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

SUPPORTING INFORMATION

One-pot construction of sterically challenging polyarylphenols *via* transition-metal-free benzannulation and their *in-vitro* antioxidant activity

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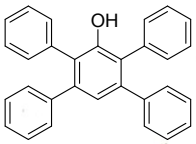
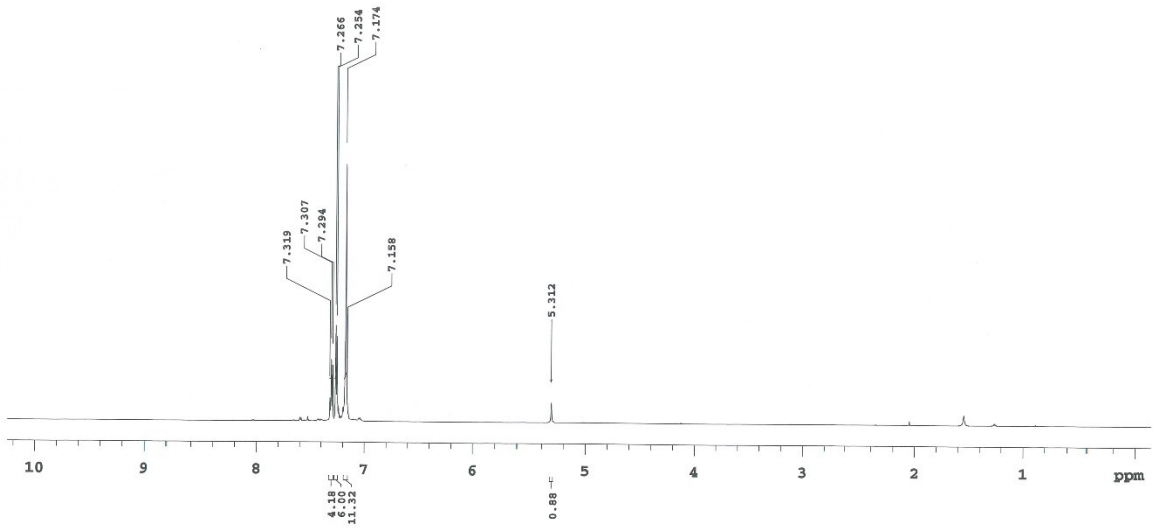
Compound-**3a**

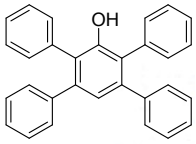
^{1}H-NMR/$CDCl_3$

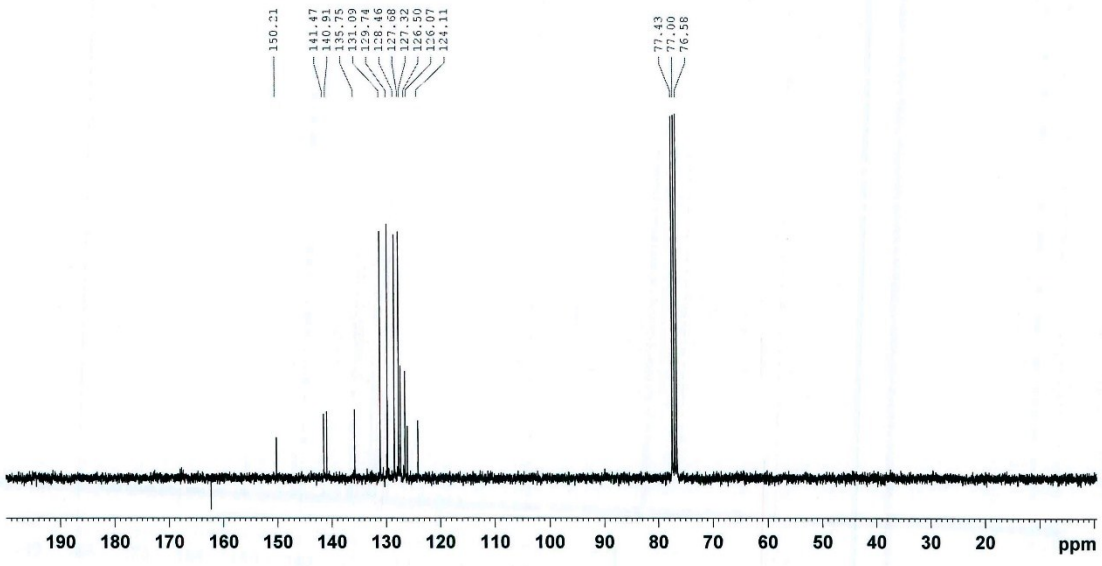




Compound-**3a**

^{13}C-NMR/$CDCl_3$





Compound-**3b**
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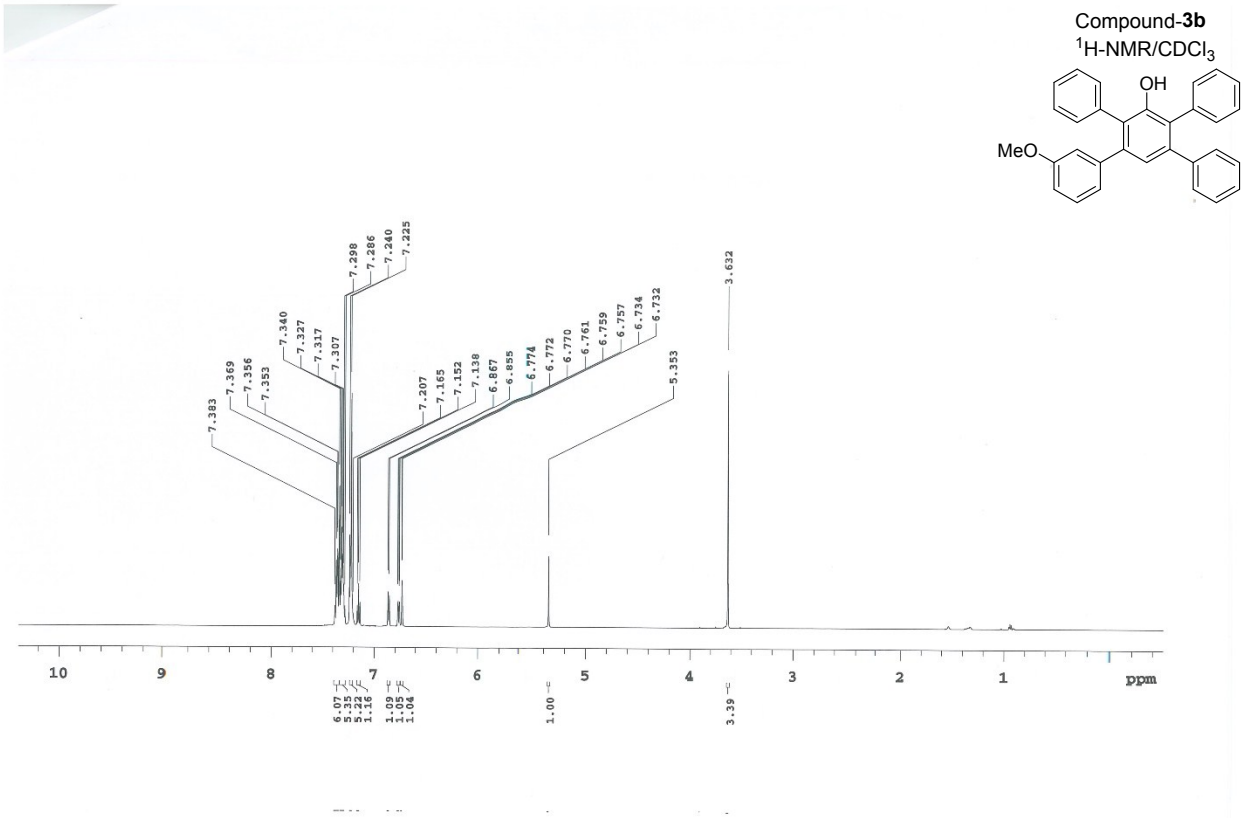

Compound-**3b**
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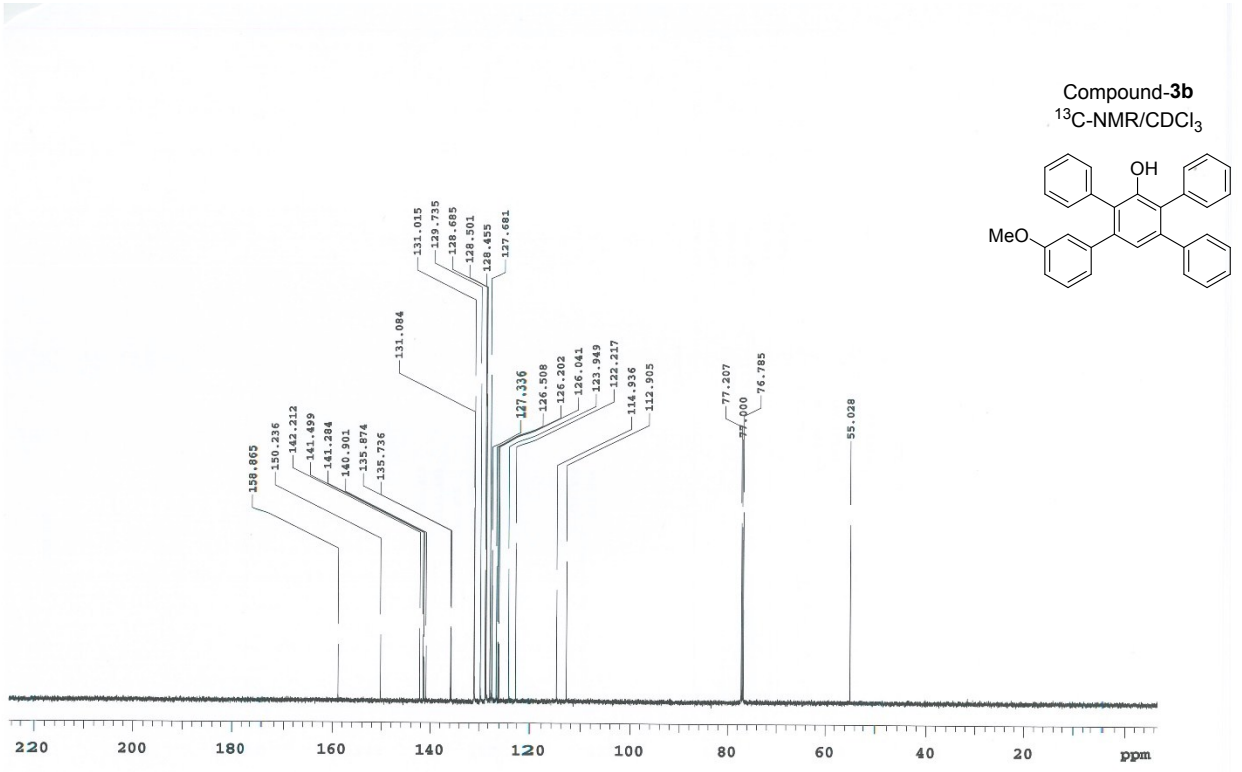

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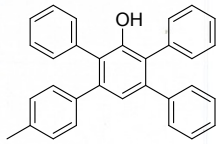

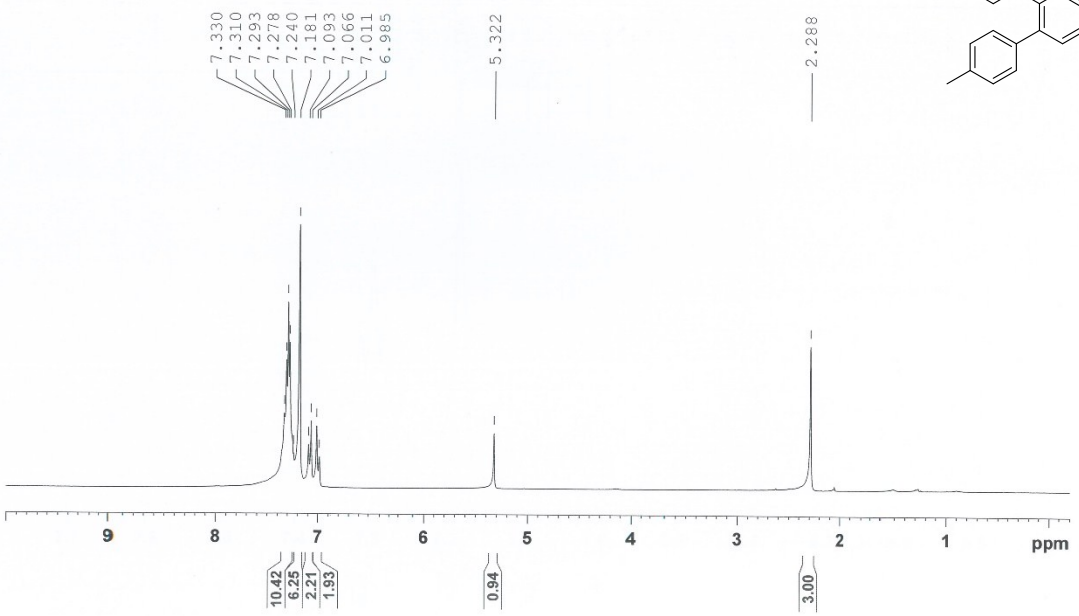

Compound-**3c**
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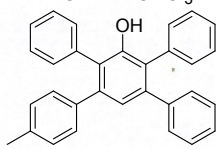

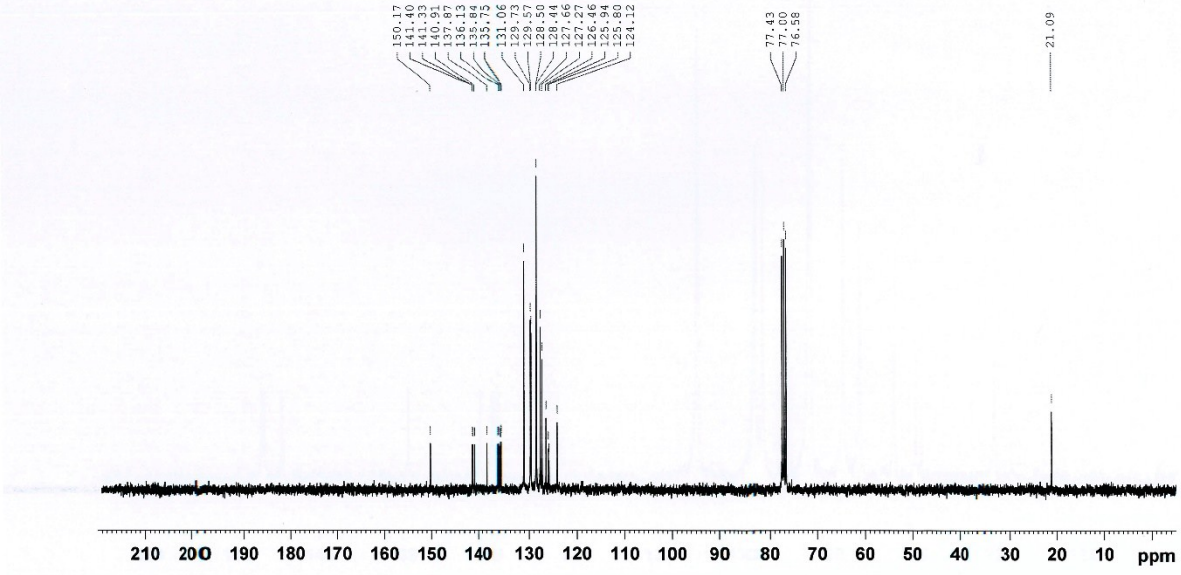

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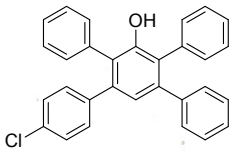
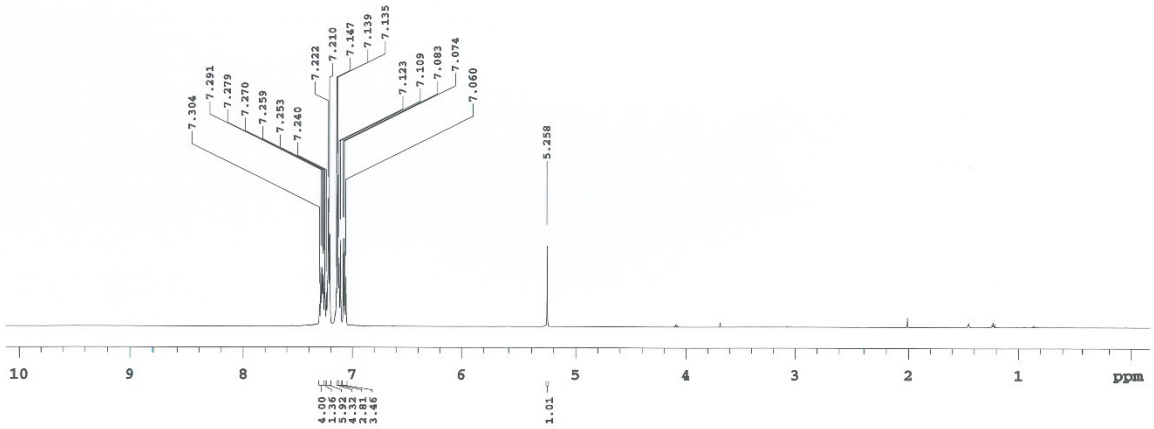
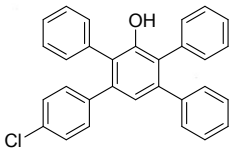
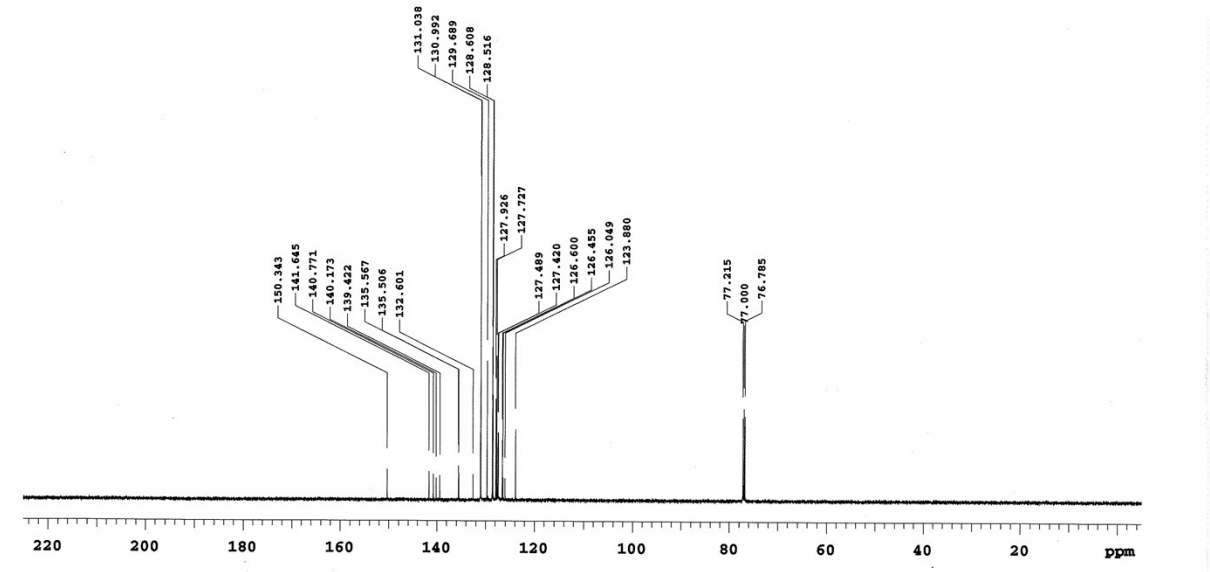




Compound-**3d**

^{13}C-NMR/$CDCl_3$





Compound-**3e**

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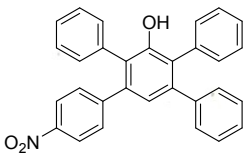
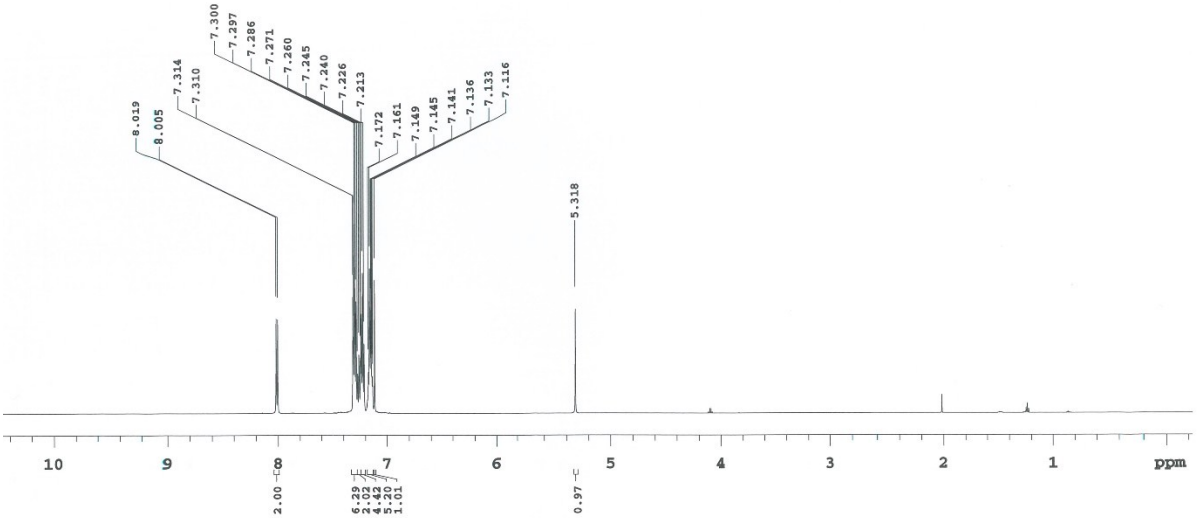
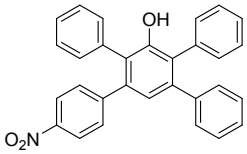
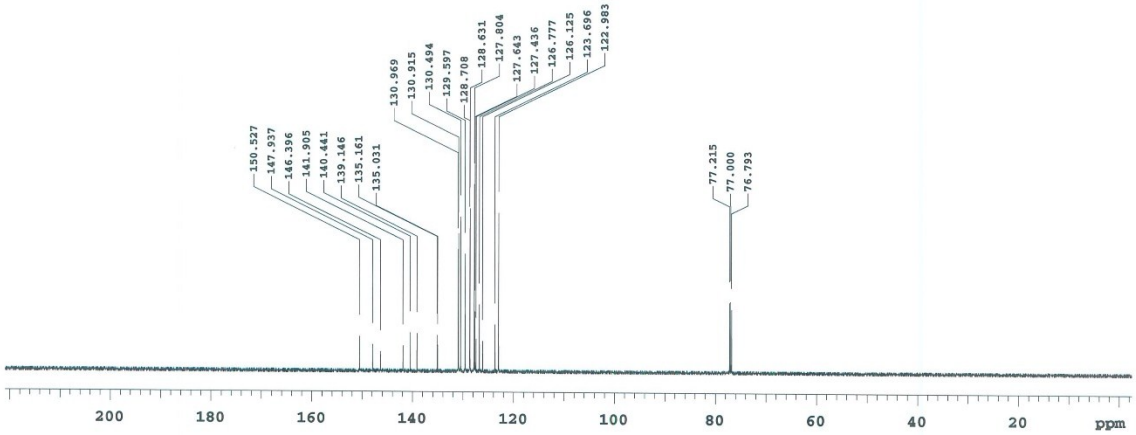




Compound-**3e**

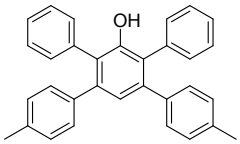
^{13}C-NMR/$CDCl_3$

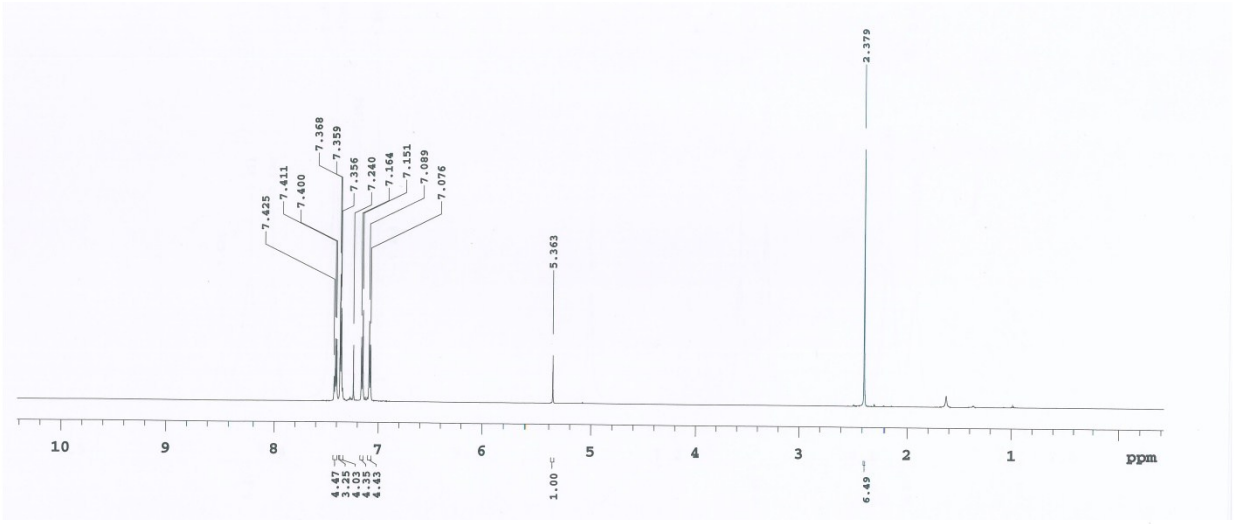




Compound-**3f**

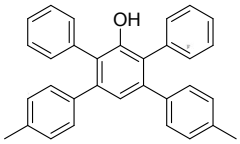
^{1}H-NMR/$CDCl_3$

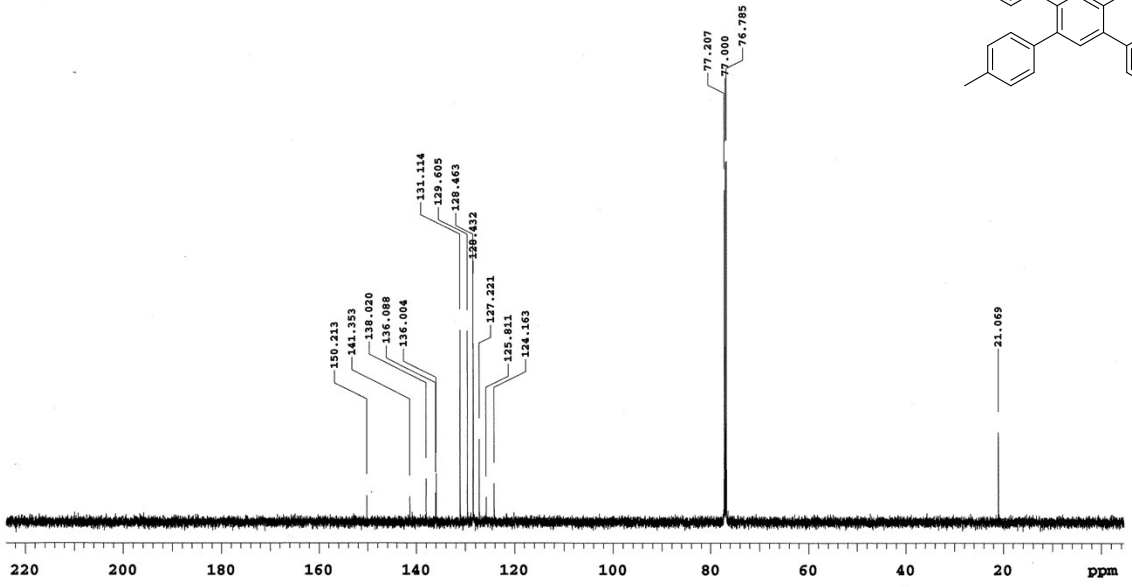




Compound-**3f**

^{13}C-NMR/$CDCl_3$





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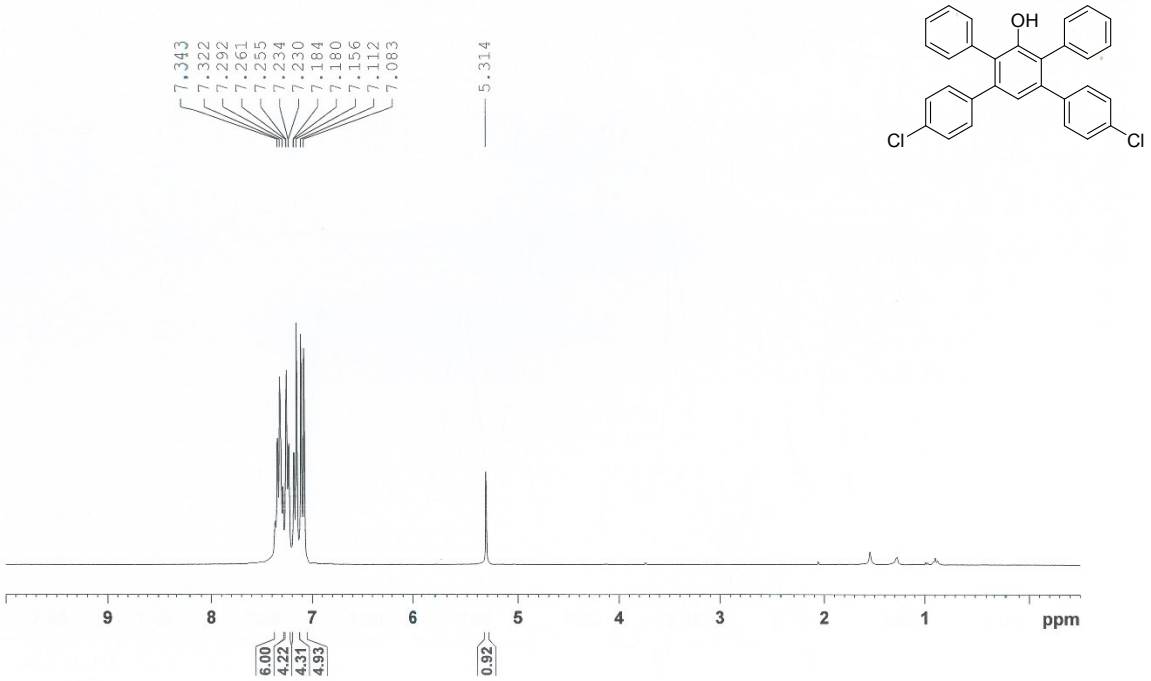
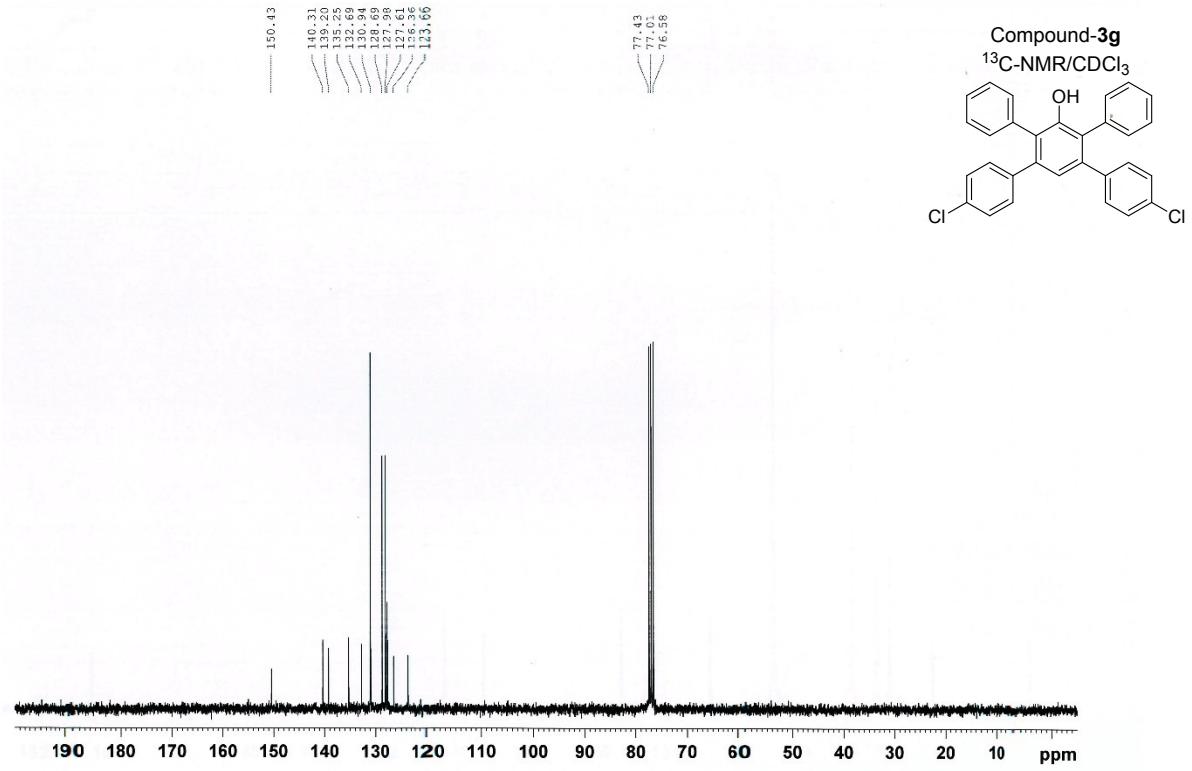
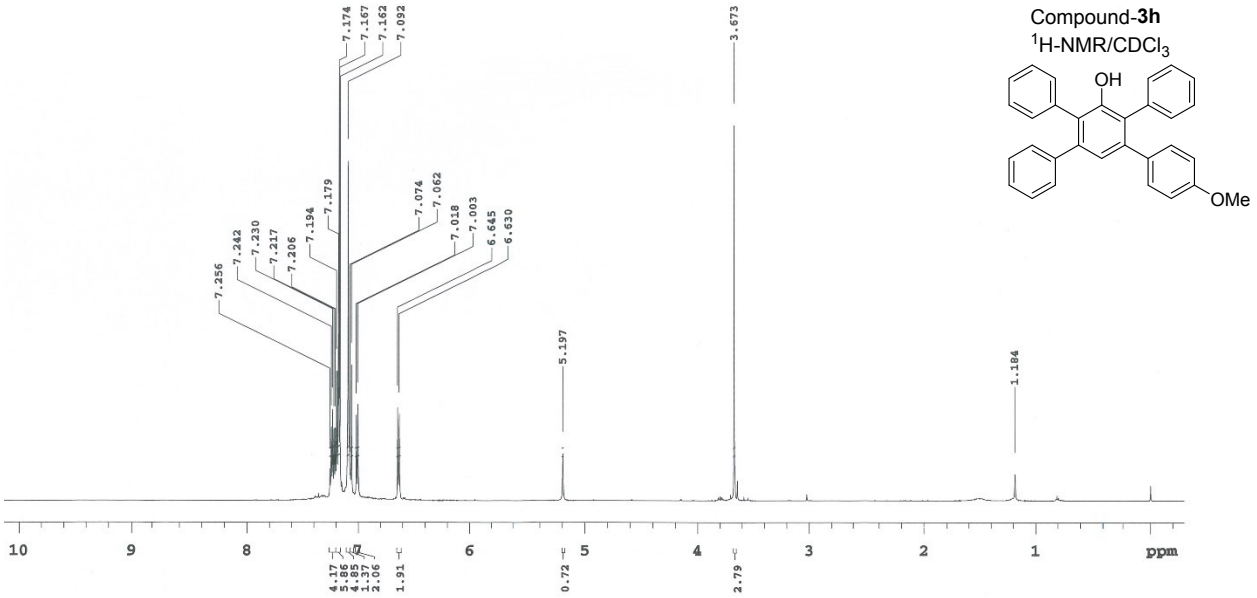
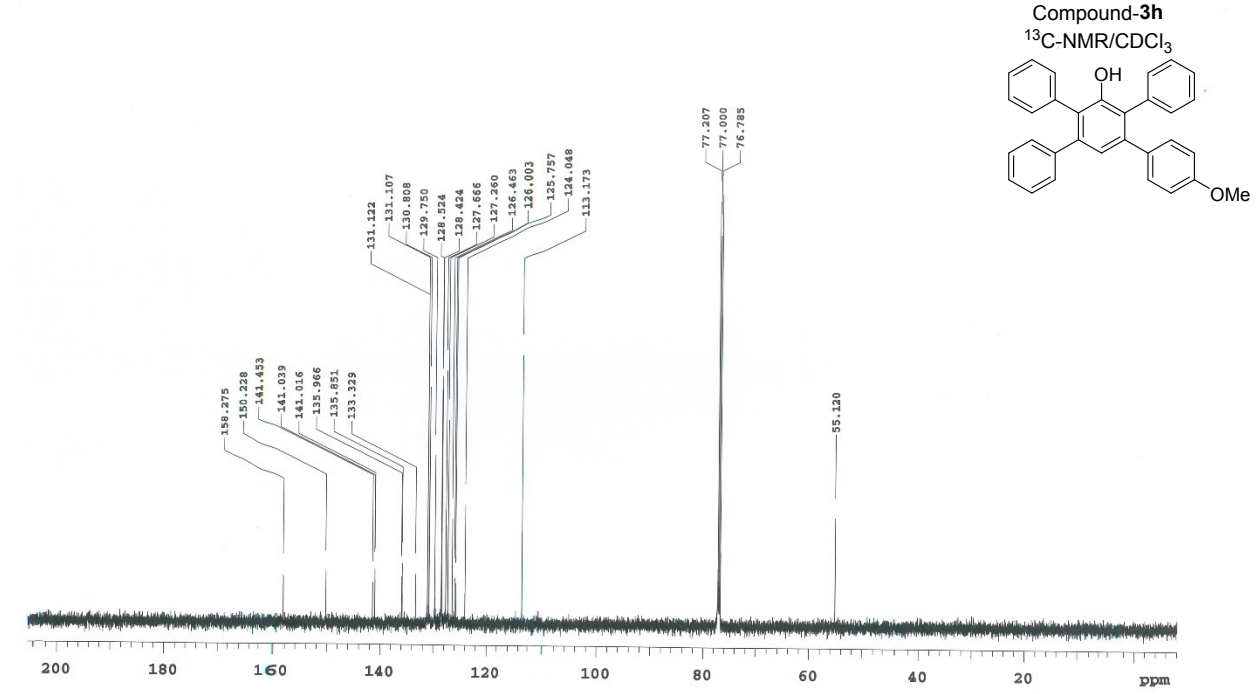
^{1}H-NMR/$CDCl_3$



Compound-**3g**
^{13}C-NMR/$CDCl_3$

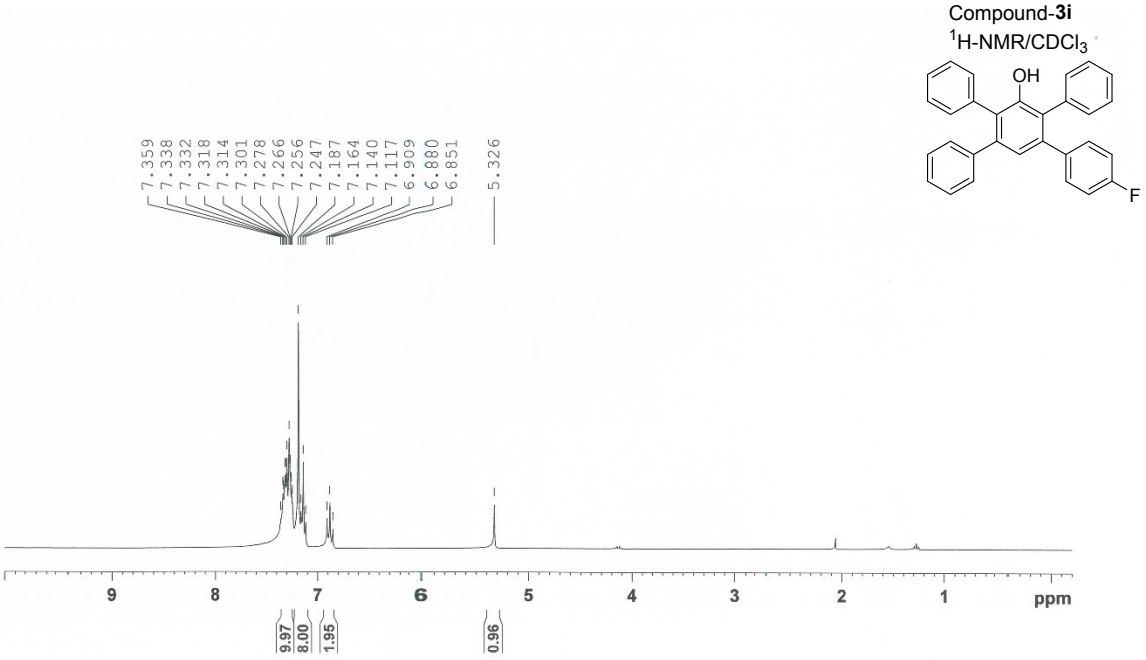



Compound-3h
1H-NMR/CDCl3
OH
OMe
7.174
7.167
7.162
7.092
3.673
7.256
7.242
7.230
7.217
7.206
7.194
7.179
7.074
7.062
7.018
7.003
6.645
6.630
5.197
1.184
10
9
8
7
6
5
4
3
2
1
ppm


Compound-3h
13C-NMR/CDCl3
OH
OMe
77.207
77.000
76.785
131.122
131.107
130.808
129.750
128.524
128.424
127.666
127.260
126.463
126.003
125.757
124.048
113.173
158.275
150.228
141.453
141.039
141.016
135.966
135.851
133.329
55.120
200
180
160
140
120
100
80
60
40
20
ppm

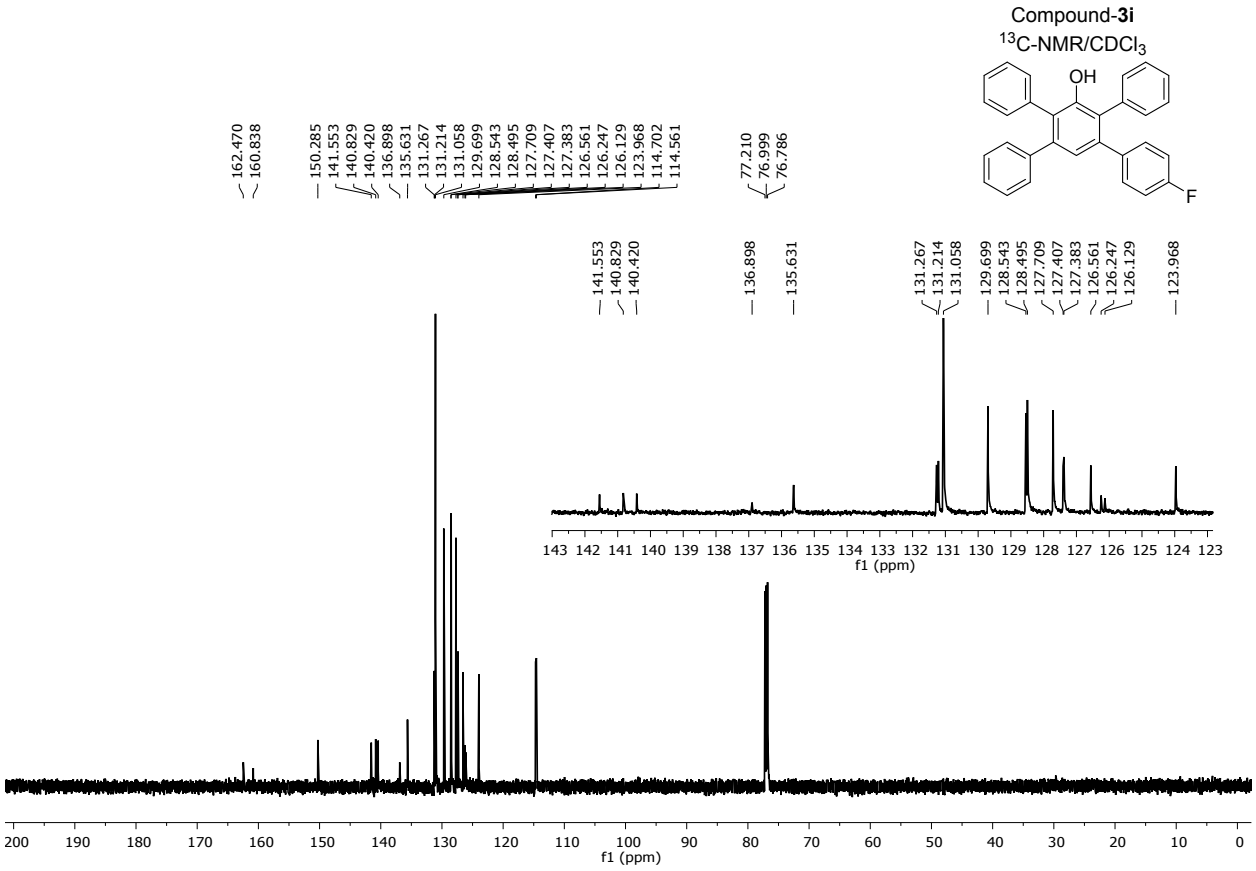
Compound-**3i**

^{1}H-NMR/CDCl$_3$



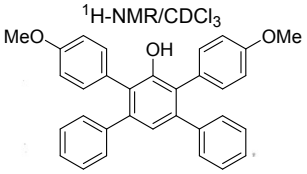
Compound-**3i**

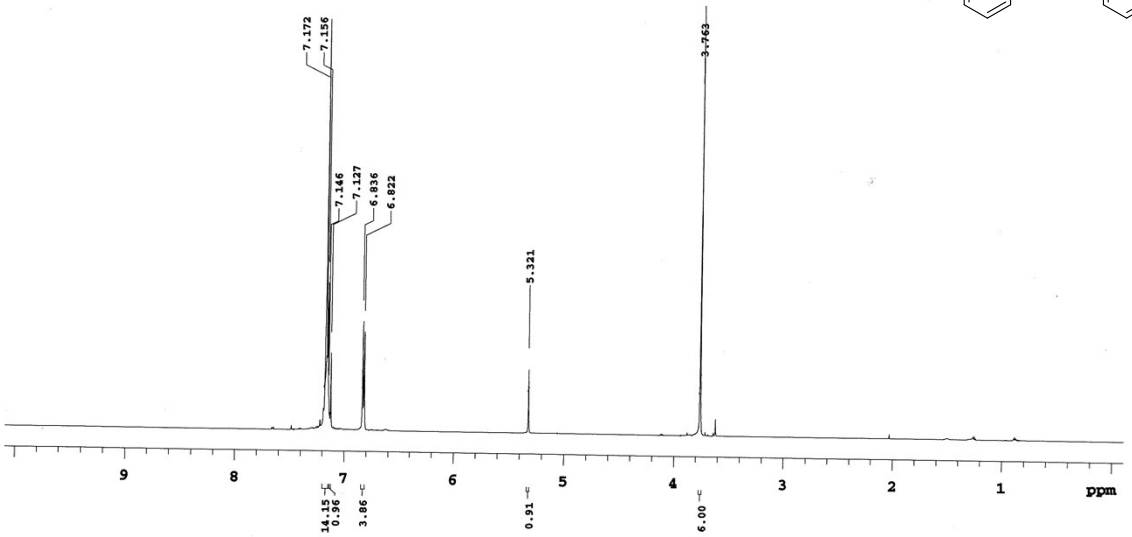
^{13}C-NMR/CDCl$_3$



Compound-**3j**

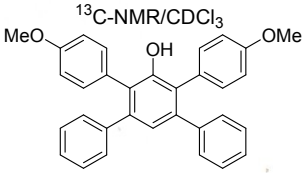
^{1}H-NMR/$CDCl_3$

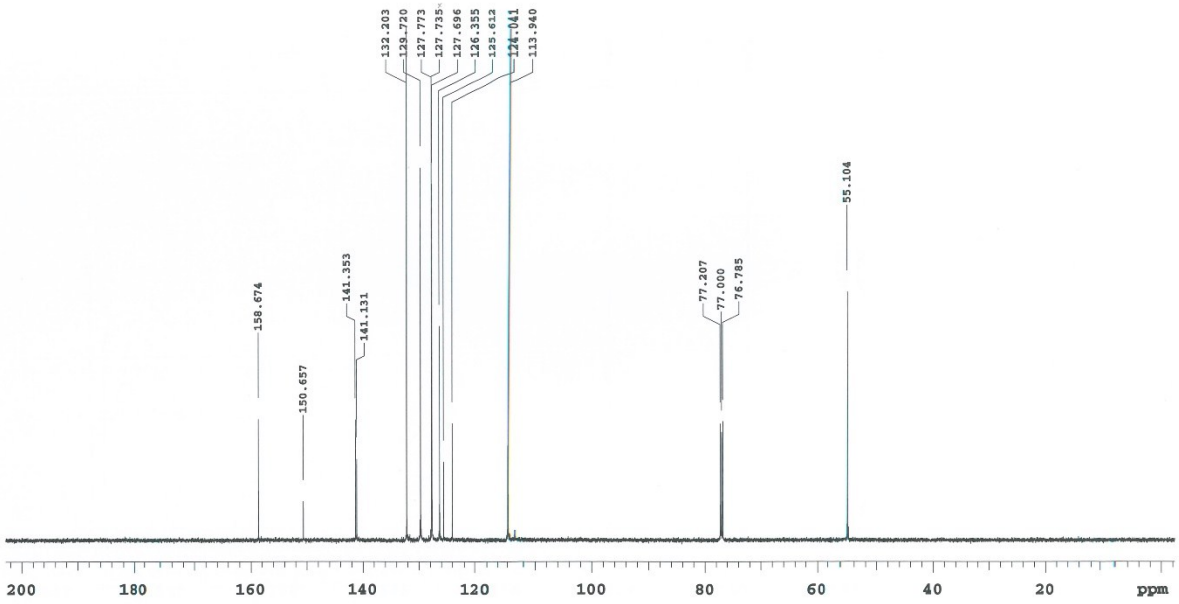




Compound-**3j**

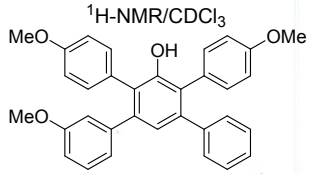
^{13}C-NMR/$CDCl_3$

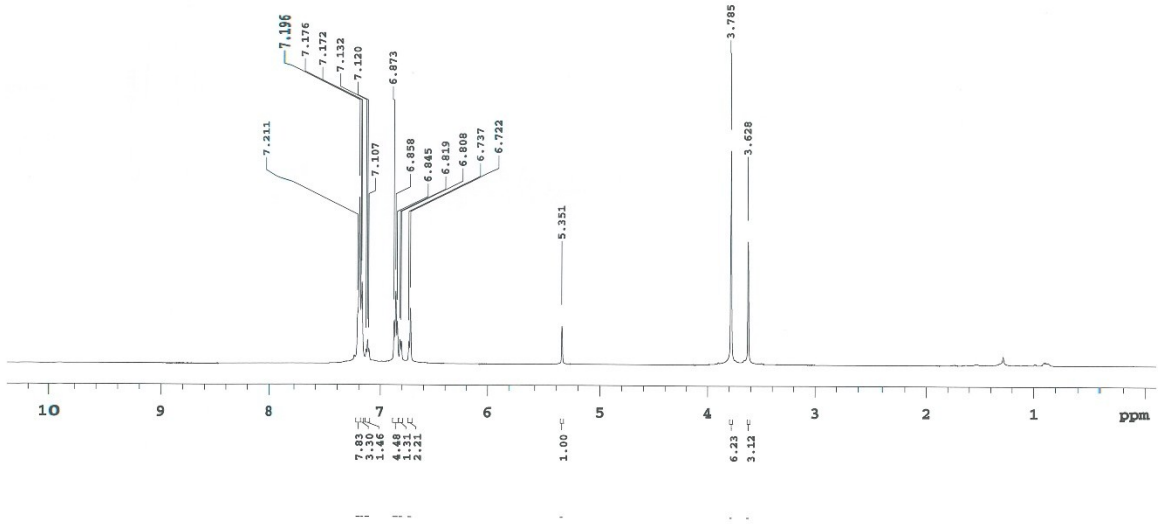




Compound-**3k**

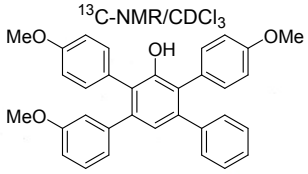
^{1}H-NMR/$CDCl_3$

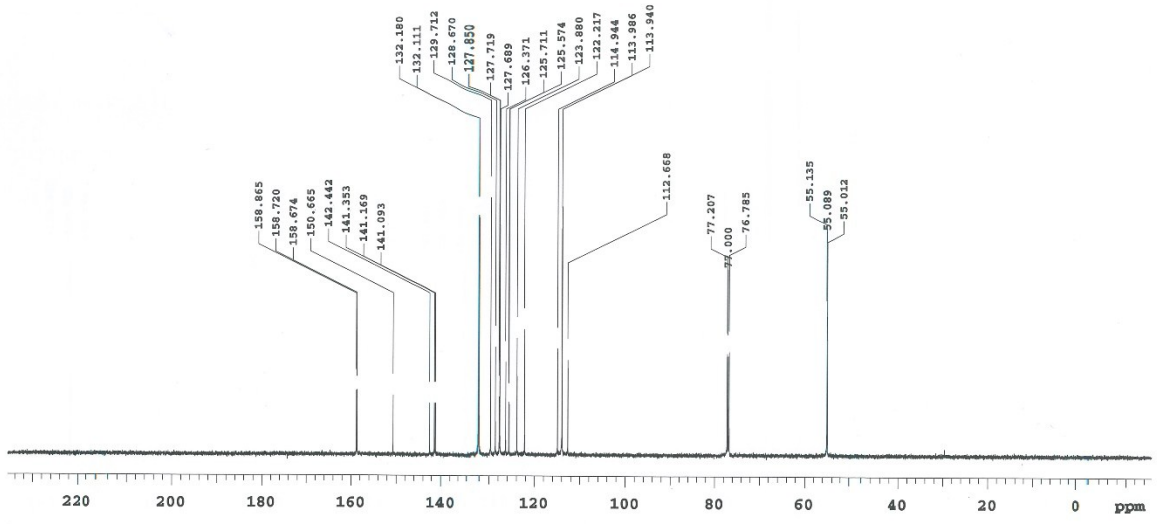


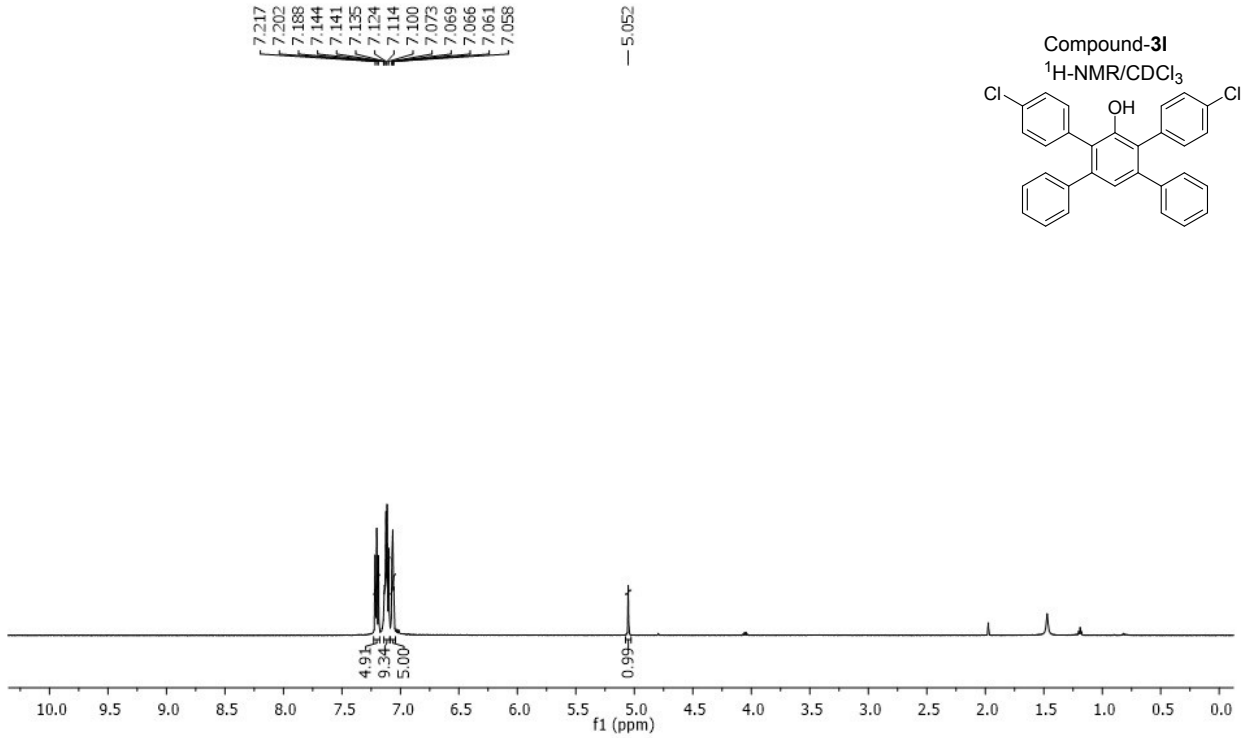


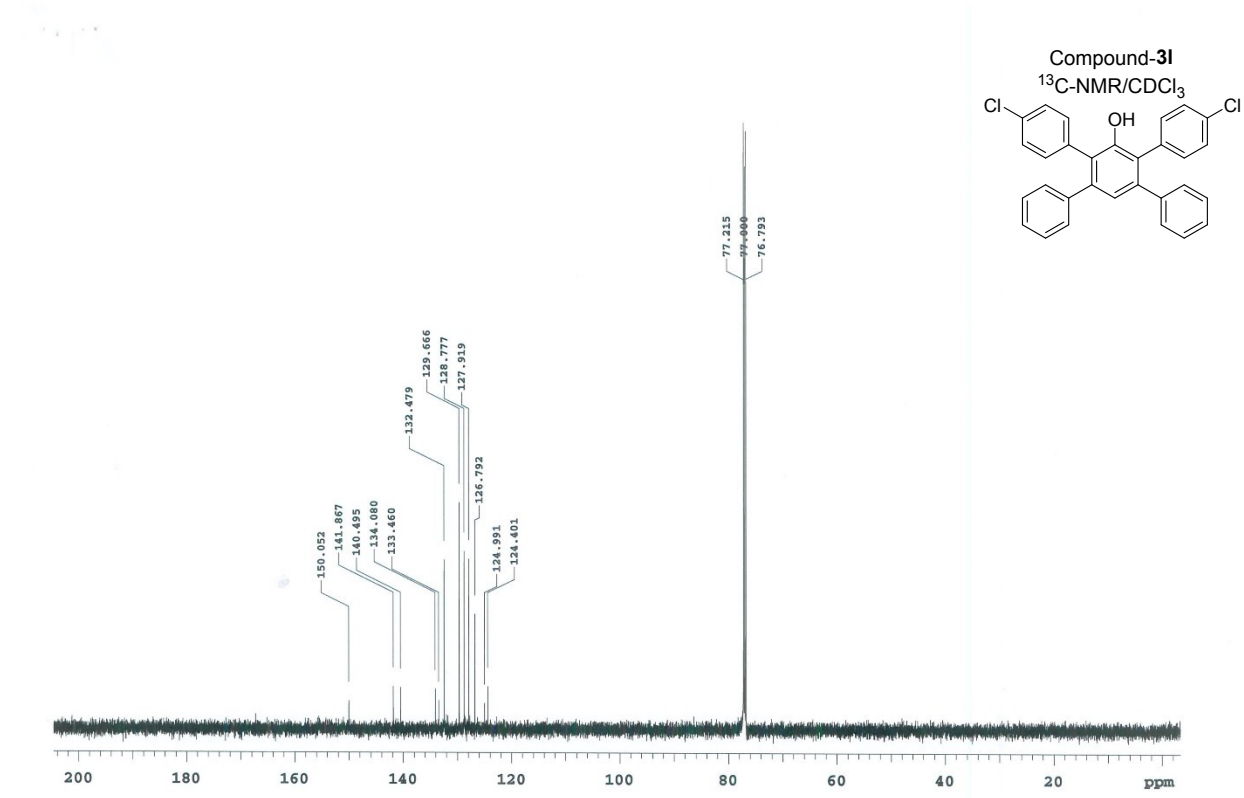
Compound-**3k**

^{13}C-NMR/$CDCl_3$



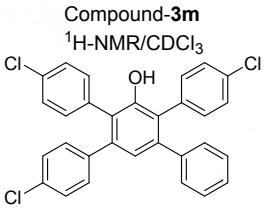


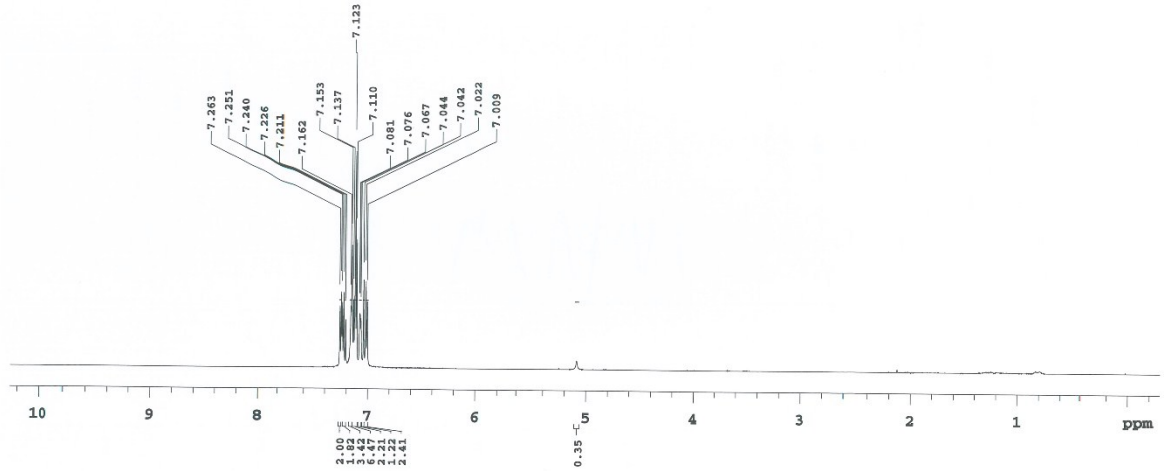

7.217
7.202
7.188
7.144
7.141
7.135
7.124
7.114
7.100
7.073
7.069
7.066
7.061
7.058
5.052
Compound-3l
1H-NMR/CDCl3
Cl
OH
Cl
4.91
9.34
5.00
0.99
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


Compound-3l
13C-NMR/CDCl3
Cl
OH
Cl
150.052
141.867
140.495
134.080
133.460
132.479
129.666
128.777
127.919
126.792
124.991
124.401
77.215
77.000
76.793
200 180 160 140 120 100 80 60 40 20
ppm

Compound-**3m**

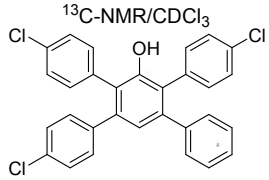
^{1}H-NMR/$CDCl_3$

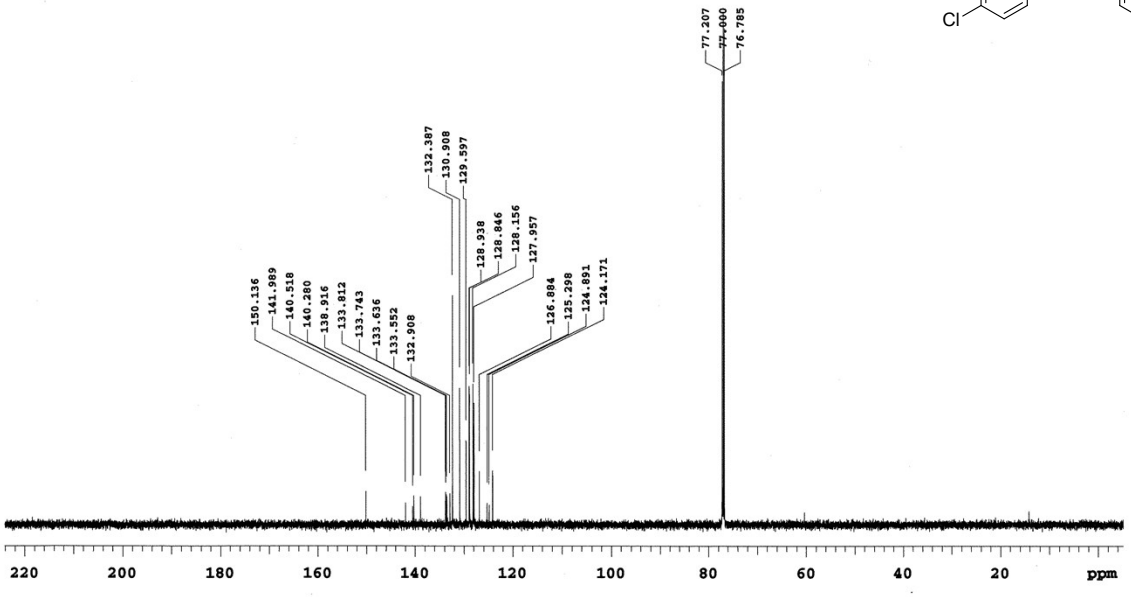




Compound-**3m**

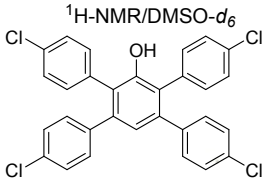
^{13}C-NMR/$CDCl_3$

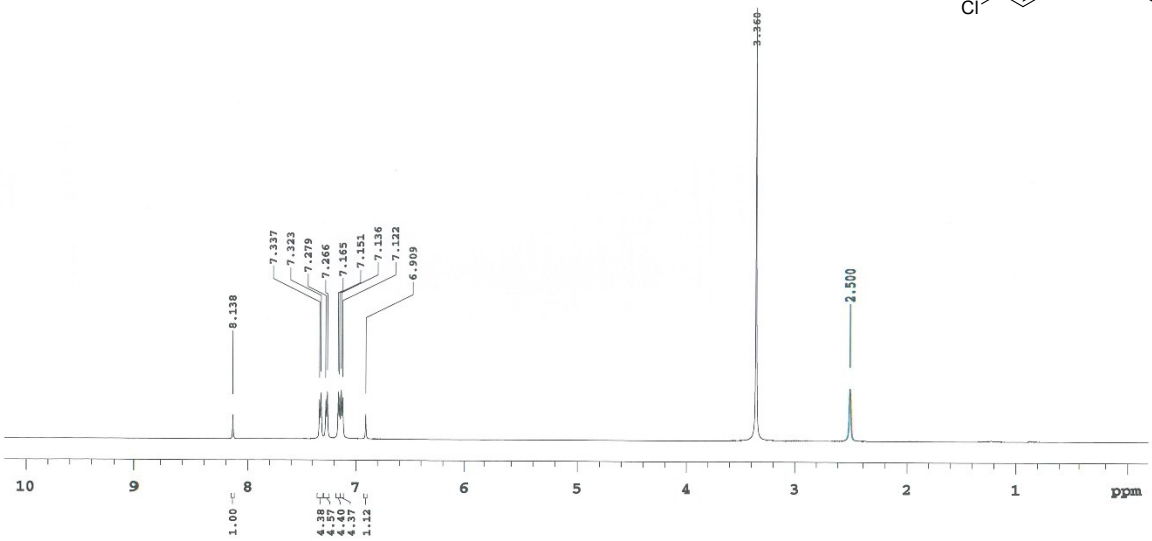




Compound-**3n**

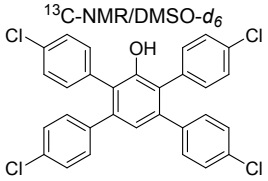
^{1}H-NMR/DMSO-d_6

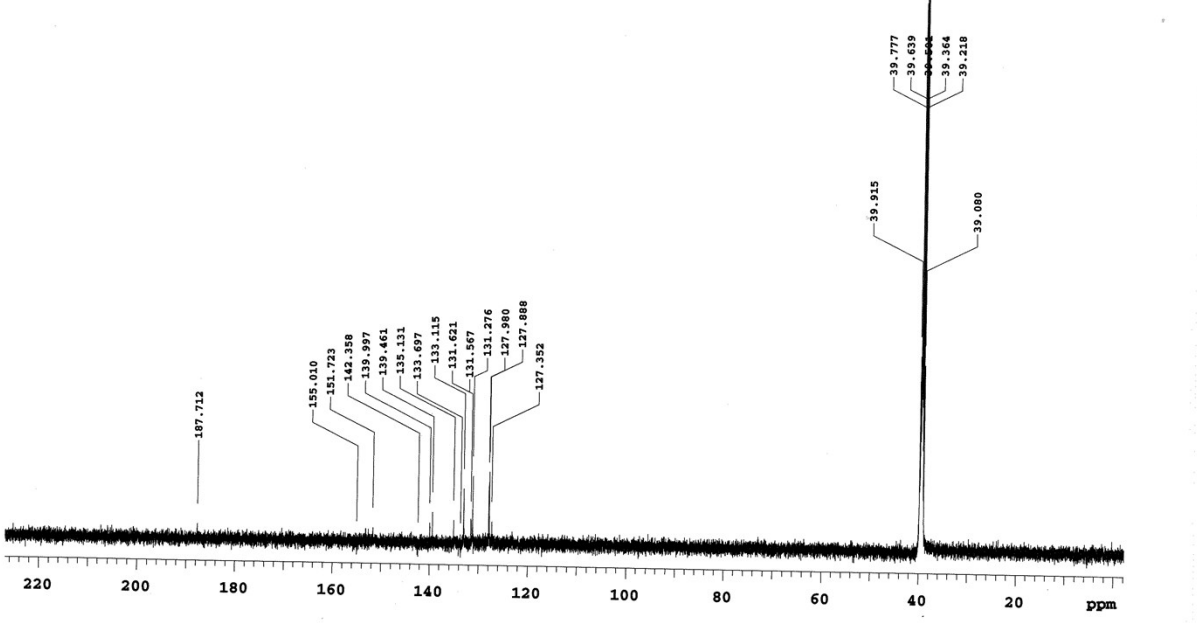




Compound-**3n**

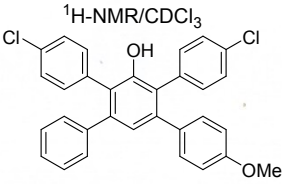
^{13}C-NMR/DMSO-d_6

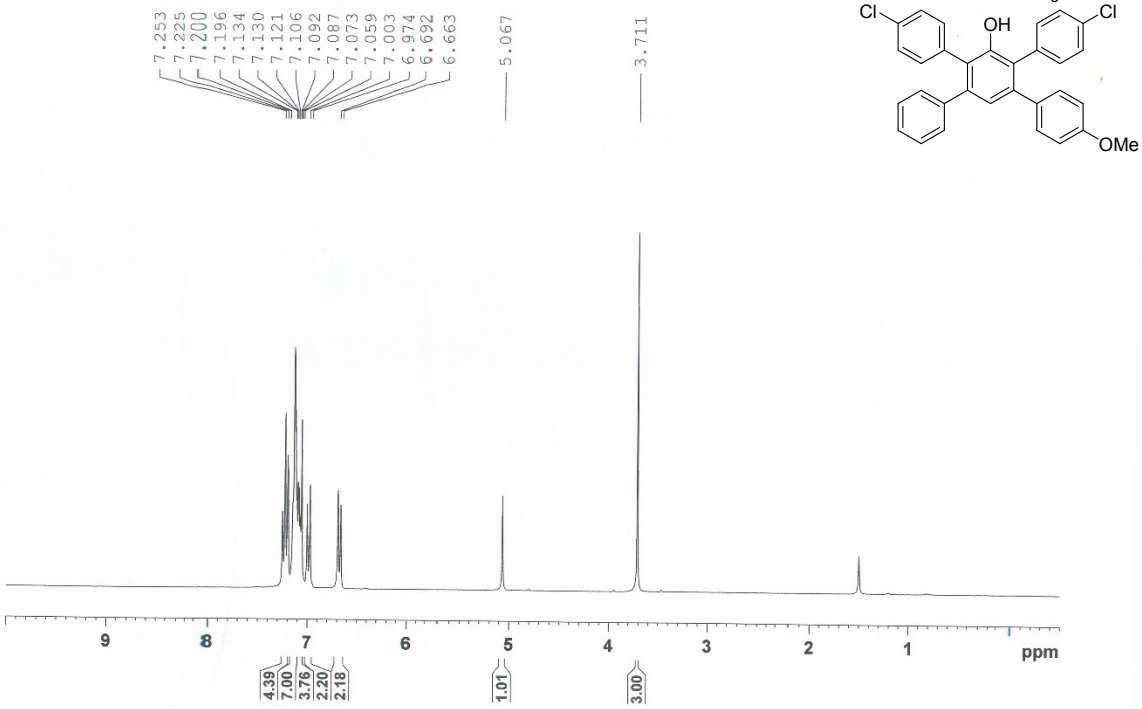




Compound-**3o**

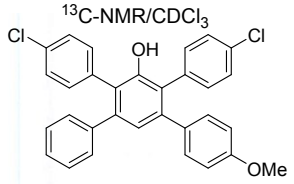
^{1}H-NMR/$CDCl_3$

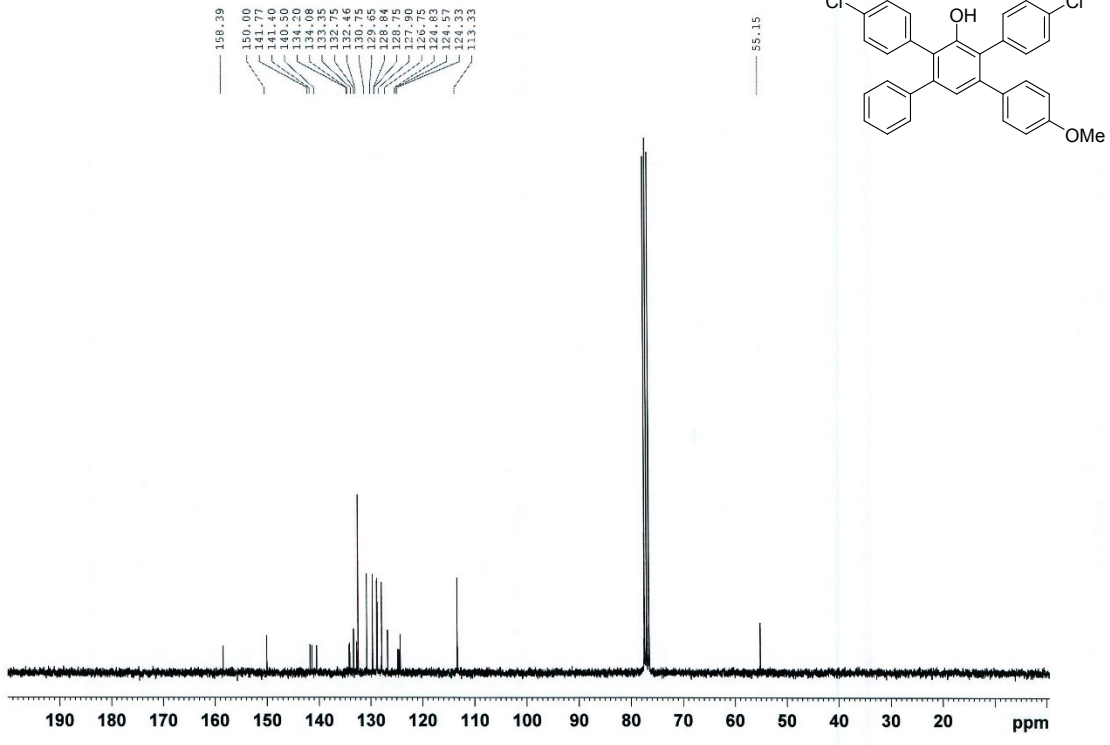




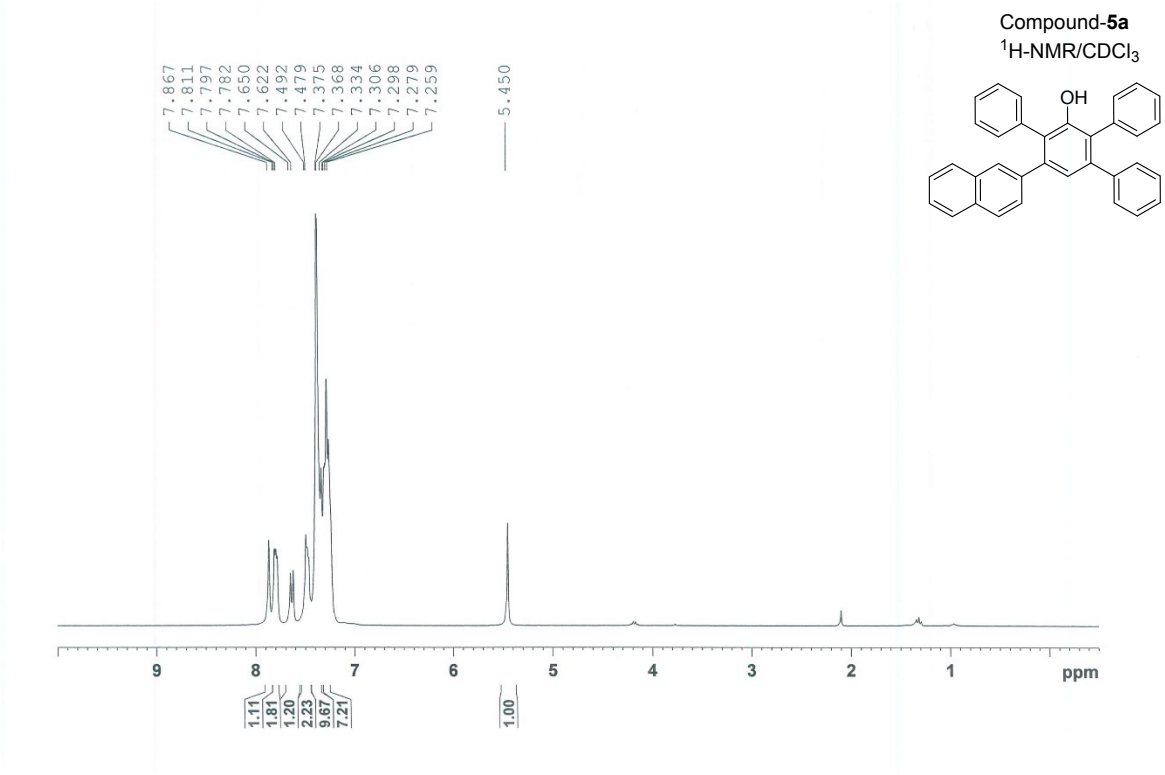
Compound-**3o**

^{13}C-NMR/$CDCl_3$

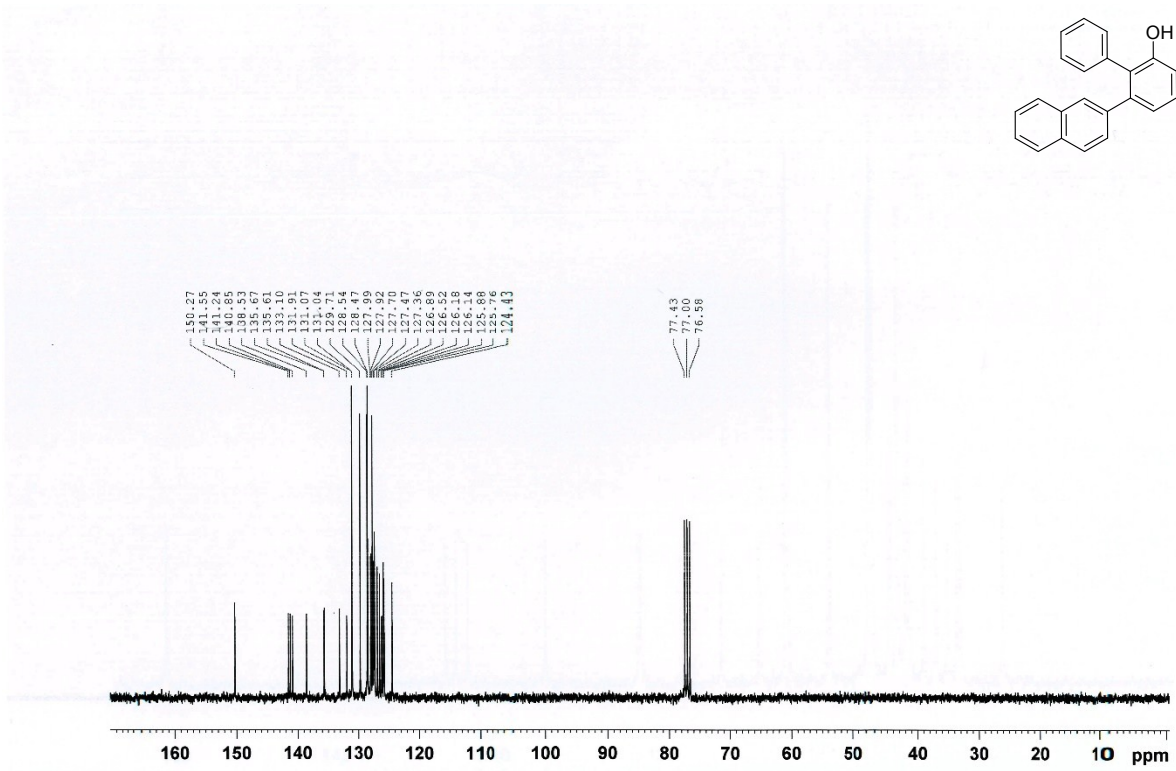


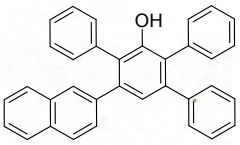


Compound-**5a**
^{1}H-NMR/CDCl$_3$



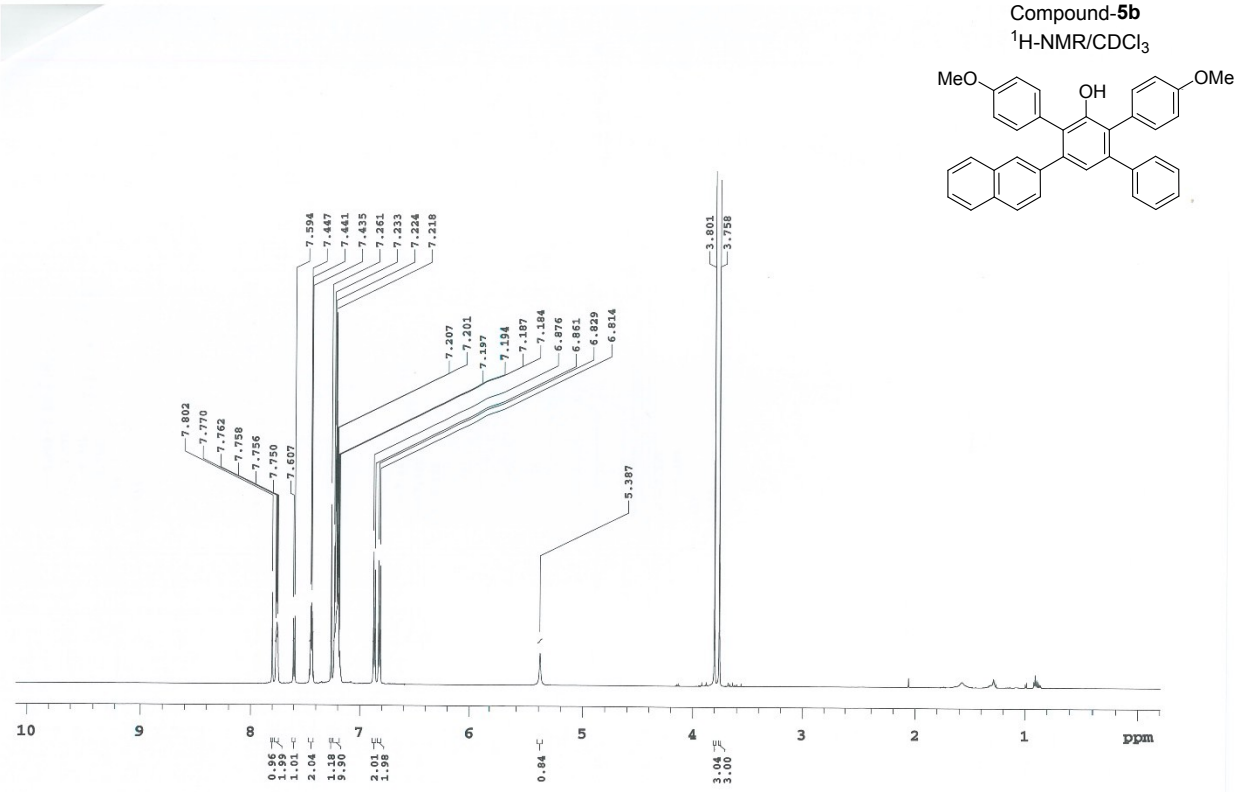
Compound-**5a**
^{13}C-NMR/CDCl$_3$





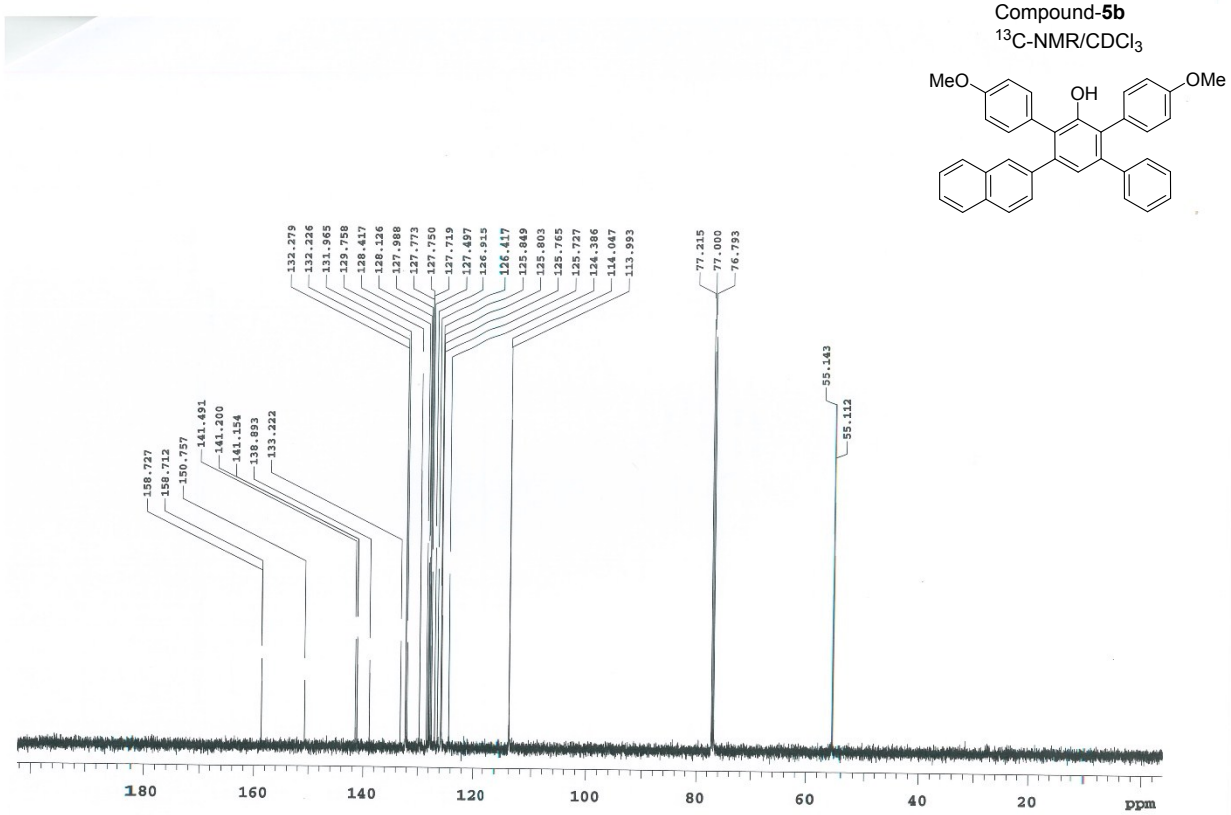
Compound-**5b**

^{1}H-NMR/$CDCl_3$

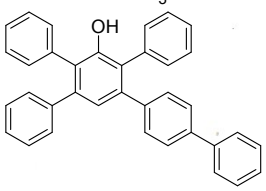


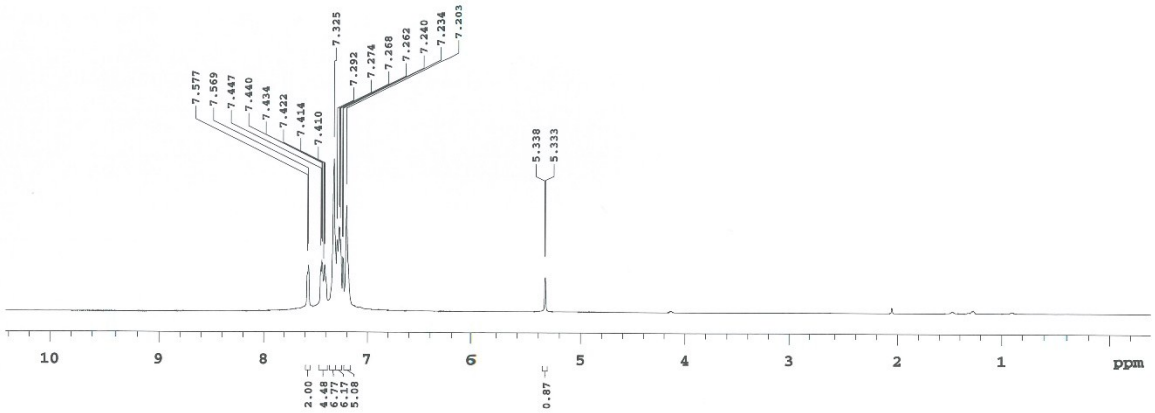
Compound-**5b**

^{13}C-NMR/$CDCl_3$

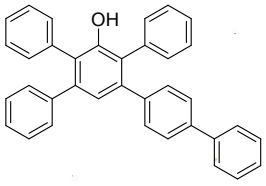


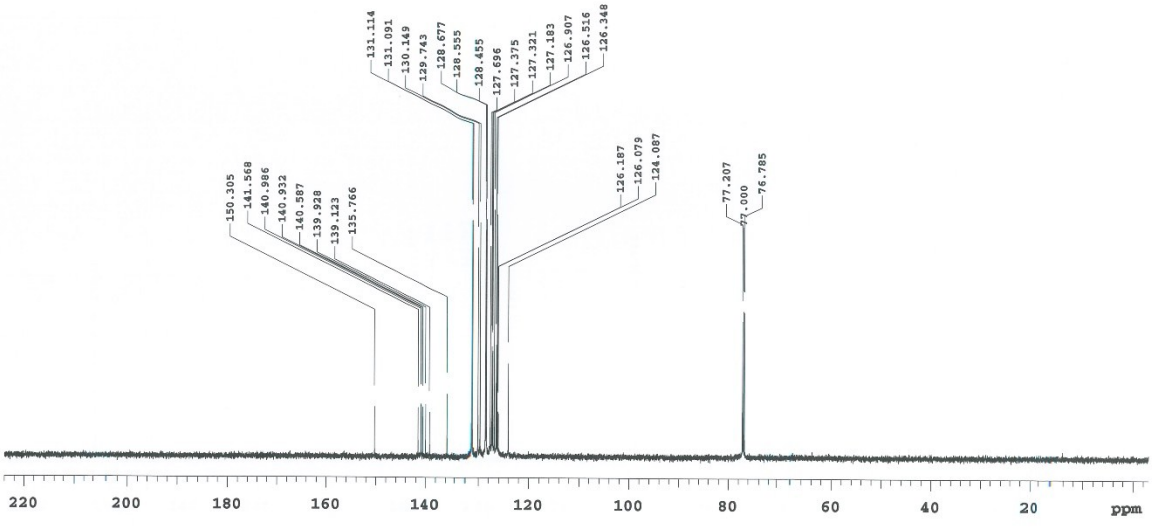
Compound-**5c**
^{1}H-NMR/$CDCl_3$





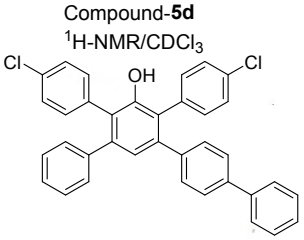
Compound-**5c**
^{13}C-NMR/$CDCl_3$

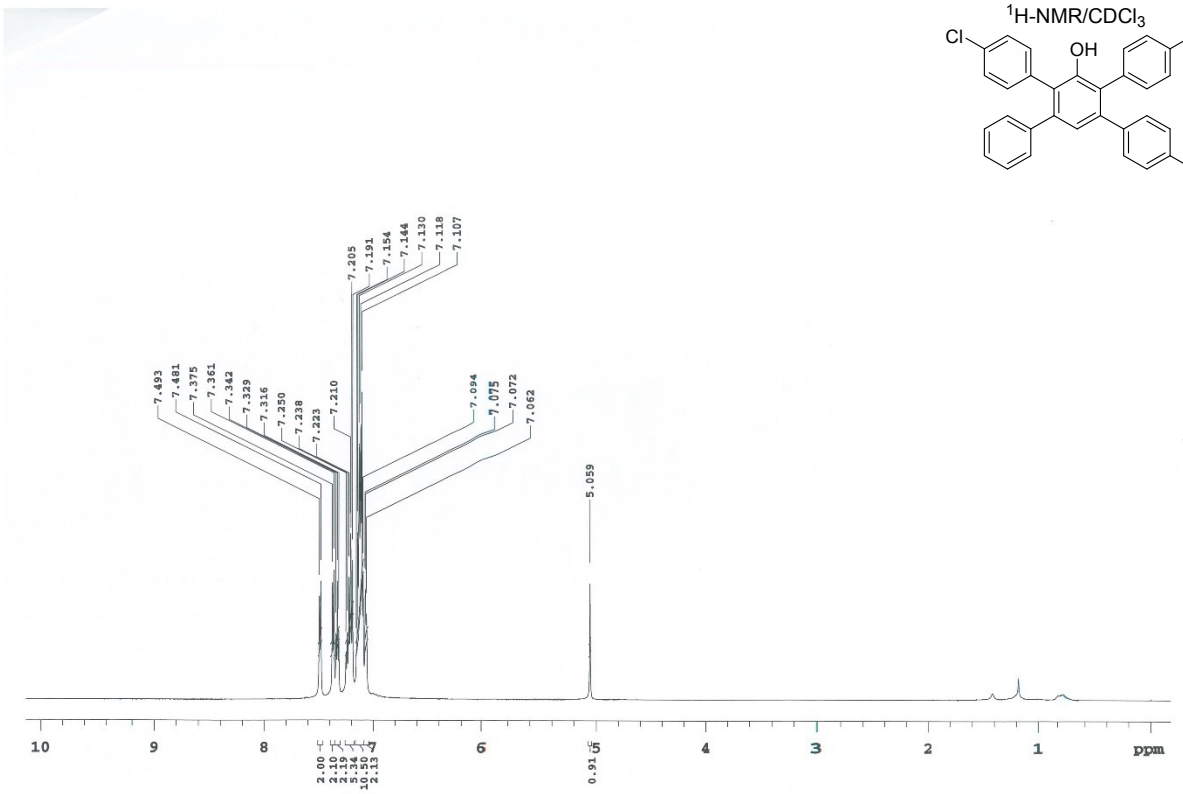




Compound-**5d**

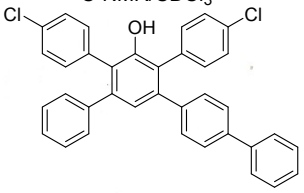
^{1}H-NMR/CDCl$_3$

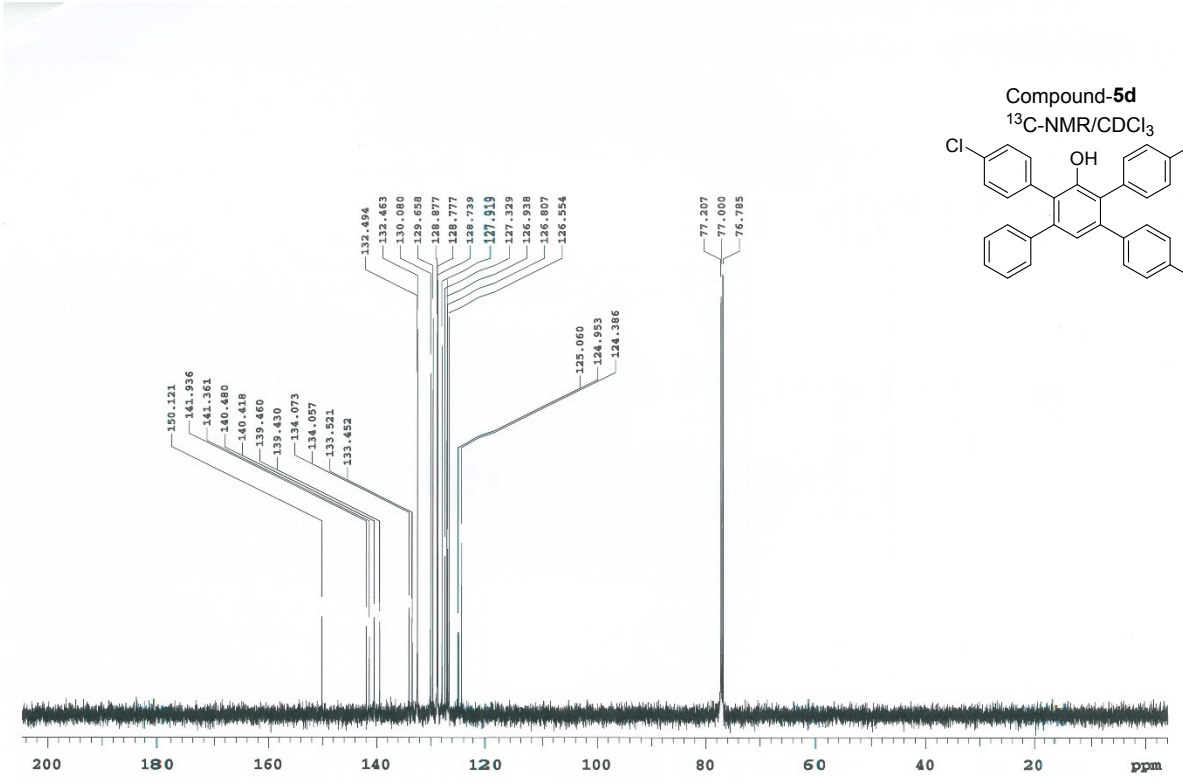




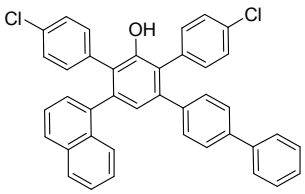
Compound-**5d**

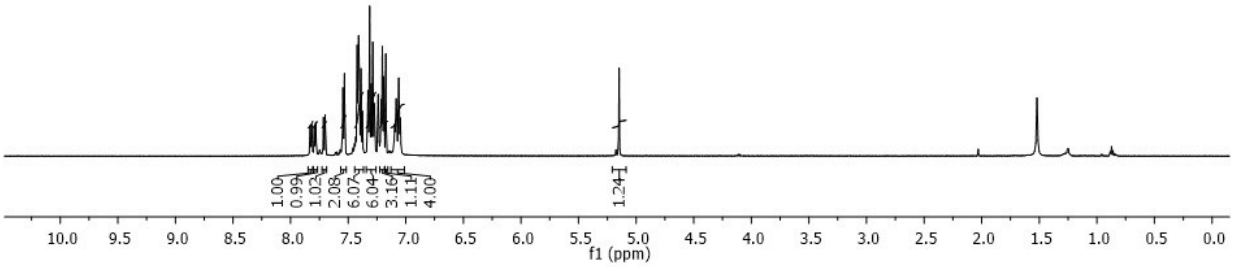
^{13}C-NMR/CDCl$_3$



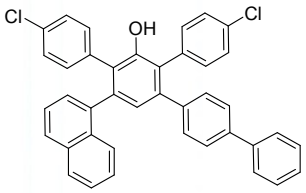


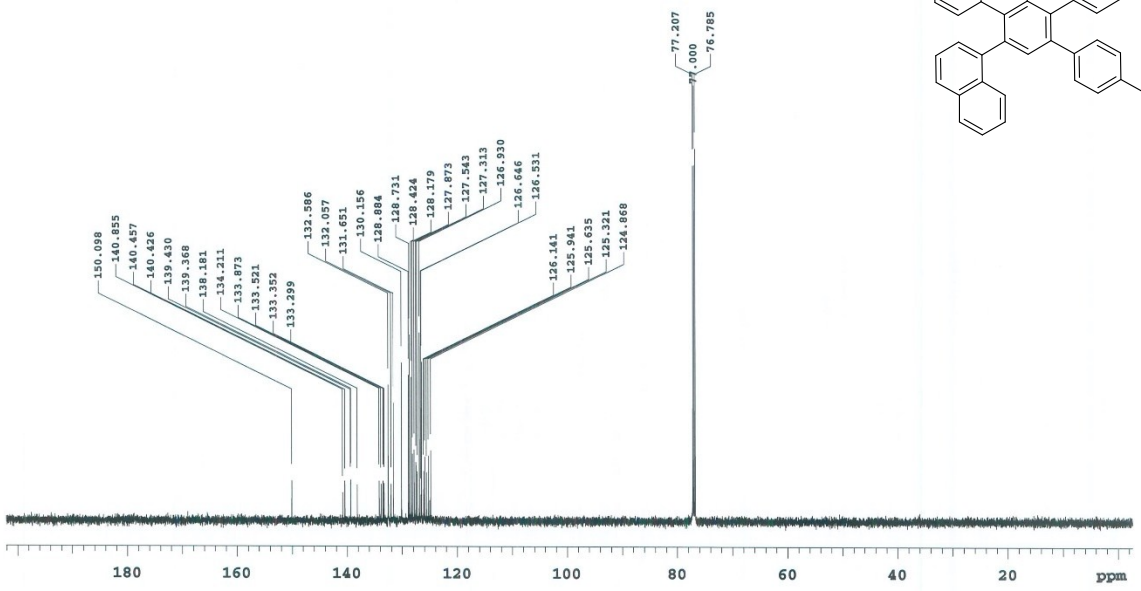
Compound-**5e**
^{1}H-NMR/CDCl$_3$



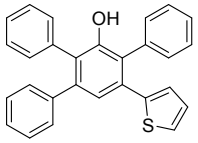


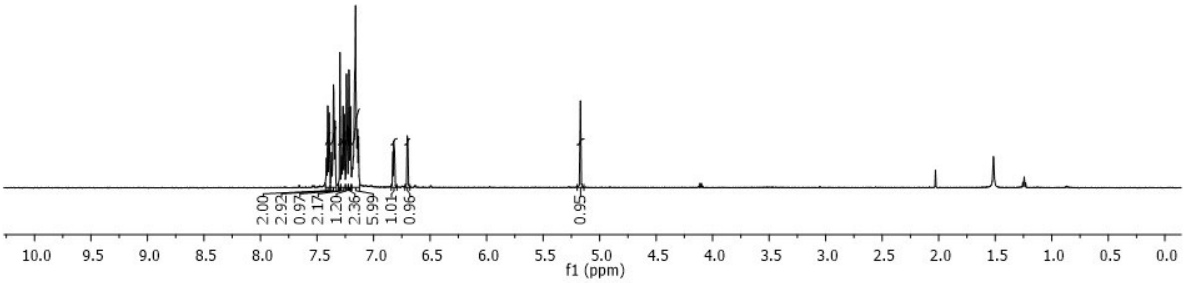
Compound-**5e**
^{13}C-NMR/CDCl$_3$



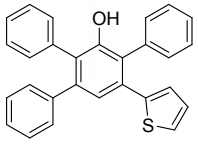


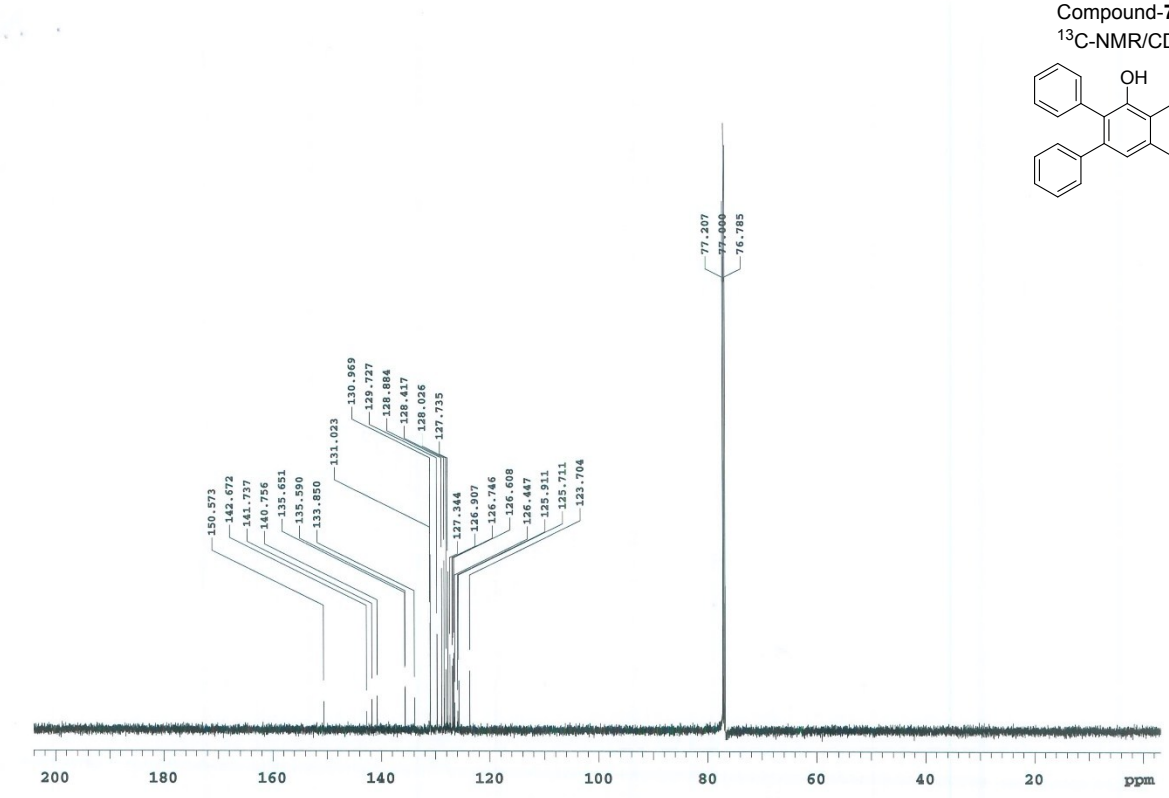
Compound-**7a**
^{1}H-NMR/CDCl$_3$



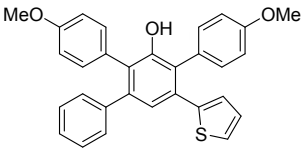


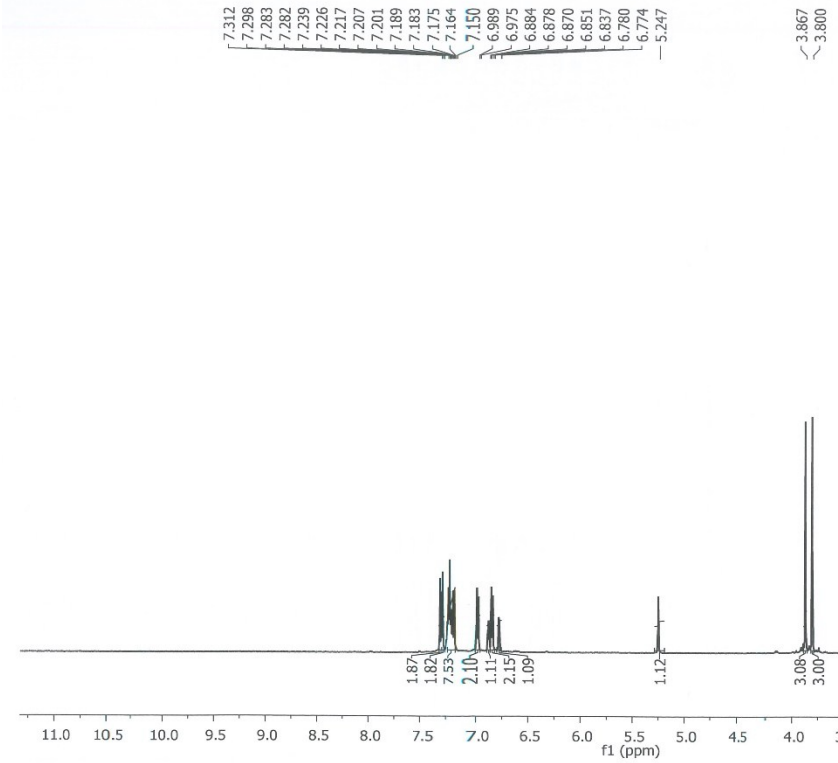
Compound-**7a**
^{13}C-NMR/CDCl$_3$





Compound-**7b**
^{1}H-NMR/CDCl$_3$





Compound-**7b**
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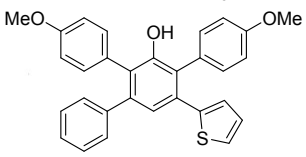
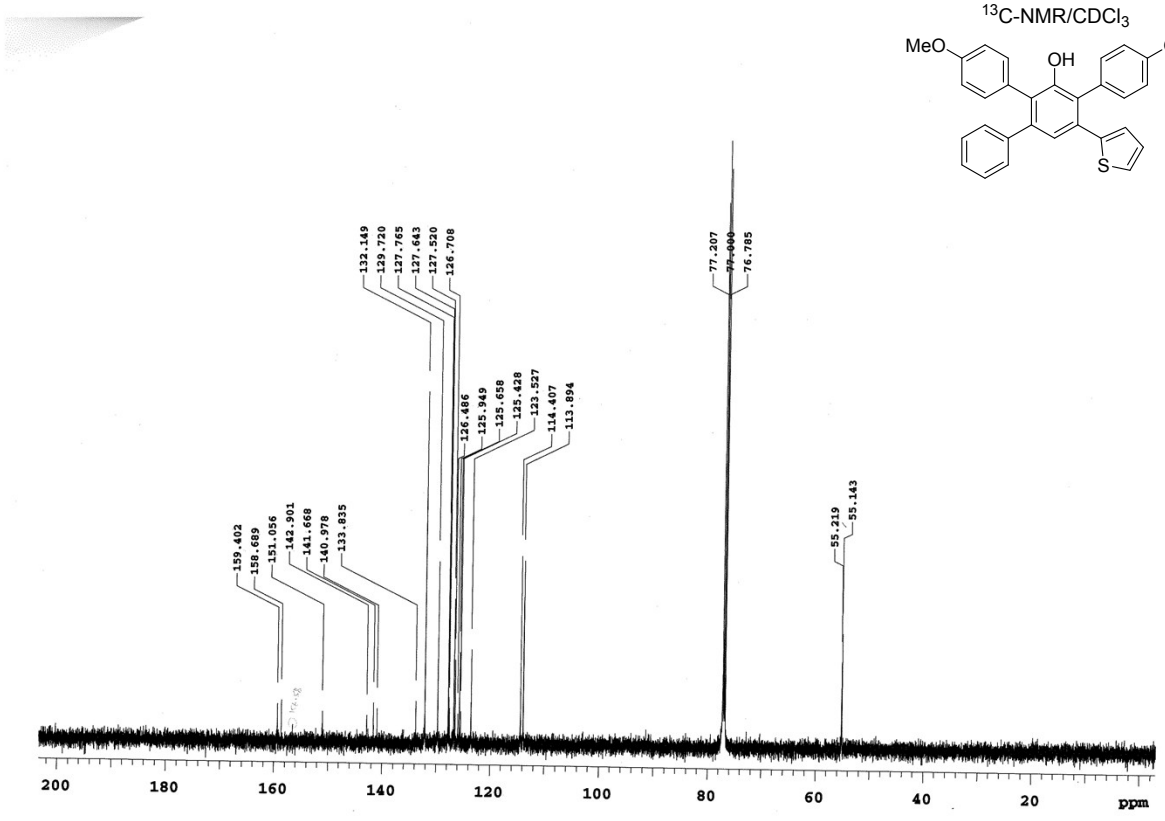
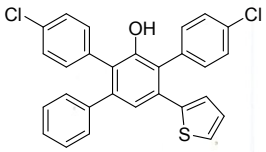
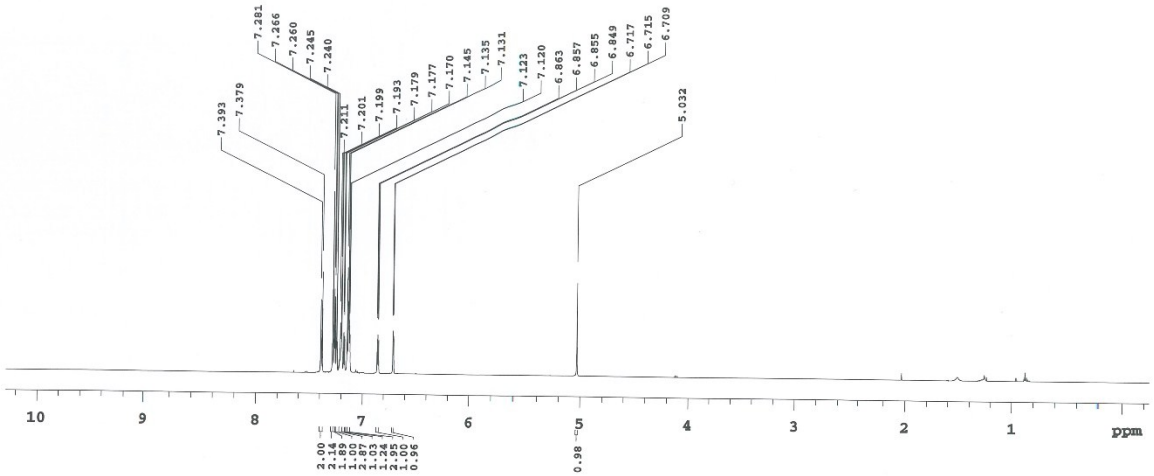




Compound-**7c**

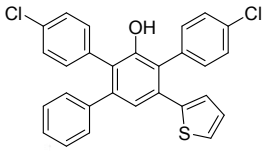
^{13}C-NMR/$CDCl_3$

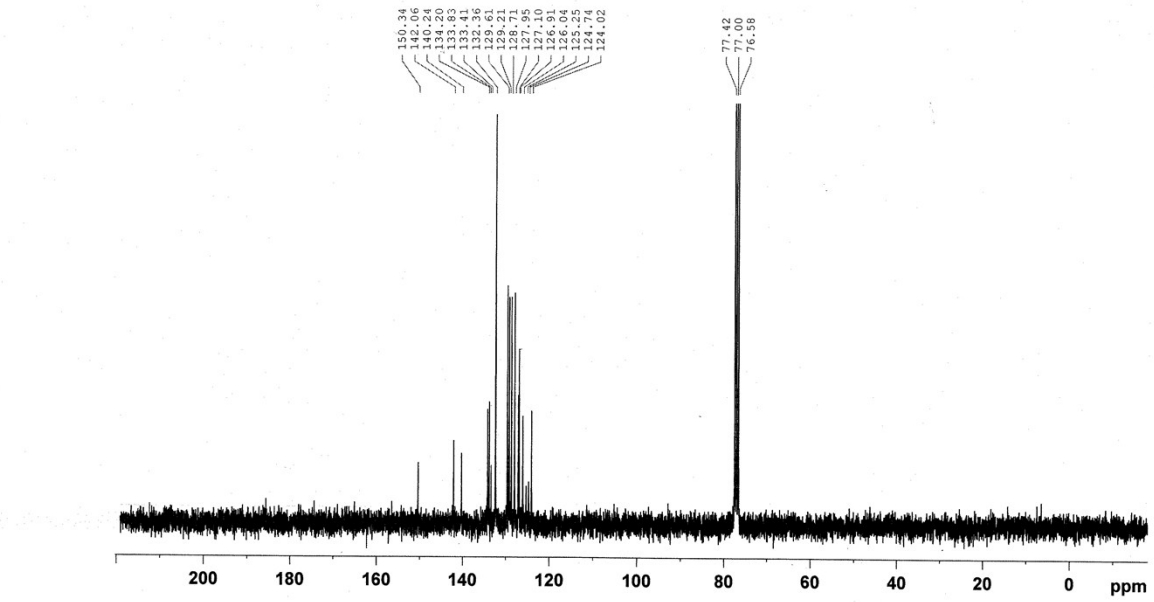




Compound-**7c**

^{1}H-NMR/$CDCl_3$





Compound-**7d**
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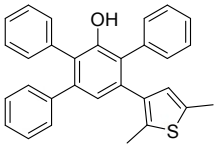

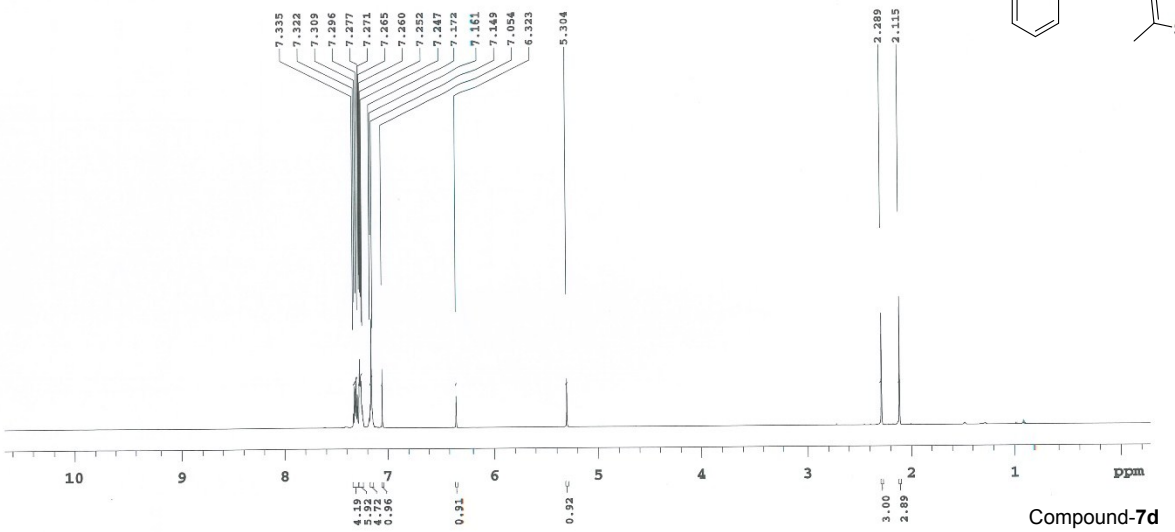

Compound-**7d**
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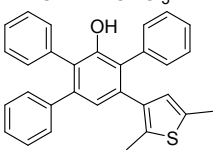
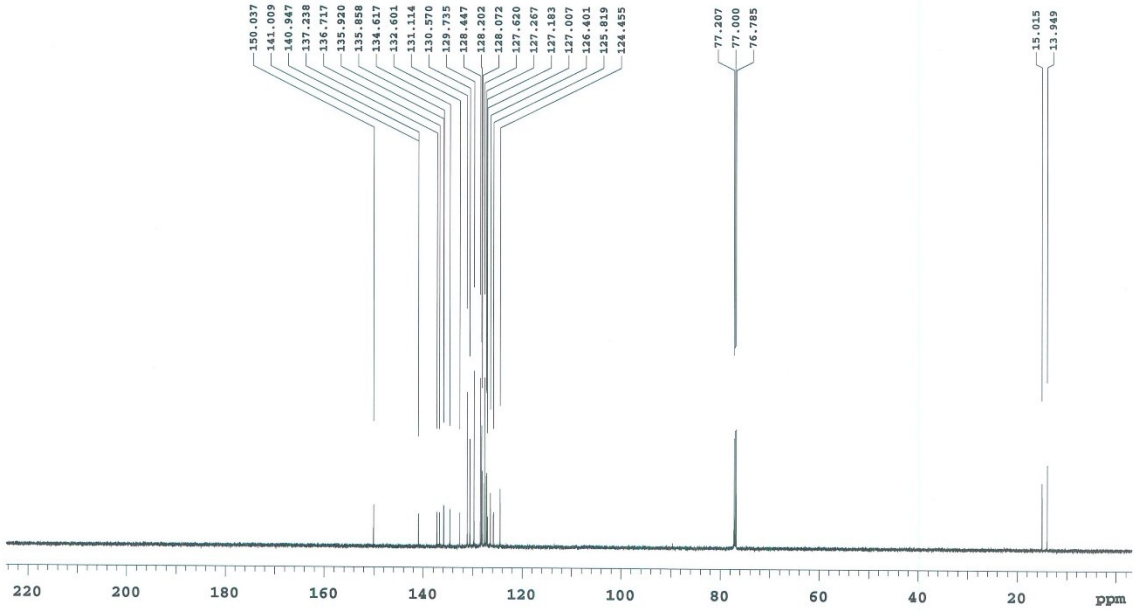
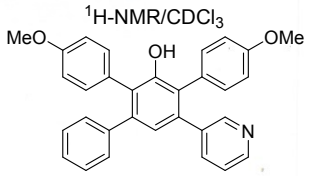
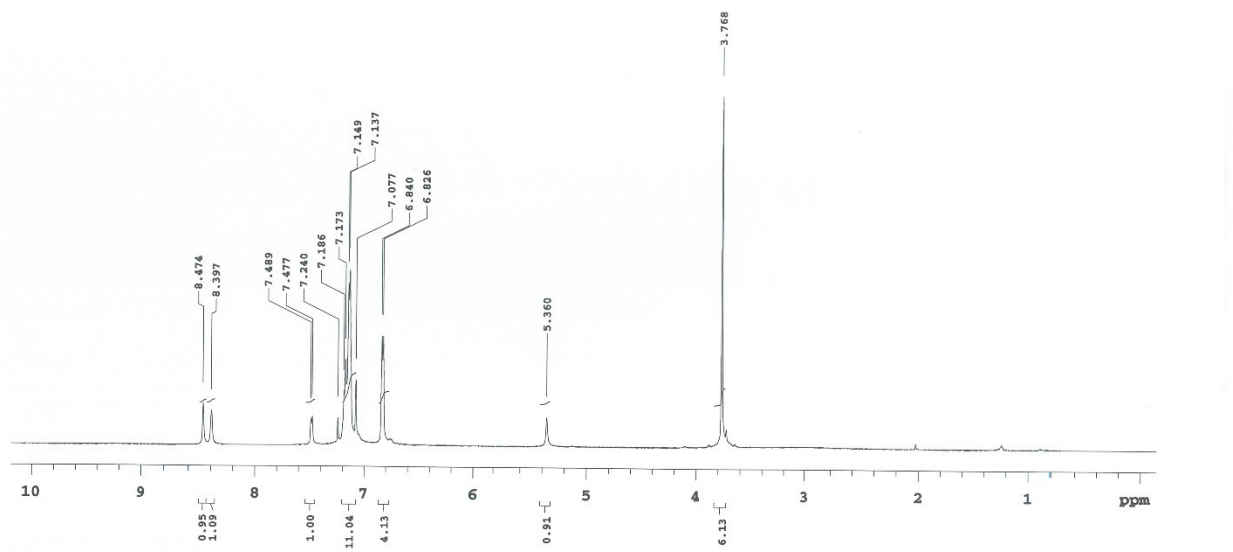




Compound-**7e**

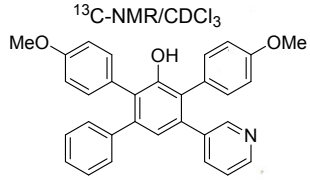
^{1}H-NMR/$CDCl_3$

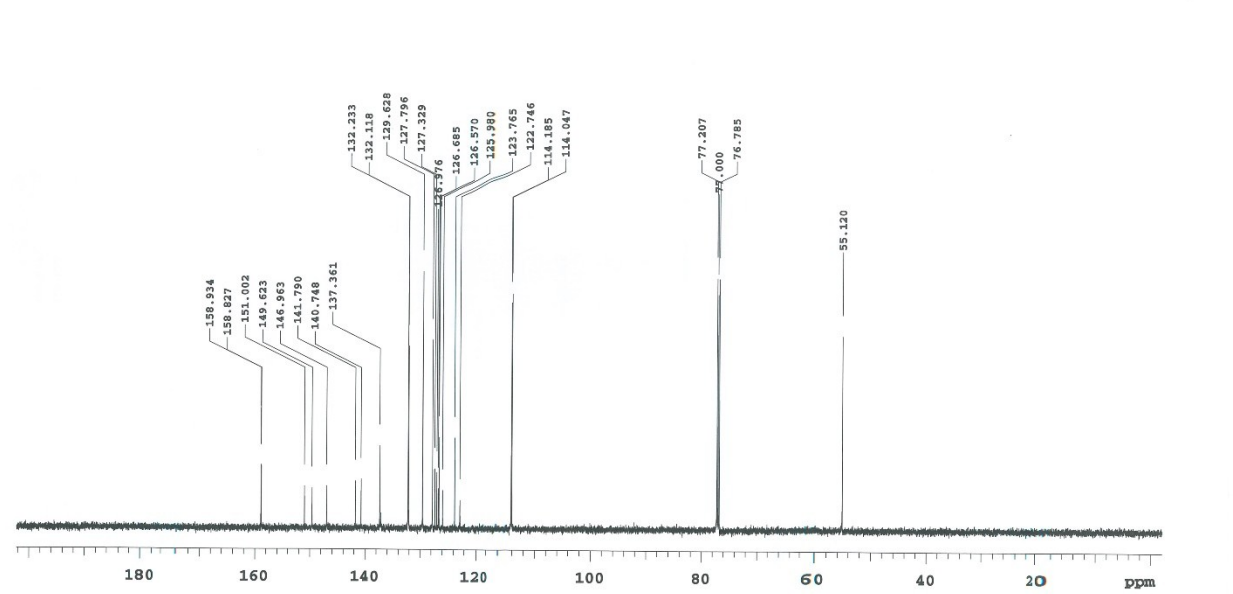




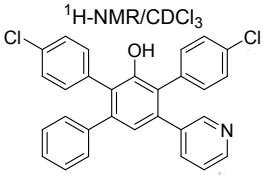
Compound-**7e**

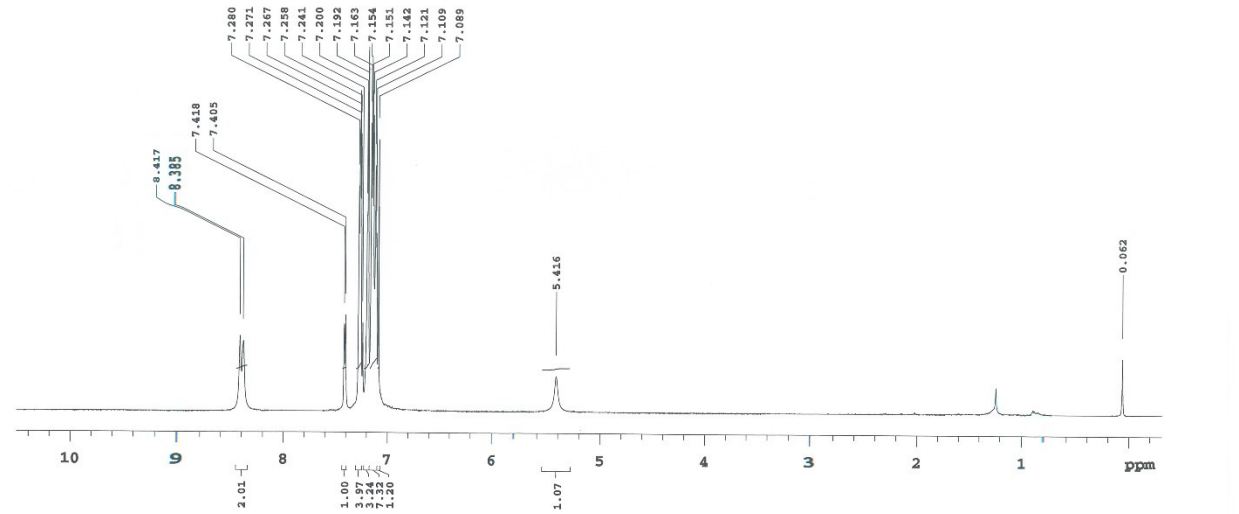
^{13}C-NMR/$CDCl_3$



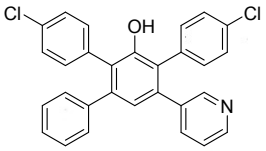


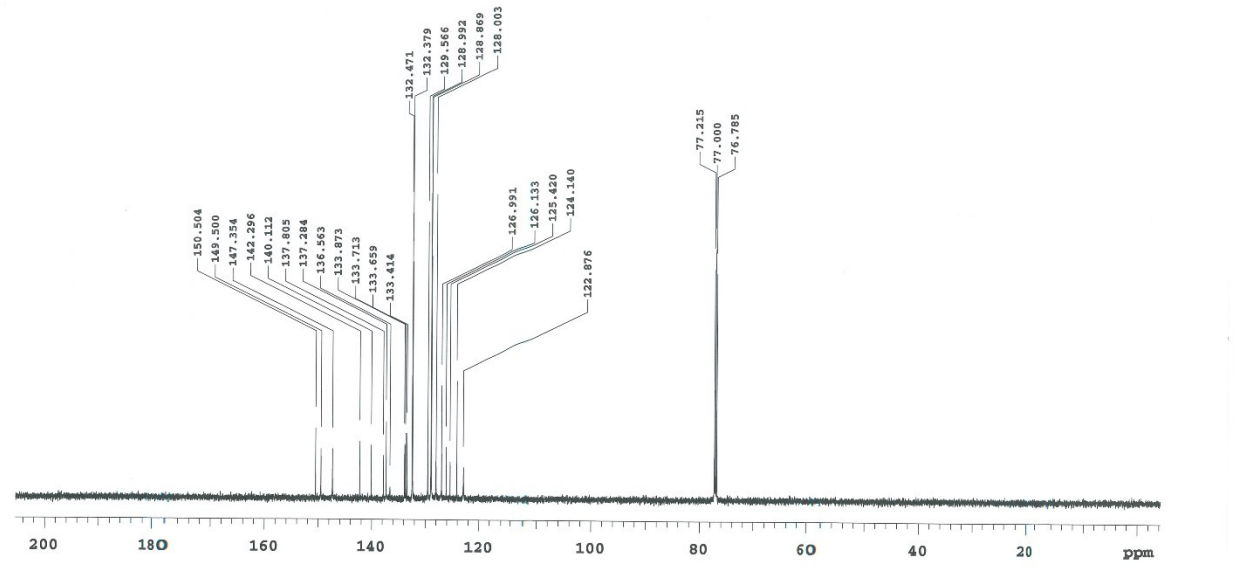
Compound-**7f**
^{1}H-NMR/$CDCl_3$

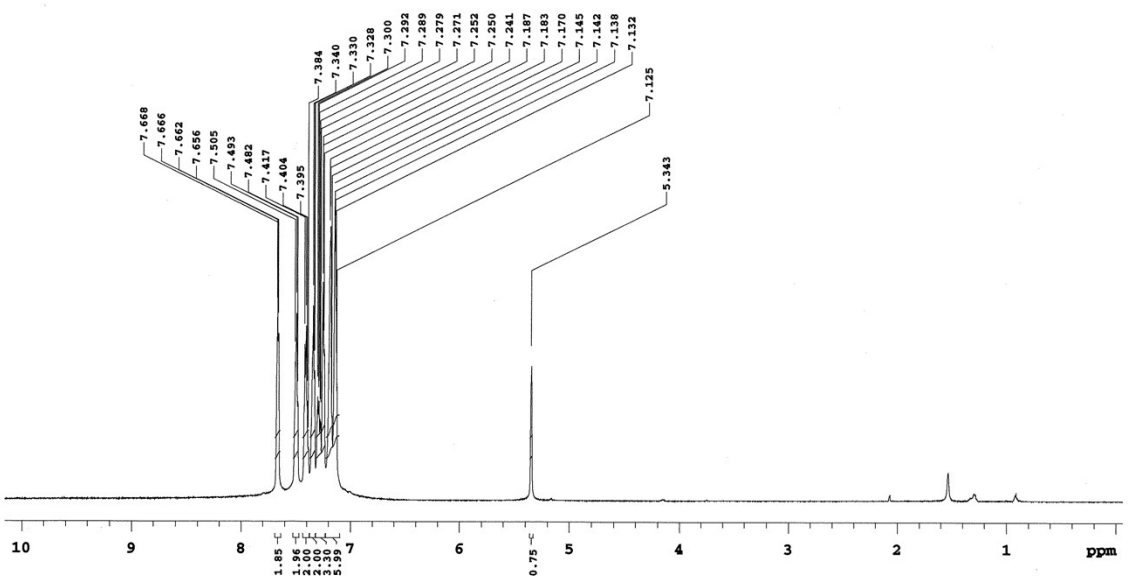




Compound-**7f**
^{13}C-NMR/$CDCl_3$

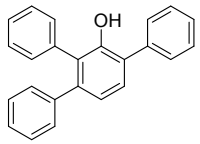


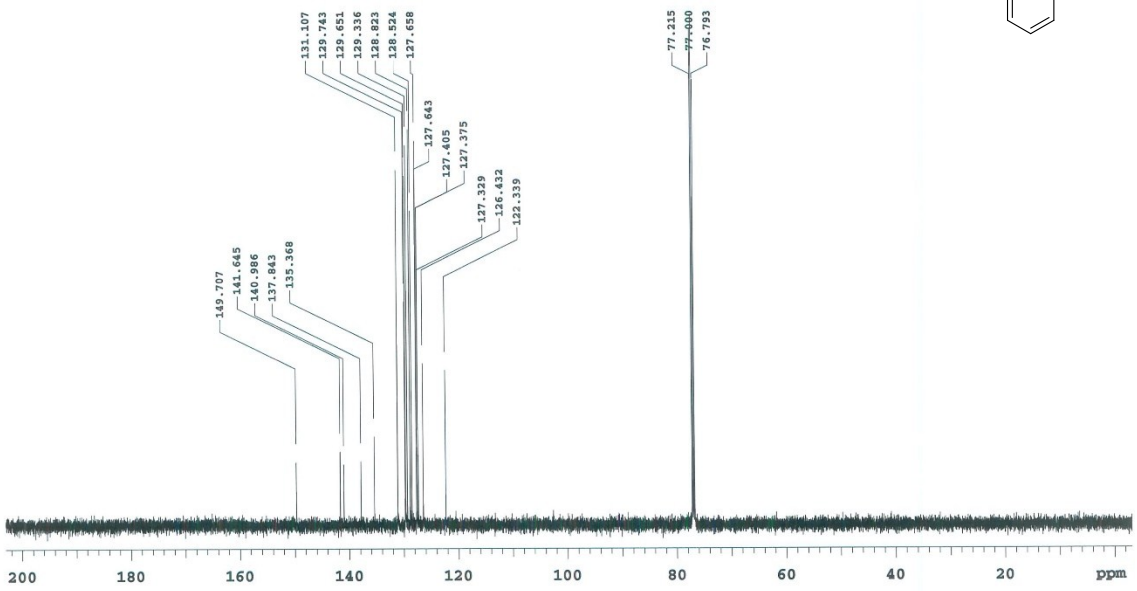




Compound-**9a**

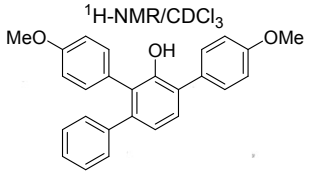
^{13}C-NMR/$CDCl_3$

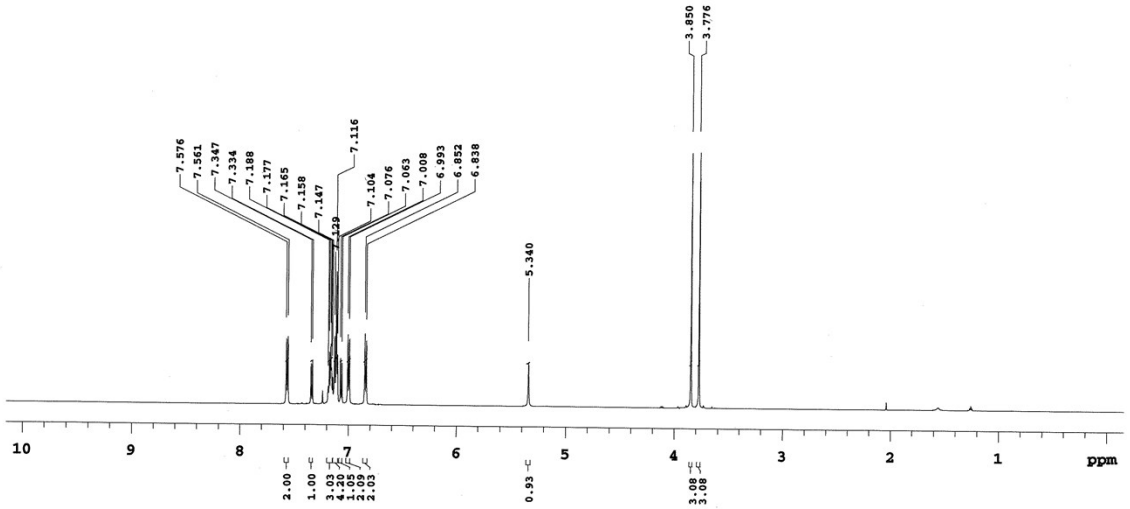




Compound-**9b**

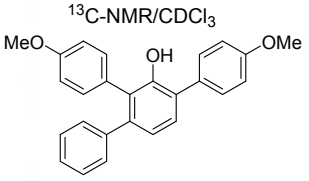
^{1}H-NMR/$CDCl_3$

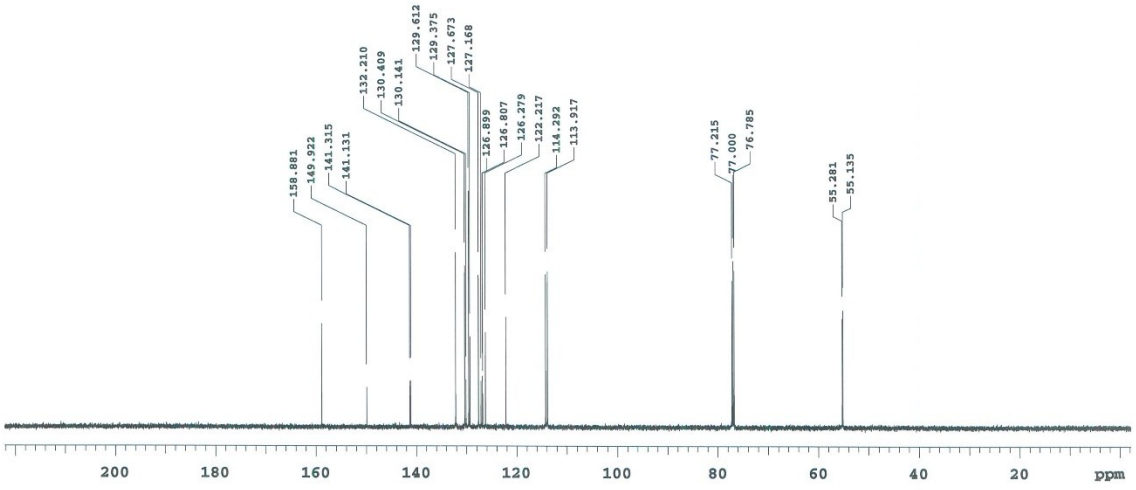




Compound-**9b**

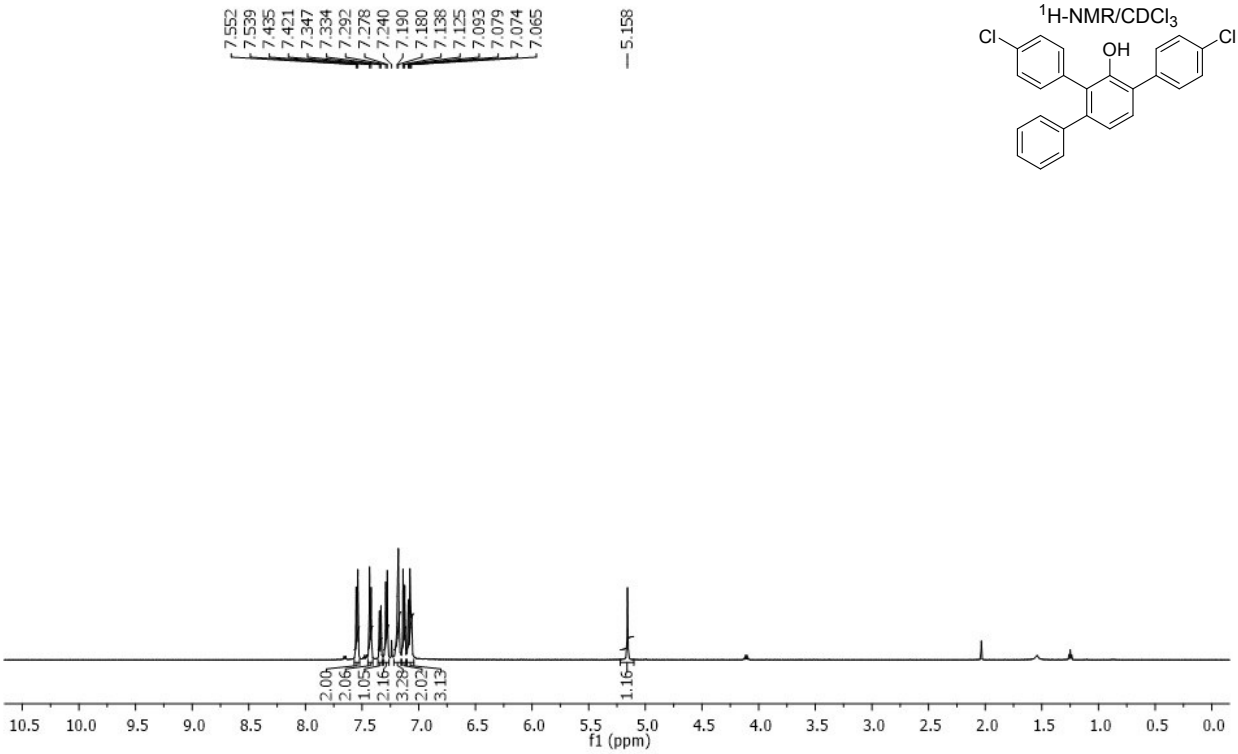
^{13}C-NMR/$CDCl_3$





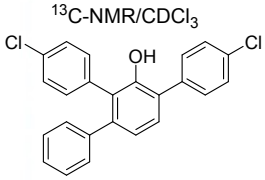
Compound-**9c**

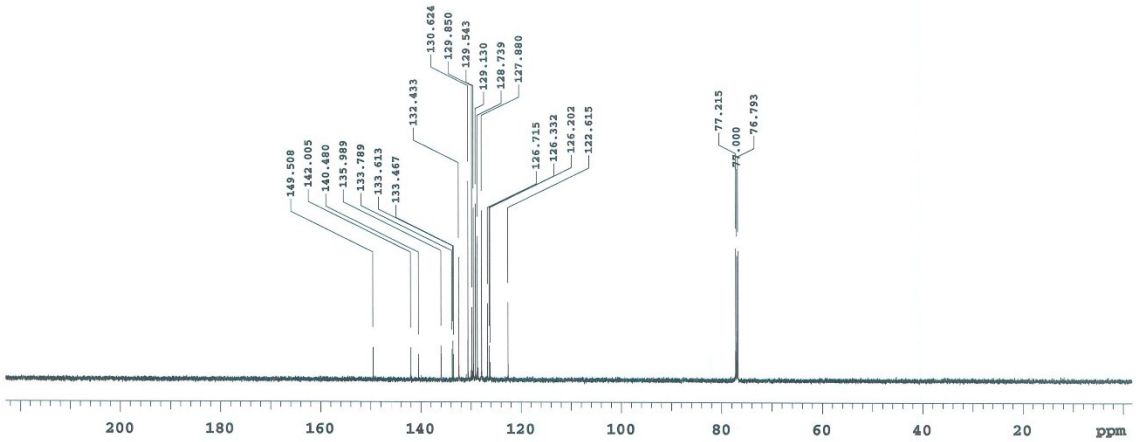
^{1}H-NMR/$CDCl_3$



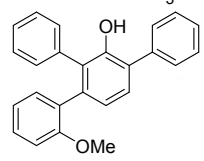
Compound-**9c**

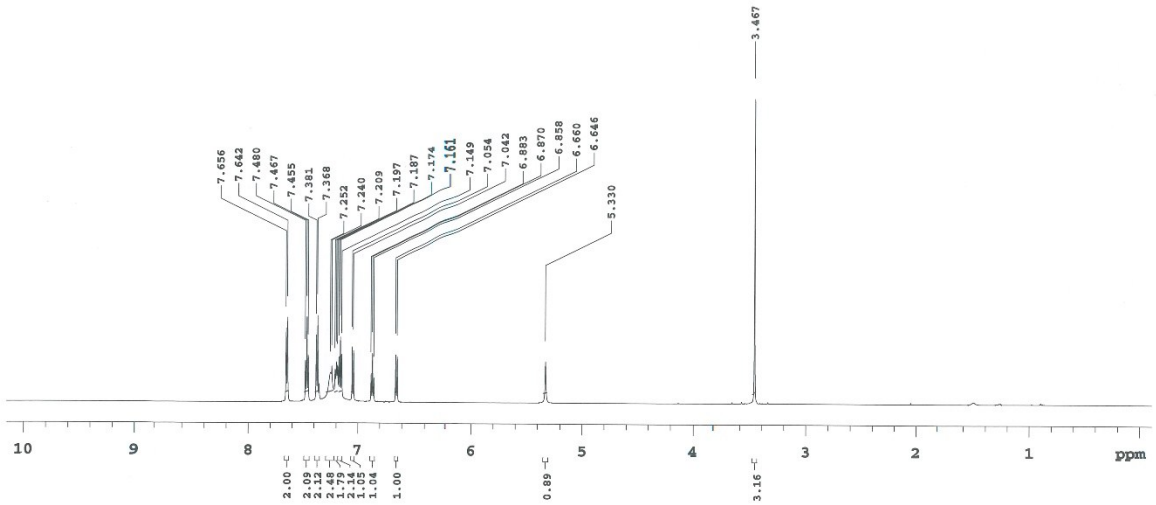
^{13}C-NMR/$CDCl_3$



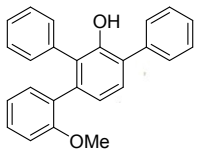


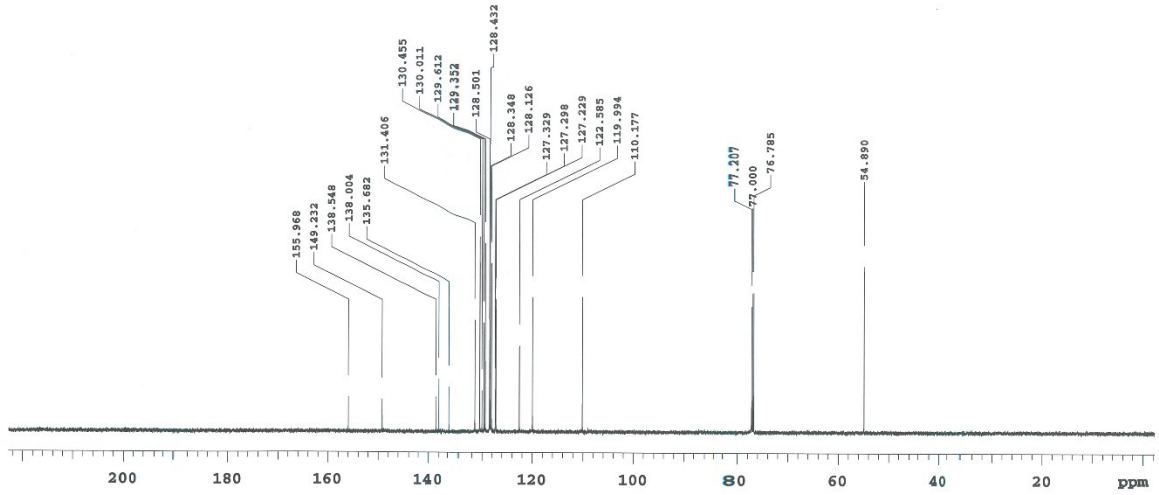
Compound-**9d**
^{1}H-NMR/$CDCl_3$



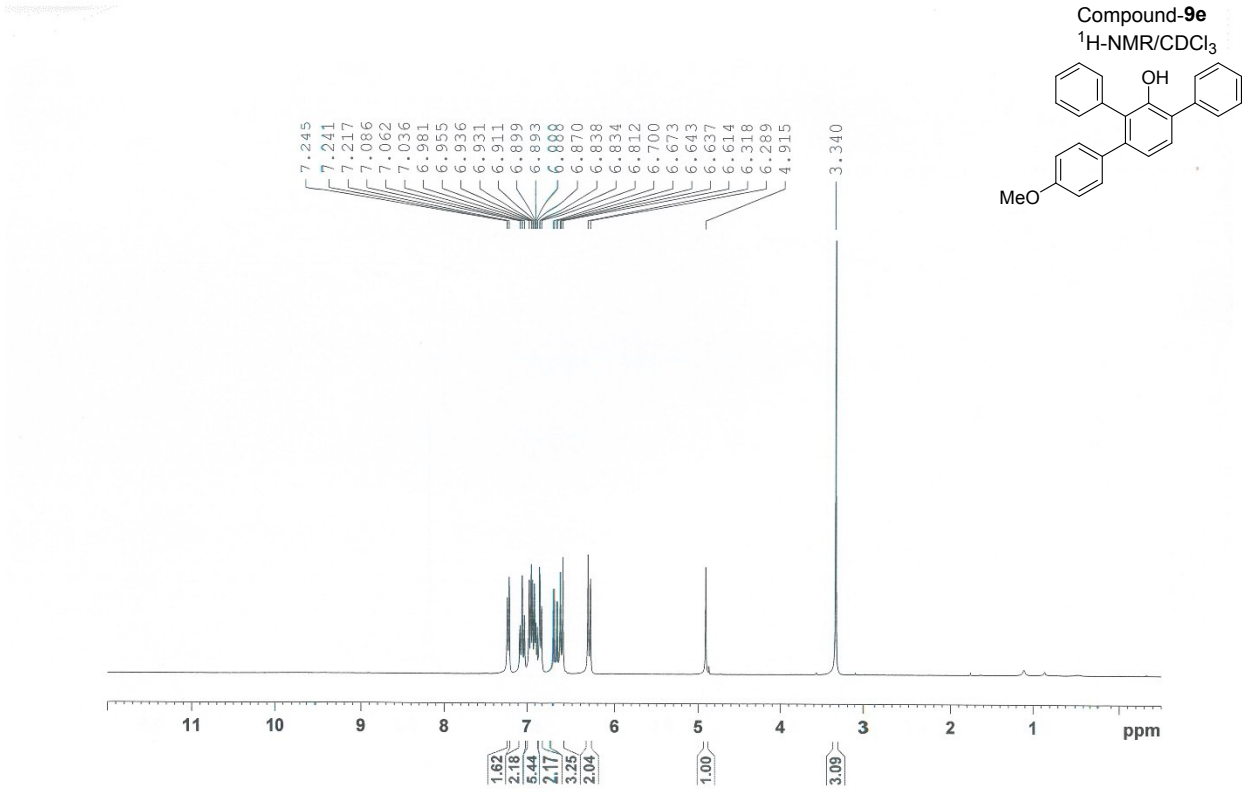


Compound-**9d**
^{13}C-NMR/$CDCl_3$

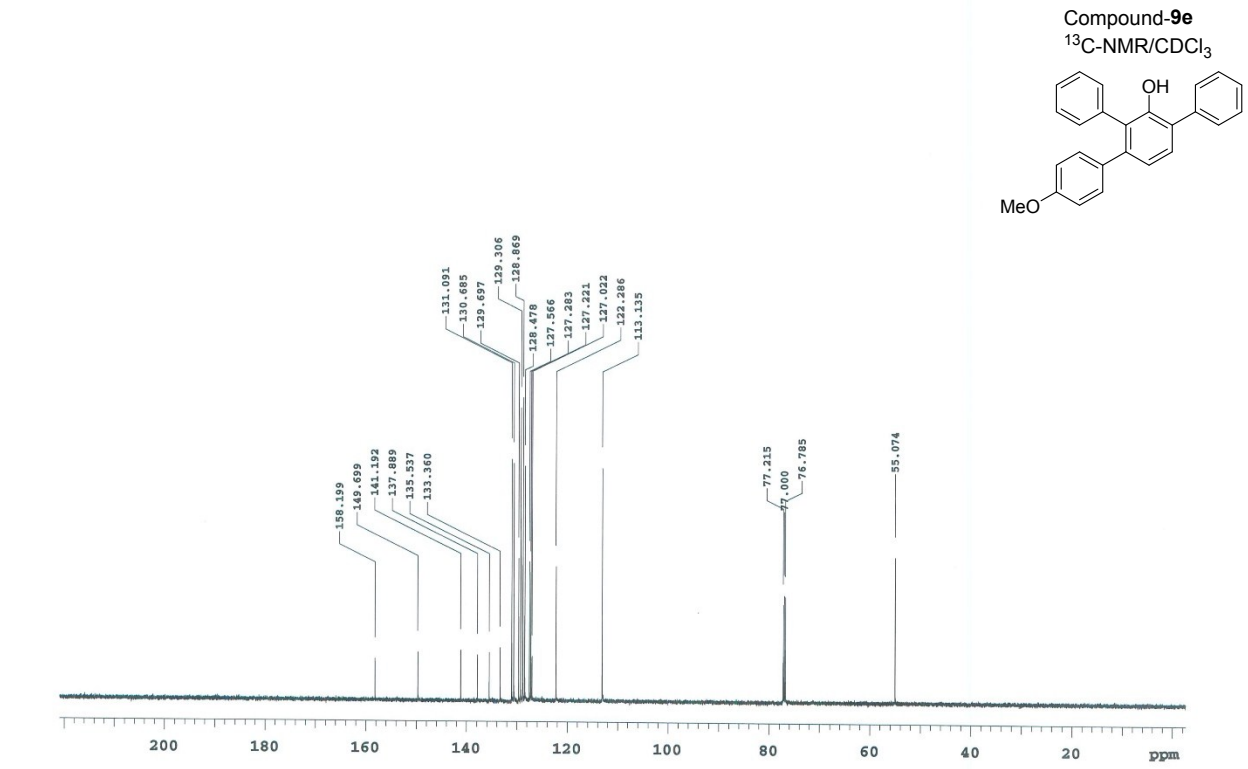




Compound-**9e**
^{1}H-NMR/$CDCl_3$

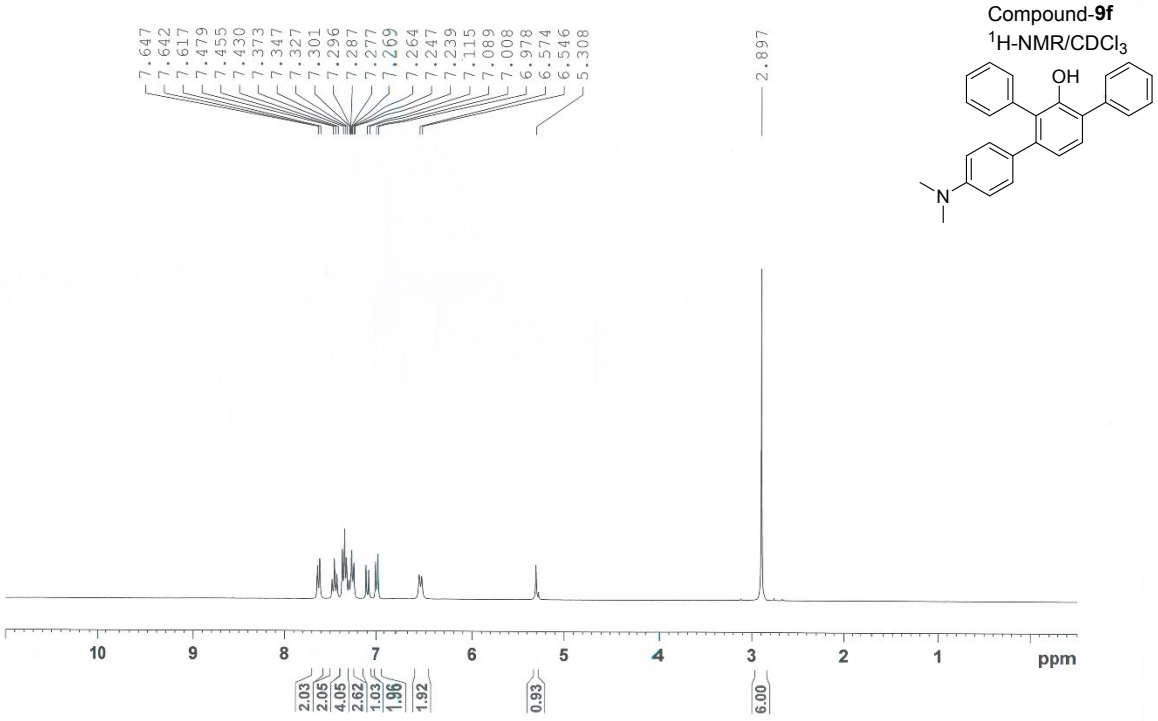


Compound-**9e**
^{13}C-NMR/$CDCl_3$



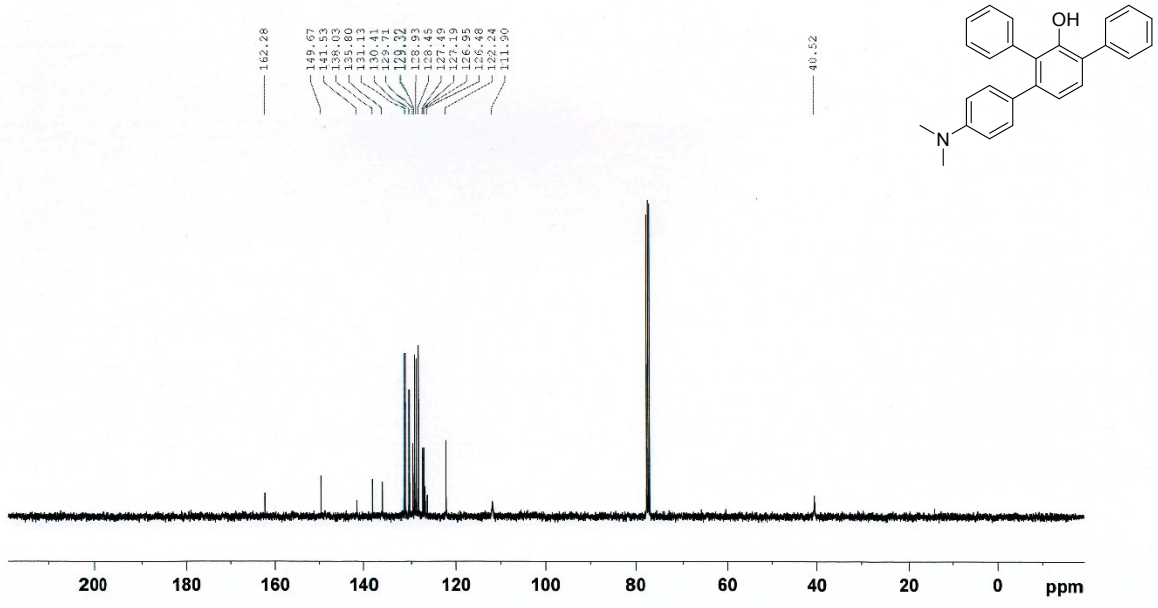
Compound-**9f**

^{1}H-NMR/$CDCl_3$

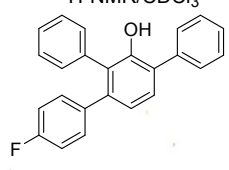


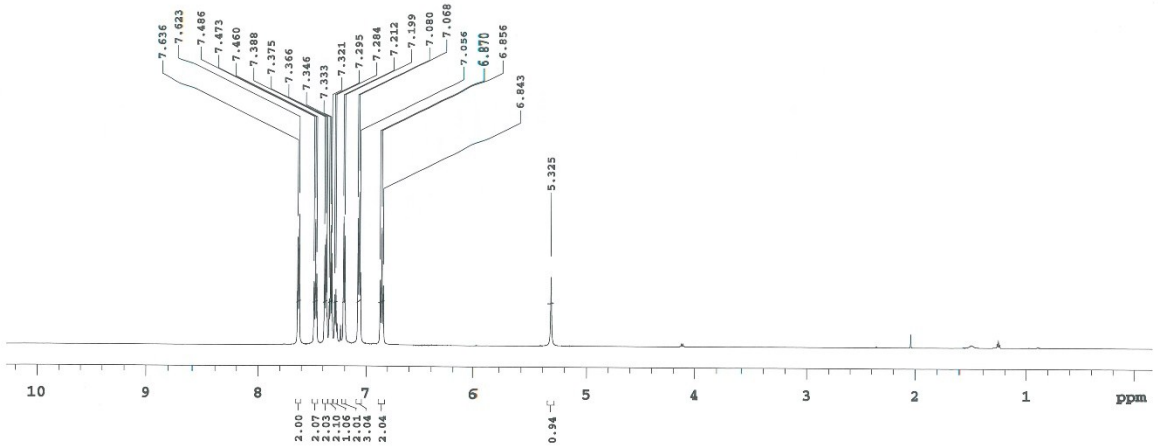
Compound-**9f**

^{13}C-NMR/$CDCl_3$

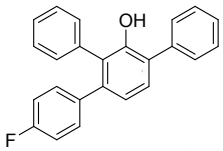


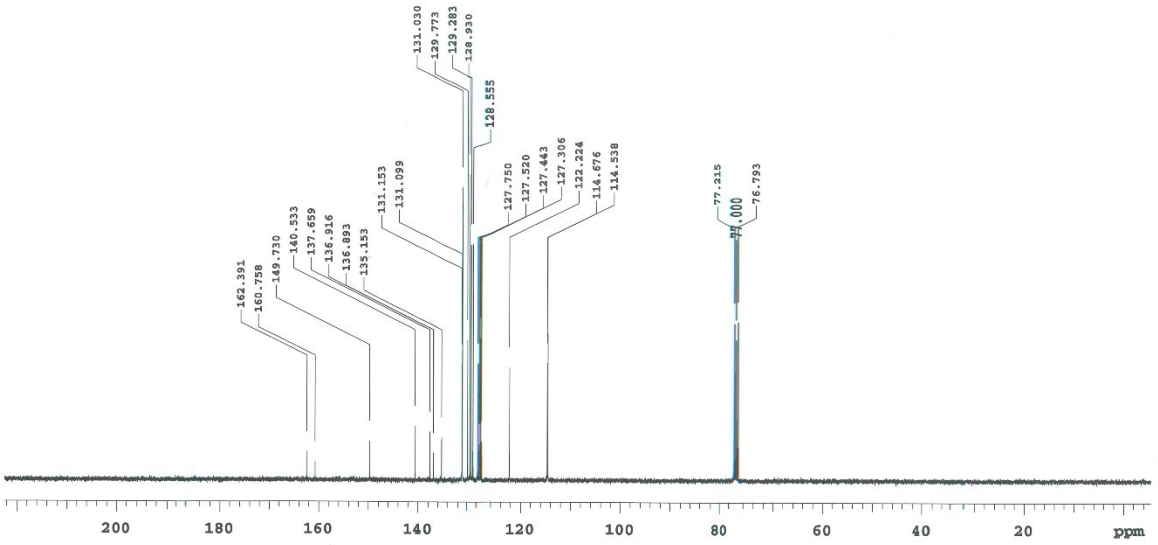
Compound-**9g**
^{1}H-NMR/$CDCl_3$

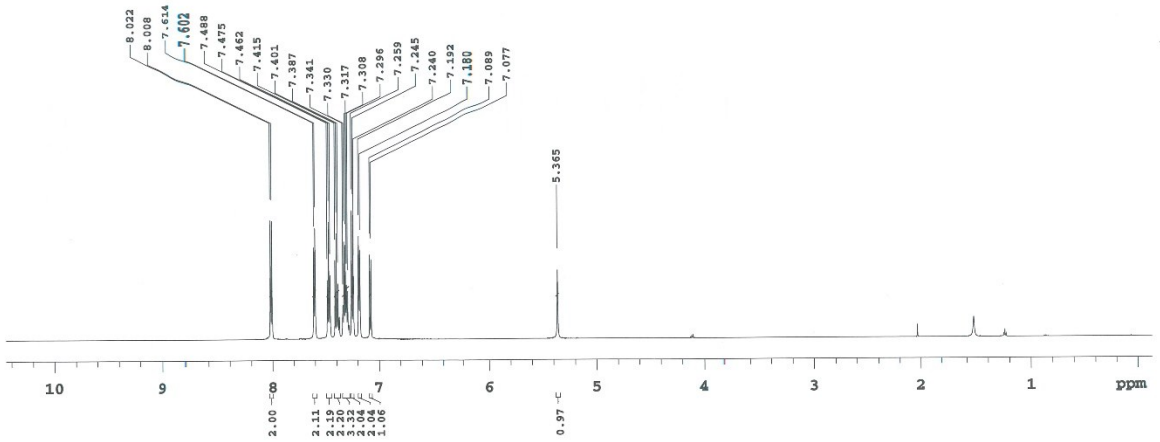




Compound-**9g**
^{13}C-NMR/$CDCl_3$

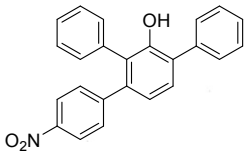


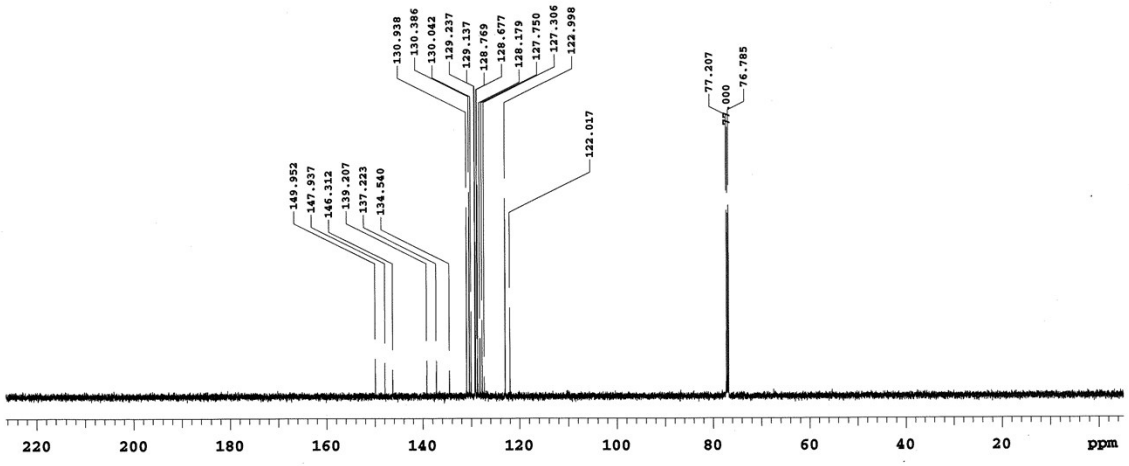




Compound-**9h**

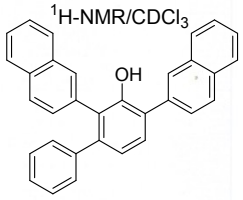
^{13}C-NMR/$CDCl_3$

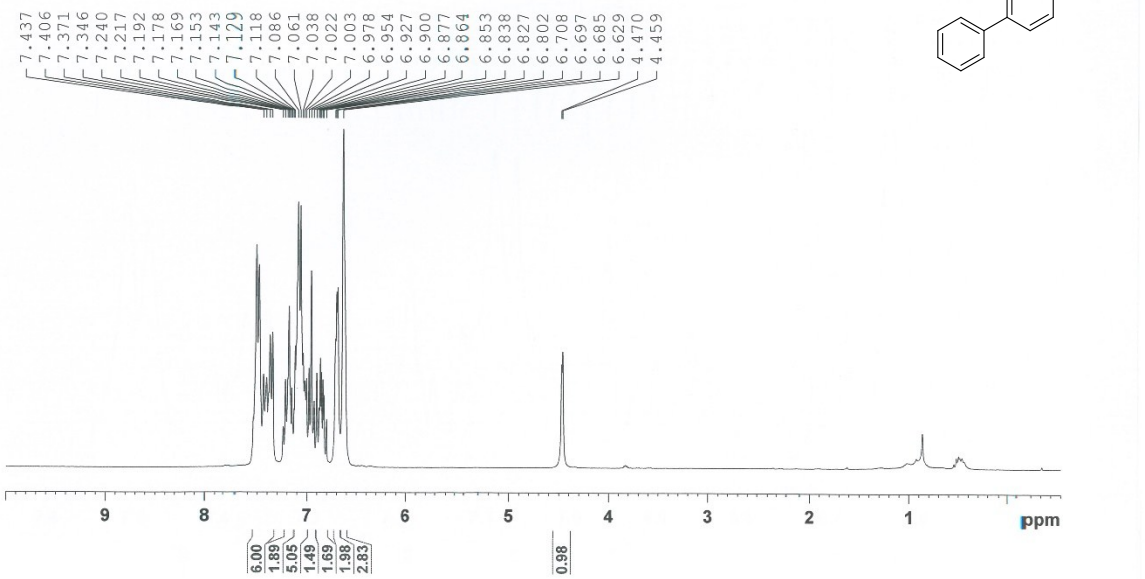




Compound-**9i**

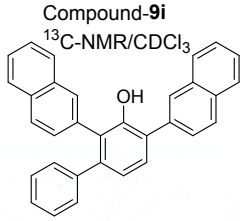
^{1}H-NMR/$CDCl_3$

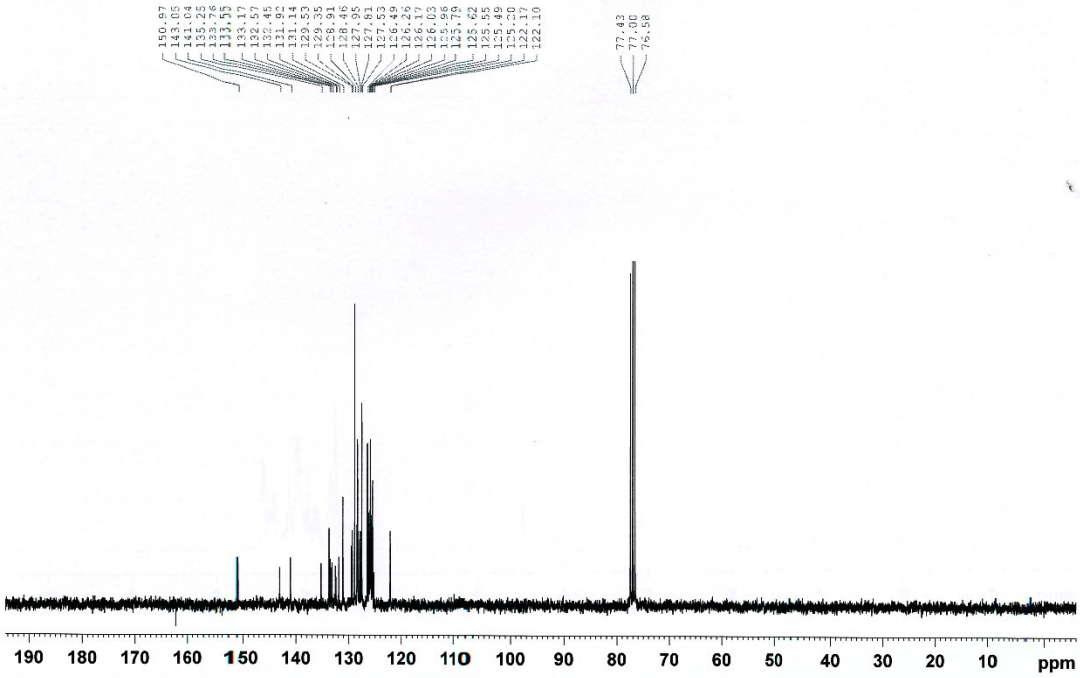




Compound-**9i**

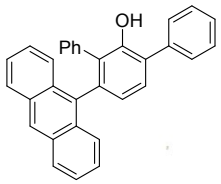
^{13}C-NMR/$CDCl_3$

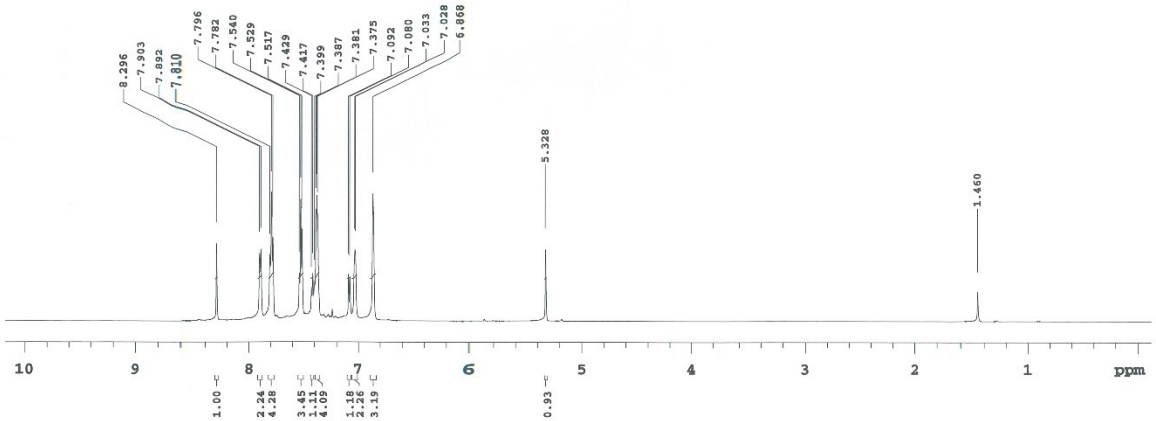




Compound-**9j**

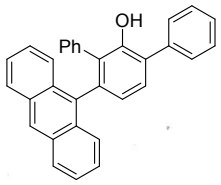
^{1}H-NMR/$CDCl_3$

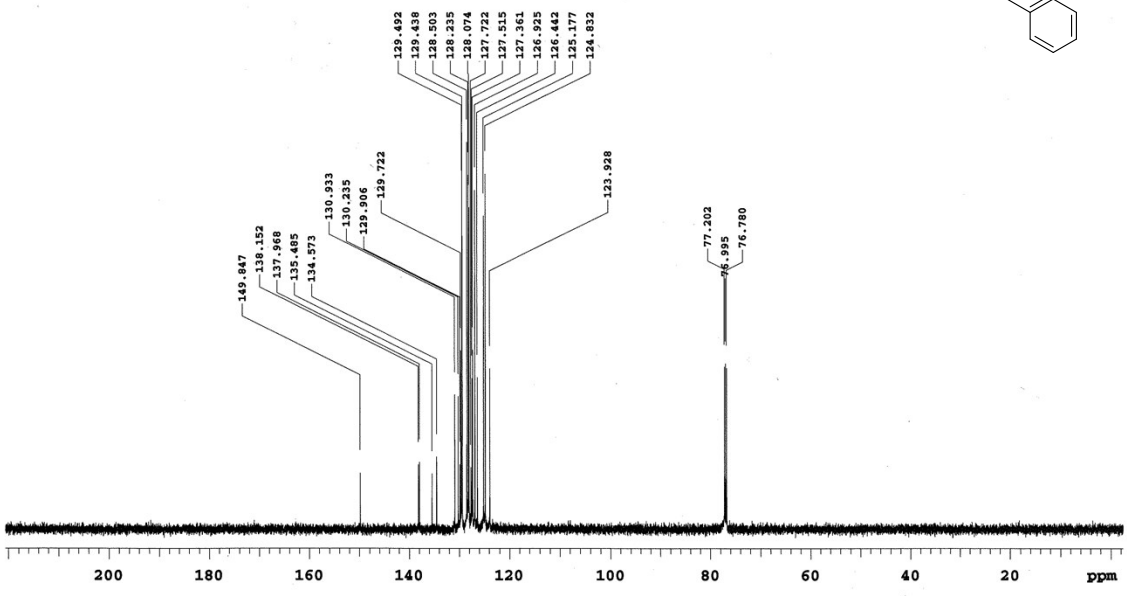




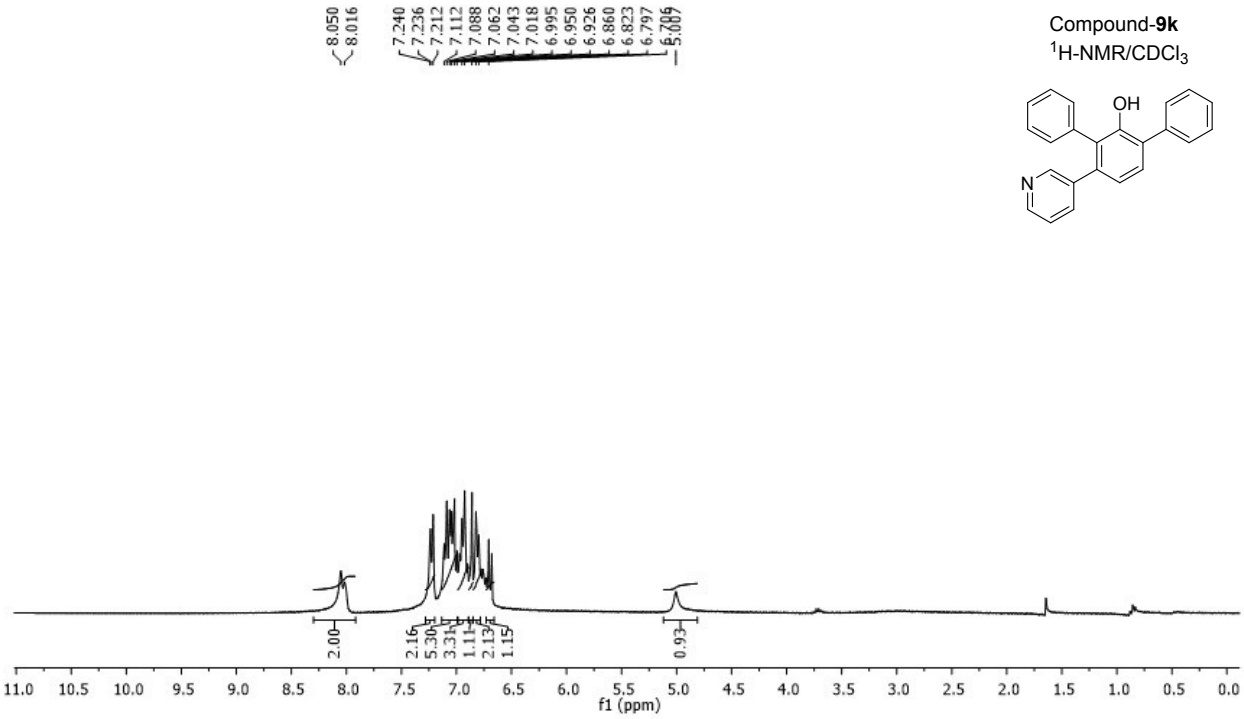
Compound-**9j**

^{13}C-NMR/$CDCl_3$

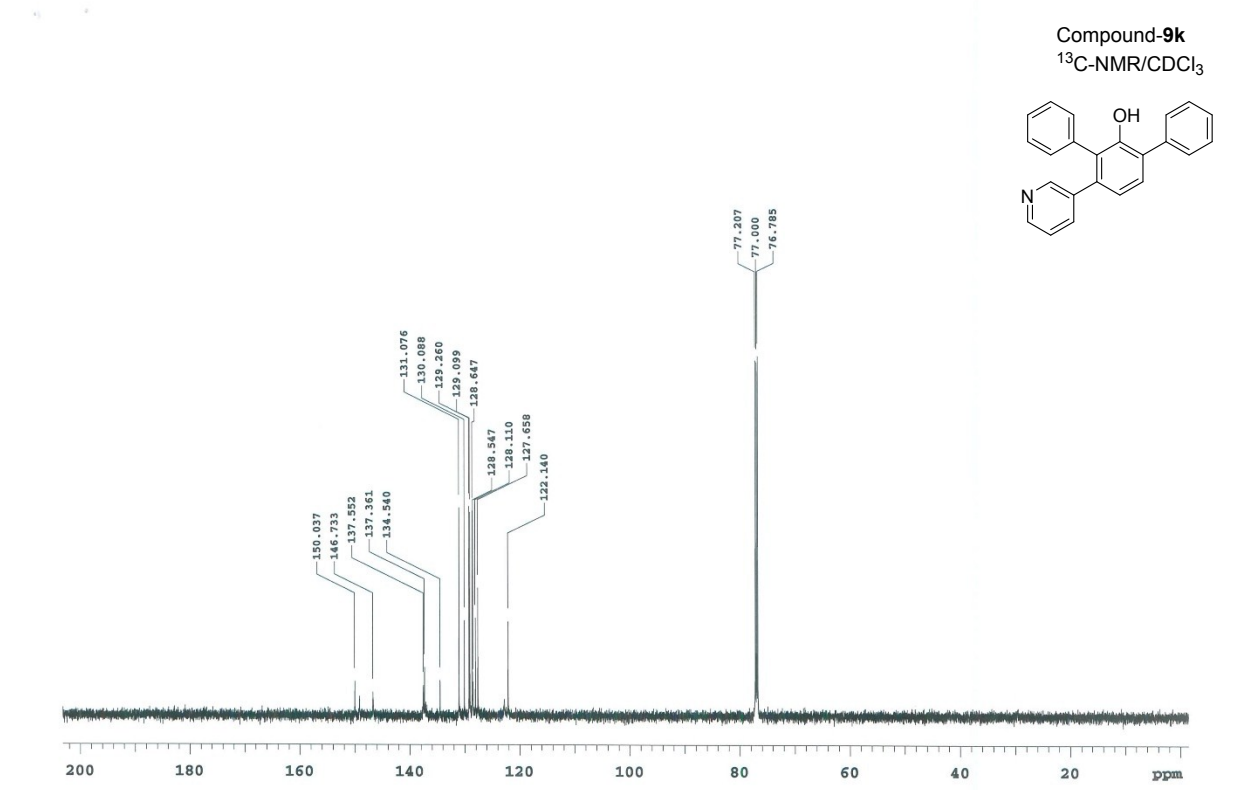


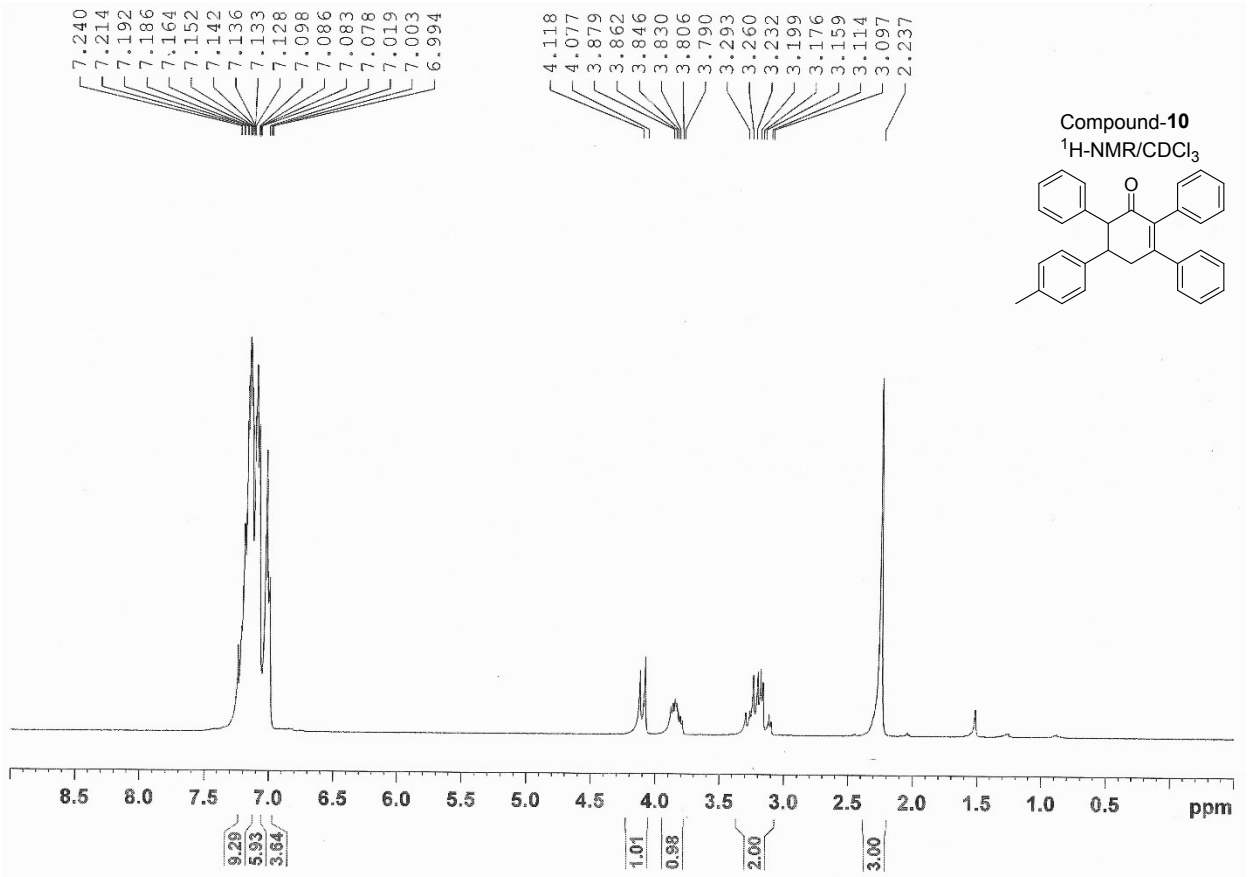


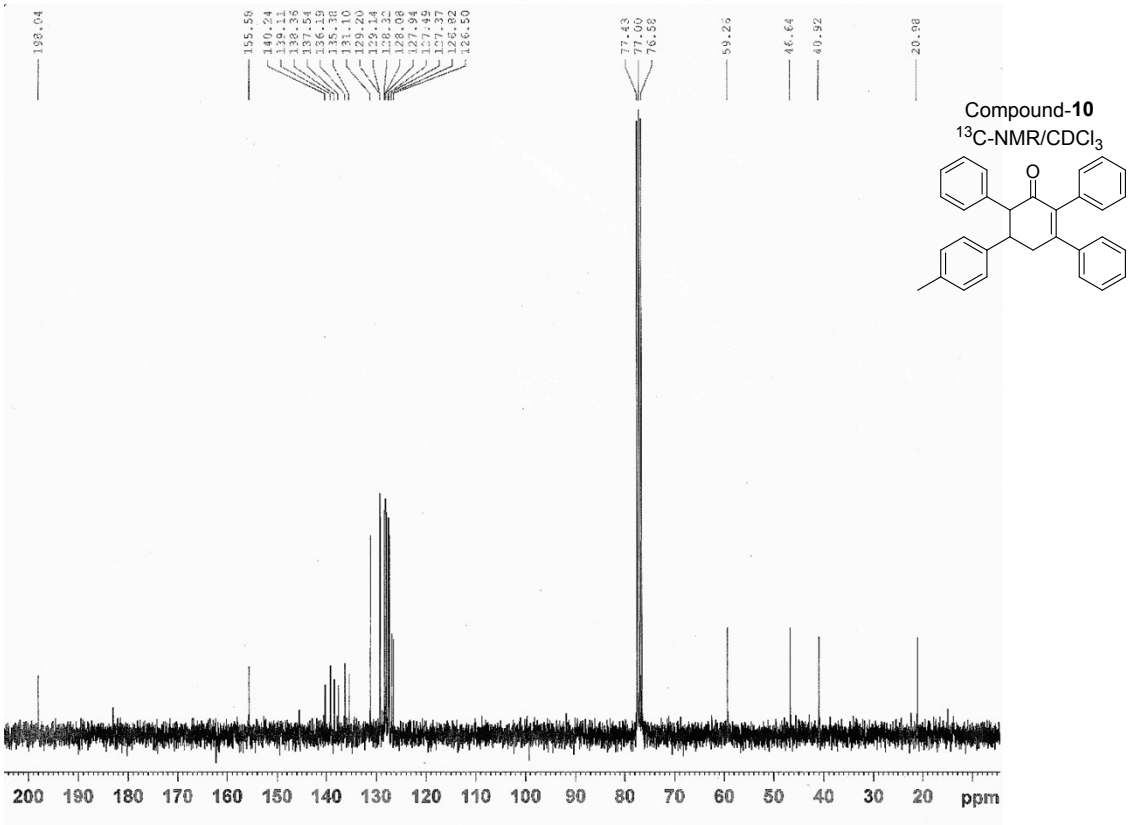
Compound-**9k**
^{1}H-NMR/$CDCl_3$



Compound-**9k**
^{13}C-NMR/$CDCl_3$

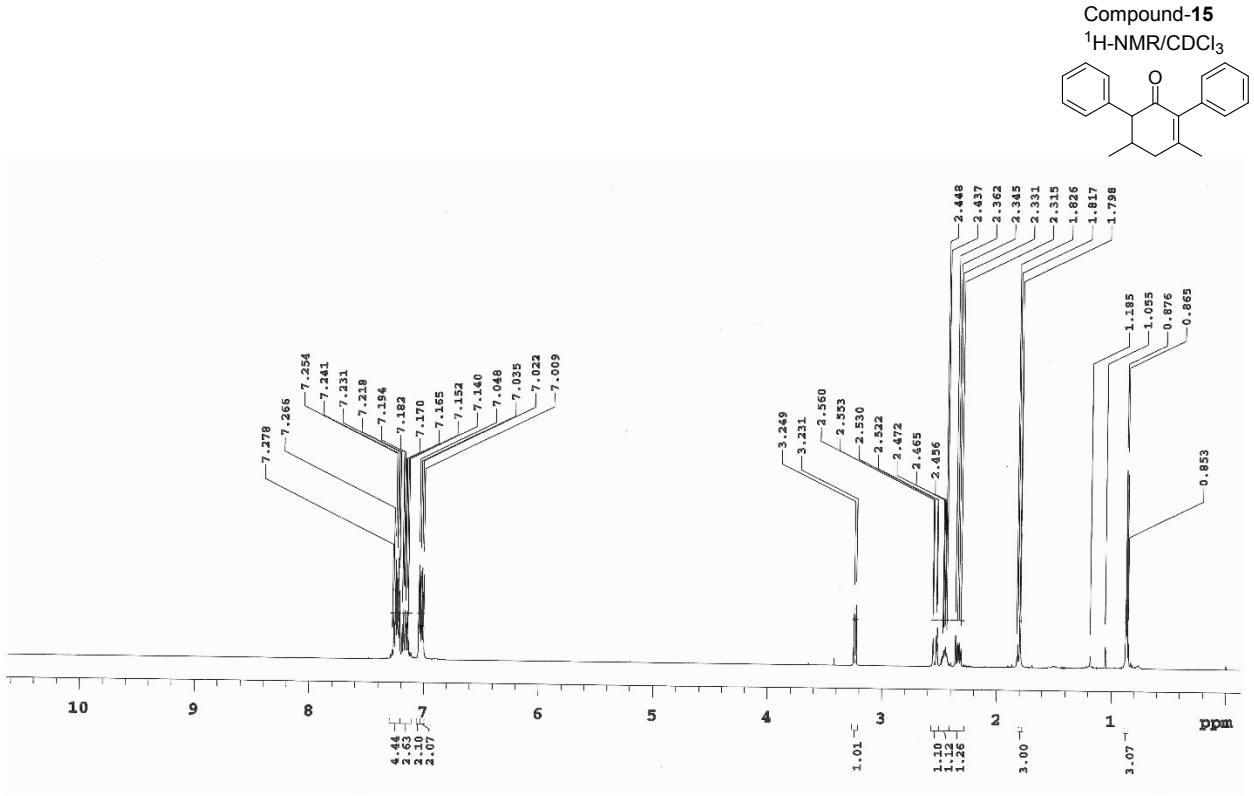



7.240
7.214
7.192
7.186
7.164
7.152
7.142
7.136
7.133
7.128
7.098
7.086
7.083
7.078
7.019
7.003
6.994
4.118
4.077
3.879
3.862
3.846
3.830
3.806
3.790
3.293
3.260
3.232
3.199
3.176
3.159
3.114
3.097
2.237
Compound-10
1H-NMR/CDCl3
O
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
9.29
5.93
3.64
1.01
0.98
2.00
3.00


198.04
155.56
140.24
139.11
138.36
137.54
136.19
135.38
131.10
129.20
129.14
128.32
128.08
127.94
127.49
127.37
126.82
126.50
77.43
77.00
76.58
59.26
46.64
40.92
20.98
Compound-10
13C-NMR/CDCl3
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

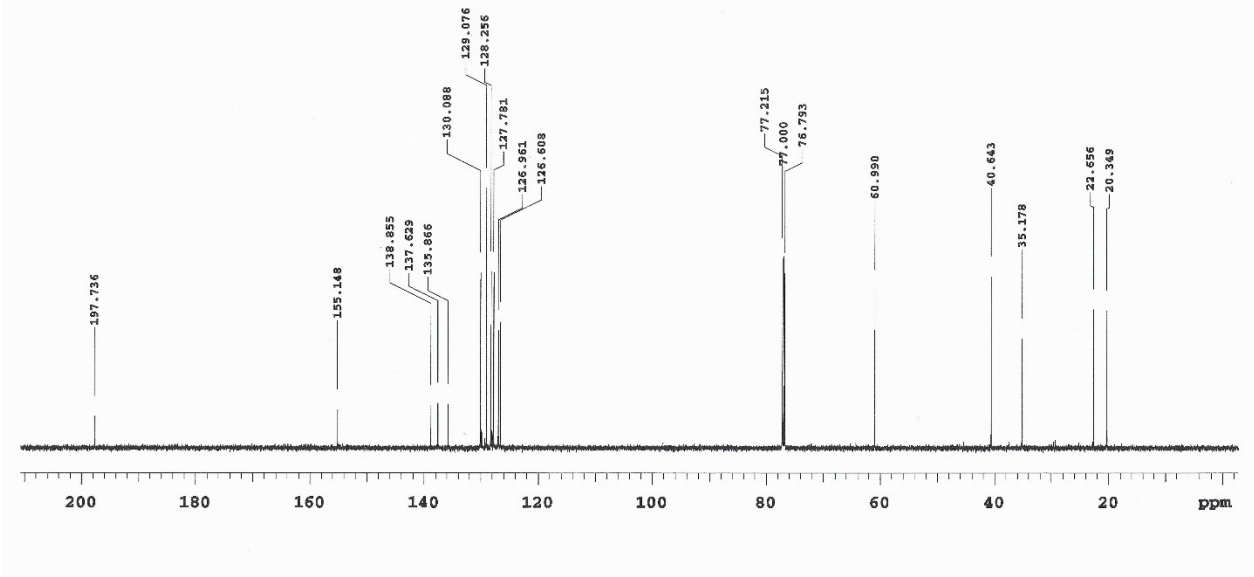
Compound-**15**

^{1}H-NMR/$CDCl_3$



Compound-**15**

^{13}C-NMR/$CDCl_3$



X-Ray crystallographic structure and data of compound 9d: Empirical Formula- $C_{25}H_{20}O_2$, M = 352.41, Triclinic, Space group P_{bca}, a = 9.5607 (9) Å, b = 10.2840 (10) Å, c = 10.9413 (10) Å, V = 916.80 (15) $Å^3$, Z = 2, T = 223(2) K, ρ_{calcd} = 1.277 Mg/m^3, $2\Theta_{max.}$ = 28.413°, Refinement of 246 parameters on 4586 independent reflections out of 54615 collected reflections (R_{int} = 0.0425) led to R_1 = 0.0429 [I >2σ(I)], wR_2 = 0.1258 (all data) and S = 1.069 with the largest difference peak and hole of 0.239 and -0.190 e. $Å^{-3}$ respectively. The crystal structure has been deposited at the Cambridge Crystallographic Data Centre (CCDC 1526470). The data can be obtained free of charge via the Internet at www.ccdc.cam.ac.uk/data_request/cif.

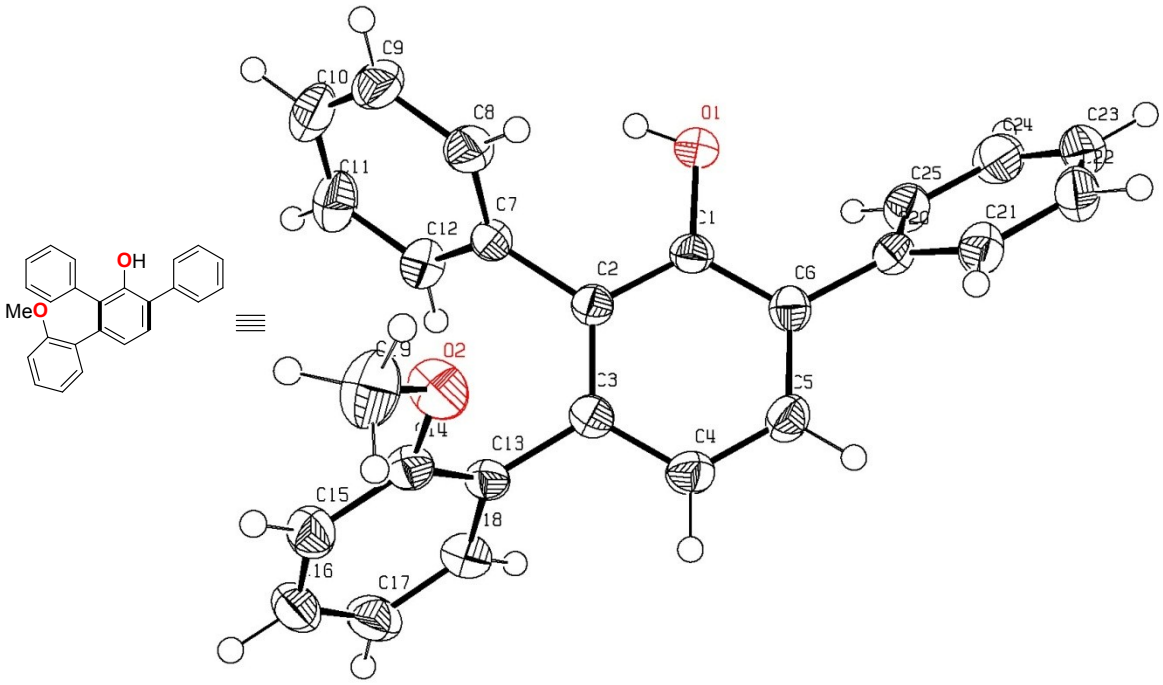


Fig. S1 X-Ray Structure of Compound **9d**.

Table 1. Crystal data and structure refinement for **9d**

Identification code	**9d**	
Empirical formula	$C_{25}\ H_{20}\ O_2$	
Formula weight	352.41	
Temperature	223(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.5607(9) Å	□= 100.114(4)°.
	b = 10.2840(10) Å	□= 114.210(4)°.
	c = 10.9413(10) Å	□ = 102.160(4)°.
Volume	916.80(15) Å^3	
Z	2	
Density (calculated)	1.277 Mg/m^3	
Absorption coefficient	0.080 mm^{-1}	
F(000)	372	
Crystal size	0.180 x 0.150 x 0.100 mm^3	
Theta range for data collection	2.119 to 28.413°.	
Index ranges	-12<=h<=12, -13<=k<=13, -14<=l<=14	
Reflections collected	54615	
Independent reflections	4586 [R(int) = 0.0425]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4586 / 0 / 246	
Goodness-of-fit on F^2	1.069	
Final R indices [I>2sigma(I)]	R1 = 0.0429, wR2 = 0.1164	
R indices (all data)	R1 = 0.0621, wR2 = 0.1258	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.239 and -0.190 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)
for **9d**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	7188(1)	2846(1)	438(1)	29(1)
C(2)	7528(1)	1863(1)	1165(1)	28(1)
C(3)	8095(1)	842(1)	677(1)	29(1)
C(4)	8344(2)	846(1)	-491(1)	35(1)
C(5)	8045(2)	1847(1)	-1164(1)	35(1)
C(6)	7440(1)	2852(1)	-736(1)	30(1)
O(1)	6592(1)	3847(1)	845(1)	40(1)
C(7)	7232(1)	1929(1)	2412(1)	30(1)
C(8)	8074(2)	3099(1)	3580(1)	39(1)
C(9)	7750(2)	3208(2)	4709(2)	46(1)
C(10)	6593(2)	2151(2)	4698(2)	49(1)
C(11)	5764(2)	971(2)	3561(2)	48(1)
C(12)	6072(2)	858(2)	2416(1)	38(1)
C(13)	8398(2)	-287(1)	1344(1)	31(1)
C(14)	9658(2)	-20(1)	2691(1)	33(1)
C(15)	9916(2)	-1106(2)	3260(2)	41(1)
C(16)	8941(2)	-2460(2)	2475(2)	45(1)
C(17)	7727(2)	-2747(1)	1141(2)	45(1)
C(18)	7462(2)	-1657(1)	586(2)	39(1)
O(2)	10594(1)	1343(1)	3359(1)	47(1)
C(19)	12081(2)	1622(2)	4568(2)	55(1)
C(20)	7071(2)	3899(1)	-1502(1)	31(1)
C(21)	8269(2)	4791(1)	-1650(1)	37(1)
C(22)	7935(2)	5789(2)	-2328(2)	46(1)
C(23)	6391(2)	5880(2)	-2906(2)	50(1)
C(24)	5185(2)	4981(2)	-2801(2)	47(1)
C(25)	5520(2)	4006(2)	-2093(1)	39(1)

Table 3. Bond lengths [Å] and angles [°] for **9d**.

C(1)-O(1)	1.3705(14)
C(1)-C(6)	1.4019(16)
C(1)-C(2)	1.4027(16)
C(2)-C(3)	1.4005(16)
C(2)-C(7)	1.4955(16)
C(3)-C(4)	1.3936(17)
C(3)-C(13)	1.4935(16)
C(4)-C(5)	1.3790(18)
C(4)-H(4)	0.9400
C(5)-C(6)	1.3875(17)
C(5)-H(5)	0.9400
C(6)-C(20)	1.4898(16)
O(1)-H(1)	0.8300
C(7)-C(12)	1.3911(18)
C(7)-C(8)	1.3921(18)
C(8)-C(9)	1.3835(19)
C(8)-H(8)	0.9400
C(9)-C(10)	1.373(2)
C(9)-H(9)	0.9400
C(10)-C(11)	1.380(2)
C(10)-H(10)	0.9400
C(11)-C(12)	1.3907(19)
C(11)-H(11)	0.9400
C(12)-H(12)	0.9400
C(13)-C(18)	1.3873(18)
C(13)-C(14)	1.4000(18)
C(14)-O(2)	1.3699(16)
C(14)-C(15)	1.3891(18)
C(15)-C(16)	1.387(2)
C(15)-H(15)	0.9400
C(16)-C(17)	1.371(2)
C(16)-H(16)	0.9400
C(17)-C(18)	1.3866(19)
C(17)-H(17)	0.9400

C(18)-H(18)	0.9400
O(2)-C(19)	1.4161(18)
C(19)-H(19A)	0.9700
C(19)-H(19B)	0.9700
C(19)-H(19C)	0.9700
C(20)-C(25)	1.3921(18)
C(20)-C(21)	1.3932(17)
C(21)-C(22)	1.3847(19)
C(21)-H(21)	0.9400
C(22)-C(23)	1.379(2)
C(22)-H(22)	0.9400
C(23)-C(24)	1.377(2)
C(23)-H(23)	0.9400
C(24)-C(25)	1.3825(19)
C(24)-H(24)	0.9400
C(25)-H(25)	0.9400

O(1)-C(1)-C(6)	116.81(10)
O(1)-C(1)-C(2)	121.40(10)
C(6)-C(1)-C(2)	121.79(11)
C(3)-C(2)-C(1)	118.79(10)
C(3)-C(2)-C(7)	122.62(10)
C(1)-C(2)-C(7)	118.57(10)
C(4)-C(3)-C(2)	119.49(11)
C(4)-C(3)-C(13)	118.41(11)
C(2)-C(3)-C(13)	122.07(10)
C(5)-C(4)-C(3)	120.60(11)
C(5)-C(4)-H(4)	119.7
C(3)-C(4)-H(4)	119.7
C(4)-C(5)-C(6)	121.62(11)
C(4)-C(5)-H(5)	119.2
C(6)-C(5)-H(5)	119.2
C(5)-C(6)-C(1)	117.66(11)
C(5)-C(6)-C(20)	121.01(11)
C(1)-C(6)-C(20)	121.32(11)
C(1)-O(1)-H(1)	109.5

C(12)-C(7)-C(8)	118.27(12)
C(12)-C(7)-C(2)	121.33(11)
C(8)-C(7)-C(2)	120.34(11)
C(9)-C(8)-C(7)	121.02(13)
C(9)-C(8)-H(8)	119.5
C(7)-C(8)-H(8)	119.5
C(10)-C(9)-C(8)	120.26(14)
C(10)-C(9)-H(9)	119.9
C(8)-C(9)-H(9)	119.9
C(9)-C(10)-C(11)	119.65(13)
C(9)-C(10)-H(10)	120.2
C(11)-C(10)-H(10)	120.2
C(10)-C(11)-C(12)	120.46(14)
C(10)-C(11)-H(11)	119.8
C(12)-C(11)-H(11)	119.8
C(11)-C(12)-C(7)	120.32(13)
C(11)-C(12)-H(12)	119.8
C(7)-C(12)-H(12)	119.8
C(18)-C(13)-C(14)	118.35(11)
C(18)-C(13)-C(3)	119.36(12)
C(14)-C(13)-C(3)	122.20(11)
O(2)-C(14)-C(15)	123.98(12)
O(2)-C(14)-C(13)	115.72(11)
C(15)-C(14)-C(13)	120.29(12)
C(16)-C(15)-C(14)	119.59(13)
C(16)-C(15)-H(15)	120.2
C(14)-C(15)-H(15)	120.2
C(17)-C(16)-C(15)	121.03(13)
C(17)-C(16)-H(16)	119.5
C(15)-C(16)-H(16)	119.5
C(16)-C(17)-C(18)	119.07(13)
C(16)-C(17)-H(17)	120.5
C(18)-C(17)-H(17)	120.5
C(17)-C(18)-C(13)	121.63(13)
C(17)-C(18)-H(18)	119.2
C(13)-C(18)-H(18)	119.2

C(14)-O(2)-C(19)	117.43(12)
O(2)-C(19)-H(19A)	109.5
O(2)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
O(2)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(25)-C(20)-C(21)	118.35(12)
C(25)-C(20)-C(6)	120.83(11)
C(21)-C(20)-C(6)	120.81(11)
C(22)-C(21)-C(20)	120.72(13)
C(22)-C(21)-H(21)	119.6
C(20)-C(21)-H(21)	119.6
C(23)-C(22)-C(21)	120.06(13)
C(23)-C(22)-H(22)	120.0
C(21)-C(22)-H(22)	120.0
C(24)-C(23)-C(22)	119.83(13)
C(24)-C(23)-H(23)	120.1
C(22)-C(23)-H(23)	120.1
C(23)-C(24)-C(25)	120.38(14)
C(23)-C(24)-H(24)	119.8
C(25)-C(24)-H(24)	119.8
C(24)-C(25)-C(20)	120.60(13)
C(24)-C(25)-H(25)	119.7
C(20)-C(25)-H(25)	119.7

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **9d**. 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)	32(1)	25(1)	31(1)	6(1)	16(1)	9(1)
C(2)	29(1)	26(1)	28(1)	7(1)	13(1)	8(1)
C(3)	28(1)	29(1)	31(1)	8(1)	12(1)	9(1)
C(4)	36(1)	38(1)	37(1)	12(1)	20(1)	18(1)
C(5)	35(1)	43(1)	34(1)	14(1)	20(1)	16(1)
C(6)	29(1)	30(1)	30(1)	10(1)	14(1)	7(1)
O(1)	60(1)	34(1)	41(1)	16(1)	31(1)	25(1)
C(7)	33(1)	32(1)	29(1)	11(1)	15(1)	15(1)
C(8)	44(1)	37(1)	34(1)	8(1)	16(1)	14(1)
C(9)	56(1)	53(1)	29(1)	9(1)	16(1)	26(1)
C(10)	53(1)	78(1)	33(1)	24(1)	25(1)	35(1)
C(11)	44(1)	66(1)	45(1)	26(1)	26(1)	18(1)
C(12)	37(1)	42(1)	34(1)	12(1)	16(1)	11(1)
C(13)	33(1)	30(1)	35(1)	11(1)	19(1)	15(1)
C(14)	34(1)	34(1)	36(1)	10(1)	19(1)	14(1)
C(15)	44(1)	50(1)	44(1)	23(1)	24(1)	25(1)
C(16)	57(1)	41(1)	62(1)	30(1)	39(1)	28(1)
C(17)	52(1)	30(1)	60(1)	14(1)	31(1)	15(1)
C(18)	40(1)	33(1)	42(1)	9(1)	19(1)	14(1)
O(2)	41(1)	39(1)	42(1)	9(1)	6(1)	8(1)
C(19)	40(1)	69(1)	38(1)	14(1)	9(1)	3(1)
C(20)	36(1)	30(1)	25(1)	7(1)	14(1)	10(1)
C(21)	39(1)	39(1)	32(1)	11(1)	16(1)	8(1)
C(22)	61(1)	38(1)	42(1)	16(1)	28(1)	10(1)
C(23)	79(1)	44(1)	43(1)	23(1)	32(1)	31(1)
C(24)	53(1)	57(1)	39(1)	20(1)	21(1)	32(1)
C(25)	39(1)	44(1)	36(1)	14(1)	18(1)	15(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **9d**.

	x	y	z	U(eq)
H(4)	8719	159	-824	42
H(5)	8256	1849	-1930	41
H(1)	6362	3689	1470	60
H(8)	8875	3826	3602	47
H(9)	8324	4009	5486	55
H(10)	6367	2230	5462	59
H(11)	4987	238	3560	58
H(12)	5493	55	1642	45
H(15)	10747	-923	4172	50
H(16)	9115	-3193	2863	54
H(17)	7083	-3670	610	54
H(18)	6627	-1851	-327	47
H(19A)	11875	1319	5287	83
H(19B)	12651	2613	4915	83
H(19C)	12734	1124	4331	83
H(21)	9316	4714	-1286	45
H(22)	8762	6405	-2394	55
H(23)	6163	6555	-3371	60
H(24)	4128	5031	-3212	56
H(25)	4692	3410	-2011	46

Table 6. Torsion angles [°] for **9d**.

O(1)-C(1)-C(2)-C(3)	178.34(11)
C(6)-C(1)-C(2)-C(3)	-1.70(17)
O(1)-C(1)-C(2)-C(7)	-0.20(17)
C(6)-C(1)-C(2)-C(7)	179.77(11)
C(1)-C(2)-C(3)-C(4)	1.57(17)
C(7)-C(2)-C(3)-C(4)	-179.97(11)
C(1)-C(2)-C(3)-C(13)	-176.56(11)
C(7)-C(2)-C(3)-C(13)	1.91(18)
C(2)-C(3)-C(4)-C(5)	0.31(18)
C(13)-C(3)-C(4)-C(5)	178.50(12)
C(3)-C(4)-C(5)-C(6)	-2.2(2)
C(4)-C(5)-C(6)-C(1)	2.00(19)
C(4)-C(5)-C(6)-C(20)	-177.96(12)
O(1)-C(1)-C(6)-C(5)	179.91(11)
C(2)-C(1)-C(6)-C(5)	-0.06(17)
O(1)-C(1)-C(6)-C(20)	-0.13(17)
C(2)-C(1)-C(6)-C(20)	179.90(11)
C(3)-C(2)-C(7)-C(12)	-63.18(16)
C(1)-C(2)-C(7)-C(12)	115.29(13)
C(3)-C(2)-C(7)-C(8)	119.50(13)
C(1)-C(2)-C(7)-C(8)	-62.03(16)
C(12)-C(7)-C(8)-C(9)	-1.02(19)
C(2)-C(7)-C(8)-C(9)	176.37(12)
C(7)-C(8)-C(9)-C(10)	0.5(2)
C(8)-C(9)-C(10)-C(11)	0.6(2)
C(9)-C(10)-C(11)-C(12)	-1.2(2)
C(10)-C(11)-C(12)-C(7)	0.7(2)
C(8)-C(7)-C(12)-C(11)	0.42(19)
C(2)-C(7)-C(12)-C(11)	-176.95(12)
C(4)-C(3)-C(13)-C(18)	-63.52(16)
C(2)-C(3)-C(13)-C(18)	114.62(14)
C(4)-C(3)-C(13)-C(14)	113.04(13)
C(2)-C(3)-C(13)-C(14)	-68.81(16)
C(18)-C(13)-C(14)-O(2)	176.63(11)

C(3)-C(13)-C(14)-O(2)	0.03(17)
C(18)-C(13)-C(14)-C(15)	-2.12(18)
C(3)-C(13)-C(14)-C(15)	-178.72(11)
O(2)-C(14)-C(15)-C(16)	-177.26(12)
C(13)-C(14)-C(15)-C(16)	1.38(19)
C(14)-C(15)-C(16)-C(17)	0.2(2)
C(15)-C(16)-C(17)-C(18)	-1.1(2)
C(16)-C(17)-C(18)-C(13)	0.3(2)
C(14)-C(13)-C(18)-C(17)	1.30(19)
C(3)-C(13)-C(18)-C(17)	178.00(12)
C(15)-C(14)-O(2)-C(19)	12.71(19)
C(13)-C(14)-O(2)-C(19)	-165.98(12)
C(5)-C(6)-C(20)-C(25)	121.14(14)
C(1)-C(6)-C(20)-C(25)	-58.82(16)
C(5)-C(6)-C(20)-C(21)	-58.53(17)
C(1)-C(6)-C(20)-C(21)	121.51(13)
C(25)-C(20)-C(21)-C(22)	2.15(19)
C(6)-C(20)-C(21)-C(22)	-178.17(12)
C(20)-C(21)-C(22)-C(23)	-2.1(2)
C(21)-C(22)-C(23)-C(24)	0.4(2)
C(22)-C(23)-C(24)-C(25)	1.4(2)
C(23)-C(24)-C(25)-C(20)	-1.3(2)
C(21)-C(20)-C(25)-C(24)	-0.44(19)
C(6)-C(20)-C(25)-C(24)	179.88(12)

Symmetry transformations used to generate equivalent atoms: