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Supporting Information

Effect on Orthometallation of NHC Palladium Complexes toward the Catalytic Activity Studies in Suzuki Coupling Reaction

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Experimental procedures

Unless otherwise noted, all manipulations were performed in air. All solvents and reagents were used as received. The reagents were purchased from Sigma–Aldrich, Acros, Merck, TEDIA and Alfa-Aesar. The imidazolium salt IPr·HCl, SIPr·HCl and NHC palladium complexes were prepared by following literature procedures and their identity and purity was confirmed by ^{1}H NMR spectroscopy.[1]

All aryl halides and boronic acids were used as received. Technical grade ethyl alcohol was used to carry out Suzuki-Miyaura cross-coupling reactions. All reactions were carried out in air at ambient temperature. Flash chromatography was performed on silica gel 60 (230-400 mesh) using mixtures of hexanes/ethyl acetate (10:1), unless otherwise noted.

^{1}H and ^{13}C{^{1}H} NMR spectra were recorded either on Brucker-AV-400 (400 MHz) spectrometers in chloroform-*d* at ambient temperature unless stated otherwise and referenced internally to the residual solvent peak and reported as parts per million relative to tetramethylsilane. Elemental analyses were performed by FLASH 2000 Series Nitrogen and Carbon Analyzer instrument (Thermo). The Suzuki-Miyaura cross-coupling reactions were analyzed by GC-MS on a Bruker SCION 436 SQ instrument equipped with a Bruker BR-5ms column. The MS detector was configured with an electronic impact ionization source.

Procedure of Suzuki-Miyaura cross-coupling reaction.

Complex (1 mol %), base (1.2 equiv.), and phenylboronic acid (0.6 mmol) were added in turn to a vial equipped with a magnetic bar and sealed with a screw cap. Technical grade solvent (1 mL) was injected into the vial, and the mixture stirred on a stirring plate at room temperature. Aryl chloride (0.5mmol, if liquid) was then injected (or charged if solid). The reaction was monitored by GC-MS. When finished, the solvent was evaporated under vacuum and the product isolated by flash chromatography. The amount of product shown is the average of two runs.

Characterisation of Complexes 1a-b

Synthesis of 1a. A vial was charged with [Pd(μ-Cl)Cl(IPr)]$_2$ (202 mg, 0.18 mmol) and *N*,*N*-Dimethylbenzylamine (54 μL, 0.36 mmol) and dichloromethane (2 mL) as solvent. The solution was stirred at room temperature for 20 min. The solution was filtered through a pad of Celite, and the filtrate was removed of the solvent to afford a pale yellow solid, to obtain the desired compound in 95% yield (238 mg). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.05 (d, *J*= 6.8 Hz, C*H*$_3$, 12H), 1.37 (d, *J*= 6.8 Hz, C*H*$_3$, 12H), 2.12 (s, N(C*H*$_3$)$_2$, 6H), 3.14 (septet, *J*= 6.8 Hz, C*H*, 4H), 3.60 (s, N(C*H*$_2$), 2H), 6.99 (t, *J*= 7.6 Hz, Ar*H*, 2H), 7.07 (s, C*H*=C*H*, 2H), 7.12 (t, *J*=7.6 Hz, Ar*H*, 1H), 7.39 (t, *J*= 7.2 Hz, Ar*H*, 6H), 7.54 (t, *J*= 7.6 Hz, Ar*H*, 2H). ^{13}C{^{1}H} NMR ($CDCl_3$, 100MHz) δ 22.9 (s, iPr), 26.4 (s, iPr), 28.6 (s, *C*HiPr), 49.6 (s, N(*C*H$_3$)$_2$), 65.0 (s, *C*H$_2$N(CH$_3$)$_2$), 124.0 (s, *C*H aromatic), 125 (s, *C*H aromatic), 127.3 (s, *C*H aromatic), 128.0 (s, *C*H aromatic), 130.0 (s, *C*H aromatic), 131.0 (s, *C*H aromatic), 134.9 (s, *C* aromatic), 135.2 (s, *C* aromatic), 147.0 (s, *C* aromatic), 153.6 (*C* carbene). Anal. Calcd for $C_{36}H_{49}Cl_2N_3Pd$: C, 61.67; H, 7.04; N, 5.99. Found: C, 61.25; H, 7.18; N, 5.78.

Synthesis of 1b. A vial was charged with [Pd(μ-Cl)Cl(SIPr)]$_2$ (341 mg, 0.3 mmol) and *N*,*N*-Dimethylbenzylamine (89 μL, 0.6 mmol) and dichloromethane (2 mL) as solvent. The solution was stirred at room temperature for 20 min. The solution was filtered through a pad of Celite, and the filtrate was removed of the solvent to afford a pale yellow solid, to obtain the desired compound in 78% yield (329 mg). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.18 (d, *J*= 6.8 Hz, C*H*$_3$, 12H), 1.46 (d, *J*= 6.4 Hz, C*H*$_3$, 12H), 2.08 (s, N(C*H*$_3$)$_2$, 6H), 3.60 (septet, *J*= 7.3 Hz, C*H*, 4H), 4.05 (s, N(C*H*$_2$), 2H), 6.97 (t, *J*= 7.8 Hz, Ar*H*, 2H), 7.12 (t, *J*= 7.4 Hz, Ar*H*, 1H), 7.36 (m, Ar*H*+C*H*$_2$C*H*$_2$, 8H), 7.49 (t, *J*= 7.8 Hz, Ar*H*, 2H). ^{13}C{^{1}H} NMR ($CDCl_3$, 100MHz) δ 23.9 (s, iPr), 27.0 (s, iPr), 28.7 (s, *C*HiPr), 49.3 (s, N(*C*H$_3$)$_2$), 53.6 (s, *C*H$_2$N(CH$_3$)$_2$), 64.9 (s, *C*H$_2$*C*H$_2$), 124.4 (s, *C*H aromatic), 127.2 (s, *C*H aromatic), 127.9 (s, *C*H aromatic), 130.9 (s, *C*H aromatic), 134.7 (s, *C* aromatic), 135.4 (s, *C* aromatic), 148.2 (*C*

aromatic), 185.1 (s, *C* carbene). Anal. Calcd for $C_{36}H_{51}Cl_2N_3Pd$: C, 61.49; H, 7.31; N, 5.98. Found: C, 61.44；H, 7.46；N, 5.76.

Structure determination

The Crystal **1a-b** were grown from concentrated dichloromethane solution and isolated by filtration. Data were collected on a mounted on a Bruker AXS SMART 1000 diffractometer with graphite-monochromated Mo Kα radiation (λ = 0.7107 Å). Absorption correction was applied using SADABS.[2] The structure was solved by direct methods using a SHELXTL package.[3-4] All non-H atoms were located from successive Fourier maps, and hydrogen atoms were refined using a riding model. Anisotropic thermal parameters were used for all non-H atoms, and fixed isotropic parameters were used for H atoms. Some details of the data collection and refinement are given in Table S1.

Table S1 Summary of crystal data for compounds **1a-b**

	1a	**1b**
Formula	$C_{36}H_{49}Cl_2N_3Pd$	$C_{36}H_{51}Cl_2N_3Pd$
Fw	701.08	703.09
T, K	293(2)	150(2)
Crystal system	Monoclinic	Monoclinic
Space group	*P21*	*P21*
a, Å	10.7929(8)	10.7760(5)
b, Å	12.4800(6)	12.5569(5)
c, Å	13.3567(10)	13.3141(6)
a °	90	90
β °	98.630(7)	98.3808(17)
γ °	90	90
V, Å^3	1778.7(2)	1782.33(14)
Z	2	2
ρ_{calc}, Mg/m^3	1.309	1.310
μ(MoKα), mm^{-1}	0.699	0.698
Reflections collected	8218	31750
No. of parameters	384	380
Indep. reflns (R_{int})	6767 (0.0384)	7266 (0.0398)
R indices(all data)	0.0468, 0.0874	0.0236, 0.0496
GoF [b]	1.029	1.039

[a] $R1 = [|F_0| - |F_c|]/ |F_0|]$, $wR2 = [w(F_0^2 - F_c^2)^2/ w(F_0^2)^2]^{1/2}$, w= 0.10.
[b] GoF = $[\Sigma w(F_0^2-F_c^2)^2/(N_{rflns} - N_{params})]^{1/2}$.

Spectra of Suzuki-Miyaura cross-coupling products

Biphenyl (Table 2, entry 1)[5] Crude product was purified by flash column chromatography on silica gel (hexanes/ethyl acetate= 10/1), 74 mg (96 %) of the title compound (white solid). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (t, *J*= 7.6 Hz, Ar*H*, 1H), 7.44 (t, *J*= 7.6Hz, Ar*H*, 2H), 7.60 (d, *J*= 8Hz, Ar*H*, 2H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 127.1, 127.2, 128.7, 141.2.

2-Phenylthiophene (Table 2, entry 2)[5] Crude product was purified by flash column chromatography on silica gel (hexanes/ethyl acetate= 10/1), 76.0 mg (95%) of the title compound (white solid). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.02-7.04 (m, Ar*H*, 1H), 7.21-7.35 (m, Ar*H,* 5H), 7.55-7.59 (m, Ar*H*, 2H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 123.1, 124.9, 126.0, 127.5, 128.1, 129.0, 134.5, 144.5.

4-Methoxybiphenyl (Table 2, entry 3)[5] The procedure afforded, after filtration through silica (hexanes/ethyl acetate= 10/1), 83.7 mg (91%) of the title compound (white solid). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.83 (s, OCH_3, 3H), 6.96 (d, *J*= 8.8 Hz, Ar*H*, 2H), 7.26-7.30 (m, Ar*H*, 1H), 7.38-7.41 (m, Ar*H*, 2H), 7.50-7.54 (m, Ar*H*, 4H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 55.3, 114.2, 126.6, 126.7, 128.1, 128.7, 133.8, 140.8, 159.1.

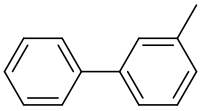
4-Methylbiphenyl (Table 2, entry 4)[5] Crude product was purified by flash column chromatography on silica gel (hexanes/ethyl acetate= 10/1), 80.8 mg (96 %) of the title compound (colorless liquid). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.36 (s, CH_3, 3H), 7.21 (d, *J*= 7.2 Hz, Ar*H*, 2H), 7.27-7.32 (m, Ar*H*, 1H), 7.37-7.40 (m, Ar*H*, 2H), 7.46 (d, *J*= 6.8 Hz, Ar*H*, 2H), 7.55-7.56 (m, Ar*H*, 2H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 21.2, 127.0, 127.2, 128.8, 129.5, 137.0, 138.4, 141.2.

2-Methylbiphenyl (Table 2, entry 5)[6] Crude product was purified by flash column chromatography on silica gel (hexanes/ethyl acetate= 10/1), 80.8 mg (96 %) of the title compound (colorless liquid). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.38 (s, CH_3, 3H),7.12-7.56 (m, Ar*H*, 9H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 21.6, 124.3, 127.2, 128.0, 128.0, 128.6, 128.7, 138.3, 141.4.

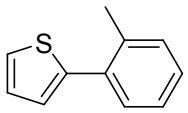
2-Methoxybiphenyl (Table 2, entry 6)[5] Crude product was purified by flash column

chromatography on silica gel (dichloromethane), 88.4 mg (96%) of the title compound (colorless liquid). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.76 (s, OCH_3, 3H), 6.94-7.02 (m, Ar*H*, 2H), 7.29 (t, *J*= 7.6 Hz, Ar*H*, 3H), 7.39 (d, *J*= 8.4 Hz, Ar*H*, 2H), 7.51 (d, *J*= 8 Hz, Ar*H*, 2H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 55.6, 111.3, 120.9, 126.9, 128.0, 128.6, 129.6, 130.8, 130.9, 138.6, 156.5.

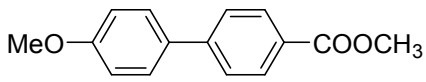
3-Methylbiphenyl (Table 2, entry 7)[5] Crude product was purified by flash column chromatography on silica gel (hexanes/ethyl acetate= 10/1), 80.7 mg (96%) of the title compound (colorless liquid). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.38 (s, CH_3, 3H), 7.12 (d, *J*= 7.6 Hz, Ar*H*, 1H), 7.27-7.30(m, Ar*H*, 2H), 7.35-7.40 (m, Ar*H*, 4H), 7.55 (d, *J*= 7.6 Hz, Ar*H*, 2H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 21.6, 124.4, 127.3, 128.0, 128.1, 128.1, 128.7, 128.8, 138.4, 141.3, 141.4.



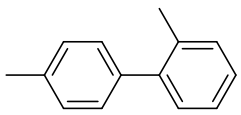
2-(*o*-Tolyl)thiophene (Table 2, entry 8)[5] Crude product was purified by flash column chromatography on silica gel (hexanes/ethyl acetate= 10/1), 82.7 mg (95%) of the title compound (yellow liquid). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.41 (s, CH_3, 3H), 7.04- 7.10 (m, Ar*H*, 2H), 7.18-7.24 (m, Ar*H*, 3H), 7.31(dd, *J*= 1.2 Hz, *J*= 1.5 Hz, Ar*H*, 1H), 7.38-7.40 (m, Ar*H*, 1H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 21.1, 125.1, 125.9, 126.4, 127.0, 127.8, 130.5, 130.7, 134.2, 136.1, 143.1.



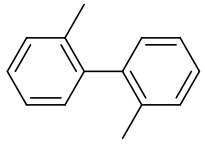
4'-methoxybiphenyl-4-carboxylate (Table 2, entry 9)[7] Crude product was purified by flash column chromatography on silica gel (hexanes/ethyl acetate= 10/1), 117.3mg (97%) of the title compound (white solid). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.84 (s, OCH_3, 3H), 3.91 (s, OCH_3, 3H), 6.98 (d, *J*= 8.8Hz, Ar*H*, 2H), 7.55 (d, *J*= 8.4 Hz, Ar*H*, 2H), 7.60 (d, *J*= 8.4 Hz, Ar*H*, 2H), 8.06 (d, *J*= 8 Hz, Ar*H*, 2H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 52.0, 55.3, 114.3, 126.4, 128.2, 128.3, 130.1, 132.4, 145.2, 159.8, 167.0.



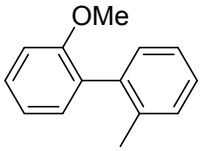
2,4'-Dimethyl-1,1'-biphenyl (Table 2, entry 10)[8] Crude product was purified by flash column chromatography on silica gel (hexanes/ethyl acetate= 10/1), 83.7 mg (92%) of the title compound (colorless liquid). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.25 (s, CH_3, 3H), 2.37 (s, CH_3, 3H), 7.19-7.23 (m, Ar*H*, 8H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 20.6, 21.2, 125.8, 127.1, 128.8, 129.1, 129.9, 130.3, 135.4, 136.4, 139.1, 141.9.



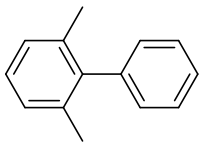
2,2'-Dimethyl-1,1'-biphenyl (Table 2, entry 11)[5] Crude product was purified by flash column chromatography on silica gel (hexanes/ethyl acetate= 10/1), 86.5 mg (95%) of the title compound (colorless liquid). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.05 (s, CH_3, 6H), 7.09 (d, J= 6.8 Hz, ArH, 2H), 7.19-7.26 (m, ArH, 6H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 19.8, 125.5, 127.1, 129.3, 129.8, 135.8, 141.6.



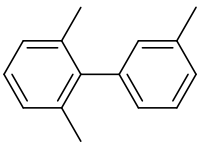
2-Methoxy-2'-methyl-1,1'-biphenyl (Table 2, entry 12)[9] Crude product was purified by flash column chromatography on silica gel (hexanes/ethyl acetate= 10/1), 85.2 mg (86%) of the title compound (colorless liquid). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.13 (s, CH_3, 3H), 3.73(s, OCH_3, 3H), 6.93-7.01 (m, ArH, 2H), 7.14-7.23 (m, ArH, 5H), 7.30-7.32 (m, ArH, 1H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 19.9, 55.4, 110.7, 120.5, 125.5, 127.3, 128.6, 129.6, 130.0, 130.9 131.0, 136.8, 138.7, 156.5.



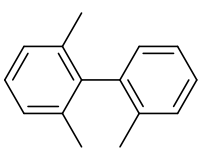
2,6-Dimethyl-biphenyl (Table 2, entry 13)[5] Crude product was purified by flash column chromatography on silica gel (hexanes/ethyl acetate= 10/1), 79.2 mg (87%) of the title compound (colorless liquid). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.01(s, CH_3, 6H), 7.07-7.13 (m, ArH, 5H), 7.31 (d, J= 6.6Hz, ArH, 1H), 7.39 (t, J=7.2Hz, ArH, 2H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 20.9, 126.5, 127.1, 127.3, 128.5, 129.1, 136.1, 141.1, 141.9.



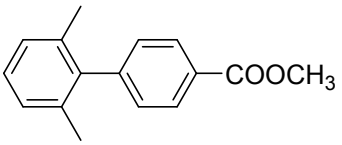
2,6,3-Trimethylbiphenyl (Table 2, entry 14)[10] Crude product was purified by flash column chromatography on silica gel (hexanes/ethyl acetate= 10/1), 82.7 mg (95%) of the title compound (colorless liquid). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.90 (s, CH_3, 6H), 2.23 (s, CH_3, 3H), 6.79-6.82 (m, ArH, 2H), 6.94-7.00 (m, ArH, 4H), 7.13-7.17(m, ArH, 1H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 20.9, 21.6, 126.1, 127.0, 127.3, 127.4, 128.4, 129.8, 136.1, 138.0, 141.1, 142.1.



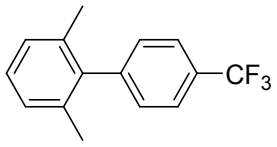
2,6,2'-Trimethylbiphenyl (Table 2, entry 15)[5] Crude product was purified by flash column chromatography on silica gel (hexanes/ethyl acetate= 10/1), 91.1 mg (93%) of the title compound (colorless liquid). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.94 (s, CH_3, 6H), 1.96 (s, CH_3, 3H), 7.02-6.99 (m, ArH, 1H), 7.29-7.09 (m, ArH, 6H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 19.4 20.3, 126.0, 126.9, 127.0, 127.2, 128.8, 130.0, 135.6, 135.8 140.5, 141.1.



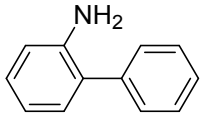
2',6'-dimethyl-[1,1'-biphenyl]-4-carboxylate (Table 2, entry 16)[11] White solid (from chloride 108 mg, 90%) obtained after column chromatography on silica gel(silica gel, hexane/EtOAc= 9:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.99 (s, CH_3, 6H), 3.92 (s, OCH_3, 3H), 7.09 (d, *J*= 7.6 Hz, Ar*H*, 2H), 7.15 (d, *J*= 6.8 Hz, Ar*H*, 1H), 7.22 (d, *J*= 8 Hz, Ar*H*, 2H), 8.10 (d, *J*= 8 Hz, Ar*H*, 2H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 20.7, 52.1, 127.4, 127.5, 128.6, 129.2, 129.8, 135.6, 140.8, 146.2, 167.1.



2,6-dimethyl-4'-trifluoromethyl-biphenyl (Table 2, entry 17)[12] Crude product was purified by flash column chromatography on silica gel (hexanes/ethyl acetate= 4/1), 106 mg (85%) of the title compound (white crystalline solid). ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.01(s, CH_3, 6H), 7.11 (d, *J*= 7.6 Hz, Ar*H*, 2H), 7.17-7.21 (m, Ar*H*, 1H), 7.27 (d, *J*= 8Hz, Ar*H*, 2H), 7.68 (d, *J*= 8 Hz, Ar*H*, 2H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 20.7, 123.0, 125.4, 125.5, 127.5, 127.6, 128.9, 129.2, 129.5, 135.7, 140.4, 145.0.

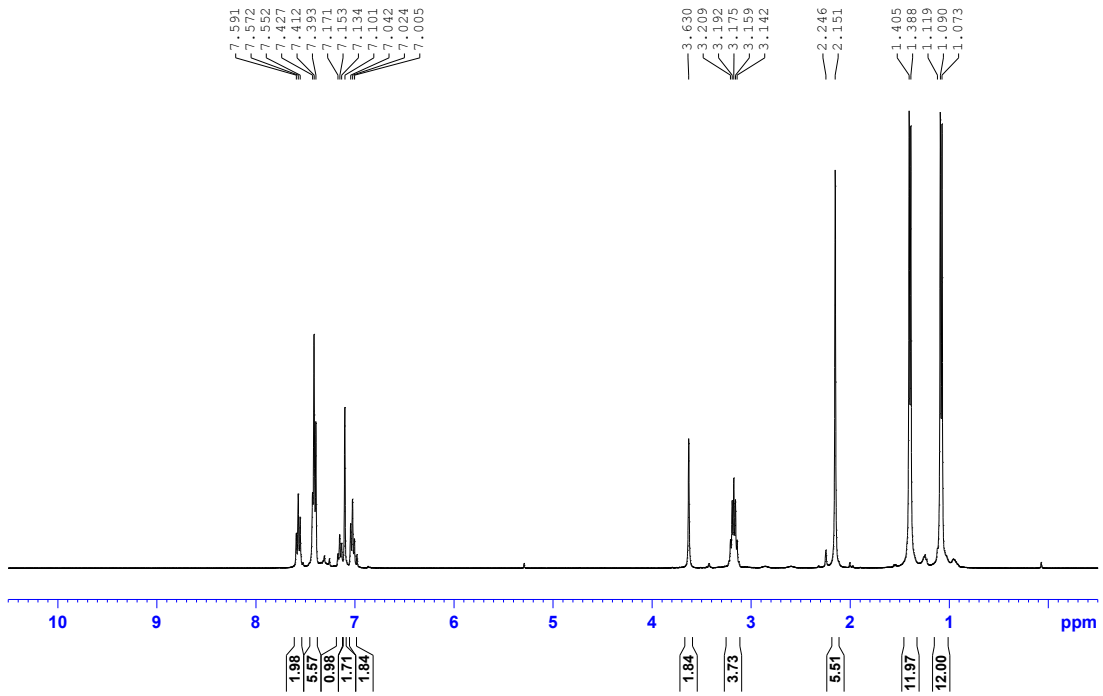


2-Amino-biphenyl (Table 2, entry 18)[13] The procedure afforded, after filtration through silica (hexanes/ethyl acetate= 10/1), 73.5 mg (87%) of the title compound (white solid). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.71-3.95 (m, NH_2, 2H), 6.62-7.21 (m, Ar*H*, 5H), 7.28-7.43 (m, Ar*H*, 4H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 115.7, 118.7, 127.2, 127.7, 128.5, 128.9, 129.1, 130.5, 139.6, 143.5.

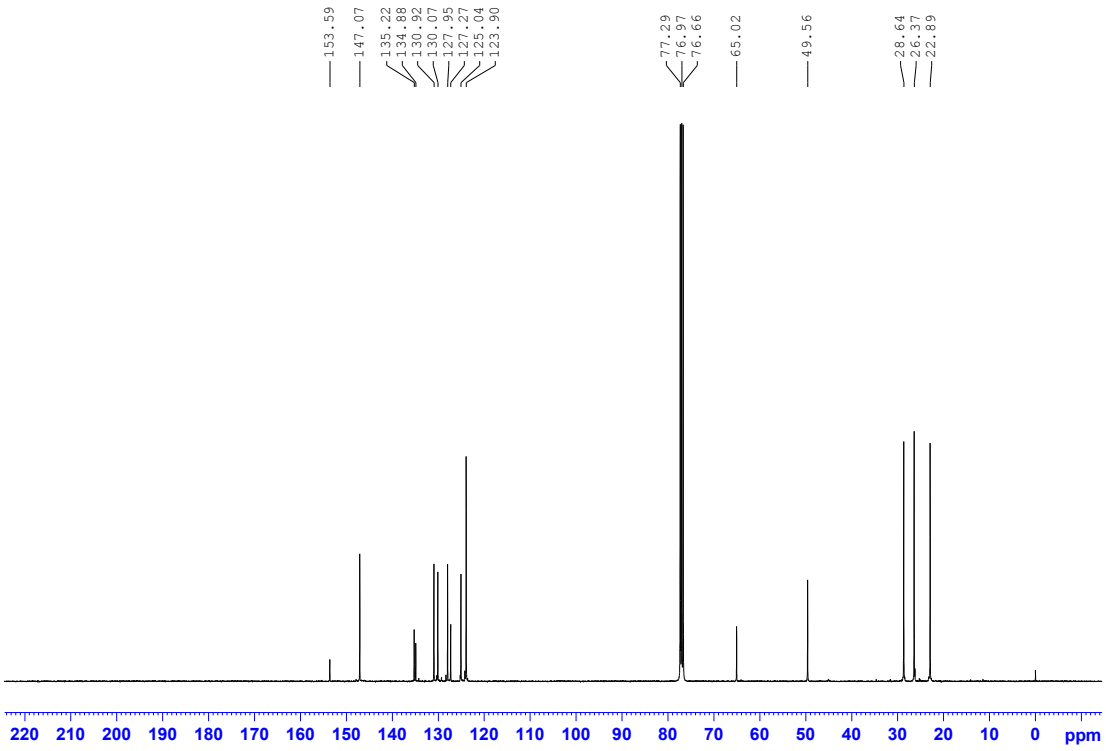


Complex 1a ^{1}H NMR

IPr-Pd-NMe2-CH2Ph-box

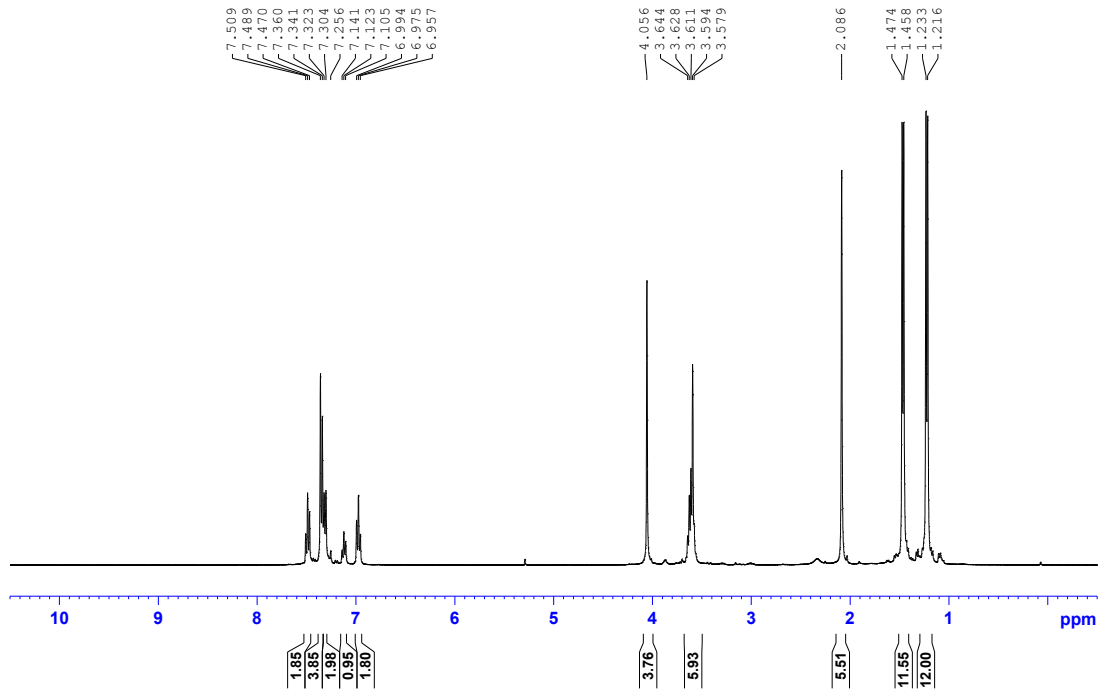


Complex 1a ^{13}C NMR



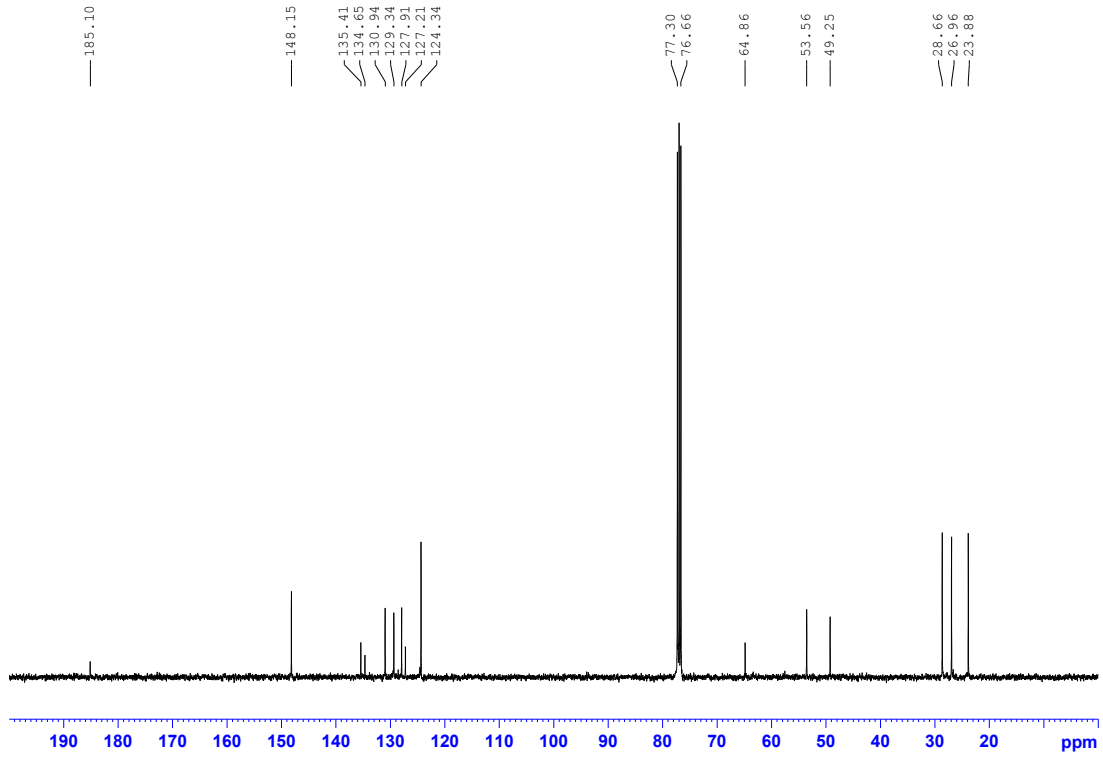
Complex 1b ^{1}H NMR

SIPrPdCl2-NMe2-CHPh-box

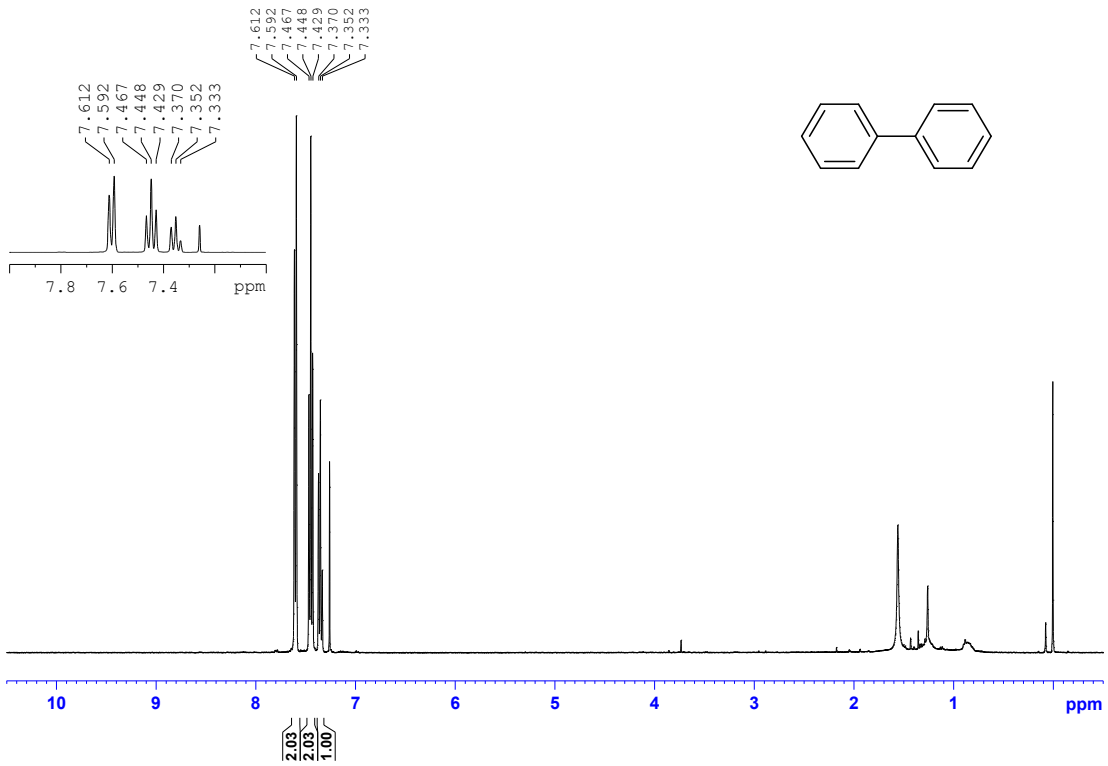


Complex 1b ^{13}C NMR

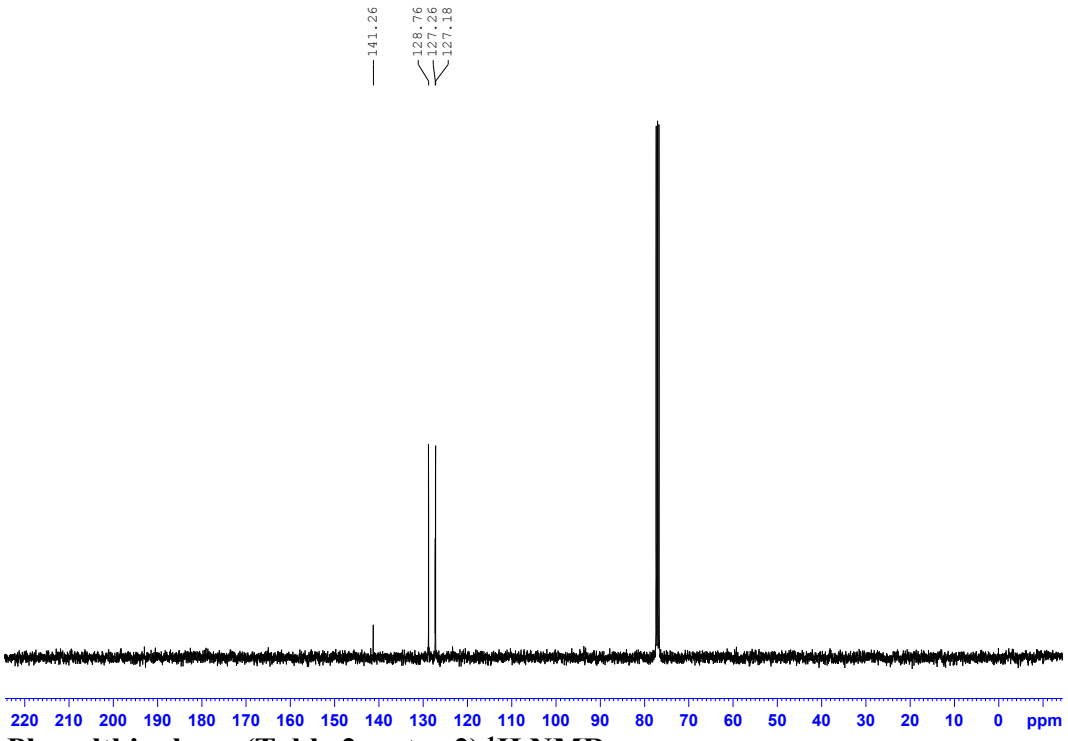
SIPrPdCl2-NMe2-CHPh-13C



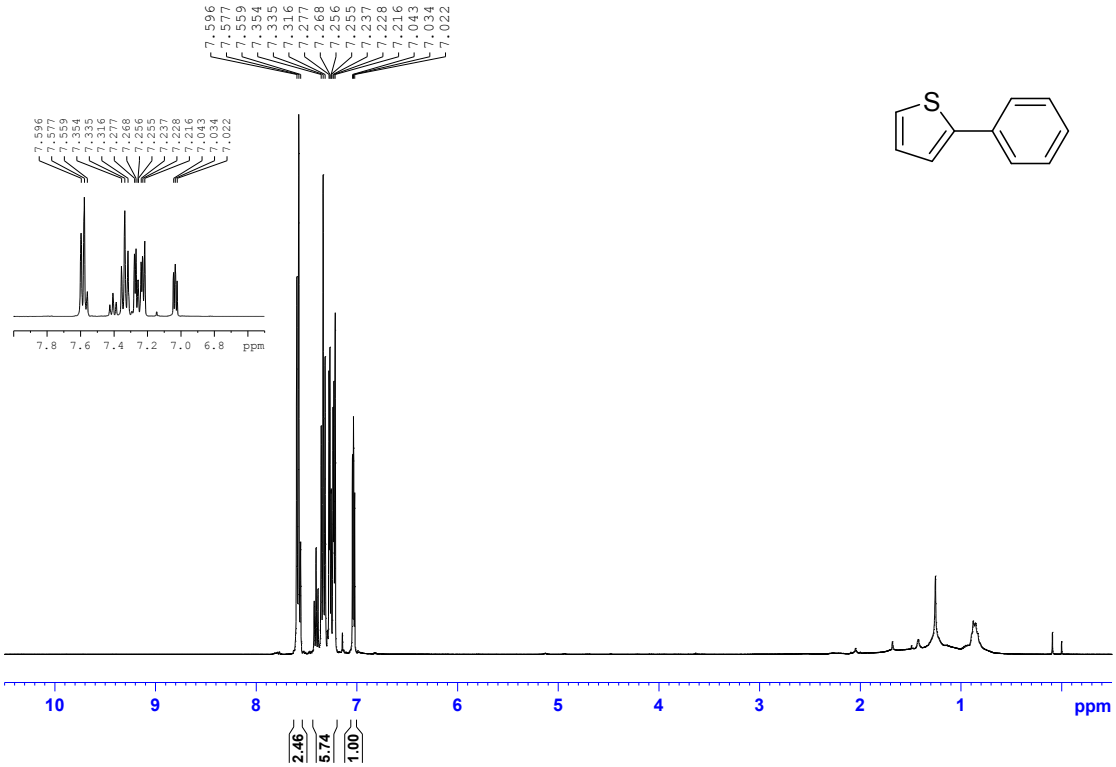
Biphenyl (Table 2, entry 1) ^{1}H NMR



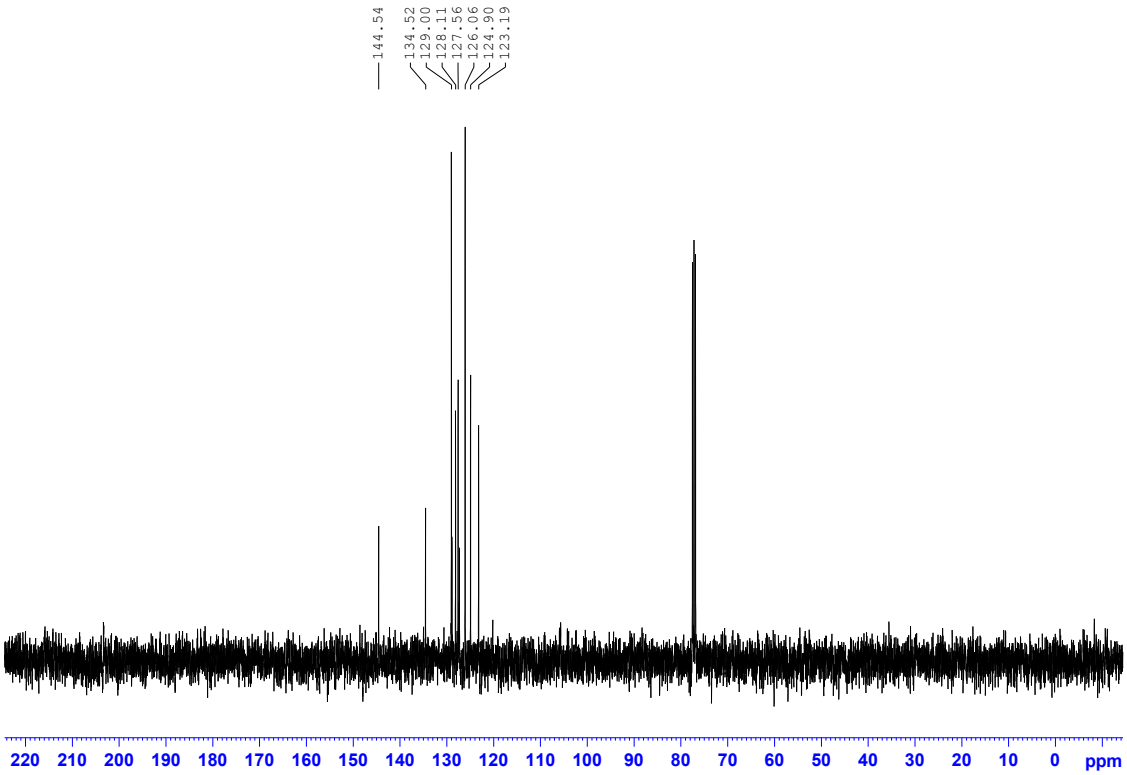
Biphenyl (Table 2, entry 1) ^{13}C NMR



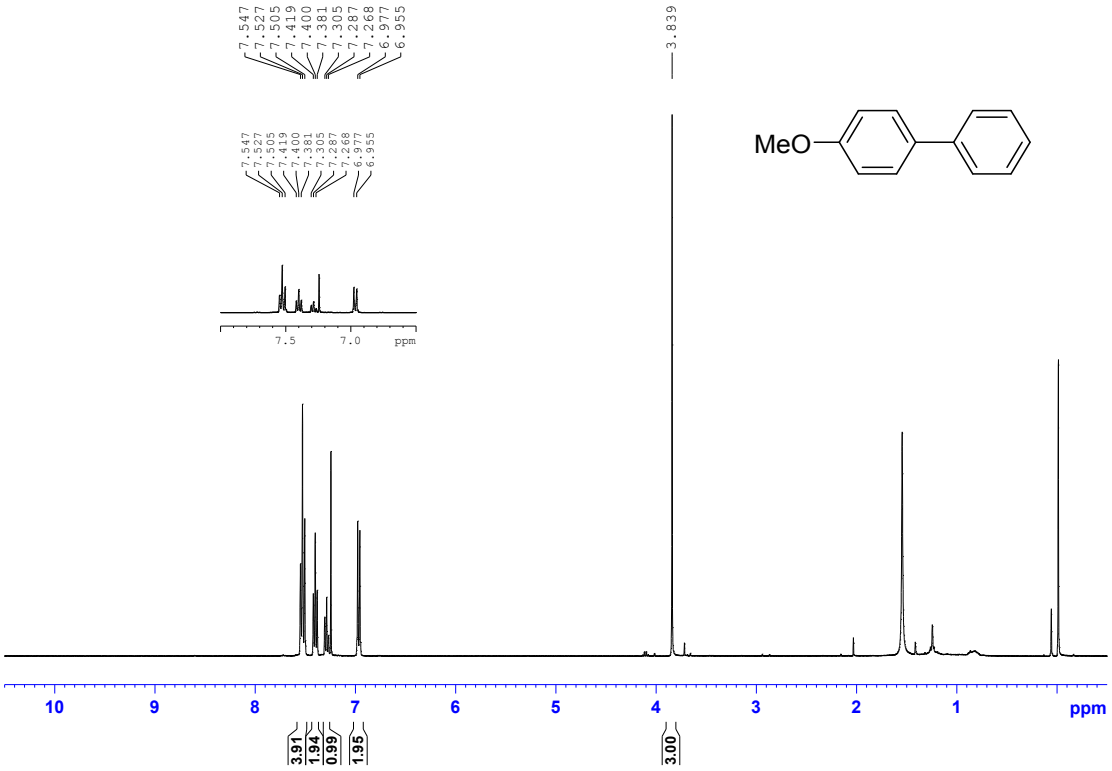
2-Phenylthiophene (Table 2, entry 2) ^{1}H NMR



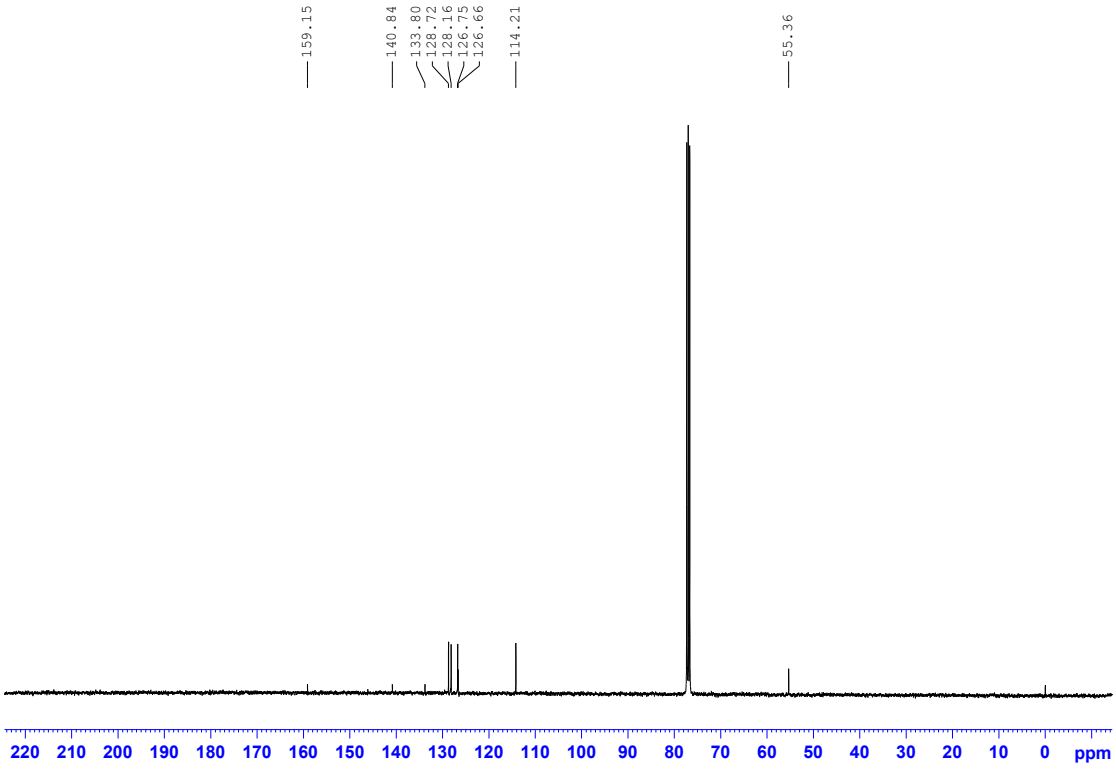
2-Phenylthiophene (Table 2, entry 2) ^{13}C NMR



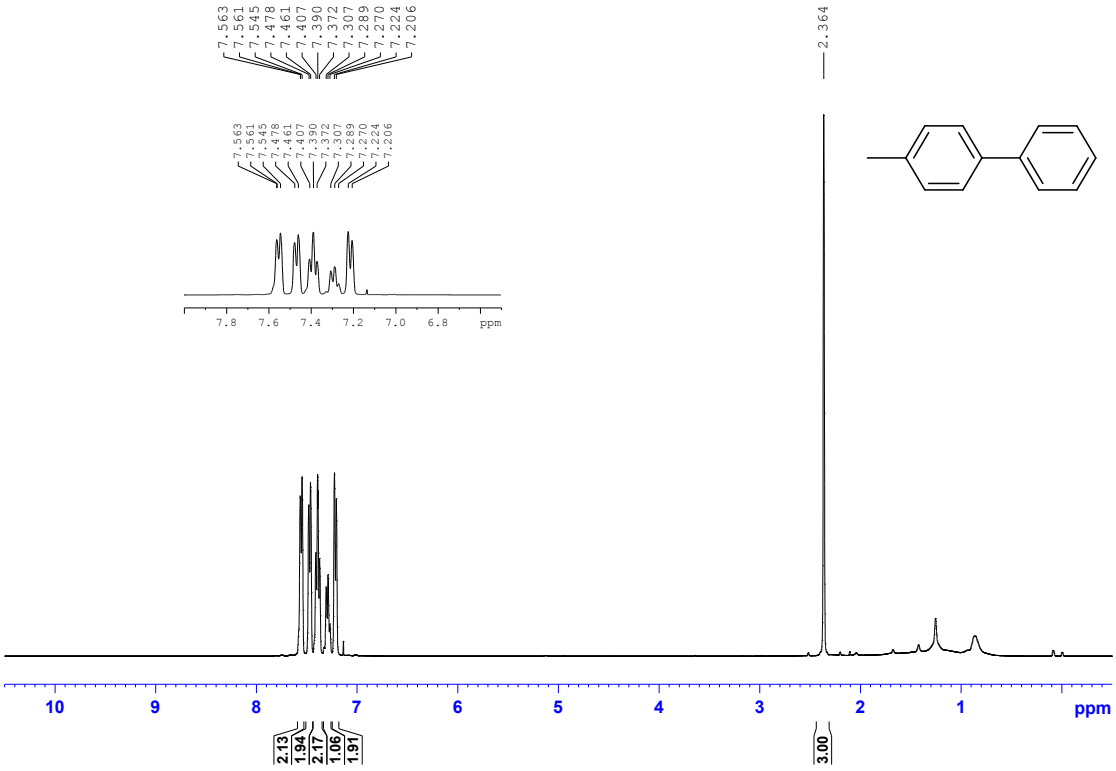
4-Methoxybiphenyl (Table 2, entry 3) ^{1}H NMR



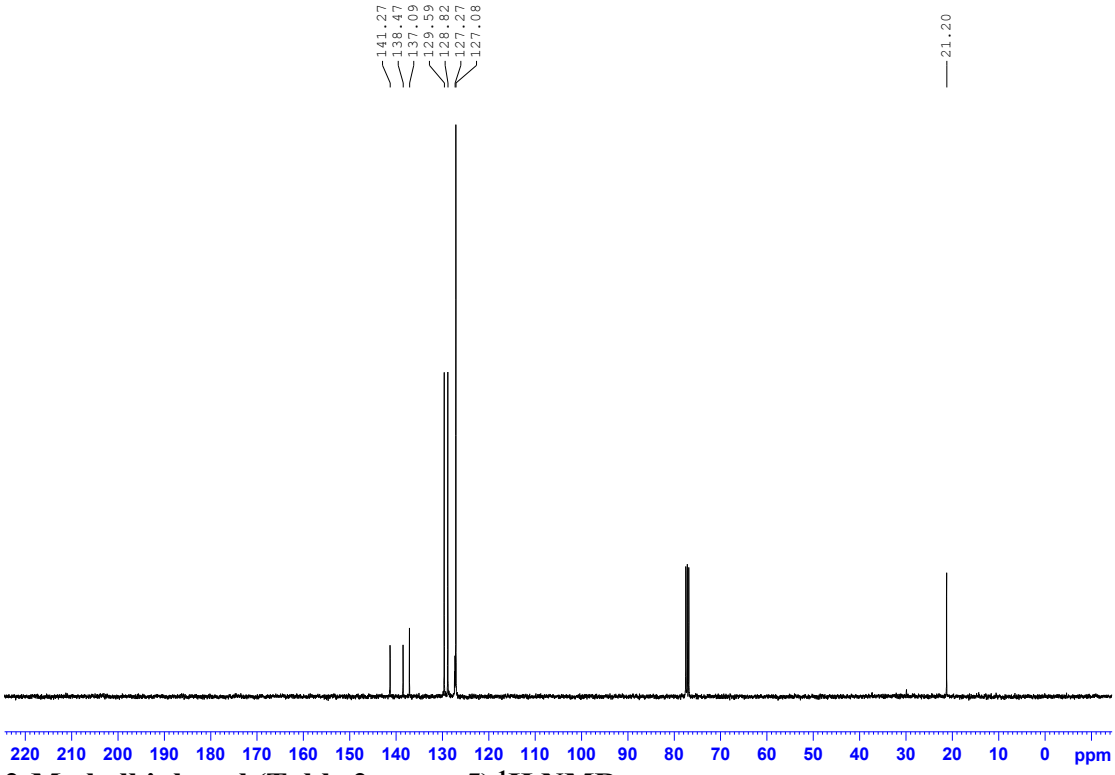
4-Methoxybiphenyl (Table 2, entry 3) ^{13}C NMR



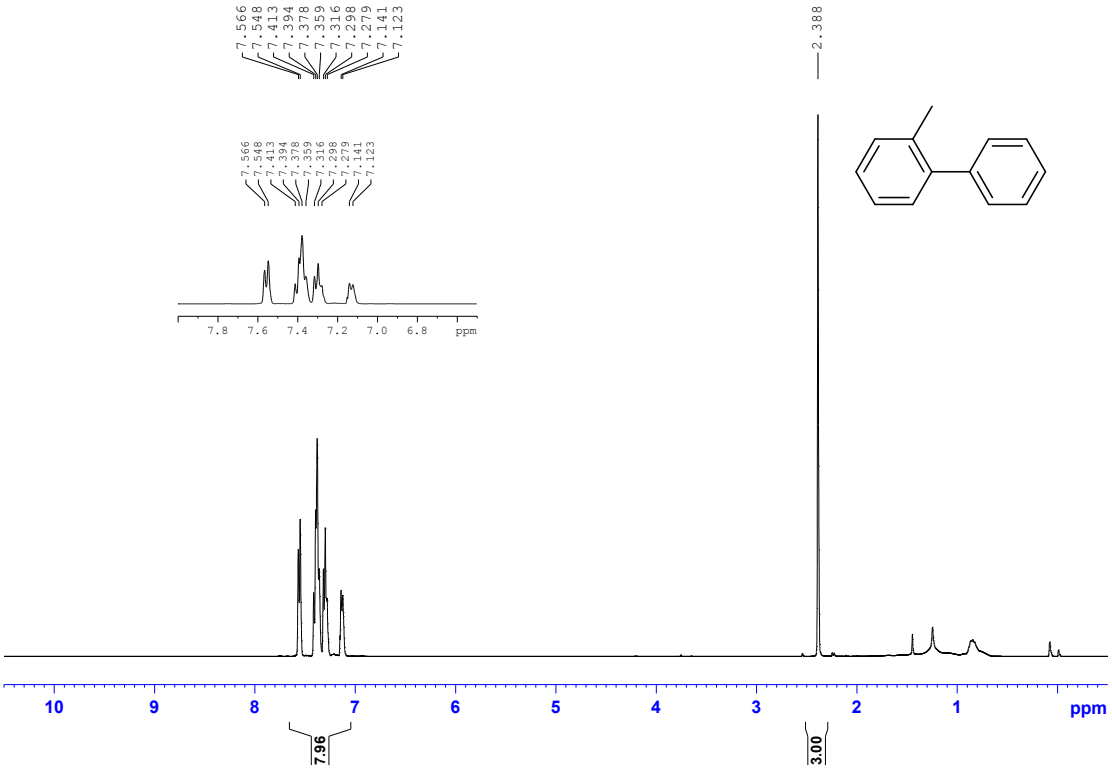
4-Methylbiphenyl (Table 2, entry 4) ^{1}H NMR



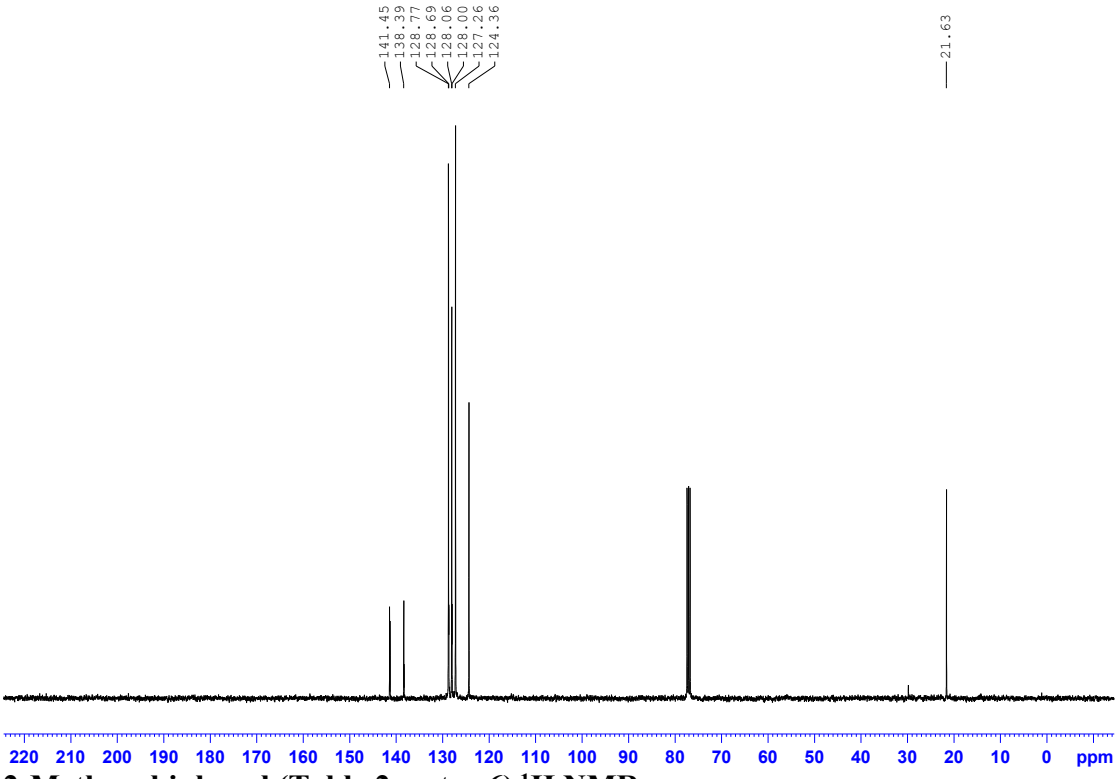
4-Methylbiphenyl (Table 2, entry 4) ^{13}C NMR



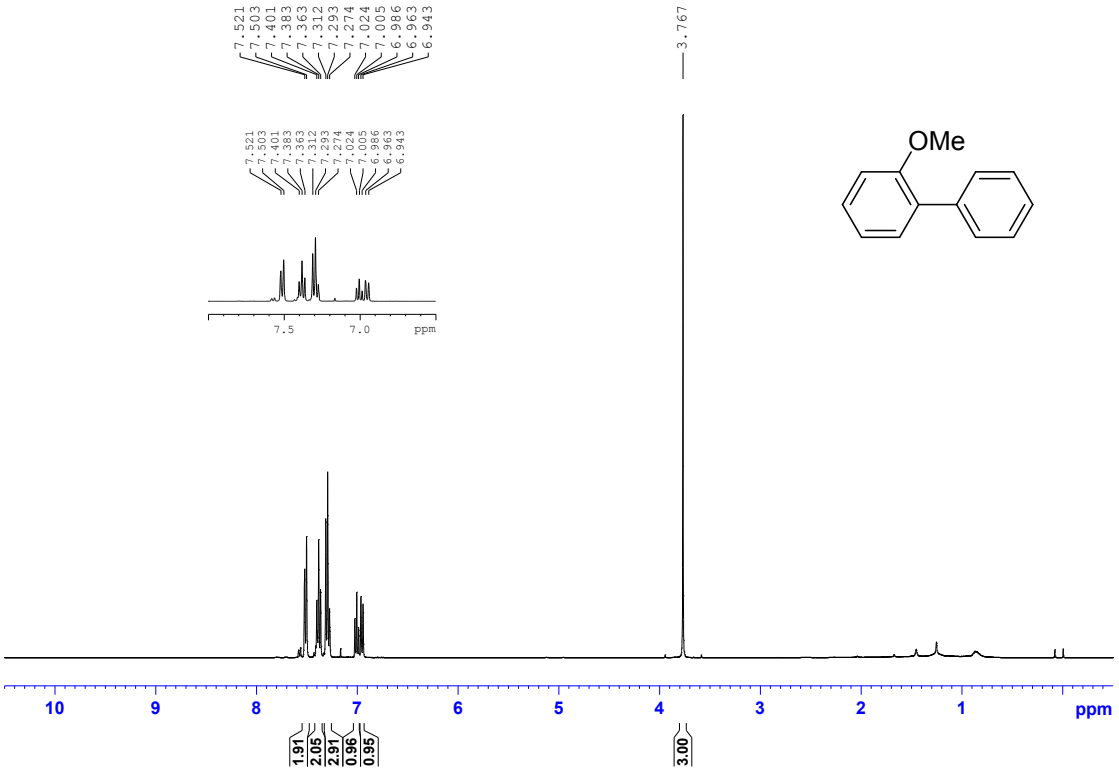
2-Methylbiphenyl (Table 2, entry 5) ^{1}H NMR



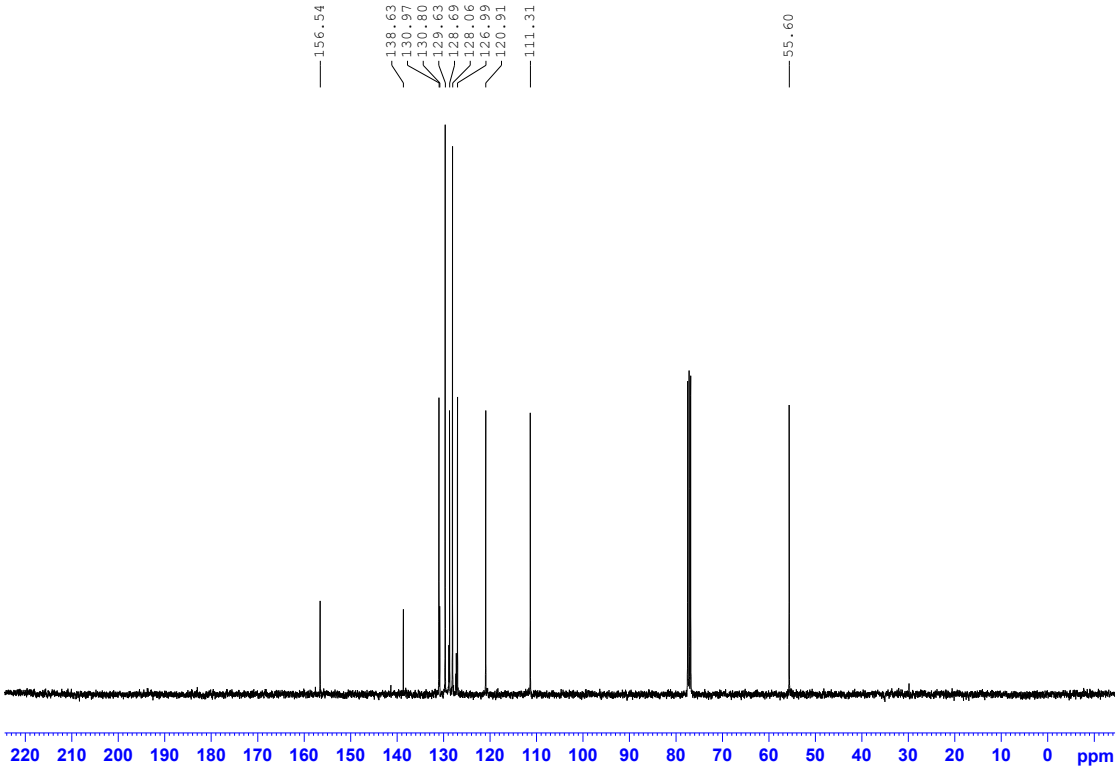
2-Methylbiphenyl (Table 2, entry 5) ^{13}C NMR



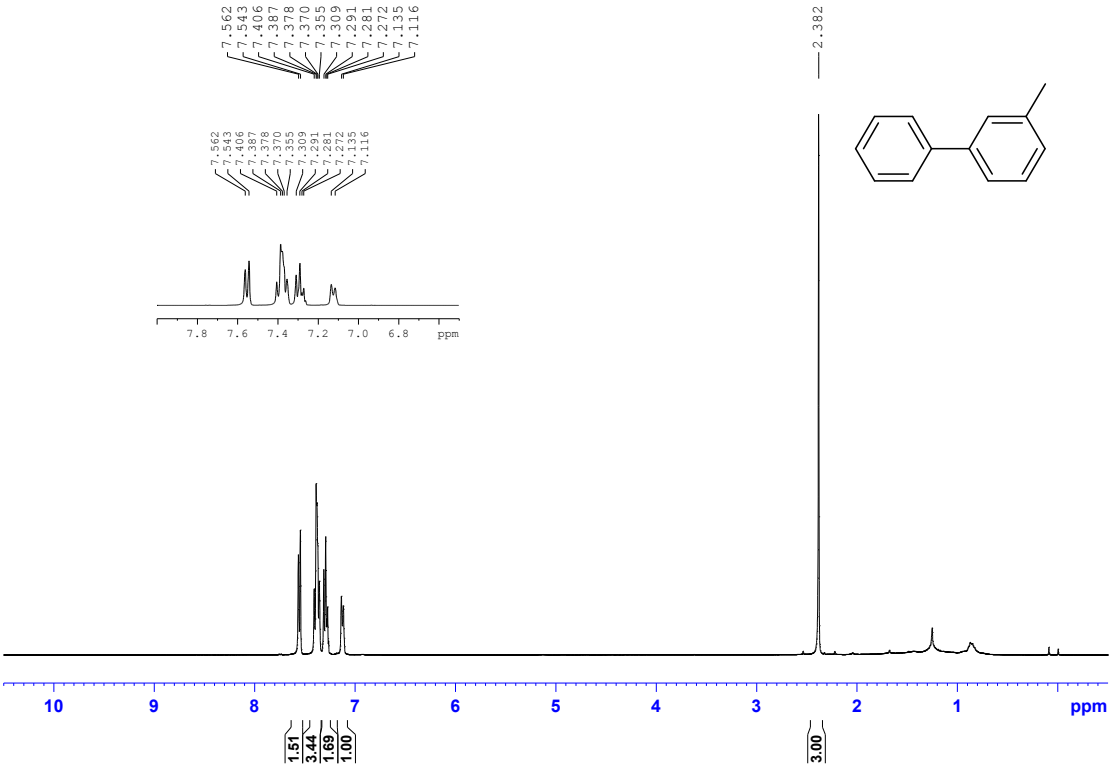
2-Methoxybiphenyl (Table 2, entry 6) ^{1}H NMR



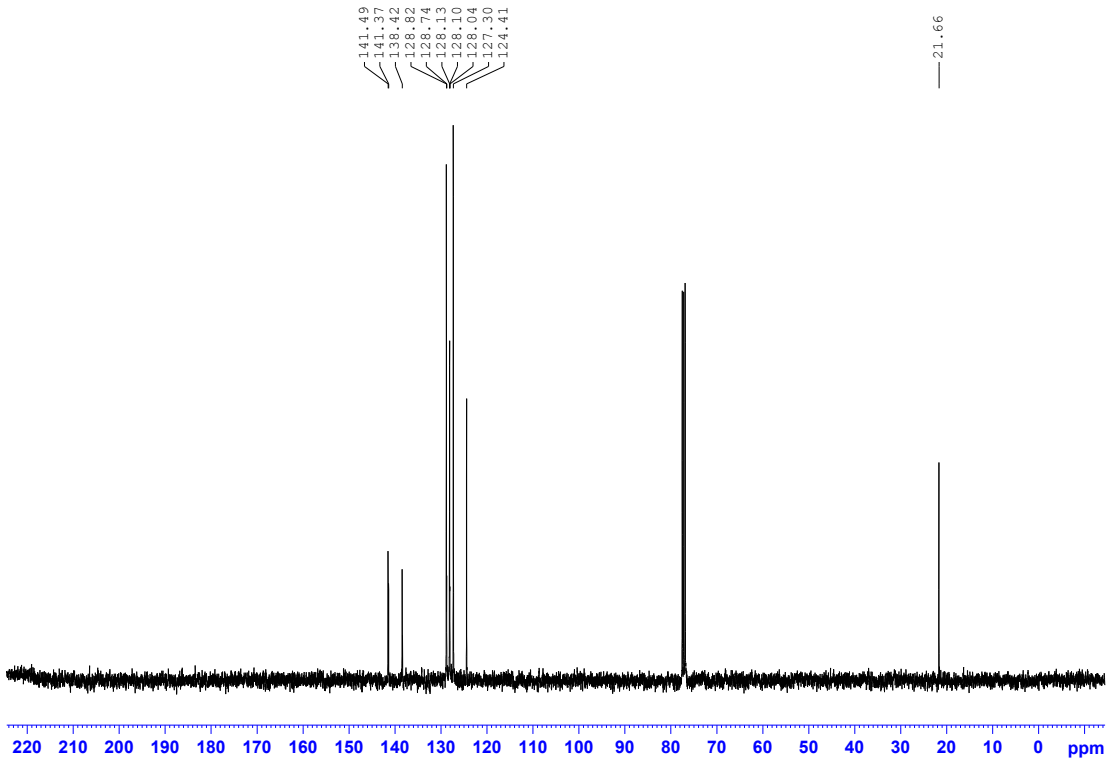
2-Methoxybiphenyl (Table 2, entry 6) ^{13}C NMR



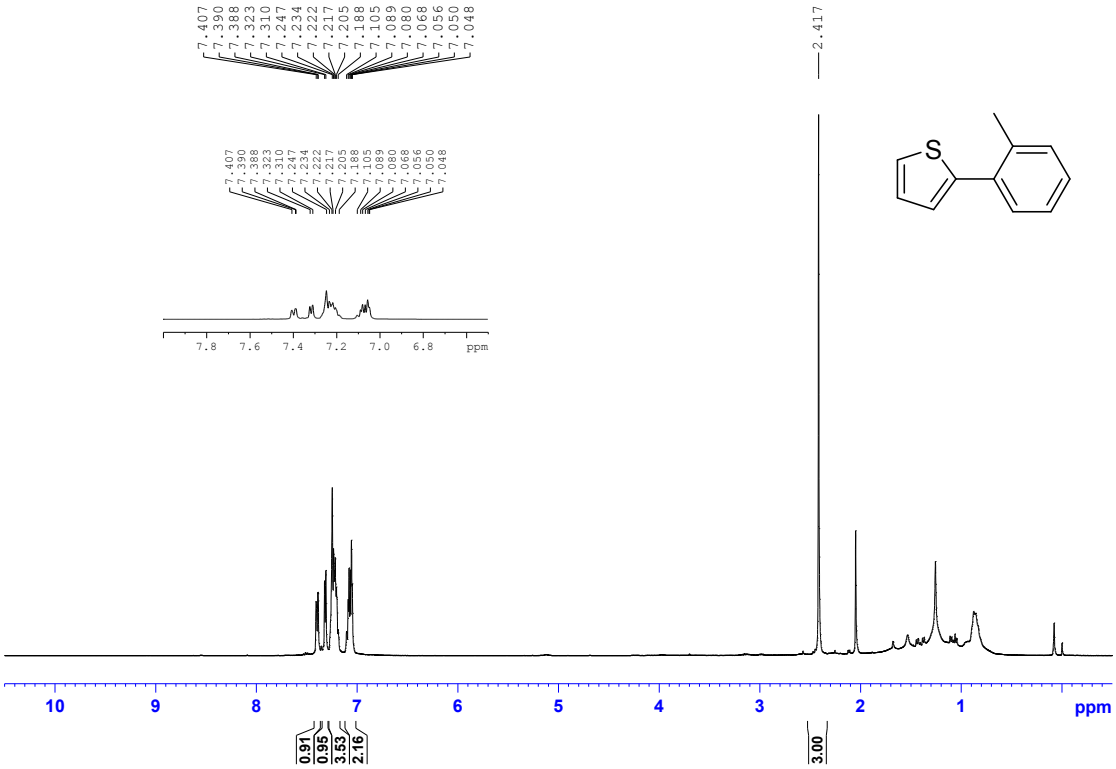
3-Methylbiphenyl (Table 2, entry 7) ^{1}H NMR



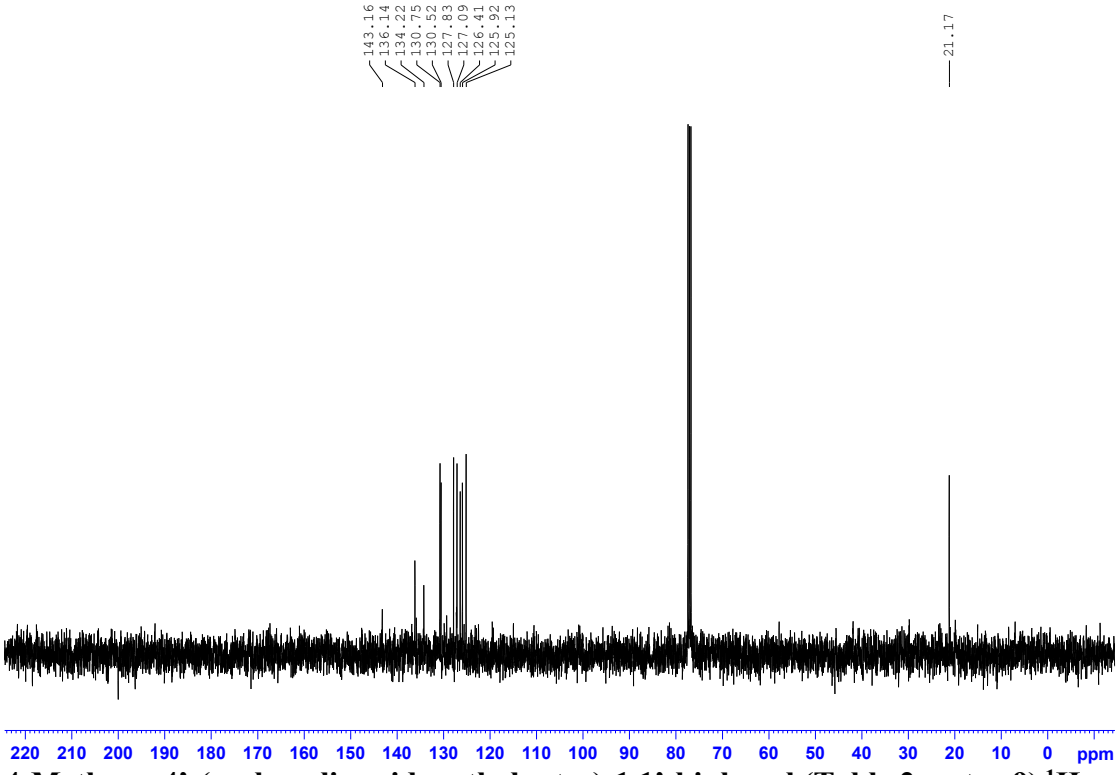
3-Methylbiphenyl (Table 2, entry 7) ^{13}C NMR



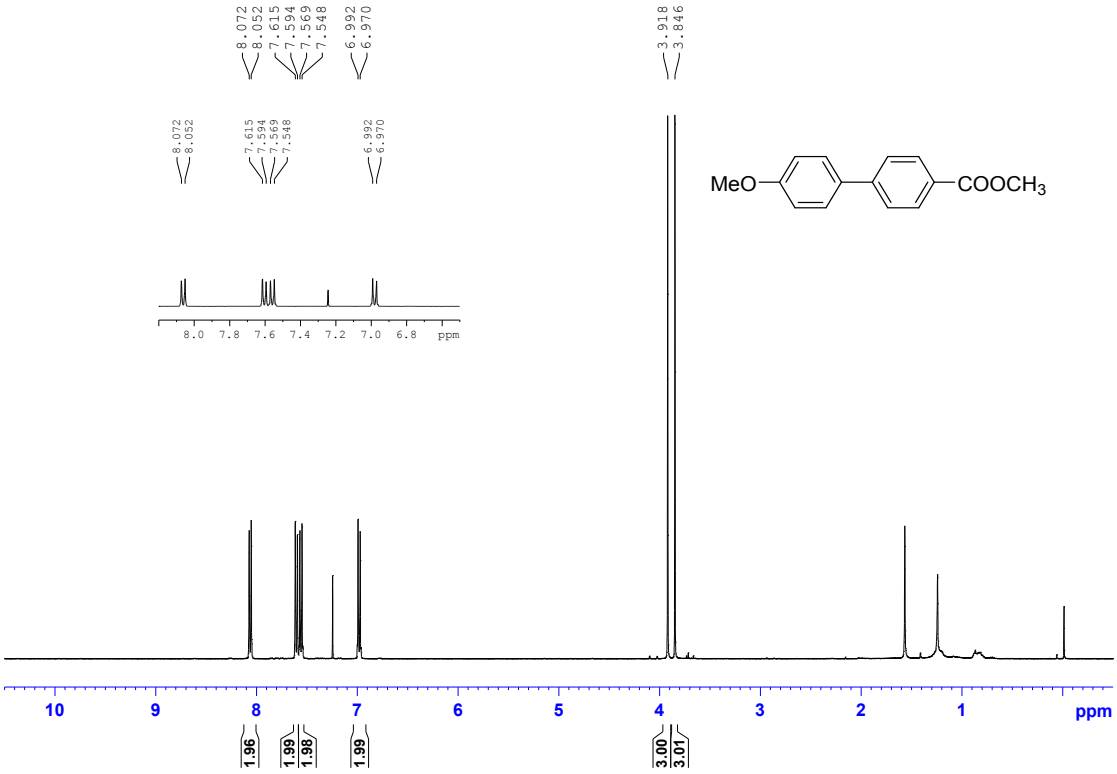
2-(*o*-Tolyl)thiophene (Table 2, entry 8) ^{1}H NMR



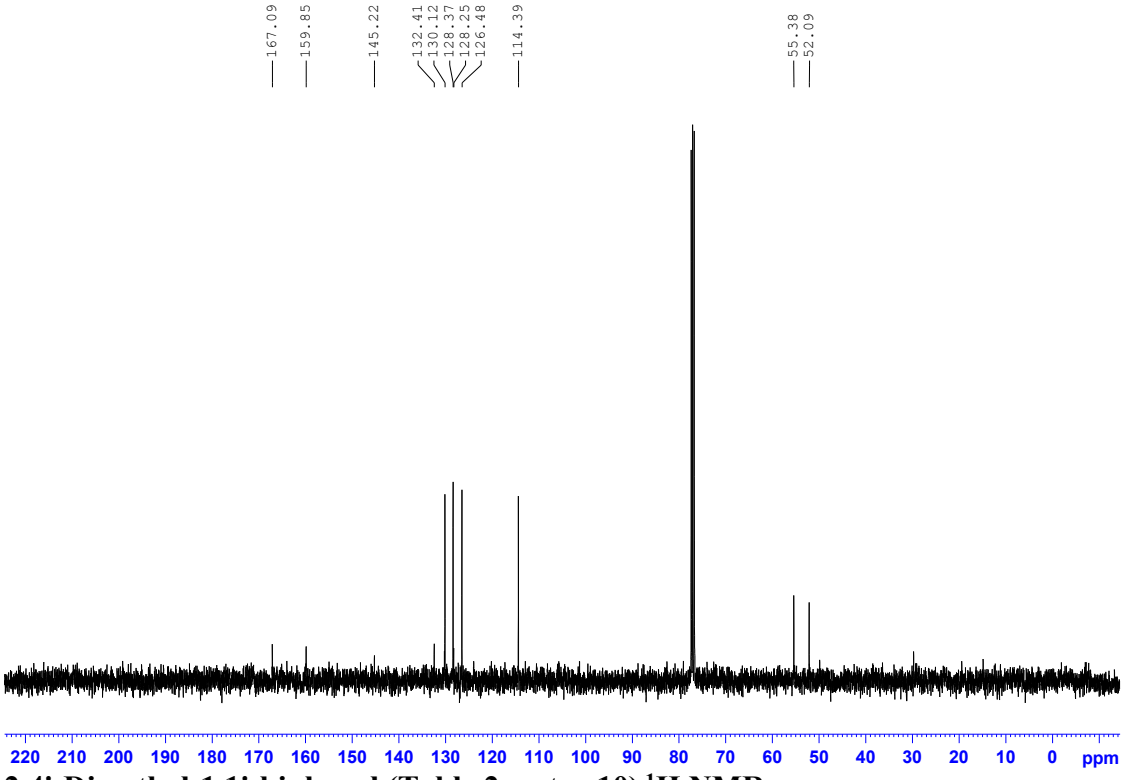
2-(*o*-Tolyl)thiophene (Table 2, entry 8) ^{13}C NMR



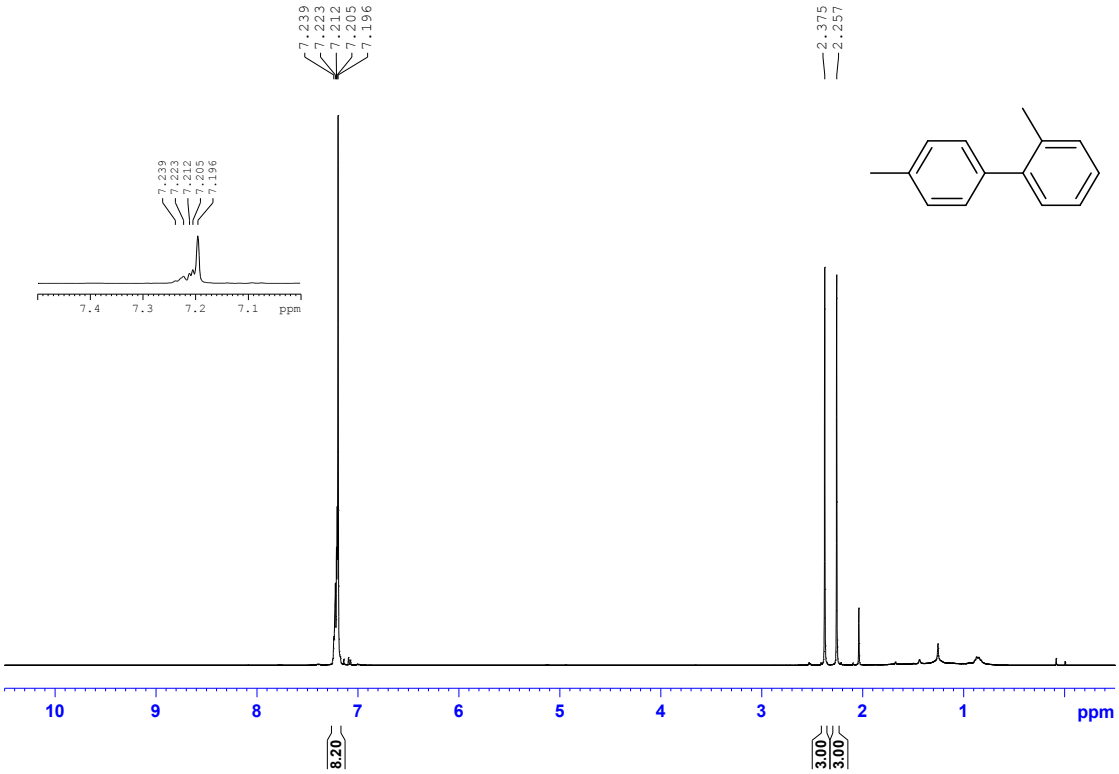
4-Methoxy-4'-(carboxylic acid methyl ester)-1,1'-biphenyl (Table 2, entry 9) ^{1}H NMR



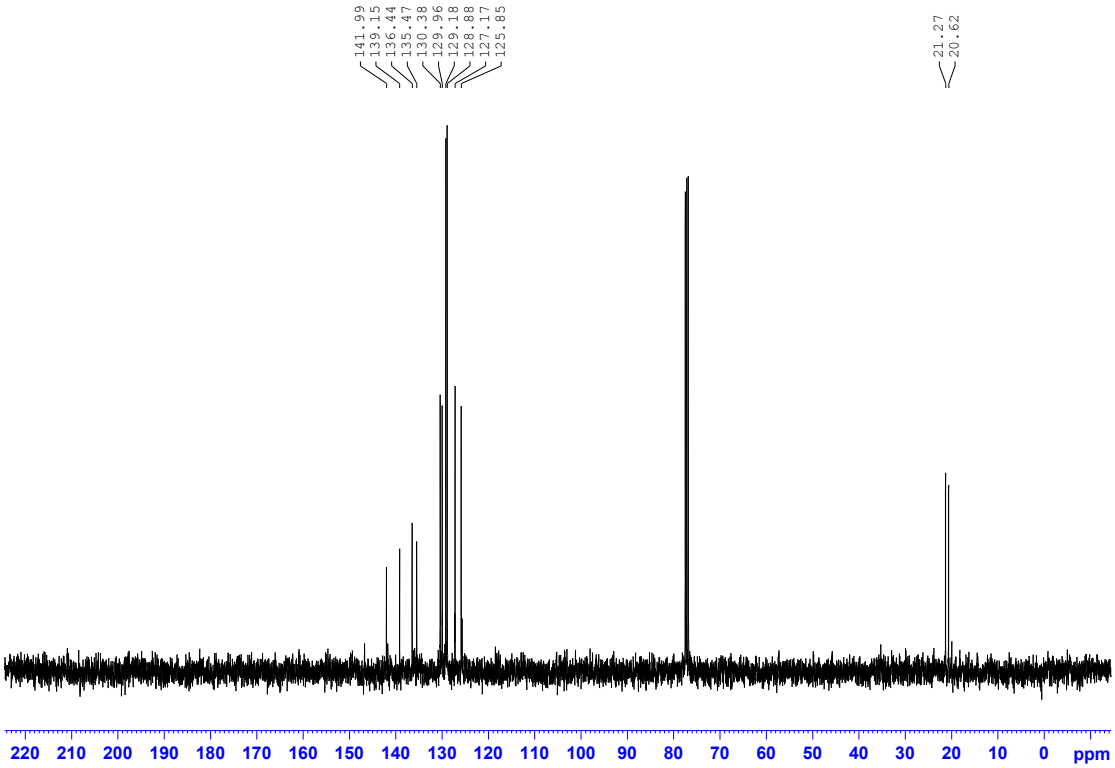
4-Methoxy-4'-(carboxylic acid methyl ester)-1,1'-biphenyl (Table 2, entry 9) ^{13}C NMR



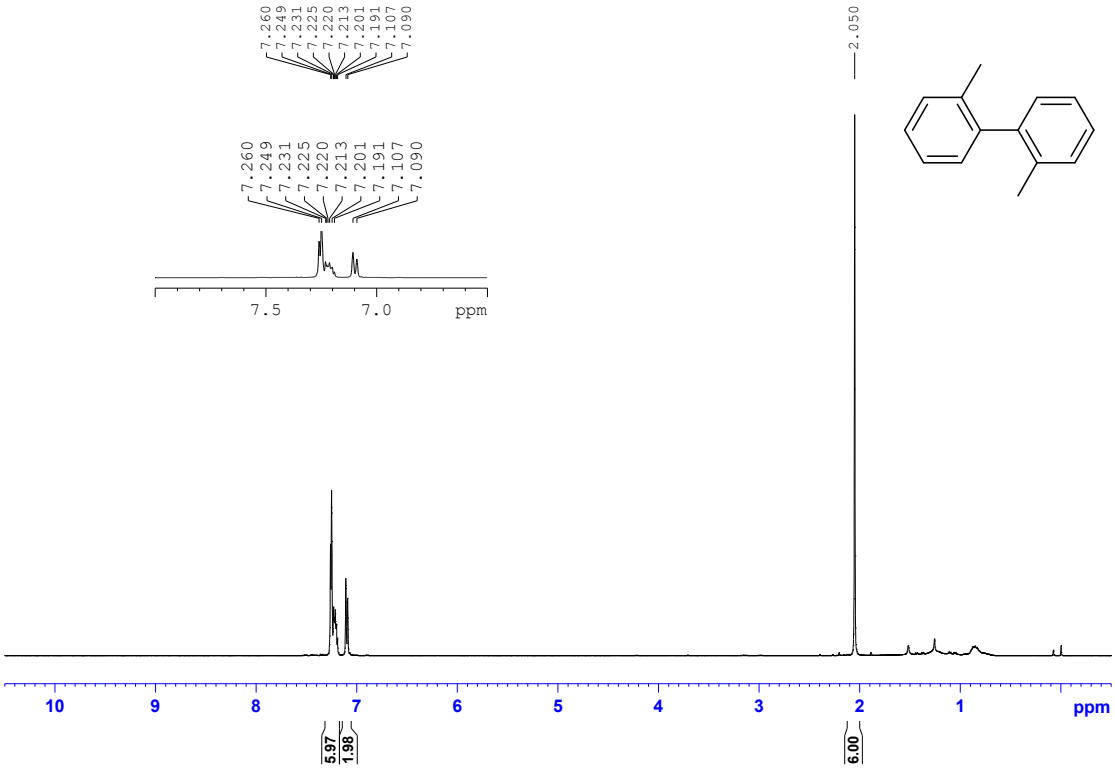
2,4'-Dimethyl-1,1'-biphenyl (Table 2, entry 10) ^{1}H NMR



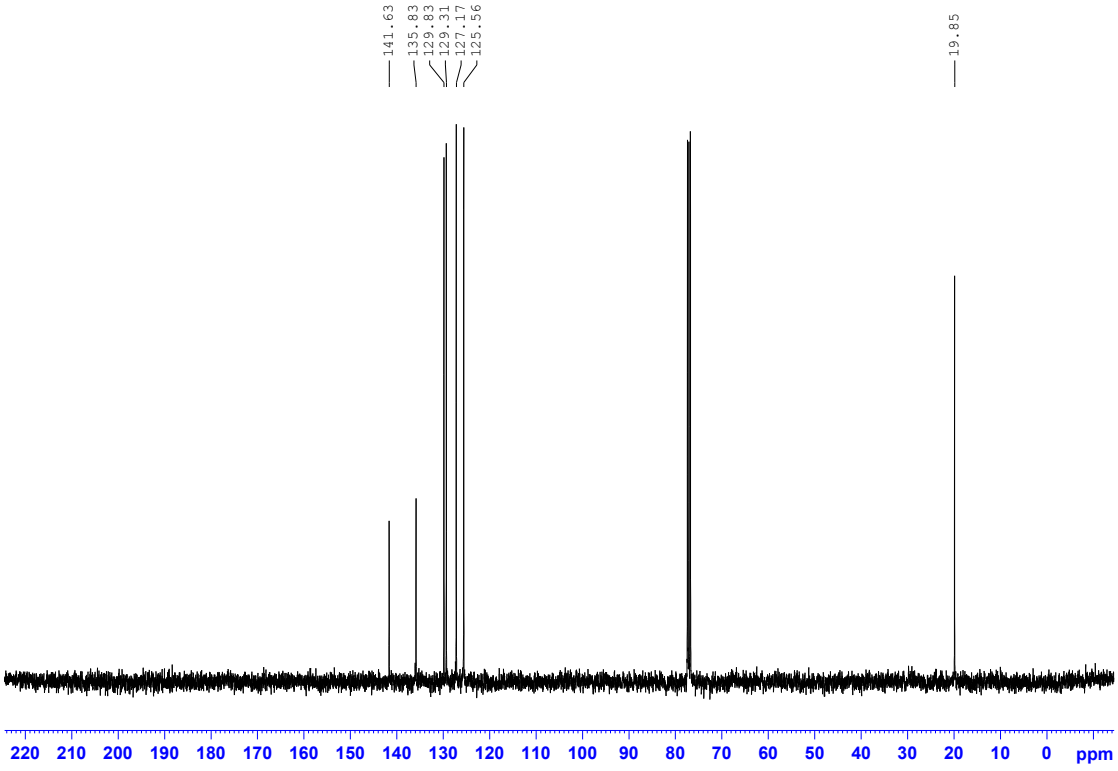
2,4'-Dimethyl-1,1'-biphenyl (Table 2, entry 10) ^{13}C NMR



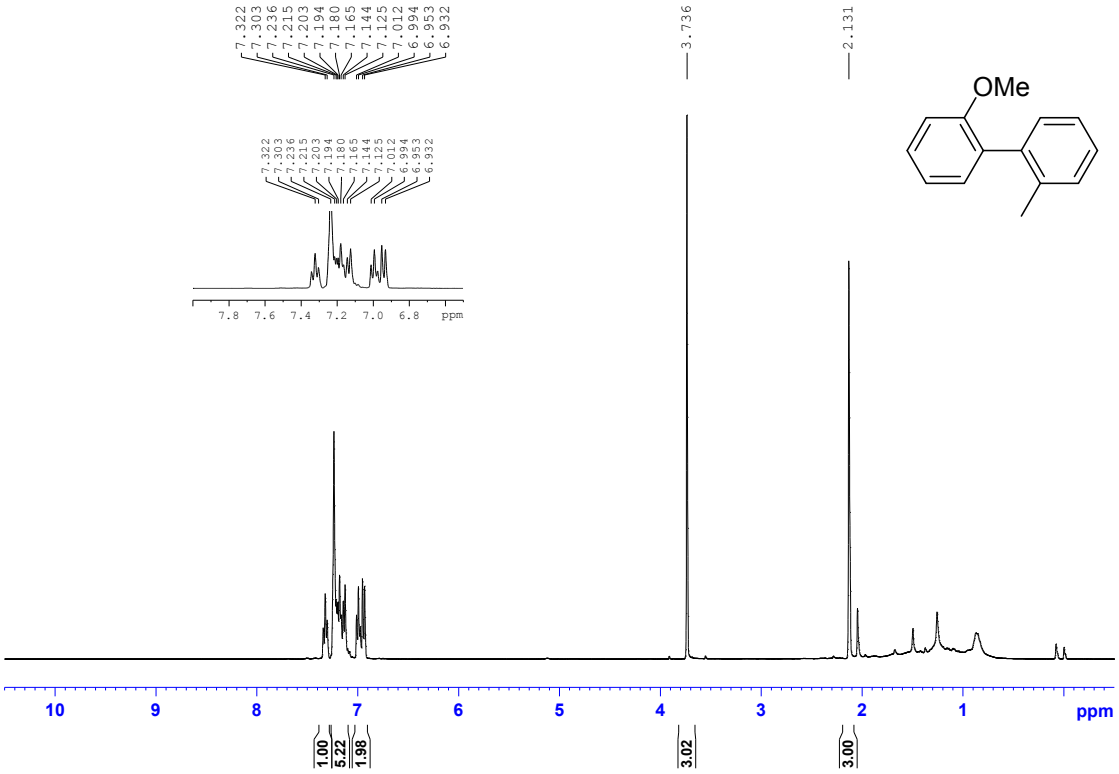
2,2'-Dimethyl-1,1'-biphenyl (Table 2, entry 11) ^{1}H NMR



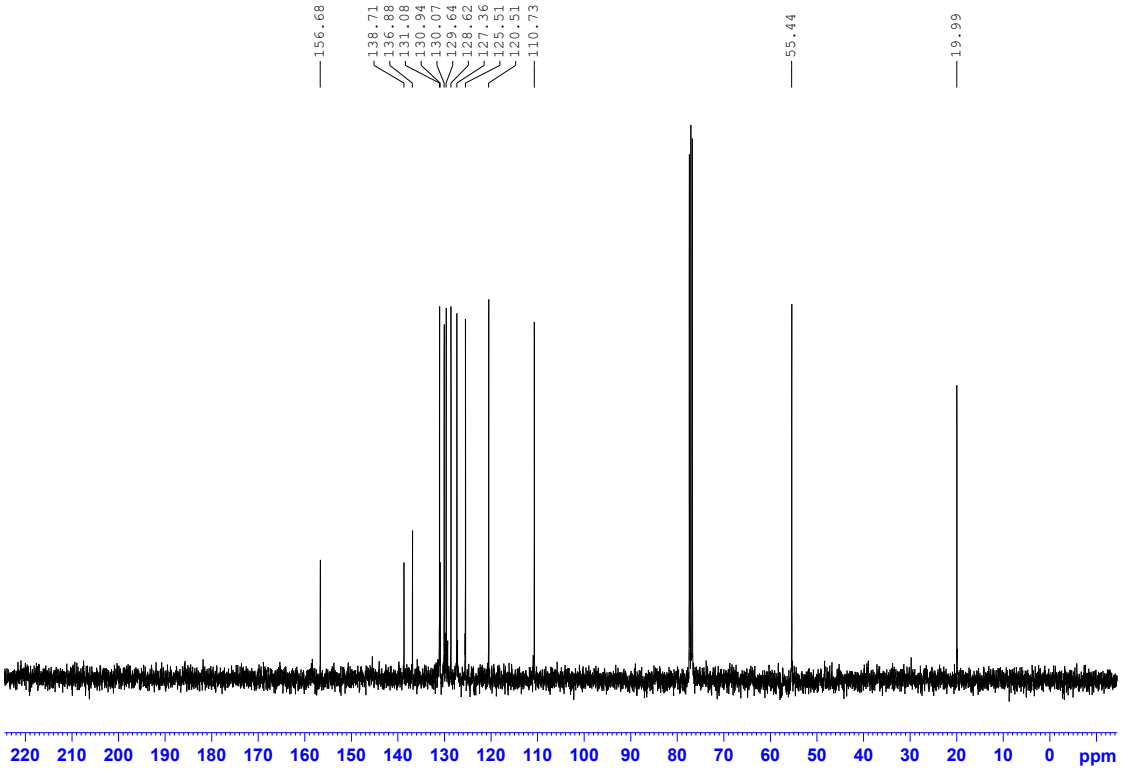
2,2'-Dimethyl-1,1'-biphenyl (Table 2, entry 11) ^{13}C NMR



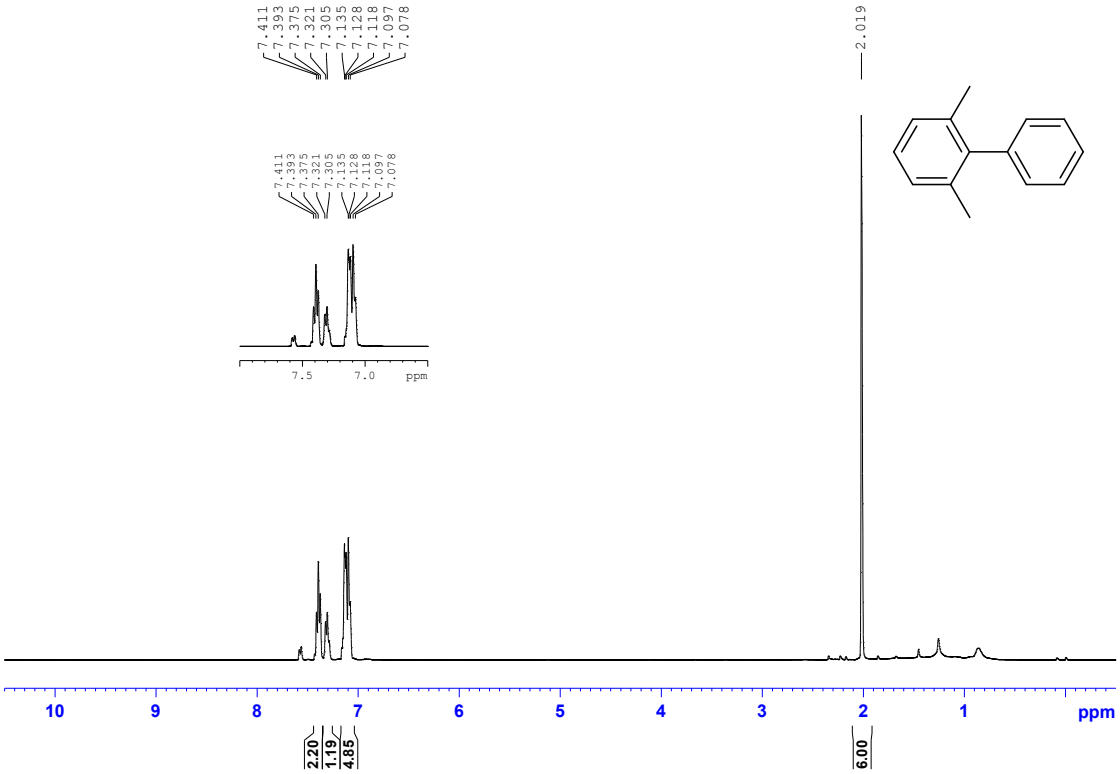
2-Methoxy-2'-methyl-1,1'-biphenyl (Table 2, entry 12) ^{1}H NMR



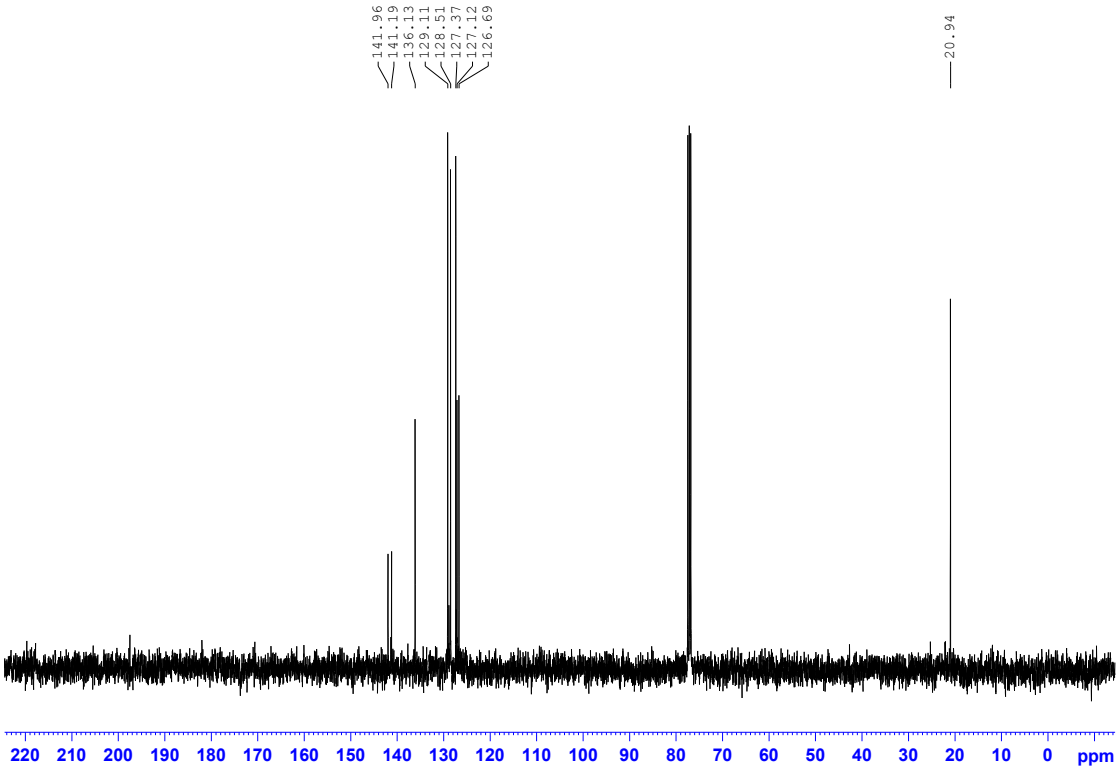
2-Methoxy-2'-methyl-1,1'-biphenyl (Table 2, entry 12) ^{13}C NMR



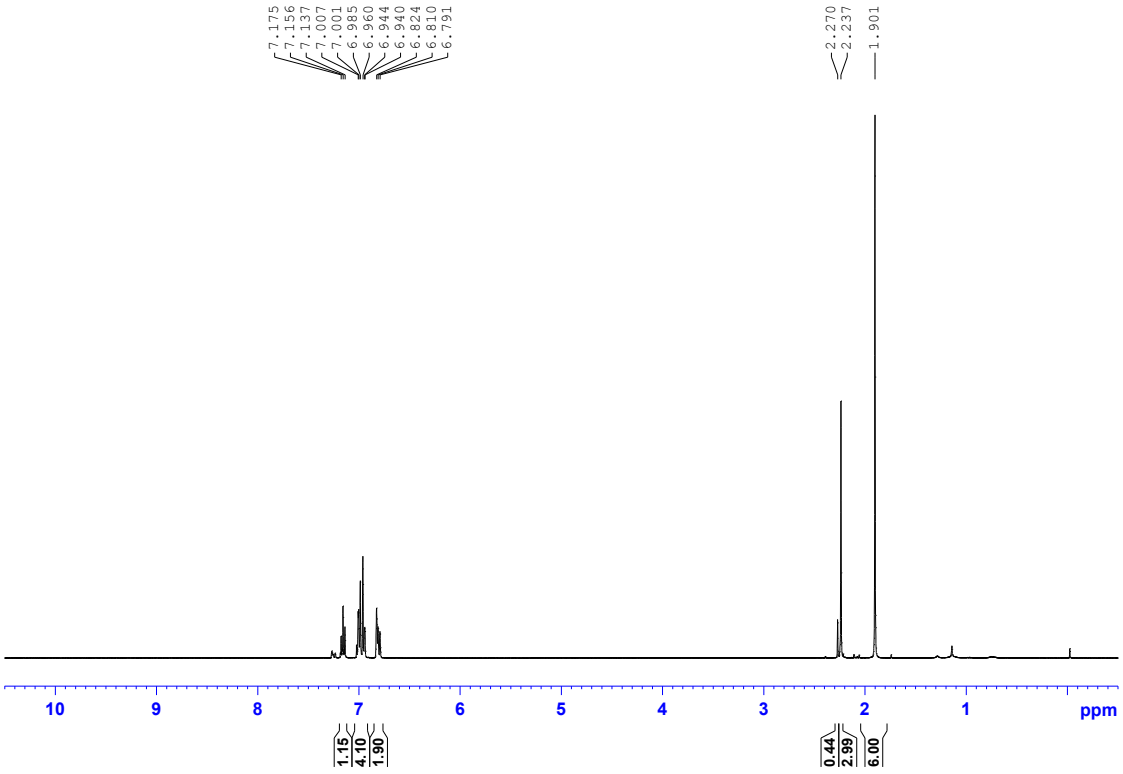
2,6-Dimethyl-biphenyl (Table 2, entry 13) ^{1}H NMR



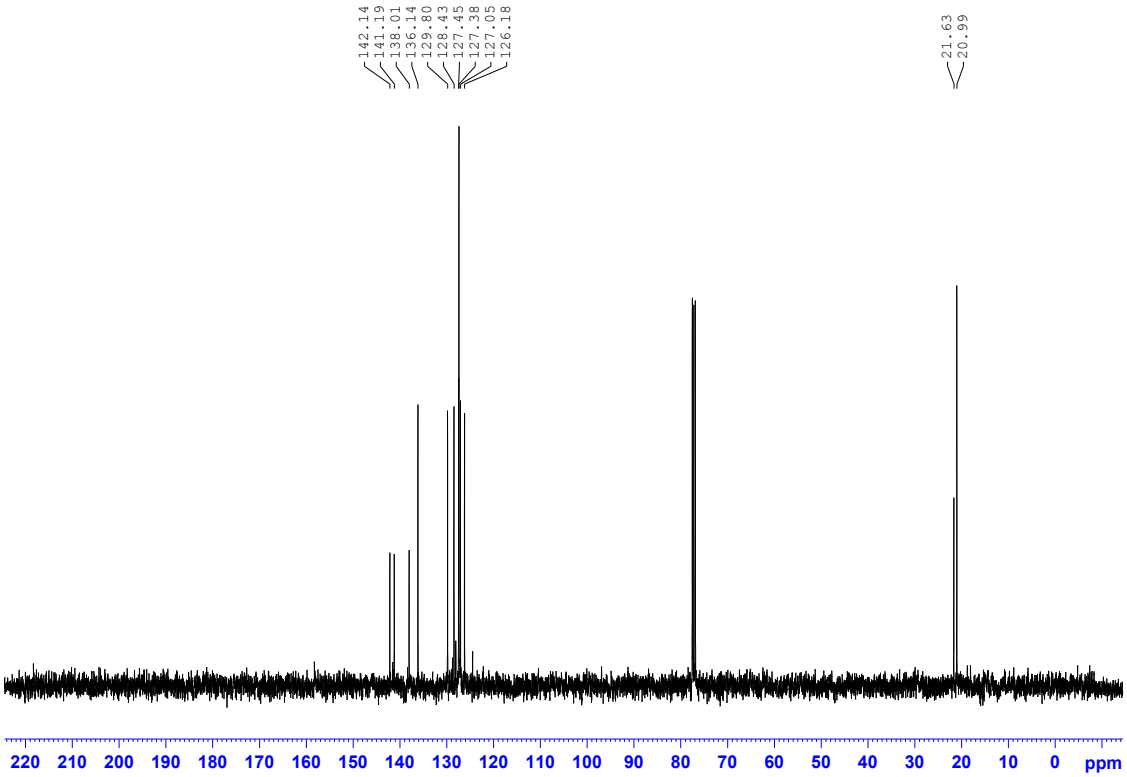
2,6-Dimethyl-biphenyl (Table 2, entry 13) ^{13}C NMR



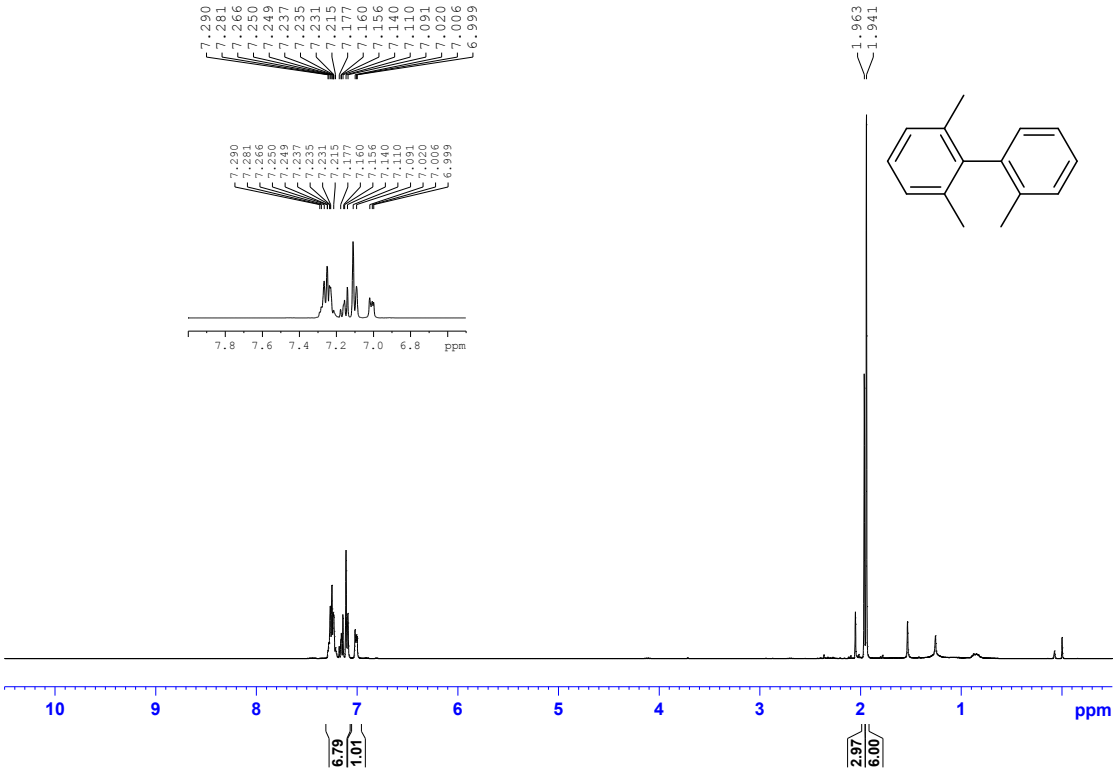
2,6,3-Trimethylbiphenyl (Table 2, entry 14) ^{1}H NMR



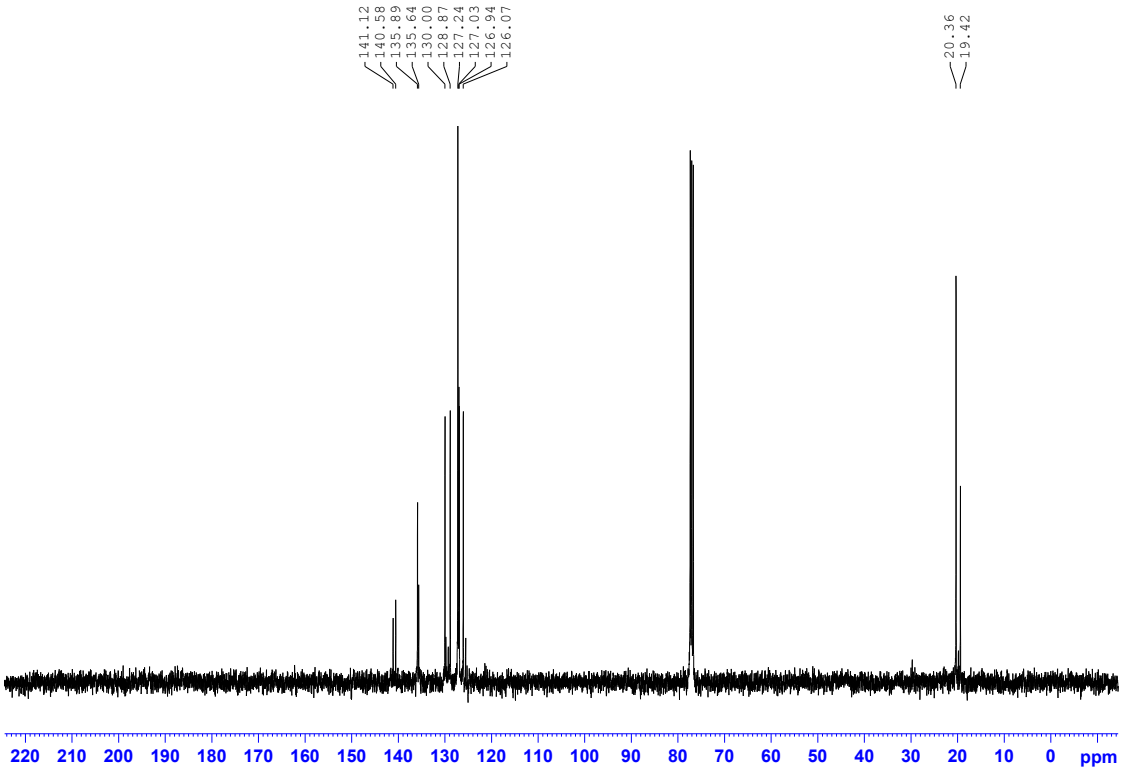
2,6,3-Trimethylbiphenyl (Table 2, entry14) ^{13}C NMR



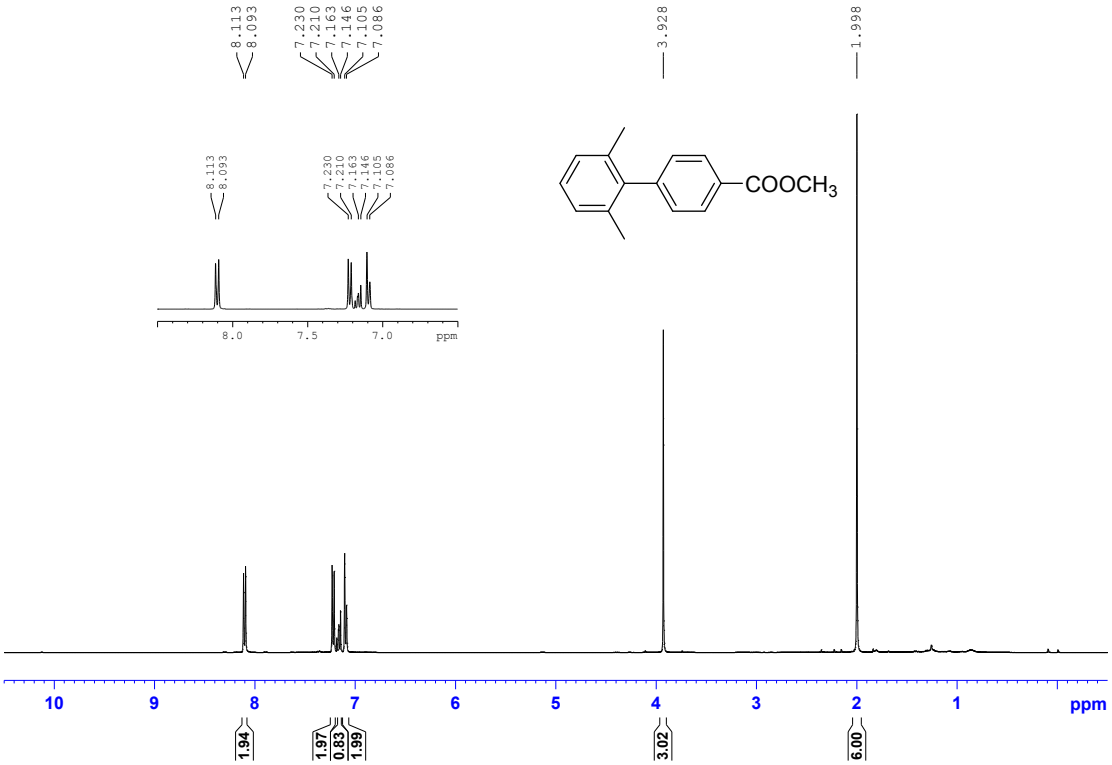
2,6,2'-Trimethylbiphenyl (Table 2, entry 15) ^{1}H NMR



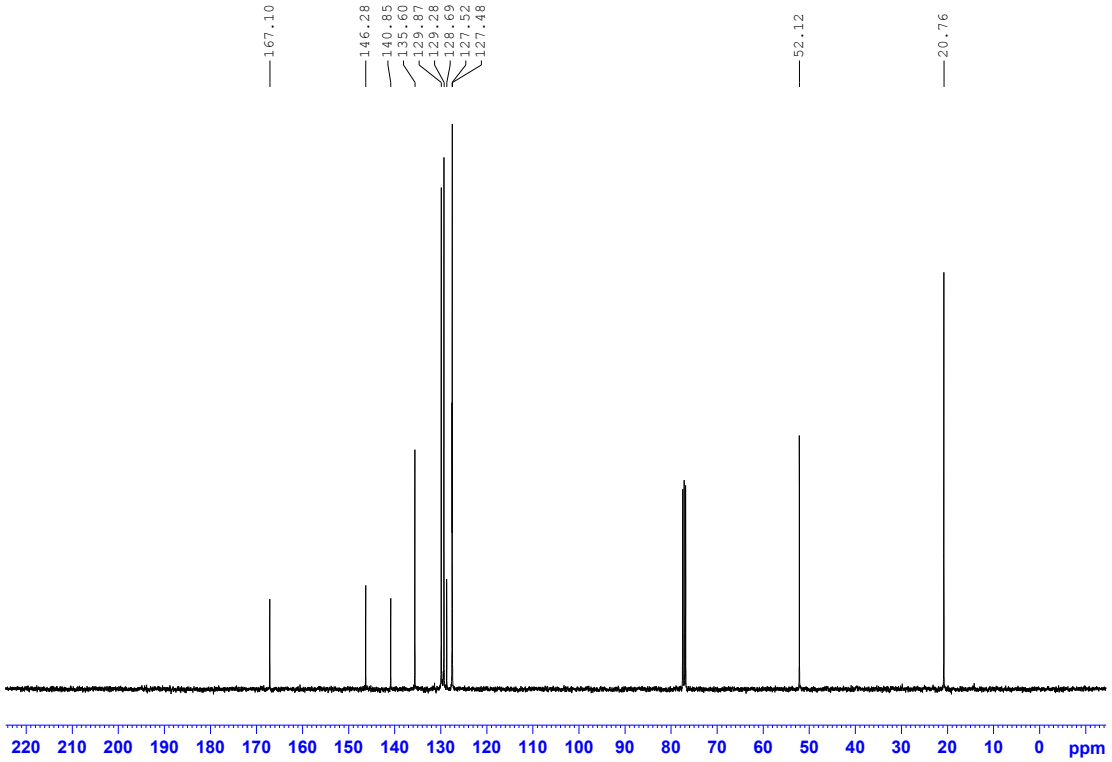
2,6,2'-Trimethylbiphenyl(Table 2, entry 15) ^{13}C NMR



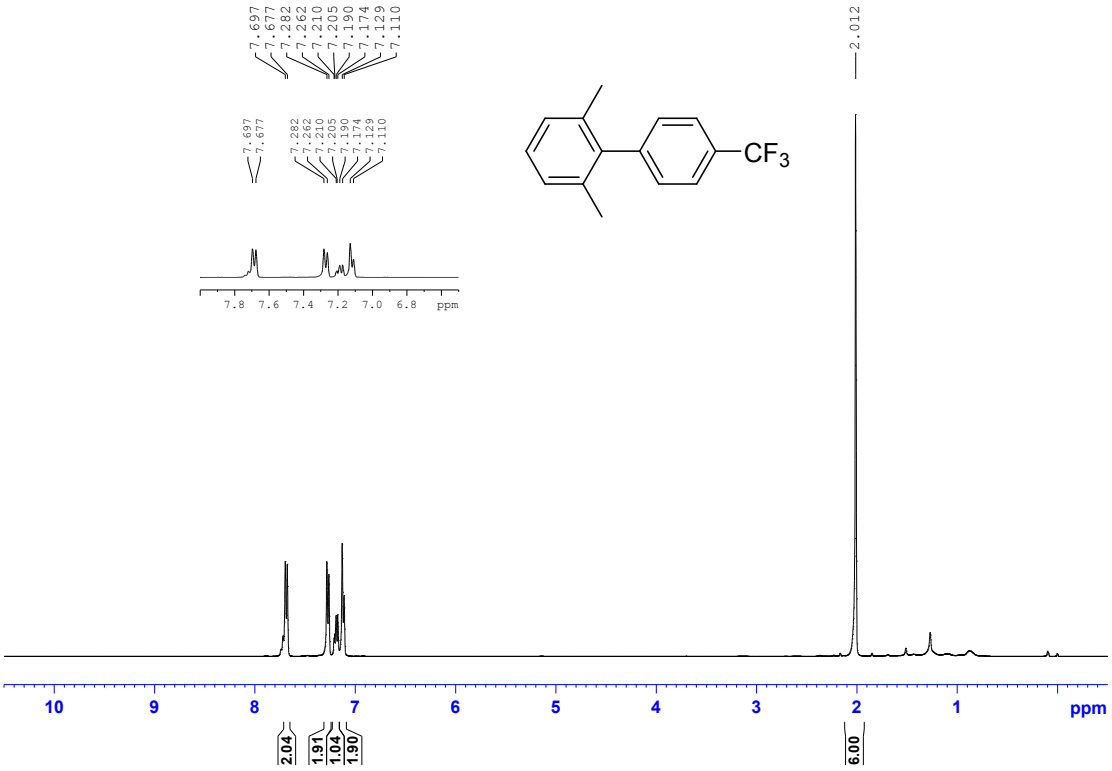
2',6'-dimethyl-[1,1'-biphenyl]-4-carboxylate (Table 2, entry 16) ^{1}H NMR



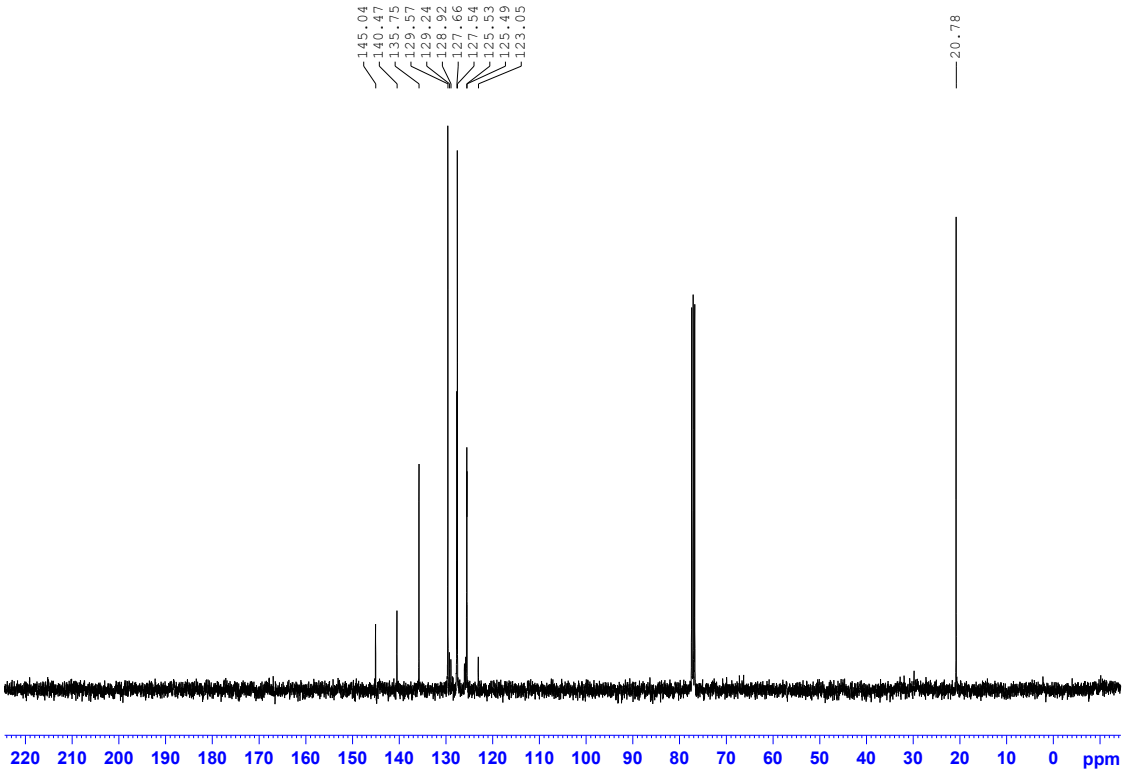
2',6'-dimethyl-[1,1'-biphenyl]-4-carboxylate (Table 2, entry 16) ^{13}C NMR



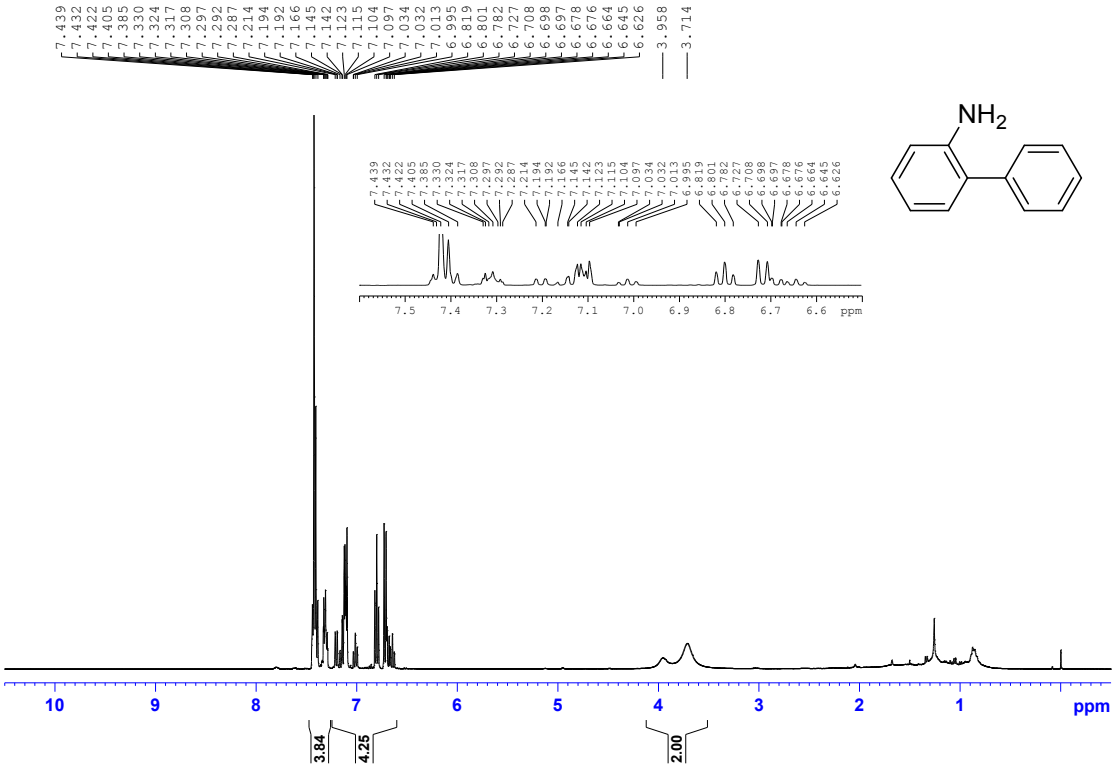
2,6-dimethyl-4'-trifluoromethyl-biphenyl (Table 2, entry 17) ^{1}H NMR



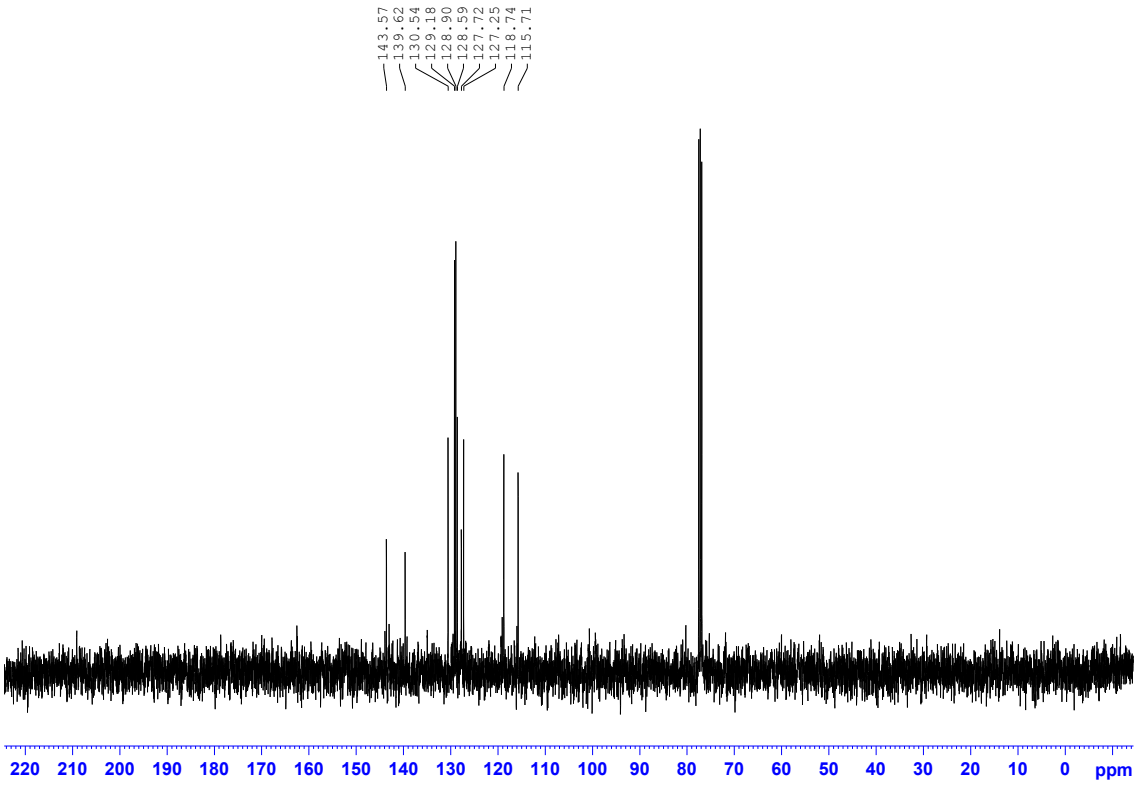
2,6-dimethyl-4'-trifluoromethyl-biphenyl (Table 2, entry 17) ^{13}C NMR



2-Aminobiphenyl (Table 2, entry 18) ^{1}H NMR



2-Aminobiphenyl (Table 2, entry 18) ^{13}C NMR



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