)	121.60(18)
C(19)-C(18)-C(23)	118.21(19)
C(19)-C(18)-C(5)	120.80(18)
C(23)-C(18)-C(5)	120.93(18)
O(1)-C(7)-C(8)	117.3(2)
O(1)-C(7)-C(6)	122.63(18)
C(8)-C(7)-C(6)	120.0(2)
C(13)-C(12)-C(17)	118.15(19)
C(13)-C(12)-C(3)	120.74(18)
C(17)-C(12)-C(3)	121.11(18)
C(20)-C(19)-C(18)	120.7(2)
C(16)-C(17)-C(12)	120.7(2)
C(8)-C(9)-C(10)	120.5(2)
C(22)-C(23)-C(18)	120.5(2)
C(21)-C(20)-C(19)	120.4(2)
C(9)-C(8)-C(7)	121.0(2)
C(11)-C(10)-C(9)	118.9(2)
C(21)-C(22)-C(23)	120.4(2)
C(14)-C(13)-C(12)	120.6(2)
C(13)-C(14)-C(15)	120.8(2)
C(20)-C(21)-C(22)	119.8(2)
C(10)-C(11)-C(6)	122.4(2)
C(16)-C(15)-C(14)	119.3(2)
C(15)-C(16)-C(17)	120.5(2)

Symmetry transformations used to generate equivalent atoms:

Table S11. Anisotropic displacement parameters (A^2 x 10^3) for **3d**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
N(1)	40(1)	42(1)	44(1)	2(1)	20(1)	2(1)
C(2)	41(1)	40(1)	48(1)	0(1)	21(1)	4(1)
C(4)	40(1)	44(1)	44(1)	2(1)	21(1)	2(1)
C(5)	38(1)	41(1)	38(1)	1(1)	17(1)	1(1)
C(1)	35(1)	43(1)	38(1)	3(1)	15(1)	3(1)
C(3)	38(1)	40(1)	36(1)	1(1)	14(1)	0(1)
C(6)	37(1)	47(1)	41(1)	-1(1)	18(1)	-1(1)
O(1)	92(2)	53(1)	122(2)	5(1)	69(1)	-4(1)
C(18)	45(1)	41(1)	36(1)	3(1)	18(1)	2(1)
C(7)	41(1)	50(1)	51(1)	-5(1)	21(1)	-5(1)
C(12)	35(1)	39(1)	41(1)	3(1)	13(1)	1(1)
C(19)	47(1)	43(1)	50(1)	2(1)	24(1)	3(1)
C(17)	50(1)	44(1)	49(1)	-1(1)	25(1)	-2(1)
C(9)	50(2)	83(2)	79(2)	-20(2)	43(2)	-13(1)
C(23)	49(1)	43(1)	59(2)	0(1)	22(1)	-2(1)
C(20)	55(1)	52(1)	55(1)	4(1)	27(1)	12(1)
C(8)	55(1)	64(2)	66(2)	-6(1)	36(1)	-17(1)
C(10)	63(2)	66(2)	98(2)	-12(2)	53(2)	5(1)
C(22)	66(2)	44(1)	58(2)	-2(1)	20(1)	-7(1)
C(13)	58(1)	49(1)	48(1)	-2(1)	24(1)	-1(1)
C(14)	72(2)	41(1)	67(2)	-10(1)	25(1)	-8(1)
C(21)	75(2)	43(1)	52(2)	4(1)	26(1)	12(1)
C(11)	58(2)	51(1)	84(2)	0(1)	44(1)	3(1)
C(15)	59(2)	46(1)	73(2)	5(1)	22(1)	-12(1)
C(16)	55(1)	55(1)	60(2)	9(1)	30(1)	-3(1)

Table S12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **3d**.

	x	y	z	U(eq)
H(2)	4398	8579	10147	49
H(4)	7406	7585	8494	49
H(1)	3661	6459	10617	120
H(19)	8804	6667	9118	54
H(17)	7350	8516	7237	55
H(9)	-468	7496	12508	79
H(23)	4436	5875	8716	59
H(20)	9786	5646	8818	62
H(8)	846	6565	12247	69
H(10)	192	8485	11660	83
H(22)	5436	4860	8380	67
H(13)	6381	9314	10671	60
H(14)	7604	10267	10306	71
H(21)	8120	4742	8479	66
H(11)	2251	8521	10624	71
H(15)	8674	10358	8400	71
H(16)	8518	9485	6858	65

Table S13. Torsion angles [deg] for **3d**.

C(1)-N(1)-C(5)-C(4)	0.0(3)
C(1)-N(1)-C(5)-C(18)	177.67(18)
C(3)-C(4)-C(5)-N(1)	1.2(3)
C(3)-C(4)-C(5)-C(18)	-176.36(19)
C(5)-N(1)-C(1)-C(2)	-1.6(3)
C(5)-N(1)-C(1)-C(6)	-179.84(18)
C(3)-C(2)-C(1)-N(1)	2.0(3)
C(3)-C(2)-C(1)-C(6)	-179.86(19)
C(1)-C(2)-C(3)-C(4)	-0.8(3)
C(1)-C(2)-C(3)-C(12)	-179.72(19)
C(5)-C(4)-C(3)-C(2)	-0.7(3)
C(5)-C(4)-C(3)-C(12)	178.2(2)
N(1)-C(1)-C(6)-C(11)	-170.1(2)
C(2)-C(1)-C(6)-C(11)	11.7(4)
N(1)-C(1)-C(6)-C(7)	9.2(3)
C(2)-C(1)-C(6)-C(7)	-169.0(2)
N(1)-C(5)-C(18)-C(19)	-151.1(2)
C(4)-C(5)-C(18)-C(19)	26.5(3)
N(1)-C(5)-C(18)-C(23)	26.3(3)
C(4)-C(5)-C(18)-C(23)	-156.1(2)
C(11)-C(6)-C(7)-O(1)	176.7(2)
C(1)-C(6)-C(7)-O(1)	-2.7(4)
C(11)-C(6)-C(7)-C(8)	-2.7(4)
C(1)-C(6)-C(7)-C(8)	178.0(2)
C(2)-C(3)-C(12)-C(13)	30.3(3)
C(4)-C(3)-C(12)-C(13)	-148.6(2)
C(2)-C(3)-C(12)-C(17)	-150.3(2)
C(4)-C(3)-C(12)-C(17)	30.8(3)
C(23)-C(18)-C(19)-C(20)	-0.5(3)
C(5)-C(18)-C(19)-C(20)	176.9(2)
C(13)-C(12)-C(17)-C(16)	0.5(3)
C(3)-C(12)-C(17)-C(16)	-178.9(2)
C(19)-C(18)-C(23)-C(22)	-0.1(3)
C(5)-C(18)-C(23)-C(22)	-177.5(2)
C(18)-C(19)-C(20)-C(21)	0.2(4)
C(10)-C(9)-C(8)-C(7)	0.0(4)
O(1)-C(7)-C(8)-C(9)	-177.3(3)
C(6)-C(7)-C(8)-C(9)	2.1(4)
C(8)-C(9)-C(10)-C(11)	-1.3(5)

C(18)-C(23)-C(22)-C(21)	1.0(4)
C(17)-C(12)-C(13)-C(14)	-1.3(4)
C(3)-C(12)-C(13)-C(14)	178.2(2)
C(12)-C(13)-C(14)-C(15)	1.0(4)
C(19)-C(20)-C(21)-C(22)	0.8(4)
C(23)-C(22)-C(21)-C(20)	-1.3(4)
C(9)-C(10)-C(11)-C(6)	0.6(5)
C(7)-C(6)-C(11)-C(10)	1.4(4)
C(1)-C(6)-C(11)-C(10)	-179.3(3)
C(13)-C(14)-C(15)-C(16)	0.0(4)
C(14)-C(15)-C(16)-C(17)	-0.7(4)
C(12)-C(17)-C(16)-C(15)	0.5(4)

Symmetry transformations used to generate equivalent atoms:

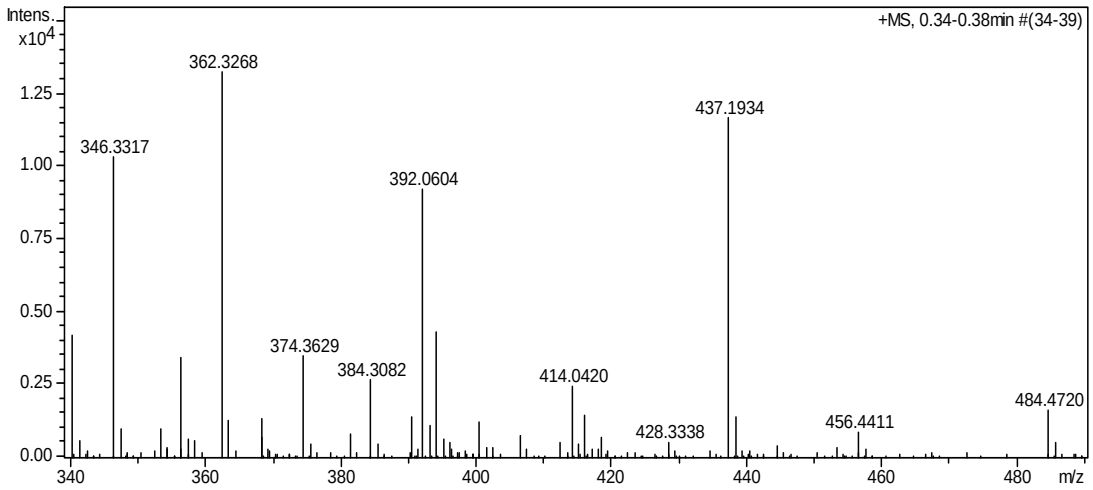
Table S14. Hydrogen bonds for **3d** [A and deg.].

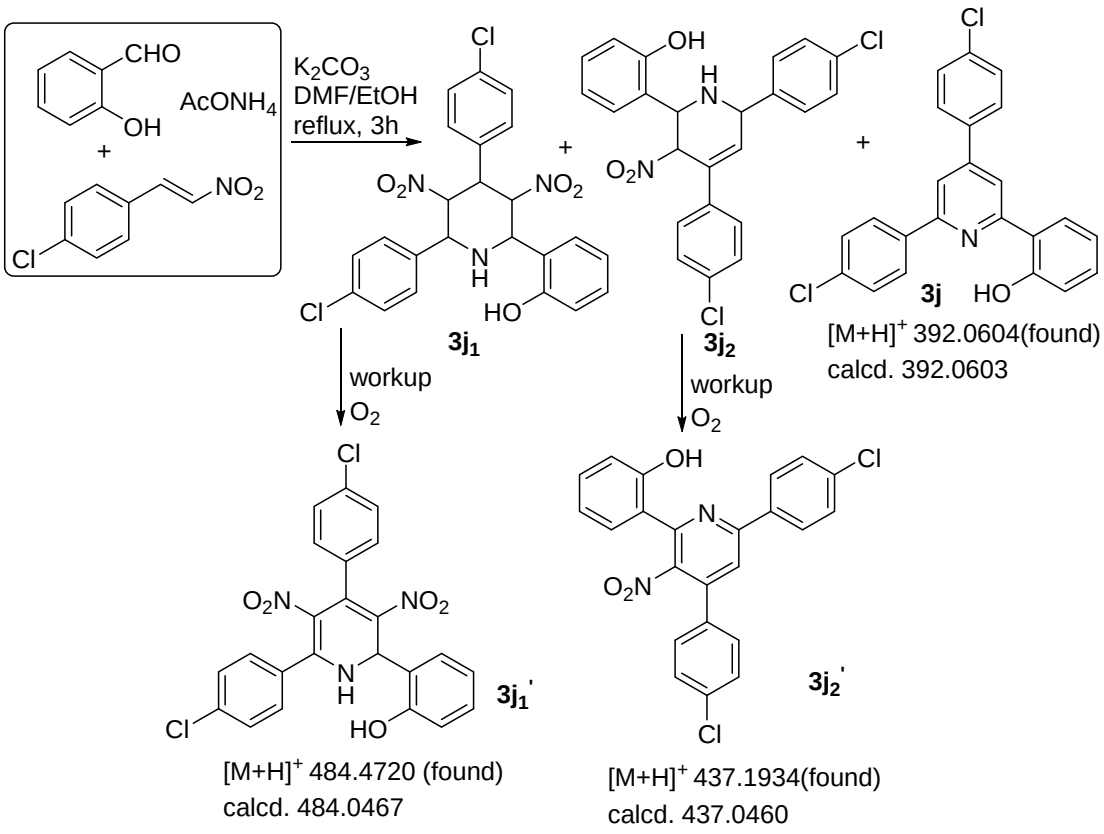
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...N(1)	0.84	1.81	2.554(2)	147.3

Symmetry transformations used to generate equivalent atoms:

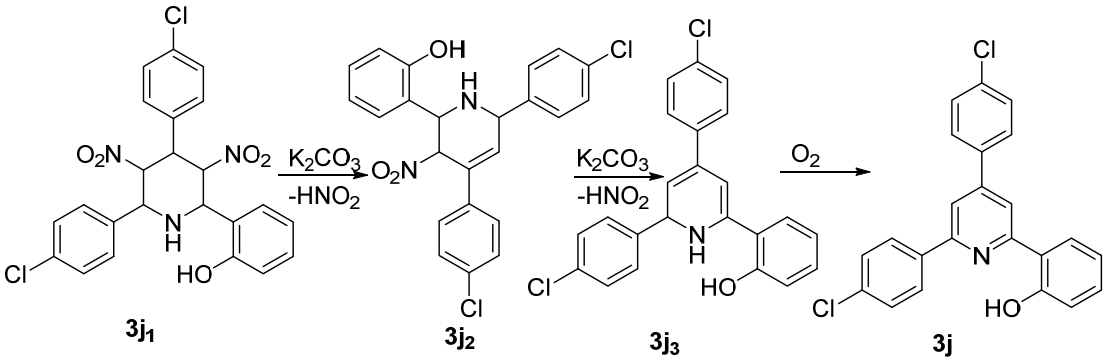
3 Control experiments

Some control experiments were tested for our proposed mechanism. Under the optimized conditions, the model reaction of salicylic aldehyde, 1-chloro-4-(2-nitrovinyl)benzene and ammonium acetate was carried out in the optimized reaction conditions for 3 h aimed at yielding some key intermediates and supporting the mechanistic proposal, but the reaction system was very complicated after workup, the desired intermediates were not isolated by flash chromatography. After workup, the solid mixture was measured by High-resolution ESI mass spectra to afford a stronger ion peak: 392.0904 (m/z), which corresponded to the mass of the molecular ion (M+1) for the final product 2-(4,6-bis(4-chlorophenyl)pyridin-2-yl)phenol (**3j**) (Scheme 1, **3j**). Additionally, the two mass of the molecular ion (M+1): 484.4720 and 437.1934, should belong to dinitrodihydropyridine (**3j$_1$**') (Scheme 1, **3j$_1$**') from the desired intermediate dinitropiperidine (**3j$_1$**) (Scheme 1, **3j$_1$**) and nitropyridine (**3j$_2$**') (Scheme 1, **3j$_2$**') from the desired intermediate nitrotetrahydropyridine (**3j$_2$**) (Scheme 1, **3j$_2$**). The results indicated there was a path that leads to the final product which the intermolecular [4+2] cyclization gave the desired intermediate dinitropiperidine (**3j$_1$**) (Scheme 2, **3j$_1$**), next HNO_2 was removed by K_2CO_3 to give the desired intermediate nitrotetrahydropyridine (**3j$_2$**) (Scheme 2, **3j$_2$**), then another HNO_2 was removed by K_2CO_3 to give the desired intermediate dihydropyridine (**3j$_3$**) (Scheme 2, **3j$_3$**), the final aromatization yielded to the product 2-(4,6-bis(4-chlorophenyl)pyridin-2-yl)phenol (**3j**) (Scheme 2, **3j**) by air.





Scheme 1



Scheme 2