Supplementary Materials: Condensation of Diacetyl with Alkyl Amines: Synthesis and Reactivity of *p*-Iminobenzoquinones and *p*-Diiminobenzoquinones

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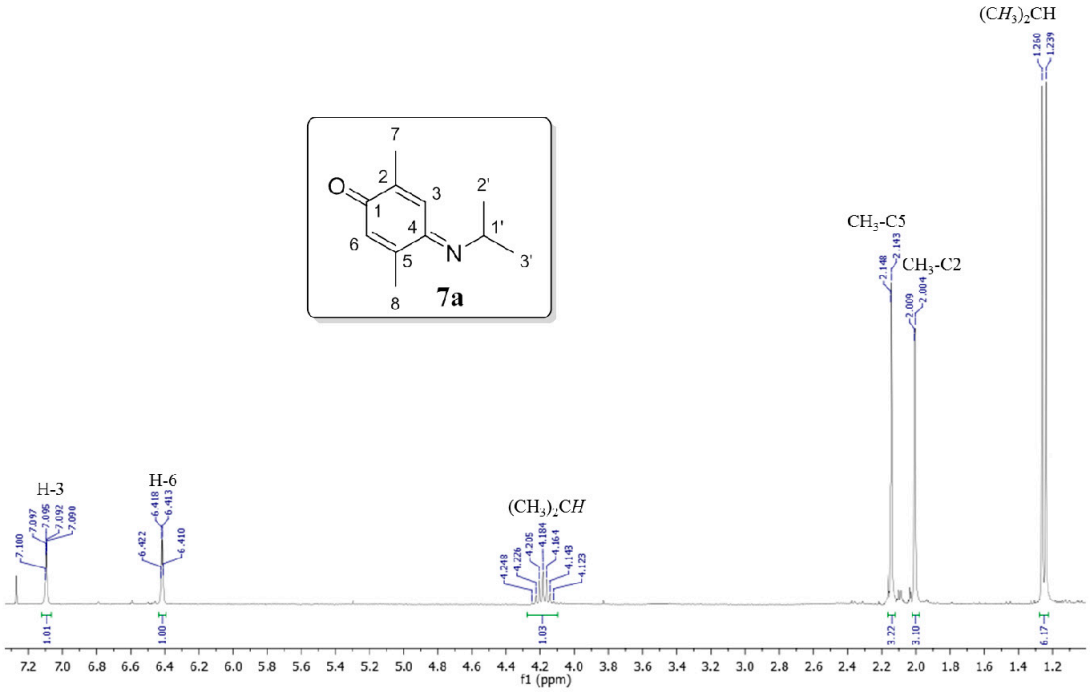
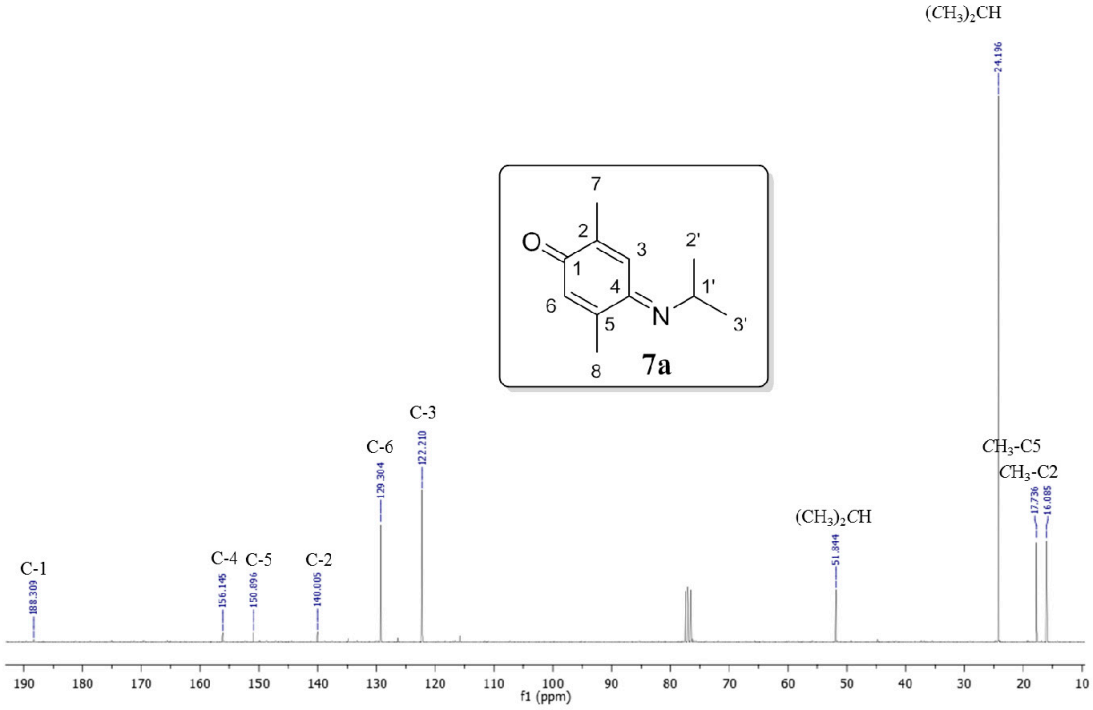
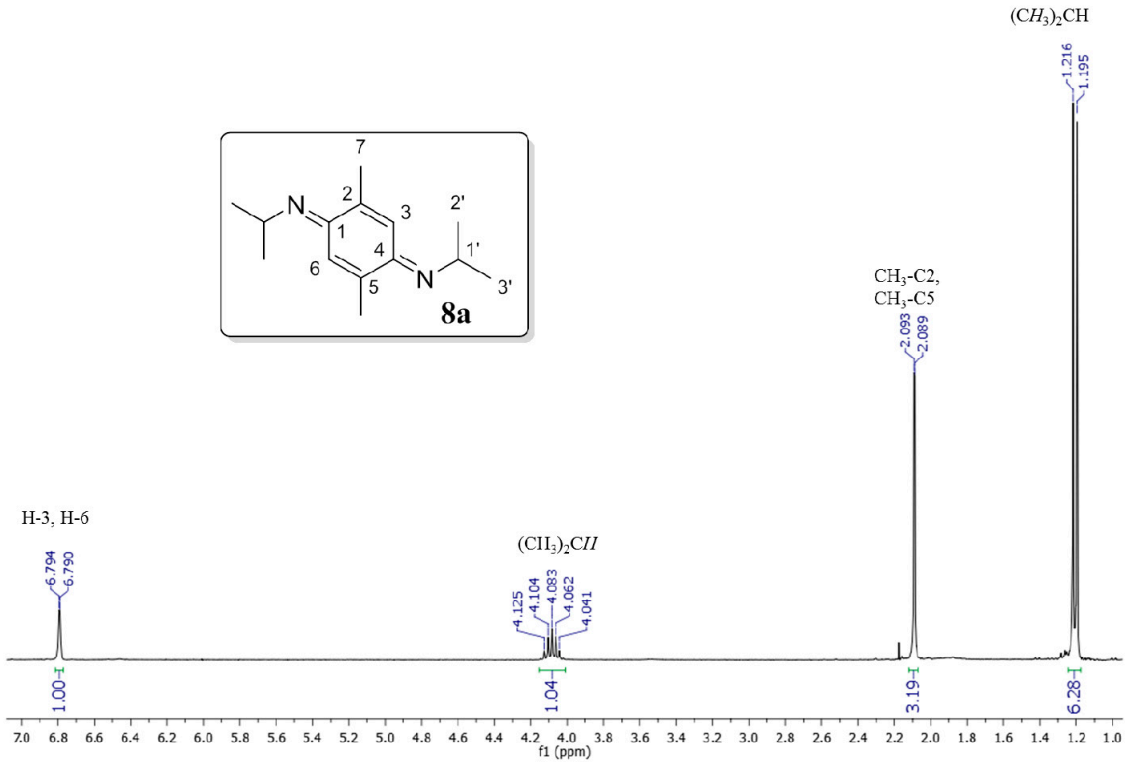
1. ^{1}H-NMR and ^{13}C-NMR of the New Compounds



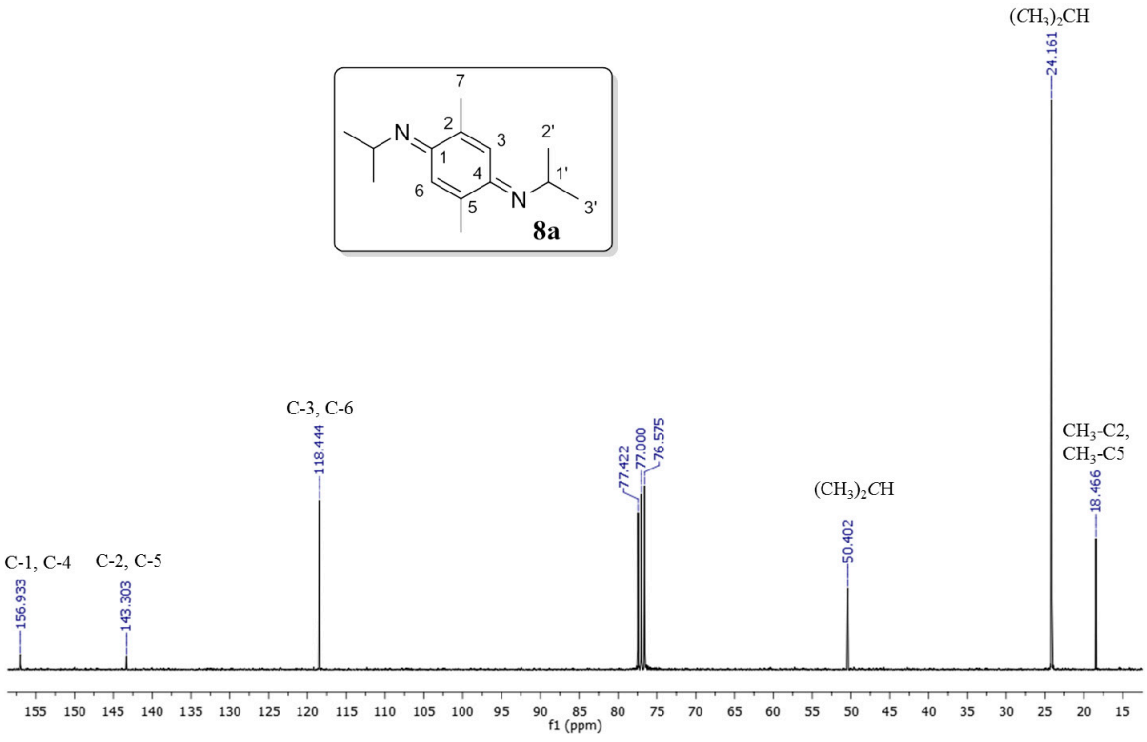
^{1}H-NMR ($CDCl_3$, 500 MHz) spectrum of **7a**.



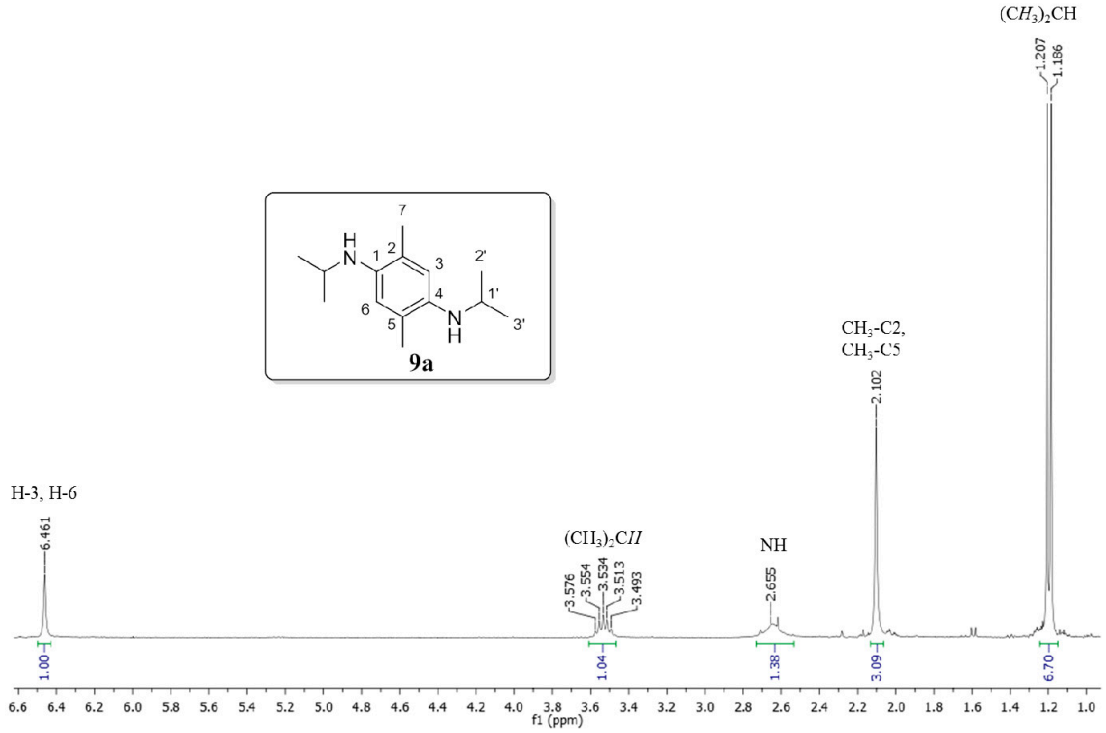
^{13}C-NMR ($CDCl_3$, 125 MHz) spectrum of **7a**.



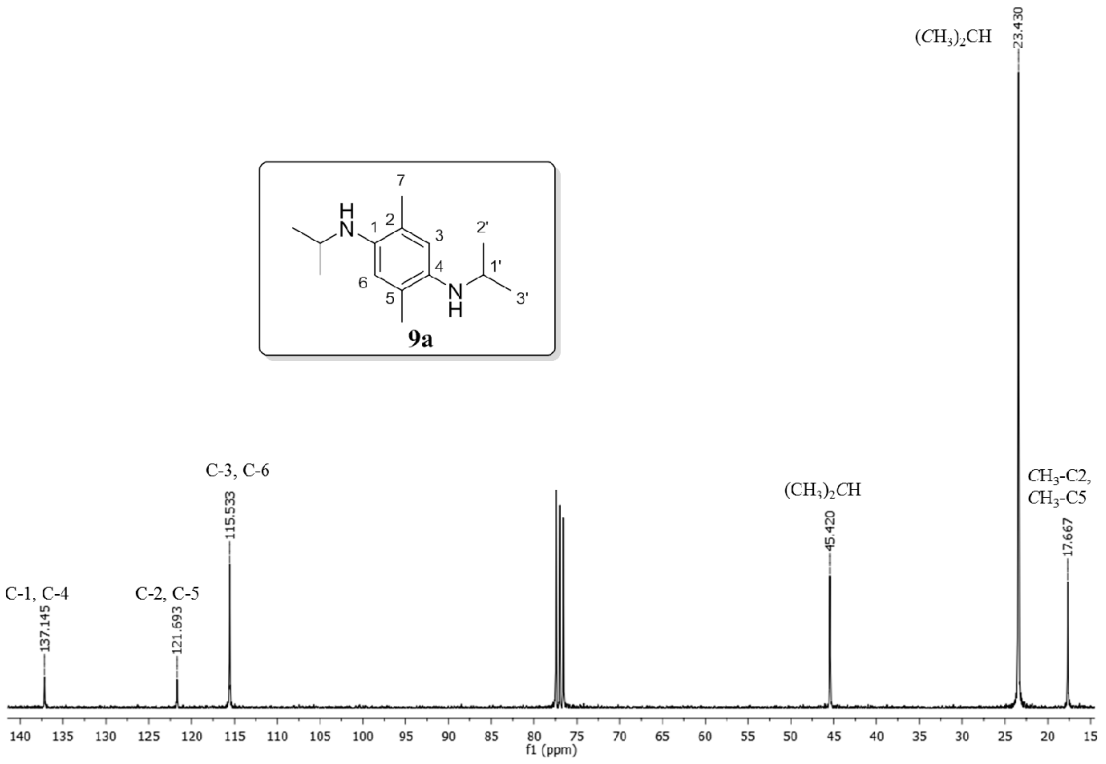
^{1}H-NMR ($CDCl_3$, 500 MHz) spectrum of **8a**.



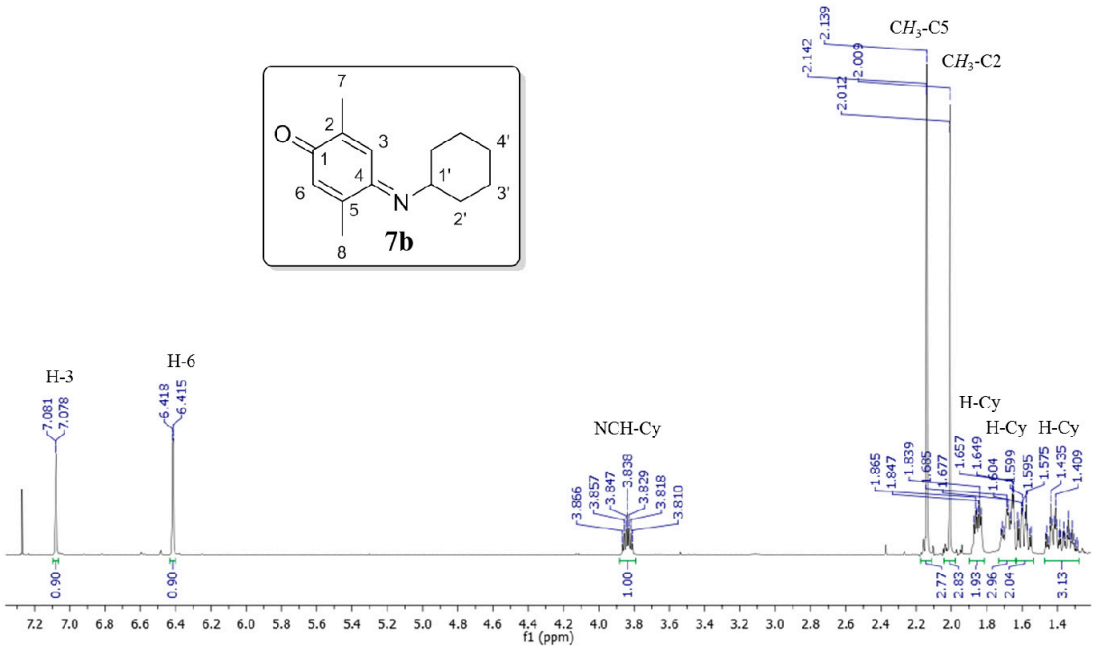
^{13}C-NMR ($CDCl_3$, 125 MHz) spectrum of **8a**.



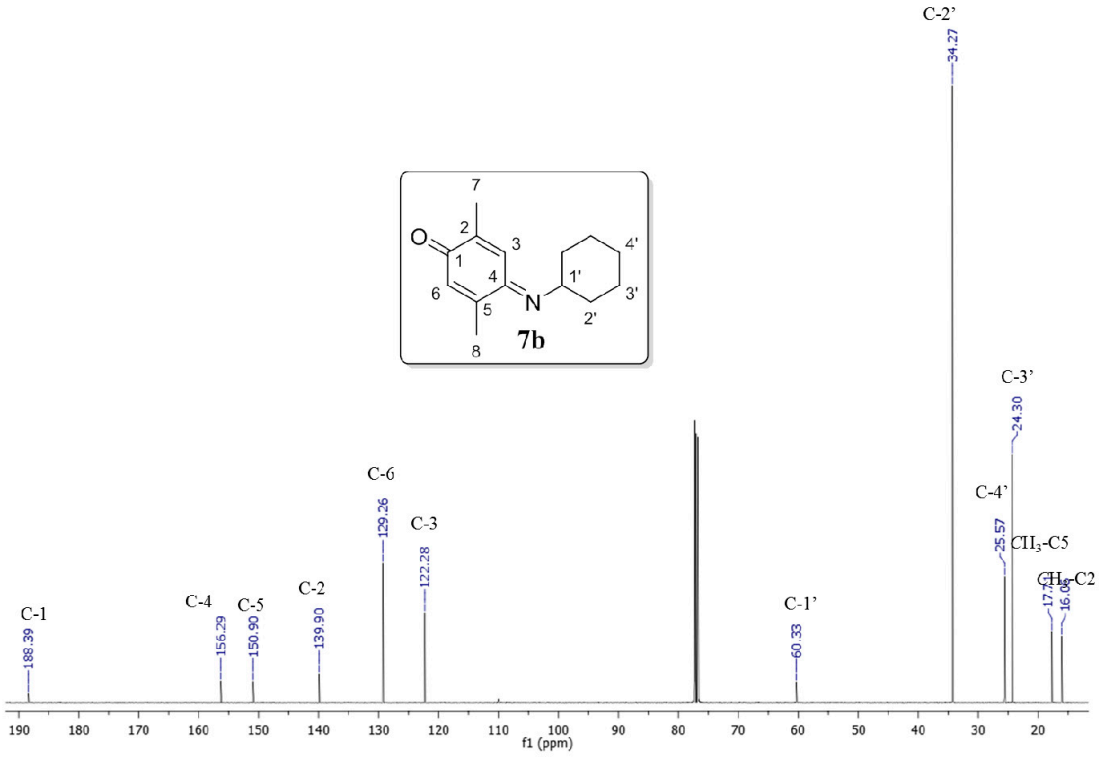
^{1}H-NMR ($CDCl_3$, 500 MHz) spectrum of **9a**.



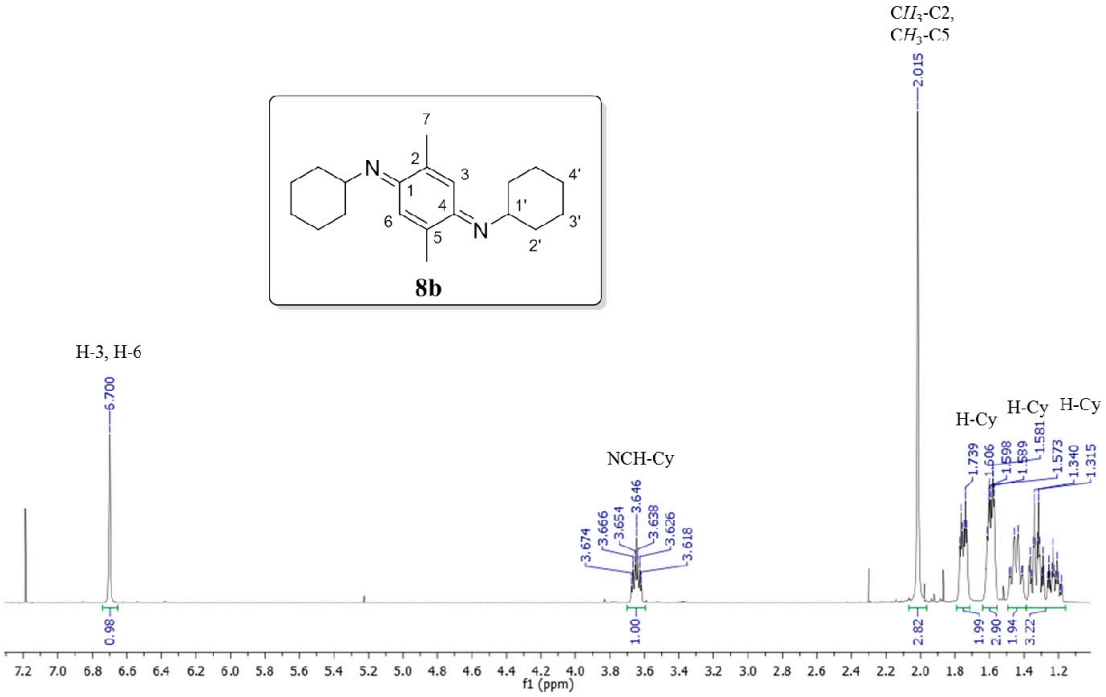
^{13}C-NMR ($CDCl_3$, 125 MHz) spectrum of **9a**.

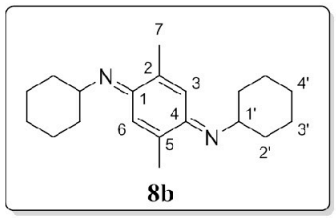


^{1}H-NMR ($CDCl_3$, 500 MHz) spectrum of **7b**.



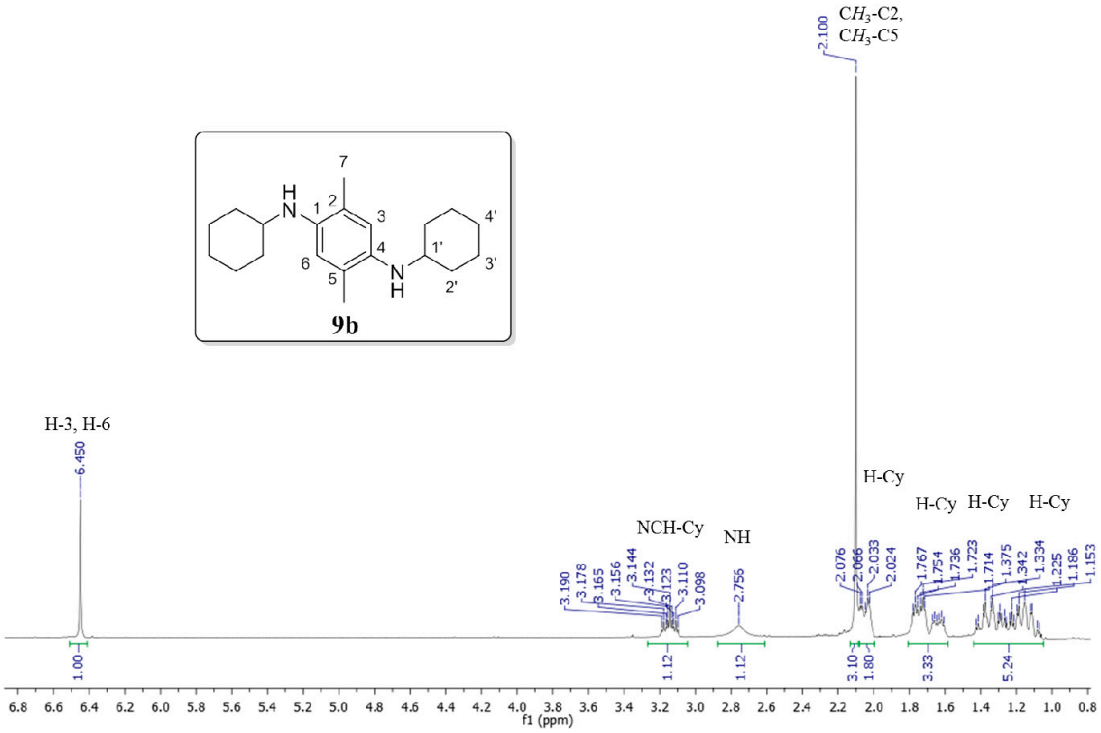
^{13}C-NMR ($CDCl_3$, 125 MHz) spectrum of **7b**.



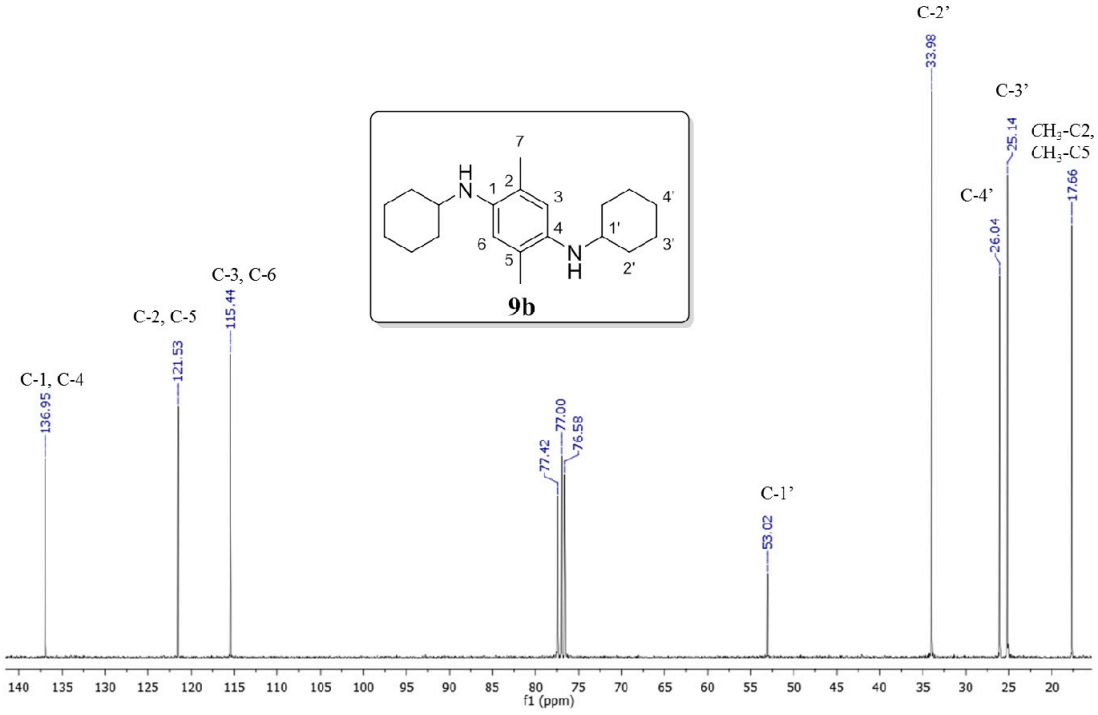


^{1}H-NMR ($CDCl_3$, 500 MHz) spectrum of **8b**.

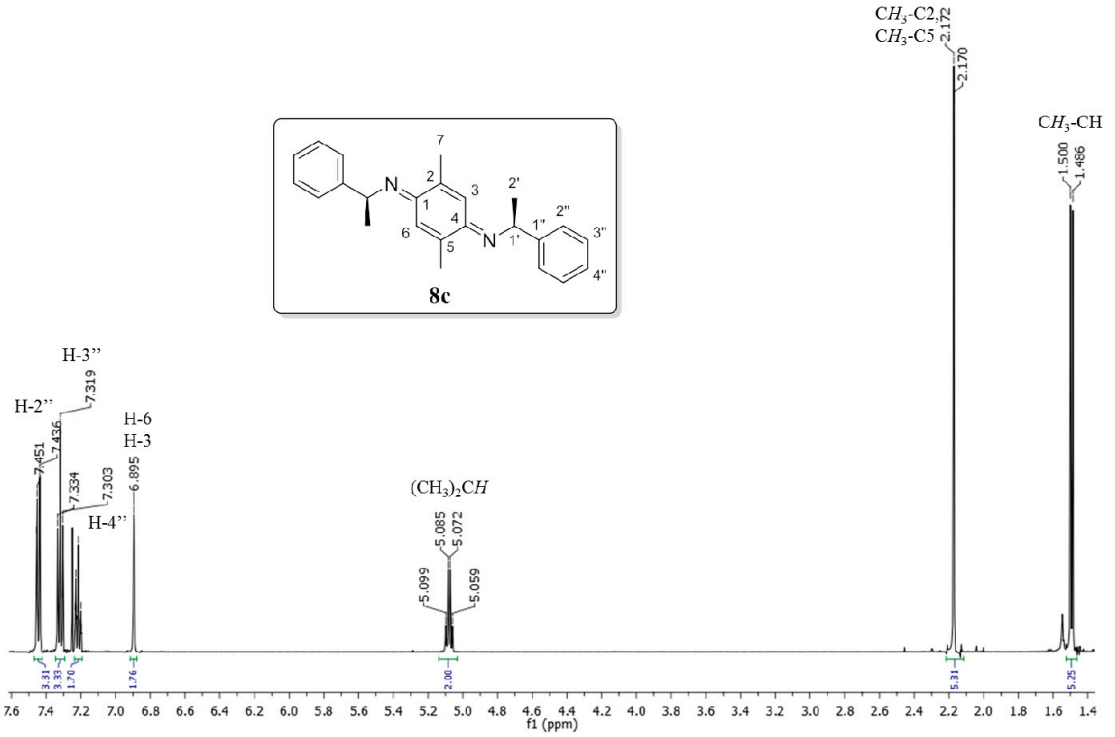
^{1}H-NMR ($CDCl_3$, 125 MHz) spectrum of **8b**.



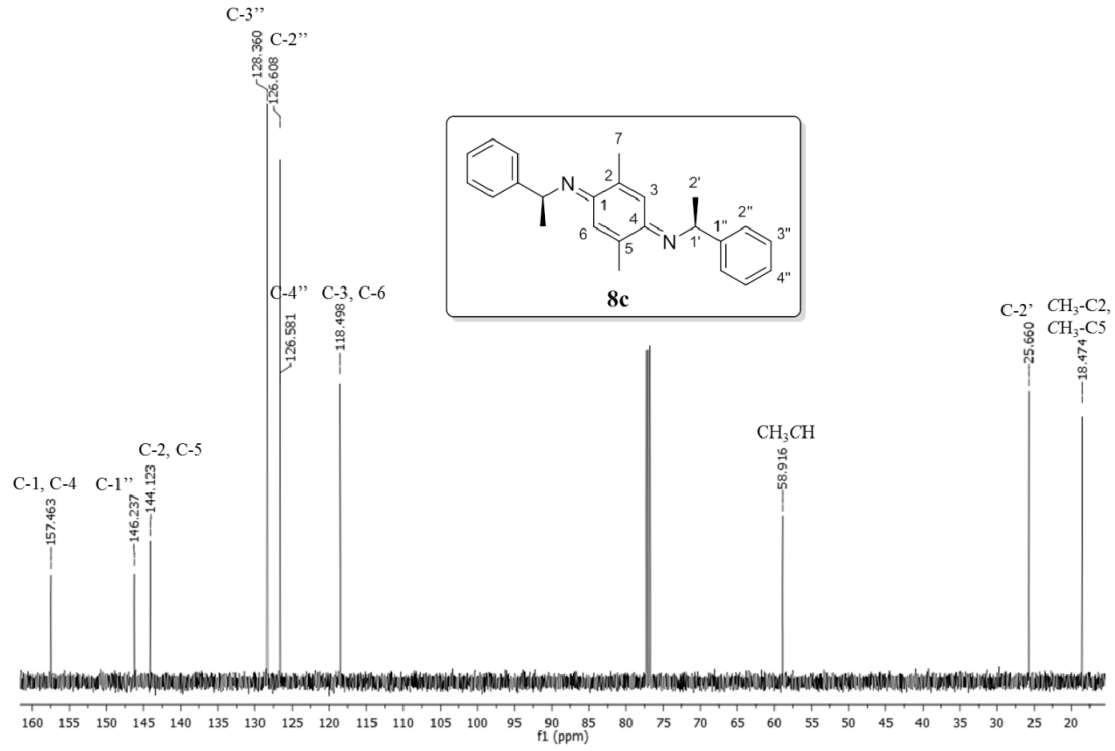
^{1}H-NMR ($CDCl_3$, 300 MHz) spectrum of **9b**.



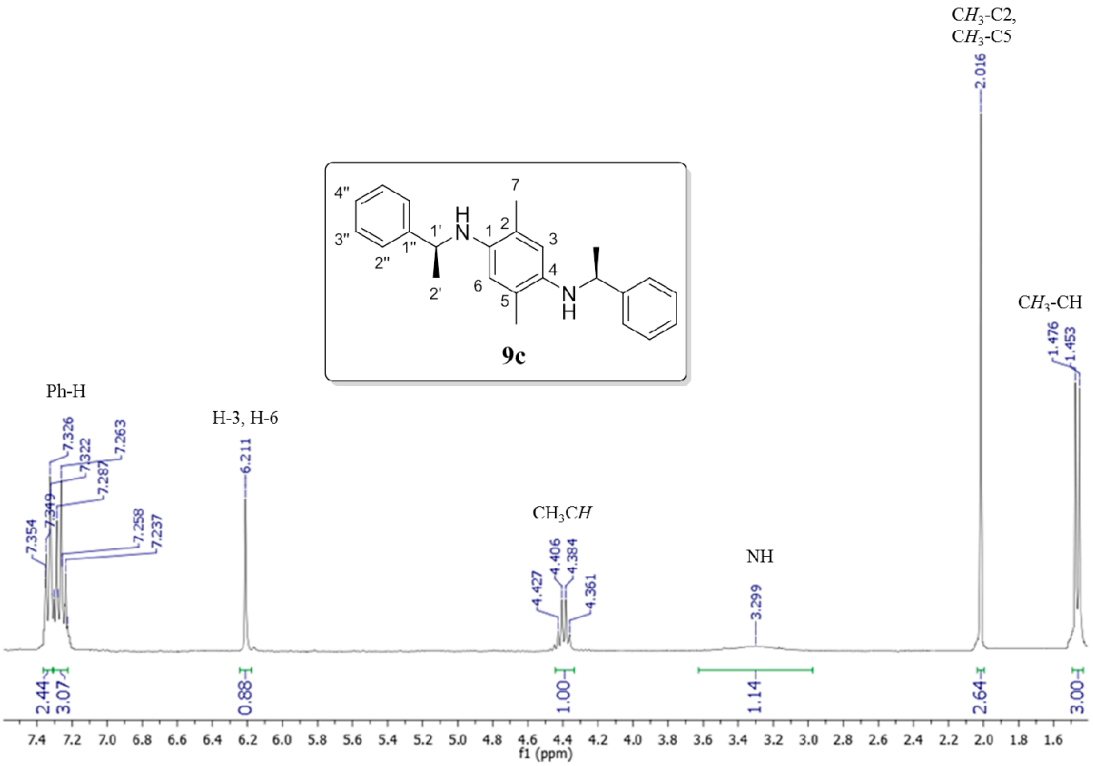
^{13}C-NMR ($CDCl_3$, 75 MHz) spectrum of **9b**.



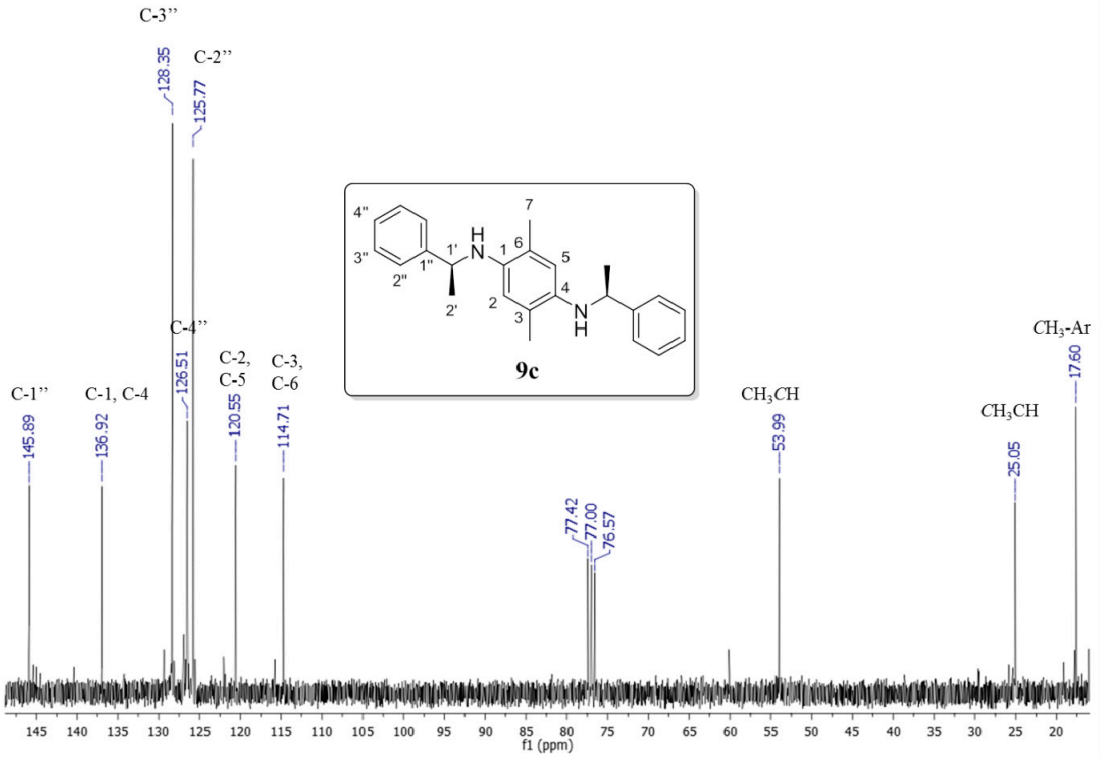
^{1}H-NMR ($CDCl_3$, 500 MHz) spectrum of **8c**.



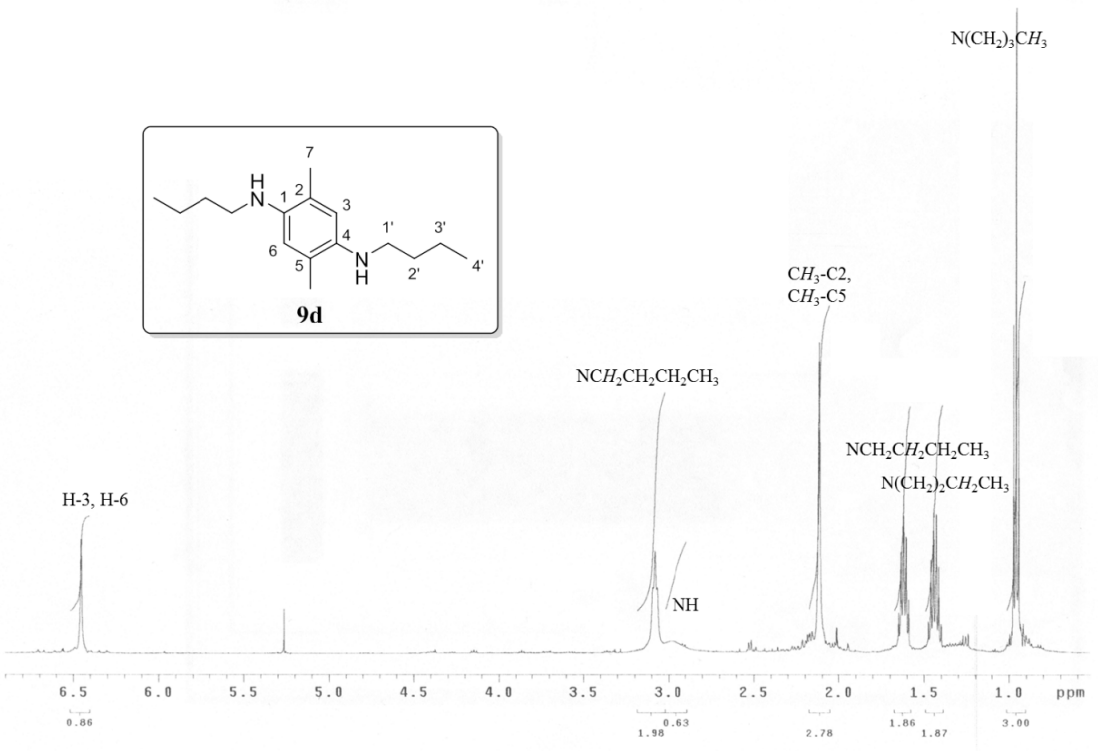
^{13}C-NMR ($CDCl_3$, 125 MHz) spectrum of **8c**.



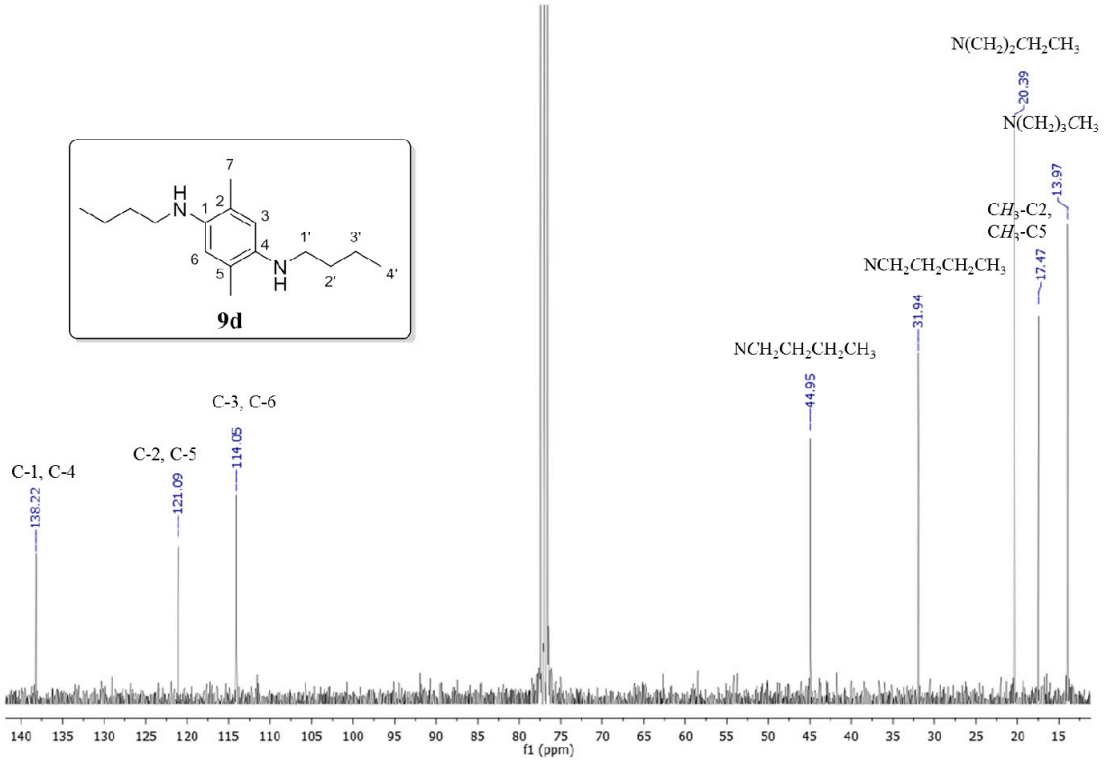
^{1}H-NMR ($CDCl_3$, 300 MHz) spectrum of **9c**.



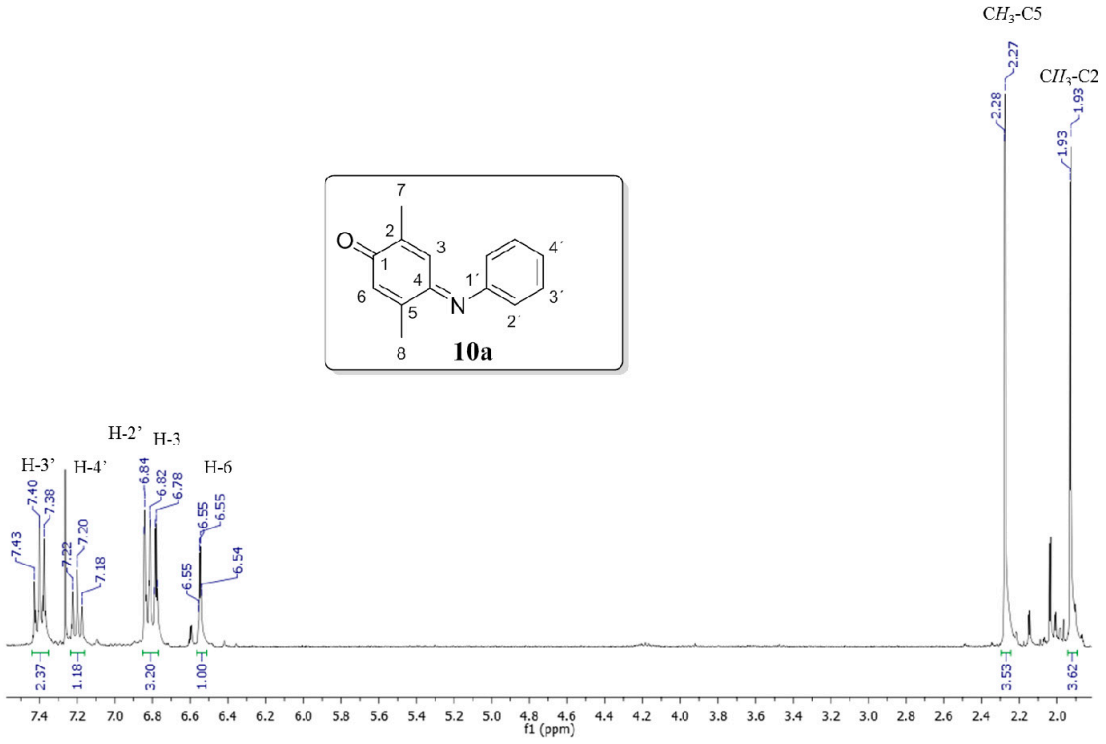
^{13}C-NMR ($CDCl_3$, 75 MHz) spectrum of **9c**.



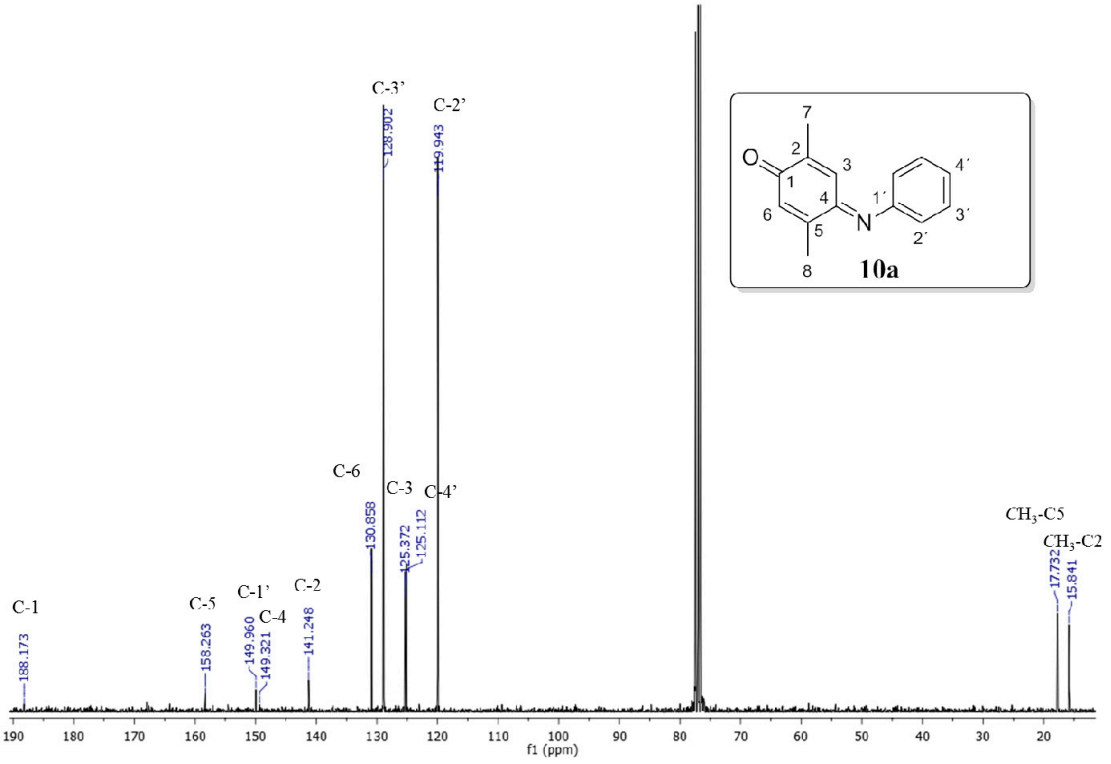
^{1}H-NMR ($CDCl_3$, 500 MHz) spectrum of **9d**.



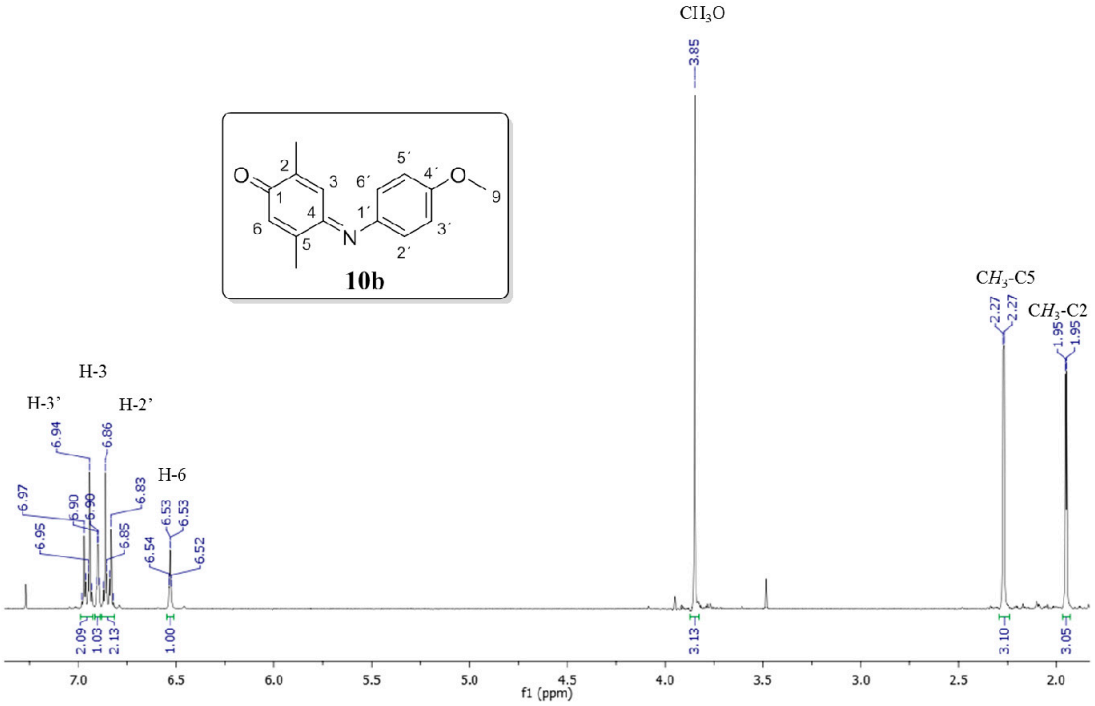
^{13}C-NMR ($CDCl_3$, 125 MHz) spectrum of **9d**.



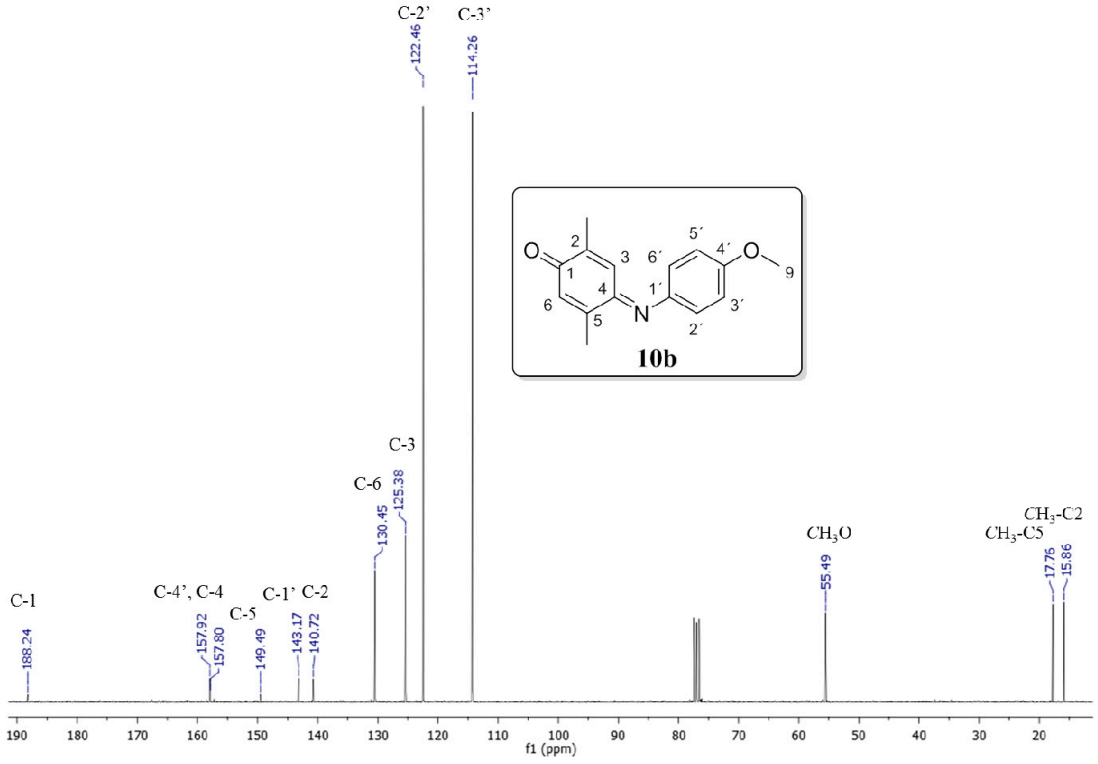
^{1}H-NMR ($CDCl_3$, 300 MHz) spectrum of **10a**



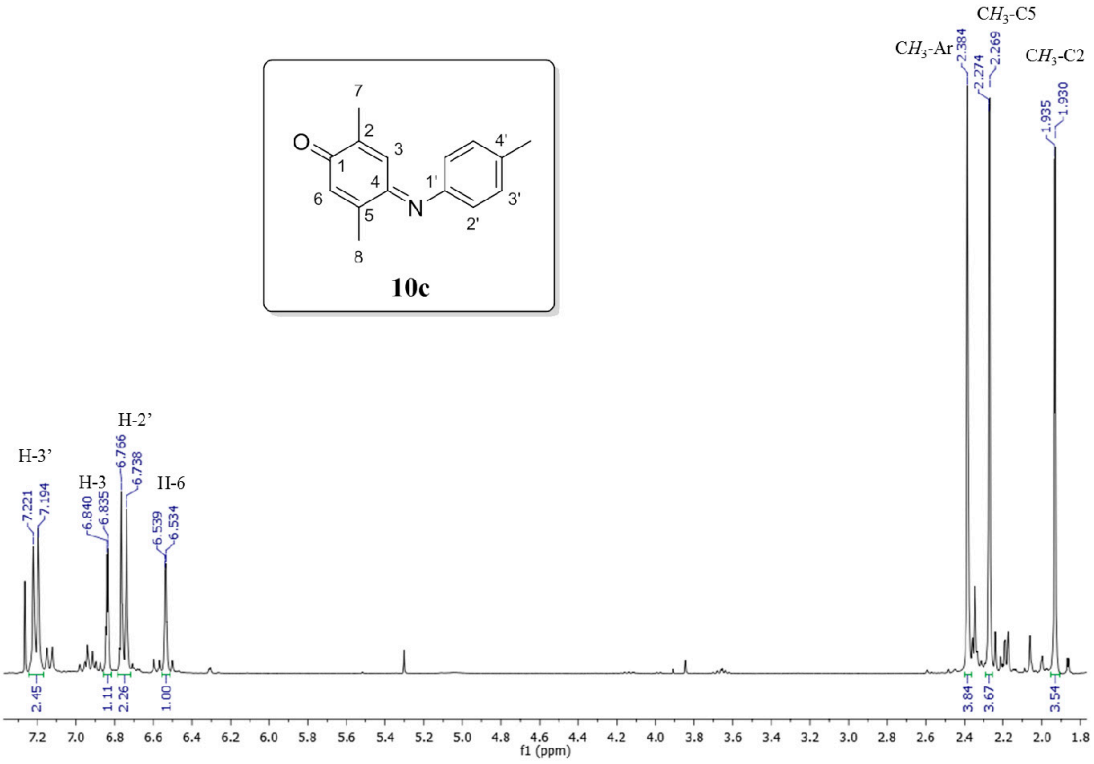
^{13}C-NMR ($CDCl_3$, 75 MHz) spectrum of **10a**



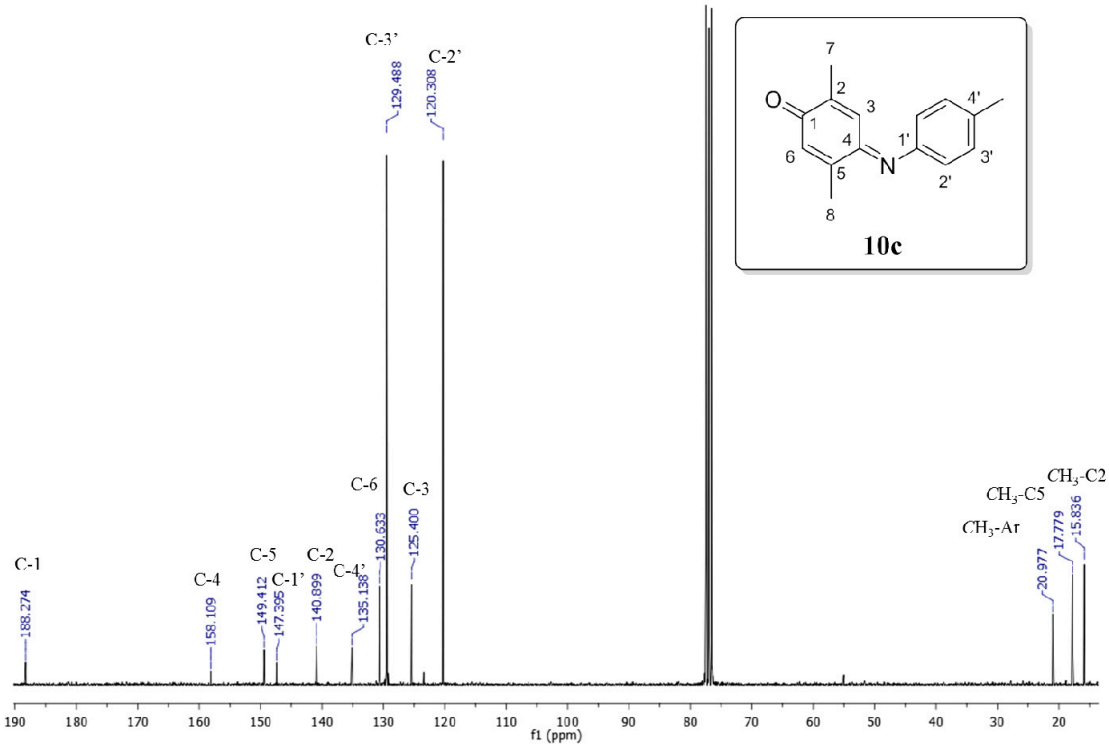
^{1}H-NMR ($CDCl_3$, 500 MHz) spectrum of 10b.



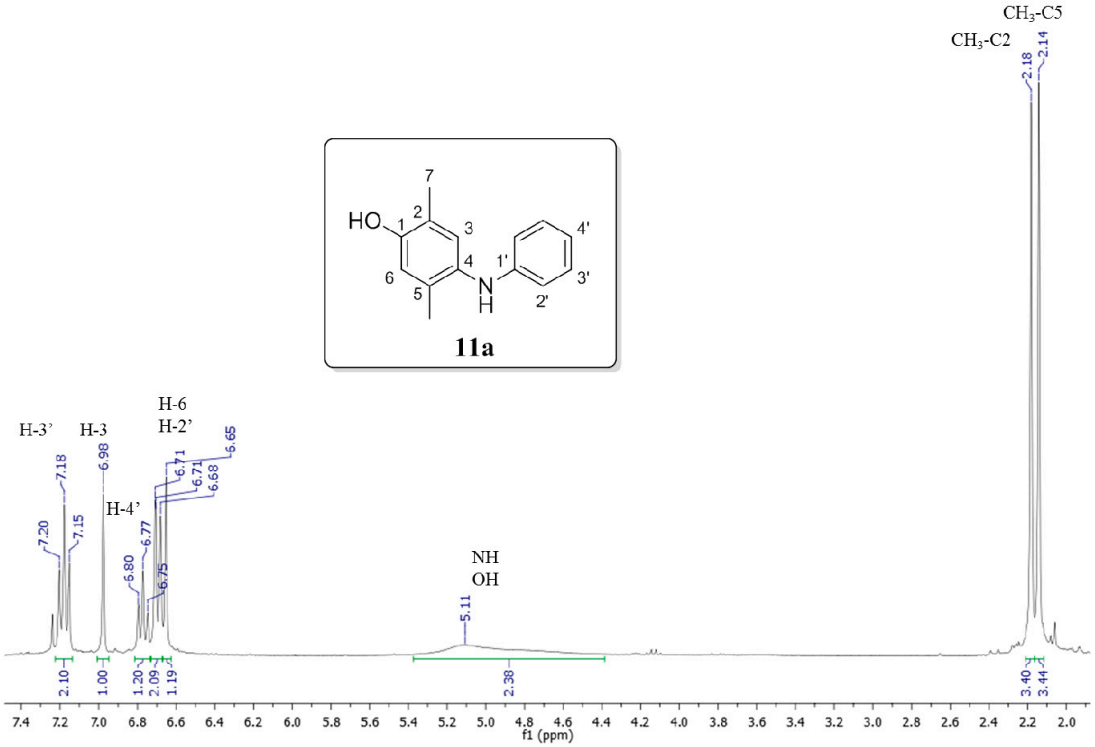
^{13}C-NMR ($CDCl_3$, 125 MHz) spectrum of 10b.



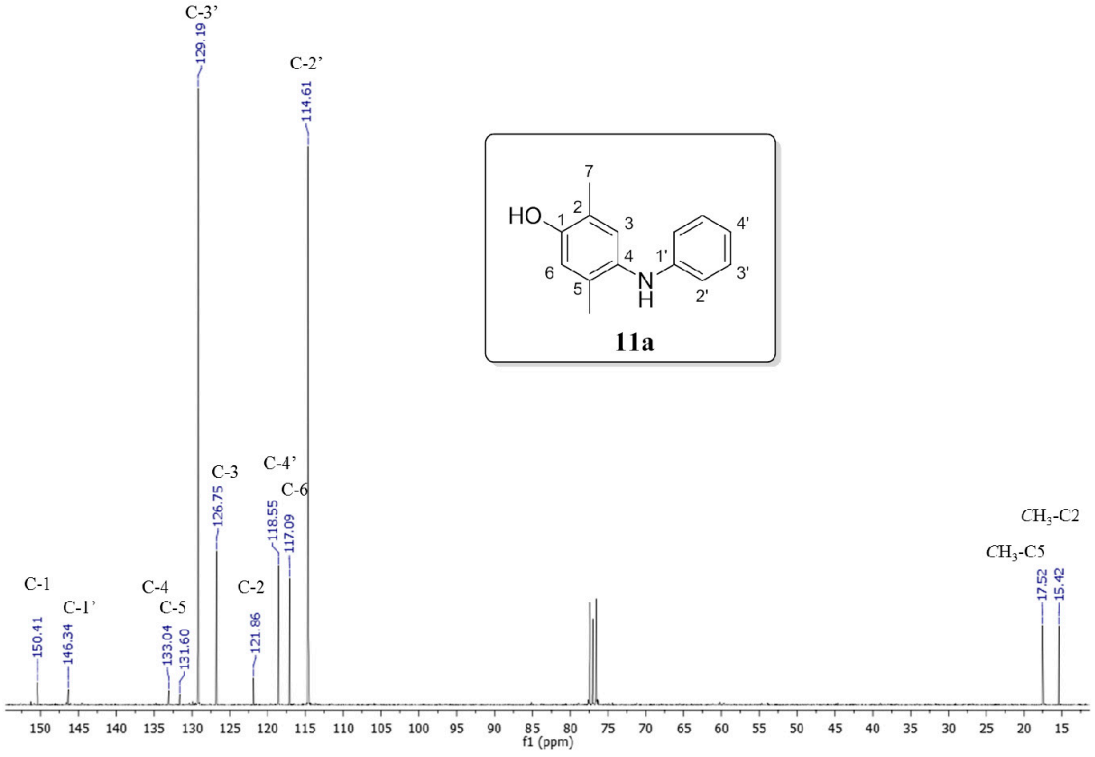
^{1}H-NMR ($CDCl_3$, 300 MHz) spectrum of **10c**.



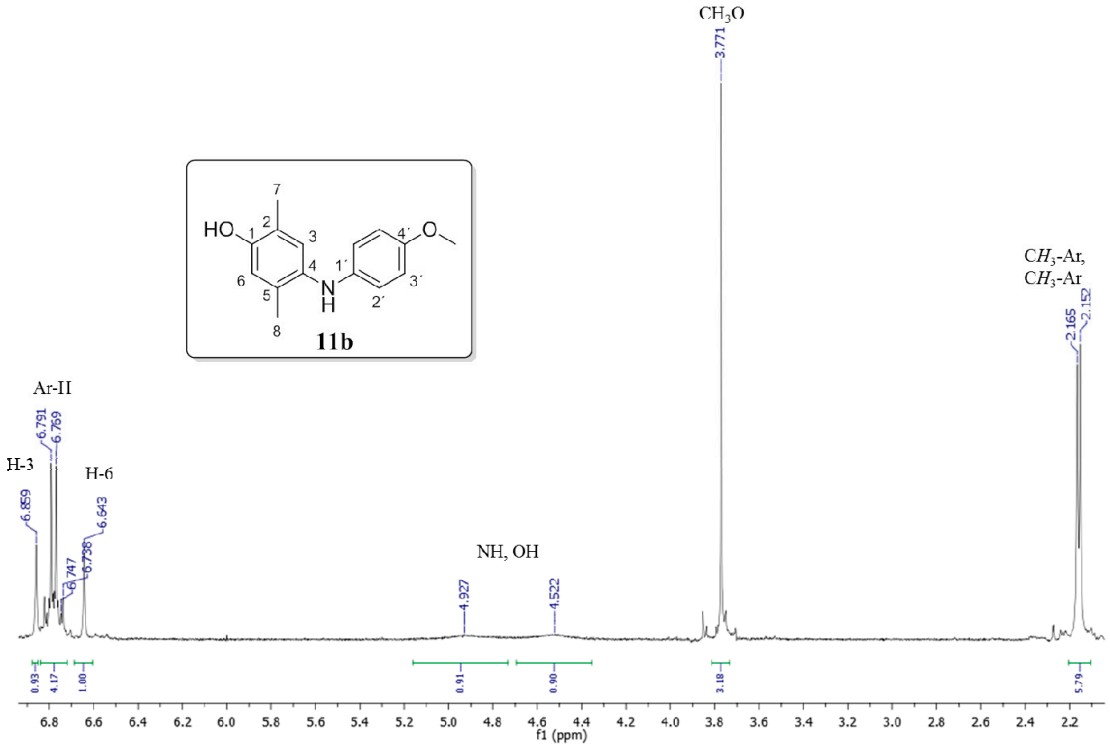
^{13}C-NMR ($CDCl_3$, 75 MHz) spectrum of **10c**.



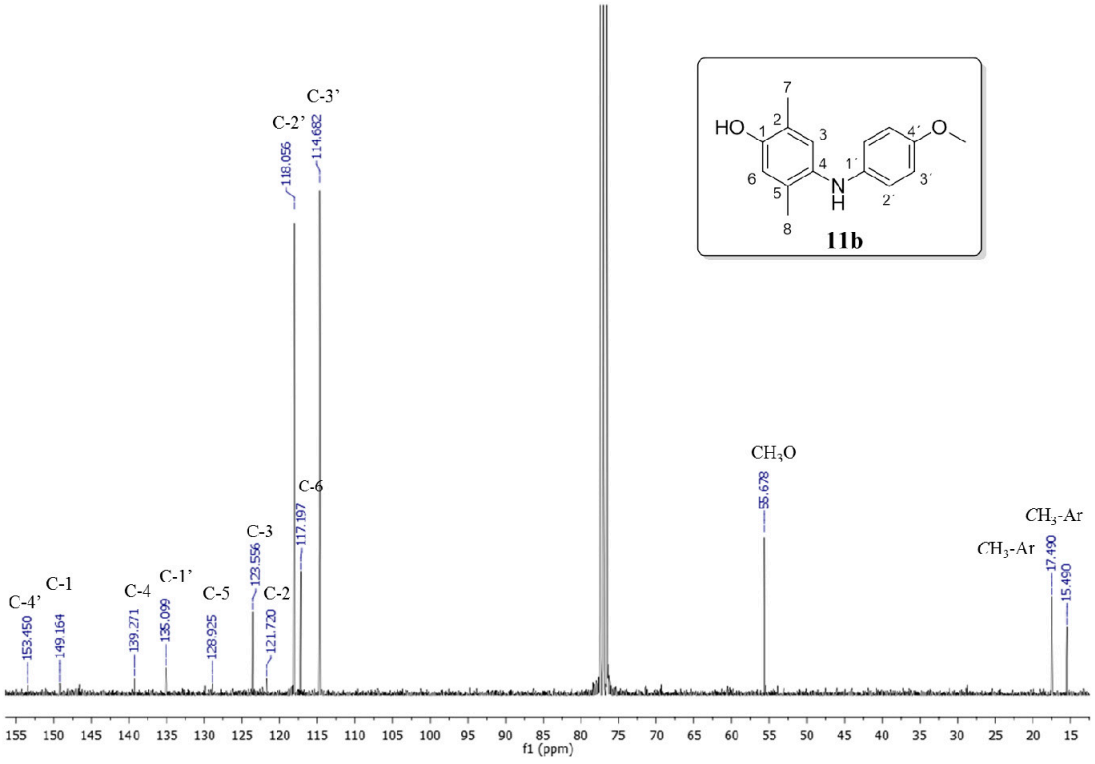
^{1}H-NMR ($CDCl_3$, 300 MHz) spectrum of **11a**



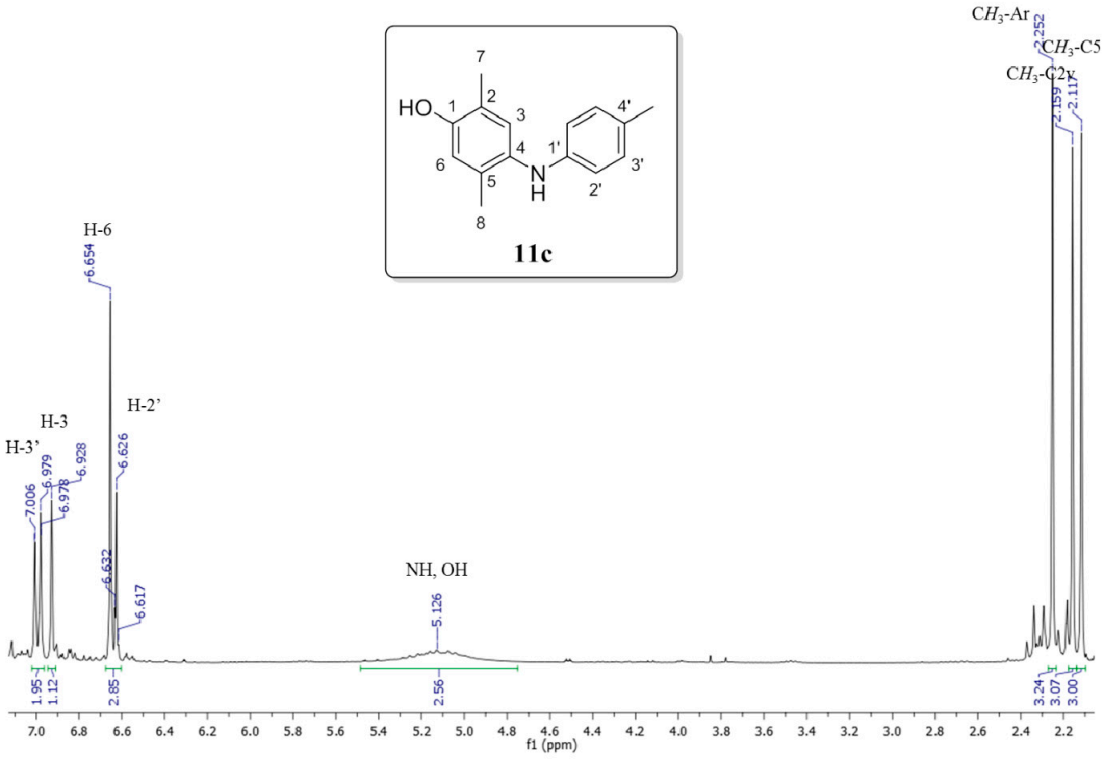
^{13}C-NMR ($CDCl_3$, 75 MHz) spectrum of **11a**



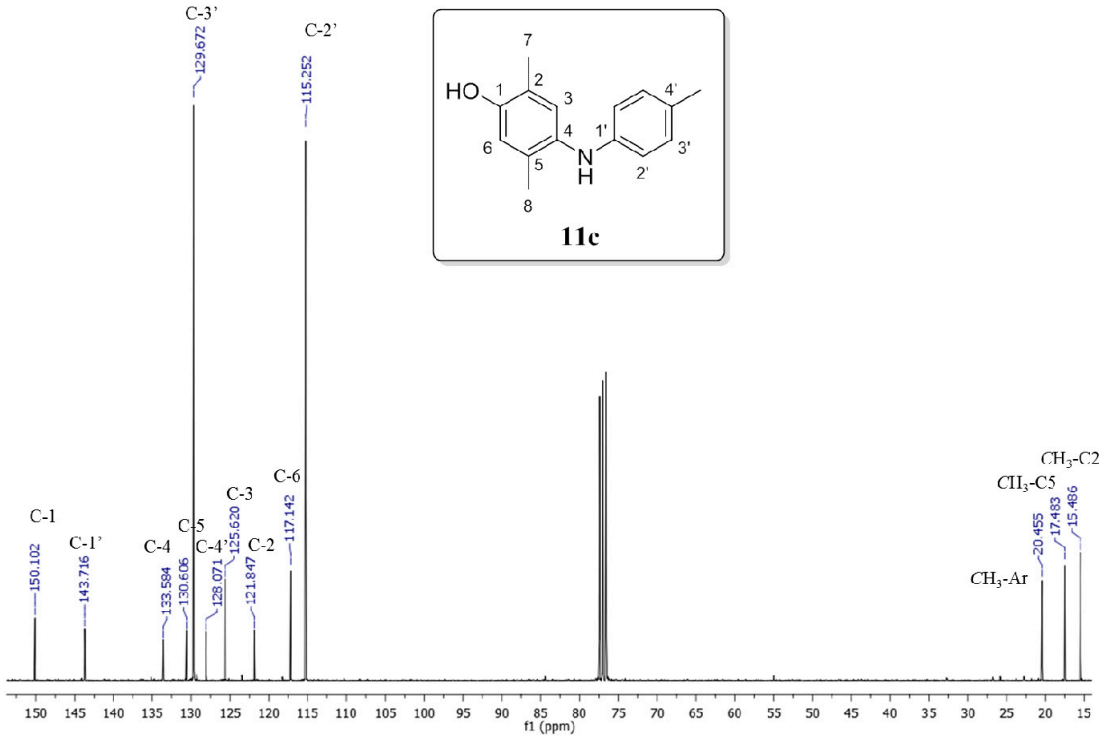
^{1}H-NMR ($CDCl_3$, 300 MHz) spectrum of 11b



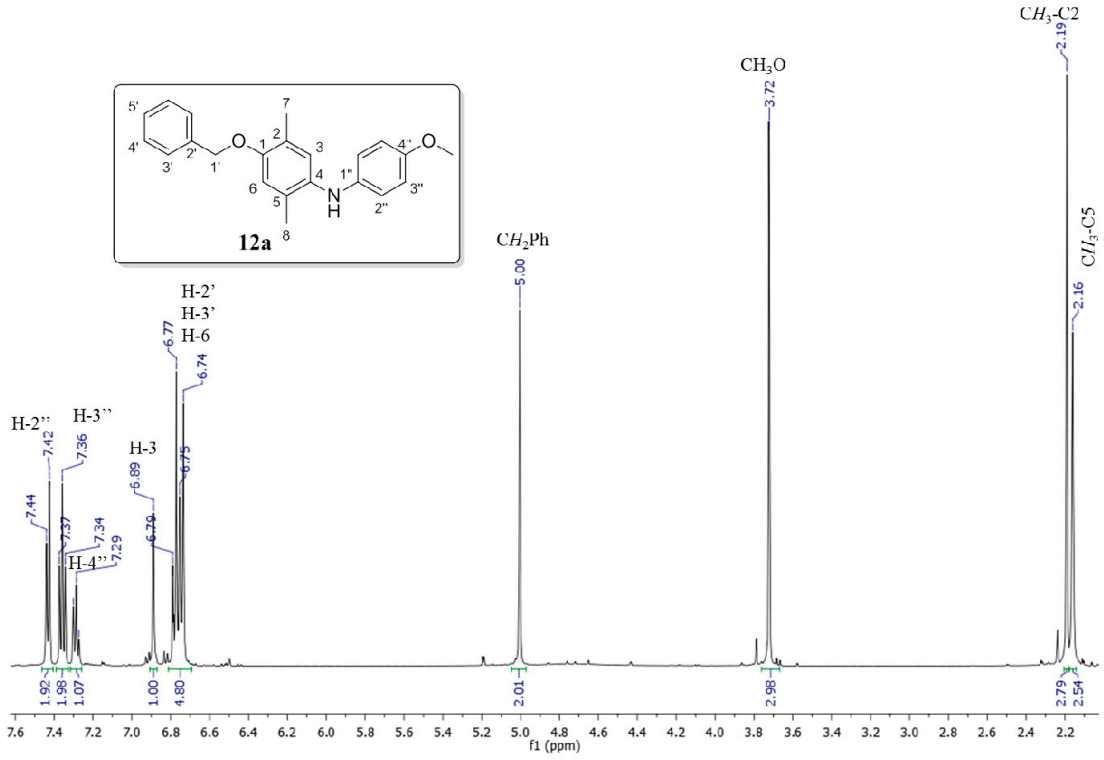
^{13}C-NMR ($CDCl_3$, 75 MHz) spectrum of 11b



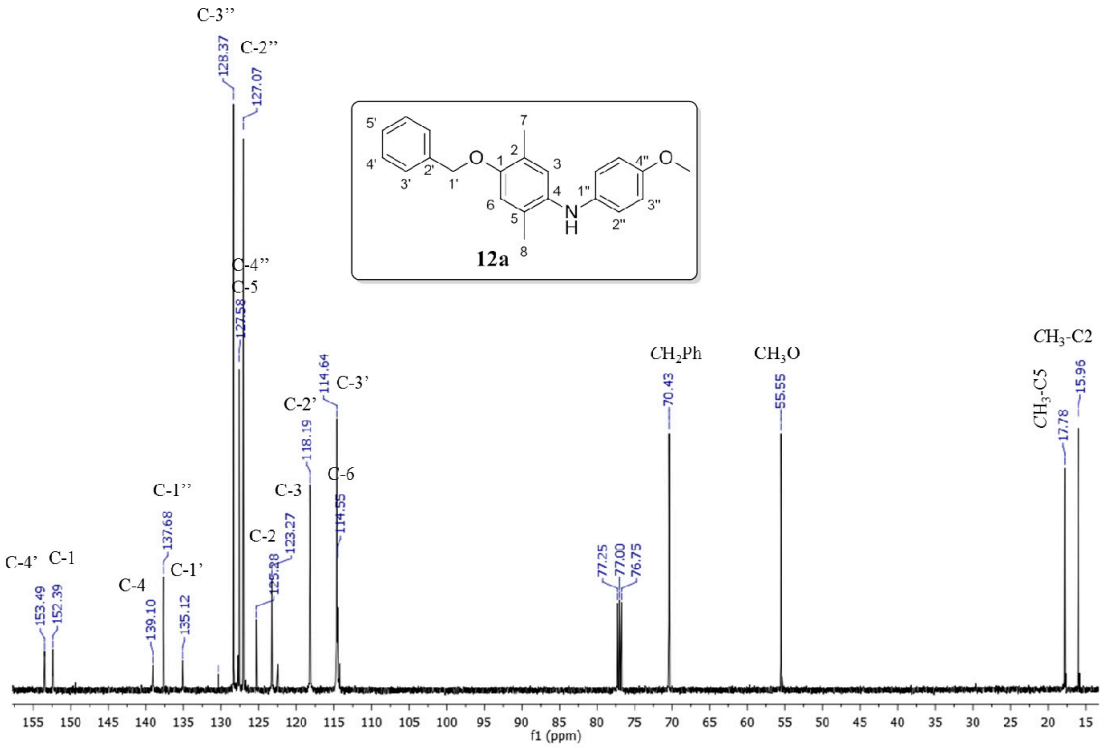
^{1}H-NMR ($CDCl_3$, 300 MHz) spectrum of **11c**.



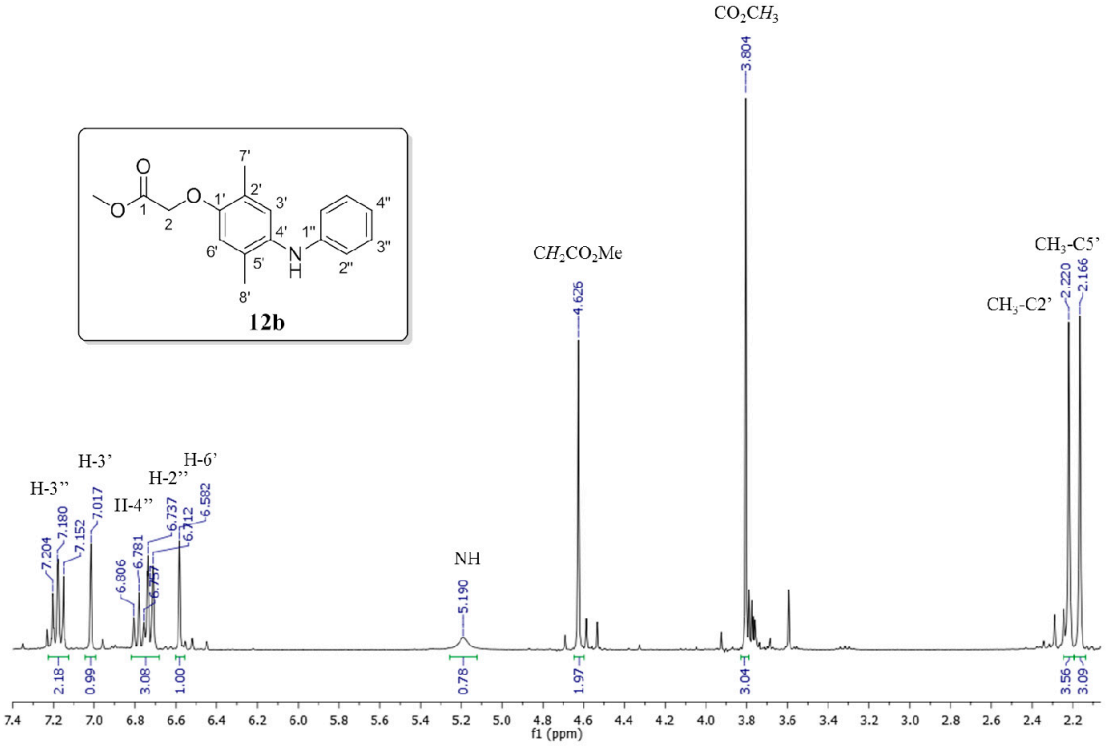
^{13}C-NMR ($CDCl_3$, 75 MHz) spectrum of **11c**.



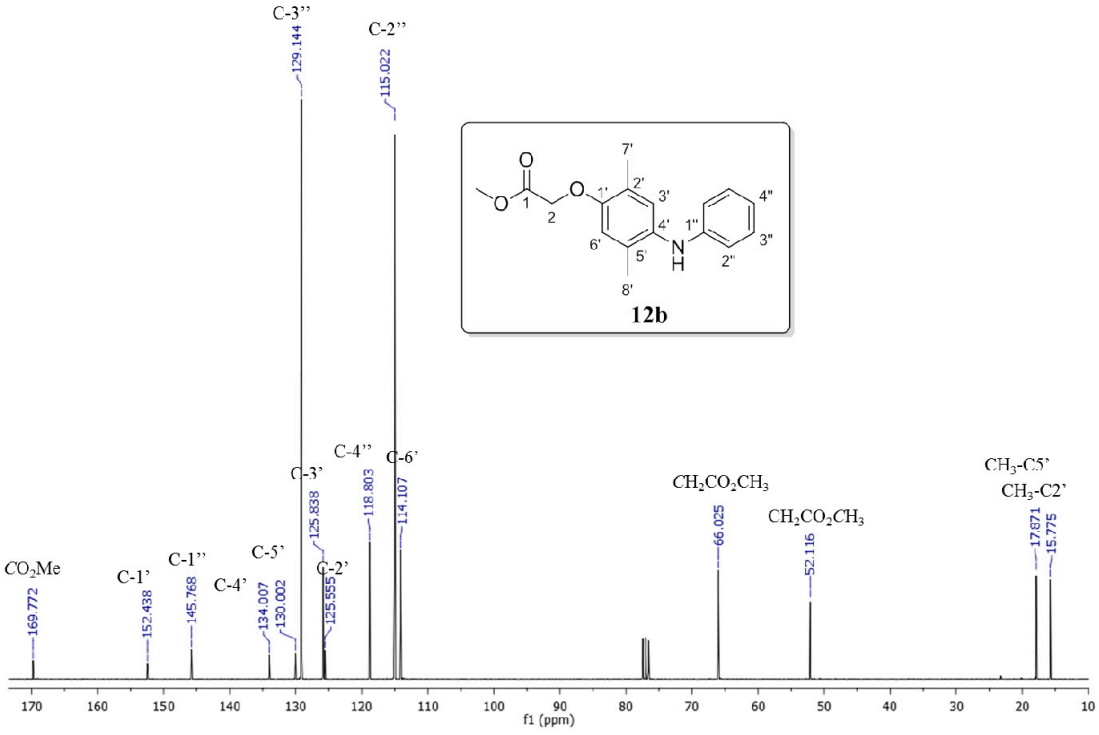
^{1}H-NMR ($CDCl_3$, 500 MHz) spectrum of **12a**



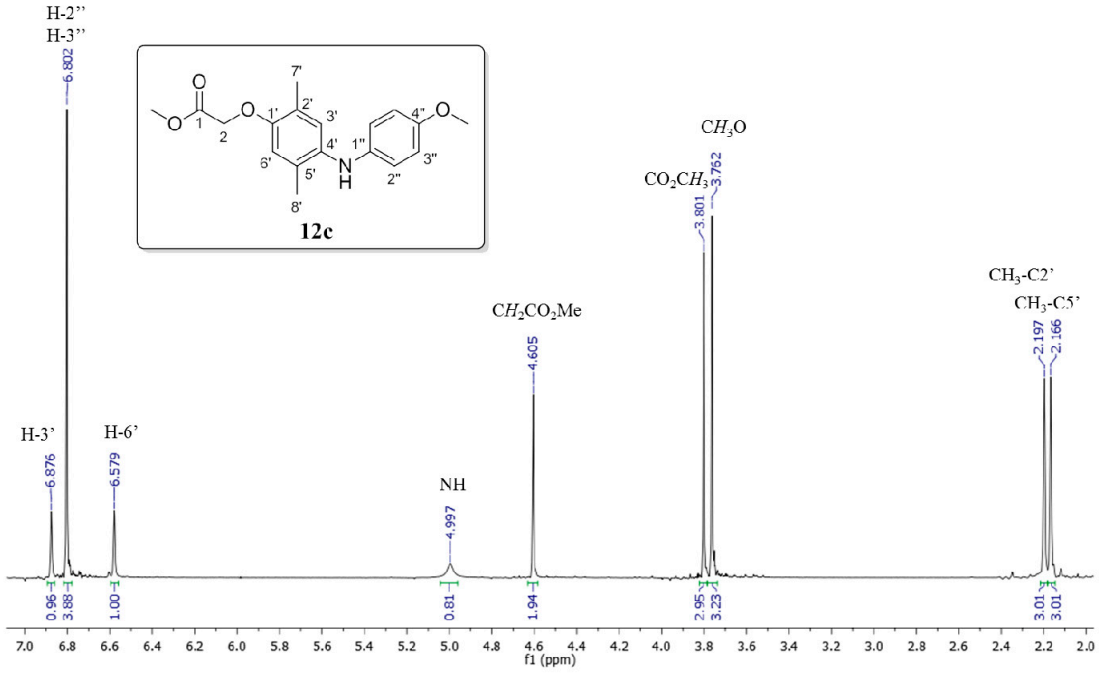
^{13}C-NMR ($CDCl_3$, 125 MHz) spectrum of **12a**



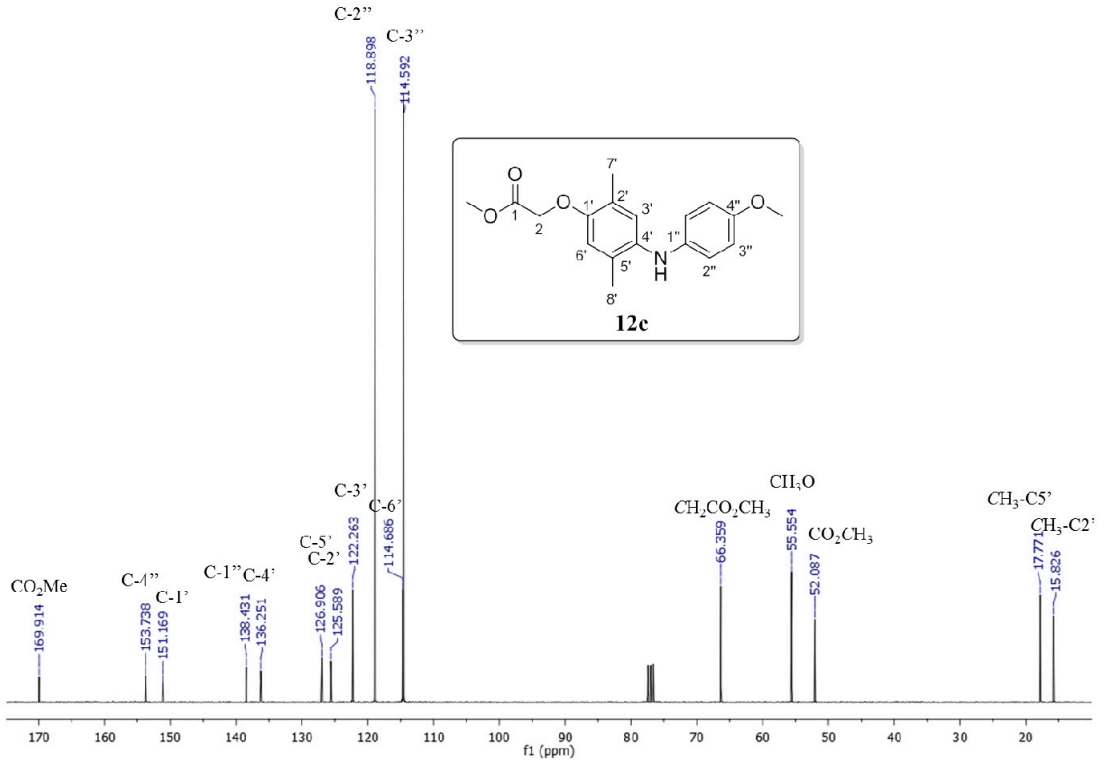
^{1}H-NMR ($CDCl_3$, 300 MHz) spectrum of **12b**



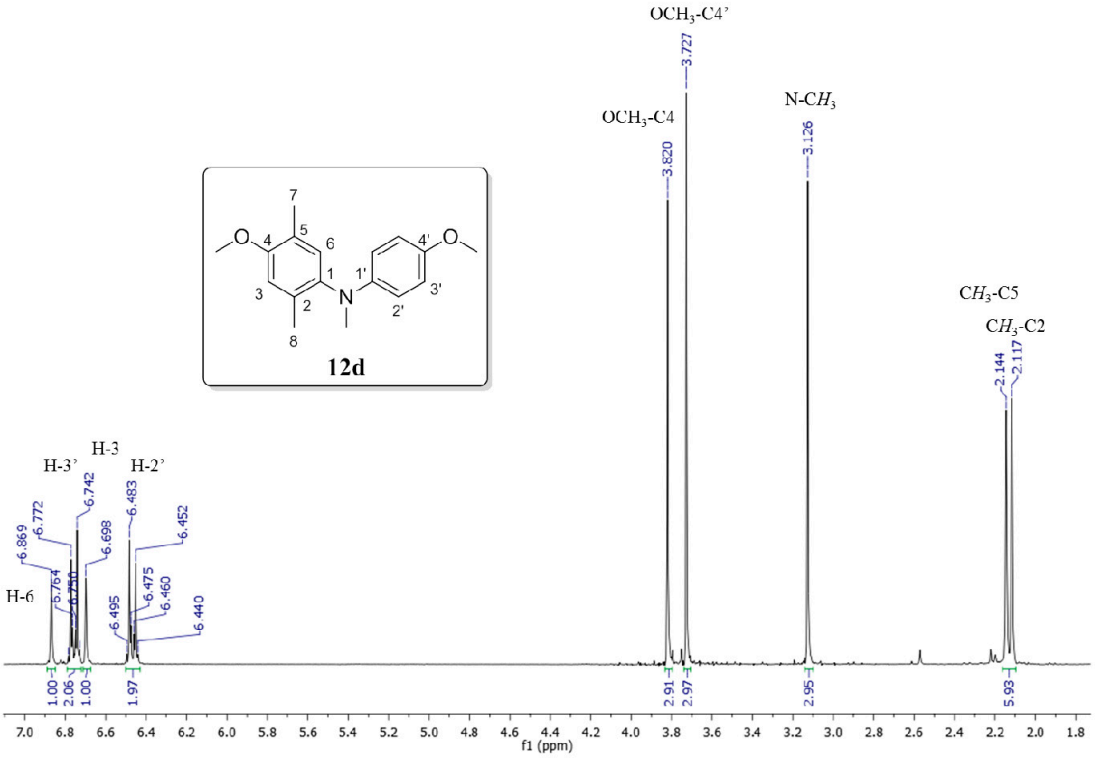
^{13}C-NMR ($CDCl_3$, 75 MHz) spectrum of **12b**



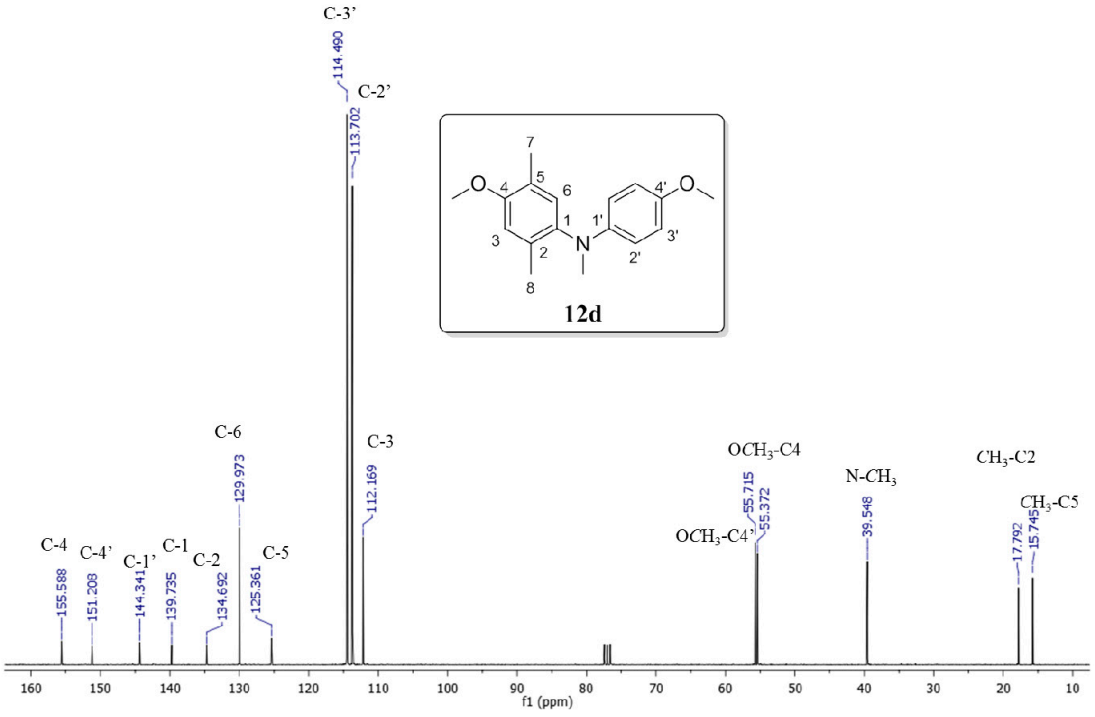
^{1}H-NMR ($CDCl_3$, 300 MHz) spectrum of **12c**



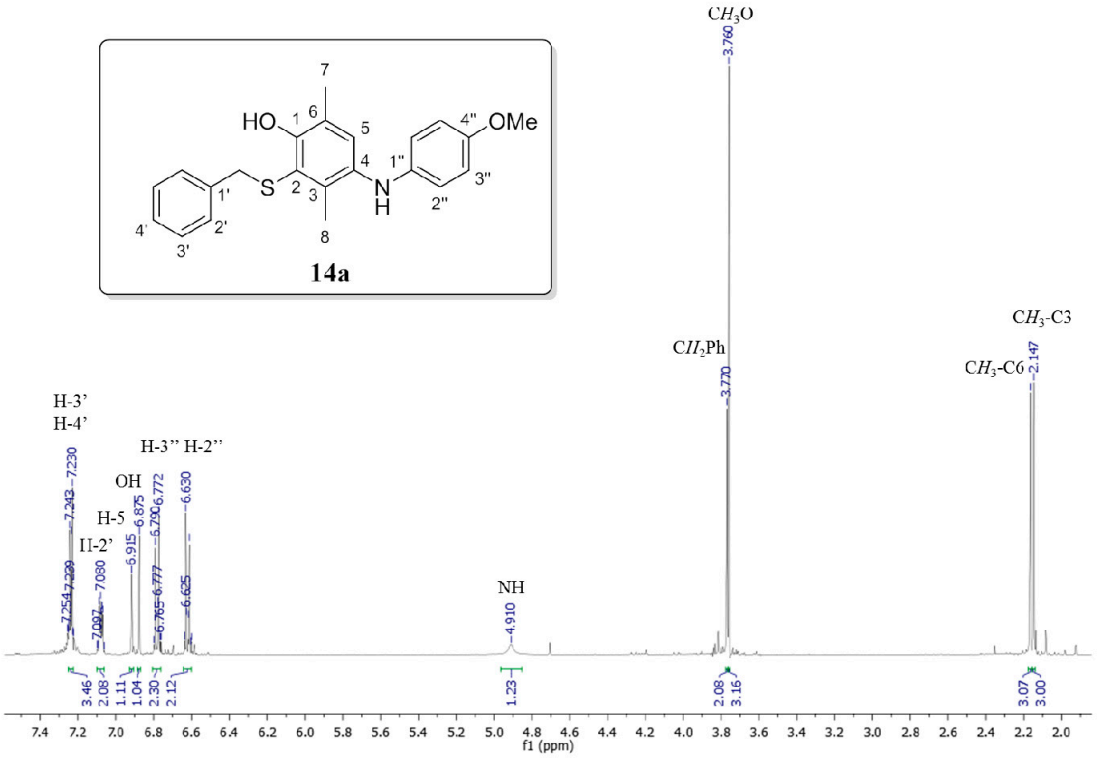
^{13}C-NMR ($CDCl_3$, 75 MHz) spectrum of **12c**



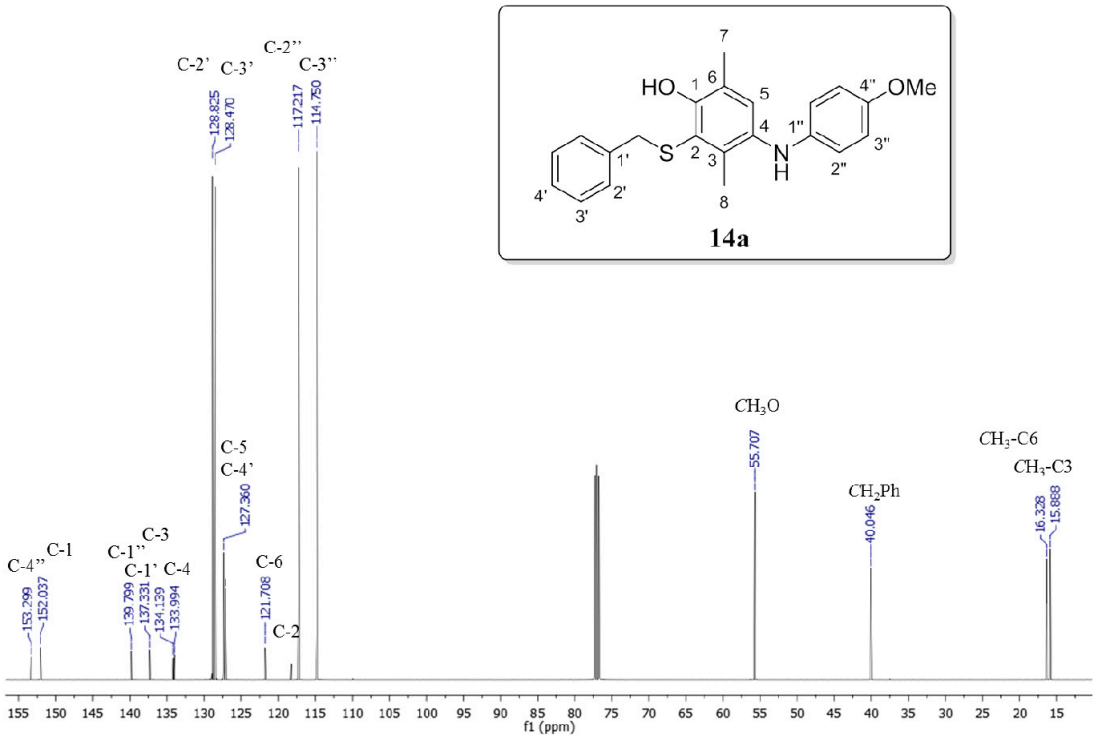
^{1}H-NMR ($CDCl_3$, 500 MHz) spectrum of **12d**



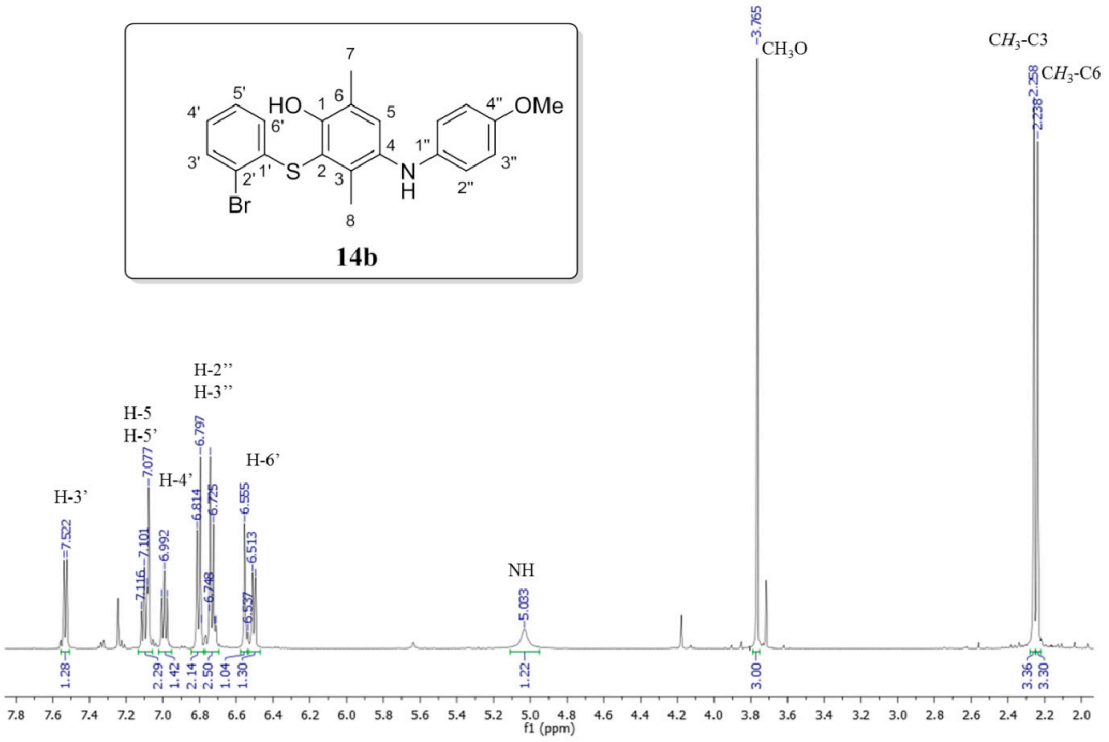
^{13}C-NMR ($CDCl_3$, 125 MHz) spectrum of **12d**



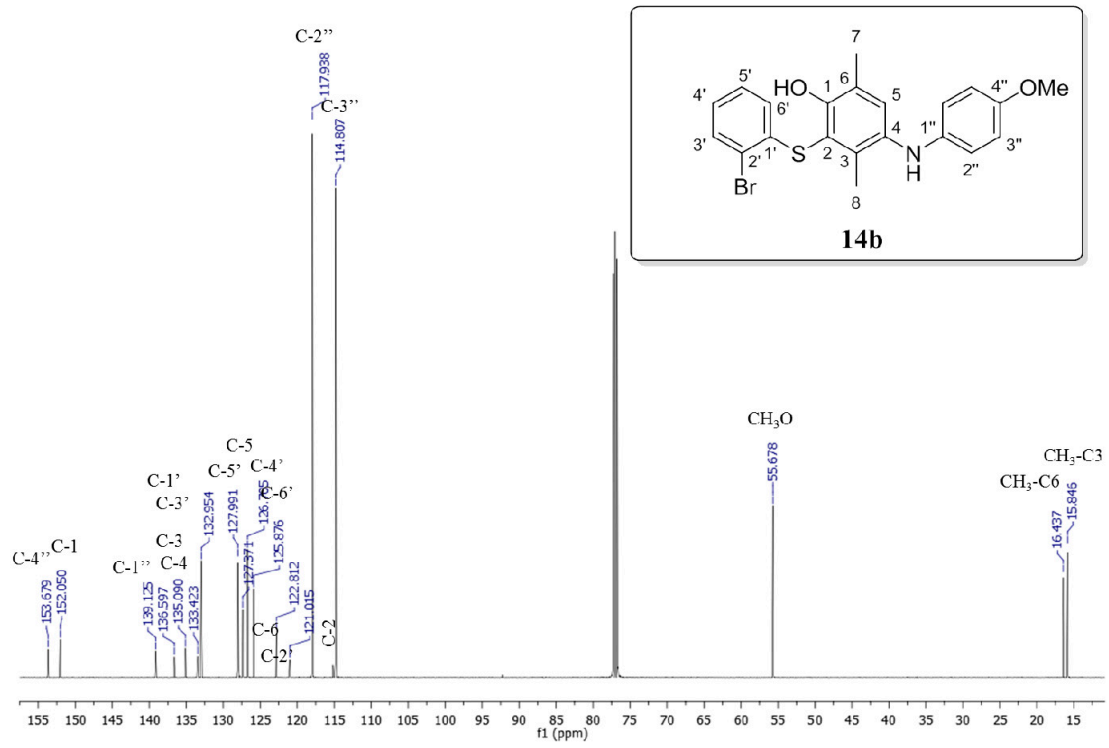
^{1}H-NMR ($CDCl_3$, 500 MHz) spectrum of **14a**



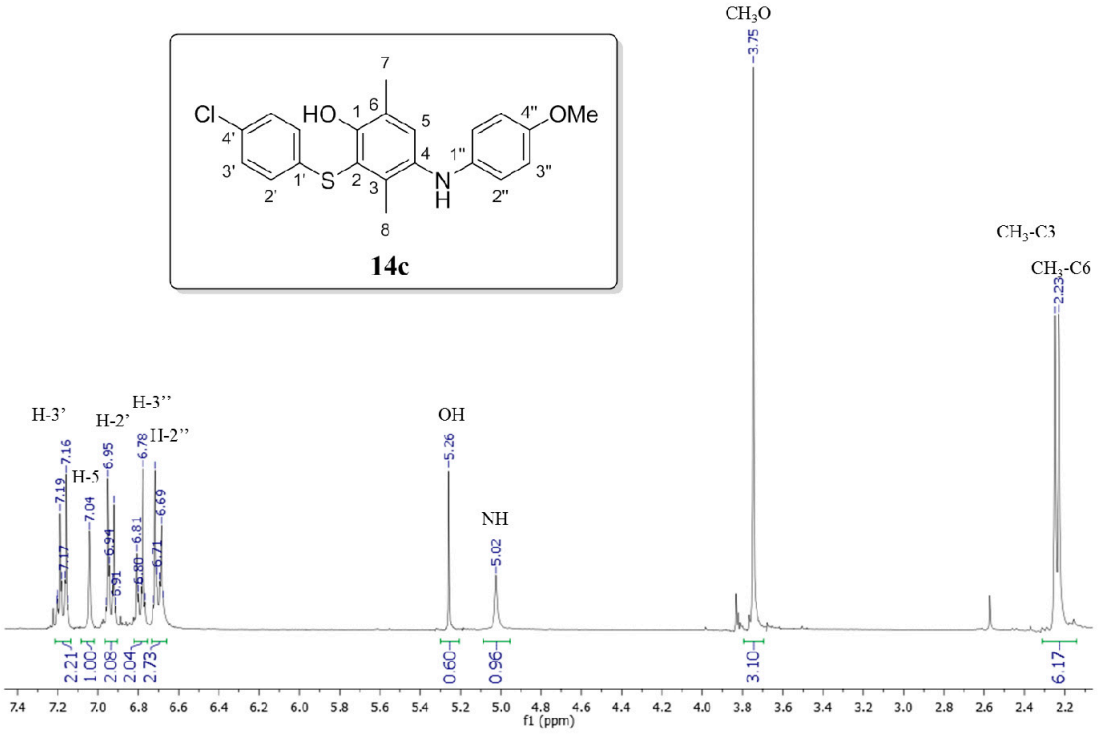
^{13}C-NMR ($CDCl_3$, 125 MHz) spectrum of **14a**



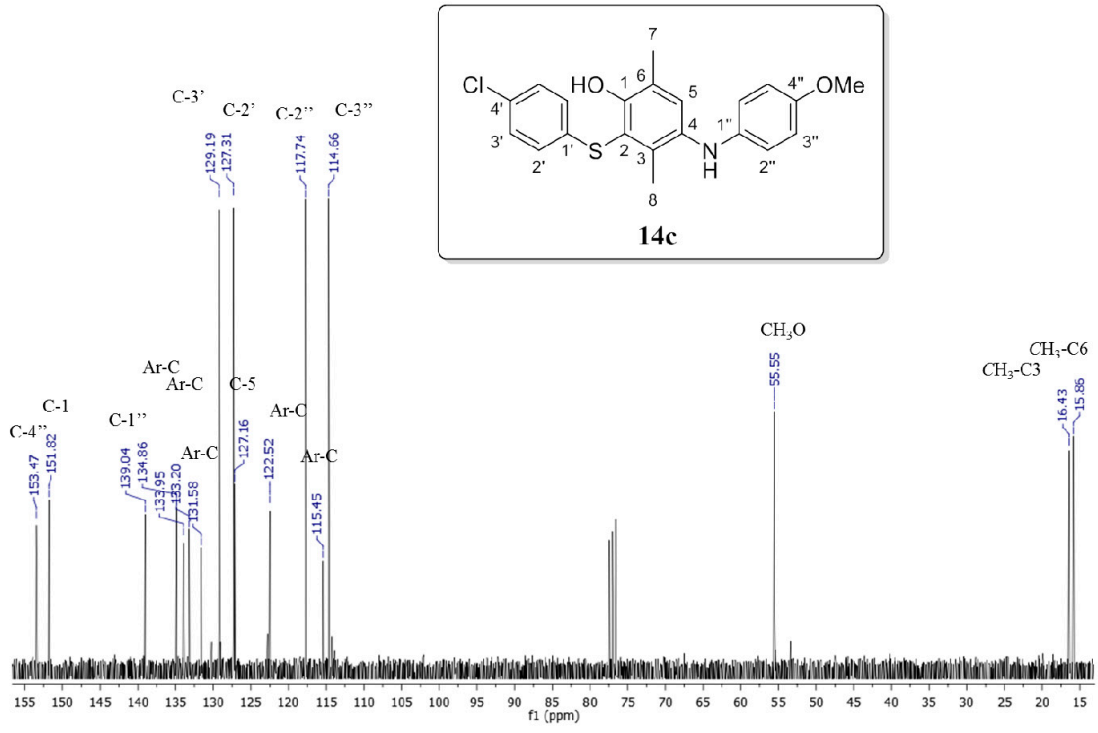
^{1}H-NMR ($CDCl_3$, 500 MHz) spectrum of **14b**



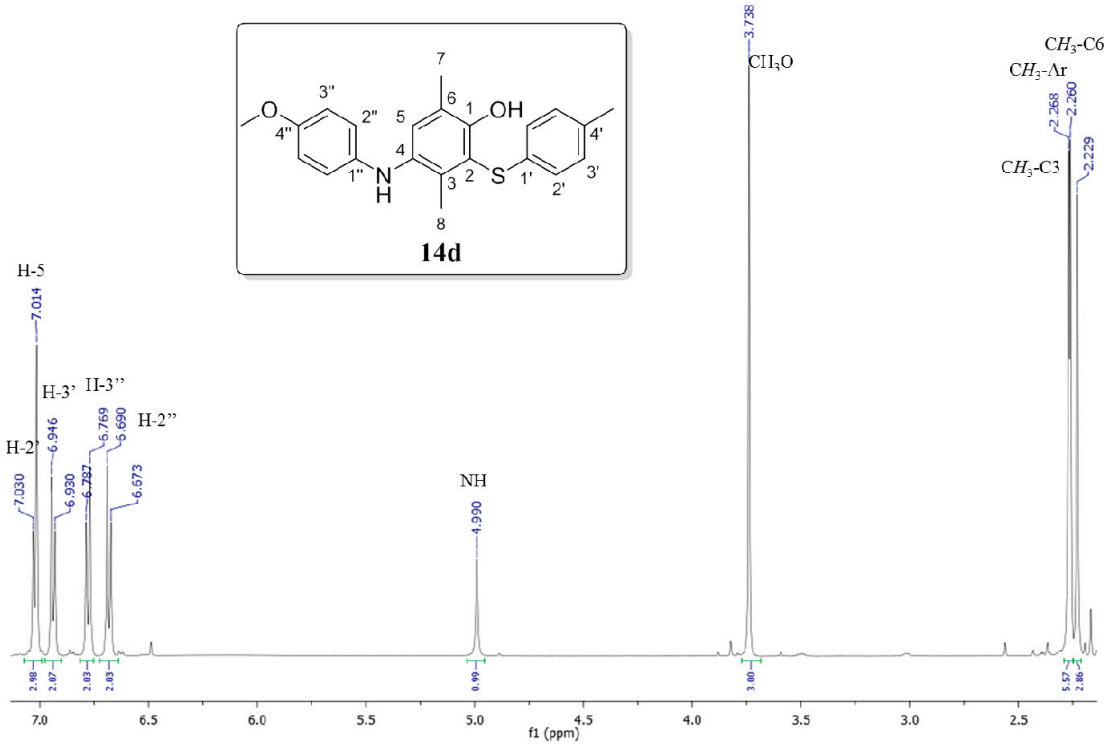
^{13}C-NMR ($CDCl_3$, 125 MHz) spectrum of **14b**



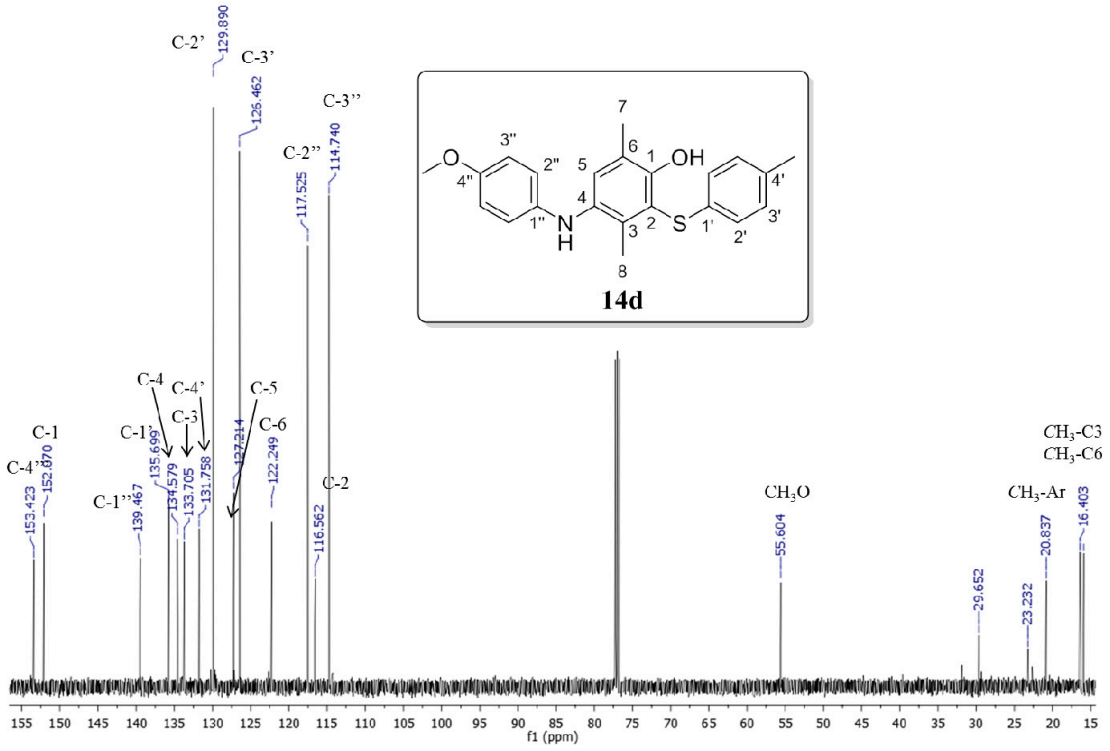
^{1}H-NMR ($CDCl_3$, 300 MHz) spectrum of **14c**



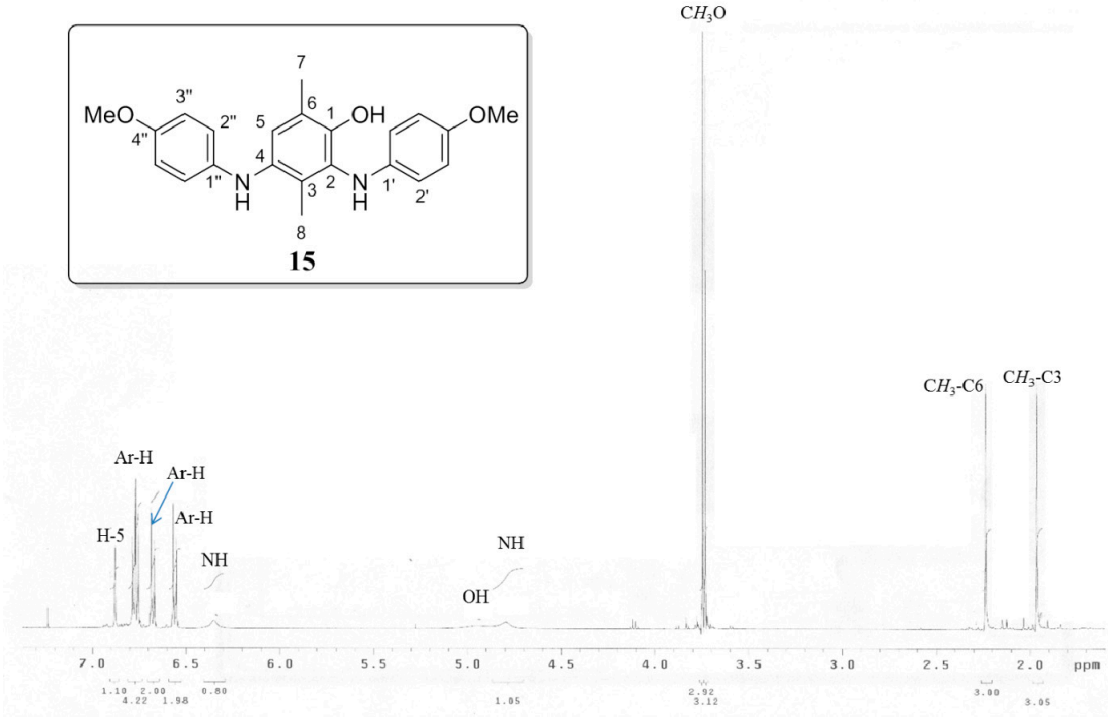
^{13}C-NMR ($CDCl_3$, 75 MHz) spectrum of **14c**



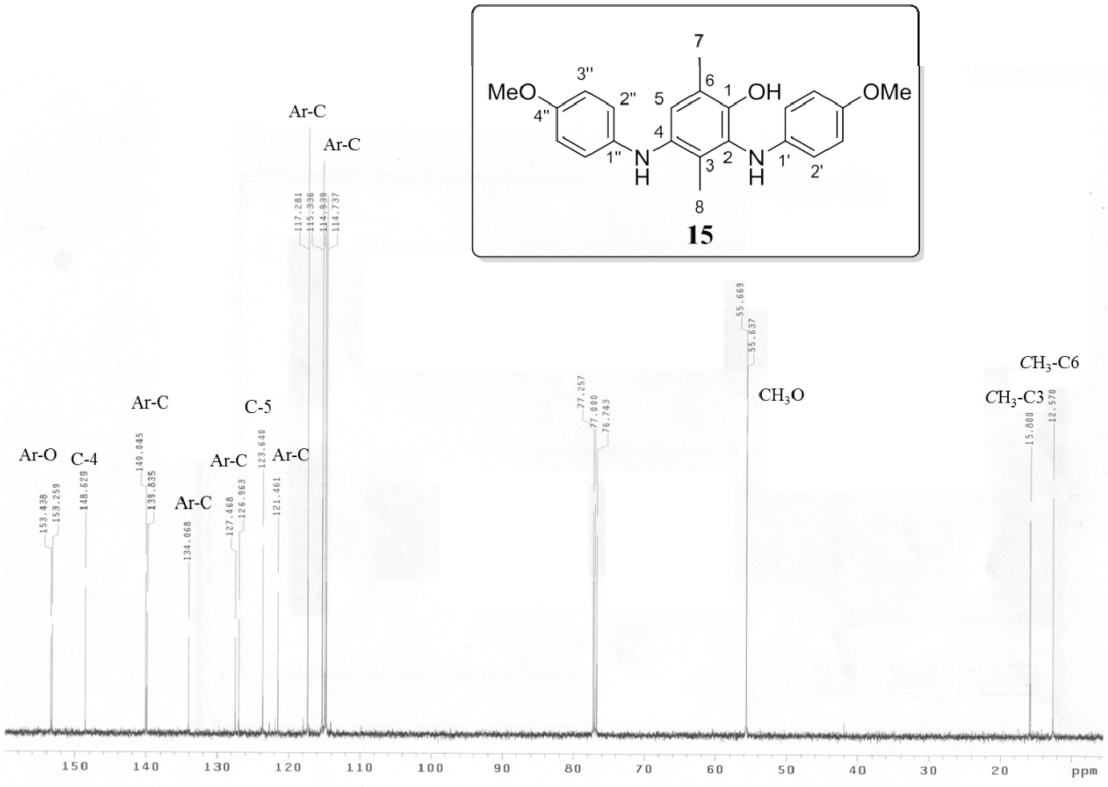
^{1}H-NMR ($CDCl_3$, 500 MHz) spectrum of **14d**.



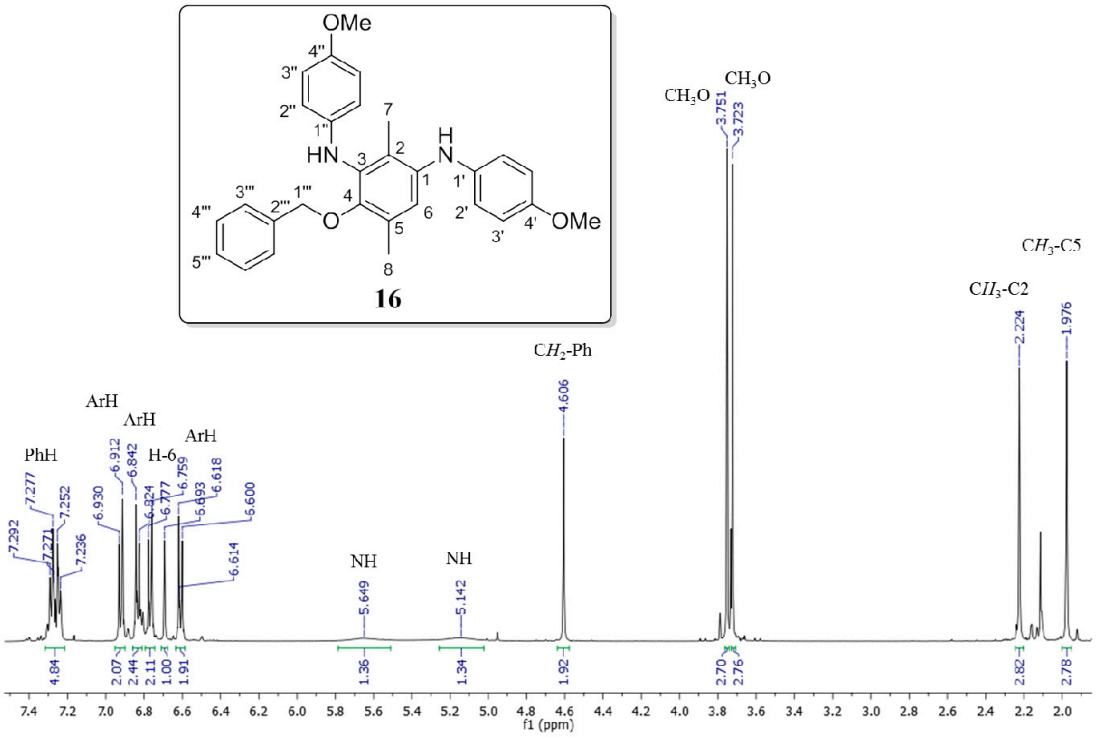
^{13}C-NMR ($CDCl_3$, 125 MHz) spectrum of **14d**.



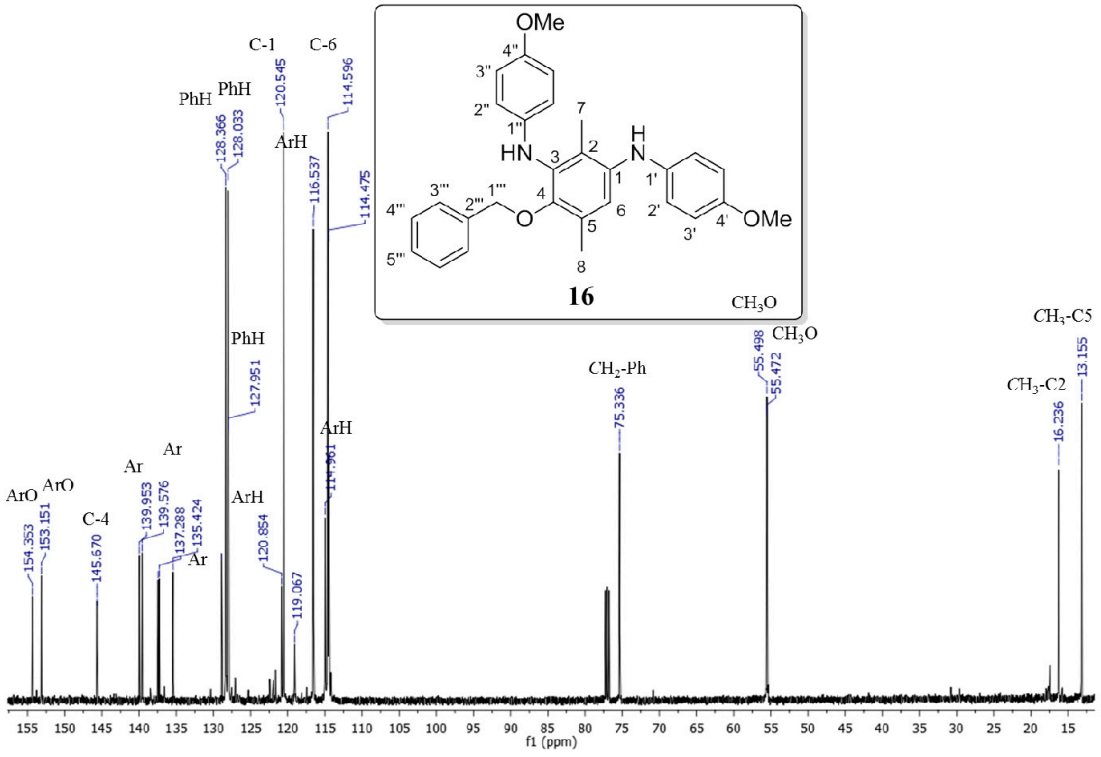
^{1}H-NMR ($CDCl_3$, 500 MHz) spectrum of **15**.



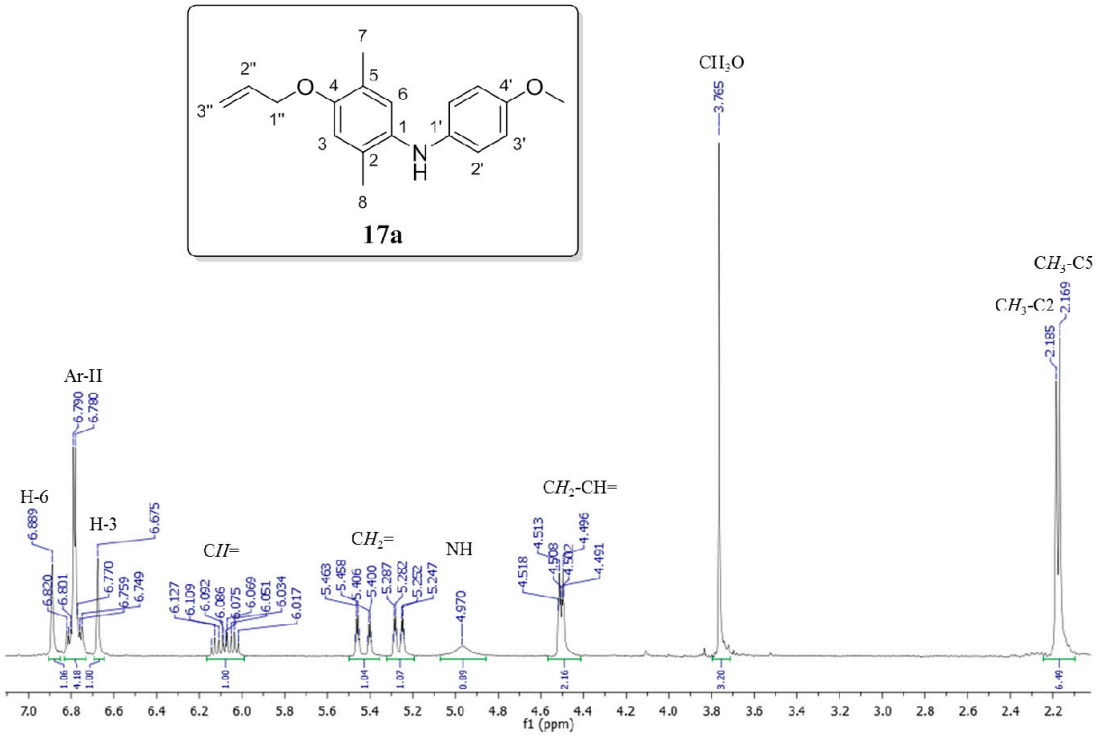
^{13}C-NMR ($CDCl_3$, 125 MHz) spectrum of **15**.



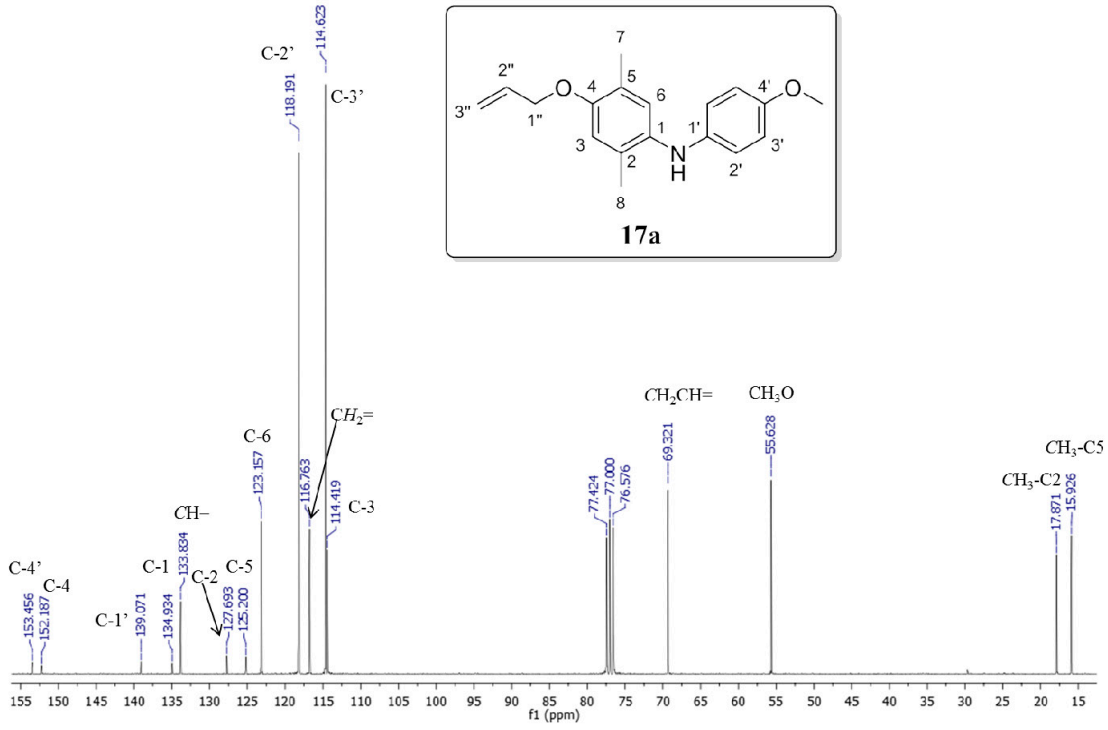
^{1}H-NMR ($CDCl_3$, 300 MHz) spectrum of **16**



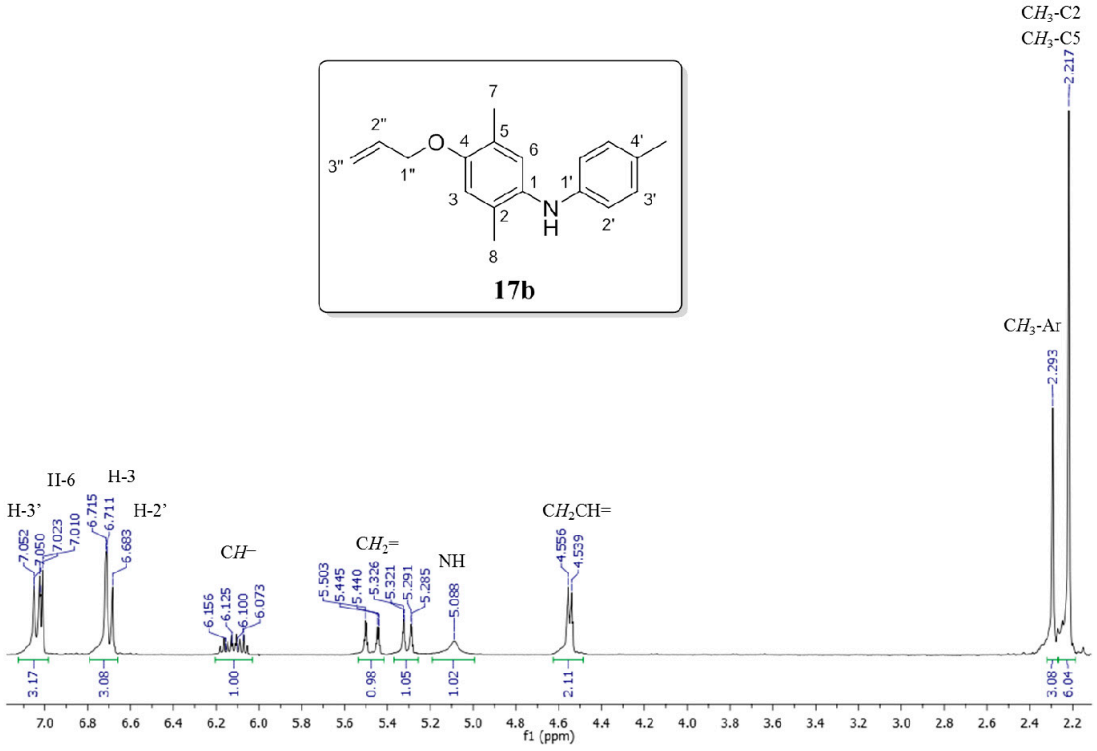
^{13}C-NMR ($CDCl_3$, 75 MHz) spectrum of **16**



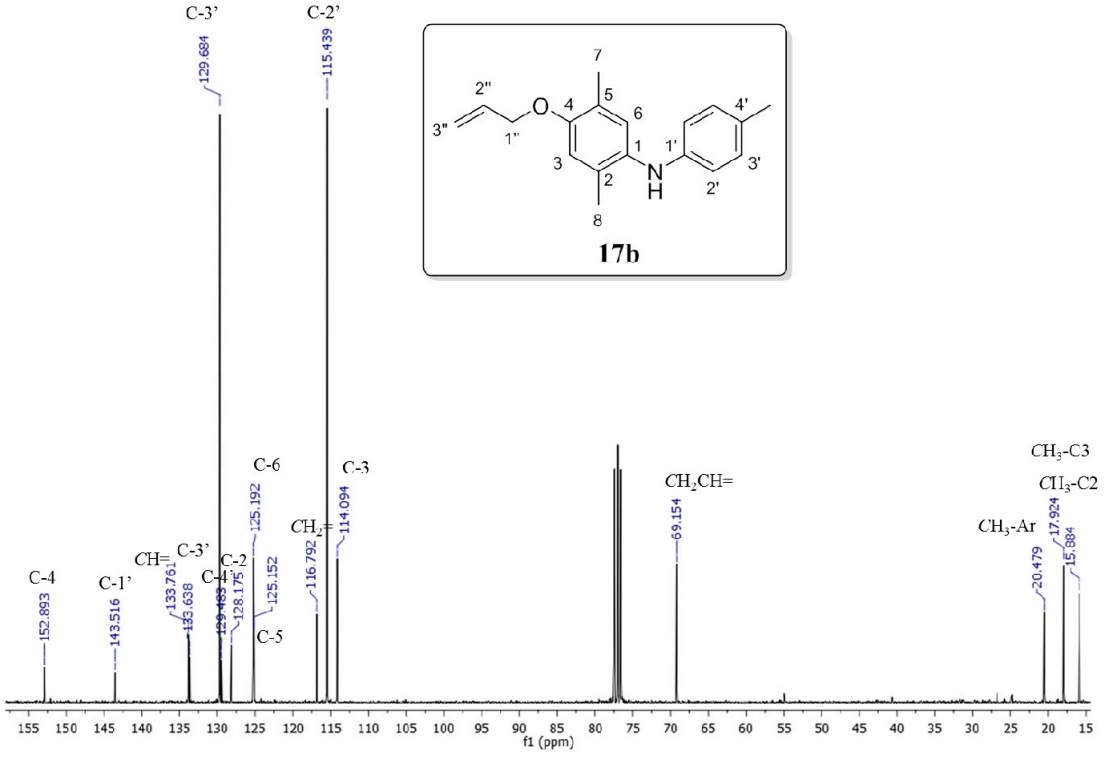
^{1}H-NMR ($CDCl_3$, 500 MHz) spectrum of **17a**.



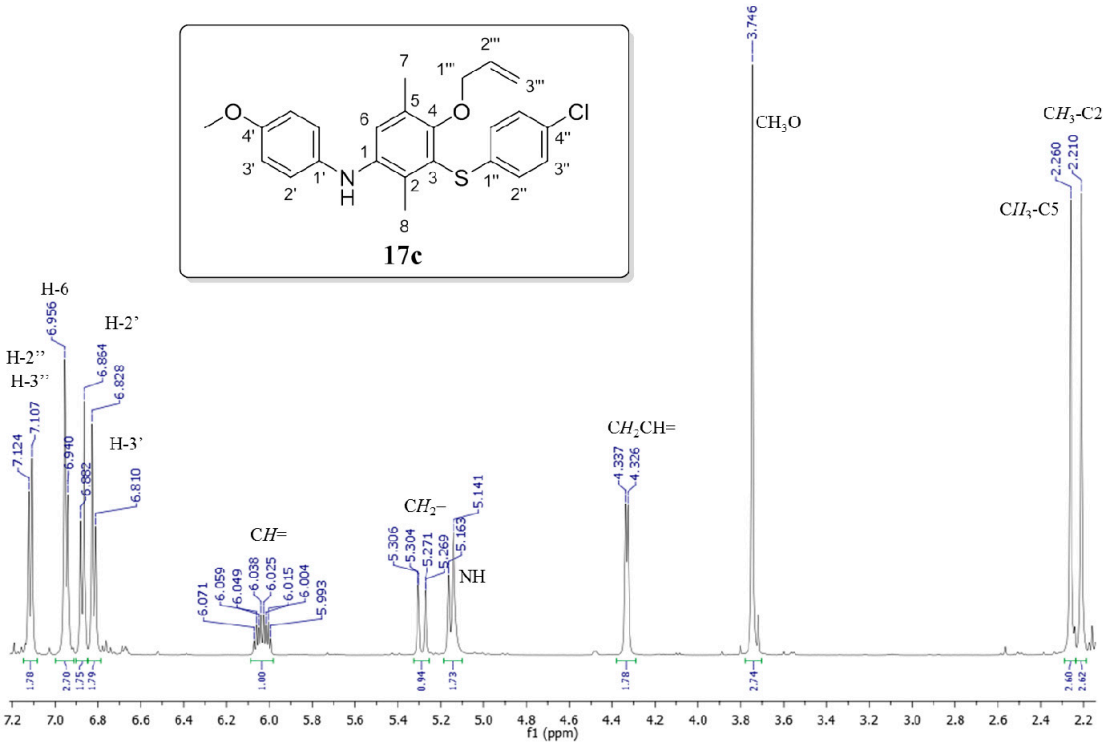
^{13}C-NMR ($CDCl_3$, 500 MHz) spectrum of **17a**.



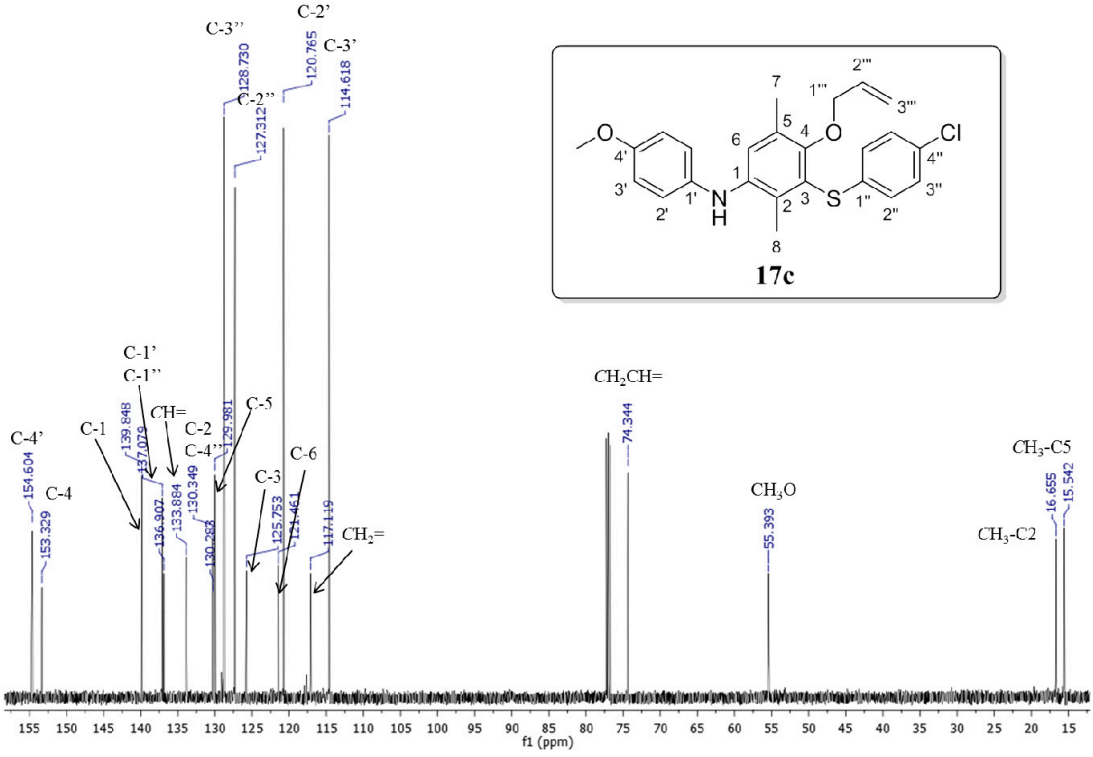
^{1}H-NMR ($CDCl_3$, 300 MHz) spectrum of **17b**.



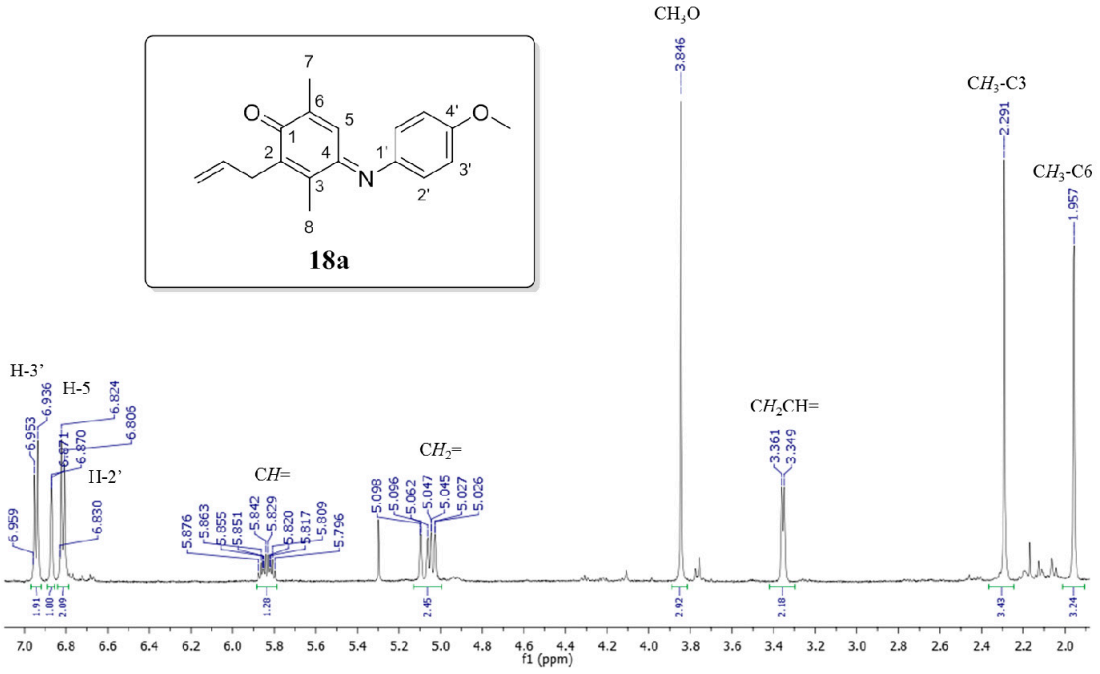
^{13}C-NMR ($CDCl_3$, 75 MHz) spectrum of **17b**.



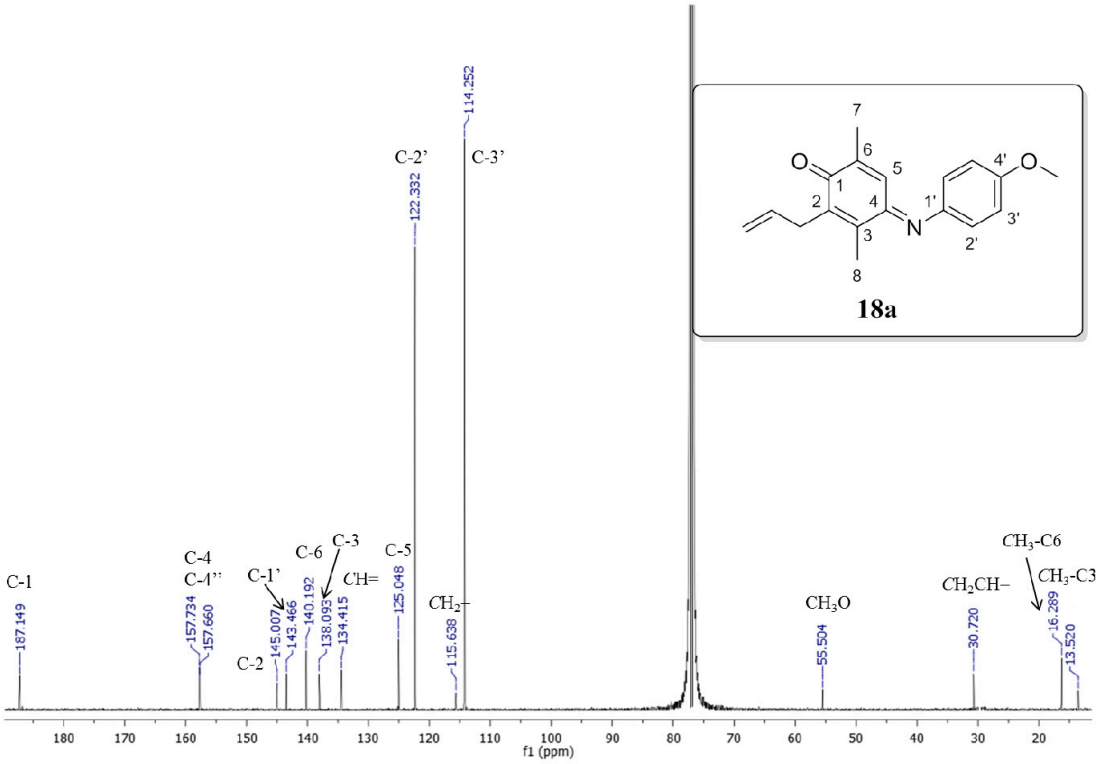
^{1}H-NMR ($CDCl_3$, 500 MHz) spectrum of **17c**.



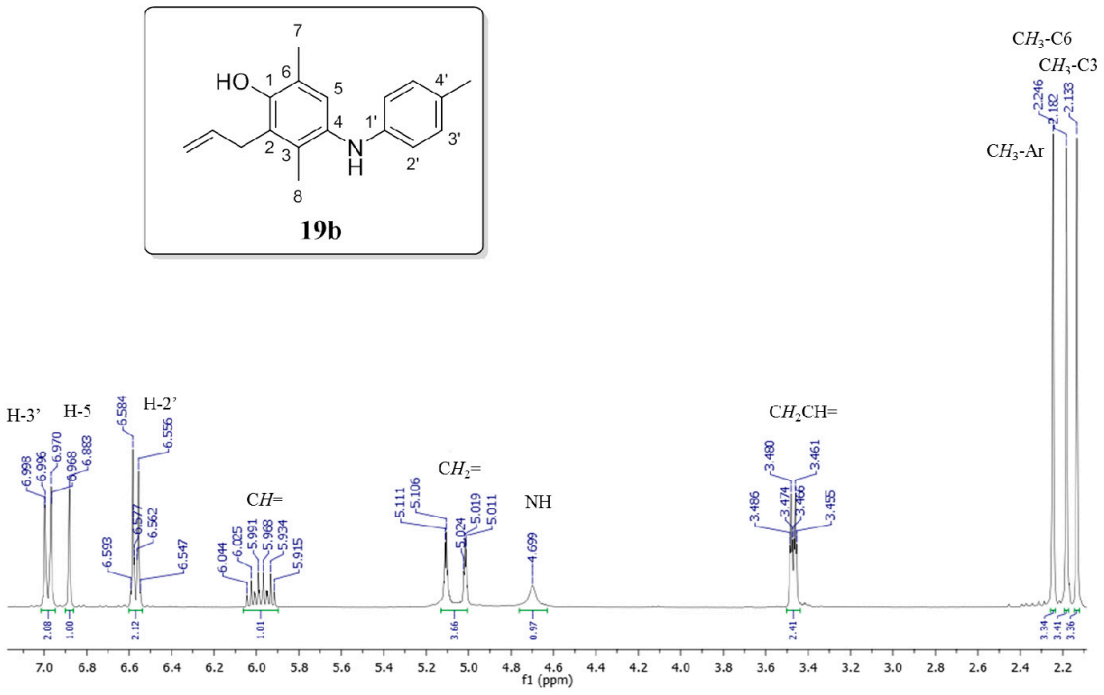
^{13}C-NMR ($CDCl_3$, 125 MHz) spectrum of **17c**.



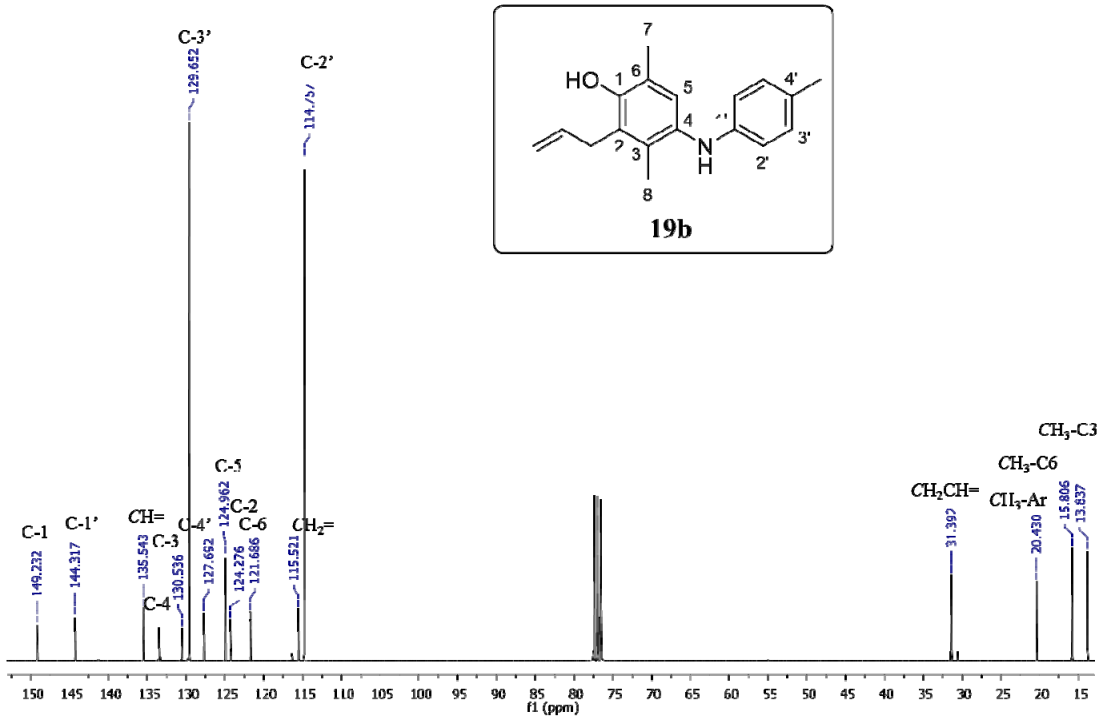
^{1}H-NMR ($CDCl_3$, 500 MHz) spectrum of **18a**.



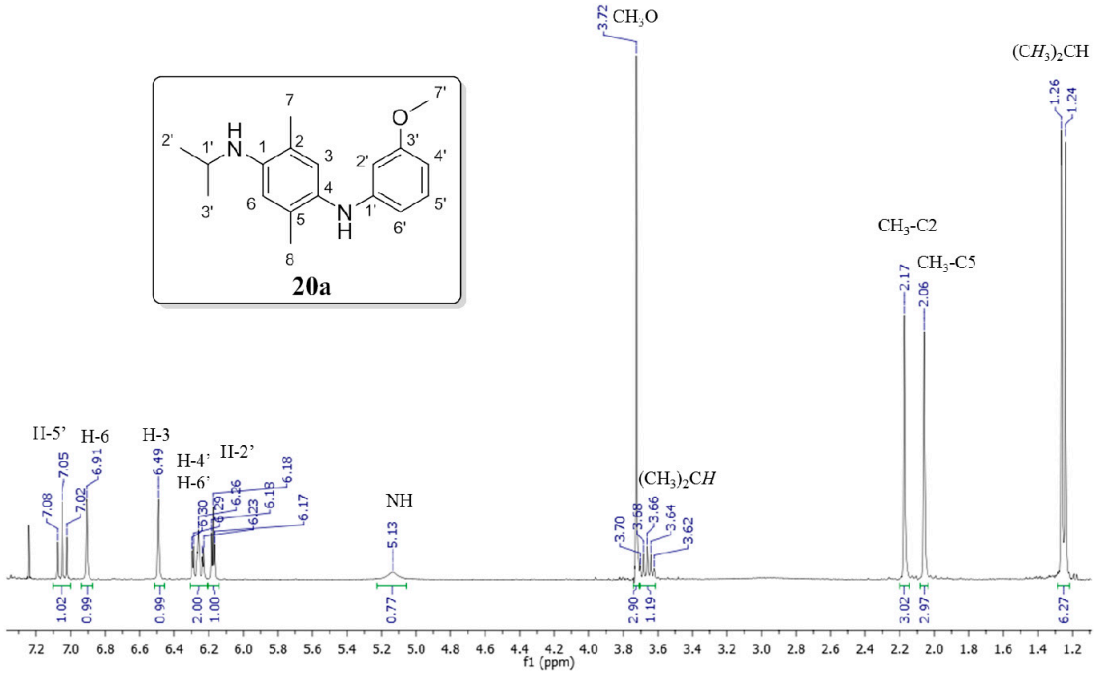
^{13}C-NMR ($CDCl_3$, 500 MHz) spectrum of **18a**.



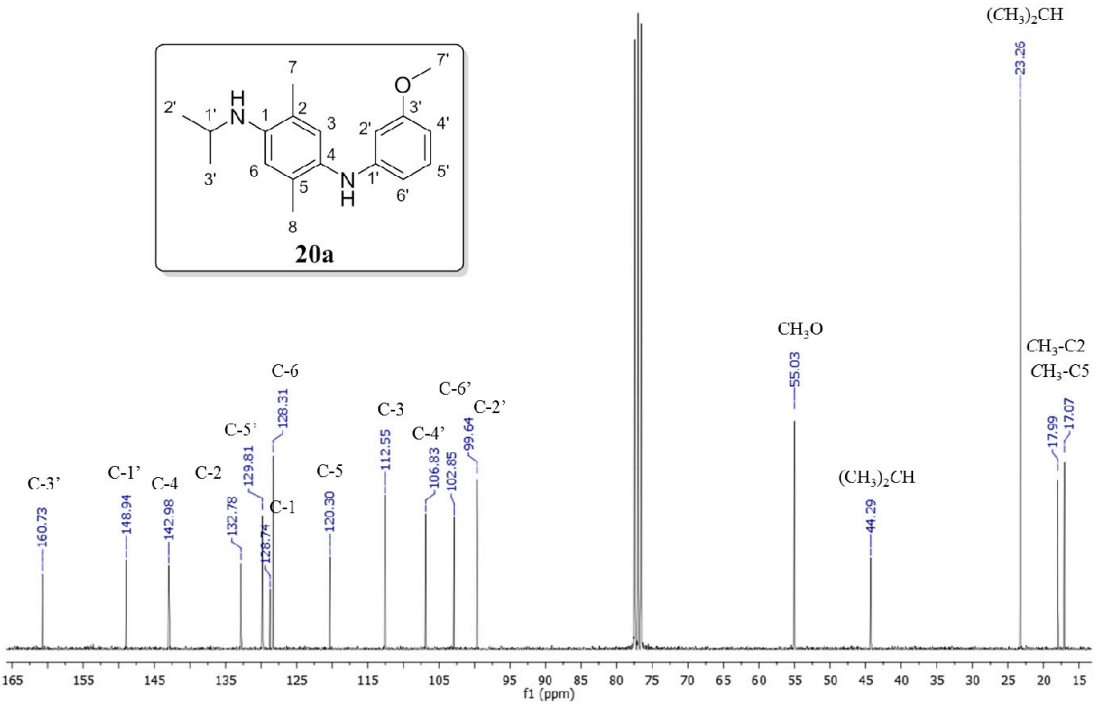
^{1}H-NMR ($CDCl_3$, 300 MHz) spectrum of **19b**.



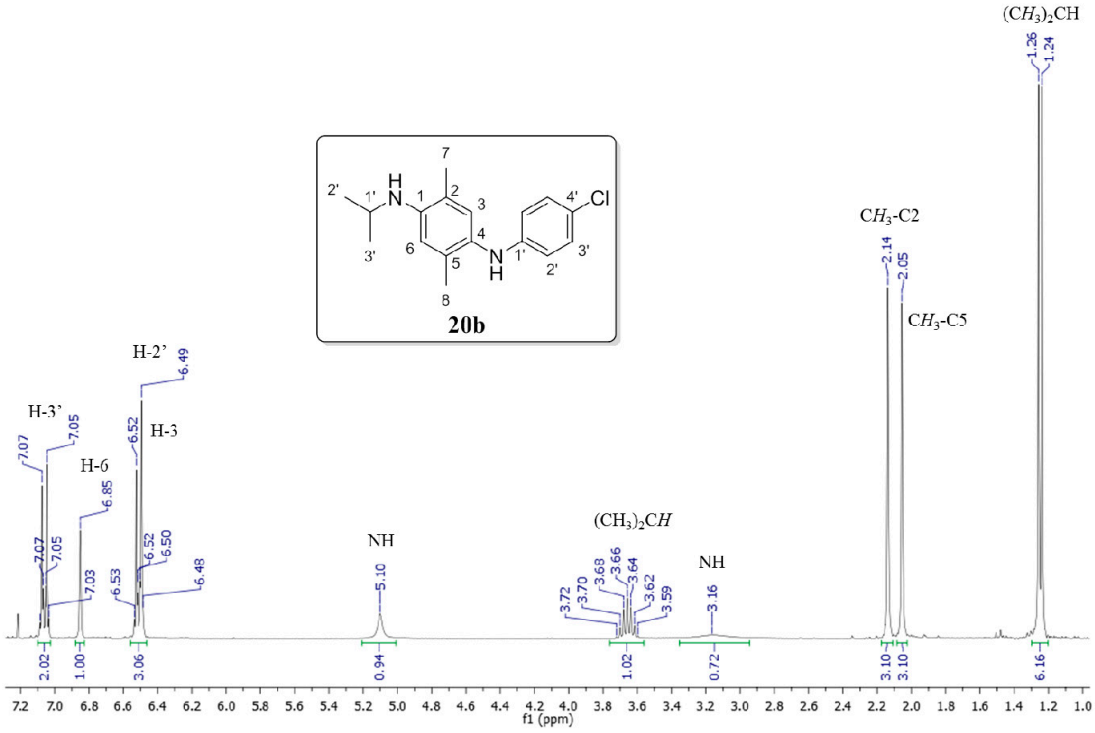
^{13}C-NMR ($CDCl_3$, 75 MHz) spectrum of **19b**.



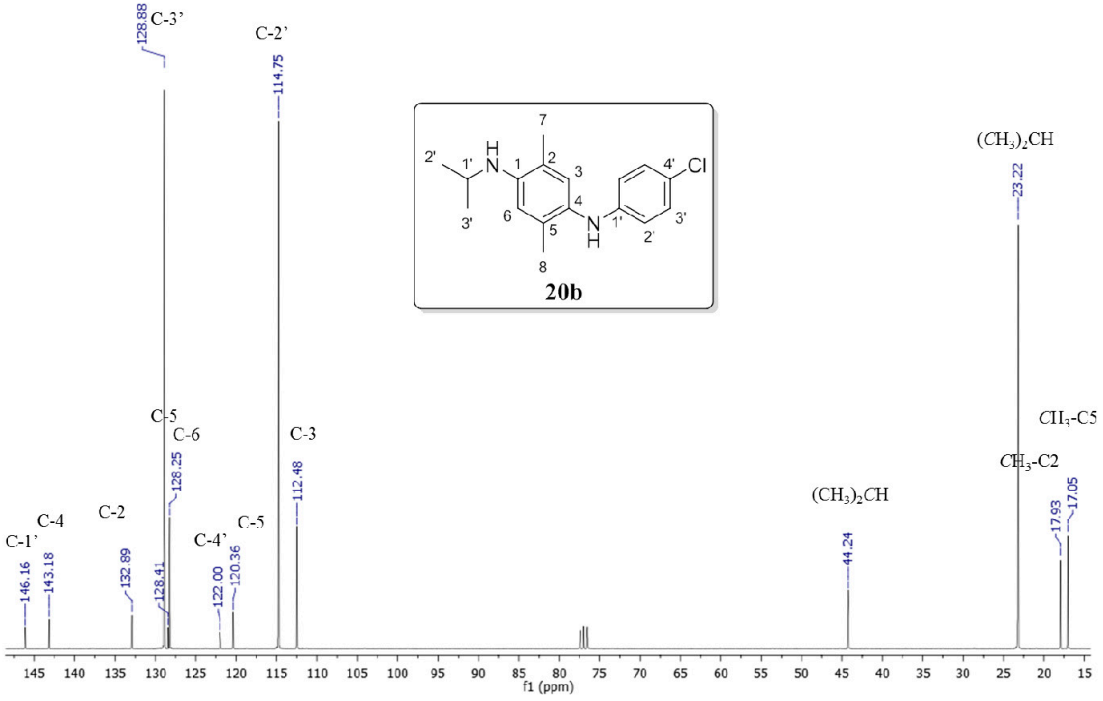
^{1}H-NMR ($CDCl_3$, 300 MHz) spectrum of **20a**



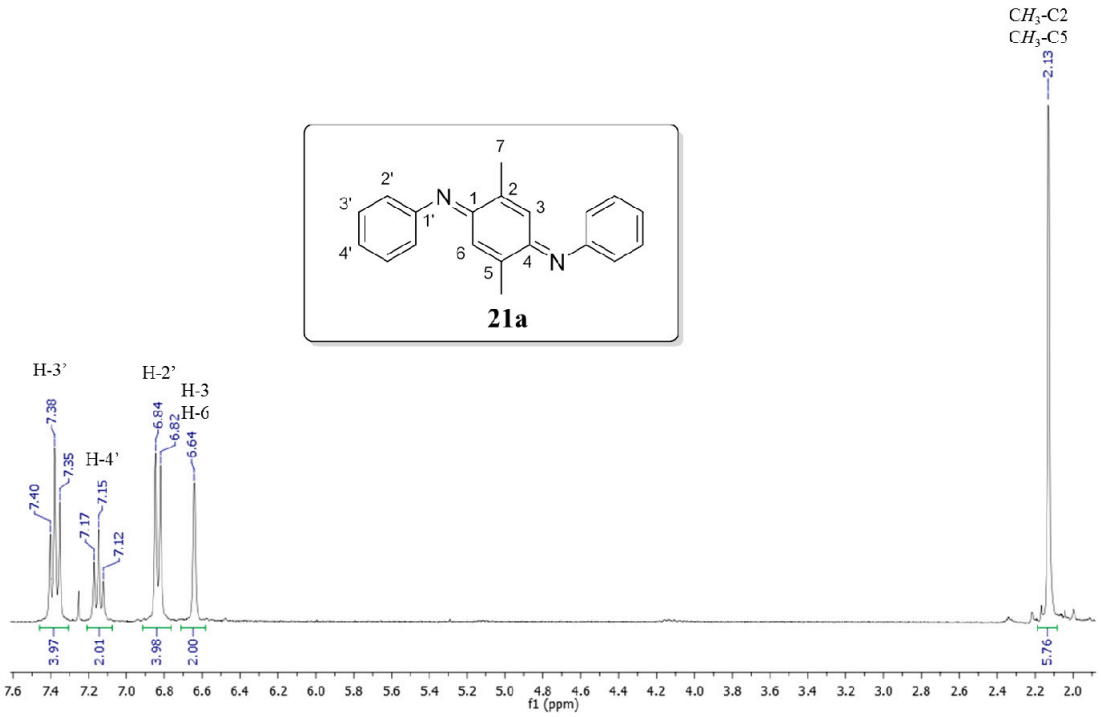
^{13}C-NMR ($CDCl_3$, 75 MHz) spectrum of **20a**



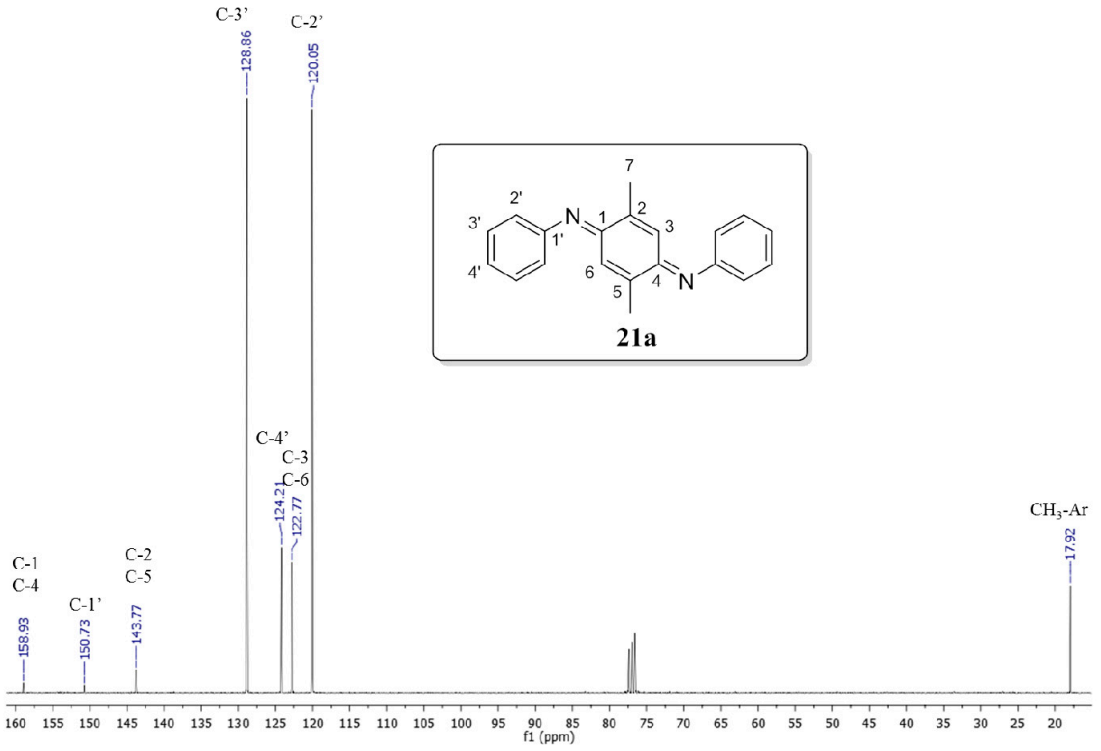
^{1}H-NMR ($CDCl_3$, 300 MHz) spectrum of **20b**



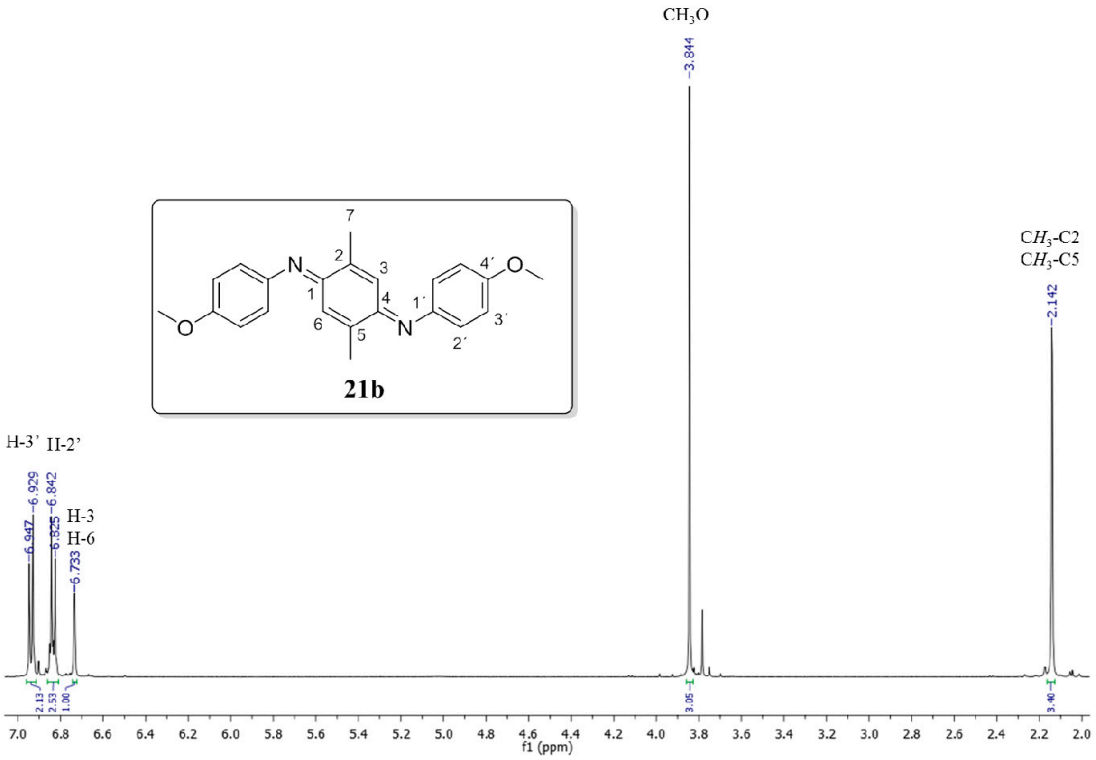
^{13}C-NMR ($CDCl_3$, 75 MHz) spectrum of **20b**



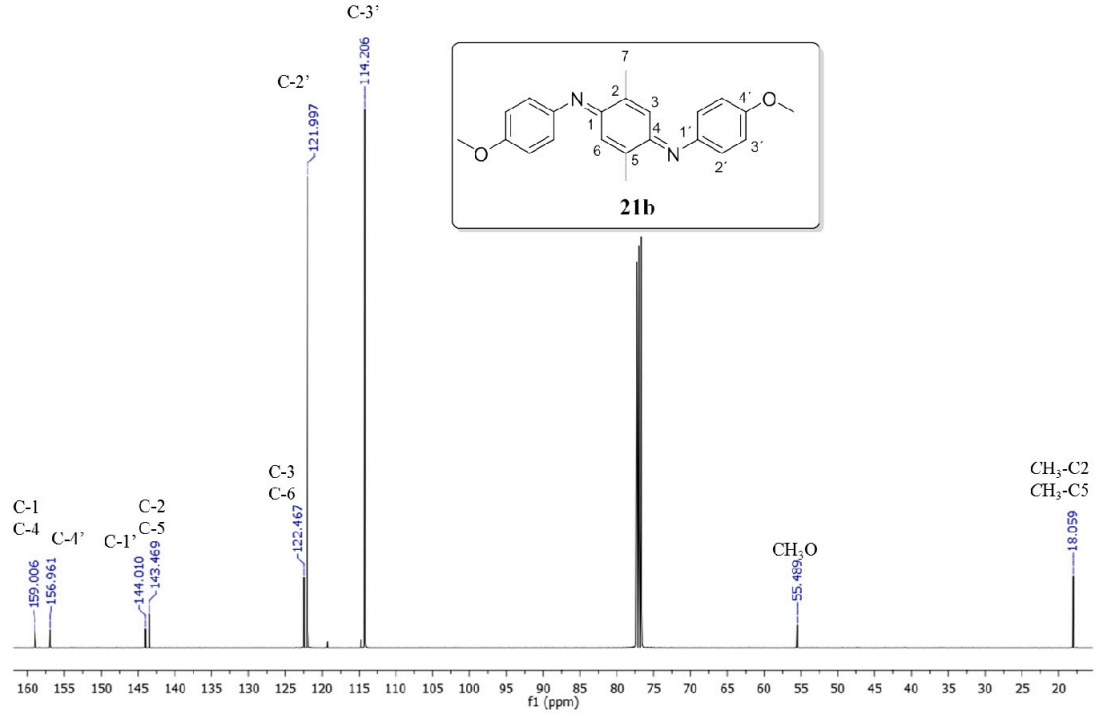
^{1}H-NMR ($CDCl_3$, 300 MHz) spectrum of **21a**



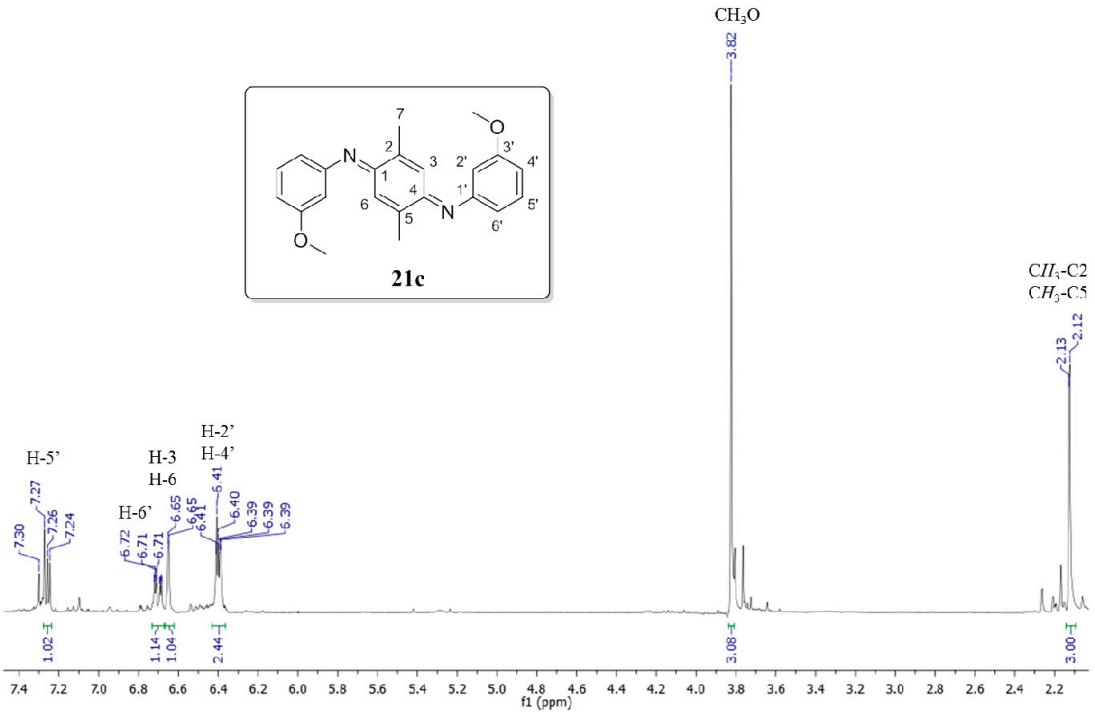
^{13}C-NMR ($CDCl_3$, 75 MHz) spectrum of **21a**



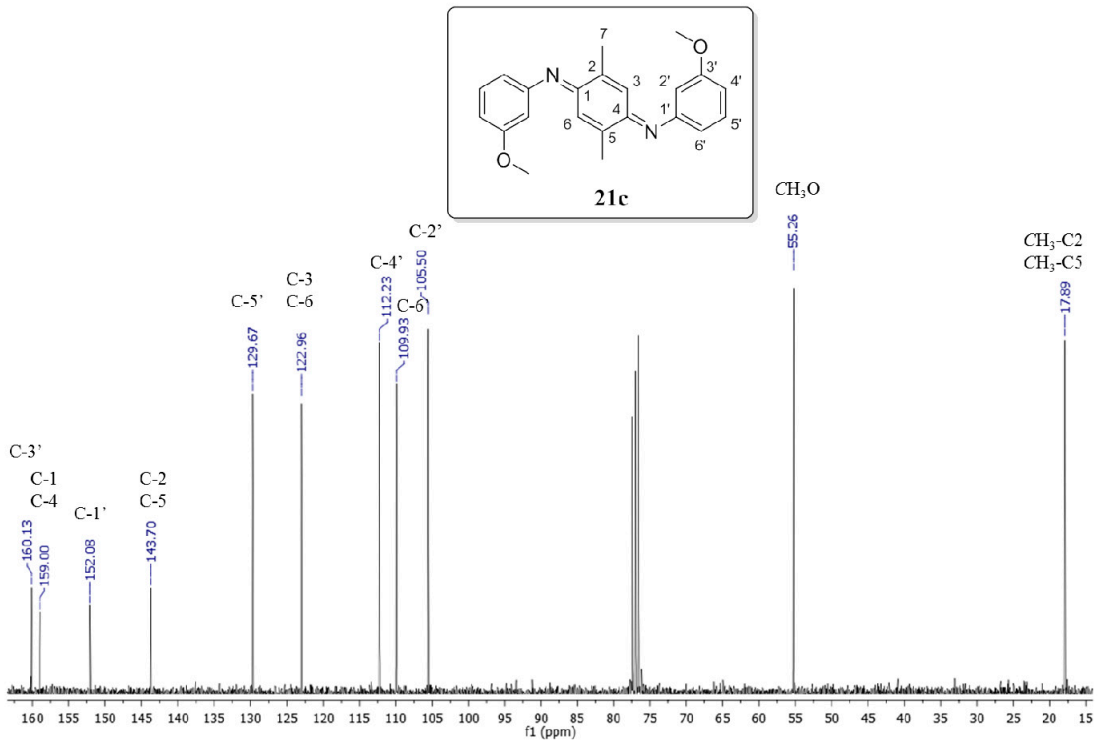
^{1}H-NMR ($CDCl_3$, 500 MHz) spectrum of **21b**



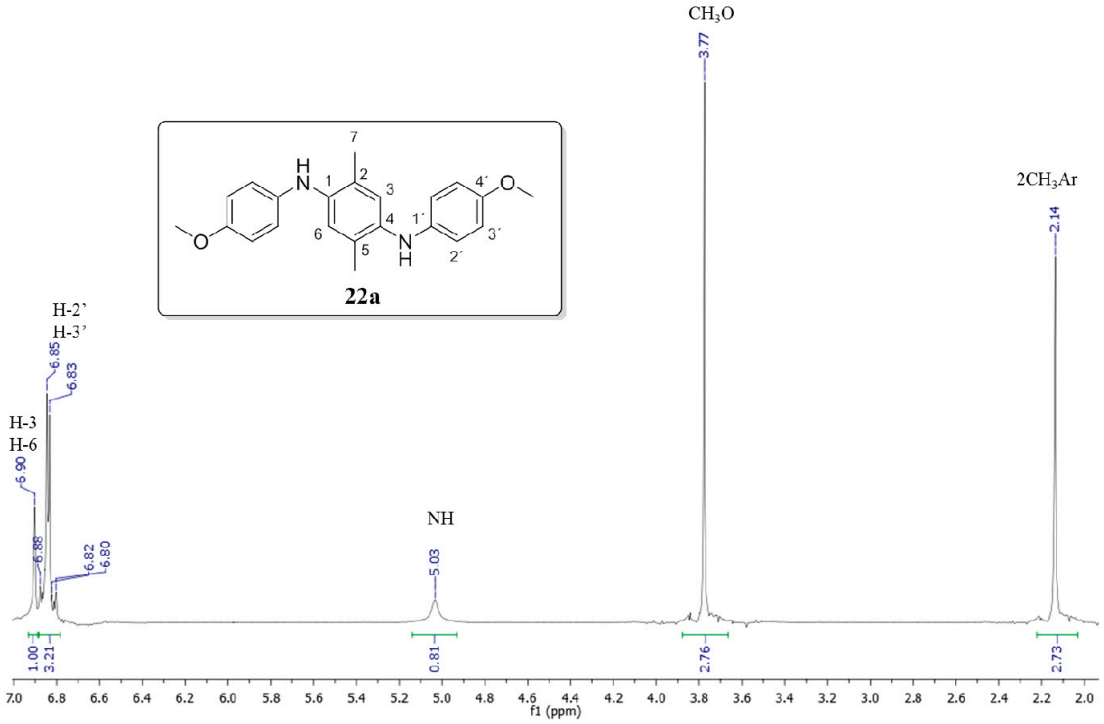
^{13}C-NMR ($CDCl_3$, 125 MHz) spectrum of **21b**



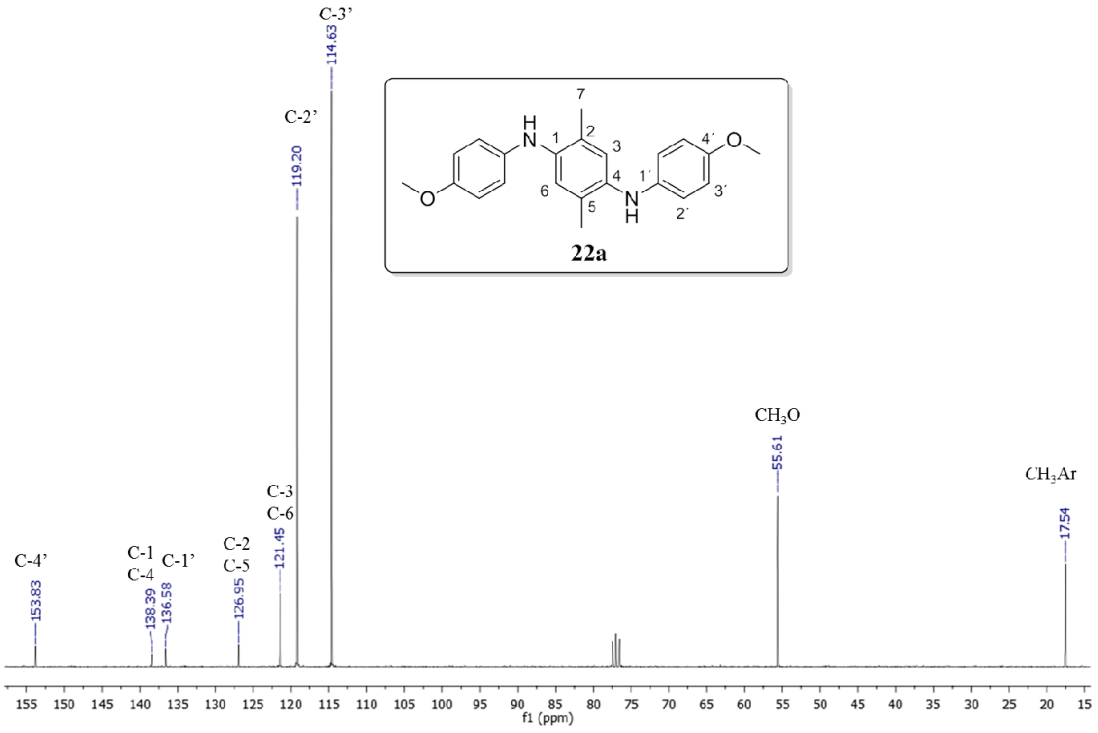
^{1}H-NMR ($CDCl_3$, 300 MHz) spectrum of **21c**



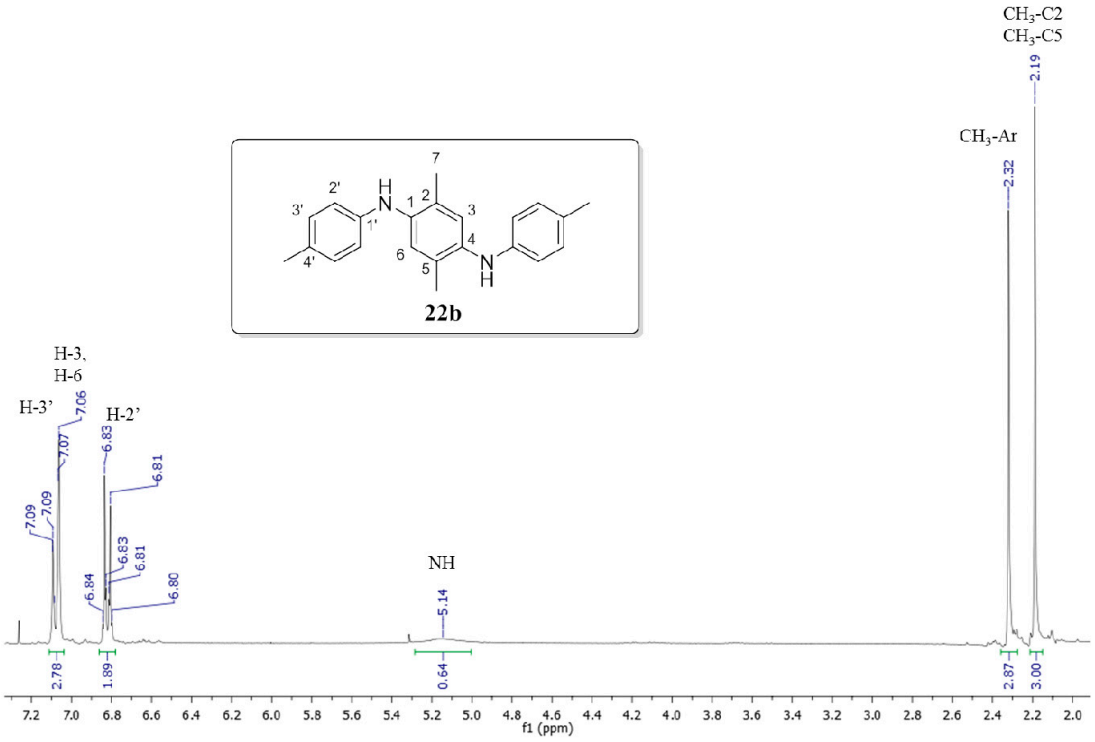
^{13}C-NMR ($CDCl_3$, 75 MHz) spectrum of **21c**



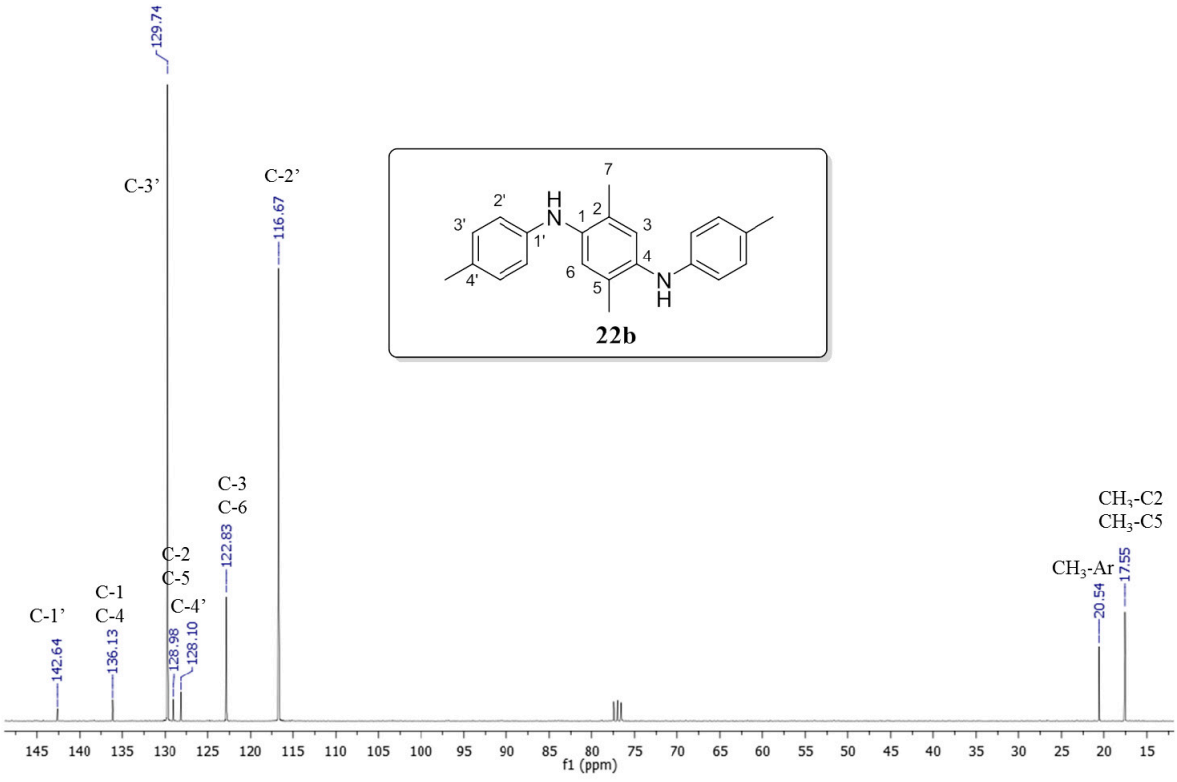
^{1}H-NMR ($CDCl_3$, 500 MHz) spectrum of **22a**



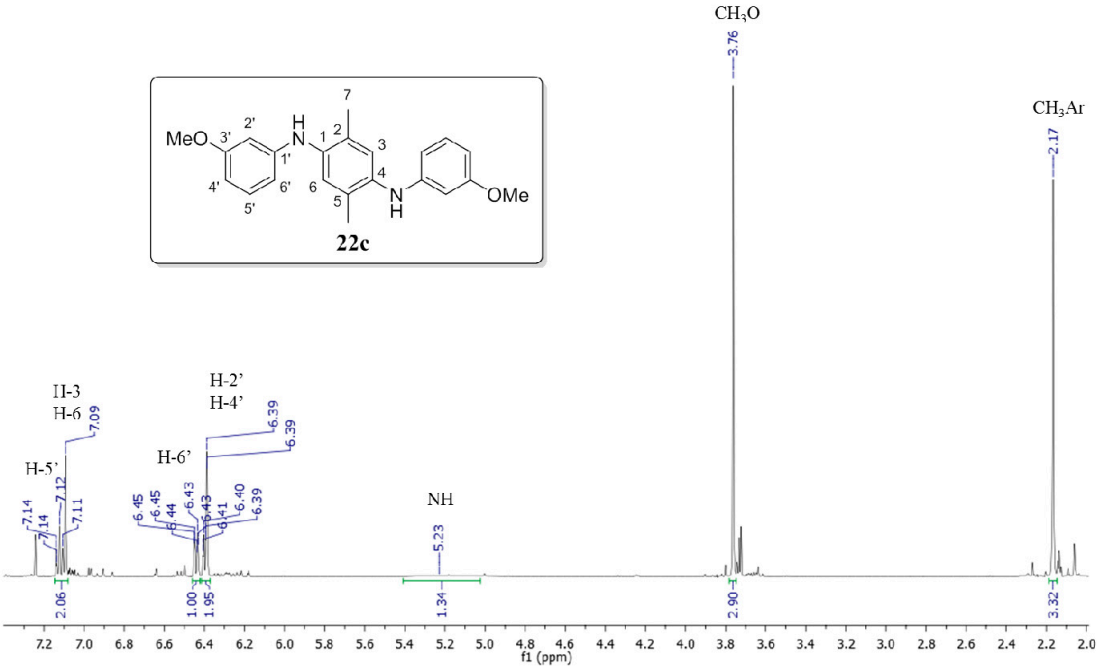
^{13}C-NMR ($CDCl_3$, 125 MHz) spectrum of **22a**



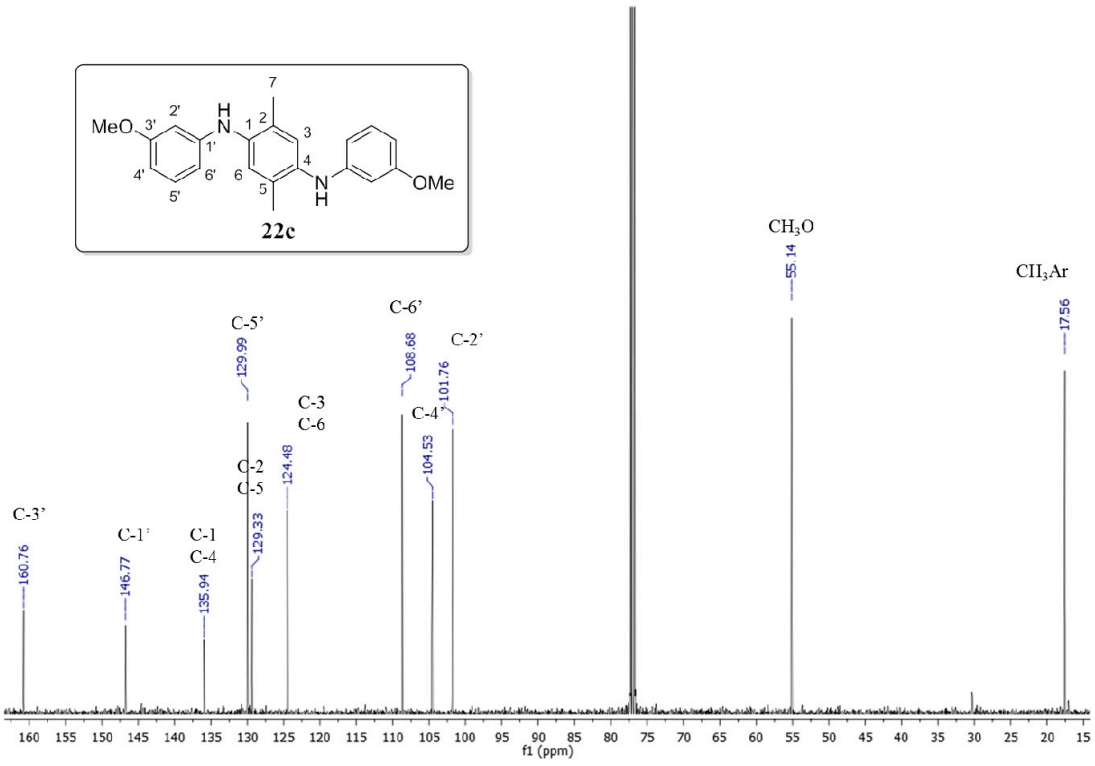
^{1}H-NMR ($CDCl_3$, 300 MHz) spectrum of **22b**



^{13}C-NMR ($CDCl_3$, 75 MHz) spectrum of **22b**



^{1}H-NMR ($CDCl_3$, 500 MHz) spectrum of **22c**



^{13}C-NMR ($CDCl_3$, 125 MHz) spectrum of **22c**

2. X-ray tables and crystallographic data of 8a

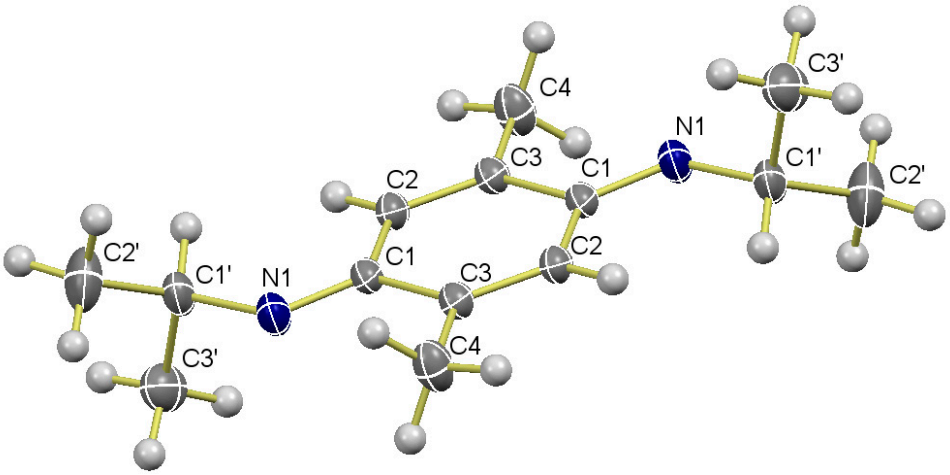


Table S1. Crystal data and structure refinement for **8a** (**CCDC 1429959**).

Identification code	0117-jt	
Empirical formula	C9.33 H14.67 N1.33	
Formula weight	24/May/1900	
Temperature	292(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	P 1 21/a 1	
Unit cell dimensions	a = 9.3369(19) Å	a = 90°
	b = 7.7080(4) Å	b = 142.07 (4)°
	c = 15.920(3) Å	g = 90°
Volume	704.3(2) Å3	
Z	3/Jan/1900	
Density (calculated)	1.030 Mg/m^3	
Absorption coefficient	0.061 mm^{-1}	
F(000)	27/Aug/1900	
Crystal size	0.57 × 0.55 × 0.51 mm^3	
Theta range for data collection	3.36 to 32.79°.	
Index ranges	−13 ≤ h ≤ 13, −11 ≤ k ≤ 11, −22 ≤ l ≤ 24	
Reflections collected	14/Jan/1921	
Independent reflections	2391 [R(int) = 0.0188]	
Completeness to theta = 27.50°	0/Jan/1900	
Max. and min. transmission	0.9697 and 0.9662	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	2391/0/117	
Goodness-of-fit on F^2	1/Jan/1900	
Final R indices [I > 2sigma(I)]	R^1 = 0.0590, wR^2 = 0.1484	
R indices (all data)	R^1 = 0.0817, wR^2 = 0.1652	
Largest diff. peak and hole	0.294 and −0.136 e·Å^{-3}	

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **8a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	1262(2)	9300(1)	1287(1)	37(1)
C(2)	1573(2)	8640(1)	579(1)	39(1)
C(3)	405(2)	9262(1)	-628(1)	39(1)
N(1)	2291(2)	8739(1)	2432(1)	48(1)
C(4)	759(3)	8542(2)	-1328(2)	59(1)
C(1′)	3999(2)	7330(2)	3183(1)	51(1)
C(3′)	2789(3)	5649(2)	2820(2)	68(1)
C(2′)	5890(4)	7746(3)	4697(2)	85(1)

Table S3. Bond lengths [Å] and angles [°] for **8a**.

C(1)-N(1)	1.2918(15)
C(1)-C(2)	1.4594(16)
C(1)-C(3)#1	1.4756(16)
C(2)-C(3)	1.3428(17)
C(2)-H(11)	0.945(15)
C(3)-C(1)#1	1.4756(16)
C(3)-C(4)	1.4969(18)
N(1)-C(1')	1.4644(17)
C(4)-H(10)	0.97(2)
C(4)-H(8)	0.99(2)
C(4)-H(9)	0.97(3)
C(1′)-C(3′)	1.504(2)
C(1′)-C(2')	1.522(3)
C(1′)-H(1′)	0.990(15)
C(3′)-H(4)	1.01(2)
C(3′)-H(2)	0.95(2)
C(3′)-H(3)	0.98(2)
C(2′)-H(5)	1.00(3)
C(2′)-H(6)	0.97(2)
C(2′)-H(7)	1.00(3)
N(1)-C(1)-C(2)	126.43(10)
N(1)-C(1)-C(3)#1	116.60(11)
C(2)-C(1)-C(3)#1	116.97(9)
C(3)-C(2)-C(1)	123.26(10)
C(3)-C(2)-H(11)	119.0(8)
C(1)-C(2)-H(11)	117.7(8)
C(2)-C(3)-C(1)#1	119.76(11)
C(2)-C(3)-C(4)	121.69(11)
C(1)#1-C(3)-C(4)	118.54(10)
C(1)-N(1)-C(1′)	121.24(11)
C(3)-C(4)-H(10)	111.9(11)
C(3)-C(4)-H(8)	109.9(12)
H(10)-C(4)-H(8)	108.1(17)
C(3)-C(4)-H(9)	111.0(15)
H(10)-C(4)-H(9)	109.5(18)
H(8)-C(4)-H(9)	106.3(19)
N(1)-C(1′)-C(3′)	108.72(12)

N(1)-C(1′)-C(2′)	107.00(14)
C(3')-C(1′)-C(2′)	111.80(15)
N(1)-C(1′)-H(1′)	112.8(9)
C(3′)-C(1′)-H(1′)	107.7(9)
C(2′)-C(1′)-H(1′)	108.9(9)
C(1′)-C(3′)-H(4)	108.1(11)
C(1′)-C(3′)-H(2)	110.4(11)
H(4)-C(3′)-H(2)	106.8(15)
C(1')-C(3′)-H(3)	112.8(12)
H(4)-C(3′)-H(3)	108.7(16)
H(2)-C(3′)-H(3)	109.8(16)
C(1′)-C(2′)-H(5)	110.5(16)
C(1′)-C(2′)-H(6)	110.3(14)
H(5)-C(2′)-H(6)	105.8(19)
C(1')-C(2′)-H(7)	111.0(17)
H(5)-C(2′)-H(7)	106(2)
H(6)-C(2′)-H(7)	113(2)

Symmetry transformations used to generate equivalent atoms: #1 − x, −y + 2, −z.

Table S4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **8a**. The anisotropic displacement factor exponent takes the form: $-2 \times \pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

	U11	**U22**	**U33**	**U23**	**U13**	**U12**
C(1)	35(1)	35(1)	36(1)	7(1)	27(1)	1(1)
C(2)	38(1)	34(1)	42(1)	9(1)	31(1)	6(1)
C(3)	41(1)	34(1)	41(1)	5(1)	32(1)	2(1)
N(1)	49(1)	49(1)	42(1)	14(1)	35(1)	10(1)
C(4)	75(1)	54(1)	60(1)	14(1)	57(1)	19(1)
C(1′)	48(1)	57(1)	44(1)	21(1)	35(1)	16(1)
C(3′)	70(1)	53(1)	85(1)	21(1)	62(1)	17(1)

Table S5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for**8a**.

	x	**y**	**z**	**U(eq)**
H(11)	2600(30)	7698(19)	978(14)	51(4)
H(1′)	4720(30)	7213(19)	2956(15)	54(4)
H(4)	2170(30)	5720(20)	3127(19)	89(6)
H(10)	1740(30)	7510(30)	-867(19)	87(6)

Table S6. Torsion angles [°] for **8a**.

N(1)-C(1)-C(2)-C(3)	178.54(11)
C(3)#1-C(1)-C(2)-C(3)	−0.88(18)
C(1)-C(2)-C(3)-C(1)#1	0.90(19)
C(1)-C(2)-C(3)-C(4)	−179.53(12)
C(2)-C(1)-N(1)-C(1′)	1.28(19)
C(3)#1-C(1)-N(1)-C(1′)	−179.29(10)
C(1)-N(1)-C(1')-C(3′)	−95.84(16)
C(1)-N(1)-C(1')-C(2′)	143.26(16)

Symmetry transformations used to generate equivalent atoms: #1 − x, −y + 2, −z.