Electronic Supplementary Information

P,N,N-pincer nickel-catalyzed cross-coupling of aryl fluorides and chlorides

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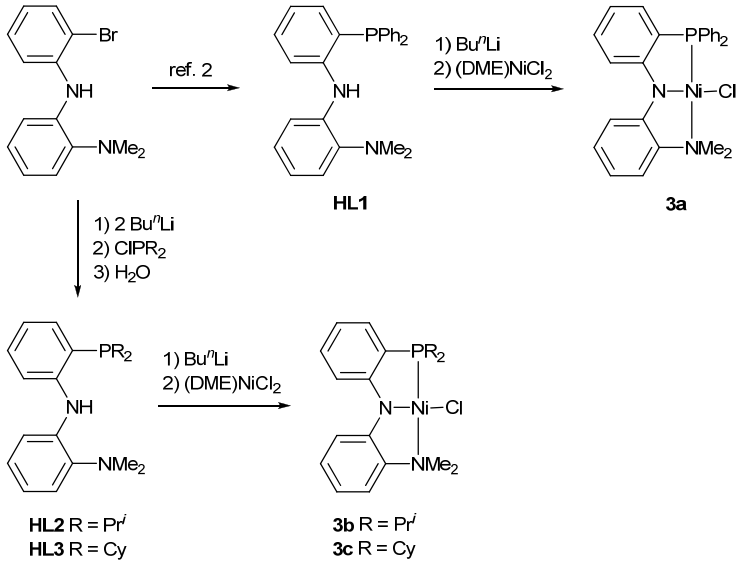
Synthesis and characterization of ligand precursors HL2 and HL3 and complexes 3a-3c



Scheme S-1. Synthesis of ligand precursors and complexes **3a-3c**

Experimental details

The reactions were performed under nitrogen atmosphere using standard Schlenk and vacuum line techniques. Solvents were distilled under nitrogen over sodium (toluene, hexane) or sodium/benzophenone (THF, Et_2O) and degassed prior to use. $CDCl_3$ was purchased from Cambridge Isotope Laboratories and used as received. $(DME)NiCl_2$,[1] 2-(Bromophenyl)-2'-(dimethylaminophenyl)amine,[2] and 2-diphenylphosphinophenyl)-2'-(dimethylaminophenyl)amine (**HL1**)[2] were prepared according to reported methods. M Other chemicals were purchased from commercial venders and used as received. NMR spectra were determined on a Bruker av300 or a Bruker Avance III 400 NMR spectrometer NMR spectrometer at room temperature using $CDCl_3$ as solvent. The chemical shifts of the ^1H

NMR spectra were referenced to TMS; the chemical shifts of the ^{13}C NMR spectra were referenced to internal solvent resonances and the chemical shifts of the ^{31}P NMR spectra were referenced to external 85% H_3PO_4. Elemental analysis was performed using an Elementar Vario EL Cube instrument.

Preparation of (2-Diisopropylphosphinophenyl)-2′-(dimethylaminophenyl)amine (HL2)

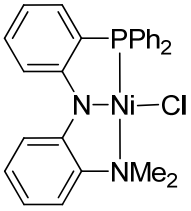
A 2.4 M solution of Bu^{n}Li in hexane (2.82 cm^3, 6.76 mmol) was added dropwise to a stirred solution of (2-bromophenyl-2'-dimethylaminophenyl)amine (0.98 g, 3.38 mmol) in Et_2O (20 cm^3) at about −80 °C. The mixture was allowed to warm to ambient temperature and stirred for 12 h. The resulting solution was recooled to −80 °C and chlorodiisopropylphosphine (0.53 cm^3, 3.38 mmol) was added into the cooled solution. The mixture was warmed to room temperature and stirred for 12 h. Degassed water (10 cm^3) and diethyl ether (10 cm^3) were added. The organic layer was separated and the aqueous phase was extracted with diethyl ether (5 cm^3 × 2). The combined organic phase was dried over $MgSO_4$ and evaporated to dryness under reduced pressure to afford a yellow oil. The yellow oil was dissolved in a mixed solvent of degassed ethanol (1 cm^3) and hexane (8 cm^3) and cooled to −80 °C to give an off-white solid of **HL2** (0.507 g, 46%). ^1H NMR ($CDCl_3$): δ 0.96 (dd, *J* = 6.8, 11.6 Hz, 6H, CH*Me*$_2$), 1.12 (dd, *J* = 6.8, 15.2 Hz, 6H, CH*Me*$_2$), 2.08-2.18 (m, 2H, C*H*Me$_2$), 2.70 (s, 6H, N*Me*$_2$), 6.86 (t, *J* = 7.4 Hz, 2H, C_6H_4), 6.95 (t, *J* = 7.6 Hz, 1H, C_6H_4), 7.08 (d, *J* = 8 Hz, 1H, C_6H_4), 7.19-7.25 (m, 1H, C_6H_4), 7.30-7.41 (m, 2H, C_6H_4), 7.59 (d, *J* = 8.4 Hz, 1H, C_6H_4). ^{13}C NMR ($CDCl_3$): δ 19.03 (d, *J* = 8.9 Hz), 20.19 (d, *J* = 18.3 Hz), 23.11 (d, *J* = 10.7 Hz), 44.04, 115.92 (d, *J* = 2.4 Hz), 116.00, 119.46 (d, *J* = 6.7 Hz), 120.50, 121.80, 121.95, 123.40, 129.55, 133.67, 137.46, 143.99, 148.63 (d, *J* = 18.4 Hz). ^{31}P NMR ($CDCl_3$): δ −13.61.

Preparation of (2-Dicyclohexylphosphinophenyl)-2′-(dimethylaminophenyl)amine (HL3)

A 2.4 M solution of Bu^{n}Li in hexane (3.46 cm^3, 8.30 mmol) was added dropwise to a stirred solution of (2-bromophenyl-2′-dimethylaminophenyl)amine (1.21 g, 4.15 mmol) in Et_2O (20 cm^3) at about −80°C. The mixture was allowed to warm to ambient temperature and stirred for 12 h. After recooling this solution to −80°C chlorodicyclohexylphosphine (0.94 cm^3, 4.15 mmol) was added. The resulting mixture was warmed to room temperature and stirred for 12 h. Degassed water (10 cm^3) and diethyl ether (10 cm^3) were added. The organic phase was separated and the aqueous phase was extracted with diethyl ether (5 cm^3 × 2). The combined organic phase was dried over $MgSO_4$ and evaporated to dryness under reduced pressure to

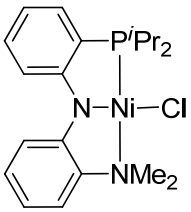
afford a yellow oil. The yellow oil was dissolved in a mixed solvent of degassed ethanol (1 cm^3) and hexane (8 cm^3). The solution was cooled to −80 °C to give an off-white solid of **HL3** (0.857 g, 51%). ^{1}H NMR ($CDCl_3$): δ 0.99-1.38 (m, 10H, Cy), 1.55-1.80 (m, 8H, Cy), 1.82-2.03 (m, 4H, Cy), 2.69 (s, 6H, NMe_2), 6.81-6.99 (m, 3H, C_6H_4), 7.07 (d, J = 8.8 Hz, 1H, C_6H_4), 7.17-7.43 (m, 3H, C_6H_4), 7.55 (d, J = 9.6 Hz, 1H, C_6H_4). ^{13}C NMR ($CDCl_3$): δ 26.52, 27.16 (d, J = 7.9 Hz), 27.37, 27.50, 28.92 (d, J = 7.5 Hz), 30.46 (d, J = 16.7 Hz), 33.02 (d, J = 10.8 Hz), 44.00, 115.73, 116.25, 119.32, 119.35, 120.54, 121.47 (d, J = 16 Hz), 123.34, 129.47, 134.09, 137.42, 144.05, 148.76 (d, J = 18 Hz). ^{31}P NMR ($CDCl_3$): δ −25.09.

Preparation of [(L1)NiCl] (3a)



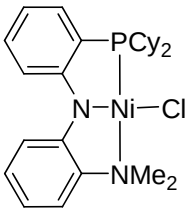
A solution of compound **HL1** (0.86 g, 2.16 mmol) in THF (25 cm^3) was cooled to about −80 °C. To the solution was added dropwise a 2.4 M solution of Bu^{n}Li in hexane (0.9 cm^3, 2.16 mmol) with stirring. The mixture was warmed to room temperature and stirred for 4 h. The resulting solution was added dropwise into a stirred suspension of (DME)$NiCl_2$ (0.48 g, 2.16 mmol) in THF (15 cm^3) at about −80 °C. The mixture was warmed to room temperature and stirred overnight. Volatiles were removed in vacuo, and the residue was dissolved in toluene. The resulting solution was filtered and concentrated to afford green powder of **3a** (0.73 g, 69%), mp 236-237 °C. Anal. Calcd for $C_{26}H_{24}N_2PNiCl{\cdot}0.1C_7H_8$: C, 64.29; H, 5.01; N, 5.62. Found: C, 64.54; H, 4.92, N, 5.70. ^{1}H NMR ($CDCl_3$): δ 3.01 (d, J = 2 Hz, 6H, NMe_2), 6.47 (t, J = 7 Hz, 1H, Ar), 6.54-6.58 (m, 1H, Ar), 6.91-6.98 (m, 2H, Ar), 7.10-7.14 (m, 1H, Ar), 7.16 (dd, J = 1.2, 8 Hz, 1H, Ar), 7.40-7.47 (m, 5H, Ar), 7.48-7.54 (m, 3H, Ar), 7.84-7.92 (m, 4H, Ar). ^{13}C NMR ($CDCl_3$): δ 49.03 (d, J = 2.3 Hz), 115.02, 115.52 (d, J = 11.8 Hz), 116.96, 117.09 (d, J = 7.7 Hz), 120.84, 122.14, 122.68, 127.38, 128.86 (d, J = 11 Hz), 129.15, 129.67, 131.06 (d, J = 2.9 Hz), 132.43 (d, J = 2 Hz), 133.50 (d, J = 10.4 Hz), 133.81, 146.52 (d, J = 2.8 Hz), 149.09 (d, J = 2 Hz), 159.89, 160.11. ^{31}P NMR ($CDCl_3$): δ 26.67.

Preparation of [(L2)NiCl] (3b)



A solution of compoud **HL2** (0.51 g, 1.54 mmol) in THF (25 cm^3) was cooled to about −80 °C. To the solution was added dropwise a 2.4 M solution Bu^{n}Li in hexane (0.64 cm^3, 1.54 mmol) with stirring. The mixture was warmed to room temperature and stirred for 4 h. The resulting solution was added dropwise into a stirred suspension of (DME)$NiCl_2$ (0.34 g, 1.54 mmol) in THF (15 cm^3) at about −80 °C. The resulting mixture was warmed to room temperature and stirred overnight. Volatiles were removed in vacuo, and the residue was dissolved in Et_2O and then filtered. Hexane was added into the filtrate to form green crystals of **3b** (0.42 g, 65%), mp 151-152 °C. Anal. Calcd for $C_{20}H_{28}N_2PNiCl·0.2C_6H_{14}$: C, 58.03; H, 7.07; N, 6.38. Found: C, 58.10; H, 6.68, N, 6.46. ^{1}H NMR ($CDCl_3$): δ 1.32 (dd, J = 6, 14.8 Hz, 6H, *i*-Pr), 1.50 (dd, J = 6, 16.4 Hz, 6H, *i*-Pr), 2.14-2.32 (m, *i*-Pr), 2.88 (s, 6H, NMe), 6.79-6.89 (m, 1H, Ar), 6.35-6.52 (m, 2H, Ar), 6.98-7.13 (m, 3H, Ar), 7.31-7.47 (m, 2H, Ar). ^{13}C NMR ($CDCl_3$): δ 17.78, 18.70, 24.62 (d, J = 24.3 Hz), 48.50, 114.80, 115.30 (d, J = 10.8 Hz), 116.23 (d, J = 6.8 Hz), 116.45, 119.59, 120.02, 120.72, 127.18, 131.54, 131.87, 146.22, 149.42, 160.94, 161.12. ^{31}P NMR ($CDCl_3$): δ 52.89.

Preparation of [(L3)NiCl] (3c)



A solution of compoud **HL3** (0.86 g, 2.10 mmol) in THF (25 cm^3) was cooled to about −80 °C. To the solution was added dropwise a 2.4 M solution of Bu^{n}Li in hexane (0.86 cm^3, 2.10 mmol) with stirring. The mixture was warmed to room temperature and stirred for 4 h. The resulting solution was added dropwise into a stirred suspension of (DME)$NiCl_2$ (0.46 g, 2.10 mmol) in THF (15 cm^3) at about −80 °C. The mixture was warmed to room temperature and stirred overnight. Volatiles were removed in vacuo. The residue was dissolved in Et_2O and then filtered. Hexane was added into the filtrate to form green crystals of **3c** (0.90 g, 86%), mp 180-181°C. Anal. Calcd for $C_{26}H_{36}N_2PNiCl$: C, 62.24; H, 7.23; N, 5.58. Found: C, 61.75; H, 7.23, N, 5.58. ^{1}H NMR ($CDCl_3$): δ 1.14-1.47 (m, 6H, C_6H_{11}), 1.55-2.16 (m, 14H, C_6H_{11}),

2.62 (b, 2H, C_6H_{11}), 2.95 (s, 6H, NMe), 6.42-6.61 (m, 2H, Ar), 6.83-6.97 (m, 1H, Ar), 7.03-7.21 (m, 3H, Ar), 7.35-7.54 (m, 2H, Ar). ^{13}C NMR ($CDCl_3$): δ 26.16, 26.99, 27.10, 27.25, 27.99, 28.53, 33.85, 34.11, 48.53, 114.77, 115.19 (d, J = 10.9 Hz), 116.16 (d, J = 6.8 Hz), 116.37, 120.02, 120.46, 120.69, 127.14, 131.65, 131.79, 146.27, 149.45, 161.00, 161.18. ^{31}P NMR ($CDCl_3$): δ 45.58.

Crystal structure determination

Single crystal of complex **3c** was mounted in Lindemann capillaries under nitrogen. Diffraction data were collected at 290(2) K on an Oxford Diffraction Gemini S Ultra diffractometer with mirror-monochromated Cu K_α radiation (λ = 1.54184 Å). The structures were solved by direct methods using SHELXS-97[3] and refined against F^2 by full-matrix least-squares using SHELXL-97.[4] Hydrogen atoms were placed in calculated positions. Crystal data and experimental details of the structure determinations are listed in Table 1. CCDC 996222 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table 1 Details of the X-ray structure detemination of complex **3c**

empirical formula	$C_{26}H_{36}ClN_2NiP$
fw	501.70
crystal system	orthorhombic
space group	P_{na21}
a (Å)	19.6835(2)
b (Å)	8.27190(10)
c (Å)	31.3730(3)
α (deg)	90.00
β (deg)	90.00
γ (deg)	90.00
V (Å^3)	5108.15(9)
Z	8
D_{calcd} (g cm^{-3})	1.305
F(000)	2128.0
μ (mm^{-1})	2.754
2θ range for data collecn (deg)	8.98 to 125.52
no. of reflns collected	29453
no. of indep reflns (R_{int})	7437 (0.0296)

no. of data/ restraints/params	7437/1/563
goodness of fit on F^2	1.033
final R indices [$I > 2\sigma(I)$]	$R1 = 0.0311$ w$R2 = 0.0840$
R indices (all data)	$R1 = 0.0326$ w$R2 = 0.0856$
largest diff peak and hole [e Å^{-3}]	0.33 and −0.19

References

1 L. G. L. Ward, *Inorg. Synth.* 1971, **13**, 154.

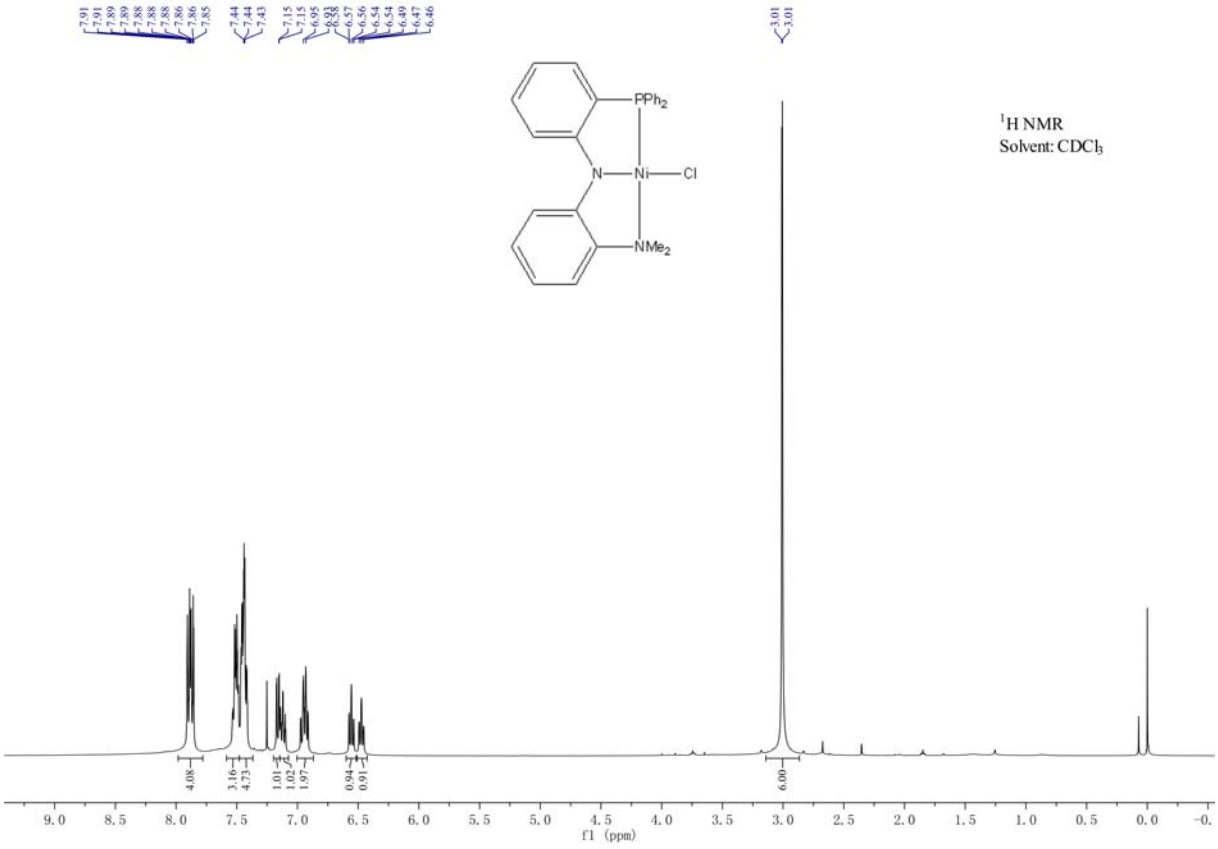
2 R. Lindner, B. van den Bosch, M. Lutz, J. N. H. Reek, J. I. van der Vlugt, *Organometallics* 2011, **30**, 499.

3 G. M. Sheldrick, Acta Crystallogr., Sect. A 1990, **46**, 467.

4 G. M. Sheldrick, SHELXL97, Programs for Structure Refinement; Universität Göttingen, Göttingen, Germany, 1997.

Copies of ^{1}H, ^{13}C and ^{31}P NMR spectra of complexes 3a-3c

1. [(L1)NiCl] (**3a**)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Cl
NMe2
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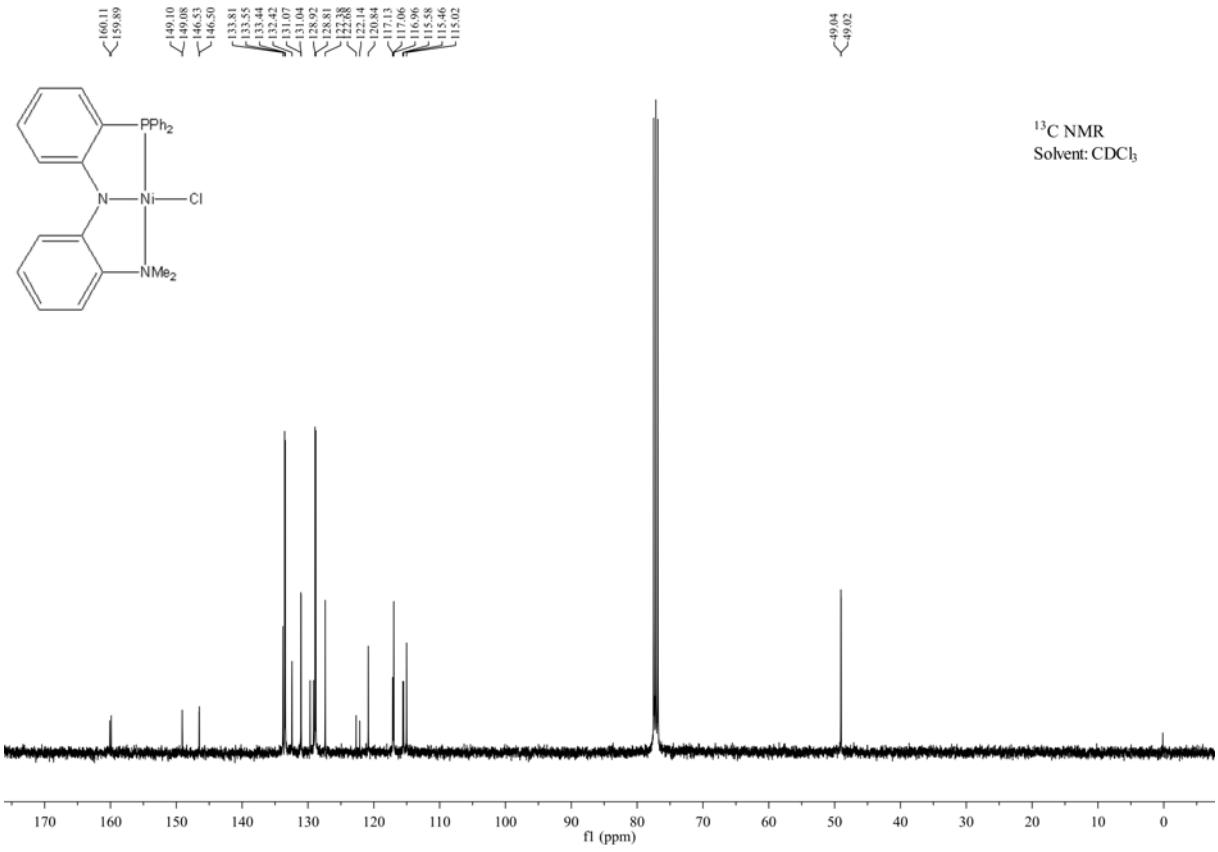
Solvent: CDCl3
f1 (ppm)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Cl
NMe2
13C NMR
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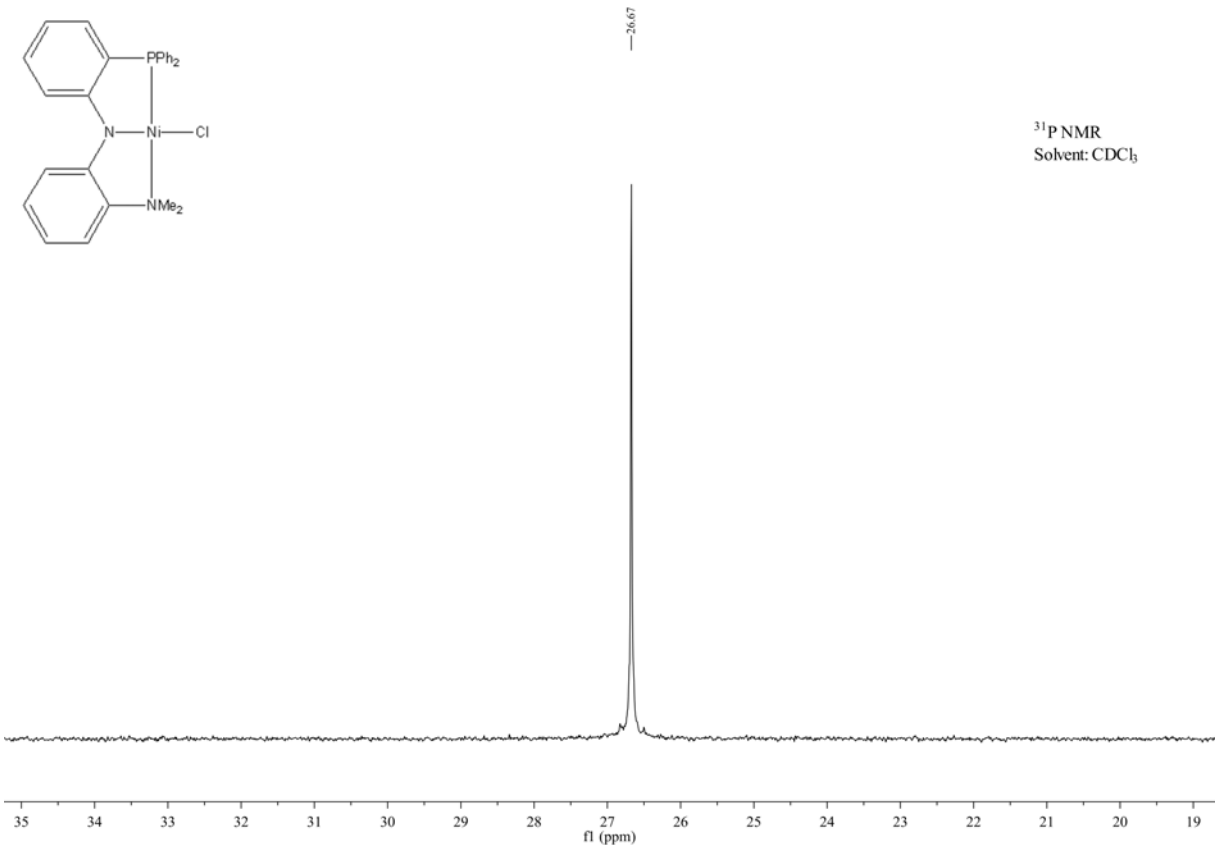
f1 (ppm)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NMe2
26.67
31P NMR
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35
34
33
32
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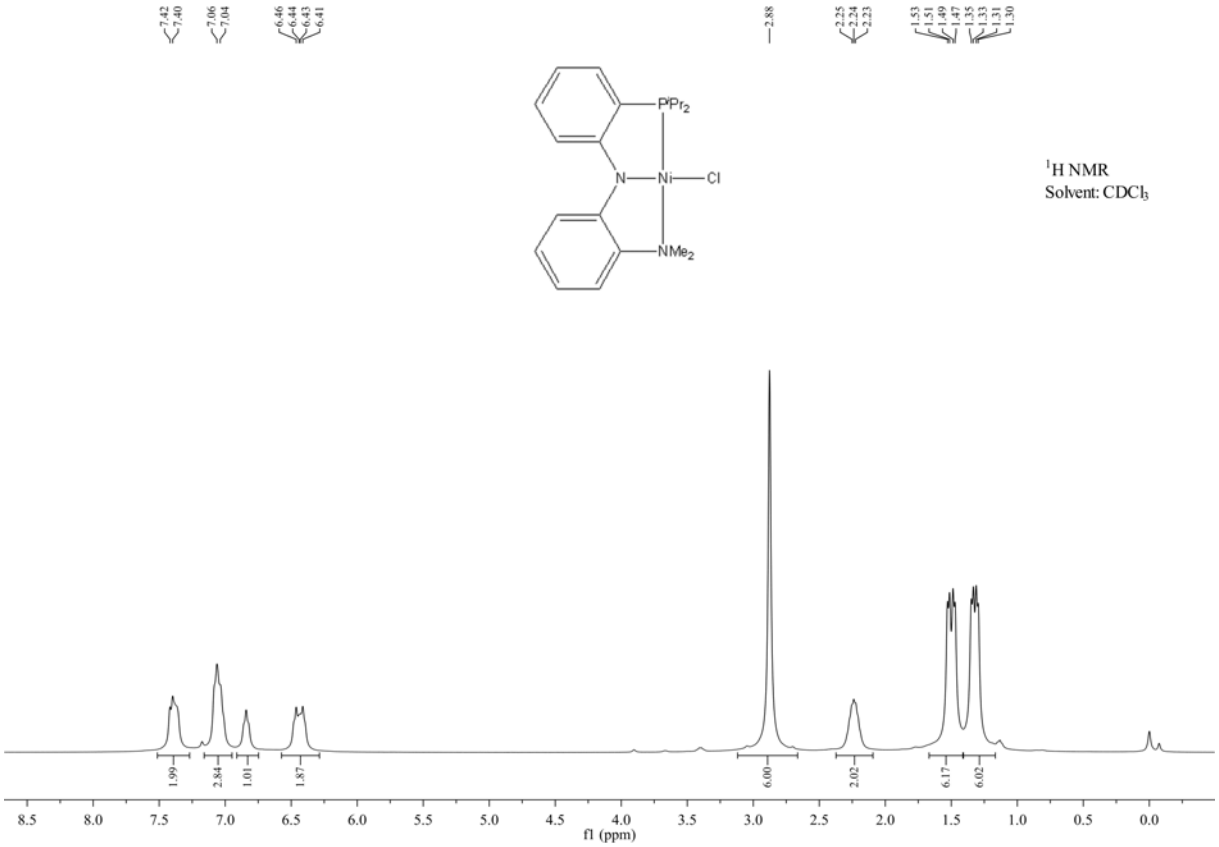
28
27
26
25
24
23
22
21
20
19
f1 (ppm)

[(L2)NiCl] (**3b**)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7.40
7.06
7.04
6.46
6.44
6.43
6.41
2.88
2.25
2.24
2.23
1.53
1.51
1.49
1.47
1.35
1.33
1.31
1.30
PiPr2
N
Ni
Cl
NMe2
1H NMR
Solvent: CDCl3
1.99
2.84
1.01
1.87
6.00
2.02
6.17
6.02
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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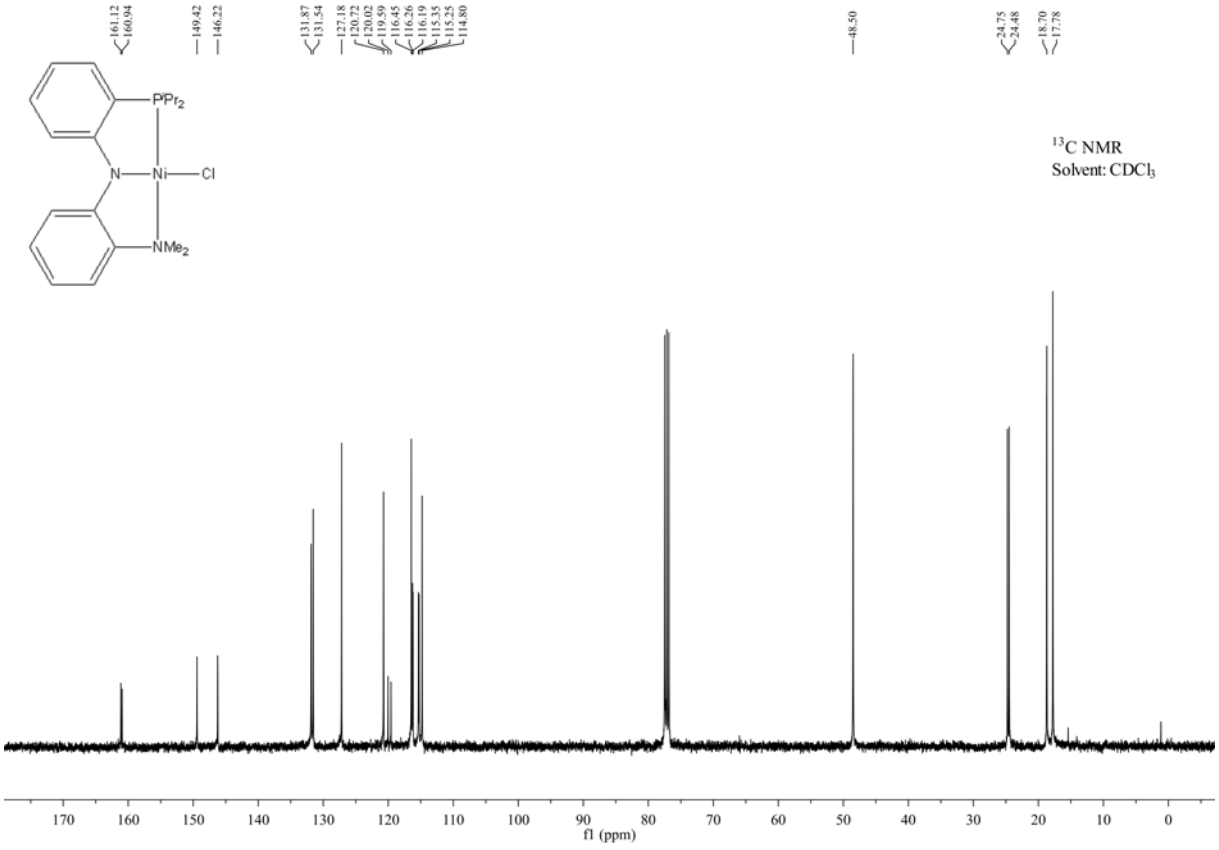
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


161.12
160.94
149.42
146.22
131.87
131.54
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120.02
119.59
116.45
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115.35
115.25
114.80
48.50
24.75
24.48
18.70
17.78
PiPr2
N
Ni
Cl
NMe2
13C NMR
Solvent: CDCl3
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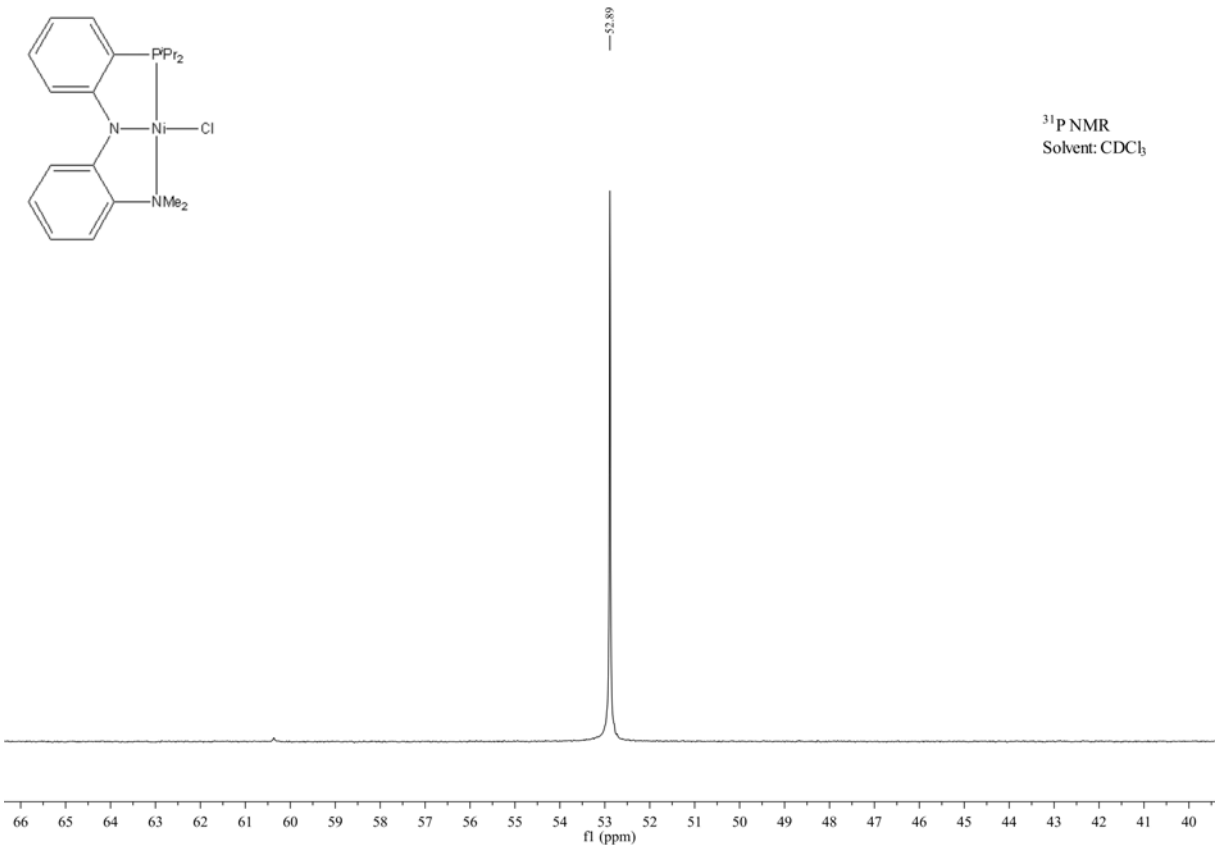
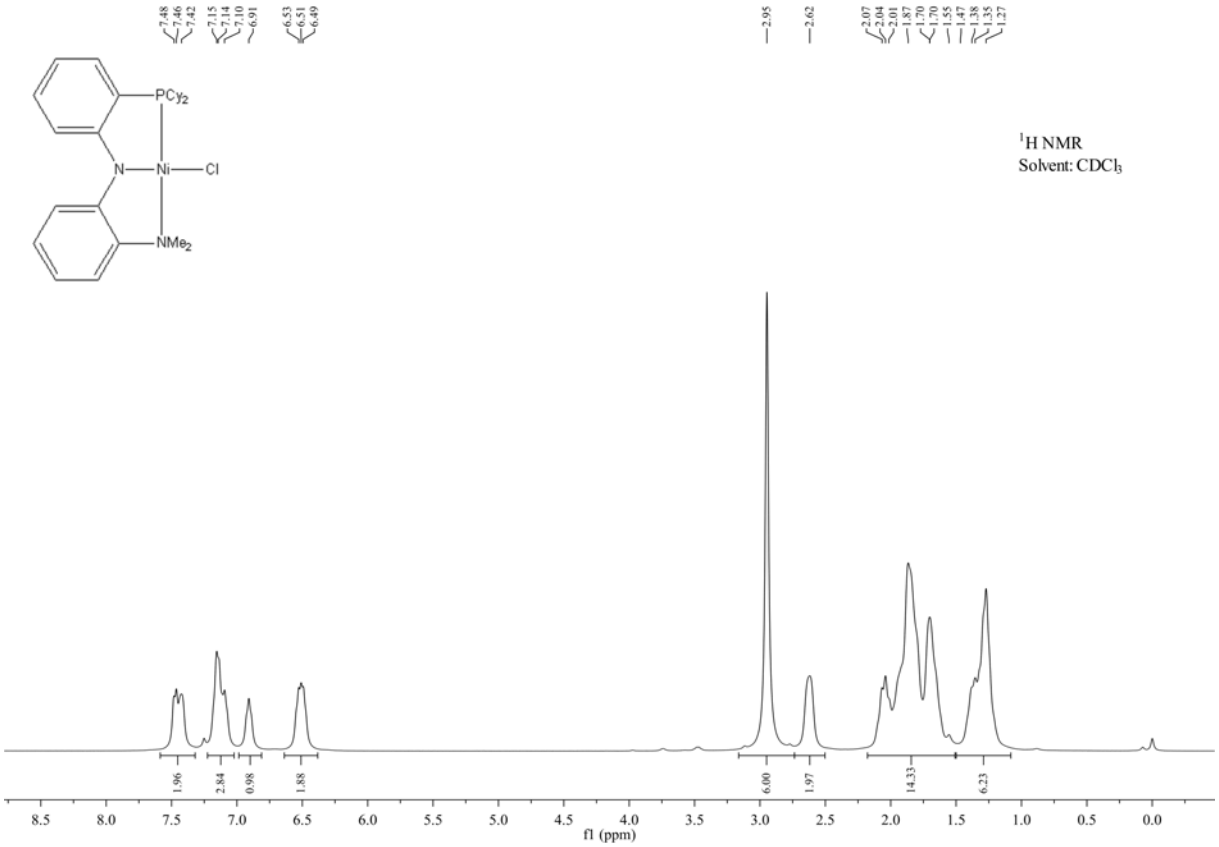
f1 (ppm)


PPr2
N
Ni
Cl
NMe2
52.89
31P NMR
Solvent: CDCl3
66 65 64 63 62 61 60 59 58 57 56 55 54 53 52 51 50 49 48 47 46 45 44 43 42 41 40
f1 (ppm)

[(L3)NiCl] (**3c**)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1H NMR
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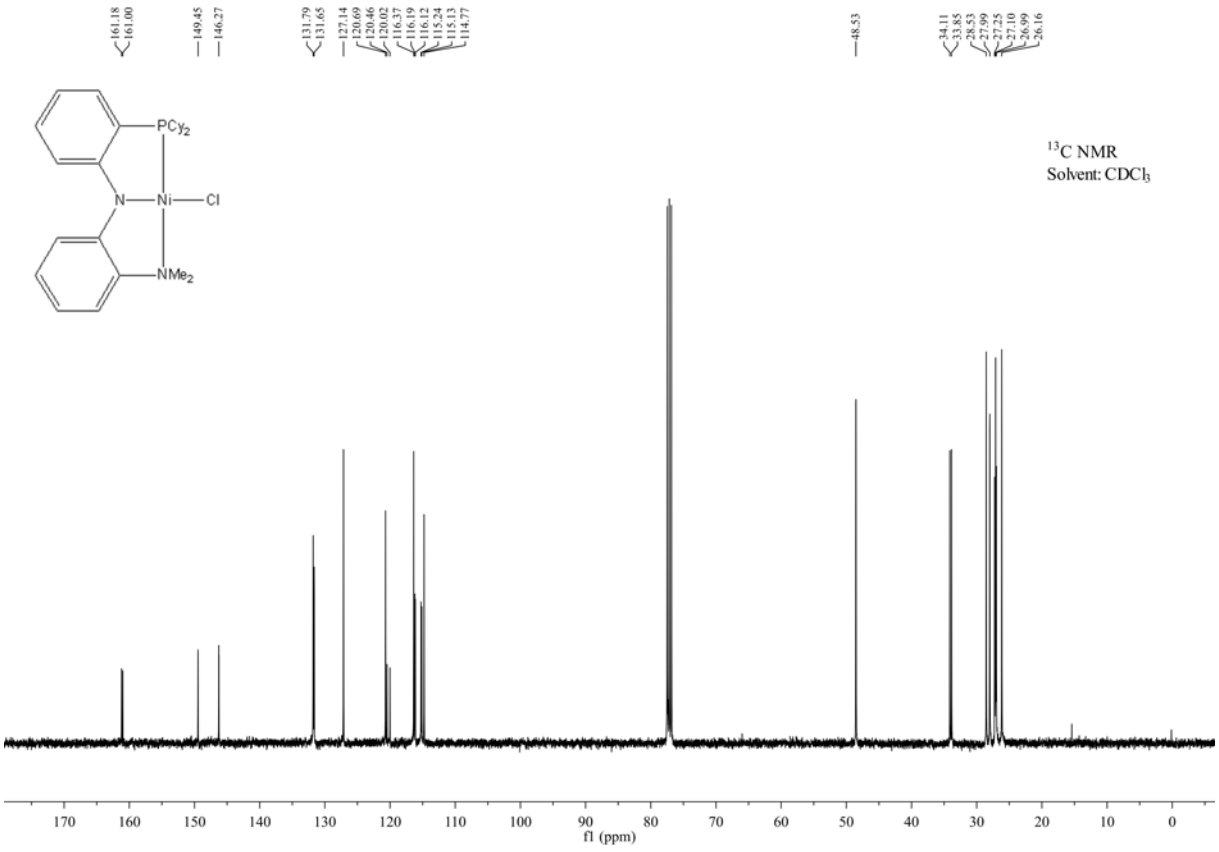
f1 (ppm)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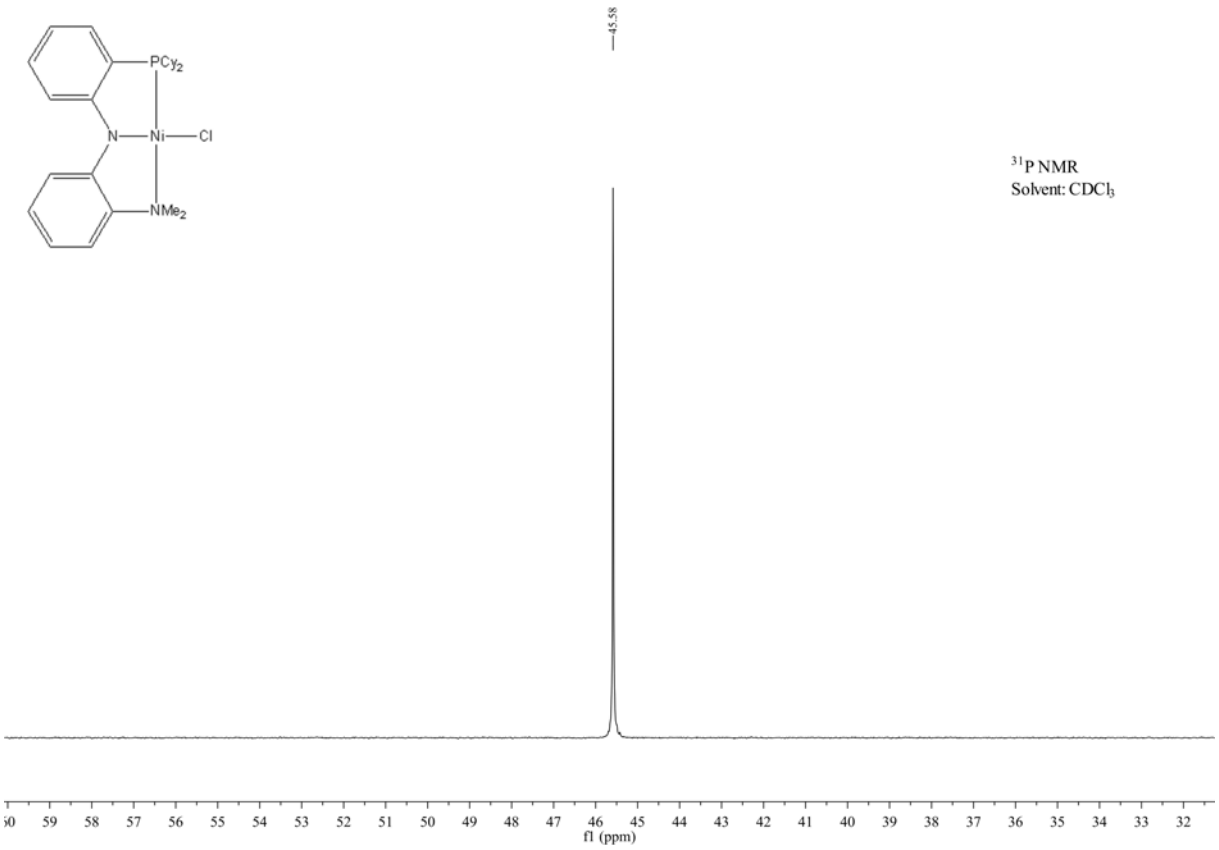
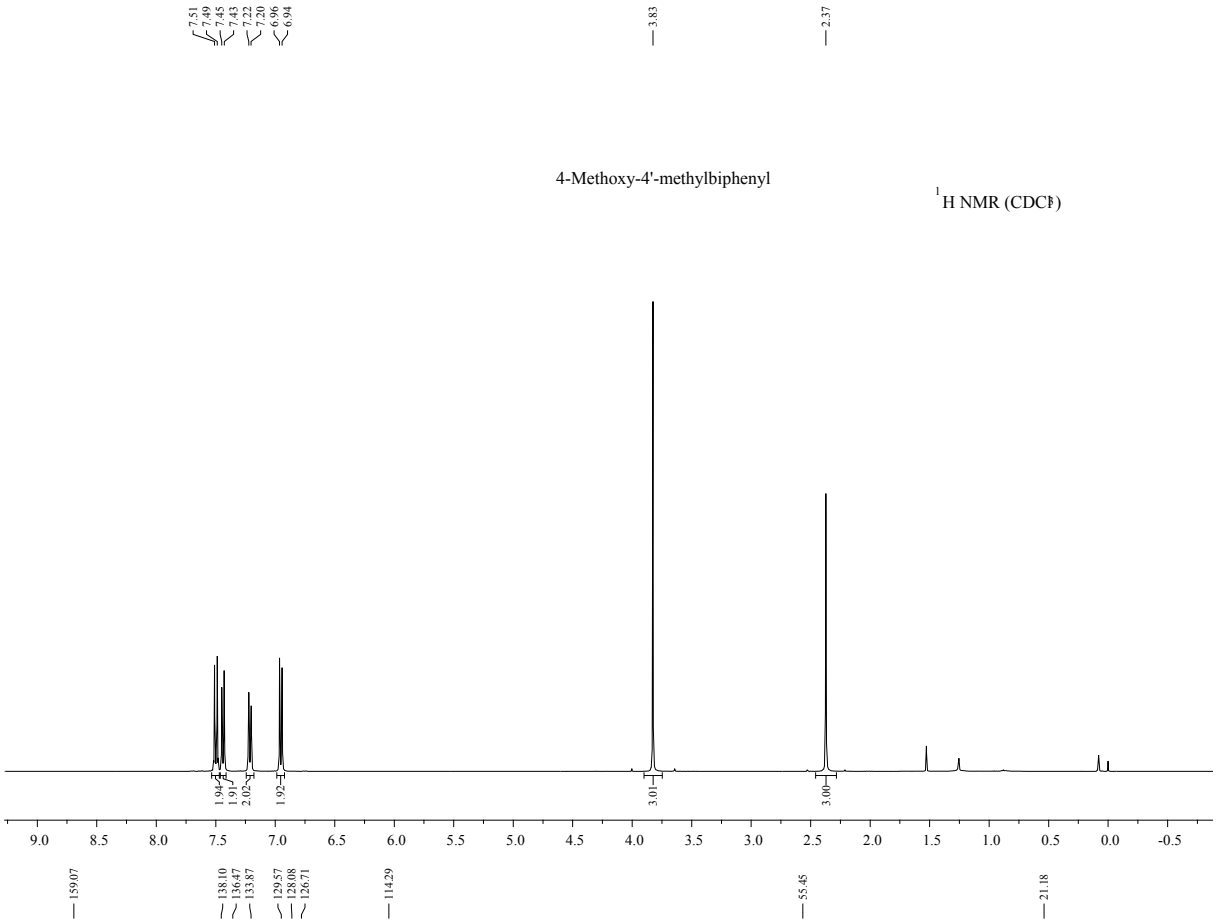
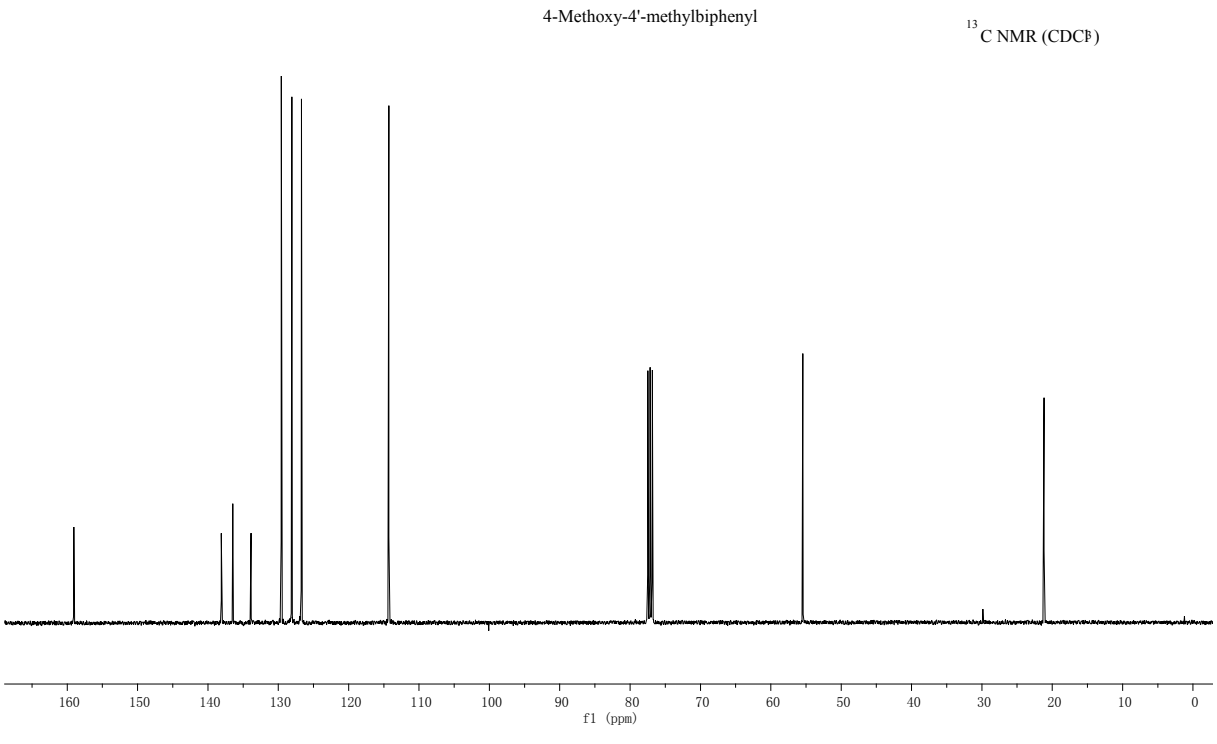
N
Ni
Cl
NMe2
13C NMR
Solvent: CDCl3
f1 (ppm)


PCy2
N
Ni
Cl
NMe2
45.58
31P NMR
Solvent: CDCl3
60 59 58 57 56 55 54 53 52 51 50 49 48 47 46 45 44 43 42 41 40 39 38 37 36 35 34 33 32
f1 (ppm)

Copies of ^{1}H and ^{13}C NMR spectra of the cross-coupling products

1. 4-Methoxy-4'-methylbiphenyl





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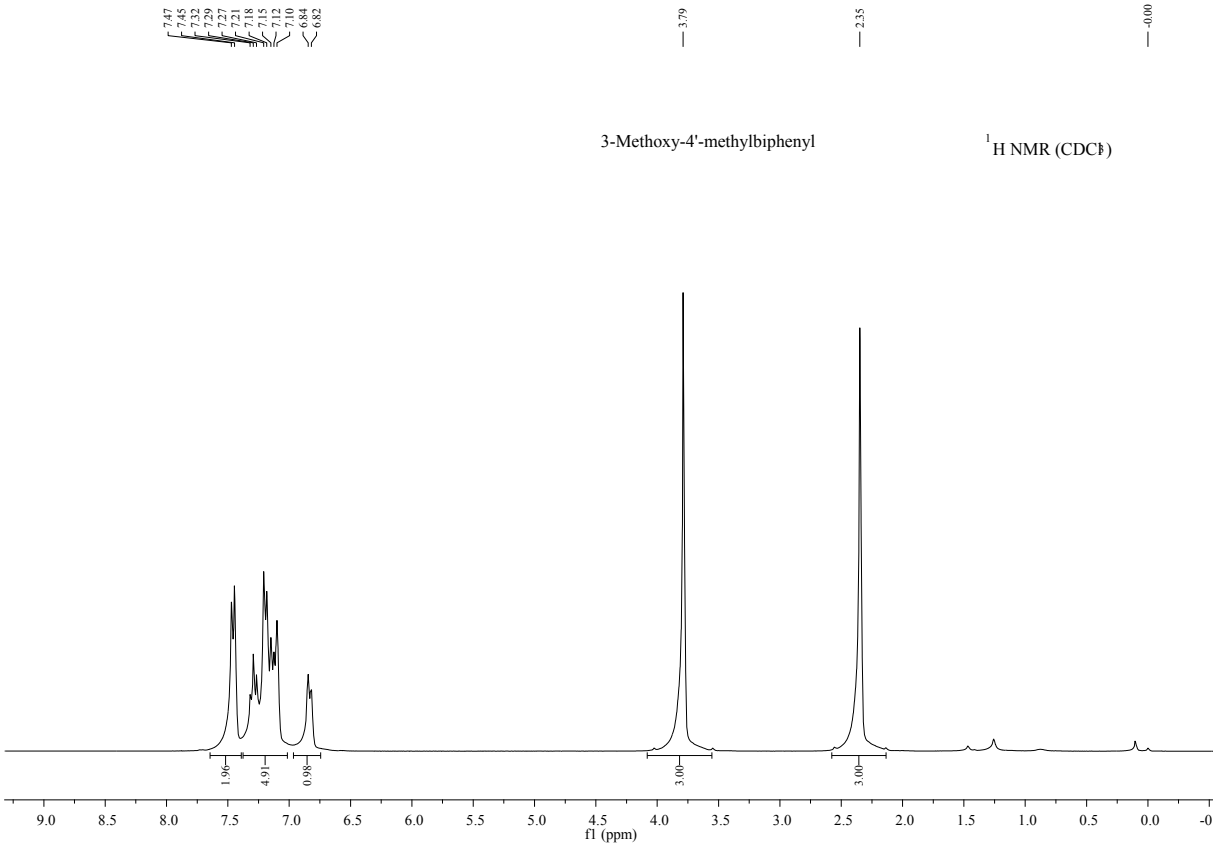
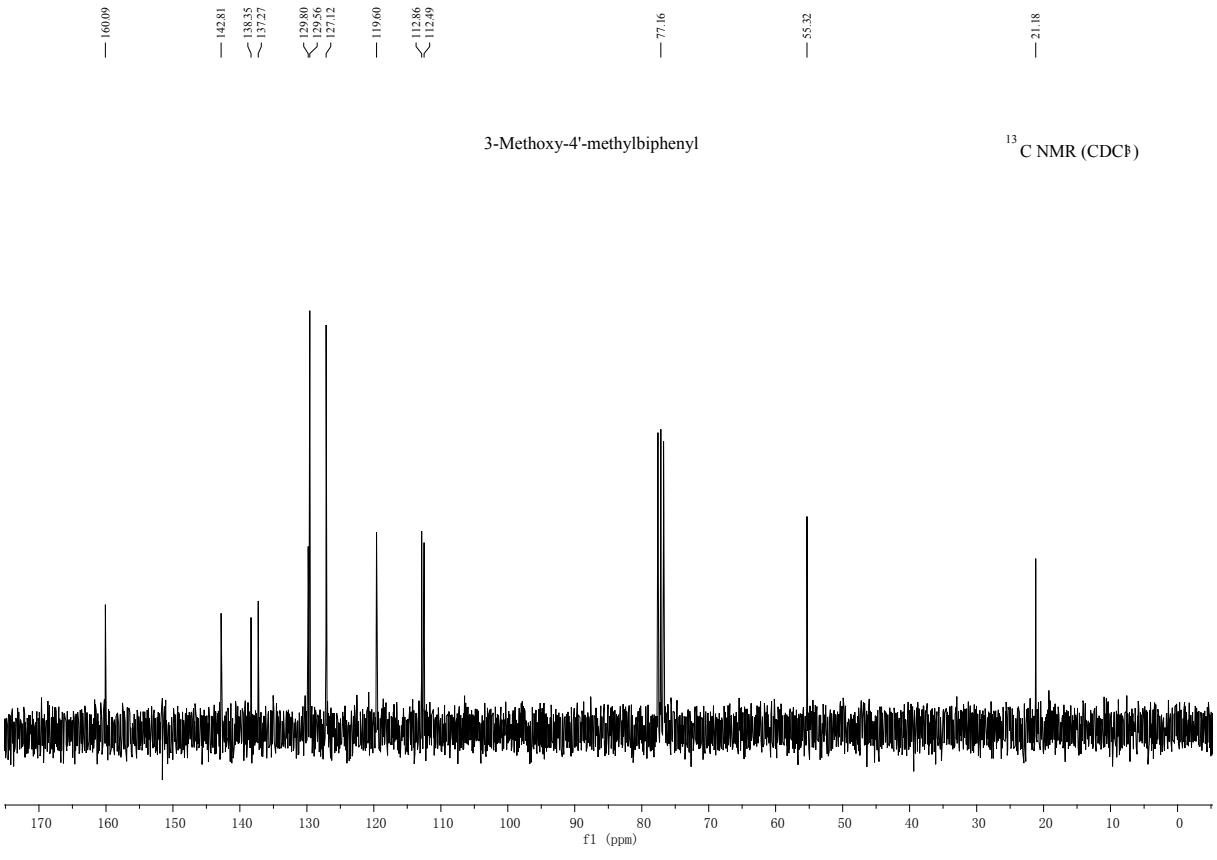
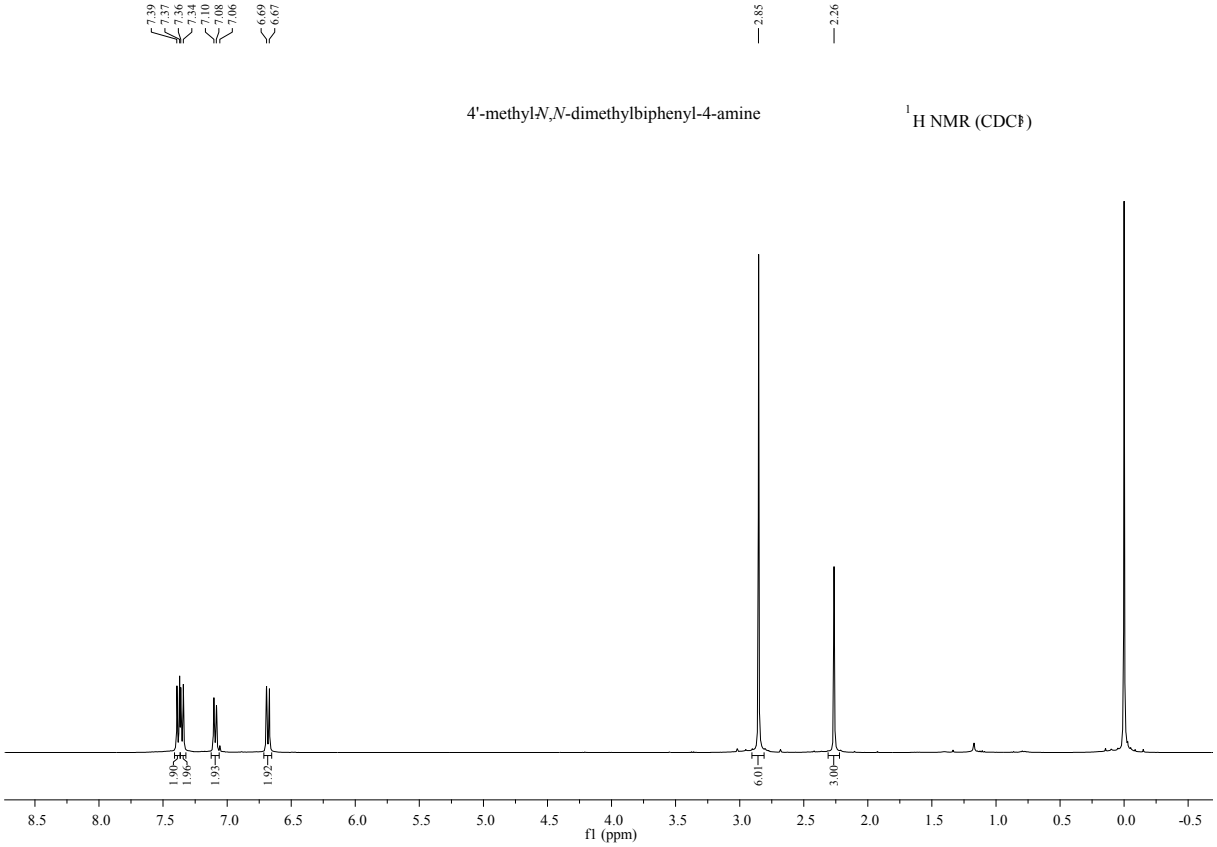
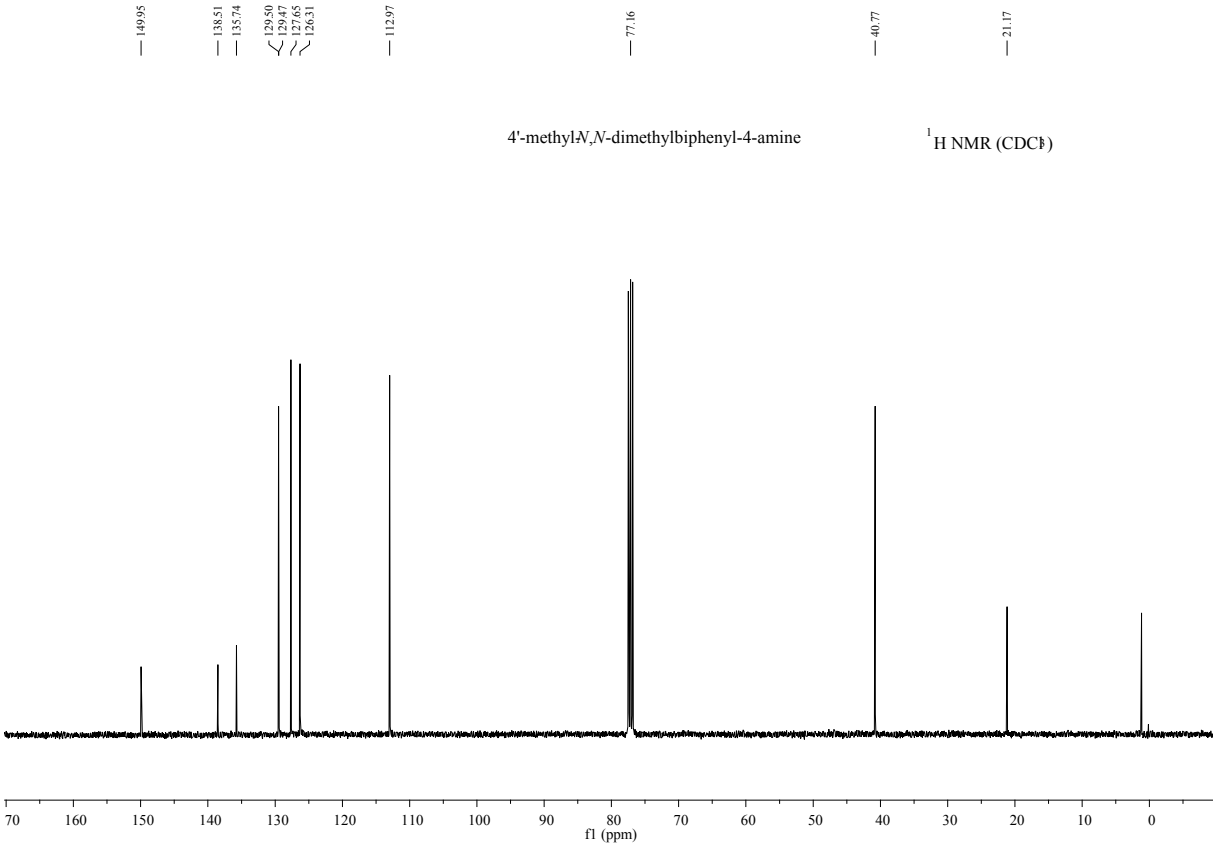




3. 4'-methyl-*N*,*N*-dimethylbiphenyl-4-amine





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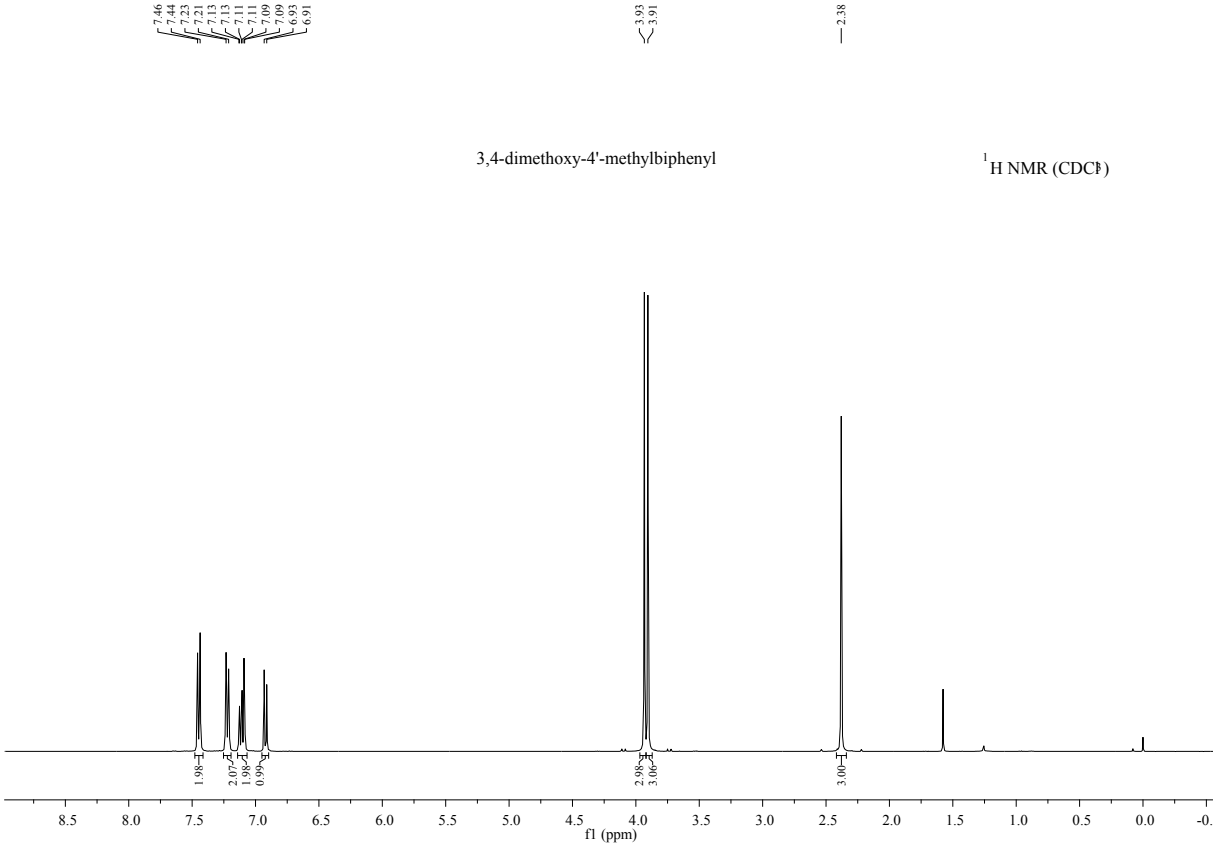
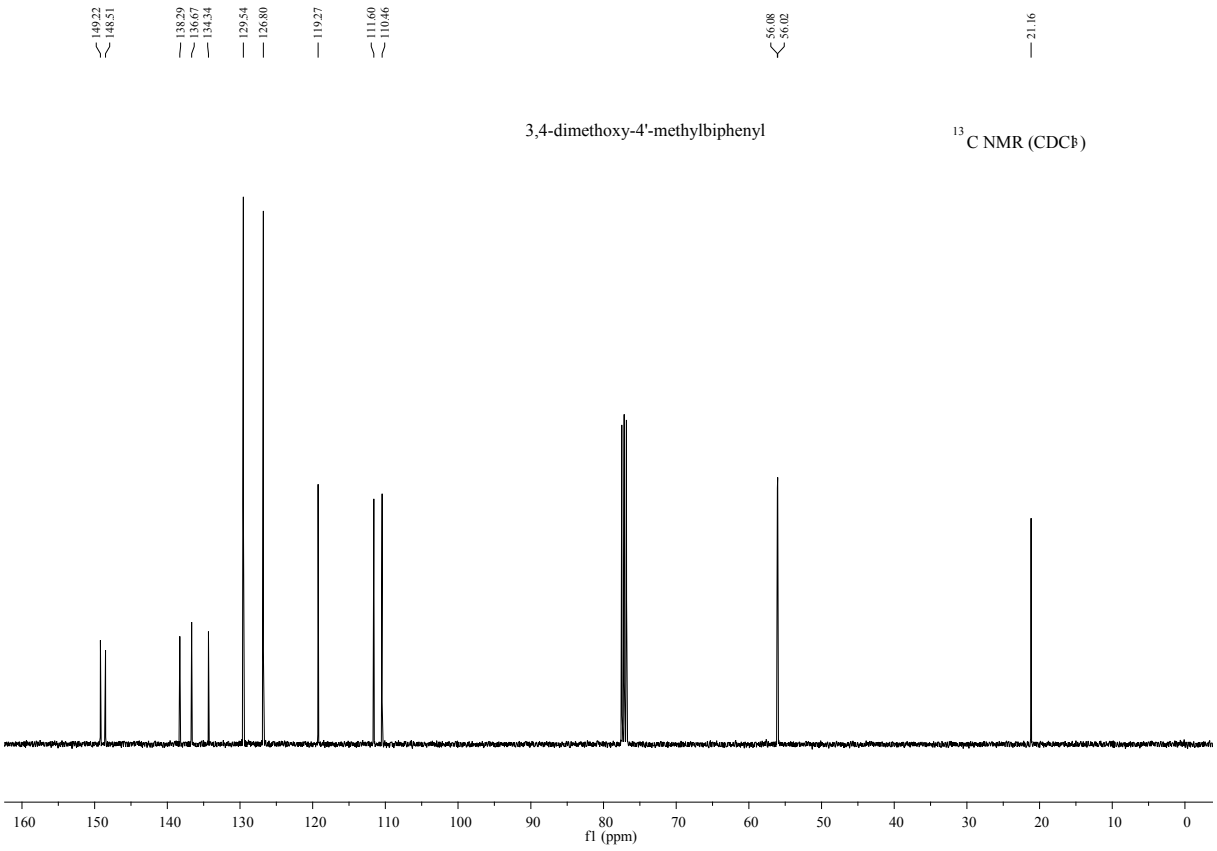
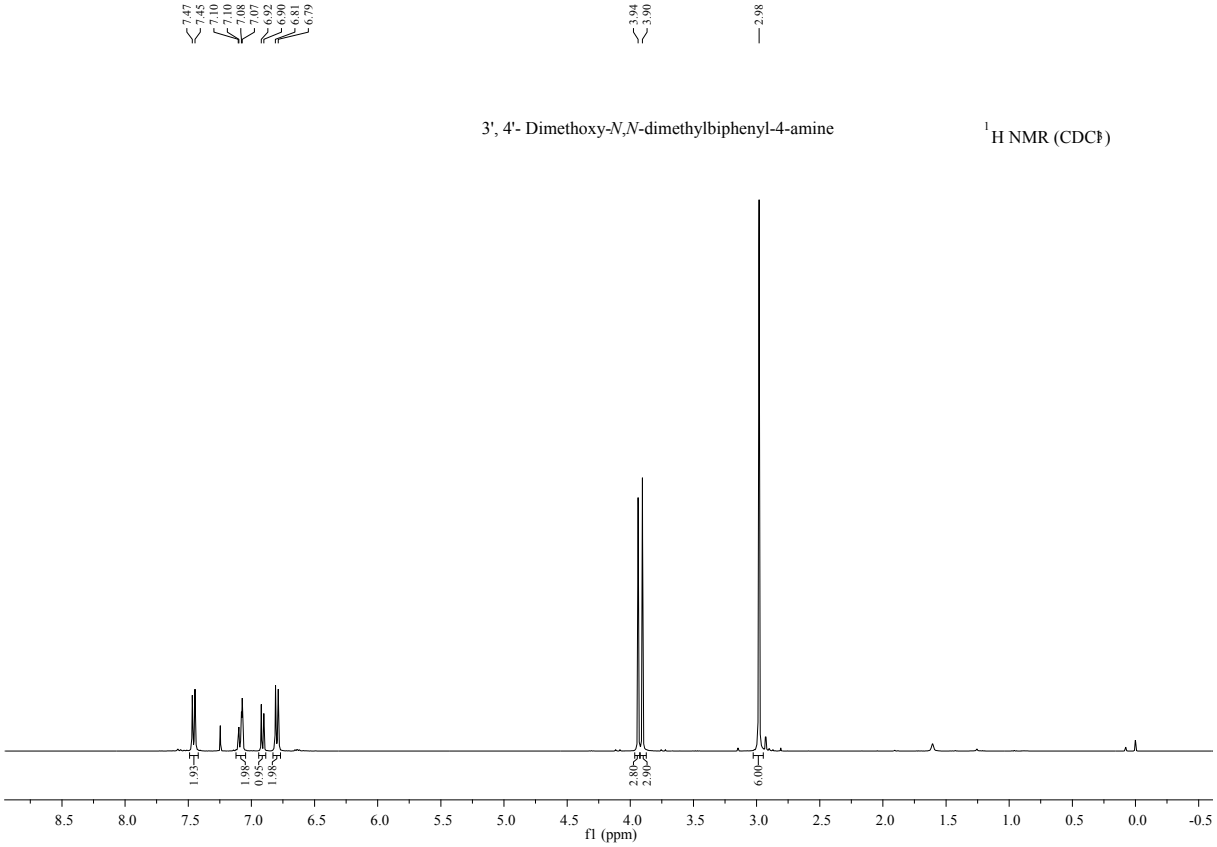
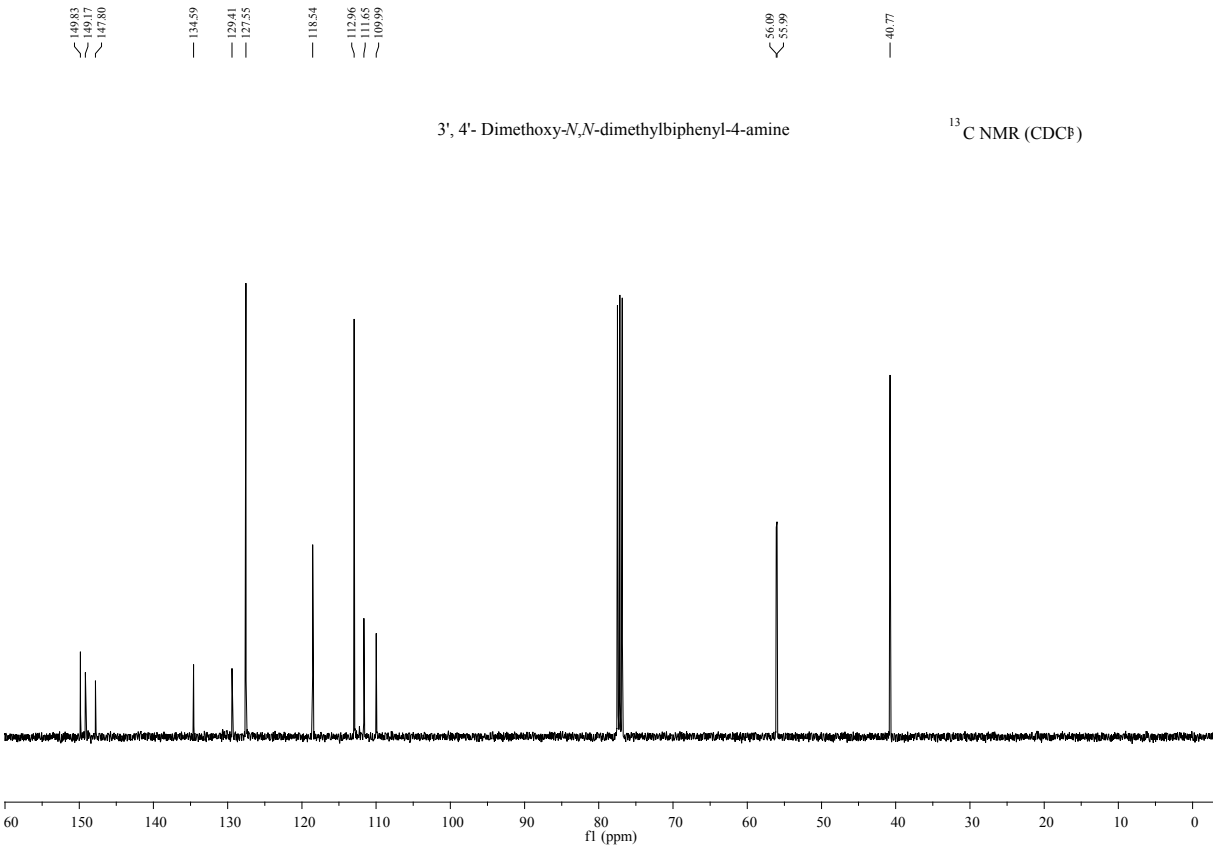


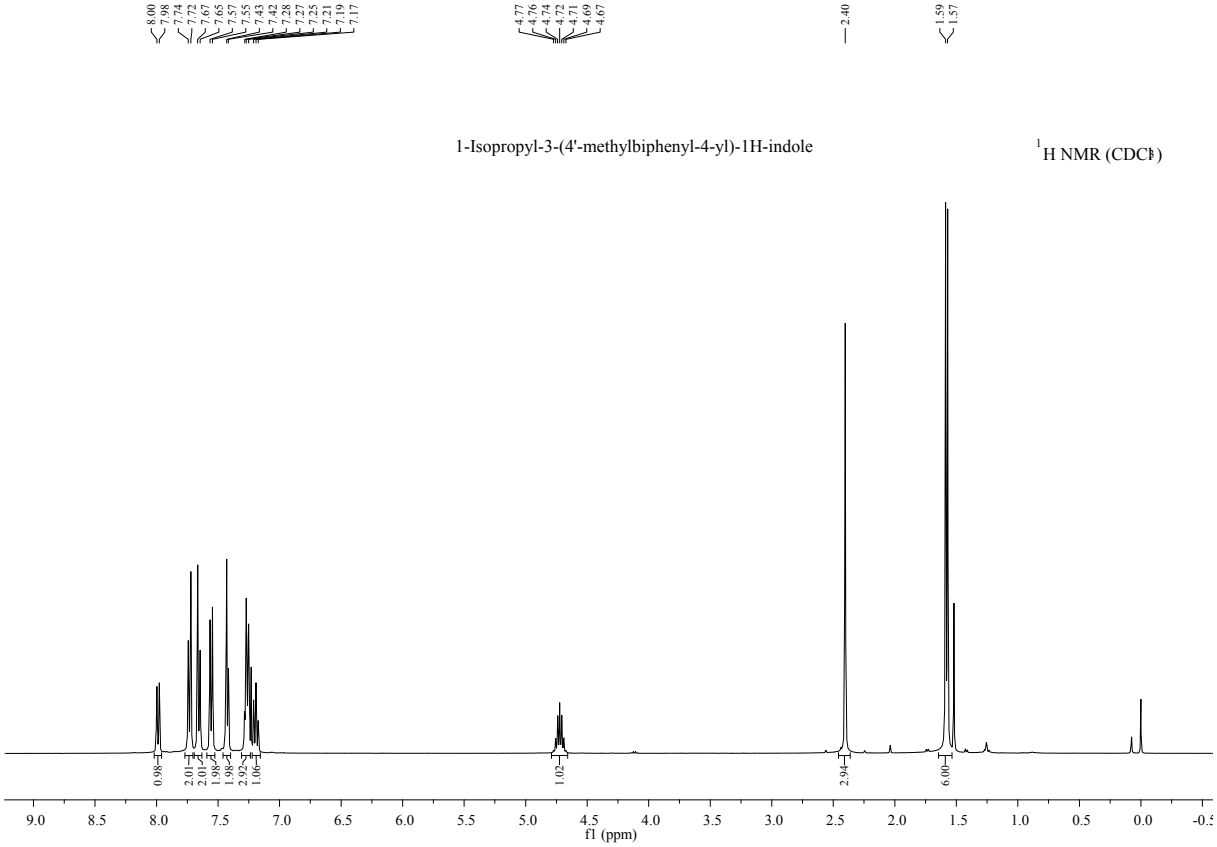


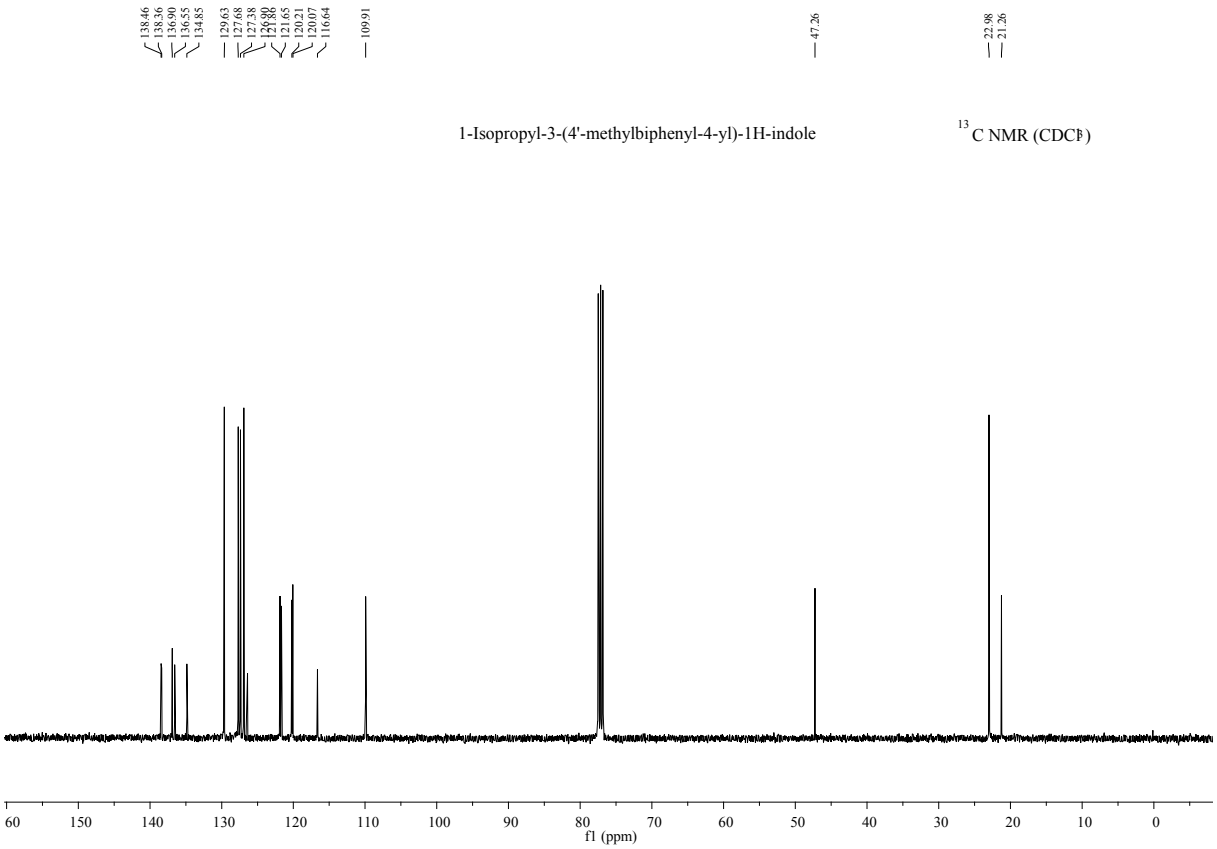
5. 3',4'- Dimethoxy- *N*,*N*-dimethylbiphenyl-4-amine



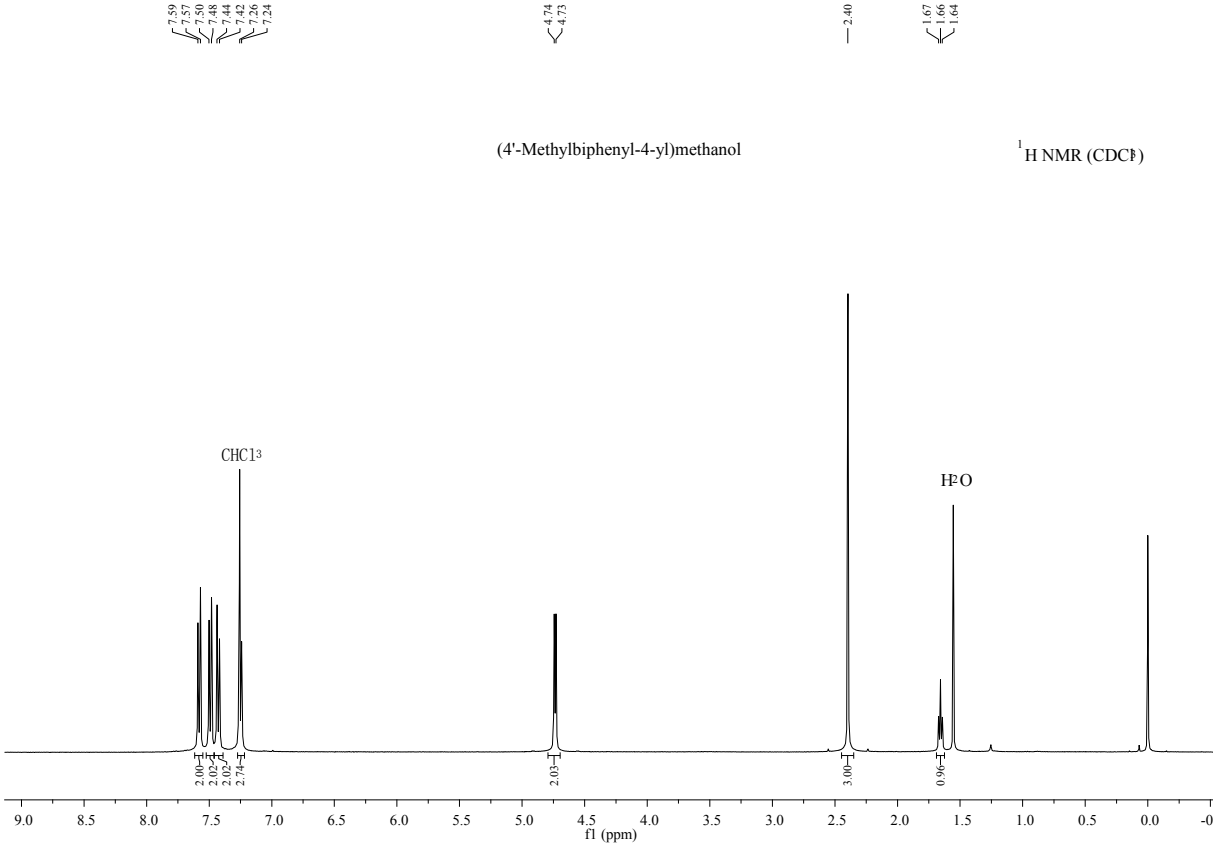


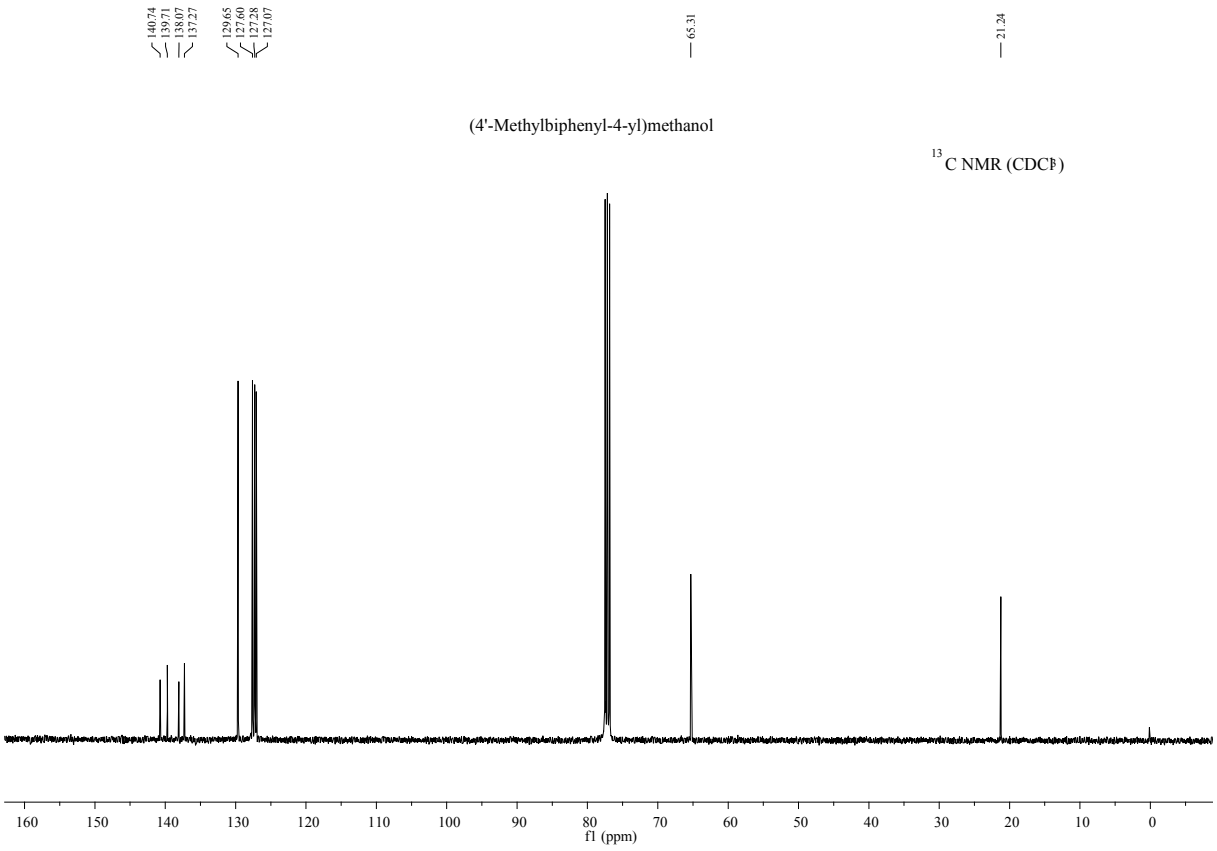
6. 1-Isopropyl-3-(4'-methylbiphenyl-4-yl)-1H-indole



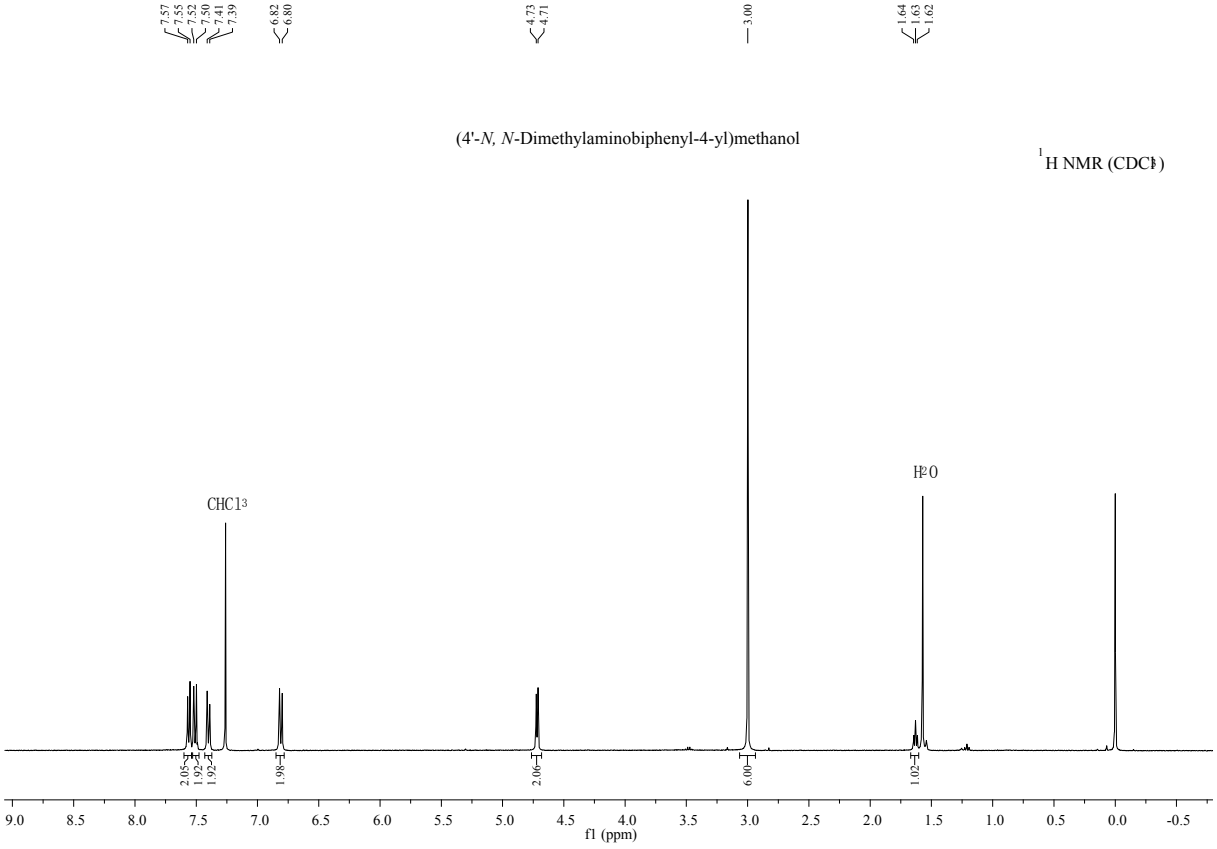


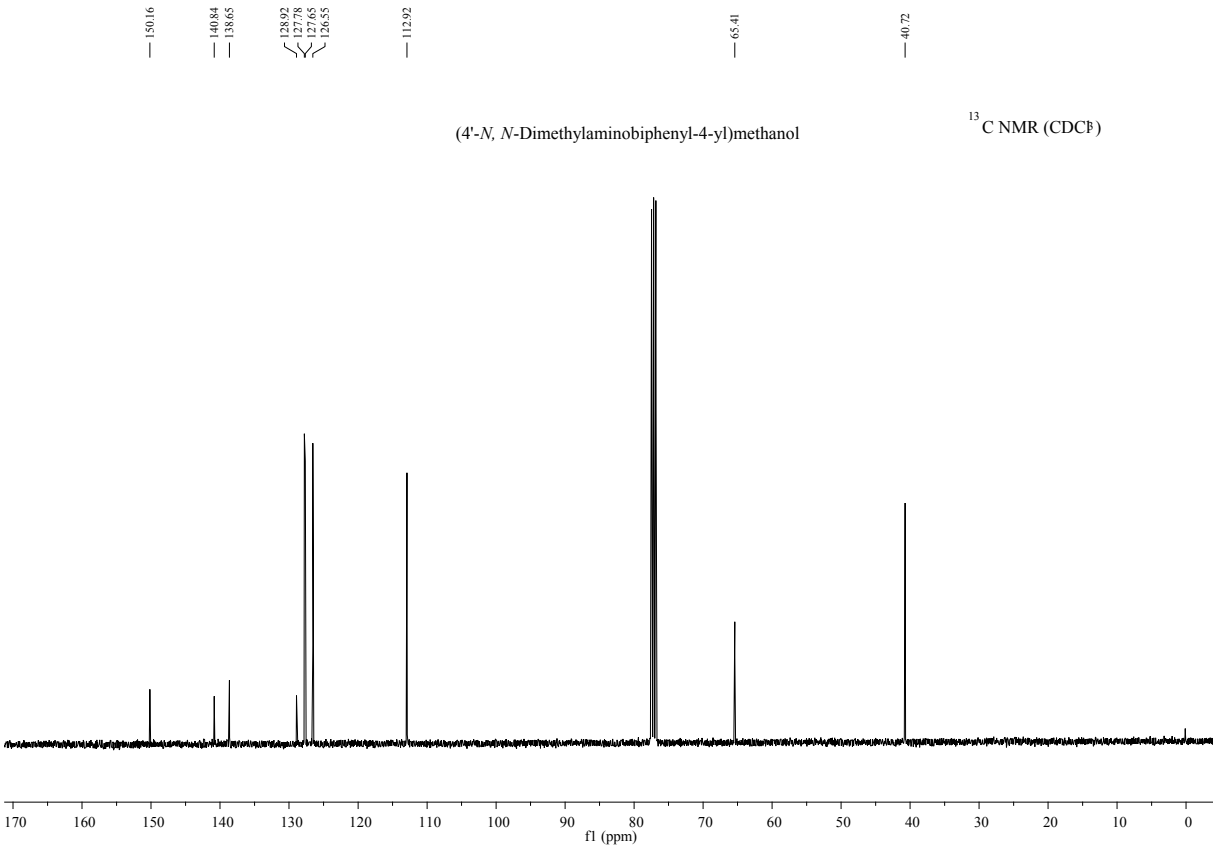
7. (4'-Methylbiphenyl-4-yl)methanol



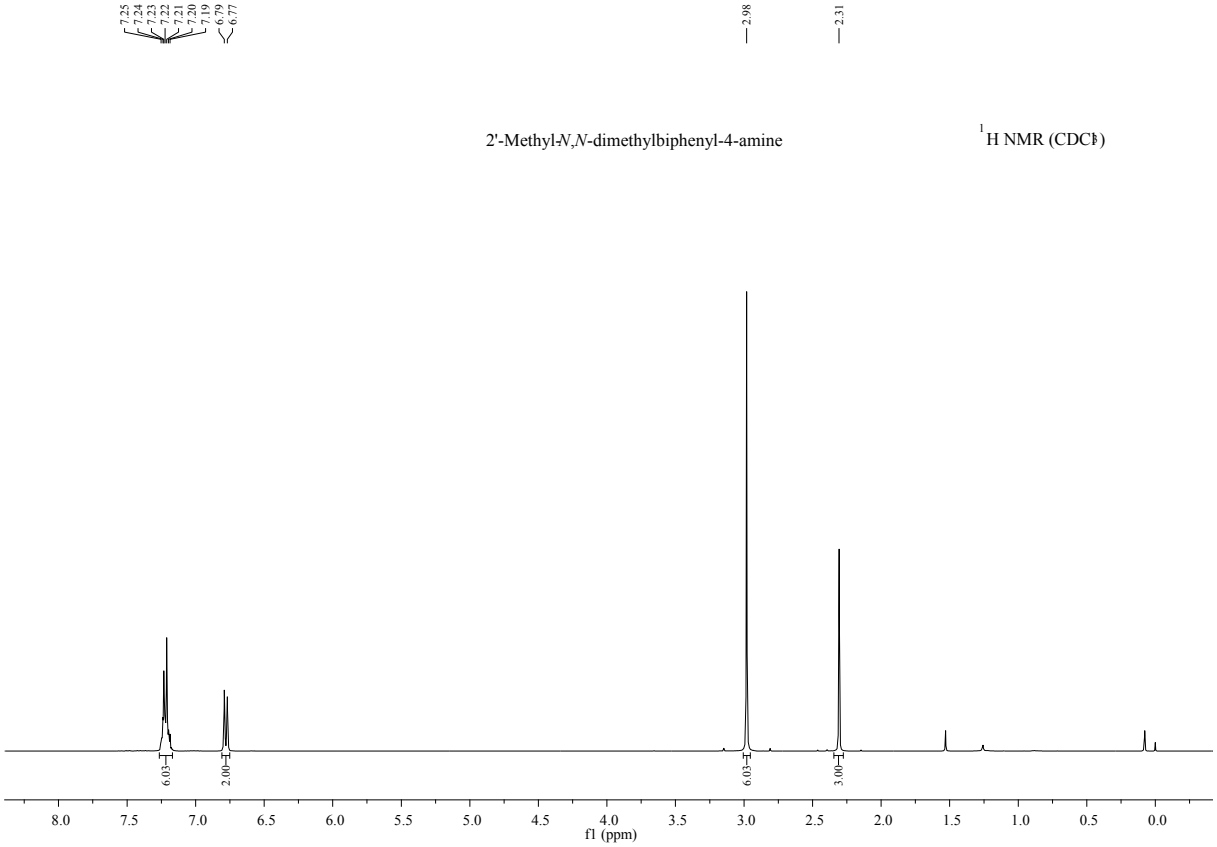


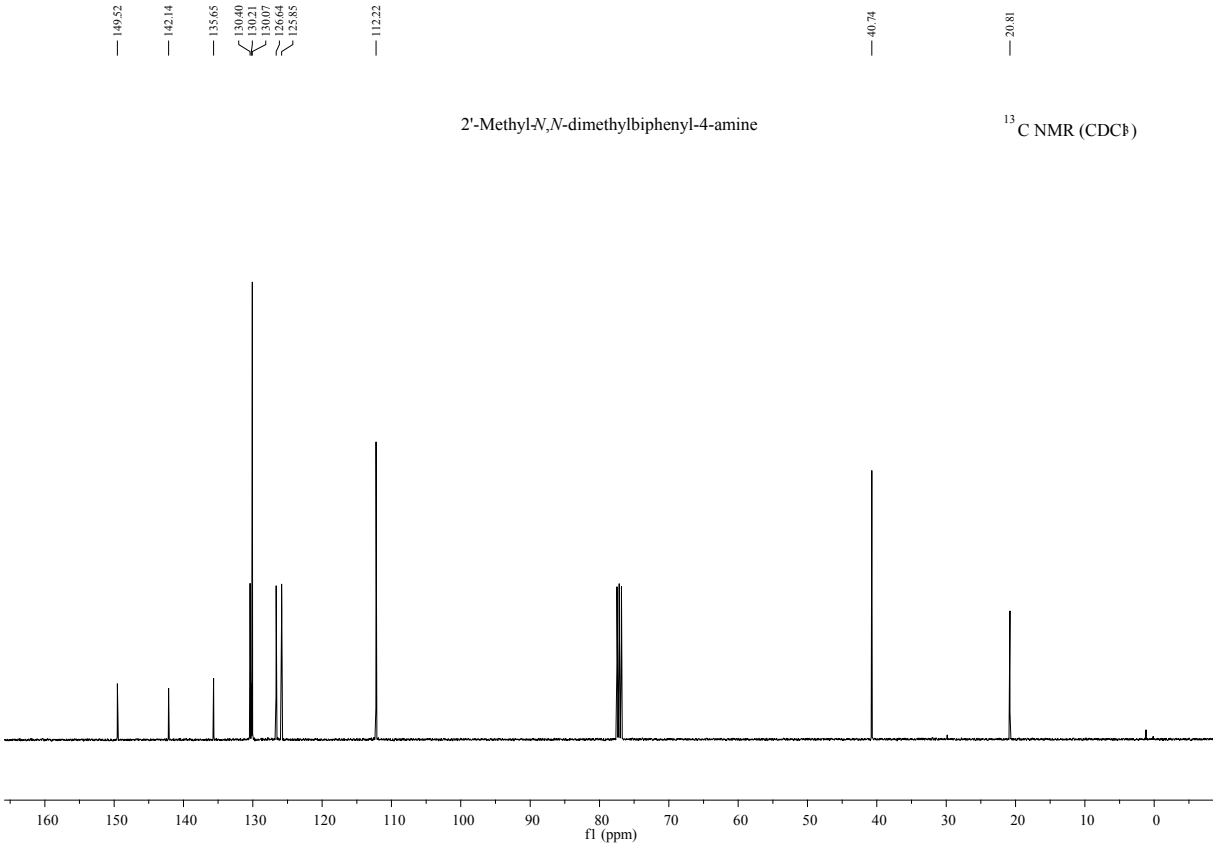
8. (4'-*N, N*-Dimethylaminobiphenyl-4-yl)methanol



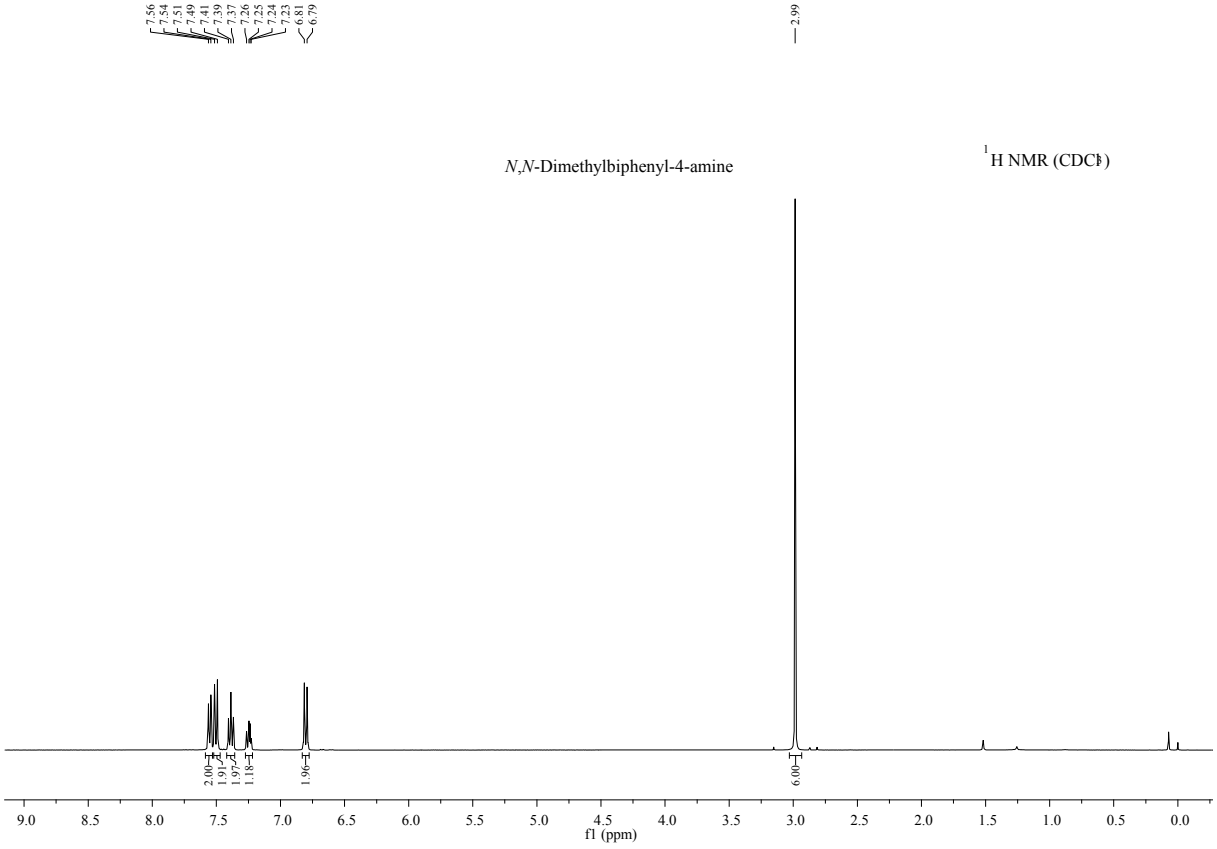


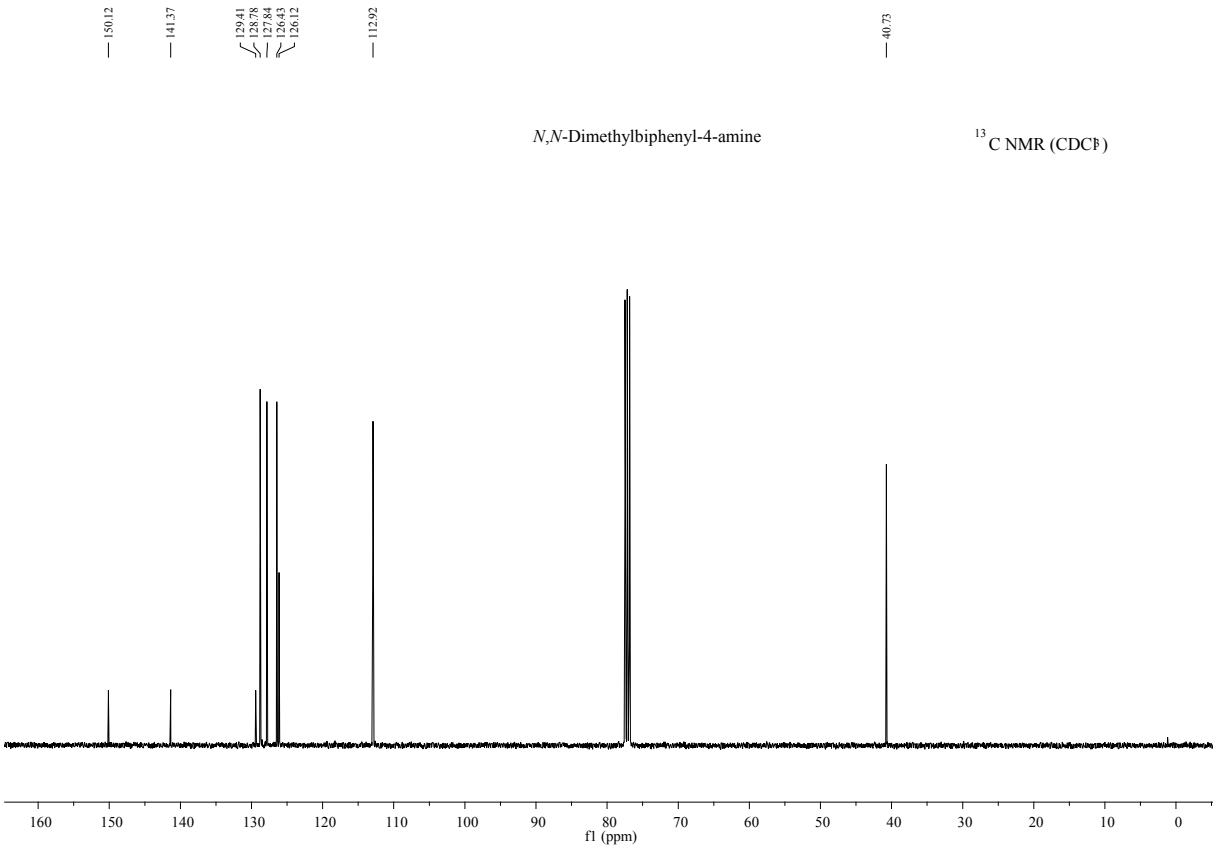
9. 2'-Methyl-*N*,*N*-dimethylbiphenyl-4-amine



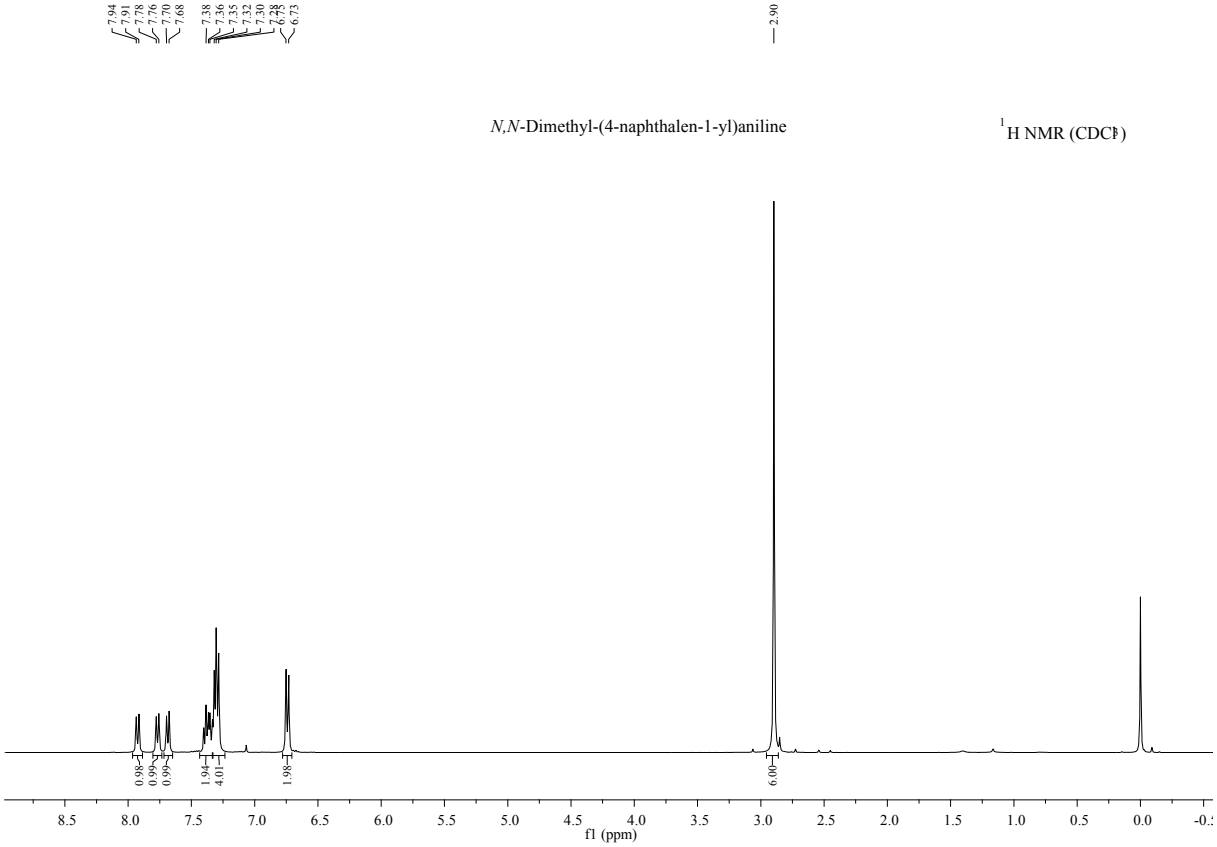


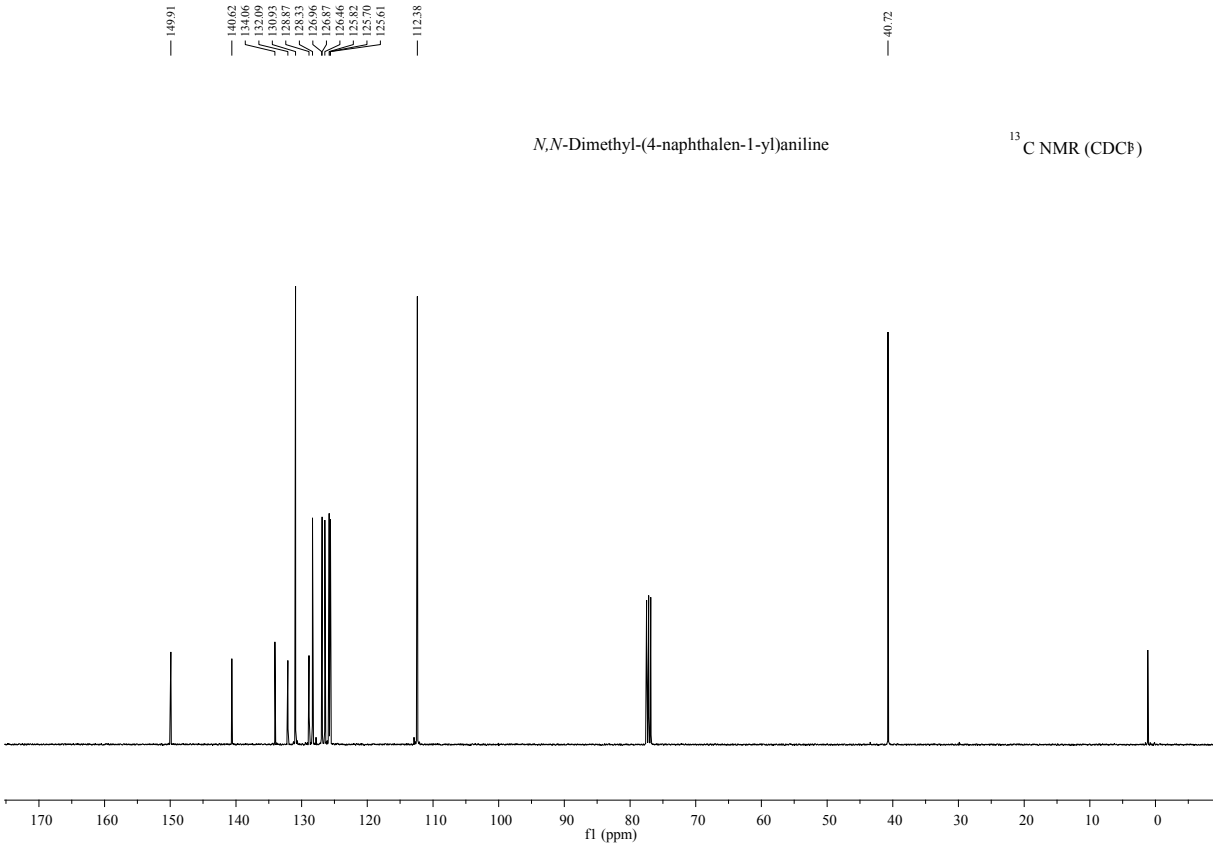
10. *N*,*N*-Dimethylbiphenyl-4-amine



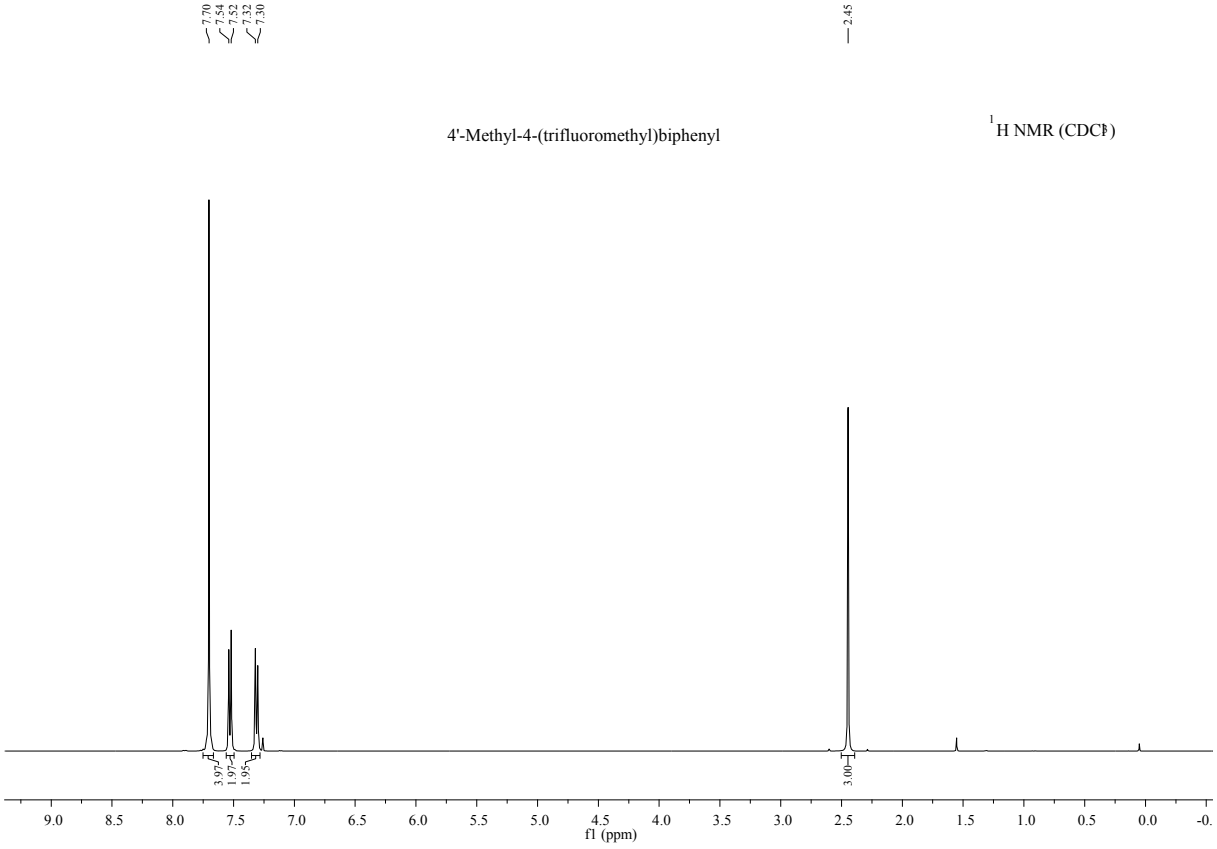


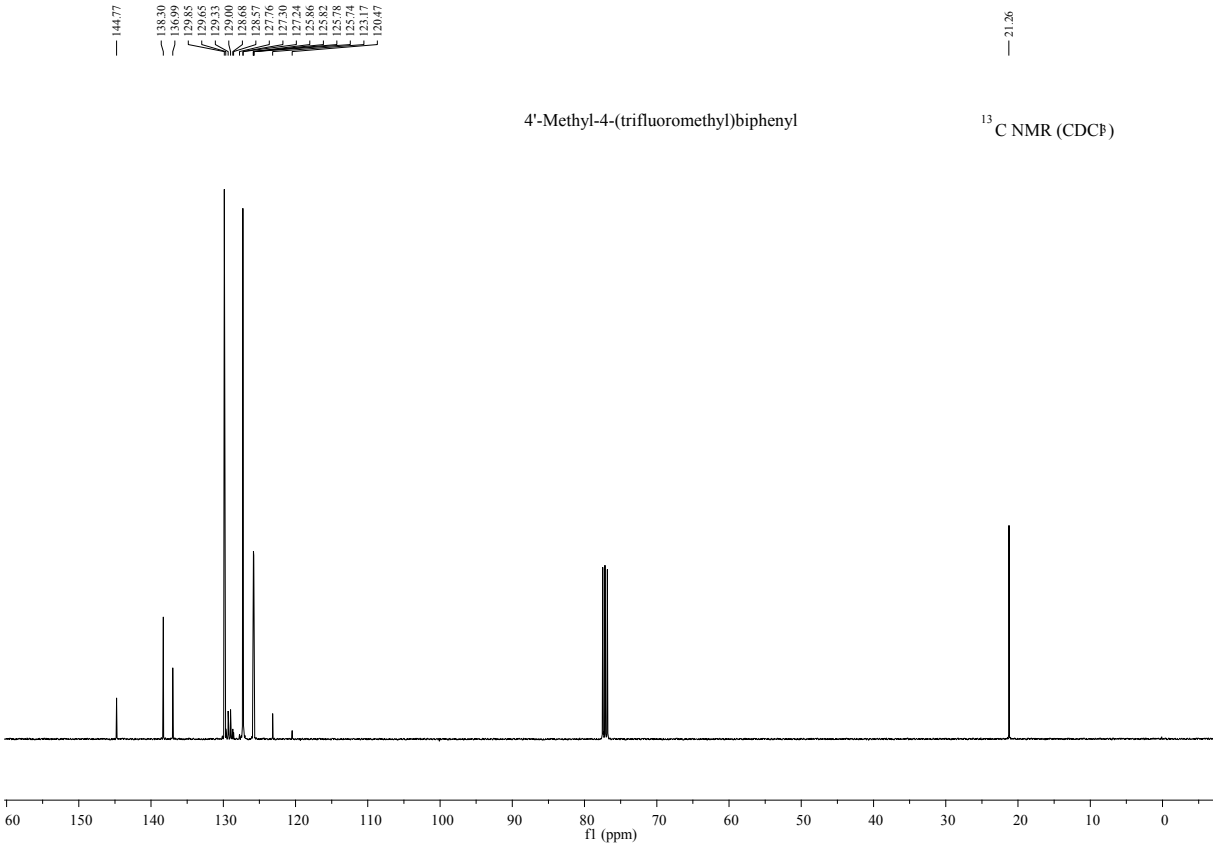
11. *N,N*-Dimethyl-(4-naphthalen-1-yl)aniline



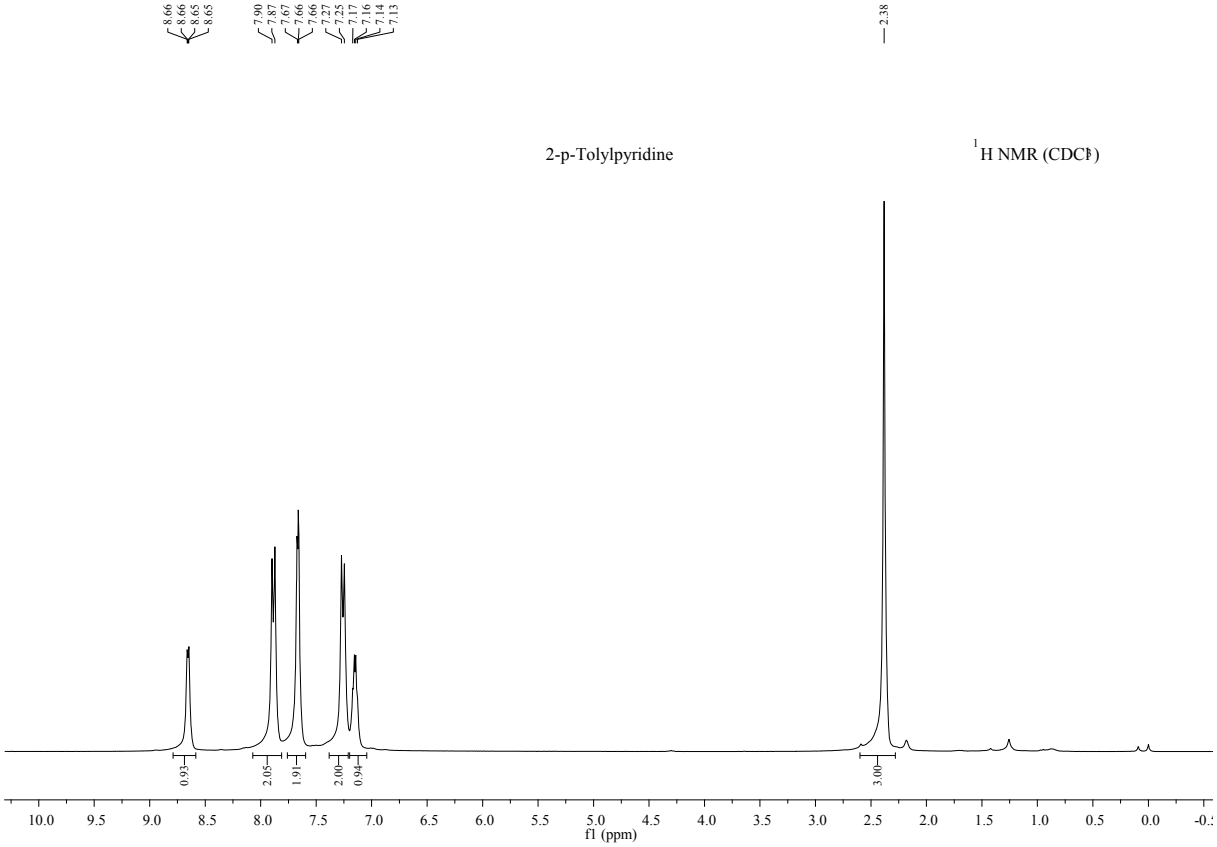


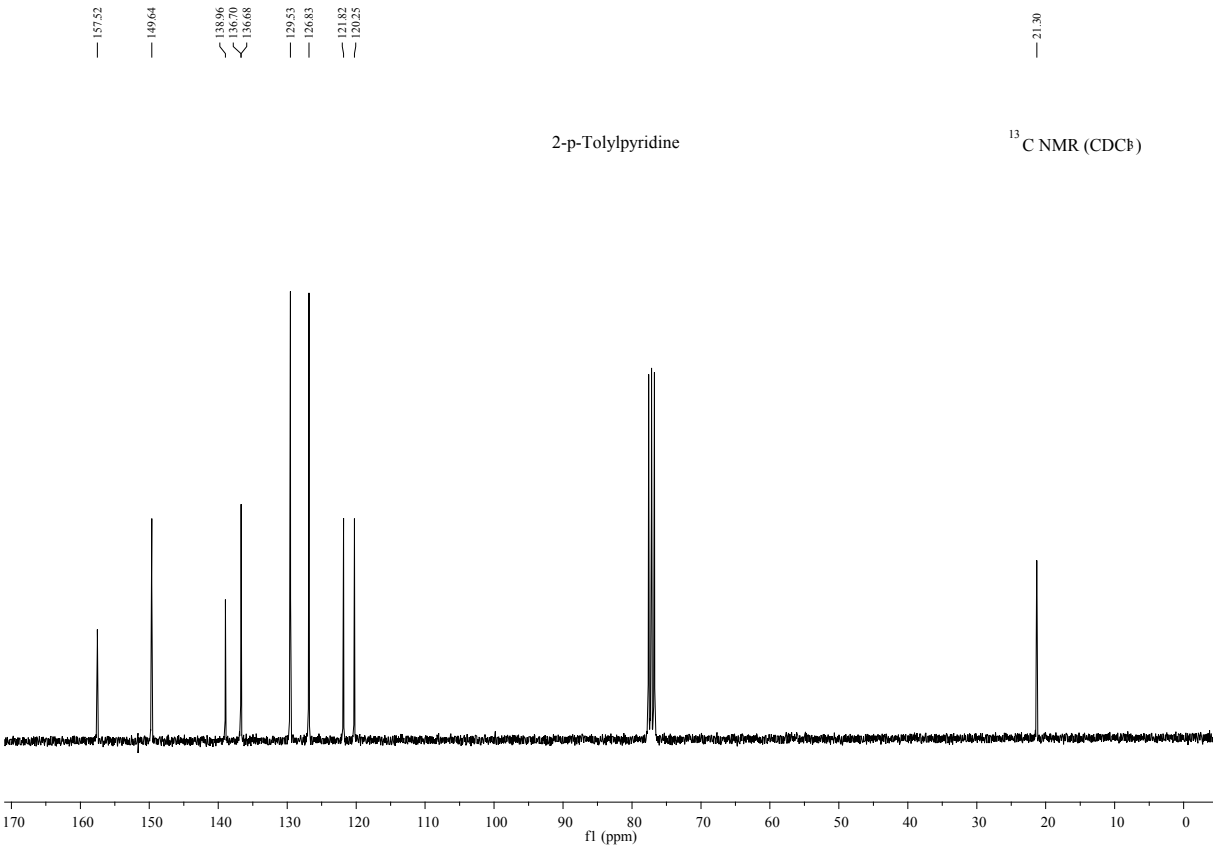
12. 4'-Methyl-4-(trifluoromethyl)biphenyl



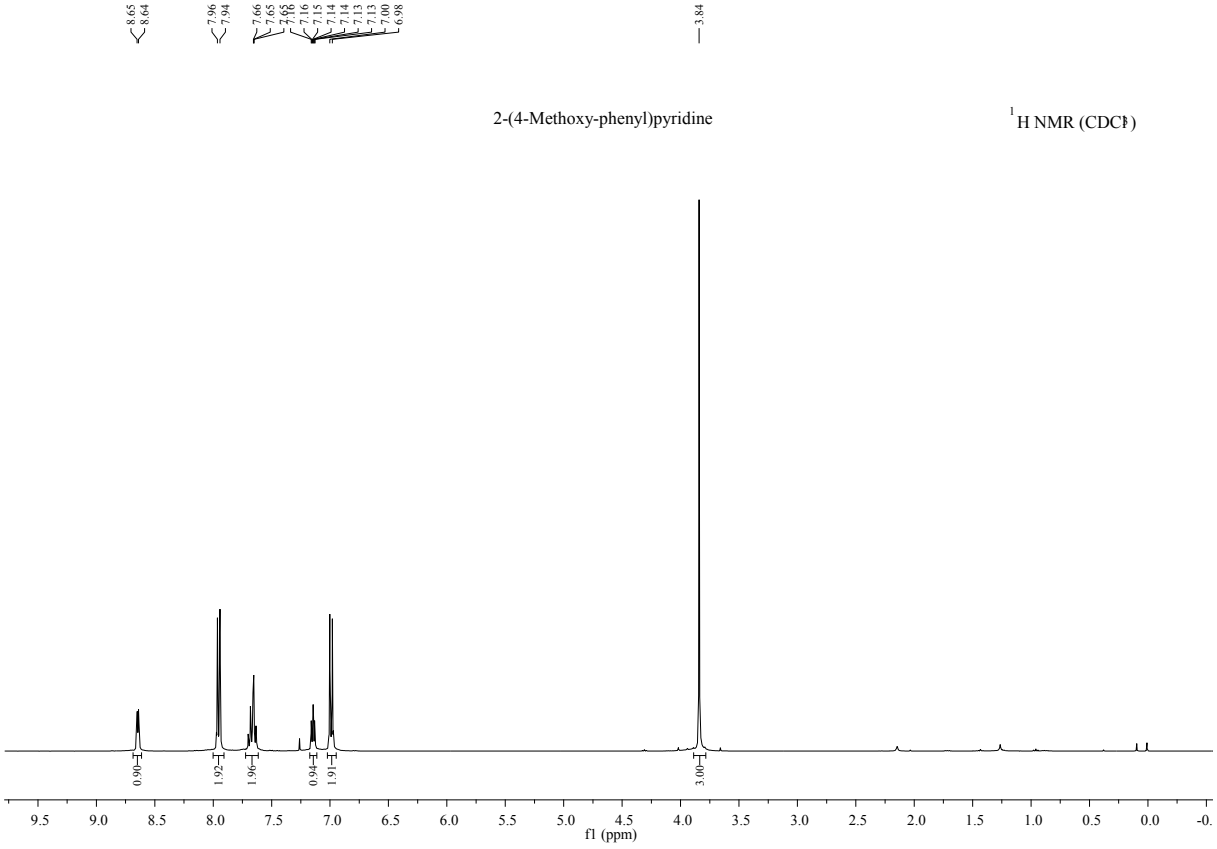


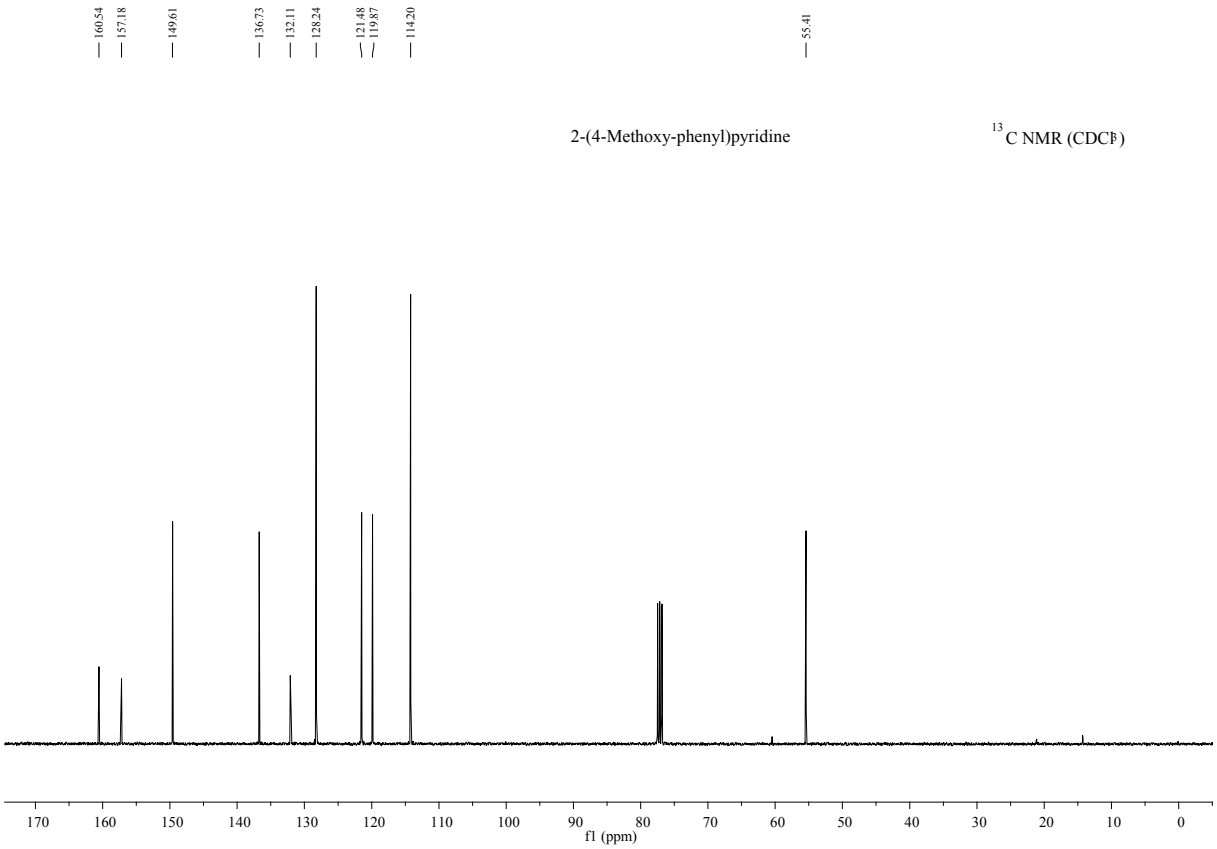
13. 2-p-Tolylpyridine



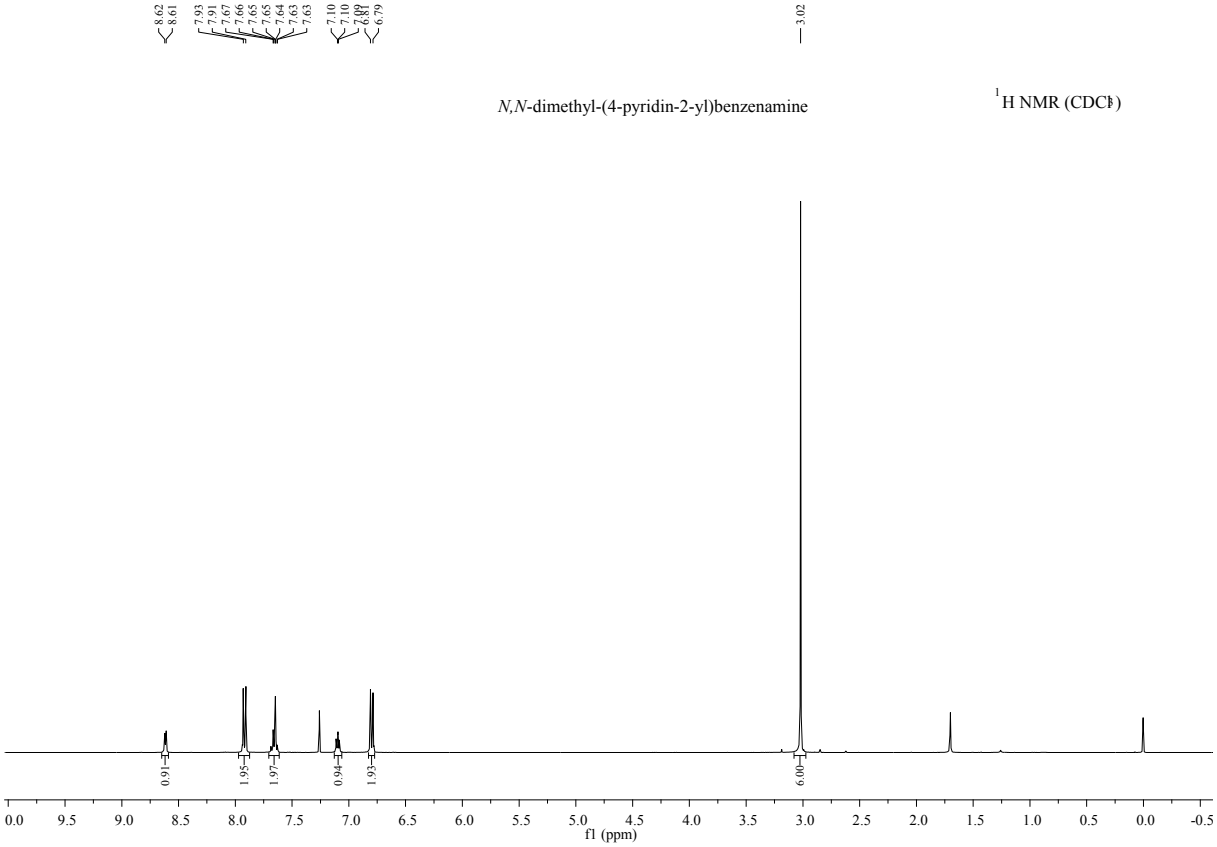


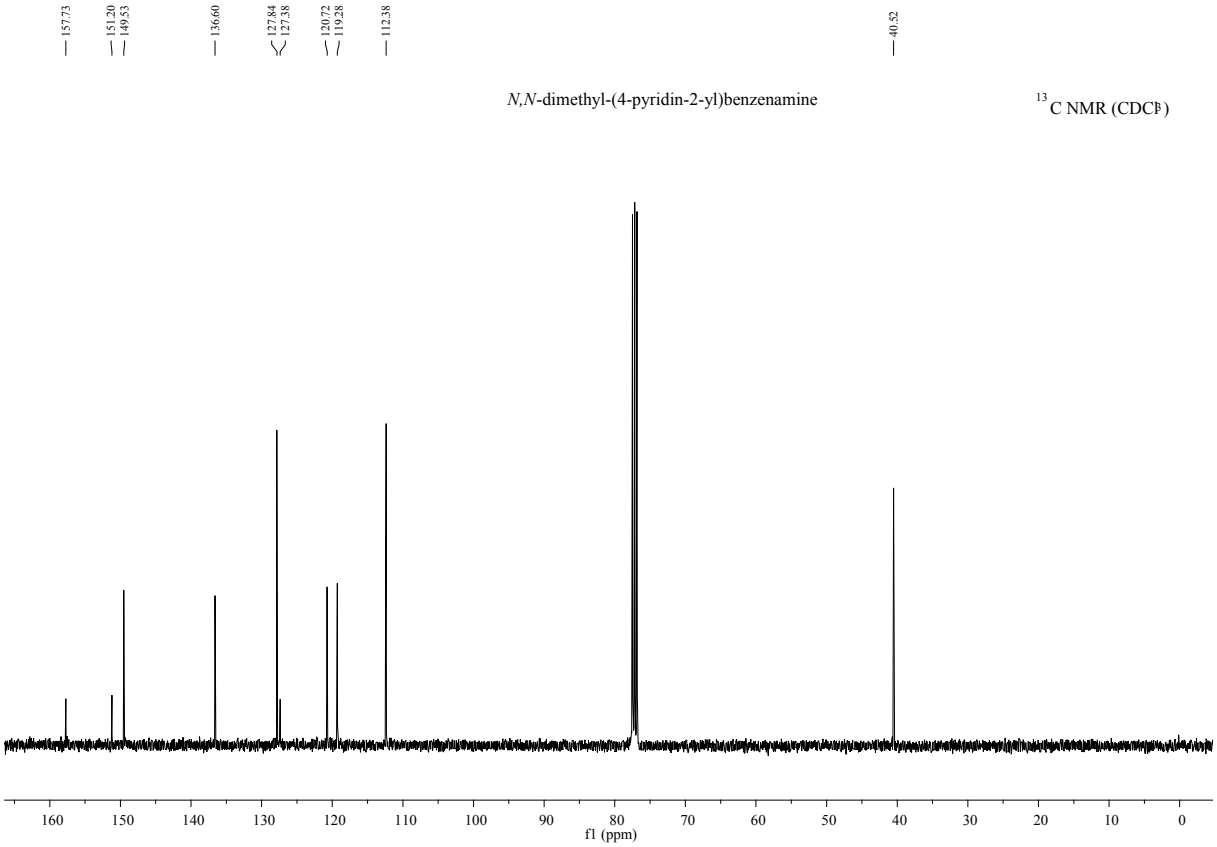
14. 2-(4-Methoxy-phenyl)pyridine



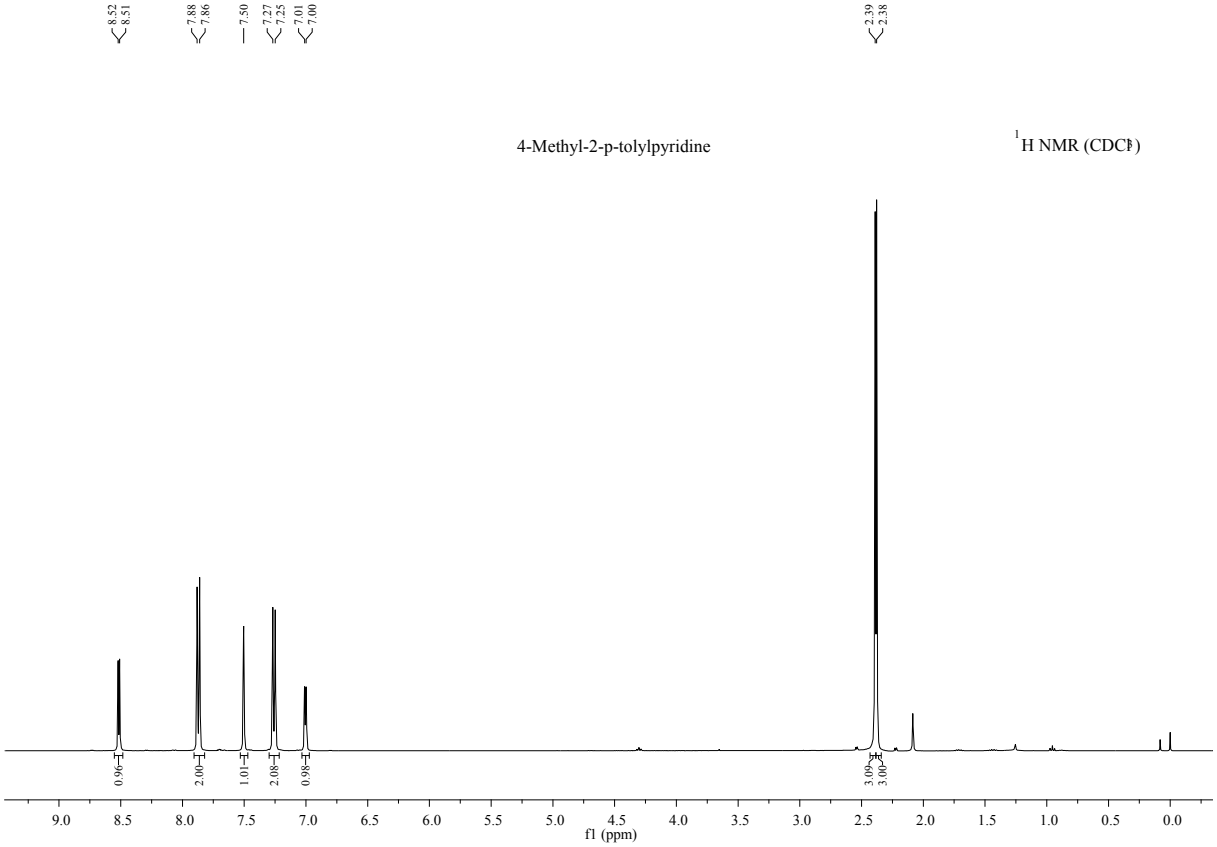


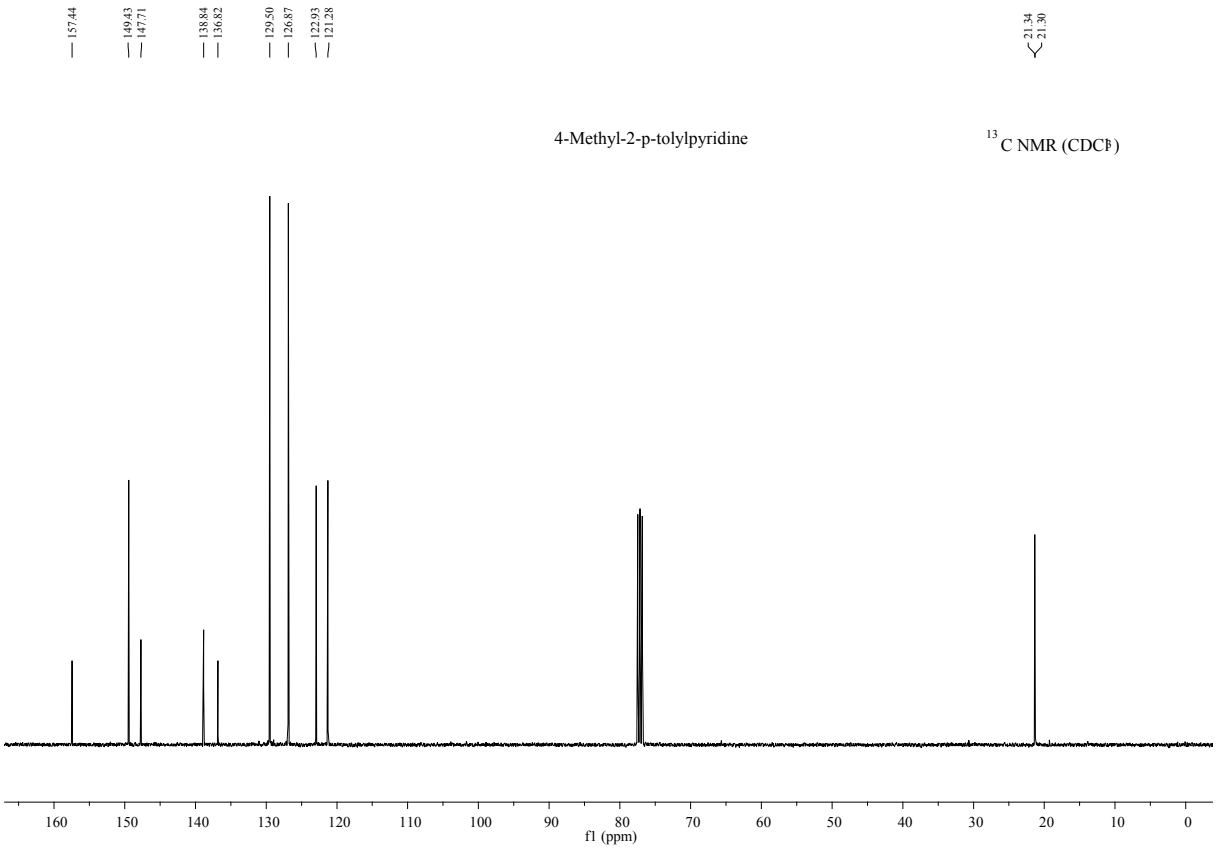
15. *N,N*-dimethyl-(4-pyridin-2-yl)benzenamine



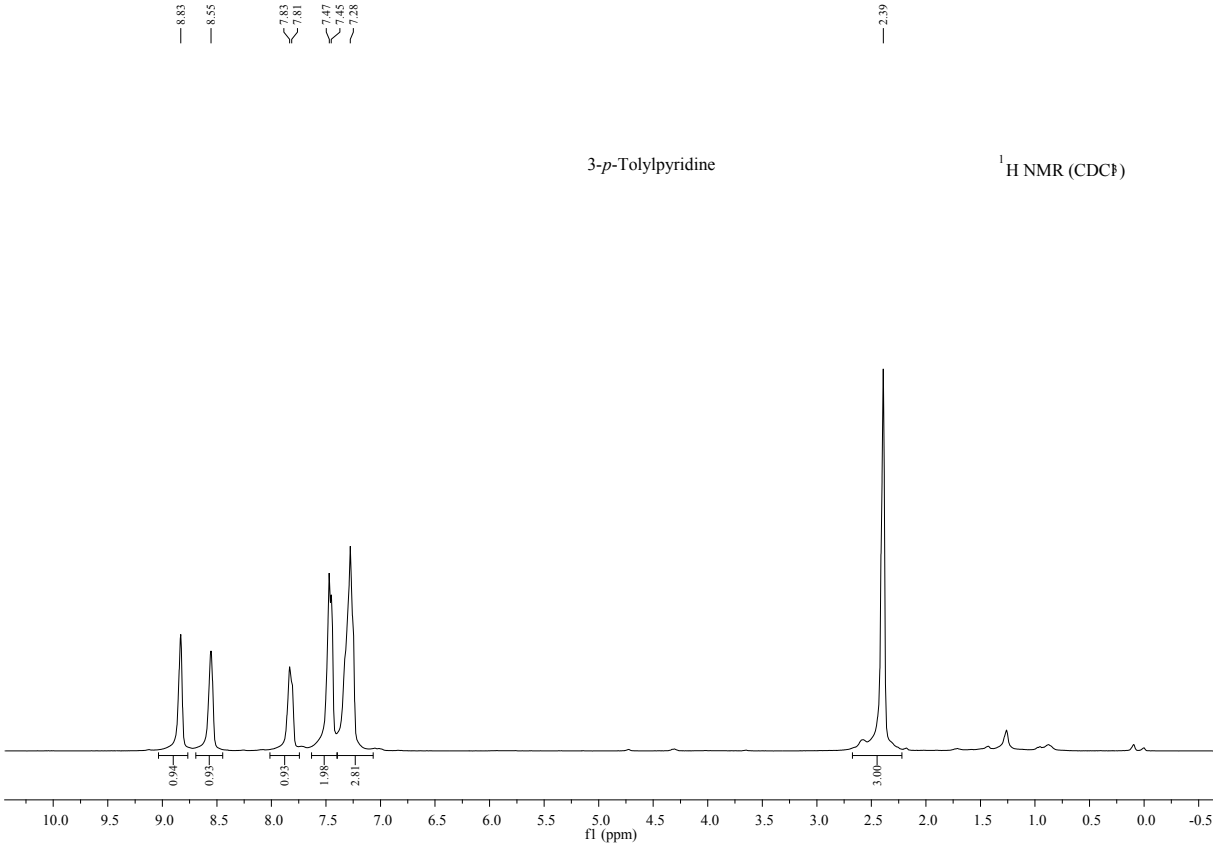


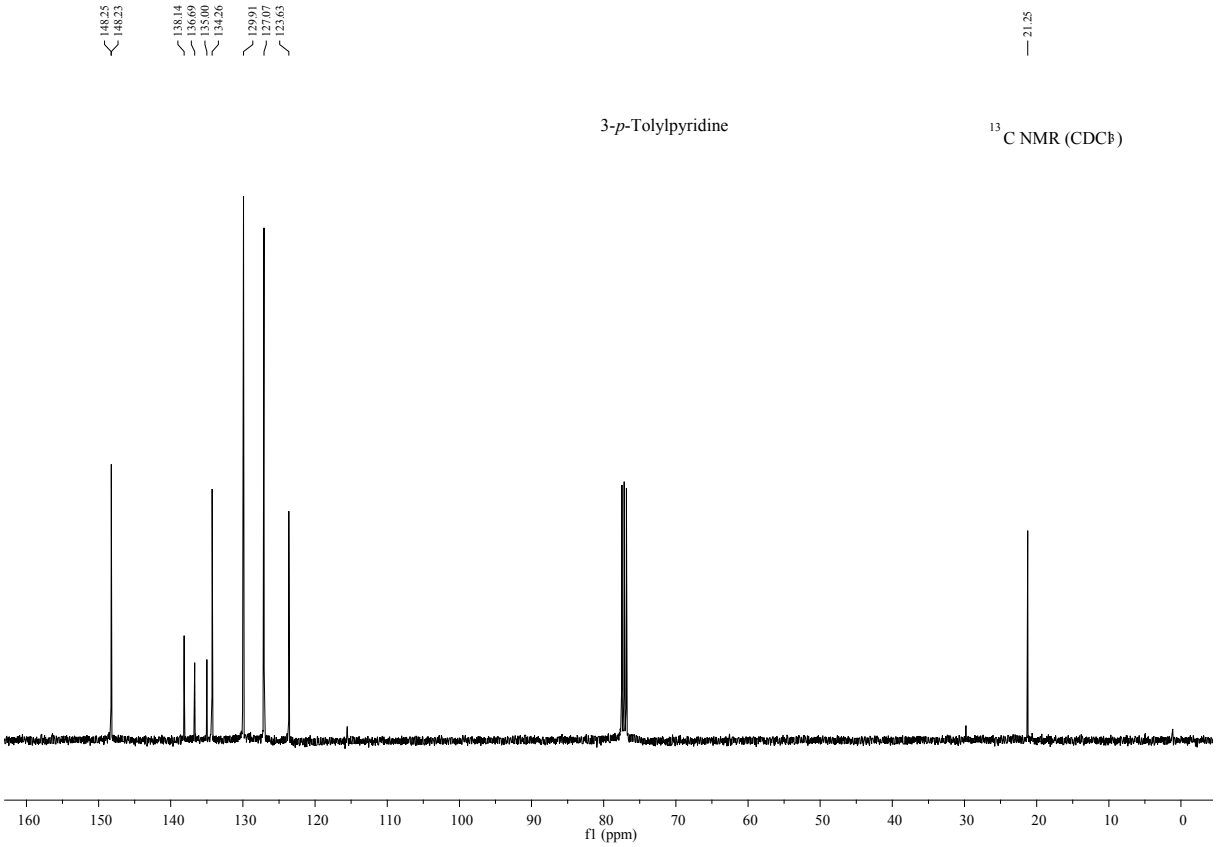
16. 4-Methyl-2-*p*-tolylpyridine



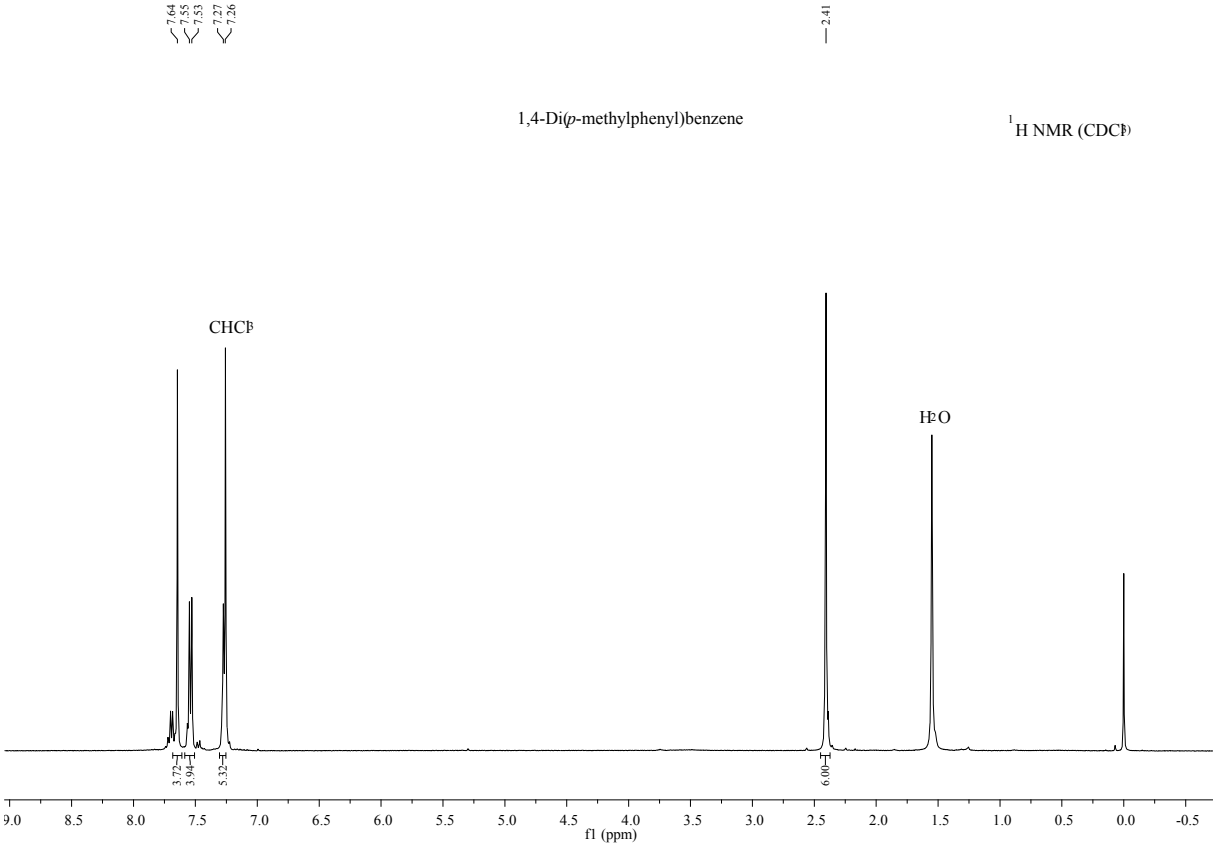


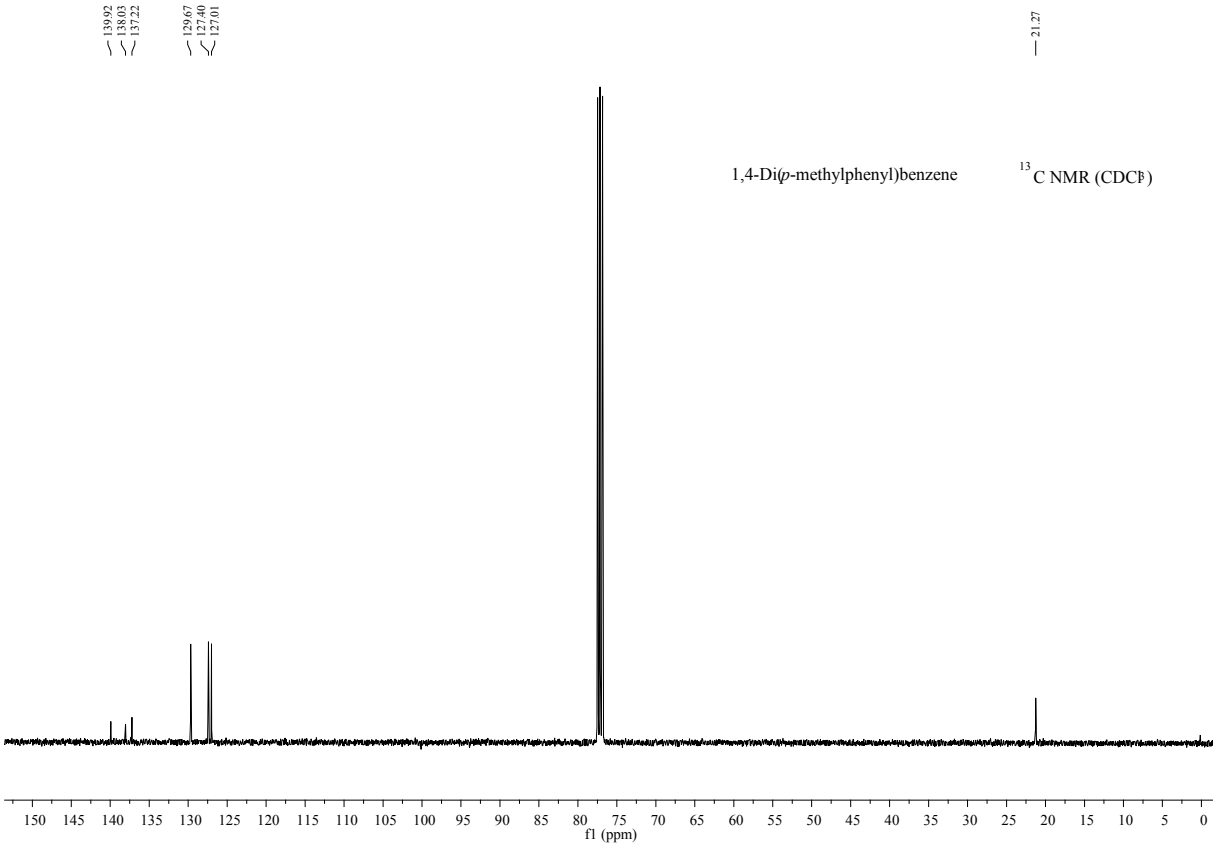
17. 3-*p*-Tolylpyridine



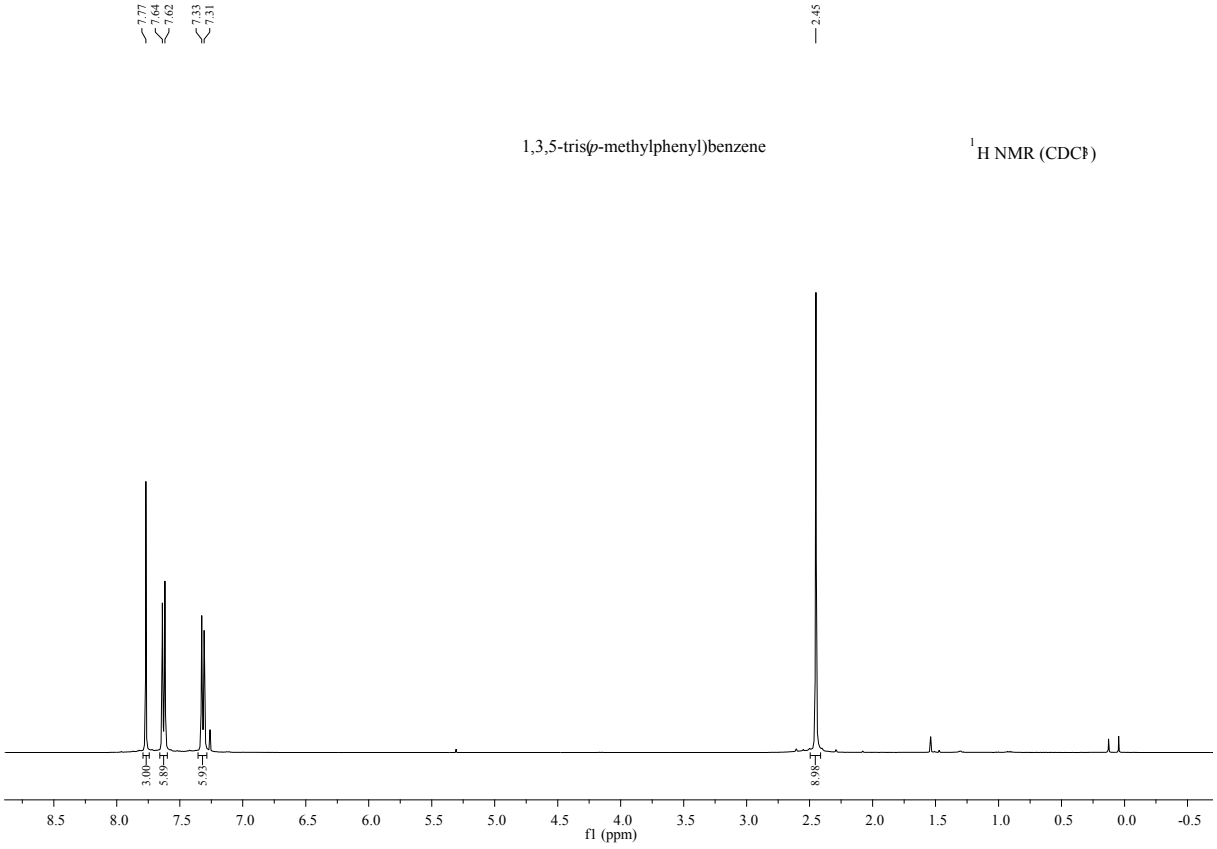


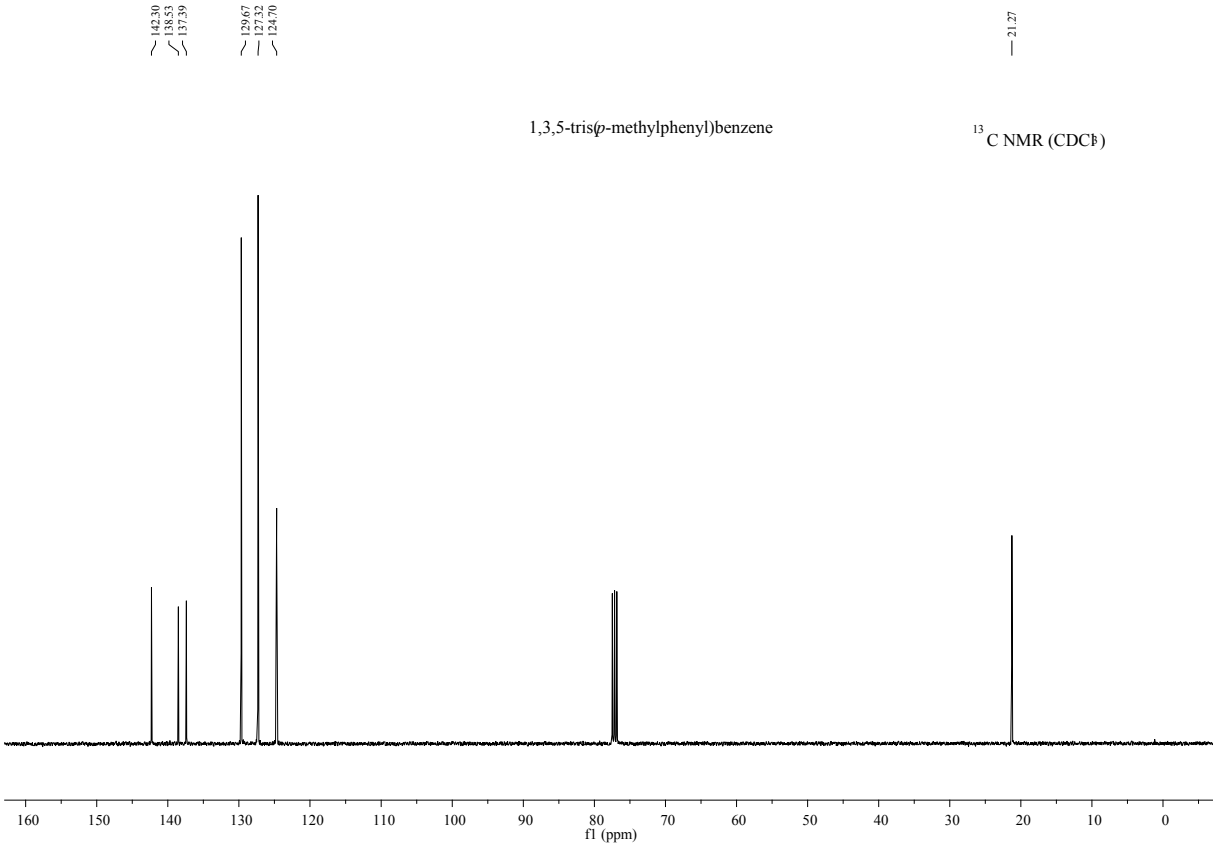
18. 1,4-Di(*p*-methylphenyl)benzene



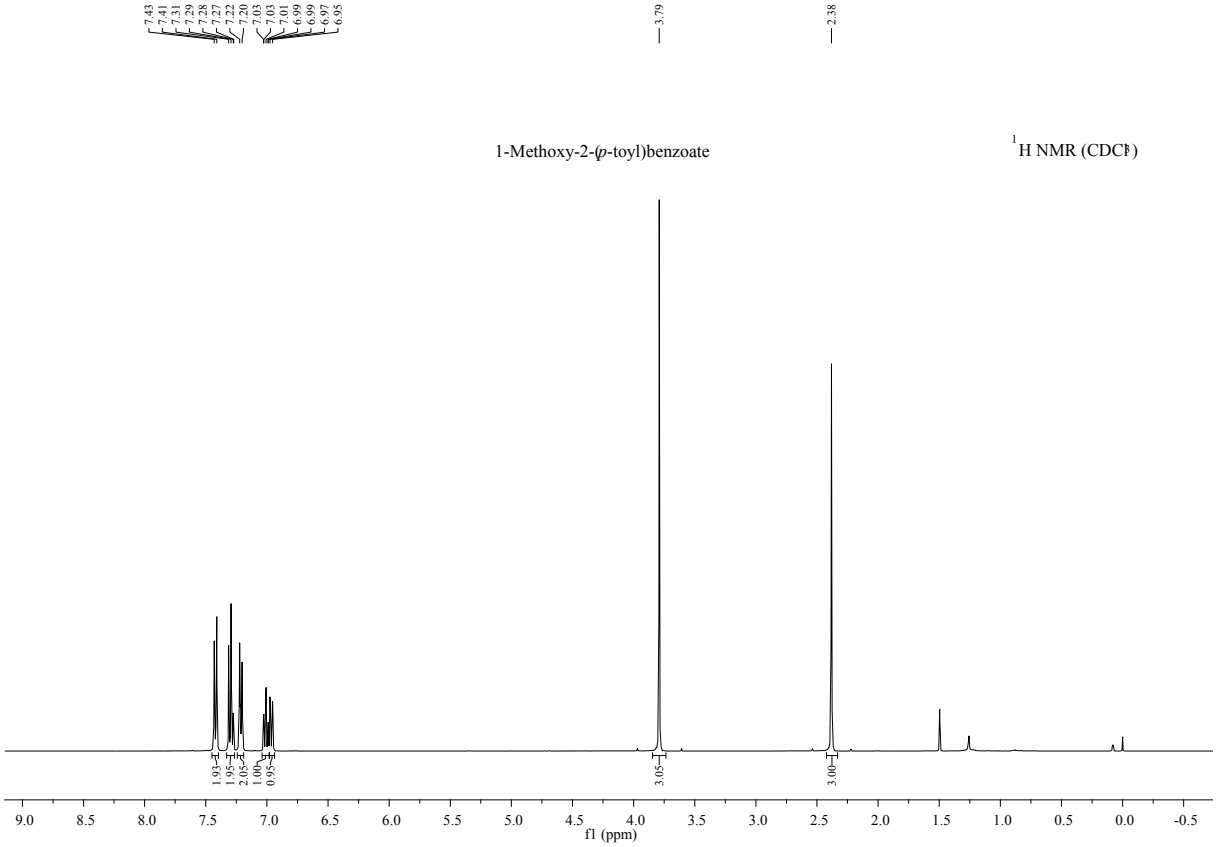


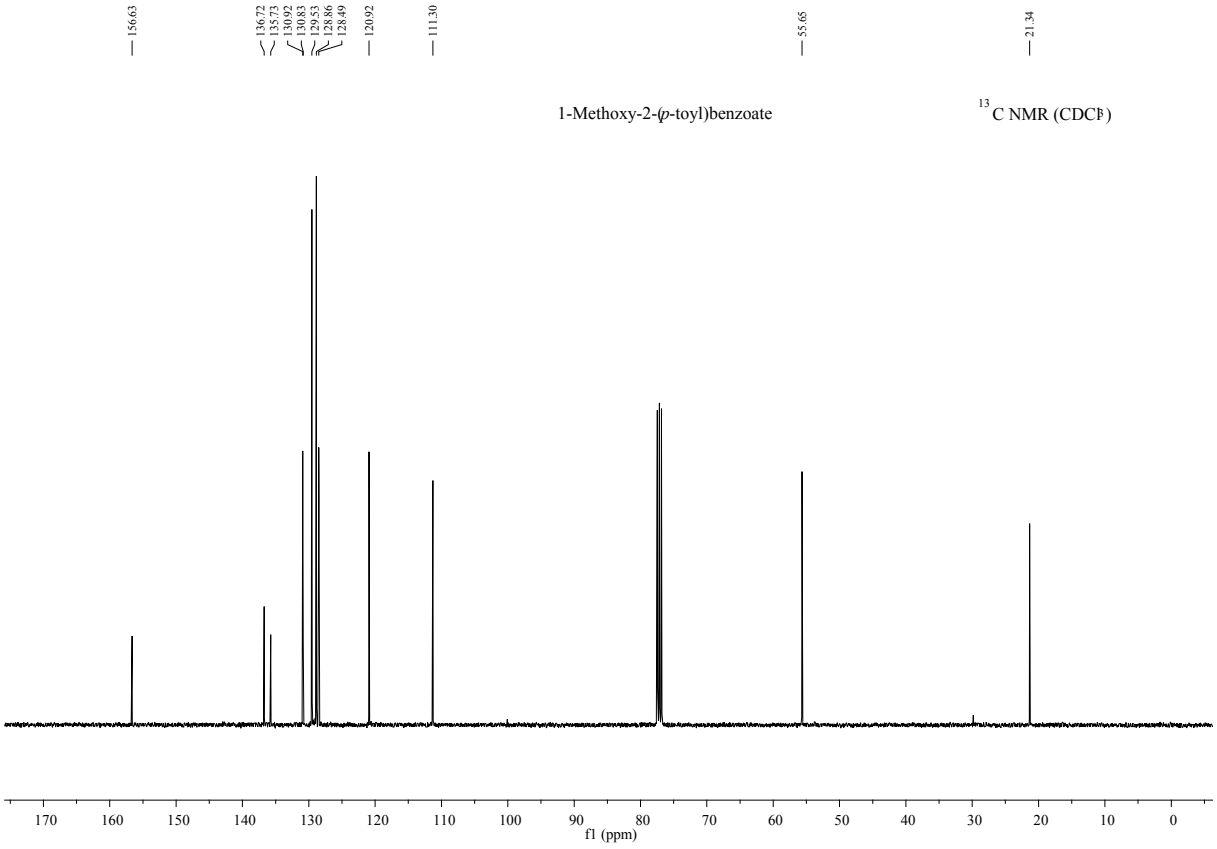
19. 1,3,5-tris(*p*-methylphenyl)benzene



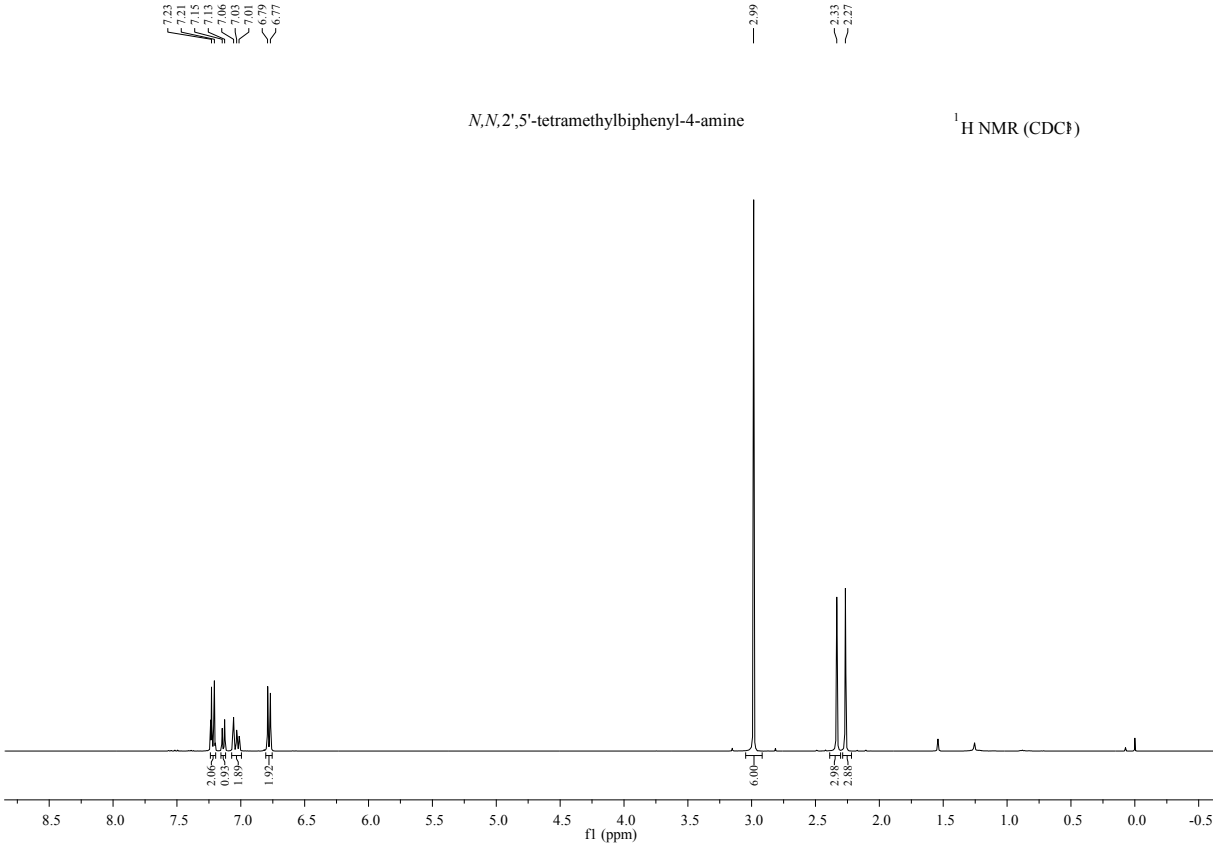


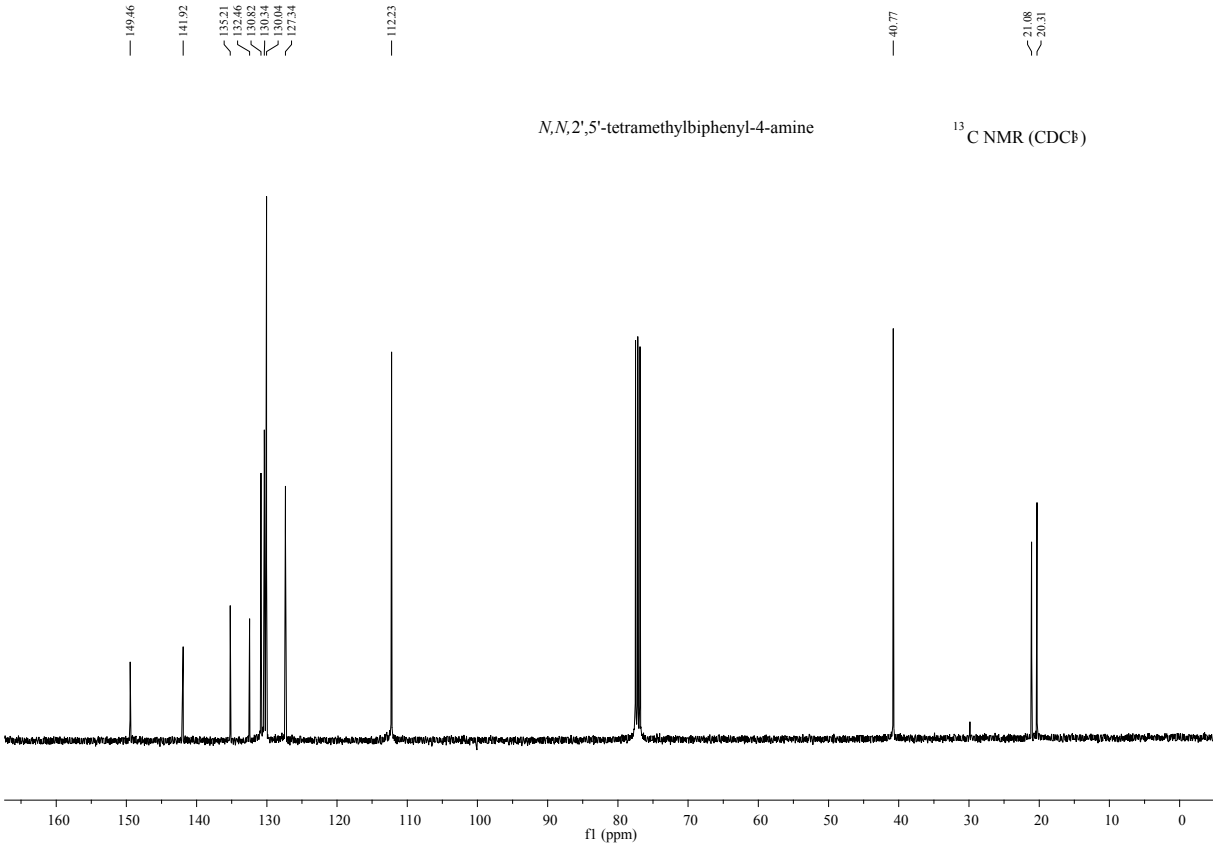
20. 1-Methoxy-2-(*p*-toyl)benzoate



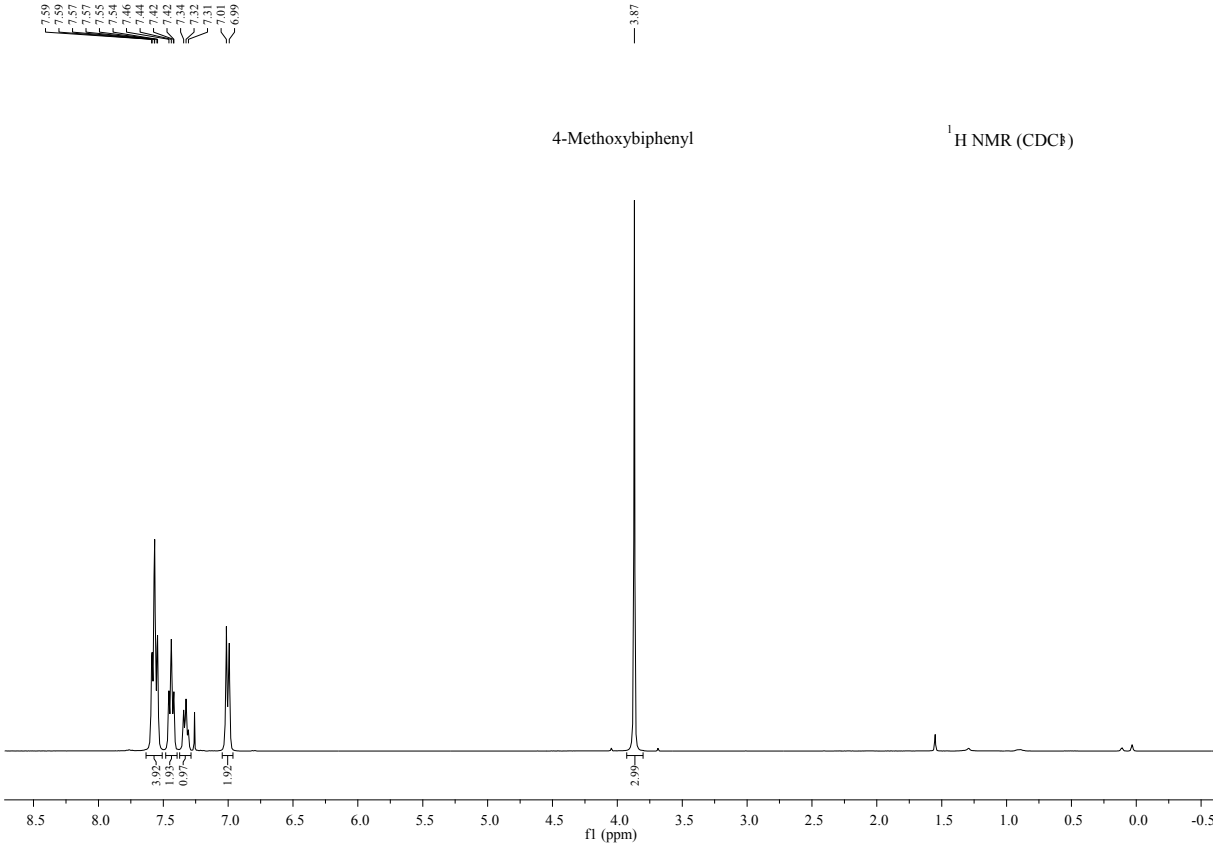


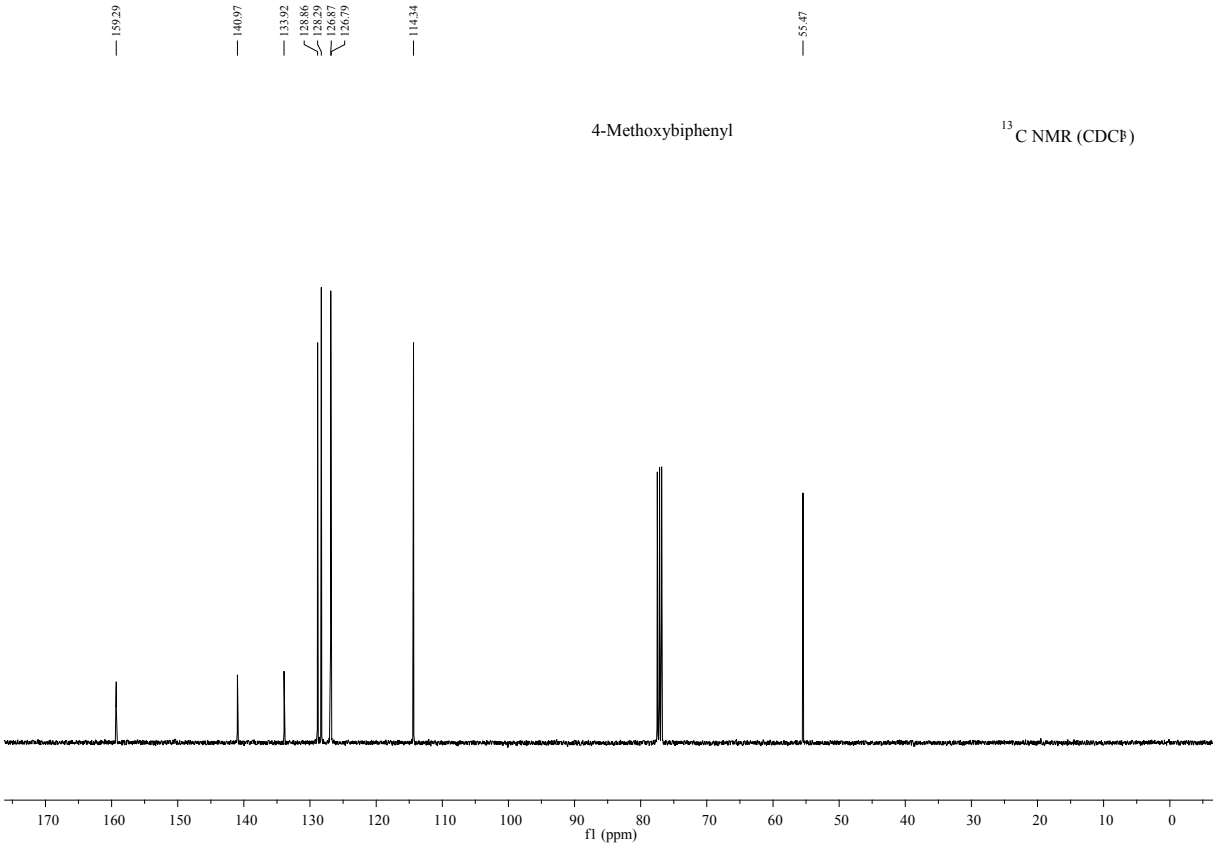
21. *N,N*,2',5'-tetramethylbiphenyl-4-amine



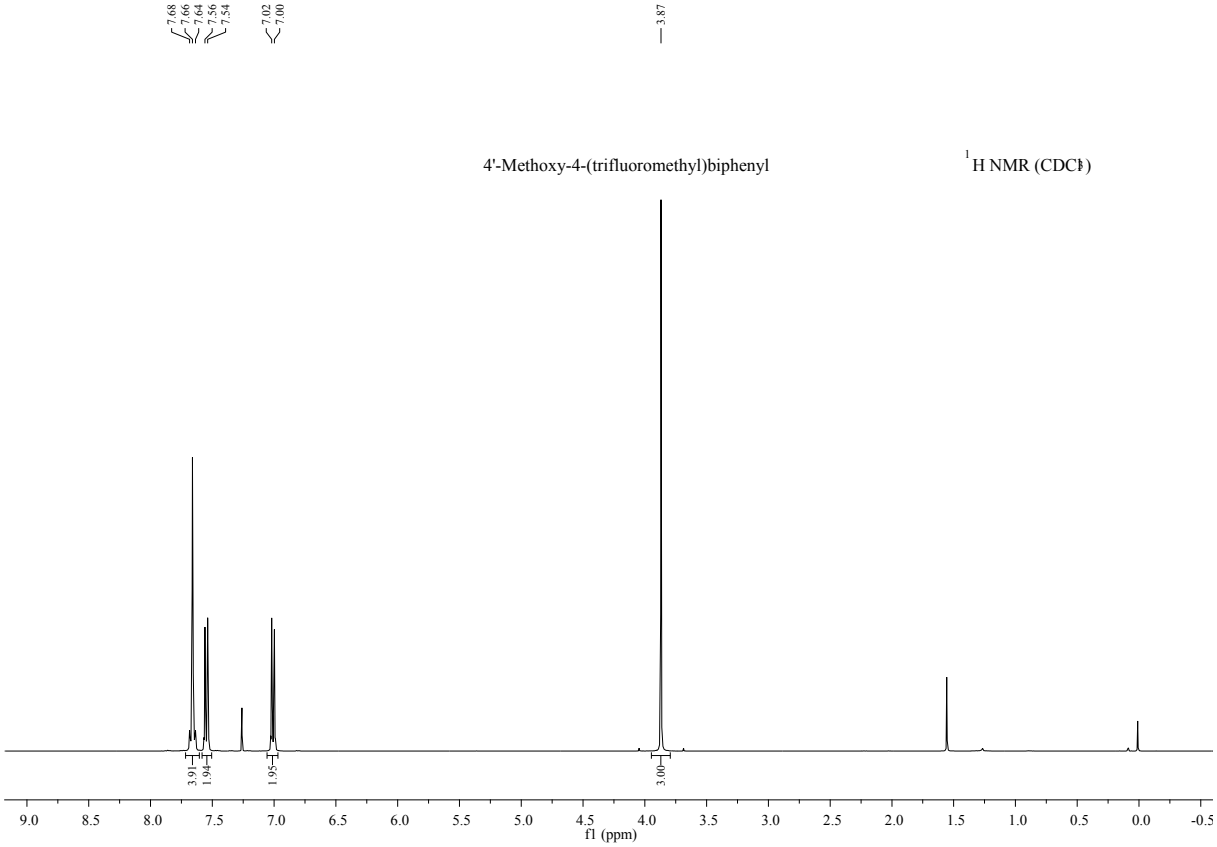


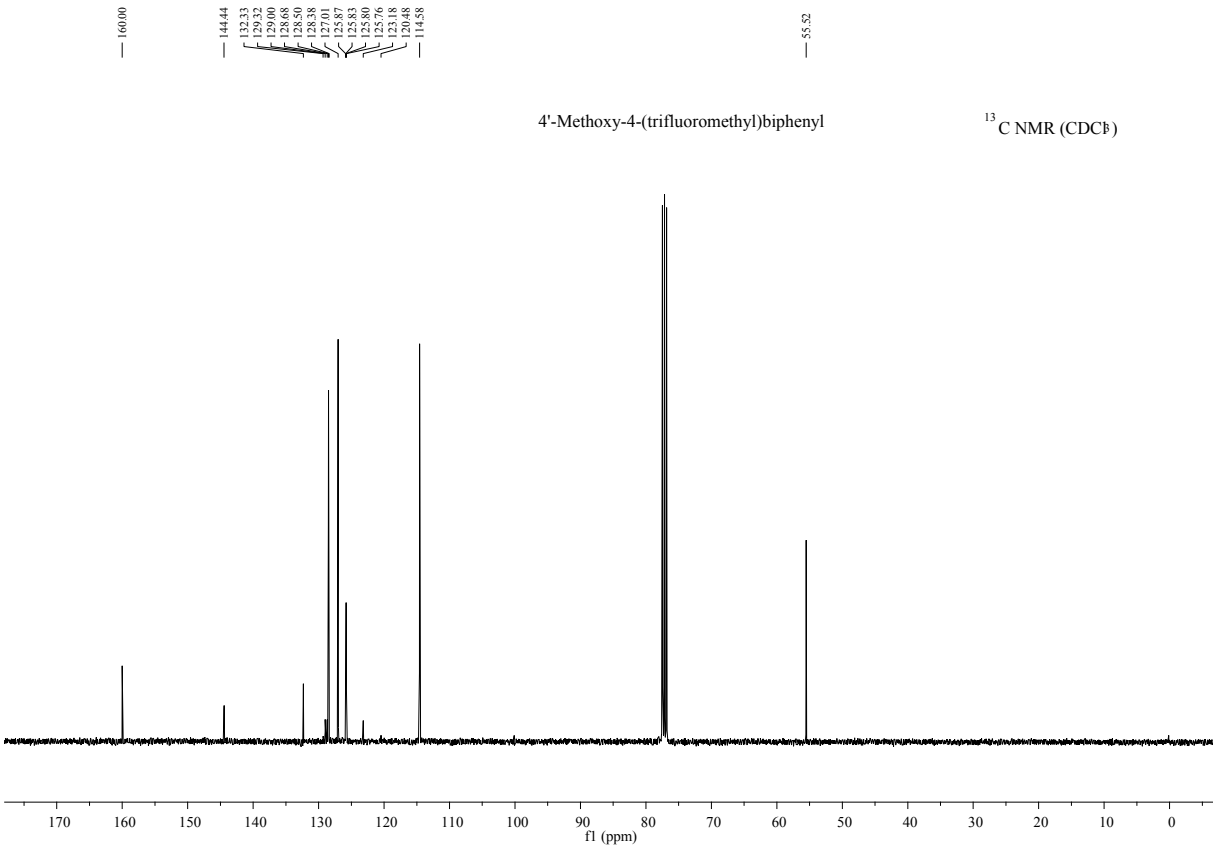
22. 4-Methoxybiphenyl



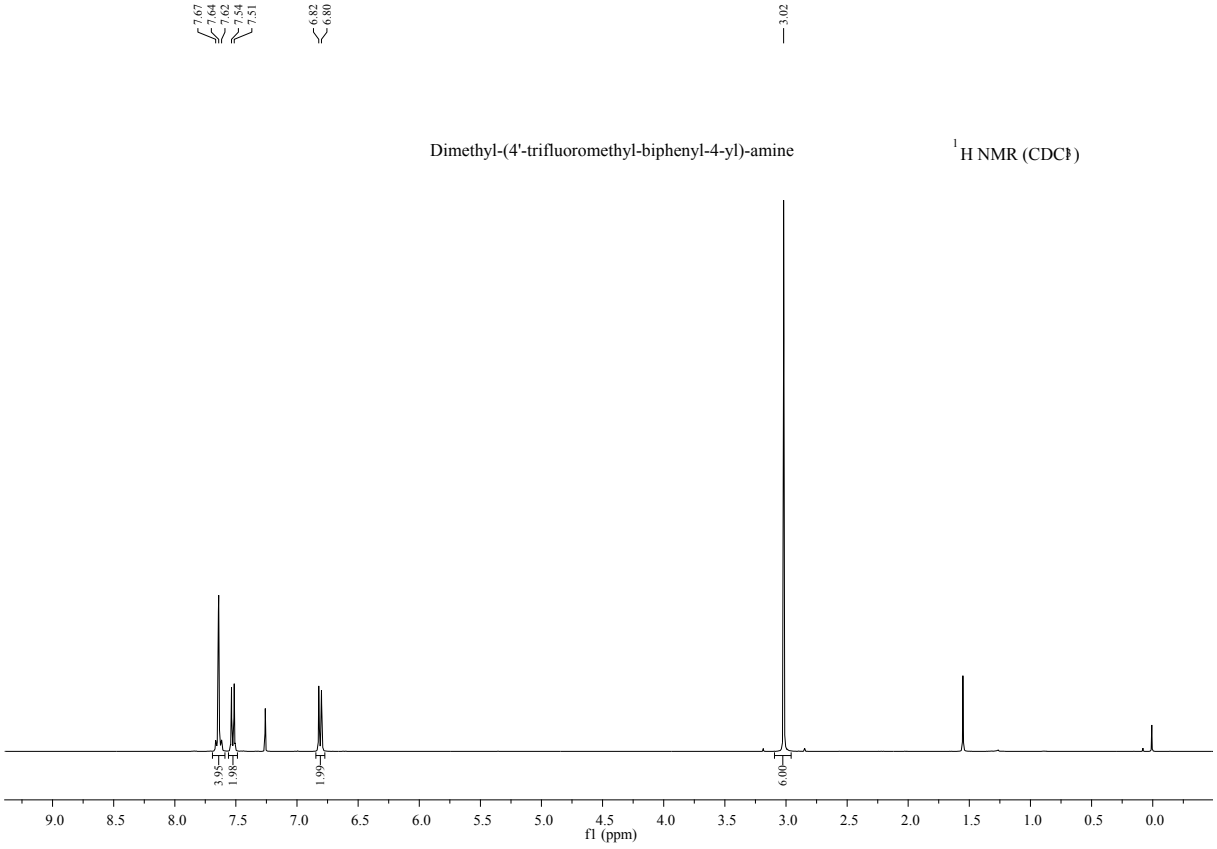


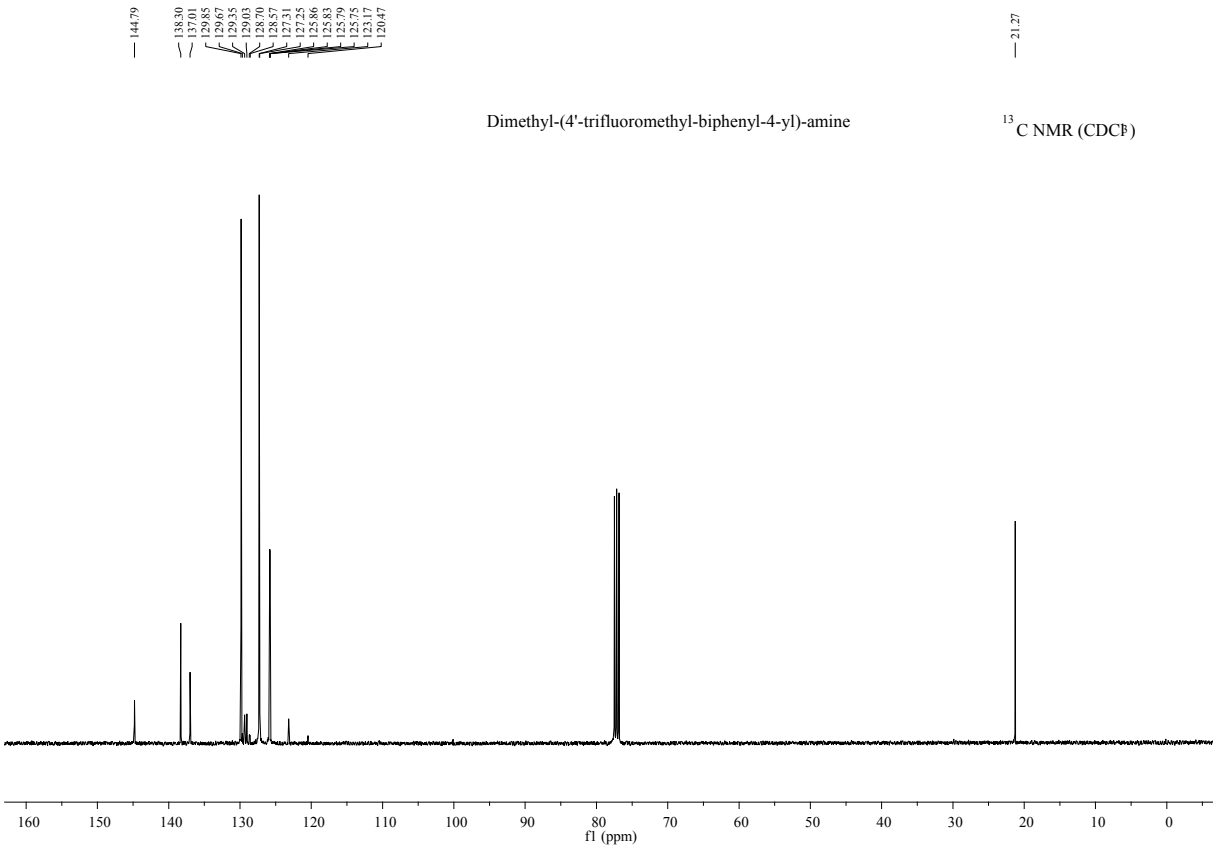
23. 4'-Methoxy-4-(trifluoromethyl)biphenyl



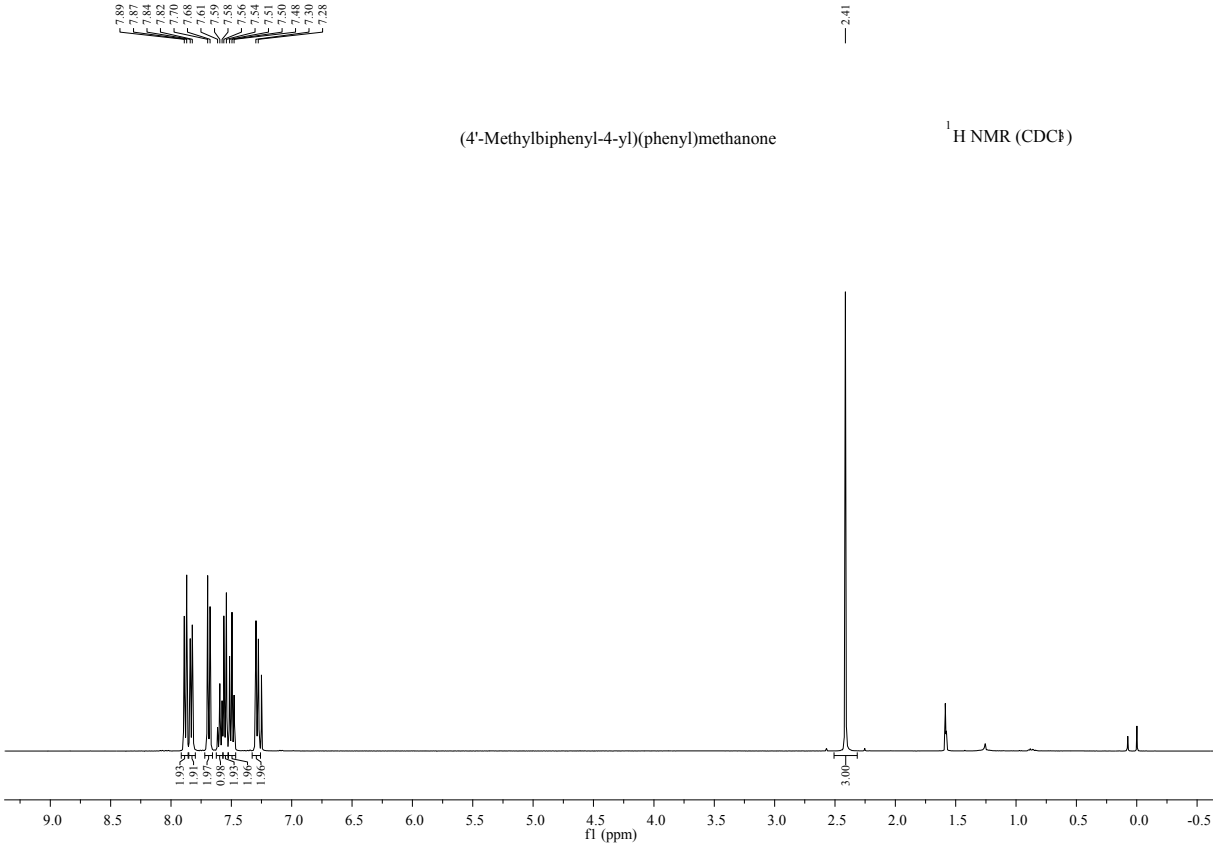


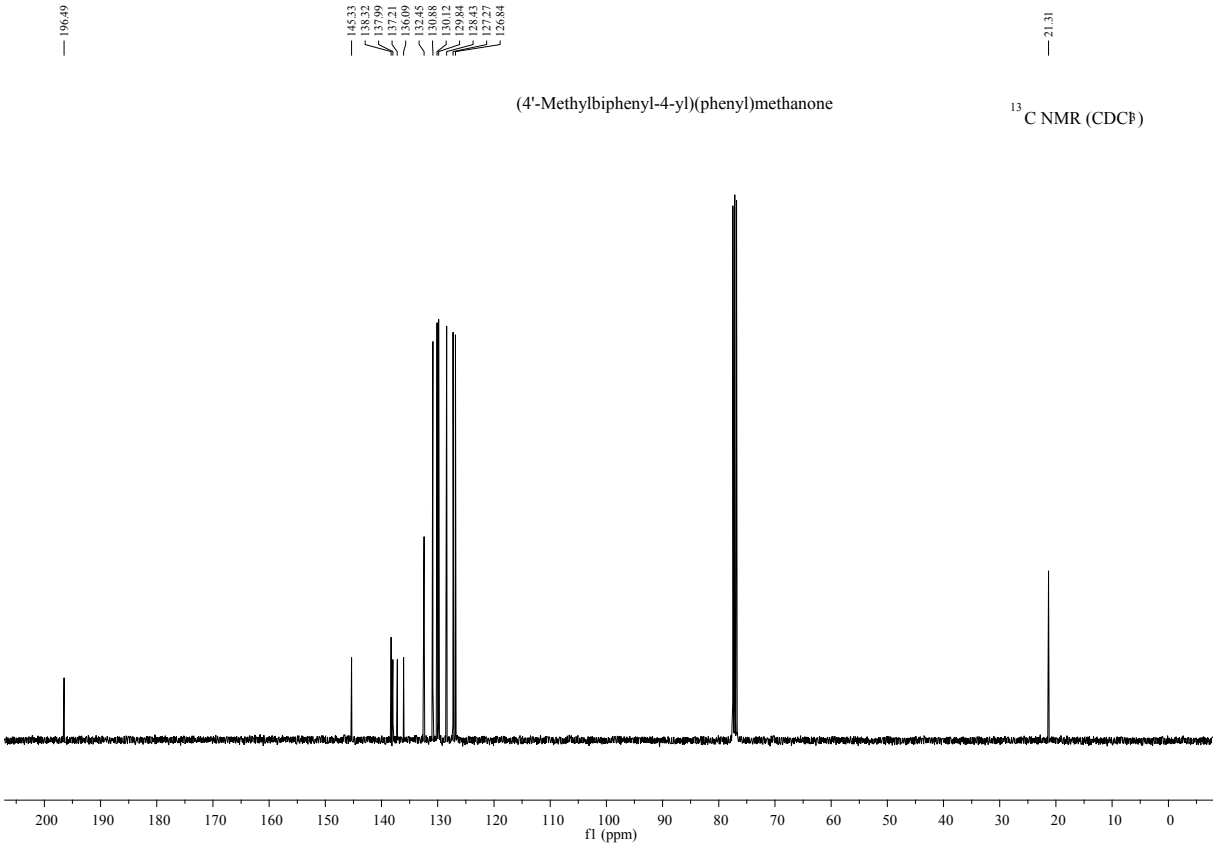
24. Dimethyl-(4'-trifluoromethylbiphenyl-4-yl)amine



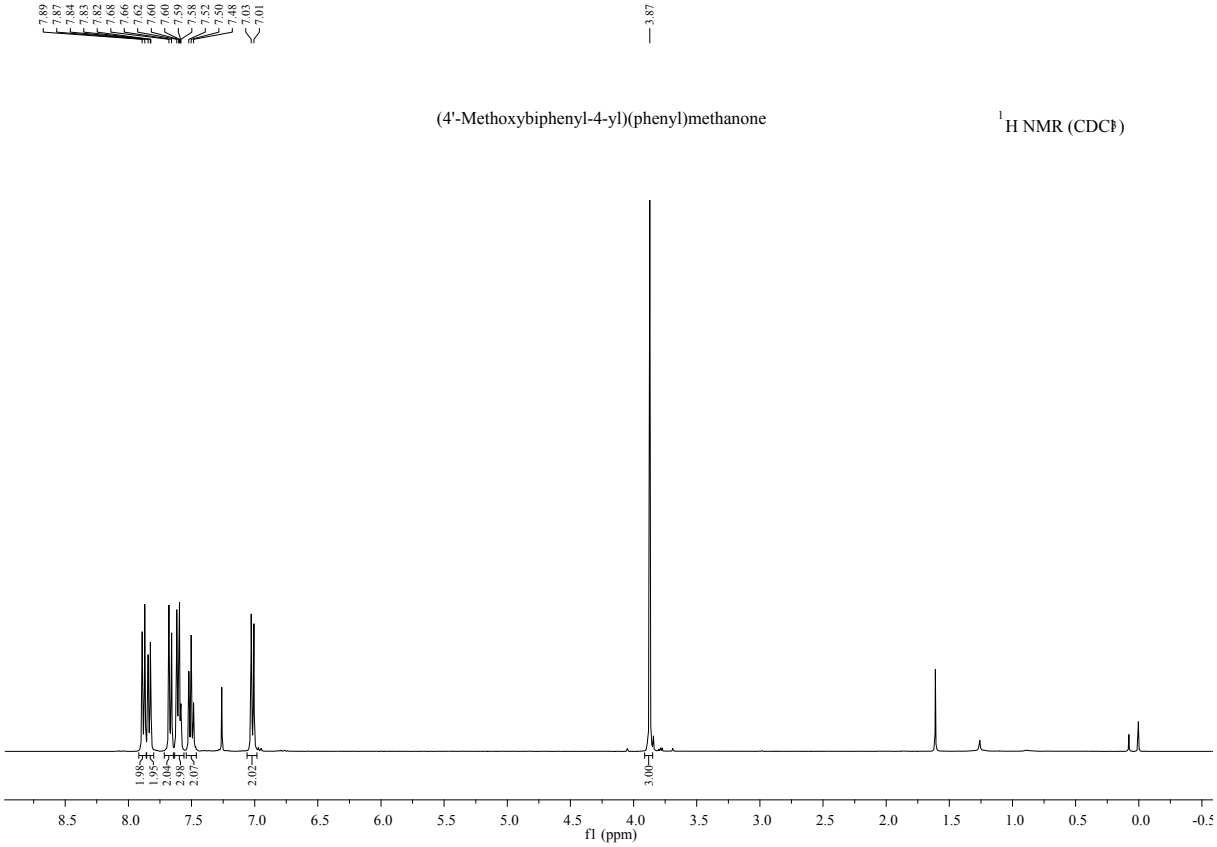


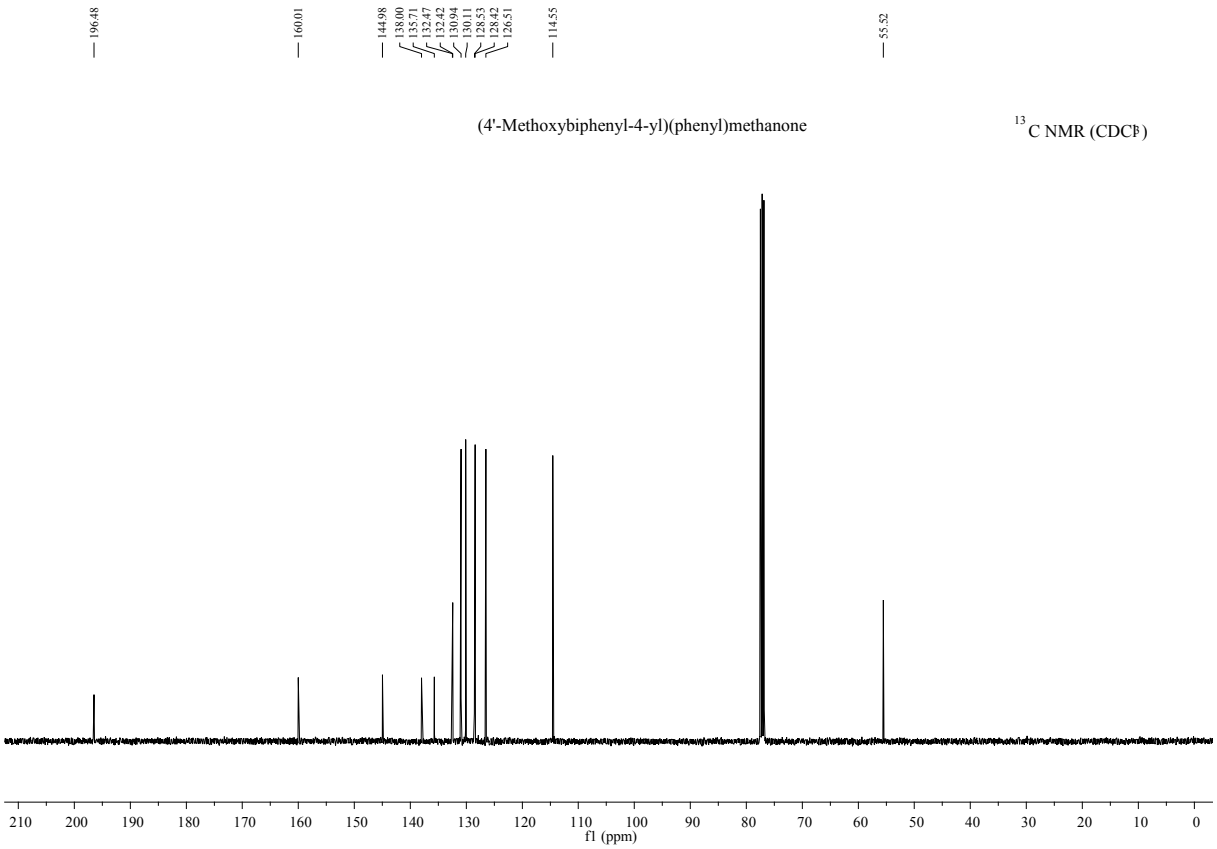
25. (4'-Methylbiphenyl-4-yl)(phenyl)methanone



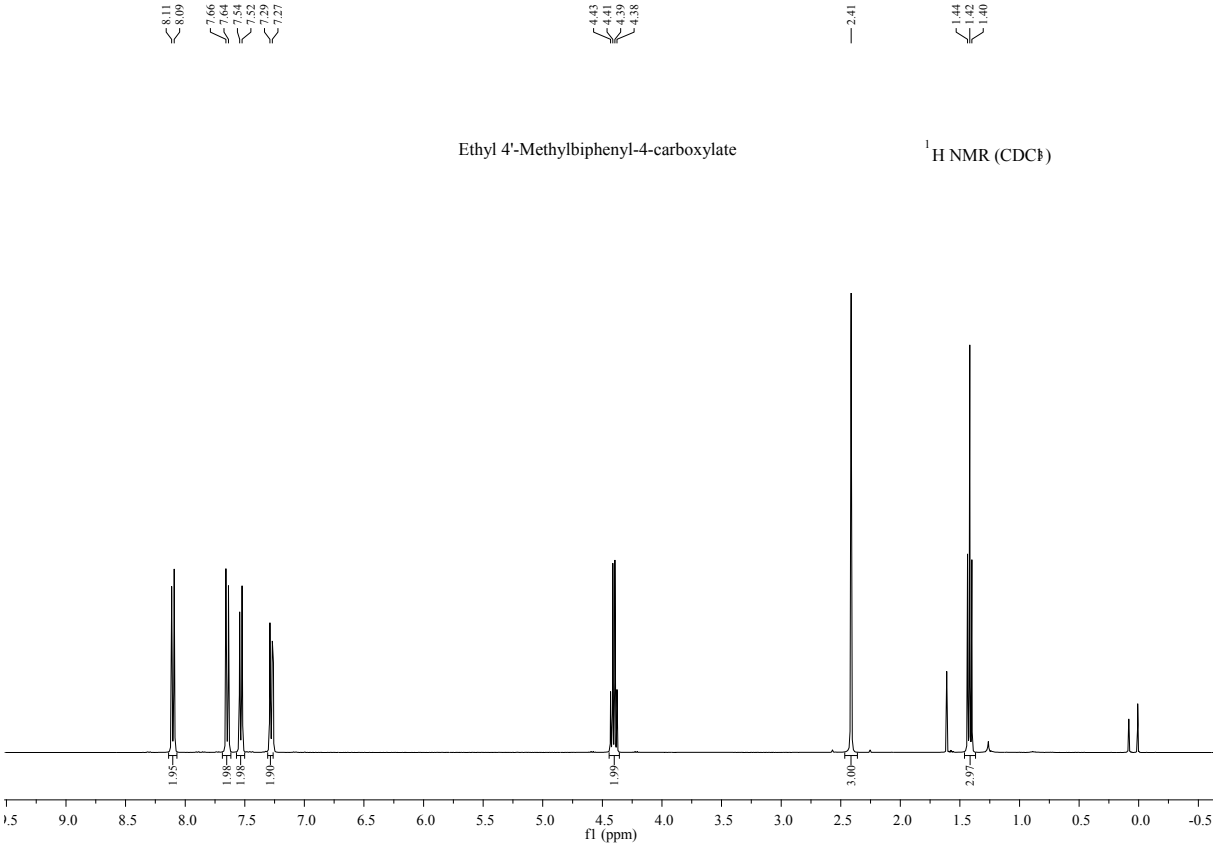


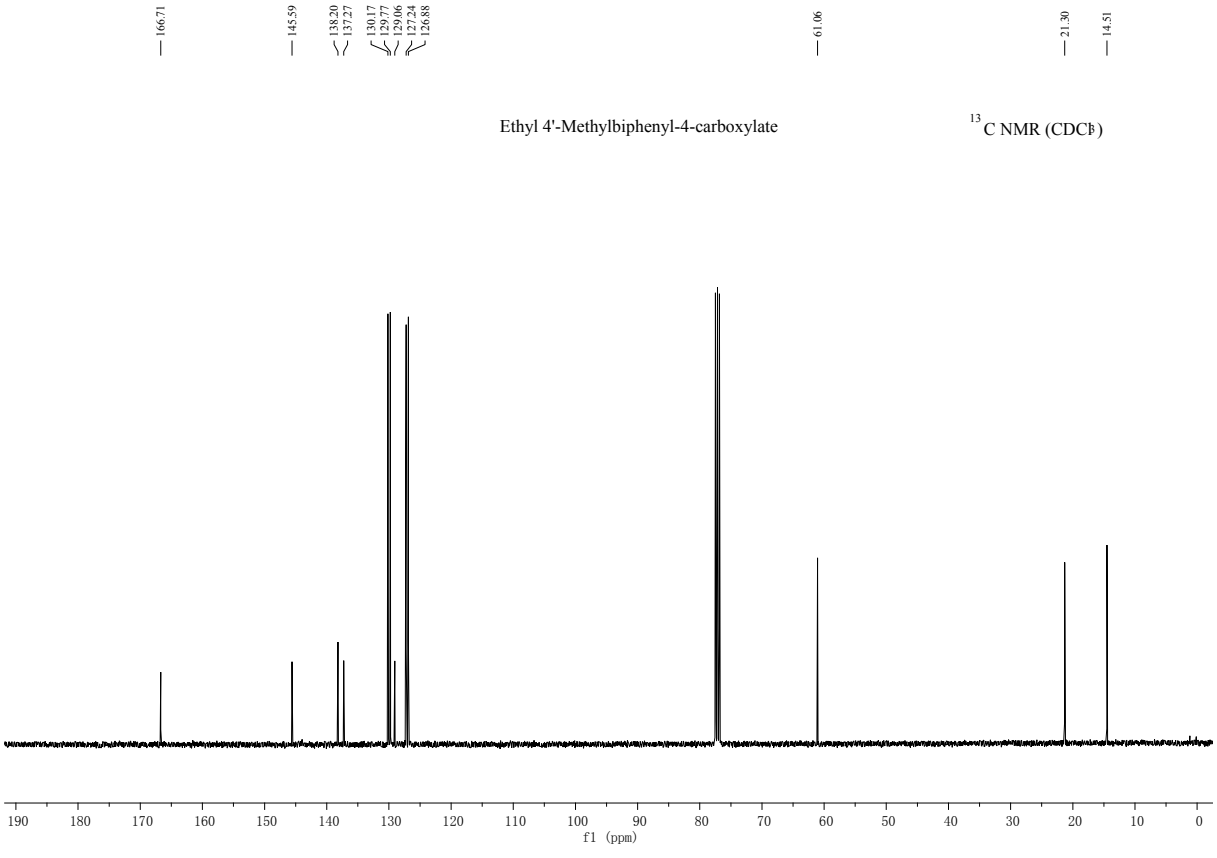
26. (4'-Methoxybiphenyl-4-yl)(phenyl)methanone



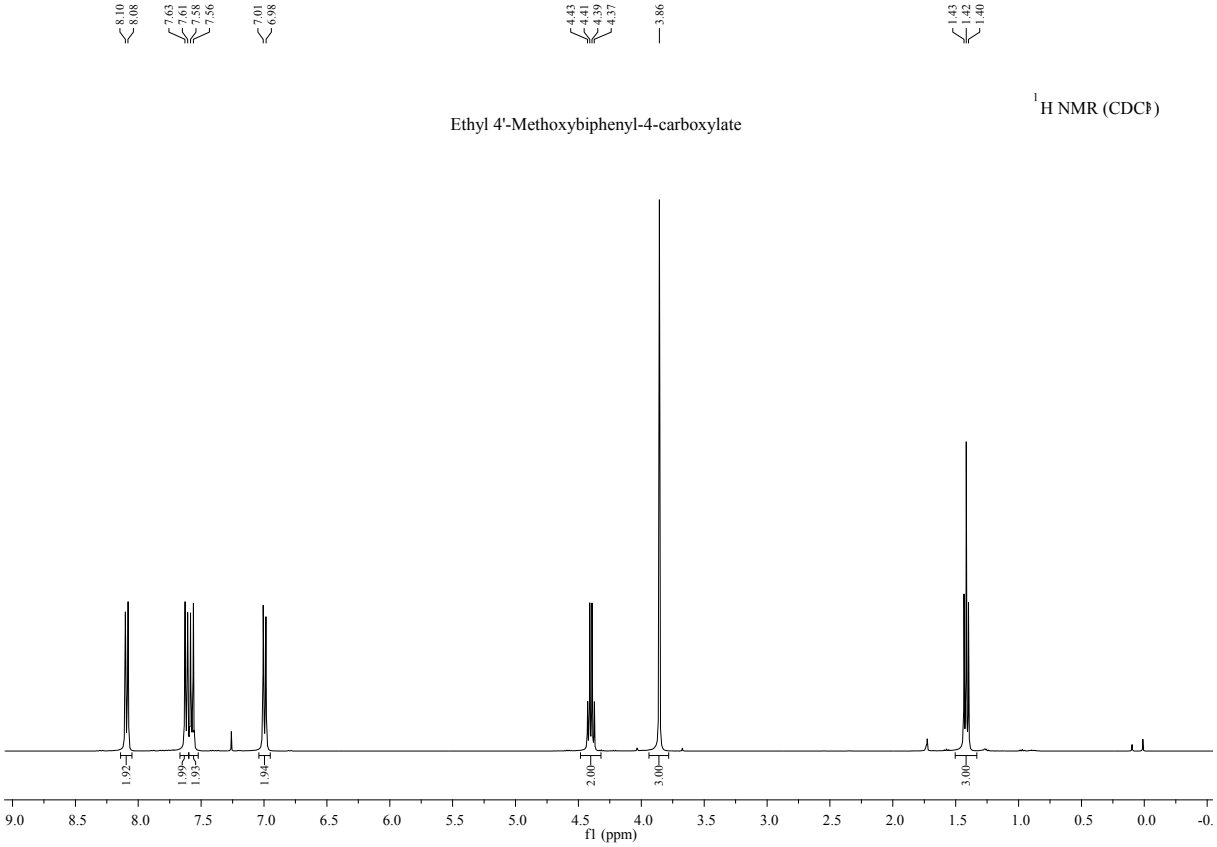


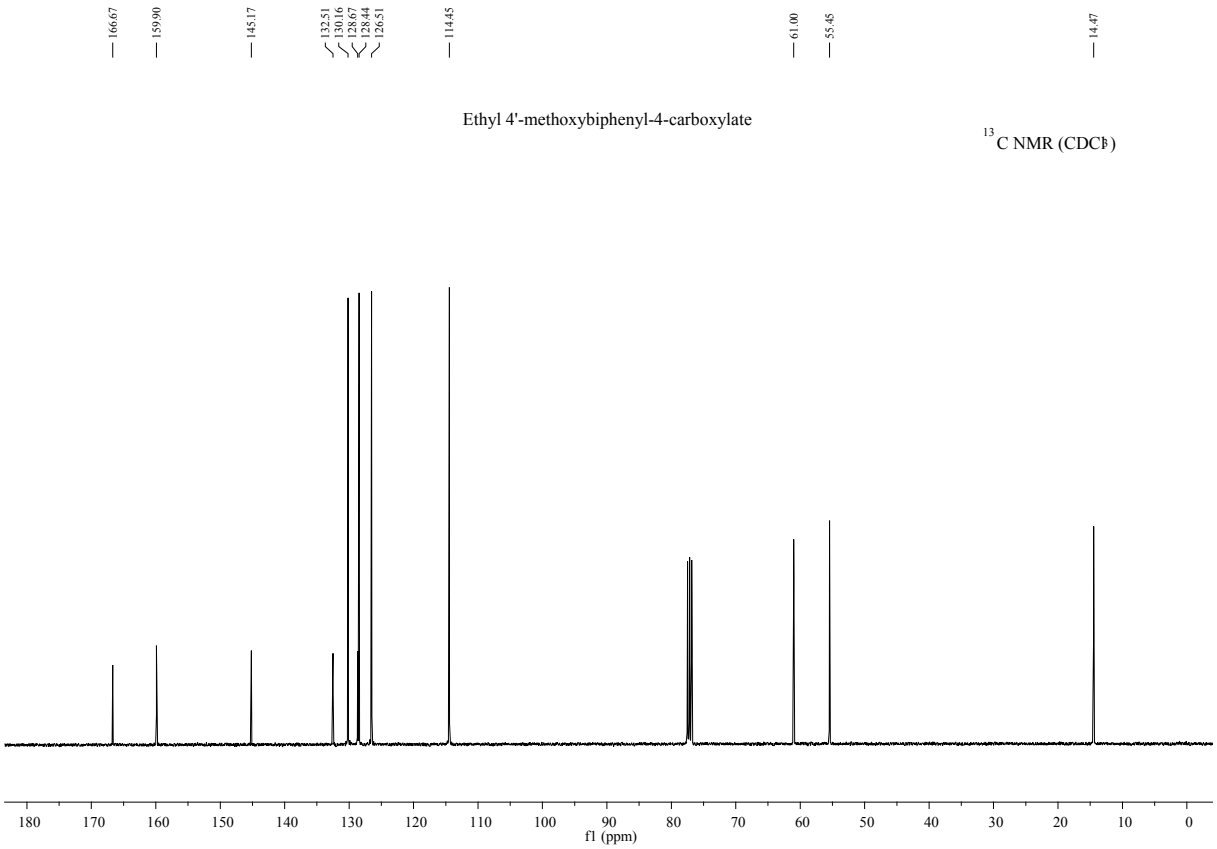
27. Ethyl 4'-methylbiphenyl-4-carboxylate



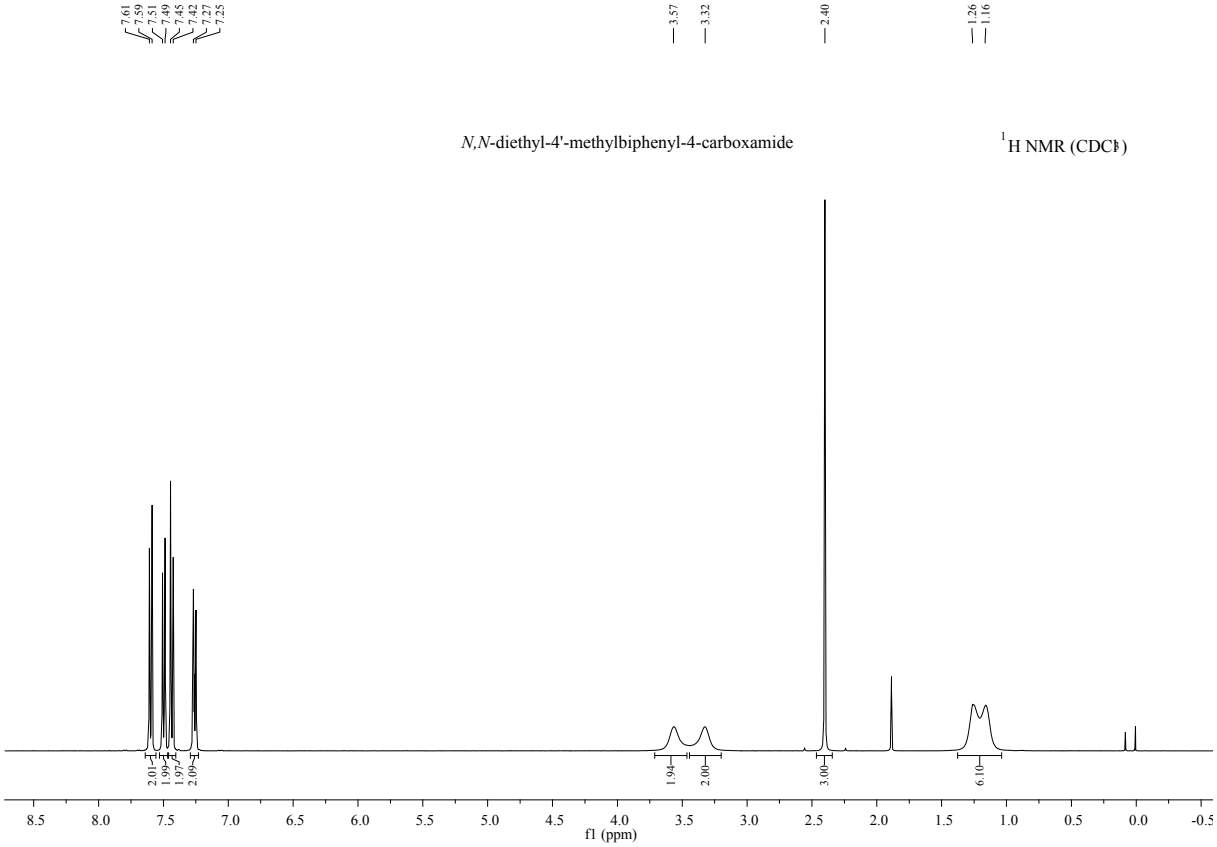


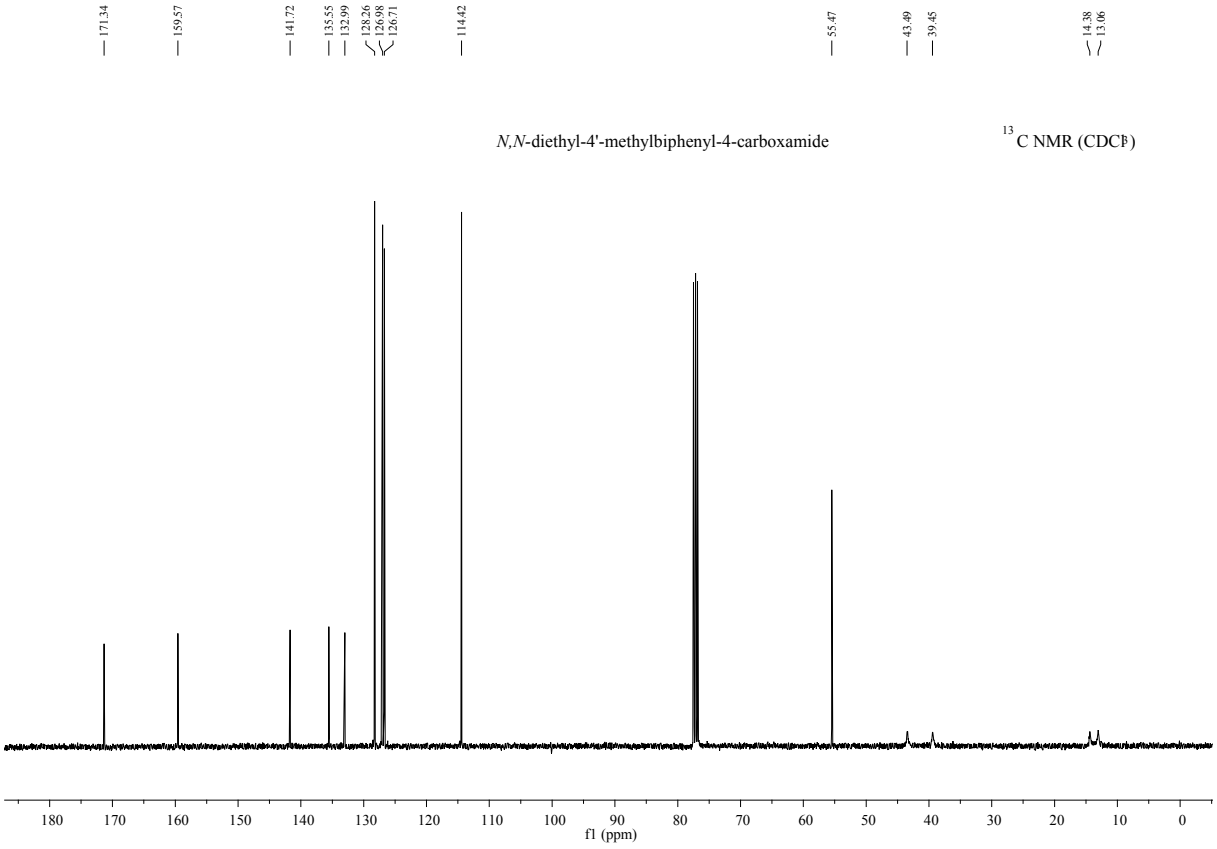
28. Ethyl 4'-methoxybiphenyl-4-carboxylate



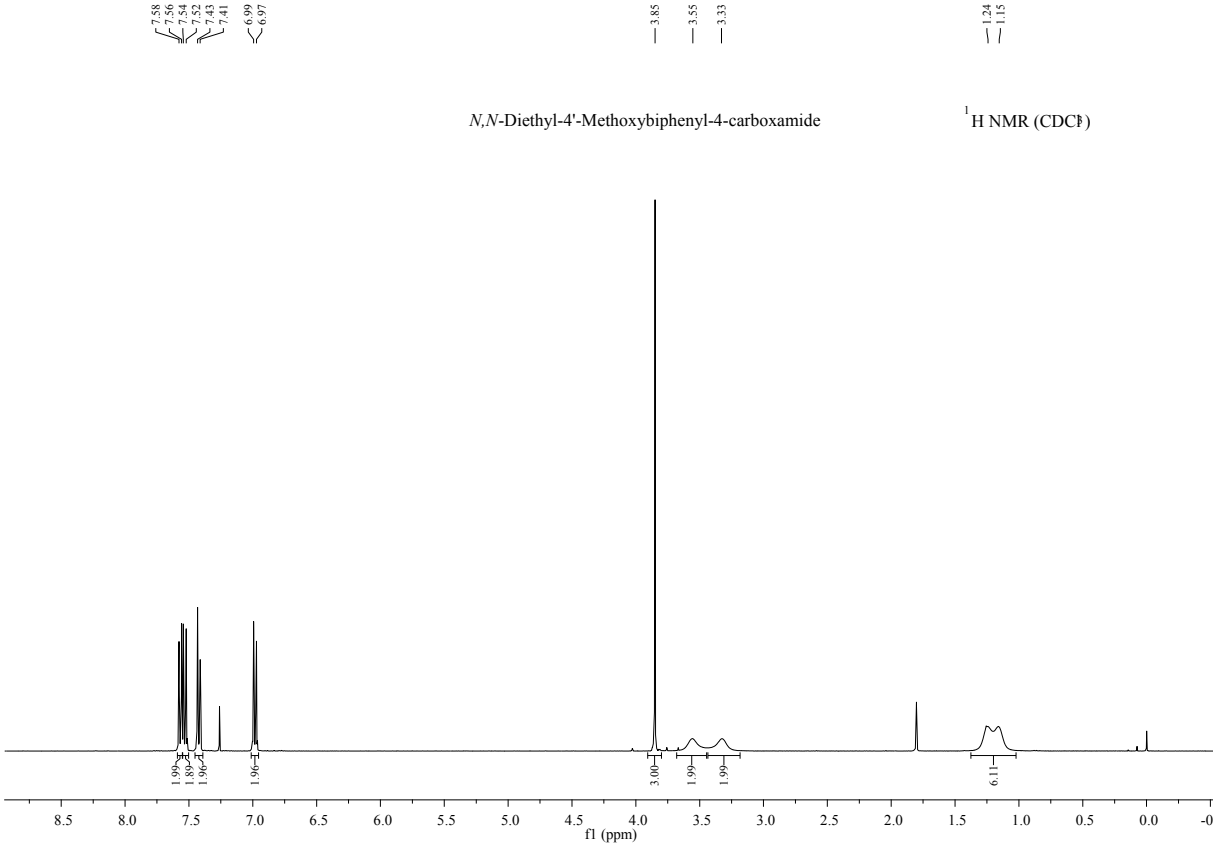


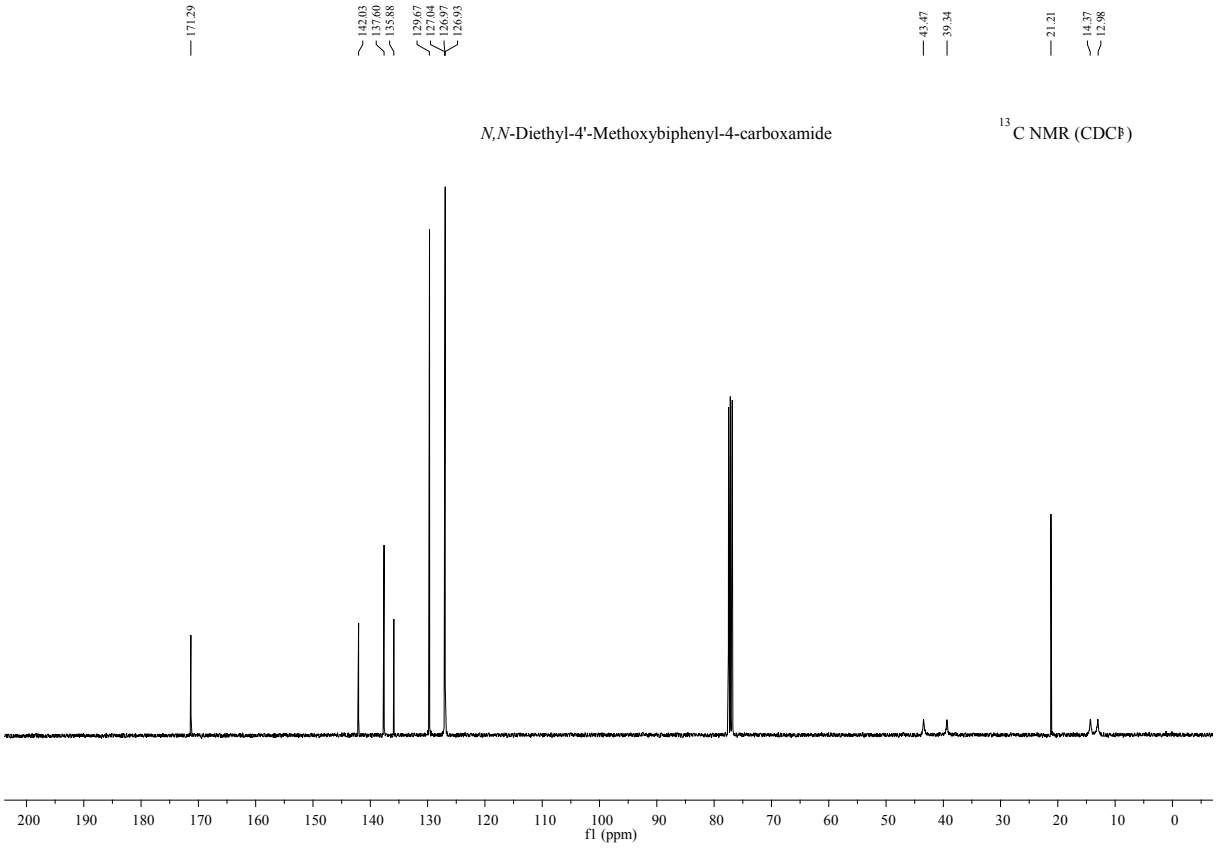
29. *N,N*-diethyl-4'-methylbiphenyl-4-carboxamide



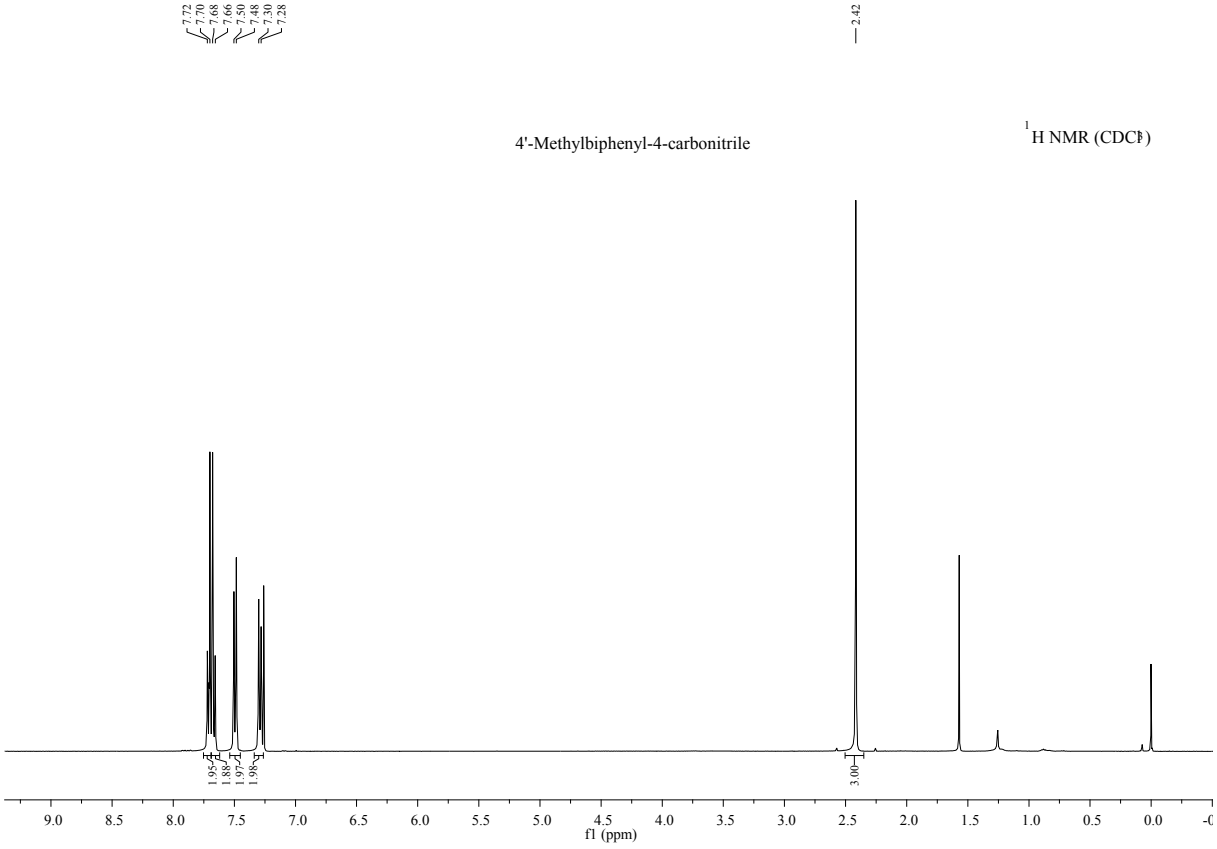


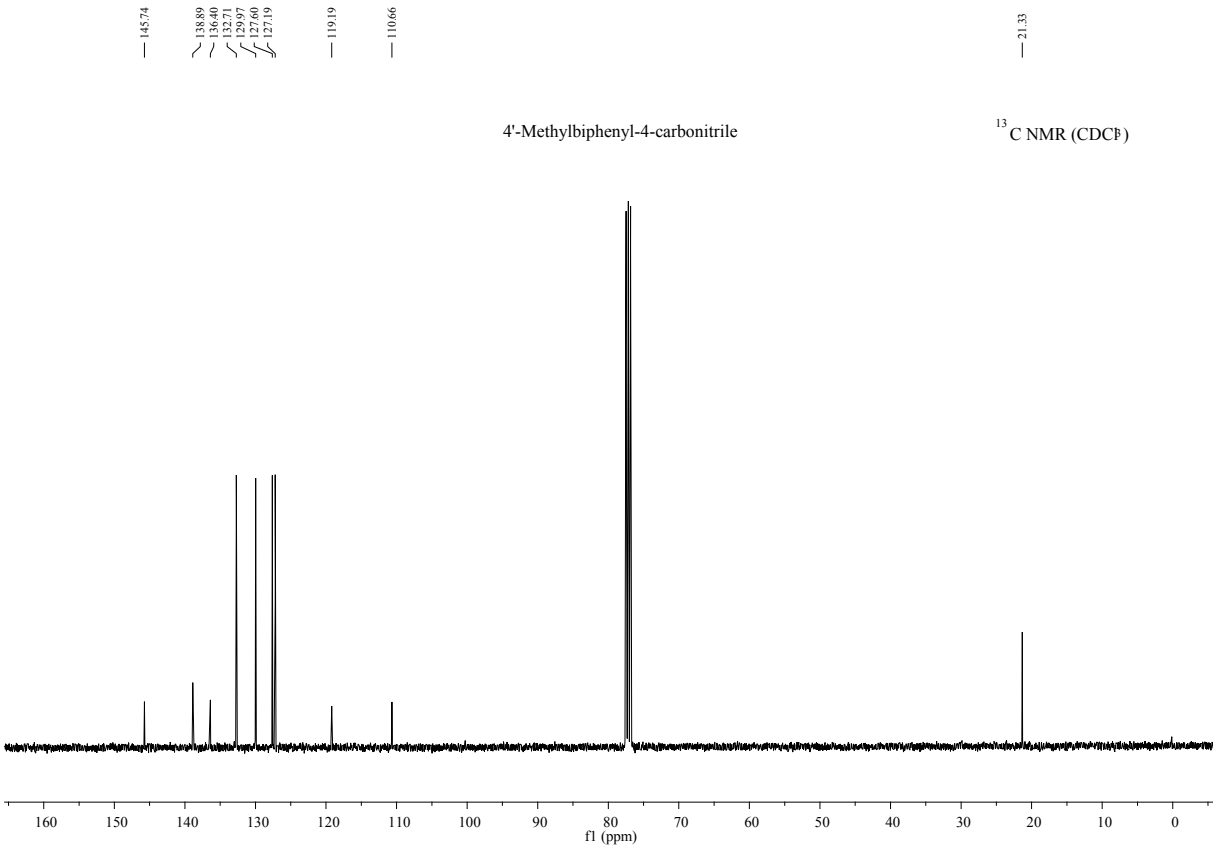
30. *N,N*-Diethyl-4'-methoxybiphenyl-4-carboxamide



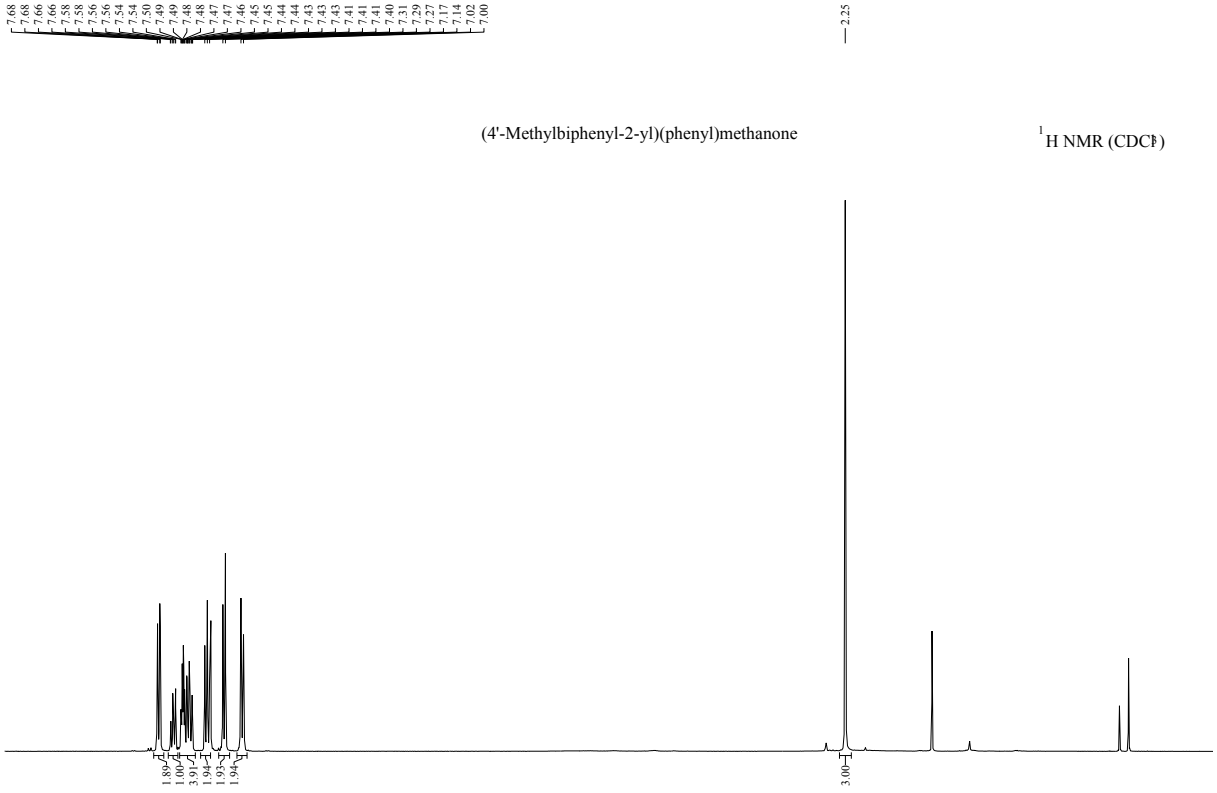


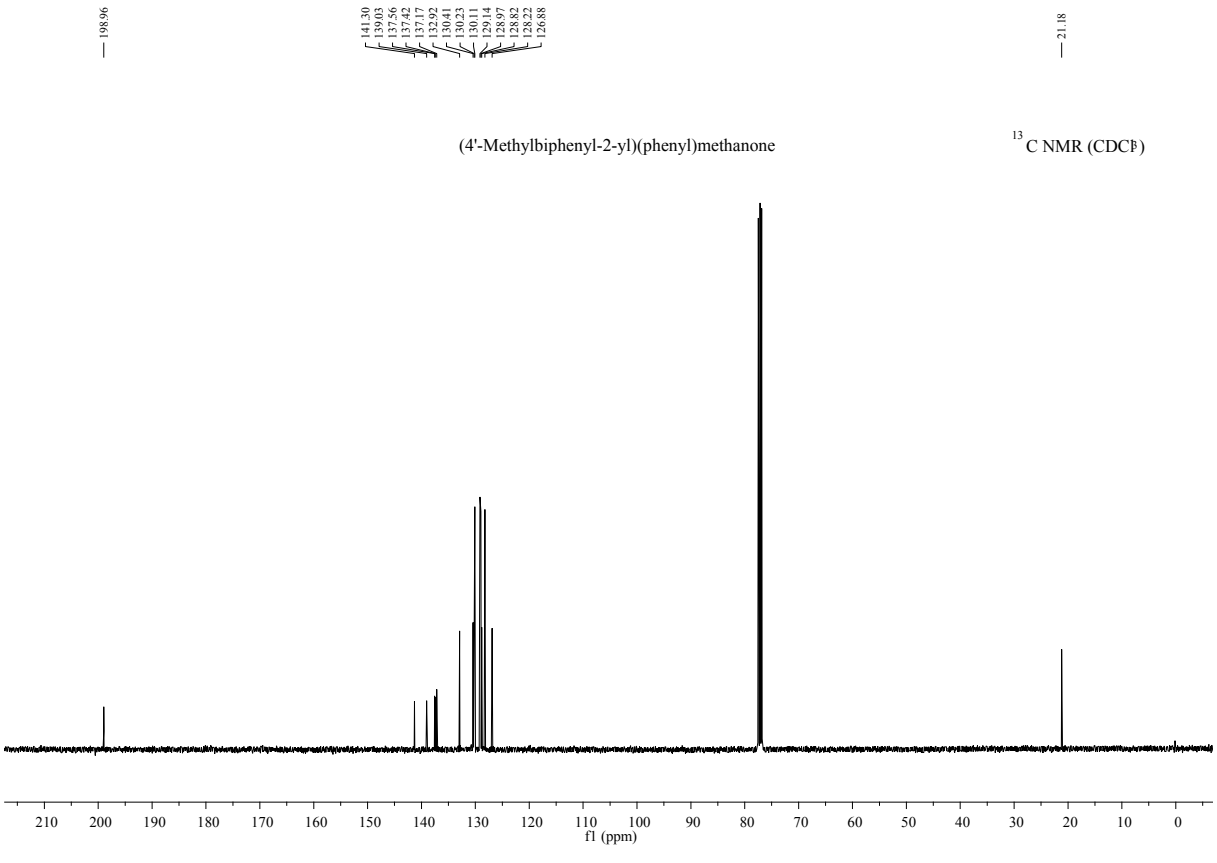
31. 4'-Methylbiphenyl-4-carbonitrile



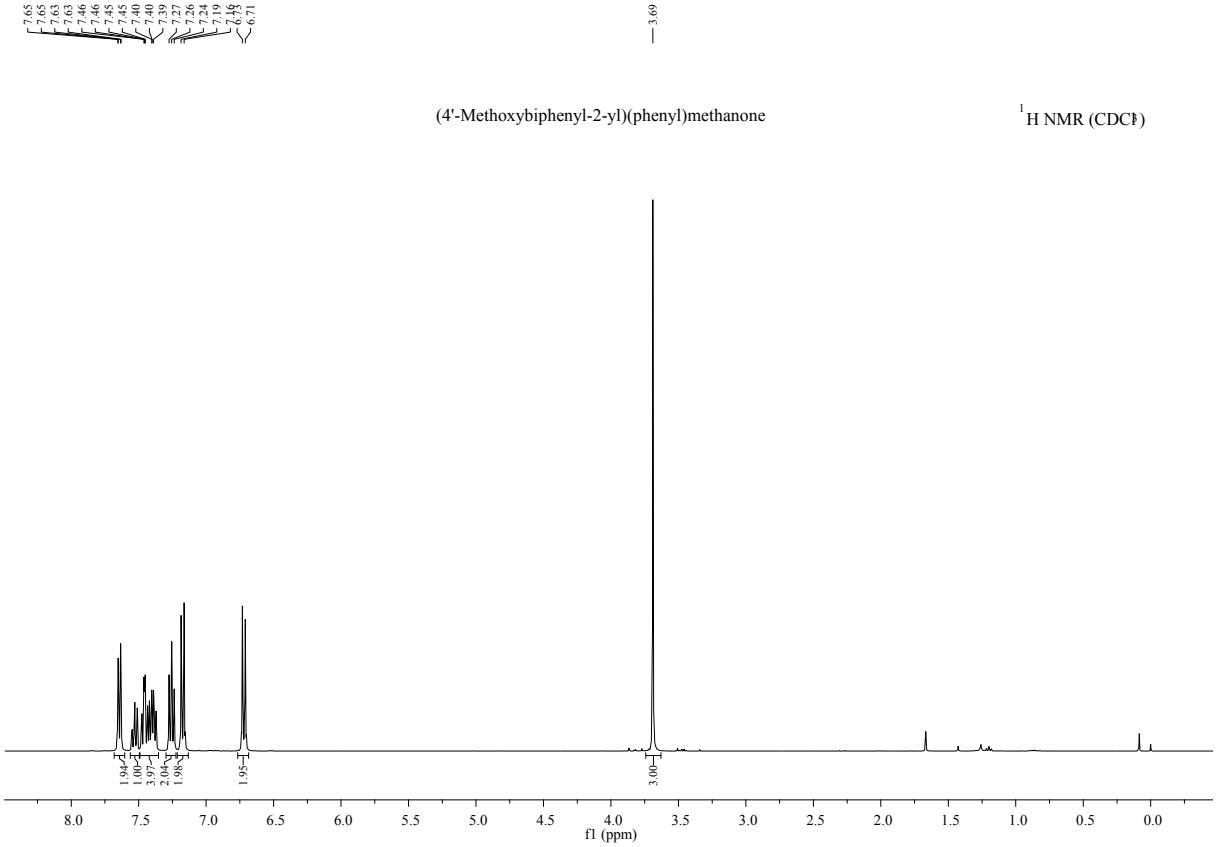


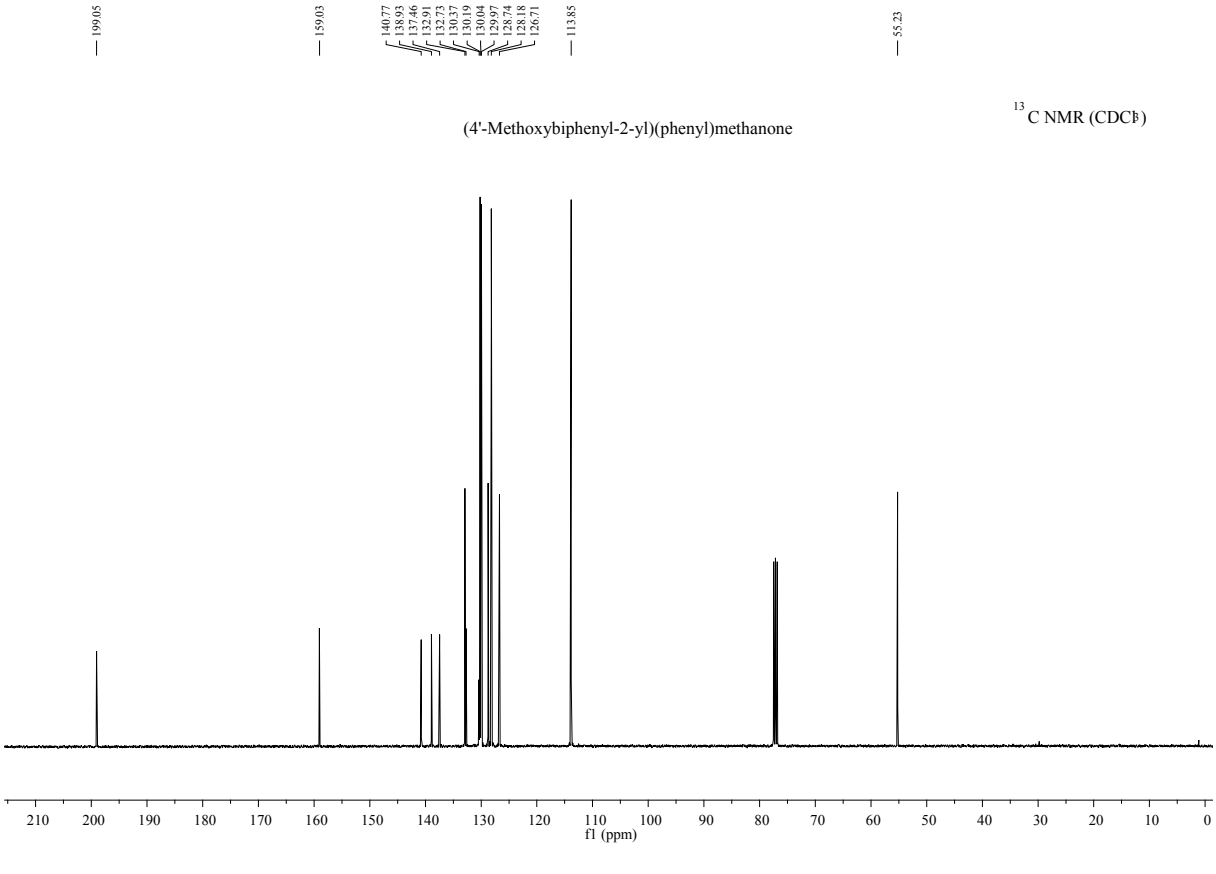
32. (4'-Methylbiphenyl-2-yl)(phenyl)methanone



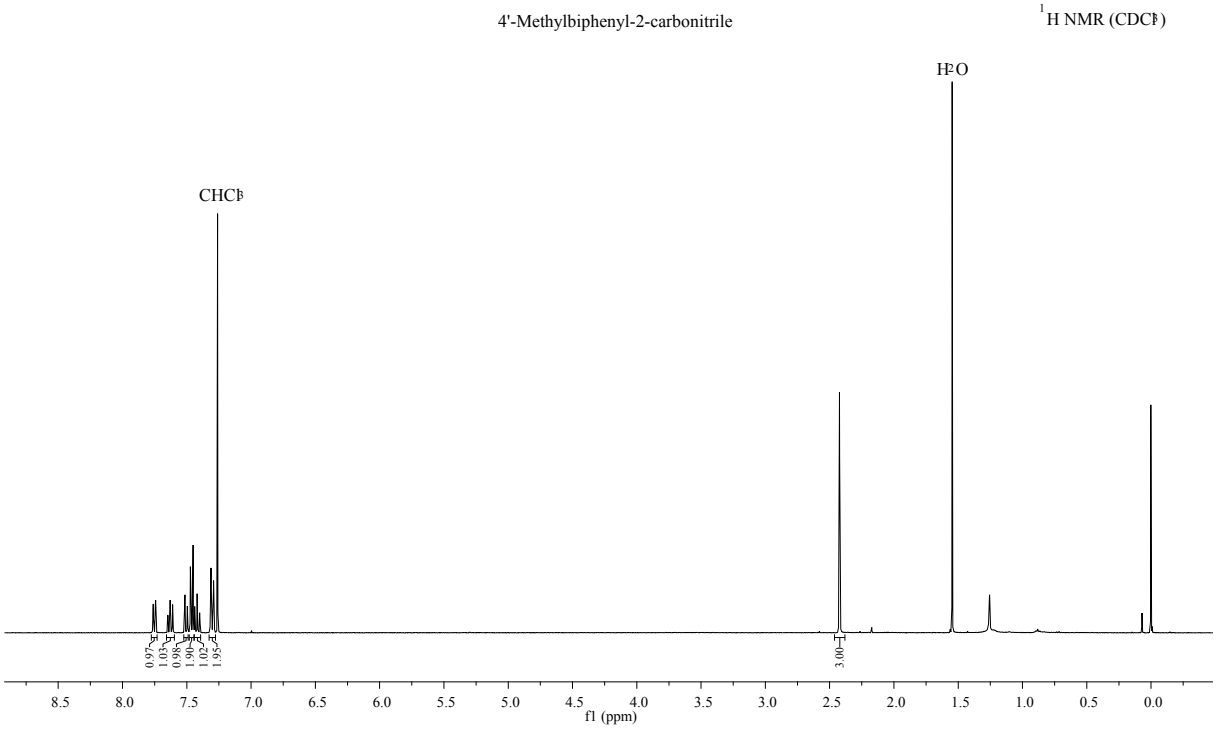


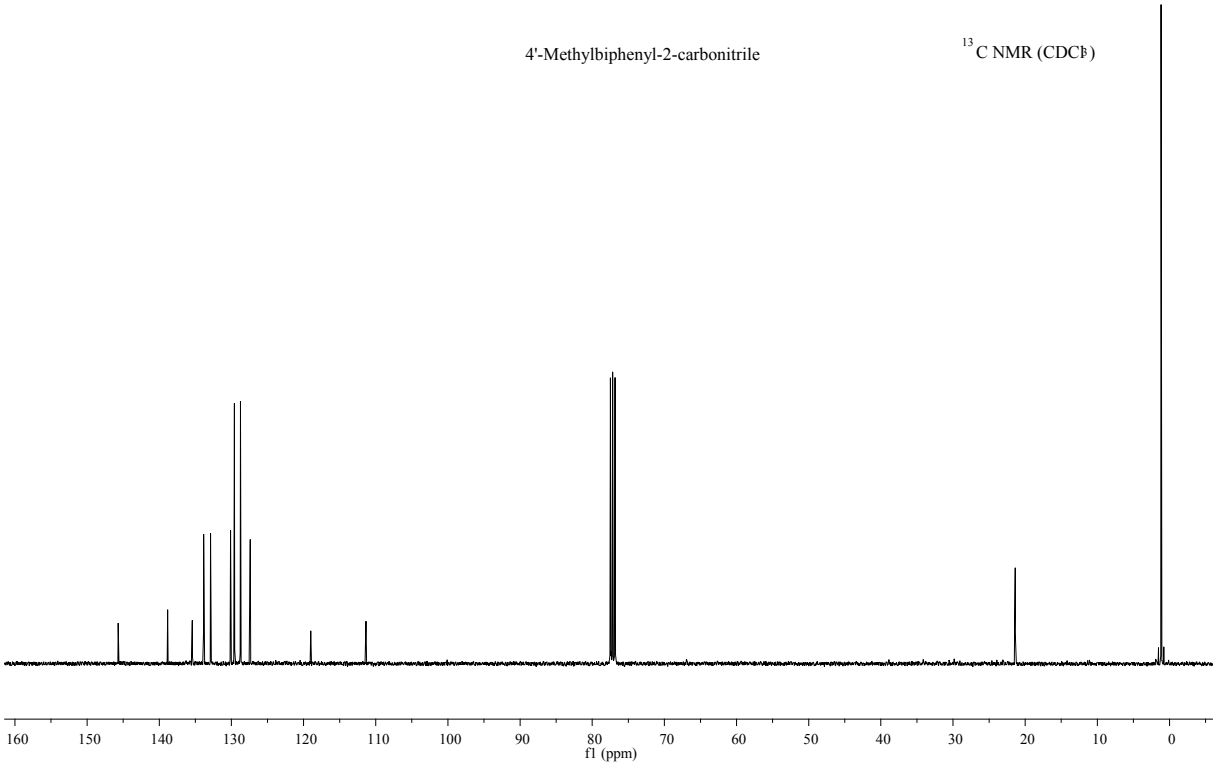
33. (4'-Methoxybiphenyl-2-yl)(phenyl)methanone



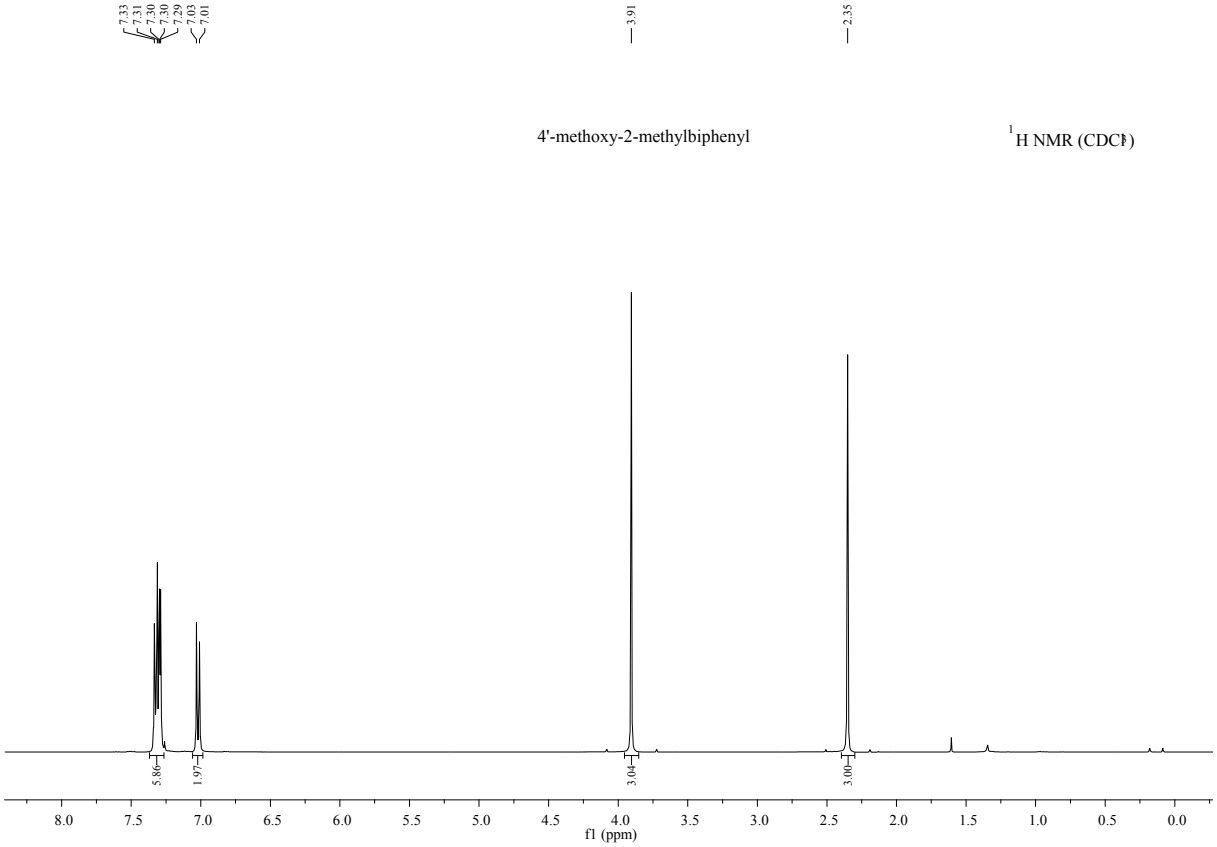


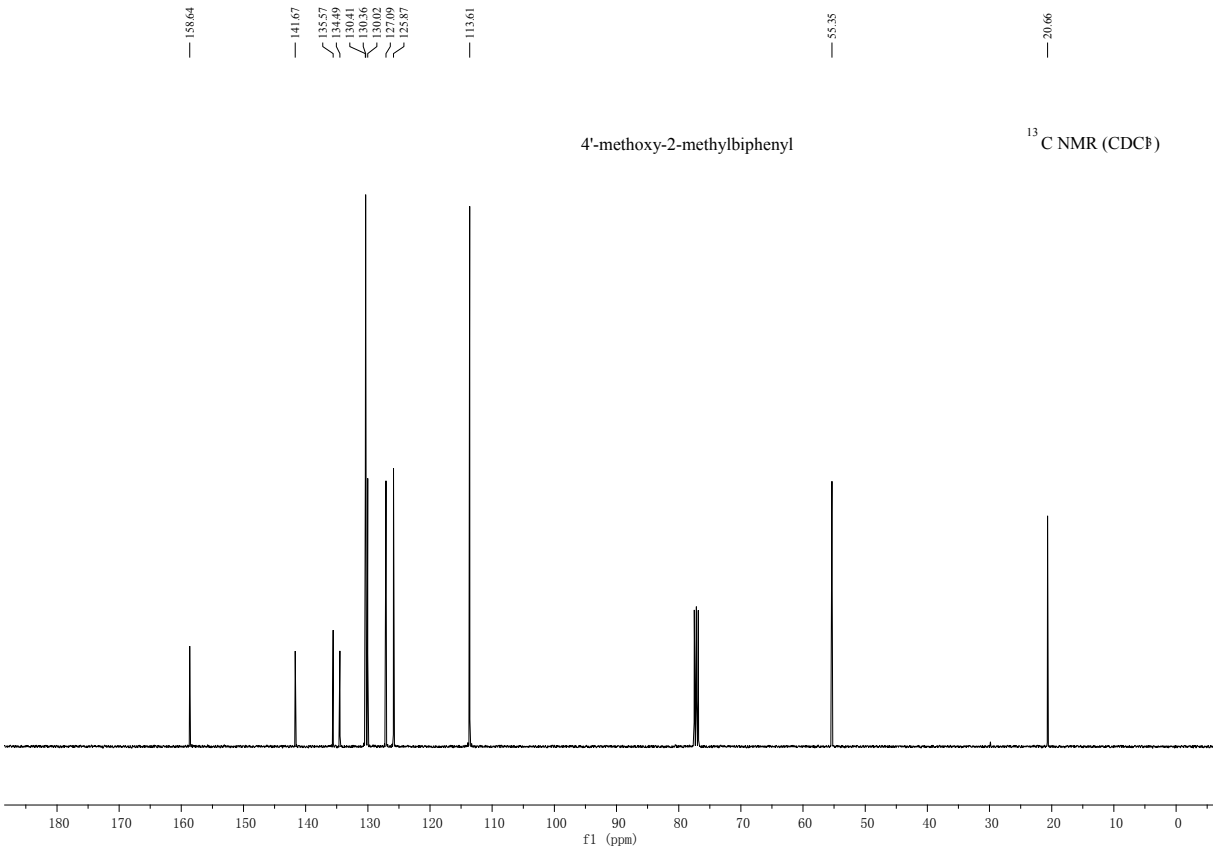
34. 4'-Methylbiphenyl-2-carbonitrile



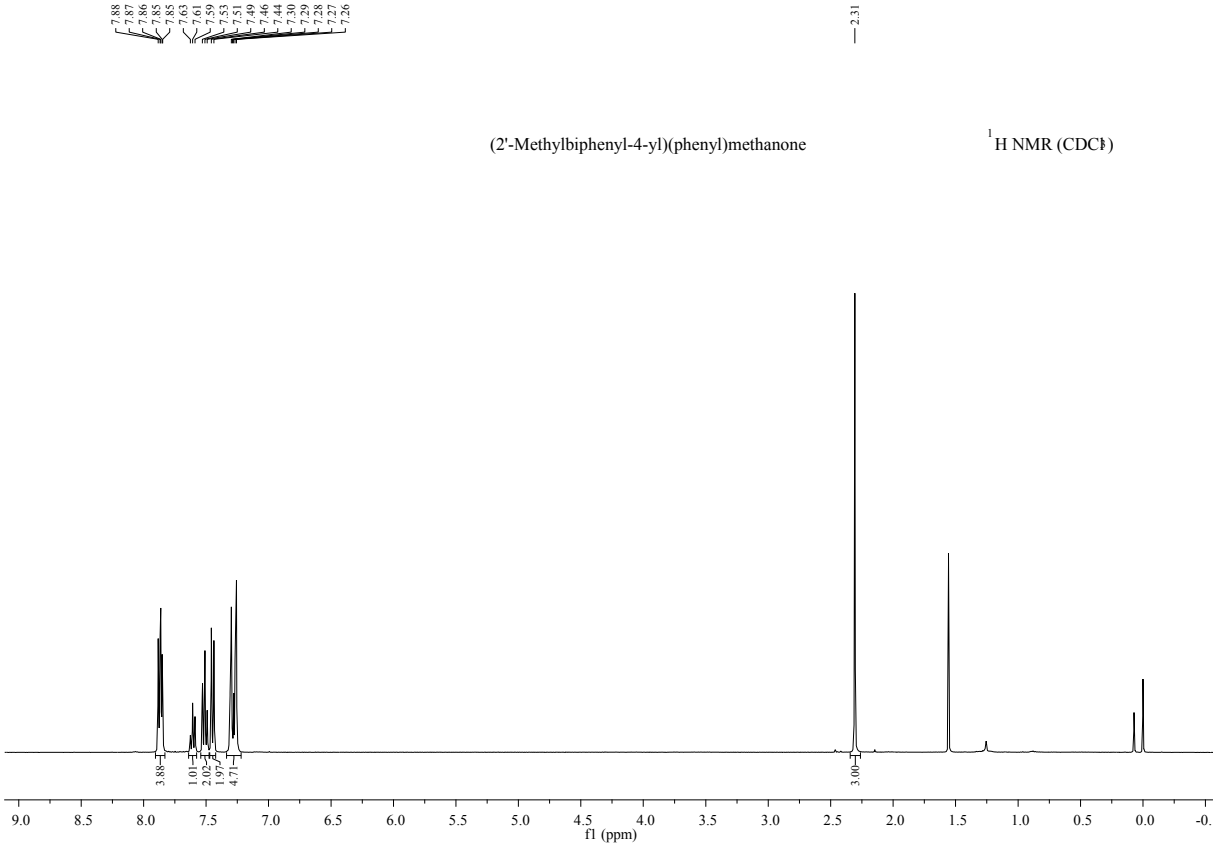


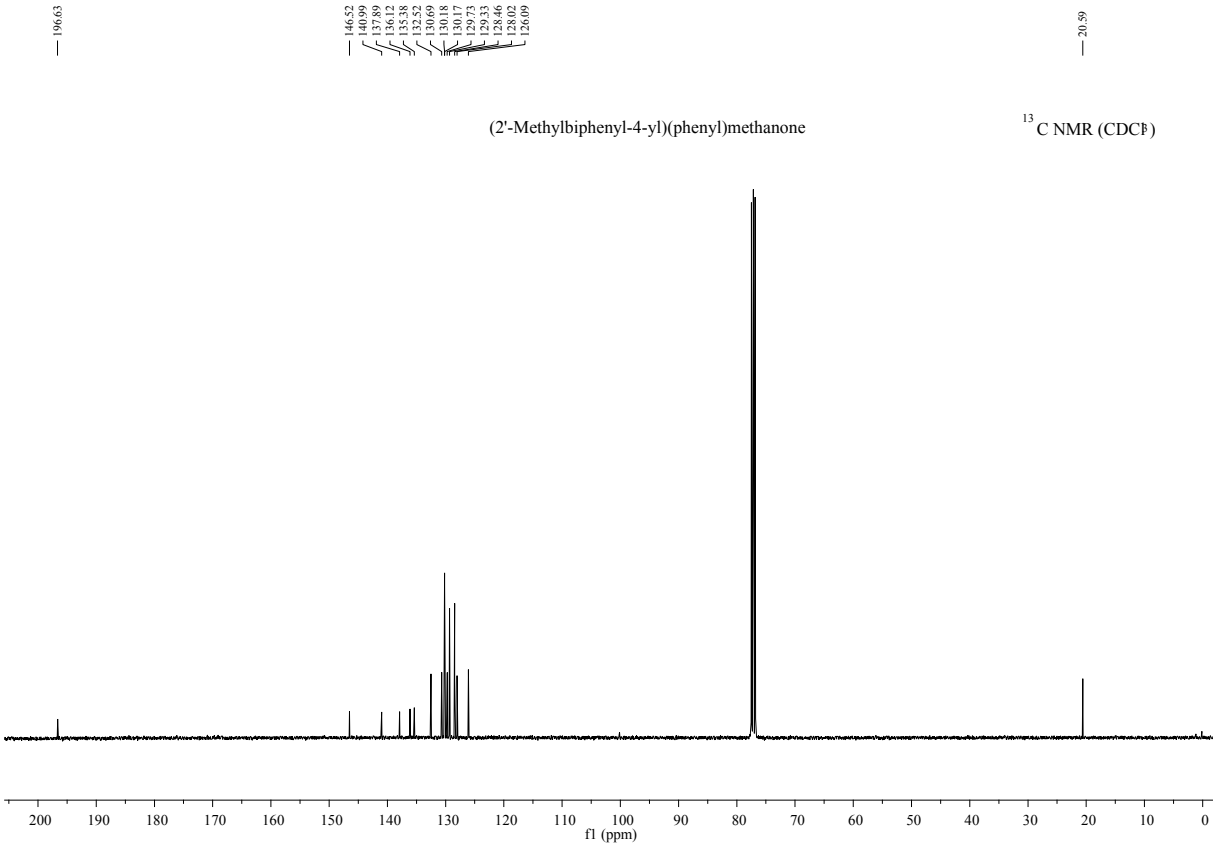
35. 4'-methoxy-2-methylbiphenyl



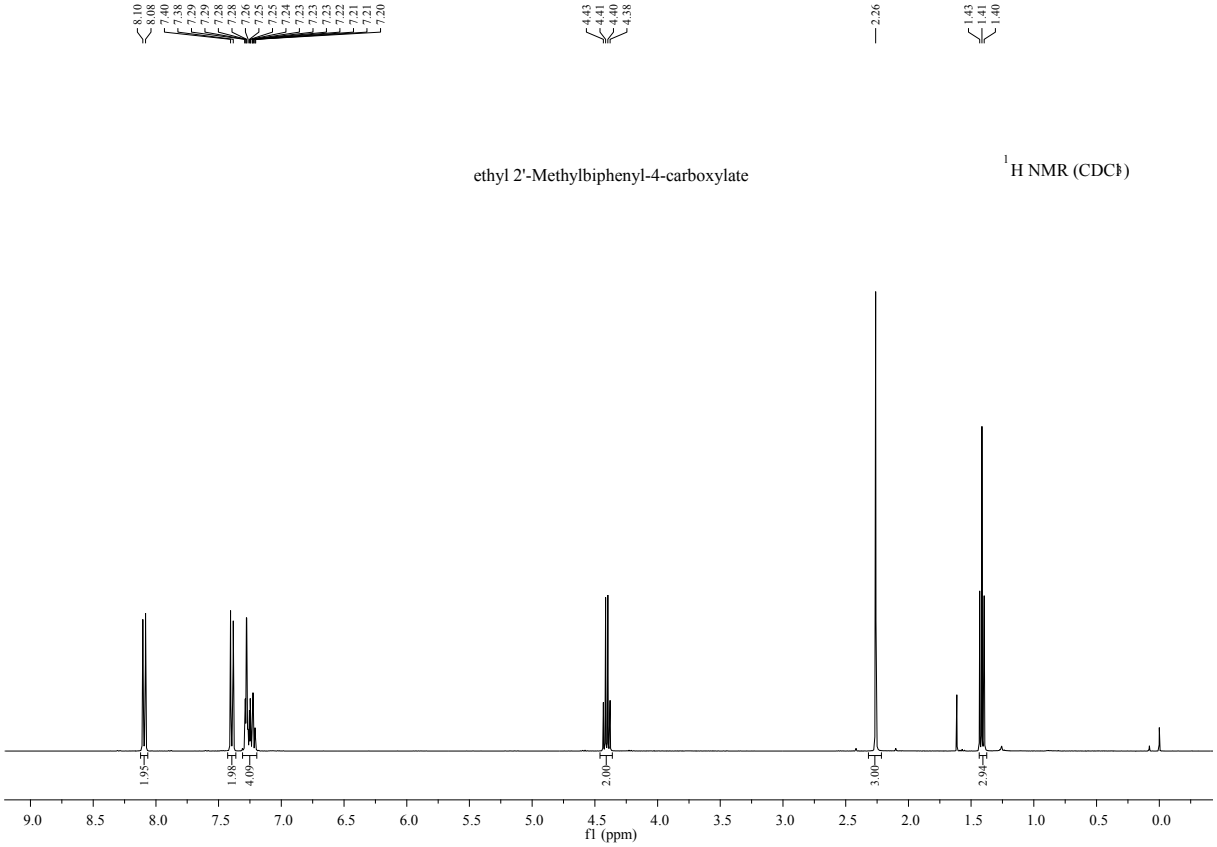


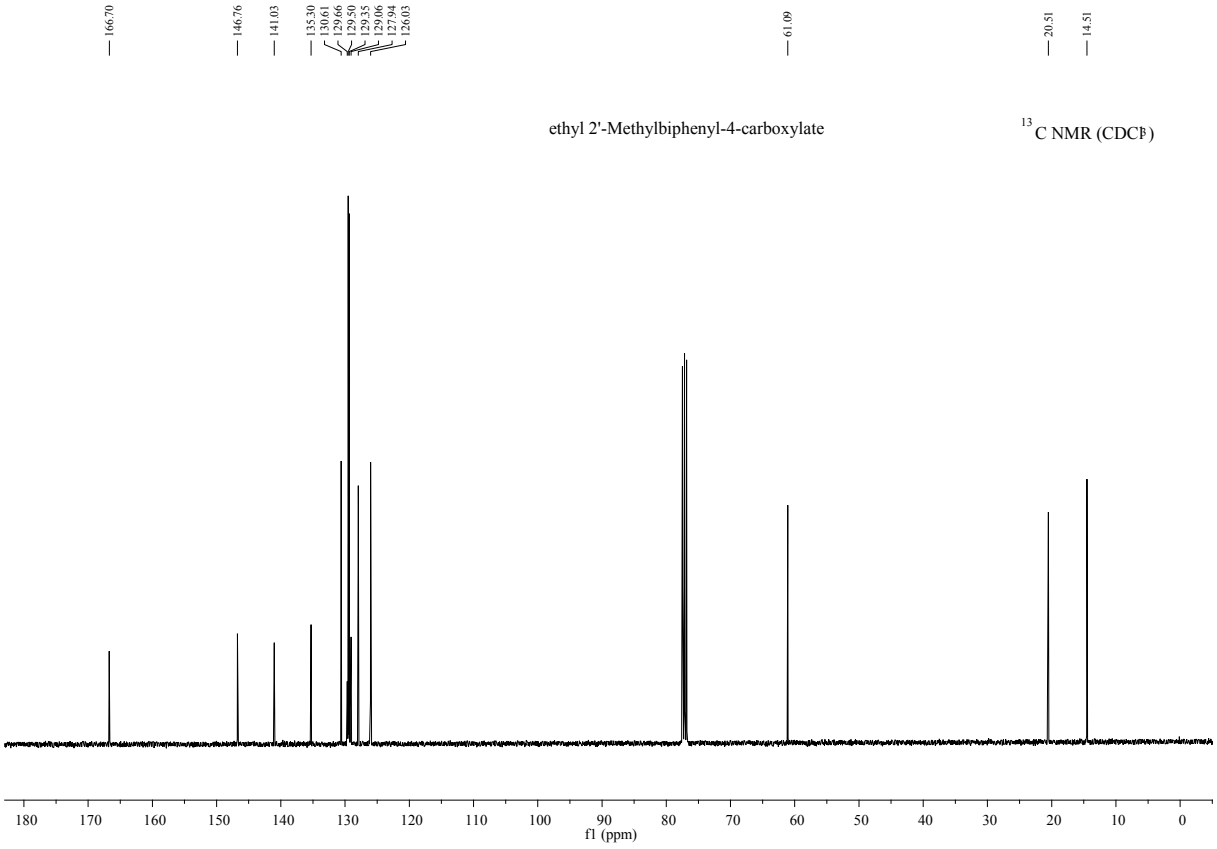
36. (2'-Methylbiphenyl-4-yl)(phenyl)methanone



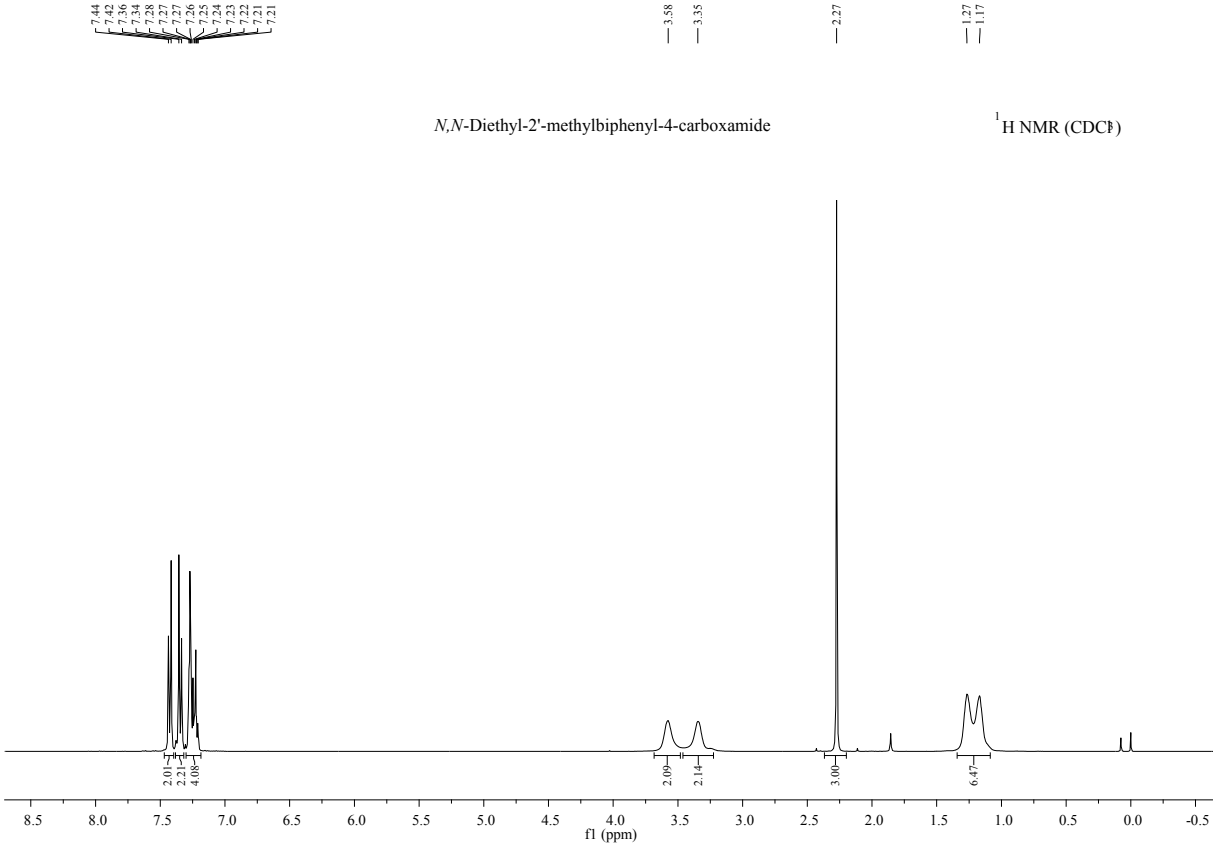


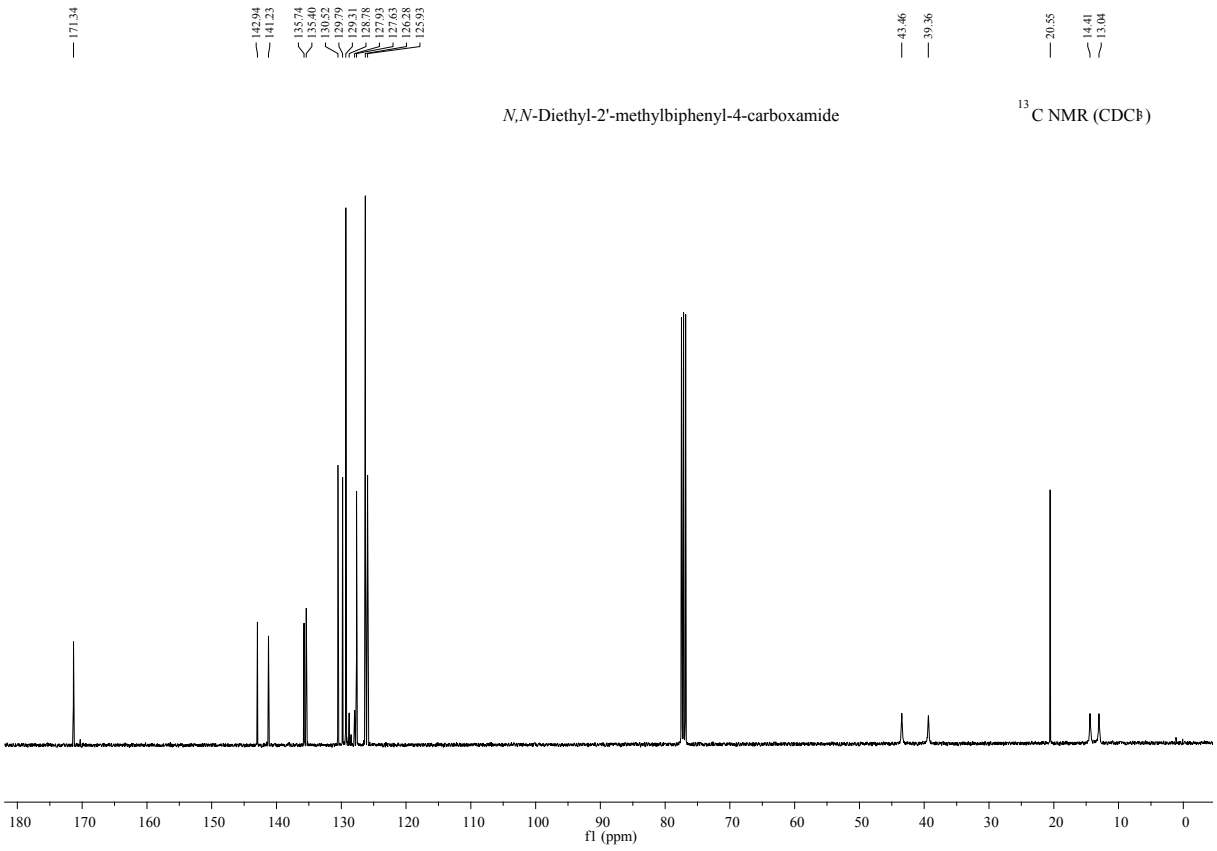
37. Ethyl 2'-methylbiphenyl-4-carboxylate



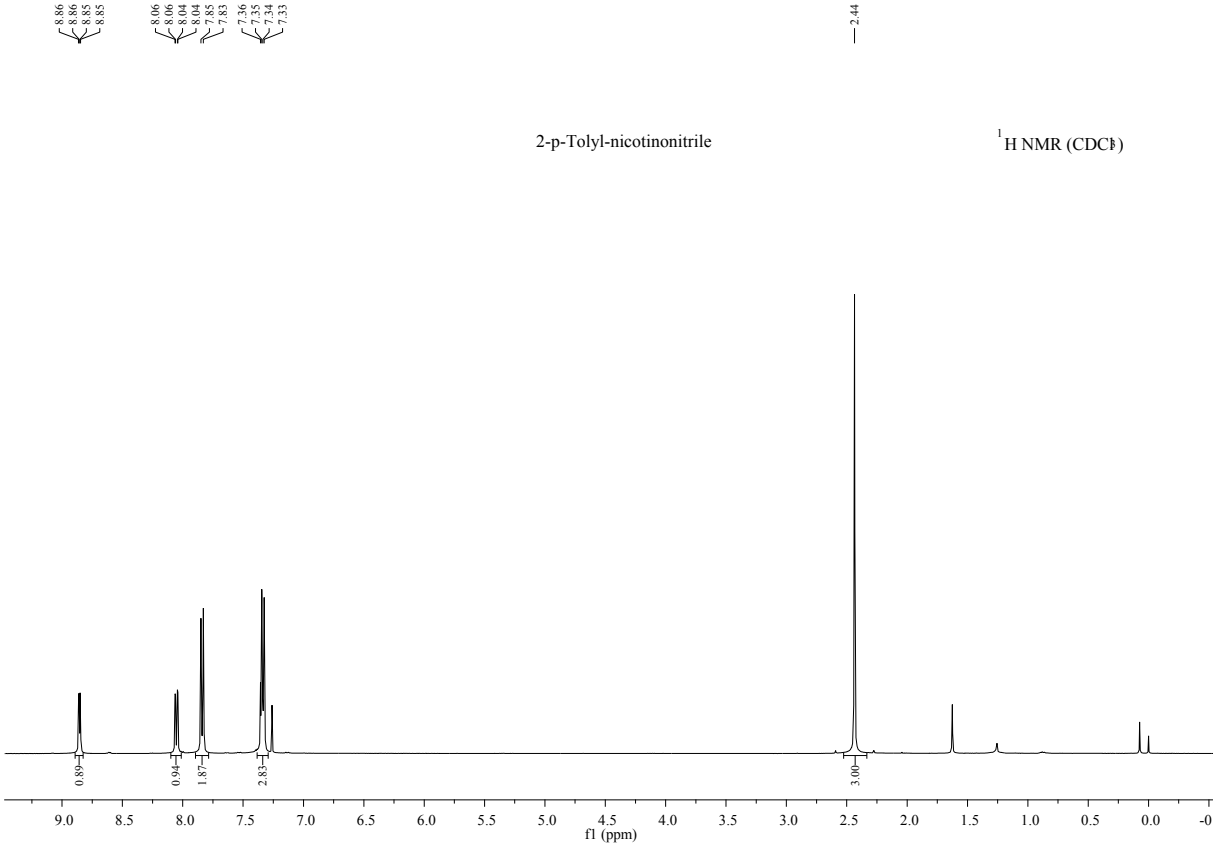


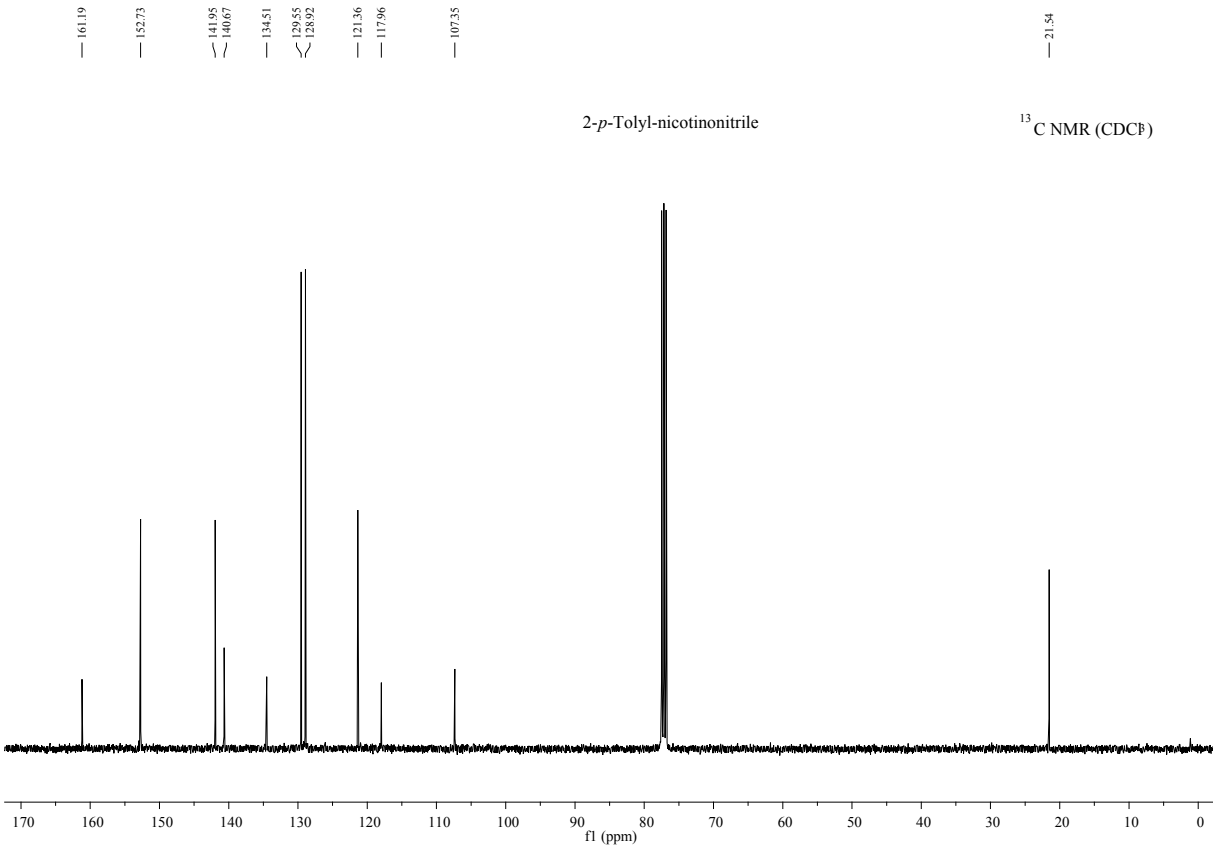
38. *N,N*-Diethyl-2'-methylbiphenyl-4-carboxamide



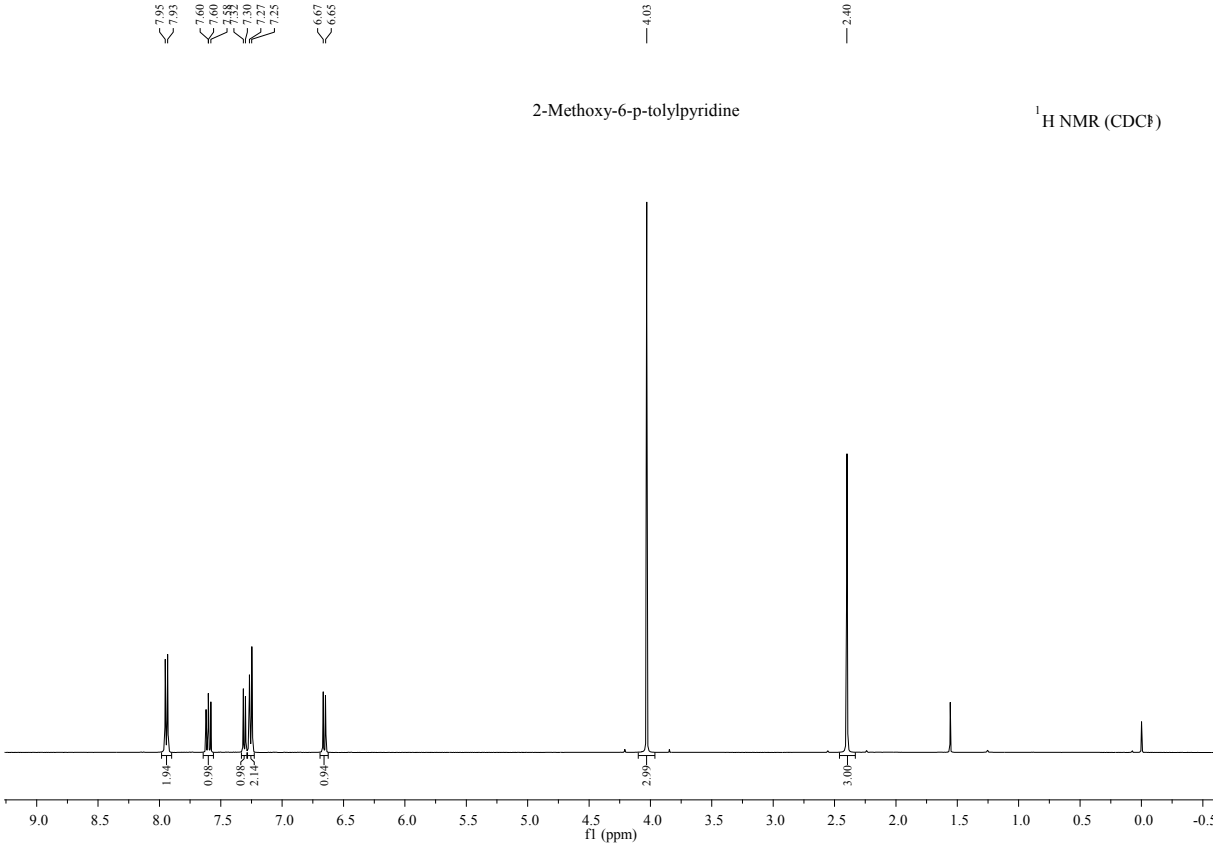


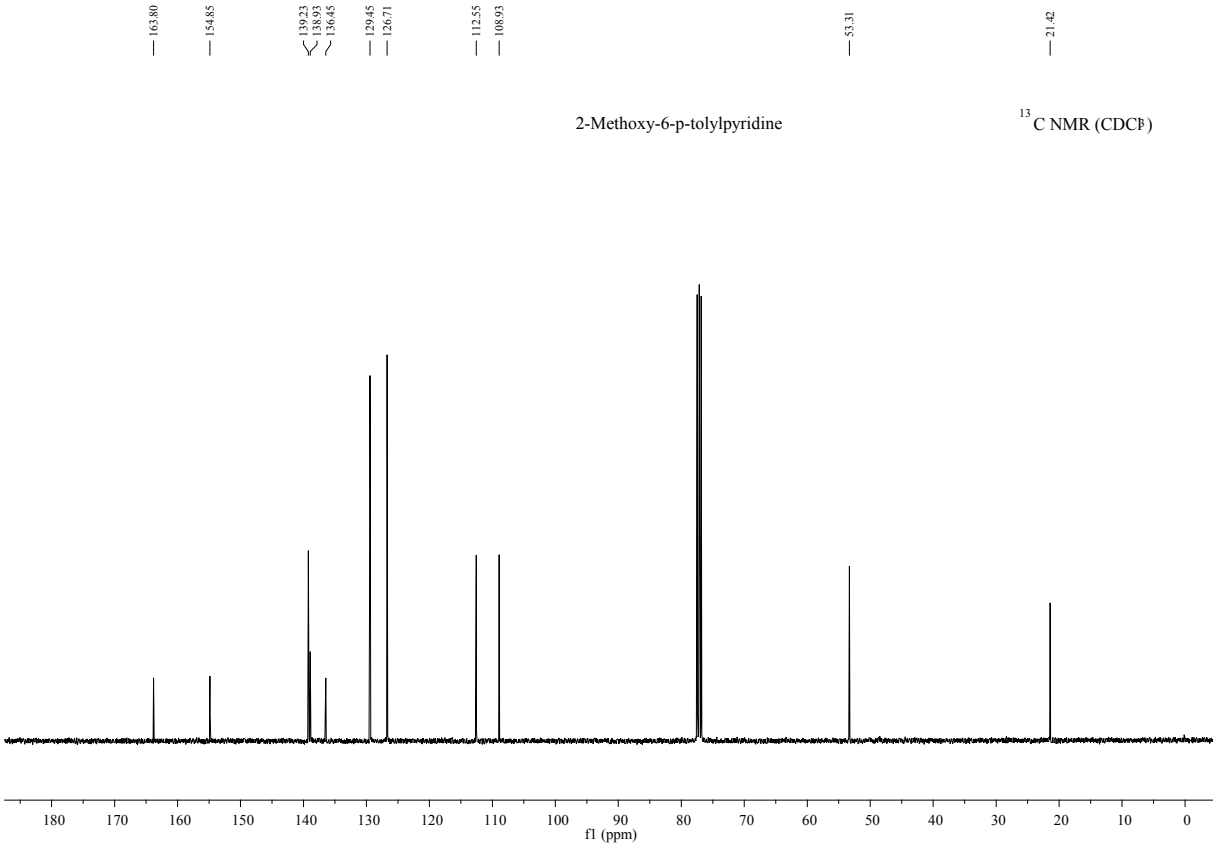
39. 2-*p*-Tolyl-nicotinonitrile



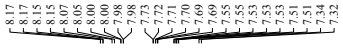


40. 2-Methoxy-6-*p*-tolylpyridine

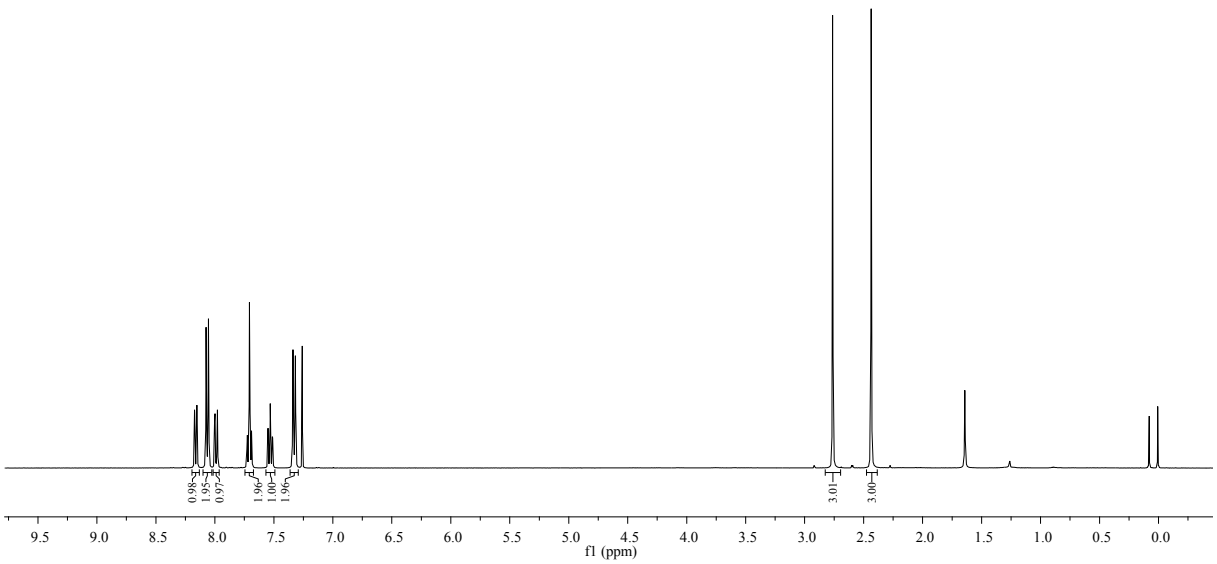




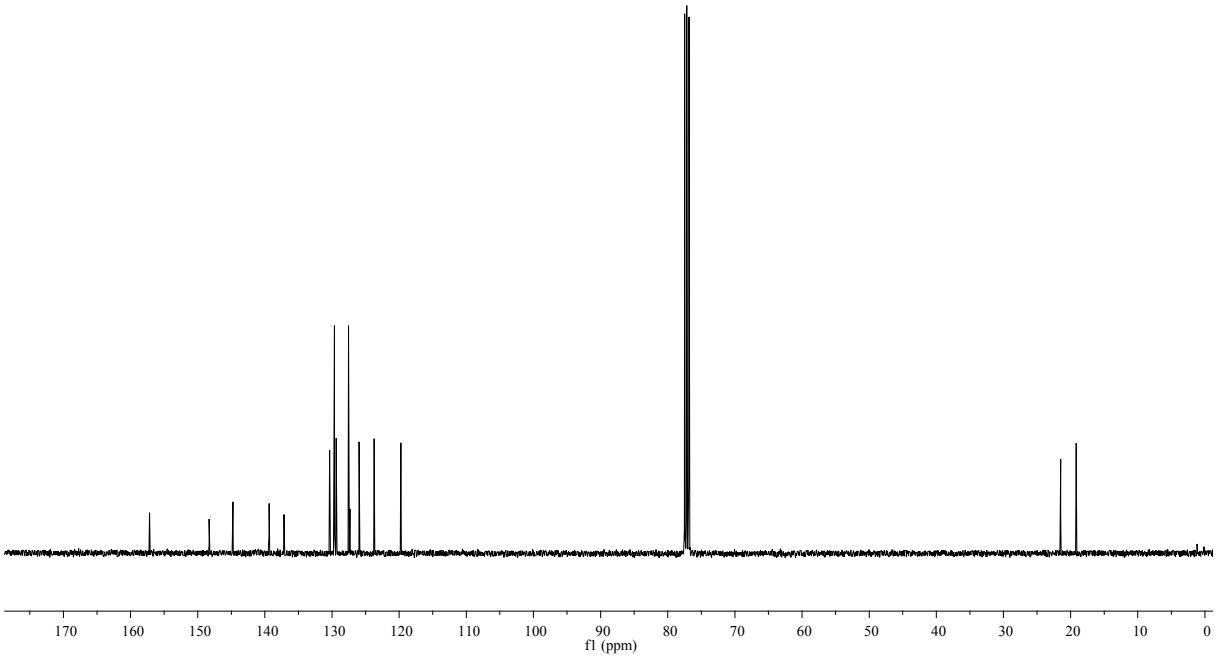
41. 2-(4-Methylphenyl)-4-methylquinoline



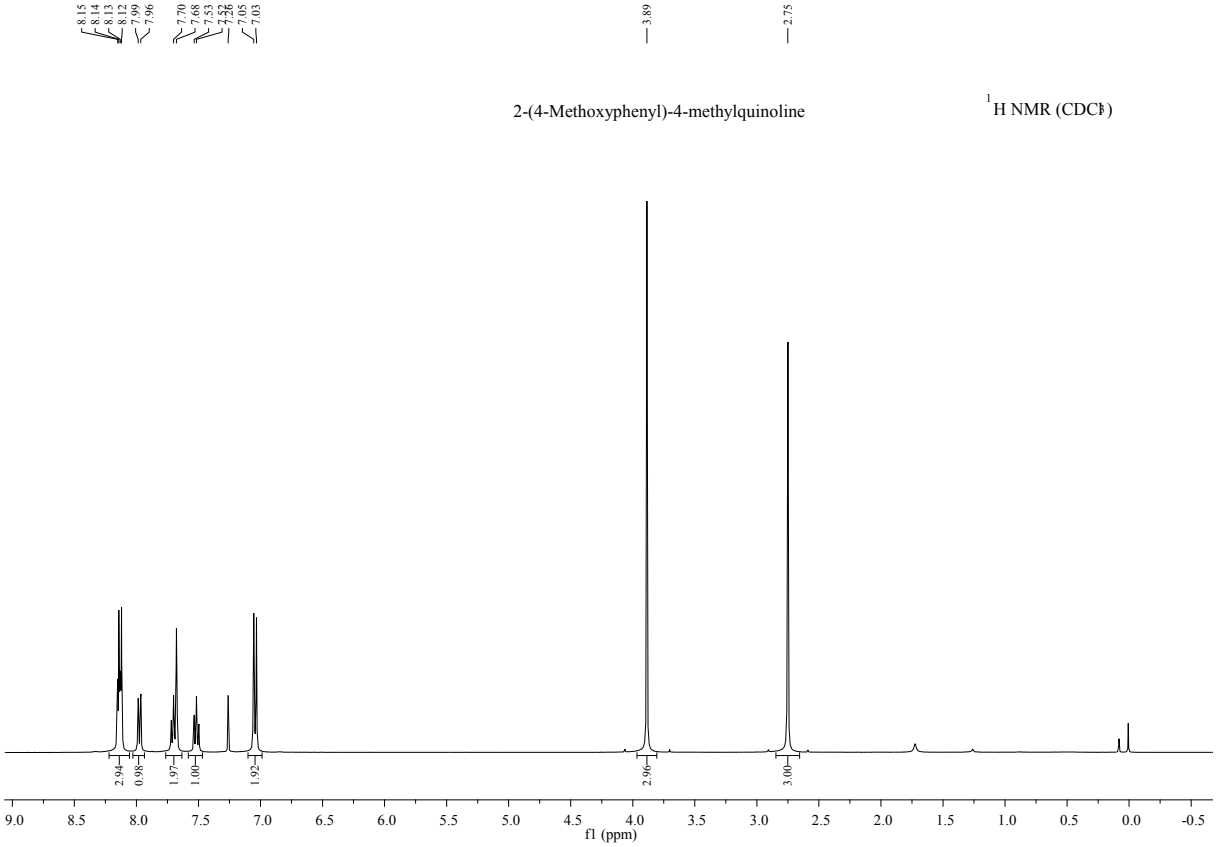
2-(4-Methylphenyl)-4-methylquinoline ^{1}H NMR (CDCl$_3$)

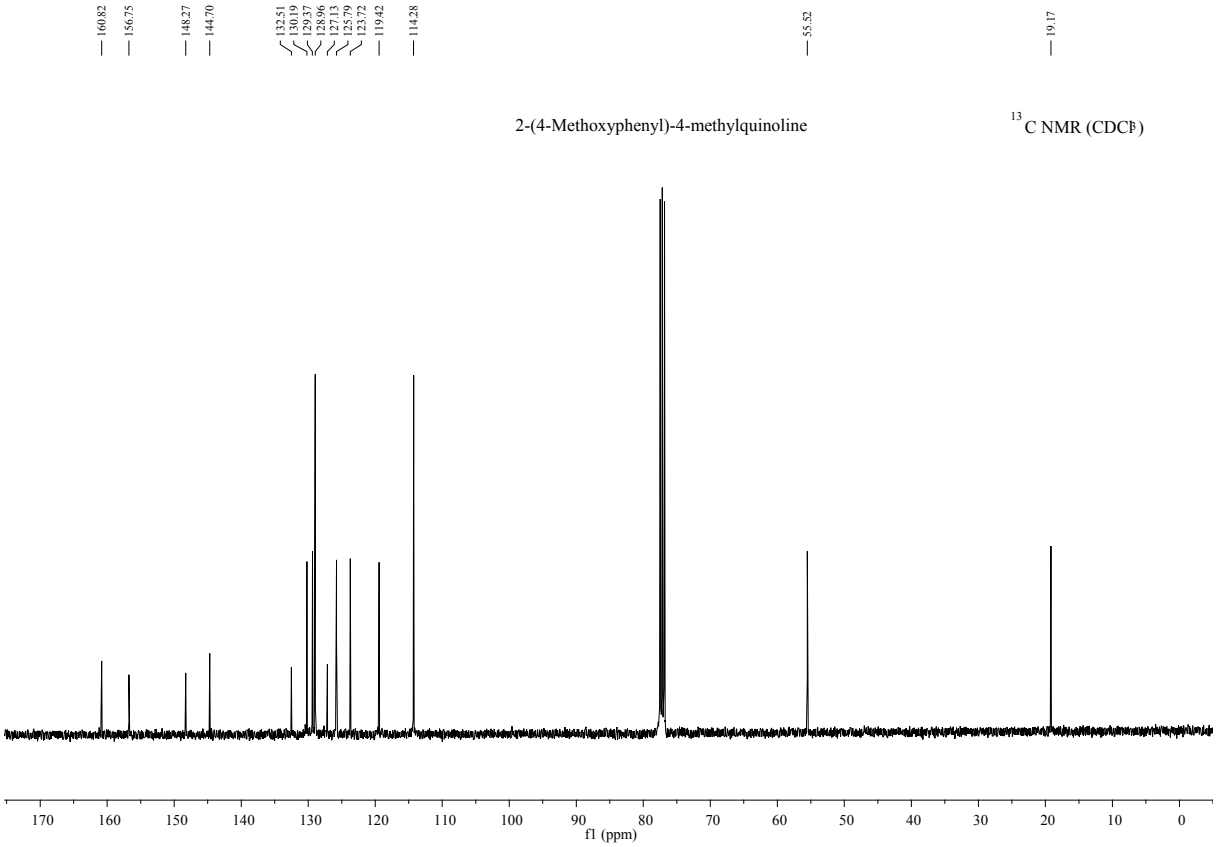


2-(4-Methylphenyl)-4-methylquinolin ^{13}C NMR (CDCl$_3$)



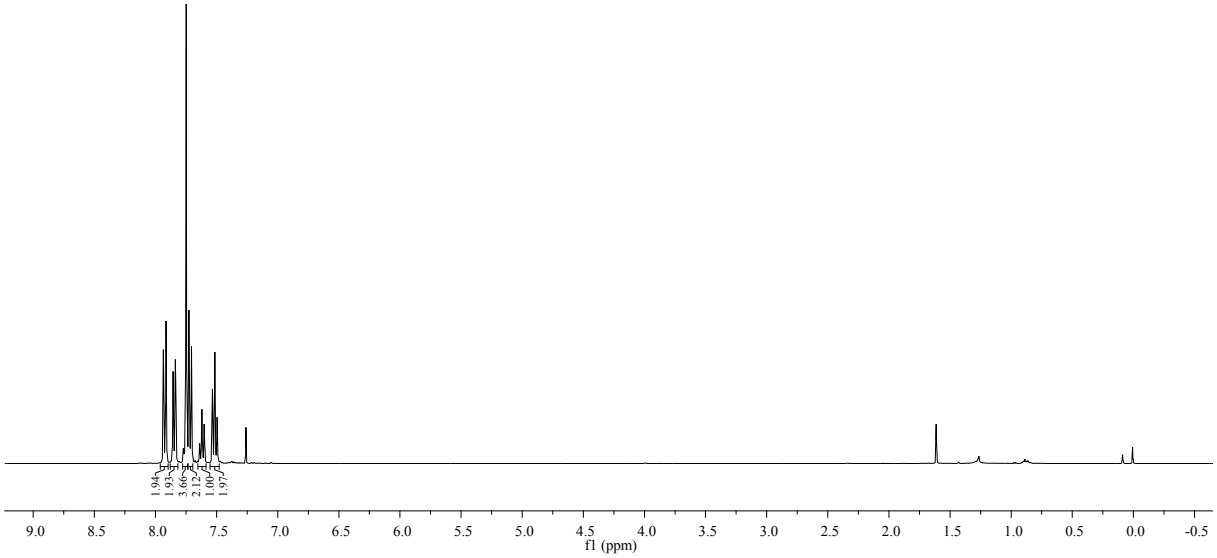
42. 2-(4-Methoxyphenyl)-4-methylquinoline

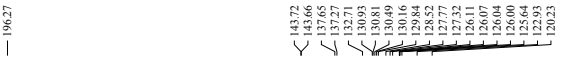




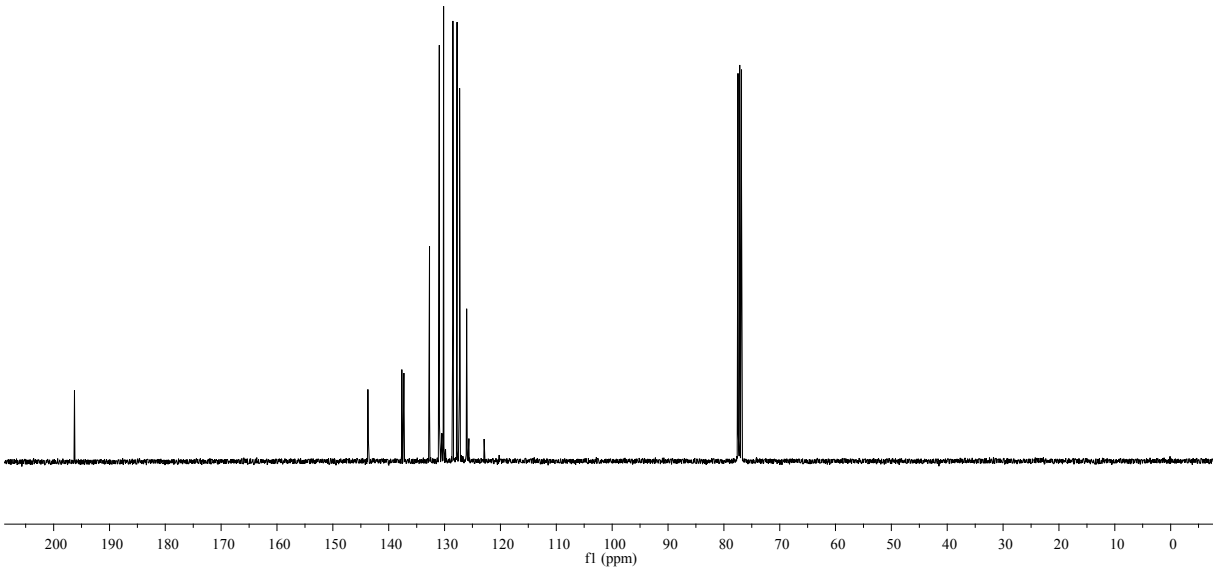
43. (4'-(Trifluoromethyl)biphenyl-4-yl)(phenyl)methanone

(4'-(trifluoromethyl)biphenyl-4-yl)(phenyl)methanone ^{1}H NMR (CDCl$_3$)

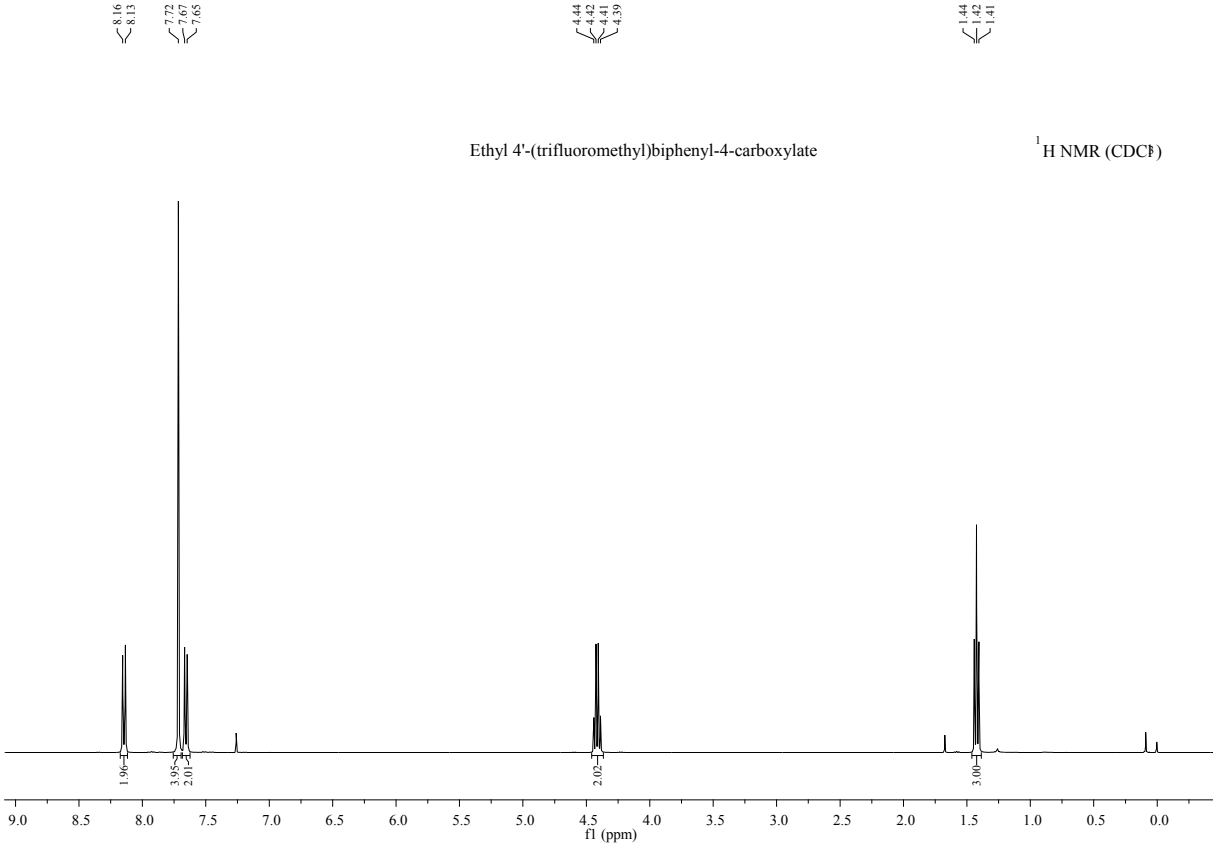


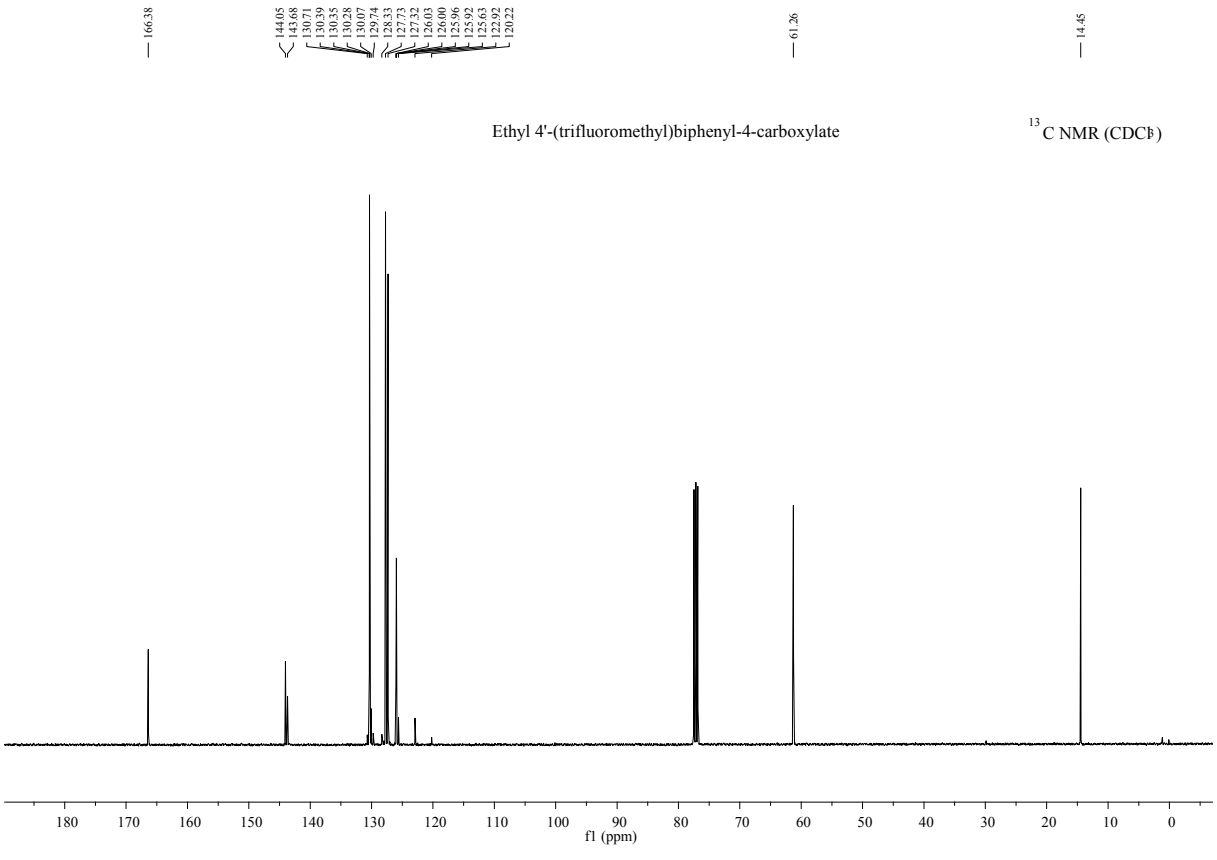


(4'-(trifluoromethyl)biphenyl-4-yl)(phenyl)methanone ^{13}C NMR (CDCl$_3$)

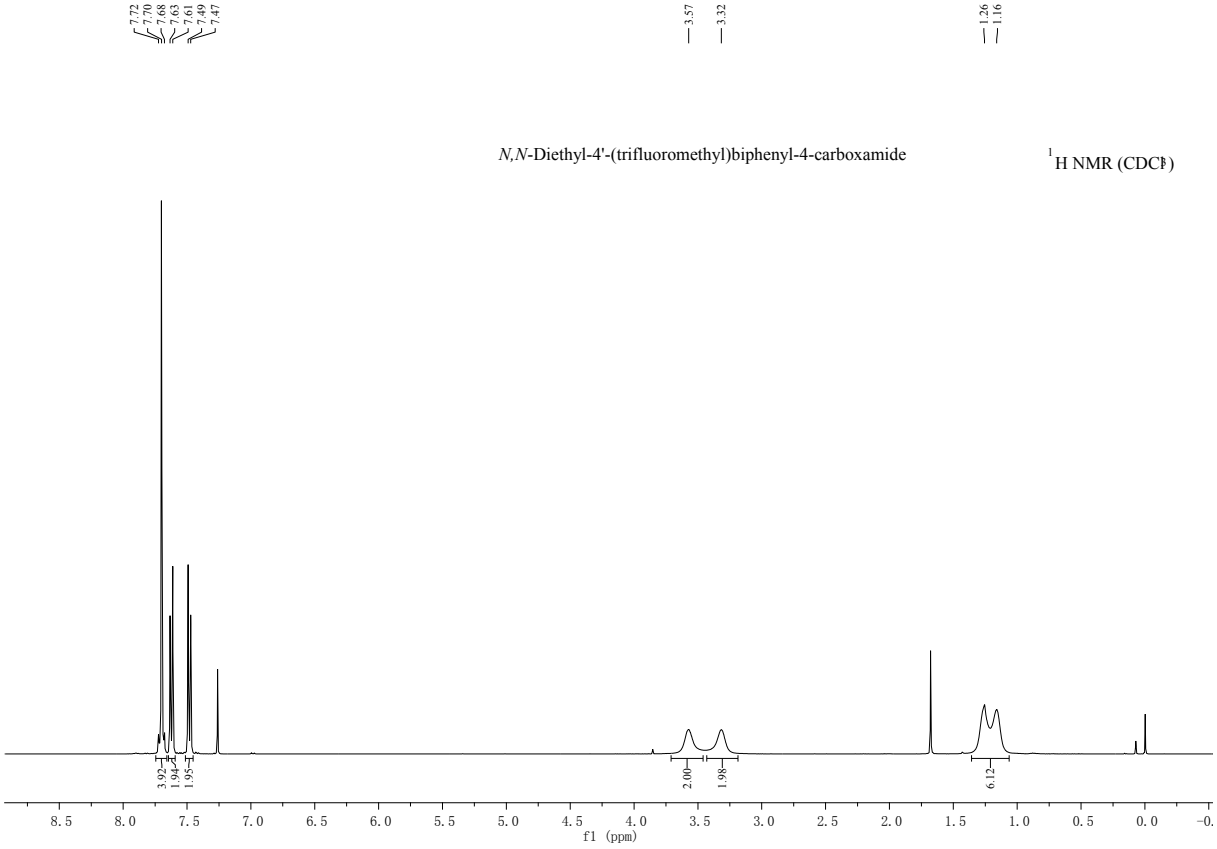


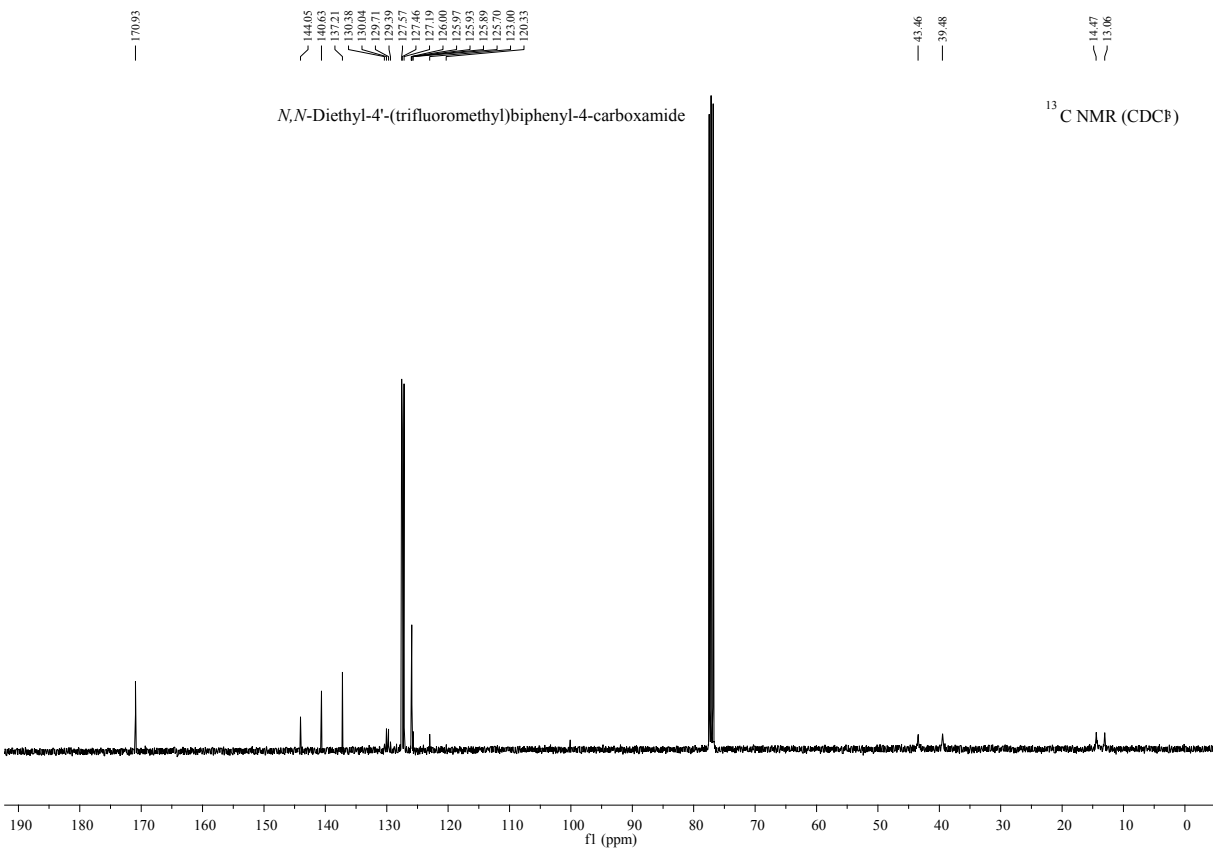
44. Ethyl 4'-(trifluoromethyl)biphenyl-4-carboxylate



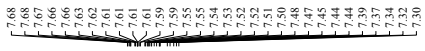


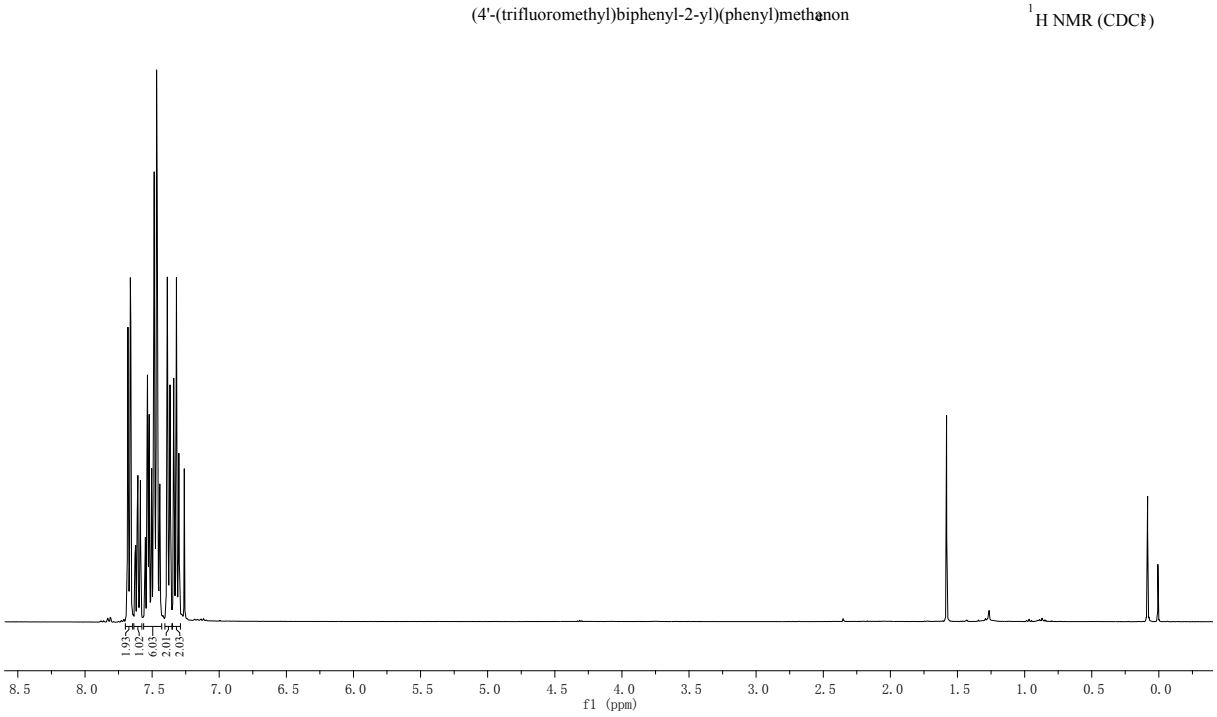
45. *N,N*-Diethyl-4'-(trifluoromethyl)biphenyl-4-carboxamide

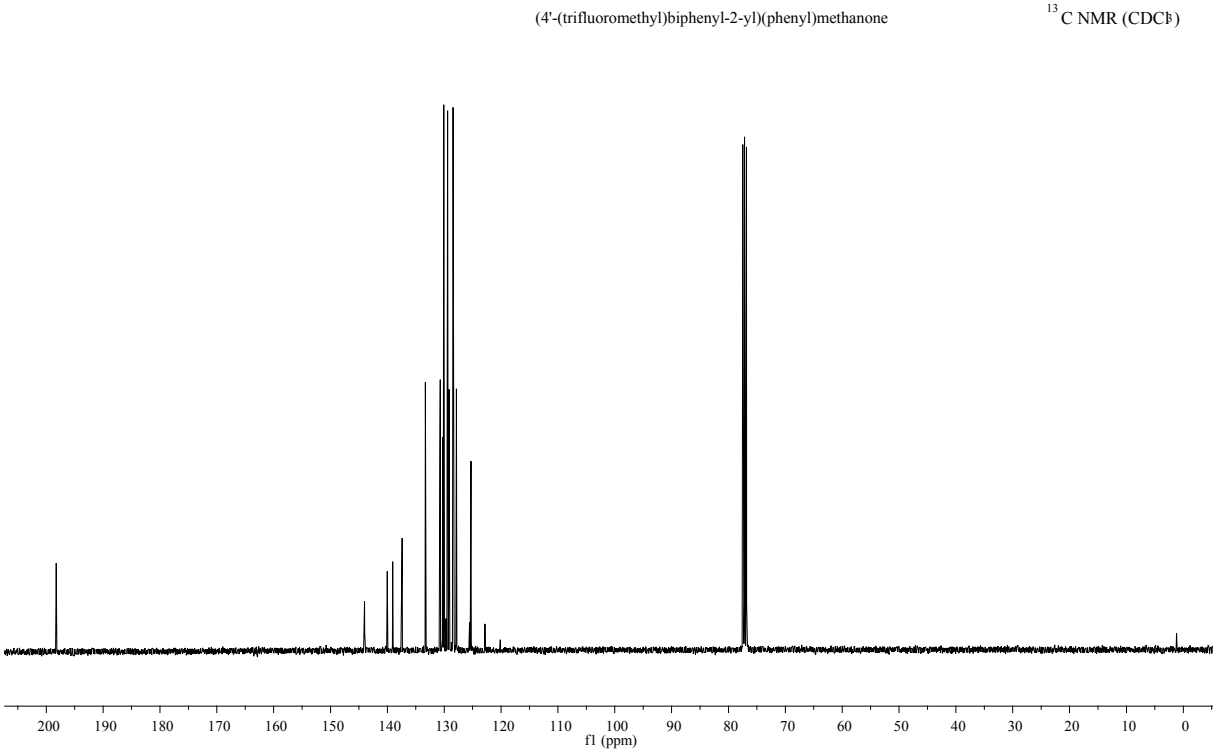




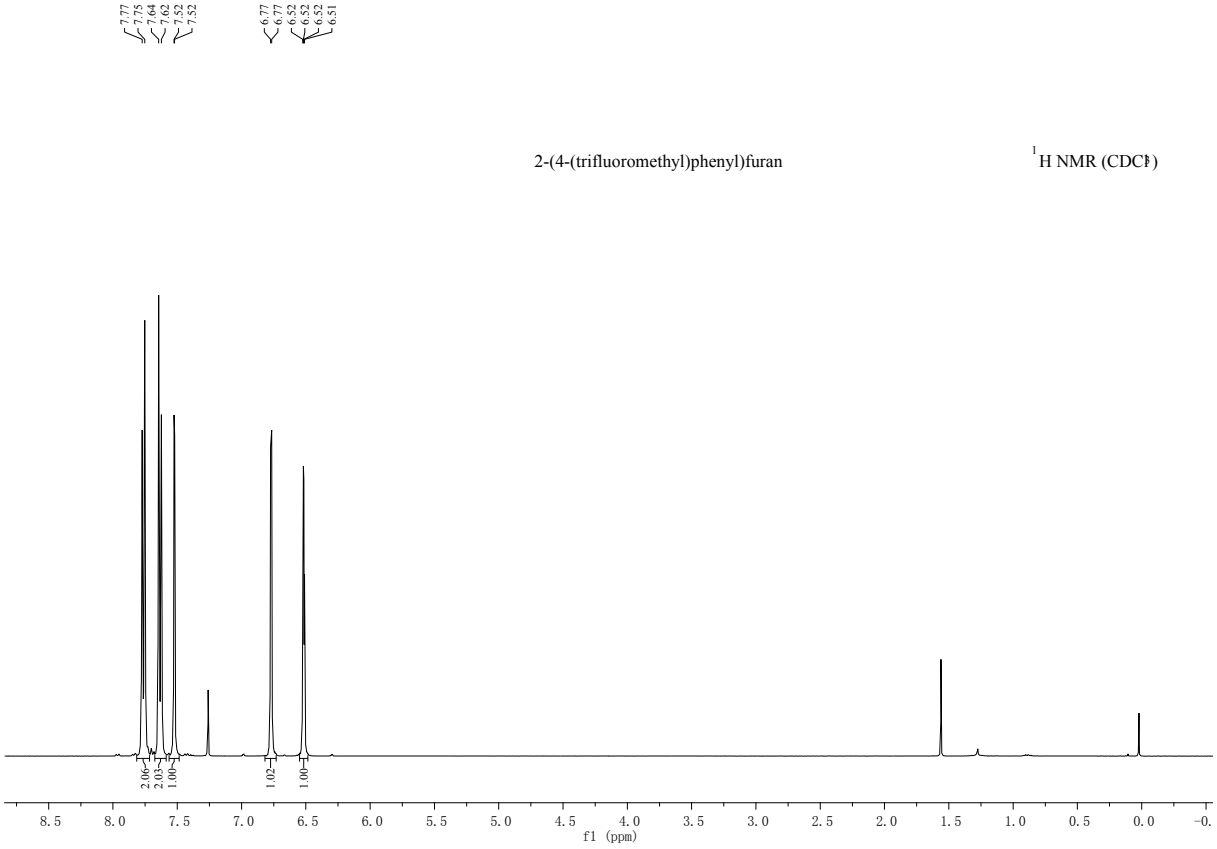
46. (4'-(trifluoromethyl)biphenyl-2-yl)(phenyl)methanone

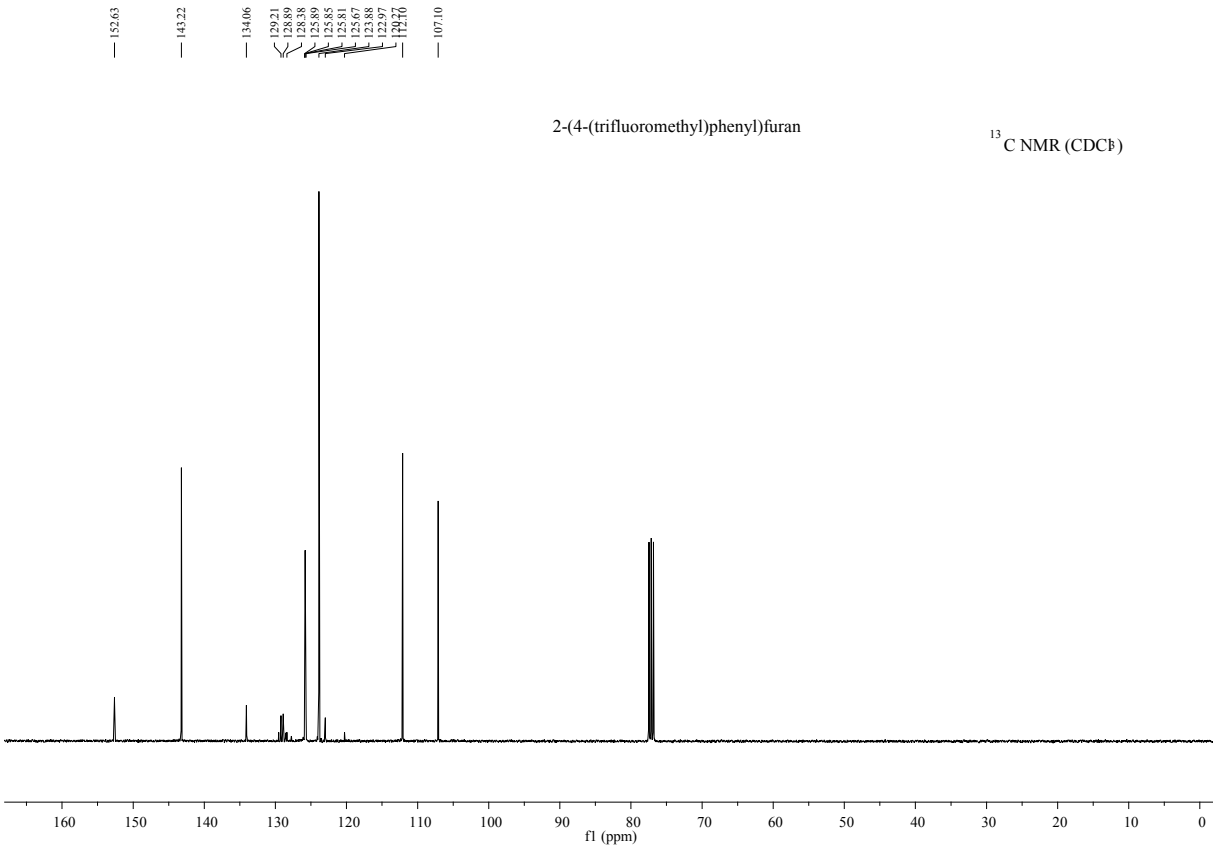






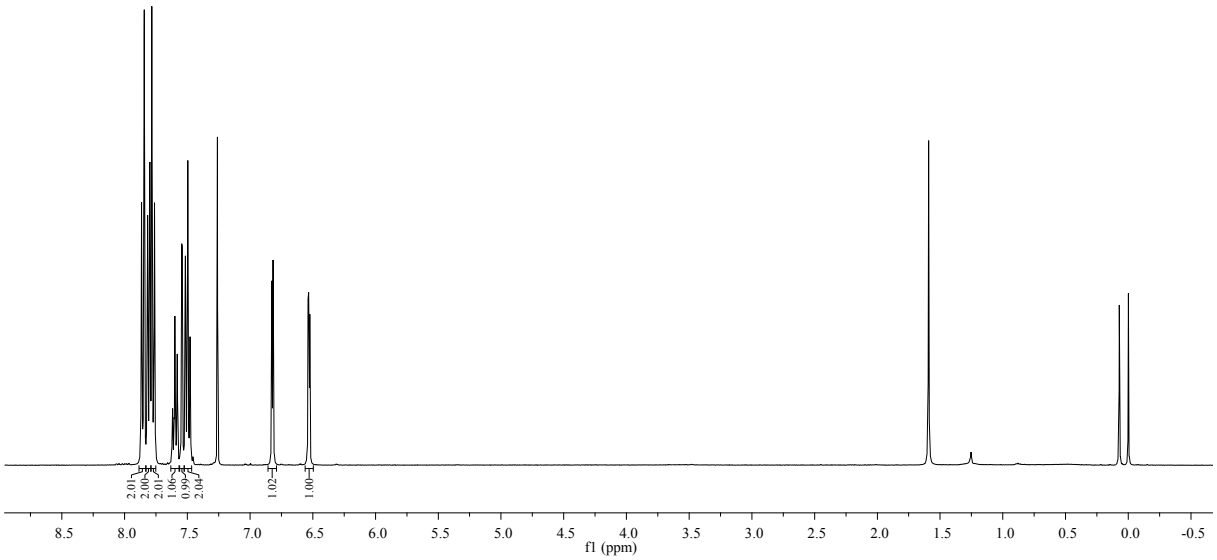
47. 2-(4-(trifluoromethyl)phenyl)furan



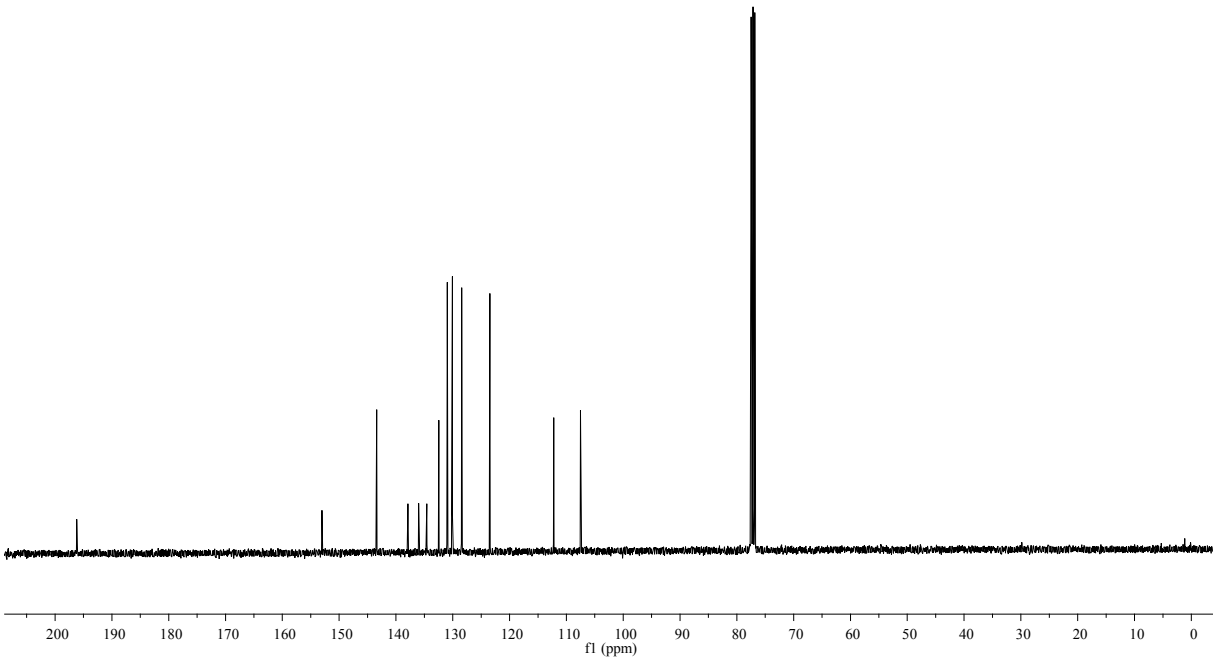


48. (4-(Furan-2-yl)phenyl)(phenyl)methanone

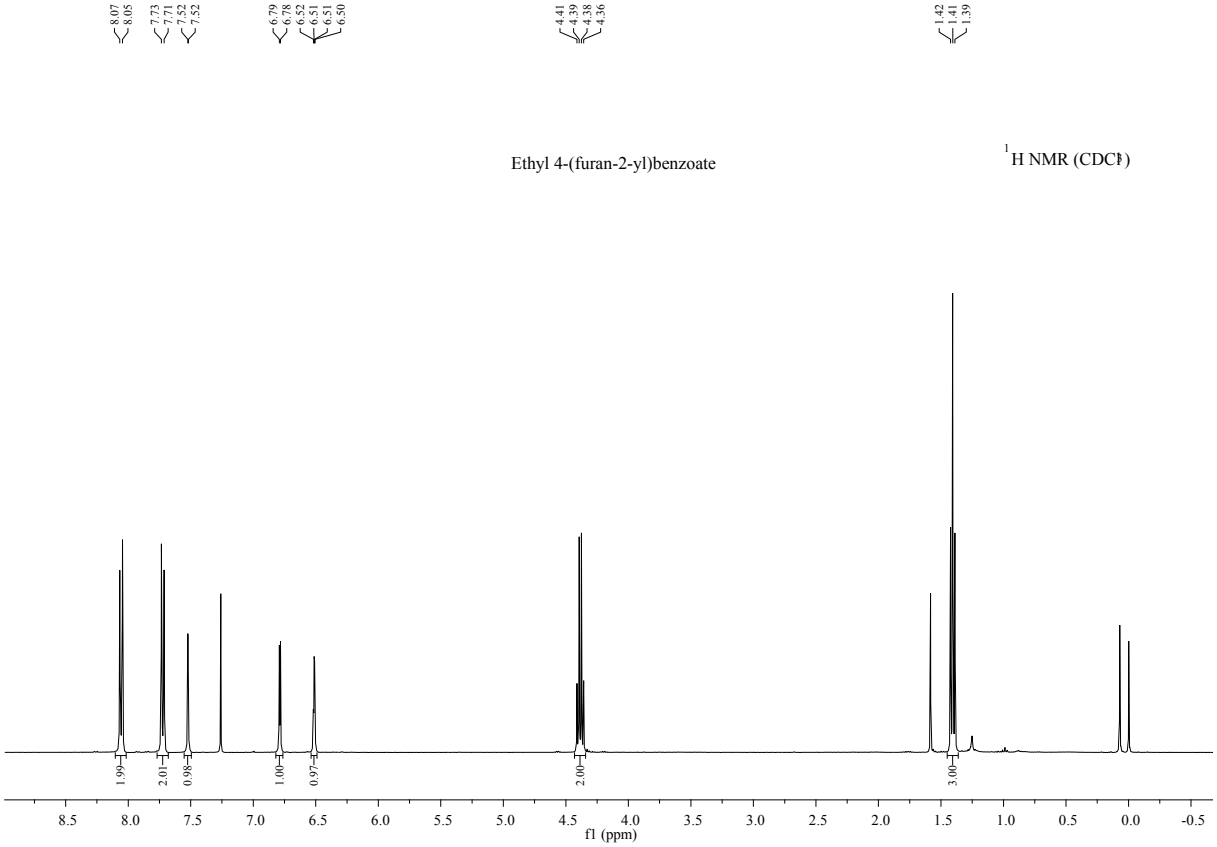
(4-(Furan-2-yl)phenyl)(phenyl)methanone ^{1}H NMR (CDCl$_3$)

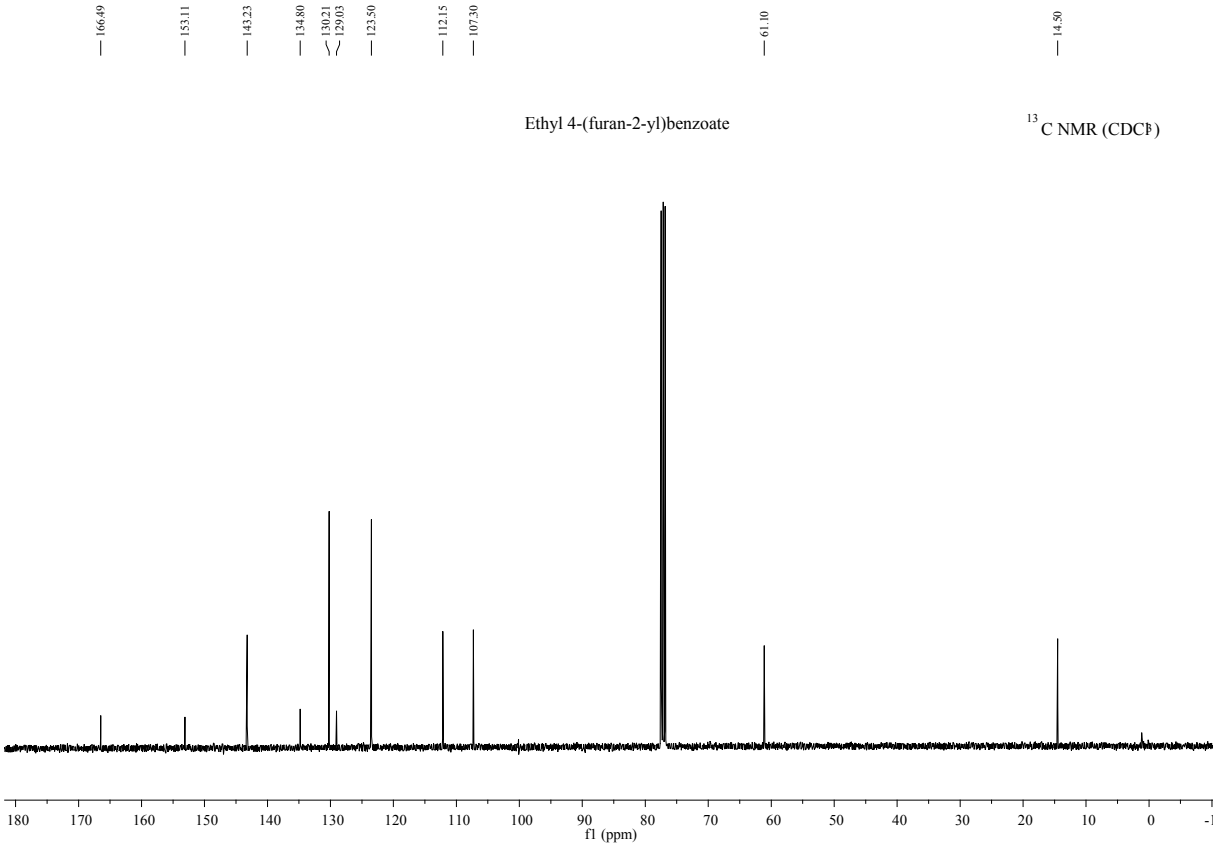


(4-(Furan-2-yl)phenyl)(phenyl)methanone ^{13}C NMR (CDCl$_3$)

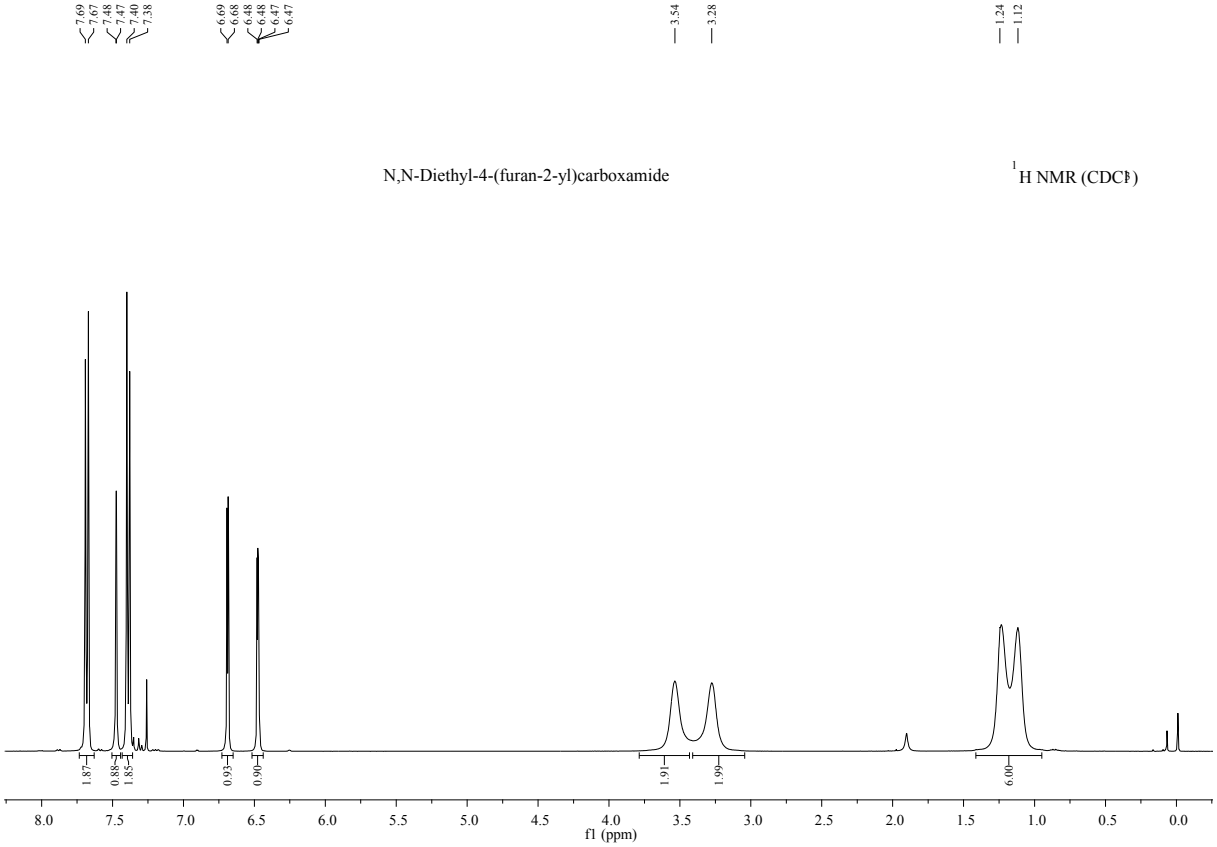


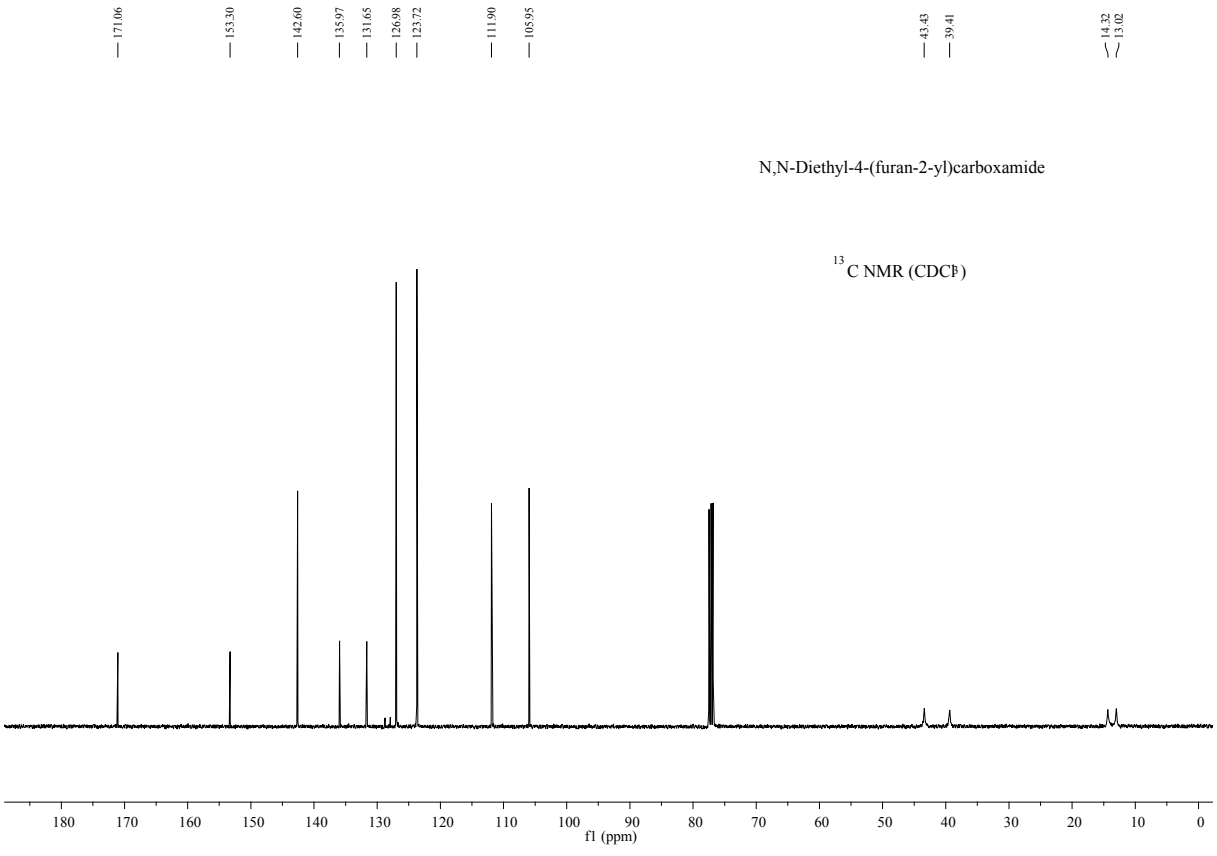
49. Ethyl 4-(furan-2-yl)benzoate





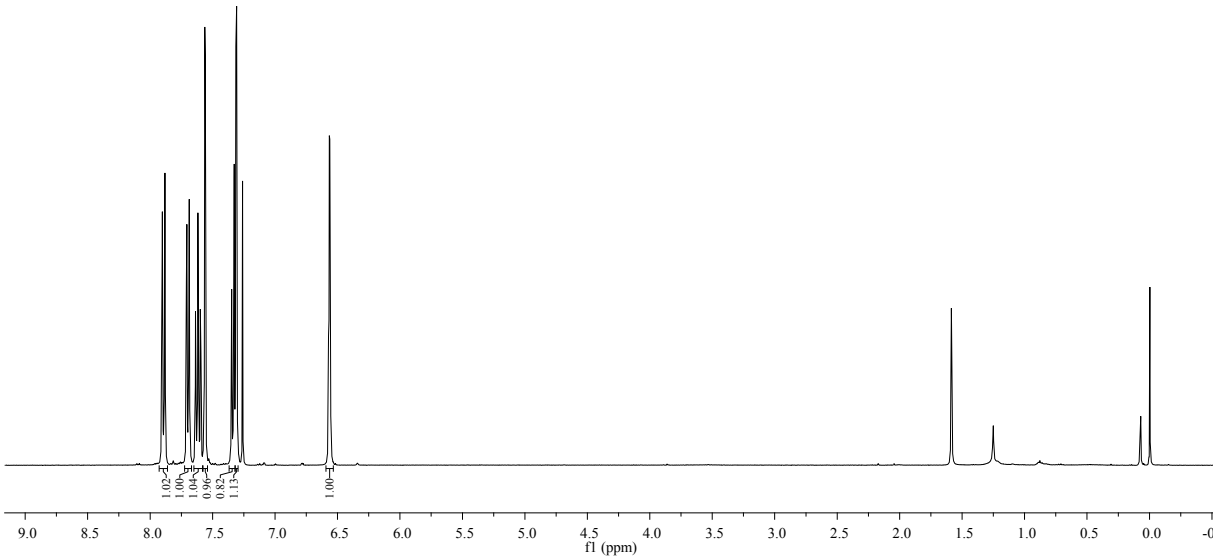
50. N,N-Diethyl-4-(furan-2-yl)carboxamide

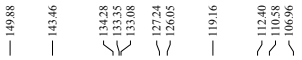




51. 2-Furan-2-yl-benzonitrile

2-Furan-2-yl-benzonitrile ^{1}H NMR (CDCl$_3$)





2-Furan-2-yl-benzonitrile ^{13}C NMR (CDCl$_3$)