Supporting Information

Cross-Coupling of Aryltrimethylammonium Iodides with Arylzinc Reagents Catalyzed by Amido Pincer Nickel Complexes

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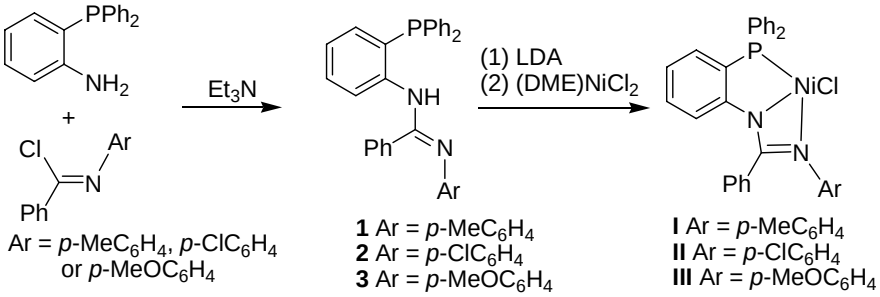
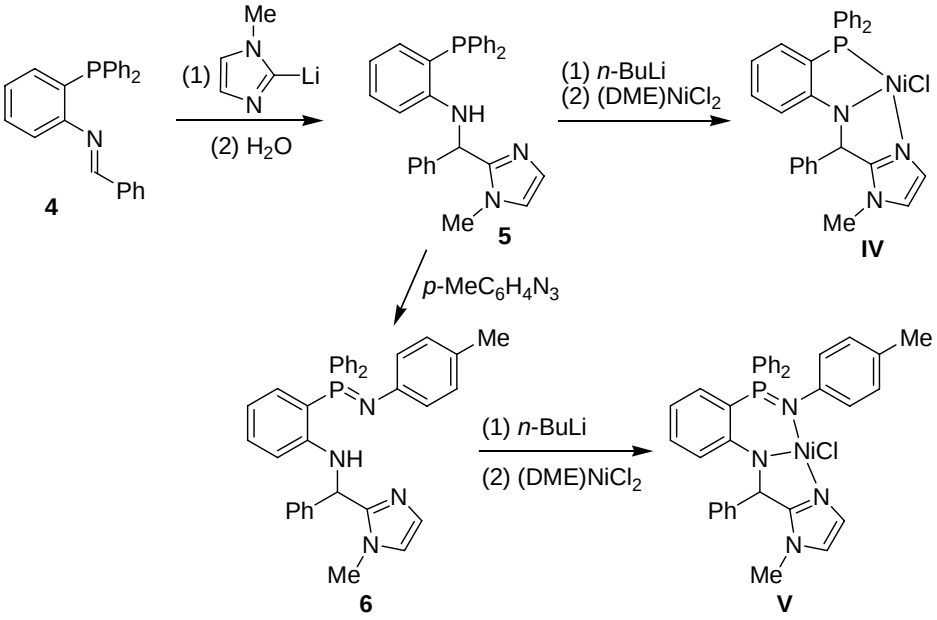
Scheme S1. Synthesis of complexes I-III



Scheme S2. Synthesis of complexes IV and V



Crystal Structure Determination: Single crystals of **I** were obtained from a mixed solvent of toluene and benzene. Single crystals of **V** were obtained by recrystallization of complex **V** from a mixed solvent of CH_2Cl_2 and toluene. The single crystals were mounted in Lindemann capillaries under nitrogen. Diffraction data were collected at 298(2) K using a area detector with graphite-monochromated Mo-K_α radiation (λ = 0.71073 Å). The structures were solved by direct methods using SHELXS-97[1] and refined against F^2 by full-matrix least squares using SHELXL-97.[2] Hydrogen atoms were placed in calculated positions. Crystal data and experimental details of the structure determinations are listed in Table S1.

Table S1. Details of the X-ray structure determinations of complexes I and V

	I·0.5C_6H_6	**V**·0.5C_7H_8
Empirical formula	$C_{35}H_{29}ClN_2NiP$	$C_{79}H_{72}Cl_2N_8Ni_2P_2$
Formula mass	602.73	1383.71
Crystal system	Triclinic	Triclinic
Space group	P-1	P-1
a (Å)	10.4293(11)	9.8520(9)
b (Å)	11.1260(14)	13.7371(14)
c (Å)	14.4551(17)	14.6279(16)
α (deg)	75.9010(10)	111.060(2)
β (deg)	87.844(2)	93.1010(10)
γ (deg)	70.9890(10)	106.5450(10)
V (Å^3)	1536.5(3)	1743.7(3)
Z	2	1
D_{calcd} (g/cm^3)	1.303	1.318
F(000)	626	722
μ (mm^{-1})	0.796	0.713
θ range for data collecn (deg)	1.45 to 25.02	1.52 to 25.02
No. of reflns collected	8096	9276
No. of indep reflns (R_{int})	5331 (R_{int} = 0.0268)	6089 (R_{int} = 0.0921)
No. of data/restraints/params	5331 / 0 / 362	6089 / 0 / 427
Goodness of fit on F^2	1.080	1.044
Final R indices[a] [I > 2σ(I)]	$R1$ = 0.0498 w$R2$ = 0.1163	$R1$ = 0.0863 w$R2$ = 0.1811
R indices (all data)	$R1$ = 0.0842 w$R2$ = 0.1266	$R1$ = 0.2567 w$R2$ = 0.2110
Largest diff peak and hole [e·Å^{-3}]	1.122 and –0.586	0.488 and –0.428

[a] $R1 = \Sigma \left| \left| Fo \right| - \left| Fc \right| \right| / \Sigma \left| Fo \right|$; $wR2 = \left[\Sigma w(Fo^2 - Fc^2)^2 / \Sigma w(Fo^4) \right]^{1/2}$

References

(1) Sheldrick, G. M. *Acta Crystallogr., Sect. A* **1990**, *46*, 467

(2) Sheldrick, G. M. *SHELXL97, Programs for structure refinement*, Universität Göttingen, **1997**.

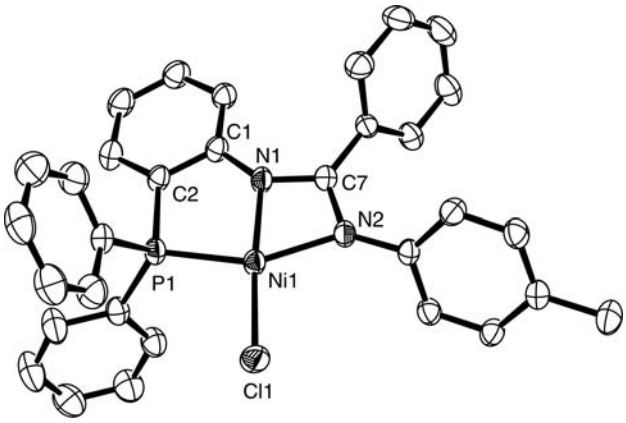


Figure S1. ORTEP drawing of complex I (30% probability. C_6H_6 molecule is omitted).

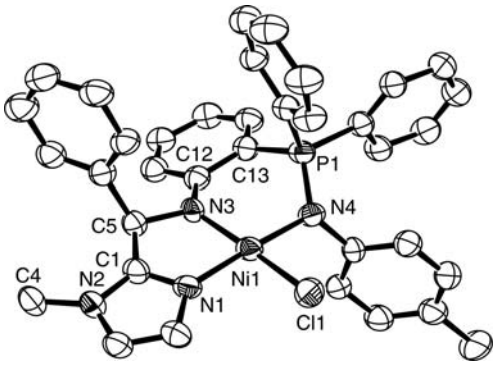
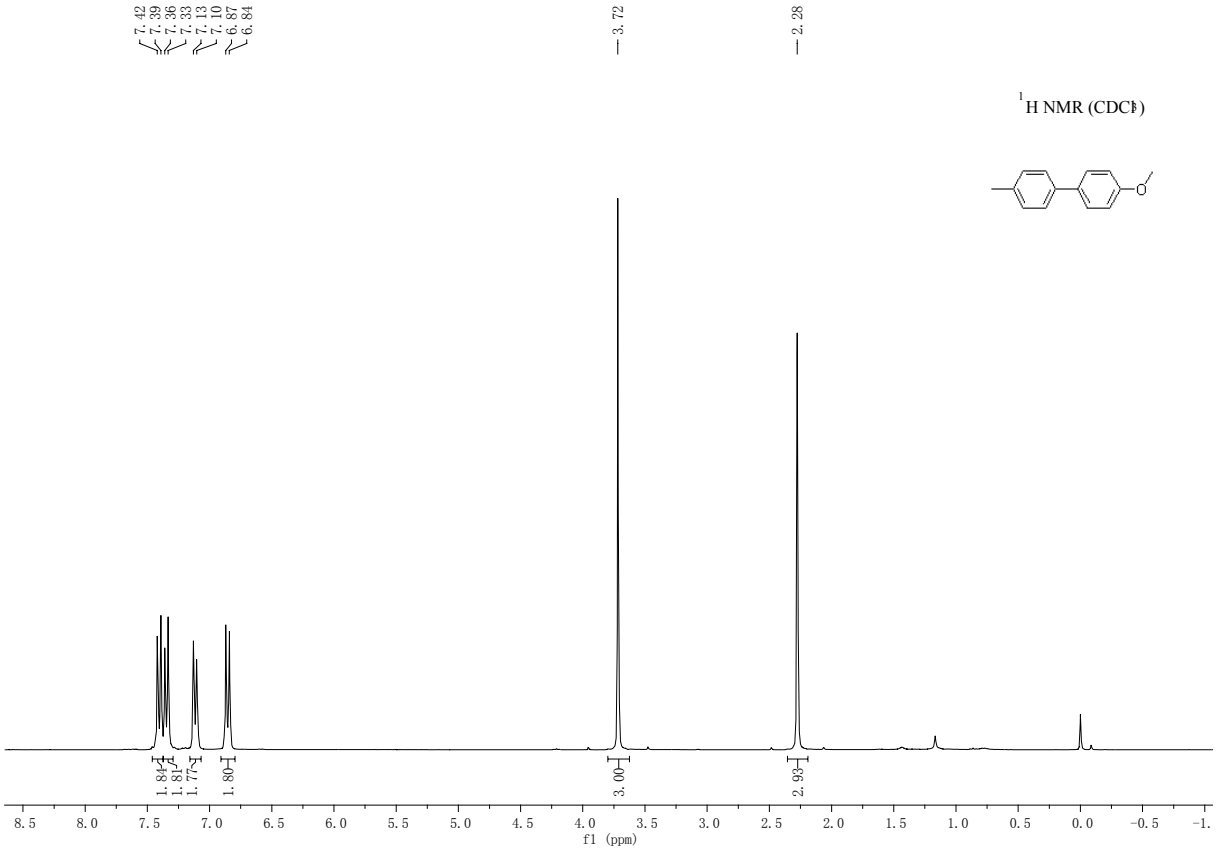
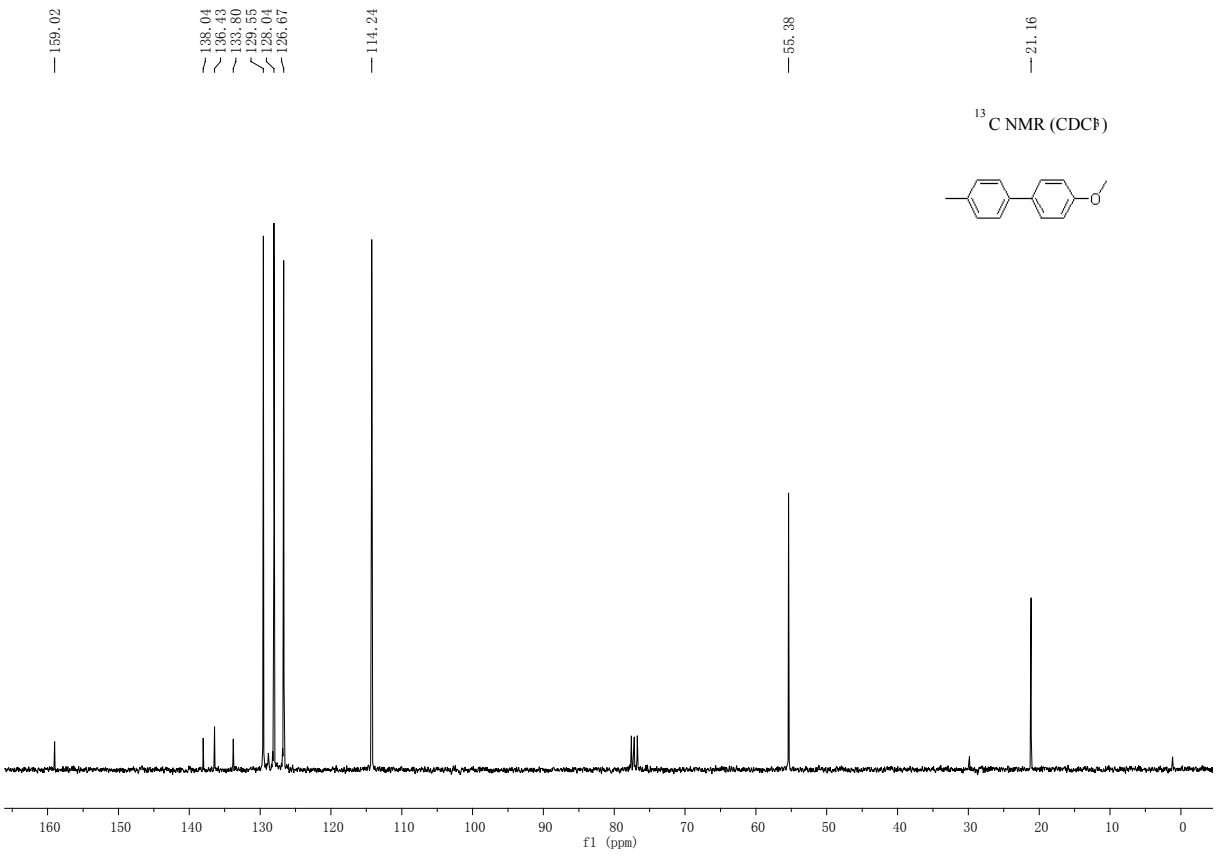


Figure S2. ORTEP drawing of complex V (30% probability. Toluene molecule is omitted).

NMR spectra

(1) 4-Methoxy-4'-methylbiphenyl





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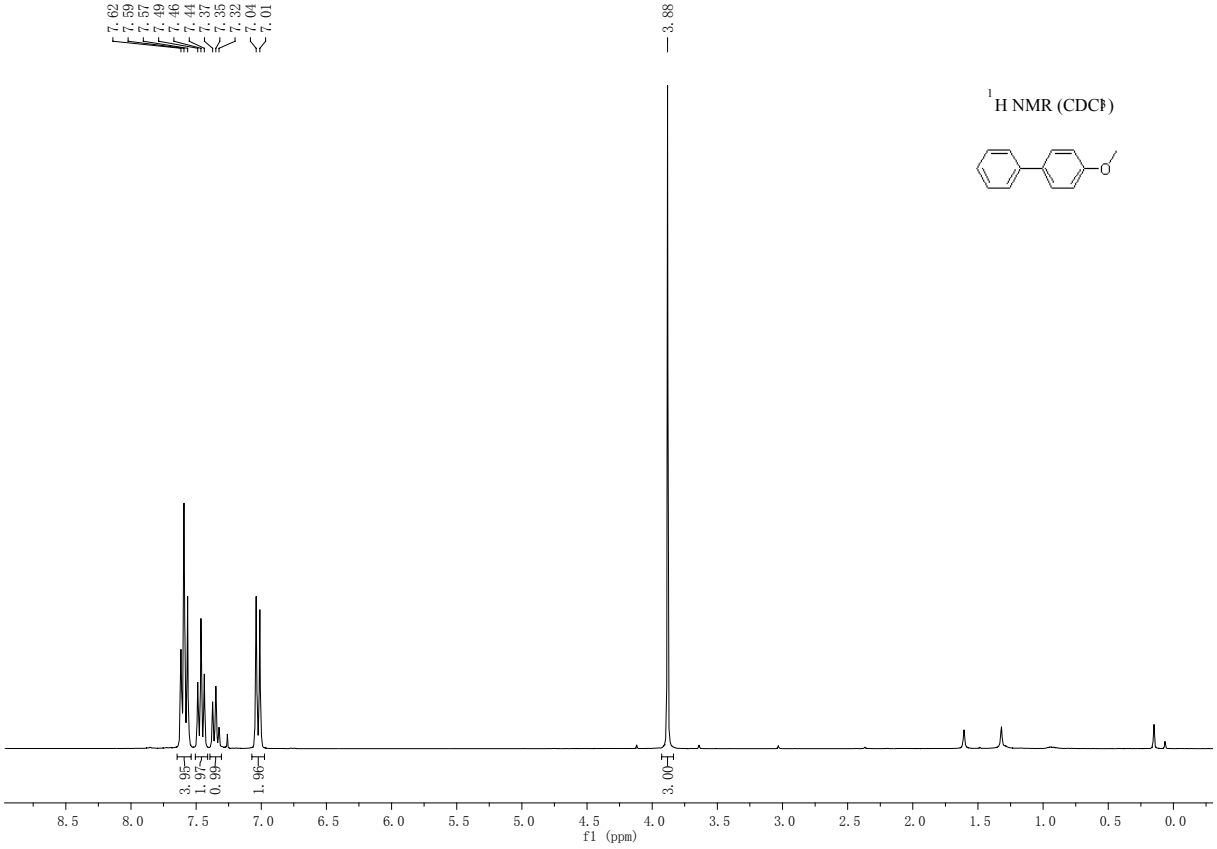

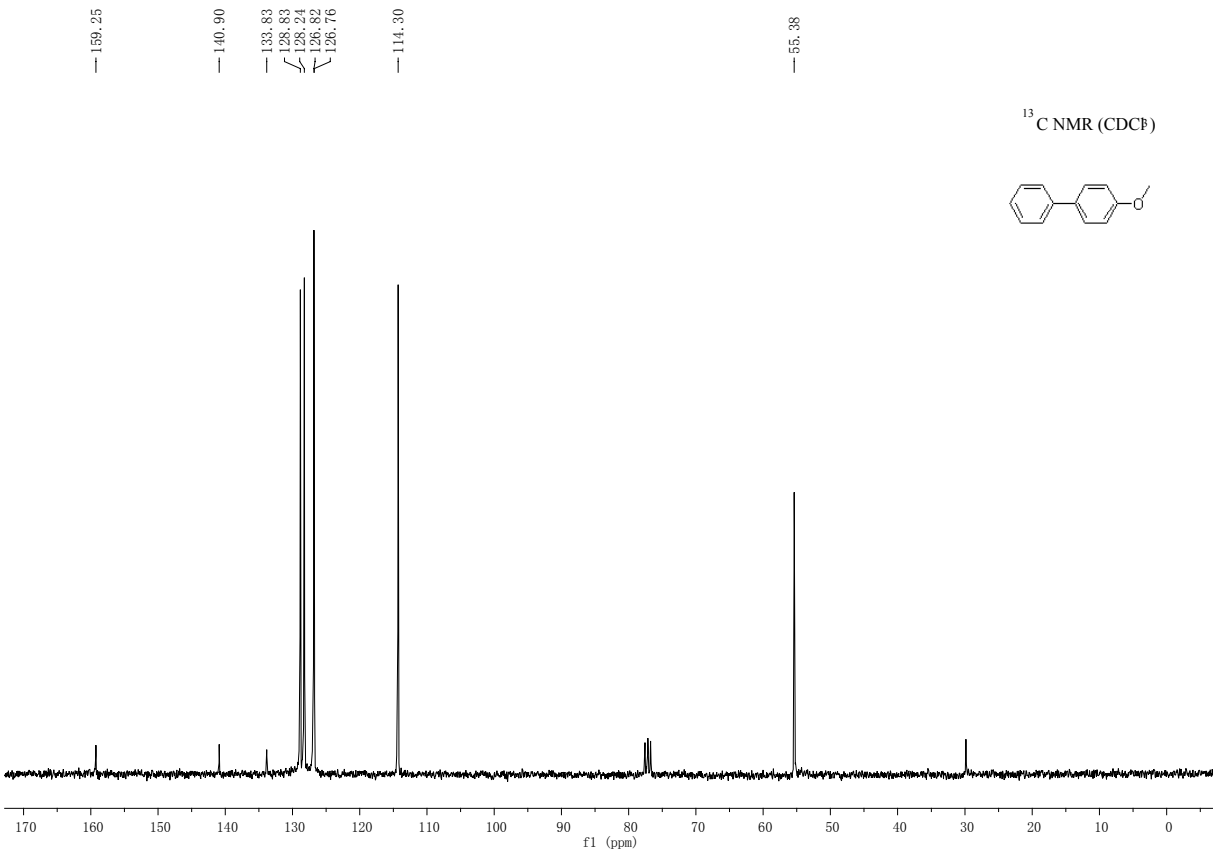

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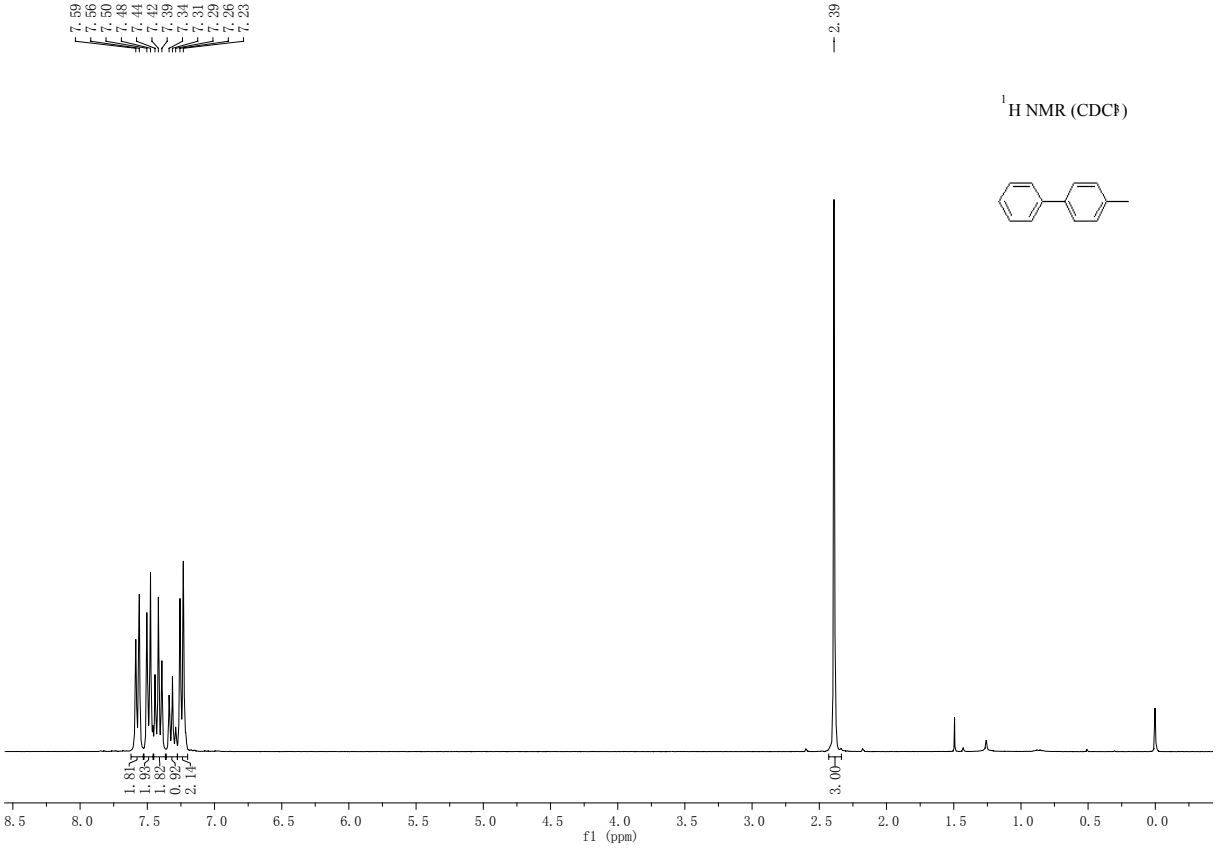

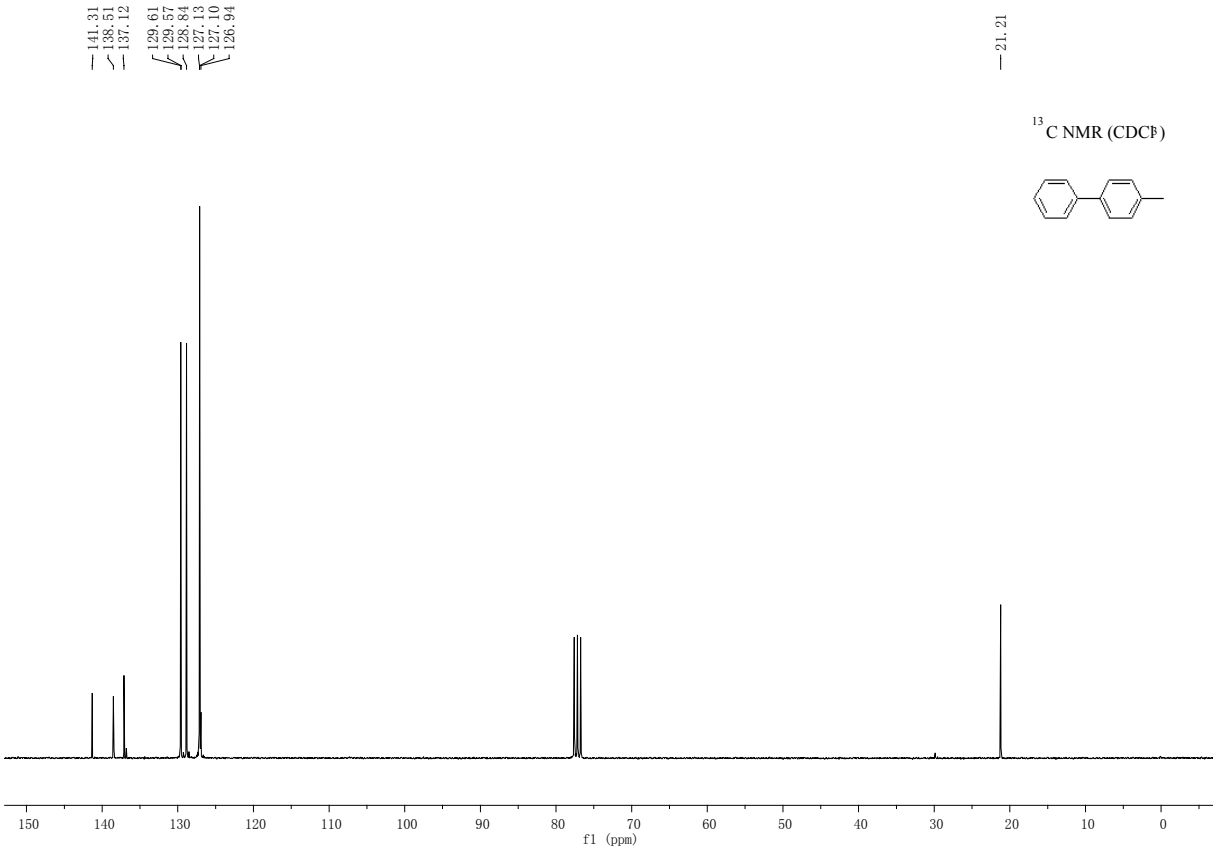

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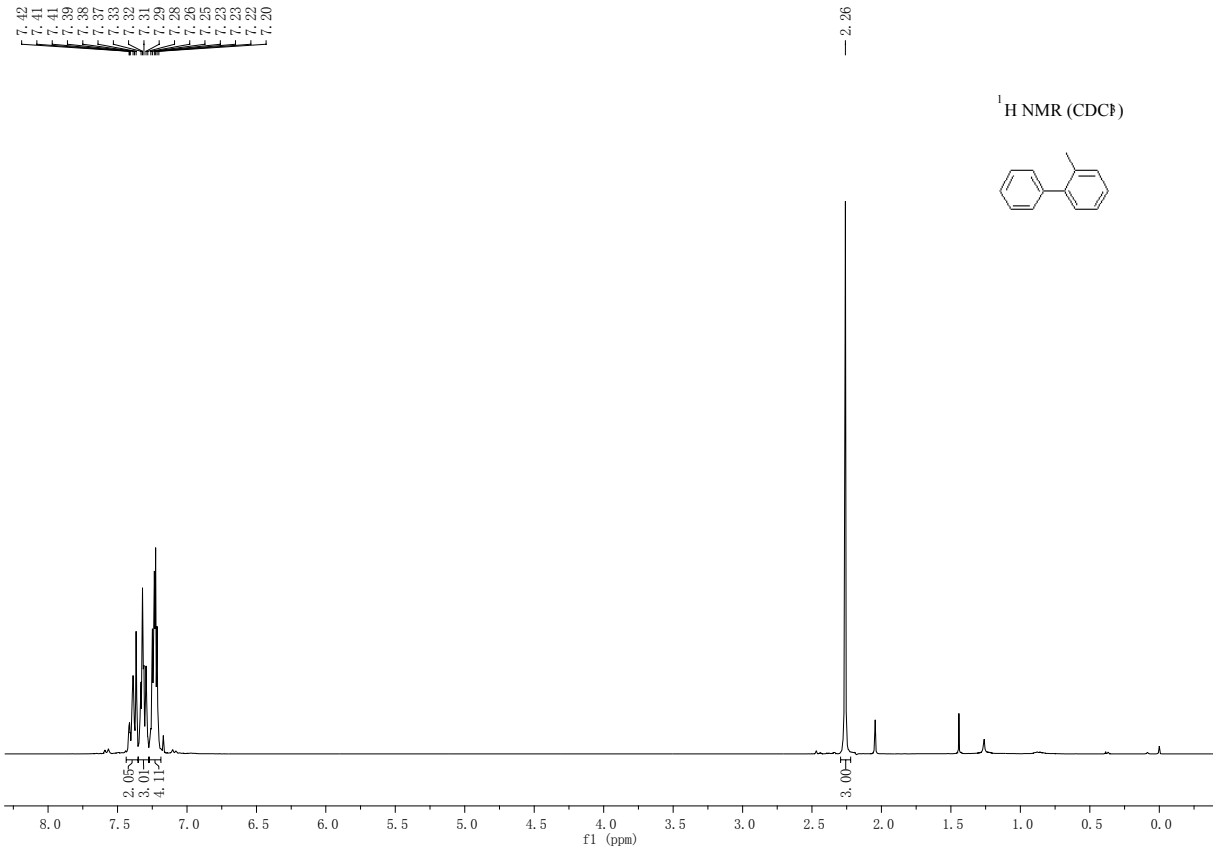

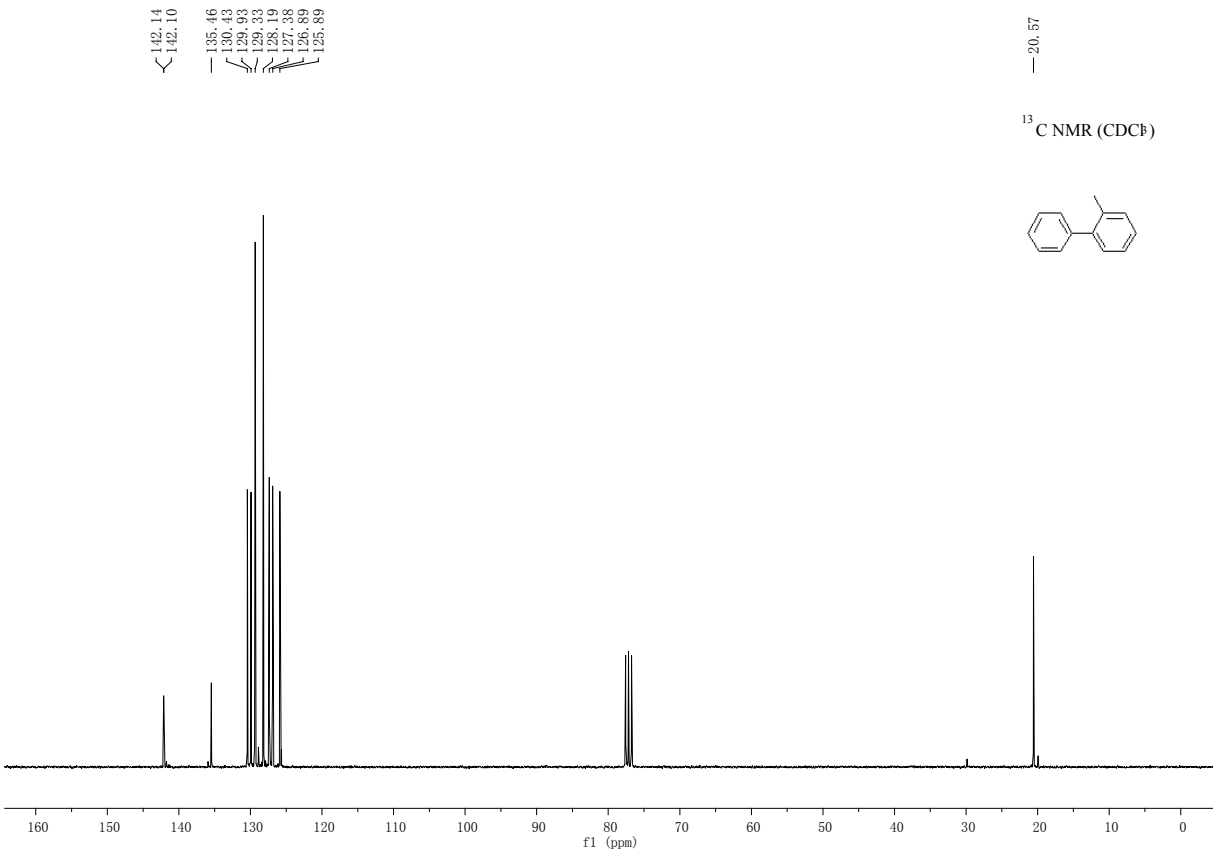

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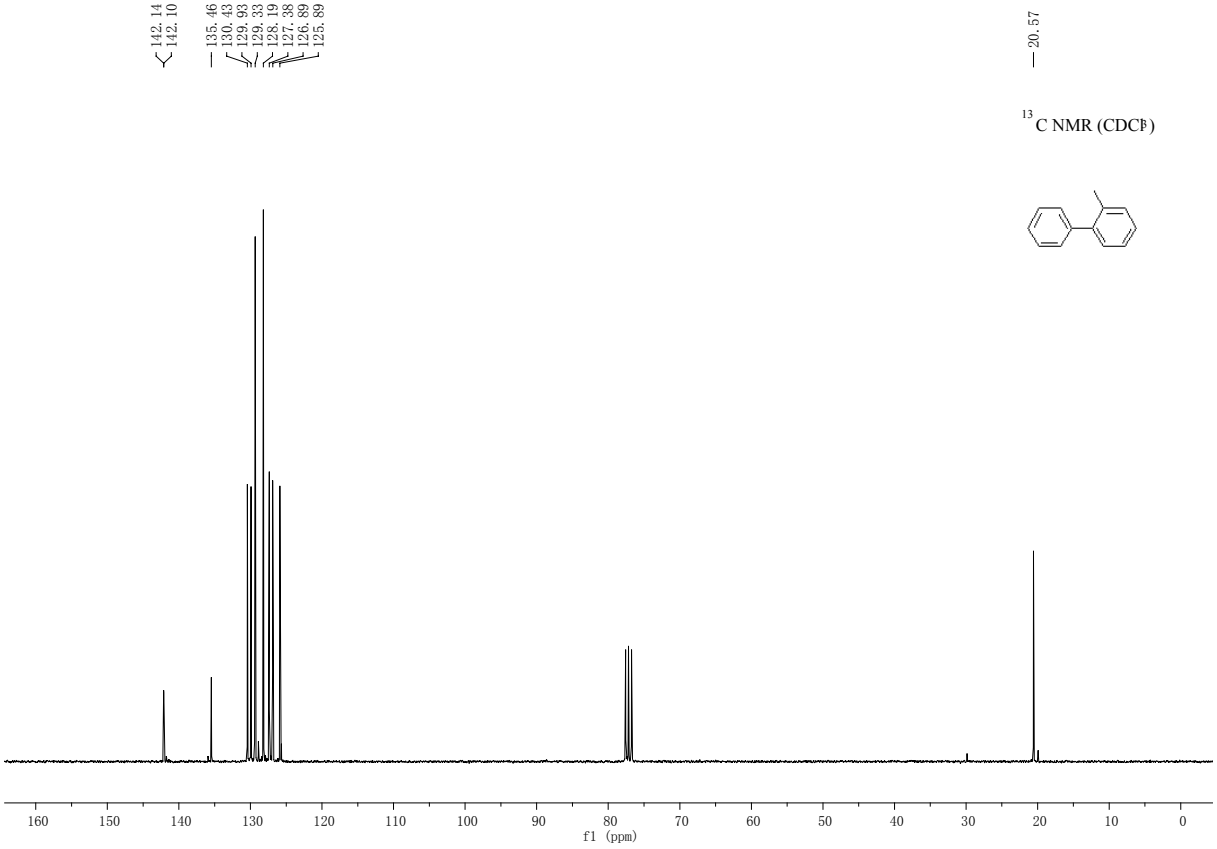

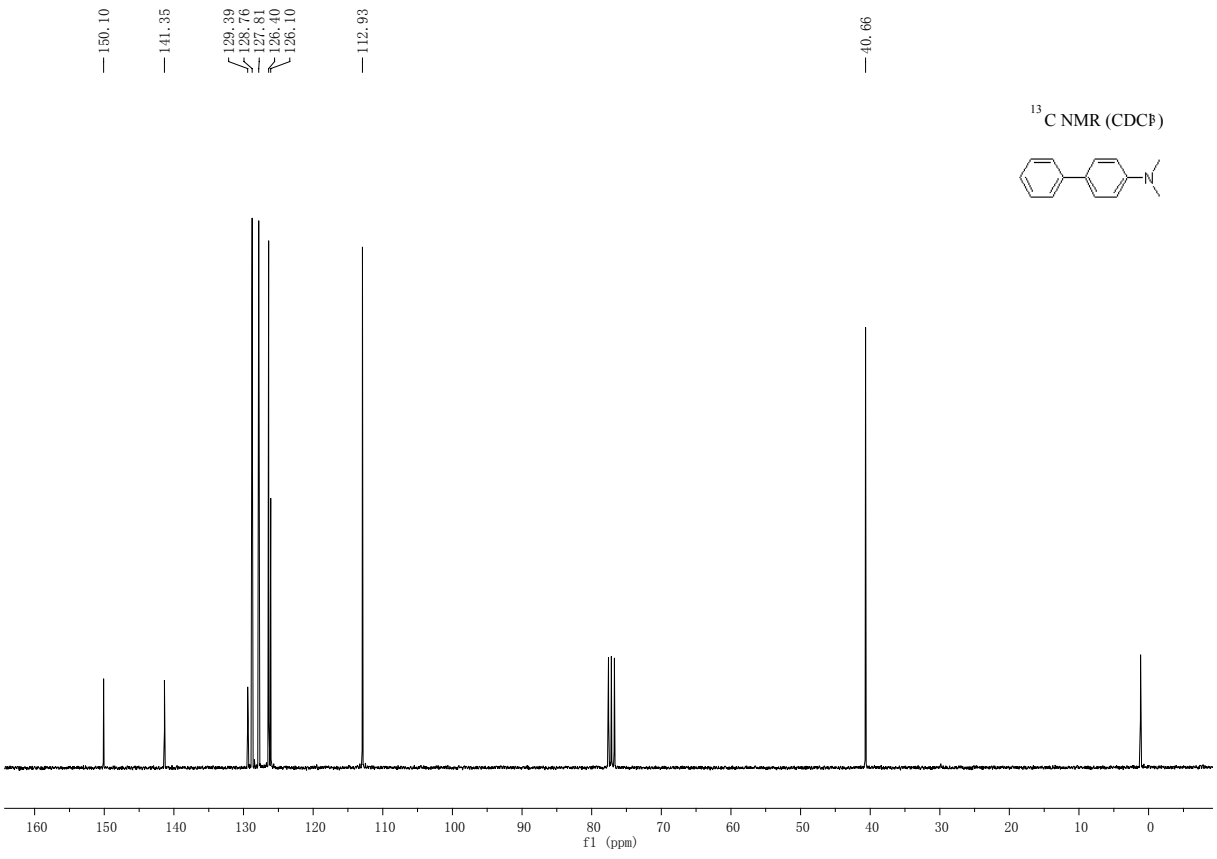

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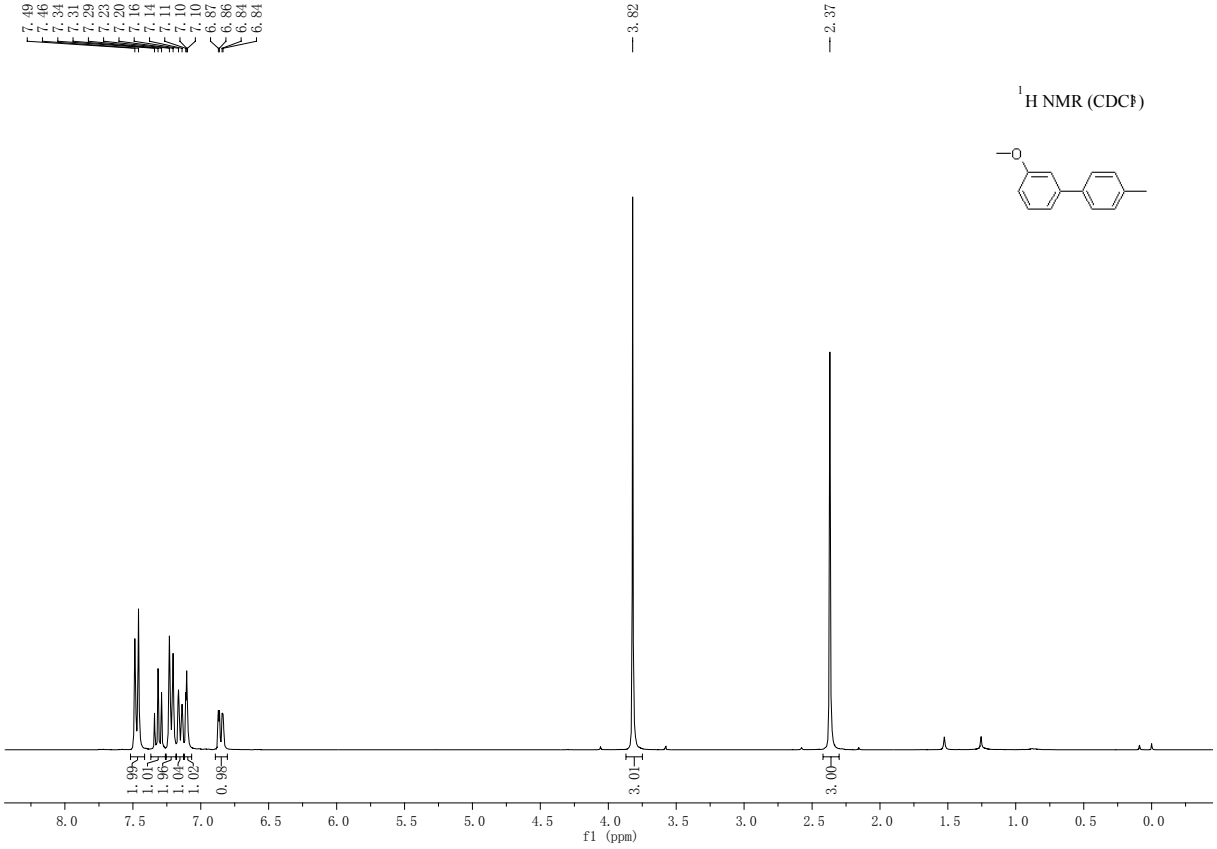
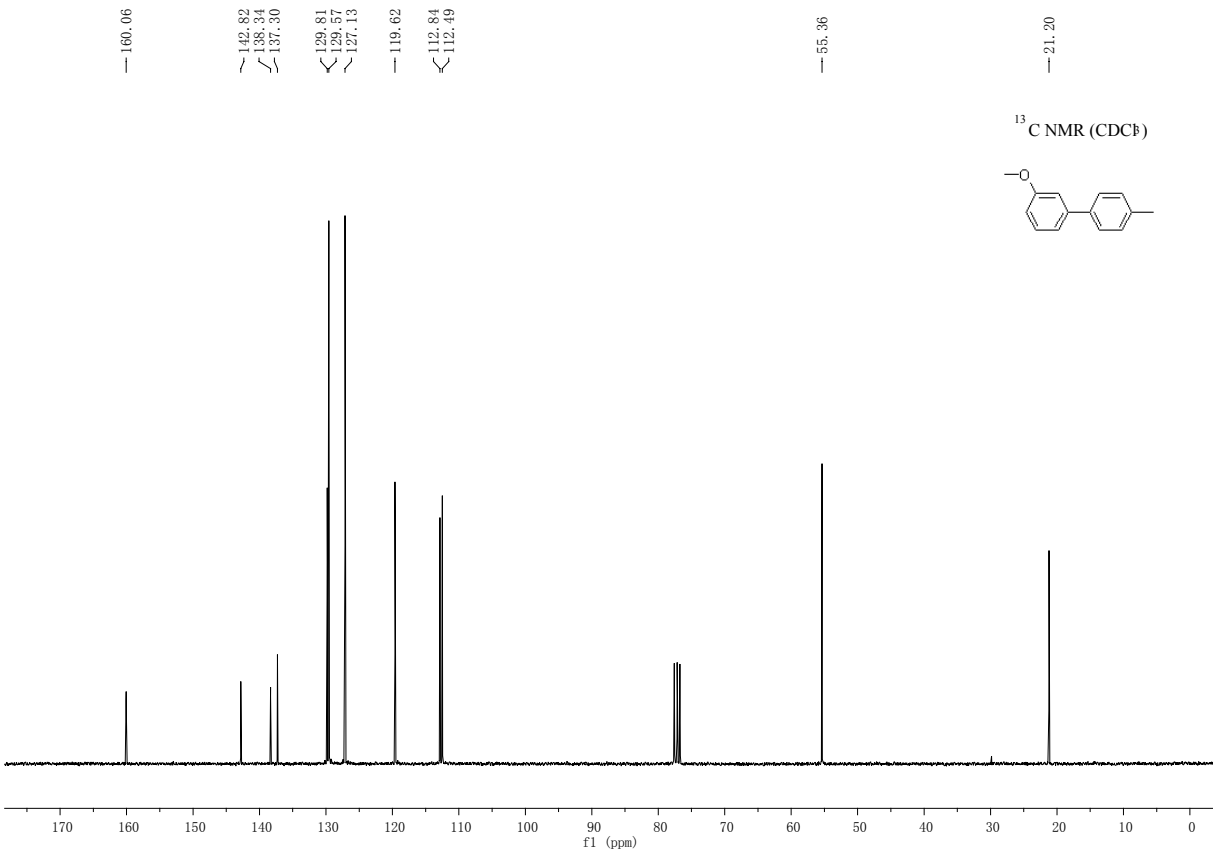
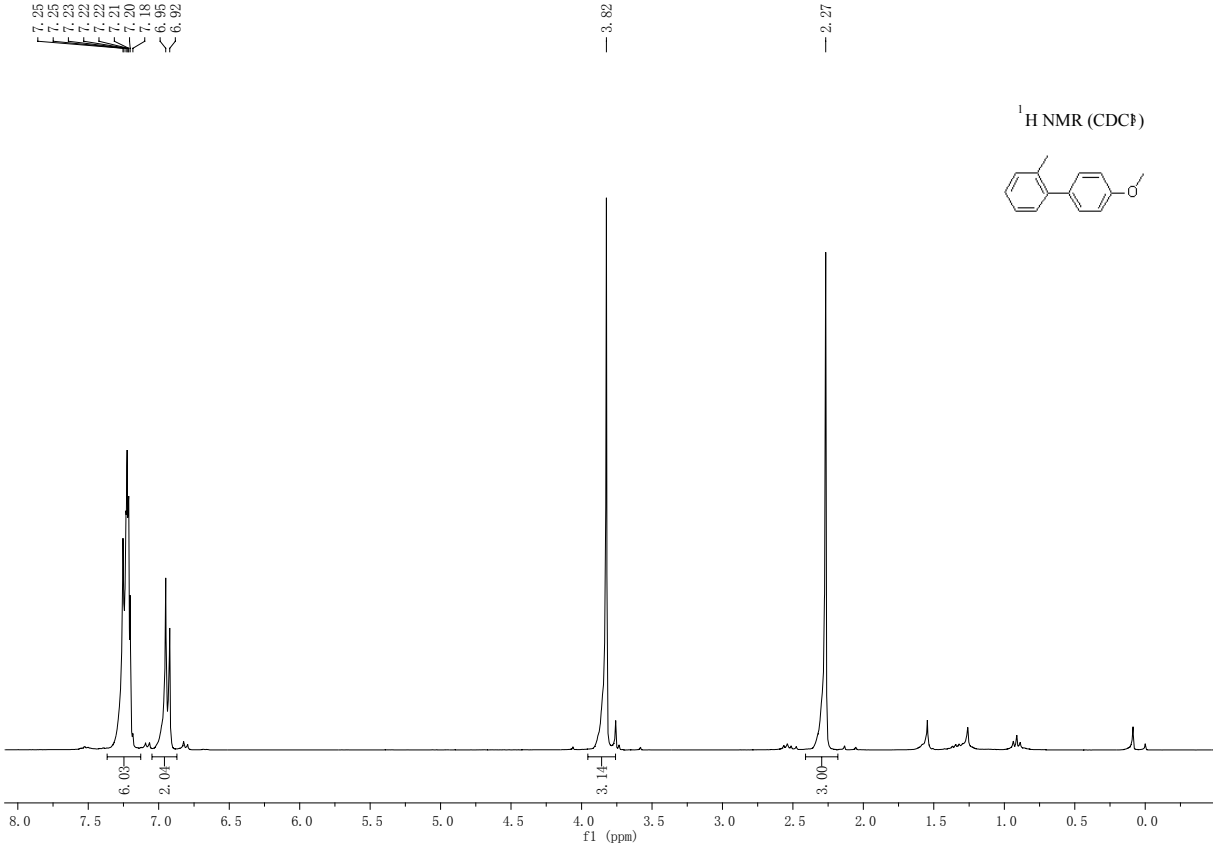
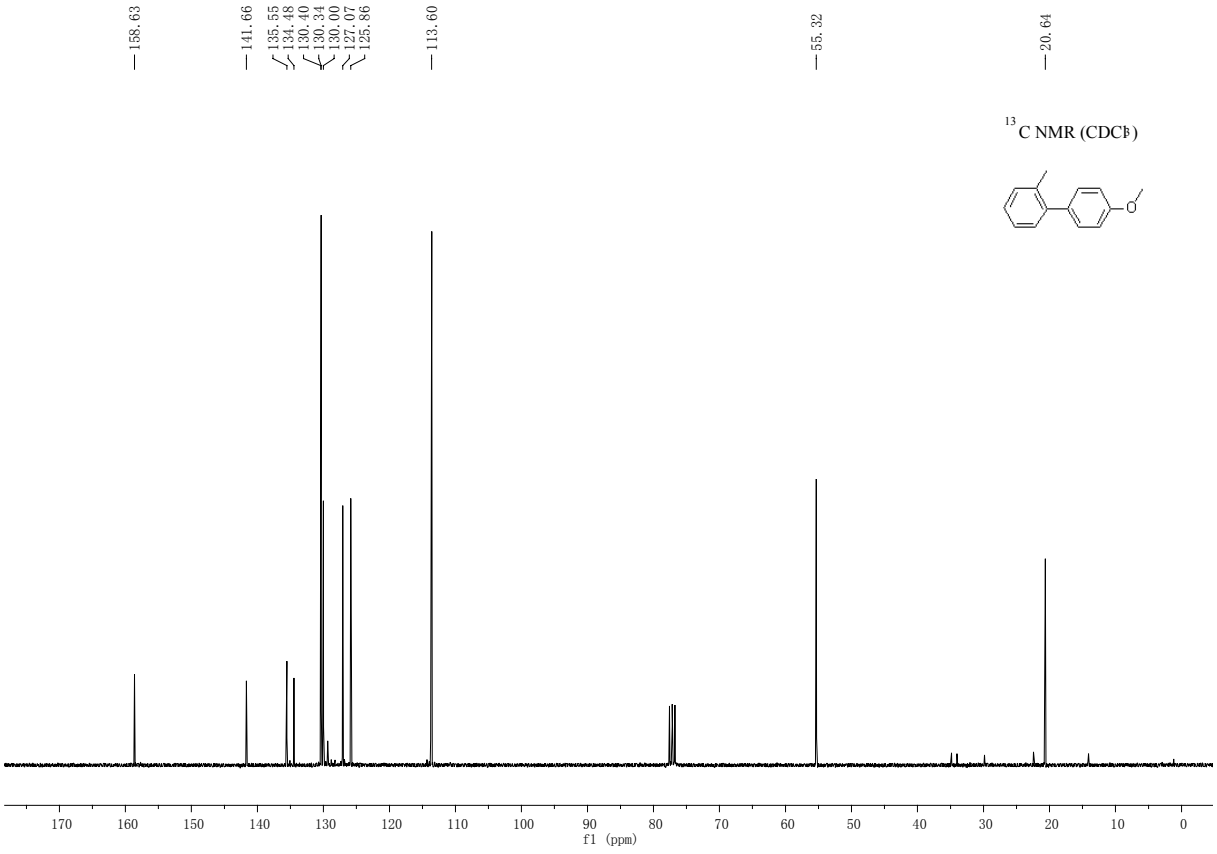


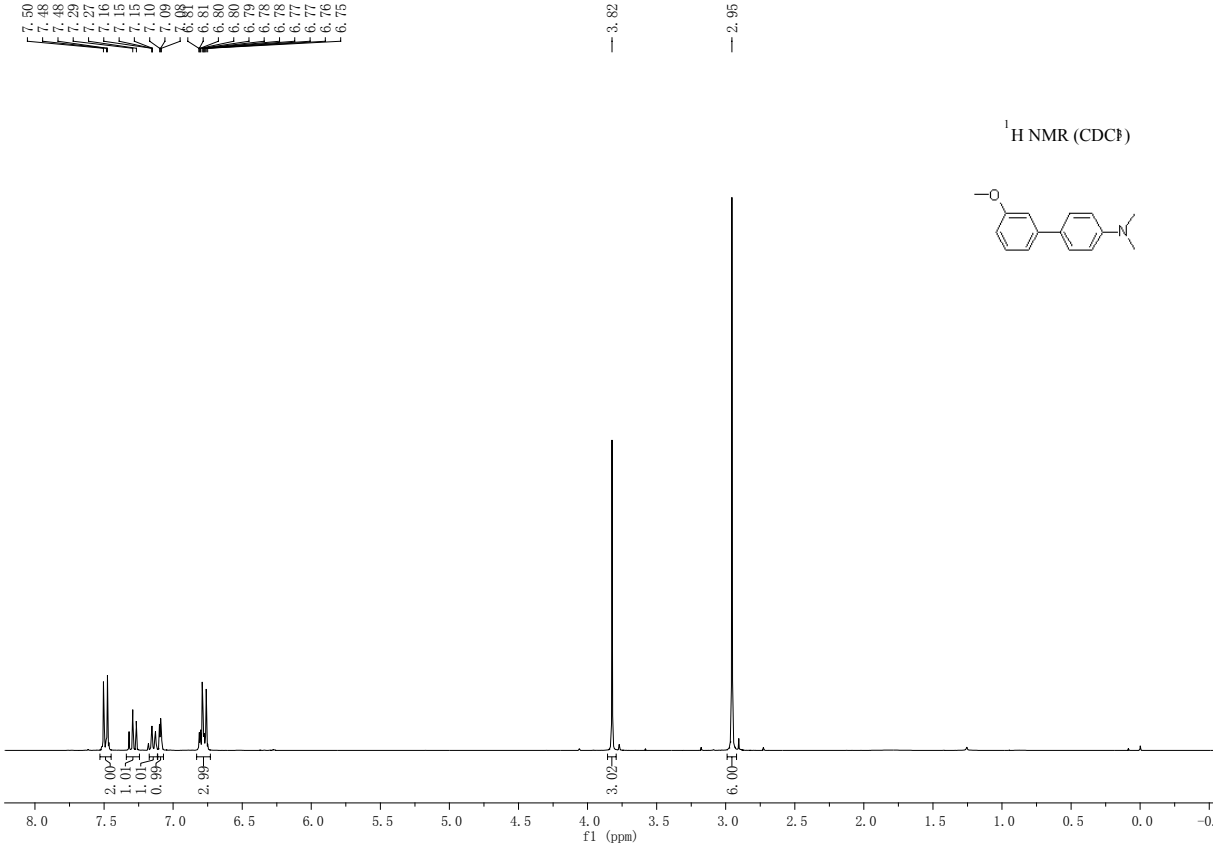


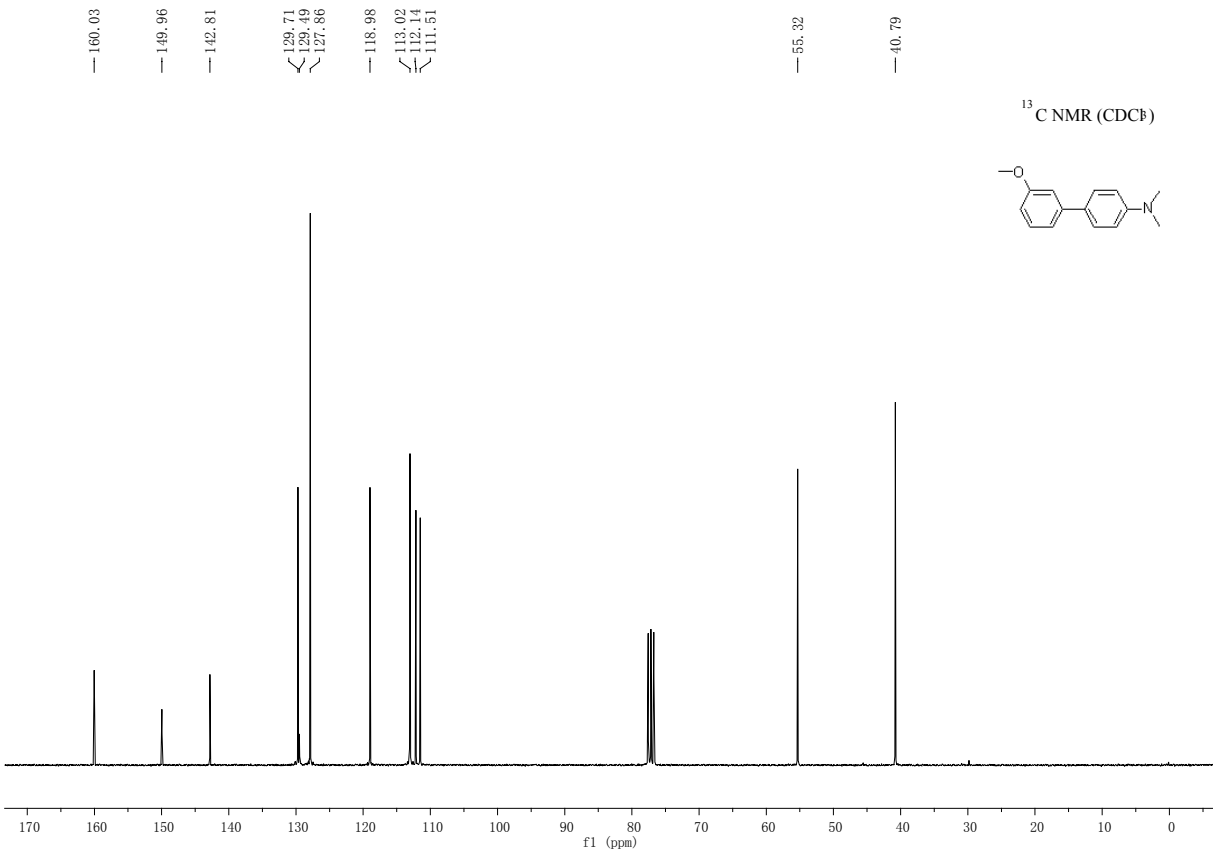
(7) 1-(4-Methoxyphenyl)-2-methylbenzene



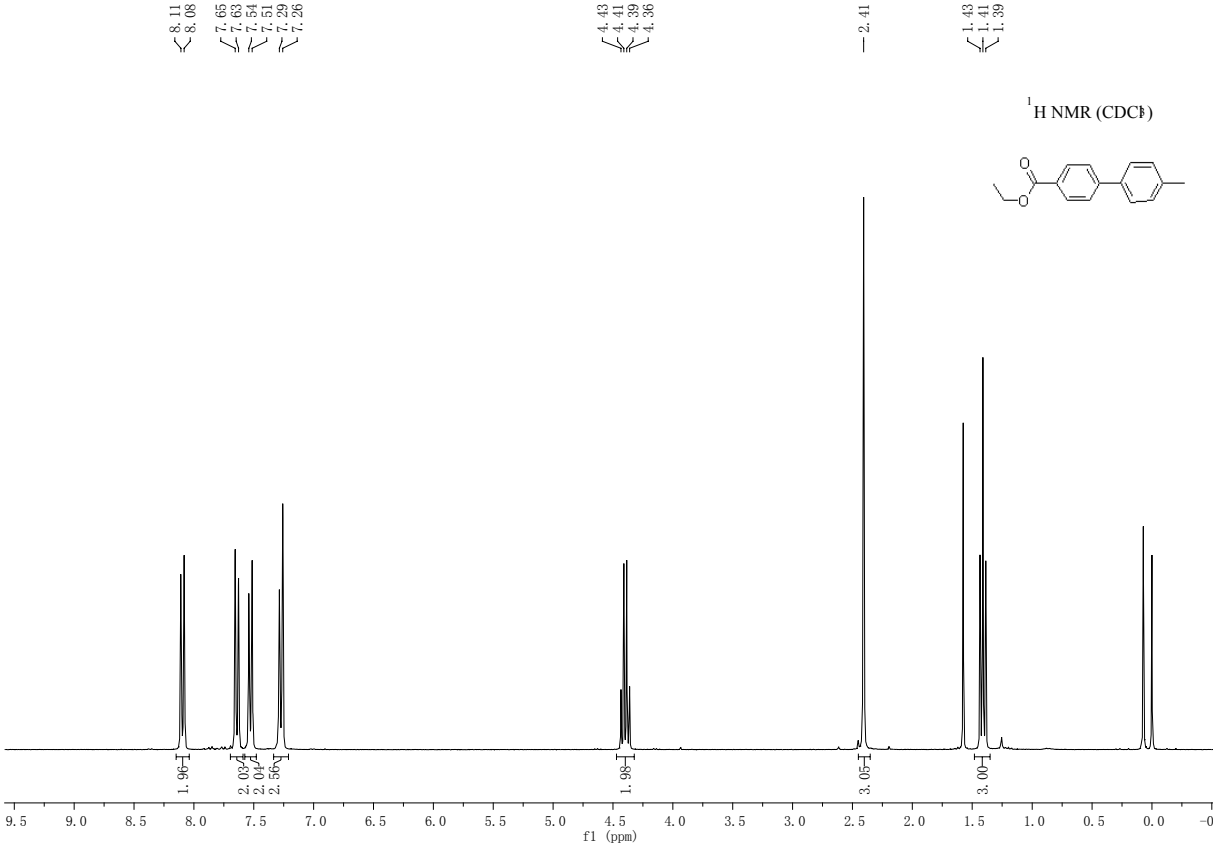


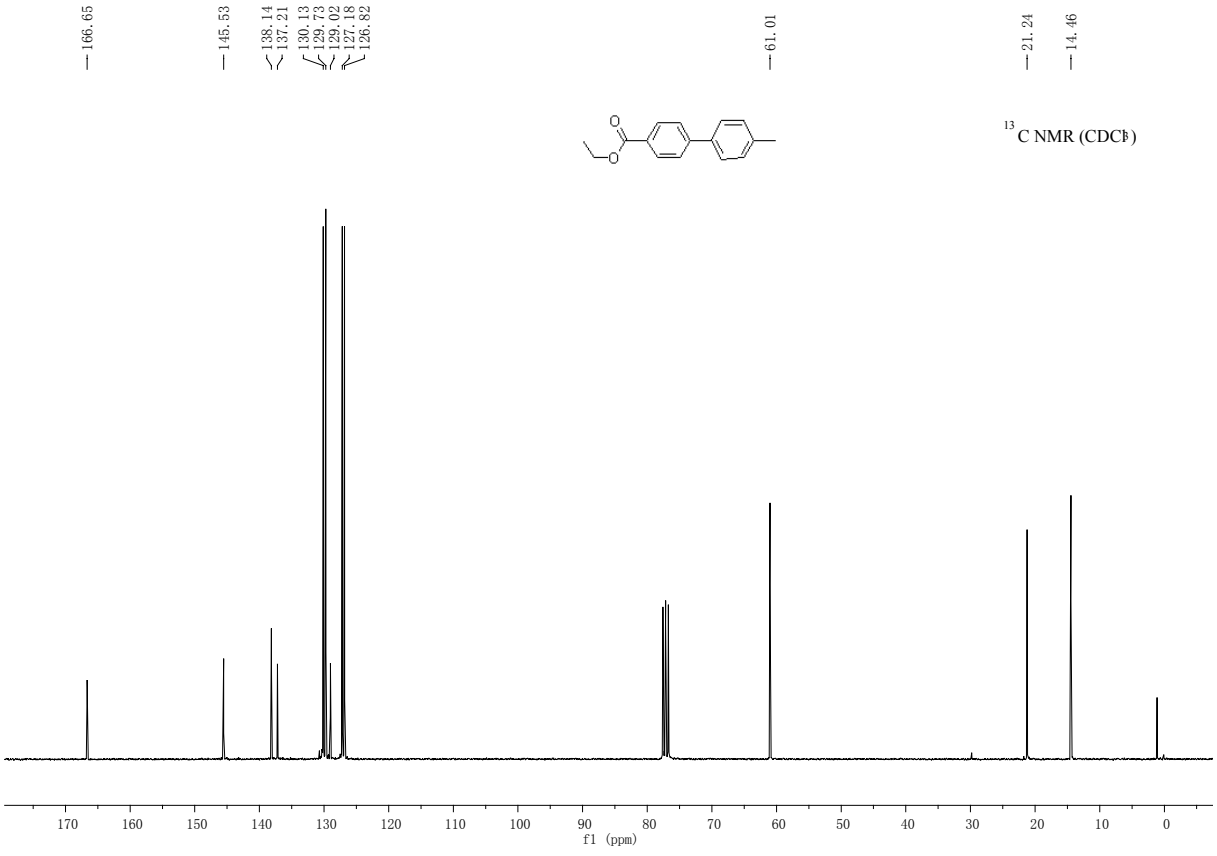
(8) 3'-Methoxy-*N*,*N*-dimethylbiphenyl-4-amine



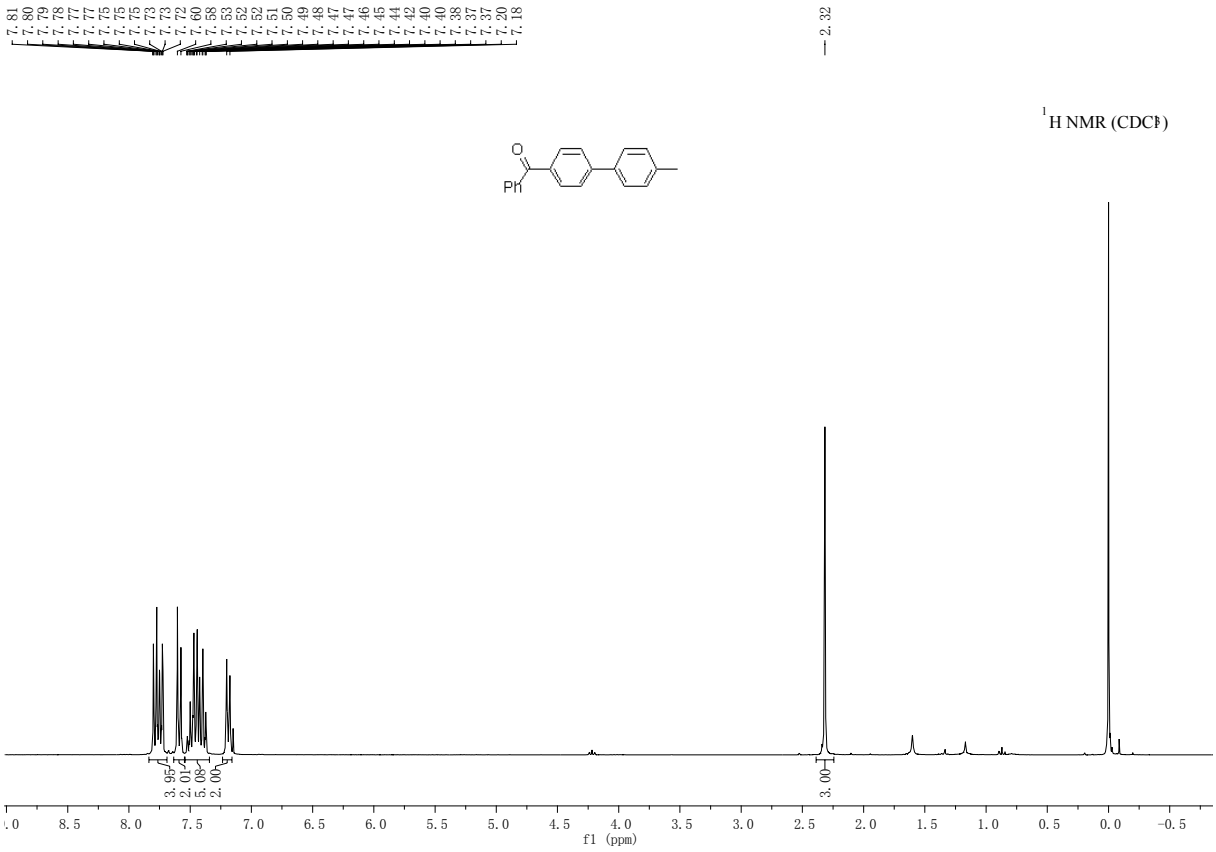


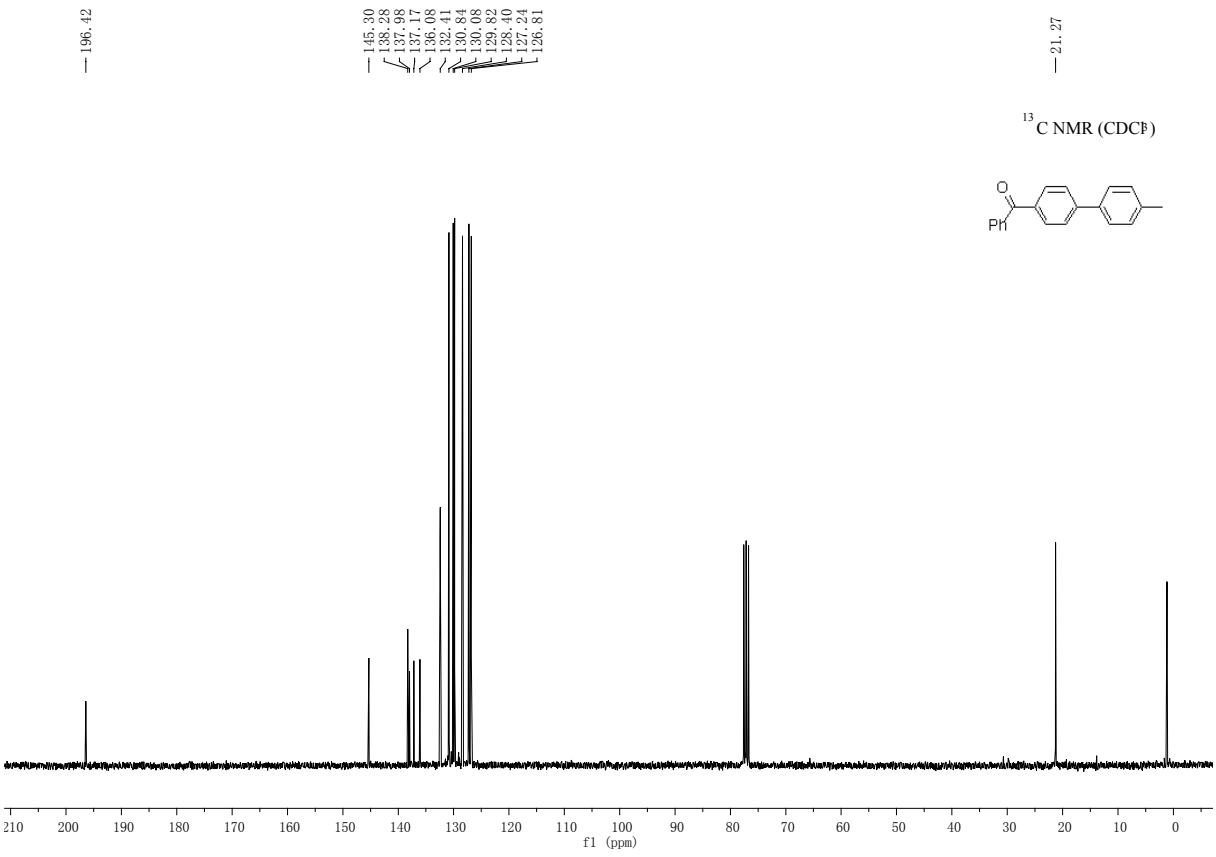
(9) Ethyl 4'-methylbiphenyl-4-carboxylate



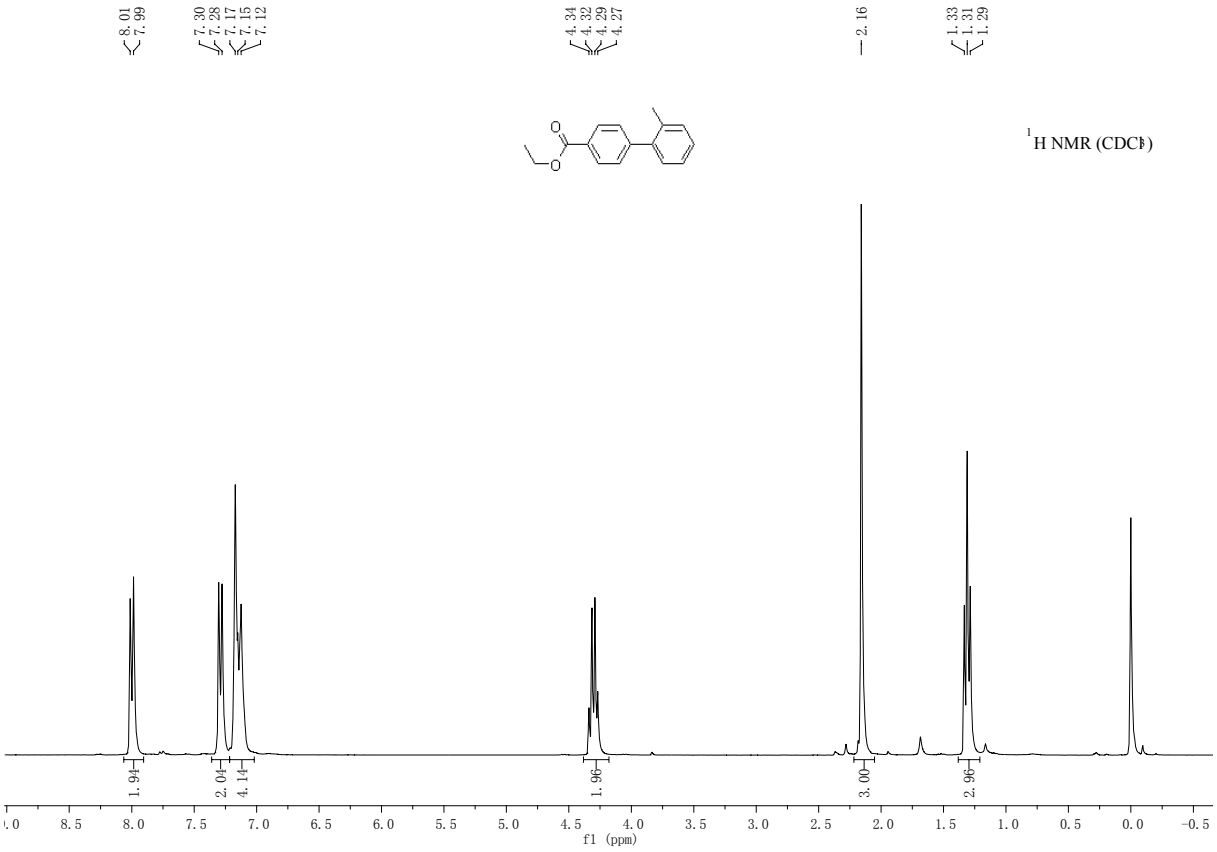


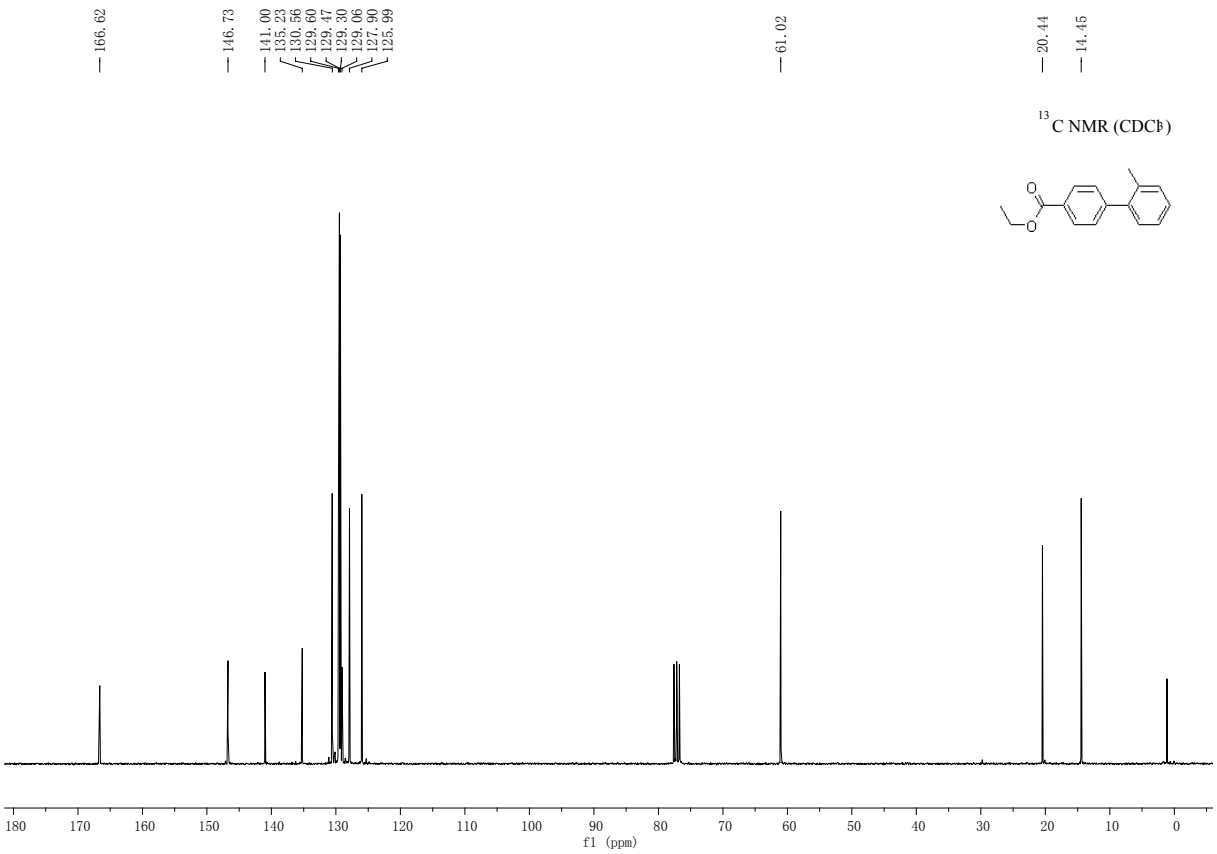
(10) Phenyl(*p*-tolyl)methanone



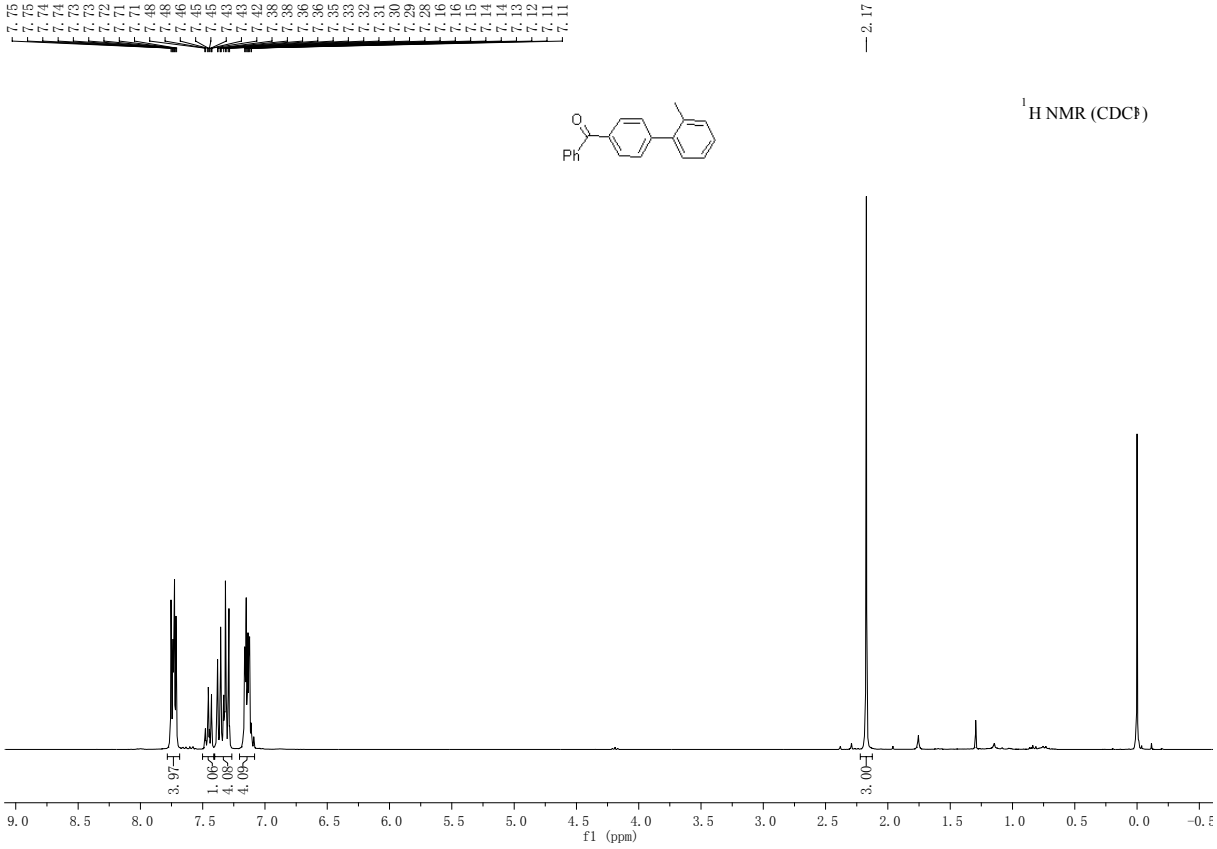


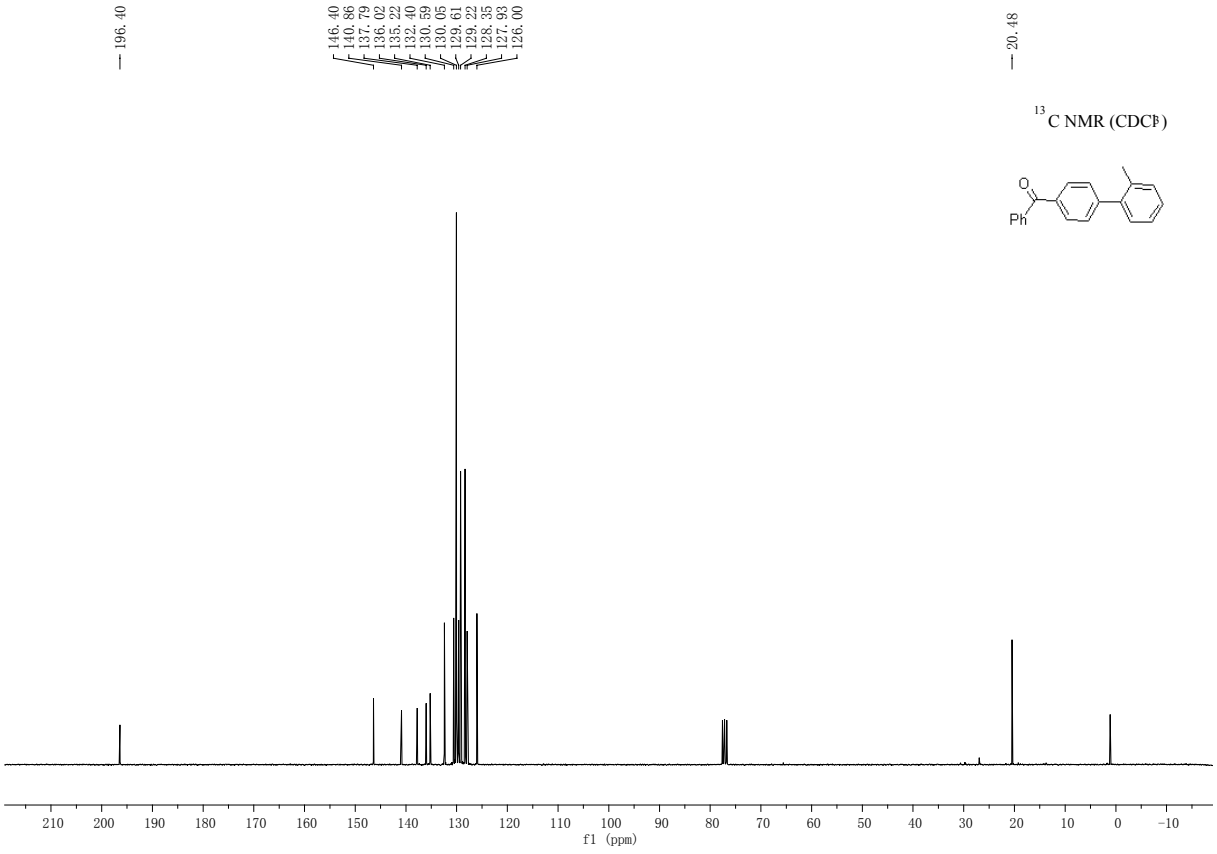
(11) Ethyl 2'-methylbiphenyl-4-carboxylate



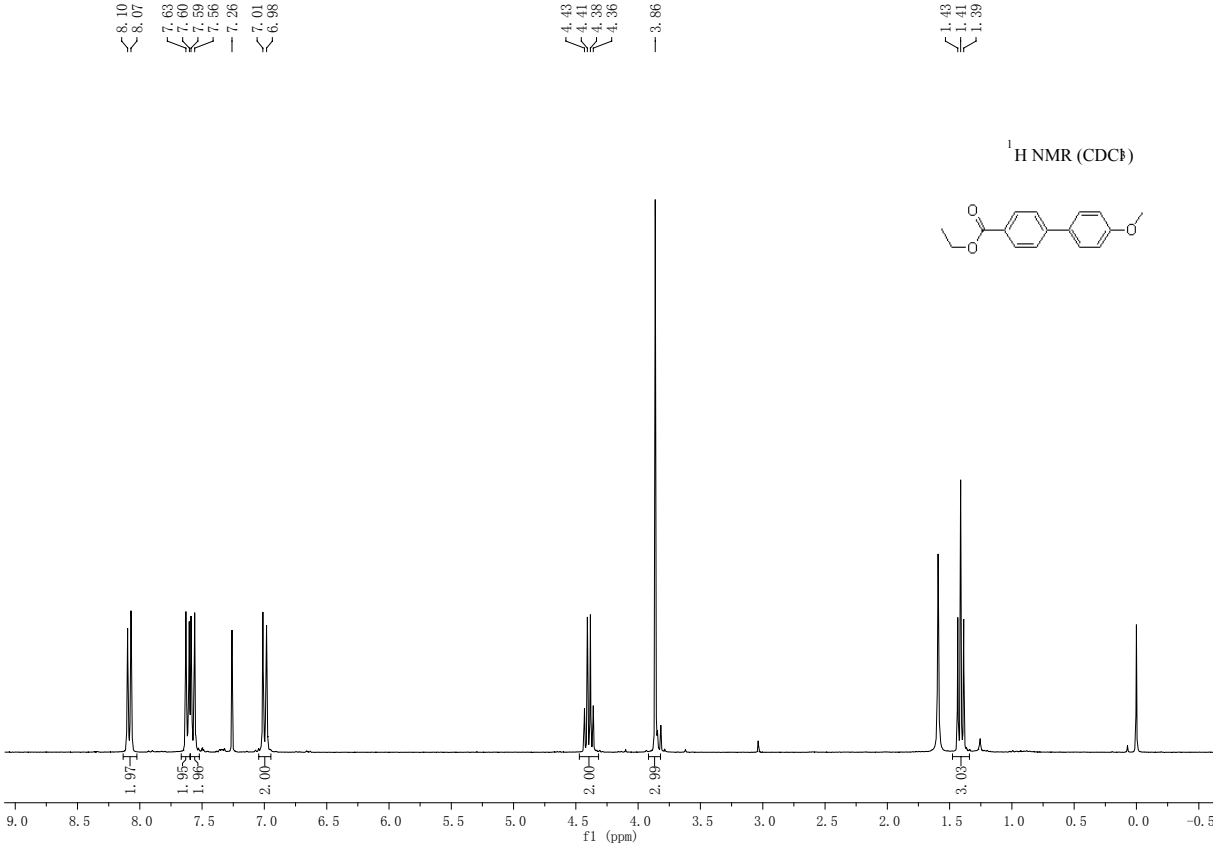


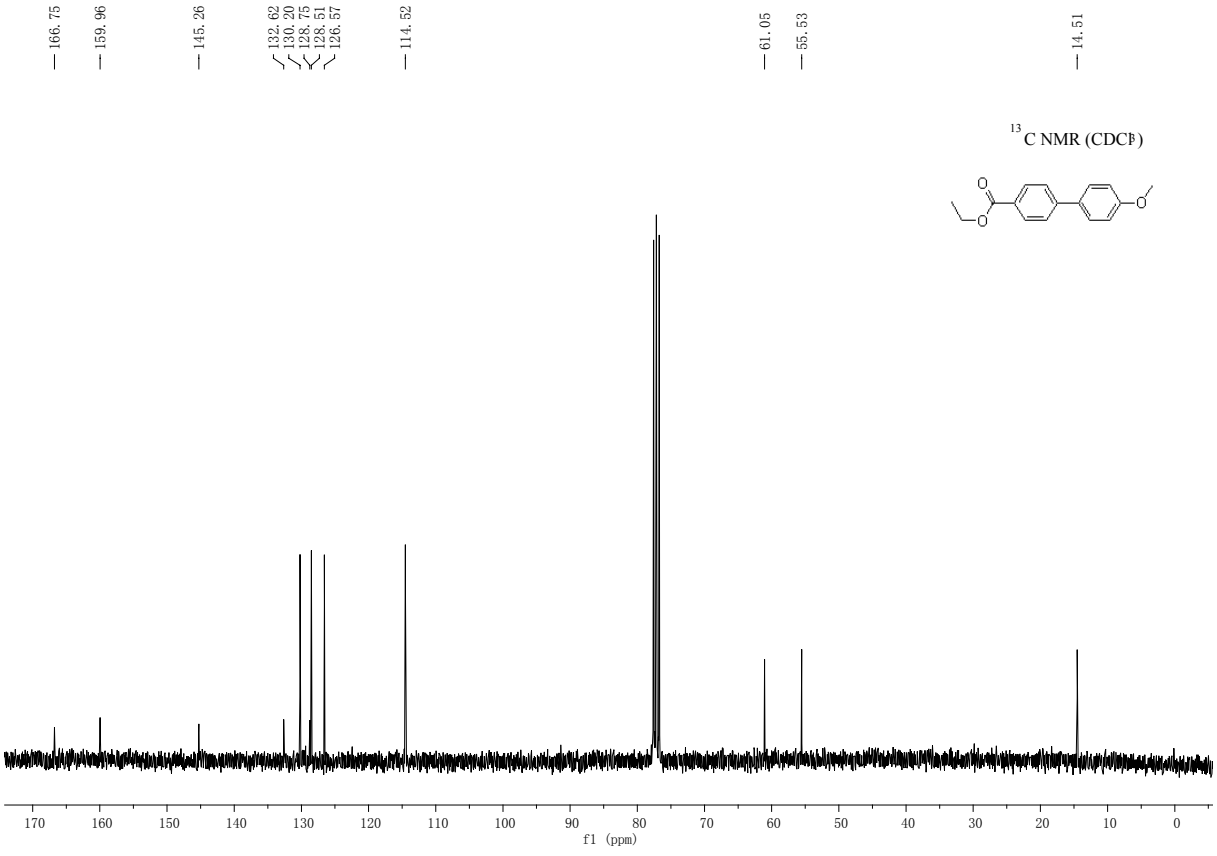
(12) (2'-Methylbiphenyl-4-yl)(phenyl)methanone



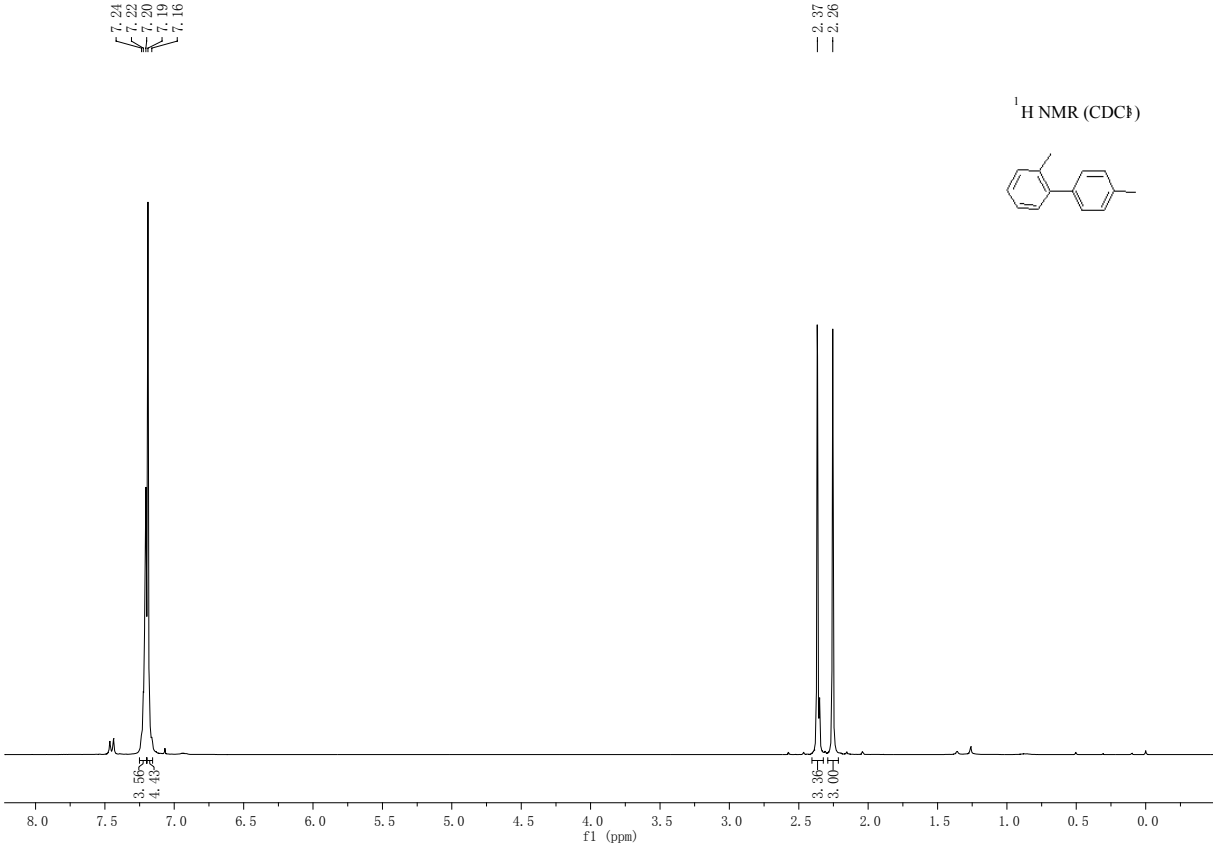


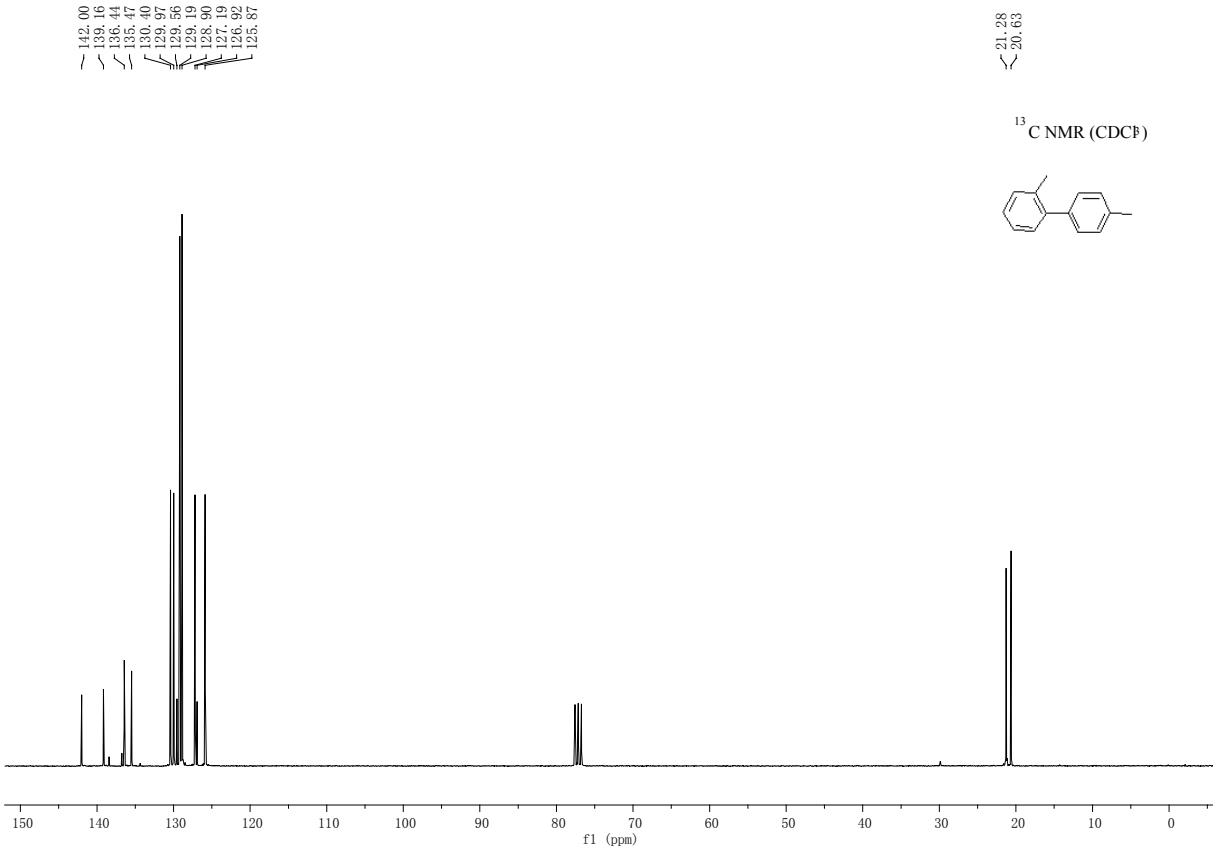
(13) Ethyl 4'-Methoxybiphenyl-4-carboxylate



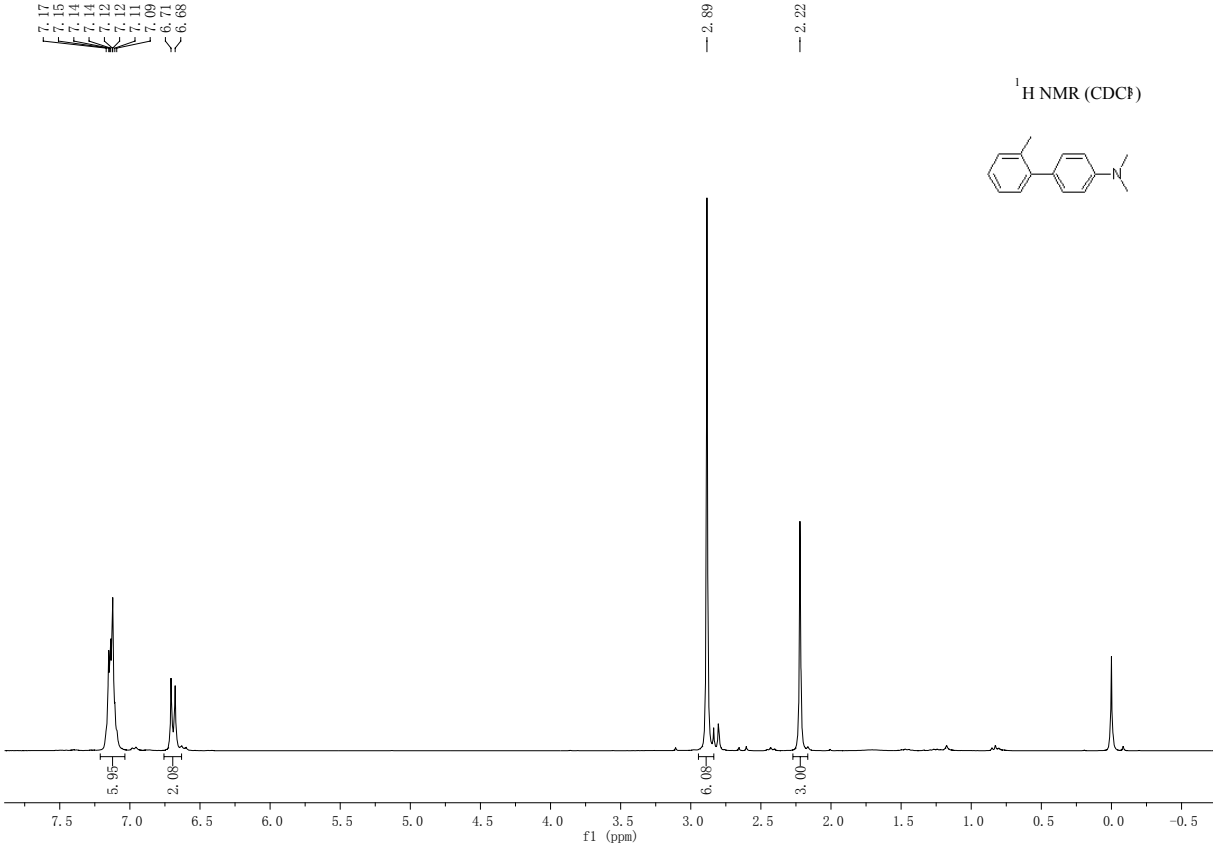


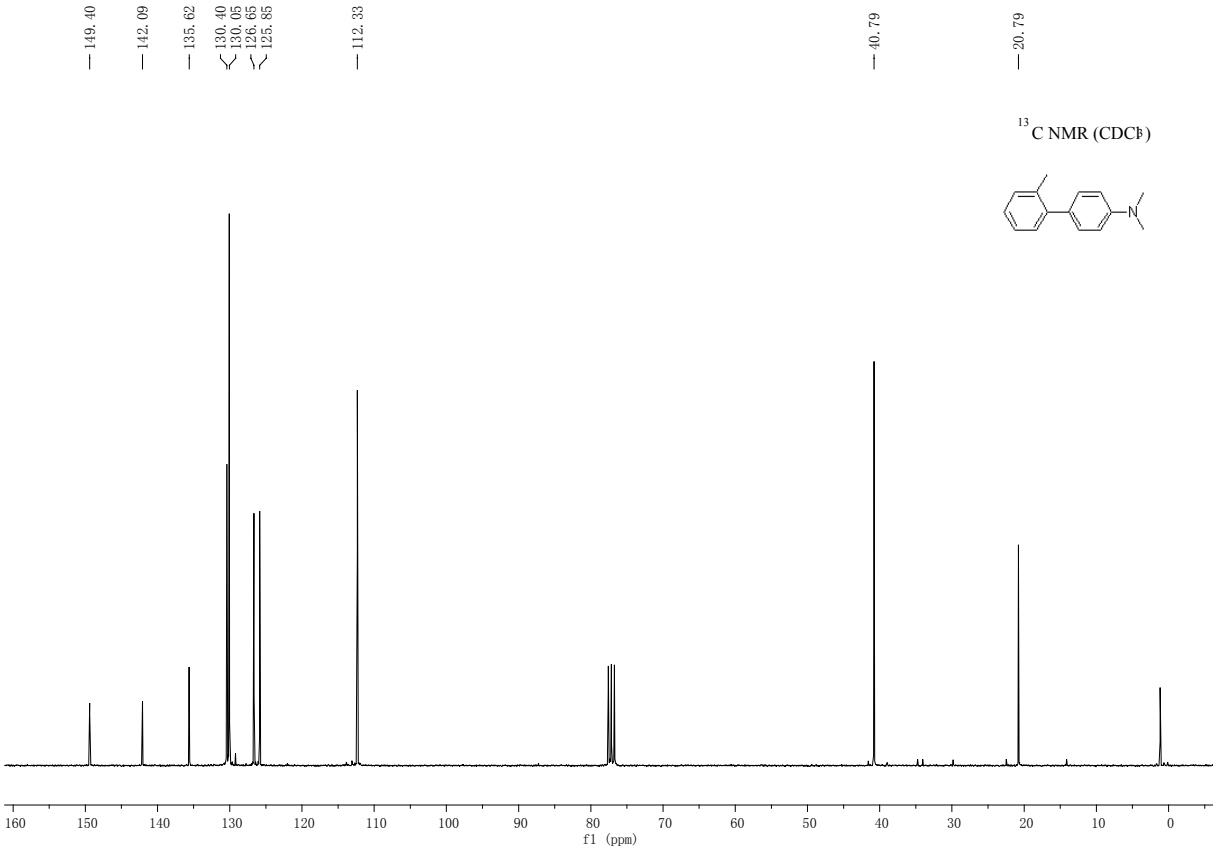
(14) 2,4'-Dimethylbiphenyl



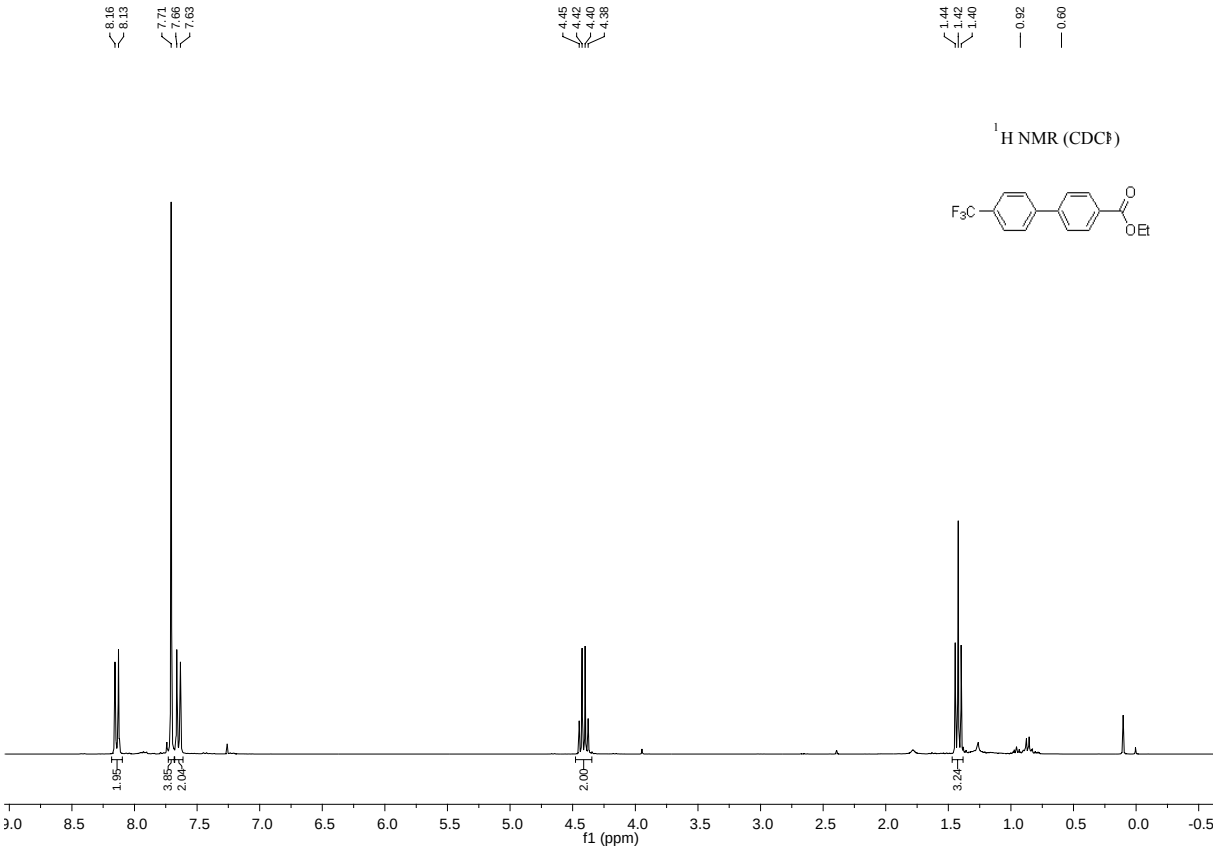


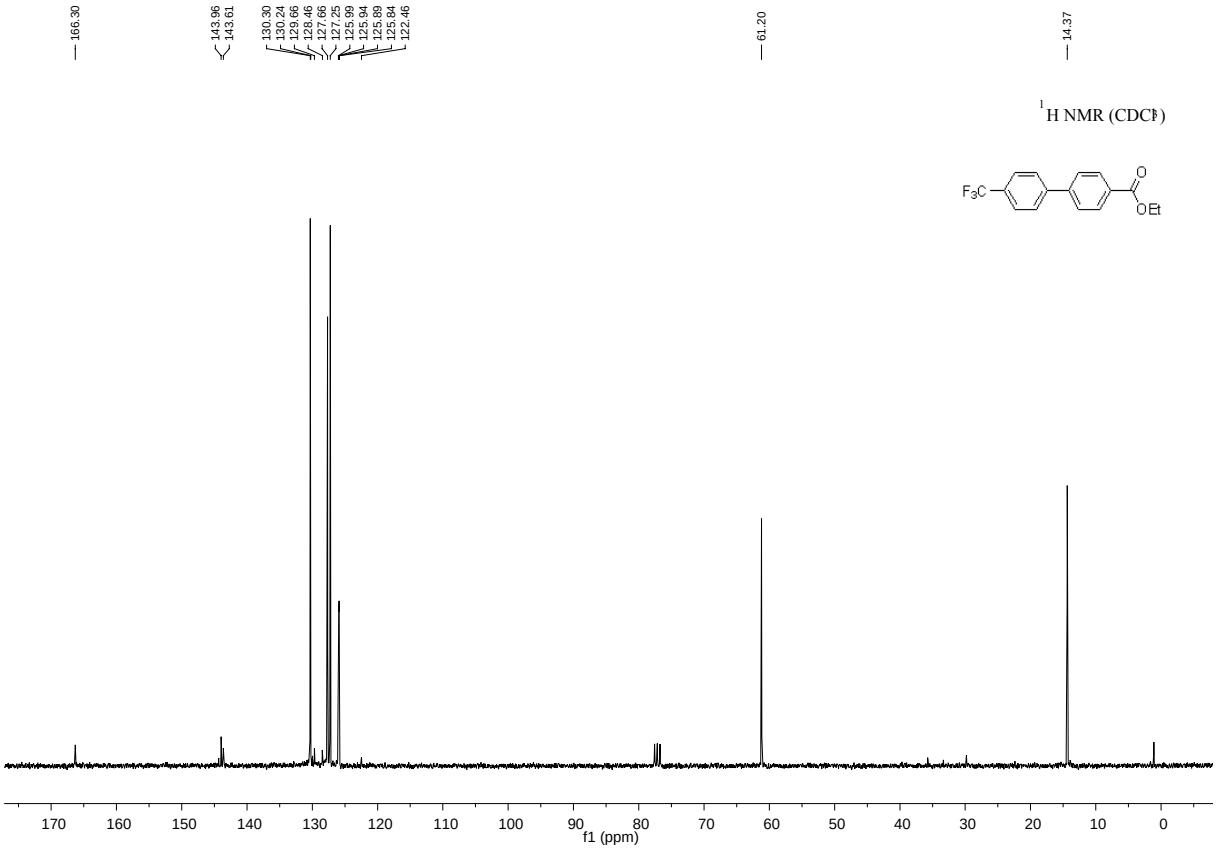
(15) 2'-Methyl-*N*,*N*-dimethylbiphenyl-4-amine



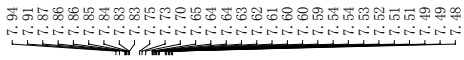


(16) Ethyl 4-[4-(trifluoromethyl)phenyl]benzoate

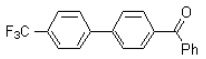


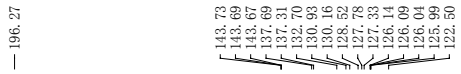


(17) Phenyl-[4-[4-(trifluoromethyl)phenyl]phenyl]methanone



^{1}H NMR ($CDCl_3$)





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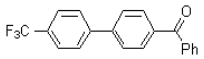
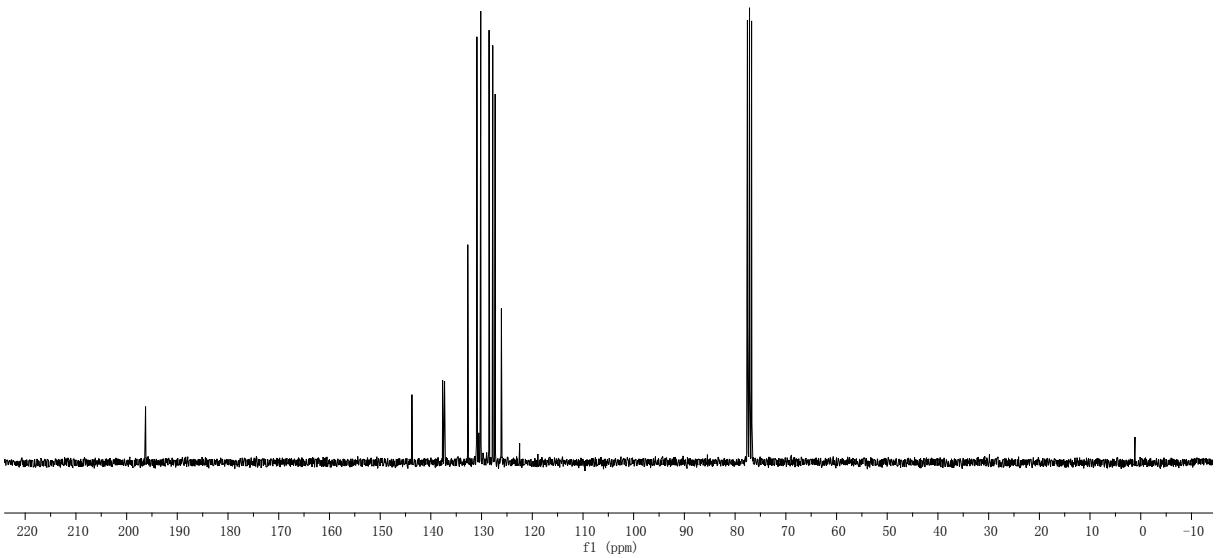
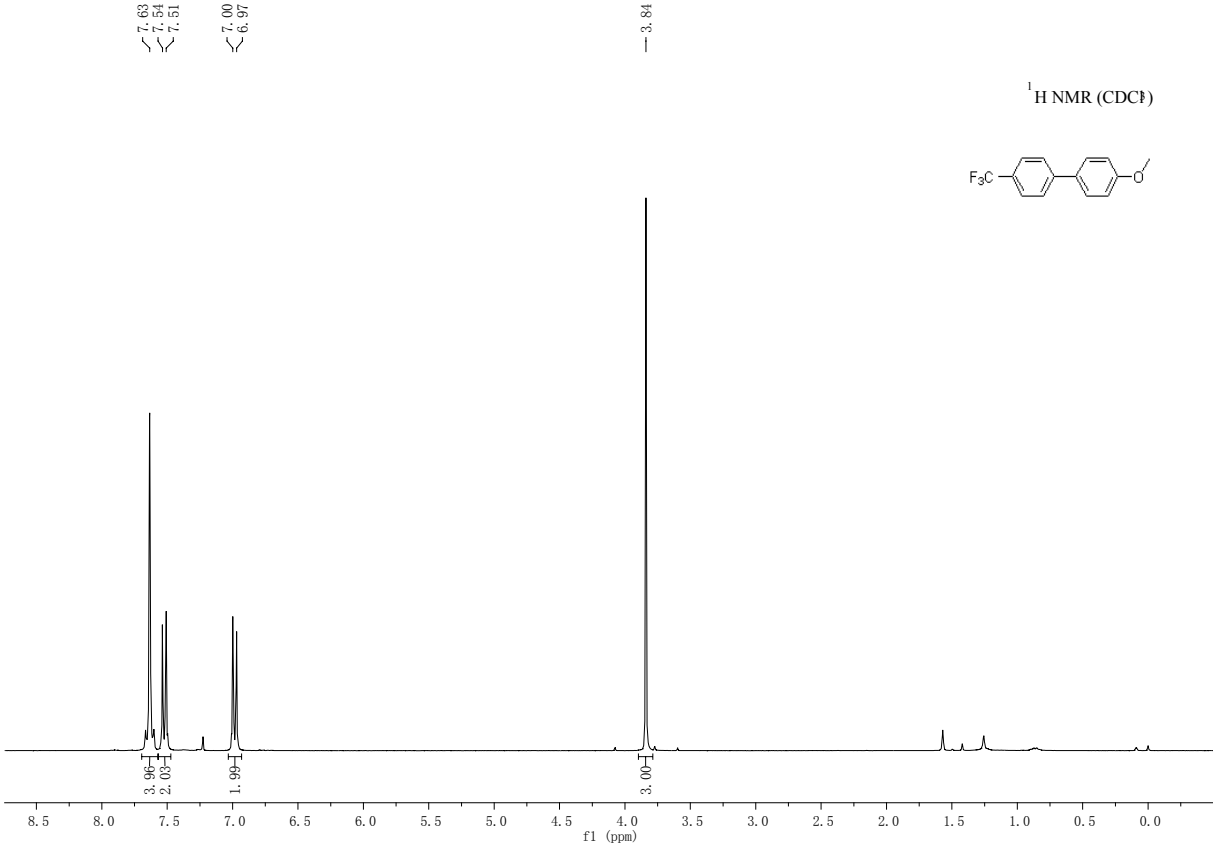
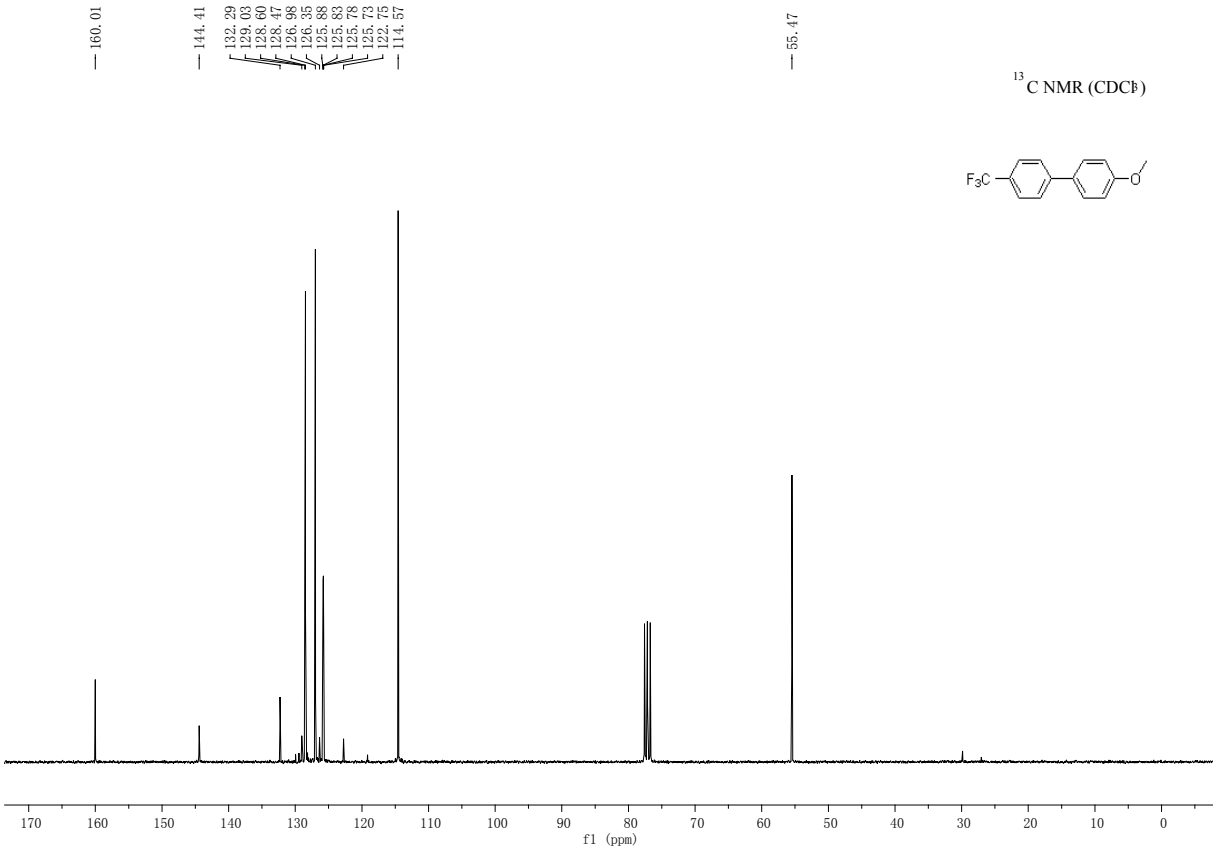


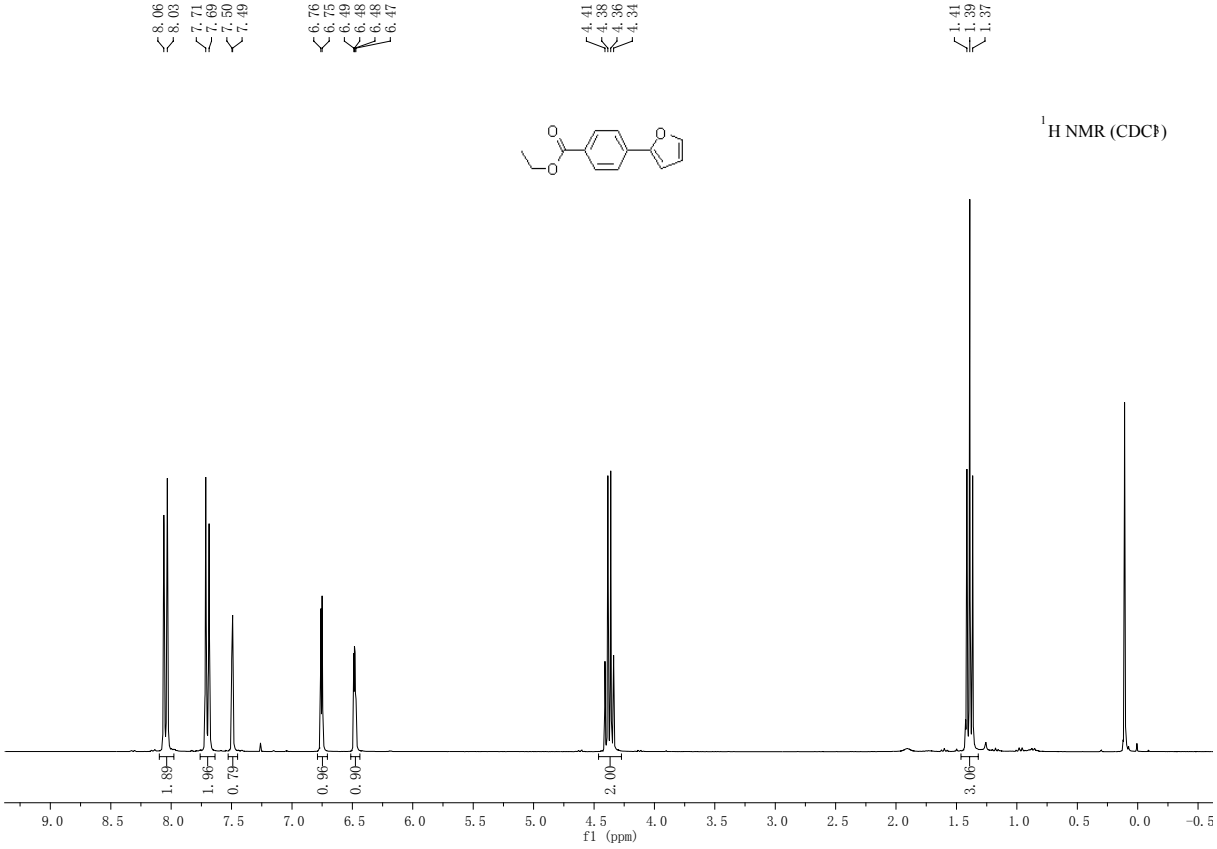


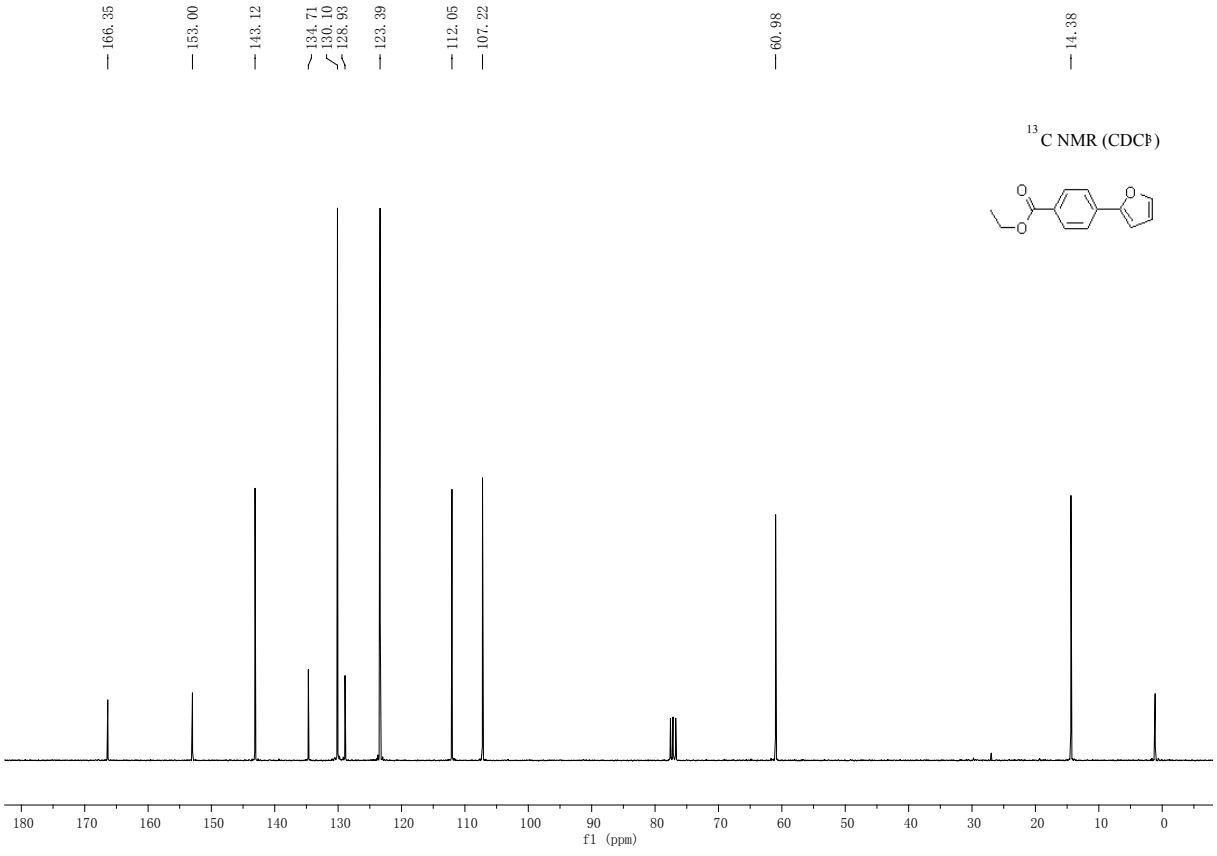
(18) 4'-Methoxy-4-(trifluoromethyl)biphenyl



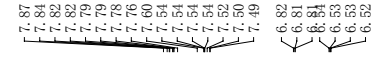


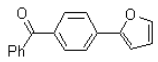
(19) Ethyl 4-(furan-2-yl)benzoate



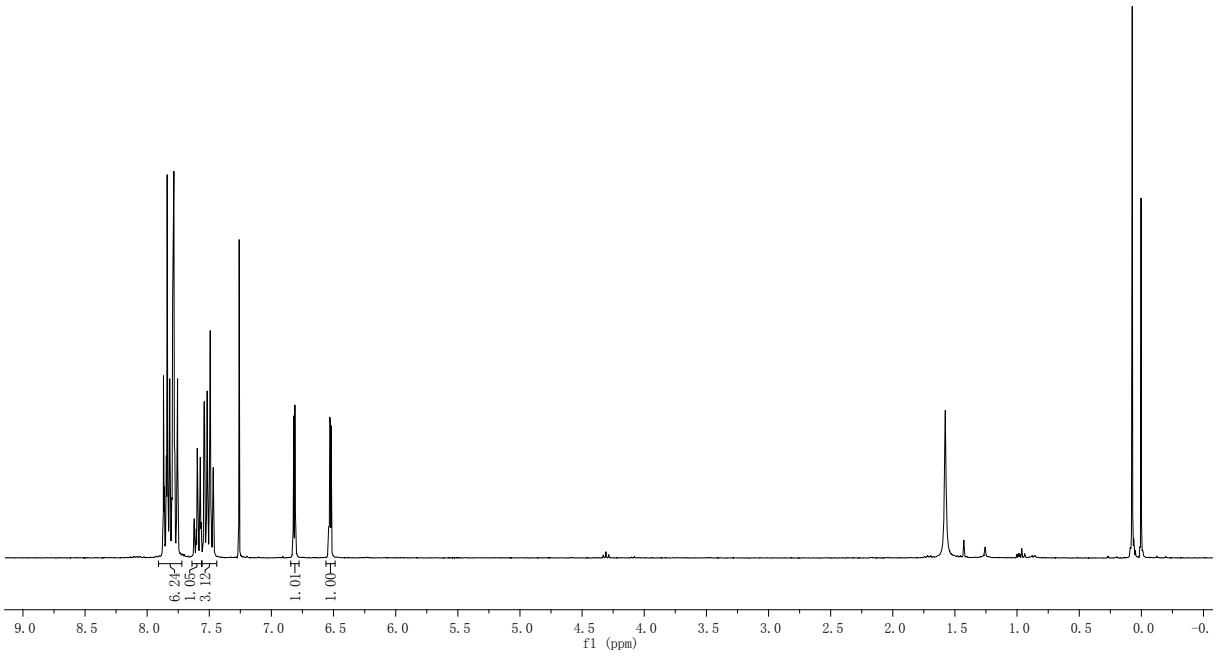


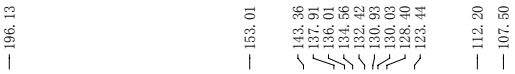
(20) (4-(Furan-2-yl)phenyl)(phenyl)methanone



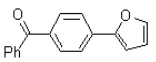


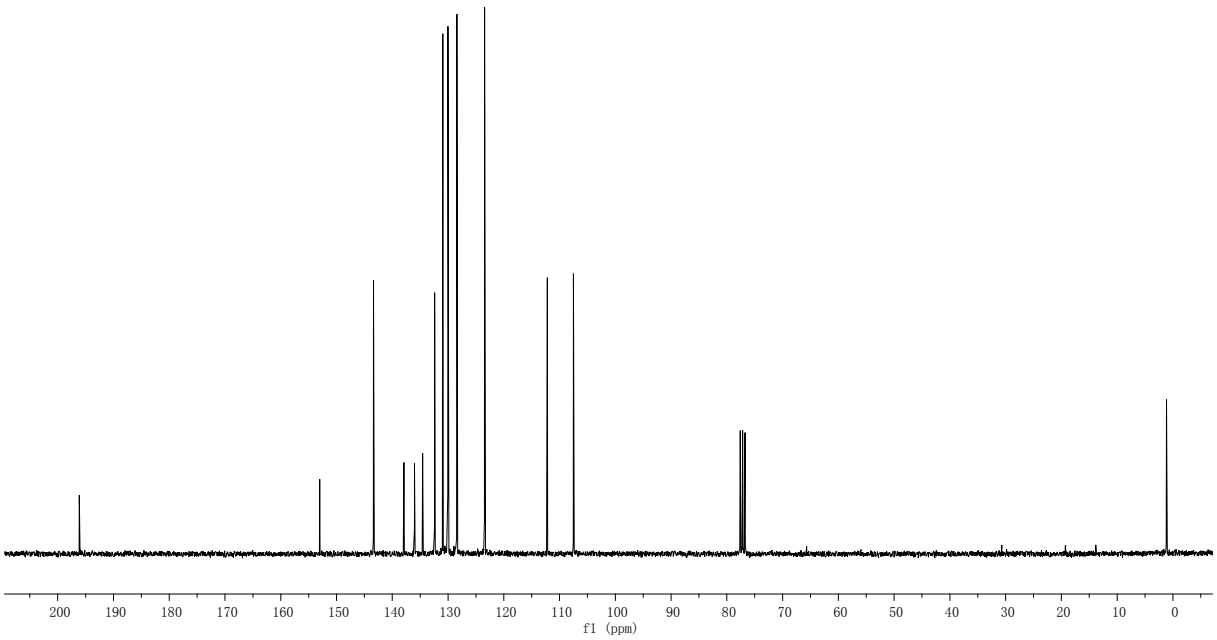
^{1}H NMR (CDCl$_3$)



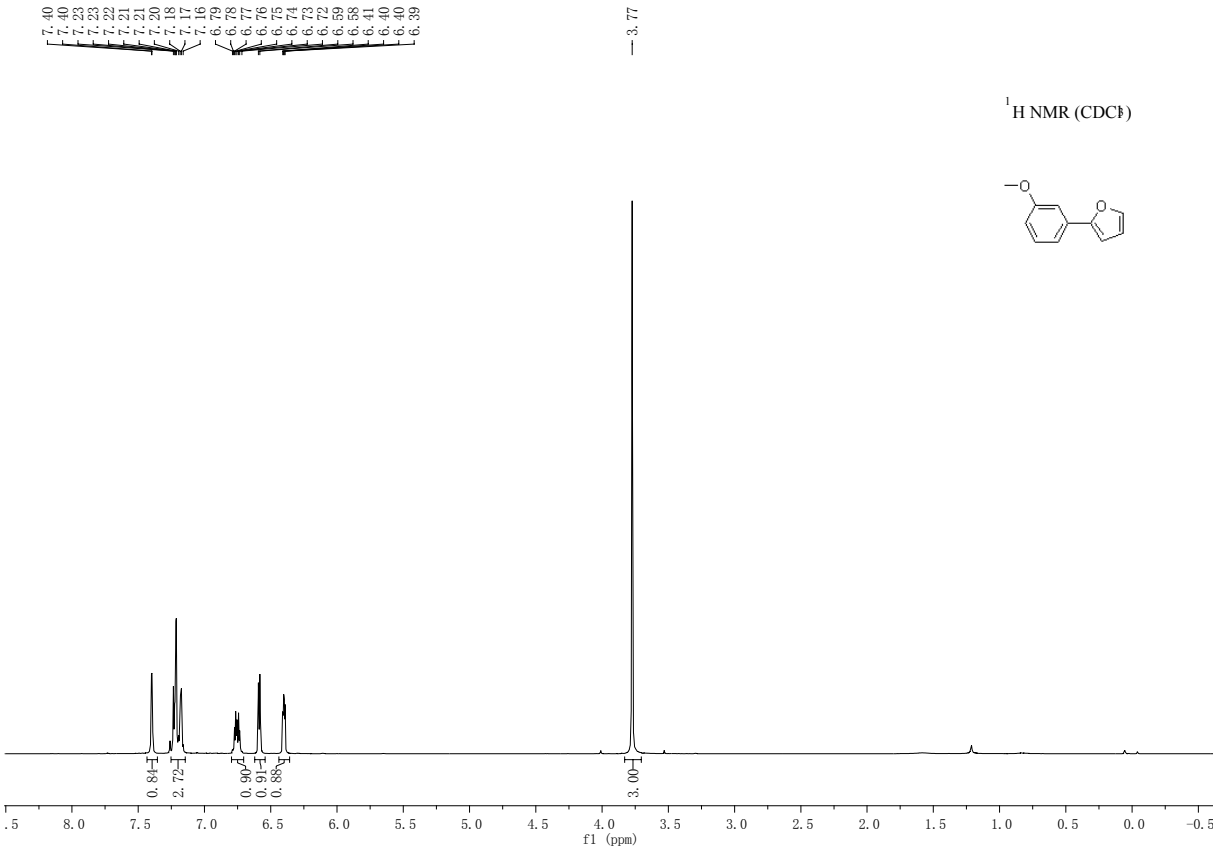


^{13}C NMR (CDCl$_3$)

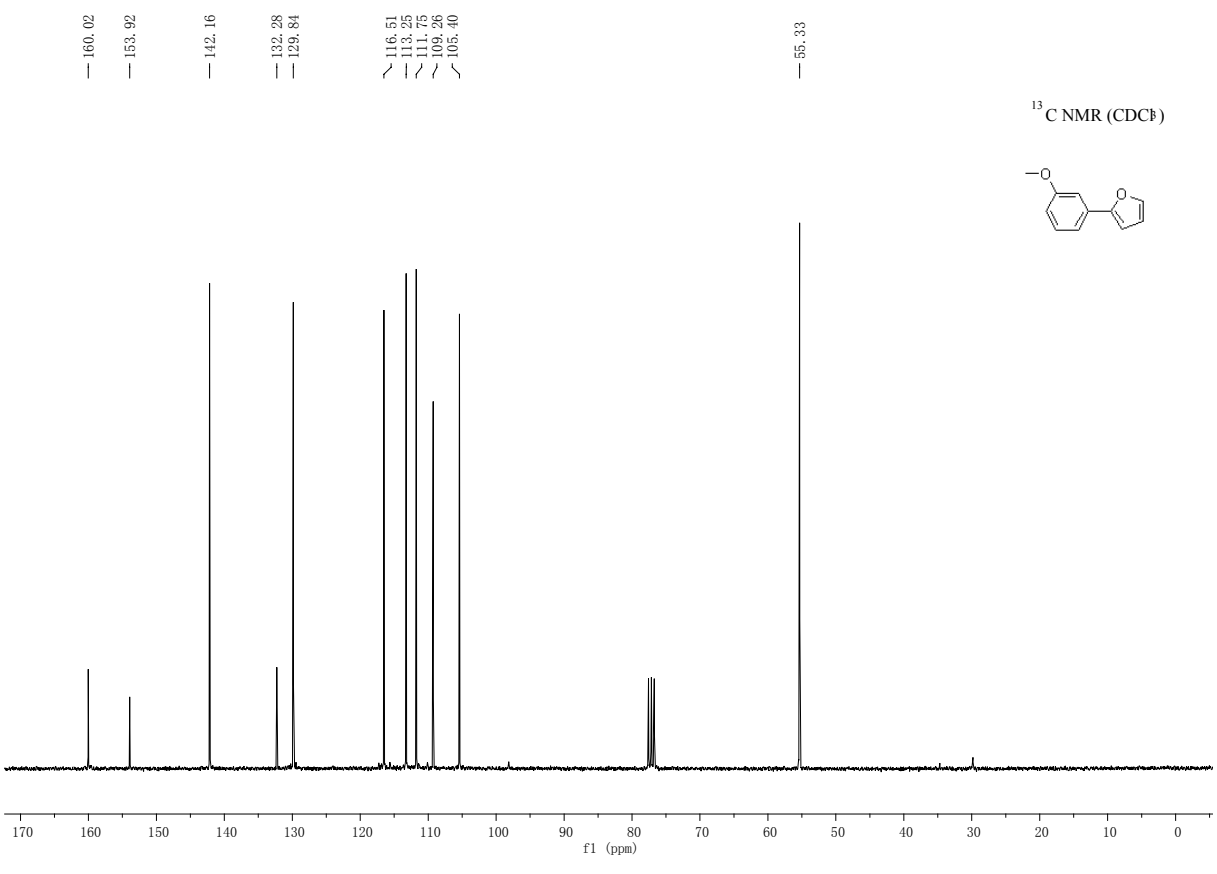




(21) 2-(3-Methoxyphenyl)furan

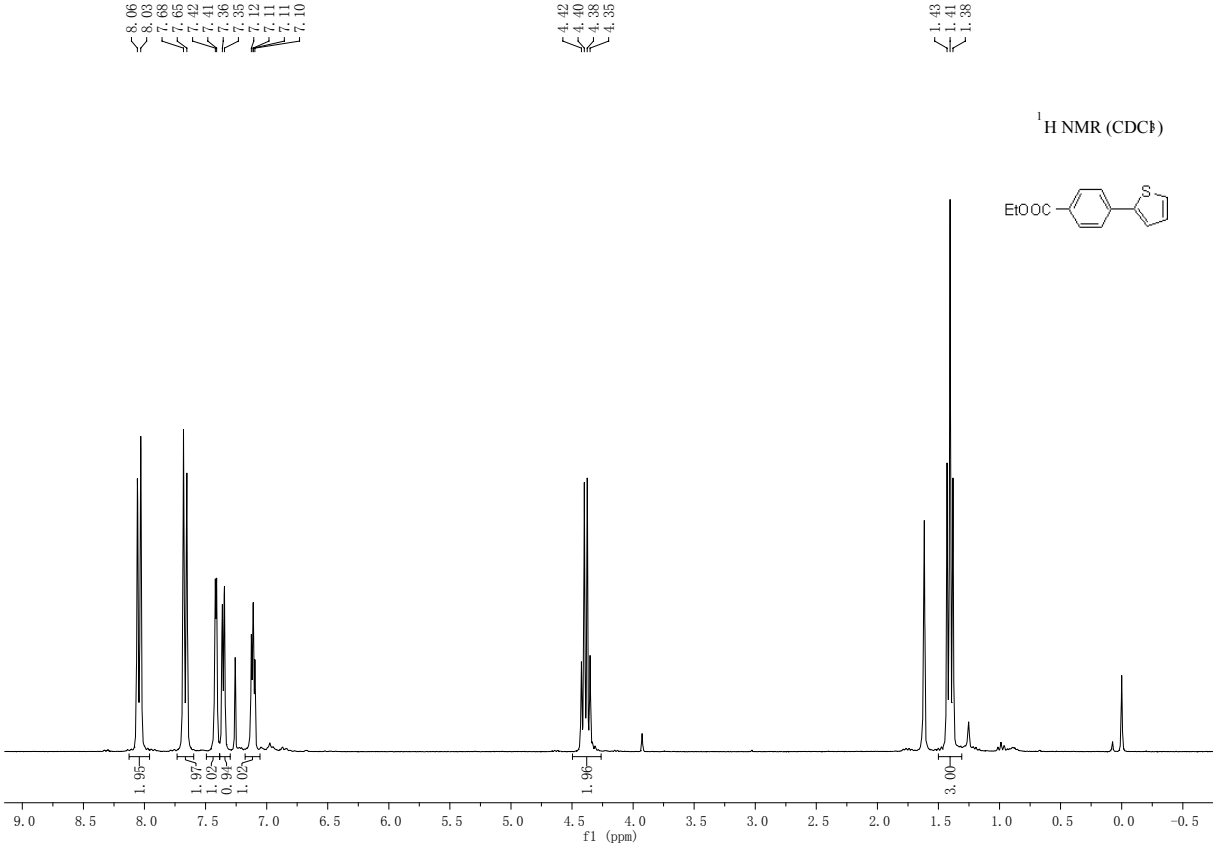


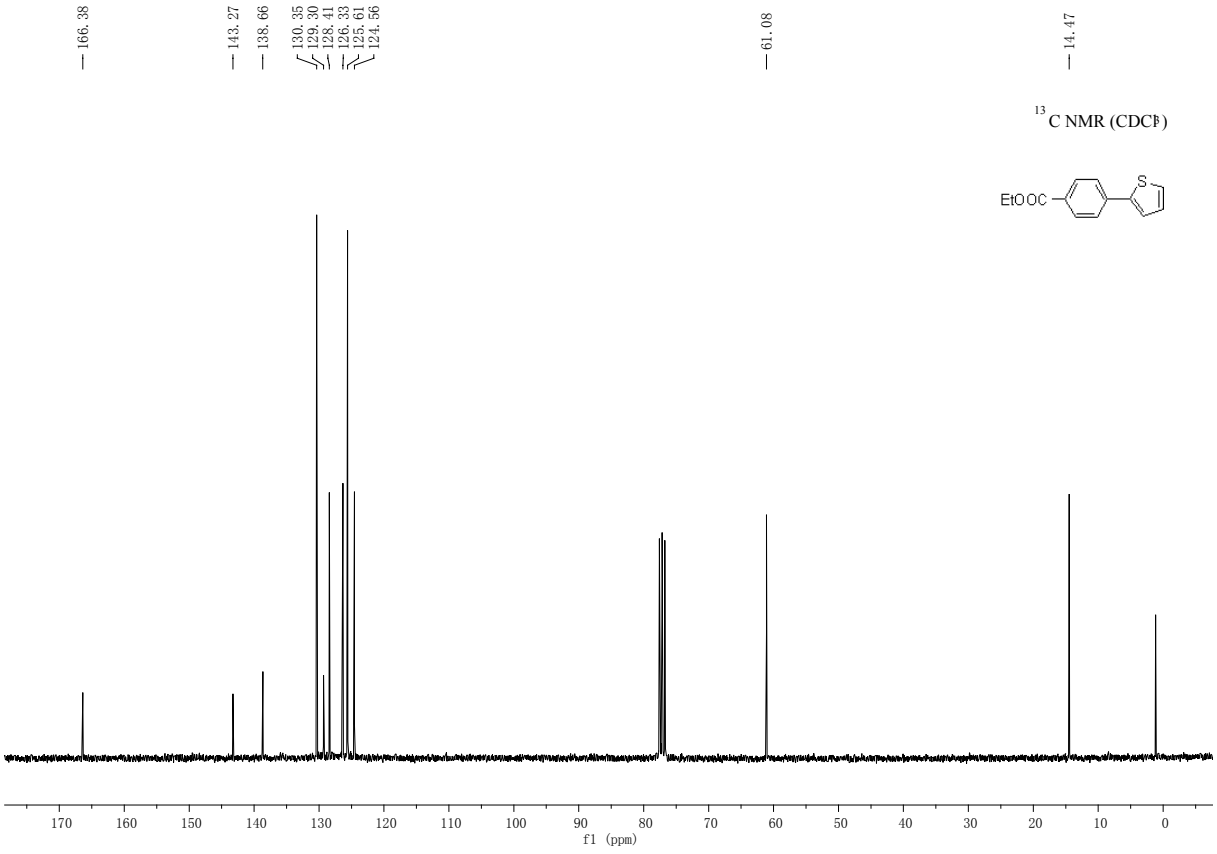
^{1}H NMR (CDCl$_3$)



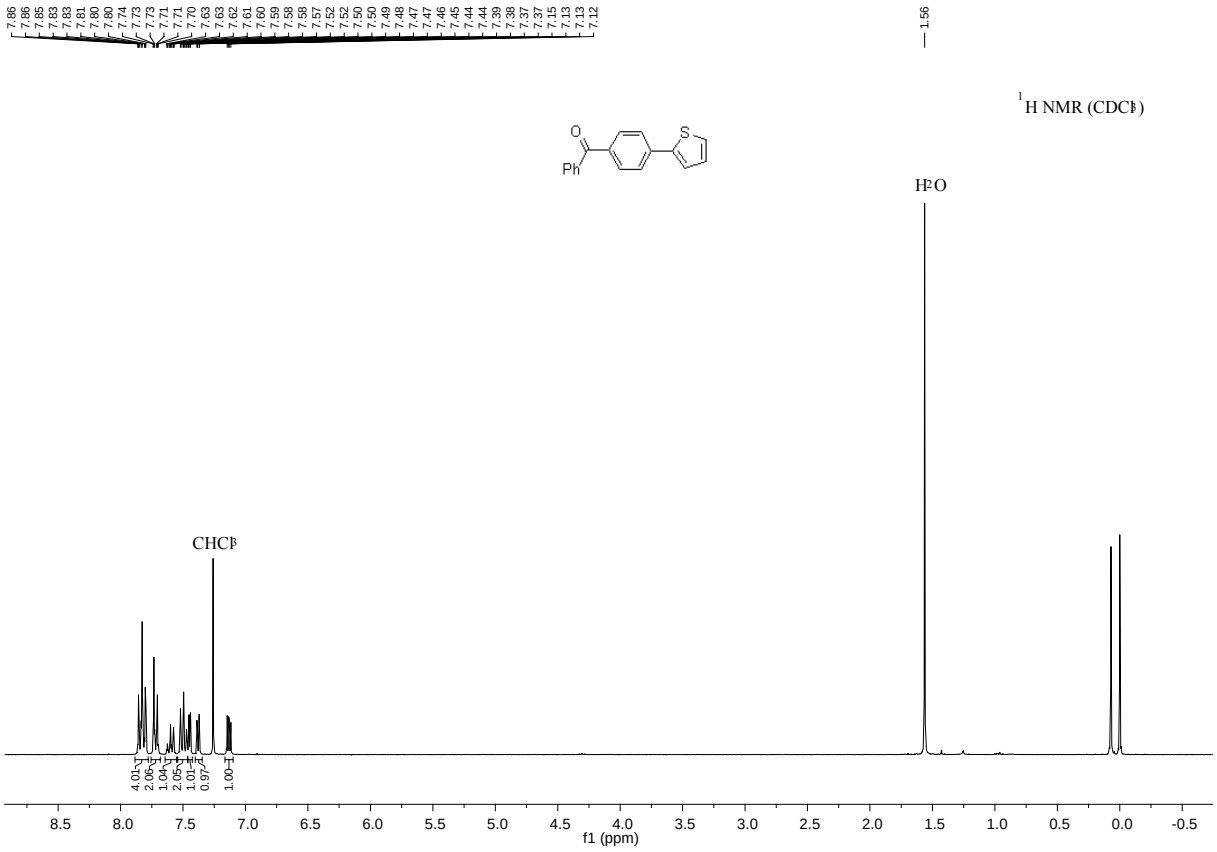
^{13}C NMR (CDCl$_3$)

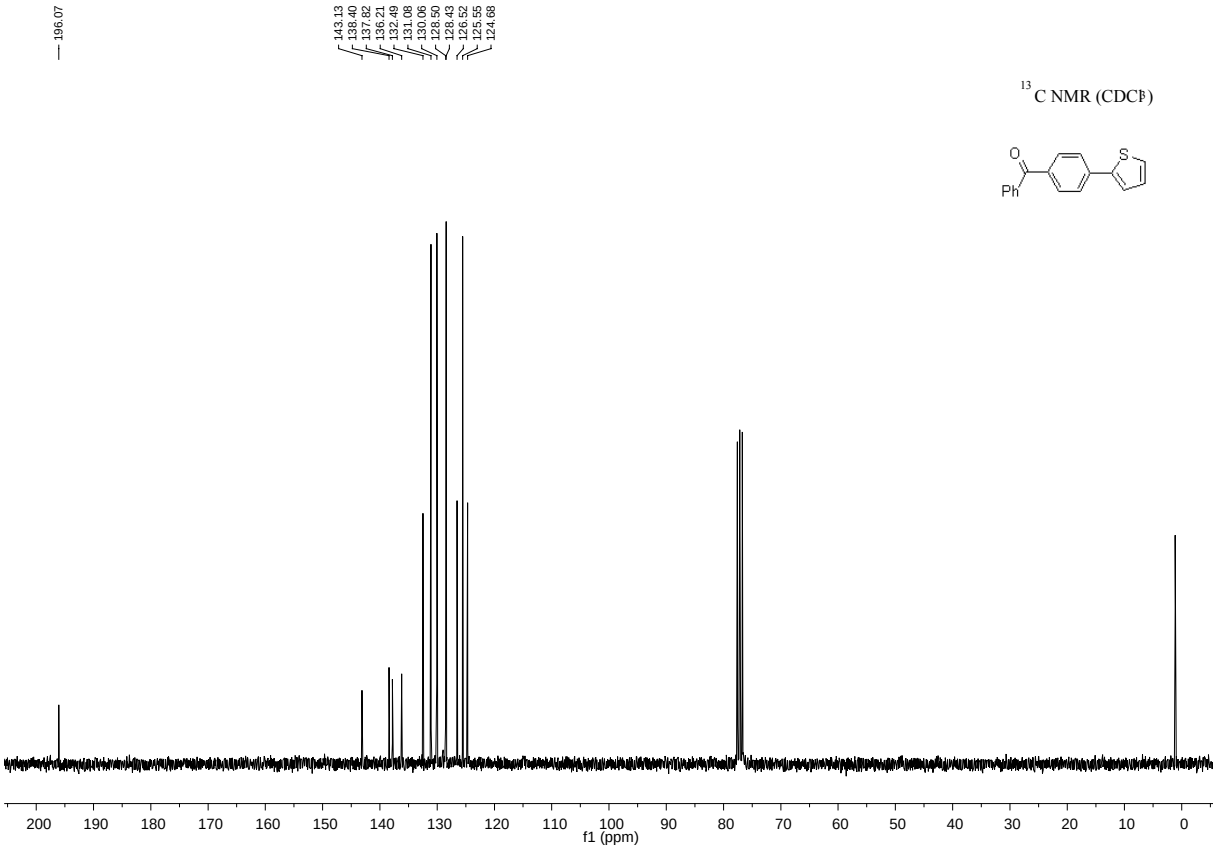
(22) 2-(4-Ethoxycarbonylphenyl)thiophene



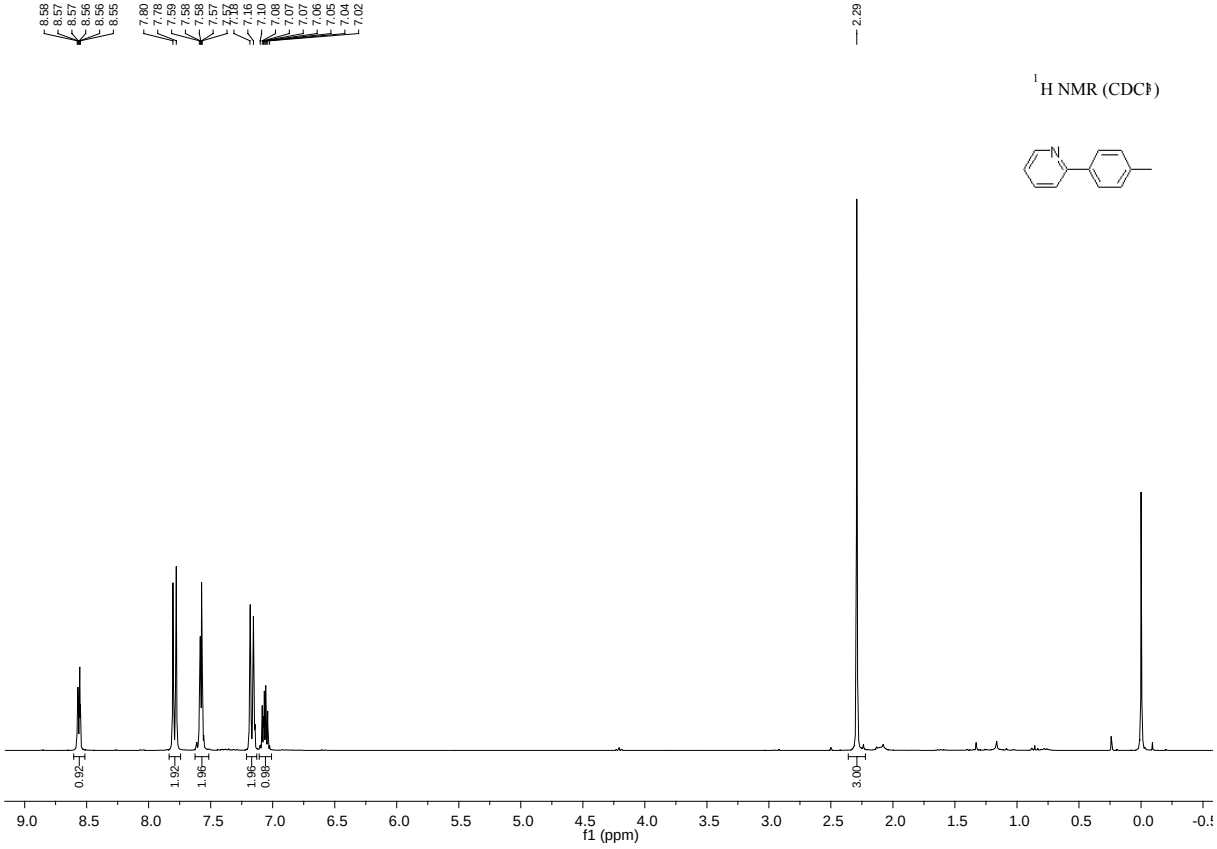


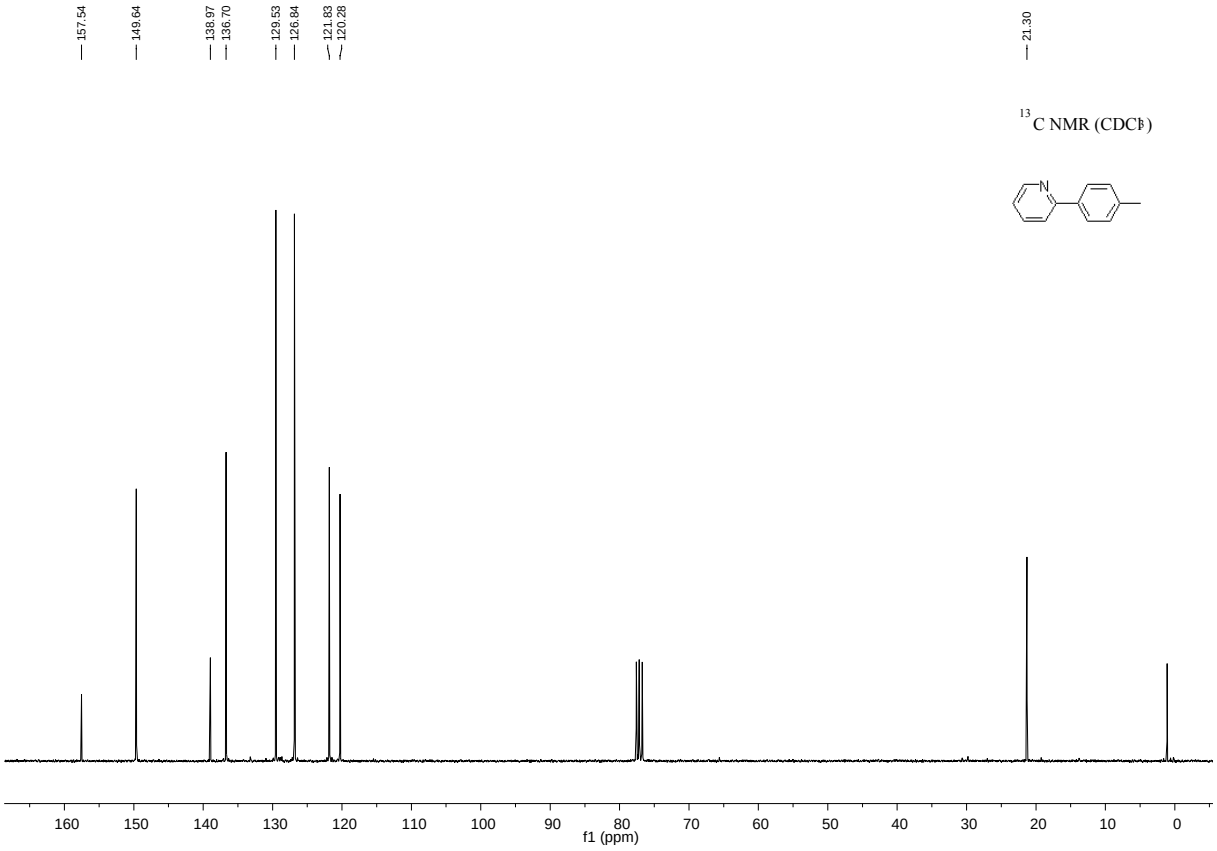
(23) Phenyl(4-(thiophen-2-yl)phenyl)methanone



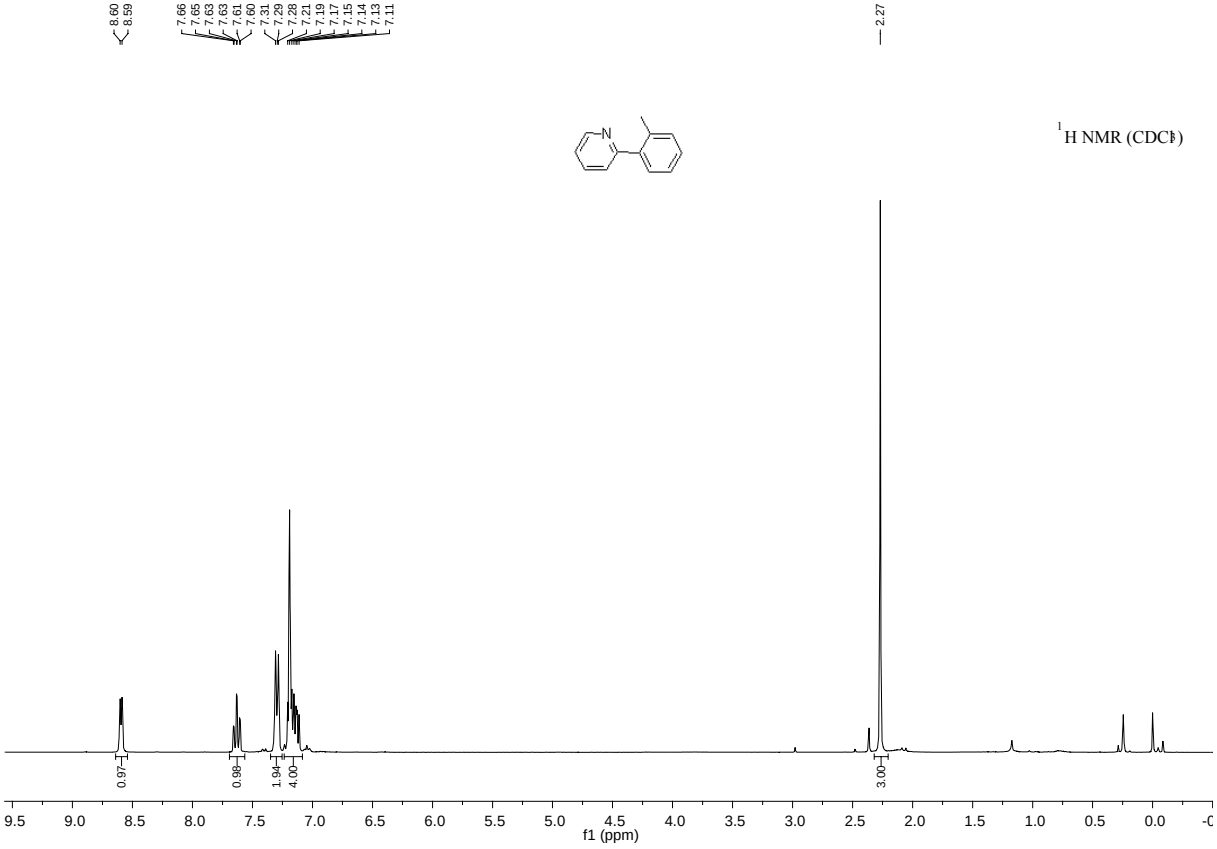


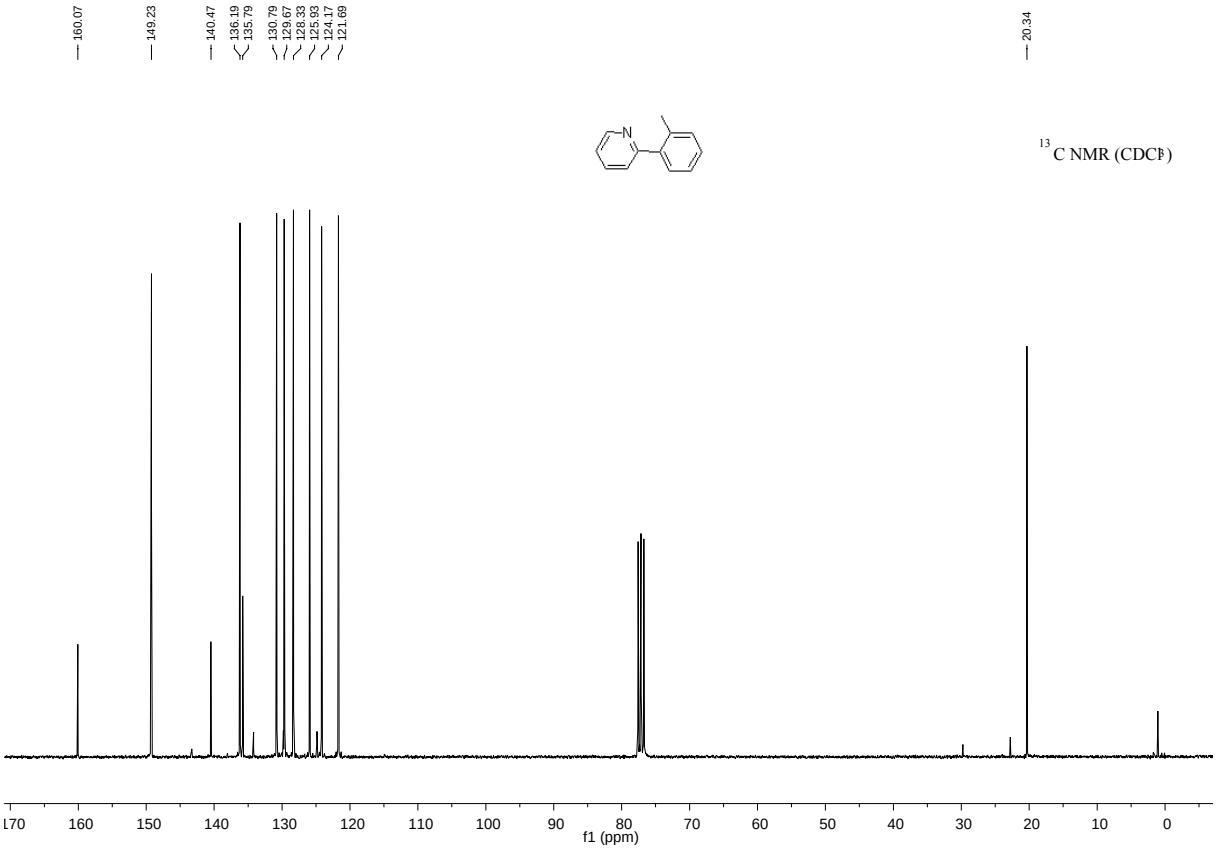
(24) *p*-Tolylpyridine



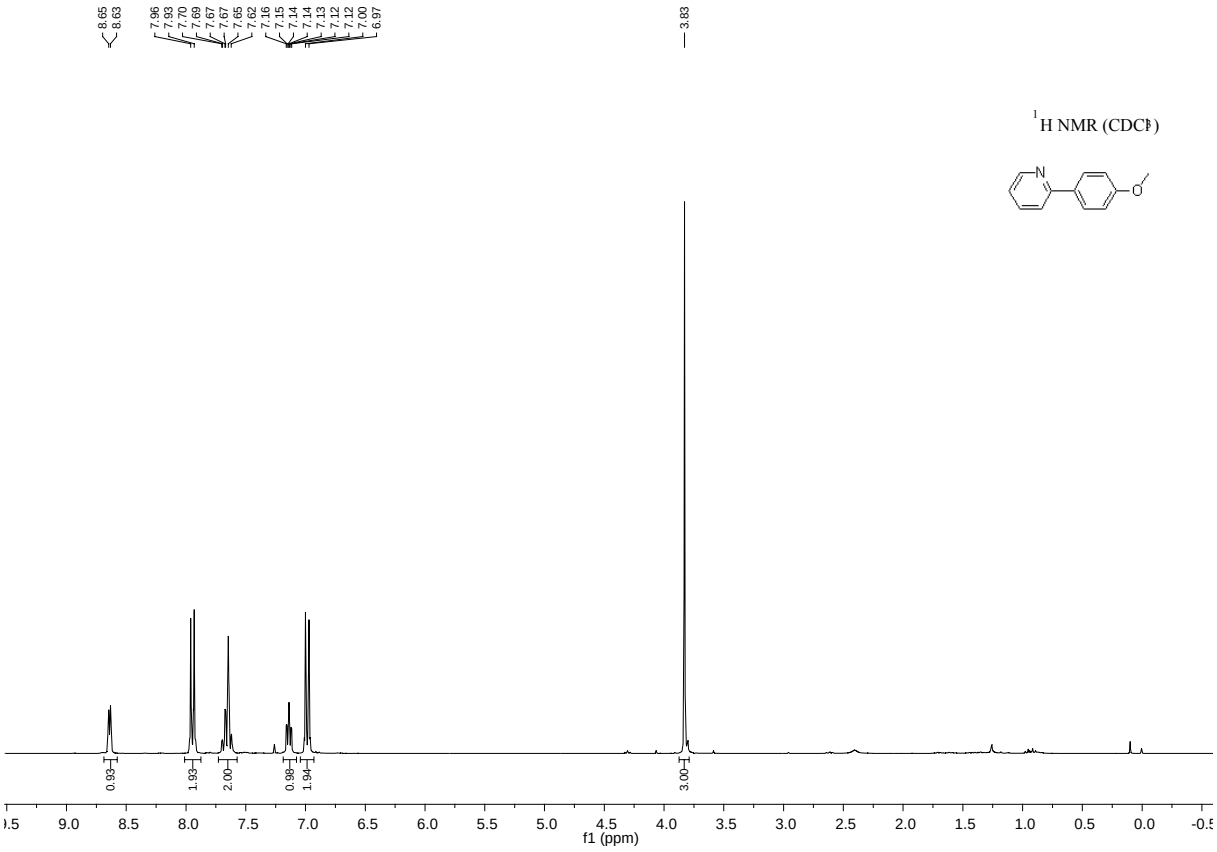


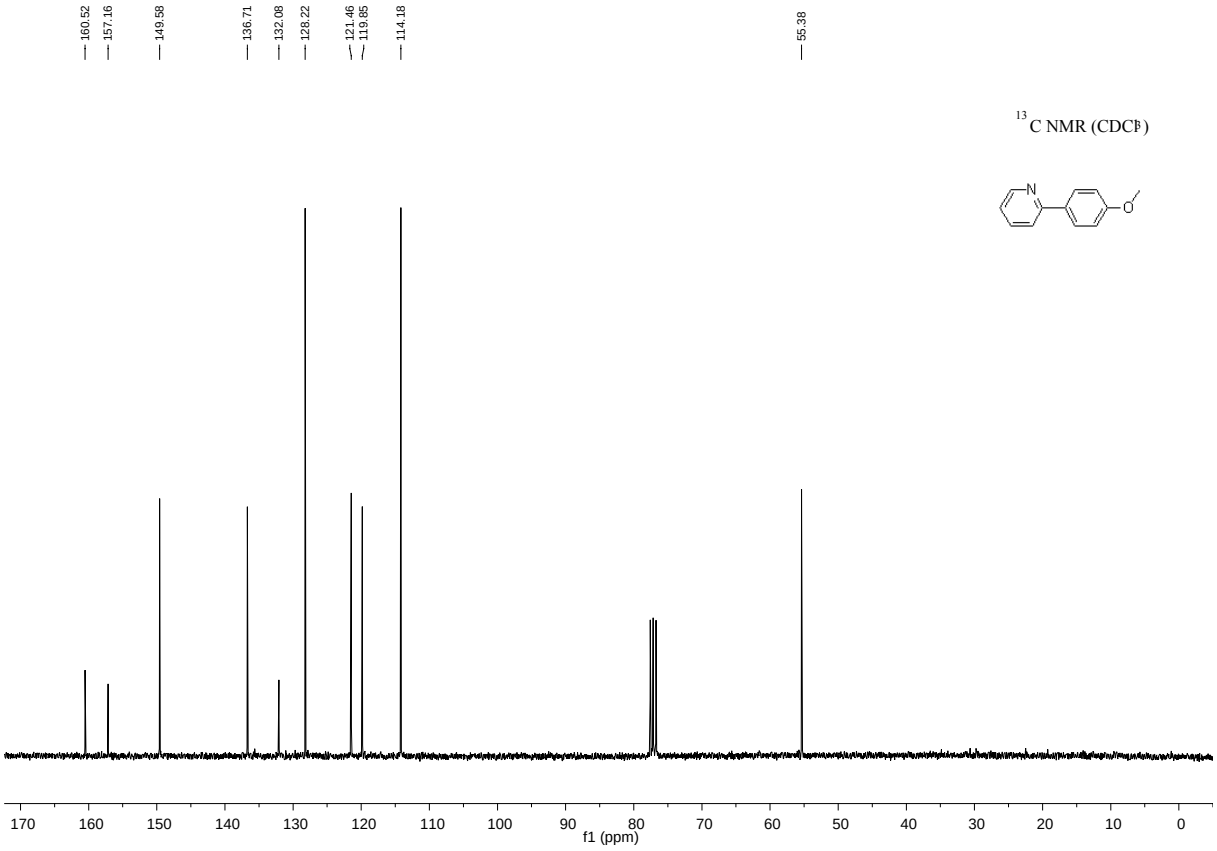
(25) *o*-Tolylpyridine



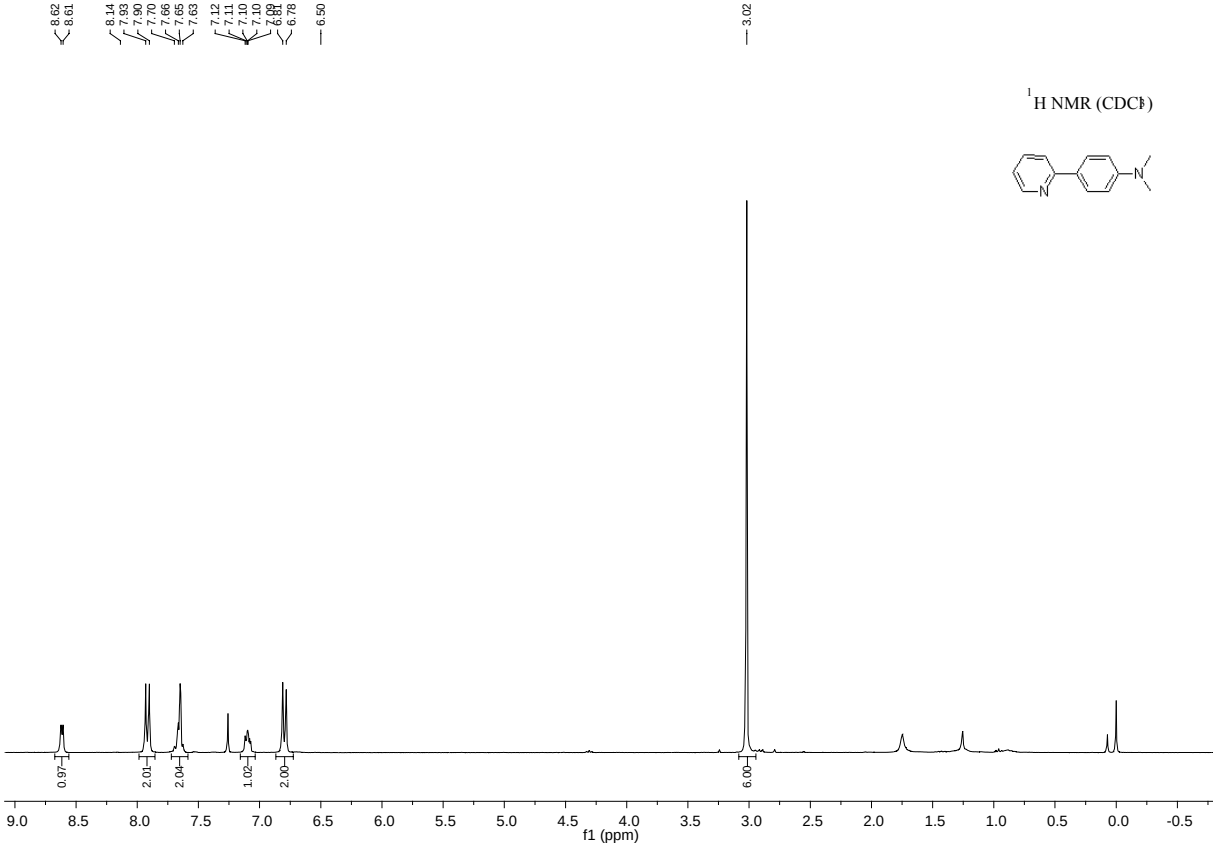


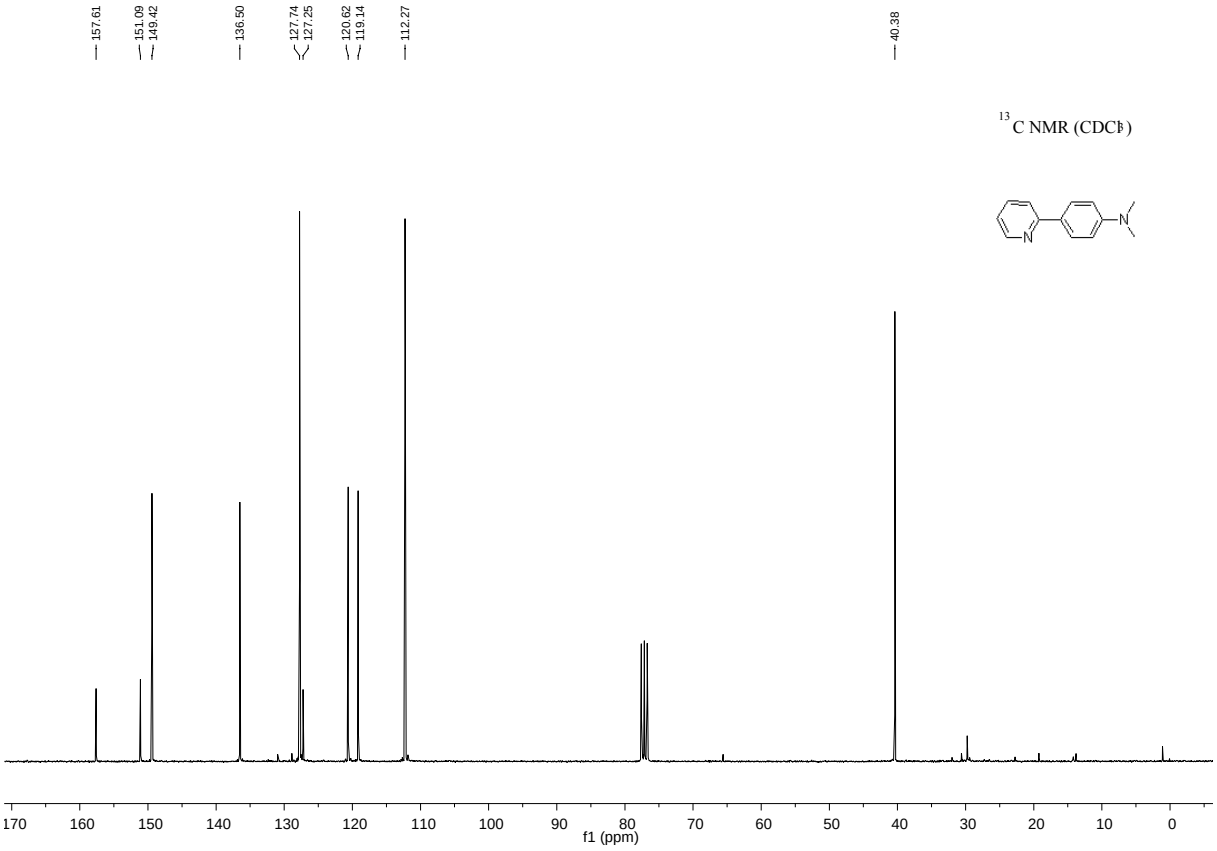
(26) 2-(4′-Methoxyphenyl)pyridine



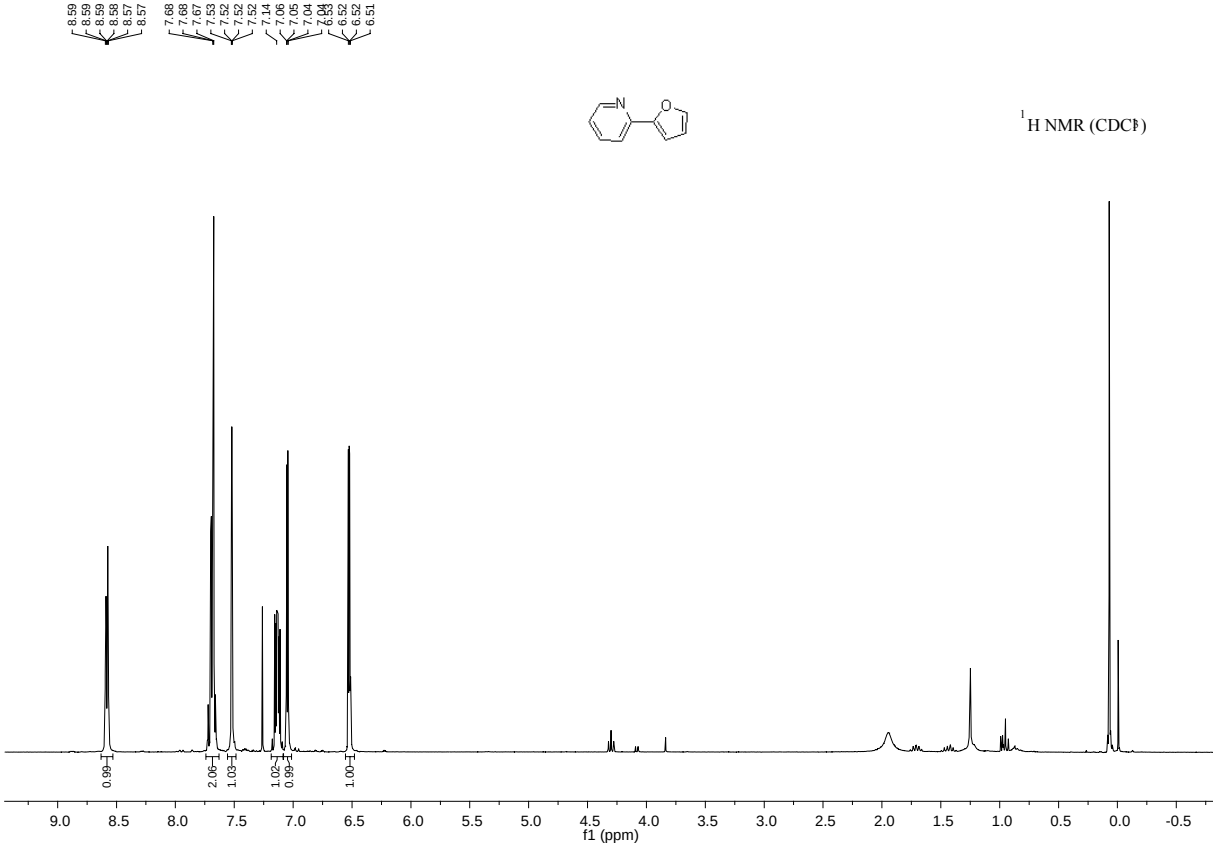


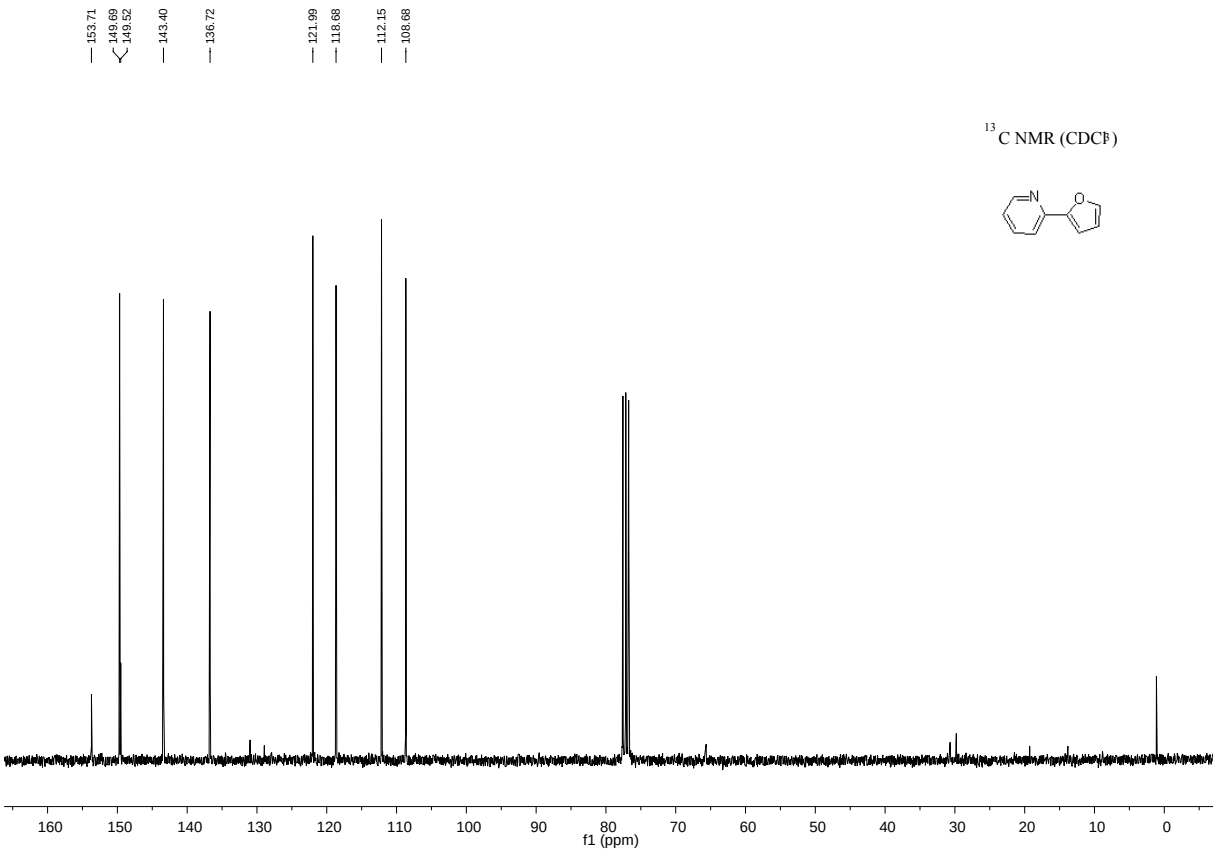
(27) *N,N*-Dimethyl-4-(pyridin-2-yl)benzenamine



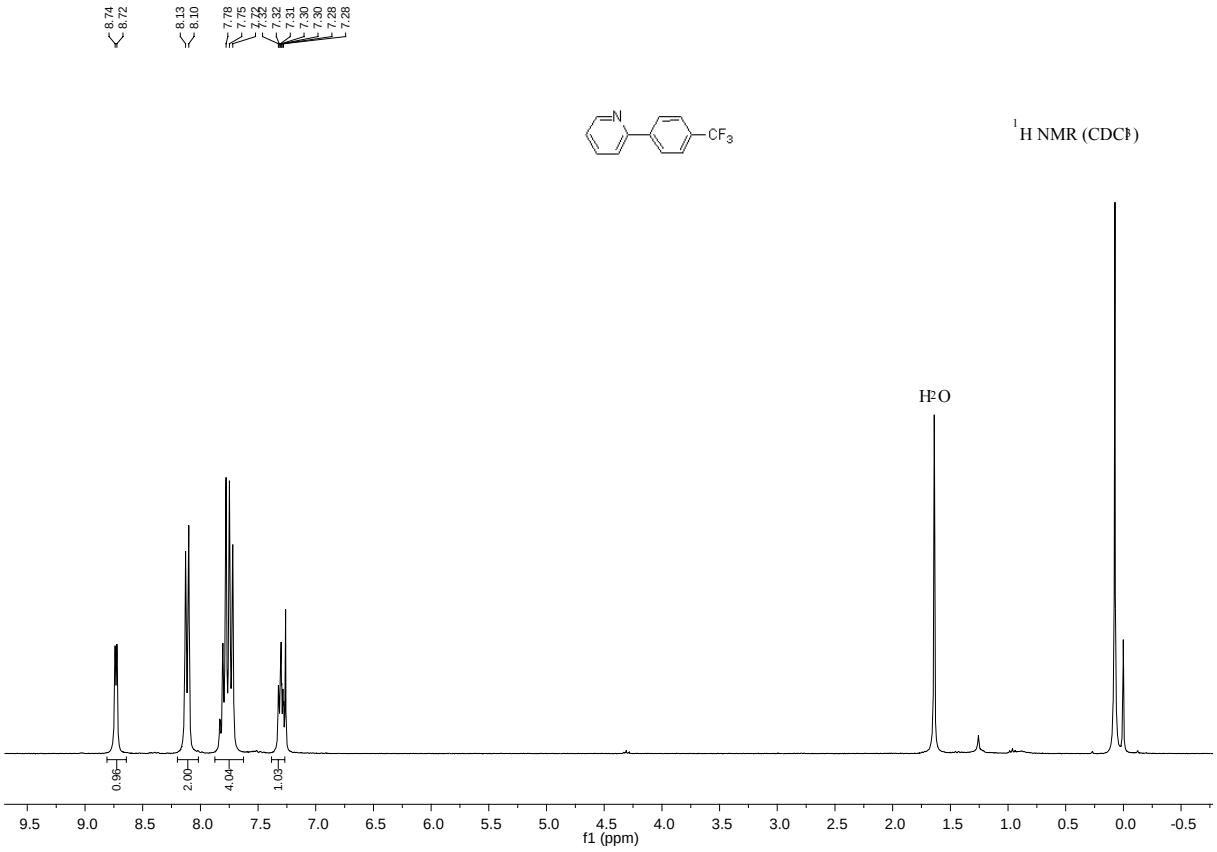


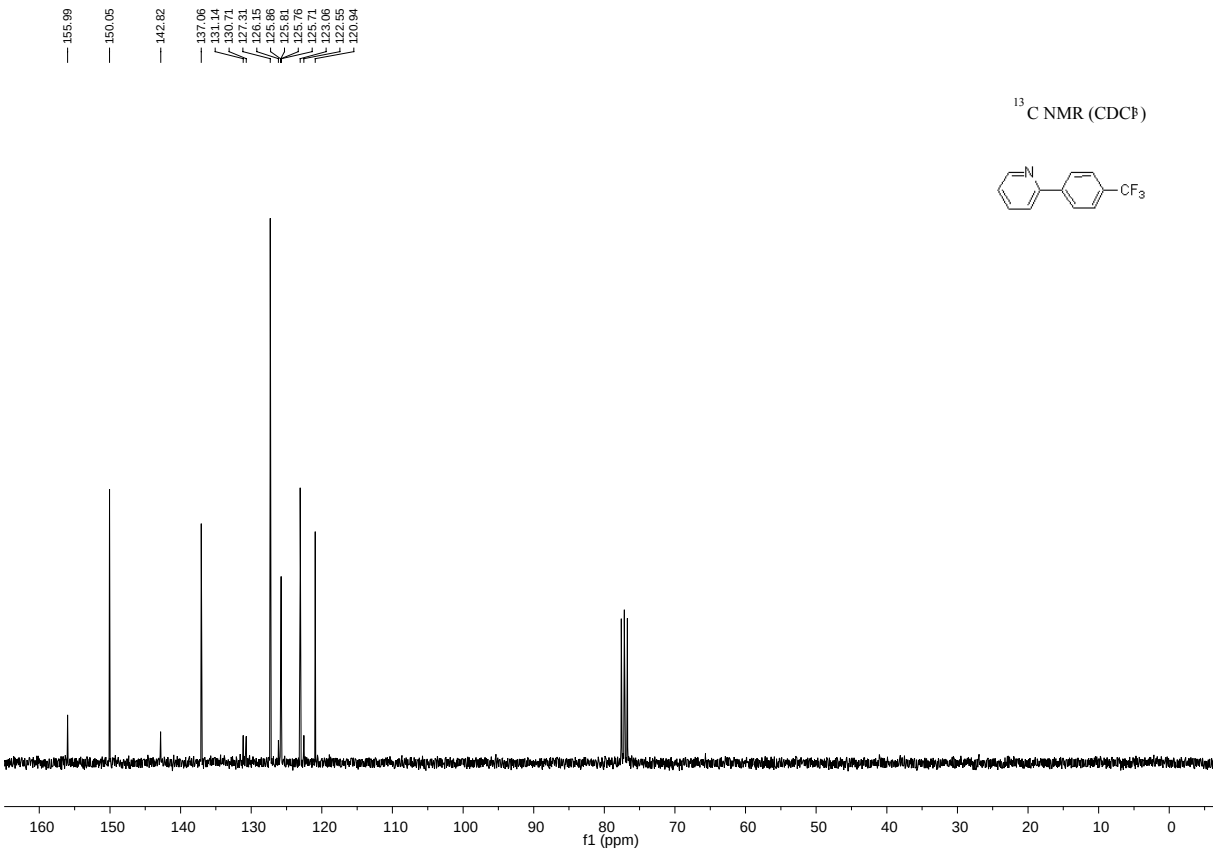
(28) 2-(Furan-2-yl)pyridine



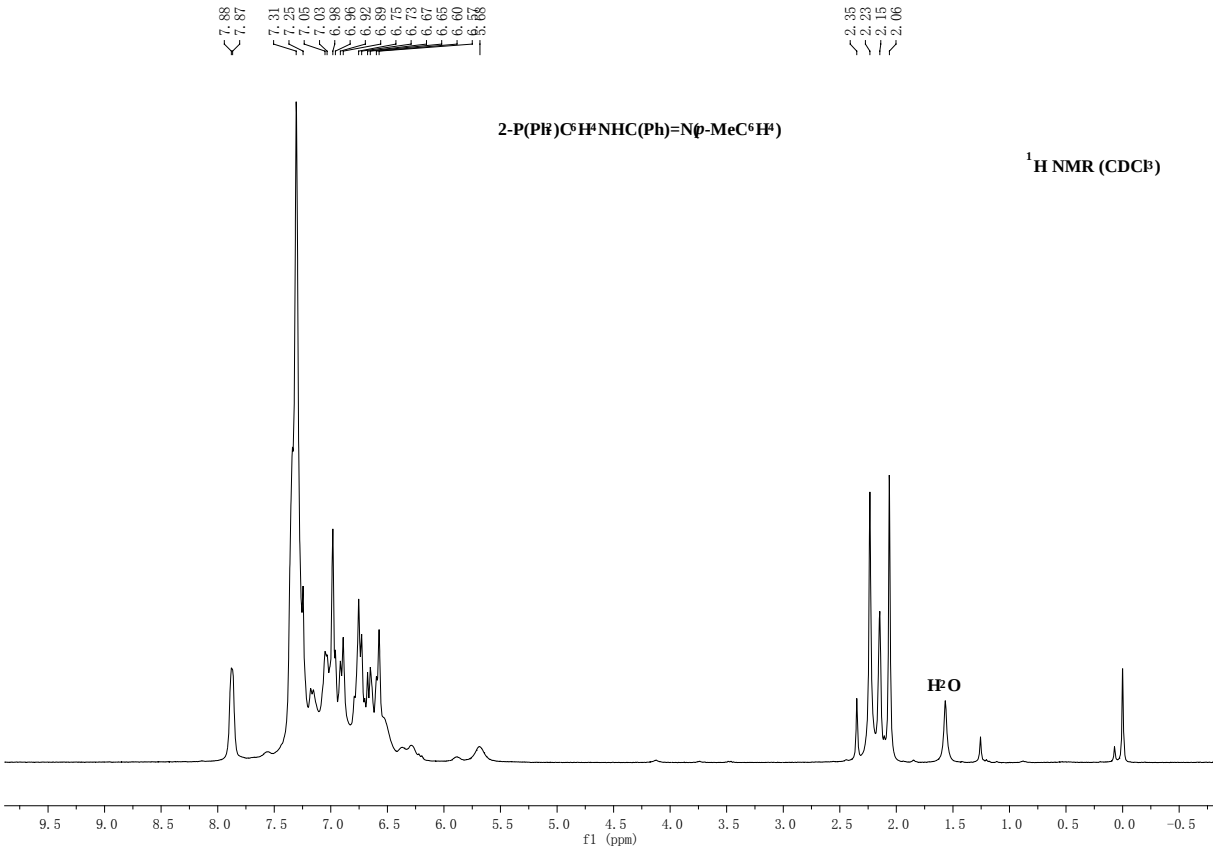


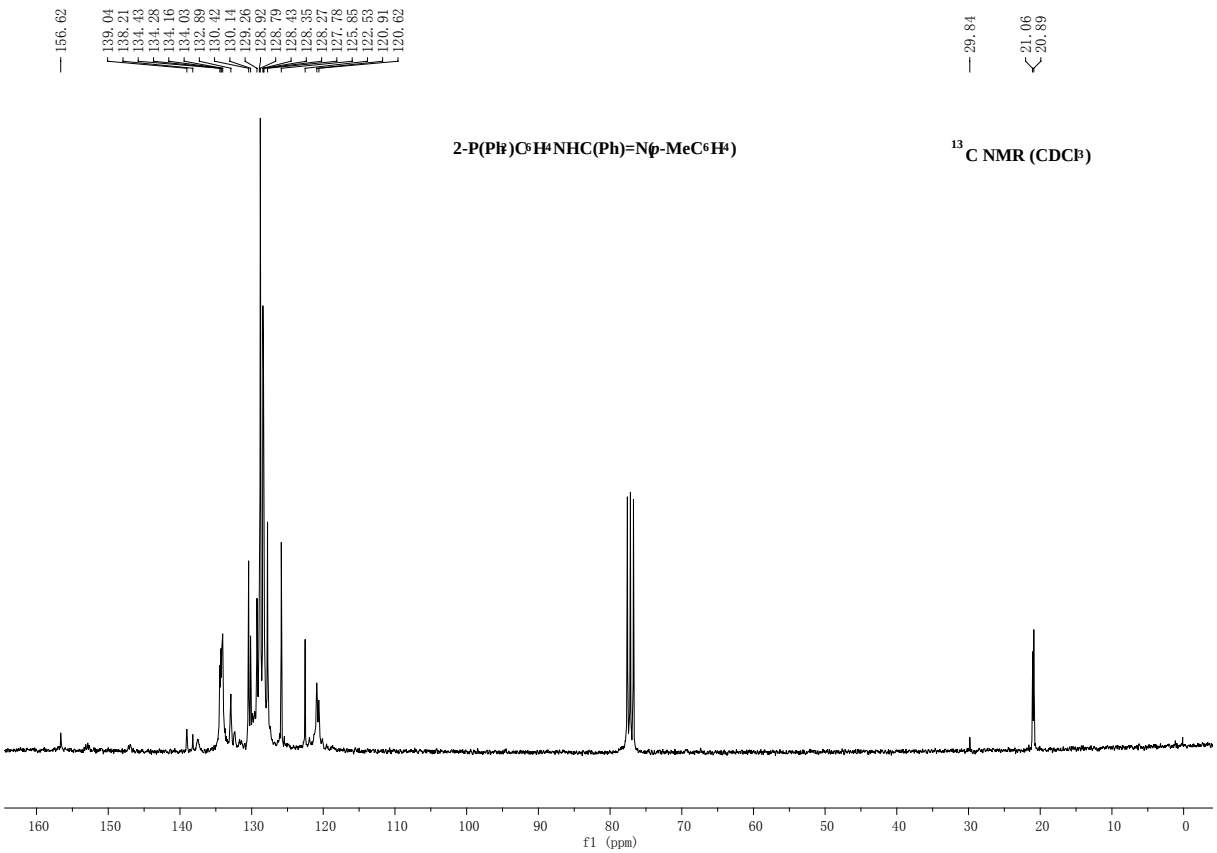
(29) 2-(4-(Trifluoromethyl)phenyl)pyridine



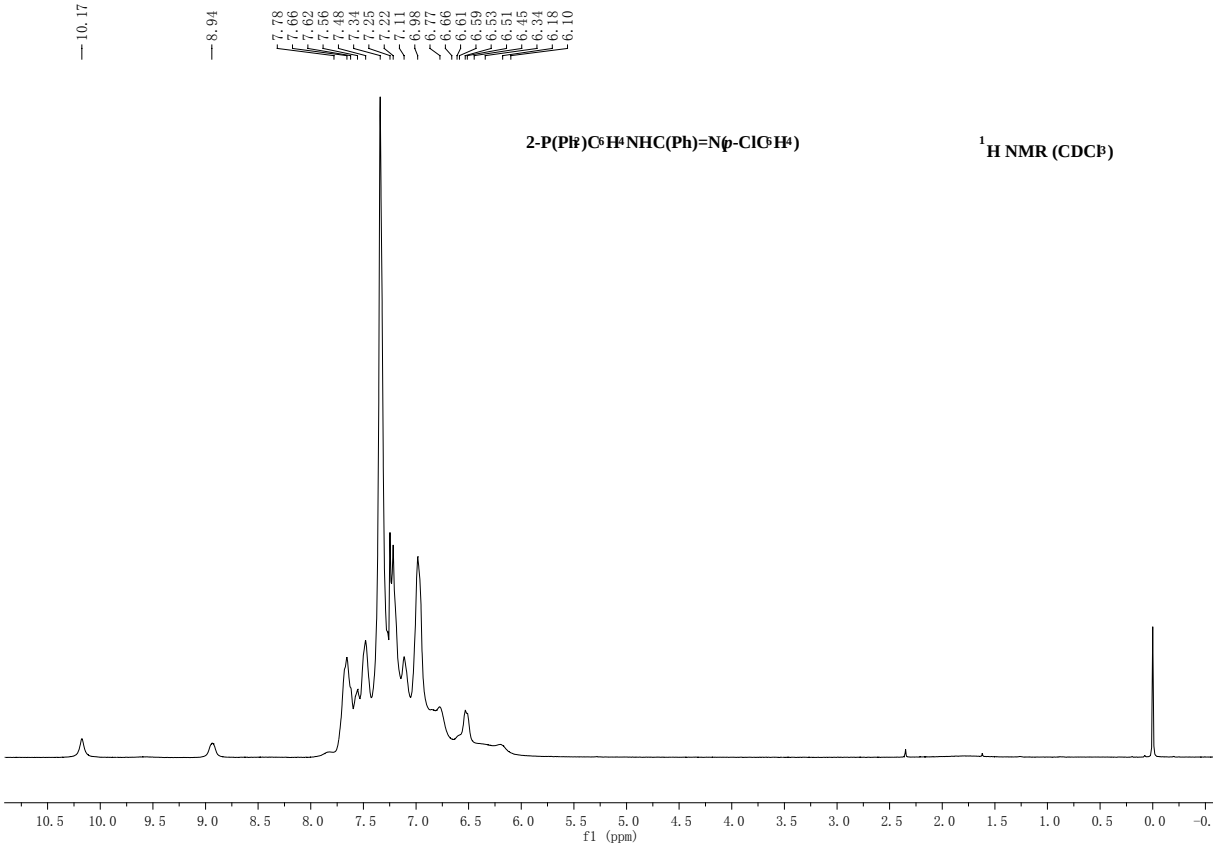


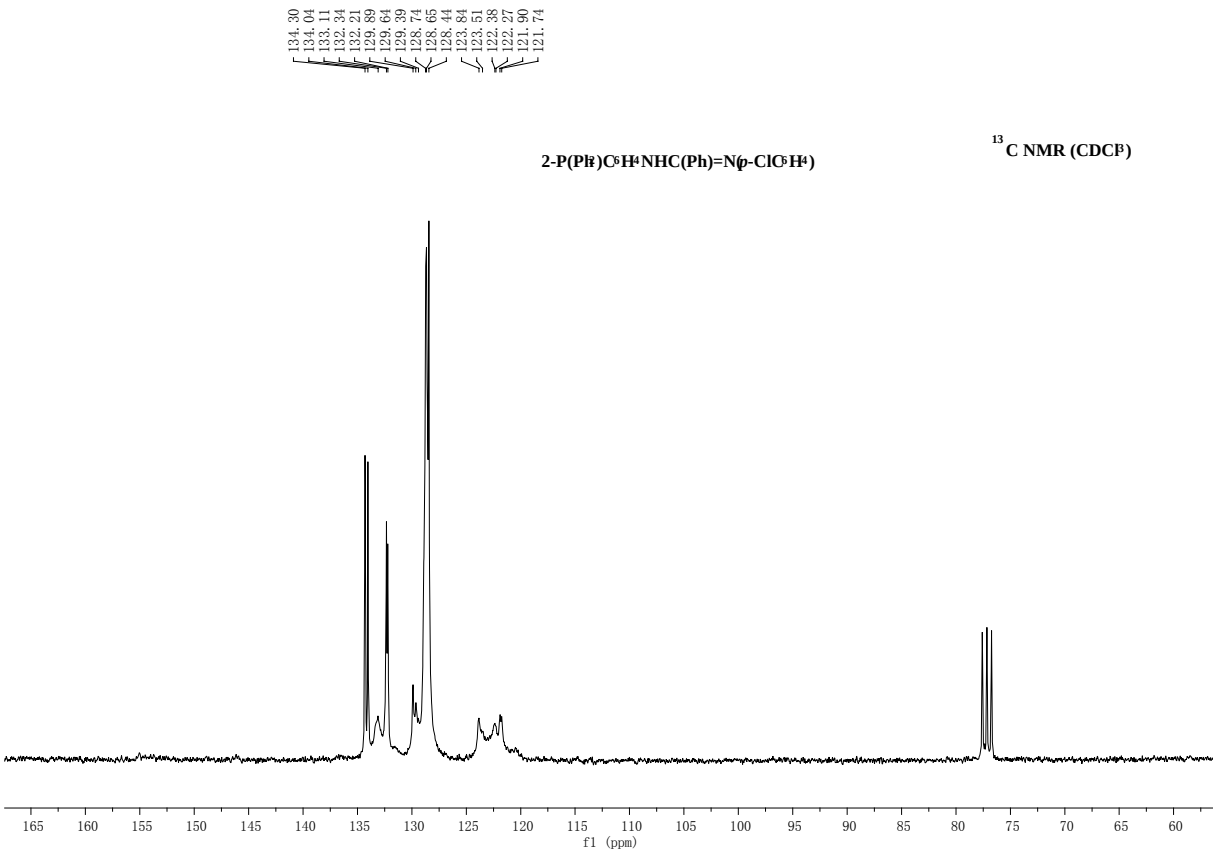
2-P(Ph_2)C_6H_4NHC(Ph)=N(*p*-MeC_6H_4) (**1**)



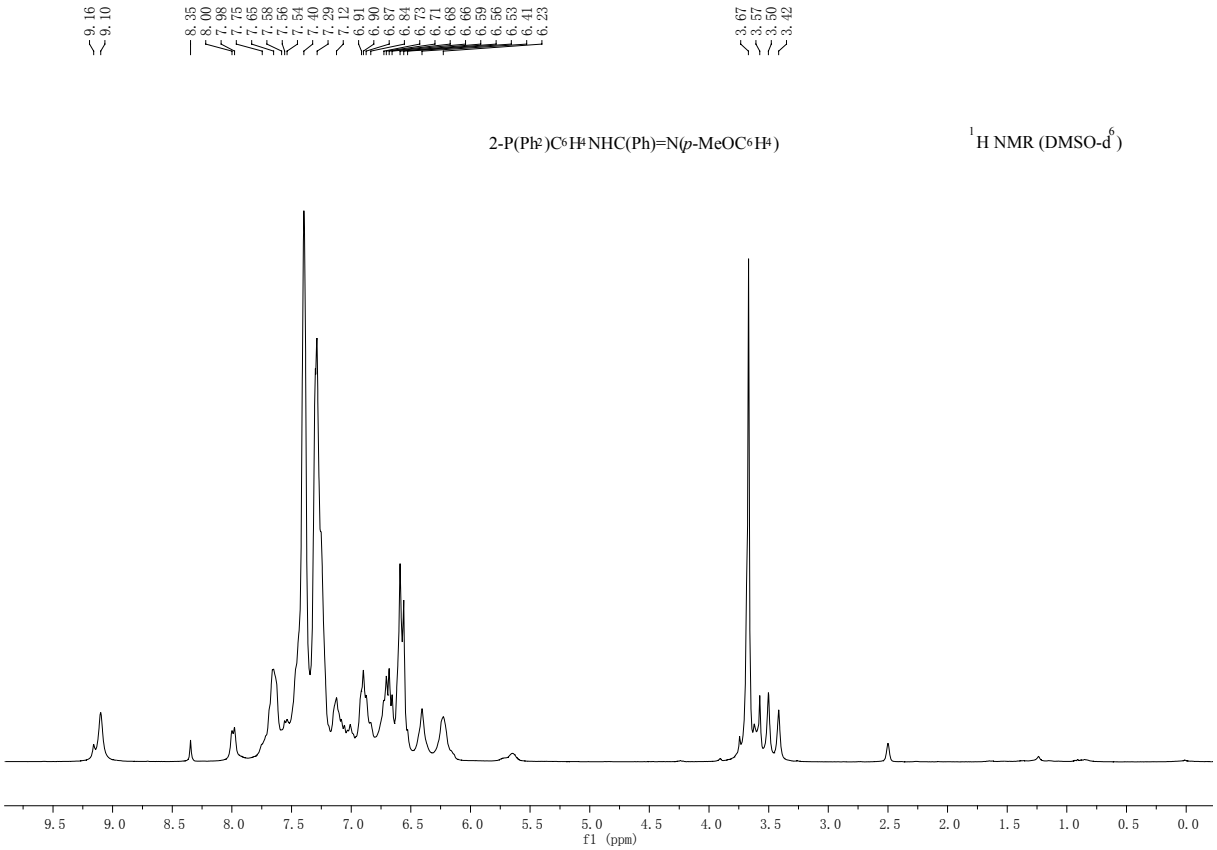


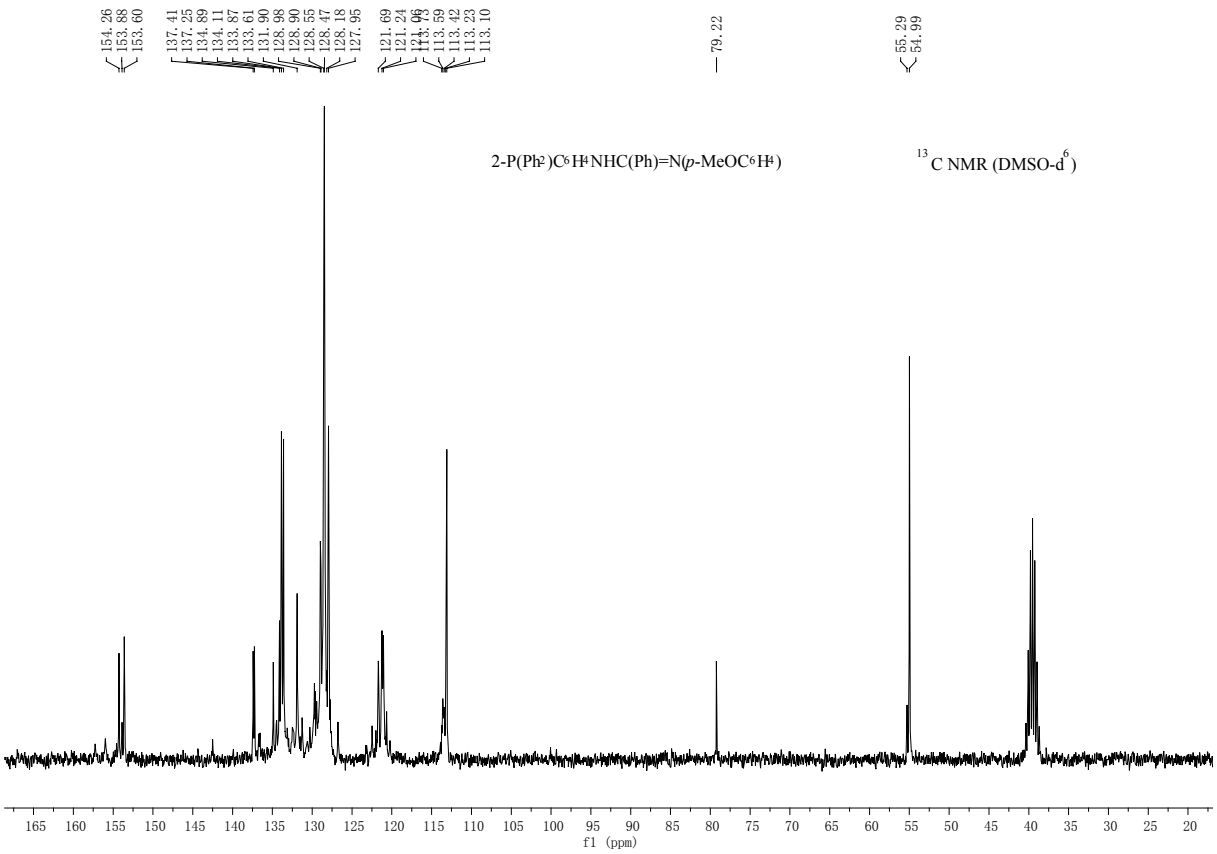
2-P(Ph_2)C_6H_4NHC(Ph)=N(*p*-ClC_6H_4) (**2**)



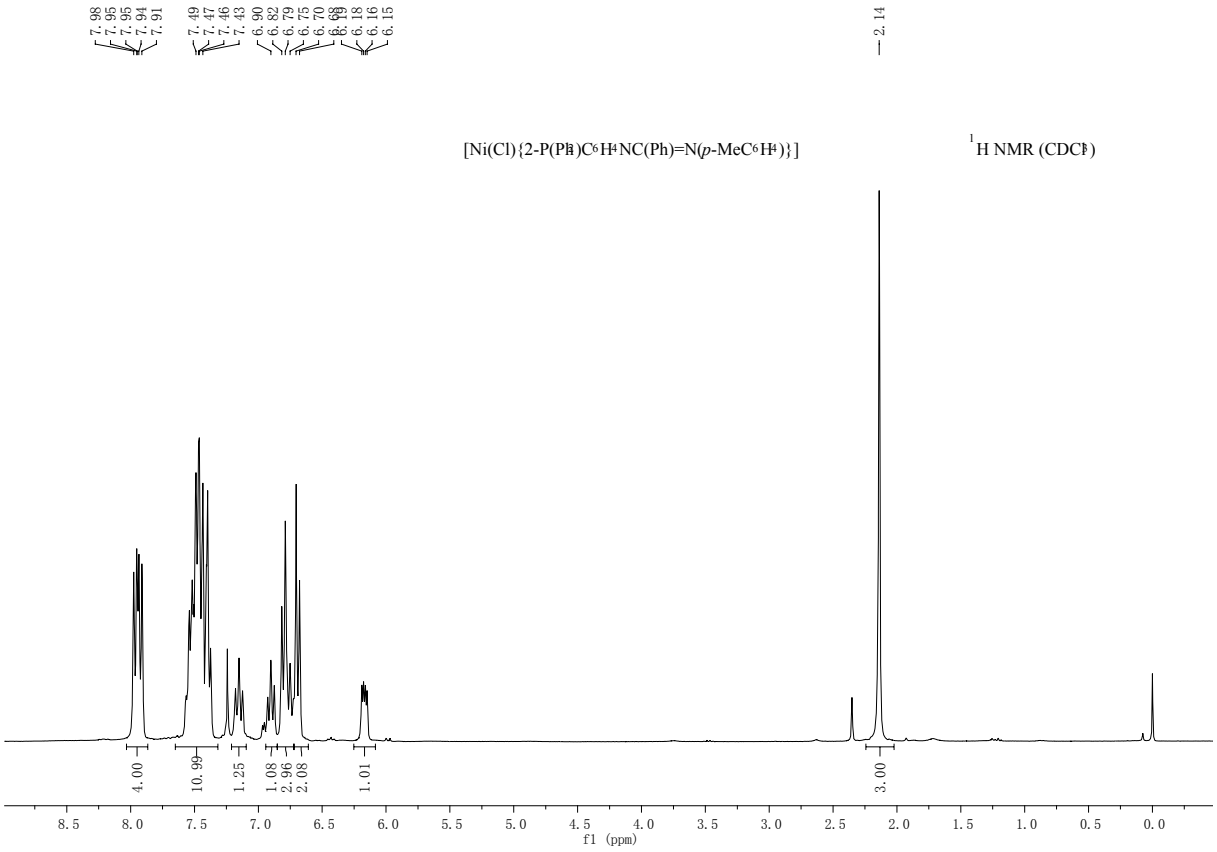


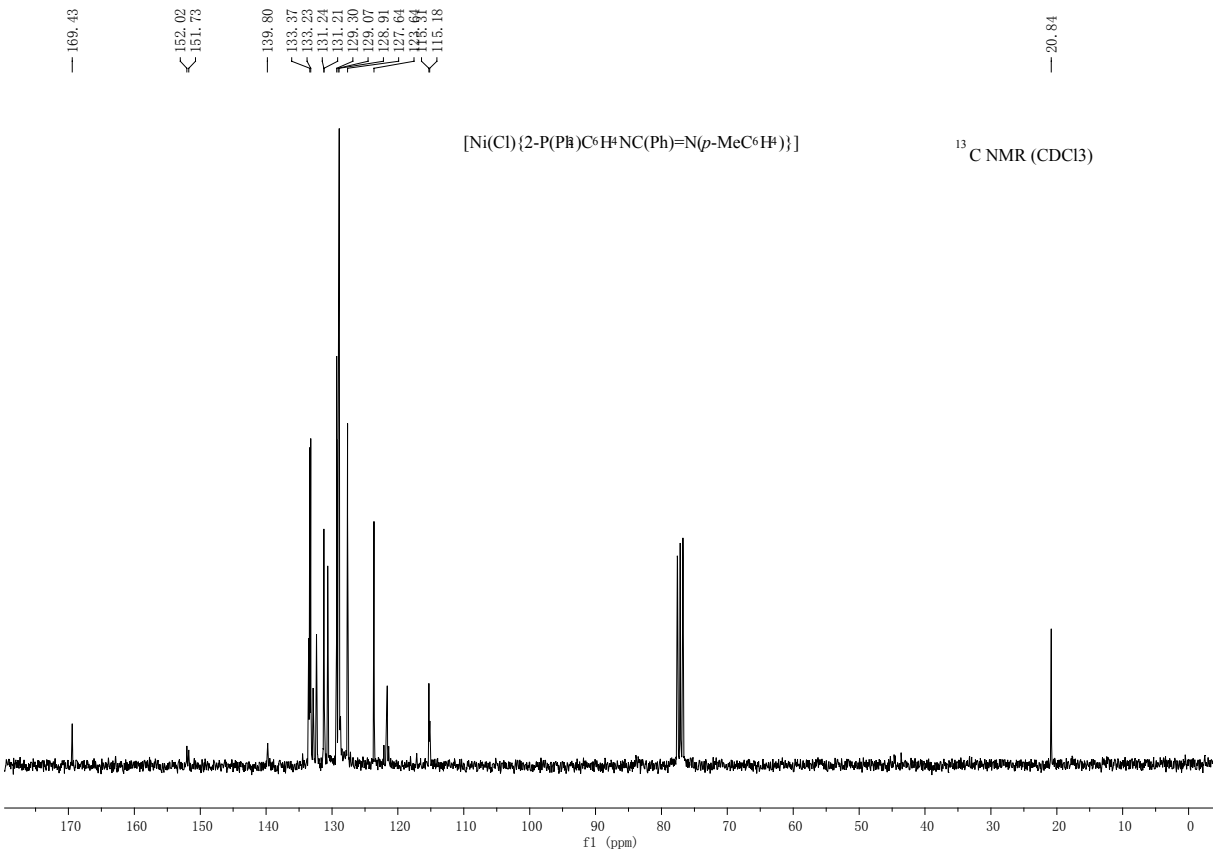
2-P(Ph_2)C_6H_4NHC(Ph)=N(*p*-MeOC_6H_4) (**3**)



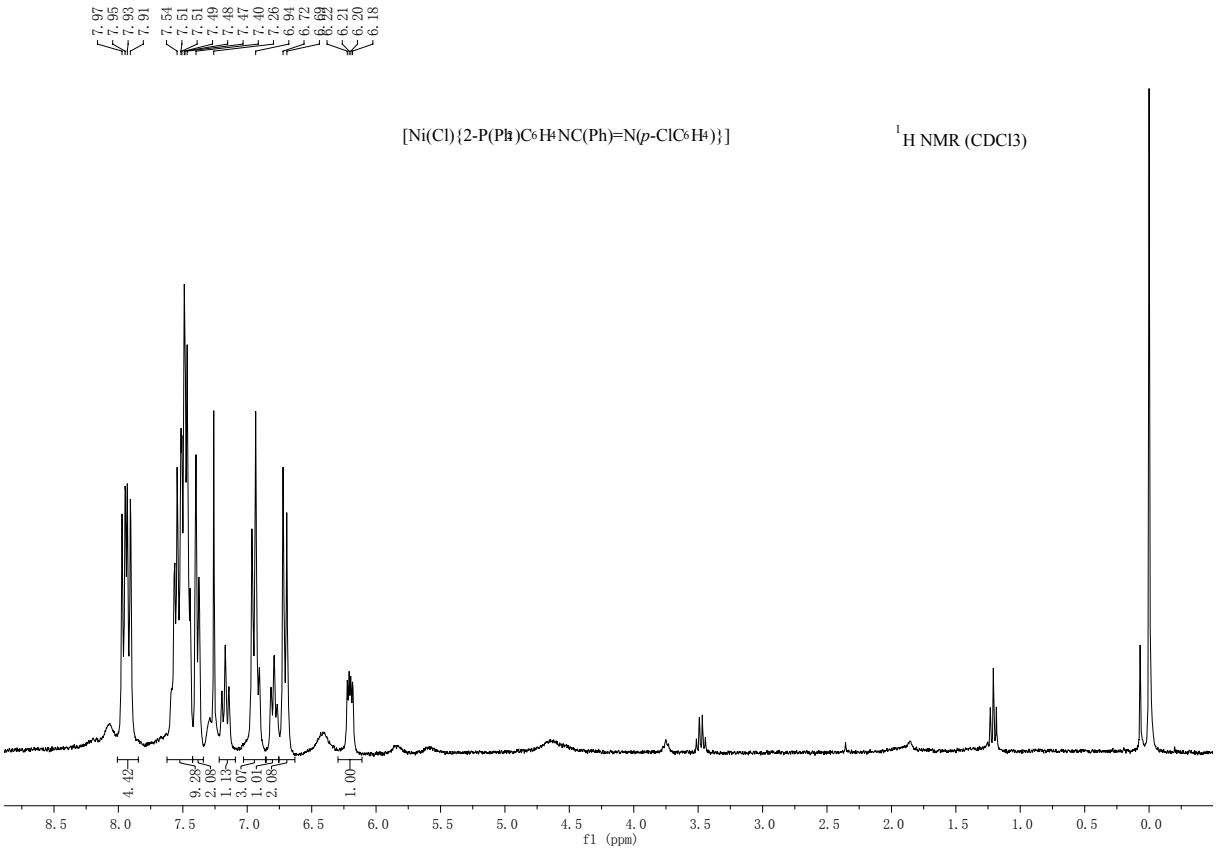


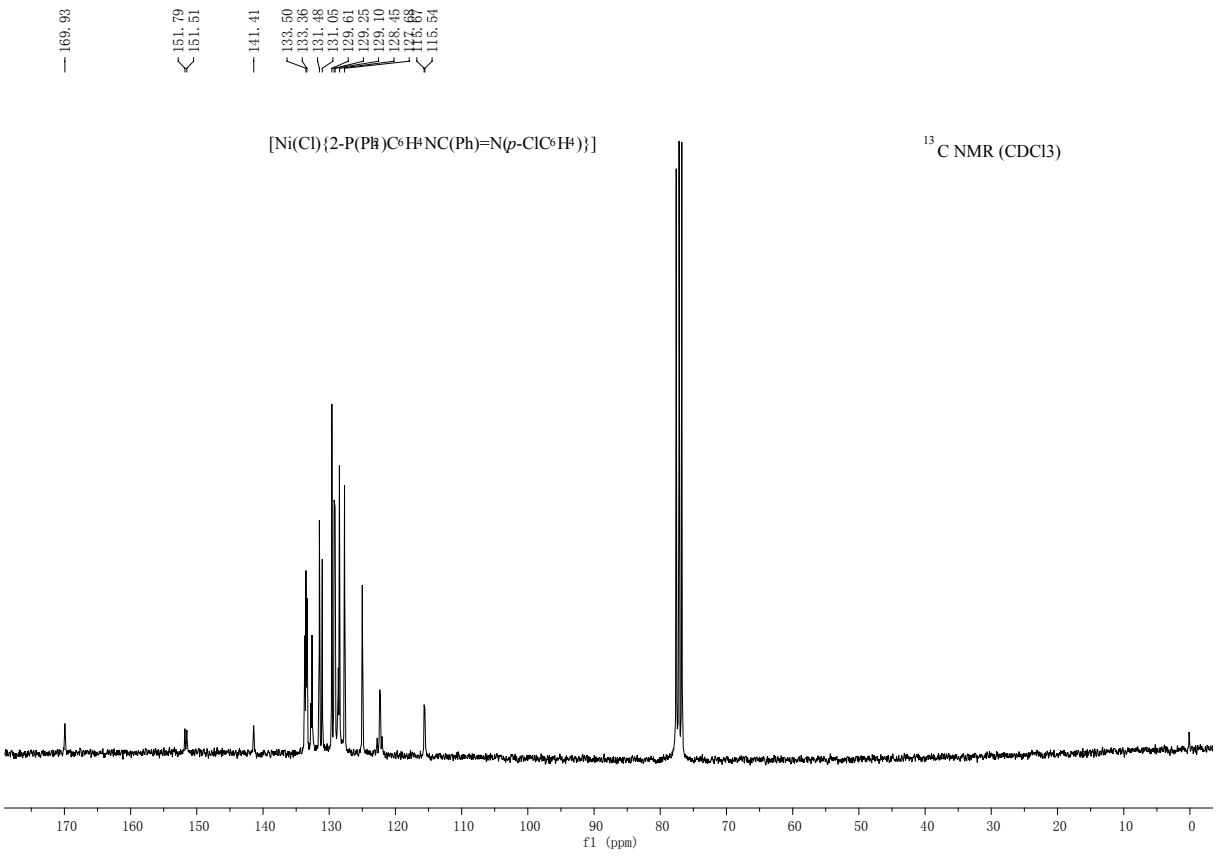
[Ni(Cl){2-P(Ph_2)C_6H_4NC(Ph)=N(*p*-MeC_6H_4)}] (**I**)



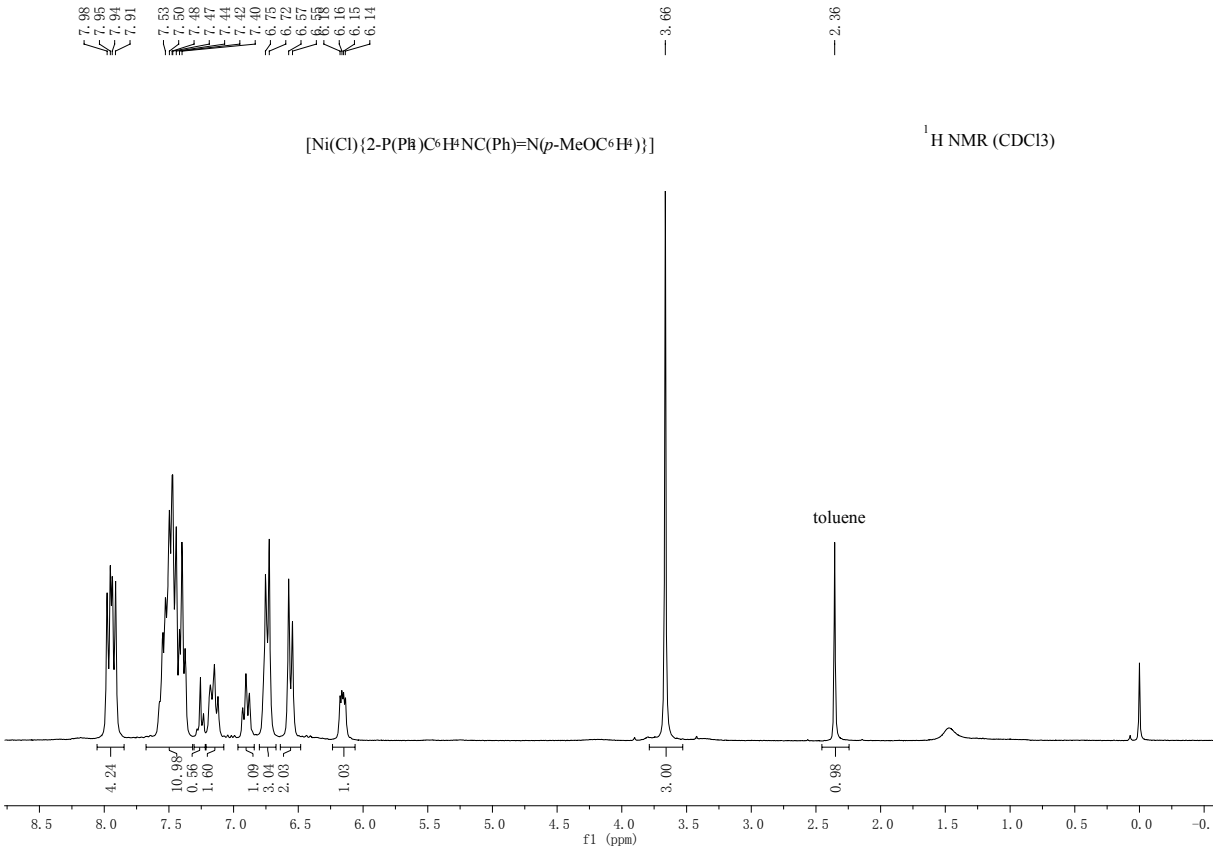


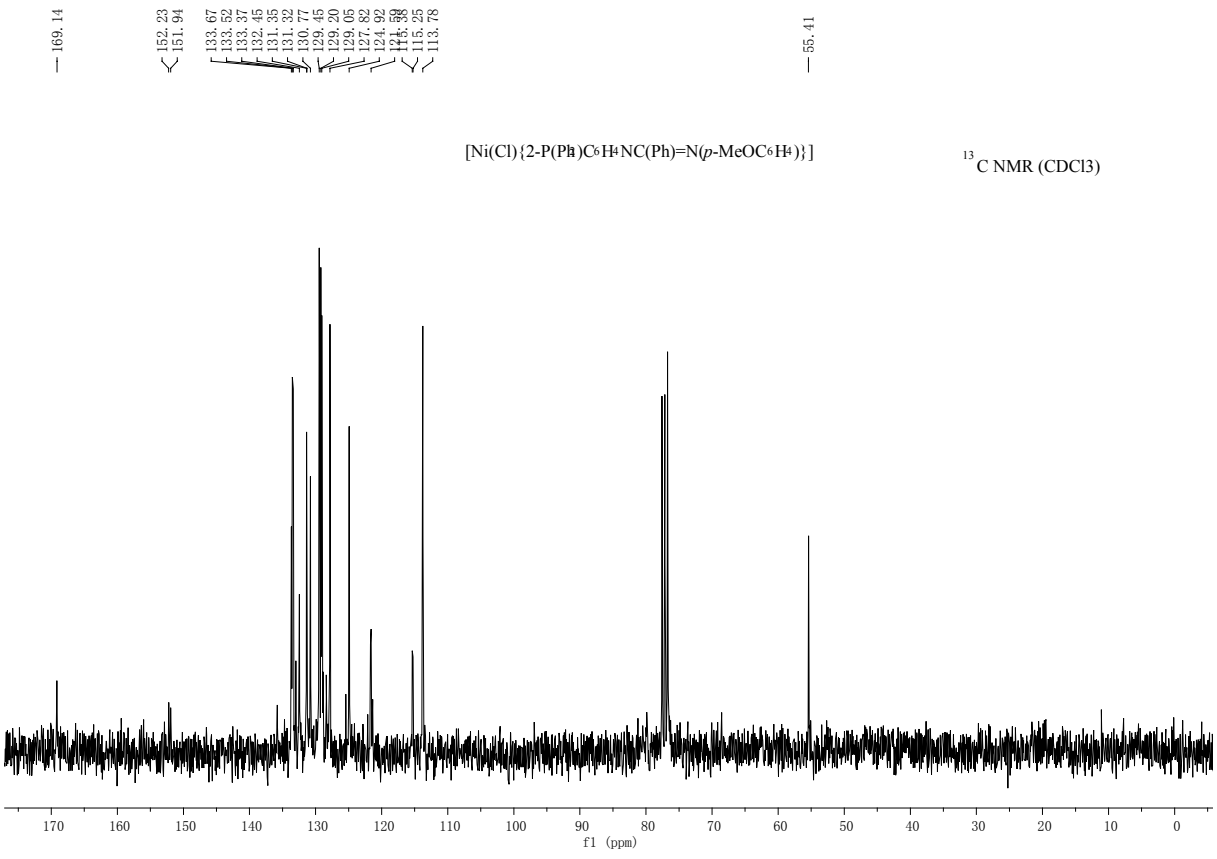
[Ni(Cl){2-P(Ph$_2$)C$_6$H$_4$NC(Ph)=N(*p*-ClC$_6$H$_4$)}] (**II**)



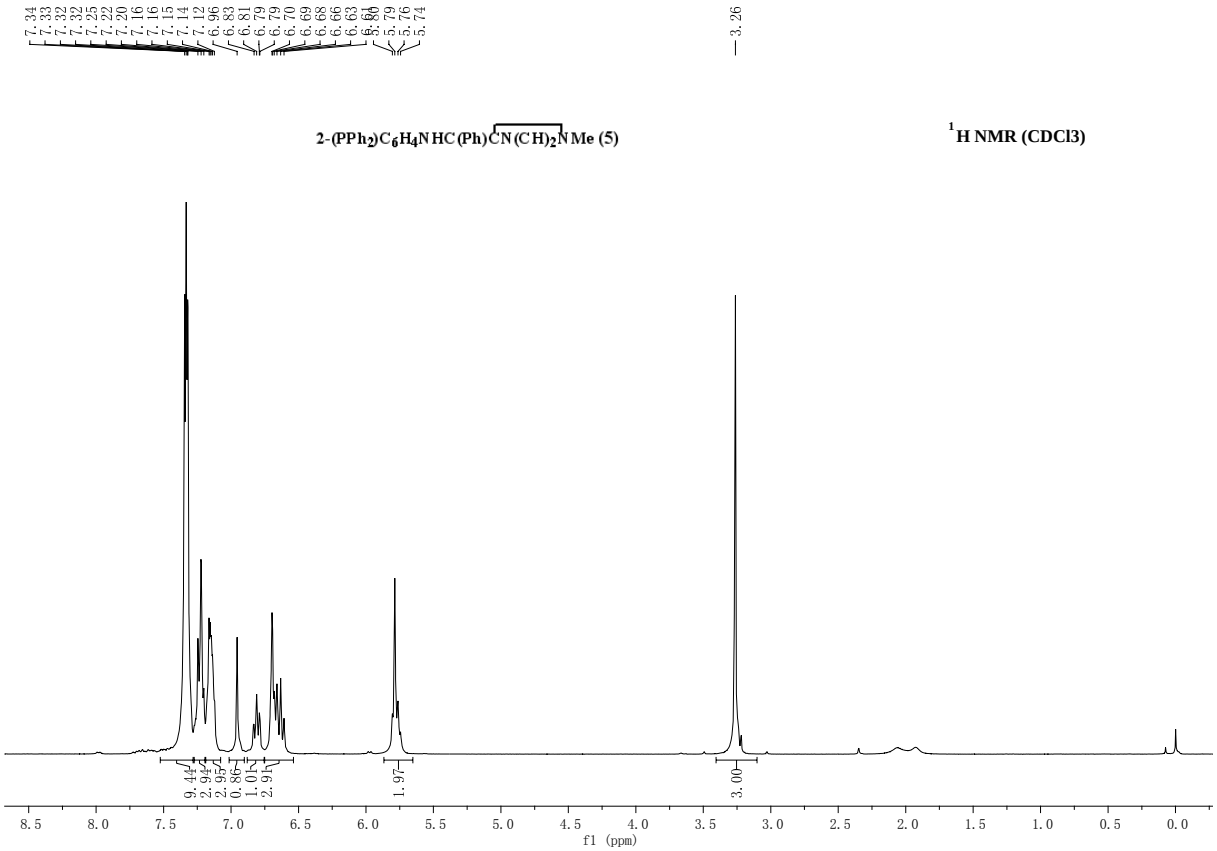


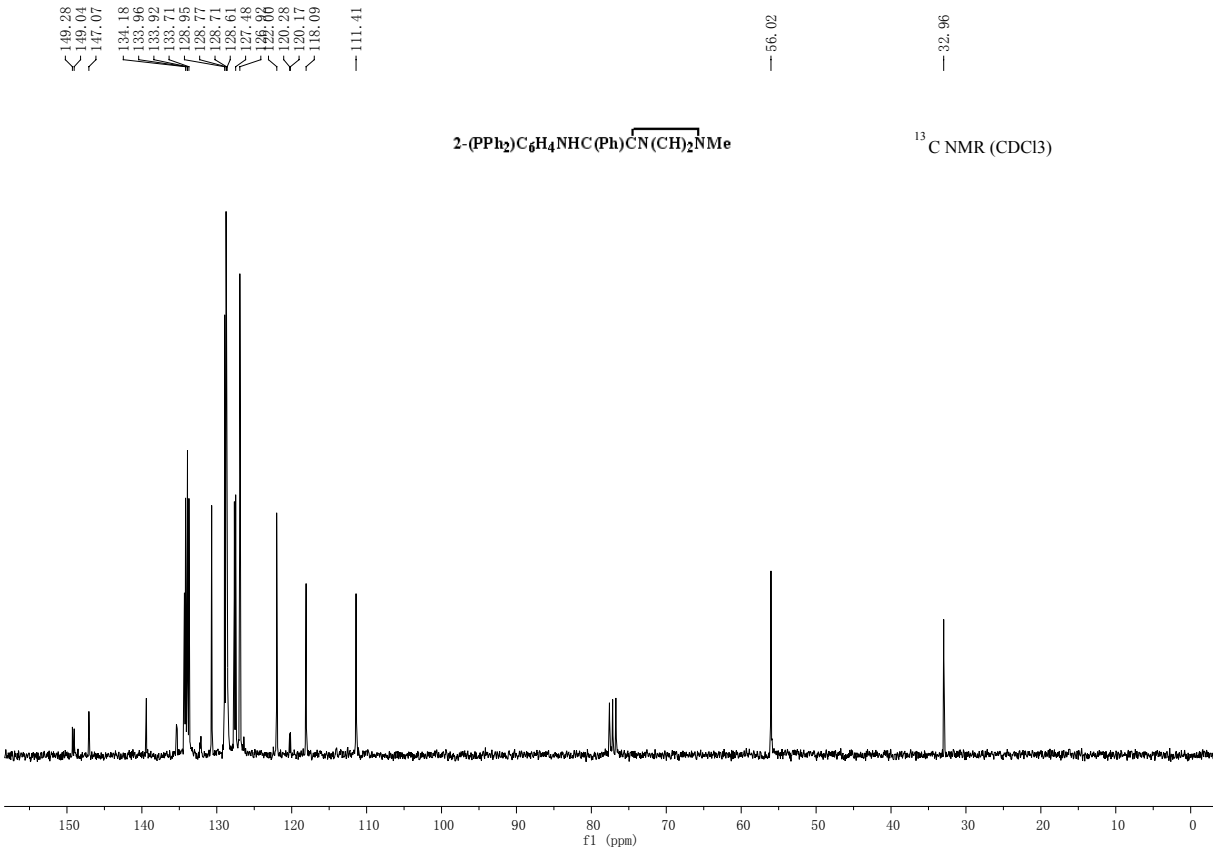
[Ni(Cl){2-P(Ph$_2$)C$_6$H$_4$NC(Ph)=N(*p*-MeOC$_6$H$_4$)}] (**III**)



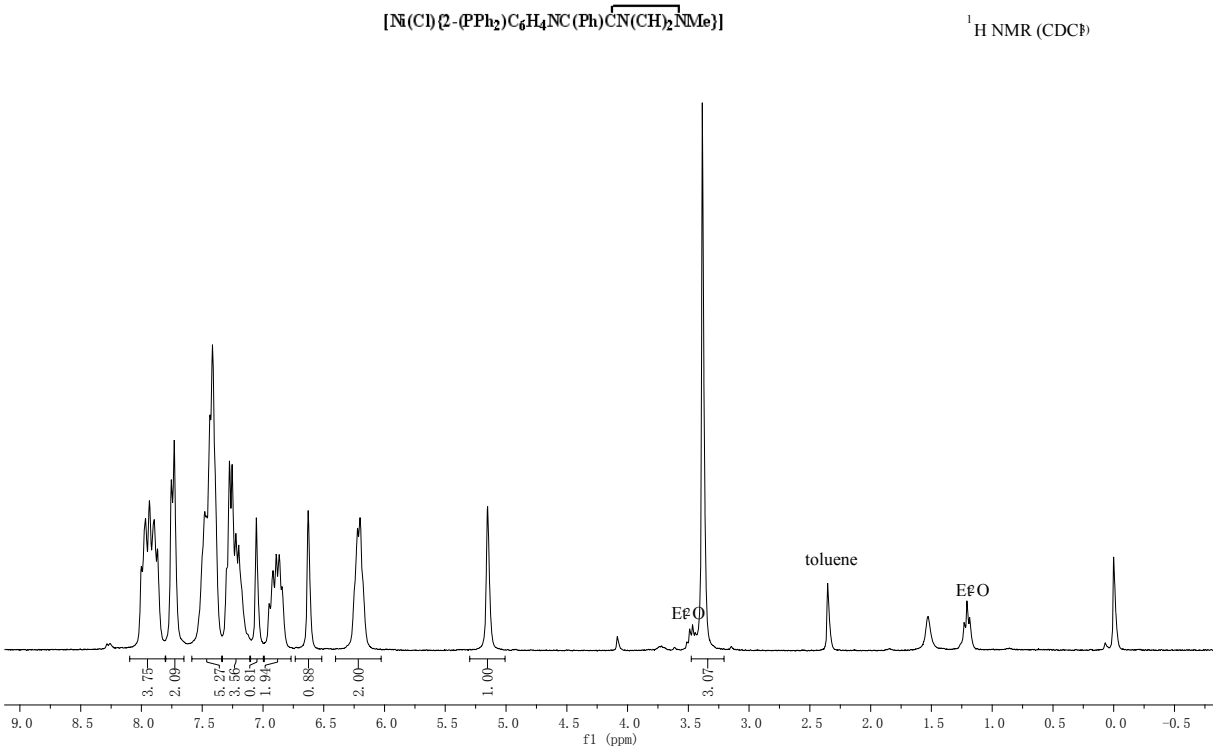


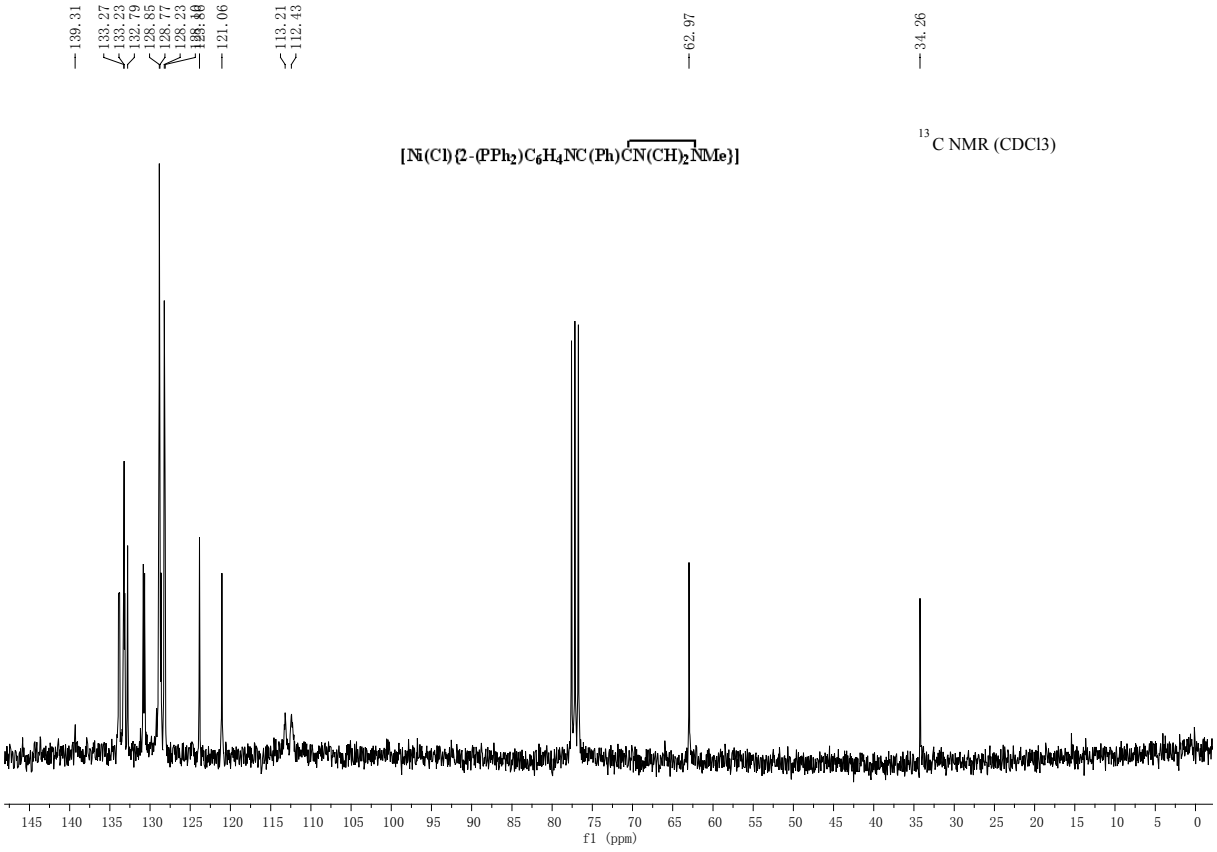
2-(PPh$_2$)C$_6$H$_4$NHC(Ph)$\overline{\text{CN(CH)}_2\text{N}}$Me (5)



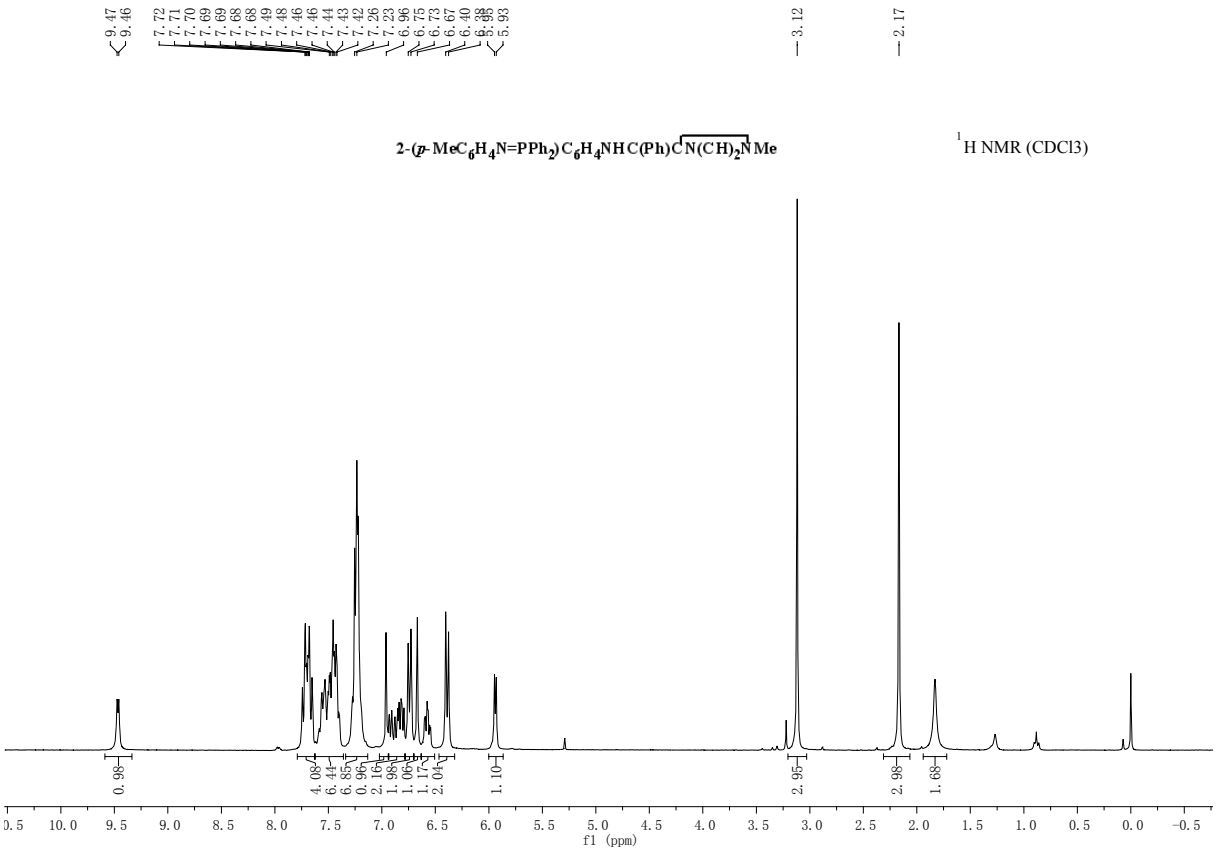


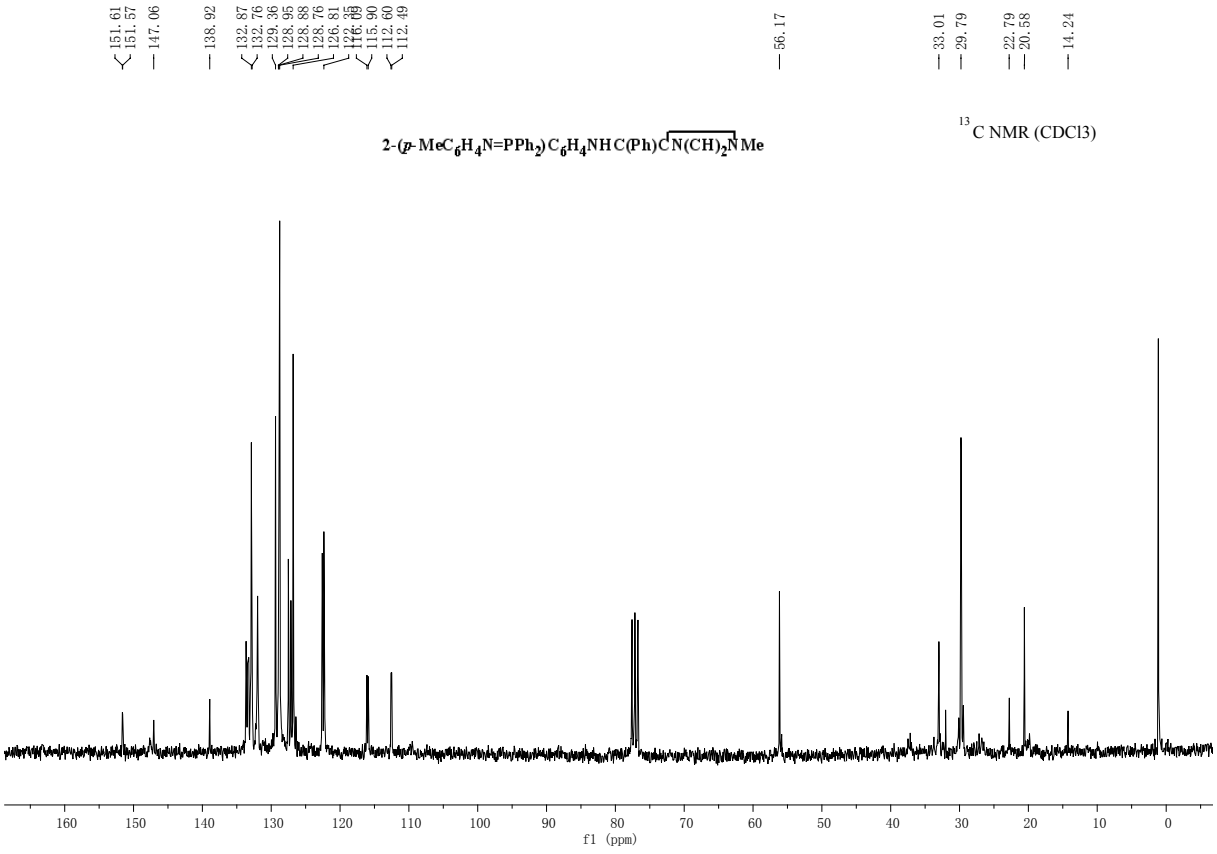
[Ni(Cl){2-(PPh$_2$)C$_6$H$_4$NC(Ph)$\overline{\text{CN(CH)}_2\text{NMe}}$}] (IV)



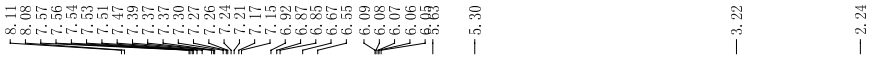


2-(*p*-MeC$_6$H$_4$N=PPh$_2$)C$_6$H$_4$NHC(Ph)C[N(CH)$_2$N]Me (6)



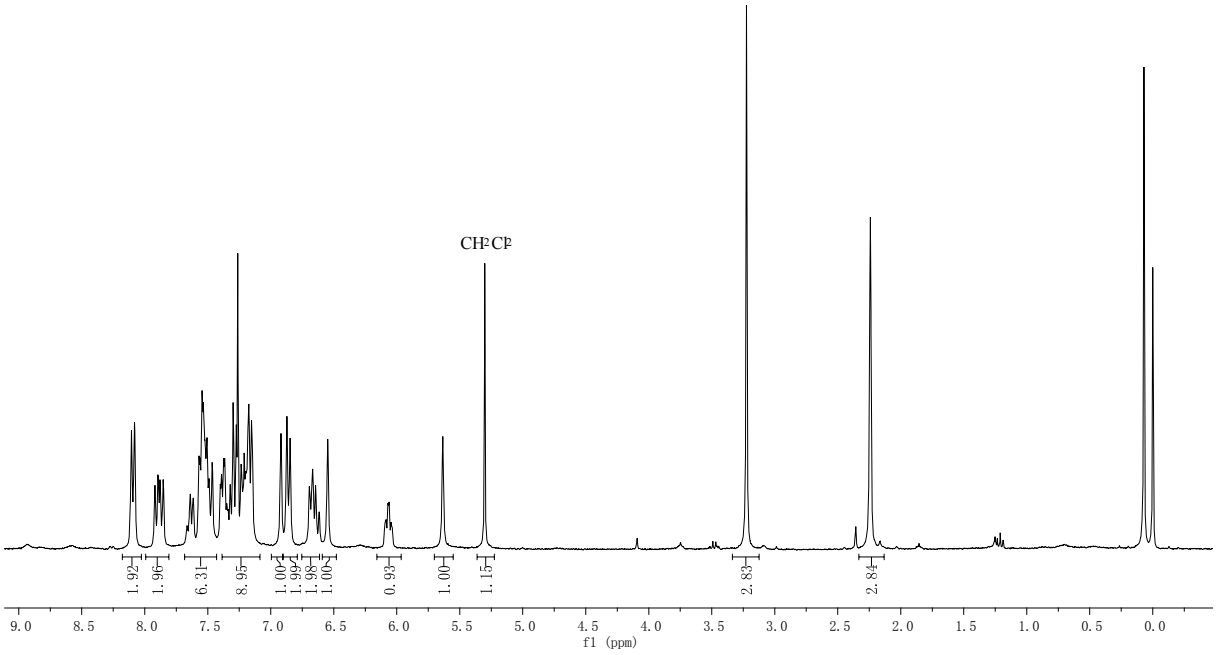


[Ni(Cl){2-(*p*-MeC$_6$H$_4$N=PPh$_2$)C$_6$H$_4$NC(Ph)$\overline{\text{CN(CH)}_2\text{N}}$Me] (V)



^{1}H NMR (CDCl$_3$)

[Ni(Cl){2-(*p*-MeC$_6$H$_4$N=PPh$_2$)C$_6$H$_4$NC(Ph)$\overline{\text{CN(CH)}_2\text{N}}$Me]



[Ni(Cl){2-(*p*-MeC$_6$H$_4$N=PPh$_2$)C$_6$H$_4$NC(Ph)$\overline{\text{CN(CH)}_2\text{N}}$Me]

^{13}C NMR (CDCl3)