Electronic Supplementary Information

Palladium(II) complexes containing ONO tridentate hydrazone for Suzuki-Miyaura coupling of aryl chlorides in aqueous-organic media

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Contents

Table 1. Selected bond lengths (Å) and angles (°) for the complexes **1, 2** and **3**

Complex	**1**	**2**	**3**
Pd(1) – N(1)	1.9674 (16)	1.9638 (12)	1.9720 (3)
Pd(1) – O(1)	1.9700 (14)	1.9724 (11)	1.9670 (2)
Pd(1) – O(2)	1.9922 (14)	1.9914 (11)	2.0000 (2)
Pd(1) – P(1)	2.2956 (5)	2.2743 (5)	2.2996 (9)
C (1) – N(1)	1.3010 (3)	1.2919 (19)	1.2940 (4)
C (1) – O(3)	1.3200 (2)	1.3179 (18)	1.3240 (4)
C(2) – O(12)	1.3140 (2)	1.3085 (17)	1.3110 (4)
N(1) – N(2)	1.4000 (2)	1.3980 (17)	1.3970 (4)
C(2) – N(12)	1.3070 (3)	1.3063 (19)	1.3040 (4)
C(1) – C(2)	1.4300 (3)	1.4310 (2)	1.4290 (5)
C(2) – C(3)	1.4120 (3)	1.4090 (2)	1.4060 (5)
N(1) – Pd(1)– O(1)	93.86 (6)	93.21 (5)	93.27 (10)
N(1) – Pd(1)– O(2)	80. 26 (6)	80.72 (5)	80.24 (10)
O(1) – Pd(1)– O(2)	173.64 (6)	173.89 (4)	173.50 (9)
N(1) – Pd(1)– P(1)	178.52 (5)	175.52 (4)	178.83 (8)
O(1) – Pd(1)– P(1)	88. 08 (4)	91.20 (4)	87.19 (7)
O(2) – Pd(1)– P(1)	98. 28 (4)	94.88 (4)	99.31 (7)
C(1) – N(1) – Pd(1)	126.31 (14)	126.72 (11)	126.10 (2)
N(2) – C(12)– O(2)	126.11 (19)	126.21 (14)	126.00 (3)
N(2) – N(1)– Pd(1)	115.37 (12)	114.66 (9)	114.90 (2)

Table 2. Crystal data and structure refinement for complexes **1, 2** and **3**

Complex	**1**	**2**	**3**
CCDC number	1005675	852732	1017037
Empirical formula	C_{34} H_{25} N_2 O_3 P Pd	C_{34} H_{25} N_2 O_2 P Pd S	C_{35} H_{26} N_3 O_2 P Pd
Formula weight	646.93	662.99	657.96
Temperature (K)	100(2)	110(2)	110(2)
Wavelength (Å)	0.71073	0.71073	1.54178
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	P 2_1/n	P 2_1/n	P 2_1/n
Unit cell dimensions			
a (Å)	15.5191(14)	15.531(5)	15.3735(13)
b (Å)	9.0388 (8)	10.833(3)	8.9176(8)
c (Å)	19.9113(17)	17.549(5)	20.6686(15)
α (°)	90	90	90
β (°)	97.858(3)	101.774(3)	97.251(5)
γ (°)	90	90	90
Volume ($Å^3$)	2766.8(4)	2890.5(14)	2810.9(4)
Z	4	4	4

Density (calculated) (Mg m^{-3})	1.553	1.523	1.555
Absorption coefficient (mm^{-1})	0.768	0.804	6.172
F(000)	1312	1344	1336
Crystal size (mm^3)	0.17 x 0.09 x 0.07	0.50 x 0.50 x 0.40	0.15 x 0.12 x 0.03
Reflections collected	88216	31660	21167
Independent reflections	6860 [R(int) = 0.0469]	6583 [R(int) = 0.0236]	3994 [R(int) = 0.0710]
Max. and min. transmission	0.9482 and 0.8805	0.7391 and 0.6892	0.8365 and 0.4579
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	6860 / 0 / 370	6583 / 0 / 370	3994 / 0 / 380
Goodness-of-fit on F^2	1.069	1.030	1.019
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0281, wR2 = 0.0705	R1 = 0.0205, wR2 = 0.0518	R1 = 0.0306, wR2 = 0.0730
R indices (all data)	R1 = 0.0375, wR2 = 0.0774	R1 = 0.0226, wR2 = 0.0531	R1 = 0.0368, wR2 = 0.0744
Largest diff. peak and hole ($e.Å^{-3}$)	1.182 and -0.895	0.352 and -0.316	0.489 and -0.749

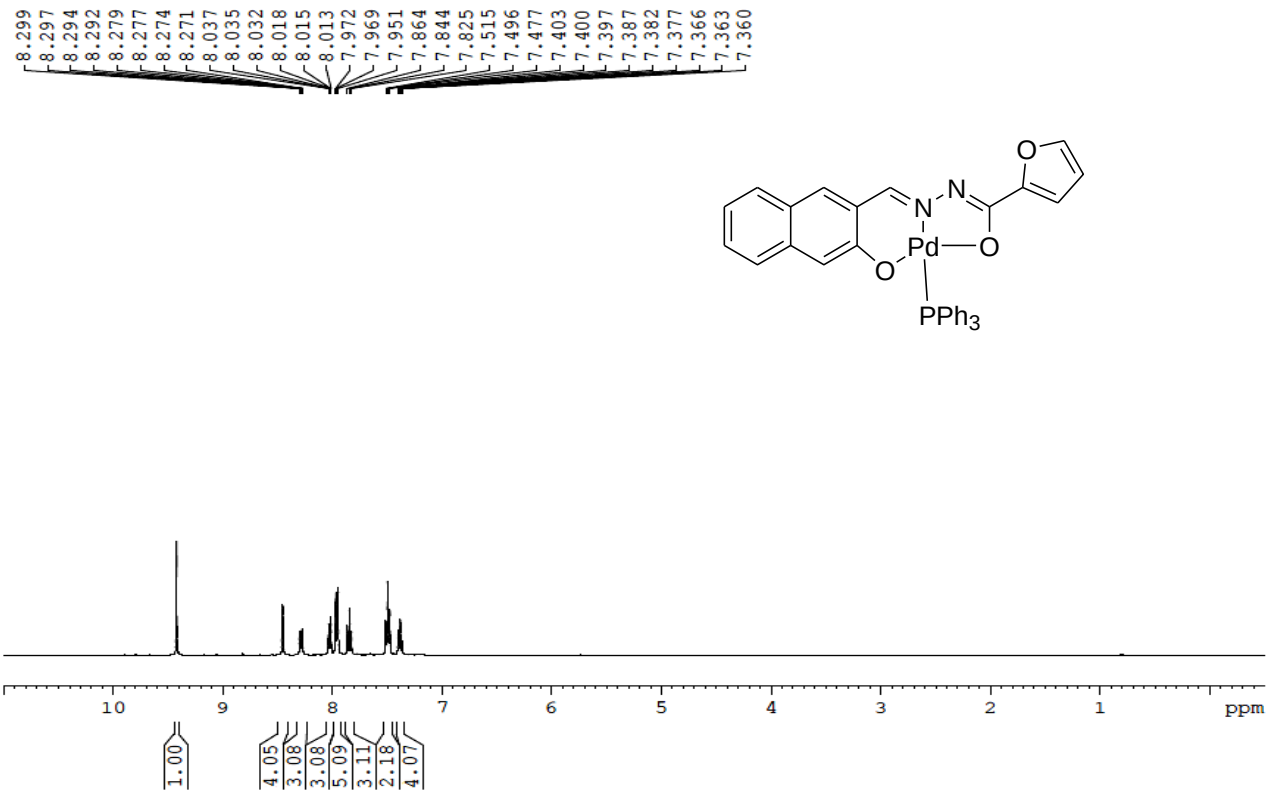

Fig. S1: ^{1}H NMR spectrum of complex 1

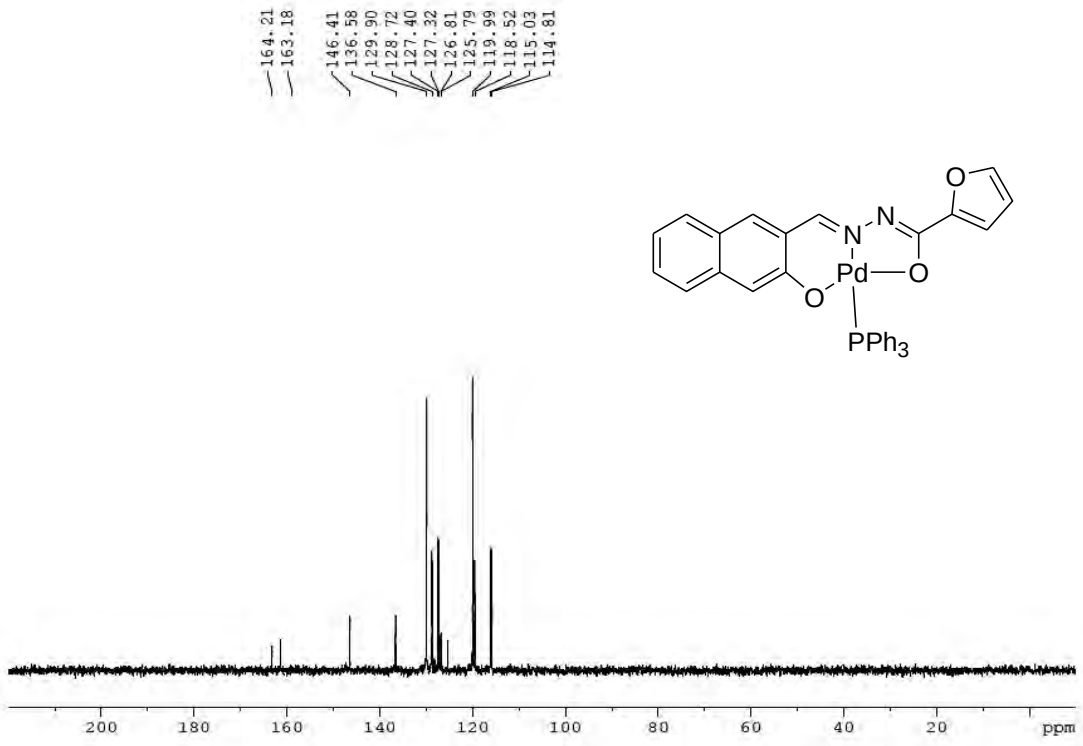

Fig. S2: ^{13}C NMR spectrum of complex 1

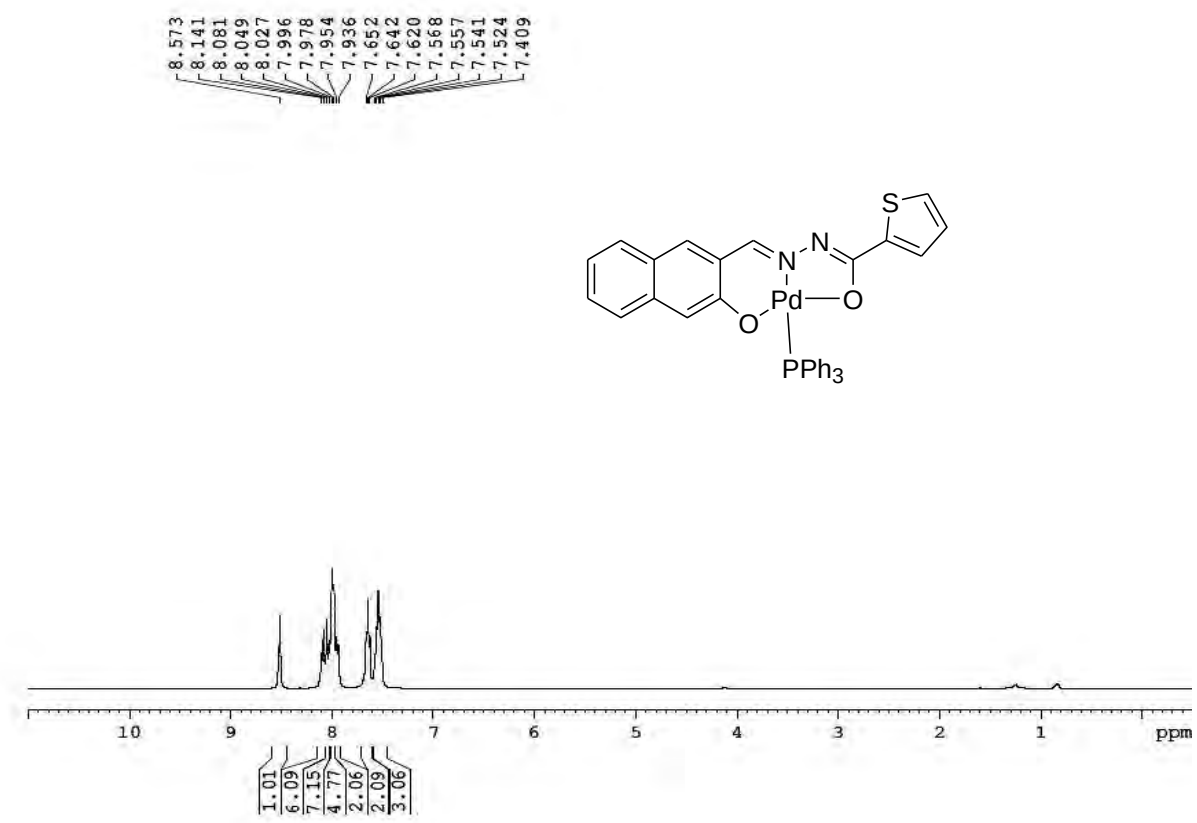

Fig. S3: ^{1}H NMR spectrum of complex 2

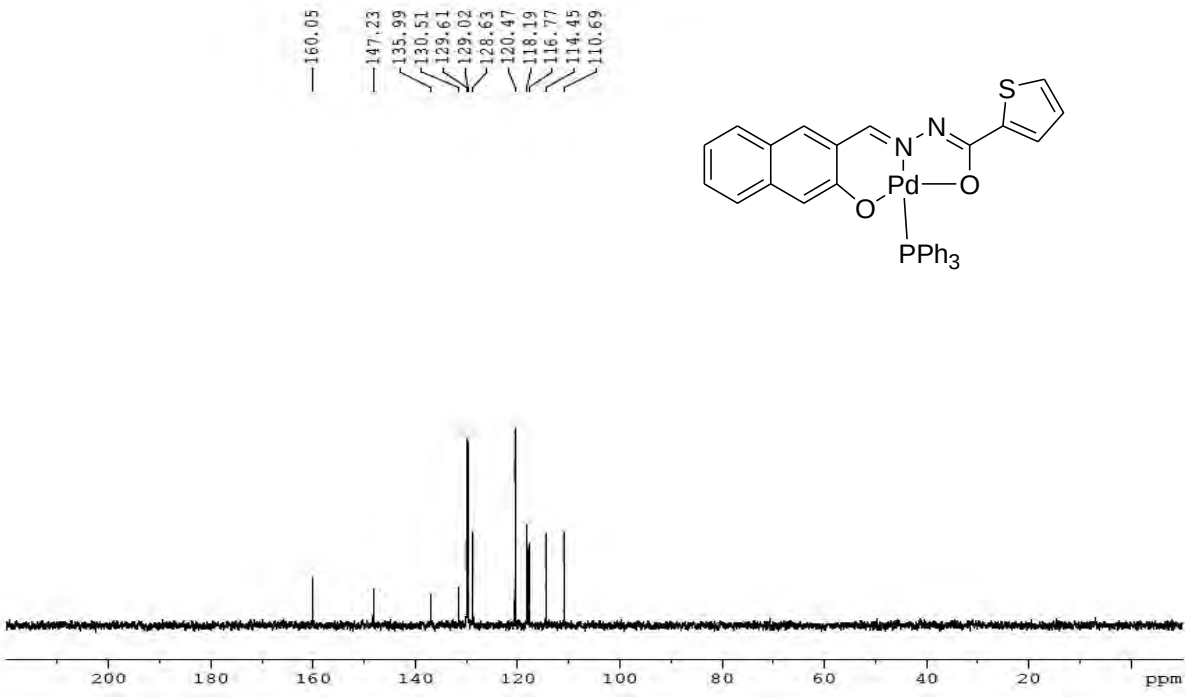

Fig. S4: ^{13}C NMR spectrum of complex 2

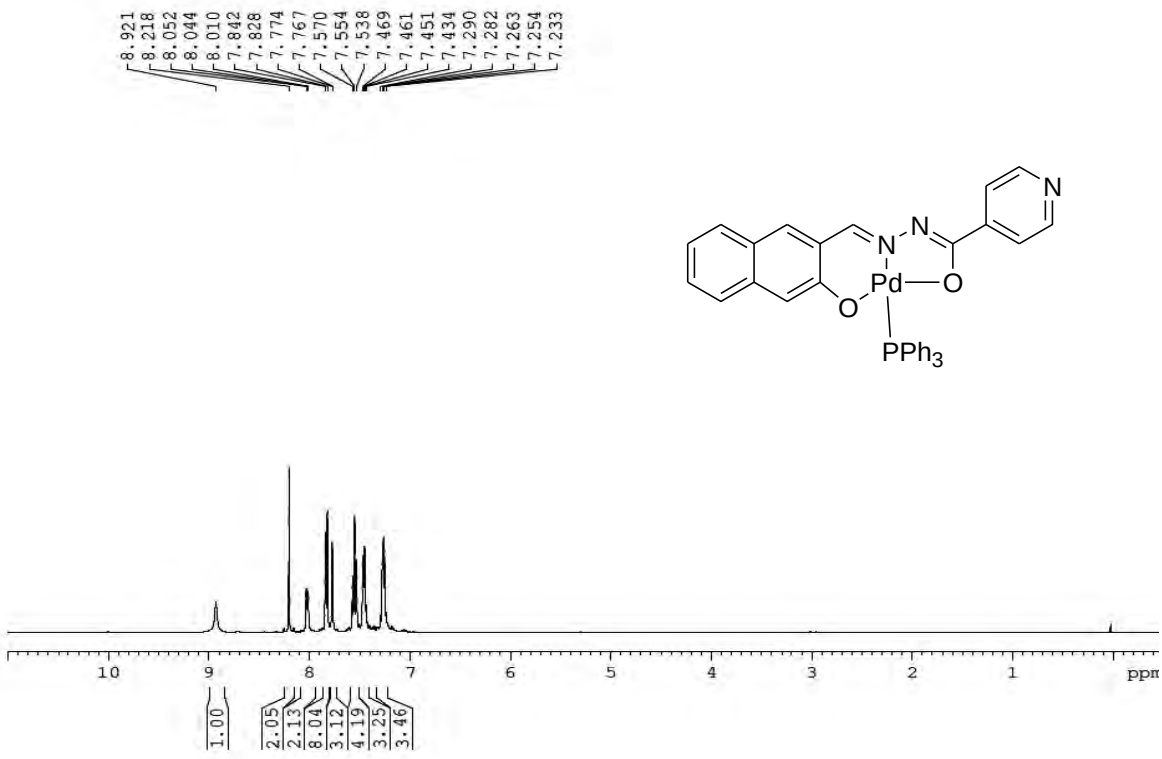

Fig. S5: ^{1}H NMR spectrum of complex 3

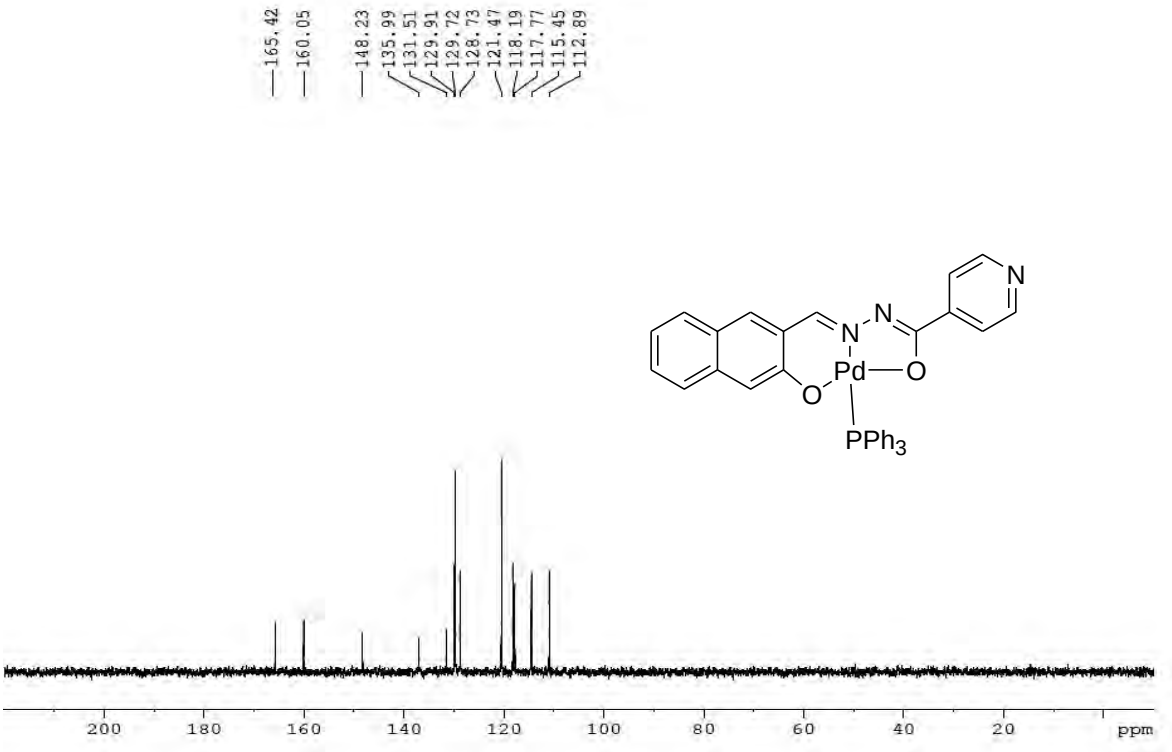

Fig. S6: ^{13}C NMR spectrum of complex 3

NMR spectral data of the coupled products listed in Table 3 and 4 .

^{1}H and ^{13}C NMR spectra were recorded in deuterated $CHCl_3$ as solvent on BRUKER 400 and 100 MHZ instruments respectively.

1) Entry 1a: biphenyl-4-carbonitrile ^{1}H NMR δ (ppm): 7.72 (d, *J* = 7.2 Hz, 2H), 7.62 (t, *J* =3.6 Hz,1H), 7.50 – 7.58 (m, 3H), 7.46 (d, *J* = 7.6 Hz,1H), 7.30 – 7. 38 (m, 2H).
   ^{13}C NMR: 147.2, 146.3, 141.4, 135.7, 135.2, 130.2, 129.7, 127.0, 125.6, 122.3.

2) Entry 1b: 2'-methyl-biphenyl-4-carbonitrile ^{1}H NMR δ (ppm): 8.19 (d, *J* = 2.8 Hz, 1H), 8.18 (d, *J* = 3.6 Hz, 1H), 7.50 – 7.93 (m, 4H), 7.51(d, *J* = 3.6 Hz,1H), 7.12(s, 1H), 2.39 (s, 3H).
   ^{13}C NMR: 158.7, 148.9, 147.1, 138.3, 133.6, 130.9, 128.4, 127.0, 126.0, 125.5, 124.9, 122.7, 20.7.

3) Entry 1c: 4'-methyl-biphenyl-4-carbonitrile ^{1}H NMR δ (ppm): 7.70 (d, *J* = 6.4 Hz, 2H), 7.55 – 7.68 (m, 4H), 7.46 (t, *J* = 6.6 Hz, 1H,), 7.30 (d, *J* = 7.2 Hz, 1H), 2.56 (s, 3H) .
   ^{13}C NMR: 149.8, 140.8, 138.2, 137.9, 128.3, 127.6, 126.5, 125.3, 123.9, 21.3.

4) Entry 1d: 2,3-dimethyl-biphenyl-4-carbonitrile ^{1}H NMR δ (ppm): 7.55 – 7.49 (2H, m), 7.39(2H, s), 7.16-7.25(m, 3H), 3.99 (s, 3H), 2.60 (3H, s).
   ^{13}C NMR: 156.4, 138.4, 137.21, 130.9, 130.7, 128.5, 128.29, 120.60, 111.0, 55.3, 21.2.

5) Entry 1e: 4'-methoxy-biphenyl-4-carbonitrile ^{1}H NMR δ (ppm): 8.35 (1H, s), 8.20 (d, *J* = 8.4 Hz, 3H), 8.09 (d, *J* = 8.4 Hz, 1H,), 7.77 – 7.79 (m, 1H,), 7. 41 – 7. 67 (m, 1H), 7.39 (d, *J* = 7.2 Hz, 1H), 7.27 (d, *J* = 8.4 Hz, 1H), 4.03 (s, 3H).
   ^{13}C NMR : 156.5, 136.1, 133.3, 132.3, 130.9, 130.5, 128.6, 127.9, 127.4, 127.0, 125.7, 125,6, 120.8, 111.1, 55.2.

6) Entry 1f: 4'-*t*-butyl-biphenyl-4-carbonitrile ^{1}H NMR δ (ppm): 7.38 – 7.40 (4H, m), 7.0 (t, *J* = 2.4 Hz, 1H), 6.94 – 6.99 (m, 1H,), 6.09(s, 2H), 2.45(s, 9H).
   ^{13}C NMR: 149.8, 140.8, 138.2, 137.9, 128.3, 127.6, 127.5, 126.5, 125.3, 123.9, 34.2, 31.5.

7) Entry 1g: 3'-hydroxy-biphenyl-4-carbonitrile ^{1}H NMR δ (ppm): 7.82 (d, *J* = 1.2 Hz, 1H, s), 7.55 – 7.60 (m, 3H), 7.48 (t, *J* = 3.6 Hz, 2H,), 7. 37 (t, *J* =4.0 Hz, 1H), 6.79(s, 1H).
   ^{13}C NMR: 143.5, 138.4, 132.3, 128.7, 126.9, 126.4, 125.8, 108.7.

8) Entry 1h: 4'-naphthalen-2-yl-benzonitrile ^{1}H NMR δ (ppm): 8.04 (1H, s), 7.95 (4H, t, *J* = 6.4), 7.73 (1H, d, *J* = 8.4 Hz), 7.57 – 7.64 (3H, m), 6.94 (2H, s).
   ^{13}C NMR: 143.7, 138.8, 133.6, 132.4, 129.7, 128.3, 127.7, 127.6, 126.4, 126.2, 125.5, 124.3, 123.9, 108.8.

9) Entry 1i: [1,1';4',1"]terphenyl-4-carbonitrile ^{1}H NMR δ (ppm): 8.84(d, *J* = 4 Hz, 1H), 8.19 (d, *J* = 6.8 Hz, 2H), 7.96 (d, *J* = 8 Hz, 2H), 7.75 – 7.79 (m, 1H), 7.57 – 7. 66 (m, 1H), 7.52 – 7.54 (4H, m), 7.31 (dd, *J* = 0.8, 4 Hz, 2H).
^{13}C NMR: 158.9, 149.2, 138.2, 136.1, 133.7, 130.9, 128.1, 127.2, 126.2, 125.3, 125.0, 124.7, 121.7.

10) Entry 1j: 4'-bromo-biphenyl-4-carbonitrile ^{1}H NMR δ (ppm): 8.70 (1H, s), 8.18 (t, *J* = 2.8 Hz, 1H), 7.93 (d, *J* = 6.8 Hz, 2H), 7.64 (t, *J* = 3.6 Hz, 2H), 7.54 – 7.58 (m, 1H m), 7.12(s,1H).
^{13}C NMR: 158.9, 149.2, 138.2, 136.1, 133.7, 130.9, 128.6, 127.2, 126.2, 125.3, 125.0, 124.7, 121.7.

11) Entry 1k: 4'-dimethylamino-biphenyl-4-carbonitrile ^{1}H NMR δ (ppm): 8.24 (s, 1H), 7.84 (d, *J* = 8 Hz, 1H), 7.56 – 7.59 (m, 1H), 7.43 (t, *J* = 3.6 Hz, 1H), 7.36 (t, *J* = 7.8 Hz, 1H), 7.0 – 7. 11 (2H, m), 2. 84 (6H, s).
^{13}C NMR: 156.4, 138.4, 137.2, 130.9, 128.5, 128.2, 127.3, 120.6, 111.6, 55.5.

12) Entry 1l: 4'-acetyl-biphenyl-4-carbonitrile ^{1}H NMR δ (ppm): 7. 59 – 7.65 (4H, m), 7.40 – 7.41 (4H, m), 2.65 (s, 3H).
^{13}C NMR: 197.2, 156.4, 137.1, 135.3, 130.5, 129.2, 127.8, 127.4, 121.4, 109.7, 26.3.

13) Entry 2a: 4-nitrobiphenyl ^{1}H NMR δ (ppm): 8.15 (t, *J* = 8.2 Hz, 1H), 7.85 (t, *J* = 10.2 Hz, 1H), 7.59 – 7.76 (m, 2H), 7.52 – 7.57 (m, 2H), 7.44 – 7.48 (m, 2H).
^{13}C NMR: 146.9, 137.6, 132.6, 132.5, 131.5, 130.3, 129.4, 128.6, 128.1.

14) Entry 2b: 2-methyl-4'-nitro-biphenyl ^{1}H NMR δ (ppm): 7.78 (d, *J* = 8.4 Hz, 2H), 7.62 (d, *J* = 7.2 Hz, 2H), 7.44 – 7.47 (m,1H) 7.36 – 7.40 (m,1H) 7.36 – 7.40 (m, 1H), 7.17 (s, 1H), 7.00 (s, 1H) 2.37 (s, 3H).
^{13}C NMR: 140.5, 140.2, 138.2, 133.1, 131.7, 130.4, 129.6, 128.8, 128.3, 122.9, 121.5, 21.3.

15) Entry 2c: 4'-methyl-4-nitro-biphenyl ^{1}H NMR δ (ppm): 7.49 – 7.51 (m, 2H), 7.33 – 7.37 (m, 2H), 7.27 (s, 2H), 7.00 (s, 2H), 2.50 (s, 3H).
^{13}C NMR: 148.6, 136.4, 131.8, 128.6, 128.4, 122.4, 116.8, 112.6, 108.9, 107.6, 22.9.

16) Entry 2d: 2,3-dimethyl-4'-nitro-biphenyl ^{1}H NMR δ (ppm): 7.78 (d, *J* = 8 Hz, 2H), 7.57 (d, *J* = 8 Hz, 2H), 7.48 – 7.53 (m, 1H) 7.25 (d, *J* = 8 Hz, 1H), 6.77 (d, *J* = 8 Hz, 1H), 2.76 (s, 3H), 2.45 (s, 3H).
^{13}C NMR: 143.9, 136.1, 132.7, 130.4, 130.1, 129.8, 128.7, 128.1, 127.1, 125.5, 21.6, 18.9.

17) Entry 2e : 2'-methoxy-4-nitro-biphenyl ^{1}H NMR δ (ppm): 8.37 (d, *J* = 7.6 Hz, 2H), 7.56 (t, *J* = 6.6 Hz, 2H), 7.53 (d, *J* = 8 Hz, 2H), 7.47 (s, 2H), 4.05 (s, 3H).
^{13}C NMR: 158.7, 139.1, 137.2, 134.9, 132.1, 131.2, 128.7, 128.4, 127.1, 55.0,

18) Entry 2f : 4'-*tert*-butyl-4-nitro-biphenyl ^{1}H NMR δ (ppm): 7.89 (d, *J* = 9.2 Hz, 2H), 7.64 (d, *J* = 7.6 Hz, 2H), 7.46 (t, *J* = 5.8 Hz, 2H), 7.38 – 7.42 (m, 2H), 2.73 (s, 9H).
^{13}C NMR: 140.2, 139.5, 133.2, 131.8, 128.5, 128.1, 121.9, 117.1, 29.5, 20.1.

19) Entry 2g: 4'-nitro-biphenyl-3-ol ^{1}H NMR δ (ppm): 8.37 (d, *J* = 7.6 Hz, 1H), 8.30 (d, *J* = 4.4 Hz, 2H), 7.68 (d, *J* = 8 Hz, 1H), 7.53 – 7.59 (m, 2H), 7.11 (s, 1H), 6.82 (d, *J* = 8 Hz, 1H), 5.80 (s, 1H).
^{13}C NMR: 152.2, 142.9, 134.5, 132.1, 130.5, 128.7, 127.2, 125.7, 125.5, 122.8.

20) Entry 2h: 2-(4-nitro-phenyl)-naphthalene ^{1}H NMR δ (ppm): 7.75 (d, *J* = 8 Hz, 2H), 7.60 (d, *J* = 7.6 Hz, 2H), 7.45 (t, *J* = 7.6 Hz, 2H), 7.39 (s, 1H), 7.37 (d, *J* = 7.2 Hz, 1H), 7.08 (t, *J* = 4 Hz, 2H), 6.98 (s, 1H) 6.81 (d, *J* = 8 Hz, 1H).
^{13}C NMR: 147.2, 140.4, 133.8, 131.4, 128.3, 127.0, 126.5, 121.3, 116.9, 111.6, 108.2, 101.8.

21) Entry 2i: 4-nitro-[1,1';4',1"]terphenyl ^{1}H NMR δ (ppm): 8.33 – 8.38 (m, 2H), 7.62 (d, *J* = 8 Hz, 2H), 7.50 – 7.58 (m, 2H), 7.49 (d, *J* = 20.8 Hz, 2H), 7.31 – 7.34 (m, 2H), 7.10 – 7.16 (m, 2H), 6.80 (d, *J* = 8 Hz, 2H).
^{13}C NMR: 140.1, 132.7, 131.3, 129.5, 128.5, 125.4, 125.1, 123.6, 122.9, 119.2, 114.3, 101.5.

22) Entry 2j: 4'-bromo-4-nitro-biphenyl ^{1}H NMR δ (ppm): 7.51 (d, *J* = 7.2 Hz, 2H), 7.46 – 7.49 (m, 2H), 7.31 – 7.37 (m, 2H), 7.02 (s, 2H), 6.97 (s, 2H).
^{13}C NMR: 142.4, 131.5, 128.2, 128.2, 123.9, 113.7, 111.0, 106.4, 101.4, 87.5.

23) Entry 2k: dimethyl-(4'-nitro-biphenyl-4-yl)-amine ^{1}H NMR δ (ppm): 7.52 (dd, *J* = 8 Hz, 2H), 7.32 – 7.39 (m, 2H), 7.09 (s, 2H), 6.99 (s, 2H), 3.44 (s, 6H).
^{13}C NMR: 147.2, 140.8, 131.4, 128.7, 128.5, 123.5, 114.4, 112.9, 108.8, 38.9.

24) Entry 2l: 1-(4'-nitro-biphenyl-4-yl)-ethanone ^{1}H NMR δ (ppm): 7.43 – 7.56 (m, 2H), 7.33 – 7.35 (m, 2H), 7.17 (d, *J* = 2.4Hz, 2H), 6.99 (dd, *J* = 2.8, 2.8 Hz, 2H), 2.71 (s, 3H).
^{13}C NMR: 197.3, 142.4, 135.5, 131.7, 128.5, 123.4, 117.7, 113.5, 112.3, 26.3.

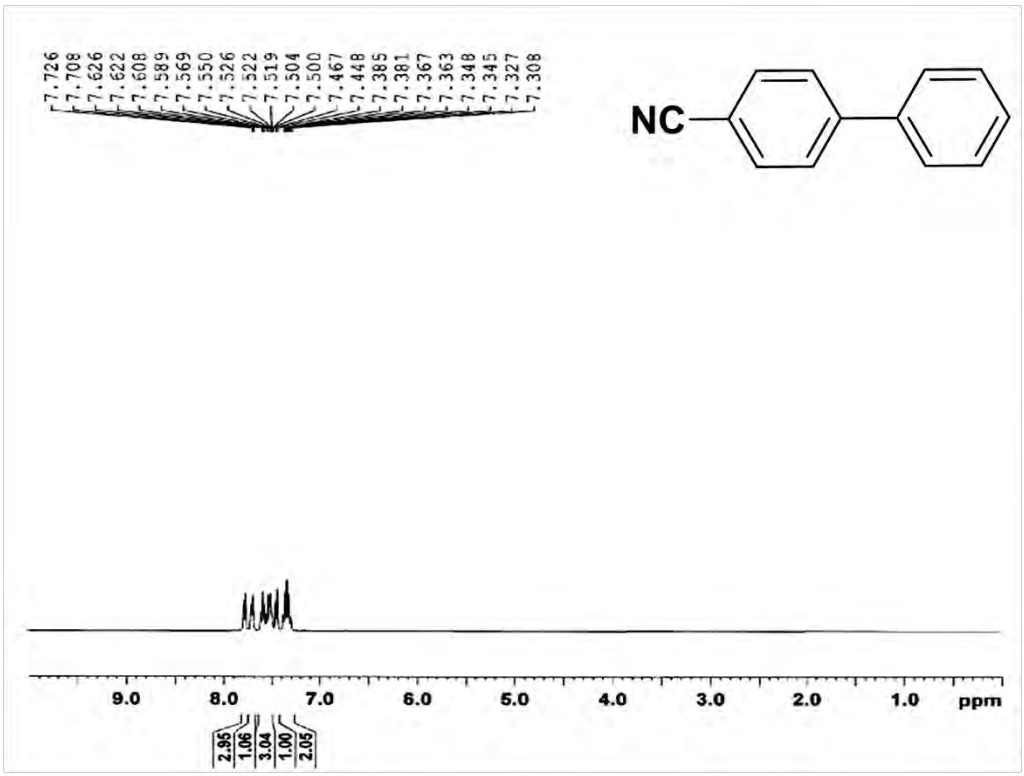

Fig. S7: ^{1}H NMR spectrum of biphenyl-4-carbonitrile

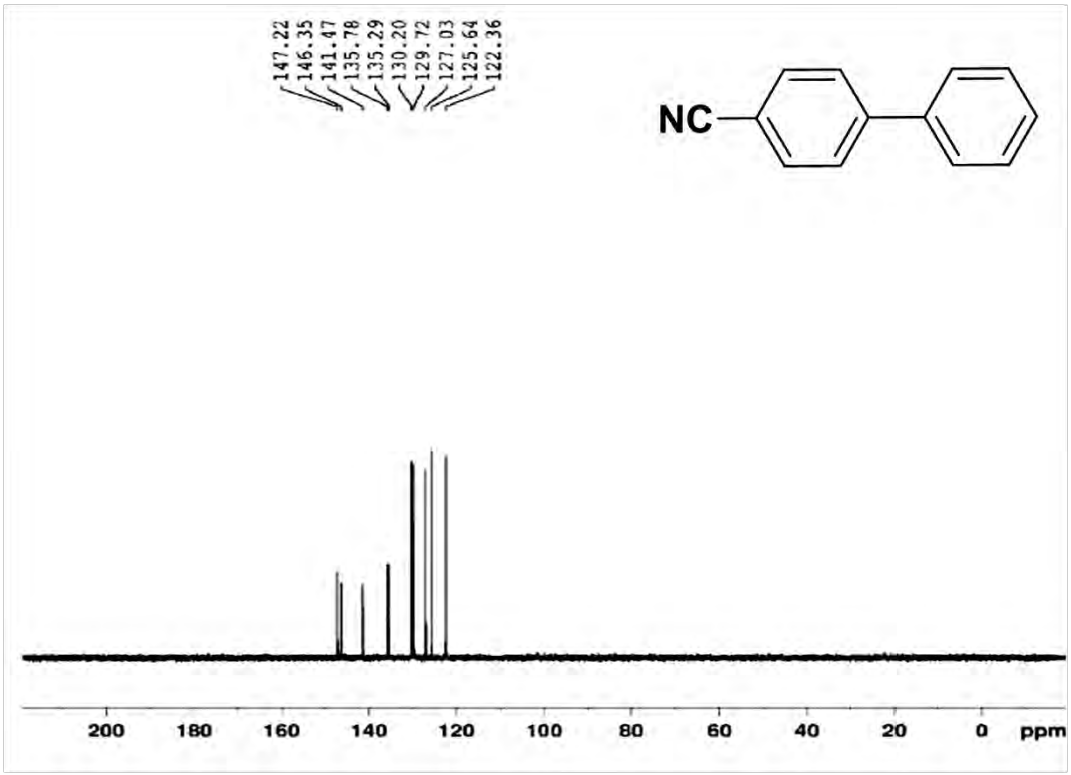

Fig. S8: ^{13}C NMR spectrum of biphenyl-4-carbonitrile

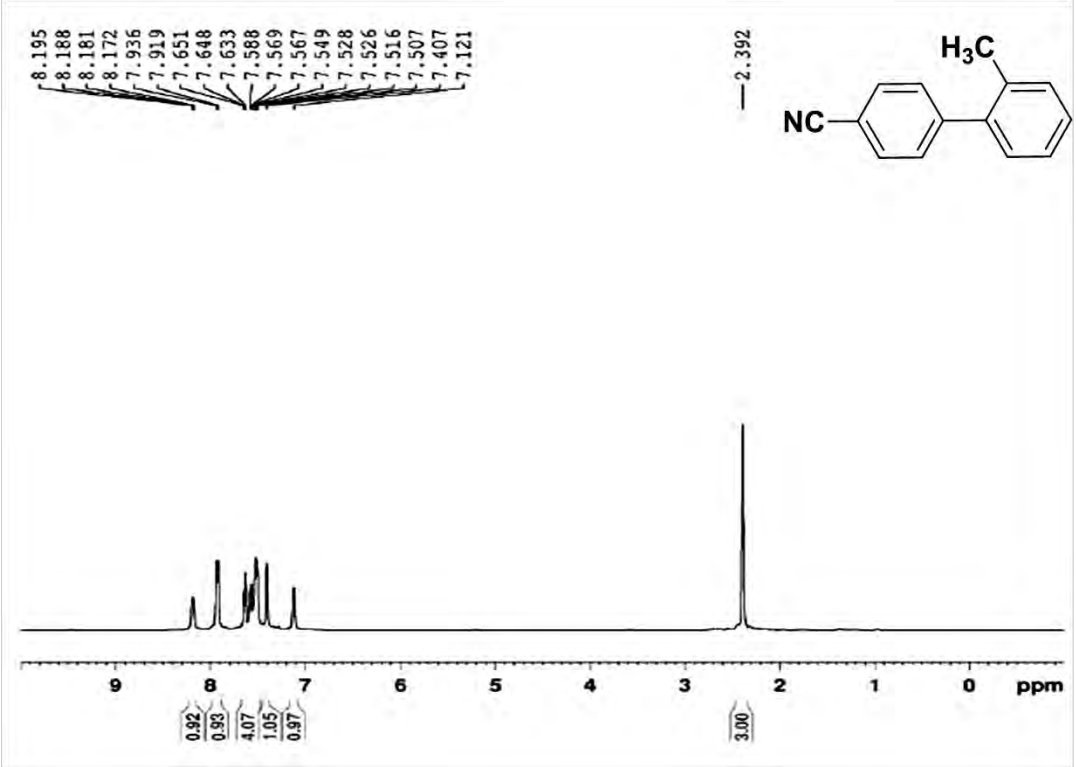

Fig. S9: ^{1}H NMR spectrum of 2'-methyl-biphenyl-4-carbonitrile

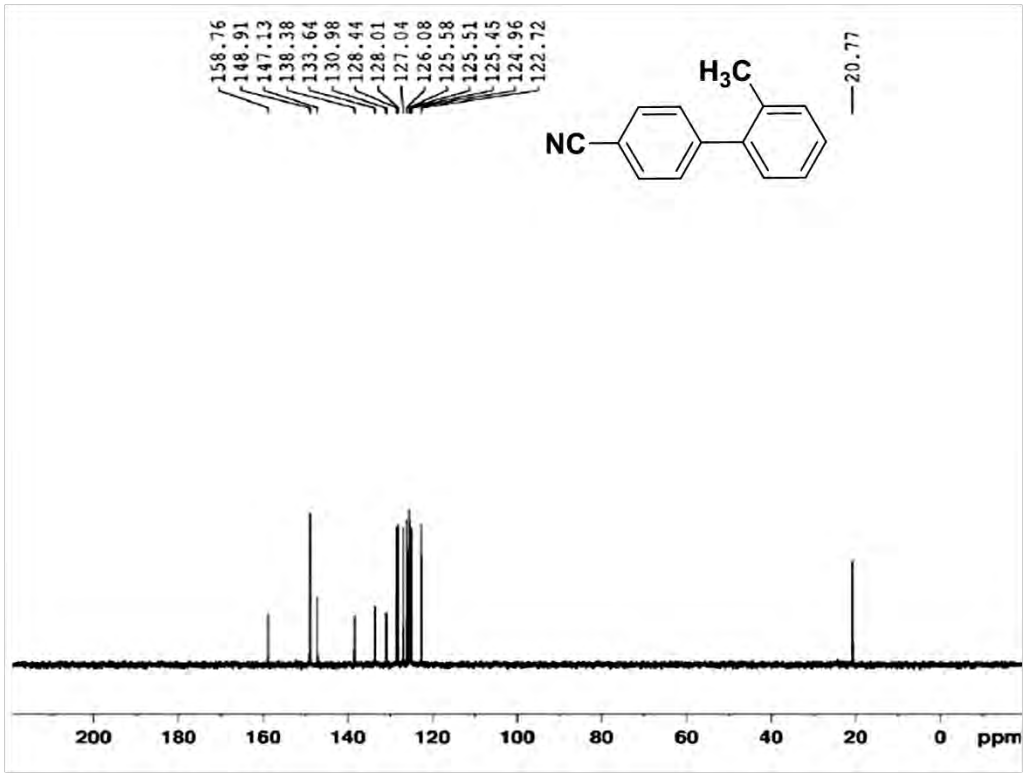

Fig. S10: ^{13}C NMR spectrum of 2'-methyl-biphenyl-4-carbonitrile

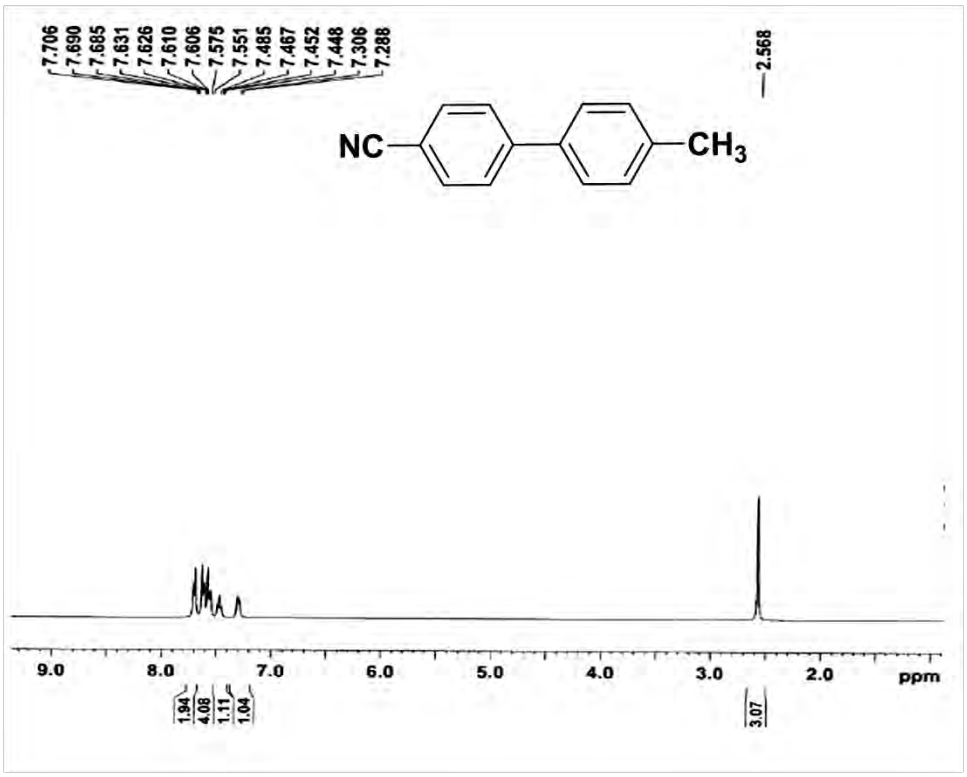

Fig. S11: ^{1}H NMR spectrum of 4'- methyl-biphenyl-4-carbonitrile

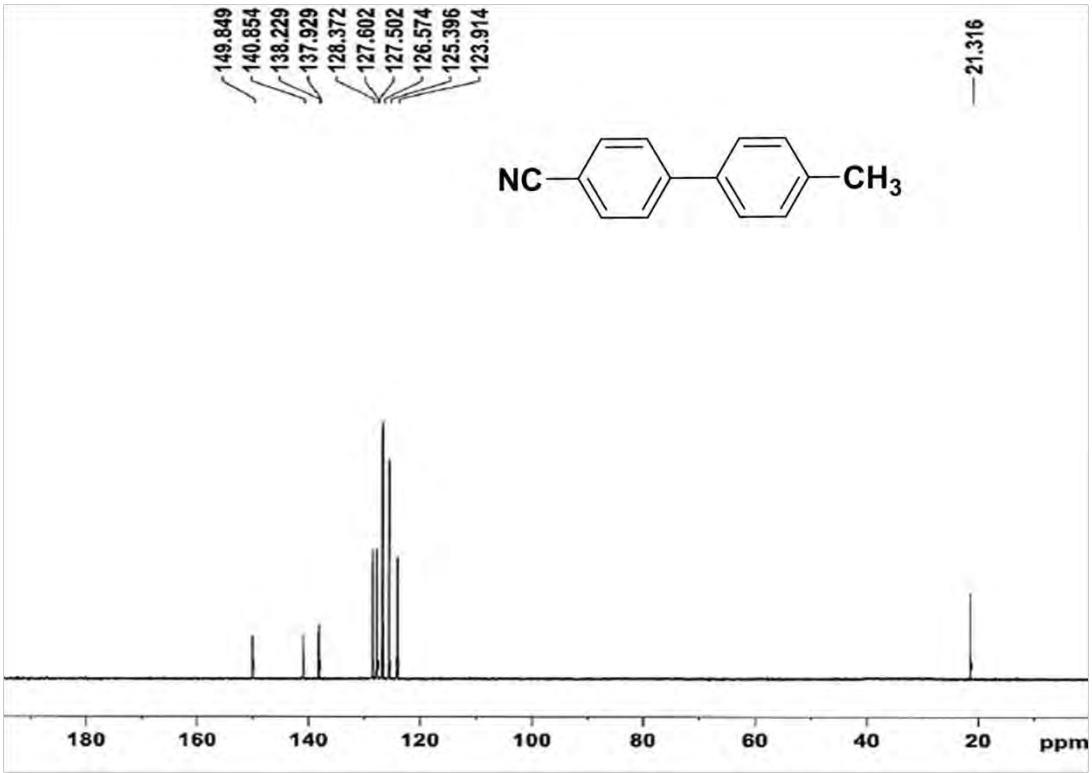

Fig. S12: ^{13}C NMR spectrum of 4'- methyl-biphenyl-4-carbonitrile

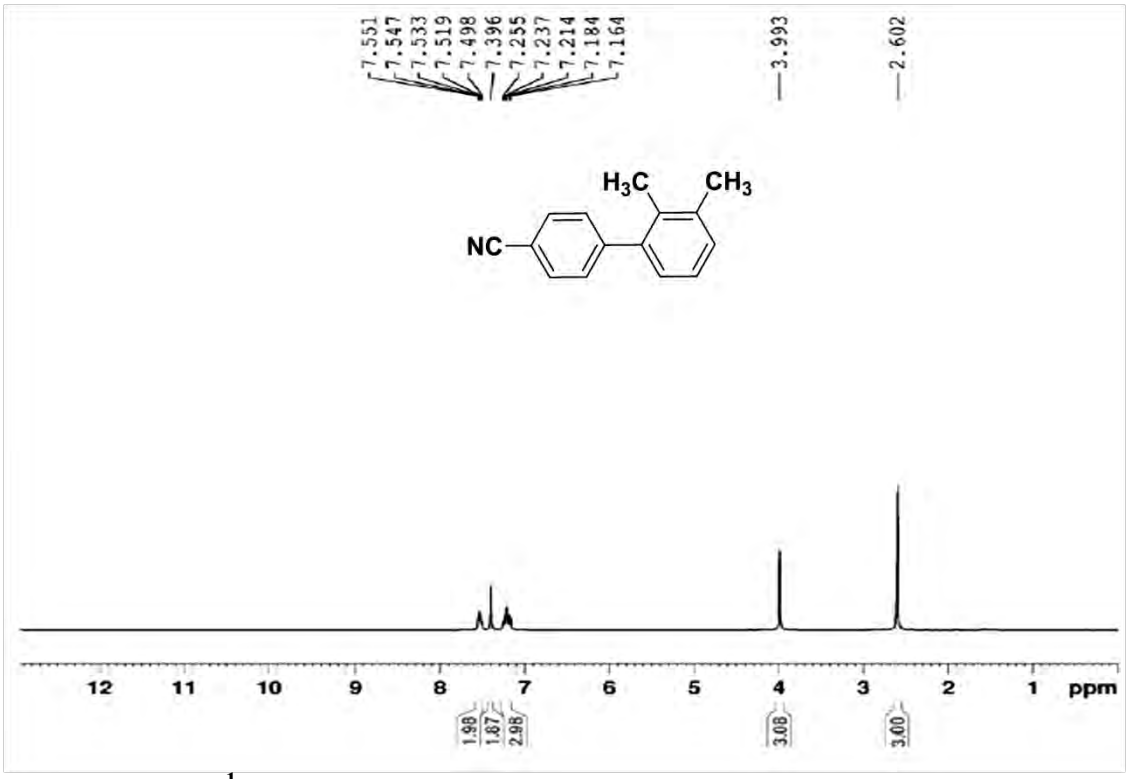

Fig. S13: ^{1}H NMR spectrum of 2,3-dimethylbiphenyl-4-carbonitrile

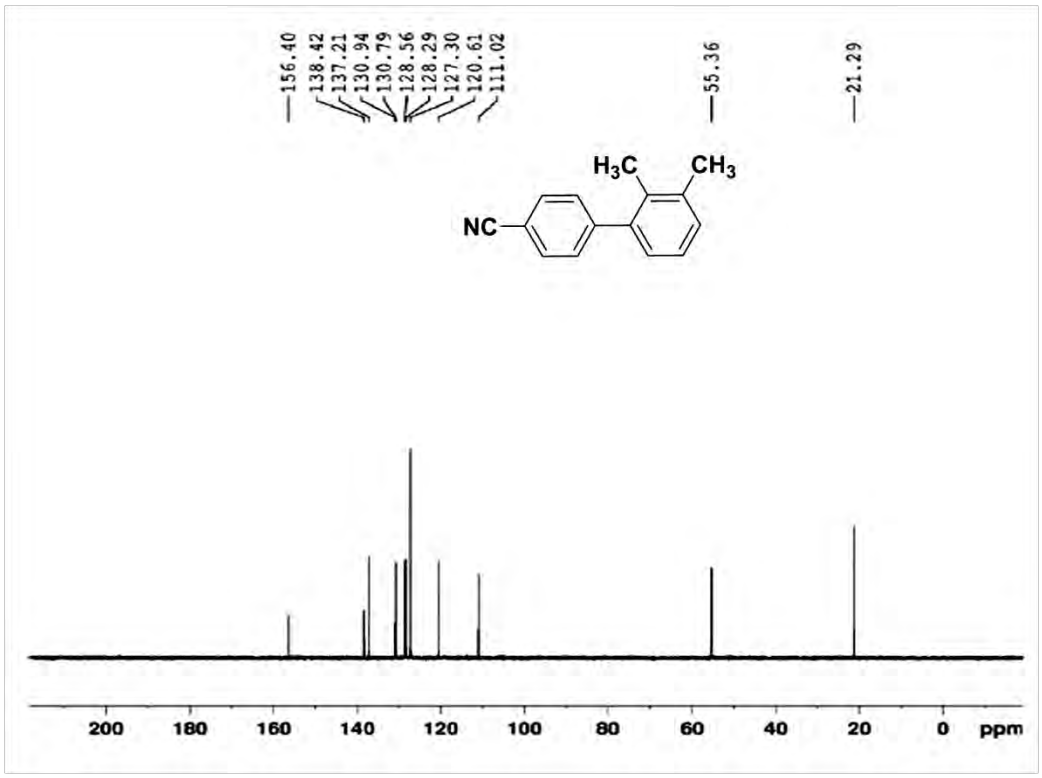

Fig. S14: ^{13}C NMR spectrum of 2',3'- dimethyl-biphenyl-4-carbonitrile

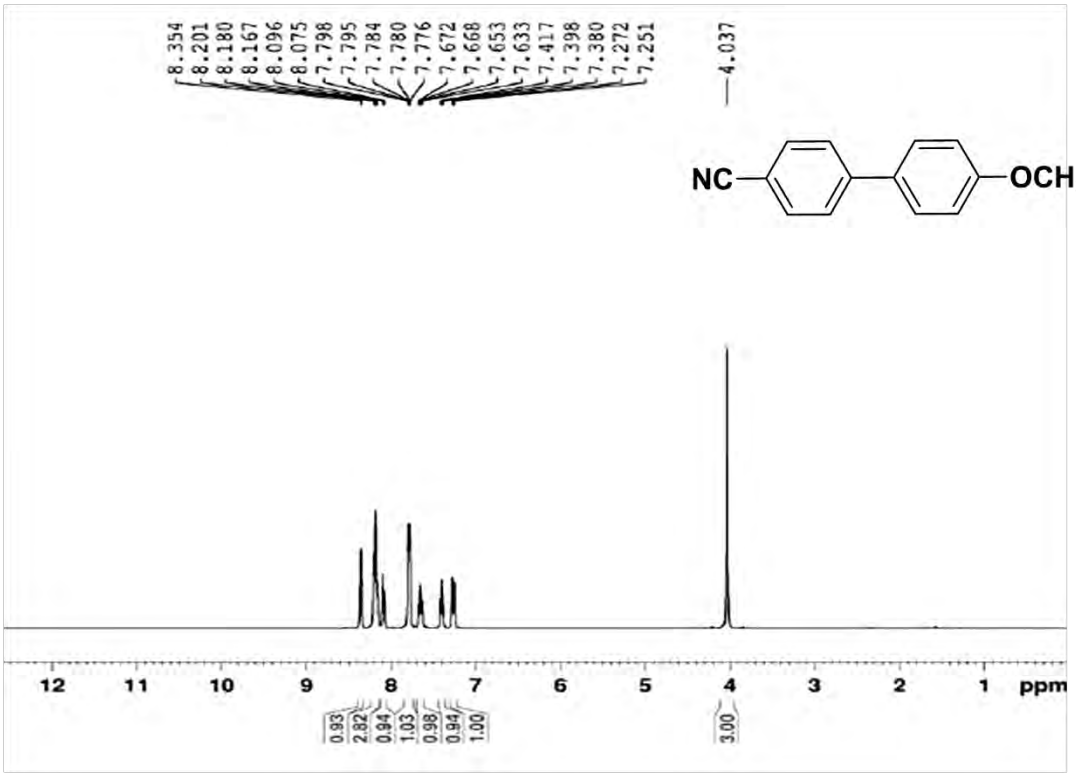

Fig. S15: ^{1}H NMR spectrum of 4'-methoxyl-biphenyl-4-carbonitrile

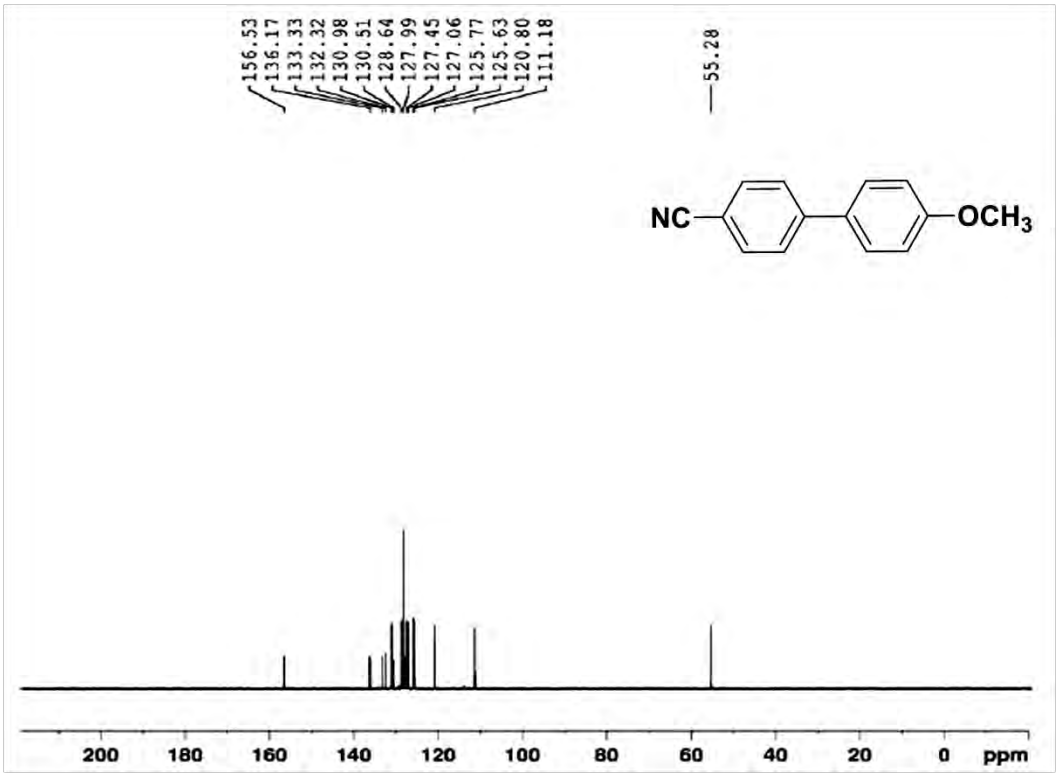

Fig. S16: ^{13}C NMR spectrum of 4'-methoxy-biphenyl-4-carbonitrile

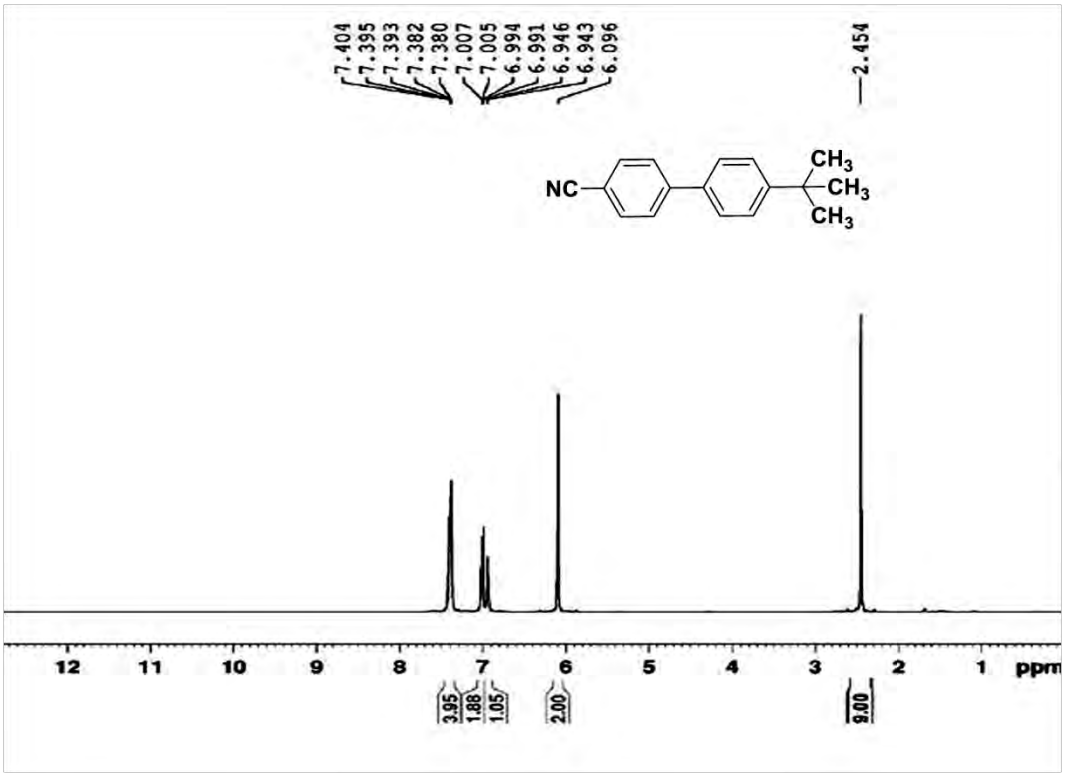

Fig. S17: ^{1}H NMR spectrum of 4'-*t*-butyl-biphenyl-4-carbonitrile

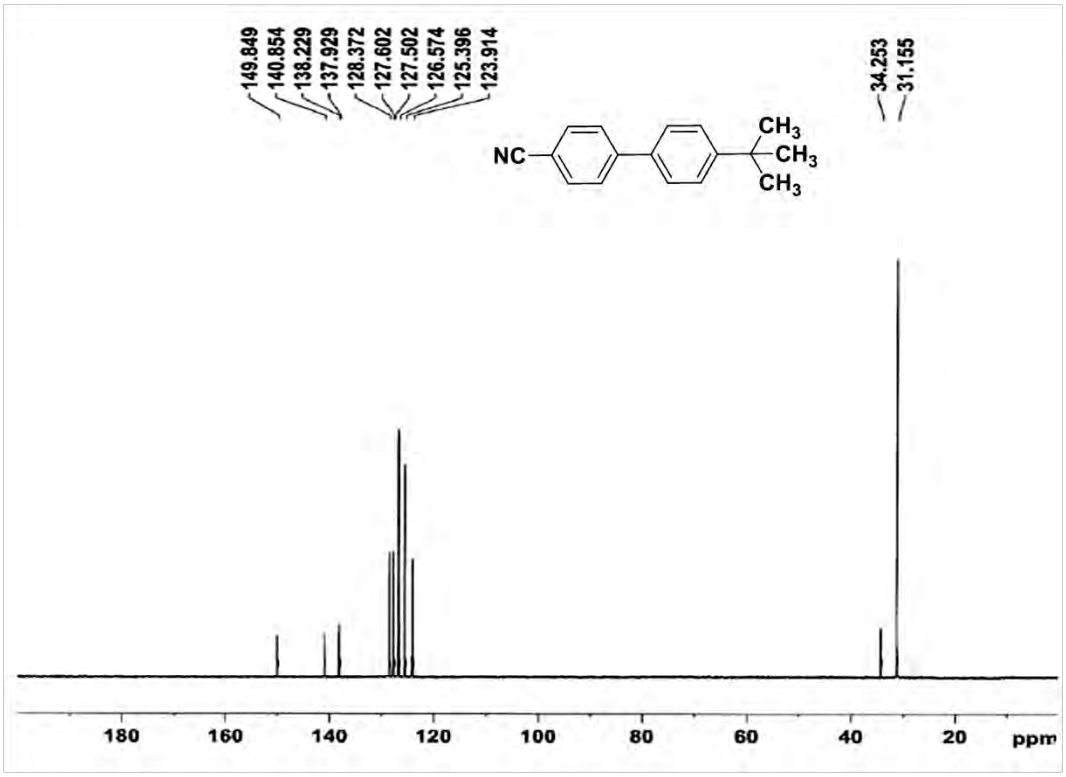

Fig. S18: ^{13}C NMR spectrum of 4'-*t*-butyl-biphenyl-4-carbonitrile

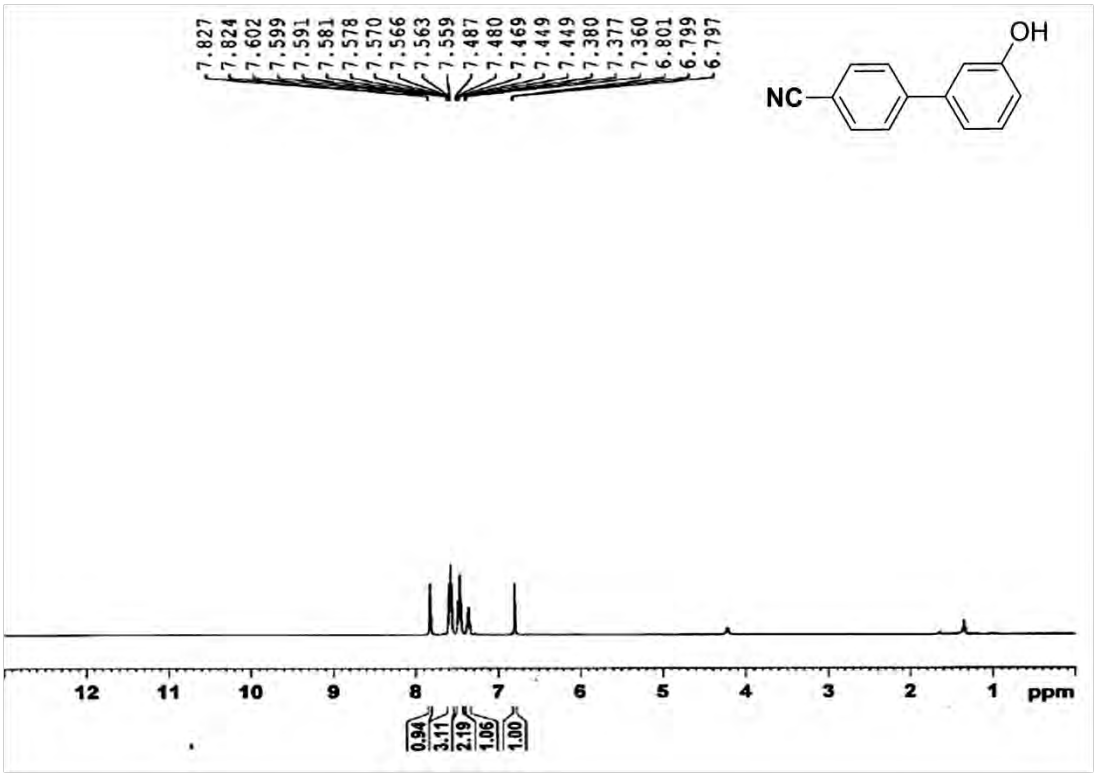

Fig. S19: ^{1}H NMR spectrum of 3'-hydroxy-biphenyl-4-carbonitrile

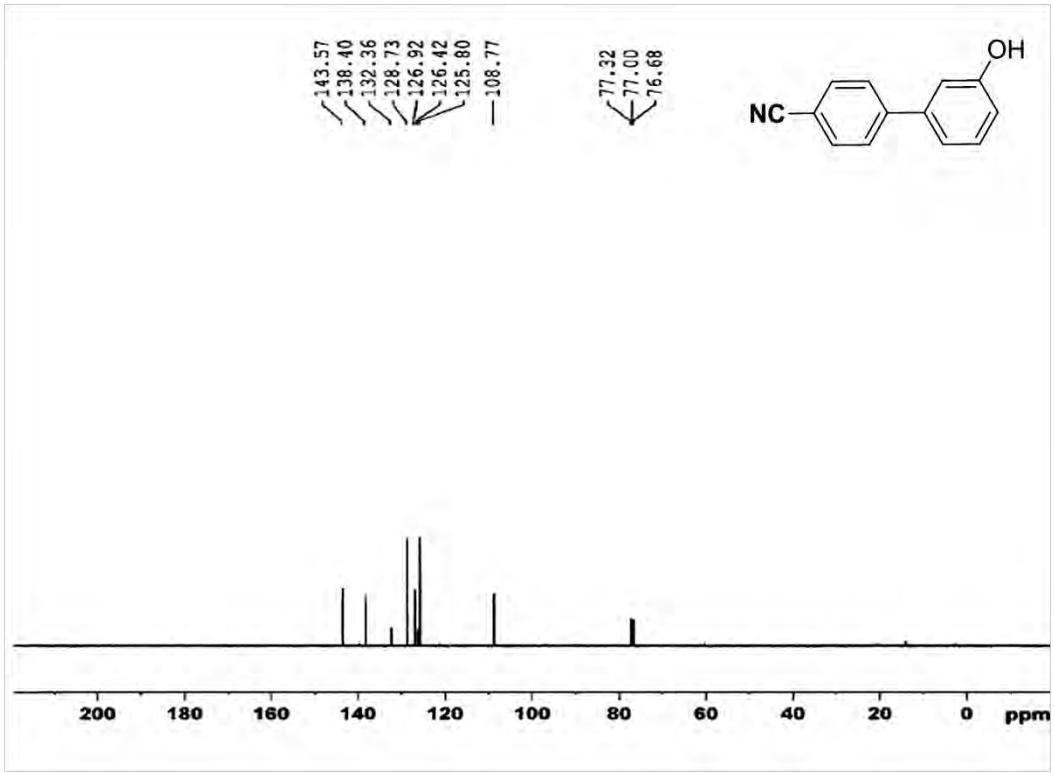

Fig. S20: ^{13}C NMR spectrum of 3'-hydroxy-biphenyl-4-carbonitrile

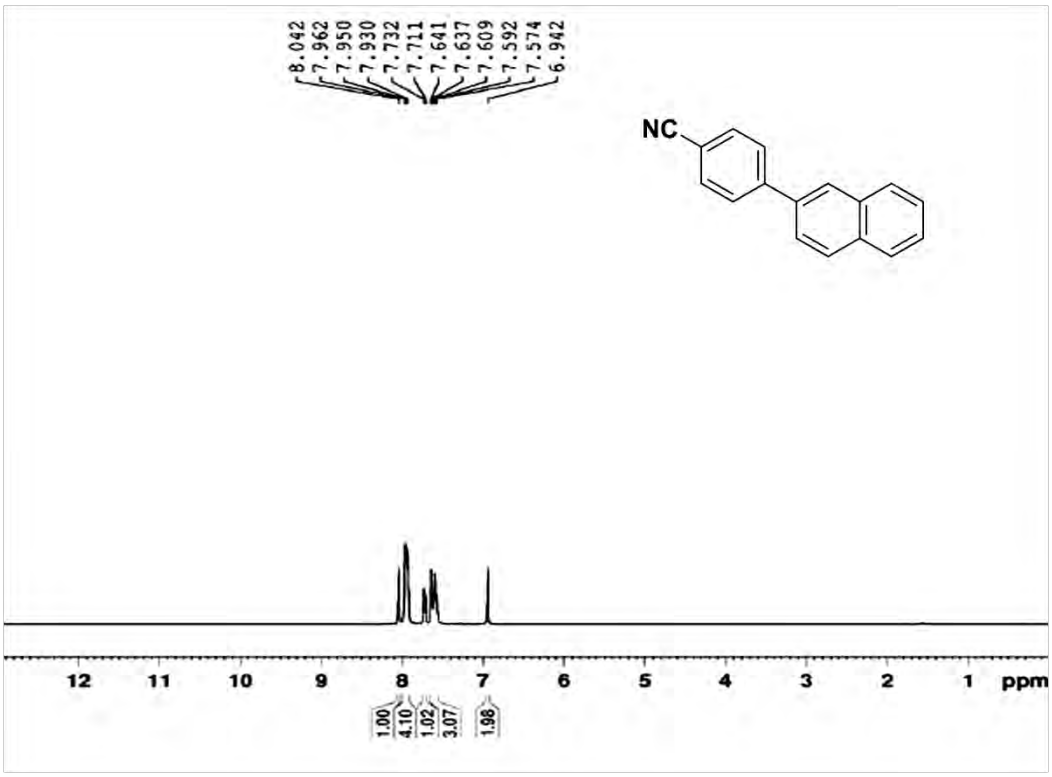

Fig. S21: ^{1}H NMR spectrum of 4'-naphthalen-2-yl-benzonitrile

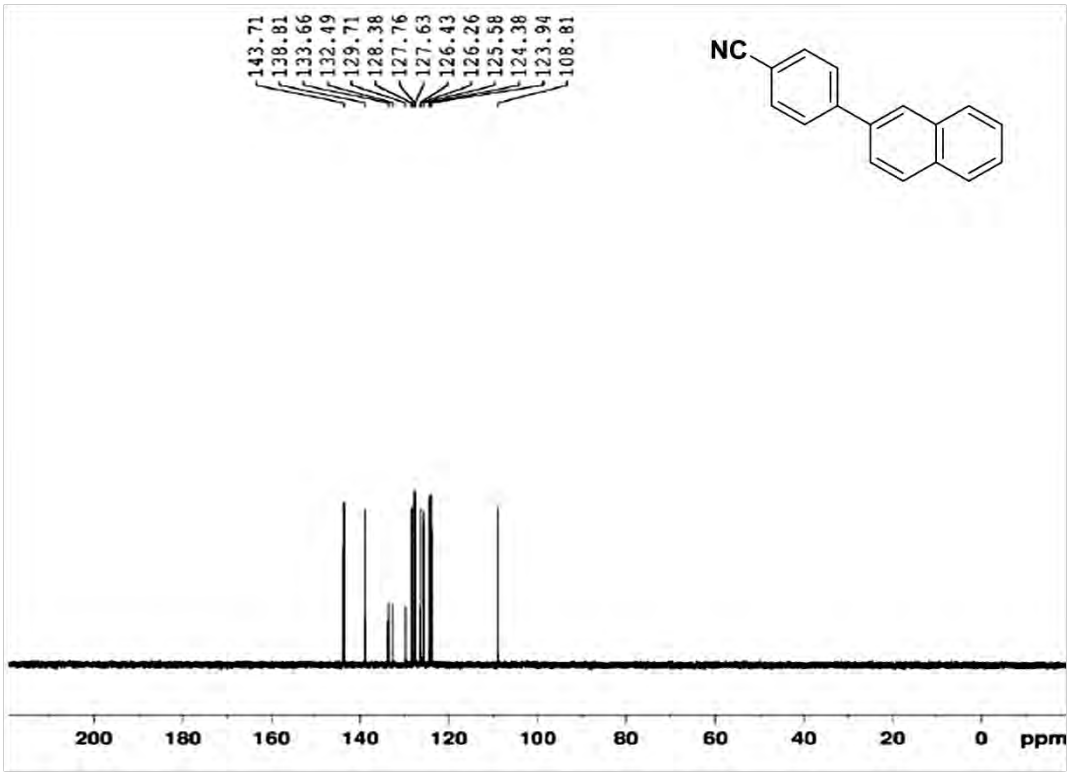

Fig. S22: ^{13}C NMR spectrum of 4'-naphthalen-2-yl-benzonitrile

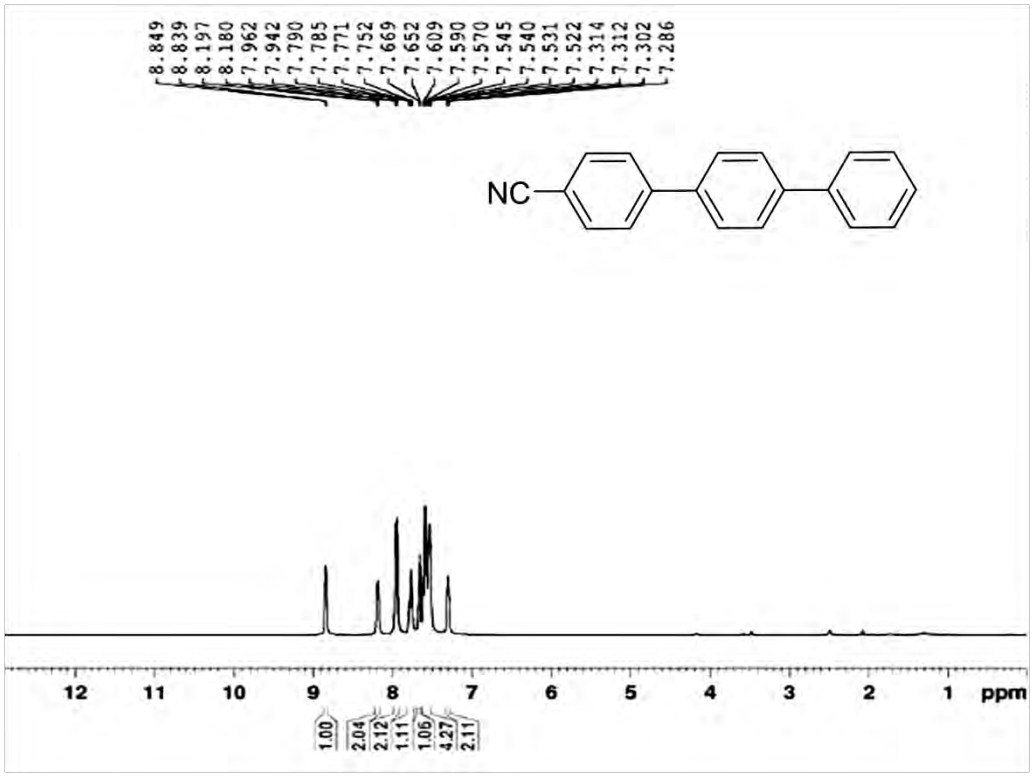

Fig. S23: ^{1}H NMR spectrum of [1,1';4',1'']terphenyl-4-carbonitrile

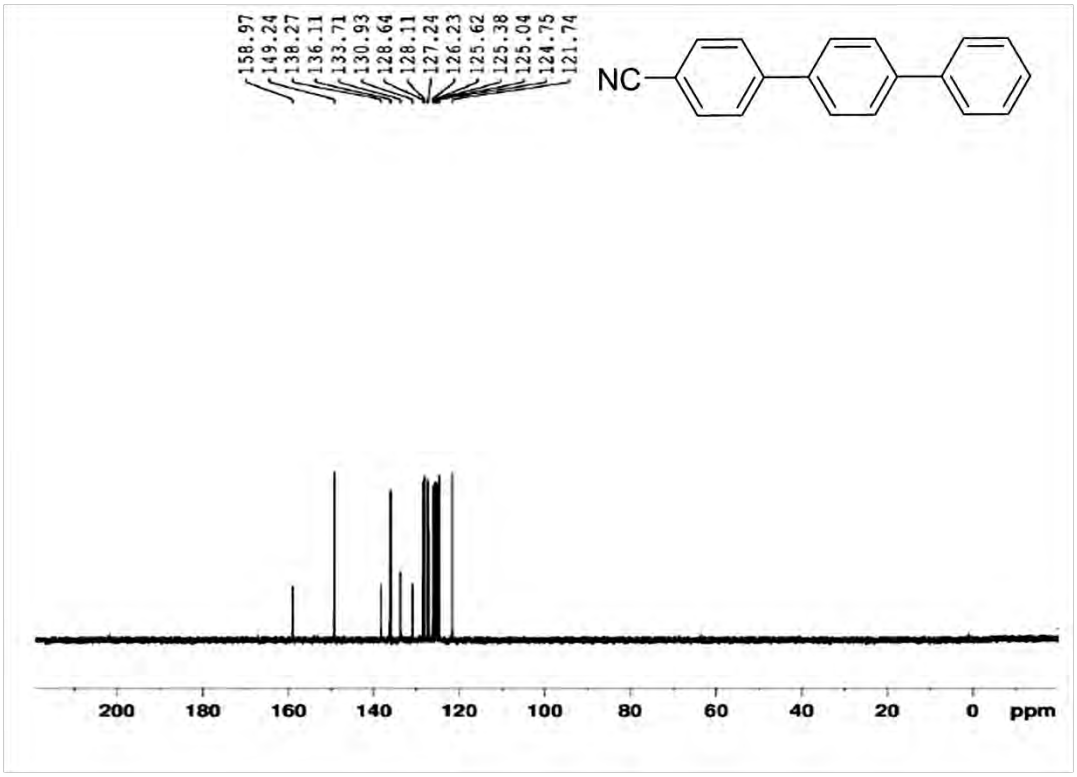

Fig. S24: ^{13}C NMR spectrum of [1,1';4',1'']terphenyl-4-carbonitrile

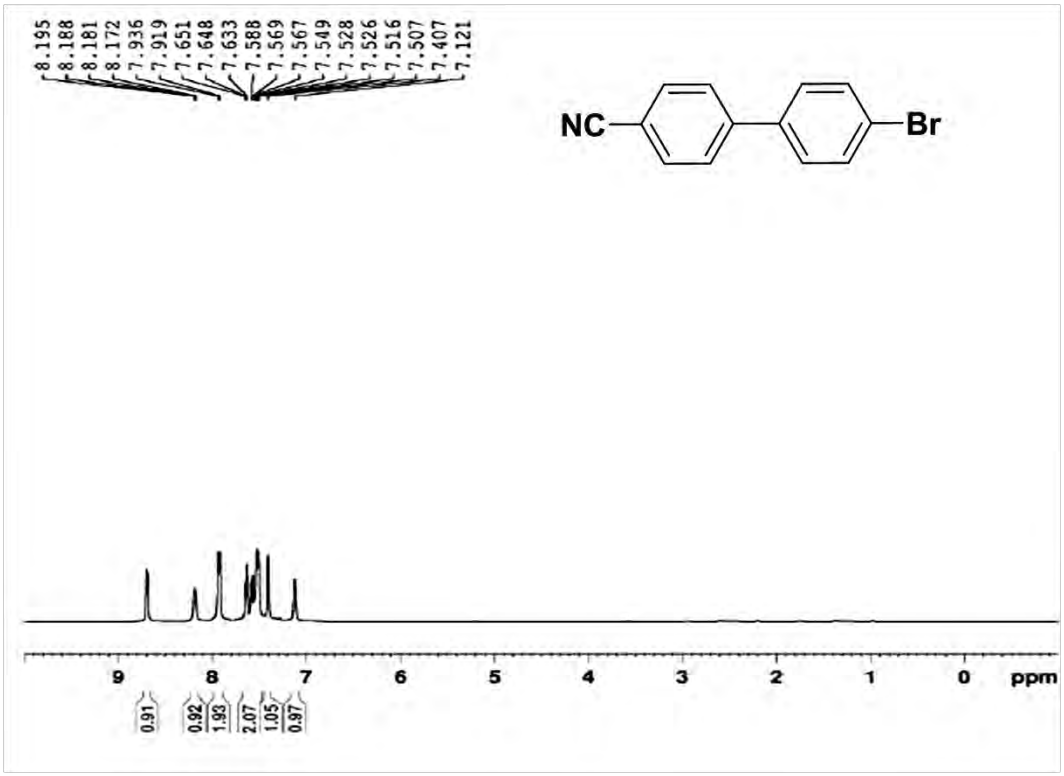

Fig. S25: ^{1}H NMR spectrum of 4'-bromo-biphenyl-4-carbonitrile

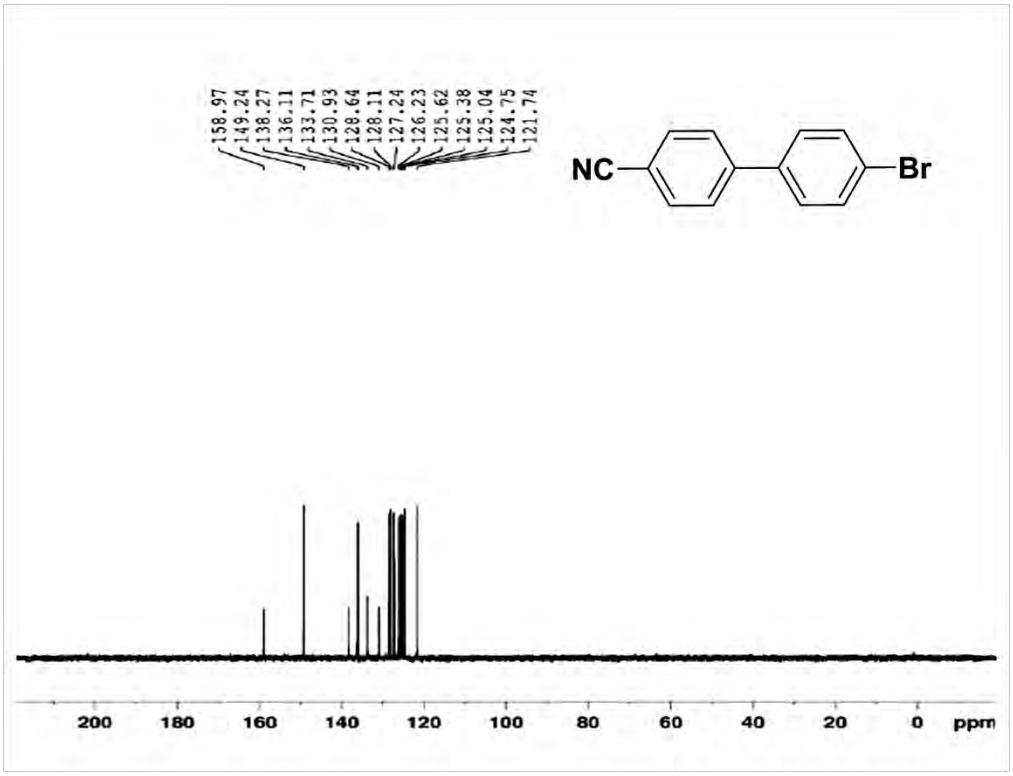

Fig. S26: ^{13}C NMR spectrum of 4'-bromo-biphenyl-4-carbonitrile

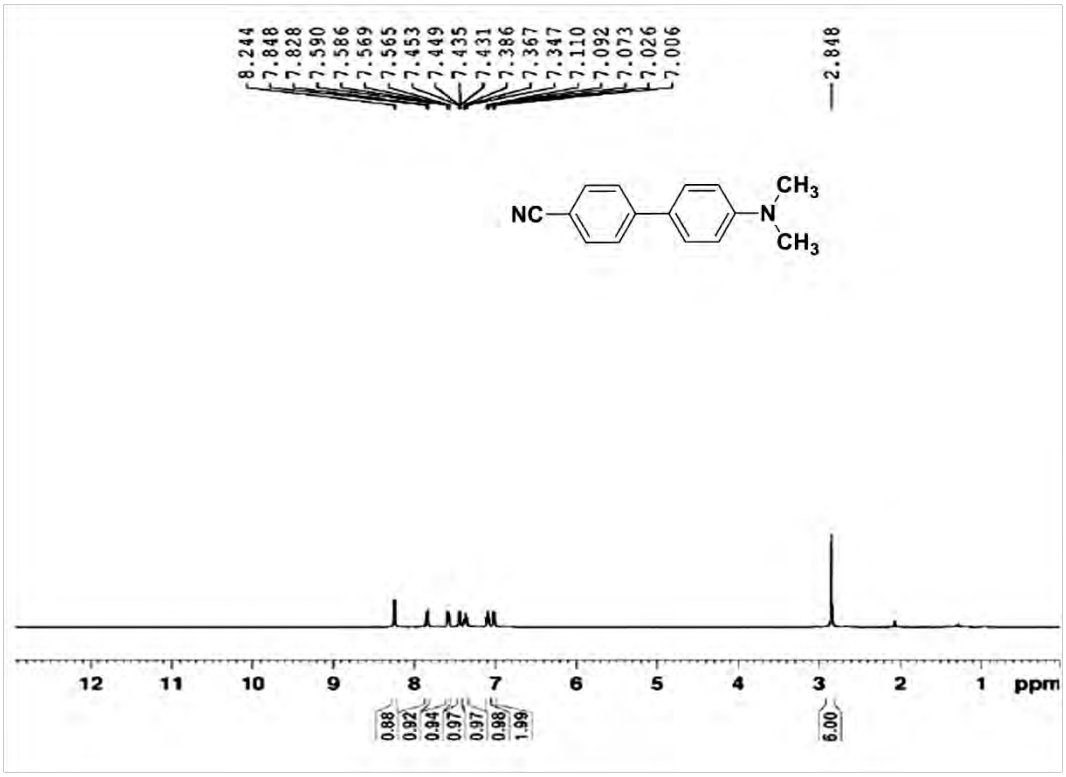

Fig. S27: ^{1}H NMR spectrum of 4'-dimethylamino-biphenyl-4-carbonitrile

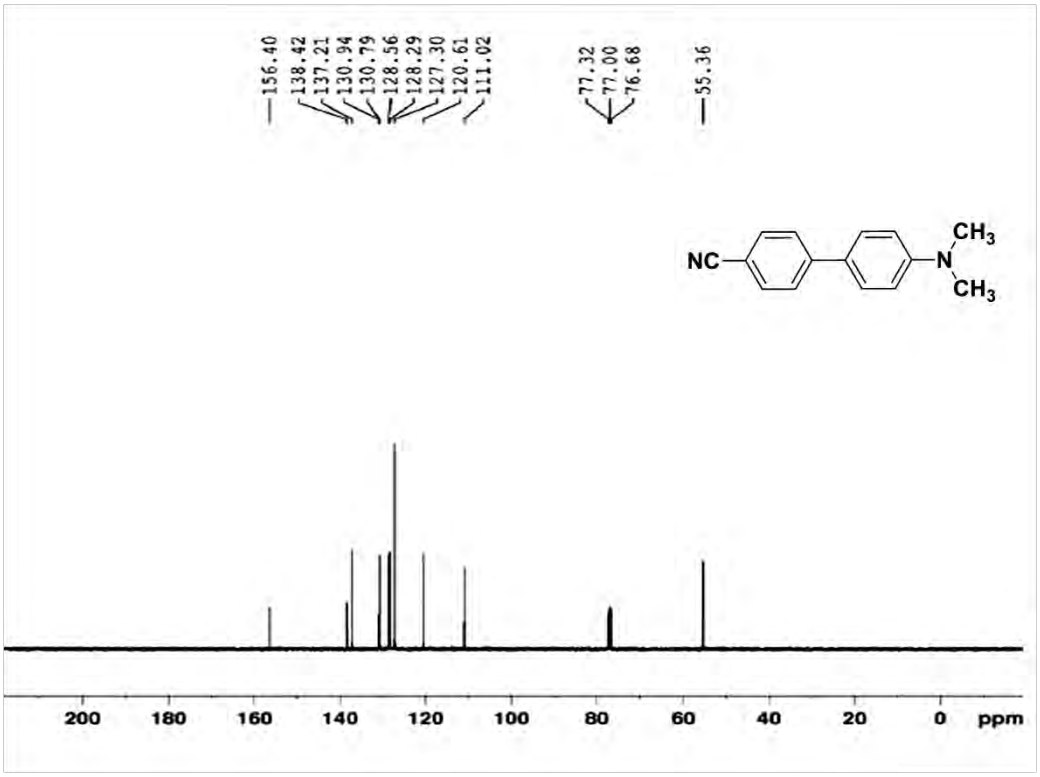

Fig. S28: ^{13}C NMR spectrum of 4'-dimethylamino-biphenyl-4-carbonitrile

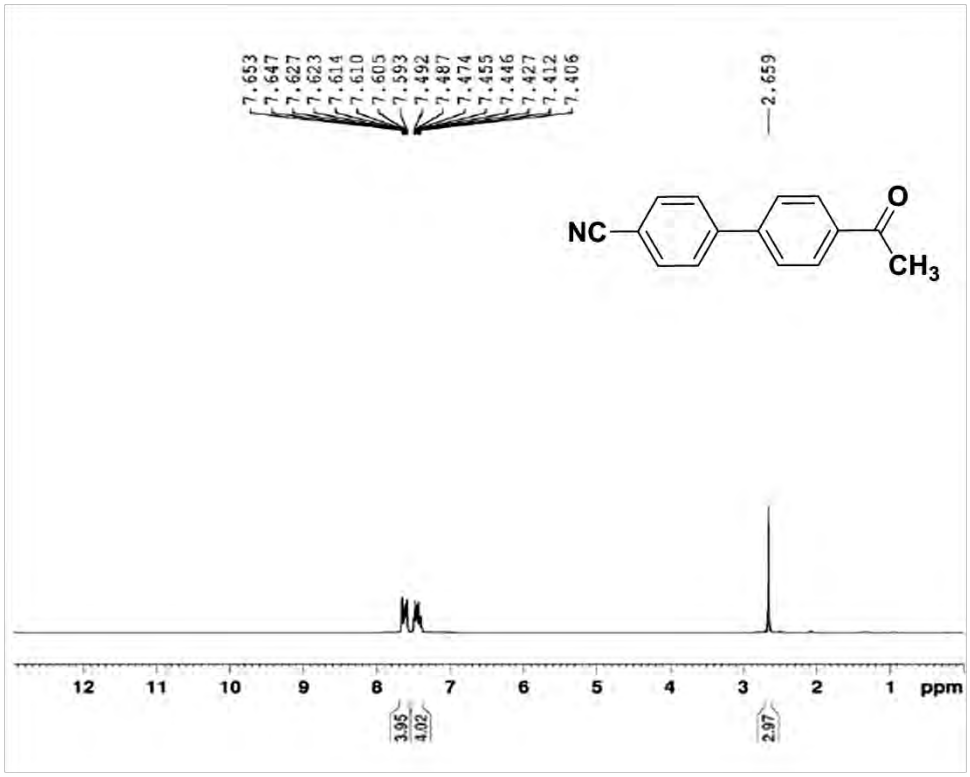

Fig. S29: ^{1}H NMR spectrum of 4'-acetyl-biphenyl-4-carbonitrile

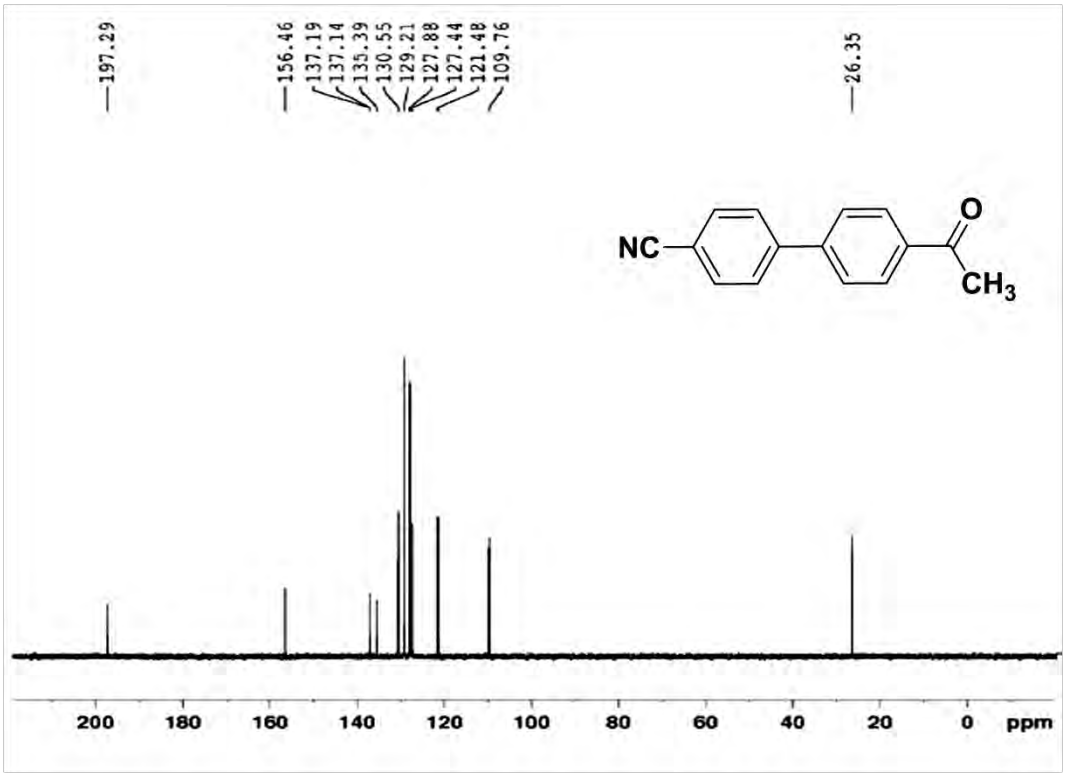

Fig. S30: ^{13}C NMR spectrum of 4'-acetyl-biphenyl-4-carbonitrile

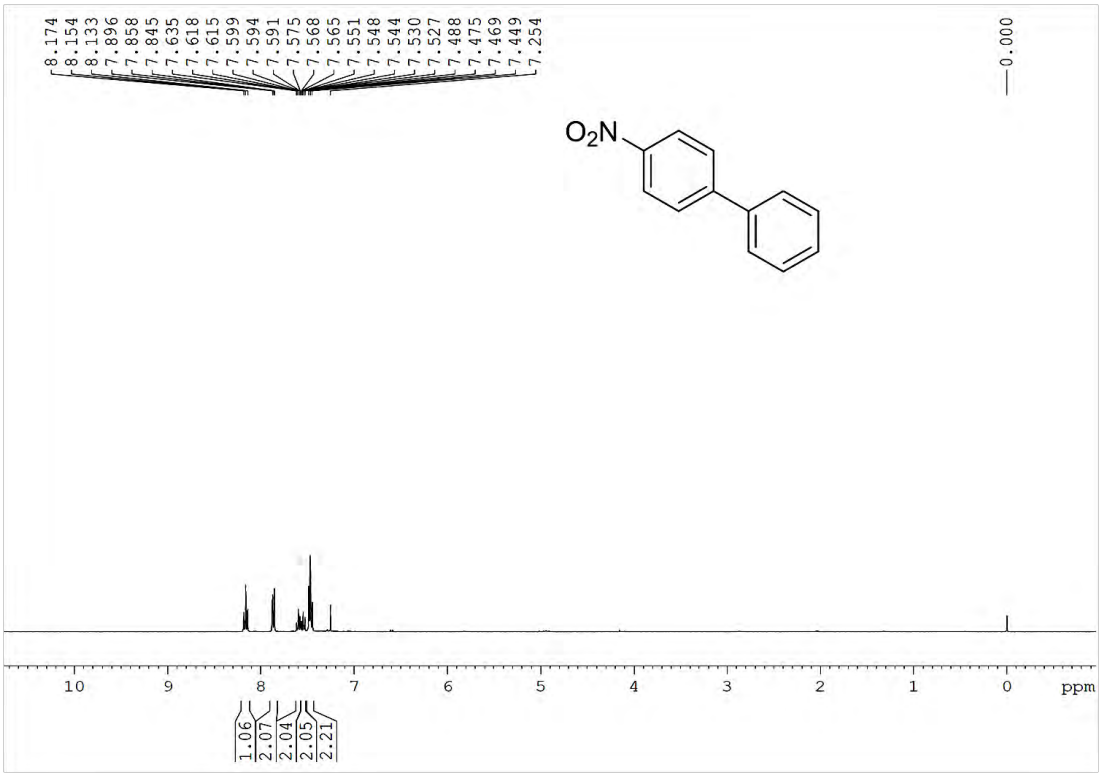

Fig. S31: [1] H NMR spectrum of 4-nitrobiphenyl

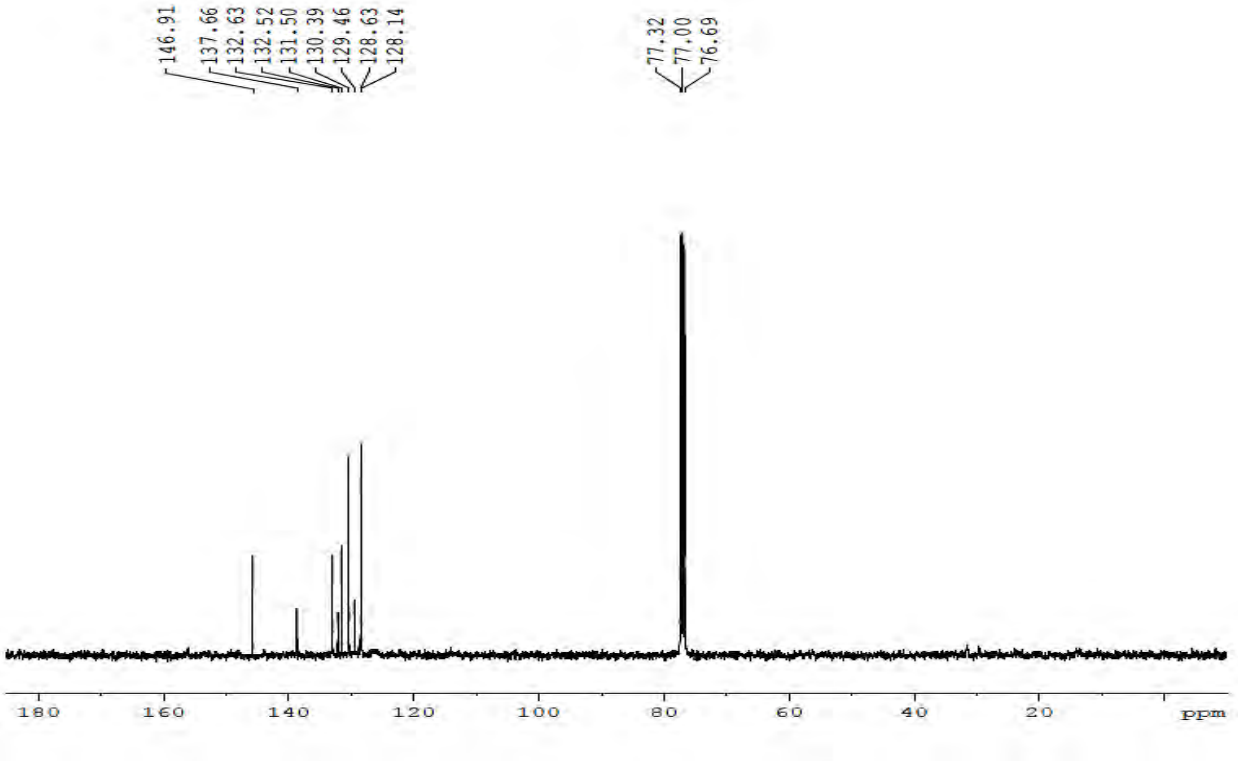

Fig. S32: [13]C NMR spectrum of 4-nitrobiphenyl

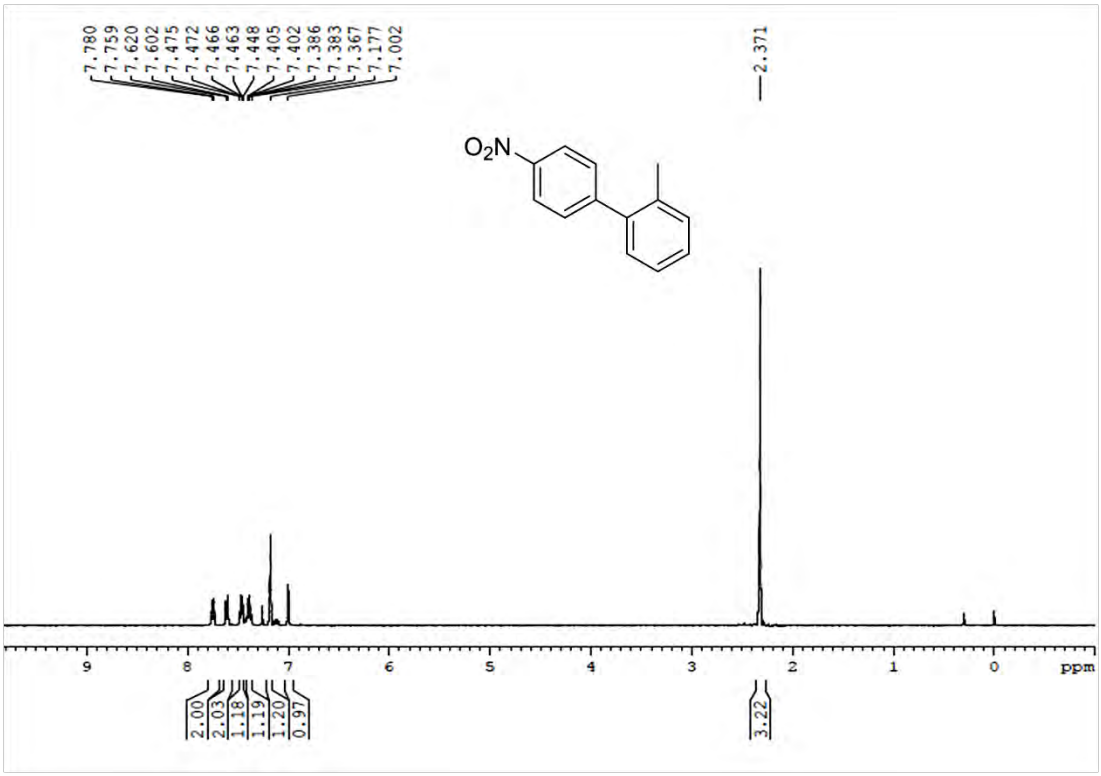

Fig. S33: ^{1}H NMR spectrum of 2-methyl-4'-nitro-biphenyl

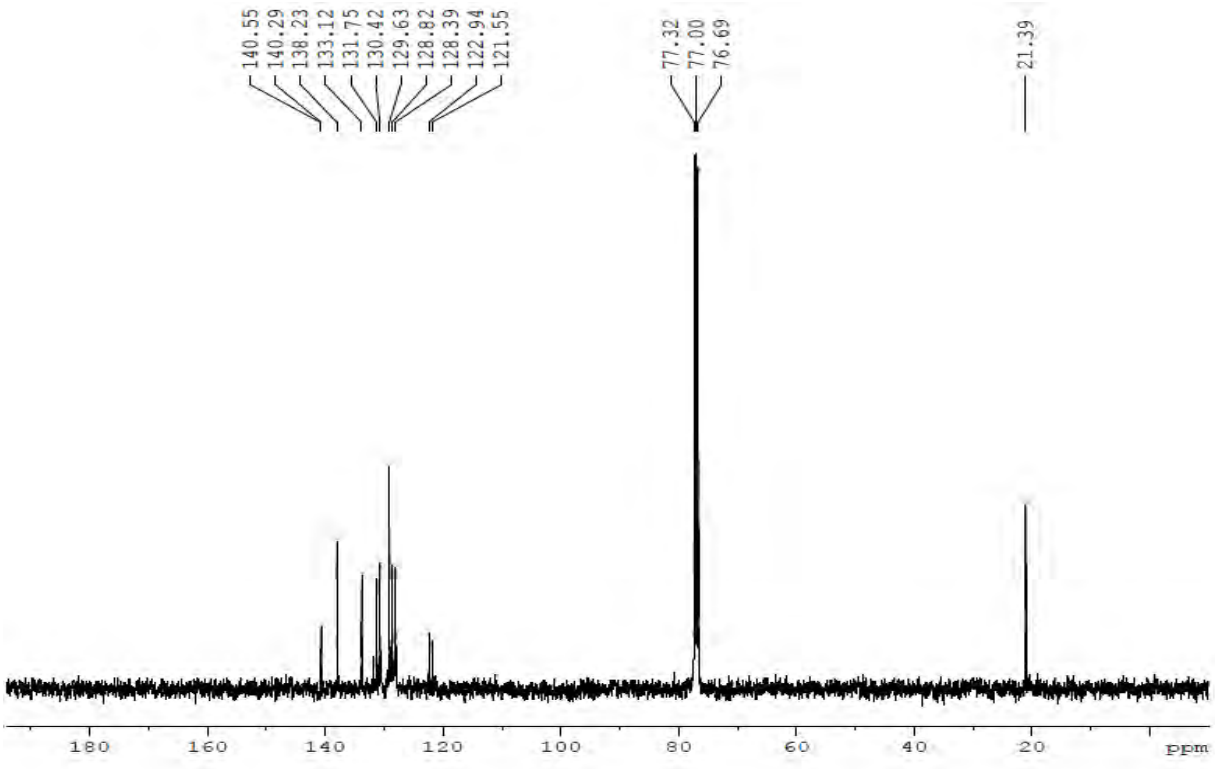

Fig. S34: ^{13}C NMR spectrum of 2-methyl-4'-nitro-biphenyl

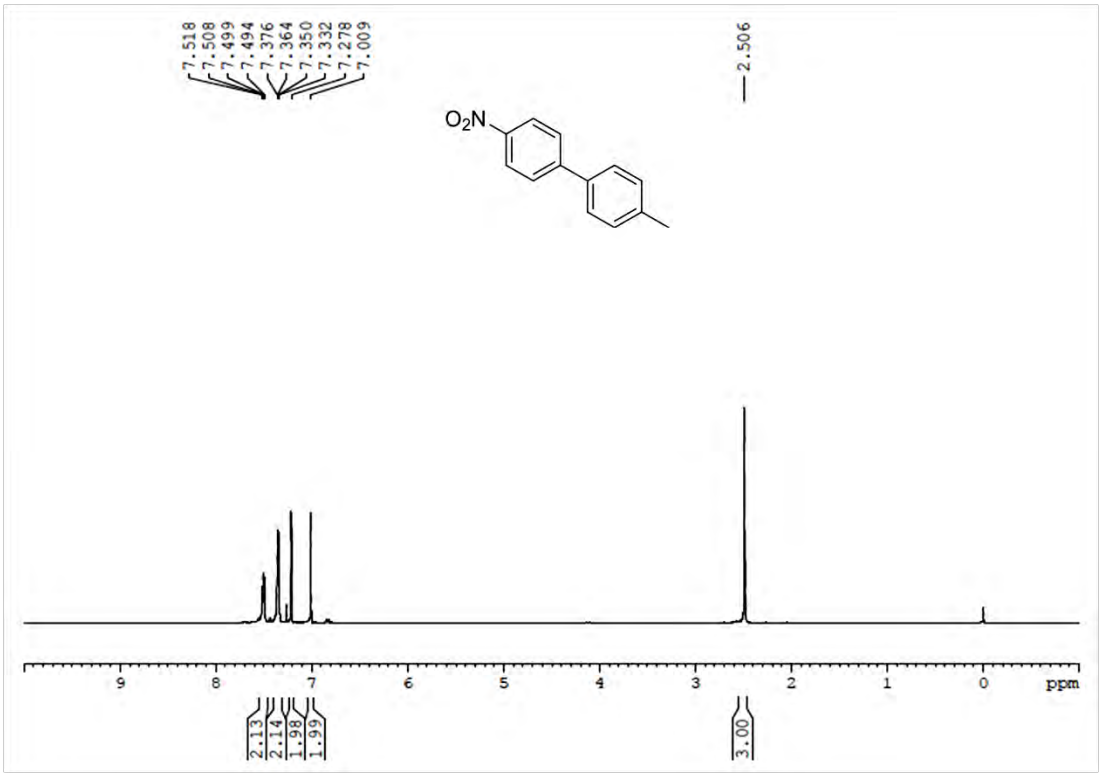

Fig. S35: ^{1}H NMR spectrum of 4'-methyl-4-nitro-biphenyl

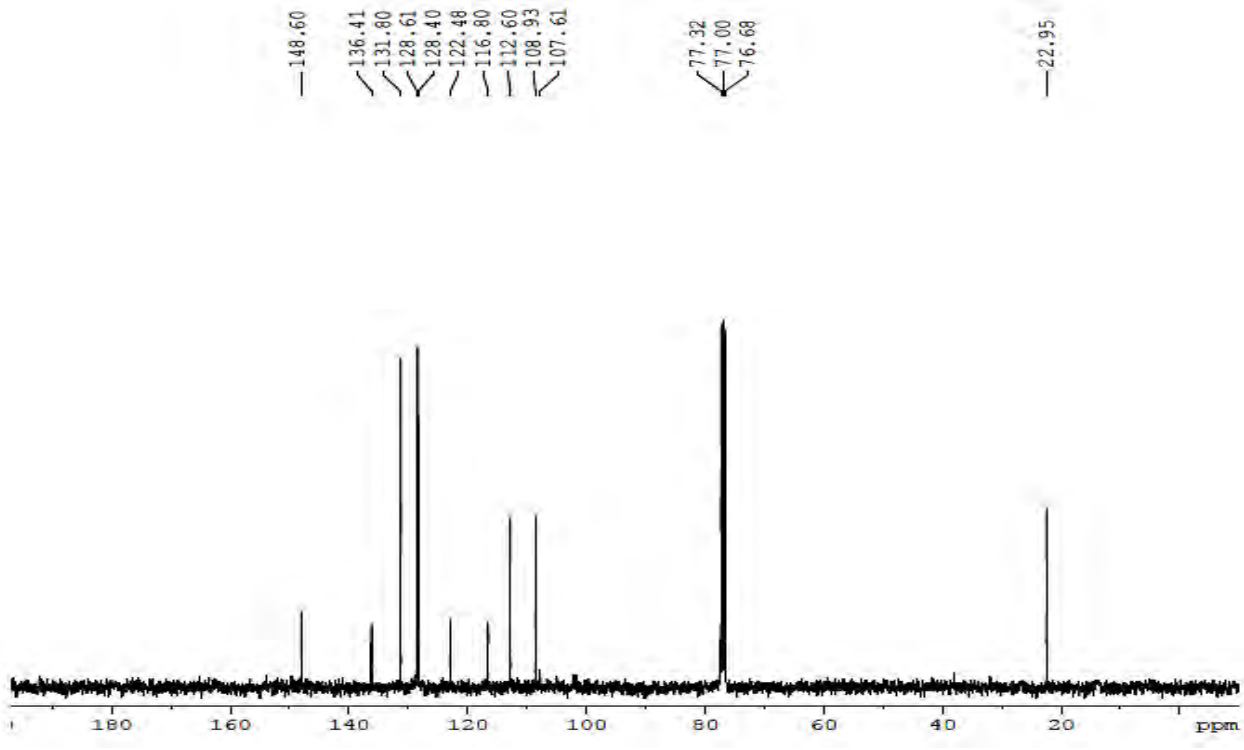

Fig. S36: ^{13}C NMR spectrum of 4'-methyl-4-nitro-biphenyl

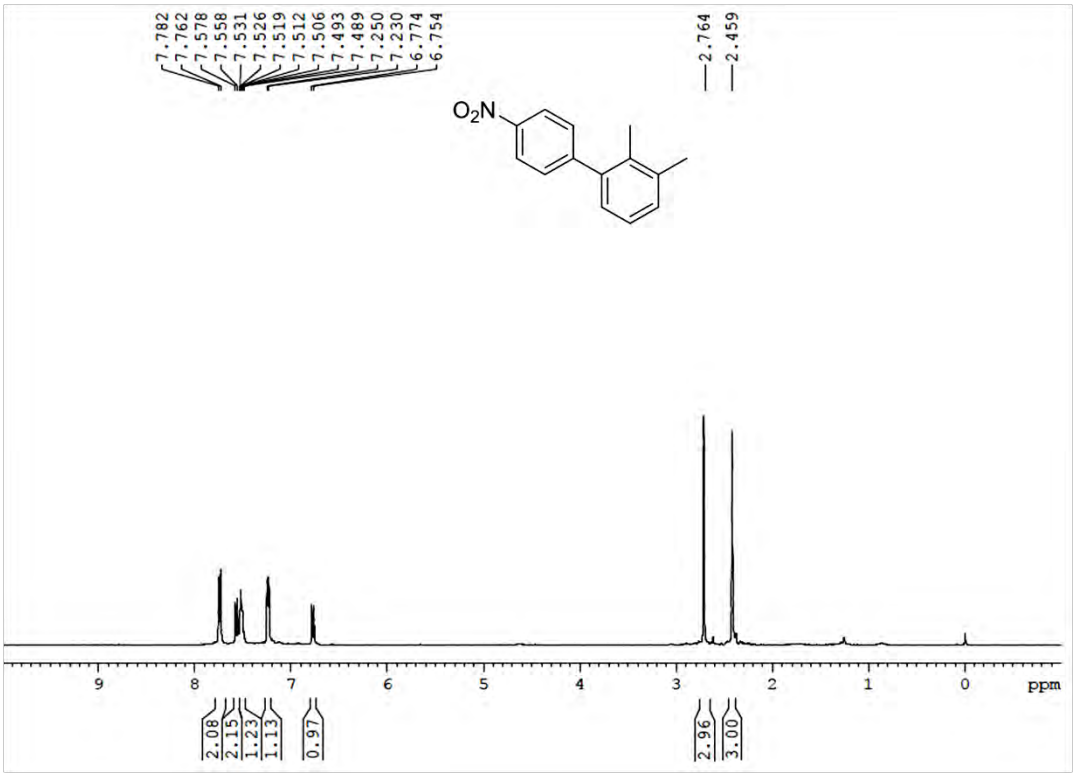

Fig. S37: ^{1}H NMR spectrum of 2, 3-dimethyl-4'-nitro-biphenyl

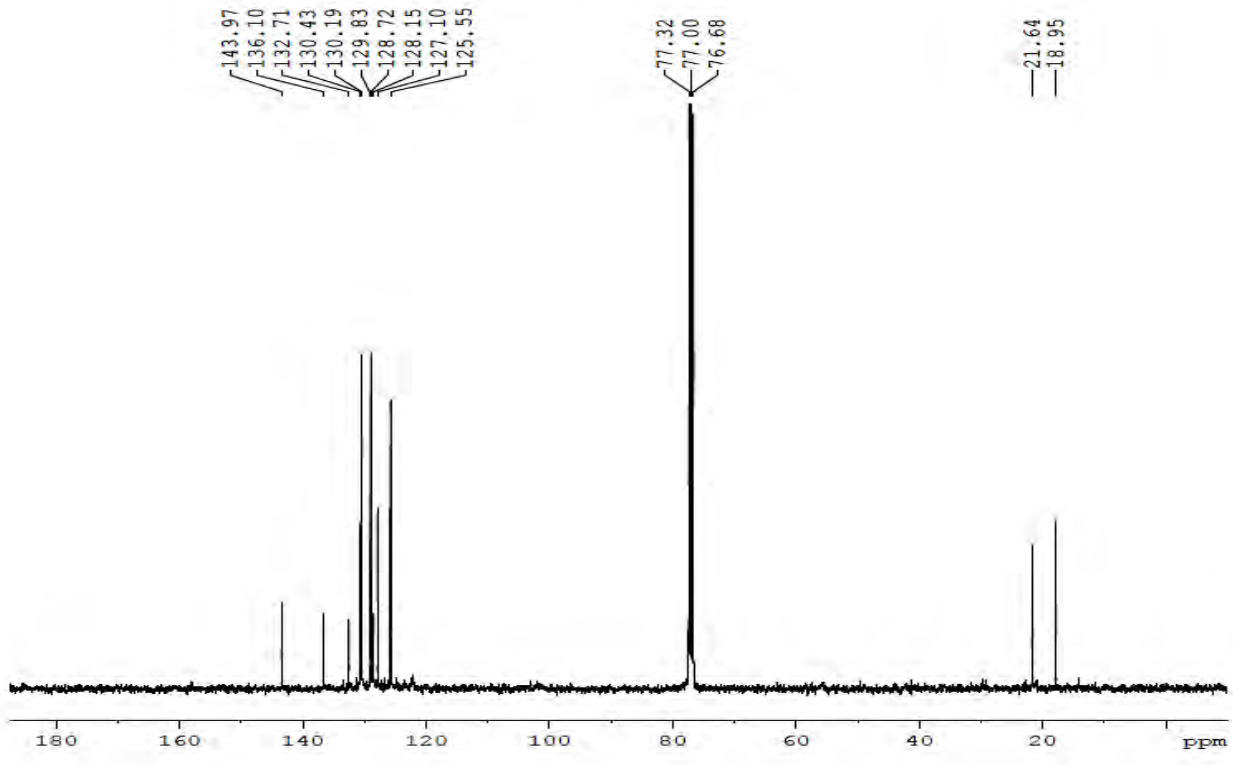

Fig. S38: ^{13}C NMR spectrum of 2, 3-dimethyl-4'-nitro-biphenyl

Fig. S39: ^{1}H NMR spectrum of 2-methoxy-4-nitro-biphenyl

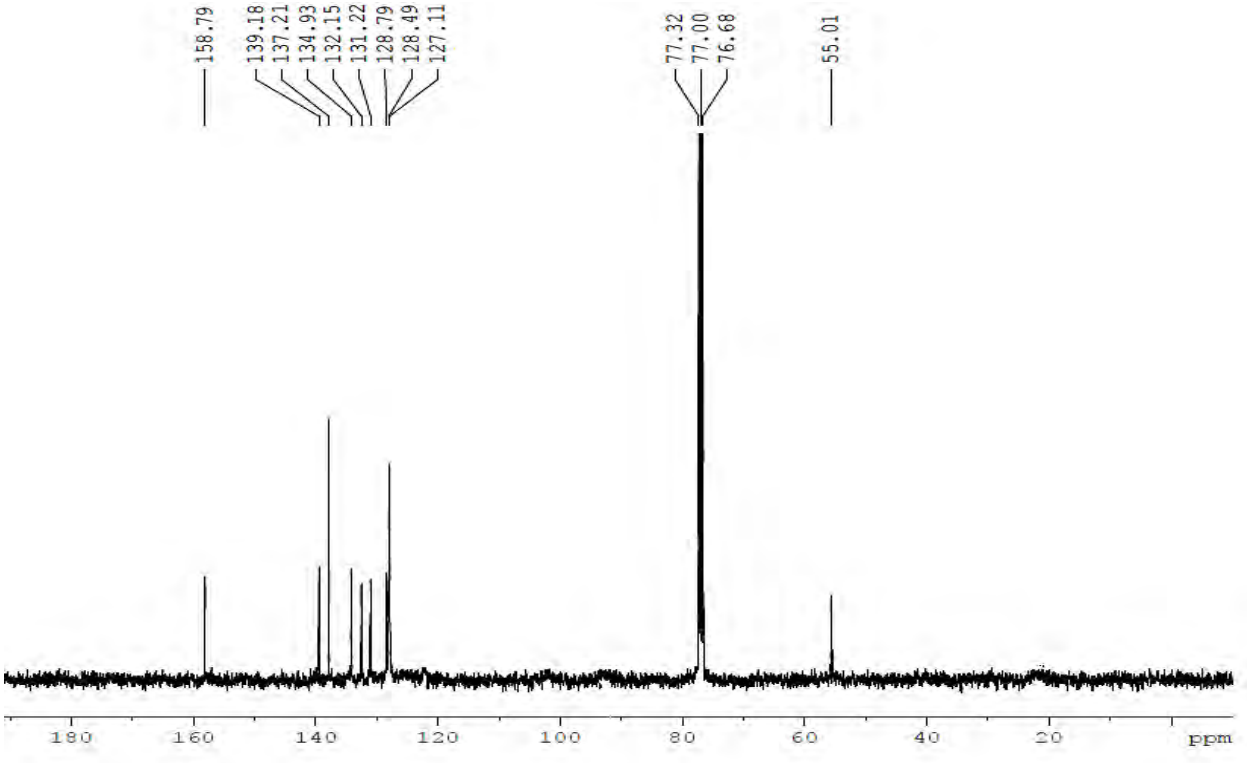

Fig. S40: ^{13}C NMR spectrum of 2-methoxy-4-nitro-biphenyl

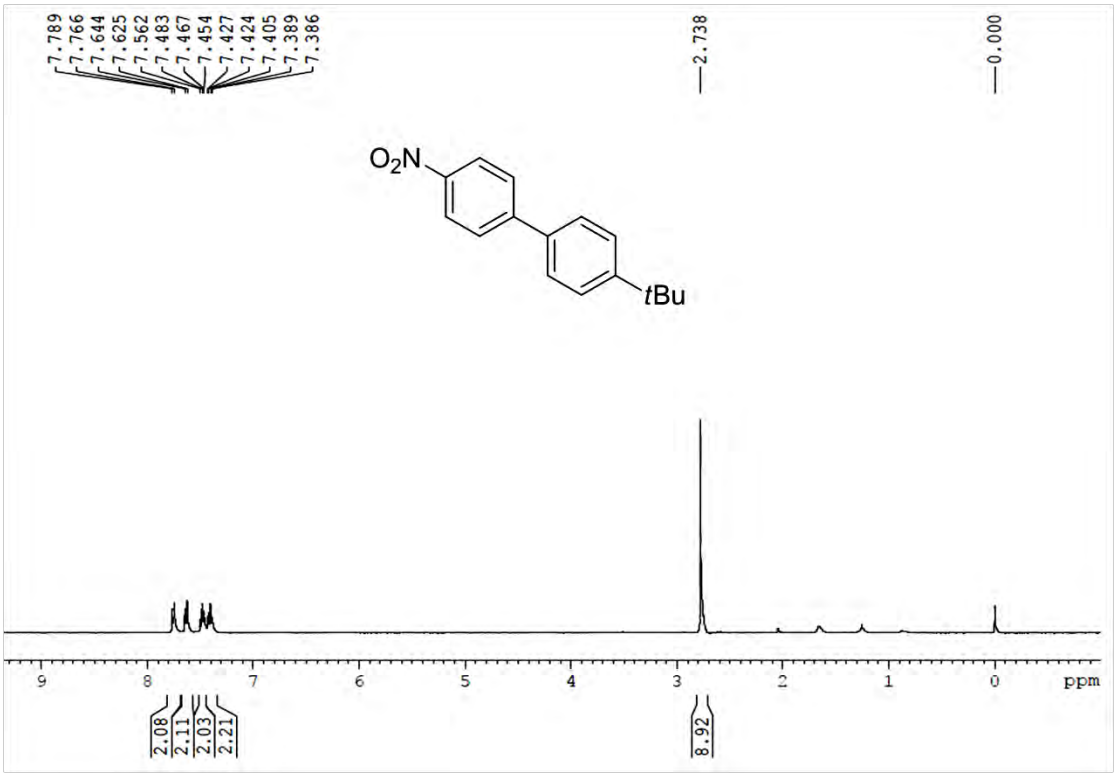

Fig. S41: ^{1}H NMR spectrum of 4'-*tert*-butyl-4-nitro-biphenyl

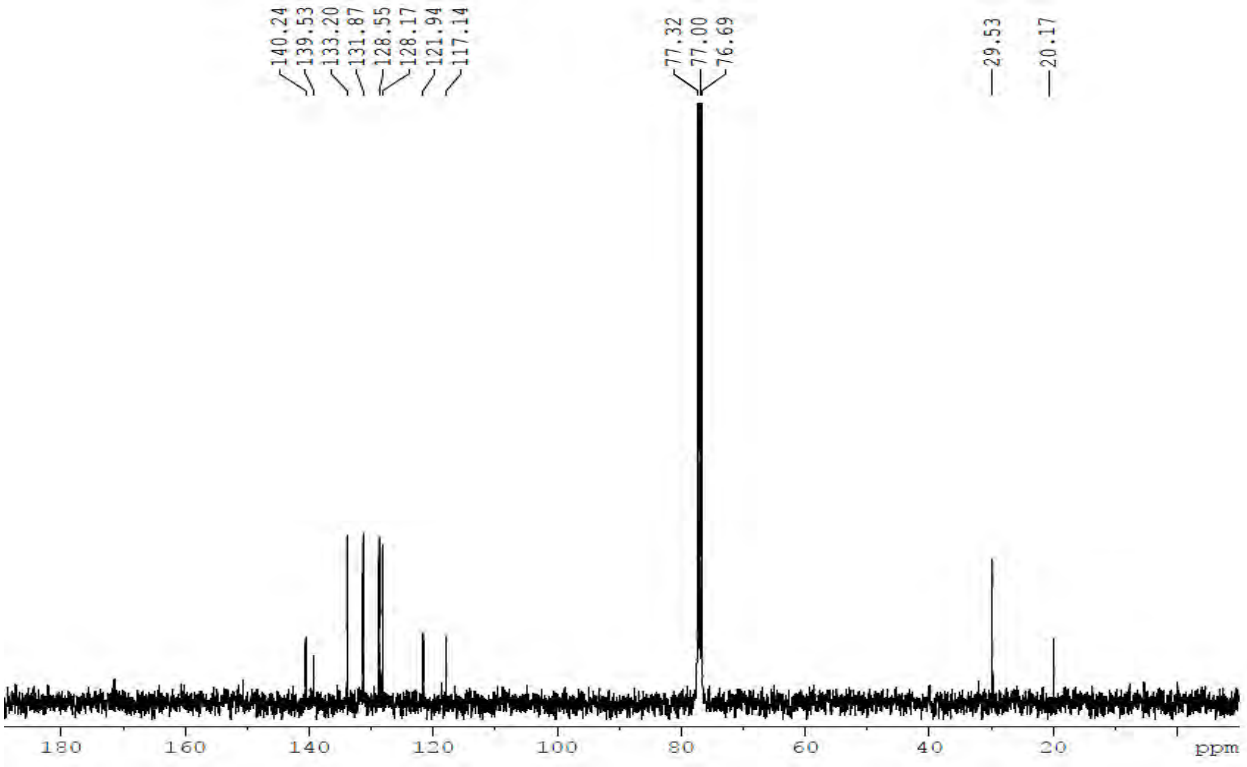

Fig. S42: ^{13}C NMR spectrum of 4'-*tert*-butyl-4-nitro-biphenyl

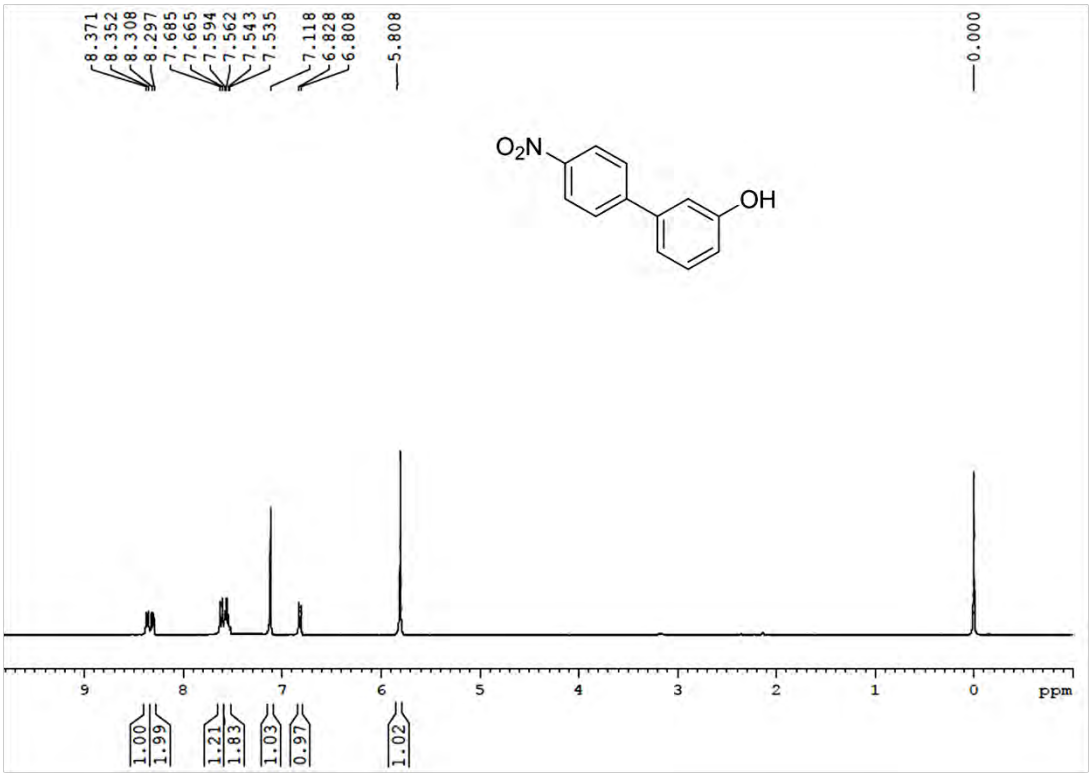

Fig. S43: ^{1}H NMR spectrum of 4'-nitro-biphenyl-3-ol

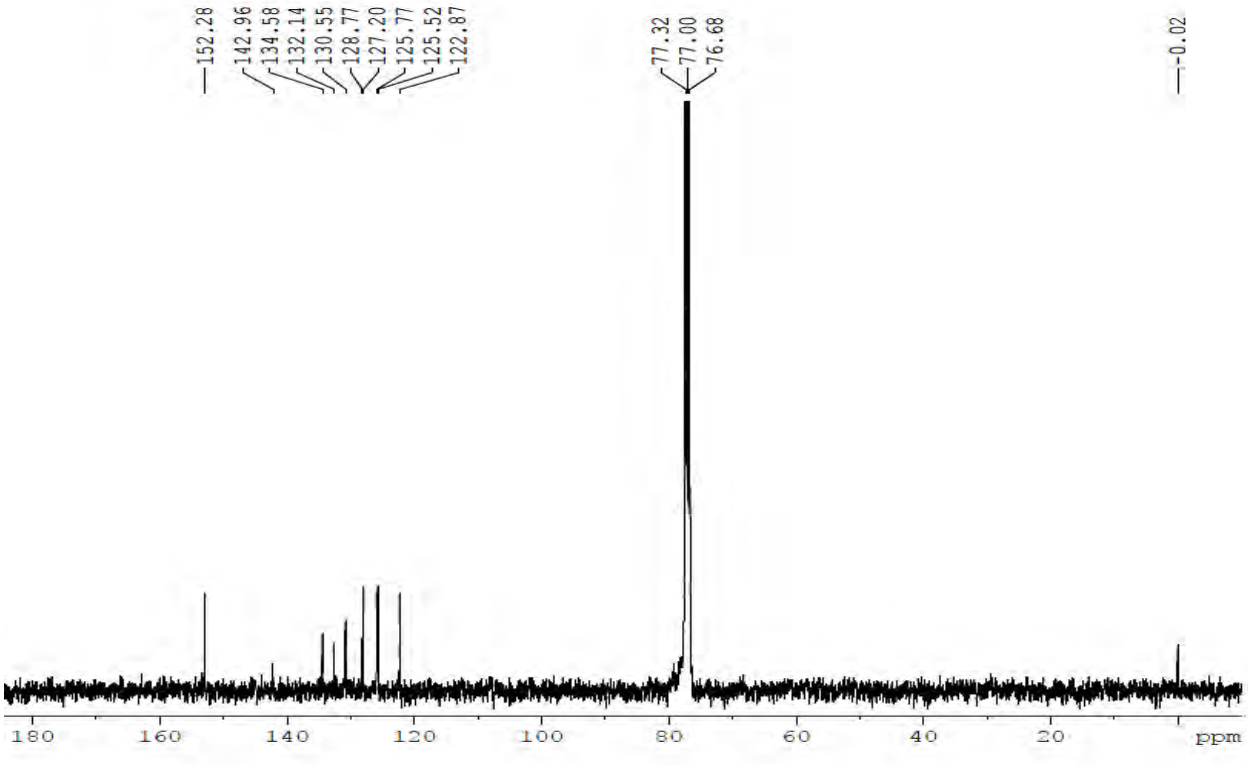

Fig. S44: ^{13}C NMR spectrum of 4'-nitro-biphenyl-3-ol

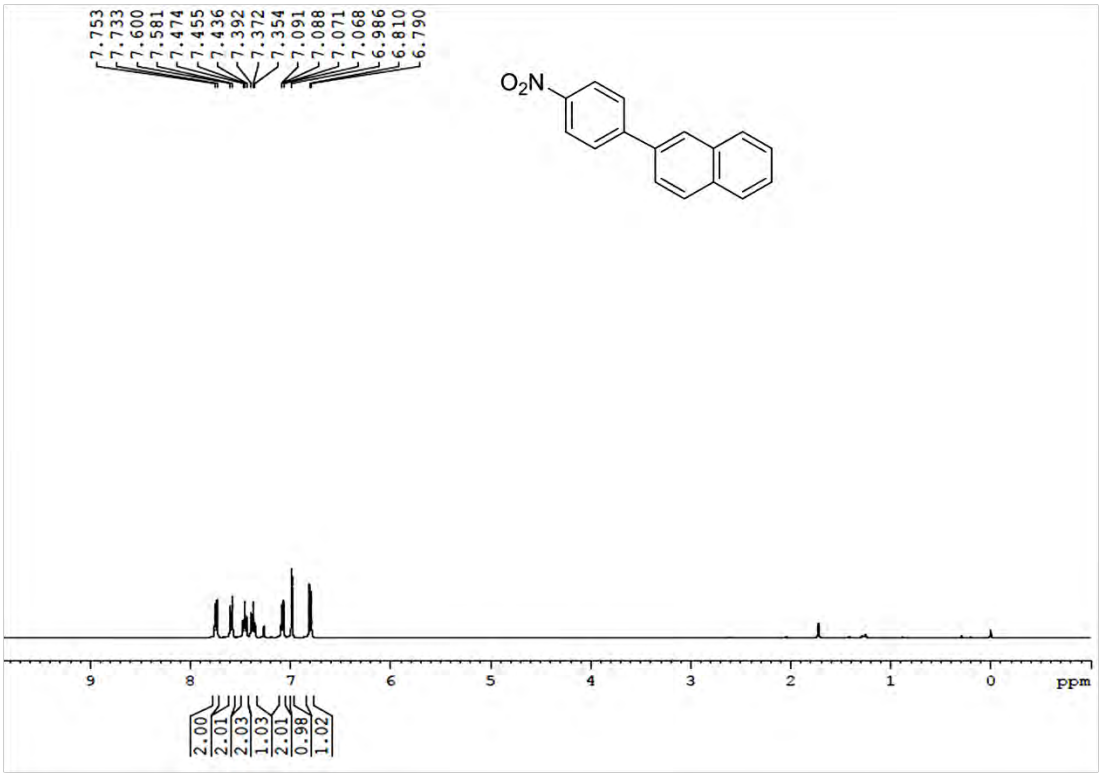

Fig. S45: ^{1}H NMR spectrum of 2-(4-nitro-phenyl)-naphthalene

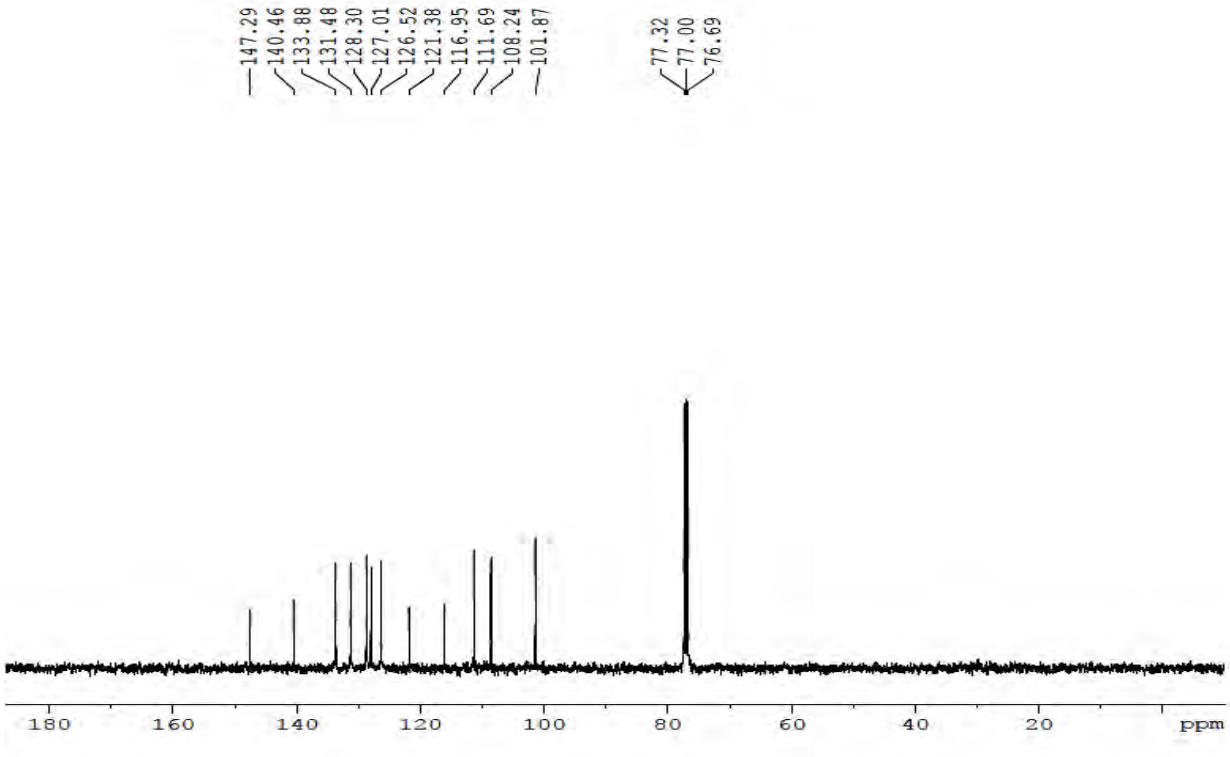

Fig. S46: ^{13}C NMR spectrum of 2-(4-nitro-phenyl)-naphthalene

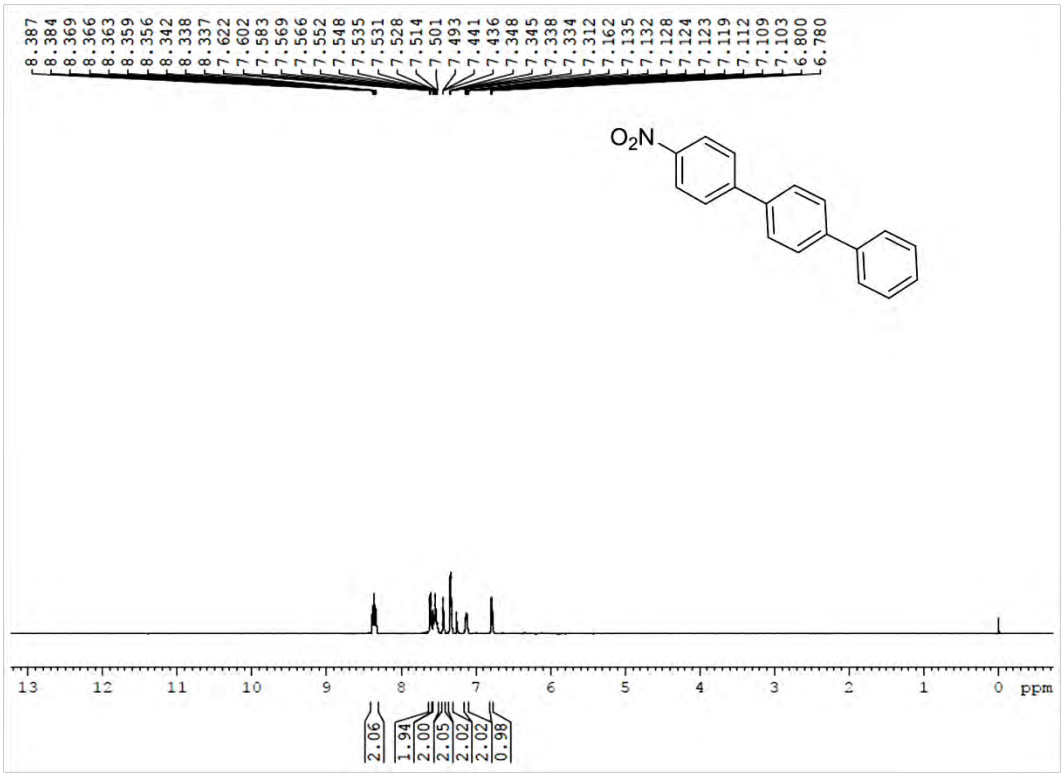

Fig. S47: ^{1}H NMR spectrum of 4-nitro-[1, 1'; 4', 1'']terphenyl

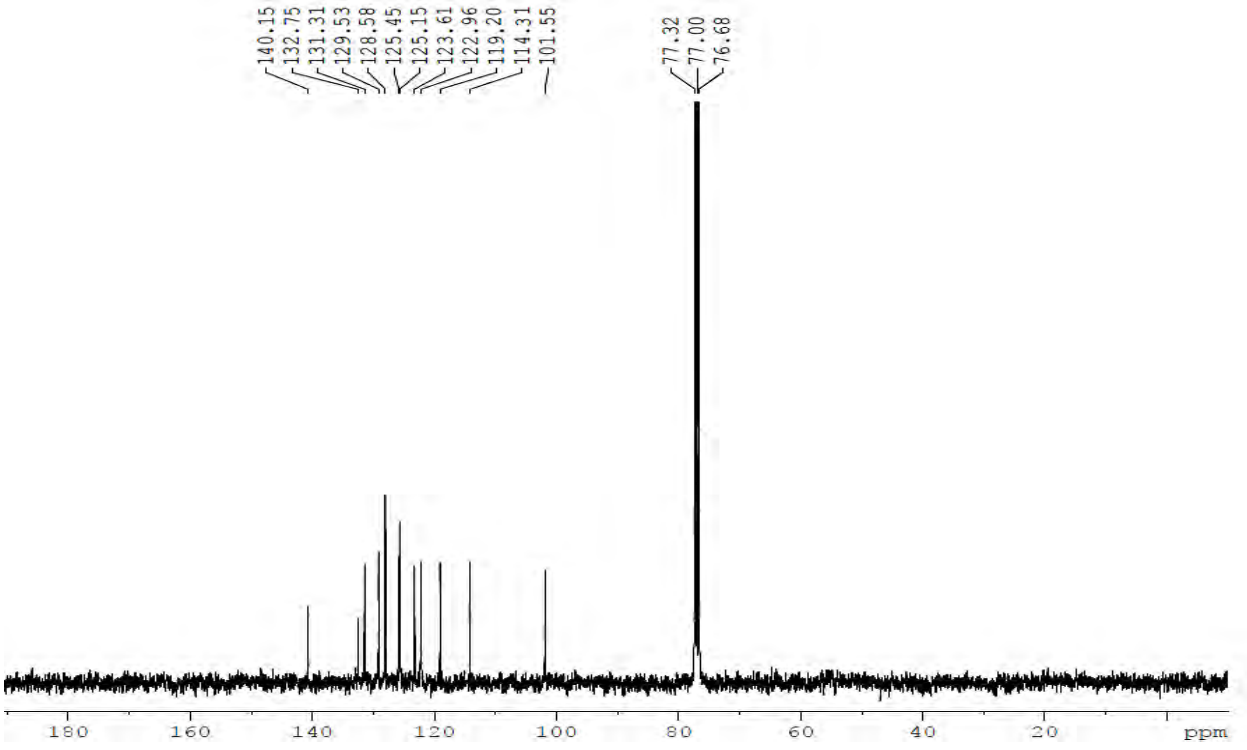

Fig. S48: ^{13}C NMR spectrum of 4-nitro-[1, 1'; 4', 1'']terphenyl

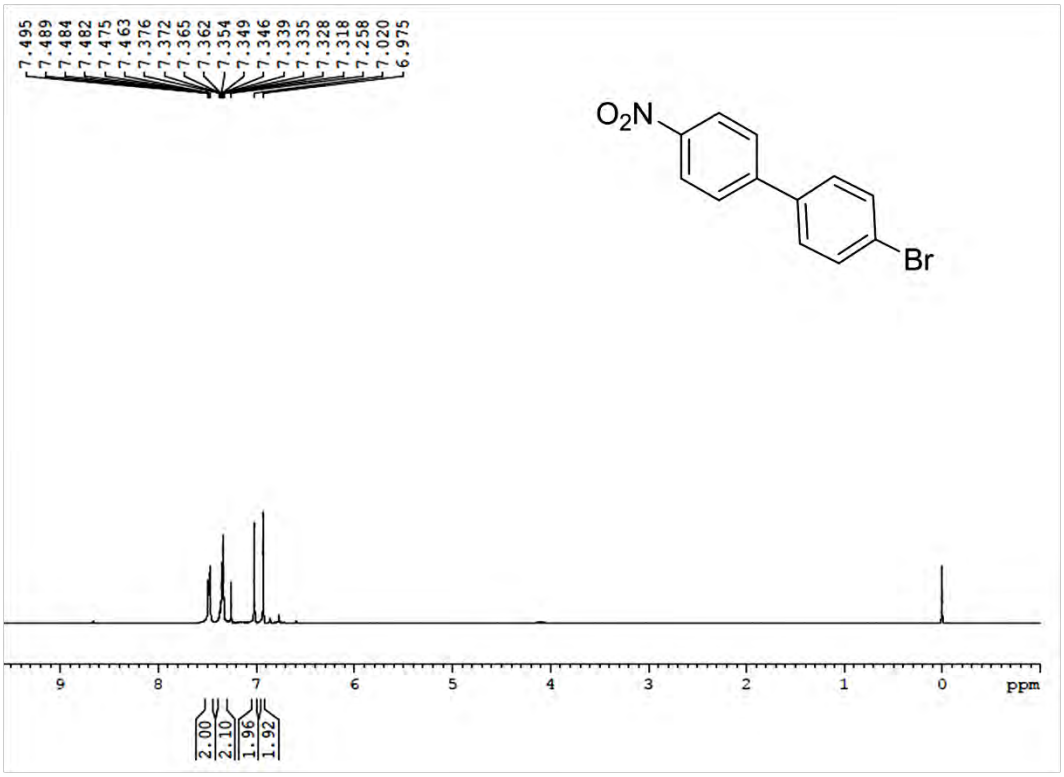

Fig. S49: ^{1}H NMR spectrum of 4'-bromo-4-nitro-biphenyl

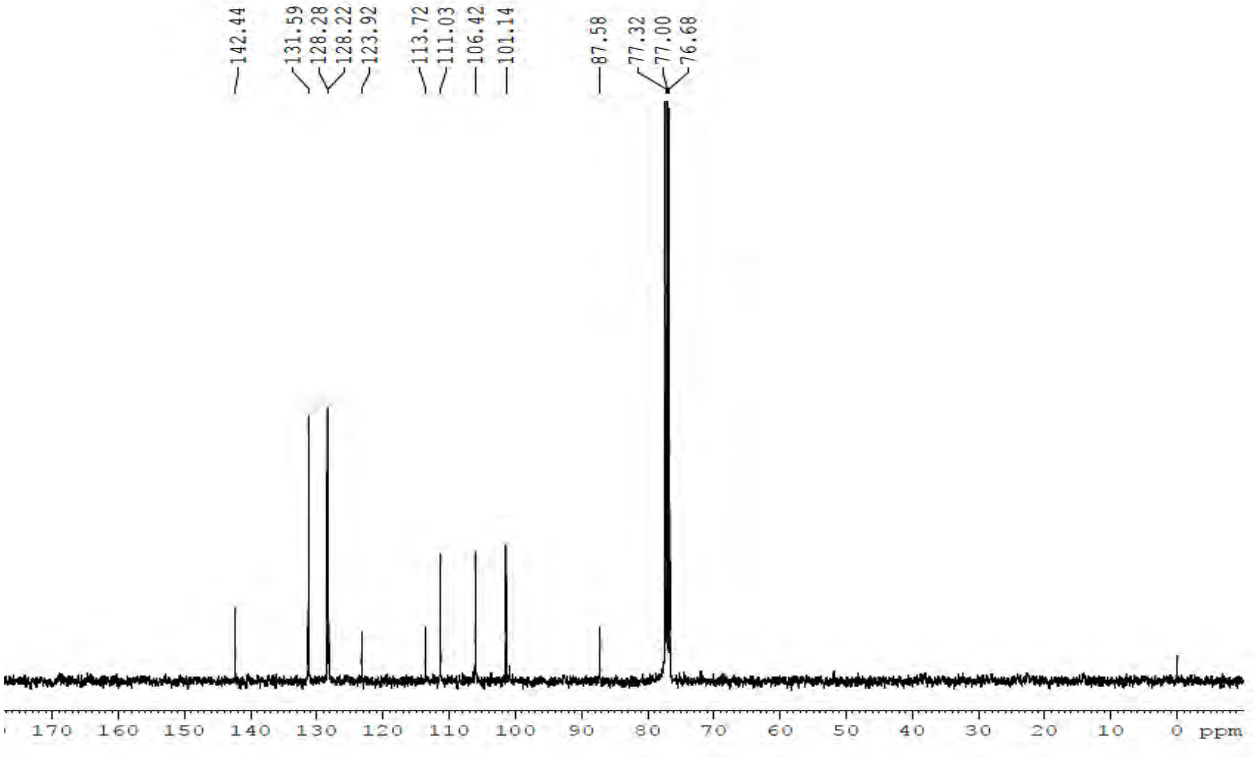

Fig. S50: ^{13}C NMR spectrum of 4'-bromo-4-nitro-biphenyl

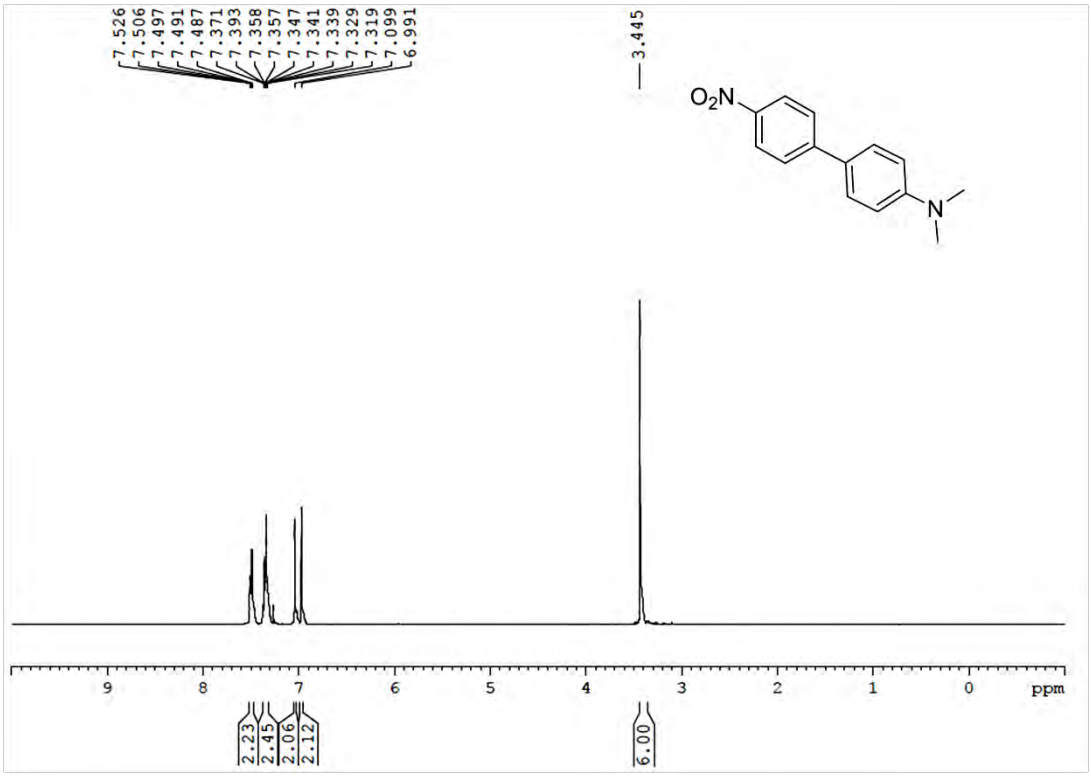

Fig. S51: ^{1}H NMR spectrum of dimethyl-(4'-nitro-biphenyl-4-yl)-amine

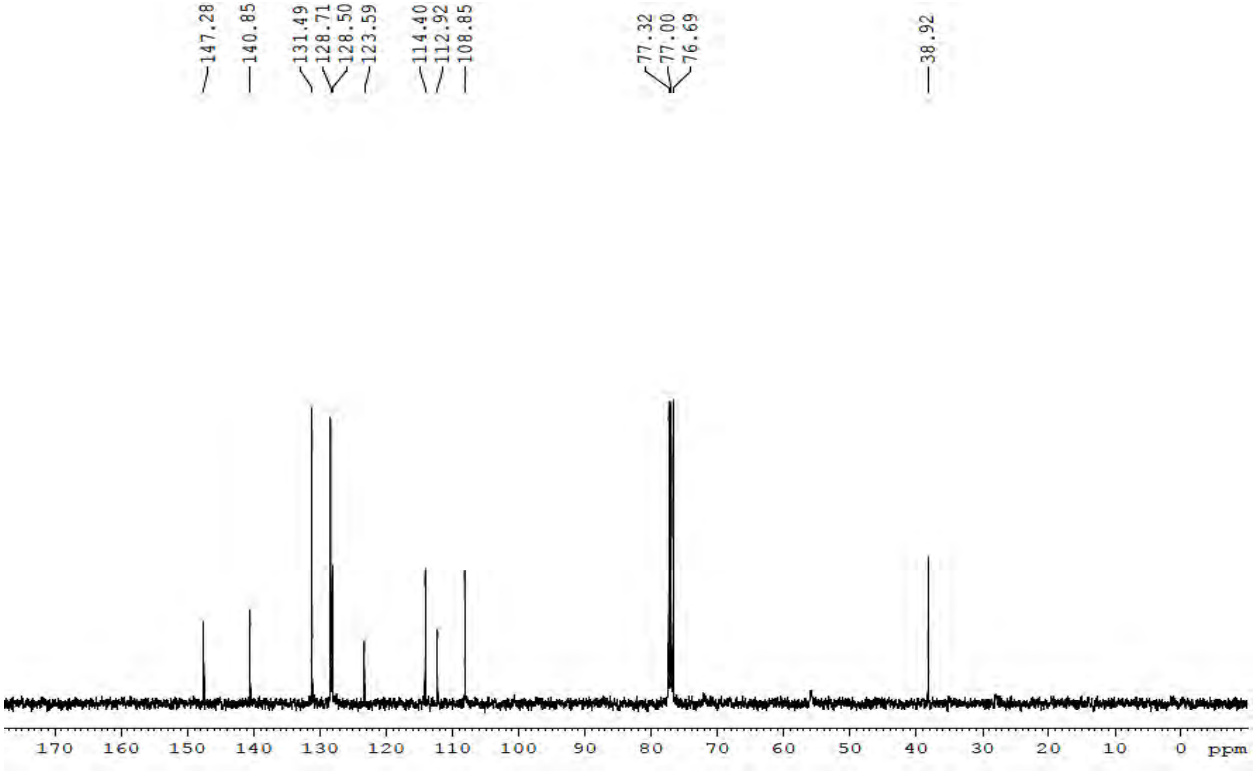

Fig. S52: ^{13}C NMR spectrum of dimethyl-(4'-nitro-biphenyl-4-yl)-amine

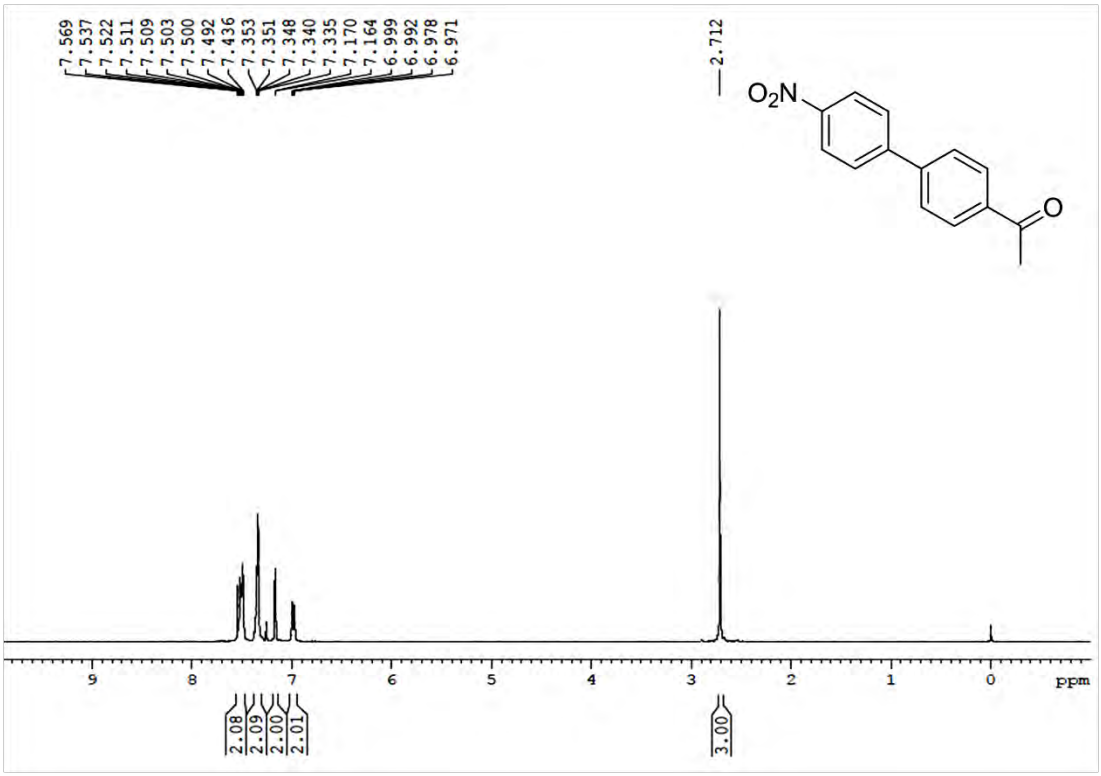

Fig. S53: ^{1}H NMR spectrum of 1-(4'-nitro-biphenyl-4-yl)-ethanone

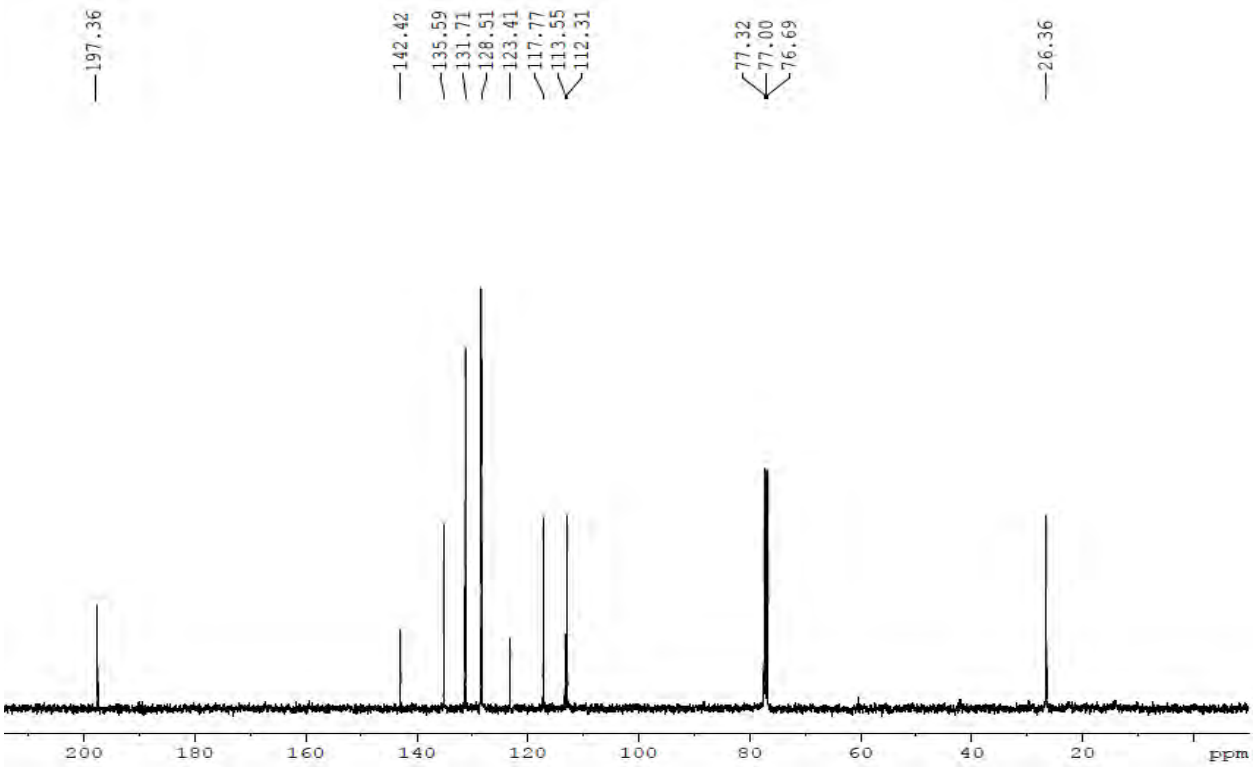

Fig. S54: ^{13}C NMR spectrum of 1-(4'-nitro-biphenyl-4-yl)-ethanone