Supplementary Information

Nickel (II) nanoparticles immobilized on EDTA-modified Fe_3O_4@SiO_2 nanospheres as efficient and recyclable catalysts for **ligand-free Suzuki-Miyaura Coupling of Aryl Carbamates and Sulfamates**

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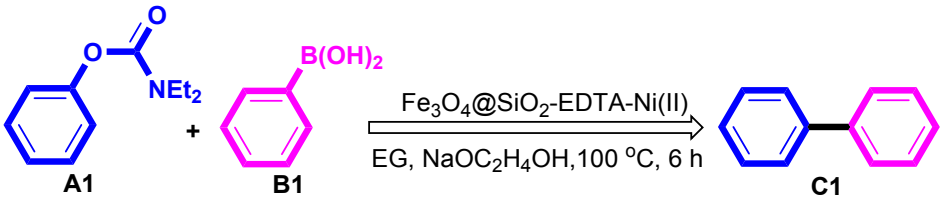
1. Reaction Optimization:

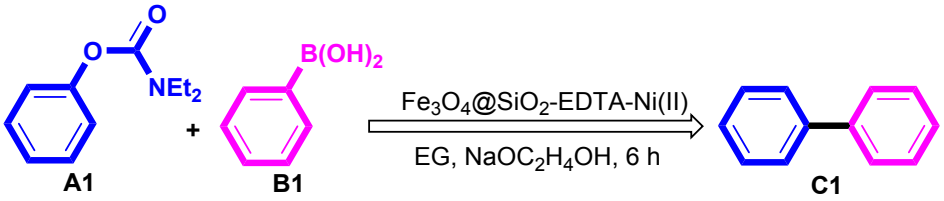
Table S1. Optimization of catalyst loading.[a]



Entry	Fe_3O_4@SiO_2-EDTA-Ni(II) (mol %)	Yield (%)[b]
1	0.5	64
2	1.0	91
3	1.5	91
4	2	91

[a] Reaction conditions: phenyl carbamate (1 mmol), phenylboronic acid (1 mmol), $NaOC_2H_4OH$ (2.0 mmol), Fe_3O_4@SiO_2-EDTA-Ni(II) catalyst, EG (3 mL), 100 °C, 6 h.
[b] Isolated yield.

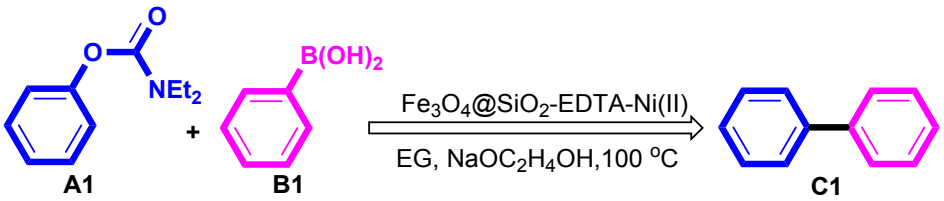
Table S2. Optimization of reaction temperature.[a]



Entry	Temperature (°C)	Yield (%)[b]
1	80	69
2	90	82
3	100	91
4	110	90
5	120	89

[a] Reaction conditions: phenyl carbamate (1 mmol), phenylboronic acid (1 mmol), $NaOC_2H_4OH$ (2.0 mmol), Fe_3O_4@SiO_2-EDTA-Ni(II) catalyst (0.018 g, 1 mol %), EG (3 mL), 6 h.
[b] Isolated yield.

Table S3. Optimization of reaction time.[a]



Entry	Time (h)	Yield (%)[b]
1	4	73
2	6	91
3	8	90
4	12	89

[a] Reaction conditions: phenyl carbamate (1 mmol), phenylboronic acid (1 mmol), $NaOC_2H_4OH$ (2.0 mmol), Fe_3O_4@SiO_2-EDTA-Ni(II) catalyst (0.018 g, 1 mol %), EG (3 mL), 100 °C.
[b] Isolated yield.

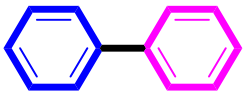
2. Experimental:

2.1 General experimental methods:

The products were characterized by comparison of their spectral and physical data such as NMR and CHNS with available literature data. ^1H and ^{13}C NMR spectra were recorded with Bruker Avance DPX 250MHz instruments with Me_4Si or solvent resonance as the internal standard. ^1H NMR spectroscopic data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q= quartet, quint = quintet, sext = sextet, sept = septet, br. = broad, m = multiplet), coupling constants (Hz), and integration. Elemental analysis was performed using Thermofinigan Flash EA-1112 CHNSO rapid elemental analyzer. Determination of the purity of the substrate and monitoring of the reaction were accomplished by thin-layer chromatography (TLC) on a silica-gel polygram SILG/UV 254 plates.

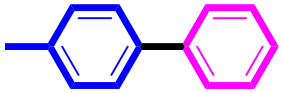
2.2 Chemicals:

All starting materials and solvents were purchased from the Merck, Flucka and Aldrich Chemical Companies in high purity.



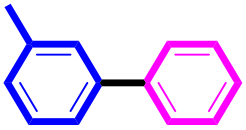
Biphenyl (C1):

Colorless crystals; mp = 69-70 ^{o}C; ^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.19-7.33 (m, 10H) ppm; ^{13}C-NMR (63 MHz, $CDCl_3$) δ: 145.3, 130.1, 127.5, 127.2 ppm; Anal. Calcd. for $C_{12}H_{10}$; C: 93.46, H: 6.54%, Found: C: 93.38, H: 6.60%.



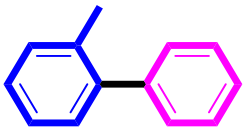
4-Methylbiphenyl (C2 and C19):

Colorless crystals; mp = 46-47 ^{o}C; ^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.62-7.74 (m, 2H), 7.37-7.55 (m, 7H), 2.53 (s, 3H) ppm; ^{13}C NMR (63 MHz, $CDCl_3$) δ: 138.1, 132.1, 131.4, 130.1, 129.4, 128.8, 127.8, 127.5, 21.6 ppm; Anal. Calcd. for $C_{13}H_{12}$; C: 92.81, H: 7.19%, Found: C: 92.78, H, 7.18%.



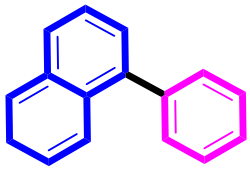
3-Methylbiphenyl (C3):

Colorless liquid; ^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.70 (, J= 9.7 Hz, 2H), 7.22-7.33 (m, 7H), 2.52 (s, 3H) ppm; ^{13}CNMR (63 MHz, $CDCl_3$) δ: 141.7, 140.4, 138.3, 129.5, 128.5, 128.2, 126.7, 124.7, 20.7 ppm; Anal. Calcd. for $C_{13}H_{12}$; C: 92.81, H, 7.19%, Found: C: 92.79, H, 7.16%.



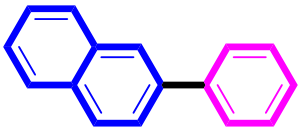
2-Methylbiphenyl (C4):

Colorless liquid; ^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.22-7.38 (m, 9H), 2.28 (s, 3H) ppm; ^{13}CNMR (63 MHz, $CDCl_3$) δ: 141.6, 141.3, 135.2, 130.3, 128.7, 128.5, 127.5, 127.0, 126.4, 125.2, 21.5 ppm; Anal. Calcd. for $C_{13}H_{12}$; C: 92.81, H, 7.19%, Found: C: 92.76, H, 7.17%.



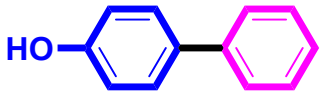
1-Phenylnaphthalene (C5):

Colorless liquid; ^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.82-7.99 (m, 7H), 7.24-7.52 (m, 5H) ppm; ^{13}C NMR (63 MHz, $CDCl_3$) δ: 141.7, 140.6, 137.3, 133.5, 131.2, 129.2, 128.6, 128.4, 126.8, 126.2, 126.0, 125.9, 125.0 ppm; Anal. Calcd. for $C_{16}H_{12}$; C: 94.08, H: 5.92%, Found: C: 93.98, H: 5.98%.



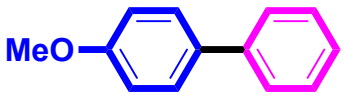
2-Phenylnaphthalene (C6):

Colorless crystals; mp = 98-100 ^{o}C;.^{1}H NMR (250 MHz, $CDCl_3$) δ: 8.02 (s, 1H), 7.87-7.90 (m, 4H), 7.68-7.79 (m, 2H), 7.41-7.49 (m, 3H), 7.36 (d, J= 9.7 Hz, 2H) ppm;^{13}C NMR (63 MHz, $CDCl_3$) δ: 141.3, 138.6, 134.2, 133.9, 132.9, 132.2, 128.7, 127.1, 127.0, 126.9, 125.9, 125.8 ppm; Anal. Calcd. for $C_{16}H_{12}$; C: 94.08%, H, 5.92, Found: C: 94.01, H: 5.91%.



Biphenyl-4-ol (C7):

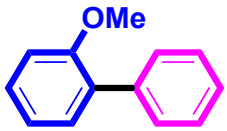
Colorless crystals, mp = 165-166 ^{o}C. ^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.33-7.17 (m, 7H), 6.94-6.88 (m, 2H), 4.00 (s, br, 1H) ppm; ^{13}CNMR (63 MHz, $CDCl_3$) δ: 156.8, 142.2, 135.8, 132.0, 128.7, 128.5, 128.4, 120.2; Anal. Calcd. for $C_{12}H_{10}O$; C: 84.68%, H, 5.92, Found: C: 84.91, H: 5.99%.



4-Methoxybiphenyl (C8):

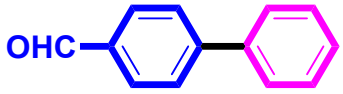
Colorless crystals, mp = 88-90 ^{o}C. ^{1}H NMR (250 MHz, $CDCl_3$) δ: 7.33-7.22 (m, 7H), 7.08-7.03 (m, 2H), 3.87 (s, 3H) ppm; ^{13}CNMR (63 MHz, $CDCl_3$) δ: 153.5, 142.8, 136.1, 133.0, 129.5,

128.5, 128.2, 118.9, 55.35 ppm; Anal. Calcd. for $C_{13}H_{12}O$; C: 84.75, H: 6.57, Found: C: 84.68, H: 6.59 %.



2-Methoxybiphenyl (C9):

Colorless liquid. ^{1}H NMR (250 MHz, $CDCl_3$) *δ:* 7.54 (d, *J*= 8.1 Hz, 2H), 7.29-7.42 (m, 5H), 6.97-7.04 (m, 2H), 3.79 (s, 3H) ppm;^{13}C NMR (63 MHz, $CDCl_3$) *δ:* 157.0, 138.9, 131.2, 129.6, 128.9, 128.1, 127.0, 121.1, 111.5, 55.6 ppm; Anal. Calcd. for $C_{13}H_{12}O$; C: 84.75, H: 6.57, Found: C: 84.67, H: 6.59%.

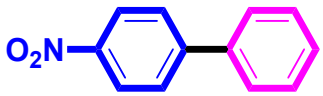


4-Biphenylcarbaldehyde (C10):

Colorless crystals, mp = 57-58 ^{o}C. ^{1}H NMR (250 MHz, $CDCl_3$) *δ:* 10.13 (s, 1H), 7.38-7.23 (m, 7H), 7.07-7.00 (m, 2H) ppm;^{13}C NMR (63MHz, $CDCl_3$) *δ:* 196.5, 153.4, 133.4, 126.3, 125.9, 125.6, 124.3, 120.8, 116.1 ppm; Anal. Calcd. for $C_{13}H_{10}O$; C: 85.69, H: 5.53, Found: C: 85.65, H: 5.54 %.

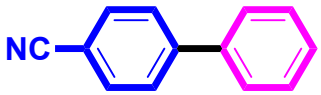
1-(4-Biphenylyl)ethanone (C11):

Colorless crystals, mp = 115-116 ^{o}C. ^{1}H NMR (250 MHz, $CDCl_3$) *δ:* 7.85 (dd, *J*= 7.5 Hz, *j*= 2 Hz, 2H), 7.41 (dd, *J*= 7.5 Hz, *j*= 2 Hz, 2H), 7.35-7.29 (m, 5H), 2.50 (m, 3H) ppm; ^{13}C NMR (63 MHz, $CDCl_3$) *δ:* 197.2, 153.1, 135.9, 130.1, 128.9, 128.8, 128.7, 123.9, 117.9, 26.6 ppm; Anal. Calcd. for $C_{14}H_{12}O$; C: 85.68, H: 6.16 %, Found: C: 85.61, H: 6.19 %.



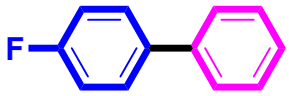
4-Nitrobiphenyl (C12):

Light yellow crystals, mp = 111-112 ^{o}C. ^{1}H NMR (250 MHz, $CDCl_3$) *δ:* 8.31 (d, *J*= 9.0 Hz, 2H), 7.45-7.76 (m, 7H) ppm; ^{13}C NMR (63 MHz, $CDCl_3$) *δ:* 147.8, 141.1, 129.7, 129.5, 128.9, 127.9, 127.6, 124.9 ppm; Anal. Calcd. for $C_{12}H_9NO_2$; C: 72.35, H: 4.55, N: 7.03, Found: C: 72.32, H: 4.51, N: 7.06 %.



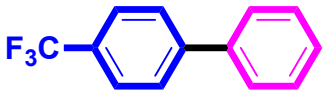
4-Biphenylcarbonitrile (C13):

Colorless crystals, mp = 81-82 °C. ^{1}H NMR (250 MHz, $CDCl_3$) *δ:* 7.58-7.76 (m, 6H), 7.41-7.48 (m, 3H) ppm; ^{13}C NMR (63 MHz, $CDCl_3$) *δ*: 146.2, 139.8, 132.1, 129.9, 129.3, 128.7, 127.3, 118.6, 110.8 ppm; Anal. Calcd. for $C_{13}H_9N$; C: 87.12, H: 5.06, N: 7.82%, Found: C: 87.08, H: 5.01, N: 7.89%.



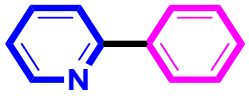
4-Fluorobiphenyl (C14):

Colorless crystals, mp = 72-74 °C. ^{1}H NMR (250 MHz, $CDCl_3$) *δ:* 7.53-7.58 (m, 2H), 7.34-7.45 (m, 5H), 7.13 (t, *J*= 9.0 Hz, 2H) ppm; ^{13}C NMR (63 MHz, $CDCl_3$) *δ:* 163.7, 161.1, 137.1, 128.8, 128.7, 127.5, 127.4, 115.3 ppm; Anal. Calcd. For: $C_{12}H_9F$; C: 83.70, H: 5.27%, Found. C: 83.55, H: 5.38%.



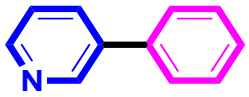
4-(Trifluoromethyl)biphenyl (C15):

Colorless crystals, mp = 64-65 °C. ^{1}H NMR (250 MHz, $CDCl_3$) *δ:* 7.46-7.37 (m, 5H), 7.28 (d, *J*= 7.5 Hz, 2H) 7.08 (d, *J*= 7.5 Hz, 2H) ppm; ^{13}C NMR (63 MHz, $CDCl_3$) *δ:* 144.5, 139.5, 132.1, 131.9, 130.9, 128.8, 128.4, 125.1, 123.4 ppm; Anal. Calcd. For: $C_{13}H_9F_3$; C: 70.27, H: 4.08%, Found. C: 70.24, H: 4.11%.



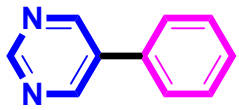
2-Phenylpyridine (C16):

Colorless crystals, mp = 75-76 °C. ^{1}H NMR (250 MHz, $CDCl_3$) *δ:* 8.71 (s, 1H), 7.43-7.99 (m, 7H), 7.23 (d, *J*= 9.0 Hz, 1H) ppm;^{13}C NMR (63 MHz, $CDCl_3$) *δ:* 157.1, 149.3, 139.5, 137.0, 127.7, 126.3, 122.4, 120.3 ppm; Anal. Calcd. For: $C_{11}H_9N$; C: 85.13, H: 5.85, N: 9.03%, Found. C: 85.31, H: 5.52, N: 9.13%.



3-Phenylpyridine (C17):

Colorless crystals, mp = 114-116 °C. ^{1}H NMR (250 MHz, $CDCl_3$) *δ:* 8.86 (s, 1H), 8.59 (d, *J*= 4.0 Hz, 1H), 7.86-7.88 (m, 1H), 7.33-7.59 (m, 6H) ppm; ^{13}C NMR (63 MHz, $CDCl_3$) *δ:* 149.4, 149.3, 137.8, 136.8, 134.5, 129.1, 128.3, 127.1, 123.4 ppm; Anal. Calcd. For: $C_{11}H_9N$; C: 85.13, H: 5.85, N: 9.03%, Found. C: 85.26, H: 5.57, N: 9.14%.

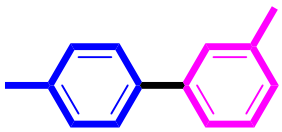


5-Phenylpyrimidine (C18):

Colorless crystals, mp = 39-41 °C. ^{1}H NMR (250 MHz, $CDCl_3$) *δ:* 9.23 (s, 1H), 8.86 (d, *J*= 8.0 Hz, 2H), 7.53-7.48 (m, 5H) ppm; ^{13}C NMR (63 MHz, $CDCl_3$) *δ:* 157.5, 153.0, 132.4, 130.9, 129.2, 128.8, 127.1; Anal. Calcd. For: $C_{10}H_8N_2$; C: 76.90, H: 5.16, N: 17.94%, Found. C: 76.84, H: 5.10, N: 18.05%.

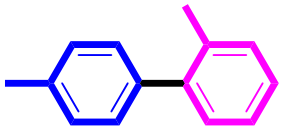
4,4'-Dimethylbiphenyl (C20):

Colorless crystals, mp = 118-120 °C. ^{1}H NMR (250 MHz, $CDCl_3$) *δ:* 7.40 (d, *J*= 6.3 Hz, 4H), 7.11 (d, *J*= 6.3 Hz, 4H), 2.33 (s, 6H) ppm; ^{13}CNMR (63MHz, $CDCl_3$) *δ:* 141.6, 136.7, 129.8, 129.3, 127.0, 126.5, 19.8 ppm; Anal. Calcd. For: $C_{14}H_{14}$; C: 92.26, H: 7.74%, Found. C: 92.35, H: 7.64%.



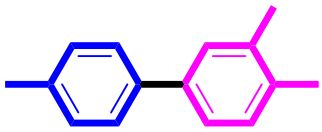
3,4'-Dimethylbiphenyl (C21):

Colorless liquid; ^{1}H NMR (250 MHz, $CDCl_3$) *δ:* 8.06 (s, 1H), 7.89 (d, *J*= 7.5 Hz, 2H), 7.55-7.47 (m, 5H), 2.47 (s, 3H), 2.28 (s, 3H) ppm; ^{13}CNMR (63 MHz, $CDCl_3$) *δ:* 158.4, 137.9, 130.9, 129.2, 129.0, 128.9, 127.0, 126.0, 123.3, 118.7, 30.3, 28.9 ppm; Anal. Calcd. For: $C_{14}H_{14}$; C: 92.26, H: 7.74%, Found. C: 92.33, H: 7.67%.



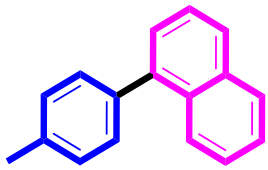
2,4'-Dimethylbiphenyl (C22):

Colorless liquid; ^{1}H NMR (250 MHz, $CDCl_3$) *δ:* 7.64 (dd, *J*= 7.5 Hz, *j*= 2 Hz, 2H), 7.46 (dd, *J*= 7.5 Hz, *j*= 2 Hz, 2H), 7.21 (m, 3H), 6.79 (s, 1H), 2.25 (s, 3H), 2.11 (s, 3H) ppm; ^{13}CNMR (63 MHz, $CDCl_3$) *δ:* 157.2, 134.1, 130.9, 128.8, 128.7, 126.2, 125.9, 125.8, 124.9, 120.5, 23.7, 22.3 ppm; Anal. Calcd. For: $C_{14}H_{14}$; C: 92.26, H: 7.74%, Found. C: 92.30, H: 7.68%.



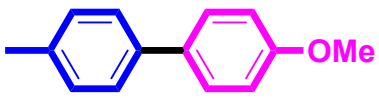
3,4,4'-Trimethylbiphenyl (C23):

Colorless crystals, mp = 75-77 ^{o}C. ^{1}H NMR (250 MHz, $CDCl_3$) *δ:* 7.25-7.18 (m, 2H), 7.00 (d, *J*= 6.3 Hz, 2H), 6.92-6.87 (m, *J*= 6.3 Hz, 3H), 2.33 (s, 3H), 2.32 (s, 3H), 2.13 (s, 3H) ppm; ^{13}CNMR (63 MHz, $CDCl_3$) *δ:* 155.5, 139.6, 133.6, 131.6, 129.1, 128.2, 126.5, 125.1, 122.3, 118.6, 29.1, 28.1, 21.3 ppm; Anal. Calcd. For: $C_{15}H_{16}$; C: 91.78, H: 8.22%, Found. C: 91.83, H: 8.25%.



1-(4-Methylphenyl)naphthalene (C24):

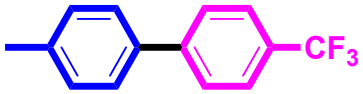
Colorless crystals, mp = 49-51 ^{o}C. ^{1}H NMR (250 MHz, $CDCl_3$) *δ:* 7.84-7.93 (m, 3H), 7.29-7.53 (m, 8H), 2.46 (s, 3H) ppm; ^{13}CNMR (62.9 MHz, $CDCl_3$) *δ:* 140.3, 137.8, 136.9, 133.7, 131.7, 129.9, 129.0, 128.2, 127.4, 126.8, 126.1, 125.9, 125.7, 125.3, 21.2 ppm; Anal. Calcd. For: $C_{17}H_{14}$; C: 93.54, H: 6.46%, Found. C: 93.39, H: 6.60%.



4-Methoxy-4'-methylbiphenyl (C25):

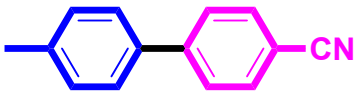
Colorless crystals, mp = 109-111 ^{o}C. ^{1}H NMR (250 MHz, $CDCl_3$) *δ:* 6.97 (d, *J*= 7.0 Hz, 2H), 6.88 (d, *J*= 7.0 Hz, 2H), 6.75-6.65 (m, 5H), 3.71 (s, 3H), 2.08 (s, 3H) ppm; ^{13}CNMR (63 MHz,

$CDCl_3$) *δ:* 158.1, 138.1, 130.1, 127.7, 126.7, 125.0, 120.9, 117.2, 66.9, 24.3 ppm; Anal. Calcd. For: $C_{14}H_{14}O$; C: 84.81, H: 7.12%, Found. C: 84.78, H: 7.13%.



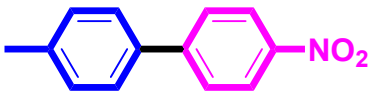
4-Methyl-4'-(trifluoromethyl)biphenyl (C26):

Colorless crystals, mp = 123-124 °C. ^{1}H NMR (250 MHz, $CDCl_3$) *δ:* 7.70 (s, 4H), 7.48 (d, *J*= 6.5 Hz, 2H), 7.27 (d, *J*= 9.2 Hz, 2H), 2.40 (s, 3H) ppm; ^{13}CNMR (63 MHz, $CDCl_3$) *δ:* 144.6, 138.0, 136.8, 129.4, 128.7, 128.4, 127.0, 125.6, 123.0, 21.1 ppm; Anal. Calcd. For: $C_{14}H_{11}F_3$; C: 71.18, H: 4.69%, Found. C: 71.01, H: 4.55%.



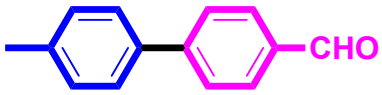
4'-Methyl-4-biphenylcarbonitrile (C27):

Colorless crystals, mp = 107-109 °C. ^{1}H NMR (250 MHz, $CDCl_3$) *δ:* 7.85 (d, *J*= 7.5 Hz, 2H), 7.66 (d, *J*= 7.5 Hz, 2H), 7.52-7.37 (m, 4H), 2.36 (s, 4H) ppm; ^{13}CNMR (63 MHz, $CDCl_3$) *δ:* 157.5, 146.3, 132.4, 130.9, 128.8, 127.8, 126.1, 124.4, 122.7, 107.0, 24.7 ppm; Anal. Calcd. For: $C_{14}H_{11}N$; C: 87.01, H: 5.74, N: 7.25%, Found. C: 86.92, H: 5.71, N: 7.27%.



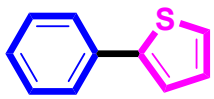
4-Methyl-4'-nitrobiphenyl (C28):

Light yellow crystals, mp = 139-140 °C. ^{1}H NMR (250 MHz, $CDCl_3$) *δ:* 8.22-8.18 (m, 2H), 7.57-7.52 (dd, *J*= 9.0 Hz, *j*= 1.7 Hz, 2H), 7.42-7.36 (m, 4H), 2.25 (s, 3H) ppm; ^{13}CNMR (63 MHz, $CDCl_3$) *δ:* 156.5, 143.7, 135.3, 131.9, 128.7, 128.5, 125.2, 117.7, 27.7 ppm; Anal. Calcd. For: $C_{13}H_{11}NO_2$; C: 73.23, H: 5.20, N: 6.57, Found. C: C: 73.16, H: 5.16, N: 6.66 %.



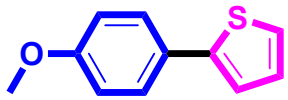
4'-Methyl-4-biphenylcarbaldehyde (C29):

Colorless crystals, mp = 105-107 ^{o}C. ^{1}H NMR (250 MHz, $CDCl_3$) *δ:* 10.27 (s, 1H), 7.92-7.86 (m, 4H), 7.51-7.45 (m, 2H), 7.28 (dd, *J*= 7.5 Hz, *j*= 2.0 Hz, 2H), 2.06 (s, 3H) ppm; ^{13}CNMR (63 MHz, $CDCl_3$) *δ:* 200.2, 156.2, 142.8, 130.9, 128.7, 126.2, 125.9, 120.5, 22.3 ppm; Anal. Calcd. For: $C_{14}H_{12}O$; C: 85.68, H: 6.16 %, Found. C: 85.61, H: 6.13 %.



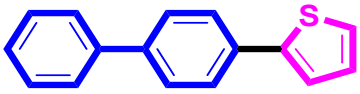
2-Phenylthiophene (C30):

Colorless liquid; ^{1}H NMR (250 MHz, $CDCl_3$) *δ:* 7.30-7.22 (m, 5H), 7.15-6.85 (m, 2H), 6.83 (s, 4H) ppm; ^{13}CNMR (63 MHz, $CDCl_3$) *δ:* 155.7, 143.5, 127.5, 127.3, 127.2, 123.8, 119.7, 107.0 ppm; Anal. Calcd. For: $C_{10}H_8S$; C: 74.96, H: 5.03, S: 20.01%, Found. C: 74.91, H: 5.01, S: 20.08%.



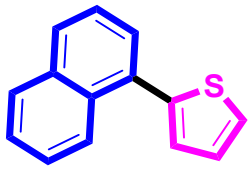
2-(4-Methoxyphenyl)thiophene (C31):

Colorless crystals, mp = 105-107 ^{o}C. ^{1}H NMR (250 MHz, $CDCl_3$) *δ:* 7.53 (d, *J*= 4.7 Hz, 2H), 7.20-7.26 (m, 2H), 6.91-7.06 (m, 3H), 3.83 (s, 3H) ppm; ^{13}C NMR (63 MHz, $CDCl_3$) *δ:* 159.1, 143.9, 127.8, 127.4, 127.2, 123.8, 122.0, 114.1, 55.4 ppm; Anal. Calcd. For: $C_{11}H_{10}OS$; C: 69.44, H: 5.30, S: 16.85 %, Found. C: 69.51, H: 5.39, S: 16.90 %.



2-(Biphenyl-4-yl)thiophene (C32):

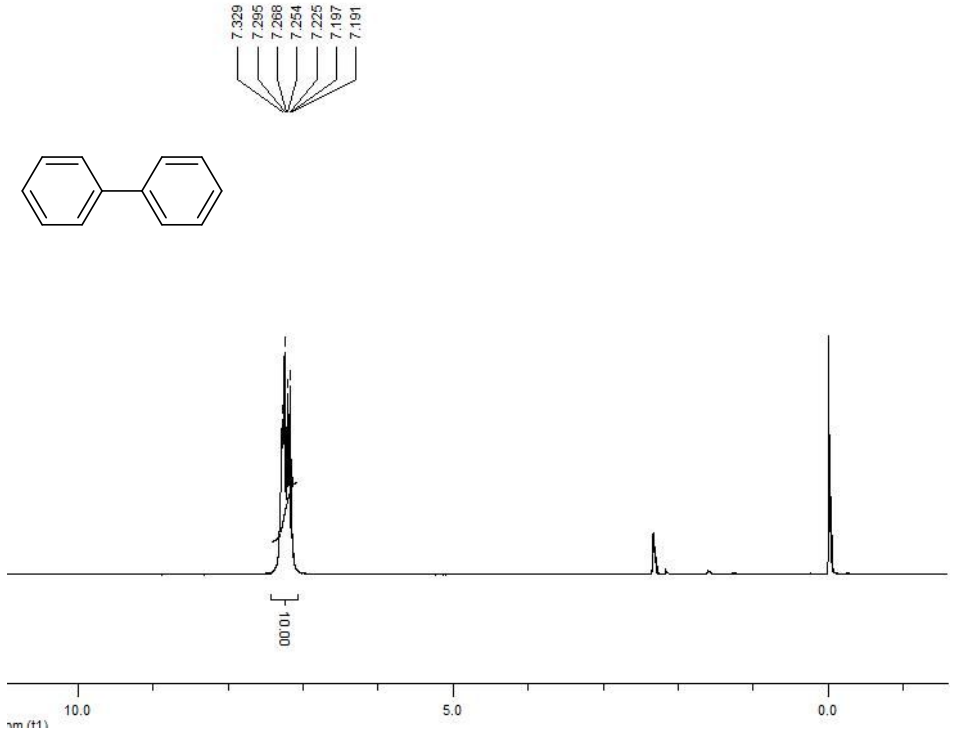
Colorless crystals, mp = 171-173 ^{o}C. ^{1}H NMR (250 MHz, $CDCl_3$) *δ:* 7.54-7.59 (m, 5H), 7.32-7.49 (m, 7H) ppm; ^{13}C NMR (63 MHz, $CDCl_3$): *δ:* 150.1, 142.4, 141.3, 133.1, 129.6, 128.8, 128.3, 128.0, 127.8, 127.5 ppm; Anal. Calcd. for $C_{16}H_{12}S$; C: 81.32, H: 5.12, S: 13.57%, Found: C: 81.21, H: 5.07, S: 13.73%.



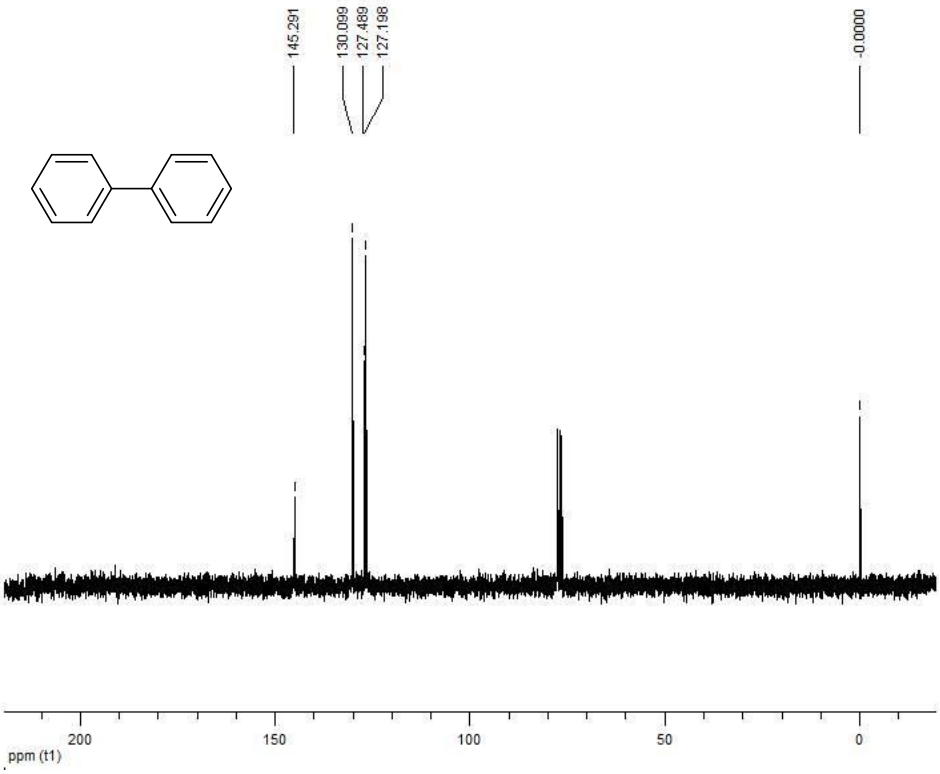
2-(Naphthalen-1-yl)thiophene (C33):

Colorless liquid; ^{1}H NMR (250 MHz, $CDCl_3$) *δ:* 8.22-8.25 (m, 1H), 7.84-7.97 (m, 2H), 7.44-7.58 (m, 3H), 7.18-7.32 (m, 4H) ppm; ^{13}C NMR (63 MHz, $CDCl_3$) *δ:* 141.1, 133.25, 132.0, 131.5, 129.3, 128.7, 127.5, 127.2, 126.8, 126.7, 125.8, 125.2 ppm; Anal. Calcd. for $C_{14}H_{10}S$; C: 79.96, H: 4.79, S: 15.25%, Found: C: 79.89, H: 4.77, S: 15.34%.

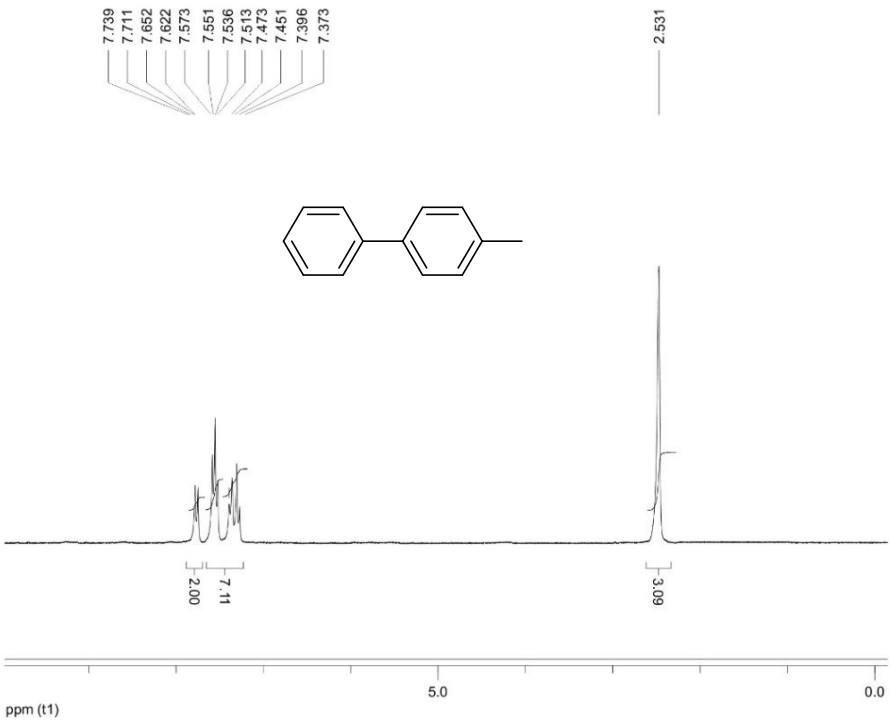
3 NMR Spectra of Compounds:



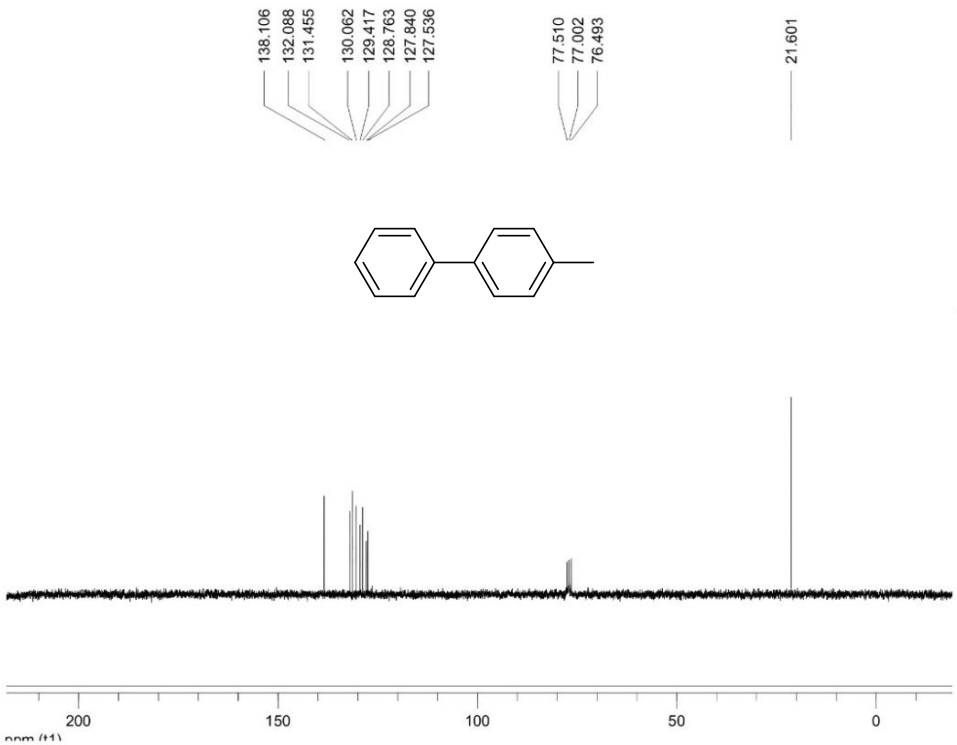
Scheme S1. ^{1}H-NMR spectra (250 MHz) of biphenyl (**C1**) in $CDCl_3$.



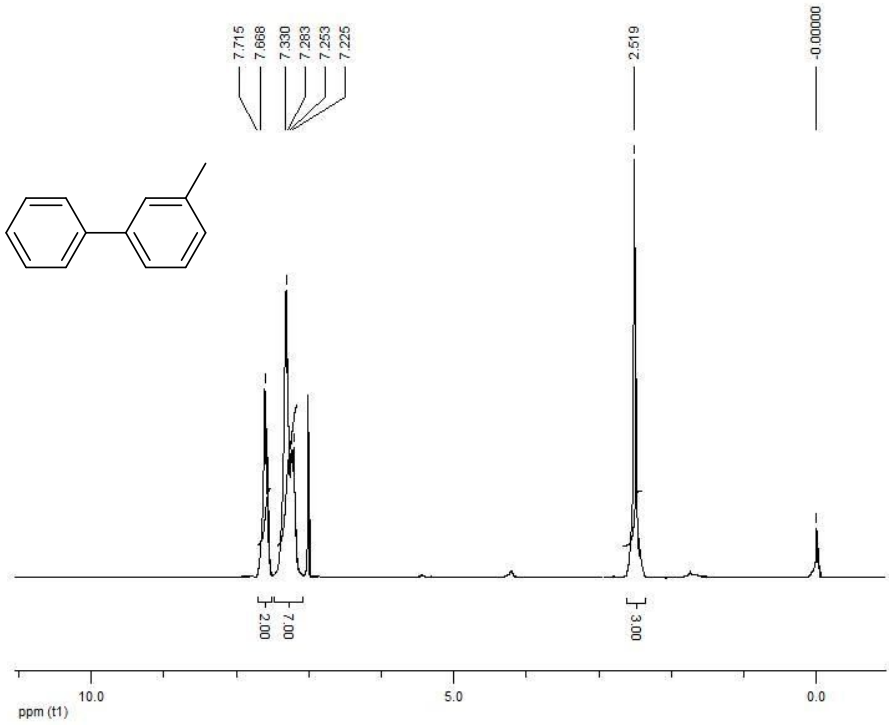
Scheme S2. ^{13}C-NMR spectra (63 MHz) of biphenyl (**C1**) in $CDCl_3$.



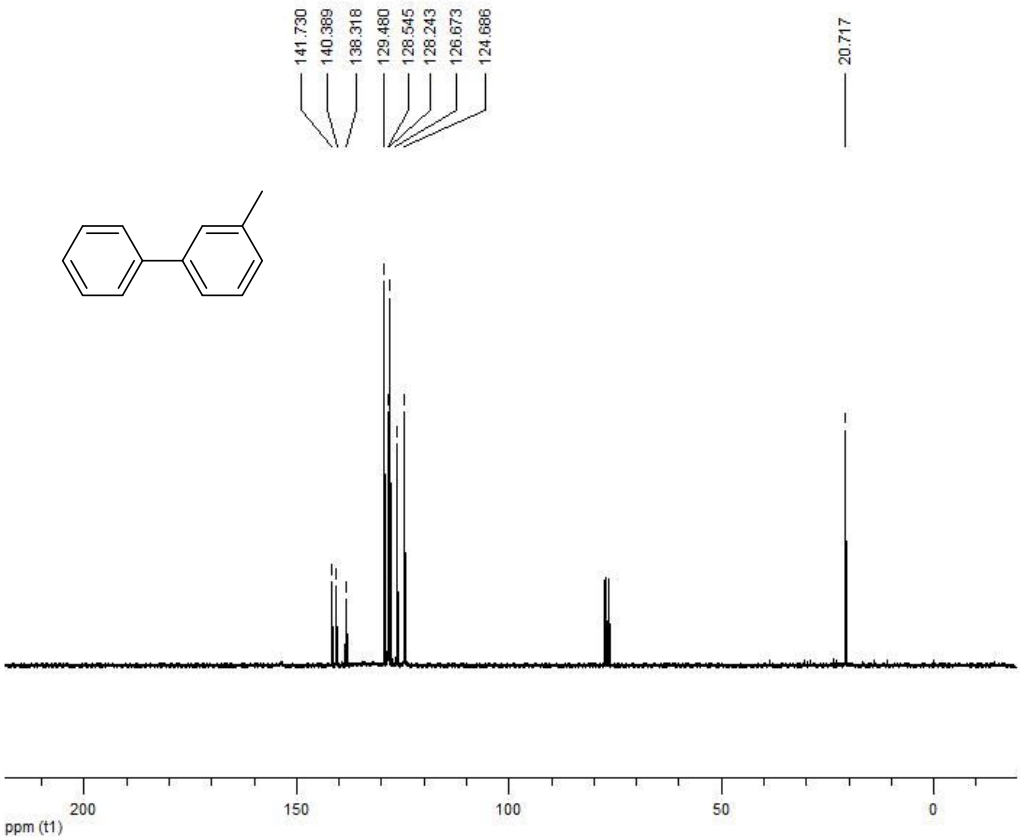
Scheme S3. ^{1}H-NMR spectra (250 MHz) of 4-methylbiphenyl **(C2 and C19)** in $CDCl_3$.



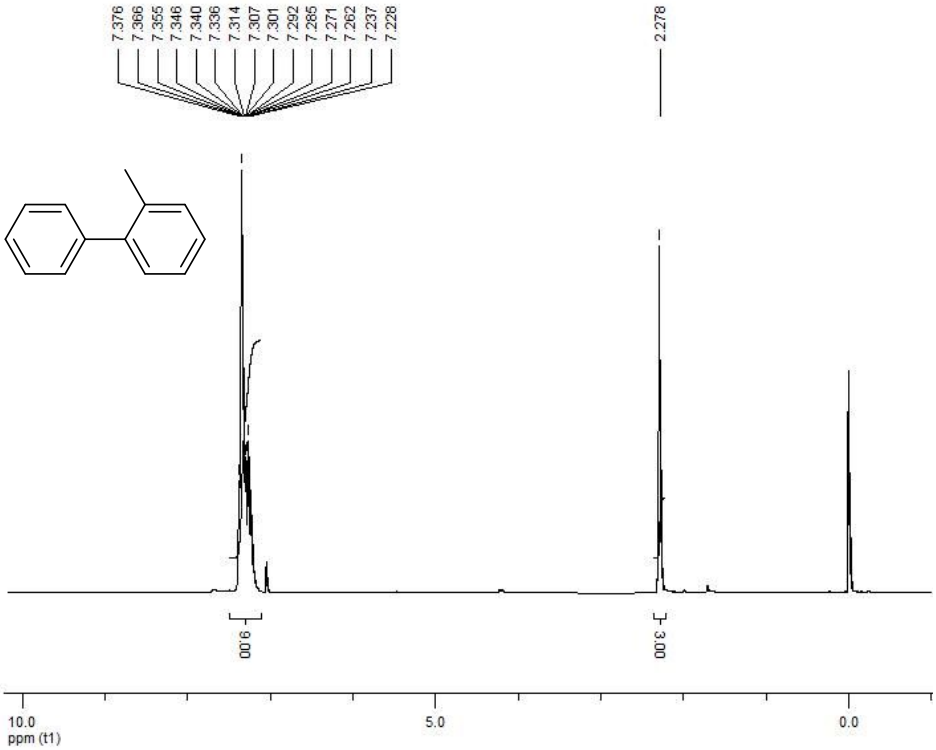
Scheme S4. ^{13}C-NMR spectra (63 MHz) of 4-methylbiphenyl **(C2 and C19)** in $CDCl_3$.



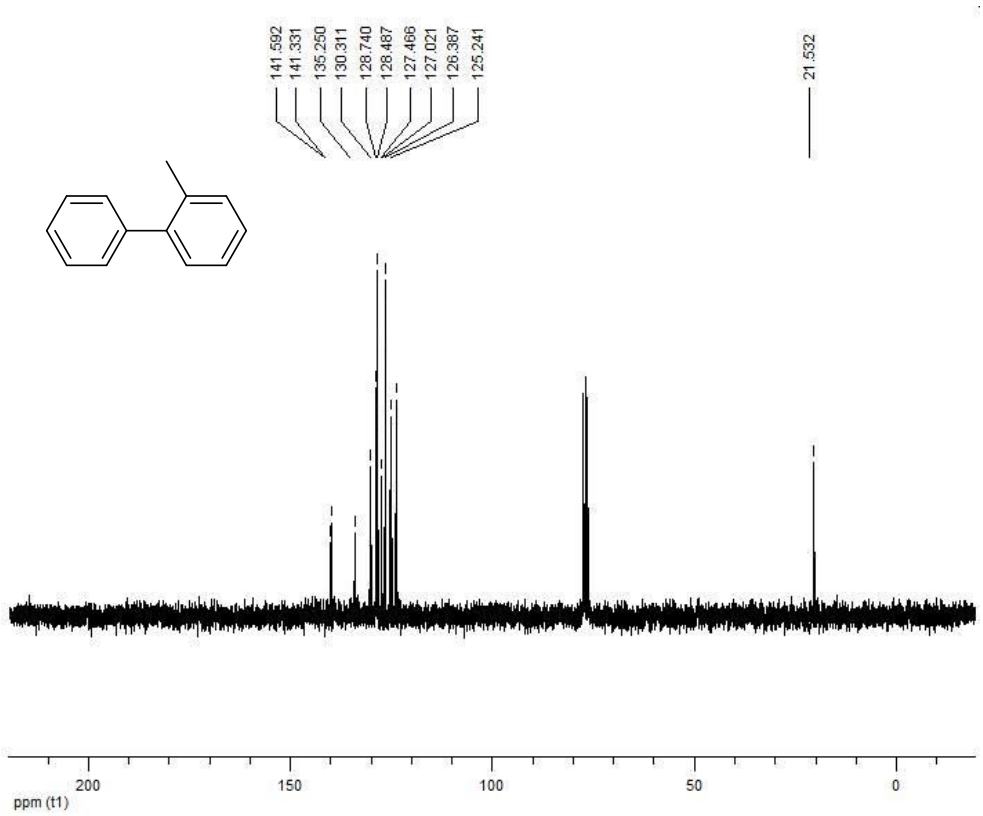
Scheme S5. ^{1}H-NMR spectra (250 MHz) of 3-methylbiphenyl **(C3)** in $CDCl_3$.



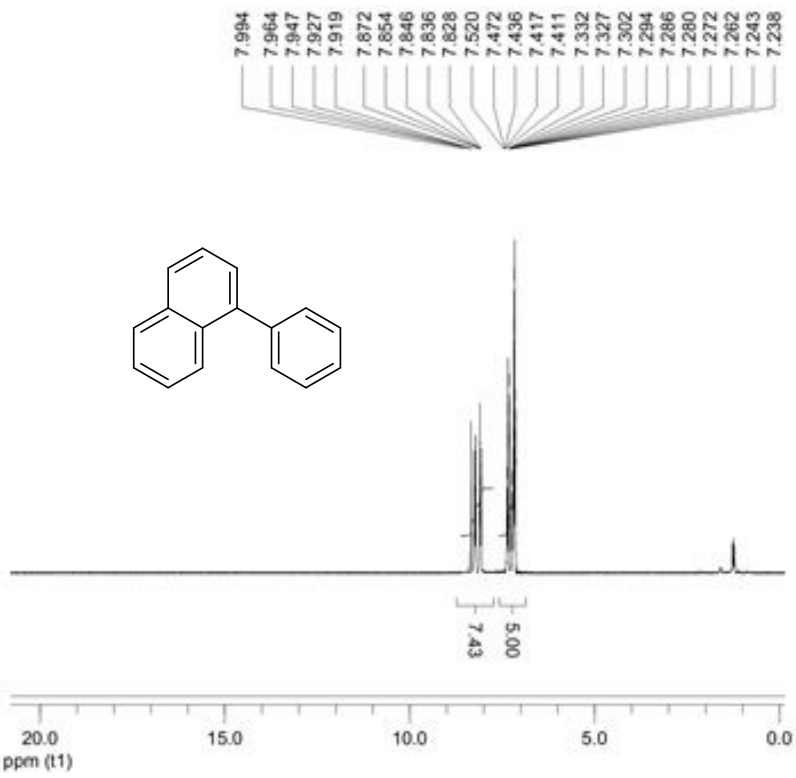
Scheme S6. ^{13}C-NMR spectra (63 MHz) of 3-methylbiphenyl **(C3)** in $CDCl_3$.



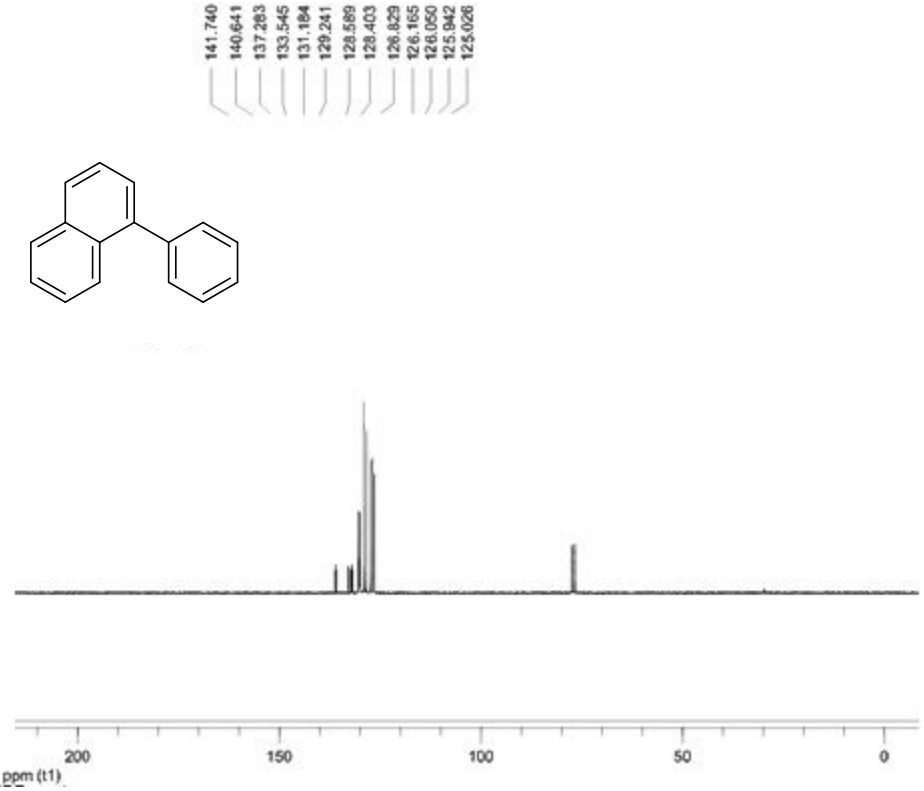
Scheme S7. ^{1}H-NMR spectra (250 MHz) of 2-methylbiphenyl **(C4)** in $CDCl_3$.



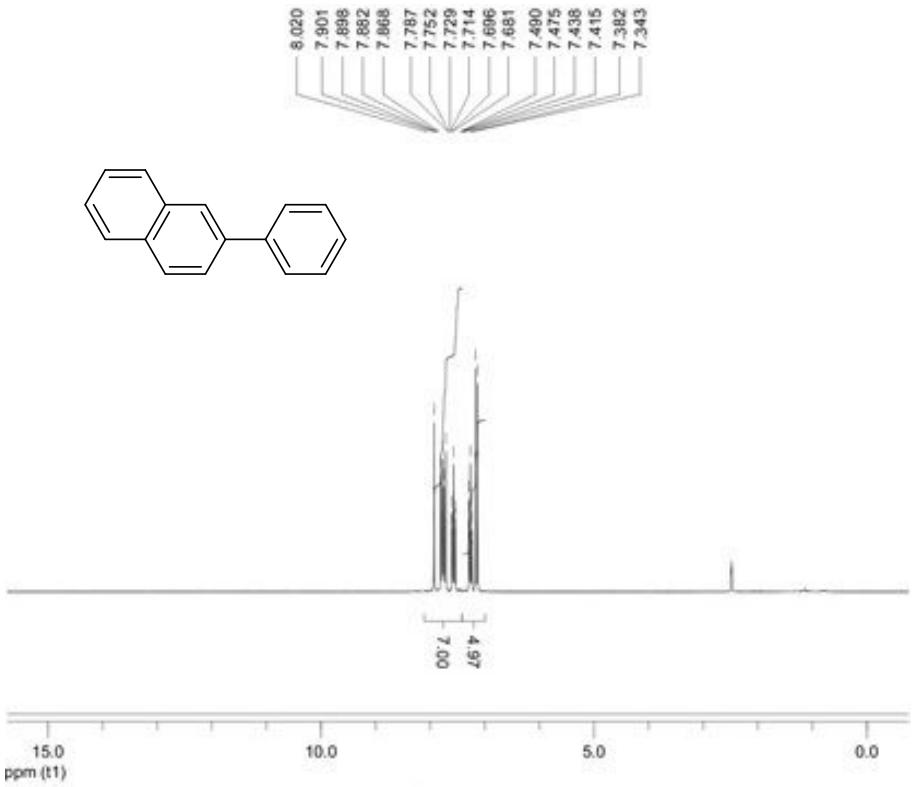
Scheme S8. ^{13}C-NMR spectra (63 MHz) of 2-methylbiphenyl **(C4)** in $CDCl_3$.



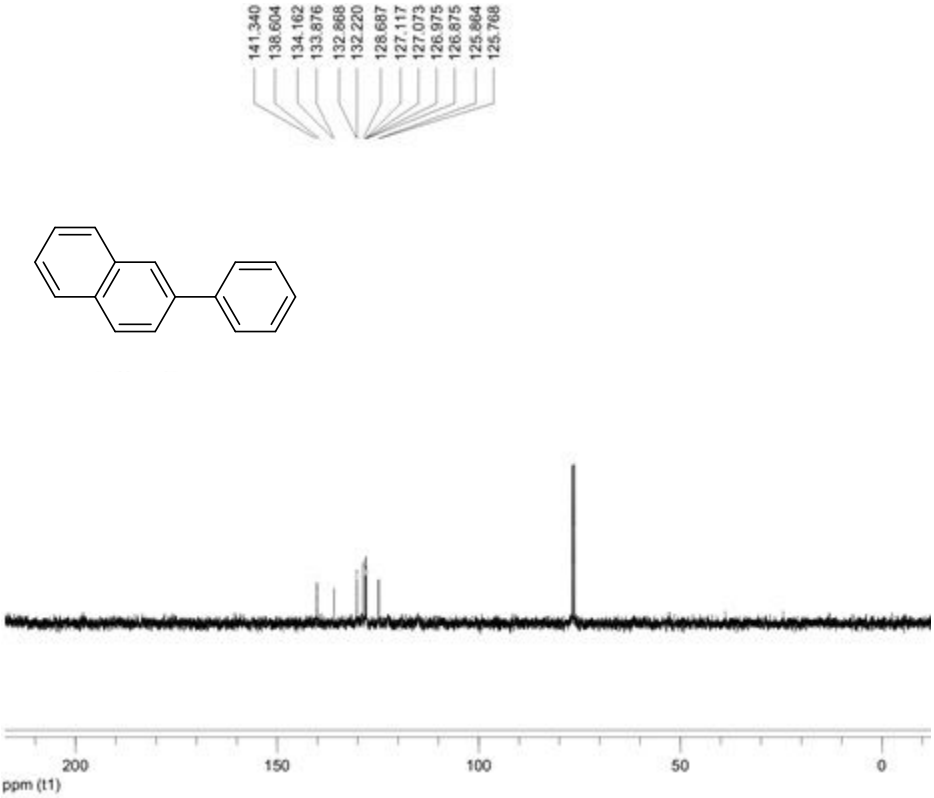
Scheme S9. ^{1}H-NMR spectra (250 MHz) of 1-phenylnaphthalene **(C5)** in $CDCl_3$.



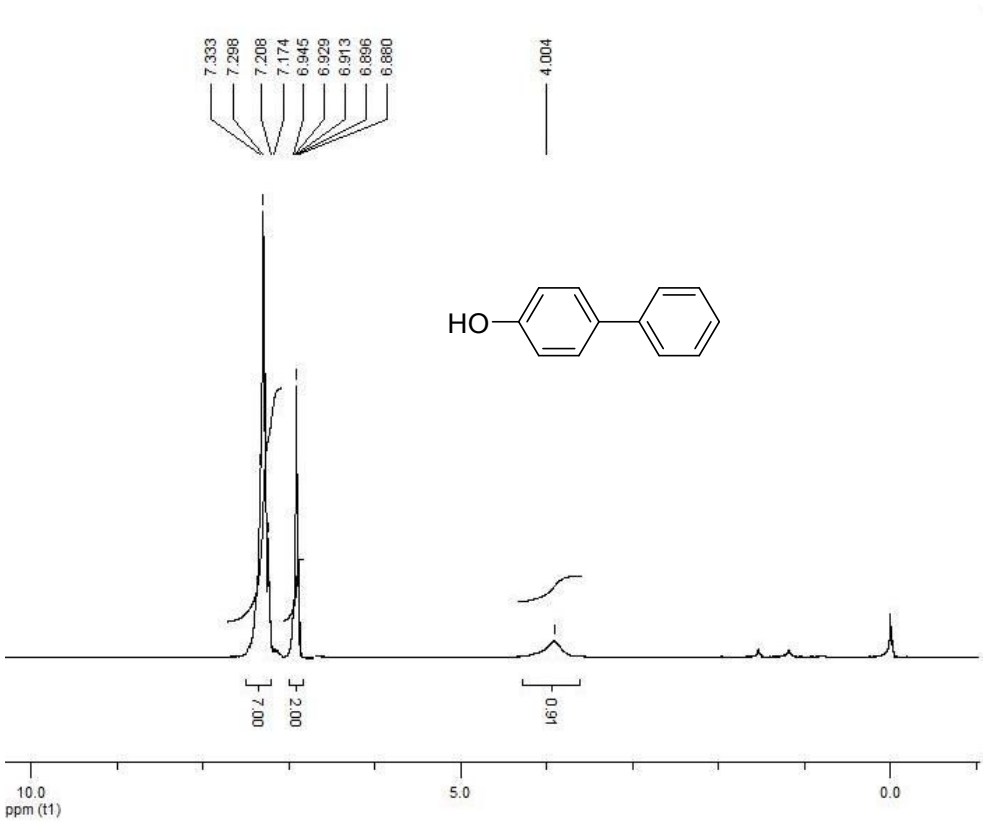
Scheme S10. ^{13}C-NMR spectra (63 MHz) of 1-phenylnaphthalene **(C5)** in $CDCl_3$.



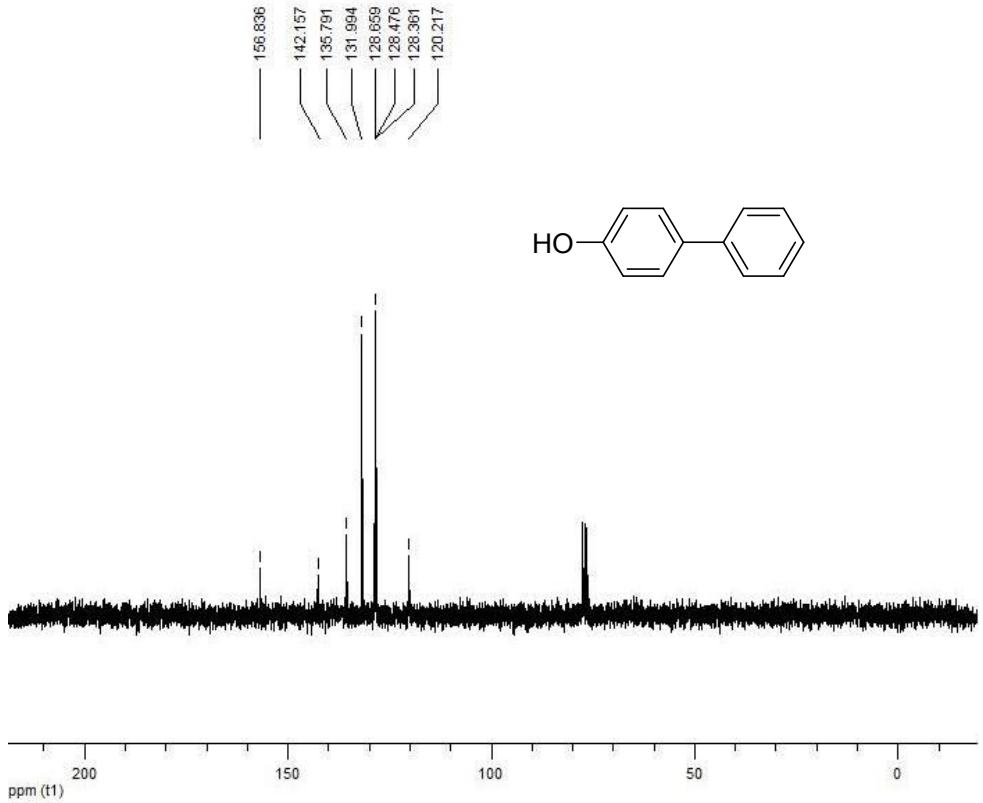
Scheme S11. ^{1}H-NMR spectra (250 MHz) of 2-phenylnaphthalene **(C6)** in $CDCl_3$.



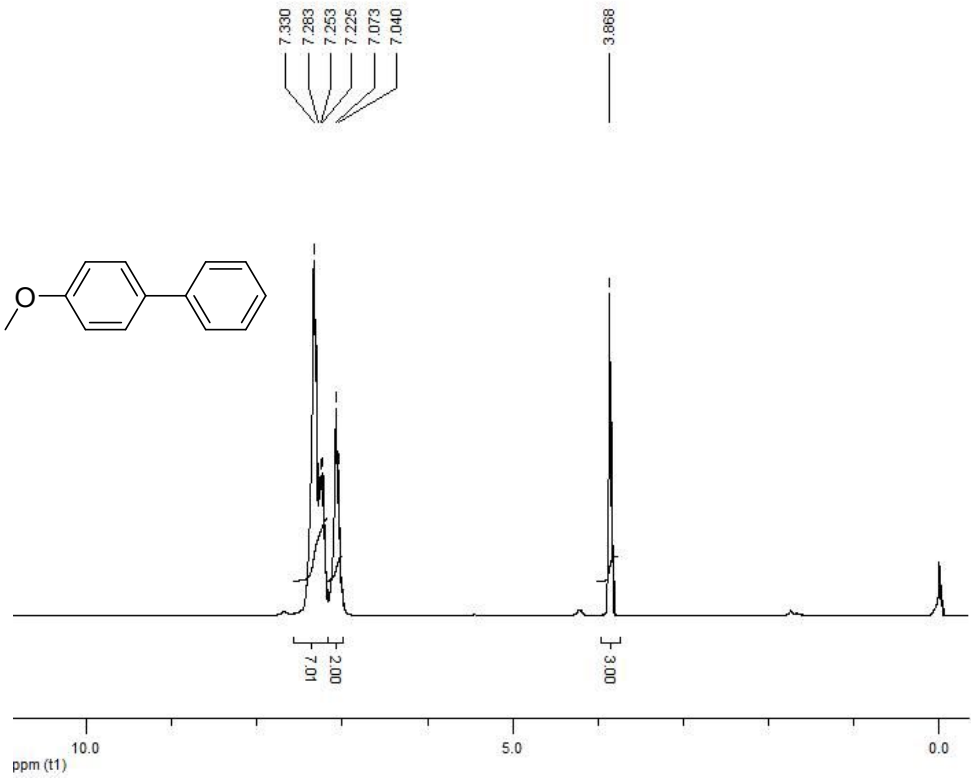
Scheme S12. ^{13}C-NMR spectra (63 MHz) of 2-phenylnaphthalene **(C6)** in $CDCl_3$.



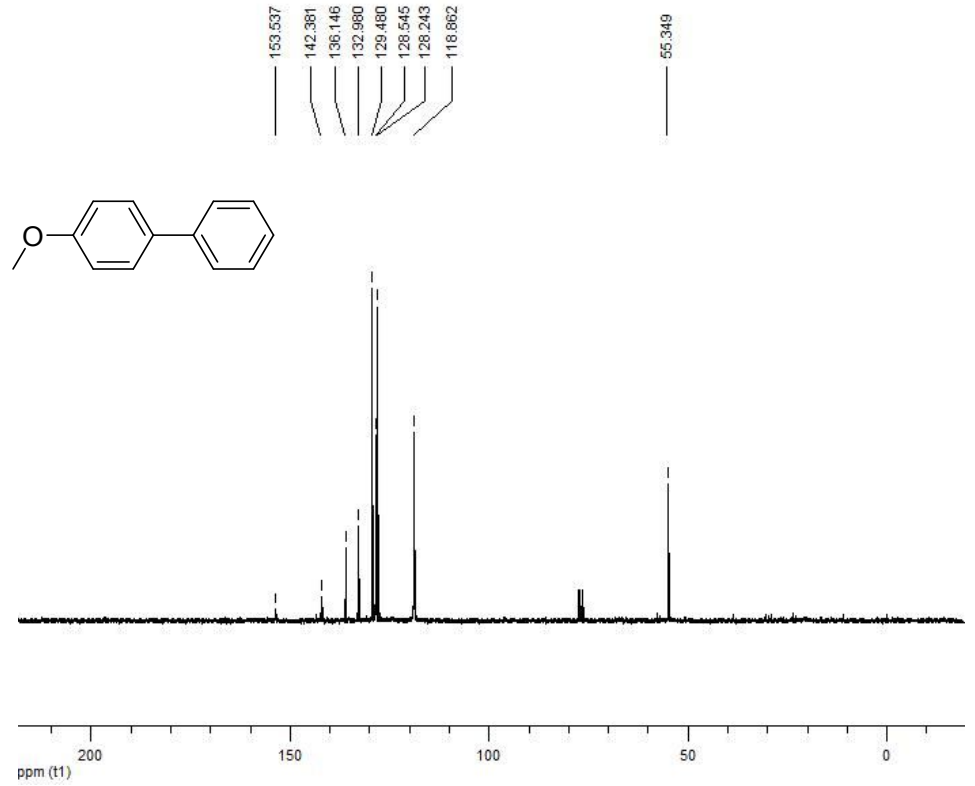
Scheme S13. ^{1}H-NMR spectra (250 MHz) of biphenyl-4-ol **(C7)** in $CDCl_3$.



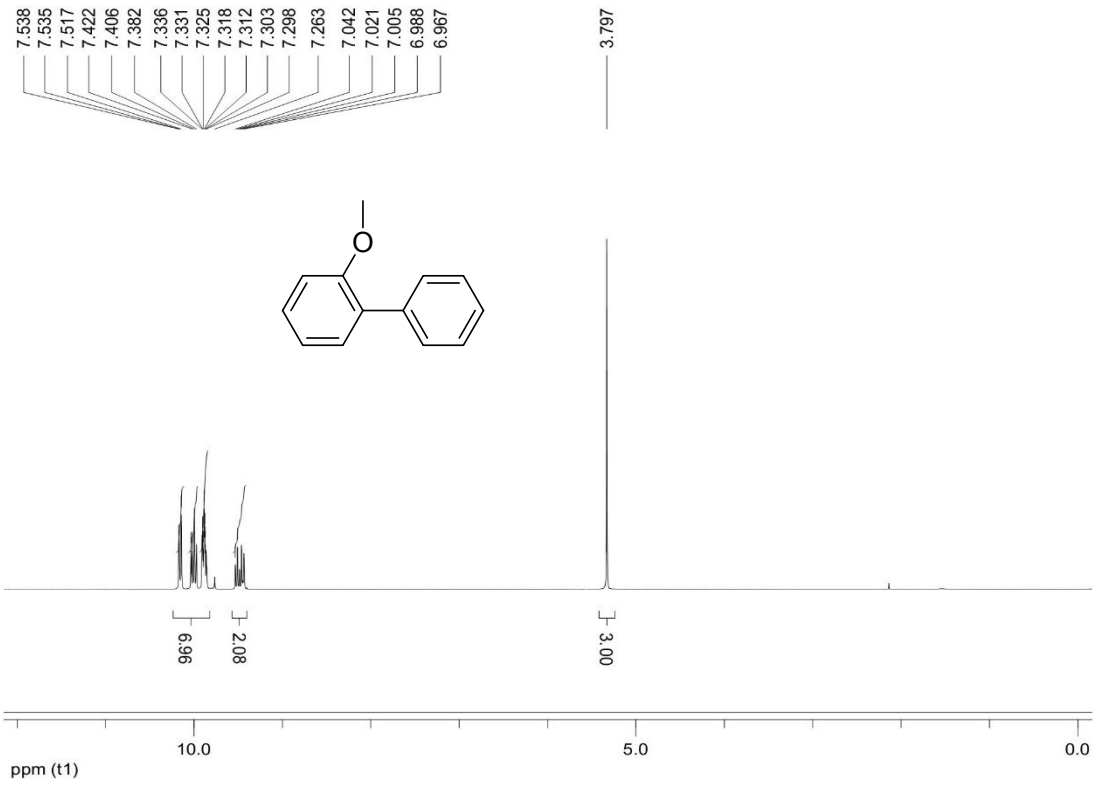
Scheme S14. ^{13}C-NMR spectra (63 MHz) of biphenyl-4-ol **(C7)** in $CDCl_3$.



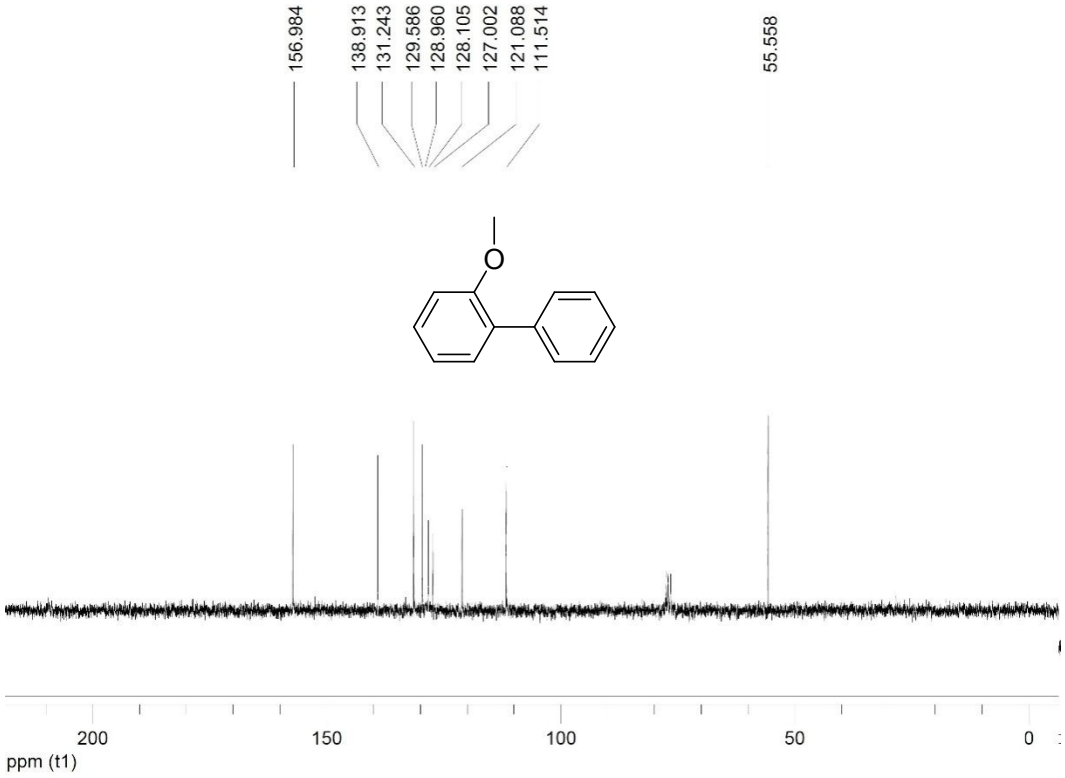
Scheme S15. ^{1}H-NMR spectra (250 MHz) of 4-methoxybiphenyl **(C8)** in $CDCl_3$.



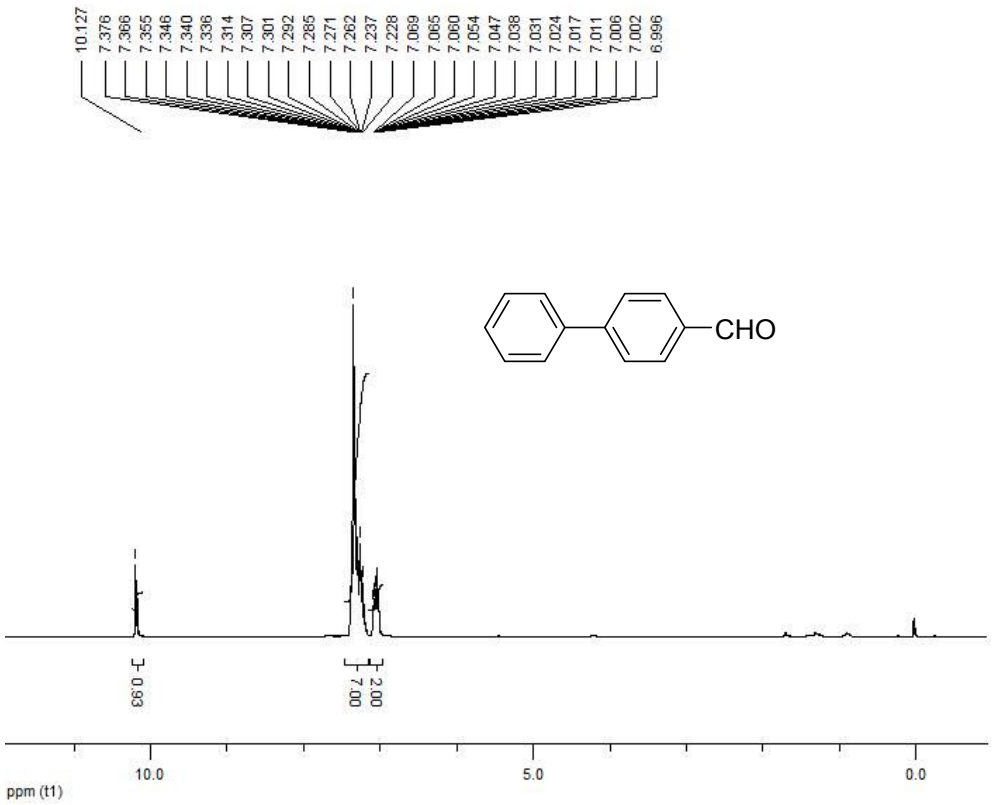
Scheme S16. ^{13}C-NMR spectra (63 MHz) of 4-methoxybiphenyl **(C8)** in $CDCl_3$.



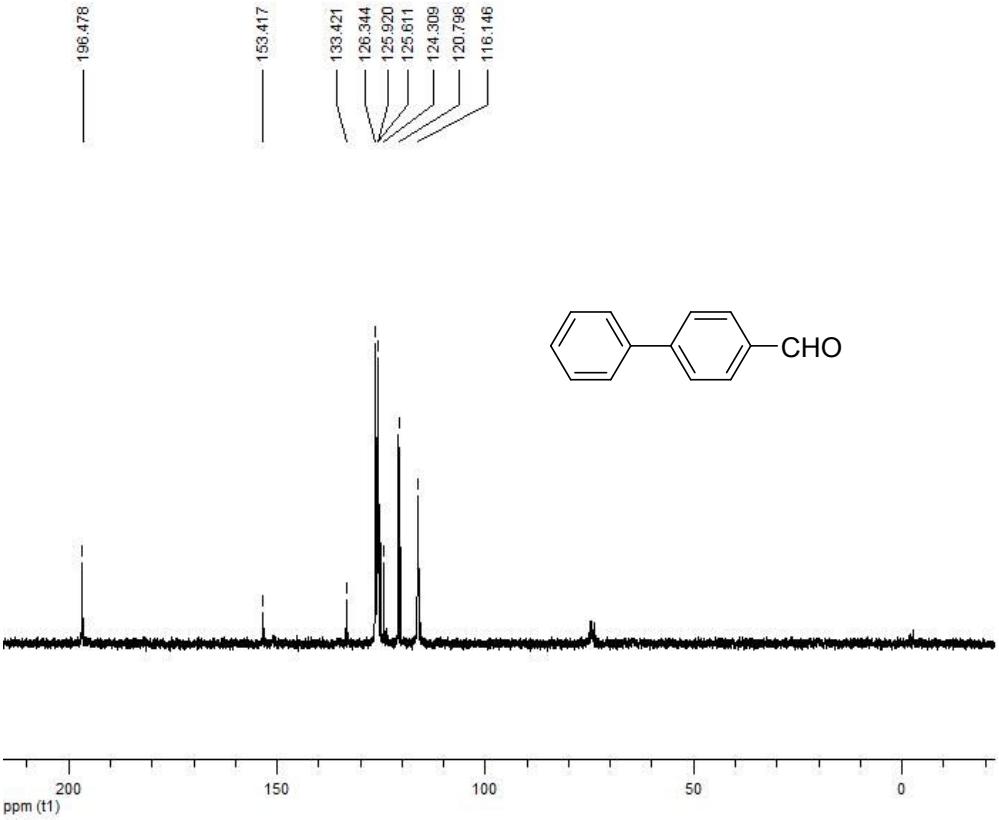
Scheme S17. ^{1}H-NMR spectra (250 MHz) of 2-methoxybiphenyl **(C9)** in $CDCl_3$.



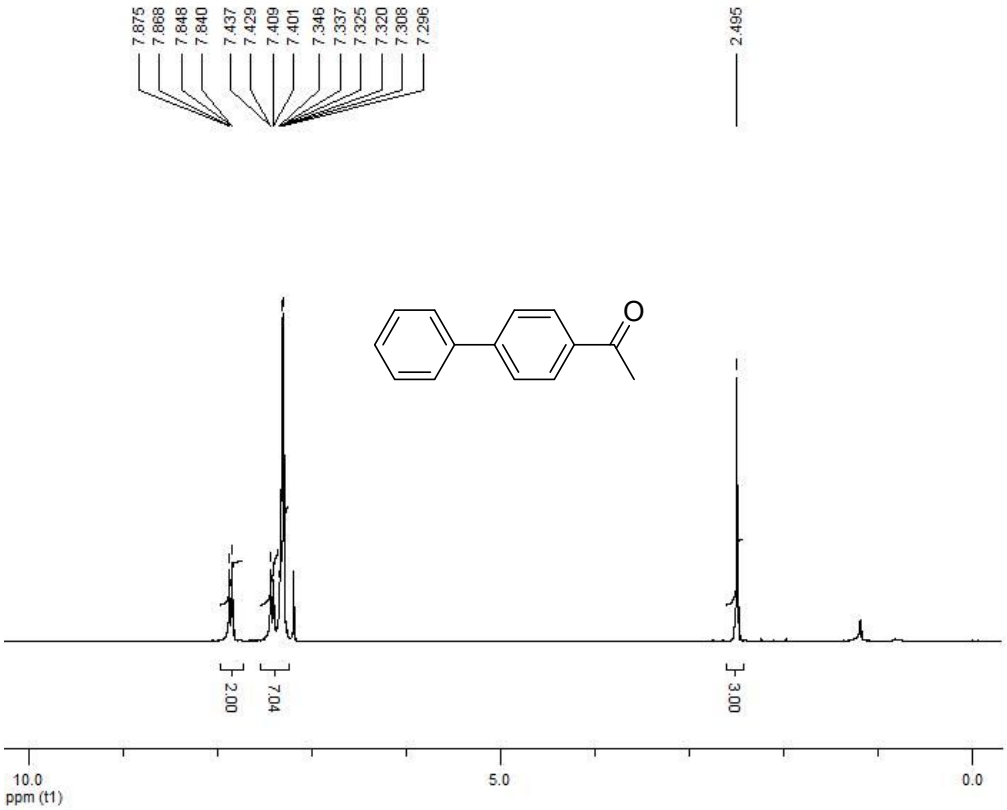
Scheme S18. ^{13}C-NMR spectra (63 MHz) of 2-methoxybiphenyl **(C9)** in $CDCl_3$.



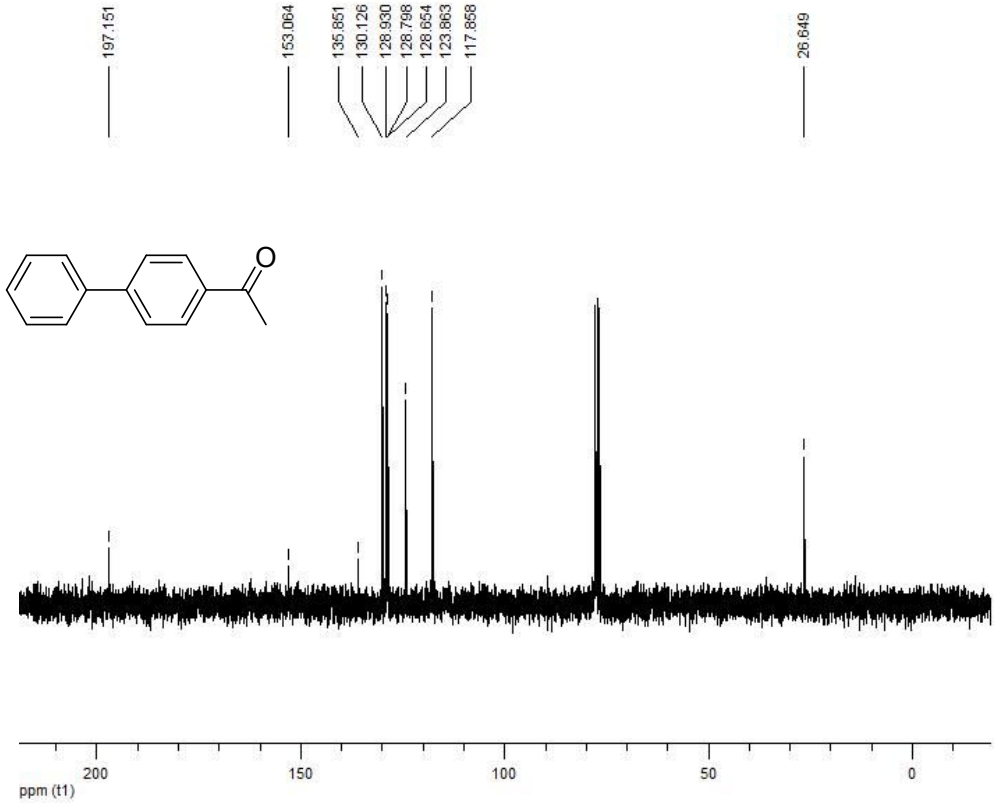
Scheme S19. ^{1}H-NMR spectra (250 MHz) of 4-biphenylcarbaldehyde **(C10)** in $CDCl_3$.



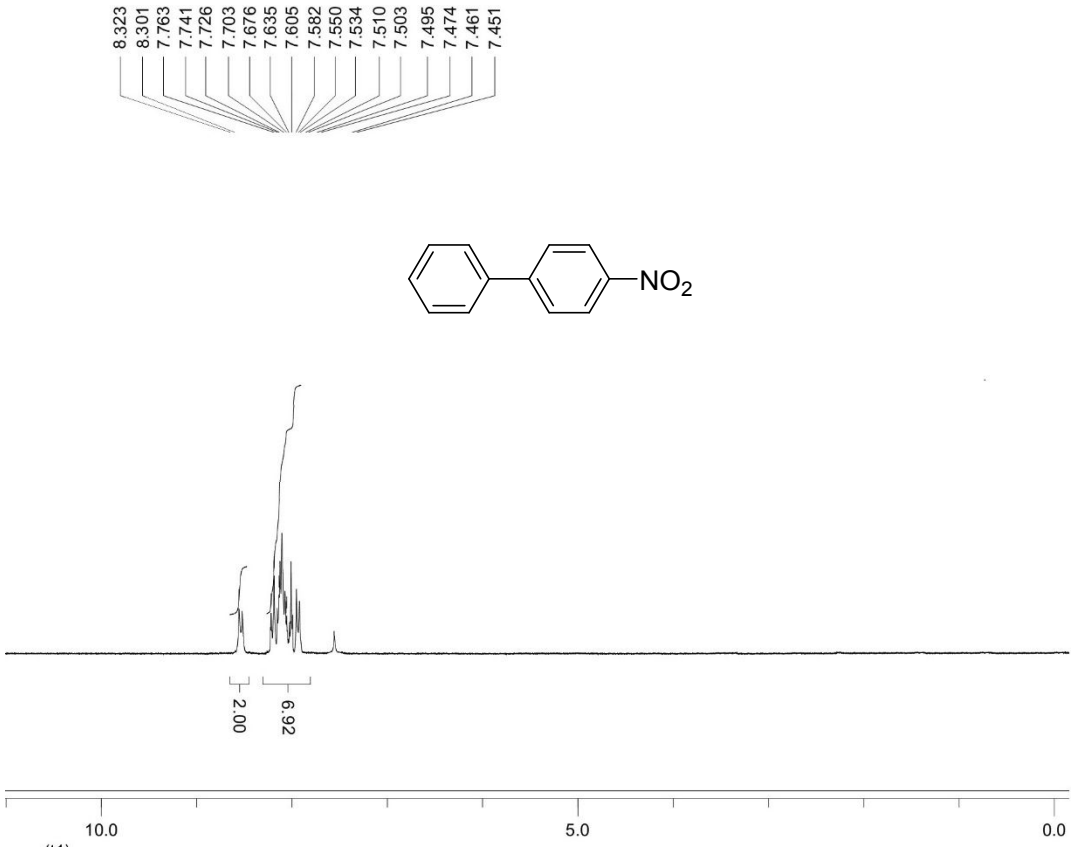
Scheme S20. ^{13}C-NMR spectra (63 MHz) of 4-biphenylcarbaldehyde **(C10)** in $CDCl_3$.



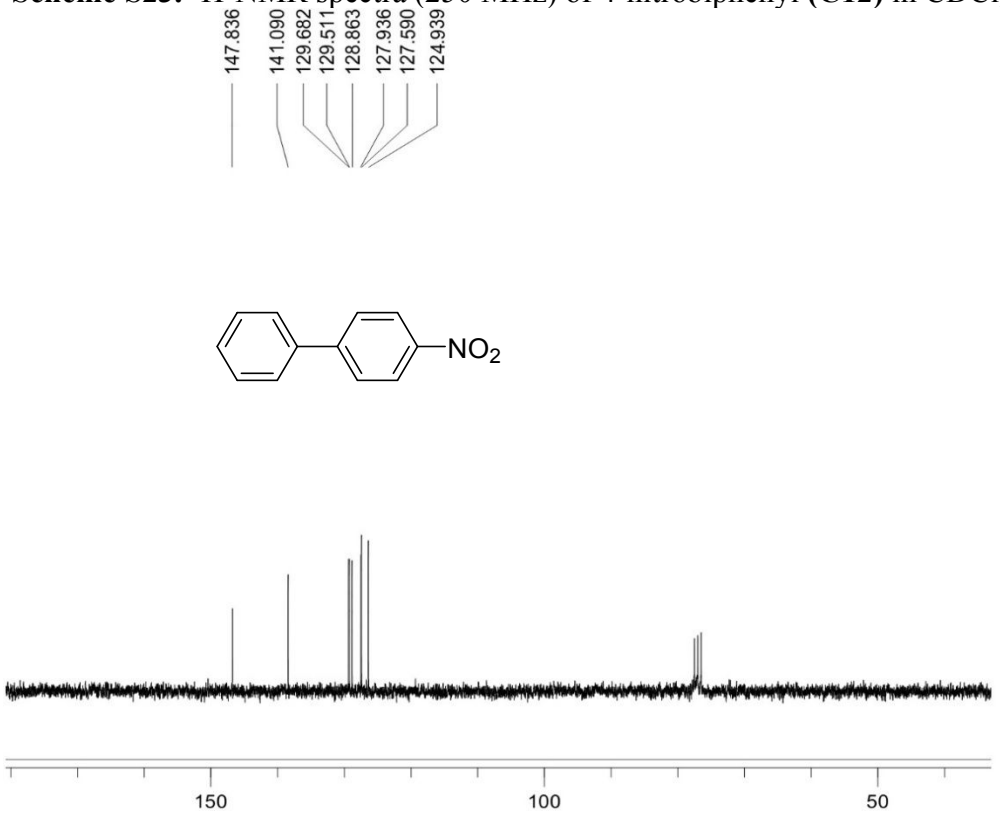
Scheme S21. ^{1}H-NMR spectra (250 MHz) of 1-(4-biphenylyl)ethanone **(C11)** in $CDCl_3$.



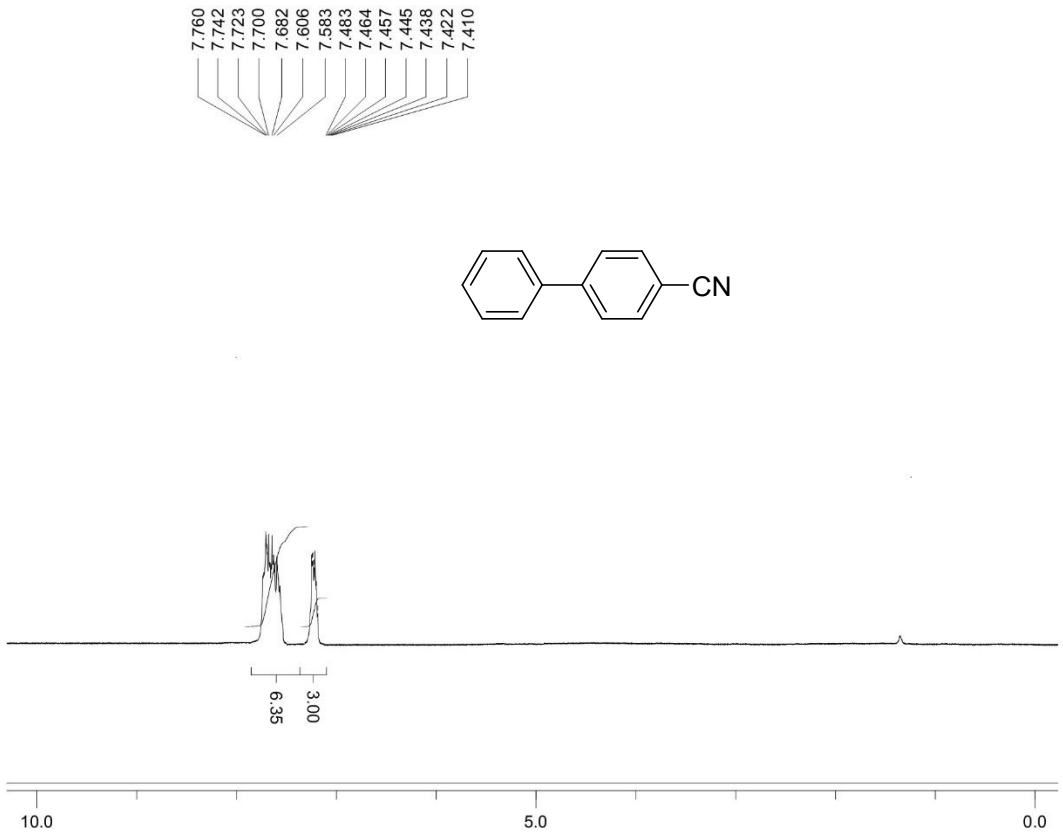
Scheme S22. ^{13}C-NMR spectra (63 MHz) of 1-(4-biphenylyl)ethanone **(C11)** in $CDCl_3$.



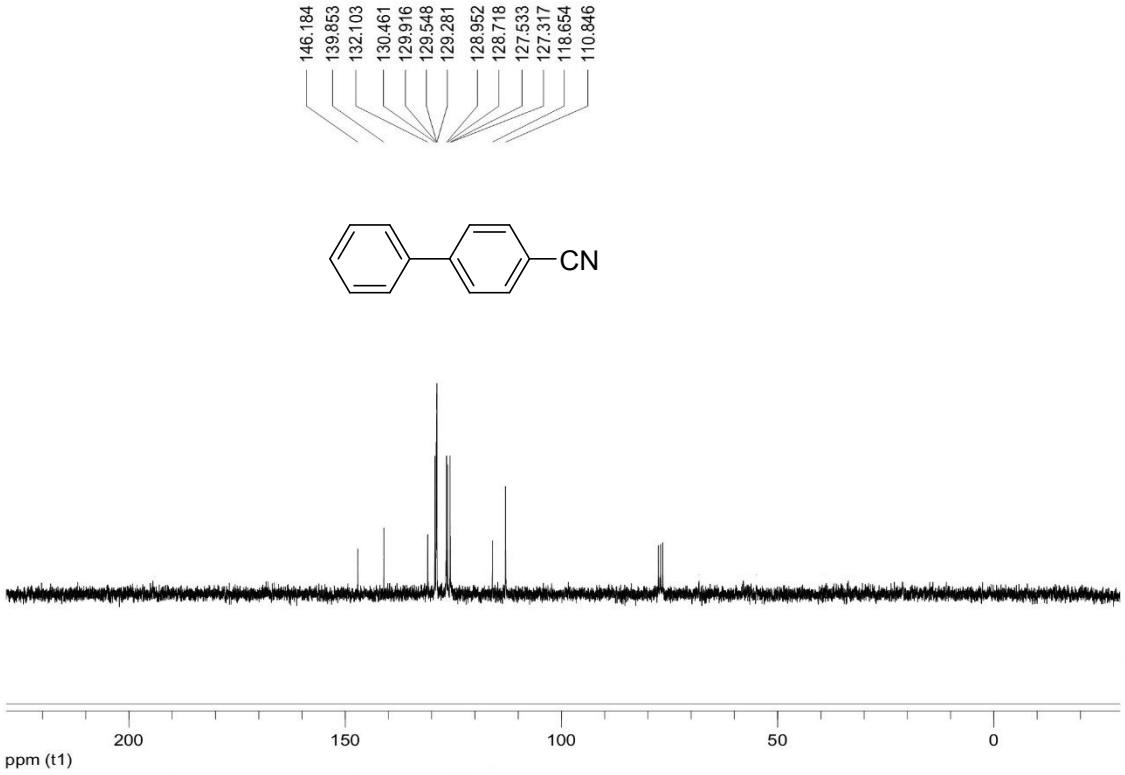
Scheme S23. ^{1}H-NMR spectra (250 MHz) of 4-nitrobiphenyl **(C12)** in $CDCl_3$.



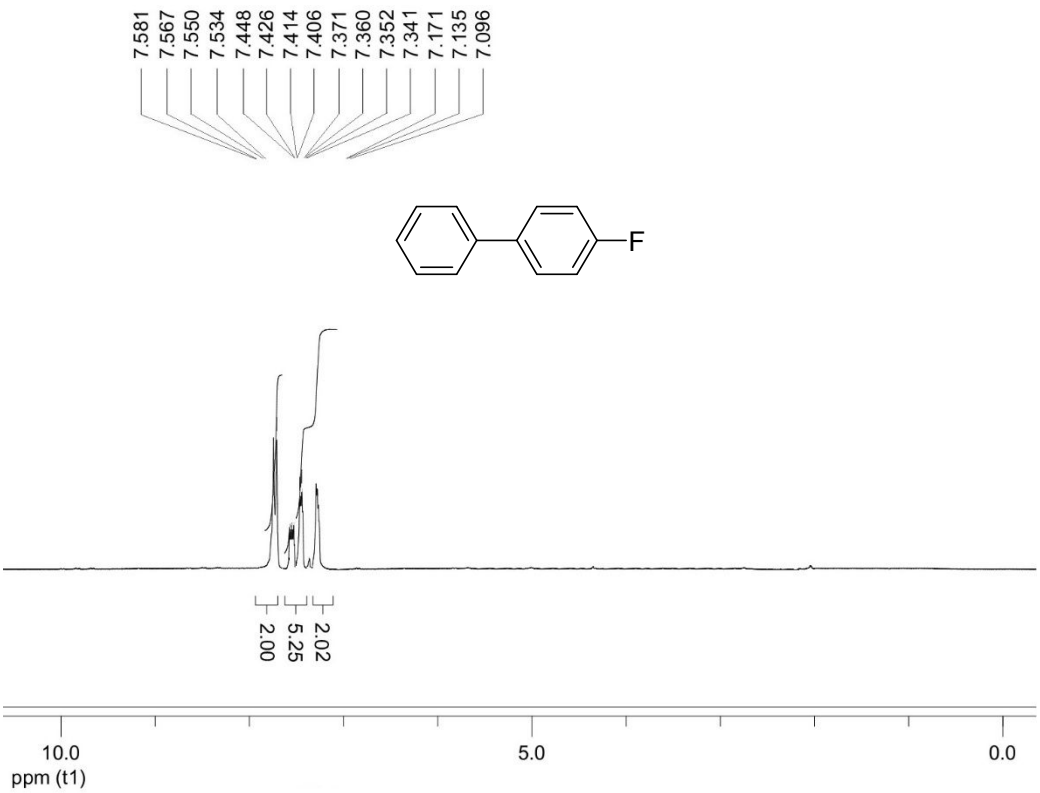
Scheme S24. ^{13}C-NMR spectra (63 MHz) of 4-nitrobiphenyl **(C12)** in $CDCl_3$.



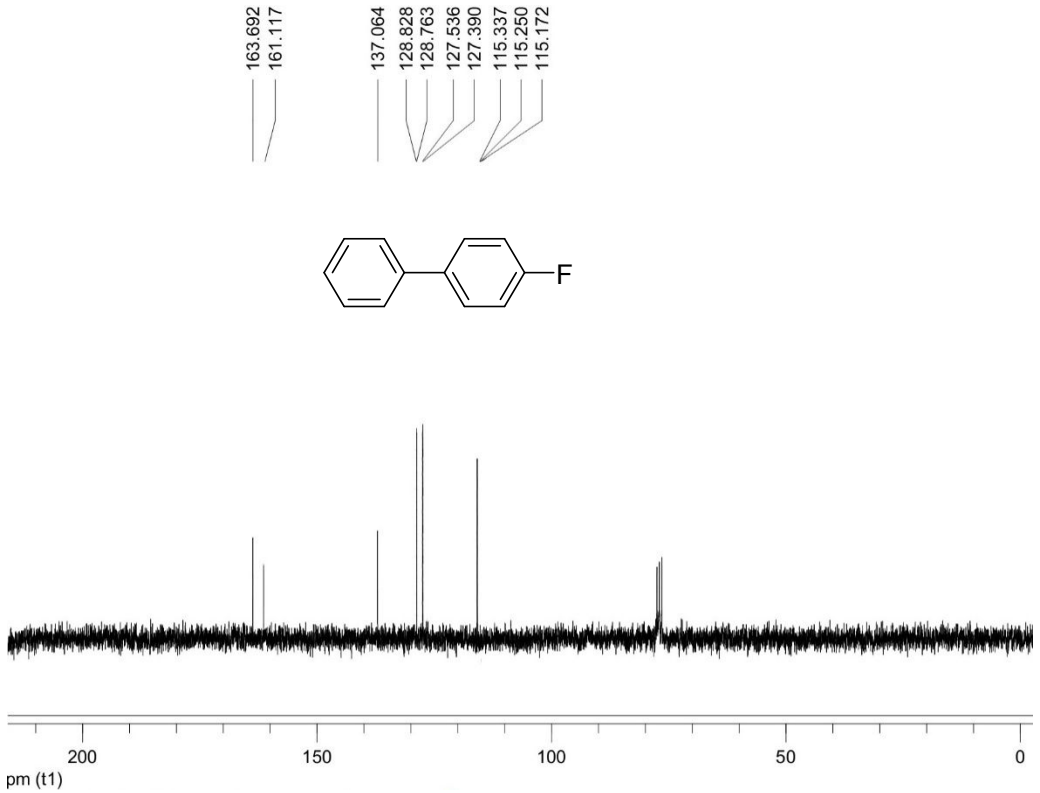
Scheme S25. ^{1}H-NMR spectra (250 MHz) of 4-biphenylcarbonitrile **(C13)** in $CDCl_3$.



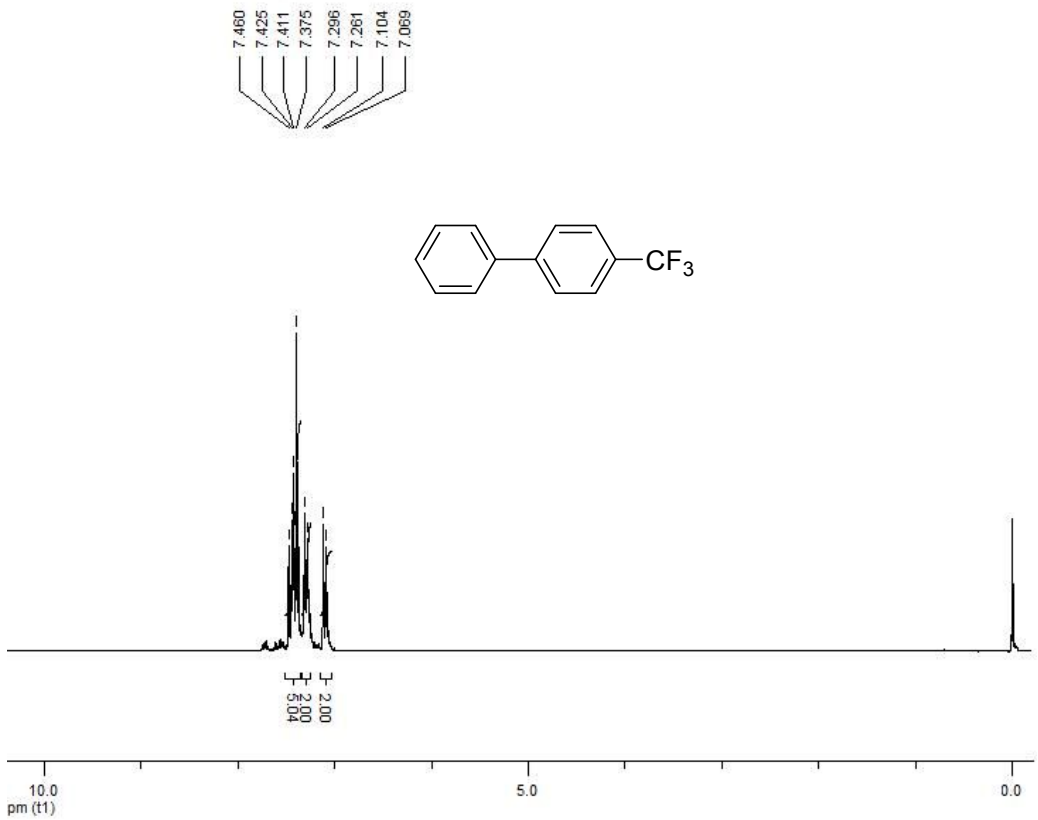
Scheme S26. ^{13}C-NMR spectra (63 MHz) of 4-biphenylcarbonitrile **(C13)** in $CDCl_3$.



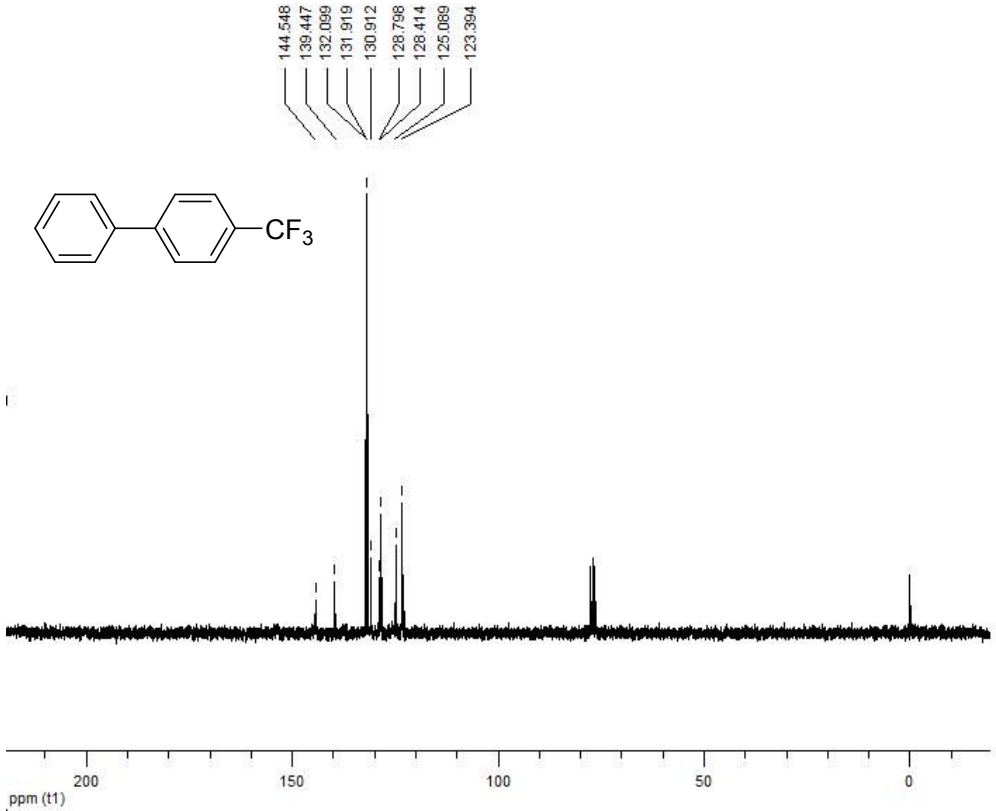
Scheme S27. ^{1}H-NMR spectra (250 MHz) of 4-fluorobiphenyl **(C14)** in $CDCl_3$.



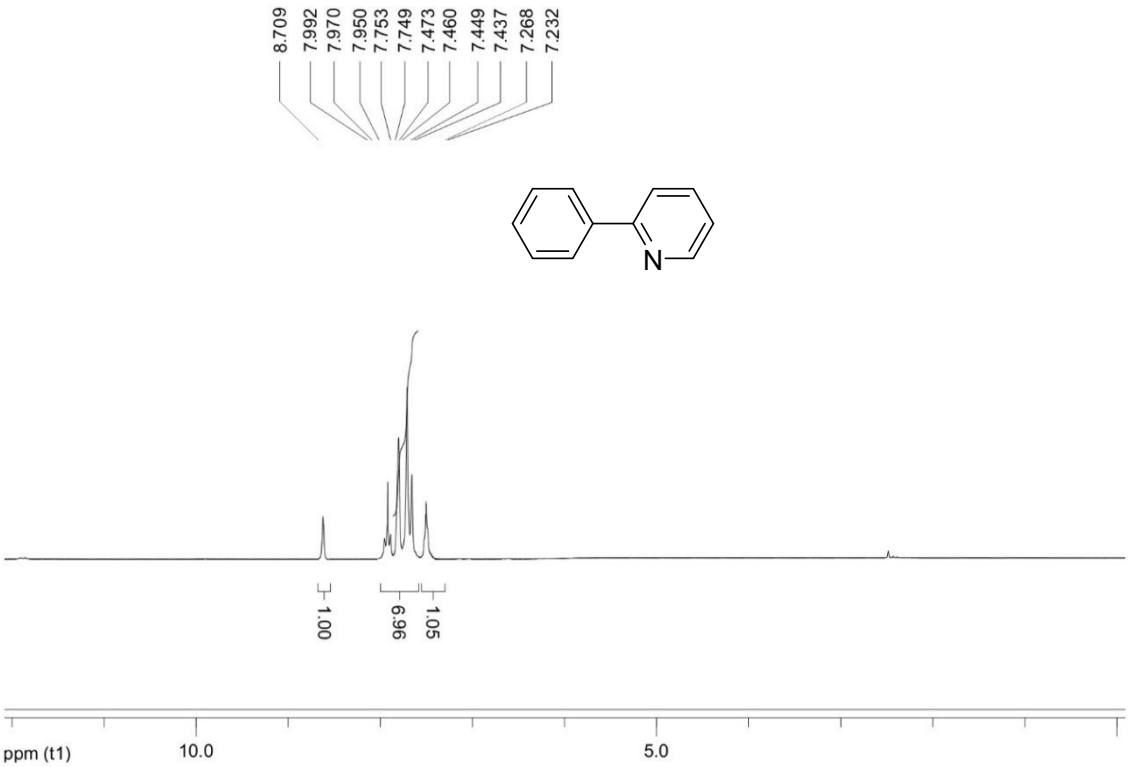
Scheme S28. ^{13}C-NMR spectra (63 MHz) of 4-fluorobiphenyl **(C14)** in $CDCl_3$.



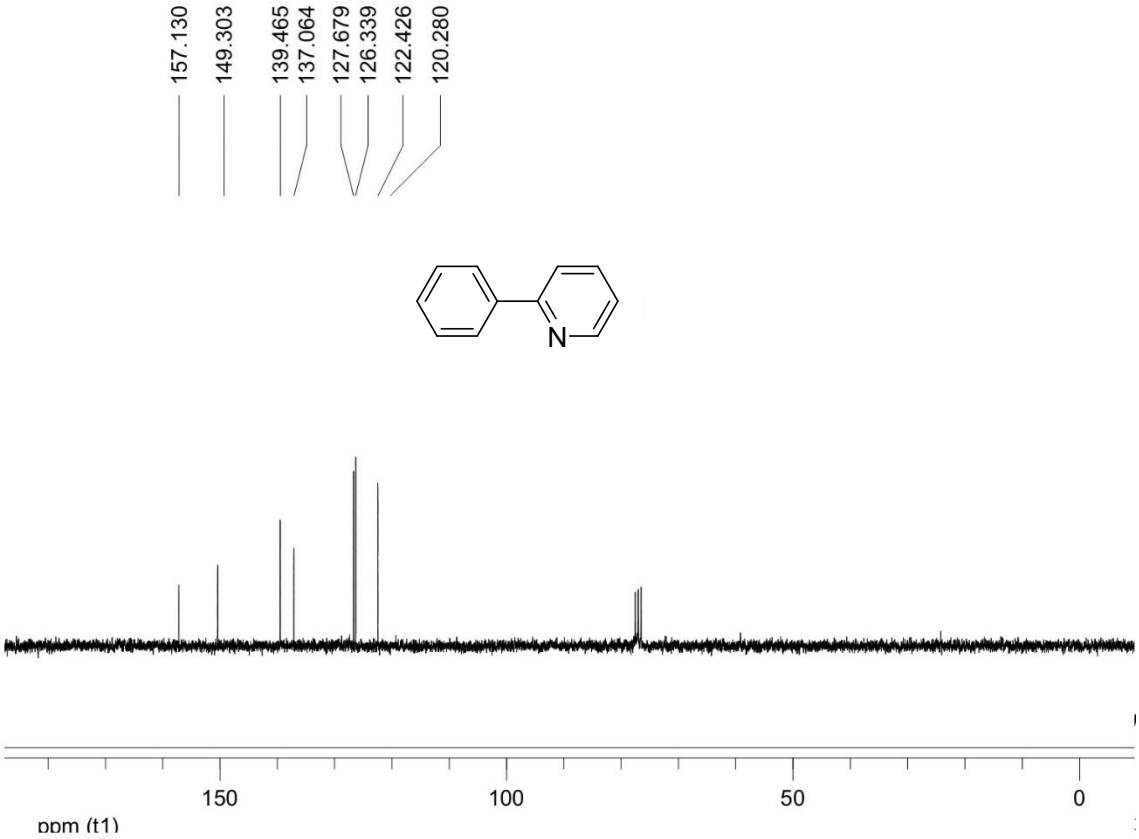
Scheme S29. ^{1}H-NMR spectra (250 MHz) of 4-(trifluoromethyl)biphenyl **(C15)** in $CDCl_3$.



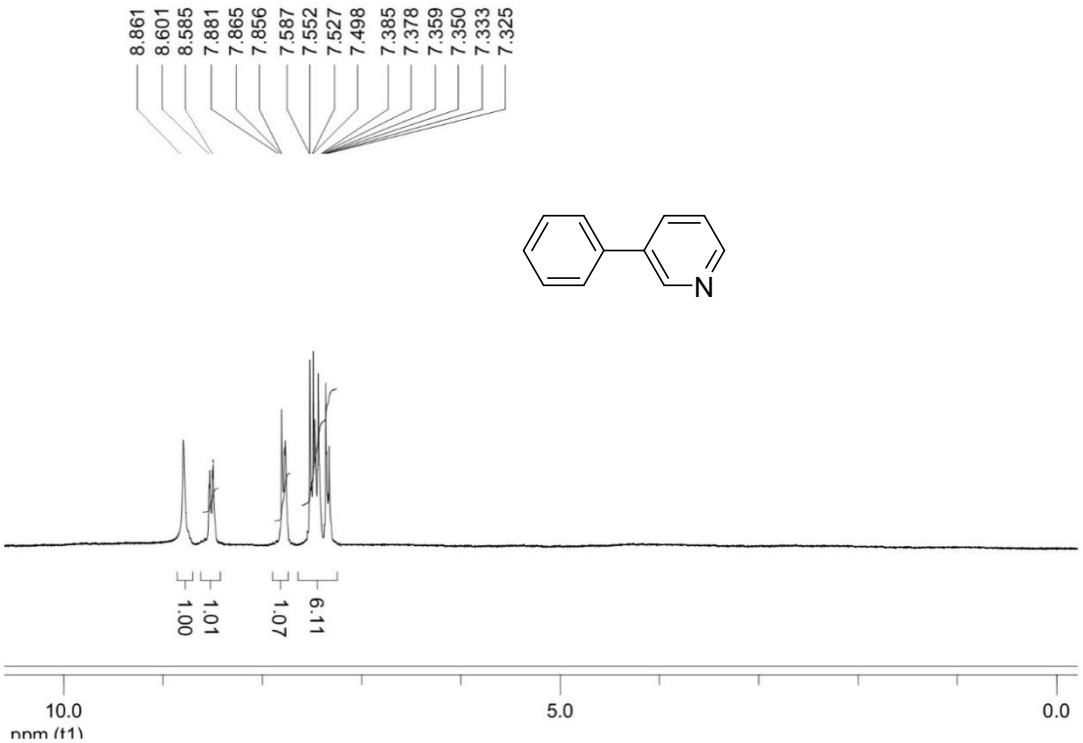
Scheme S30. ^{13}C-NMR spectra (63 MHz) of 4-(trifluoromethyl)biphenyl **(C15)** in $CDCl_3$.



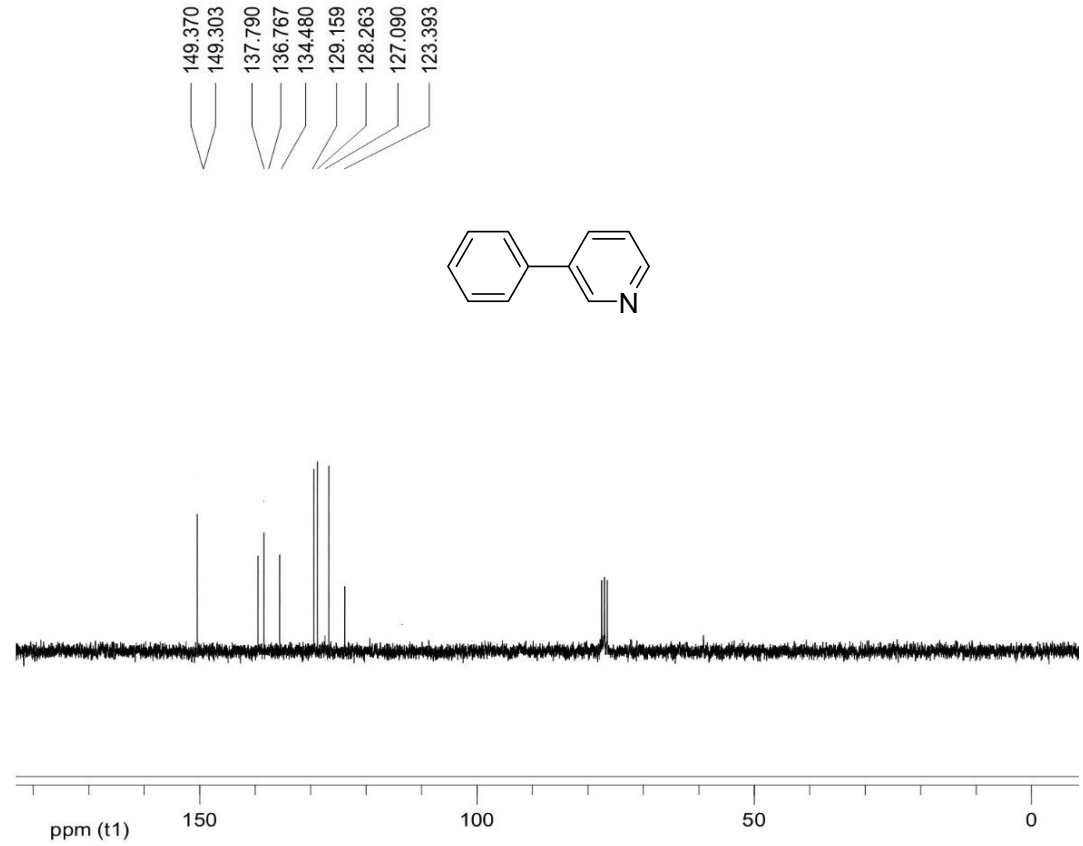
Scheme S31. ^{1}H-NMR spectra (250 MHz) of 2-phenylpyridine **(C16)** in $CDCl_3$.



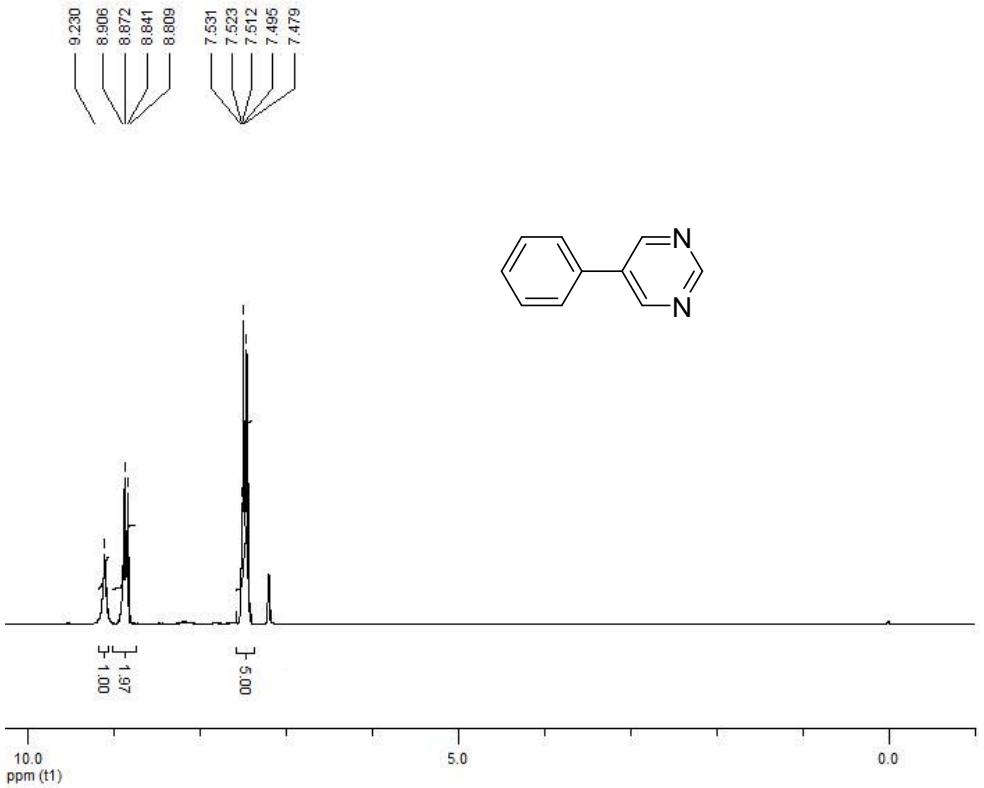
Scheme S32. ^{13}C-NMR spectra (63 MHz) of 2-phenylpyridine **(C16)** in $CDCl_3$.



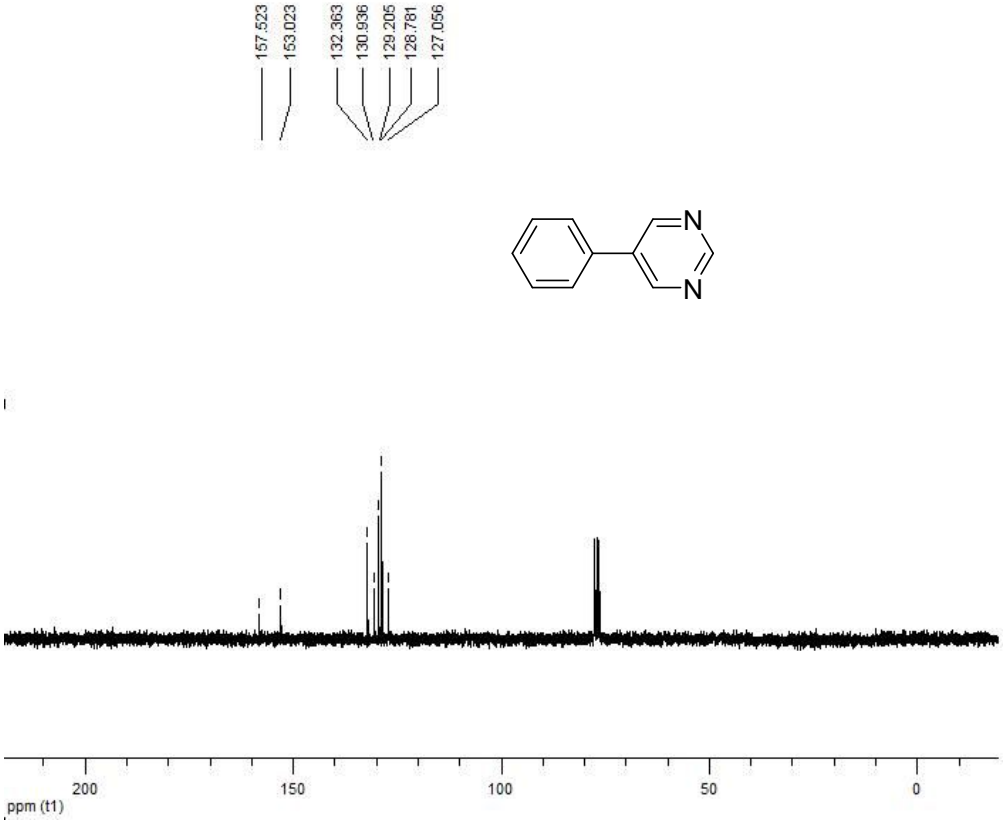
Scheme S33. ^{1}H-NMR spectra (250 MHz) of 3-phenylpyridine **(C17)** in $CDCl_3$.



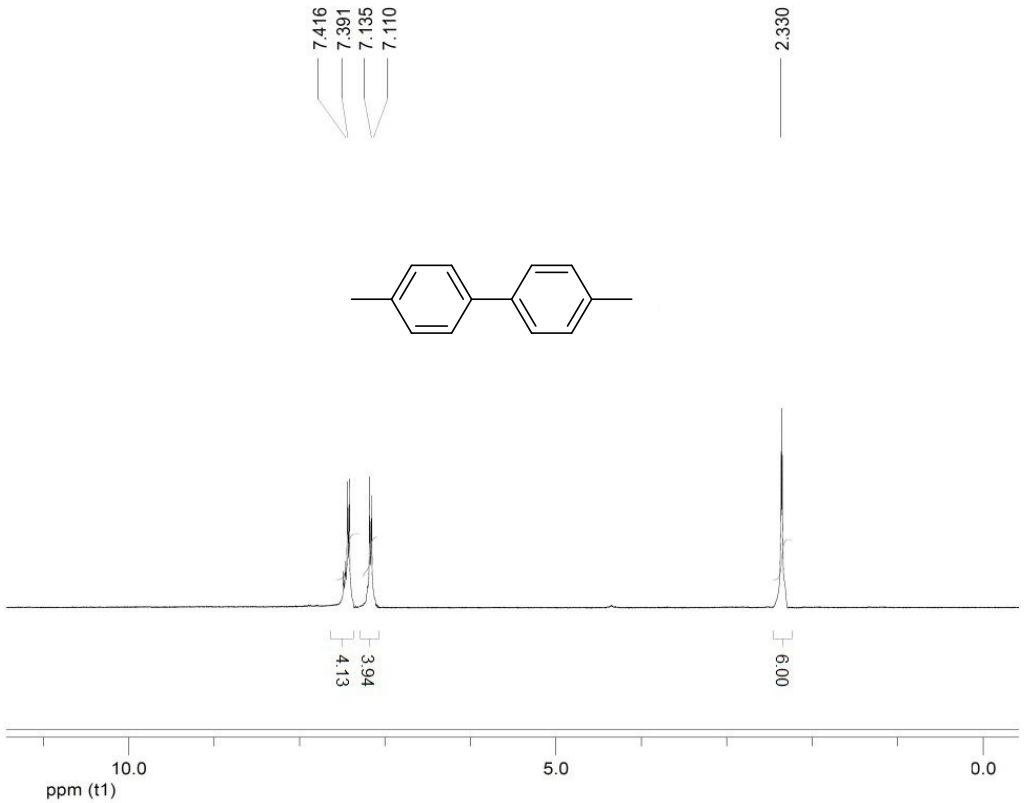
Scheme S34. ^{13}C-NMR spectra (63 MHz) of 3-phenylpyridine **(C17)** in $CDCl_3$.



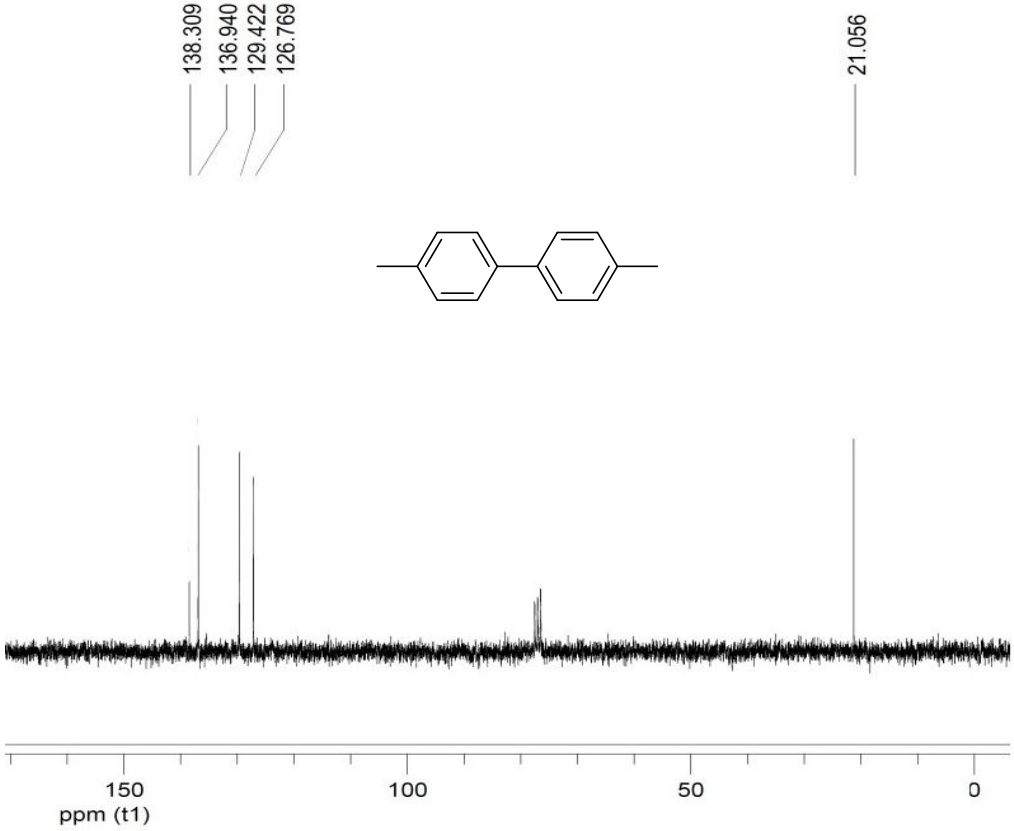
Scheme S35. ^{1}H-NMR spectra (250 MHz) of 5-phenylpyrimidine **(C18)** in $CDCl_3$.



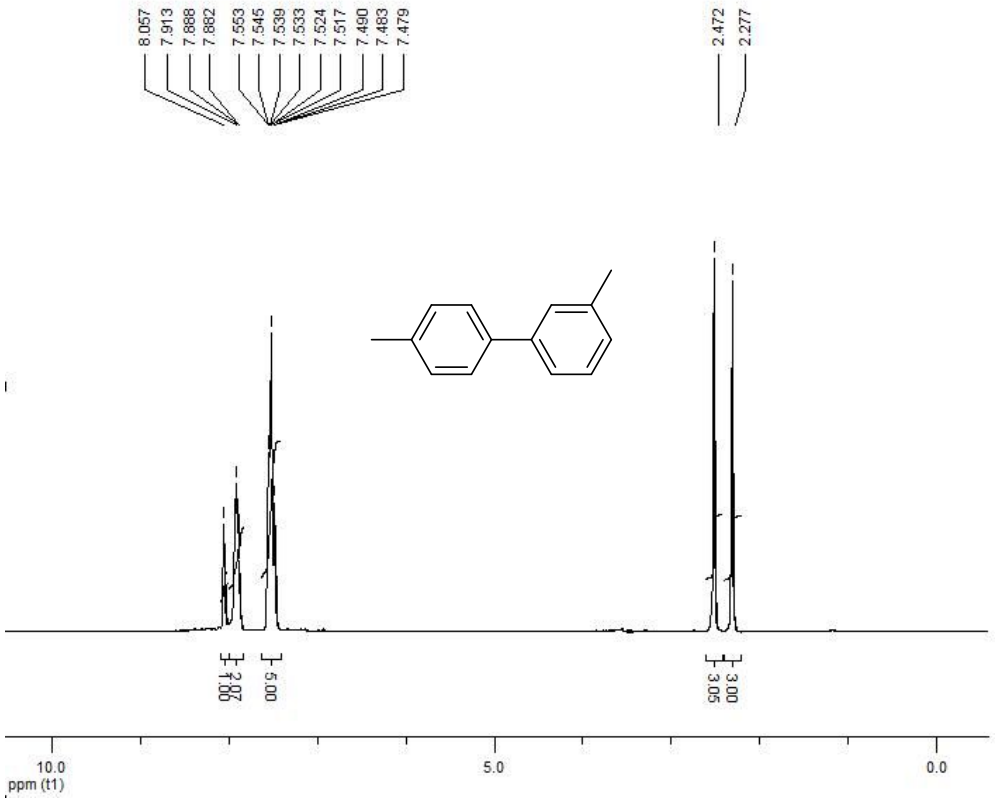
Scheme S36. ^{13}C-NMR spectra (63 MHz) of 5-phenylpyrimidine **(C18)** in $CDCl_3$.



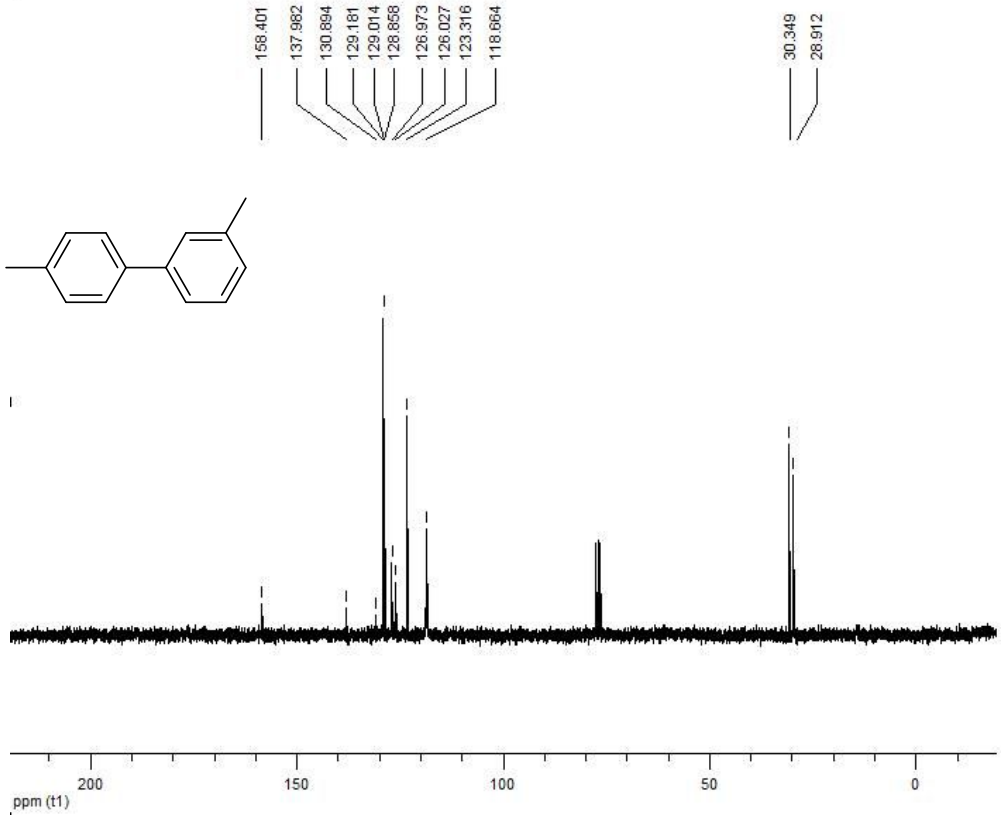
Scheme S37. ^{1}H-NMR spectra (250 MHz) of 4,4'-dimethylbiphenyl **(C20)** in $CDCl_3$.



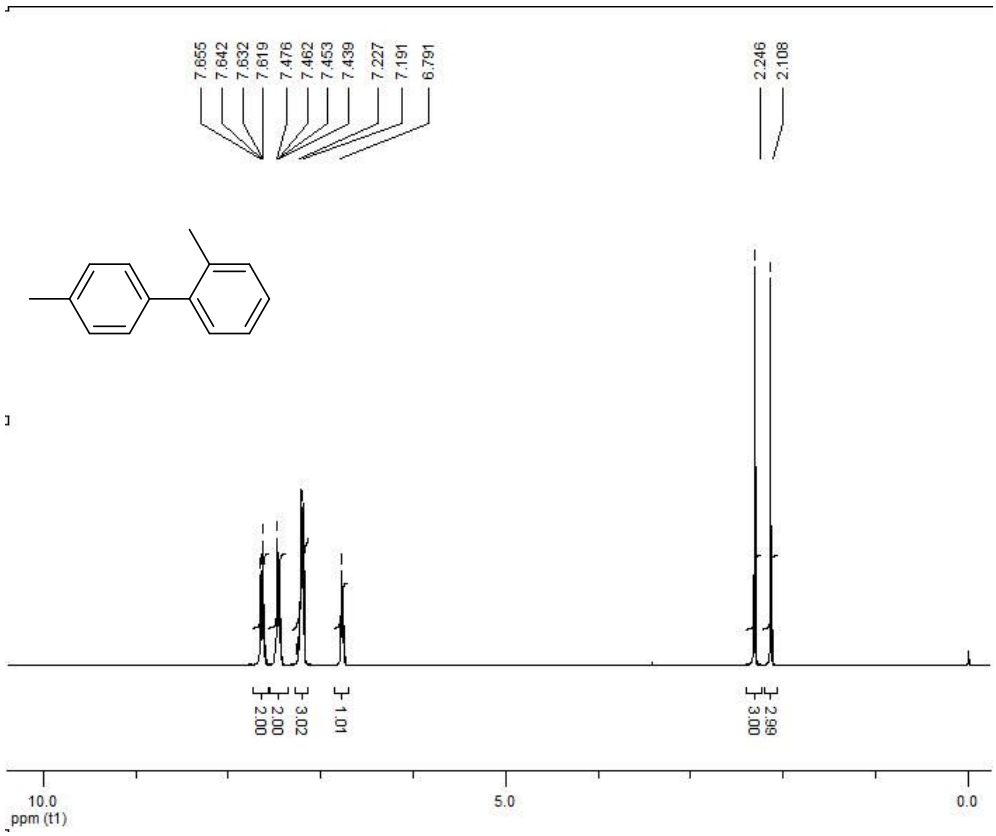
Scheme S38. ^{13}C-NMR spectra (63 MHz) of 4,4'-dimethylbiphenyl **(C20)** in $CDCl_3$.



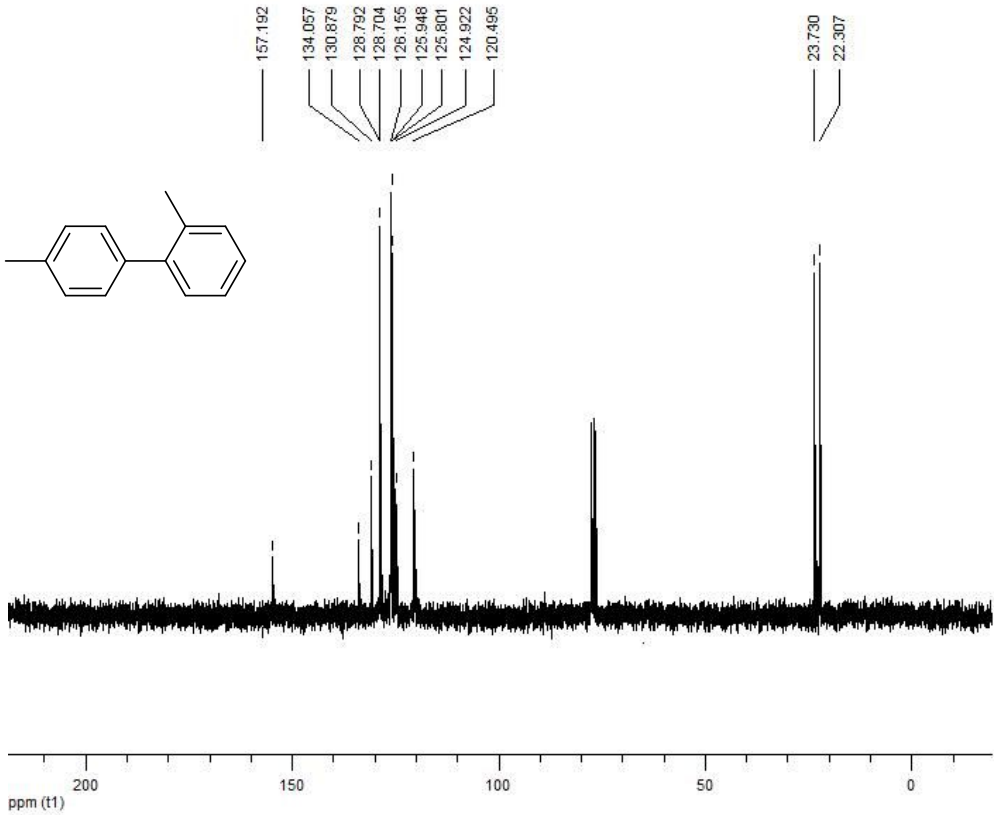
Scheme S39. ^{1}H-NMR spectra (250 MHz) of 3,4'-dimethylbiphenyl **(C21)** in $CDCl_3$.



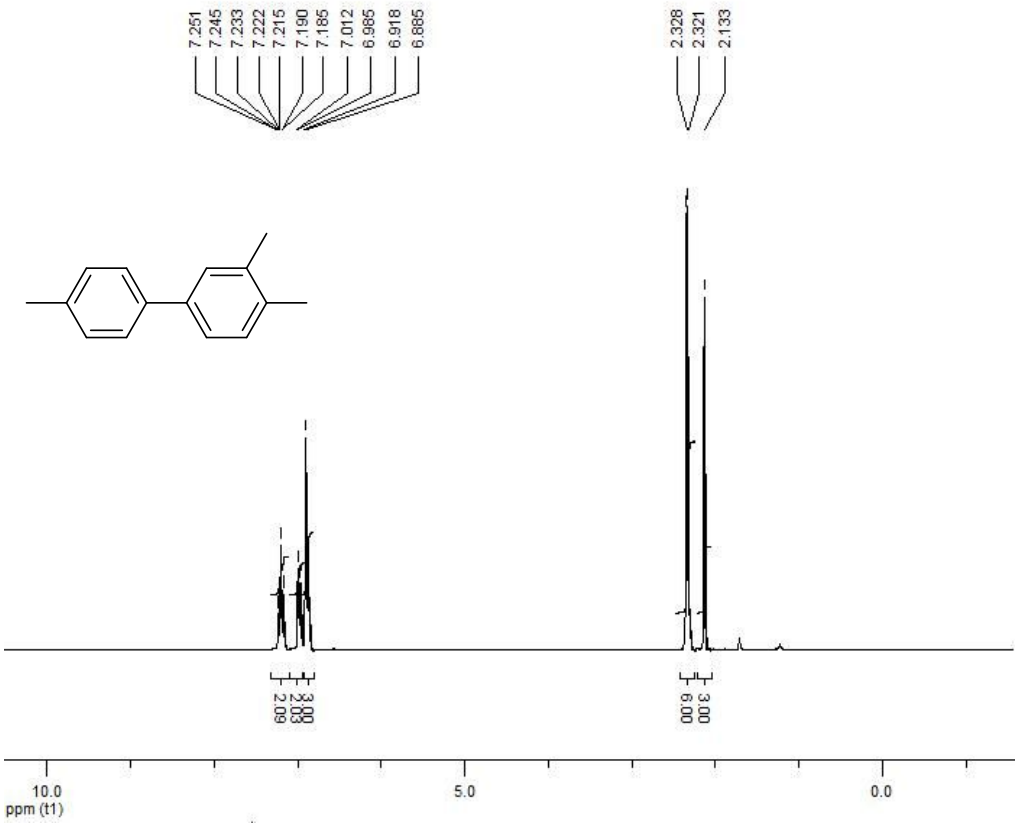
Scheme S40. ^{13}C-NMR spectra (63 MHz) of 3,4'-dimethylbiphenyl **(C21)** in $CDCl_3$.



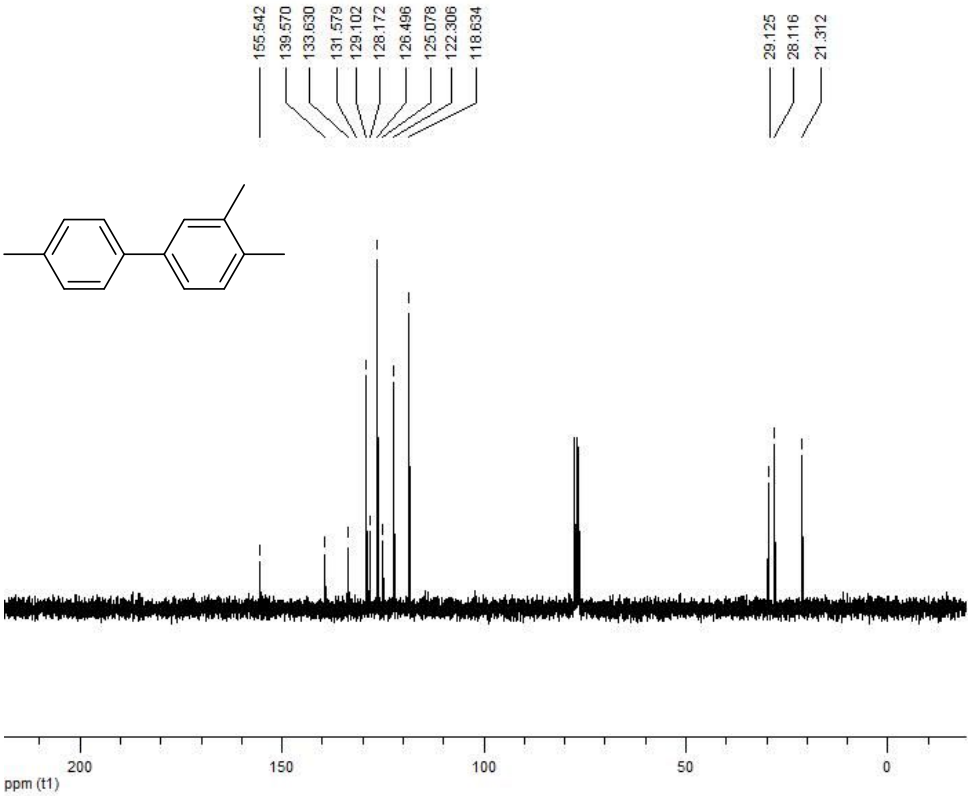
Scheme S41. ^{1}H-NMR spectra (250 MHz) of 2,4'-dimethylbiphenyl **(C22)** in $CDCl_3$.



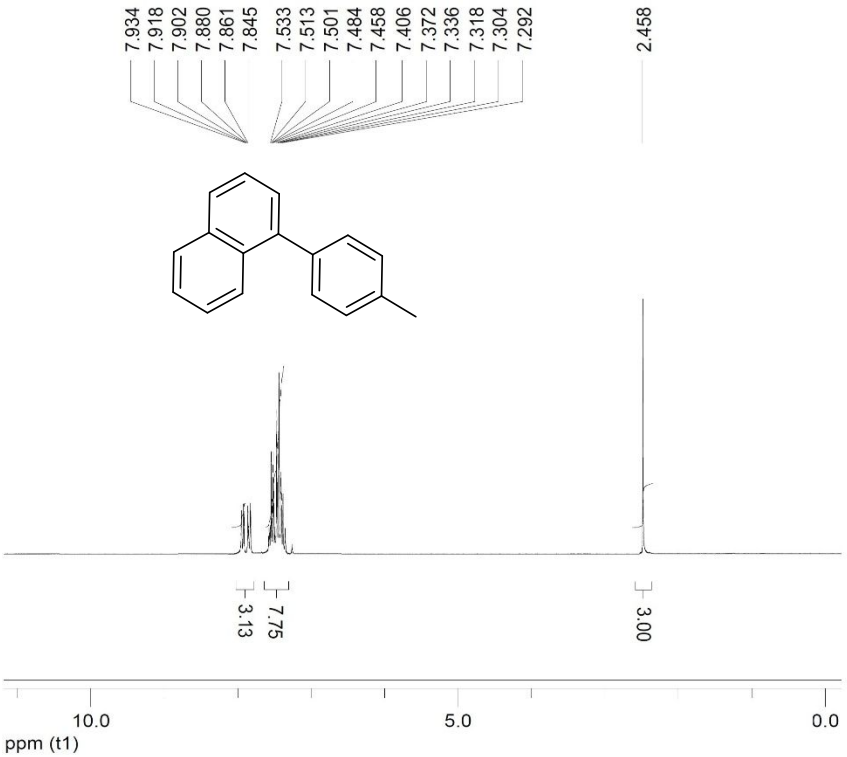
Scheme S42. ^{13}C-NMR spectra (63 MHz) of 2,4'-dimethylbiphenyl **(C22)** in $CDCl_3$.



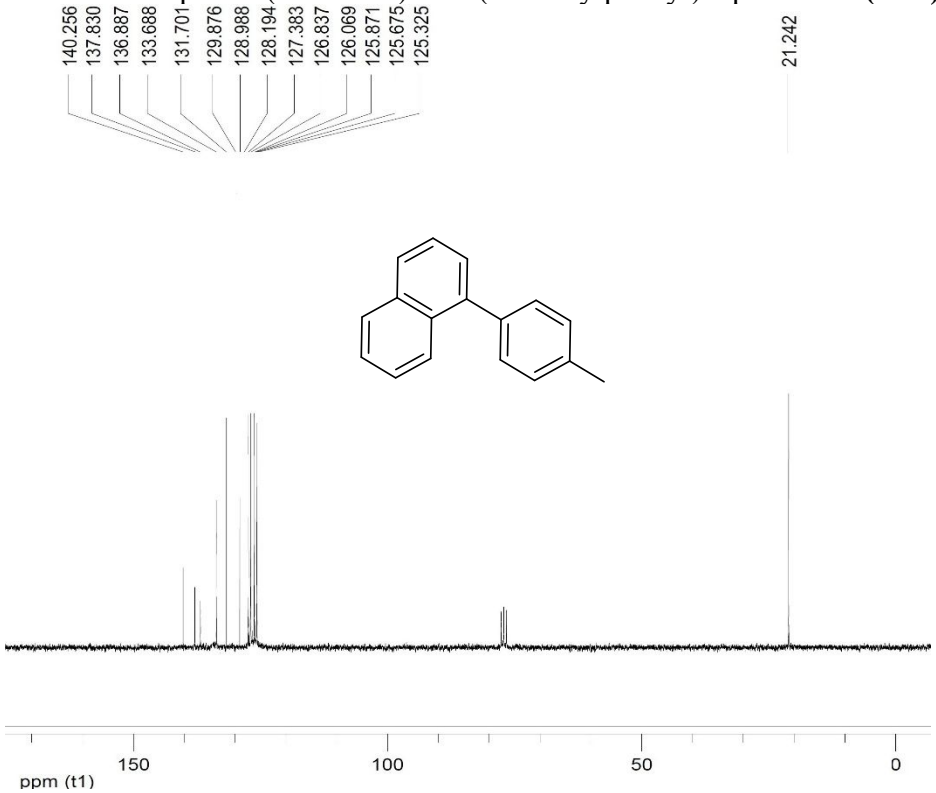
Scheme S43. ^{1}H-NMR spectra (250 MHz) of 3,4,4'-trimethylbiphenyl **(C23)** in $CDCl_3$.



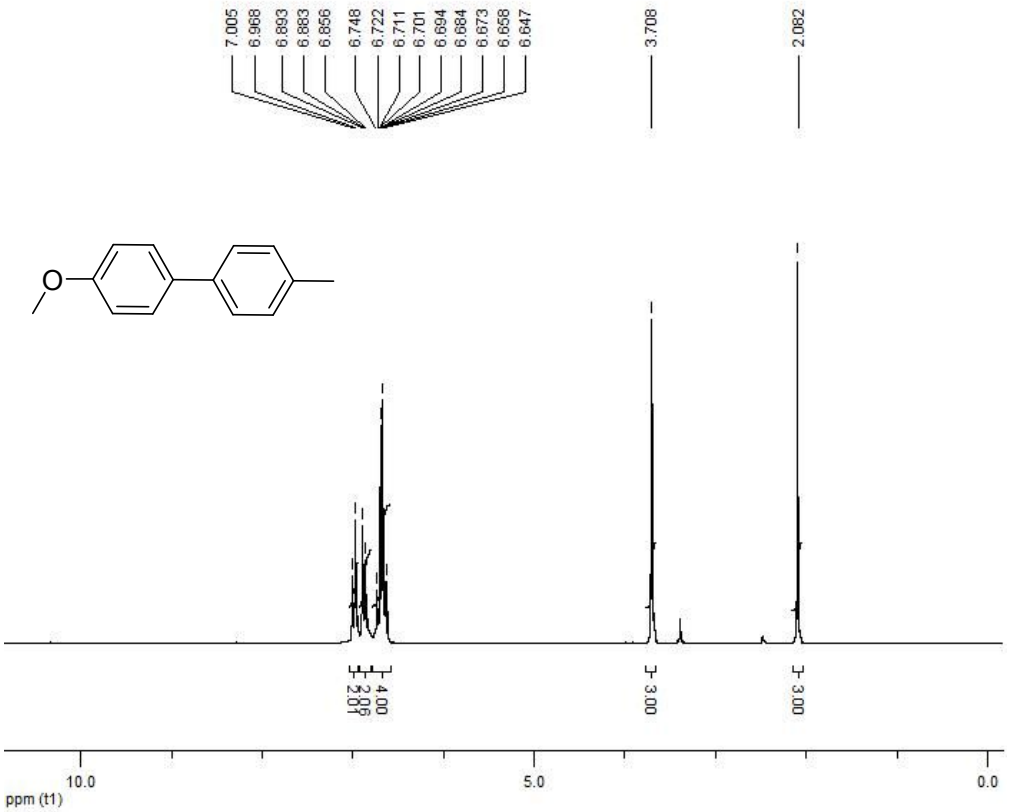
Scheme S44. ^{13}C-NMR spectra (63 MHz) of 3,4,4'-trimethylbiphenyl **(C23)** in $CDCl_3$.



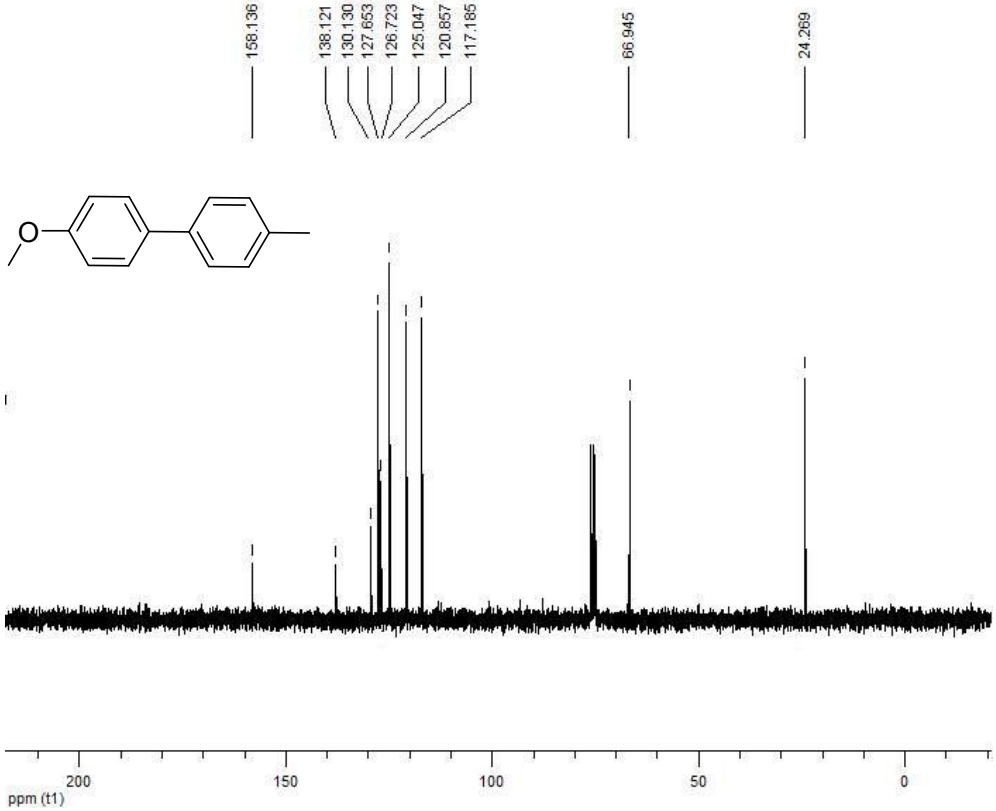
Scheme S45. ^{1}H-NMR spectra (250 MHz) of 1-(4-methylphenyl)naphthalene **(C24)** in $CDCl_3$.



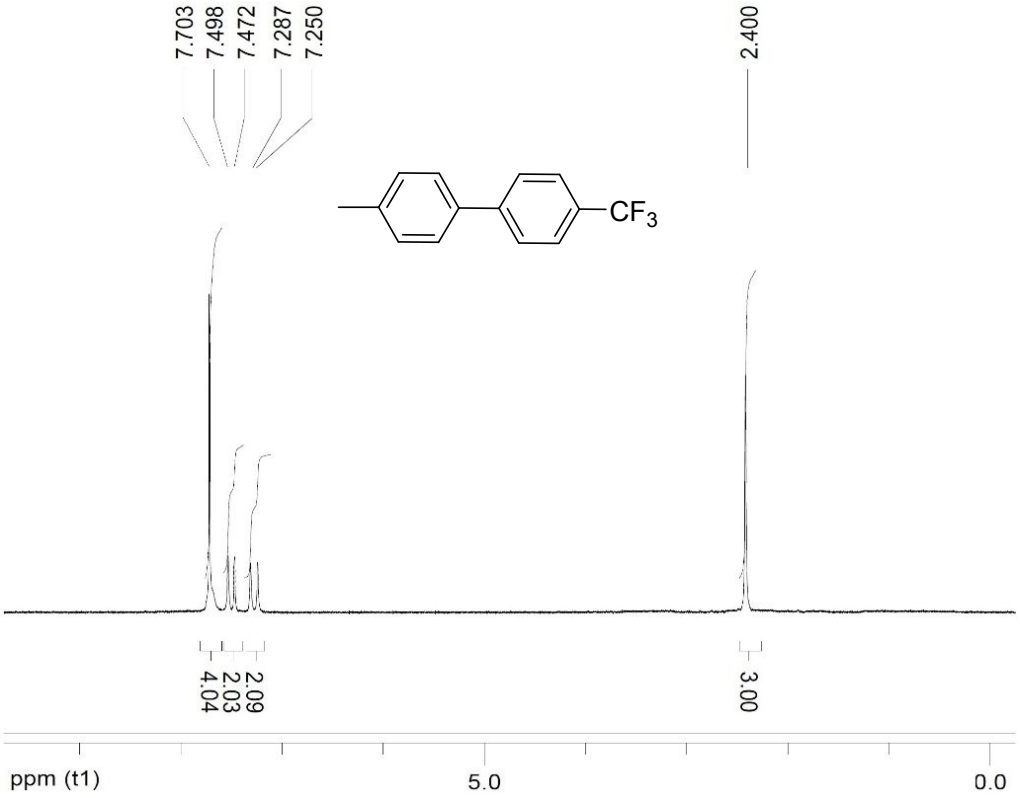
Scheme S46. ^{13}C-NMR spectra (63 MHz) of 1-(4-methylphenyl)naphthalene **(C24)** in $CDCl_3$.



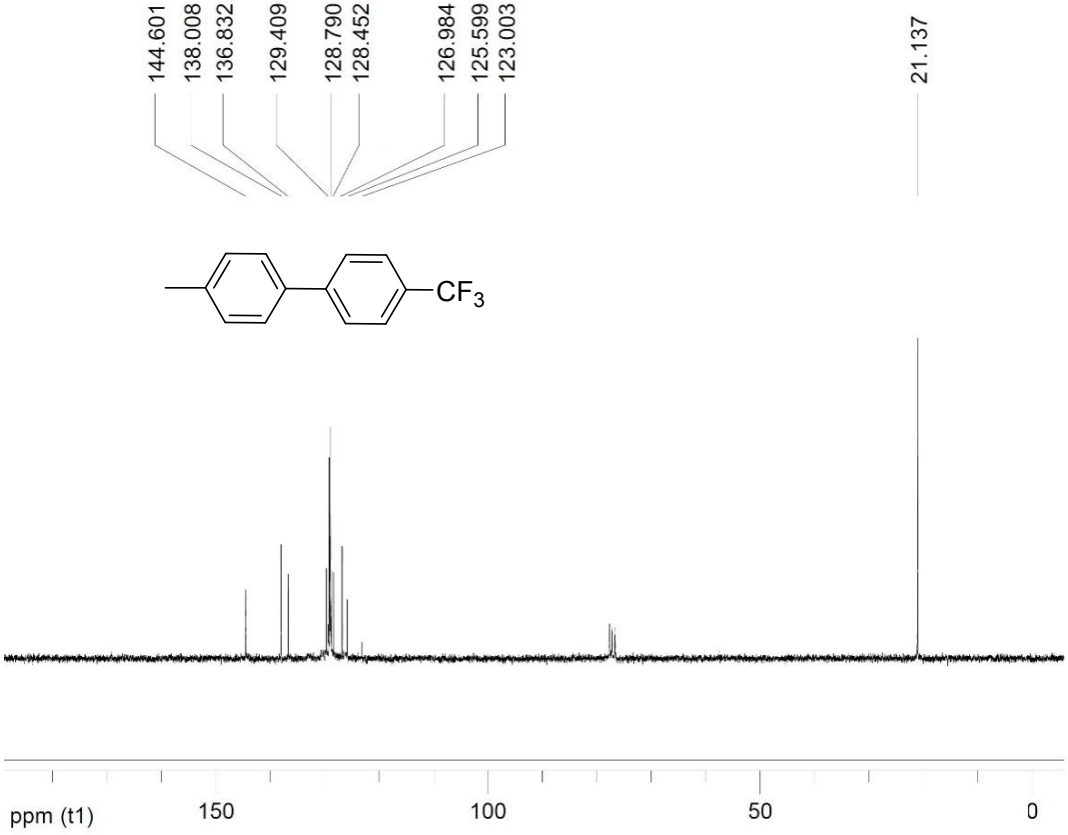
Scheme S47. ^{1}H-NMR spectra (250 MHz) of 4-methoxy-4'-methylbiphenyl **(C25)** in $CDCl_3$.



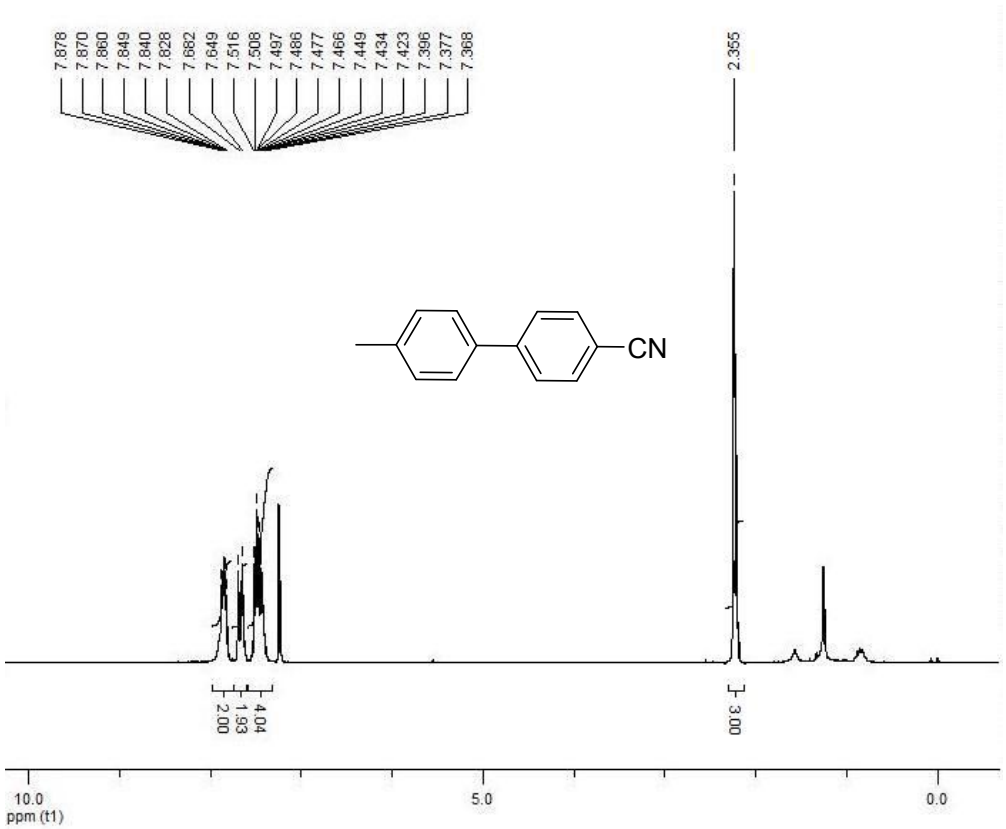
Scheme S48. ^{13}C-NMR spectra (63 MHz) of 4-methoxy-4'-methylbiphenyl **(C25)** in $CDCl_3$.



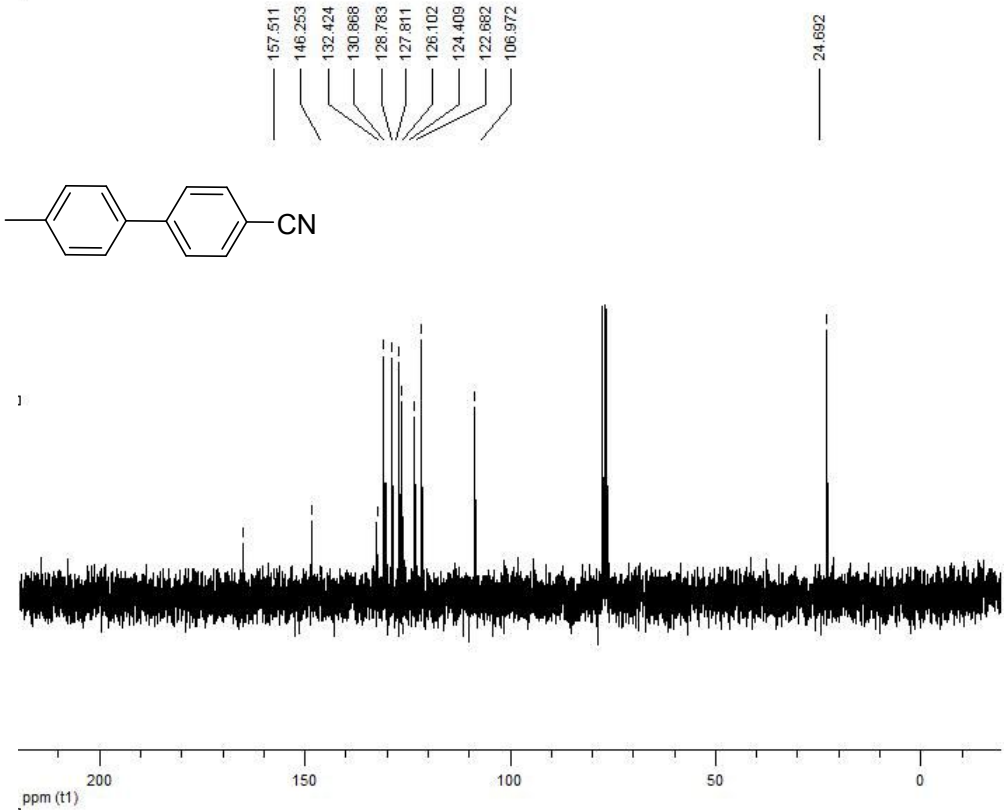
Scheme S49. ^{1}H-NMR spectra (250 MHz) of 4-methyl-4'-(trifluoromethyl)biphenyl **(C26)** in $CDCl_3$.



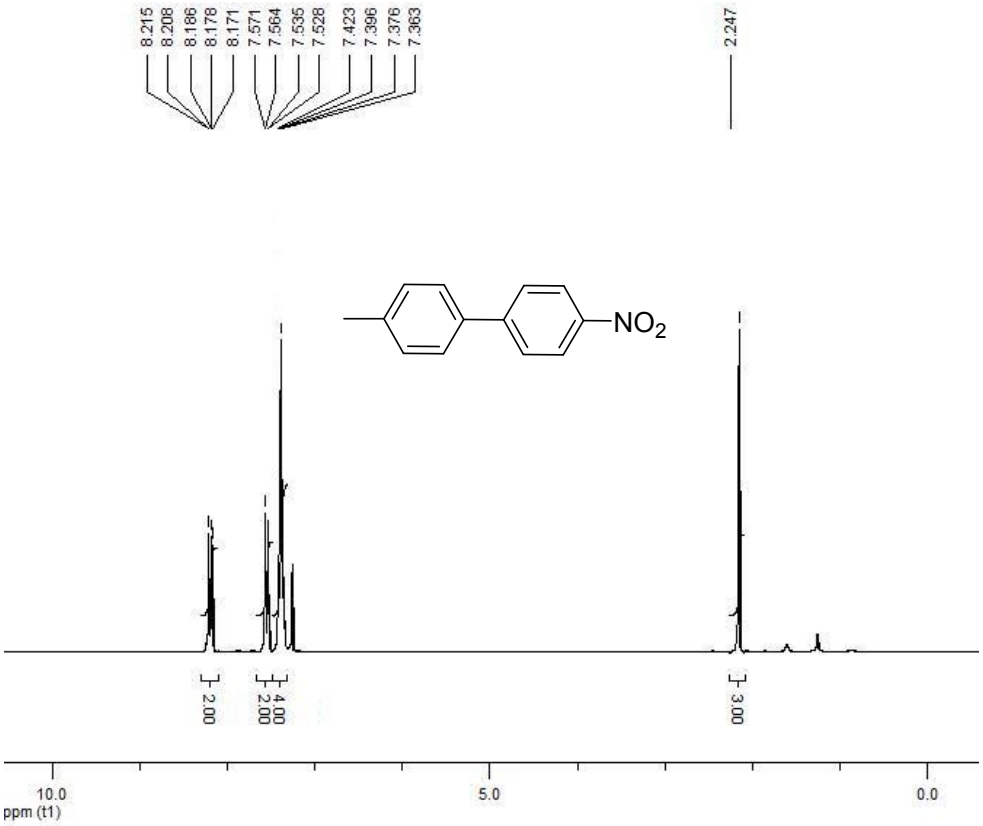
Scheme S50. ^{13}C-NMR spectra (63 MHz) of 4-methyl-4'-(trifluoromethyl)biphenyl **(C26)** in $CDCl_3$.



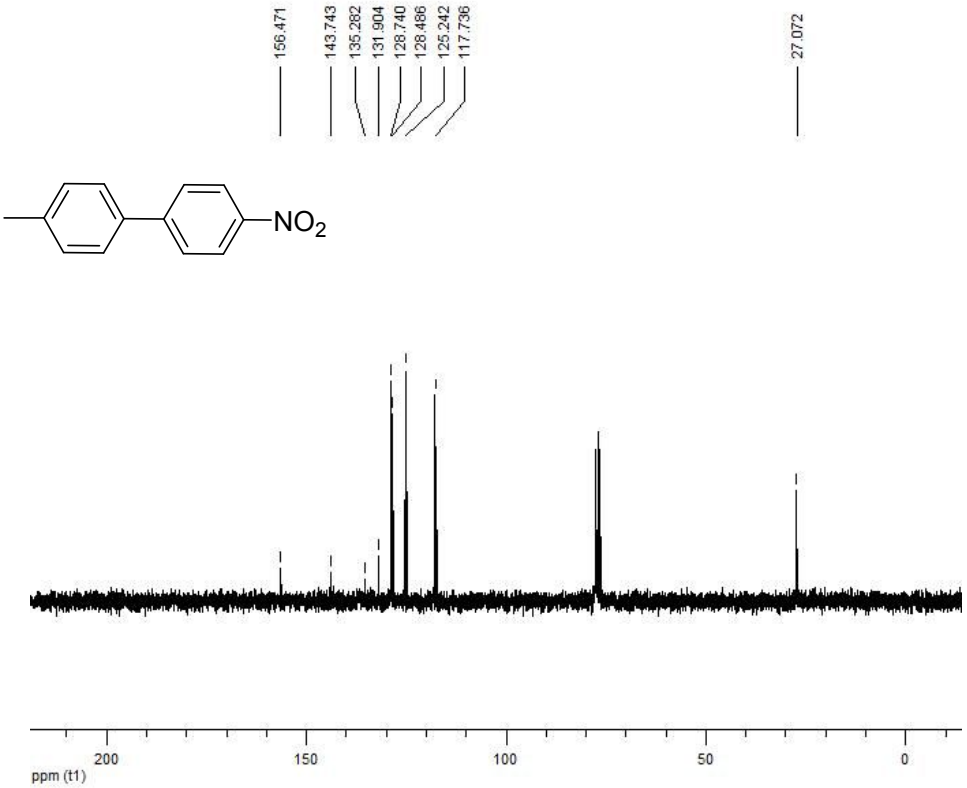
Scheme S51. ^{1}H-NMR spectra (250 MHz) of 4'-methyl-4-biphenylcarbonitrile **(C27)** in $CDCl_3$.



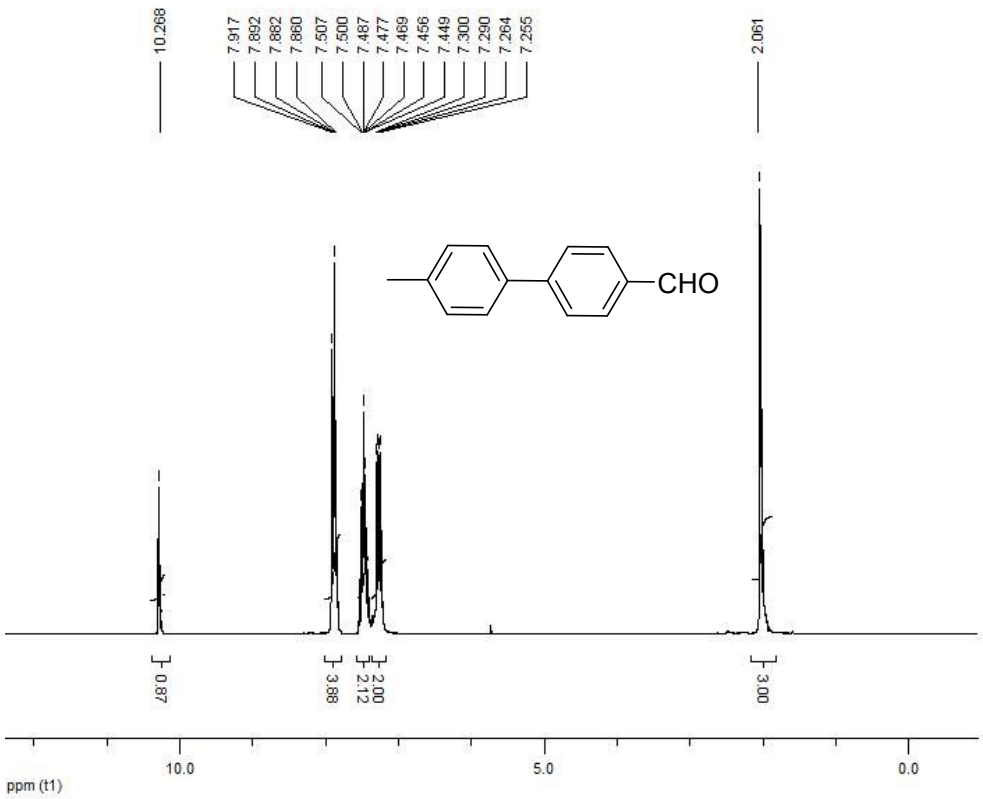
Scheme S52. ^{13}C-NMR spectra (63 MHz) of 4'-methyl-4-biphenylcarbonitrile **(C27)** in $CDCl_3$.



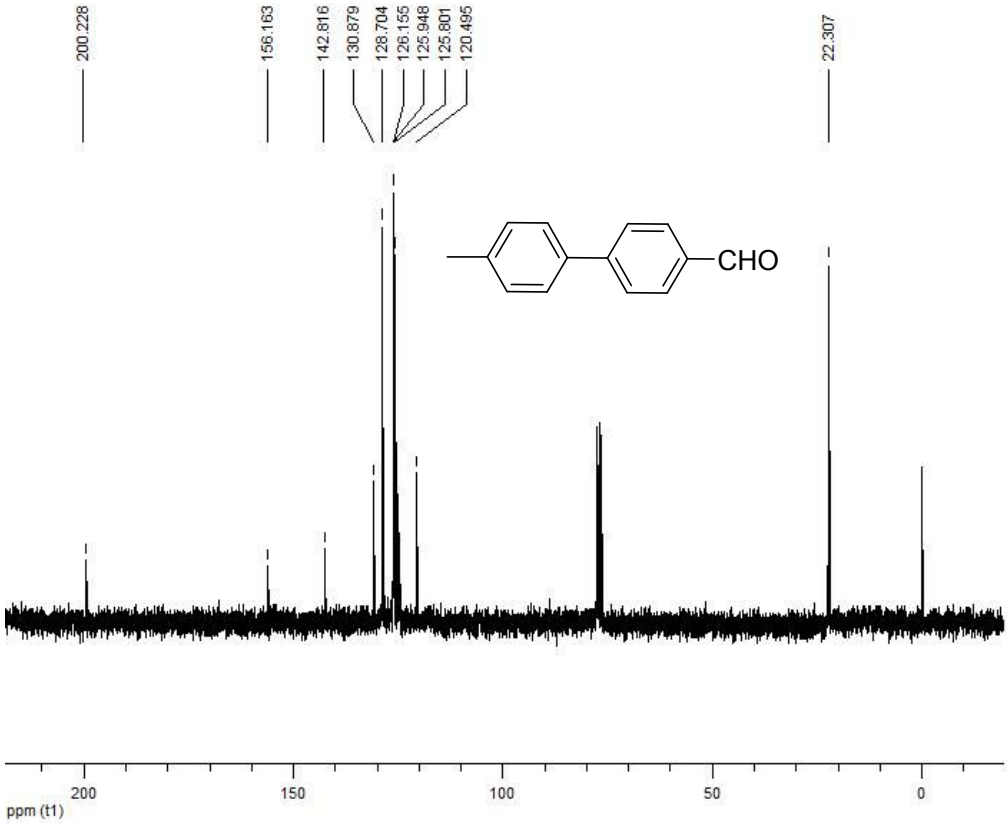
Scheme S53. ^{1}H-NMR spectra (250 MHz) of 4-methyl-4'-nitrobiphenyl **(C28)** in $CDCl_3$.



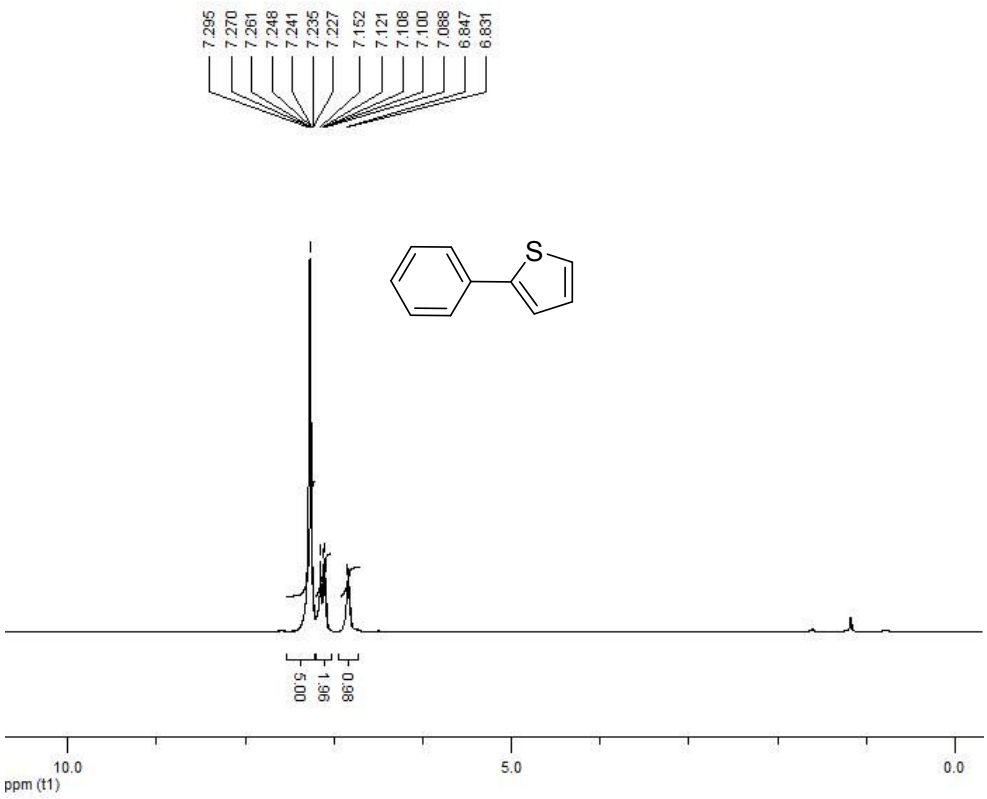
Scheme S54. ^{13}C-NMR spectra (63 MHz) of 4-methyl-4'-nitrobiphenyl **(C28)** in $CDCl_3$.



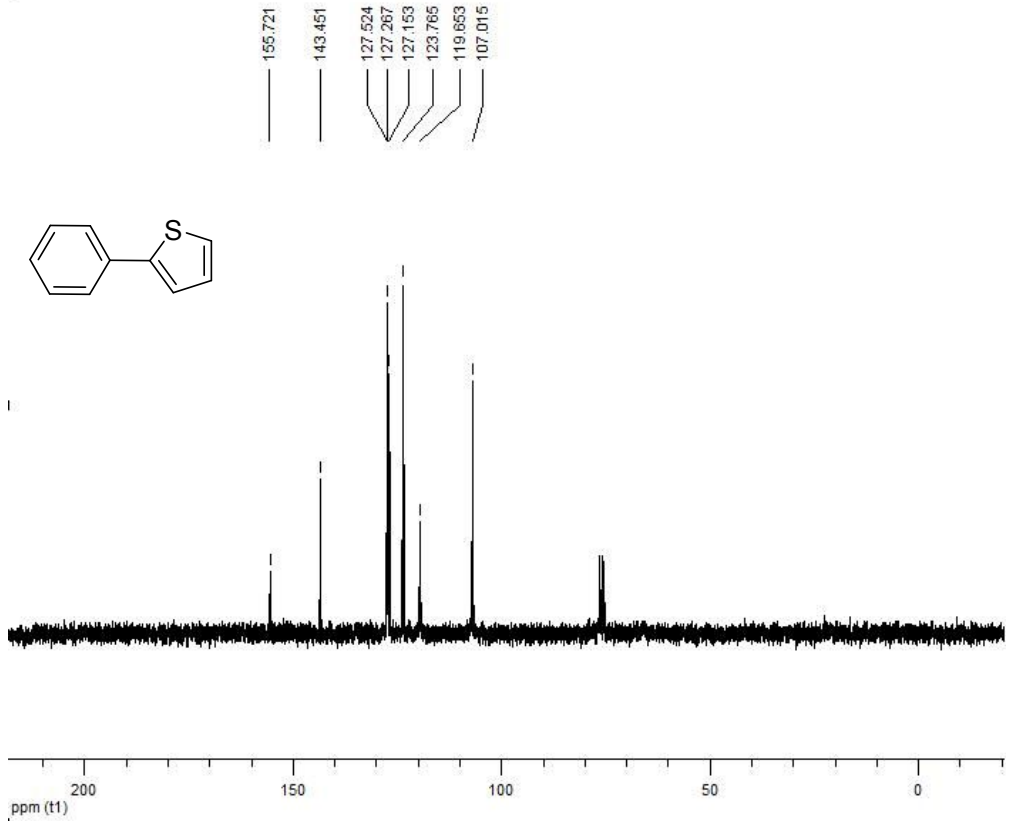
Scheme S55. ^{1}H-NMR spectra (250 MHz) of 4'-methyl-4-biphenylcarbaldehyde **(C29)** in $CDCl_3$.



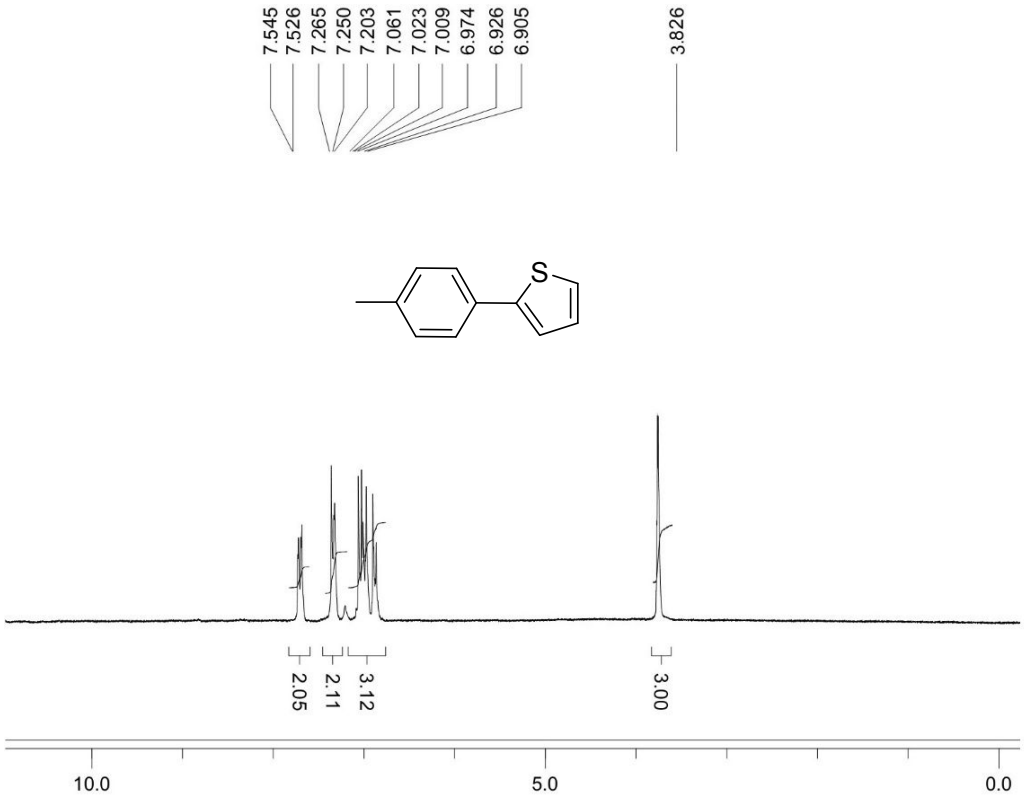
Scheme S56. ^{13}C-NMR spectra (63 MHz) of 4'-methyl-4-biphenylcarbaldehyde **(C29)** in $CDCl_3$.



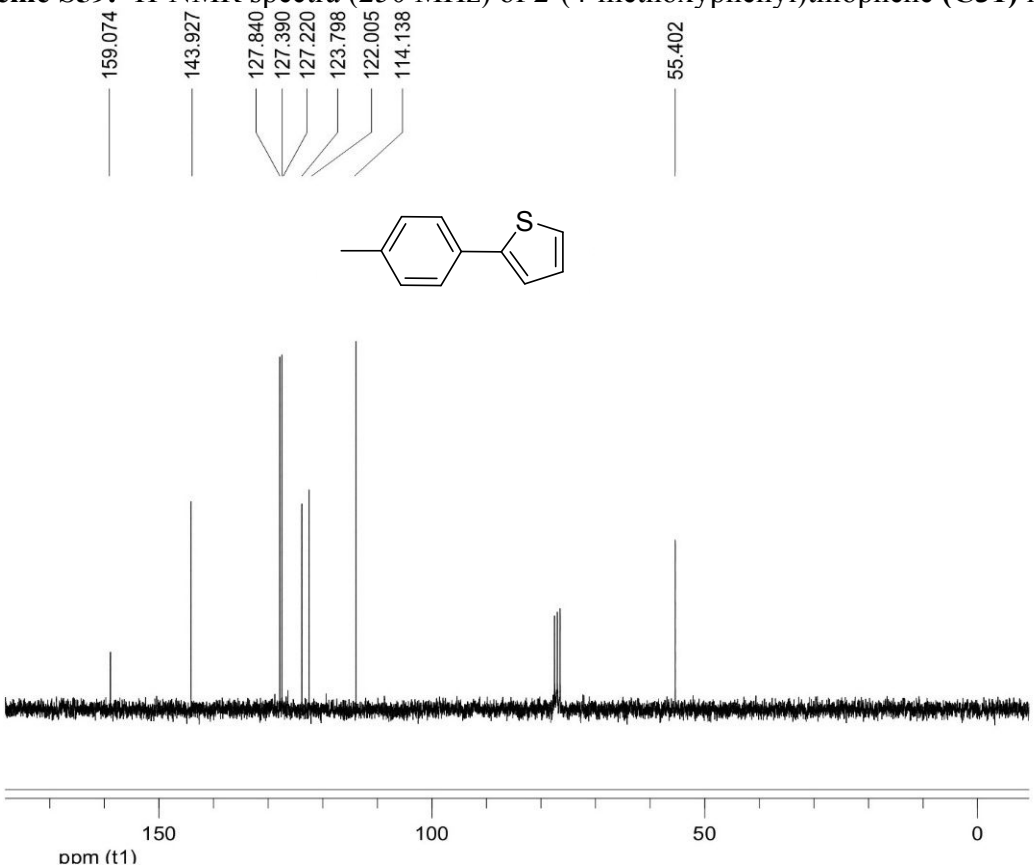
Scheme S57. ^{1}H-NMR spectra (250 MHz) of 2-phenylthiophene **(C30)** in $CDCl_3$.



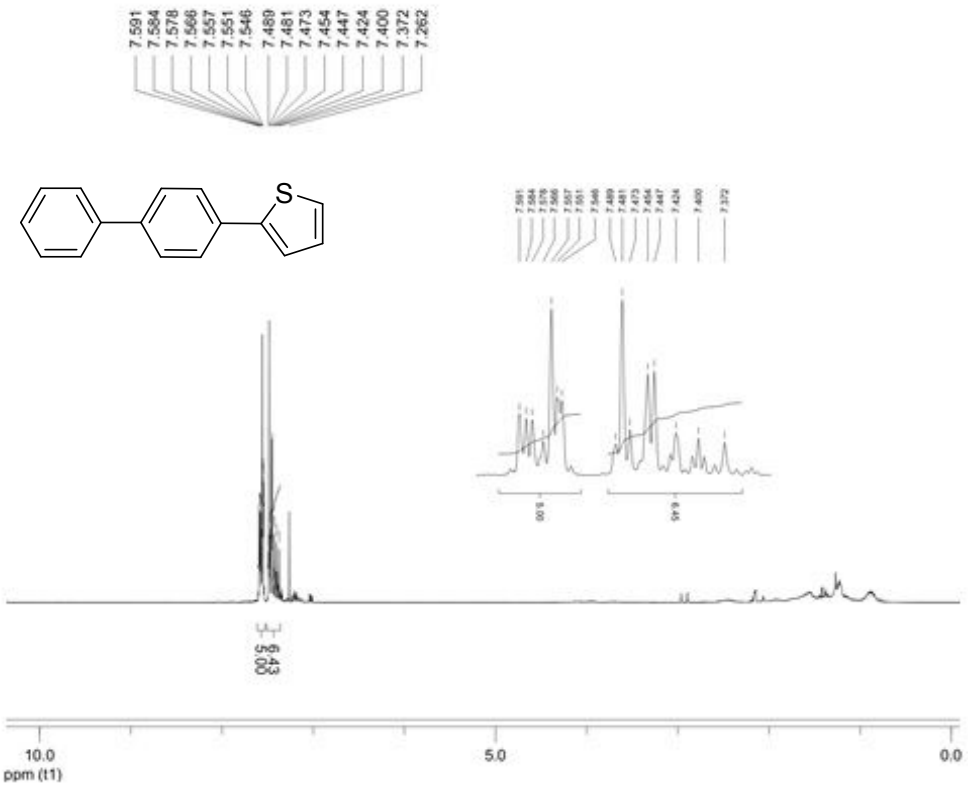
Scheme S58. ^{13}C-NMR spectra (63 MHz) of 2-phenylthiophene **(C30)** in $CDCl_3$.



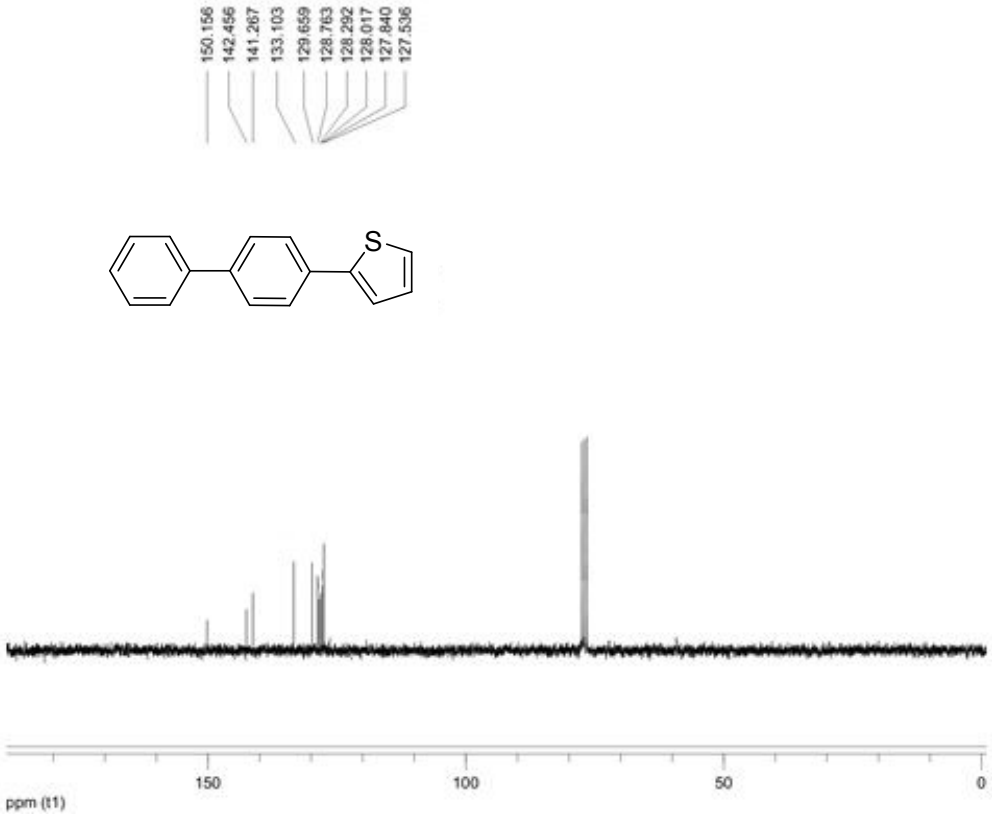
Scheme S59. ^{1}H-NMR spectra (250 MHz) of 2-(4-methoxyphenyl)thiophene **(C31)** in $CDCl_3$.



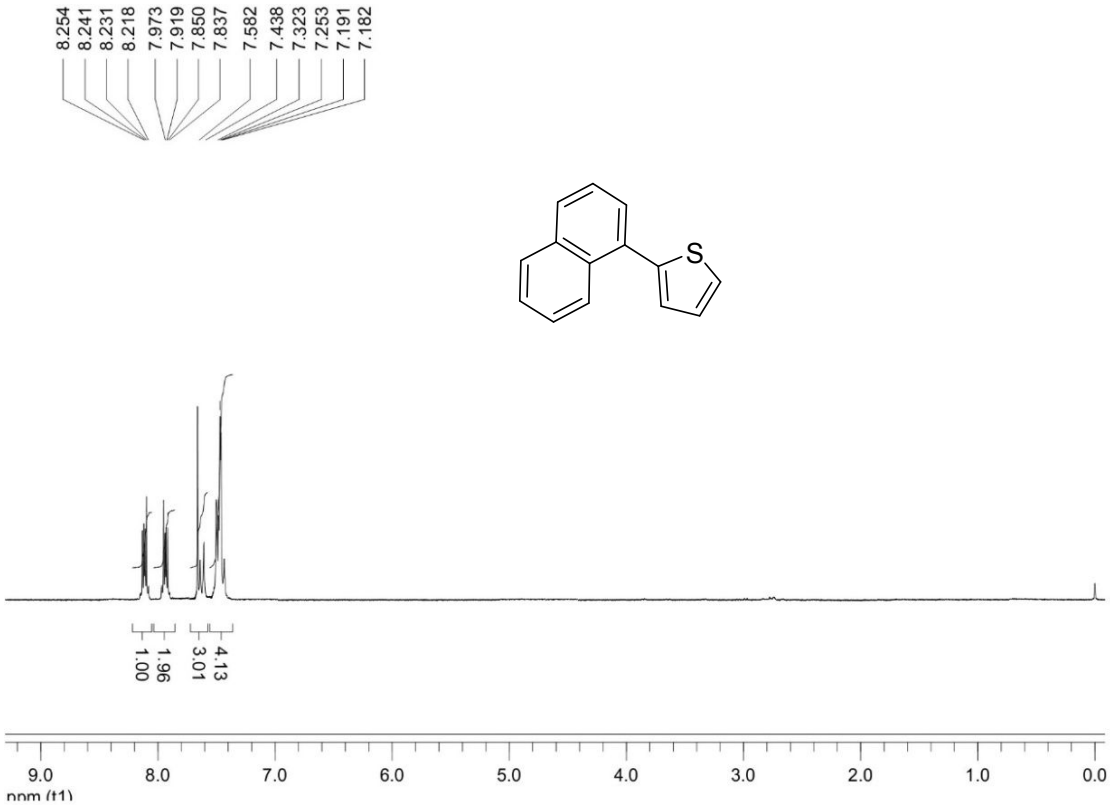
Scheme S60. ^{13}C-NMR spectra (63 MHz) of 2-(4-methoxyphenyl)thiophene **(C31)** in $CDCl_3$.



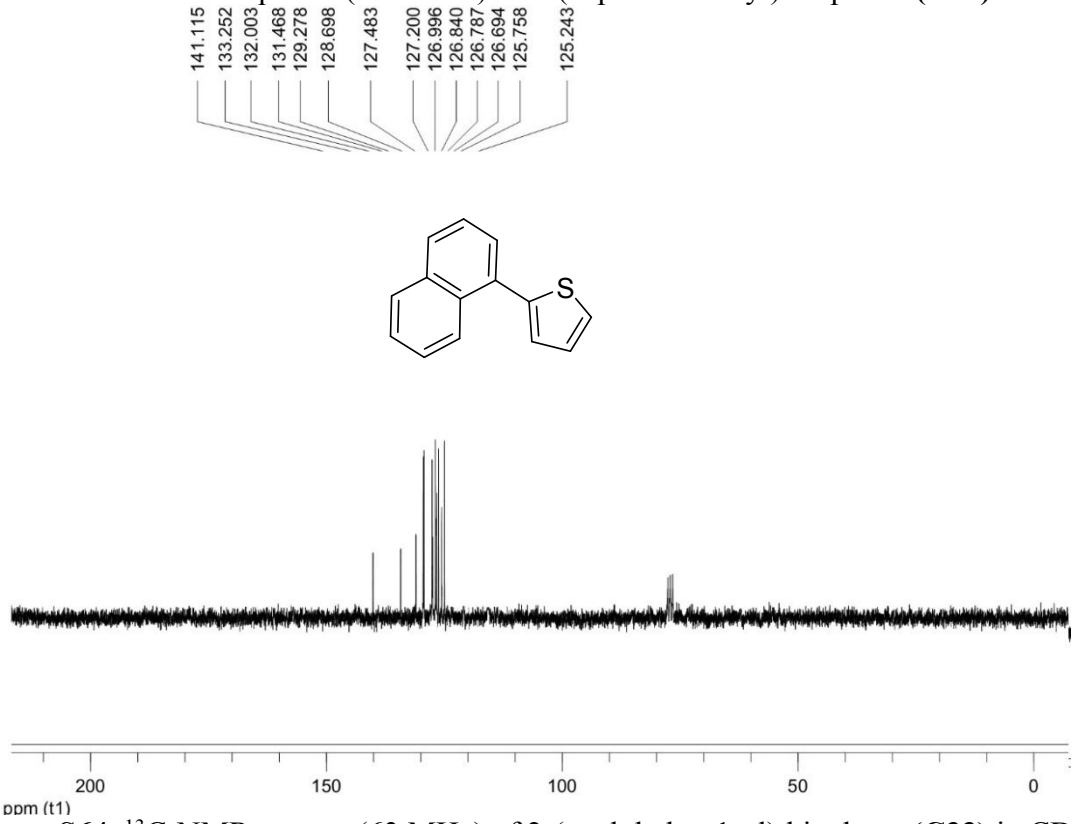
Scheme S61. ^{1}H-NMR spectra (250 MHz) of 2-(biphenyl-4-yl)thiophene **(C32)** in $CDCl_3$.



Scheme S62. ^{13}C-NMR spectra (63 MHz) of 2-(biphenyl-4-yl)thiophene **(C32)** in $CDCl_3$.



Scheme S63. ^{1}H-NMR spectra (250 MHz) of 2-(naphthalen-1-yl)thiophene **(C33)** in $CDCl_3$.



Scheme S64. ^{13}C-NMR spectra (63 MHz) of 2-(naphthalen-1-yl)thiophene **(C33)** in $CDCl_3$.