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SUPPORTING INFORMATION

Mild base-promoted benzannulation for the construction of polyfunctionalized *m*-terphenyl derivatives and their application as potent UV-filters

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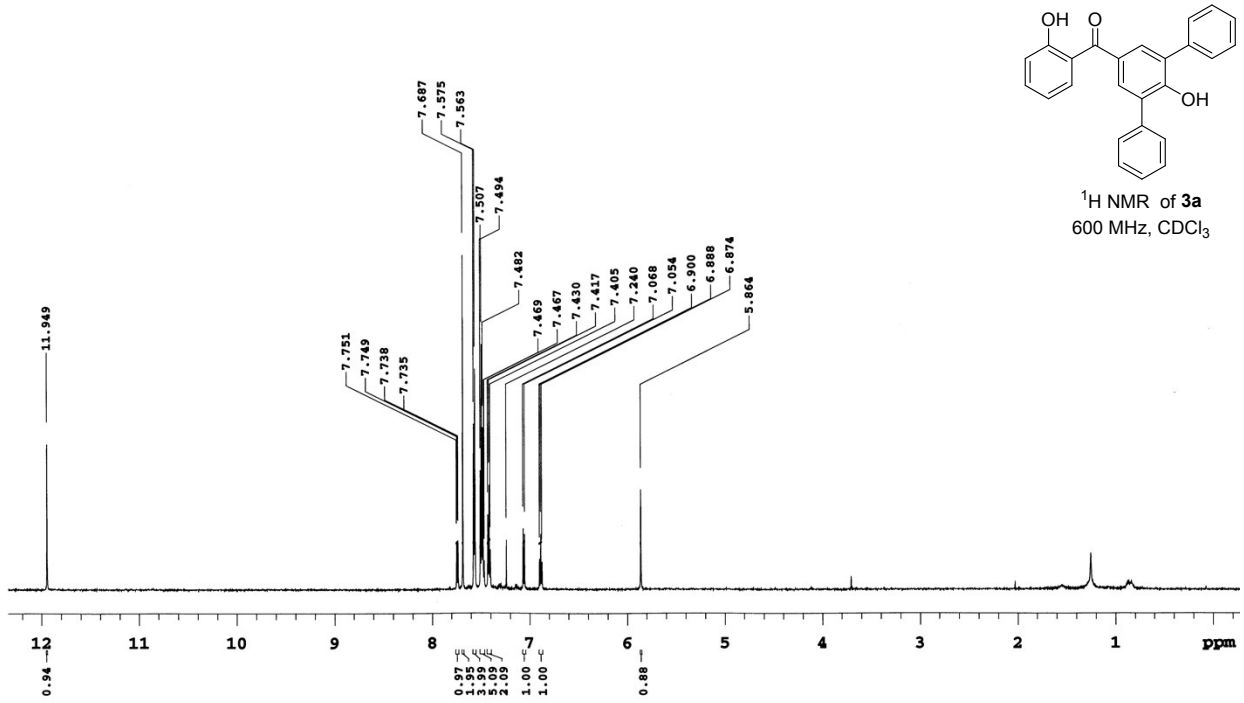
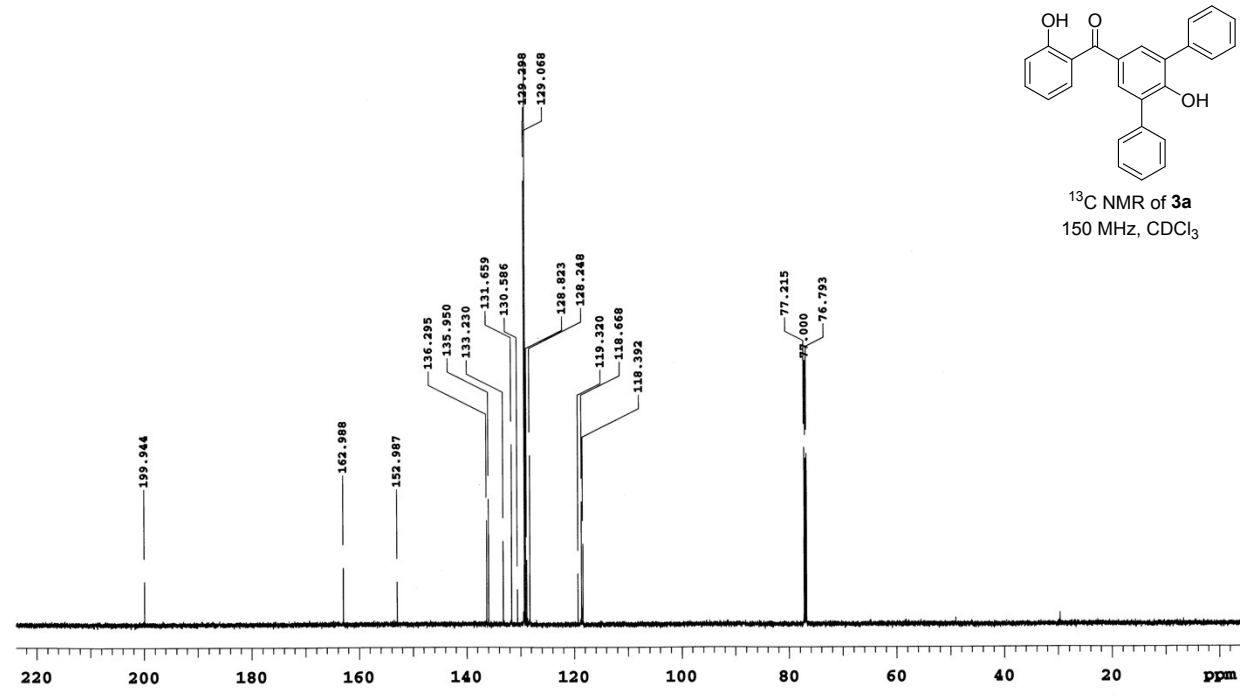
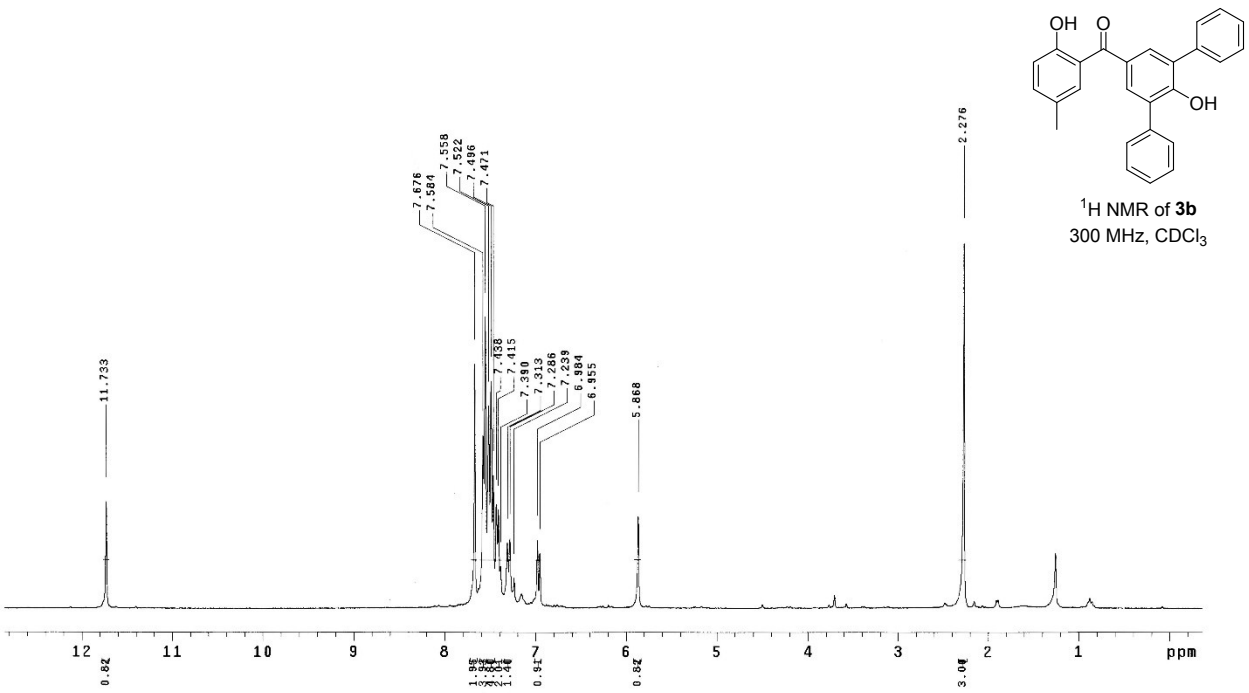
^{1}H NMR and ^{13}C NMR Spectra of compounds 3-6



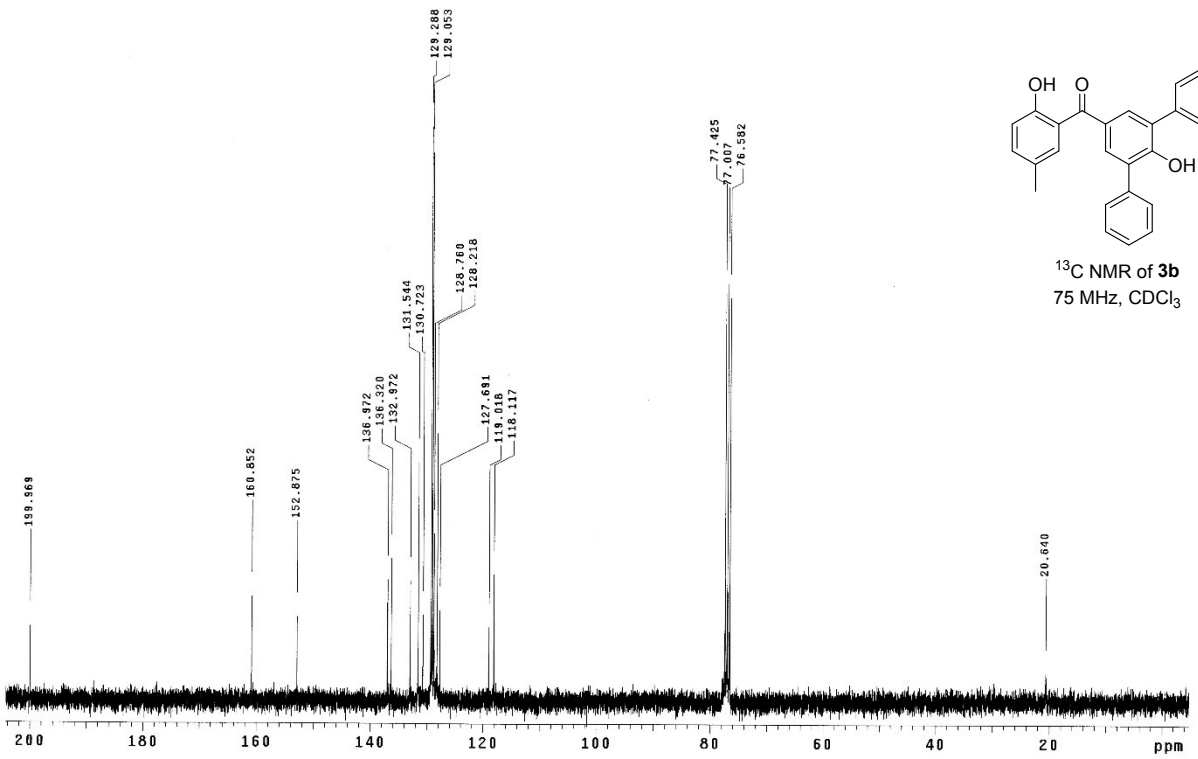
^{1}H NMR of **3a**
600 MHz, $CDCl_3$



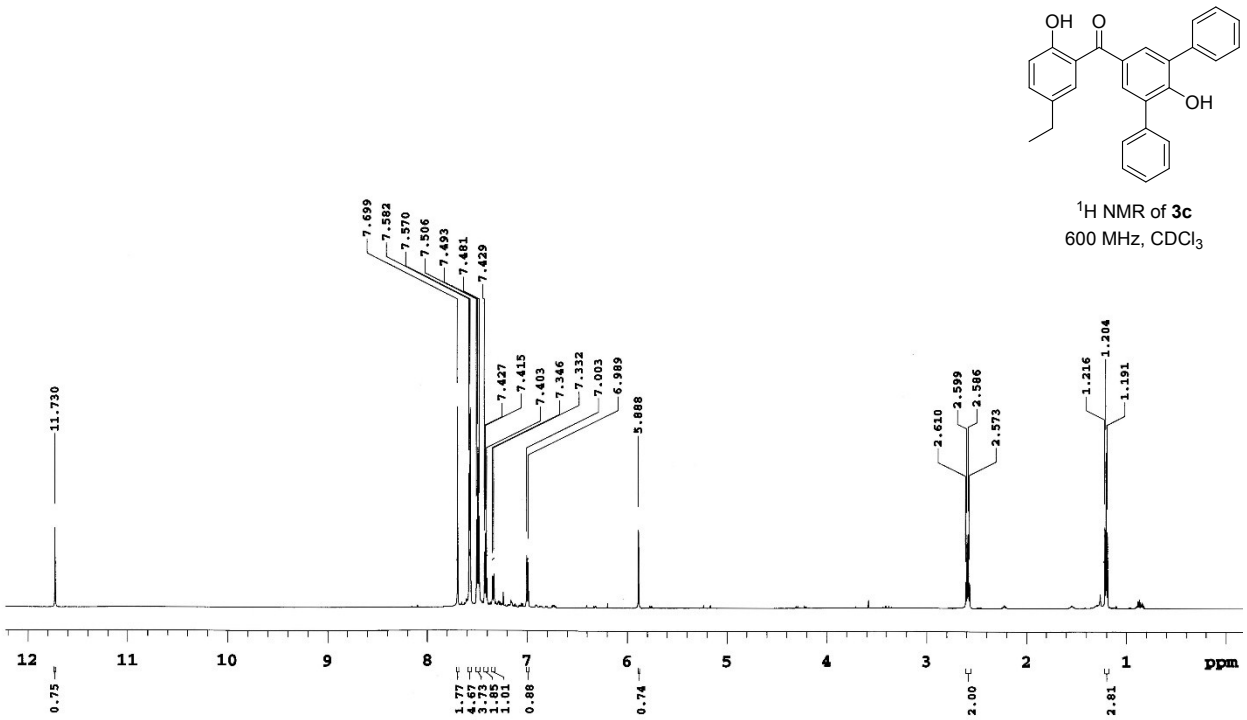
^{13}C NMR of **3a**
150 MHz, $CDCl_3$



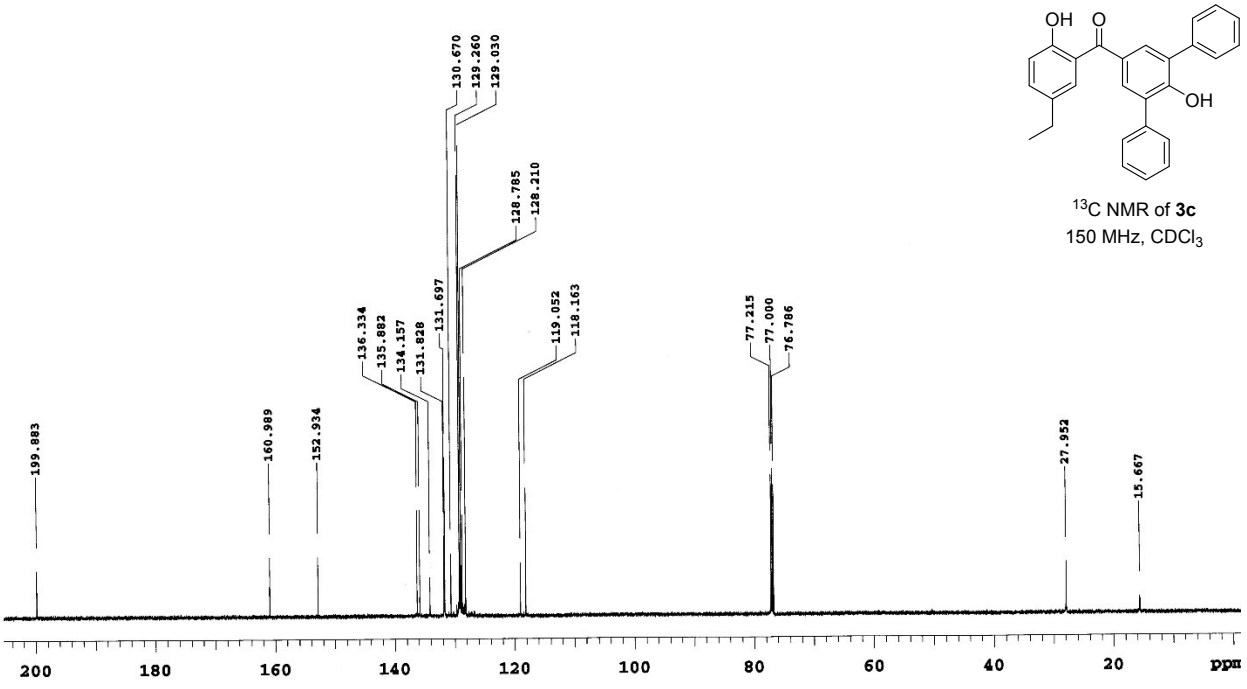
^{1}H NMR of **3b**
300 MHz, $CDCl_3$



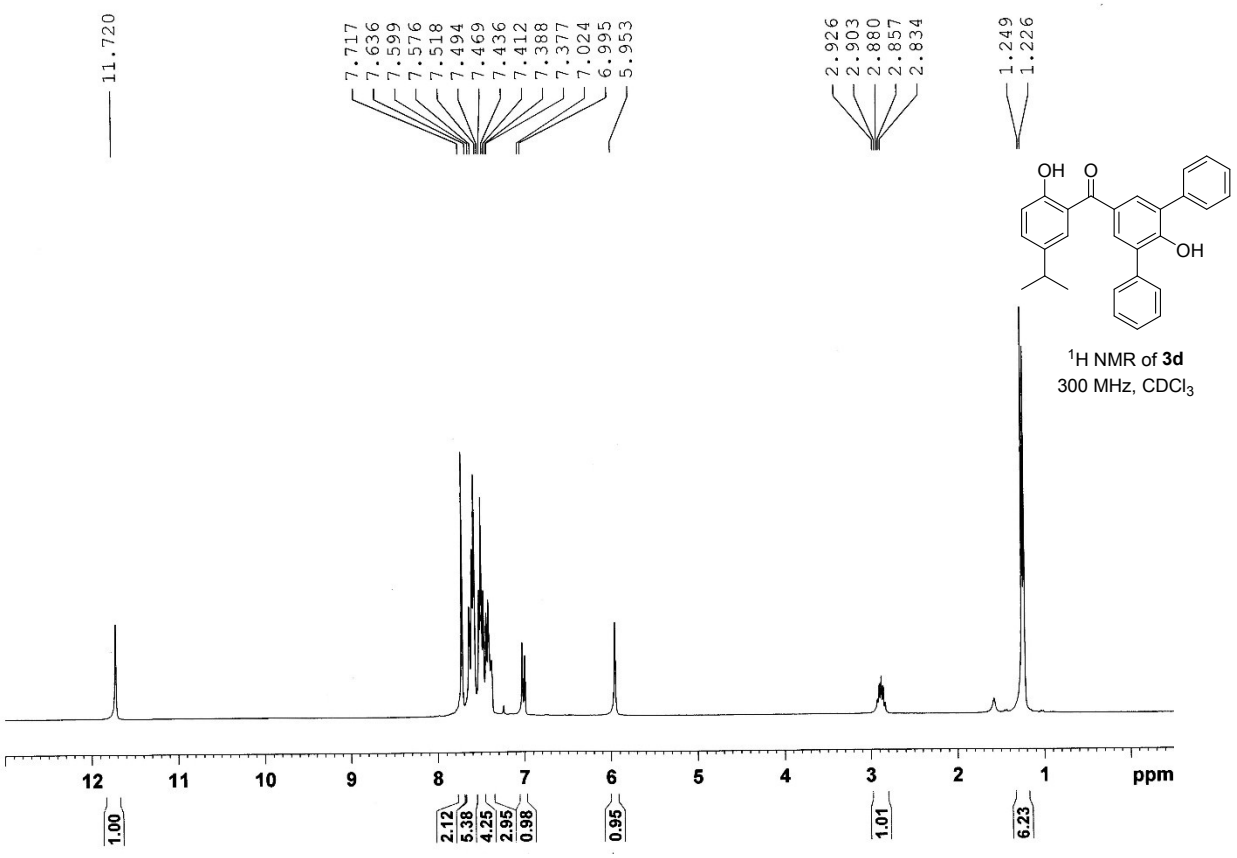
^{13}C NMR of **3b**
75 MHz, $CDCl_3$



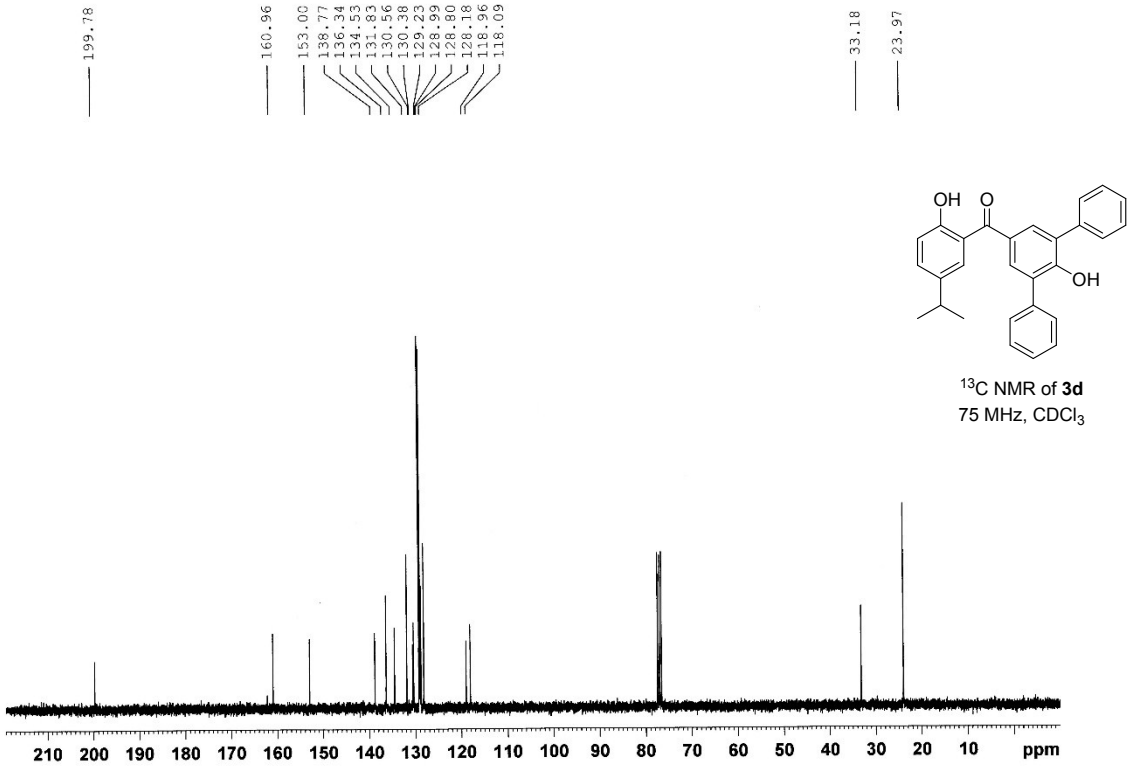
^{1}H NMR of **3c**
600 MHz, $CDCl_3$



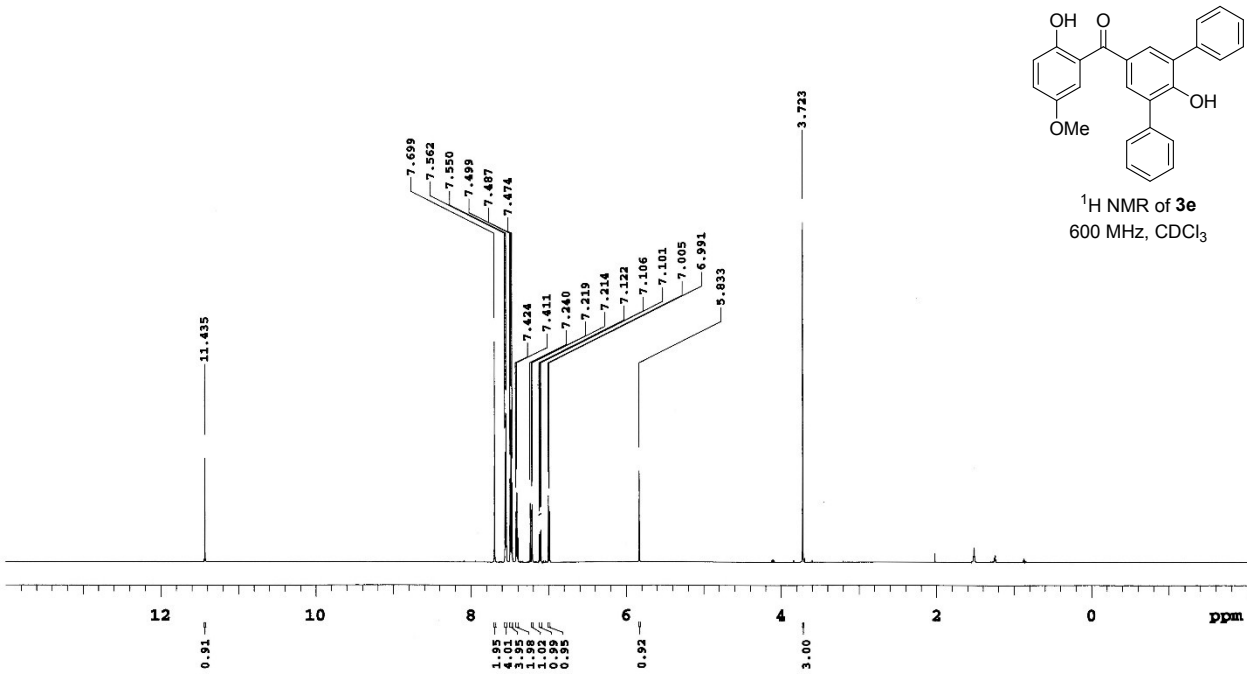
^{13}C NMR of **3c**
150 MHz, $CDCl_3$



^{1}H NMR of **3d**
300 MHz, $CDCl_3$



^{13}C NMR of **3d**
75 MHz, $CDCl_3$



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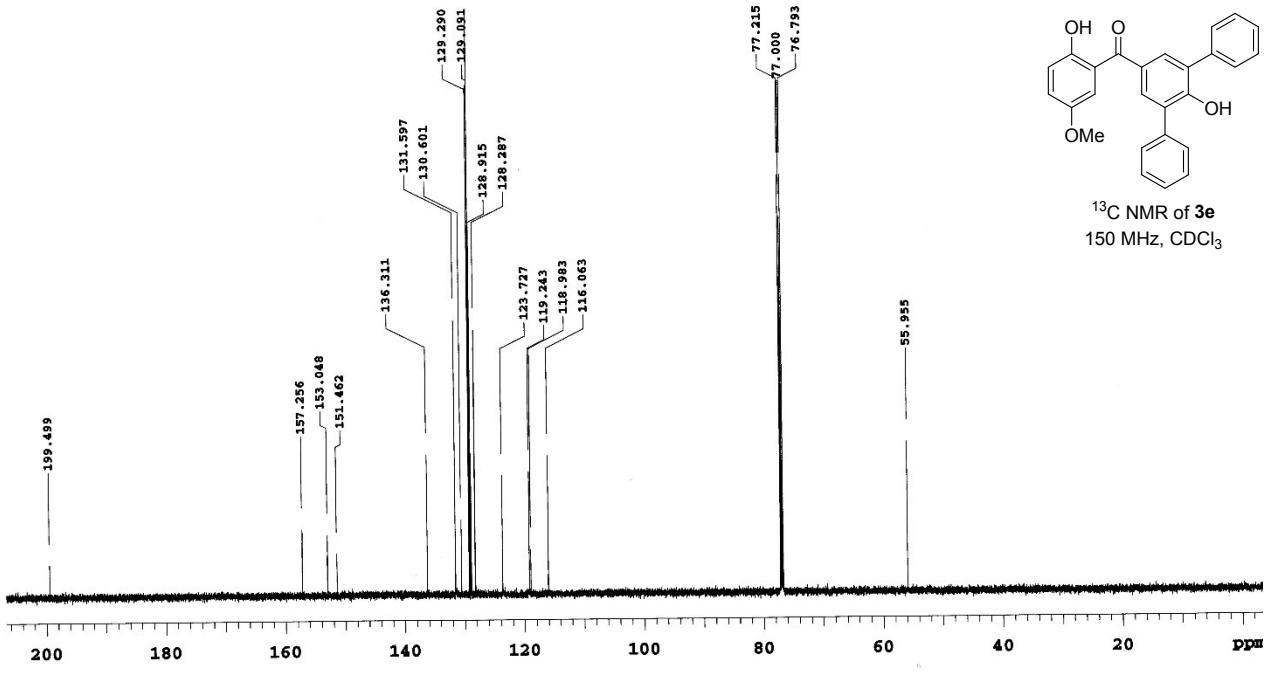
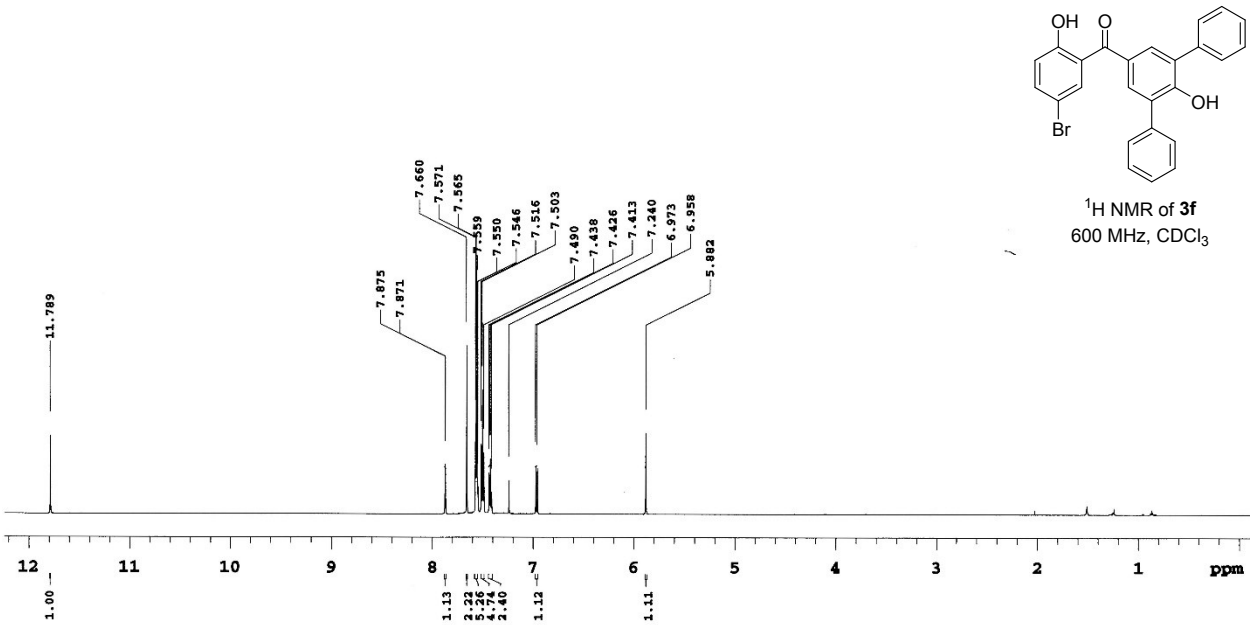
600 MHz, $CDCl_3$



^{13}C NMR of **3e**
150 MHz, $CDCl_3$



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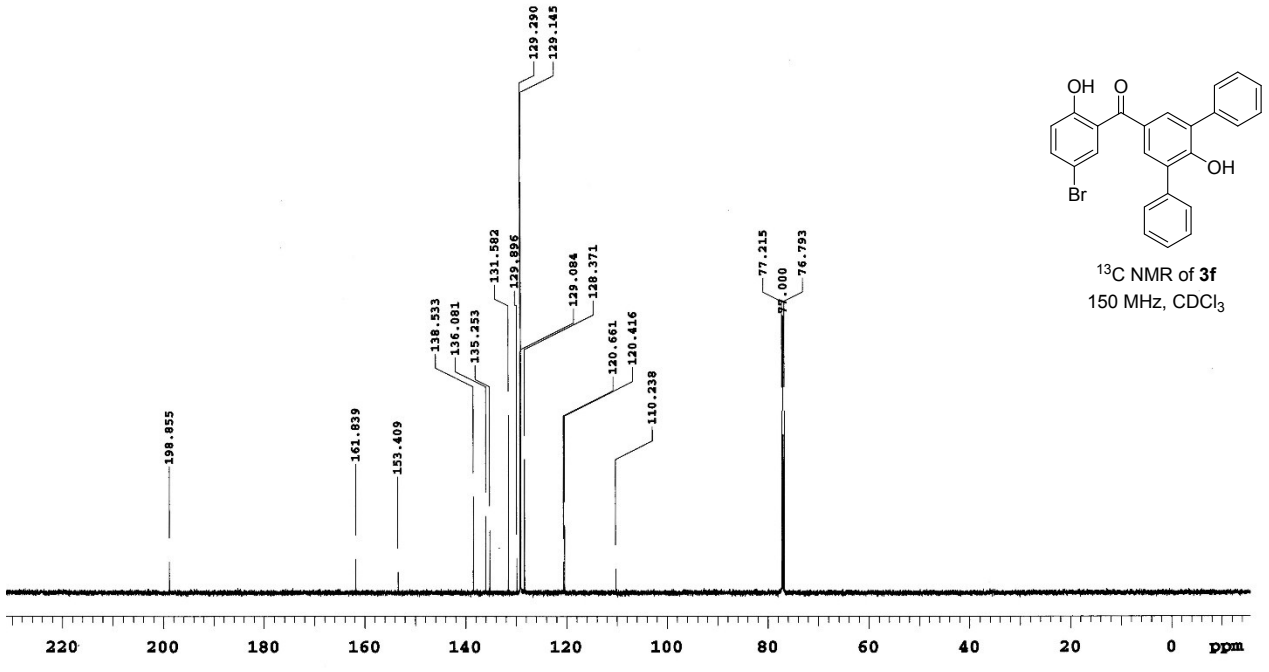
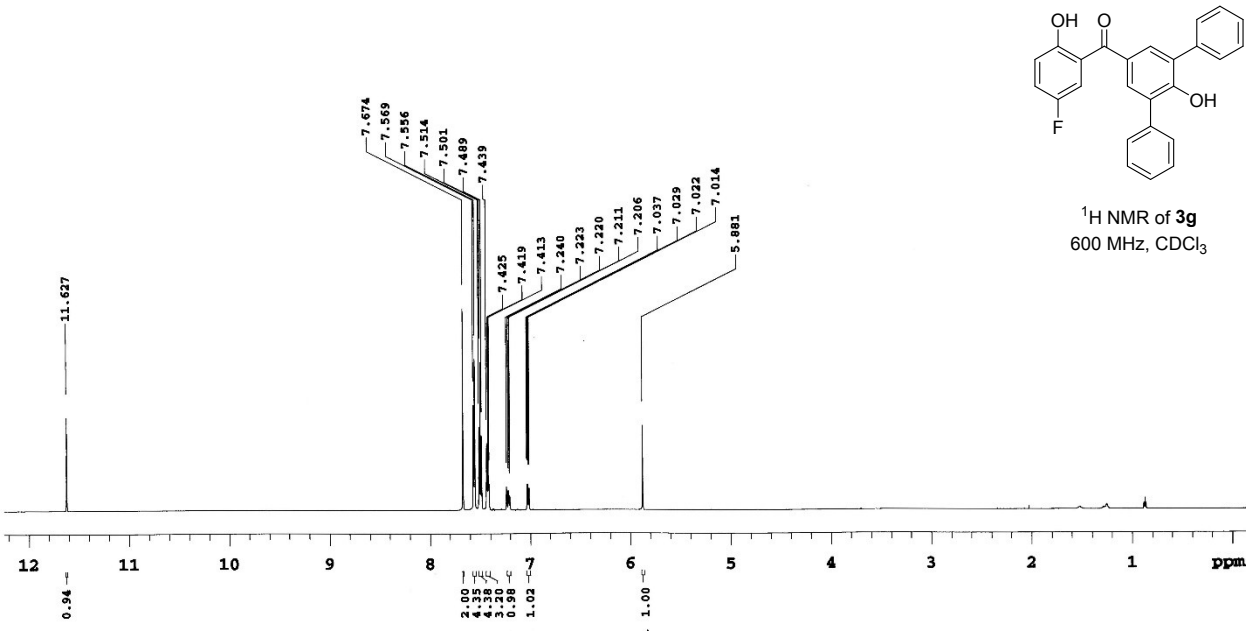


^{13}C NMR of **3f**
150 MHz, $CDCl_3$



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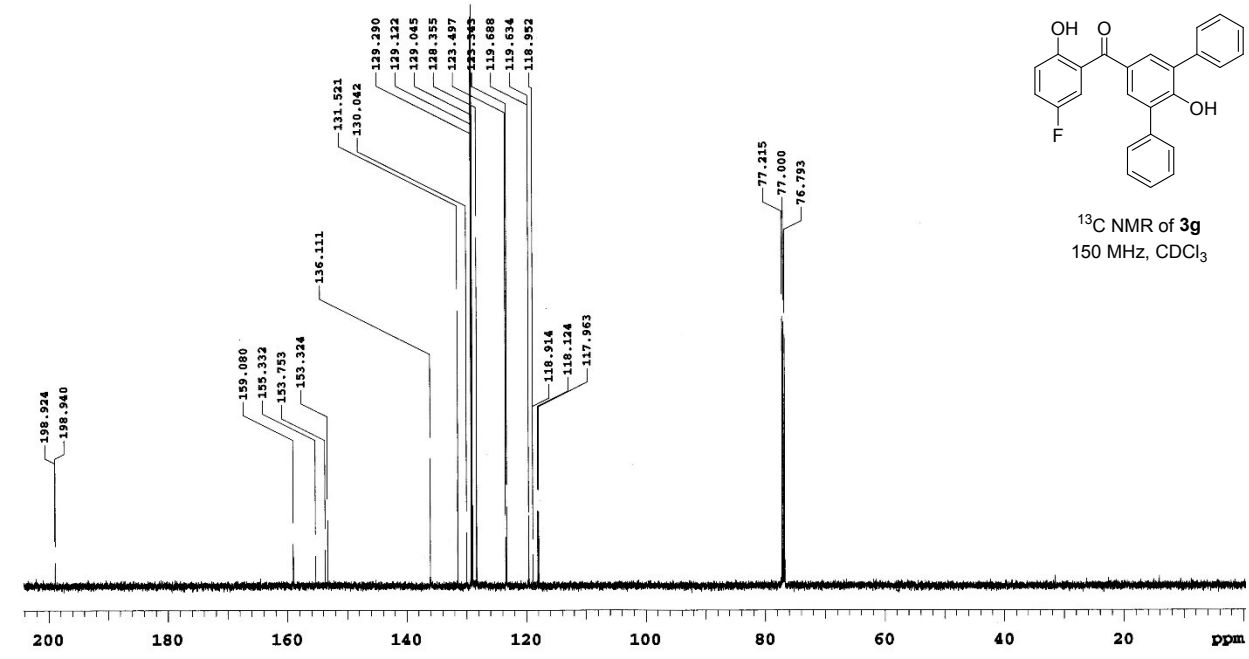
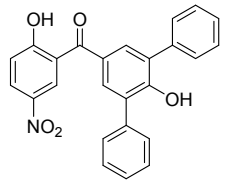


^{13}C NMR of **3g**
150 MHz, $CDCl_3$



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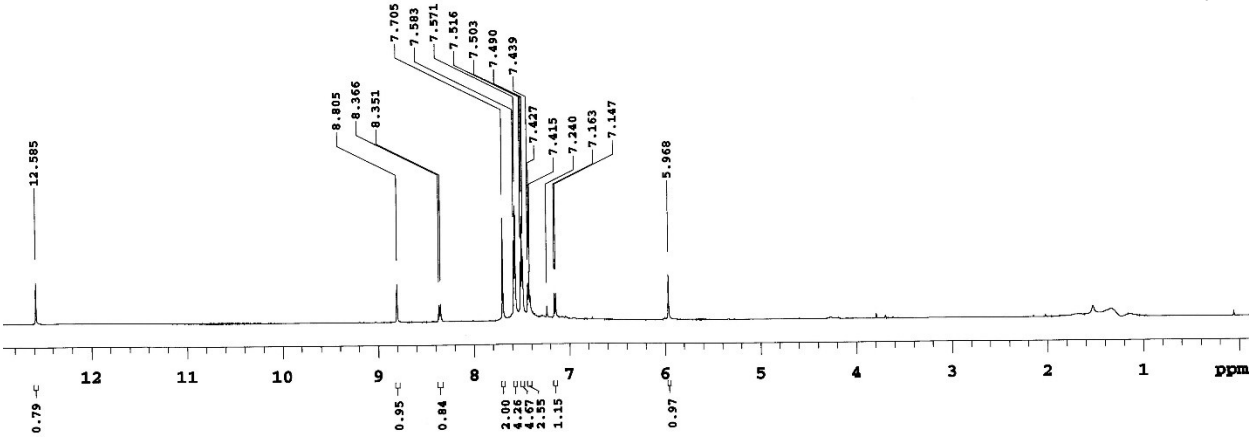
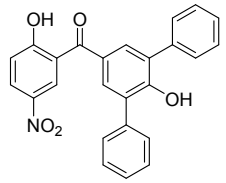
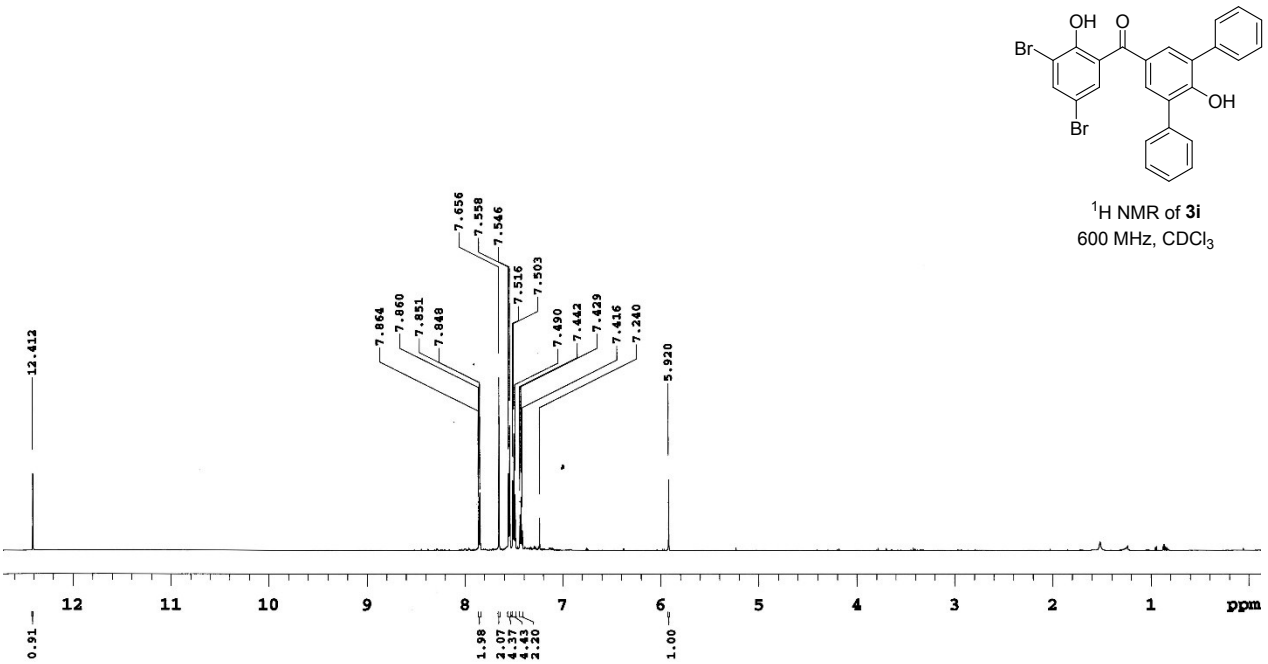
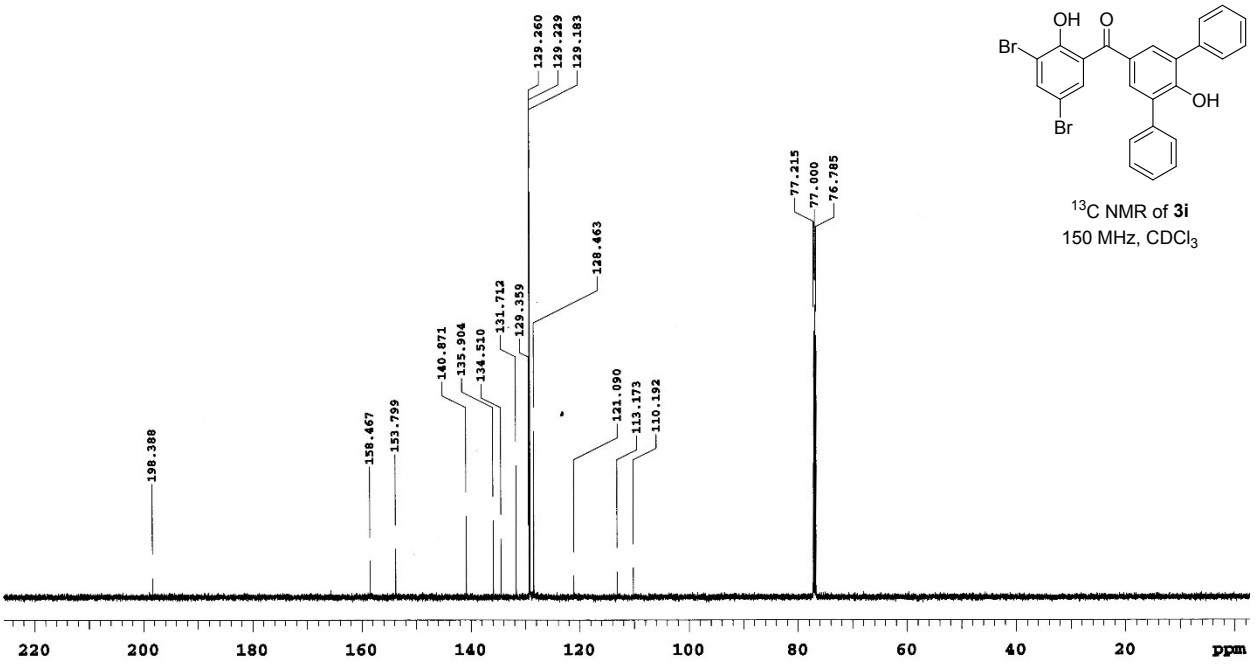




^{13}C NMR of **3h**
150 MHz, $CDCl_3$



^{1}H NMR of **3i**
600 MHz, $CDCl_3$



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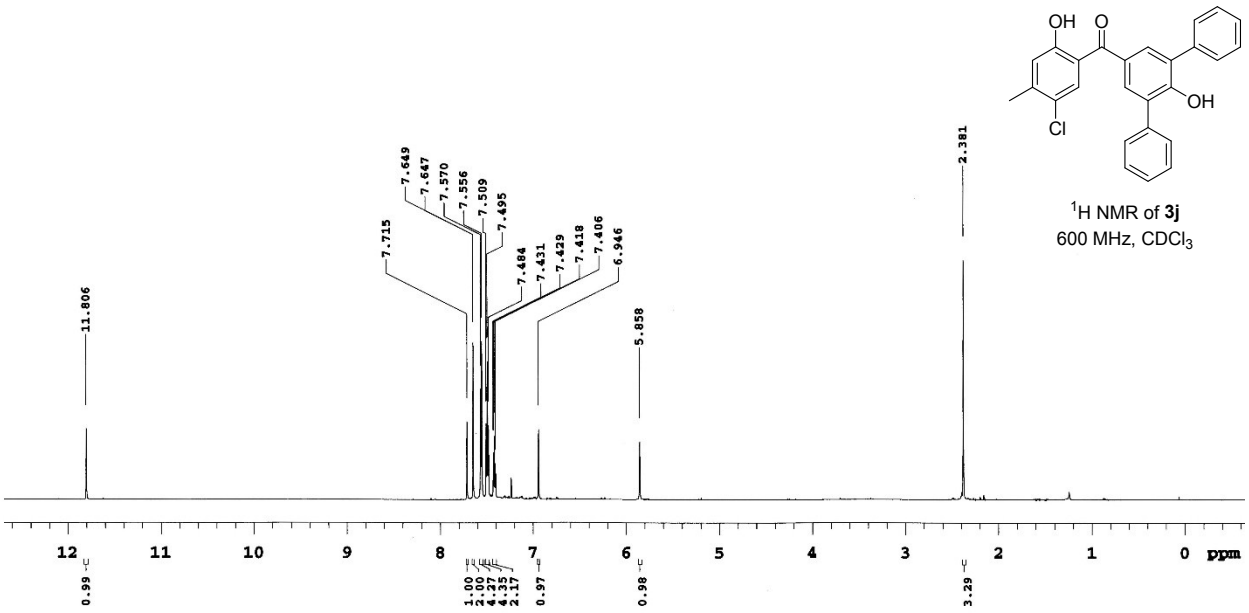

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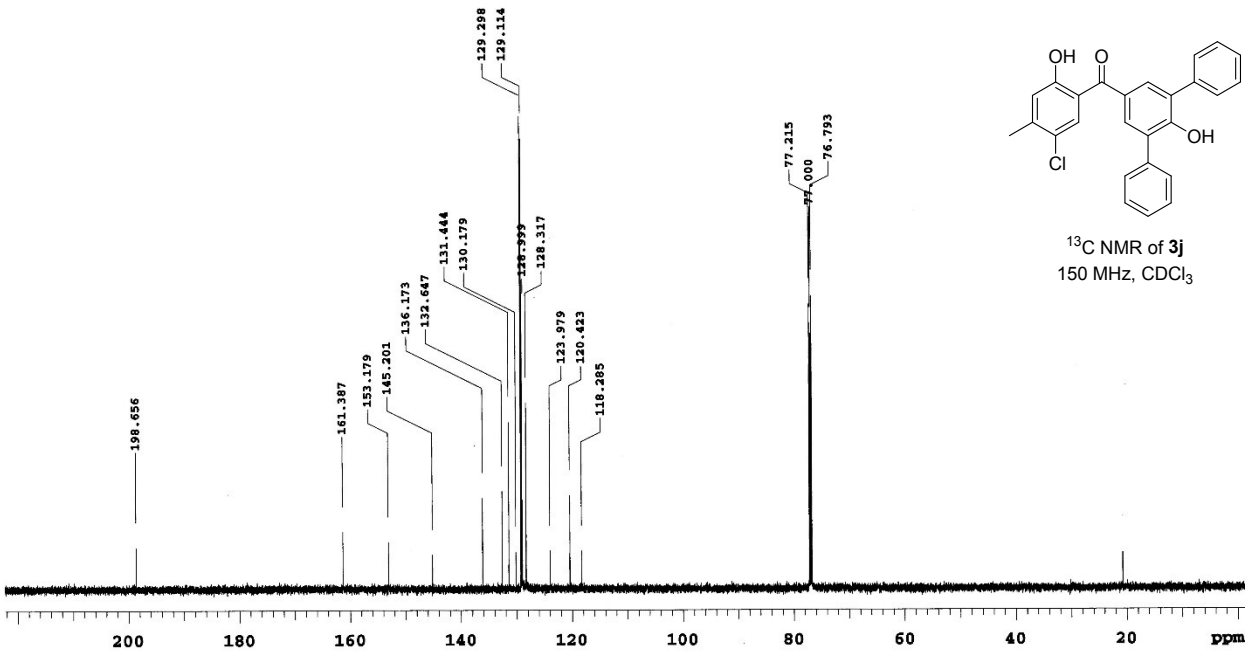
600 MHz, $CDCl_3$



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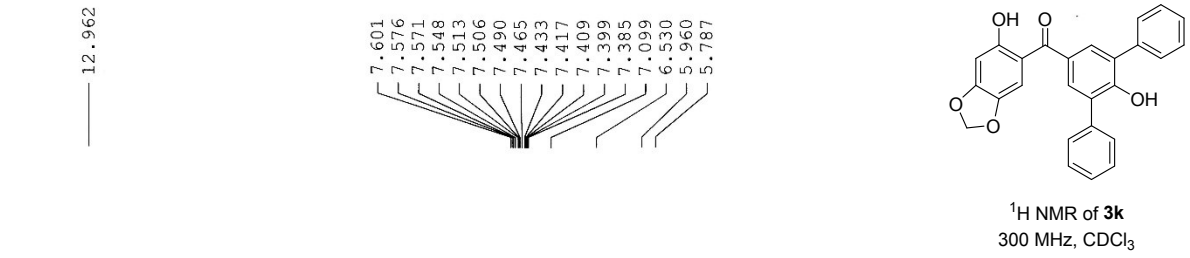
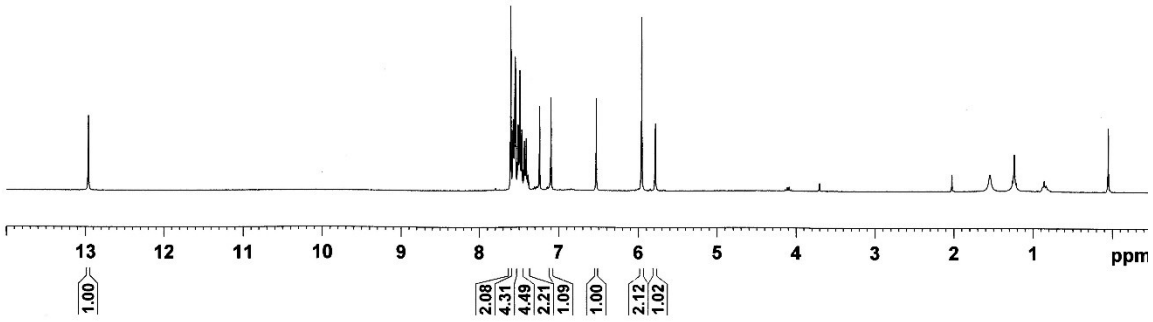
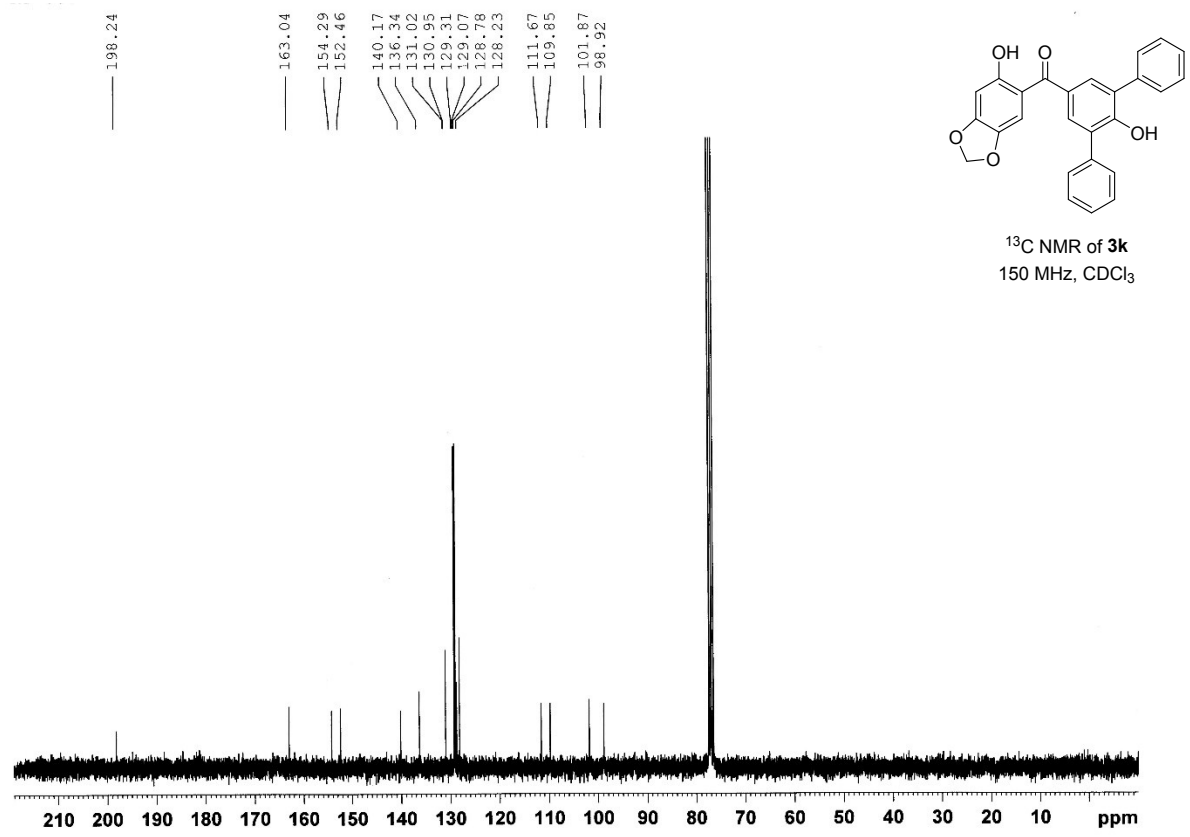
150 MHz, $CDCl_3$

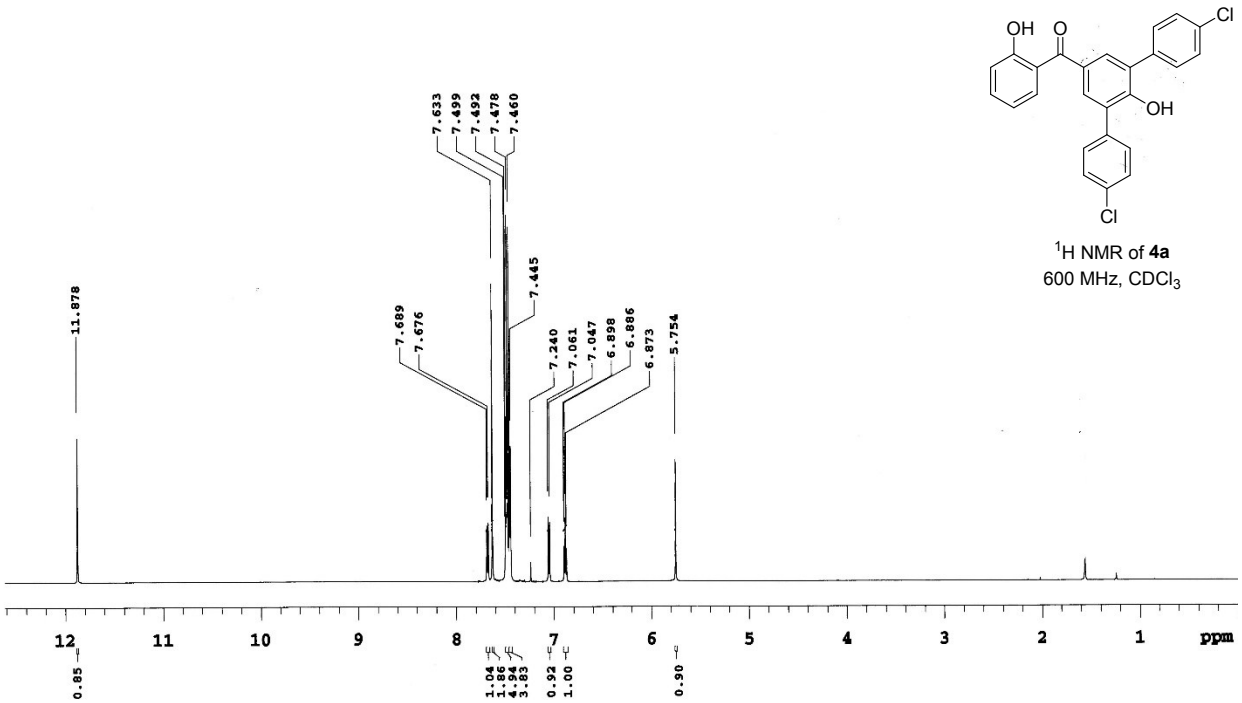


^{1}H NMR of **3k**
300 MHz, $CDCl_3$

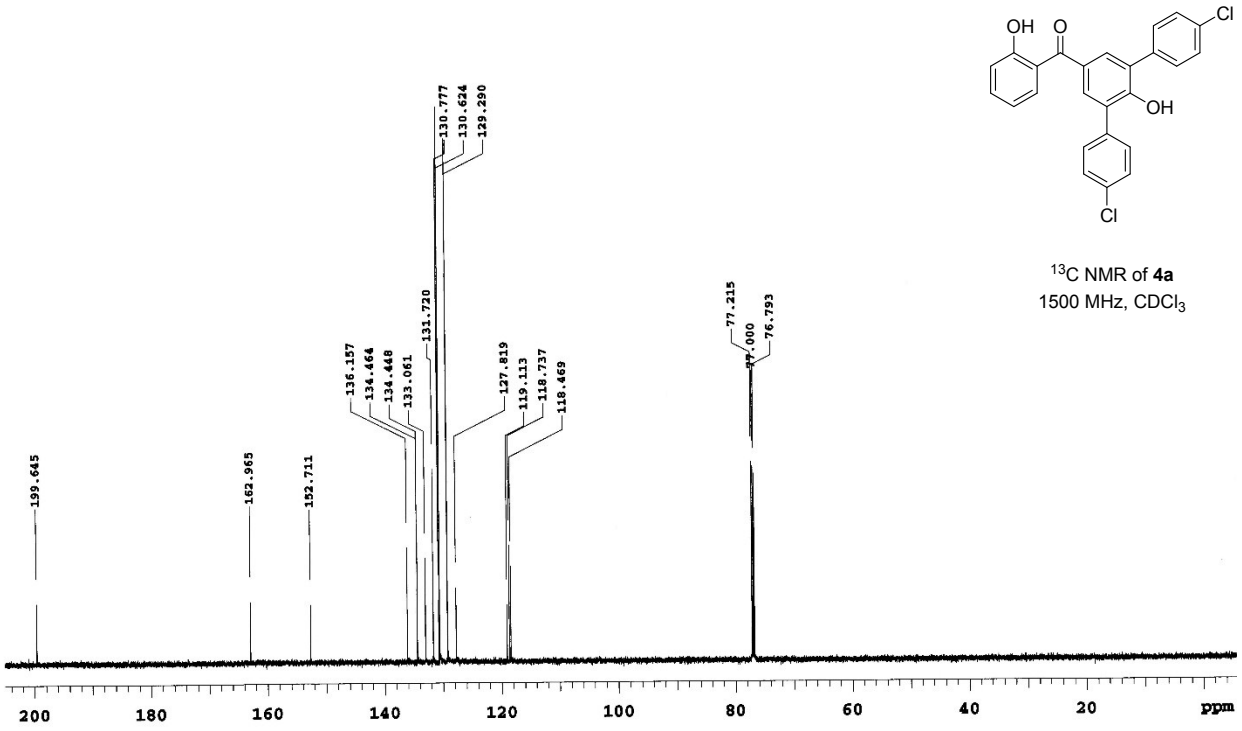




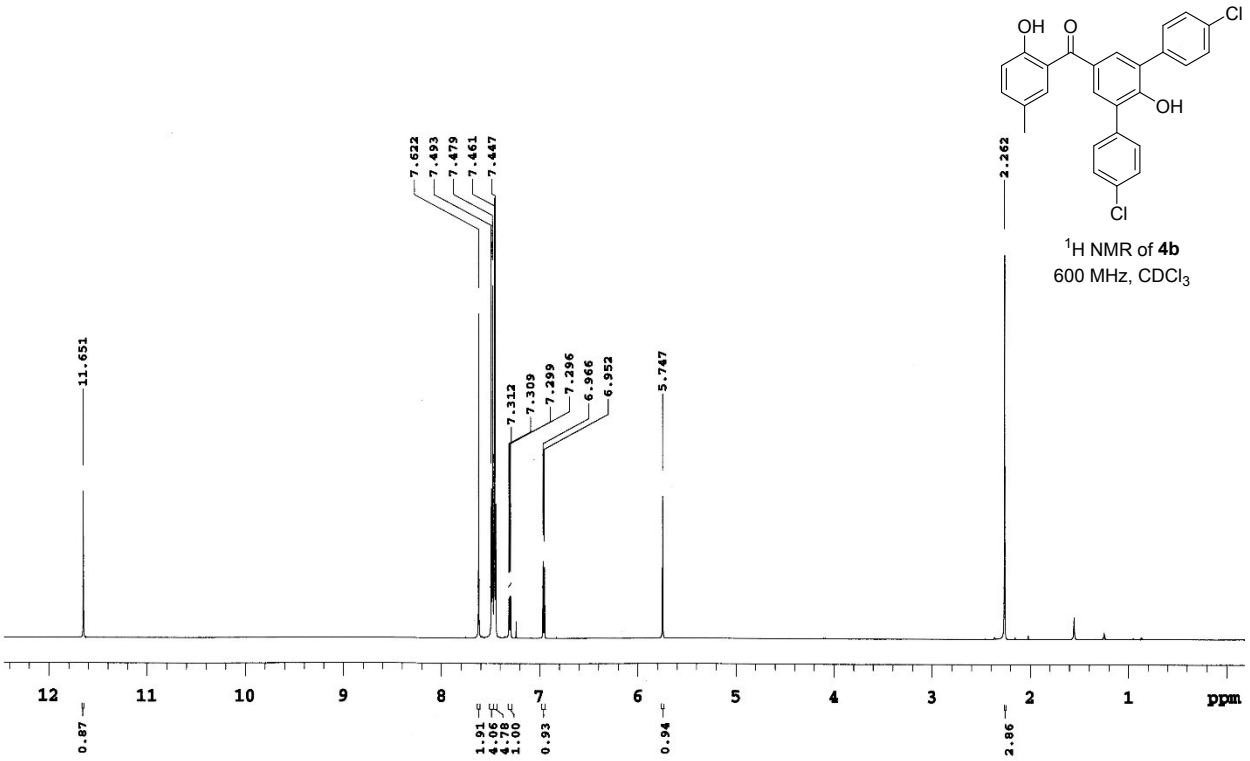
^{13}C NMR of **3k**
150 MHz, $CDCl_3$



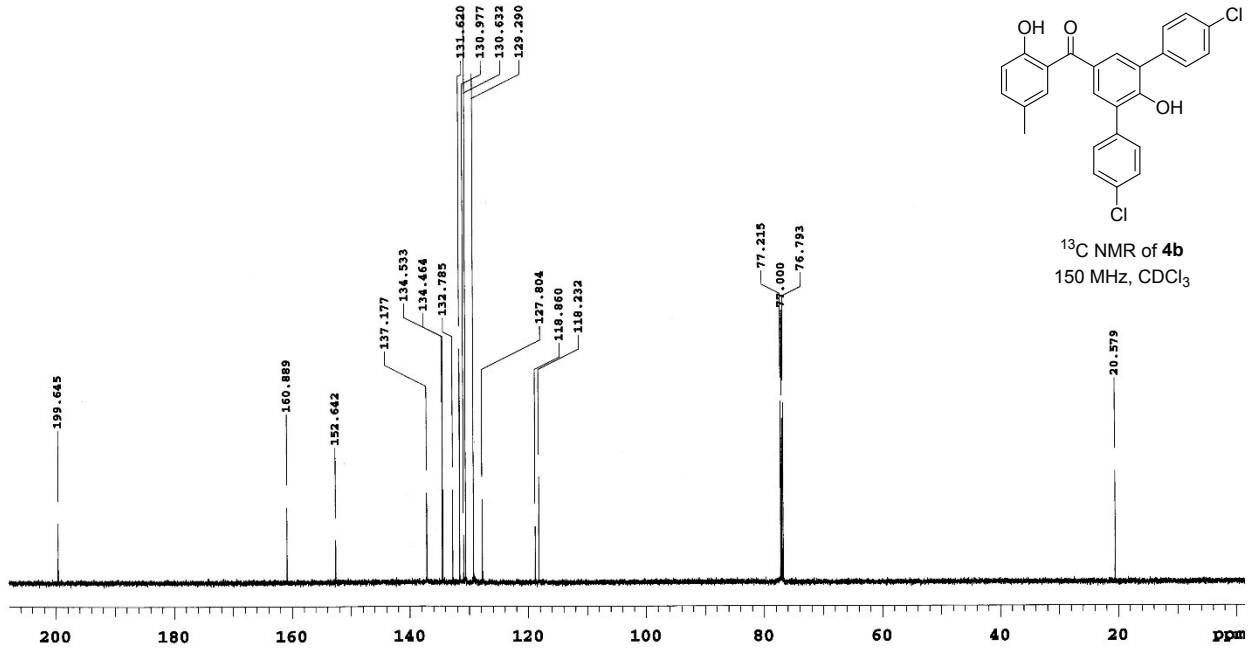
^{1}H NMR of **4a**
600 MHz, $CDCl_3$



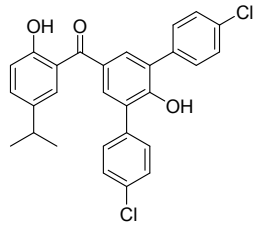
^{13}C NMR of **4a**
1500 MHz, $CDCl_3$



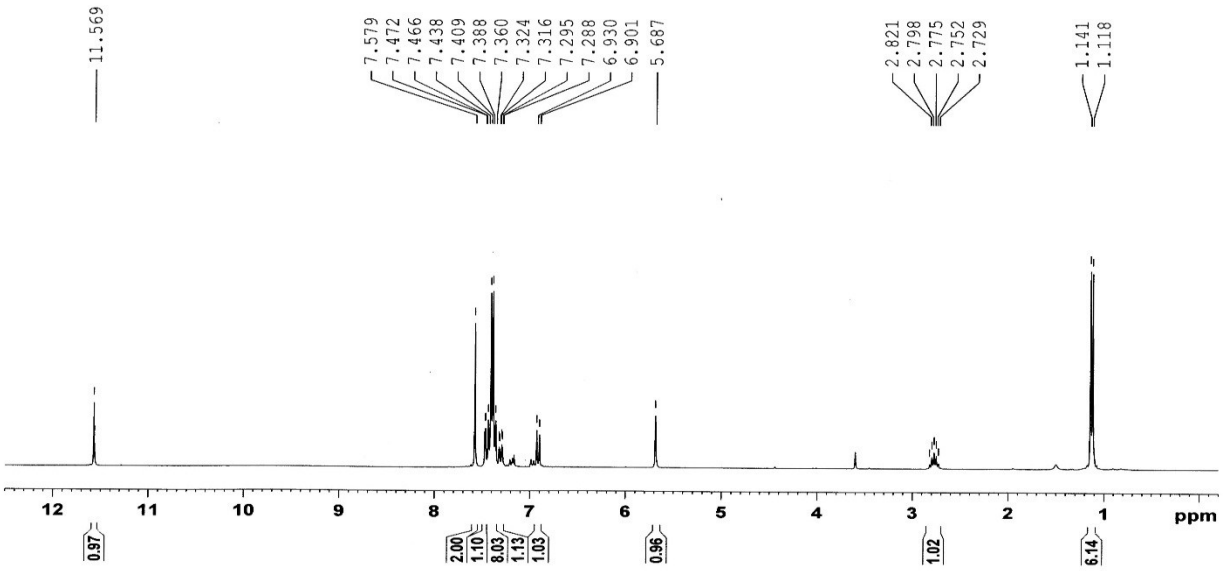
^{1}H NMR of **4b**
600 MHz, $CDCl_3$

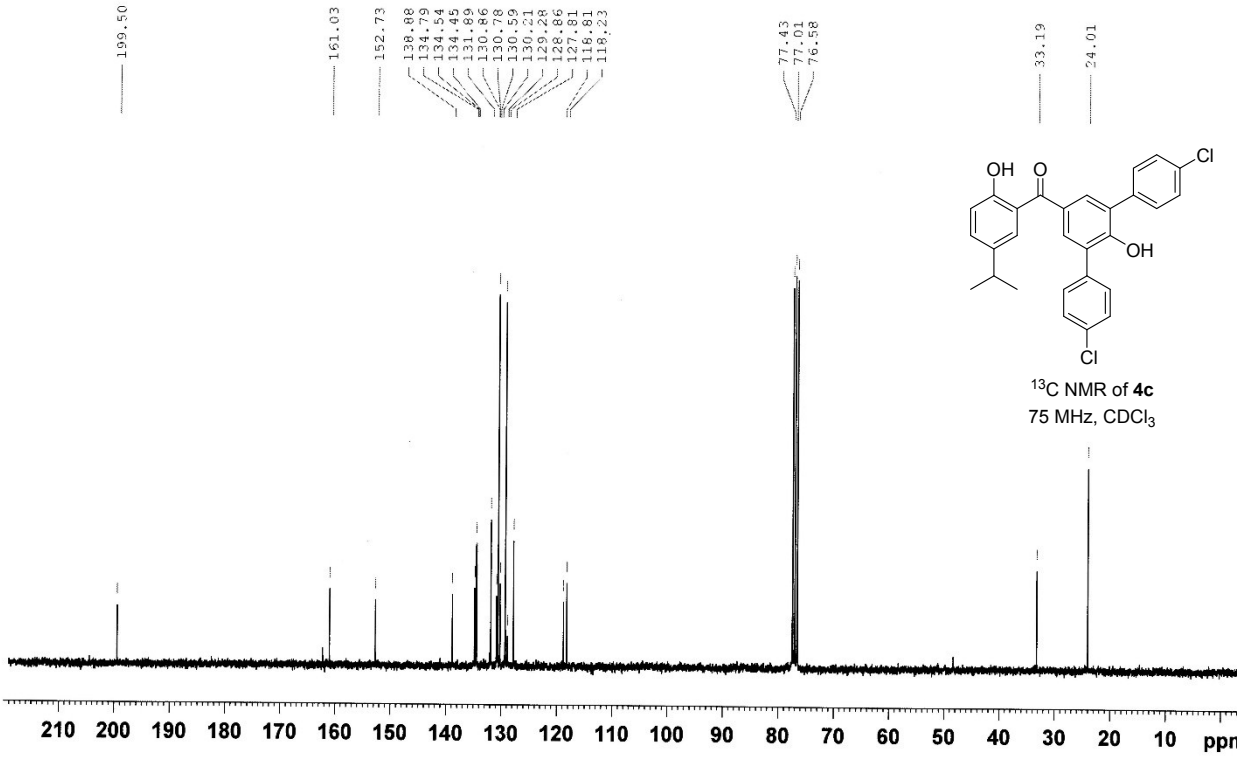


^{13}C NMR of **4b**
150 MHz, $CDCl_3$

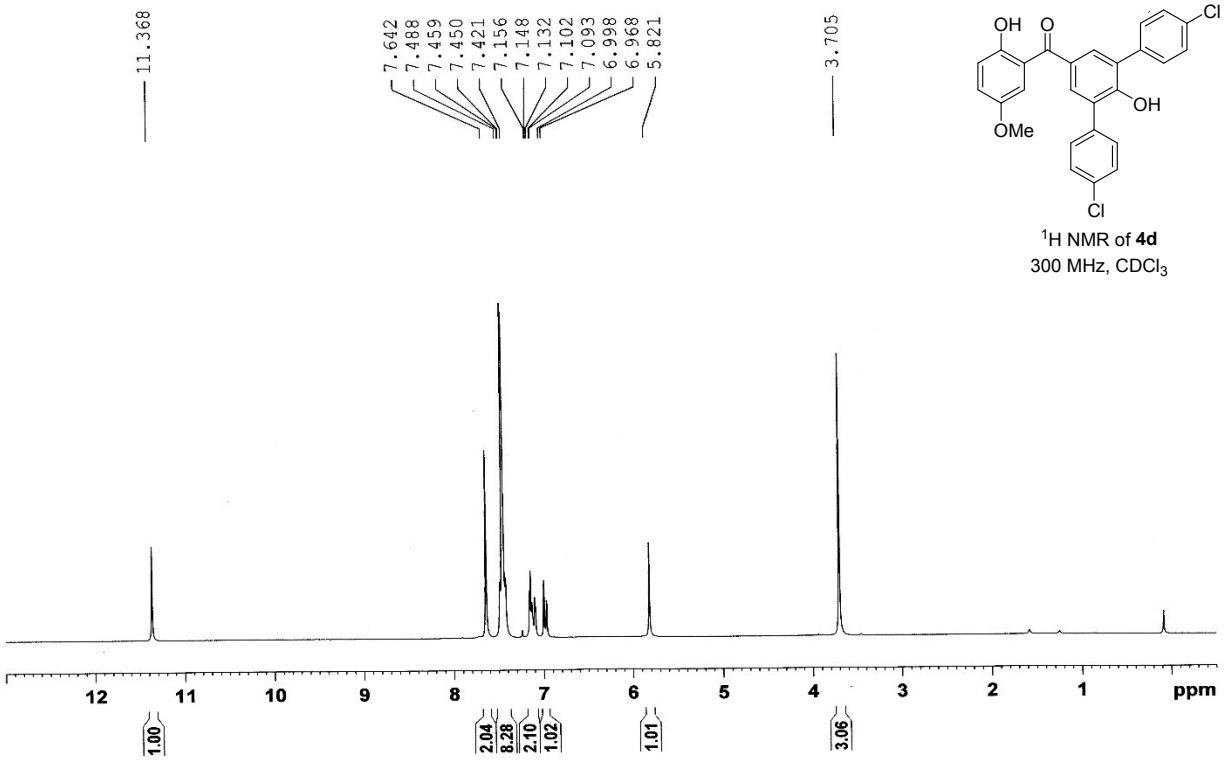


^{1}H NMR of **4c**
300 MHz, $CDCl_3$

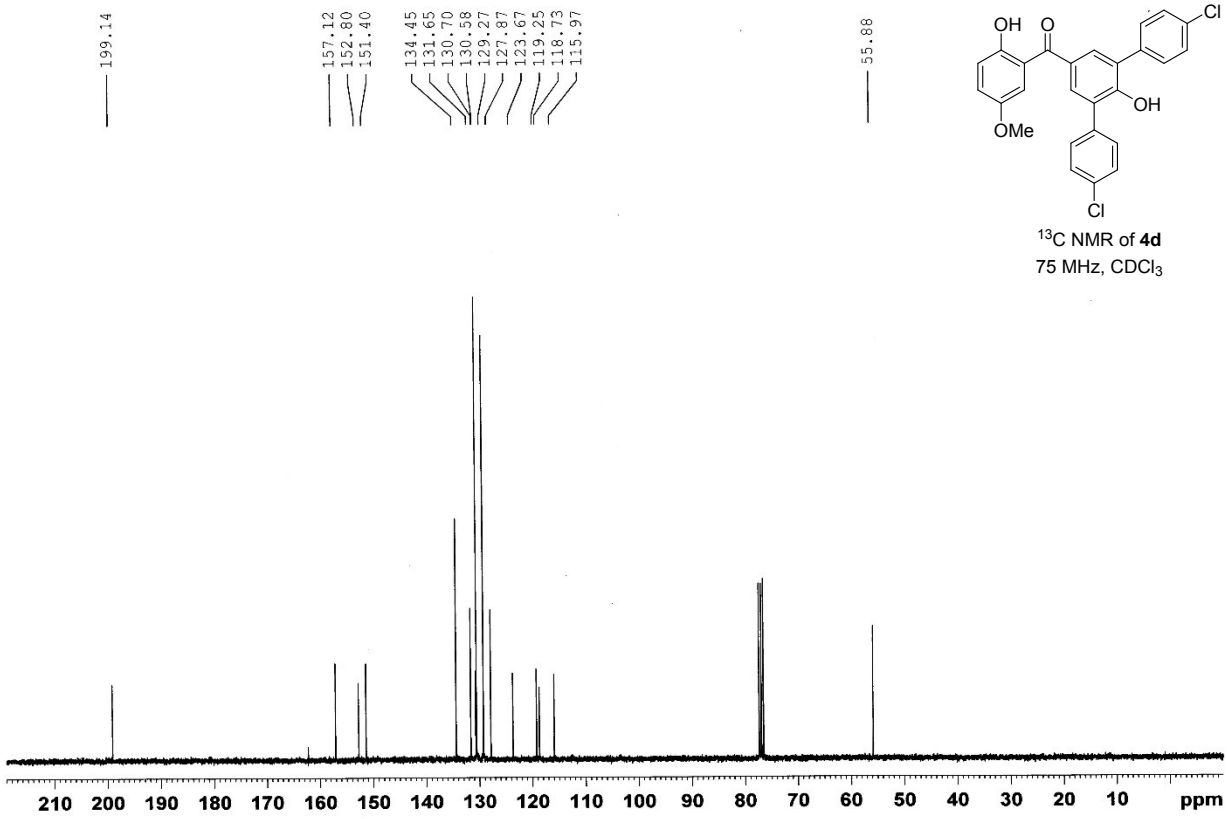




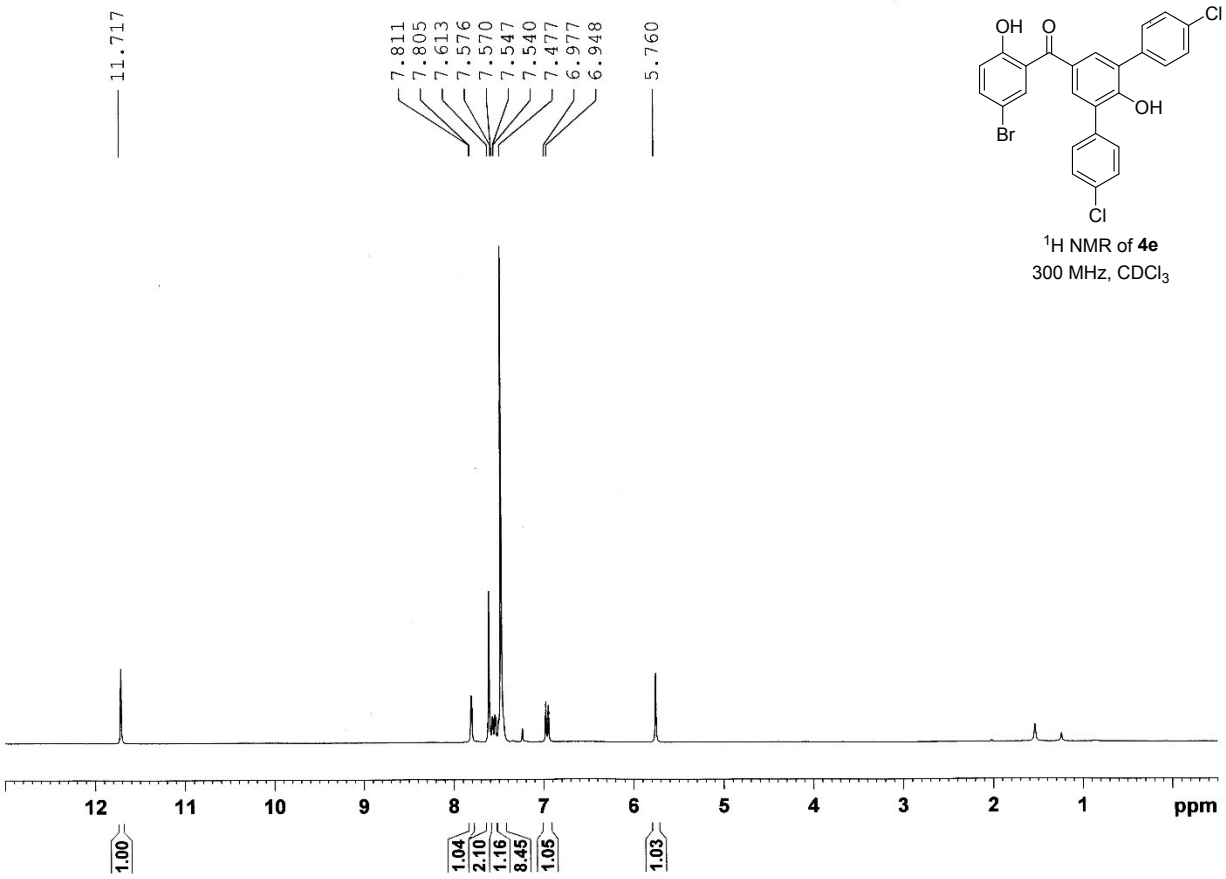
^{13}C NMR of **4c**
75 MHz, $CDCl_3$



^{1}H NMR of **4d**
300 MHz, $CDCl_3$



^{13}C NMR of **4d**
75 MHz, $CDCl_3$



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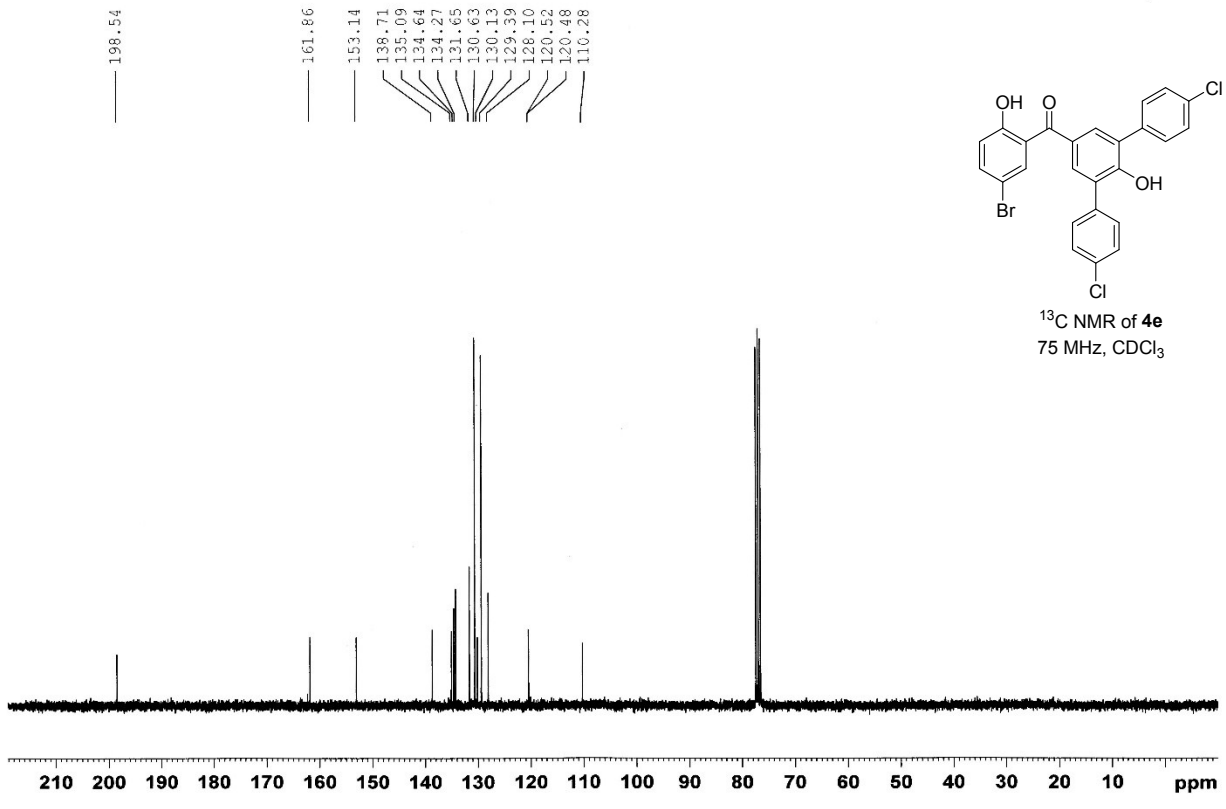
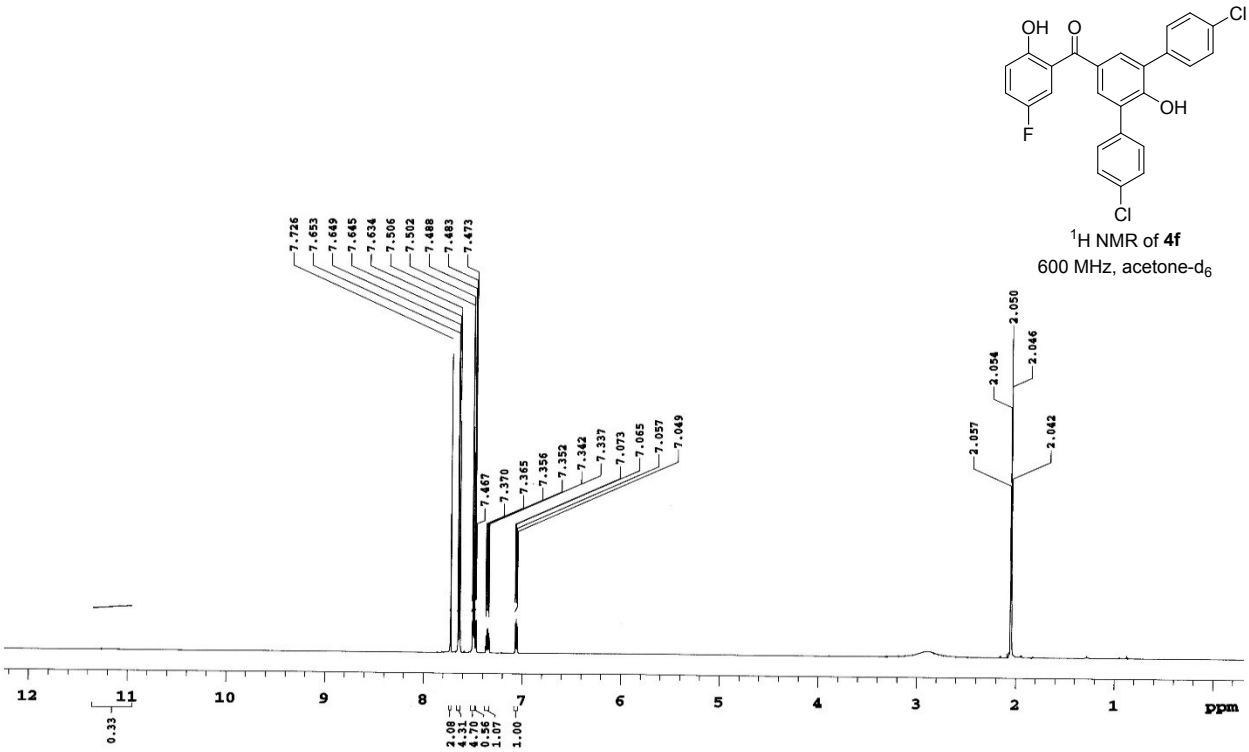
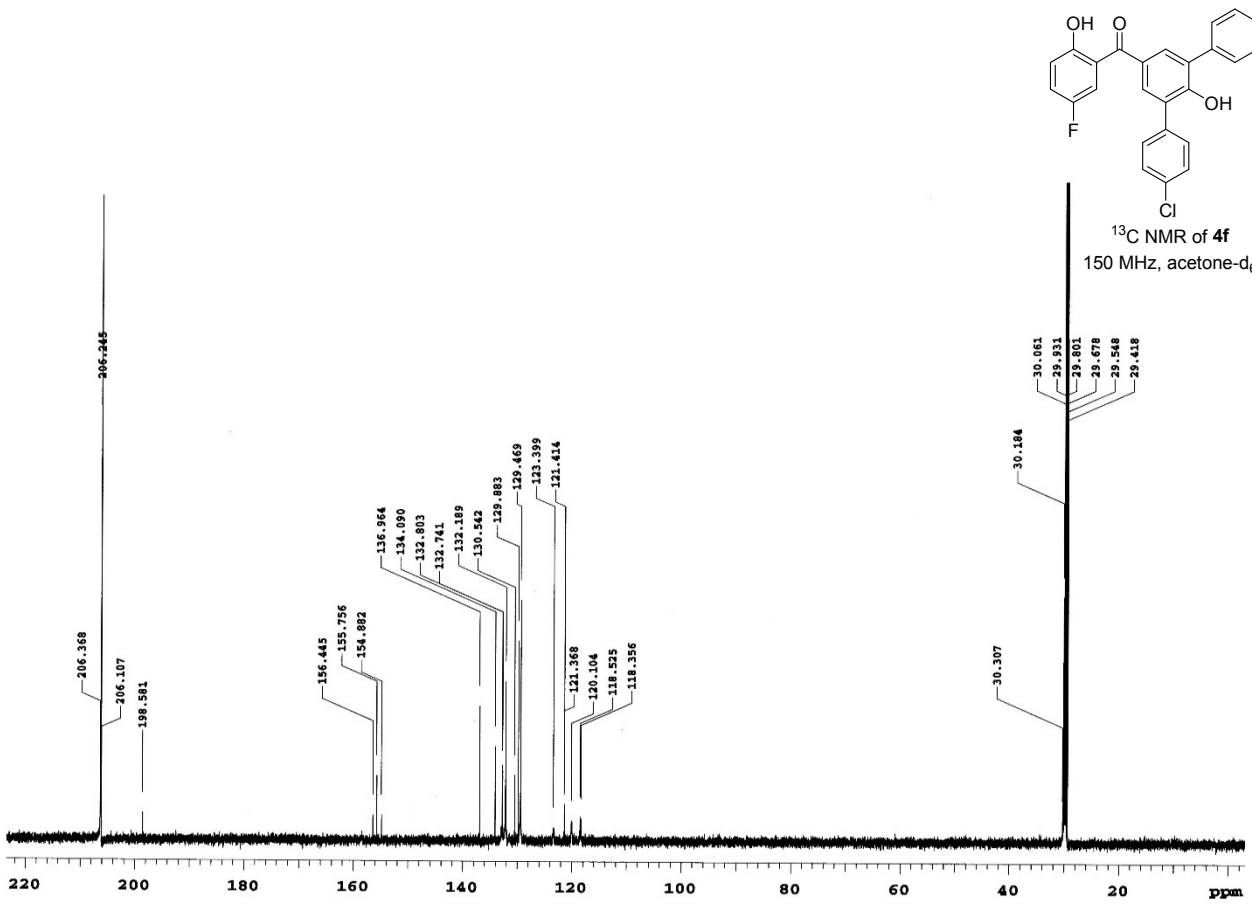


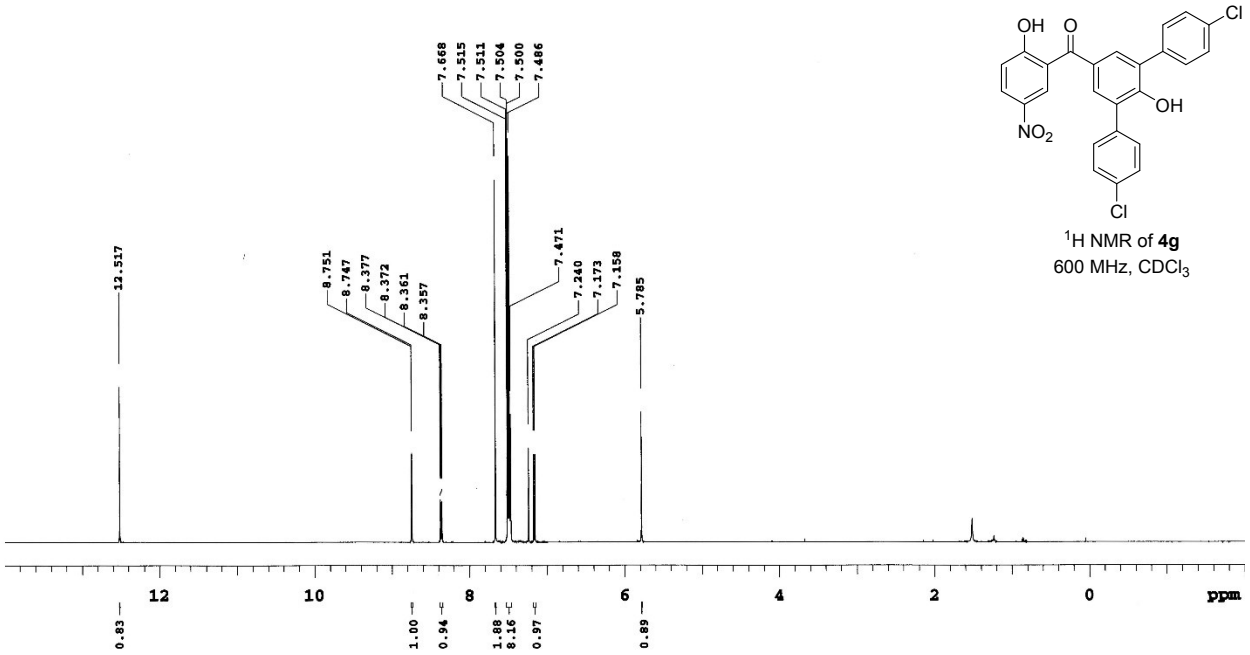
^{13}C NMR of **4e**
75 MHz, $CDCl_3$



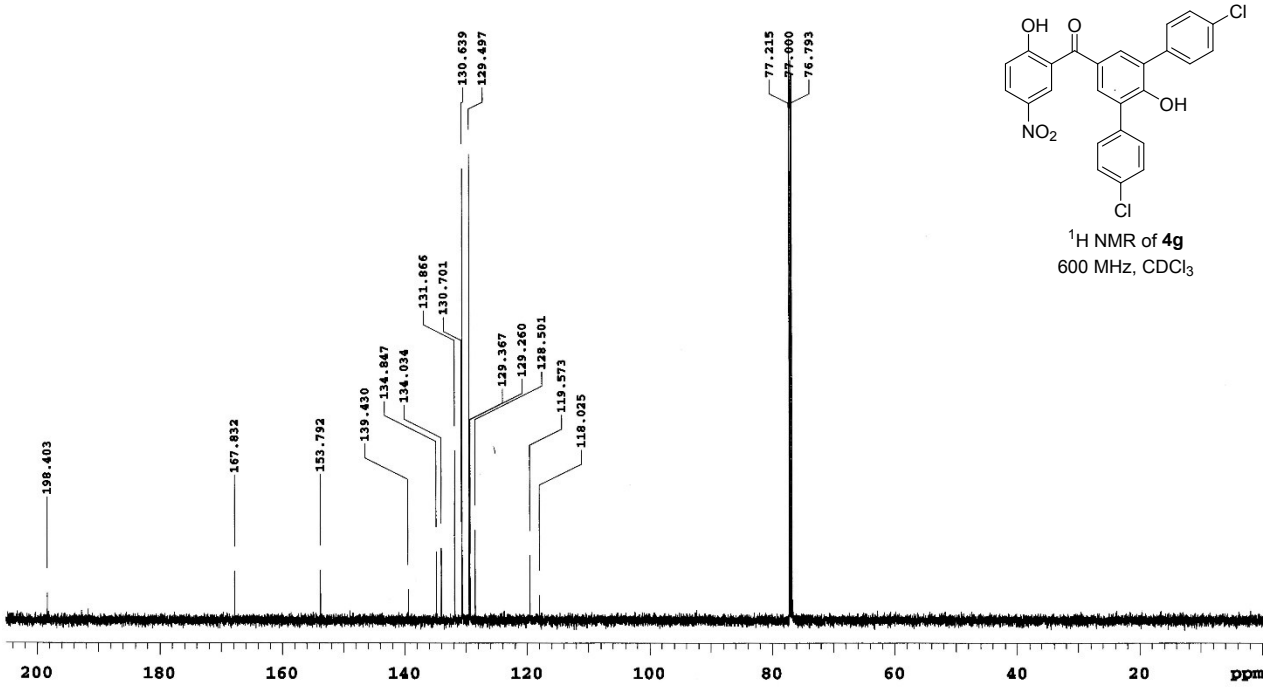
^{1}H NMR of **4f**
600 MHz, acetone-d_6



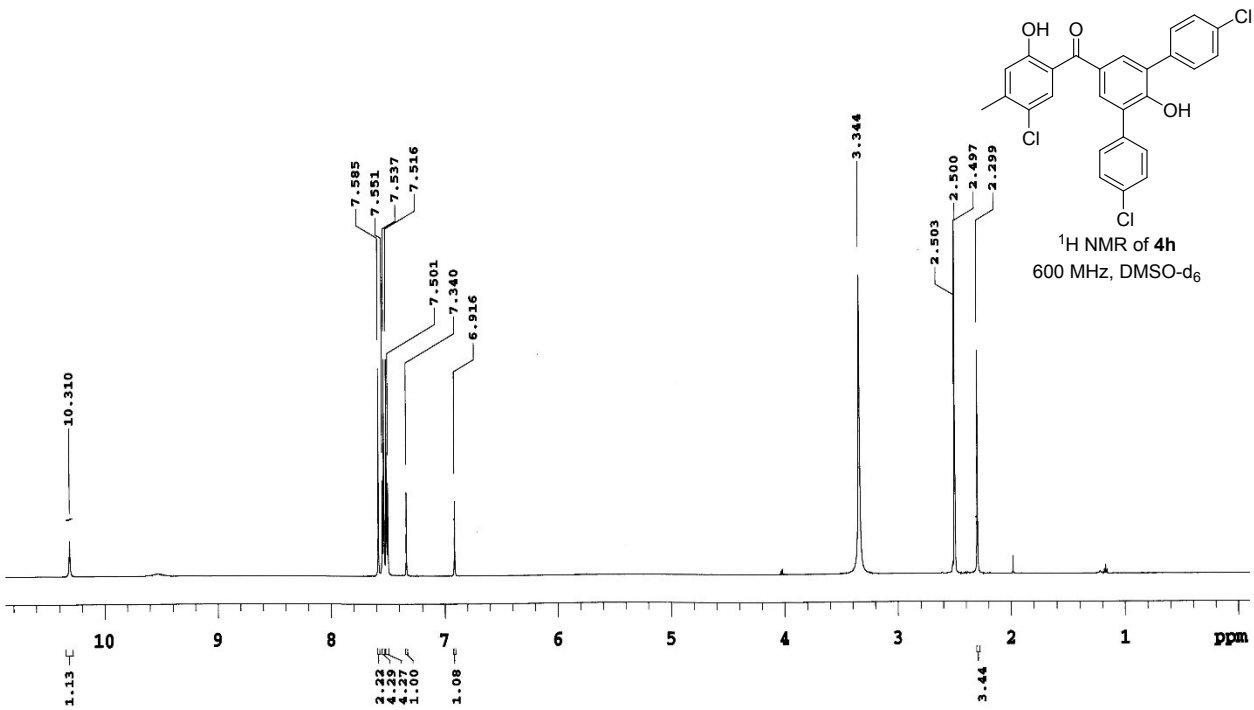
^{13}C NMR of **4f**
150 MHz, acetone-d_6



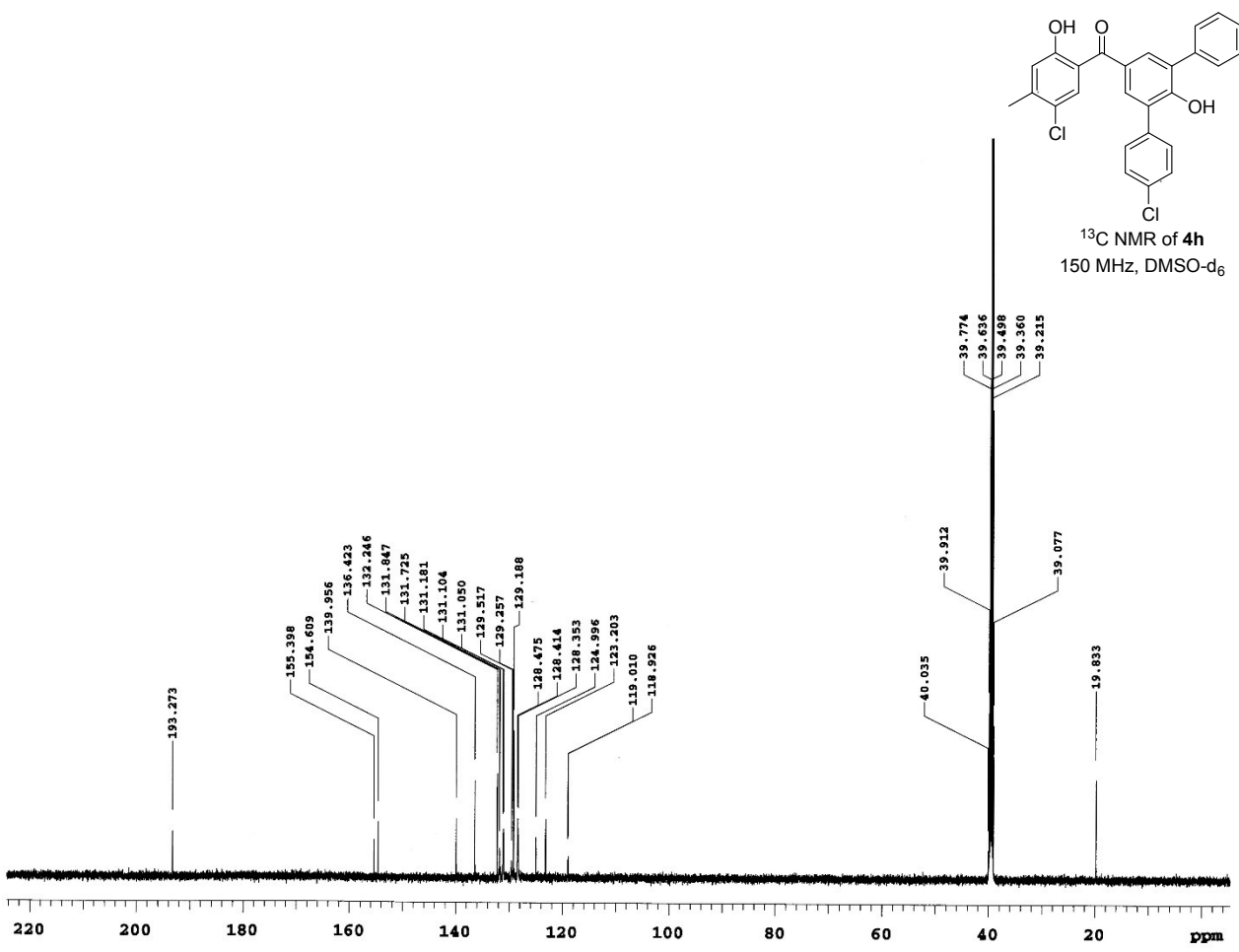
^{1}H NMR of **4g**
600 MHz, $CDCl_3$



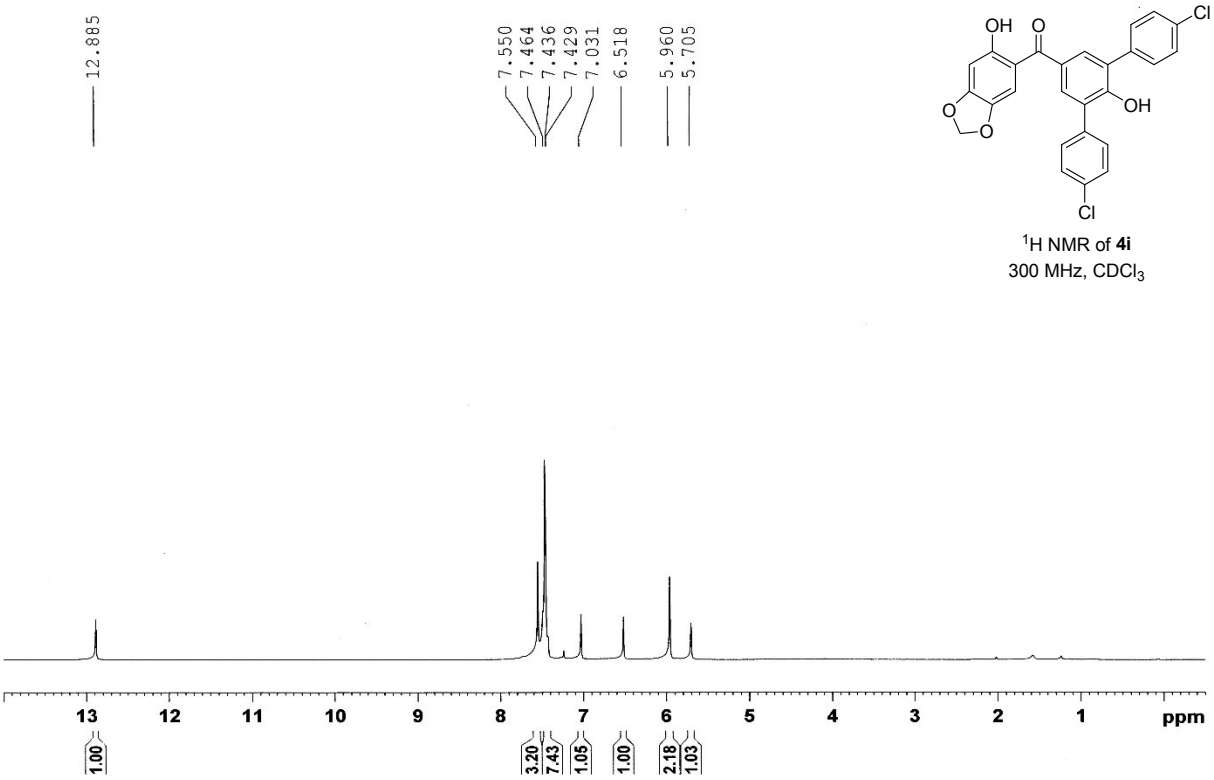
^{1}H NMR of **4g**
600 MHz, $CDCl_3$



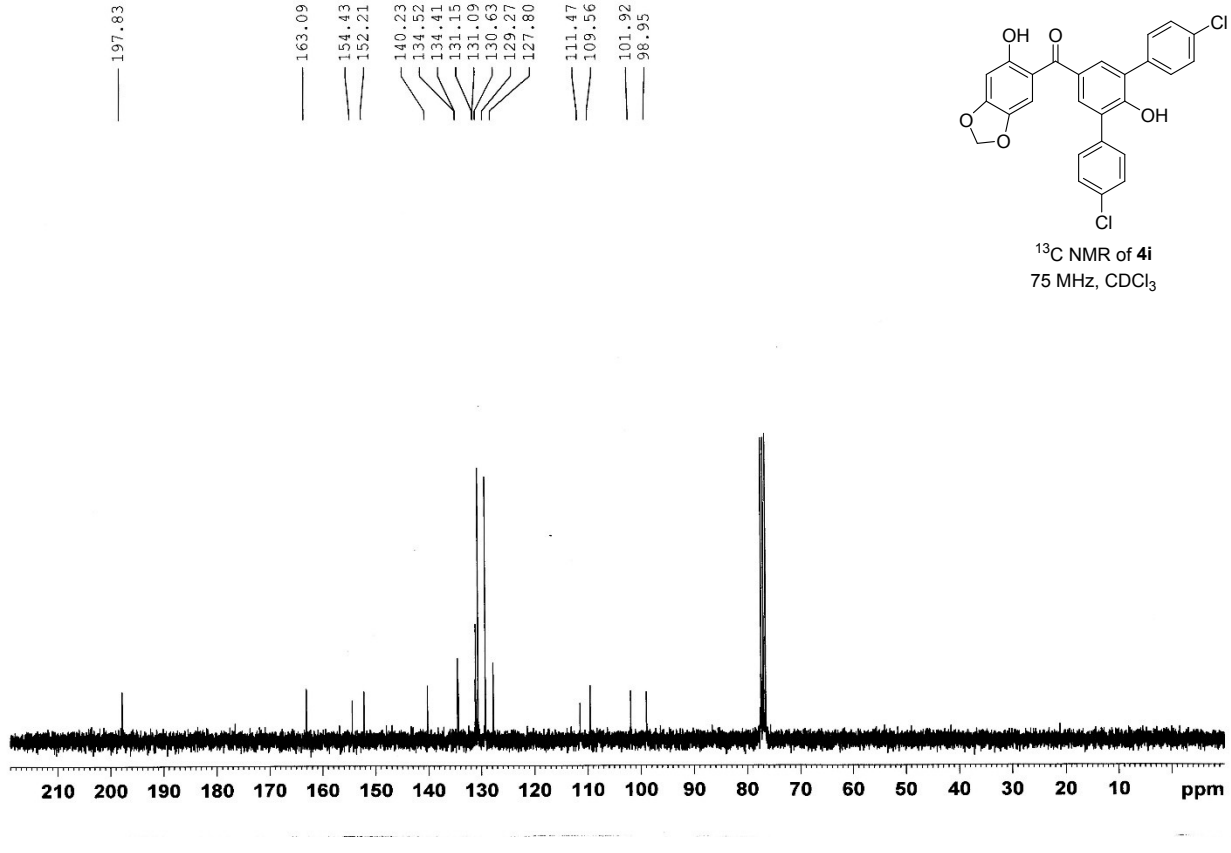
^{1}H NMR of **4h**
600 MHz, DMSO-d_6



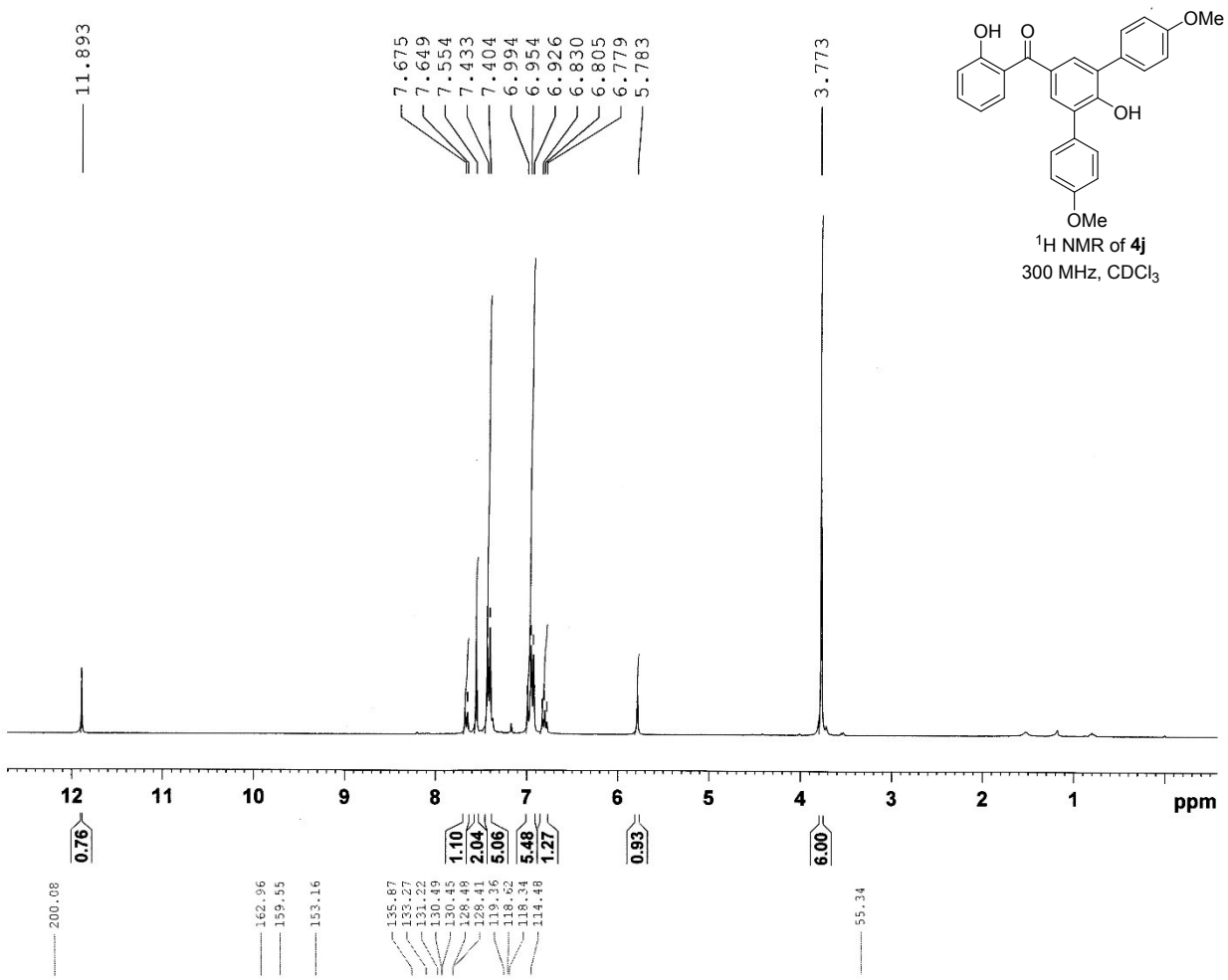
^{13}C NMR of **4h**
150 MHz, DMSO-d_6



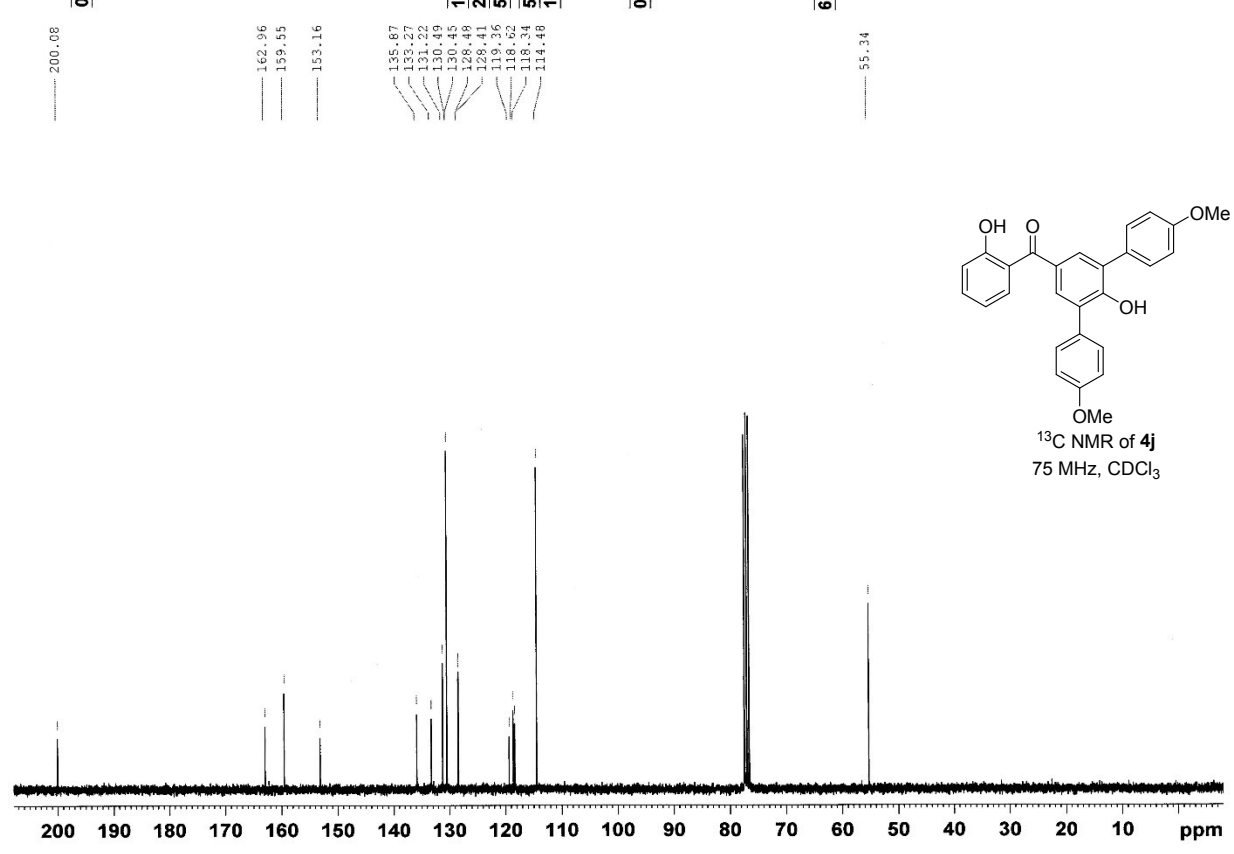
^{1}H NMR of **4i**
300 MHz, $CDCl_3$



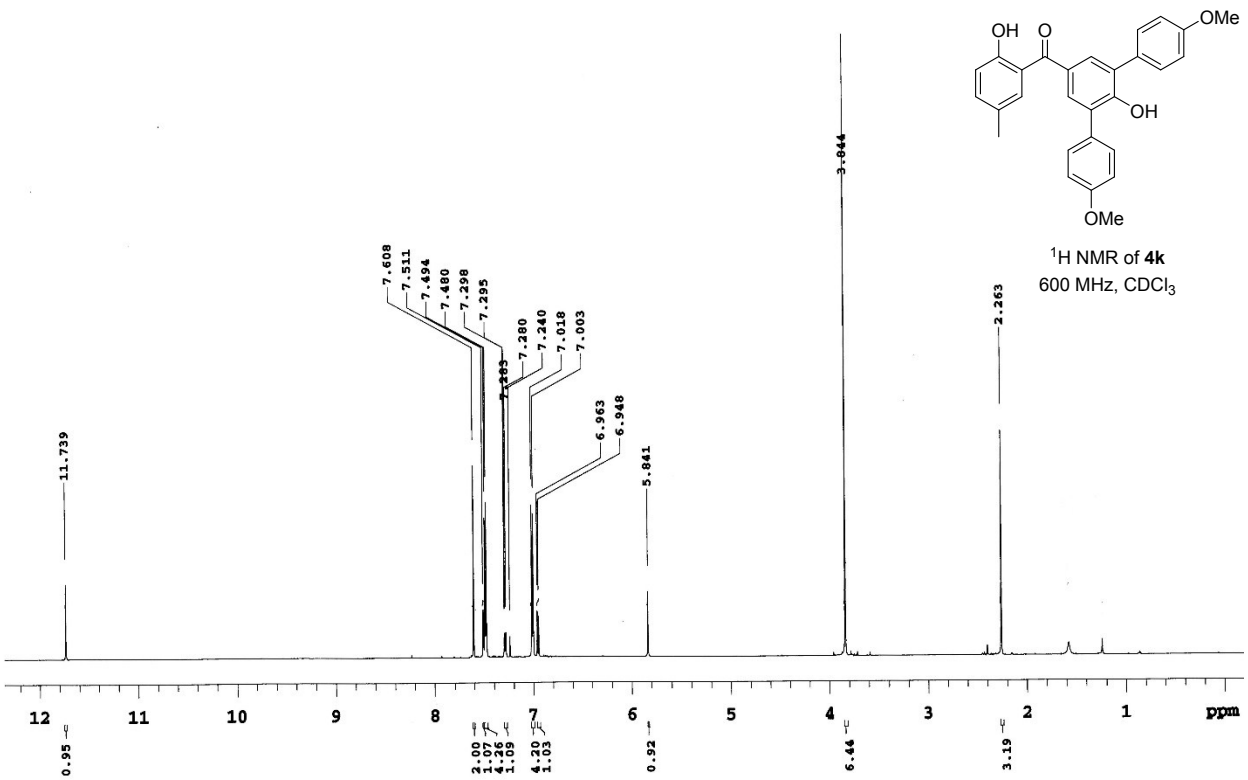
^{13}C NMR of **4i**
75 MHz, $CDCl_3$



^{1}H NMR of **4j**
300 MHz, $CDCl_3$



^{13}C NMR of **4j**
75 MHz, $CDCl_3$



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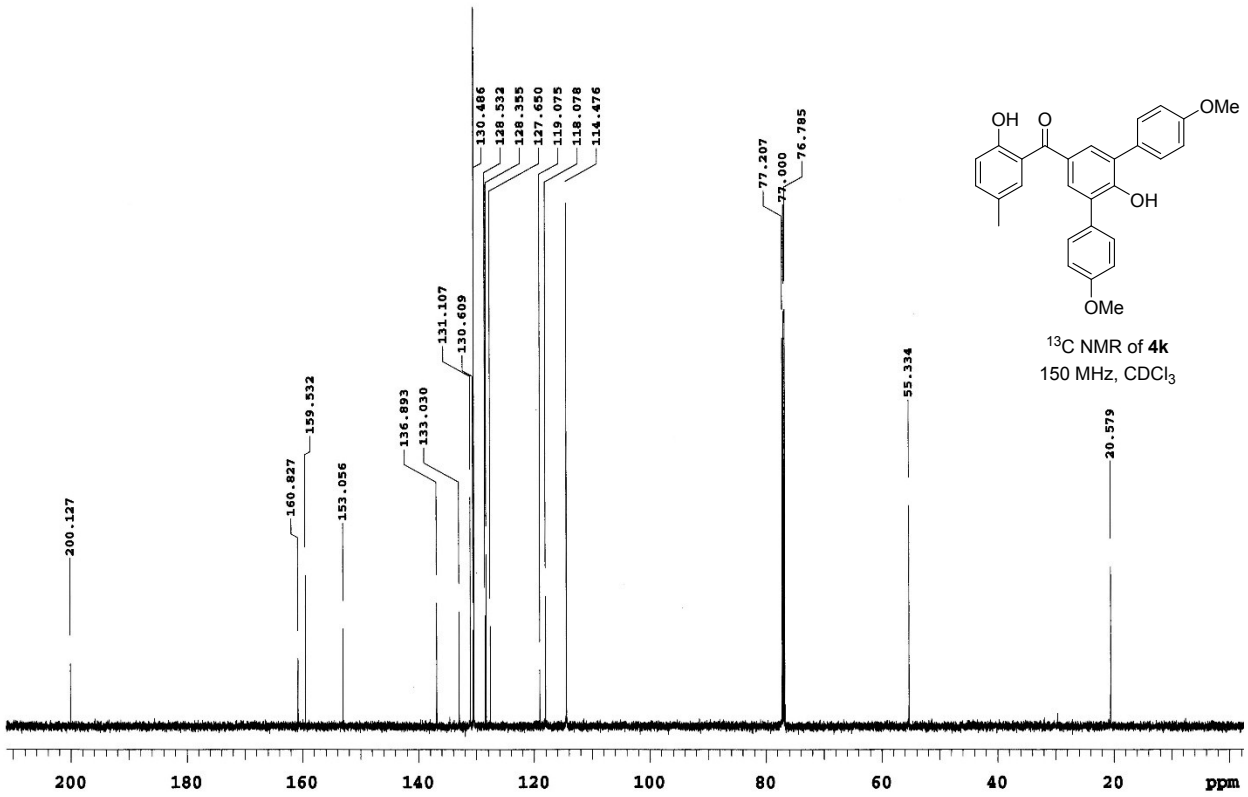
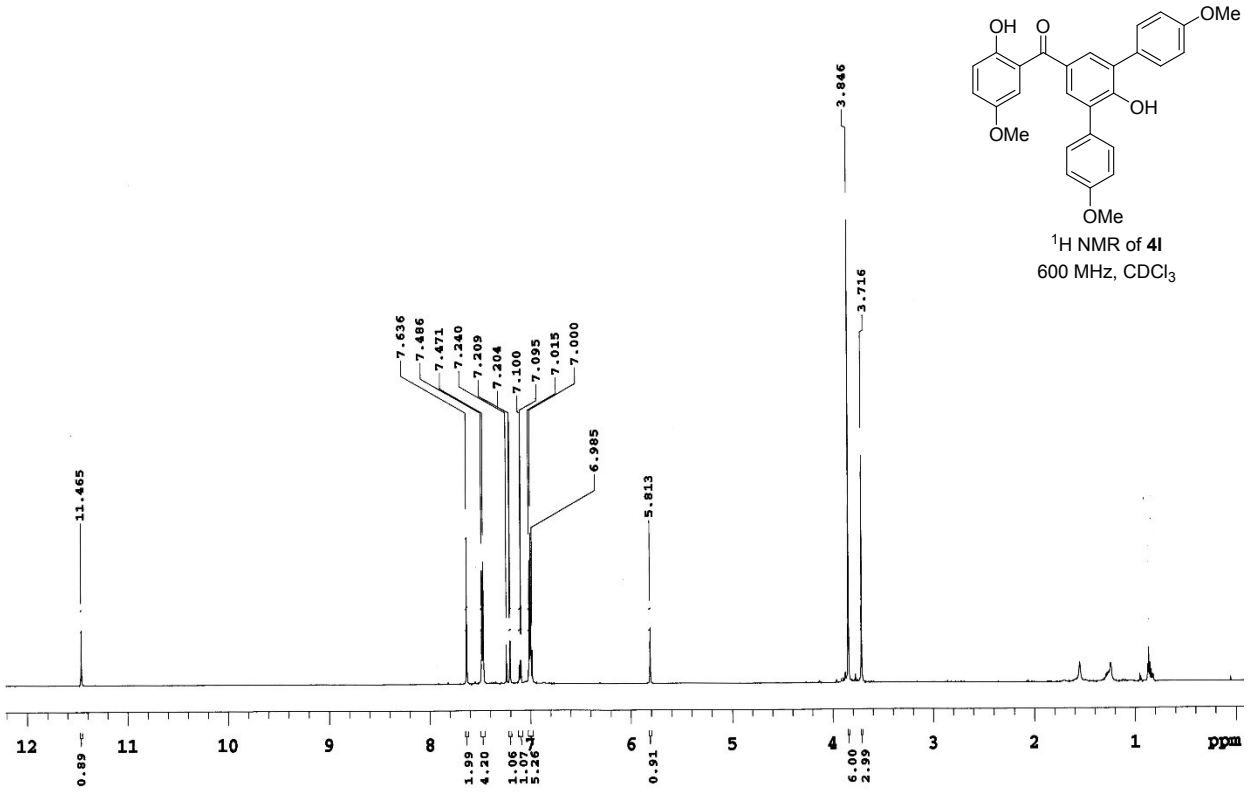
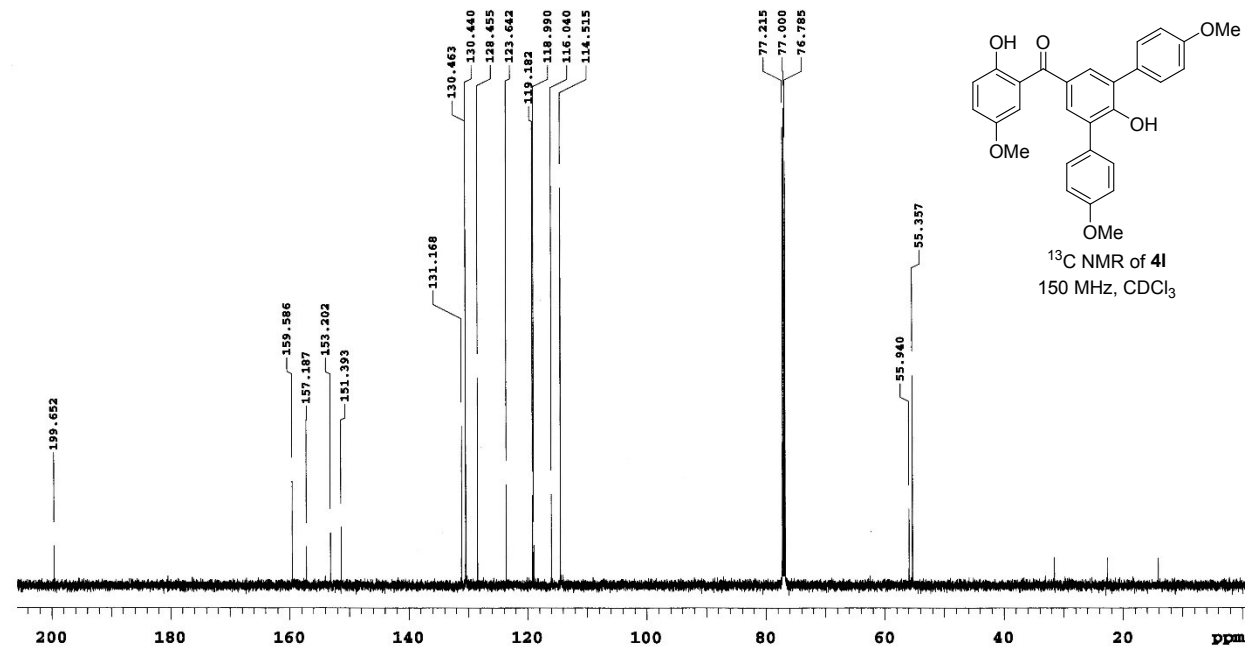
600 MHz, $CDCl_3$



^{13}C NMR of **4k**
150 MHz, $CDCl_3$



^{1}H NMR of **4l**
600 MHz, $CDCl_3$



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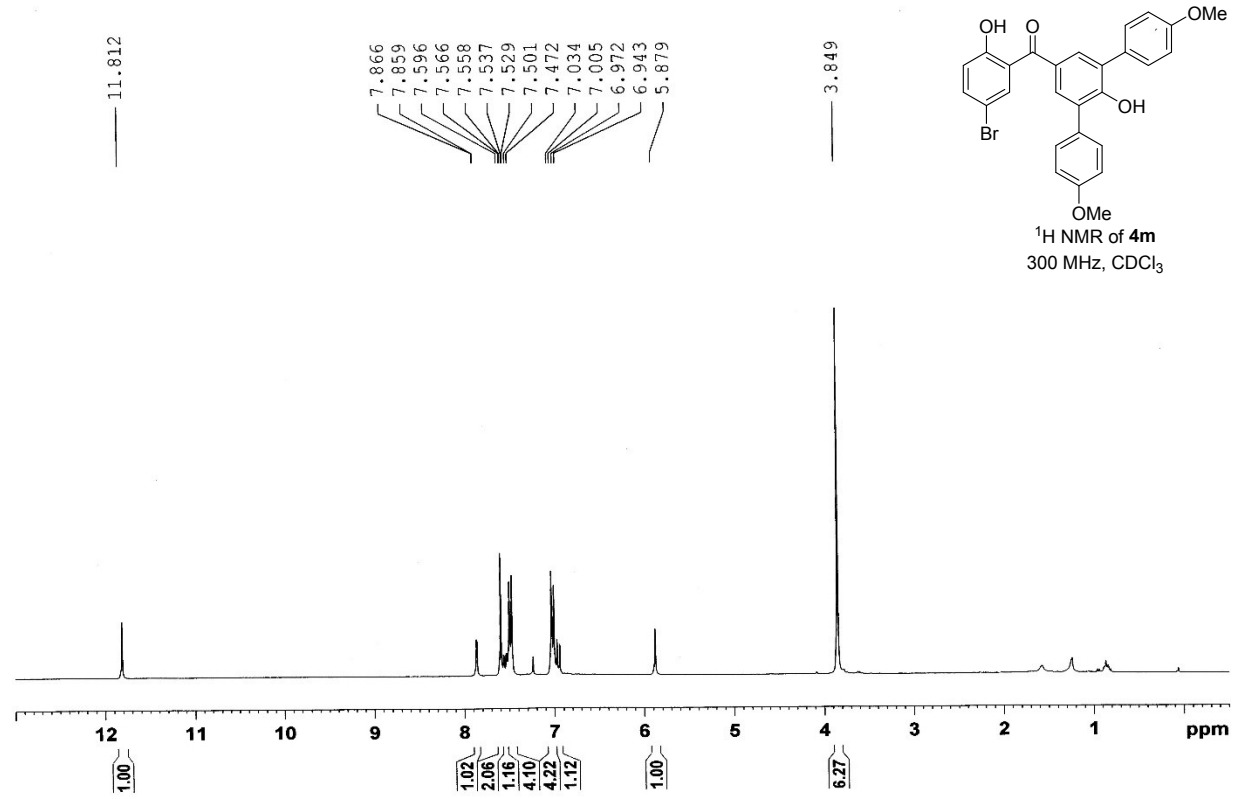
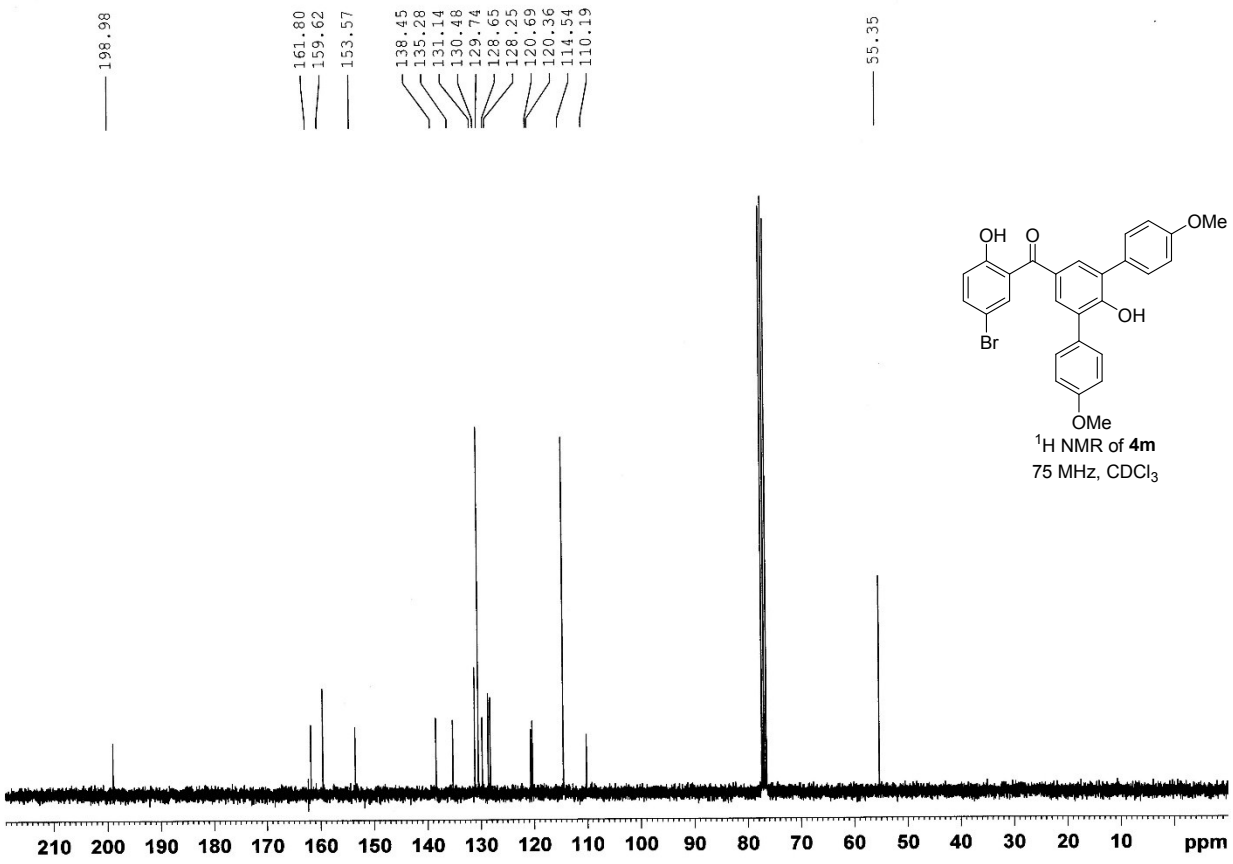
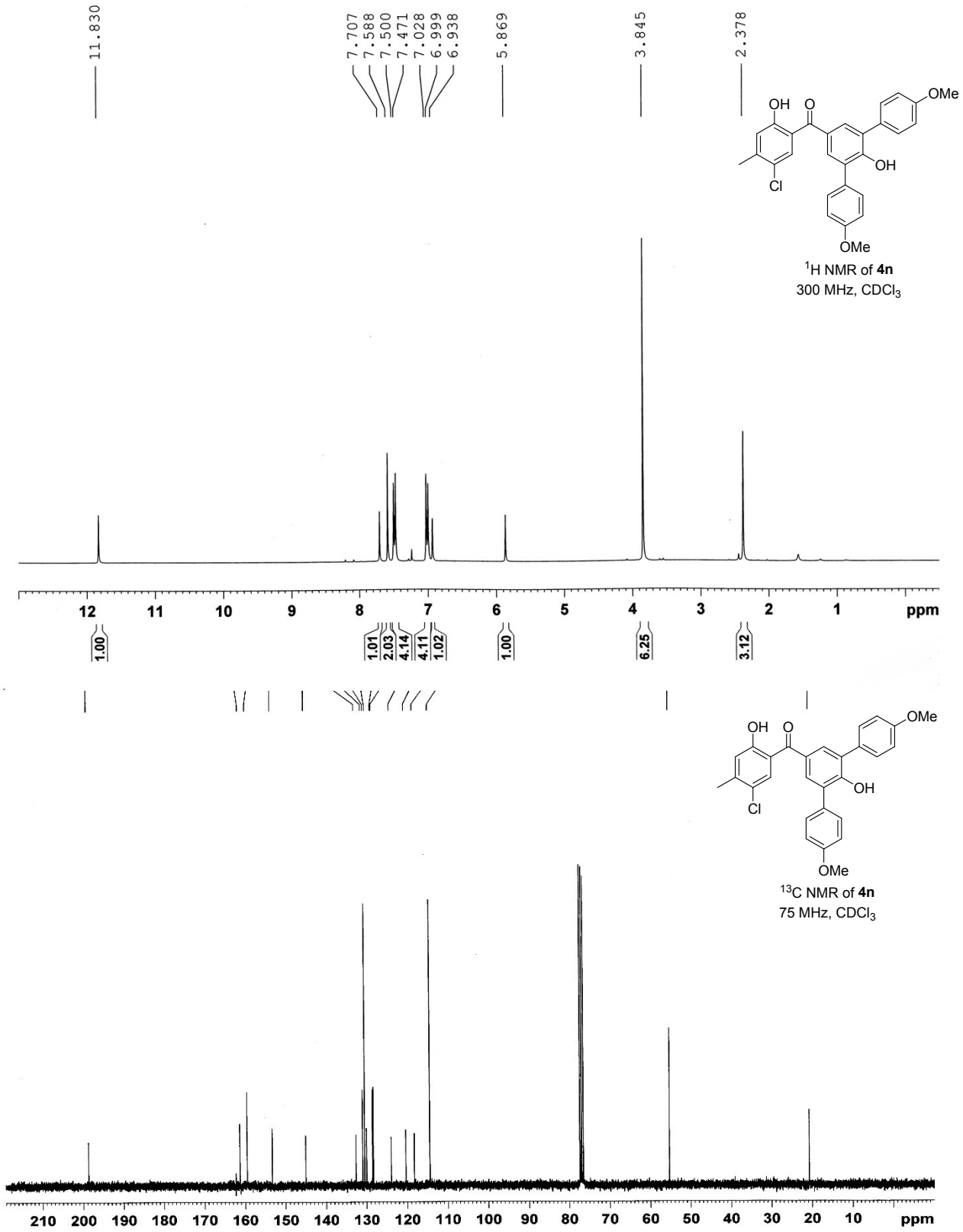


^{1}H NMR of **4m**
300 MHz, $CDCl_3$

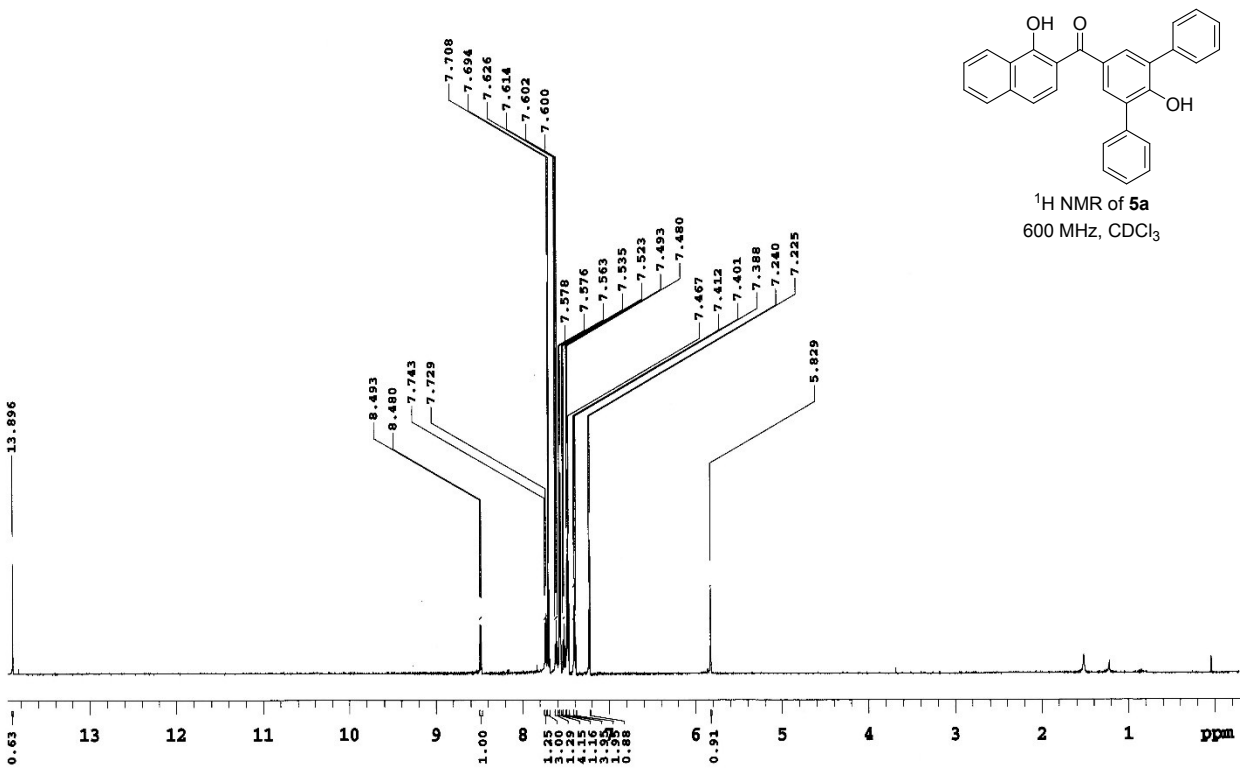


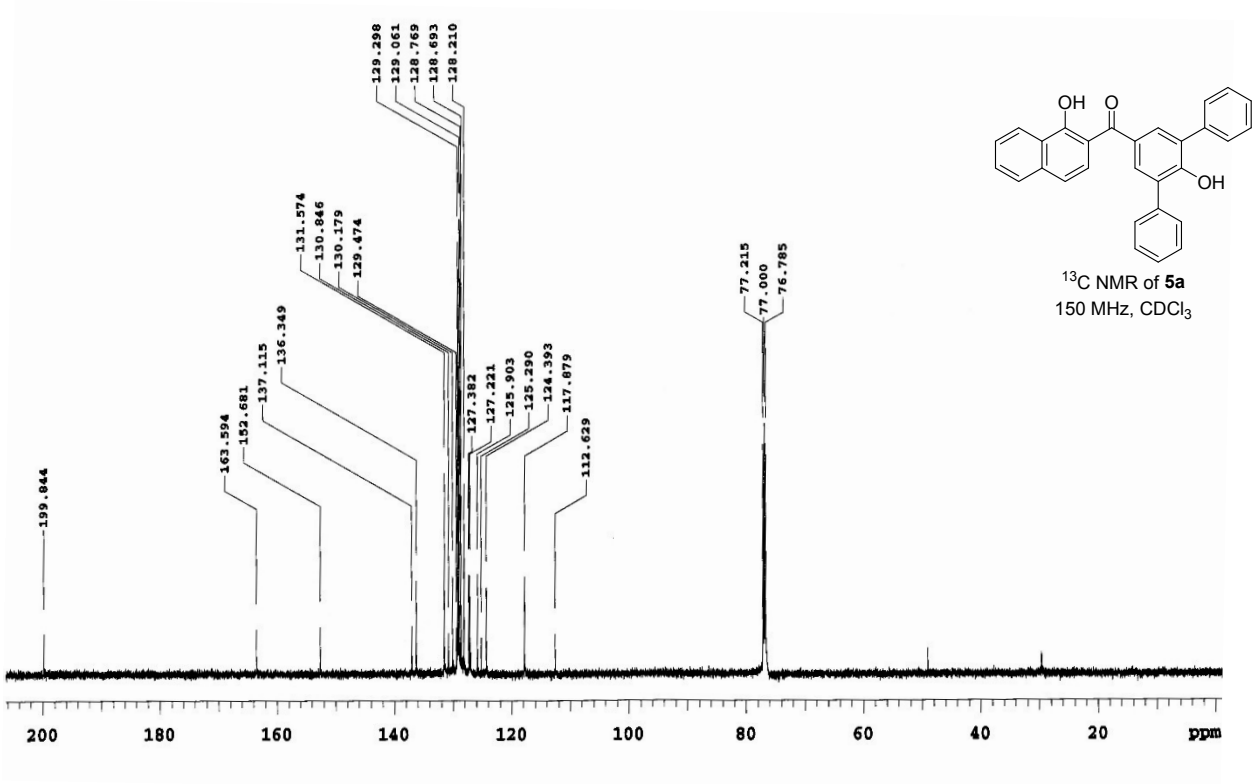
^{1}H NMR of **4m**
75 MHz, $CDCl_3$

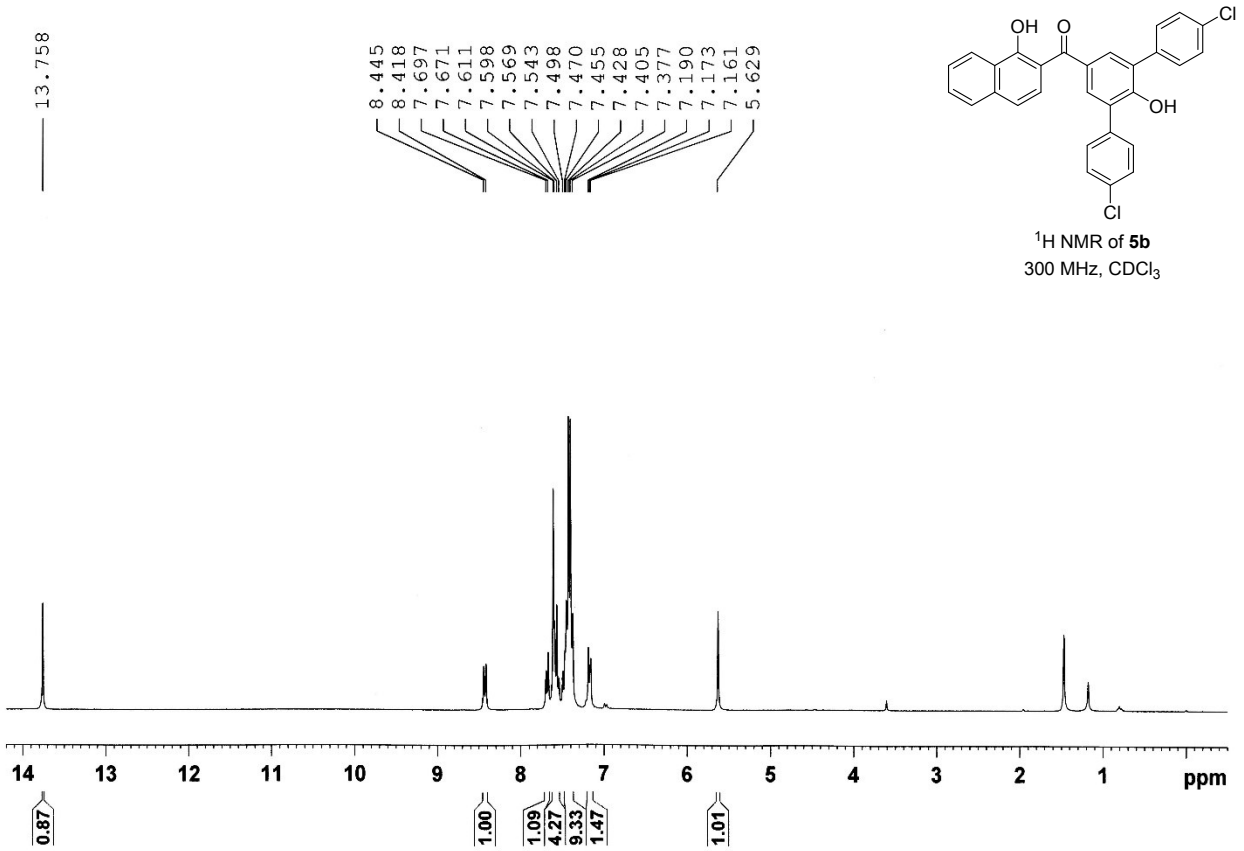


^{1}H NMR of **4n**
300 MHz, $CDCl_3$

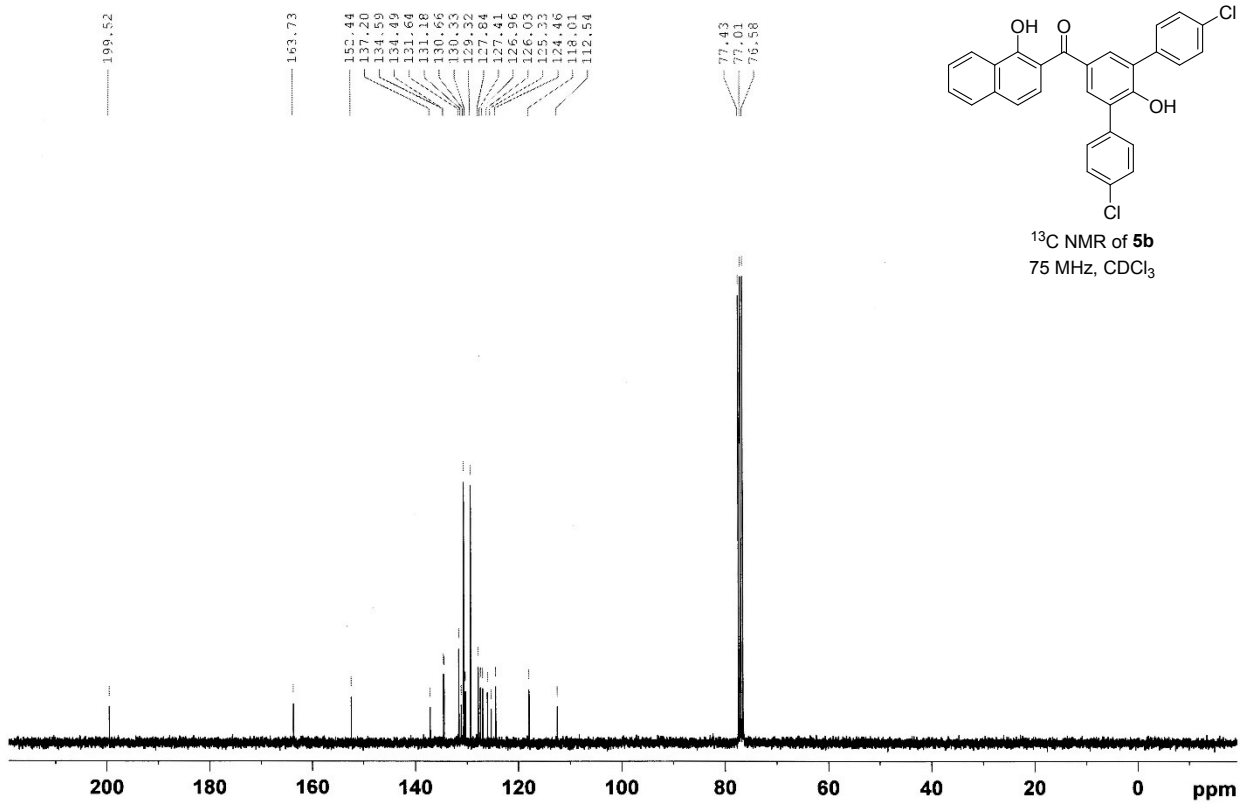
^{13}C NMR of **4n**
75 MHz, $CDCl_3$


OH
O
OH
^{1}H NMR of **5a**
600 MHz, $CDCl_3$
7.708
7.694
7.626
7.614
7.602
7.600
7.578
7.576
7.563
7.535
7.523
7.493
7.480
7.467
7.412
7.401
7.388
7.240
7.225
8.493
8.480
7.743
7.729
5.829
13.896
ppm

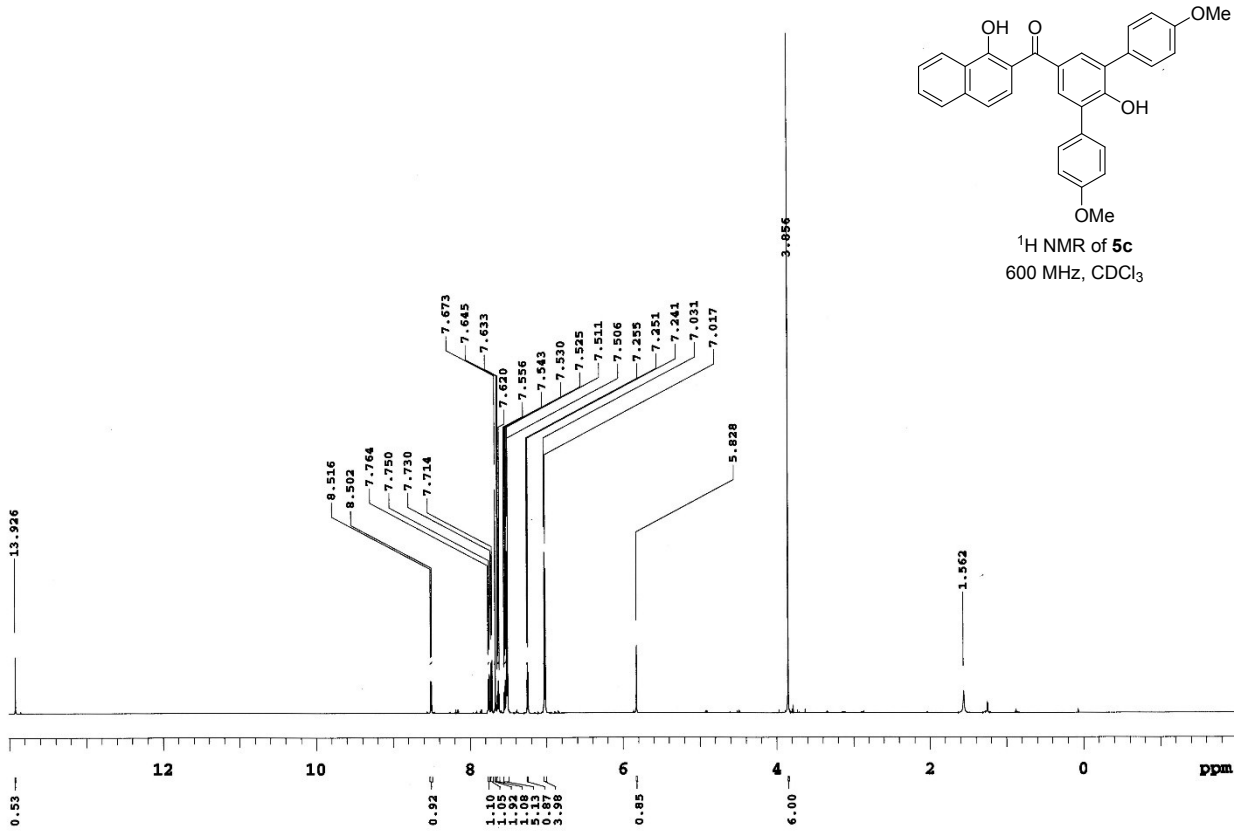

OH
O
OH
^{13}C NMR of **5a**
150 MHz, $CDCl_3$
129.298
129.061
128.769
128.693
128.210
131.574
130.846
130.179
129.474
136.349
137.115
152.681
163.594
127.382
127.221
125.903
125.290
124.393
117.879
112.629
199.844
77.215
77.000
76.785
ppm



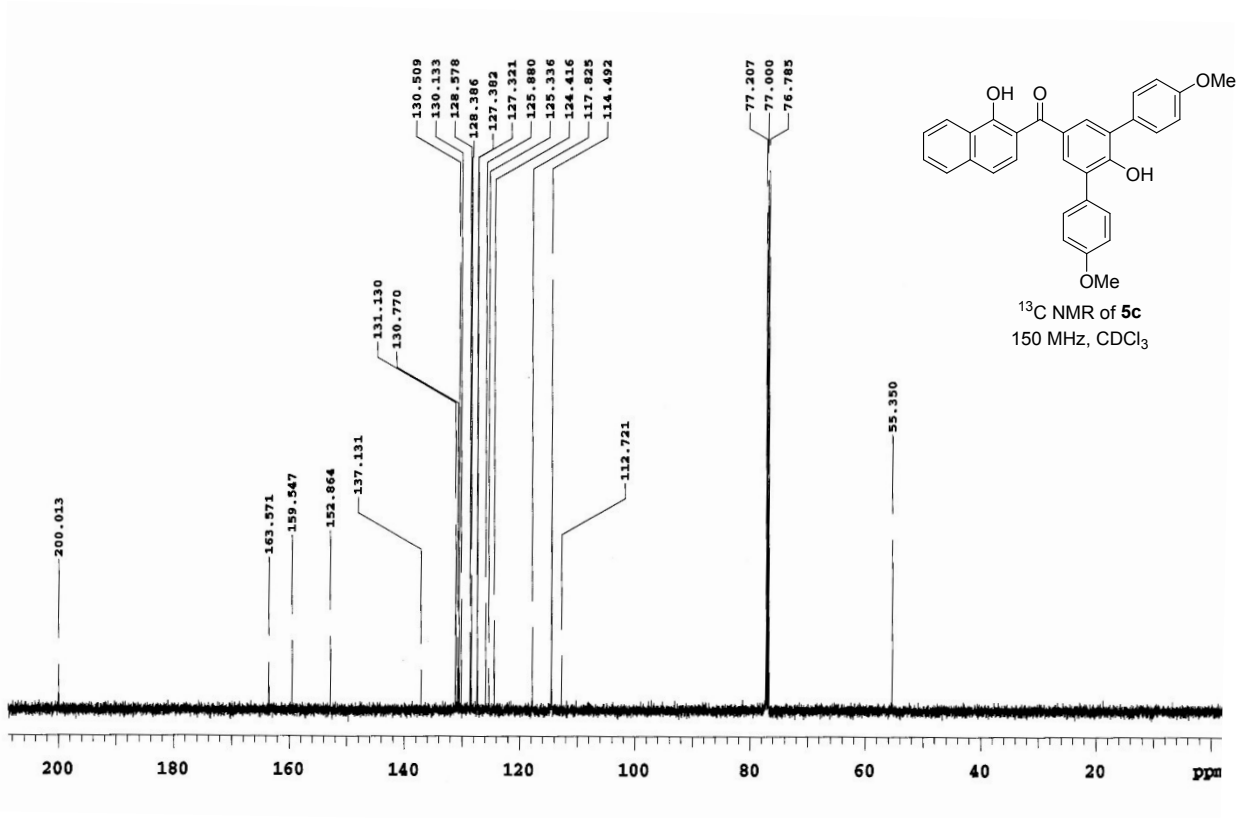
^{1}H NMR of **5b**
300 MHz, $CDCl_3$



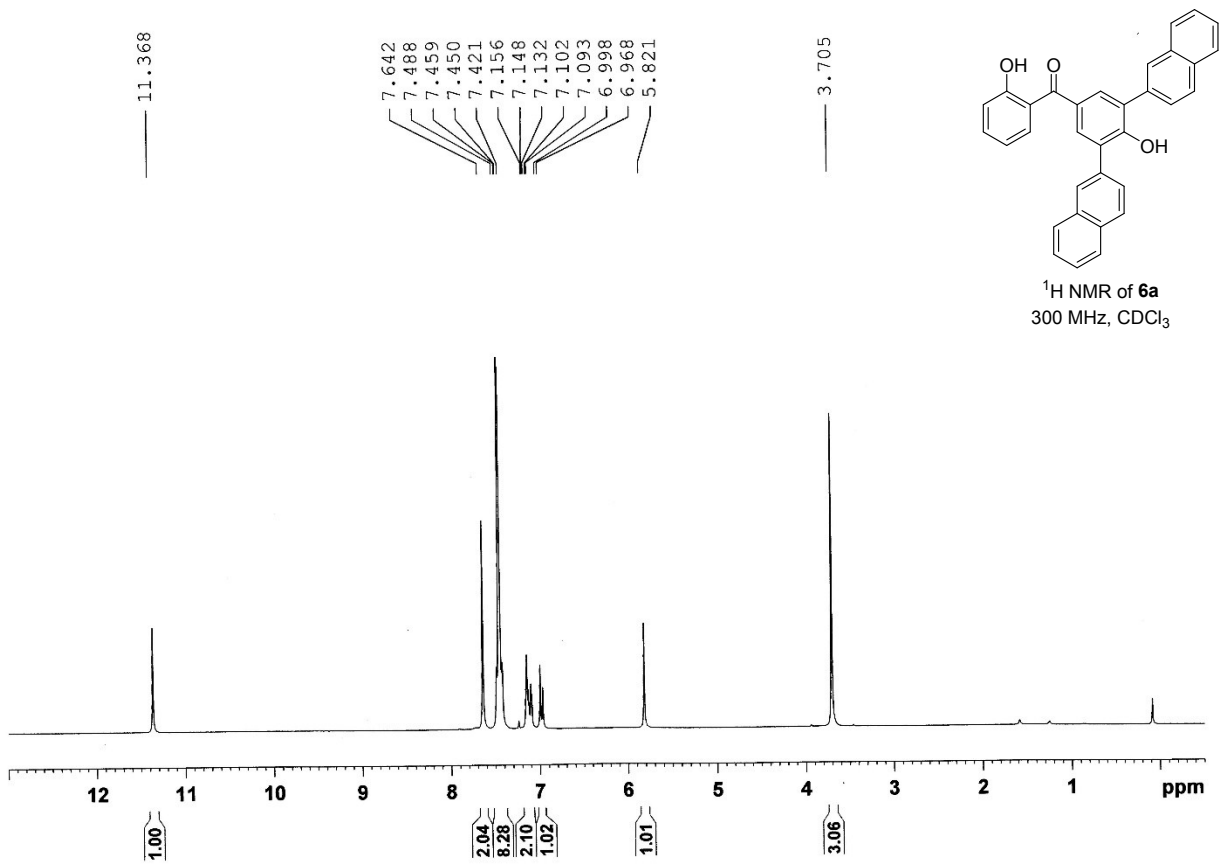
^{13}C NMR of **5b**
75 MHz, $CDCl_3$



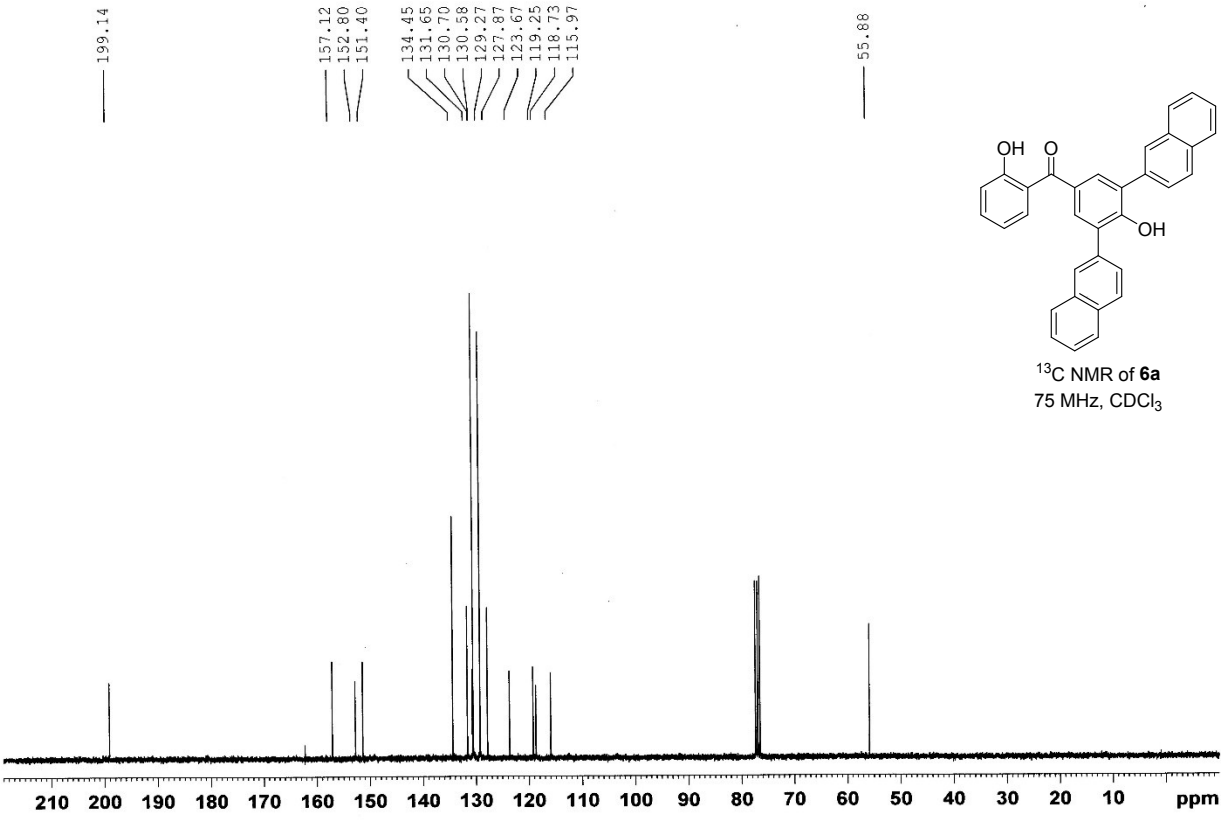
^{1}H NMR of **5c**
600 MHz, $CDCl_3$



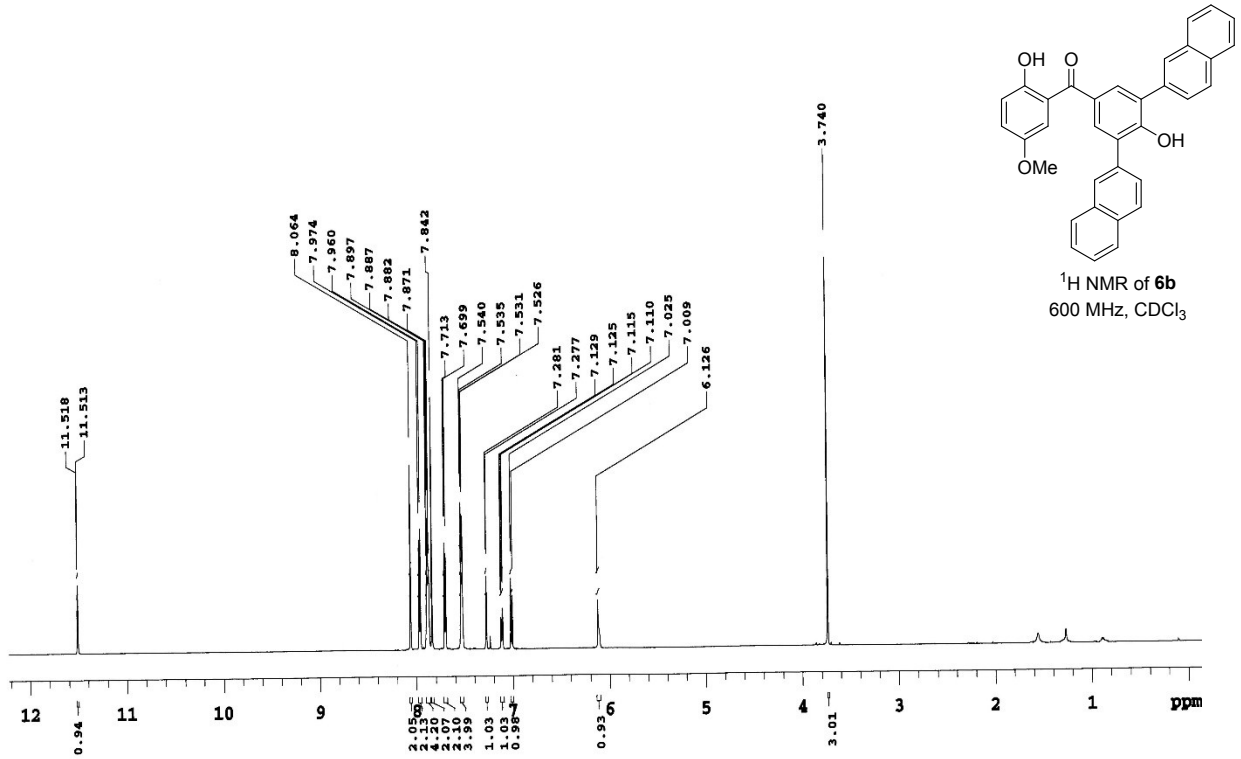
^{13}C NMR of **5c**
150 MHz, $CDCl_3$



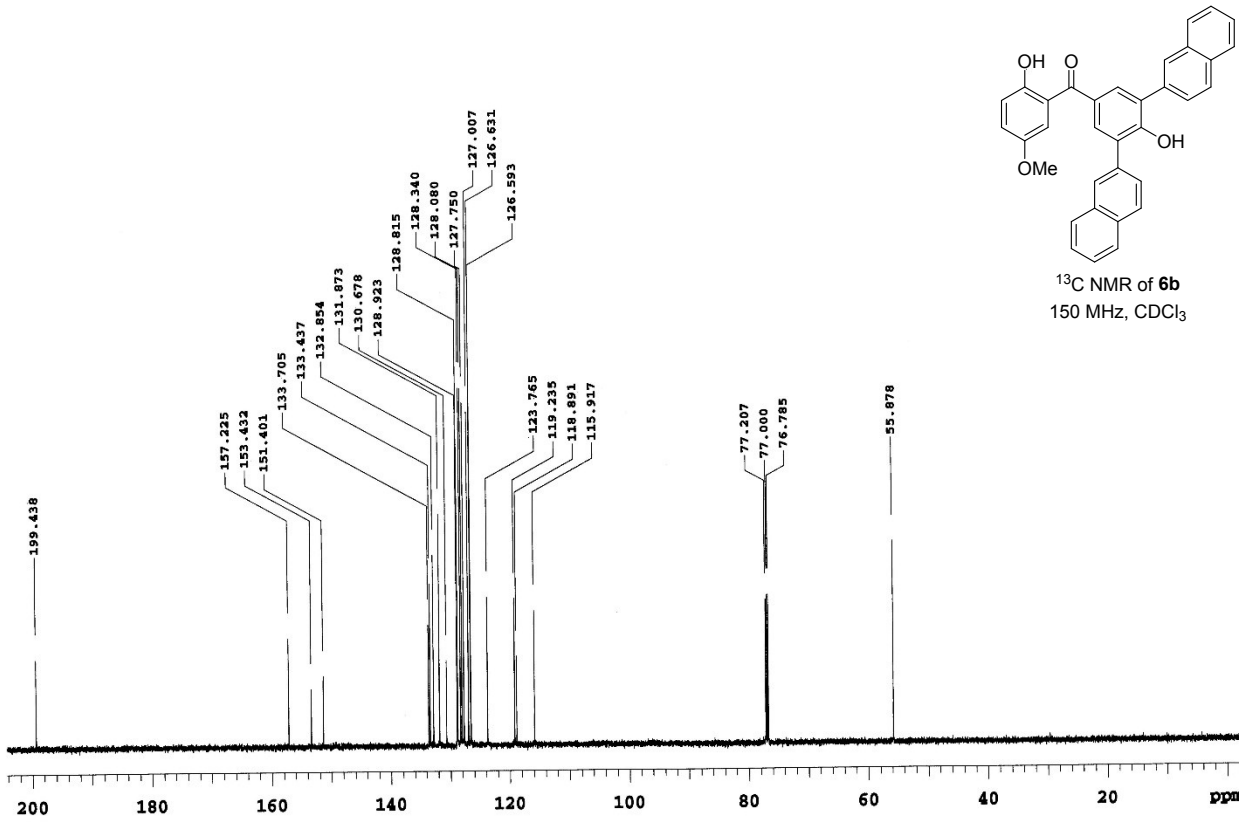
^{1}H NMR of **6a**
300 MHz, $CDCl_3$



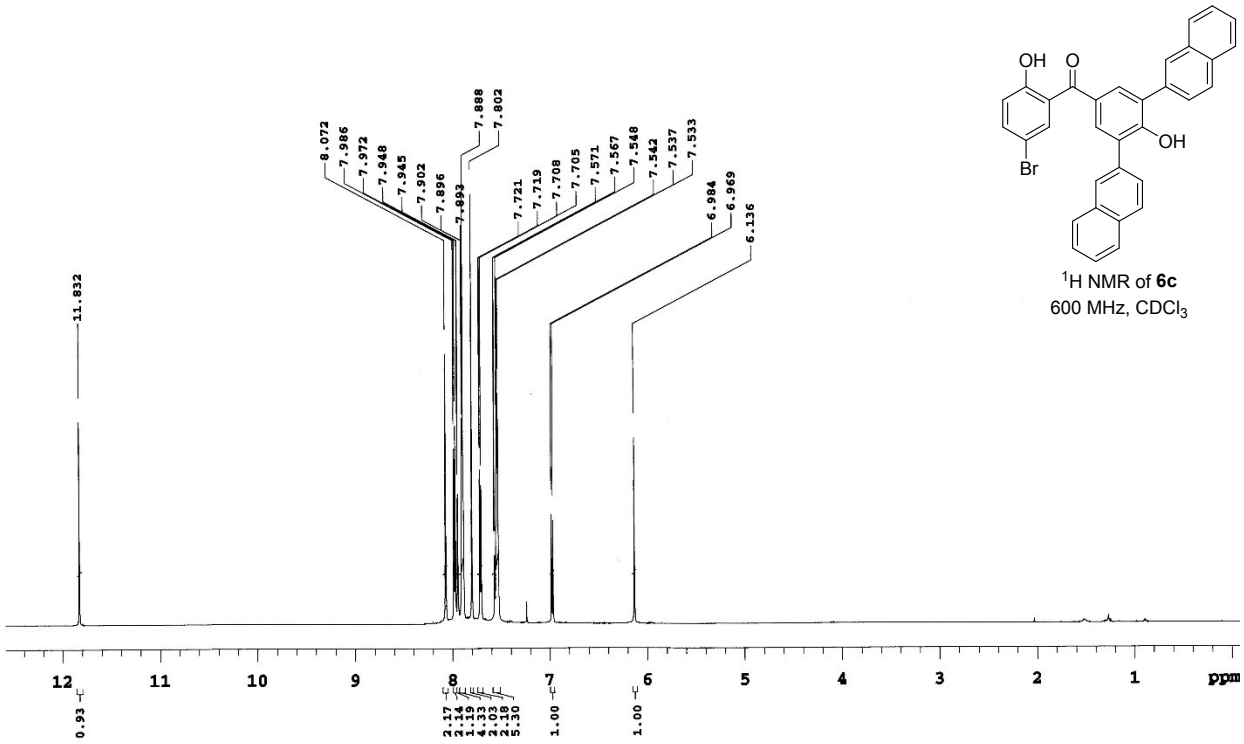
^{13}C NMR of **6a**
75 MHz, $CDCl_3$



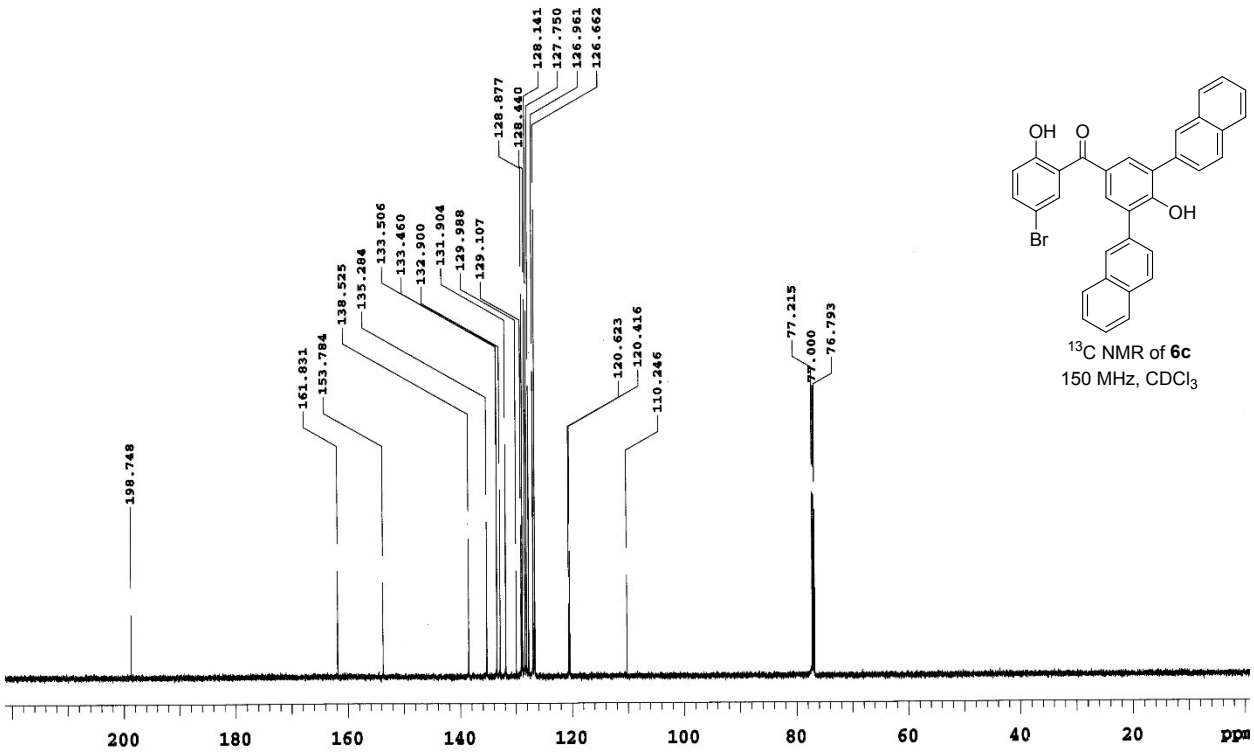
^{1}H NMR of **6b**
600 MHz, $CDCl_3$



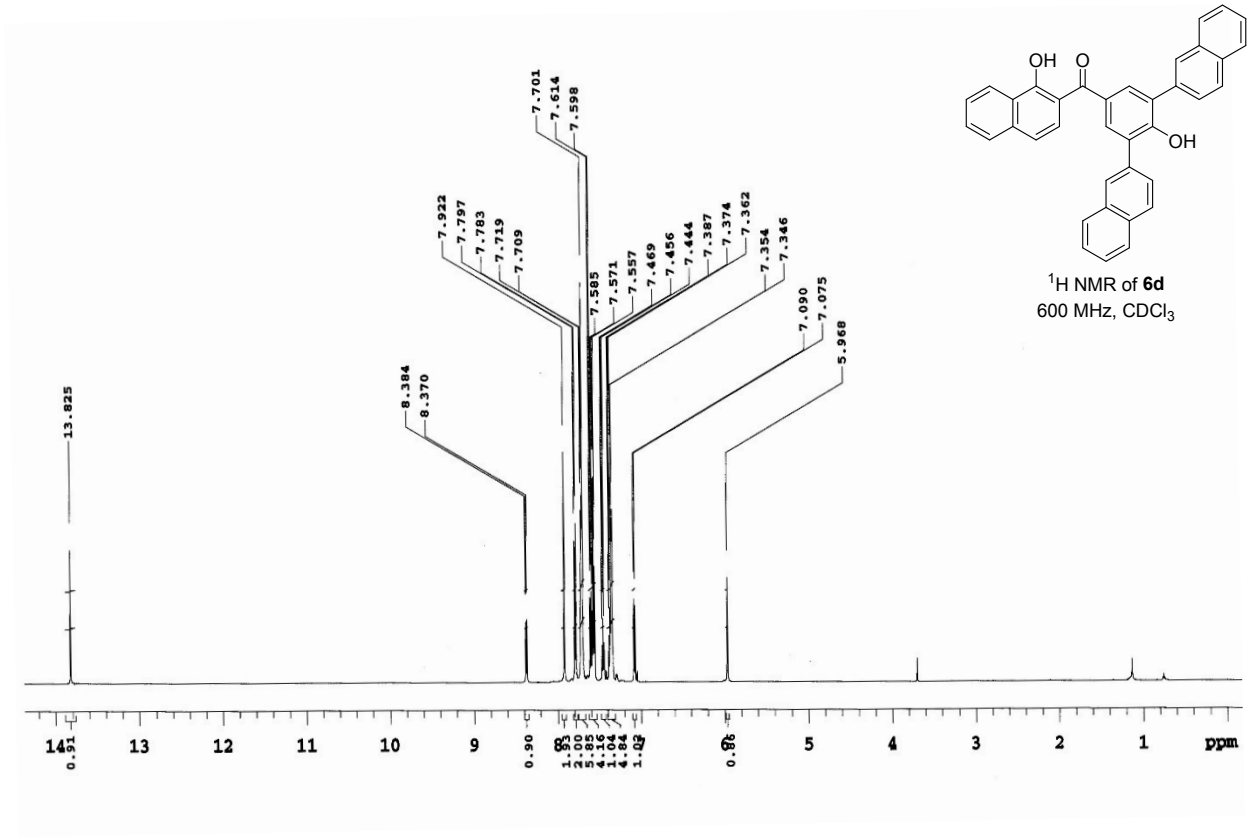
^{13}C NMR of **6b**
150 MHz, $CDCl_3$

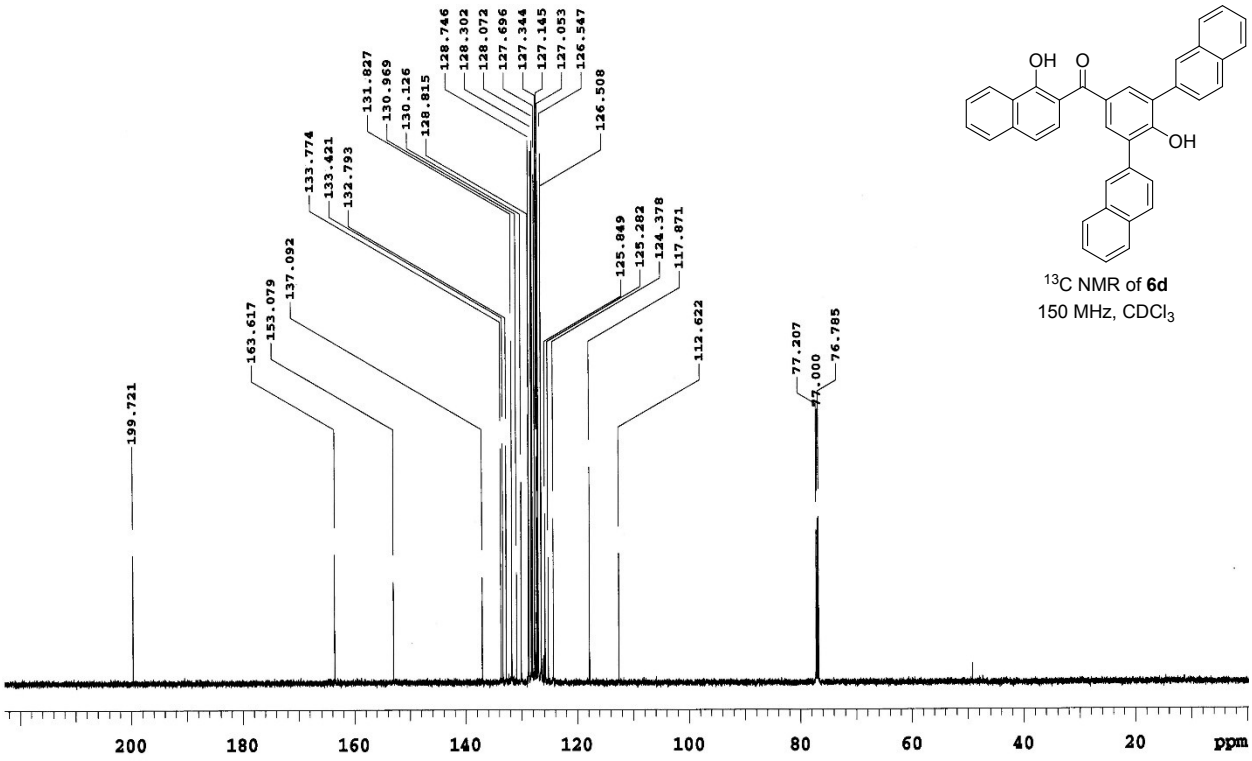


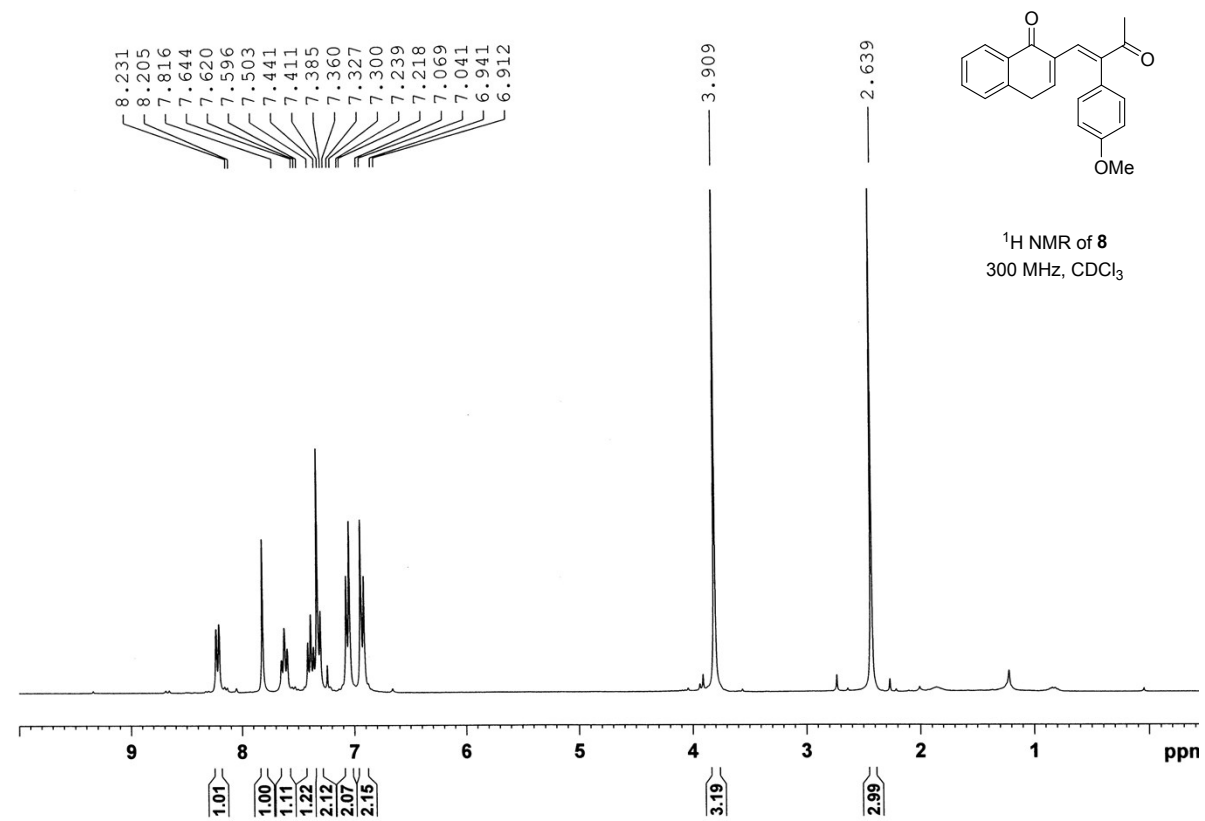
^{1}H NMR of **6c**
600 MHz, $CDCl_3$



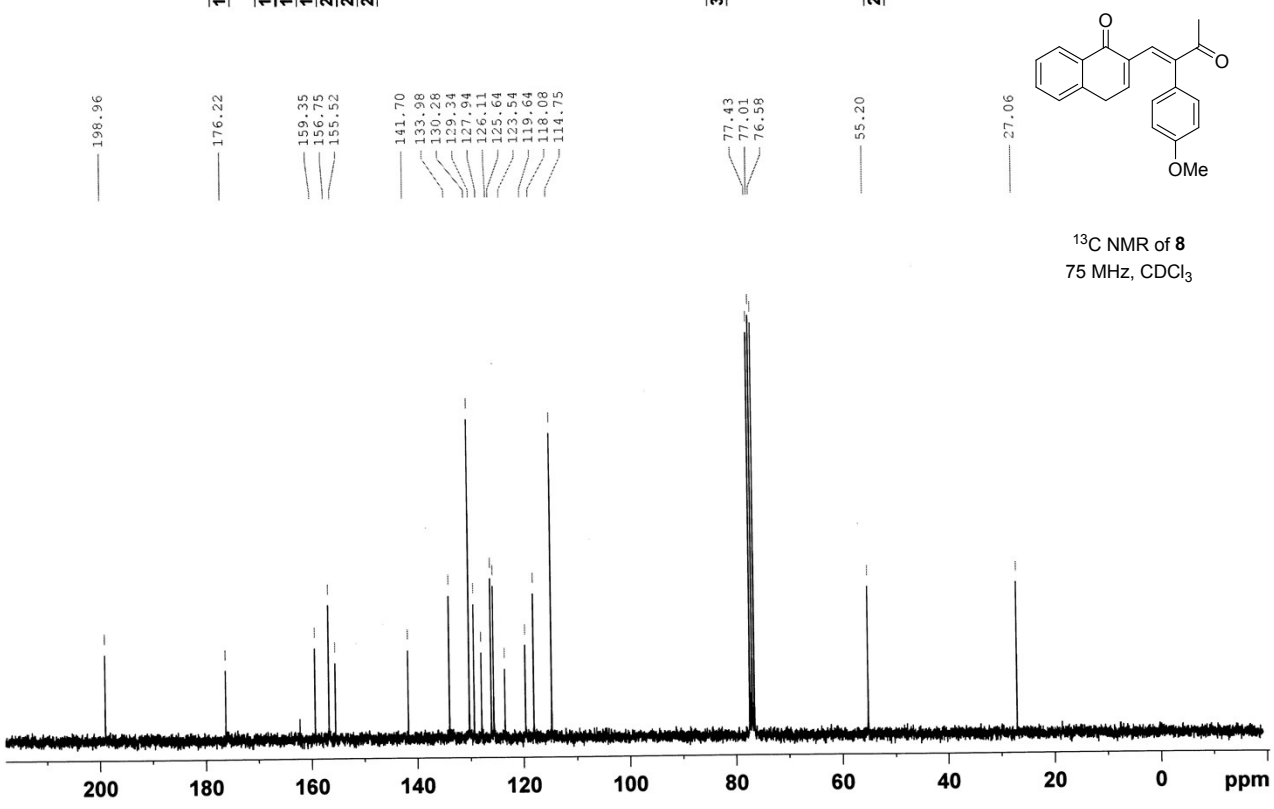
^{13}C NMR of **6c**
150 MHz, $CDCl_3$


OH
O
OH
^{1}H NMR of **6d**
600 MHz, $CDCl_3$
13.825
8.384
8.370
7.922
7.797
7.783
7.719
7.709
7.701
7.614
7.598
7.585
7.571
7.557
7.469
7.456
7.444
7.387
7.374
7.362
7.354
7.346
7.090
7.075
5.968
ppm


OH
O
OH
^{13}C NMR of **6d**
150 MHz, $CDCl_3$
199.721
163.617
153.079
137.092
133.774
133.421
132.793
131.827
130.969
130.126
128.815
128.746
128.302
128.072
127.696
127.344
127.145
127.053
126.547
126.508
125.849
125.282
124.378
117.871
112.622
77.207
77.000
76.785
ppm



^{1}H NMR of **8**
300 MHz, $CDCl_3$



^{13}C NMR of **8**
75 MHz, $CDCl_3$

Procedure for the UV absorption experiment

Absorbance spectra of the tested compounds were recorded at room temperature (298 K) using UV/Vis spectrophotometer (Optizen UV-3200). The samples were prepared in an ethanol solvent (Sigma-Aldrich, ≥ 99.8% pure) at a concentration of 50 µM. The data were corrected for solvent background by the instrument's calibration using the ethanol as a blank. The absorption spectra of samples in solution were obtained in the range of 220-600 nm at 1 nm interval in 3 determination using three trial samples. The critical wavelength (λ_c) and UVA/UVB ratio were calculated using equation 1 and 2, respectively, as shown below:

$$\int_{290}^{\lambda_c} A(\lambda)d\lambda = 0.9\int_{290}^{400} A(\lambda)d\lambda \qquad (1)$$

$$\frac{\int_{320}^{400} A(\lambda)d\lambda \Big/ \int_{320}^{400} d\lambda}{\int_{290}^{320} A(\lambda)d\lambda \Big/ \int_{290}^{320} d\lambda} \qquad (2)$$

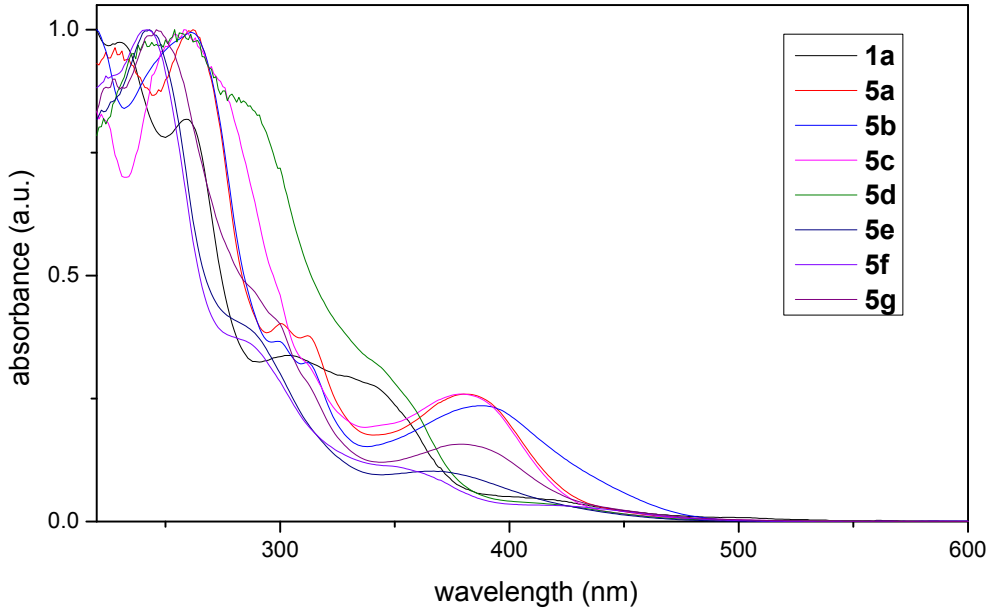


Fig. S1 Normalized UV absorbance spectra of compounds **1a**, **5a-5g** (220-600 nm)

X-Ray crystallographic structure and data of compound 3c: Empirical Formula- $C_{27}H_{22}O_3$, M = 394.45, Monoclinic, Space group P_{bca}, a = 12.4924(9) Å, b = 8.6494 (5) Å, c = 20.0211 (14) Å, V = 2086.5(2) $Å^3$, Z = 4, T = 223(2) K, ρ_{calcd} = 1.256 Mg/m^3, $2\Theta_{max.}$ = 26.07^0, Refinement of 274 parameters on 4126 independent reflections out of 58124 collected reflections (R_{int} = 0.1692) led to R_1 = 0.0487 [I >2σ(I)], wR_2 = 0.1181 (all data) and S = 1.029 with the largest difference peak and hole of 0.218 and -0.211 e. $Å^{-3}$ respectively.The crystal structure has been deposited at the Cambridge Crystallographic Data Centre (CCDC 1484692). The data can be obtained free of charge via the Internet at www.ccdc.cam.ac.uk/data_request/cif.

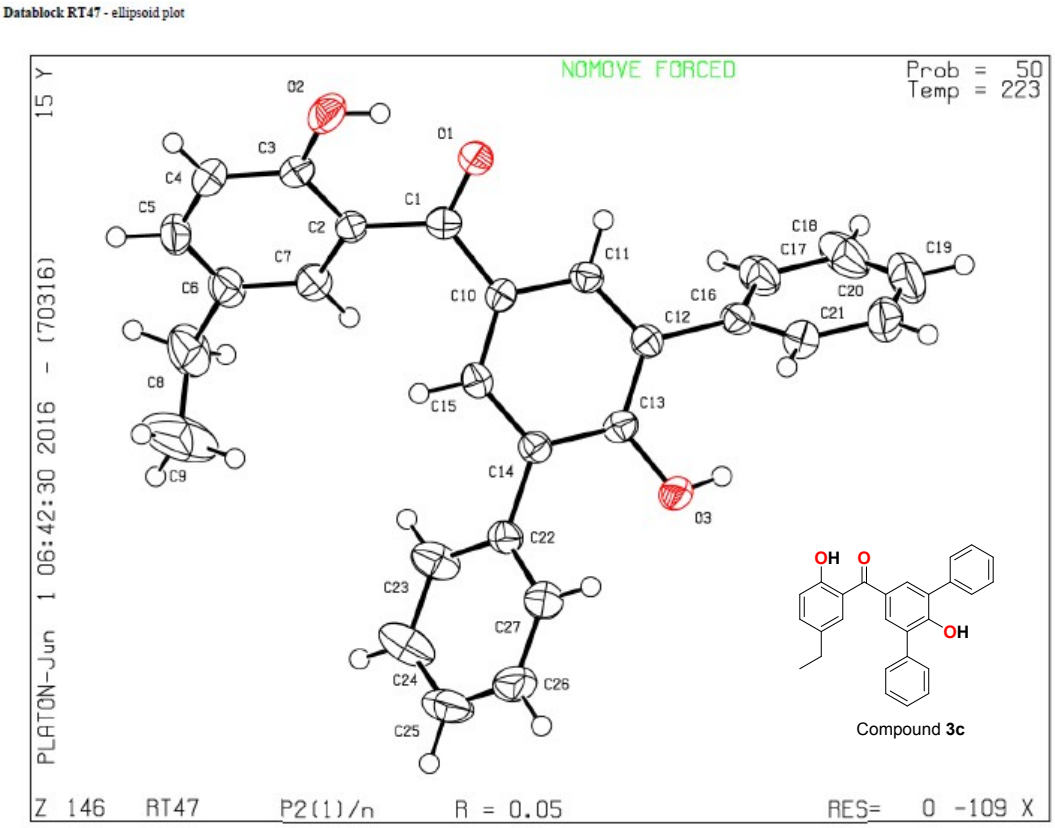


Fig. S2 X-Ray crystallographic structure of compound **3c**.

Table 1. Crystal data and structure refinement for **3c**.

Identification code	RT47	
Empirical formula	$C_{27} H_{22} O_3$	
Formula weight	394.45	
Temperature	223(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 12.4924(9) Å	α= 90°.
	b = 8.6494(5) Å	β= 105.311(4)°.
	c = 20.0211(14) Å	γ = 90°.
Volume	2086.5(2) $Å^3$	
Z	4	
Density (calculated)	1.256 Mg/m^3	
Absorption coefficient	0.081 mm^{-1}	
F(000)	832	
Crystal size	0.30 x 0.22 x 0.20 mm^3	
Theta range for data collection	2.11 to 26.07°.	
Index ranges	-15<=h<=15, -10<=k<=10, -24<=l<=24	
Reflections collected	58124	
Independent reflections	4126 [R(int) = 0.1692]	
Completeness to theta = 26.07°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9840 and 0.9762	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4126 / 0 / 274	
Goodness-of-fit on F^2	1.029	
Final R indices [I>2sigma(I)]	R1 = 0.0487, wR2 = 0.0968	
R indices (all data)	R1 = 0.1085, wR2 = 0.1181	
Largest diff. peak and hole	0.218 and -0.211 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **3c**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	4707(2)	6601(2)	4064(1)	27(1)
O(1)	4123(1)	7646(2)	4211(1)	34(1)
C(2)	5818(2)	6310(2)	4525(1)	27(1)
C(3)	6344(2)	7461(2)	4993(1)	34(1)
C(4)	7408(2)	7212(3)	5406(1)	44(1)
C(5)	7927(2)	5822(3)	5381(1)	45(1)
C(6)	7421(2)	4631(3)	4945(1)	39(1)
C(7)	6374(2)	4907(2)	4526(1)	33(1)
O(2)	5861(1)	8833(2)	5051(1)	50(1)
C(8)	8010(2)	3125(3)	4911(1)	60(1)
C(9)	8572(3)	3109(4)	4337(2)	111(1)
C(10)	4267(2)	5743(2)	3409(1)	27(1)
C(11)	3123(2)	5625(2)	3151(1)	28(1)
C(12)	2637(2)	5044(2)	2498(1)	28(1)
C(13)	3331(2)	4548(2)	2089(1)	28(1)
C(14)	4488(2)	4617(2)	2339(1)	27(1)
C(15)	4935(2)	5221(2)	2998(1)	28(1)
C(16)	1408(2)	4954(2)	2243(1)	31(1)
C(17)	801(2)	4061(3)	2585(1)	43(1)
C(18)	-349(2)	3987(3)	2342(2)	60(1)
C(19)	-880(2)	4792(3)	1757(2)	63(1)
C(20)	-291(2)	5686(3)	1419(1)	54(1)
C(21)	847(2)	5782(3)	1661(1)	42(1)
O(3)	2925(1)	3970(2)	1443(1)	37(1)
C(22)	5229(2)	3979(2)	1936(1)	30(1)
C(23)	6067(2)	2962(3)	2260(1)	47(1)
C(24)	6756(2)	2283(3)	1906(2)	61(1)
C(25)	6618(2)	2617(3)	1217(2)	55(1)
C(26)	5823(2)	3642(3)	896(1)	55(1)
C(27)	5129(2)	4310(3)	1249(1)	46(1)

Table 3. Bond lengths [Å] and angles [°] for **3c**.

C(1)-O(1)#1	1.245(2)
C(1)-O(1)	1.245(2)
C(1)-C(2)	1.471(3)
C(1)-C(10)	1.480(3)
O(1)-O(1)#1	0.000(4)
C(2)-C(7)	1.397(3)
C(2)-C(3)	1.406(3)
C(3)-O(2)	1.350(2)
C(3)-C(4)	1.384(3)
C(4)-C(5)	1.374(3)
C(4)-H(4)	0.9400
C(5)-C(6)	1.389(3)
C(5)-H(5)	0.9400
C(6)-C(7)	1.376(3)
C(6)-C(8)	1.507(3)
C(7)-H(7)	0.9400
O(2)-H(2)	0.8300
C(8)-C(9)	1.496(4)
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(9)-H(9A)	0.9700
C(9)-H(9B)	0.9700
C(9)-H(9C)	0.9700
C(10)-C(11)	1.389(3)
C(10)-C(15)	1.393(3)
C(11)-C(12)	1.382(3)
C(11)-H(11)	0.9400
C(12)-C(13)	1.407(3)
C(12)-C(16)	1.486(3)
C(13)-O(3)	1.356(2)
C(13)-C(14)	1.401(3)
C(14)-C(15)	1.391(3)
C(14)-C(22)	1.485(3)
C(15)-H(15)	0.9400

C(16)-C(17)	1.385(3)
C(16)-C(21)	1.389(3)
C(17)-C(18)	1.391(3)
C(17)-H(17)	0.9400
C(18)-C(19)	1.374(4)
C(18)-H(18)	0.9400
C(19)-C(20)	1.365(4)
C(19)-H(19)	0.9400
C(20)-C(21)	1.378(3)
C(20)-H(20)	0.9400
C(21)-H(21)	0.9400
O(3)-H(3)	0.8300
C(22)-C(27)	1.379(3)
C(22)-C(23)	1.390(3)
C(23)-C(24)	1.381(3)
C(23)-H(23)	0.9400
C(24)-C(25)	1.375(4)
C(24)-H(24)	0.9400
C(25)-C(26)	1.360(4)
C(25)-H(25)	0.9400
C(26)-C(27)	1.382(3)
C(26)-H(26)	0.9400
C(27)-H(27)	0.9400

O(1)#1-C(1)-O(1)	0.00(13)
O(1)#1-C(1)-C(2)	119.35(17)
O(1)-C(1)-C(2)	119.35(17)
O(1)#1-C(1)-C(10)	118.03(18)
O(1)-C(1)-C(10)	118.03(18)
C(2)-C(1)-C(10)	122.57(18)
O(1)#1-O(1)-C(1)	0(10)
C(7)-C(2)-C(3)	117.99(18)
C(7)-C(2)-C(1)	122.38(18)
C(3)-C(2)-C(1)	119.61(18)
O(2)-C(3)-C(4)	117.75(19)
O(2)-C(3)-C(2)	122.64(18)

C(4)-C(3)-C(2)	119.6(2)
C(5)-C(4)-C(3)	120.2(2)
C(5)-C(4)-H(4)	119.9
C(3)-C(4)-H(4)	119.9
C(4)-C(5)-C(6)	122.0(2)
C(4)-C(5)-H(5)	119.0
C(6)-C(5)-H(5)	119.0
C(7)-C(6)-C(5)	117.2(2)
C(7)-C(6)-C(8)	121.3(2)
C(5)-C(6)-C(8)	121.5(2)
C(6)-C(7)-C(2)	122.9(2)
C(6)-C(7)-H(7)	118.5
C(2)-C(7)-H(7)	118.5
C(3)-O(2)-H(2)	109.5
C(9)-C(8)-C(6)	112.1(2)
C(9)-C(8)-H(8A)	109.2
C(6)-C(8)-H(8A)	109.2
C(9)-C(8)-H(8B)	109.2
C(6)-C(8)-H(8B)	109.2
H(8A)-C(8)-H(8B)	107.9
C(8)-C(9)-H(9A)	109.5
C(8)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(8)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(11)-C(10)-C(15)	118.36(18)
C(11)-C(10)-C(1)	118.12(18)
C(15)-C(10)-C(1)	123.01(18)
C(12)-C(11)-C(10)	121.99(18)
C(12)-C(11)-H(11)	119.0
C(10)-C(11)-H(11)	119.0
C(11)-C(12)-C(13)	118.49(18)
C(11)-C(12)-C(16)	120.03(18)
C(13)-C(12)-C(16)	121.48(18)
O(3)-C(13)-C(14)	116.54(17)

O(3)-C(13)-C(12)	122.43(18)
C(14)-C(13)-C(12)	121.02(18)
C(15)-C(14)-C(13)	118.20(18)
C(15)-C(14)-C(22)	120.18(18)
C(13)-C(14)-C(22)	121.51(17)
C(14)-C(15)-C(10)	121.91(18)
C(14)-C(15)-H(15)	119.0
C(10)-C(15)-H(15)	119.0
C(17)-C(16)-C(21)	118.7(2)
C(17)-C(16)-C(12)	120.67(19)
C(21)-C(16)-C(12)	120.58(19)
C(16)-C(17)-C(18)	120.2(2)
C(16)-C(17)-H(17)	119.9
C(18)-C(17)-H(17)	119.9
C(19)-C(18)-C(17)	119.7(3)
C(19)-C(18)-H(18)	120.1
C(17)-C(18)-H(18)	120.1
C(20)-C(19)-C(18)	120.6(2)
C(20)-C(19)-H(19)	119.7
C(18)-C(19)-H(19)	119.7
C(19)-C(20)-C(21)	120.0(3)
C(19)-C(20)-H(20)	120.0
C(21)-C(20)-H(20)	120.0
C(20)-C(21)-C(16)	120.7(2)
C(20)-C(21)-H(21)	119.7
C(16)-C(21)-H(21)	119.7
C(13)-O(3)-H(3)	109.5
C(27)-C(22)-C(23)	117.0(2)
C(27)-C(22)-C(14)	124.06(19)
C(23)-C(22)-C(14)	118.89(18)
C(24)-C(23)-C(22)	121.7(2)
C(24)-C(23)-H(23)	119.2
C(22)-C(23)-H(23)	119.2
C(25)-C(24)-C(23)	119.7(3)
C(25)-C(24)-H(24)	120.1
C(23)-C(24)-H(24)	120.1

C(26)-C(25)-C(24)	119.6(2)
C(26)-C(25)-H(25)	120.2
C(24)-C(25)-H(25)	120.2
C(25)-C(26)-C(27)	120.6(2)
C(25)-C(26)-H(26)	119.7
C(27)-C(26)-H(26)	119.7
C(22)-C(27)-C(26)	121.3(2)
C(22)-C(27)-H(27)	119.3
C(26)-C(27)-H(27)	119.3

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **3c**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	31(1)	26(1)	27(1)	2(1)	11(1)	-1(1)
O(1)	32(1)	38(1)	31(1)	-5(1)	6(1)	7(1)
C(2)	25(1)	35(1)	21(1)	4(1)	7(1)	2(1)
C(3)	34(1)	44(1)	23(1)	-3(1)	7(1)	4(1)
C(4)	36(1)	62(2)	30(1)	-10(1)	2(1)	-1(1)
C(5)	26(1)	74(2)	31(1)	5(1)	3(1)	6(1)
C(6)	35(1)	48(1)	34(1)	13(1)	10(1)	10(1)
C(7)	34(1)	34(1)	31(1)	5(1)	10(1)	2(1)
O(2)	49(1)	51(1)	41(1)	-21(1)	-6(1)	12(1)
C(8)	50(2)	57(2)	68(2)	14(1)	8(1)	22(1)
C(9)	138(3)	97(3)	119(3)	17(2)	71(3)	73(3)
C(10)	27(1)	28(1)	24(1)	1(1)	4(1)	0(1)
C(11)	29(1)	32(1)	27(1)	0(1)	11(1)	2(1)
C(12)	25(1)	30(1)	29(1)	0(1)	8(1)	-2(1)
C(13)	31(1)	29(1)	25(1)	-2(1)	9(1)	-5(1)
C(14)	27(1)	29(1)	27(1)	0(1)	10(1)	-3(1)
C(15)	24(1)	28(1)	31(1)	3(1)	7(1)	0(1)
C(16)	26(1)	33(1)	34(1)	-10(1)	9(1)	-4(1)
C(17)	35(1)	41(1)	57(2)	-8(1)	18(1)	-5(1)
C(18)	42(2)	47(2)	101(2)	-19(2)	36(2)	-11(1)
C(19)	28(2)	57(2)	97(2)	-33(2)	5(2)	1(1)
C(20)	38(2)	58(2)	56(2)	-17(1)	-4(1)	13(1)
C(21)	35(1)	50(1)	38(1)	-7(1)	5(1)	2(1)
O(3)	28(1)	54(1)	31(1)	-13(1)	9(1)	-9(1)
C(22)	26(1)	32(1)	34(1)	-6(1)	13(1)	-8(1)
C(23)	52(2)	45(1)	53(2)	6(1)	30(1)	7(1)
C(24)	60(2)	50(2)	86(2)	3(2)	42(2)	15(1)
C(25)	50(2)	60(2)	69(2)	-27(2)	38(2)	-13(1)
C(26)	45(2)	89(2)	38(1)	-15(1)	22(1)	-11(2)
C(27)	37(1)	67(2)	35(1)	-3(1)	13(1)	-1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **3c**.

	x	y	z	U(eq)
H(4)	7776	7997	5704	52
H(5)	8648	5671	5668	54
H(7)	6015	4116	4228	40
H(2)	5215	8833	4800	75
H(8A)	8565	2952	5353	71
H(8B)	7472	2276	4842	71
H(9A)	8025	3275	3899	166
H(9B)	8930	2117	4329	166
H(9C)	9124	3925	4412	166
H(11)	2665	5951	3429	34
H(15)	5710	5279	3170	33
H(17)	1166	3503	2983	52
H(18)	-762	3388	2578	72
H(19)	-1655	4728	1589	75
H(20)	-662	6237	1020	64
H(21)	1247	6414	1431	50
H(3)	2254	3777	1376	56
H(23)	6168	2730	2731	56
H(24)	7315	1596	2135	73
H(25)	7072	2141	970	66
H(26)	5745	3898	429	66
H(27)	4578	5005	1015	55

Table 6. Torsion angles [°] for **3c**.

C(2)-C(1)-O(1)-O(1)#1	0.0(2)
C(10)-C(1)-O(1)-O(1)#1	0.00(17)
O(1)#1-C(1)-C(2)-C(7)	159.33(18)
O(1)-C(1)-C(2)-C(7)	159.33(18)
C(10)-C(1)-C(2)-C(7)	-23.4(3)
O(1)#1-C(1)-C(2)-C(3)	-19.4(3)
O(1)-C(1)-C(2)-C(3)	-19.4(3)
C(10)-C(1)-C(2)-C(3)	157.93(18)
C(7)-C(2)-C(3)-O(2)	-177.45(19)
C(1)-C(2)-C(3)-O(2)	1.3(3)
C(7)-C(2)-C(3)-C(4)	4.0(3)
C(1)-C(2)-C(3)-C(4)	-177.25(19)
O(2)-C(3)-C(4)-C(5)	178.3(2)
C(2)-C(3)-C(4)-C(5)	-3.1(3)
C(3)-C(4)-C(5)-C(6)	0.5(4)
C(4)-C(5)-C(6)-C(7)	1.0(3)
C(4)-C(5)-C(6)-C(8)	178.6(2)
C(5)-C(6)-C(7)-C(2)	0.1(3)
C(8)-C(6)-C(7)-C(2)	-177.5(2)
C(3)-C(2)-C(7)-C(6)	-2.6(3)
C(1)-C(2)-C(7)-C(6)	178.73(19)
C(7)-C(6)-C(8)-C(9)	82.8(3)
C(5)-C(6)-C(8)-C(9)	-94.7(3)
O(1)#1-C(1)-C(10)-C(11)	-27.5(3)
O(1)-C(1)-C(10)-C(11)	-27.5(3)
C(2)-C(1)-C(10)-C(11)	155.14(18)
O(1)#1-C(1)-C(10)-C(15)	144.08(19)
O(1)-C(1)-C(10)-C(15)	144.08(19)
C(2)-C(1)-C(10)-C(15)	-33.2(3)
C(15)-C(10)-C(11)-C(12)	-1.5(3)
C(1)-C(10)-C(11)-C(12)	170.50(18)
C(10)-C(11)-C(12)-C(13)	0.6(3)
C(10)-C(11)-C(12)-C(16)	-179.47(18)
C(11)-C(12)-C(13)-O(3)	-179.70(18)

C(16)-C(12)-C(13)-O(3)	0.3(3)
C(11)-C(12)-C(13)-C(14)	0.9(3)
C(16)-C(12)-C(13)-C(14)	-179.06(18)
O(3)-C(13)-C(14)-C(15)	179.22(17)
C(12)-C(13)-C(14)-C(15)	-1.4(3)
O(3)-C(13)-C(14)-C(22)	-4.5(3)
C(12)-C(13)-C(14)-C(22)	174.91(18)
C(13)-C(14)-C(15)-C(10)	0.4(3)
C(22)-C(14)-C(15)-C(10)	-175.96(17)
C(11)-C(10)-C(15)-C(14)	1.0(3)
C(1)-C(10)-C(15)-C(14)	-170.56(18)
C(11)-C(12)-C(16)-C(17)	-61.1(3)
C(13)-C(12)-C(16)-C(17)	118.8(2)
C(11)-C(12)-C(16)-C(21)	118.0(2)
C(13)-C(12)-C(16)-C(21)	-62.1(3)
C(21)-C(16)-C(17)-C(18)	0.8(3)
C(12)-C(16)-C(17)-C(18)	179.9(2)
C(16)-C(17)-C(18)-C(19)	0.6(3)
C(17)-C(18)-C(19)-C(20)	-1.1(4)
C(18)-C(19)-C(20)-C(21)	0.3(4)
C(19)-C(20)-C(21)-C(16)	1.1(3)
C(17)-C(16)-C(21)-C(20)	-1.6(3)
C(12)-C(16)-C(21)-C(20)	179.3(2)
C(15)-C(14)-C(22)-C(27)	-133.7(2)
C(13)-C(14)-C(22)-C(27)	50.1(3)
C(15)-C(14)-C(22)-C(23)	47.5(3)
C(13)-C(14)-C(22)-C(23)	-128.7(2)
C(27)-C(22)-C(23)-C(24)	-1.5(3)
C(14)-C(22)-C(23)-C(24)	177.5(2)
C(22)-C(23)-C(24)-C(25)	0.2(4)
C(23)-C(24)-C(25)-C(26)	1.6(4)
C(24)-C(25)-C(26)-C(27)	-2.1(4)
C(23)-C(22)-C(27)-C(26)	0.9(3)
C(14)-C(22)-C(27)-C(26)	-178.0(2)
C(25)-C(26)-C(27)-C(22)	0.9(4)

Symmetry transformations used to generate equivalent atoms:
#1 x,y,z

Table 7. Hydrogen bonds for **3c** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(2)...O(1)#1	0.83	1.86	2.582(2)	144.7
O(3)-H(3)...O(1)#2	0.83	2.06	2.7934(19)	147.5
O(2)-H(2)...O(2)#3	0.83	2.49	2.918(3)	113.4

Symmetry transformations used to generate equivalent atoms:
#1 x,y,z #2 -x+1/2,y-1/2,-z+1/2 #3 -x+1,-y+2,-z+1