Synthesis and Catalytic Activity of N-Heterocyclic Silylene (NHSi) Cobalt Hydride for Kumada Coupling Reactions

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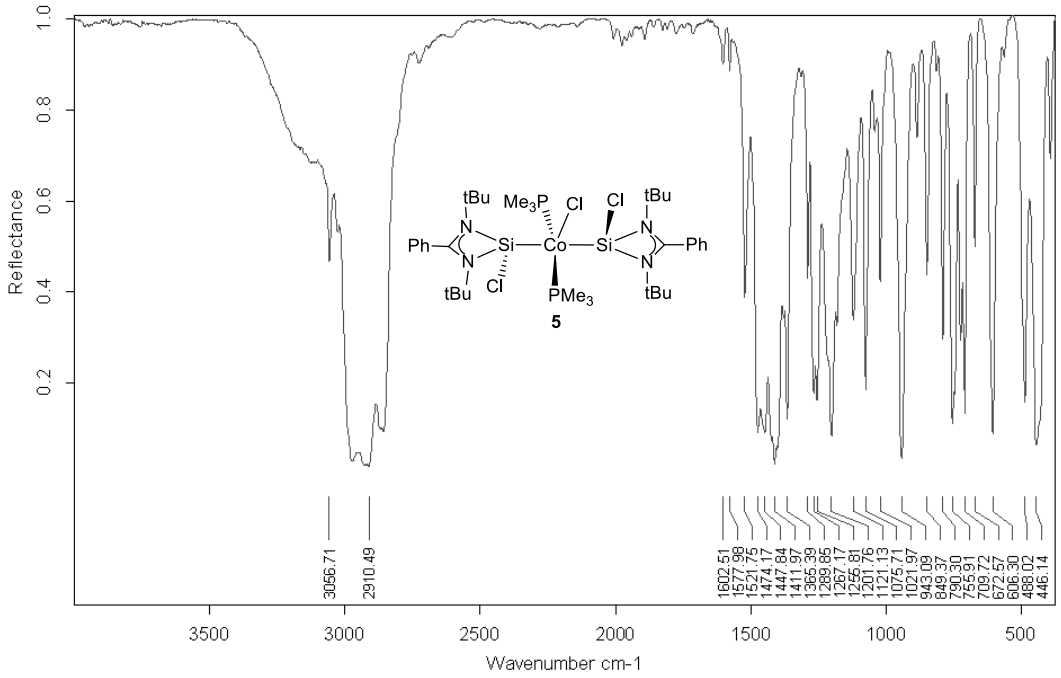
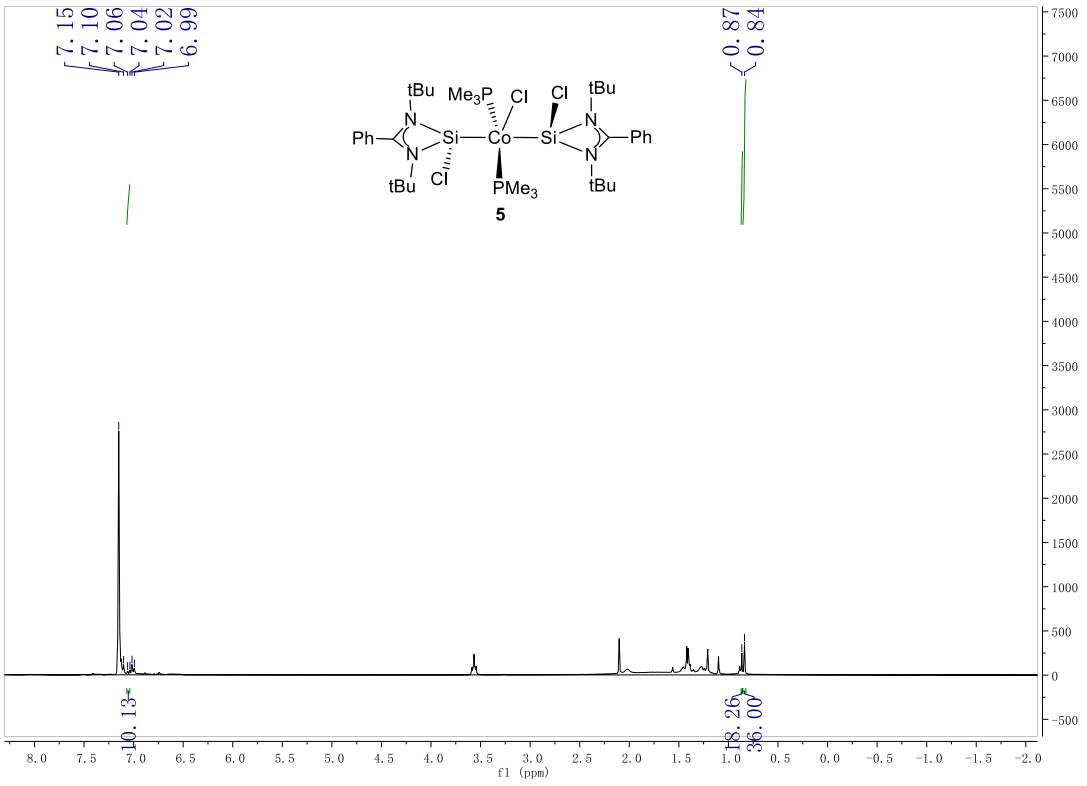
SI The table of selected crystallographic data

	5	**6**	**6d**
formula	$C_{41}H_{76}Cl_3CoN_4P_2Si_2$	$C_{106}H_{138}Cl_4Co_2N_8OP_6Si_4$	$C_{55}H_{73}Cl_2CoN_4OP_3Si_2$
M_z	908.45	2098.08	1085.09
crystal system	Monoclinic	Triclinic	Triclinic
space group	$P2_1/c$	P-1	P-1
a [Å]	13.8468(3)	13.9433(5)	13.9845(14)
b [Å]	19.5827(5)	17.2555(7)	17.415(2)
c [Å]	18.5459(4)	24.5173(10)	24.858(3)
α [°]	90	99.180(3)	98.767(9)
β [°]	103.406(2)	99.723(3)	101.053(8)
γ [°]	90	103.830(3)	103.860(8)
V [$Å^3$]	4891.8(2)	5521.0(4)	5642.2(11)
T [K]	150.15	150.15	173.15
Z	4	2	4
μ[mm^{-1}]	5.581	4.862	0.568
total reflns	22857	49093	56456
unique reflns	7980	17989	30063
R_{int}	0.0674	0.1348	0.0696
$R_1[I>2\sigma(I)]$	0.0466	0.0949	0.0838
$wR(F^2)[I>2\sigma(I)]$	0.0988	0.2452	0.2208
R_1(all data)	0.0827	0.1749	0.1409
$wR(F^2)$(all data)	0.1097	0.3026	0.2695
GOF on F^2	0.875	0.847	0.951

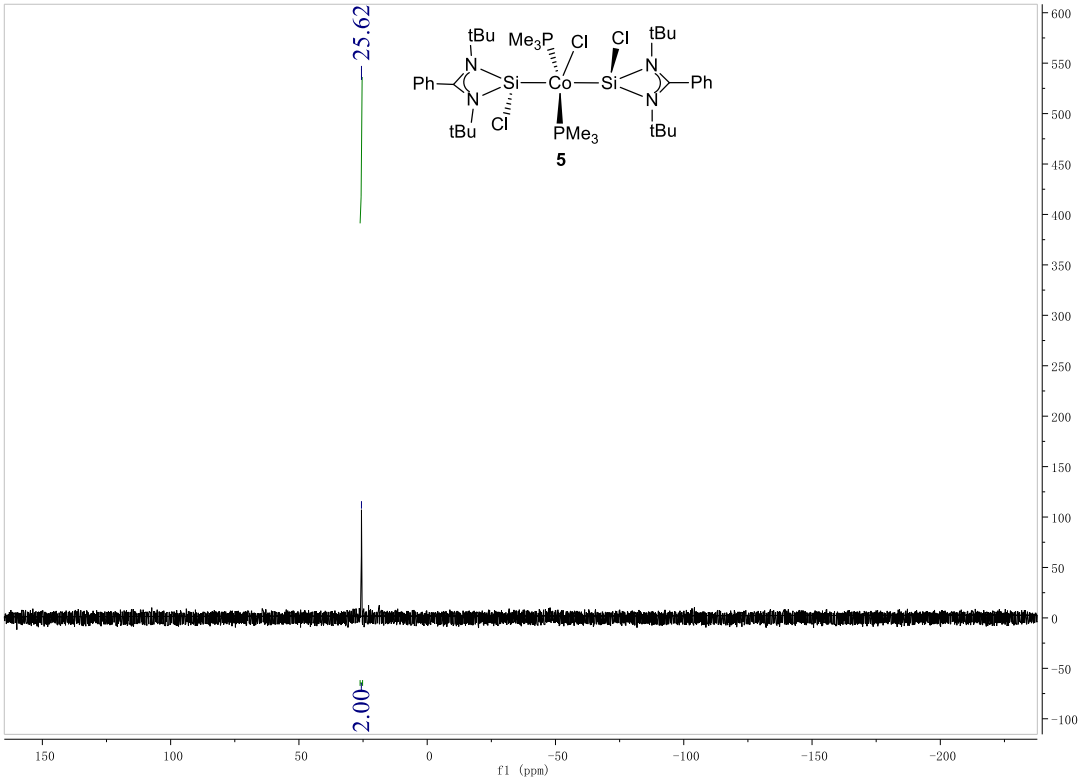
S Ⅱ IR, ^{1}H, ^{31}P and ^{13}C NMR and ^{29}Si NMR spectra of complexes 5, 6 and 6d



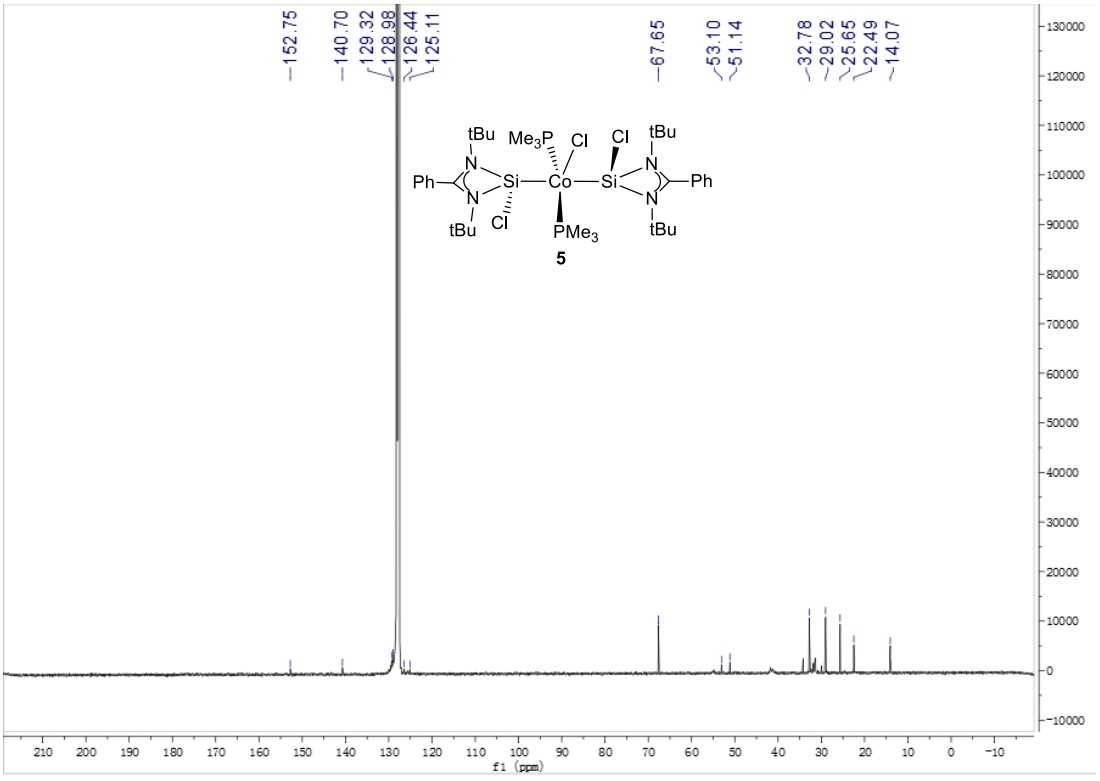
IR spectrum of complex **5**



^{1}H NMR of complex **5**

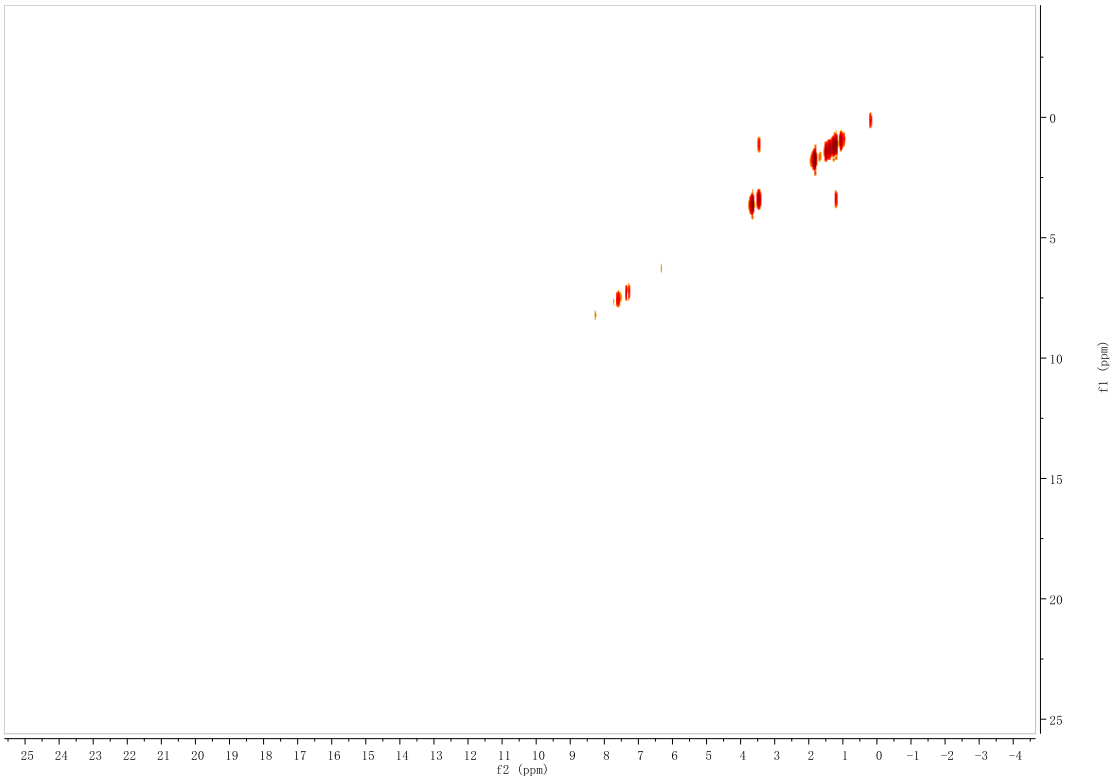


^{31}P NMR of complex **5**

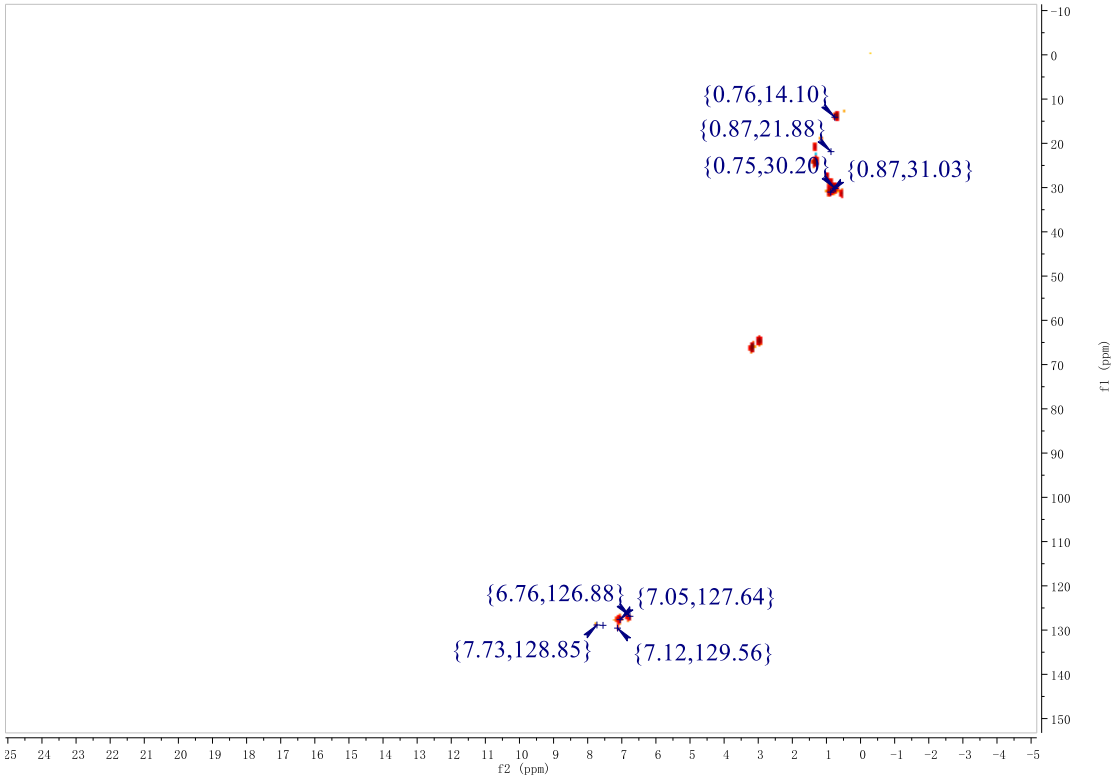


^{13}C NMR of complex **5**

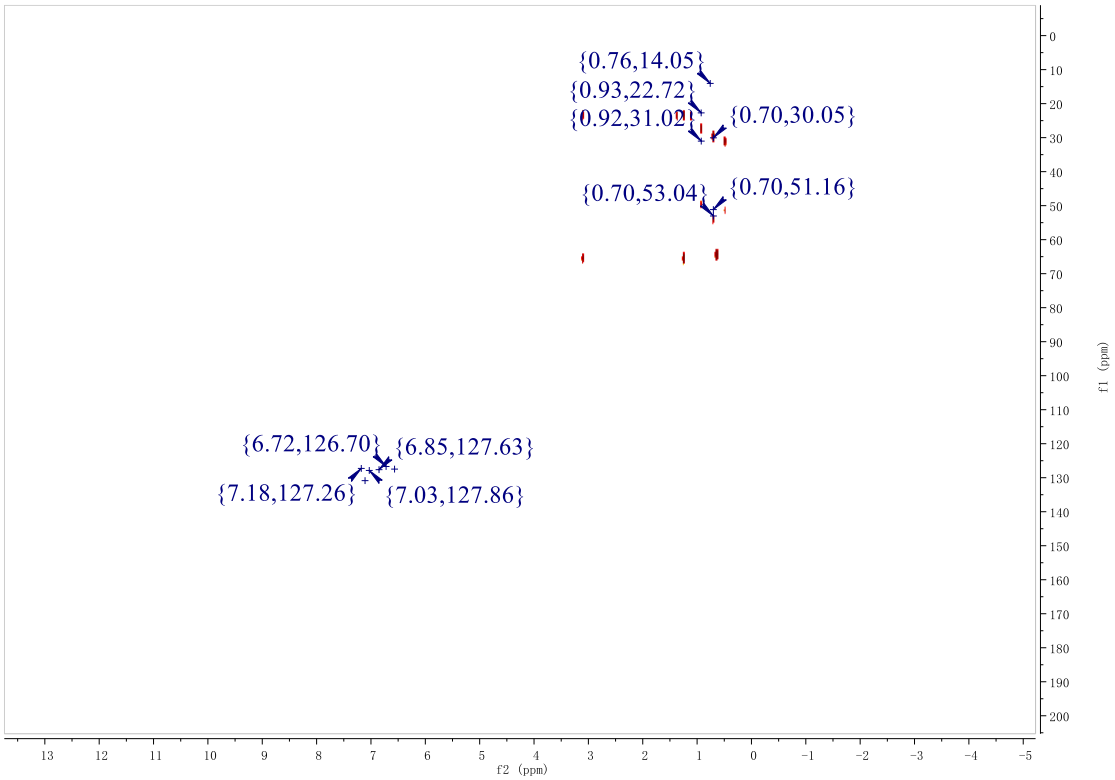
Note：The peaks at 67.65 and 25.65 ppm belong to THF.



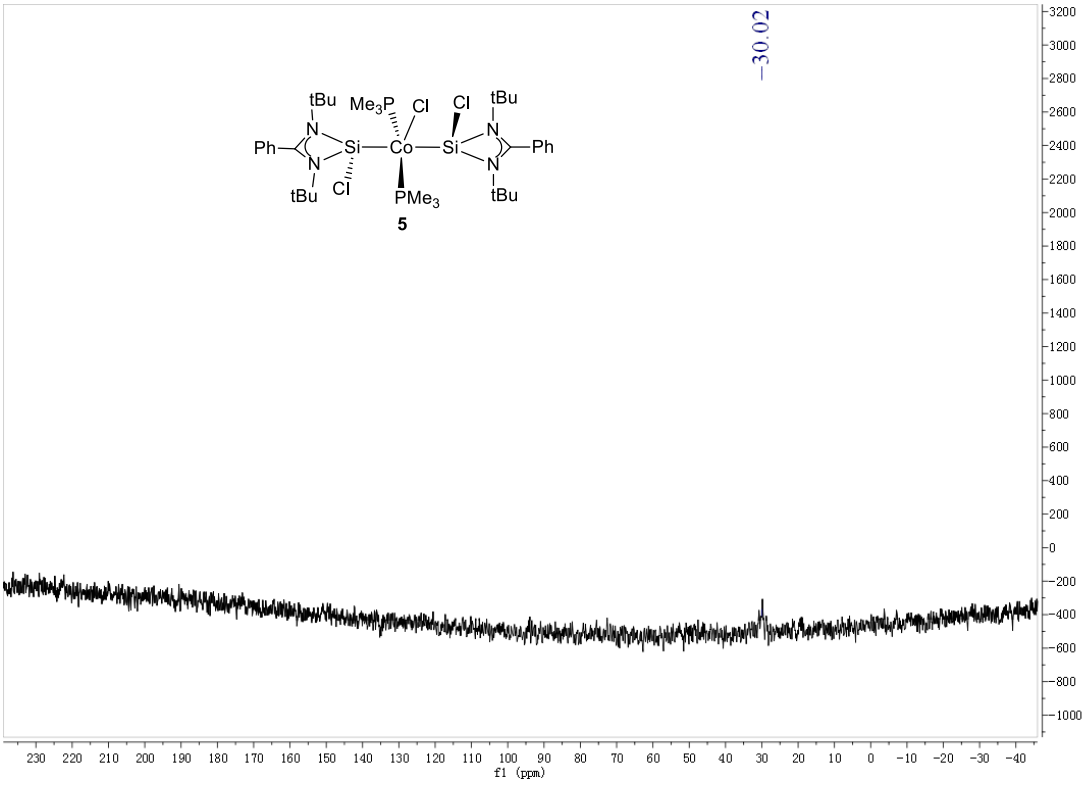
HH COSY of complex **5**



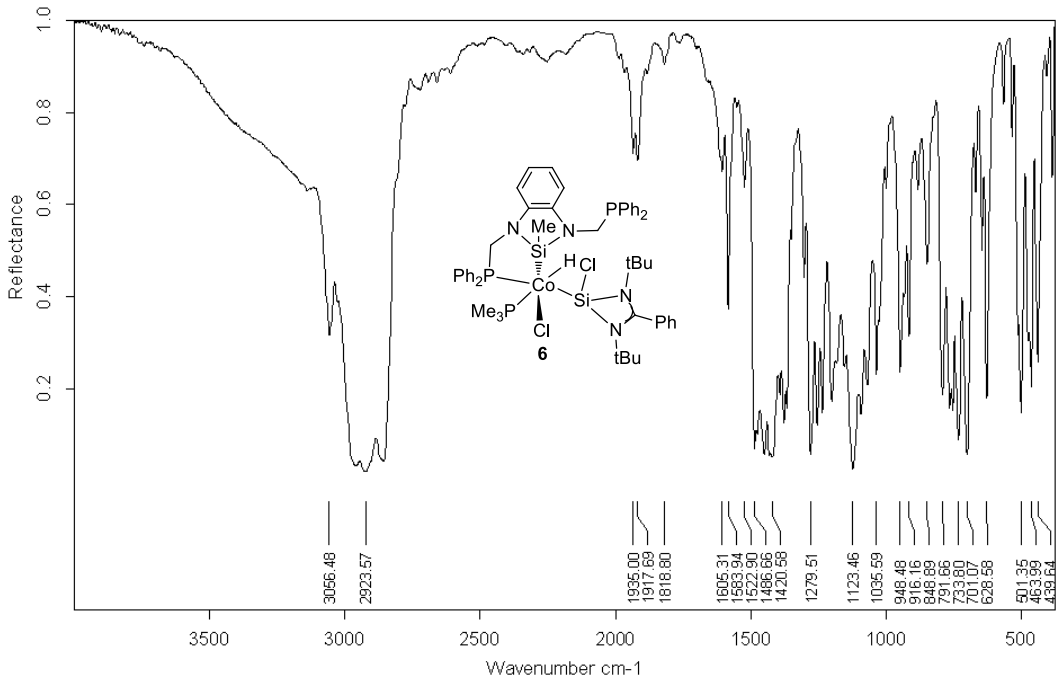
HSQC of complex **5**



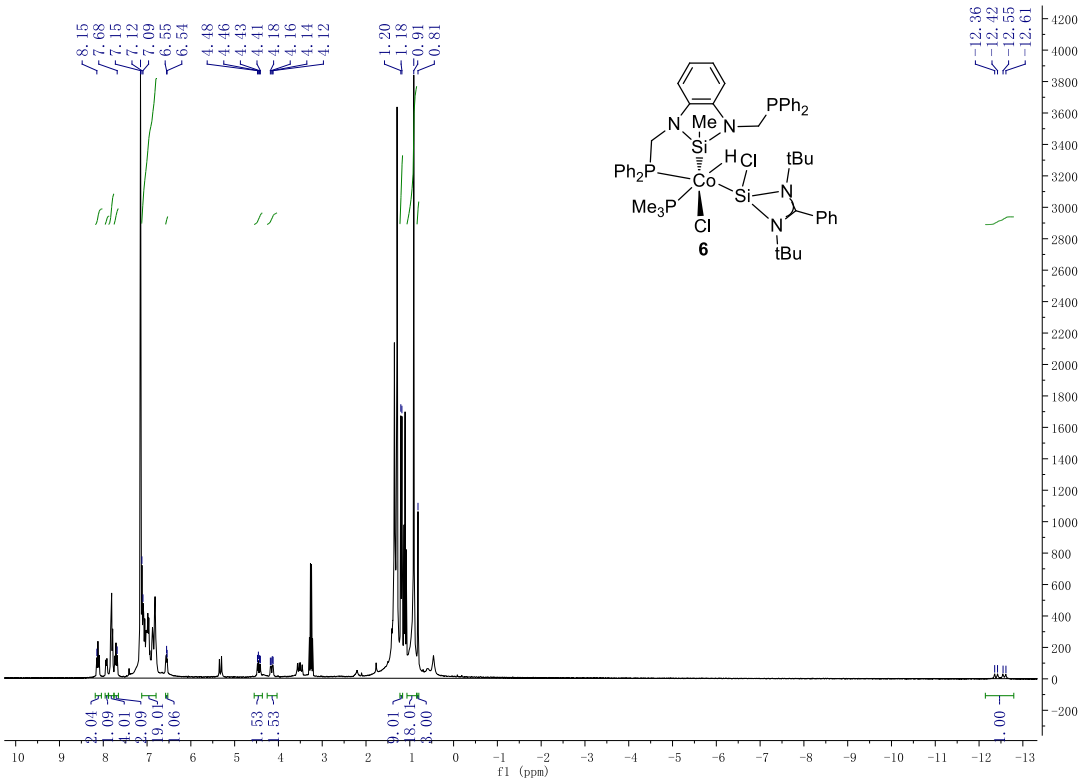
HMQC of complex **5**



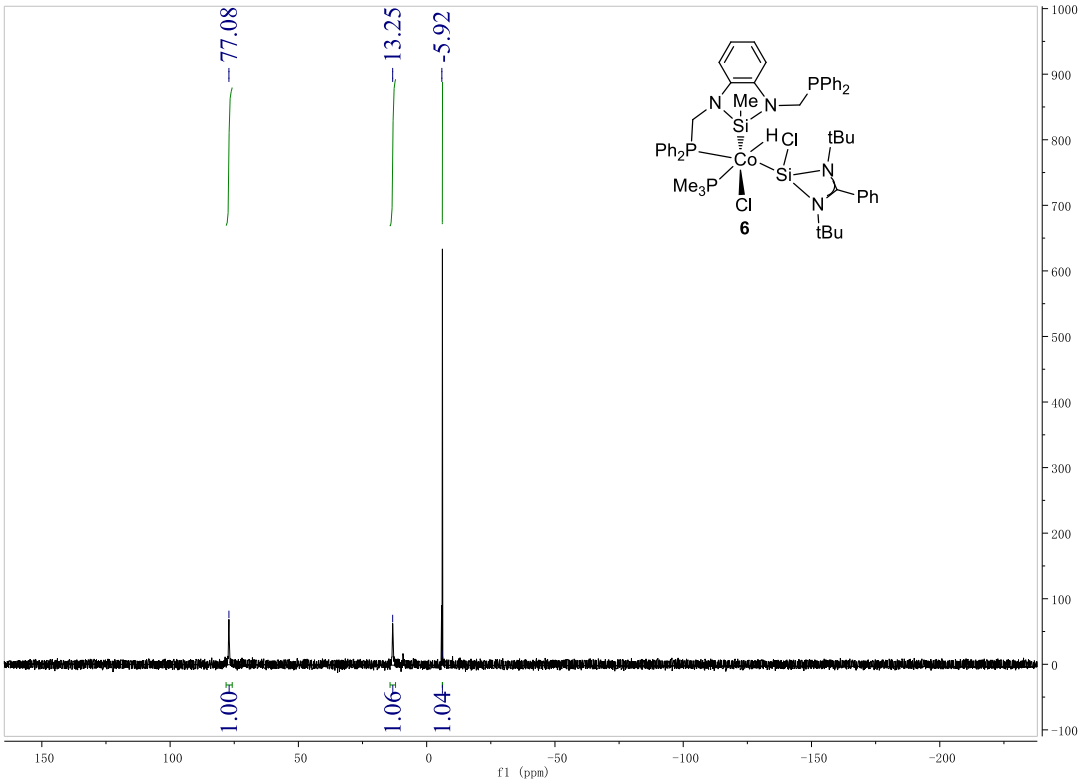
^{29}Si NMR of complex **5**



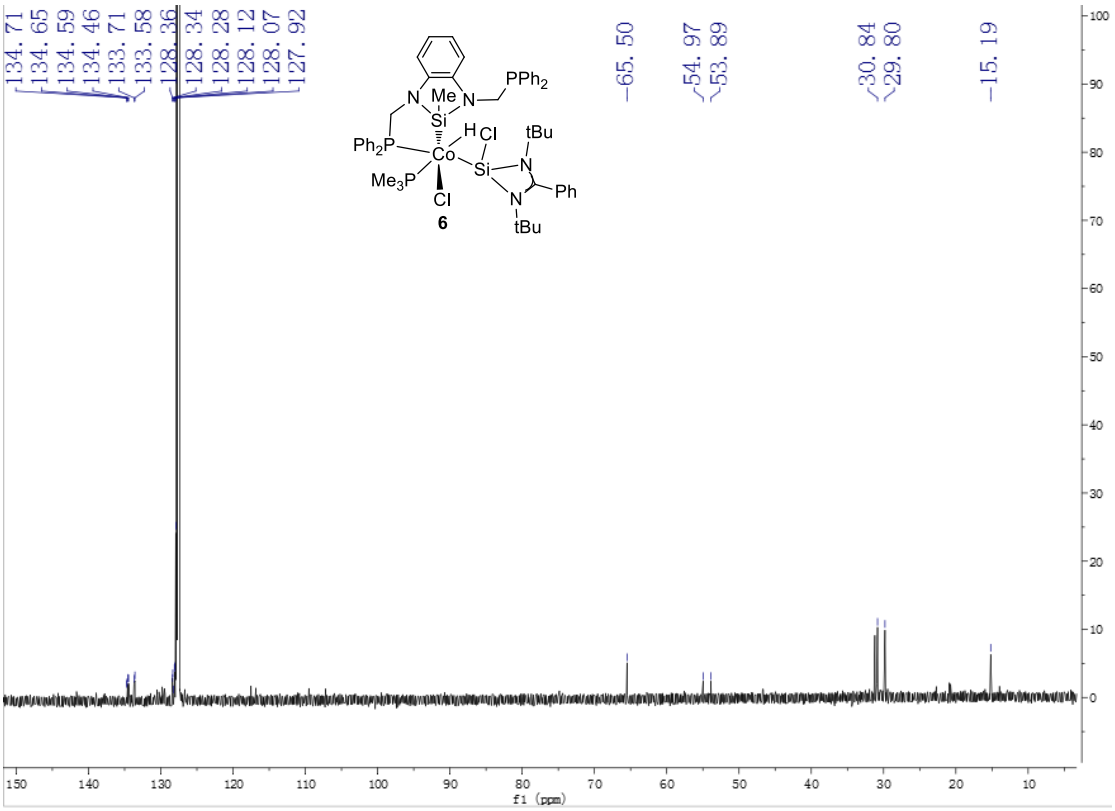
IR spectrum of complex **6**



^{1}H NMR of complex **6**

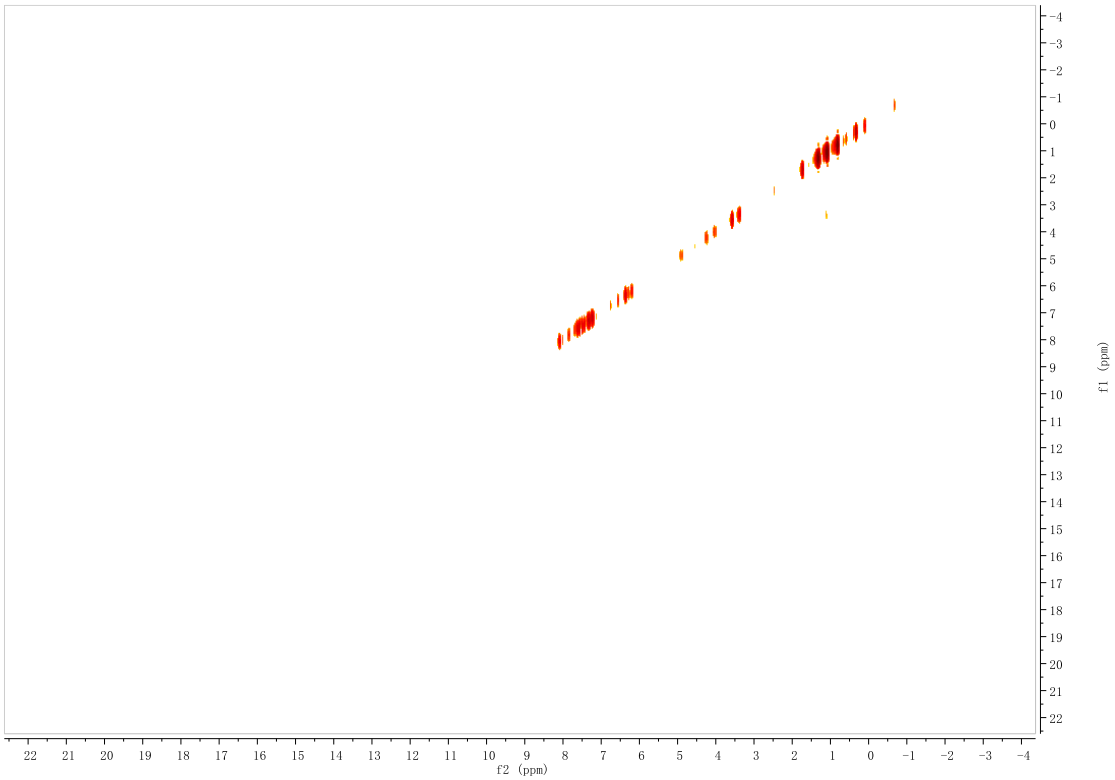


^{31}P NMR of complex **6**

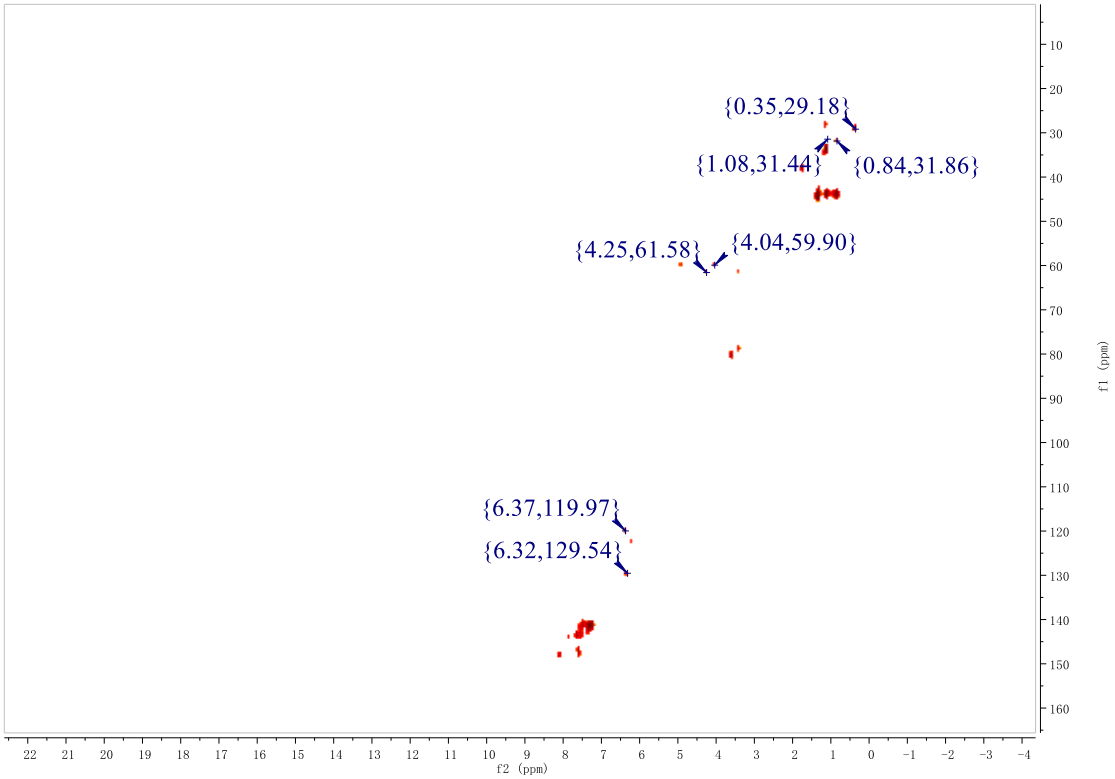


^{13}C NMR of complex **6**

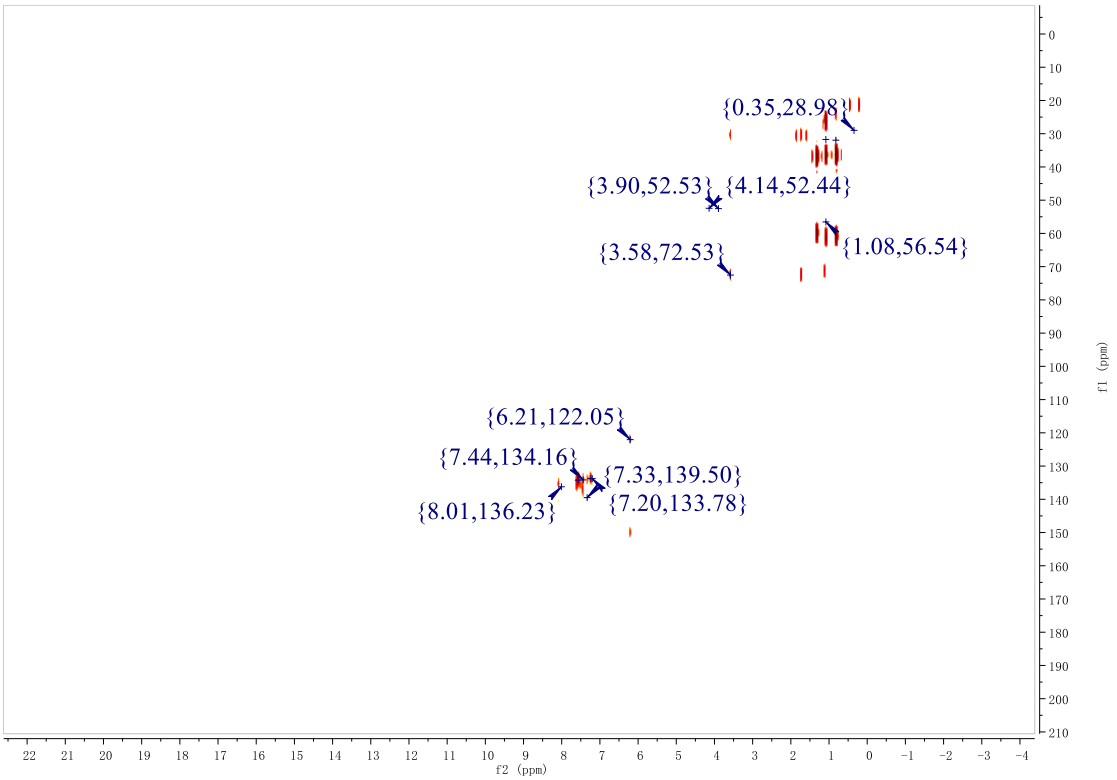
Note：The peaks at 65.50 and 15.19 ppm belong to Et_2O.



HH COSY of complex **6**



HSQC of complex **6**



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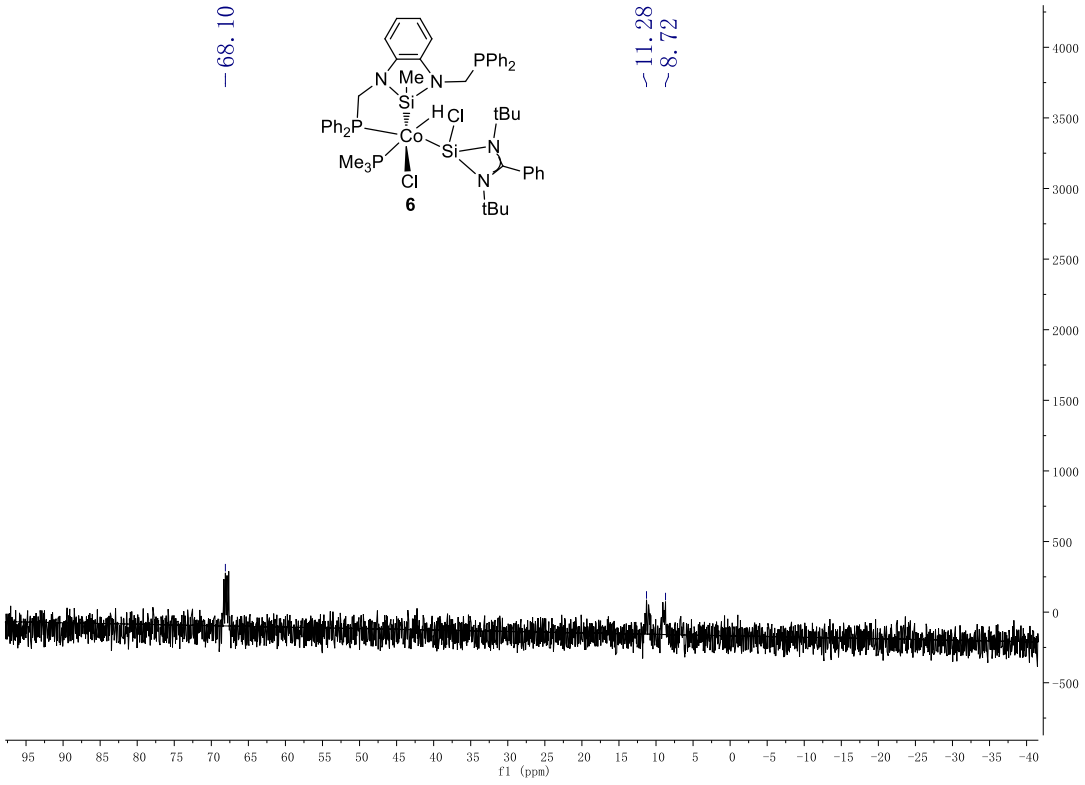
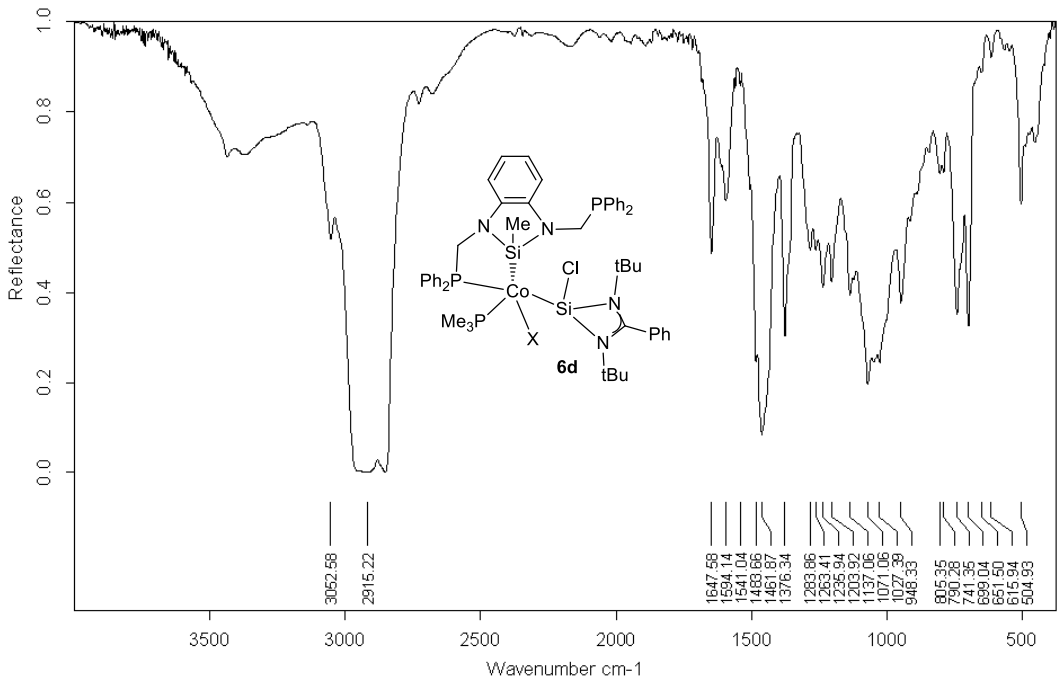
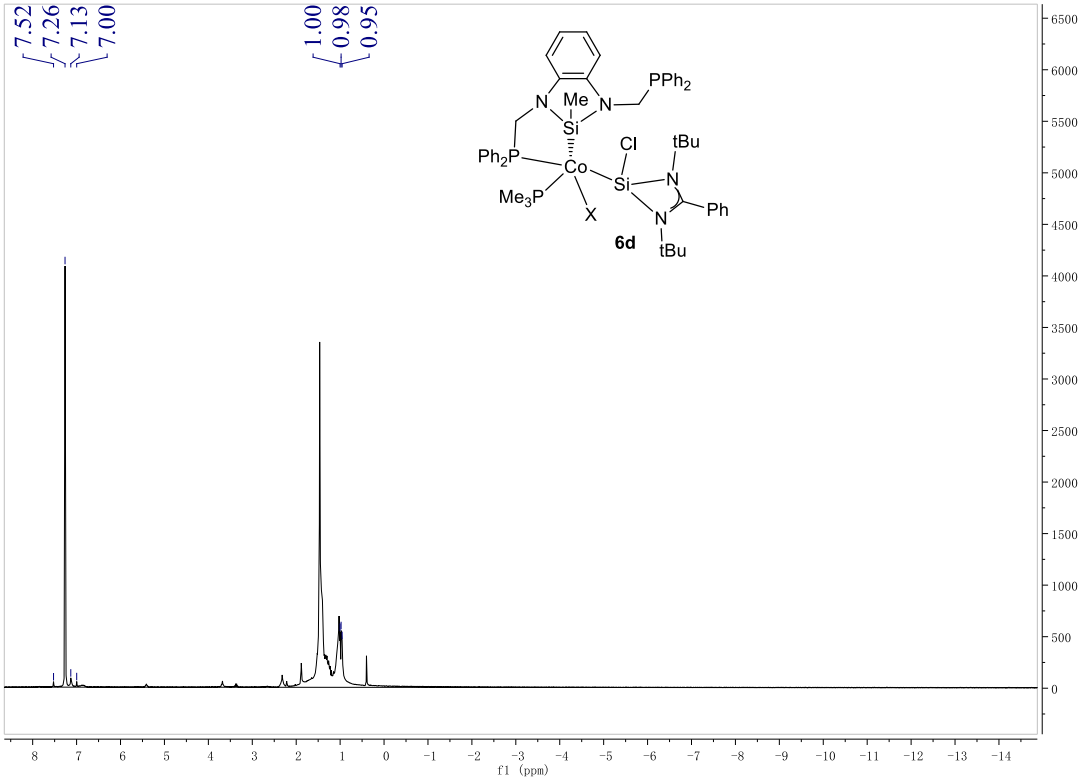


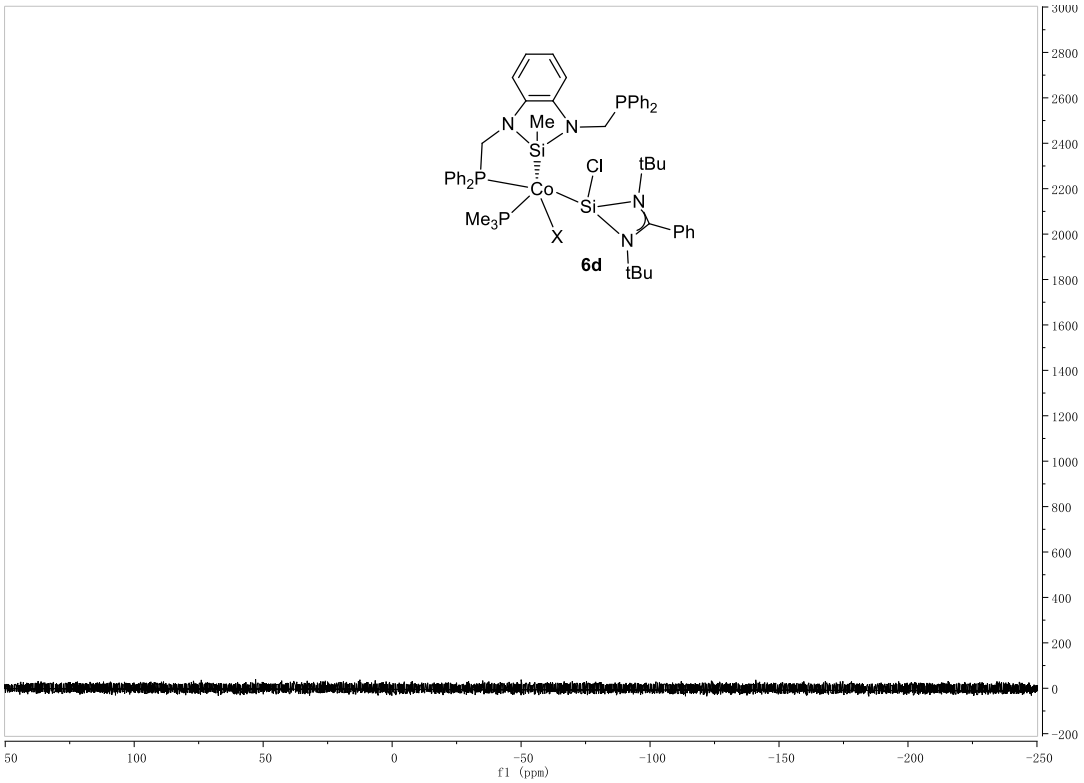
^{29}Si NMR of complex **6**



IR spectrum of complex **6d**

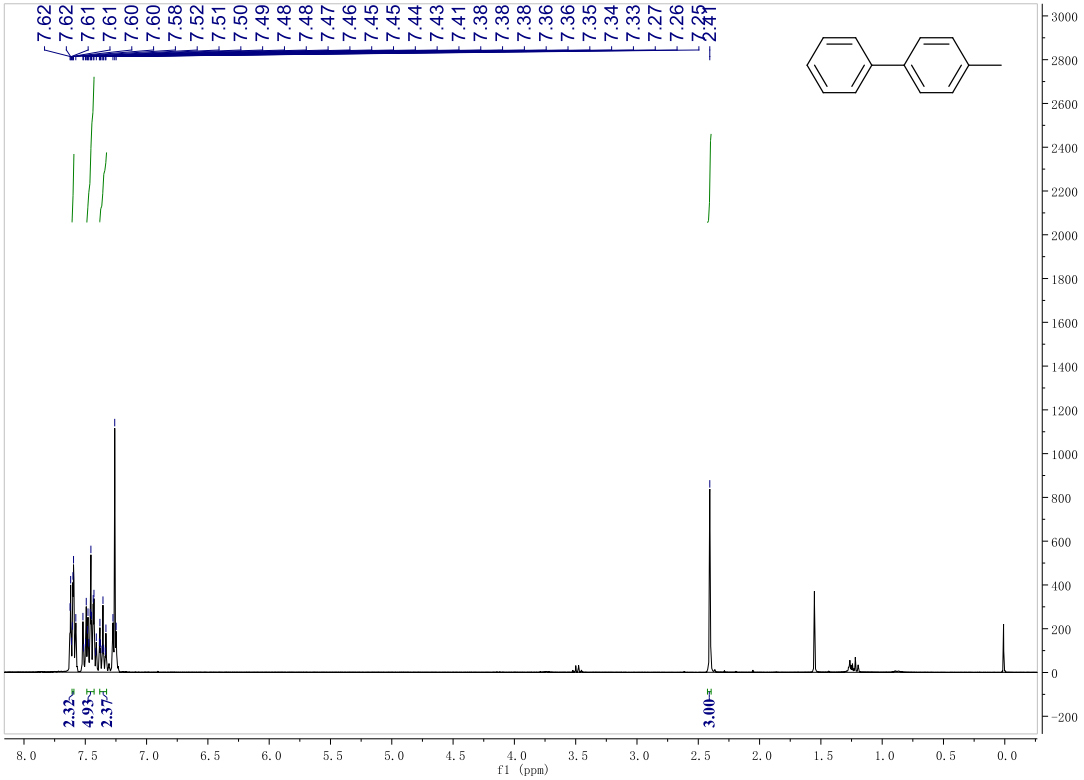


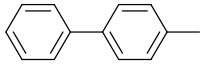
^{1}H NMR of complex **6d**

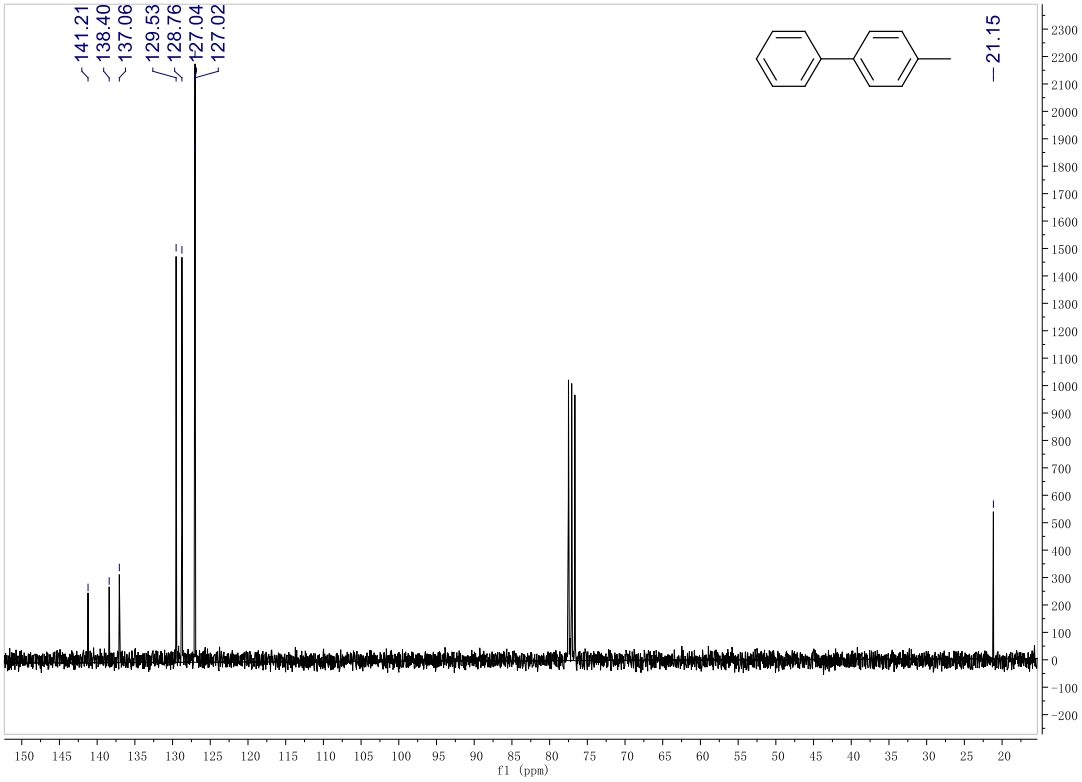


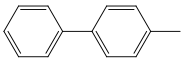
^{31}P NMR of complex **6d**

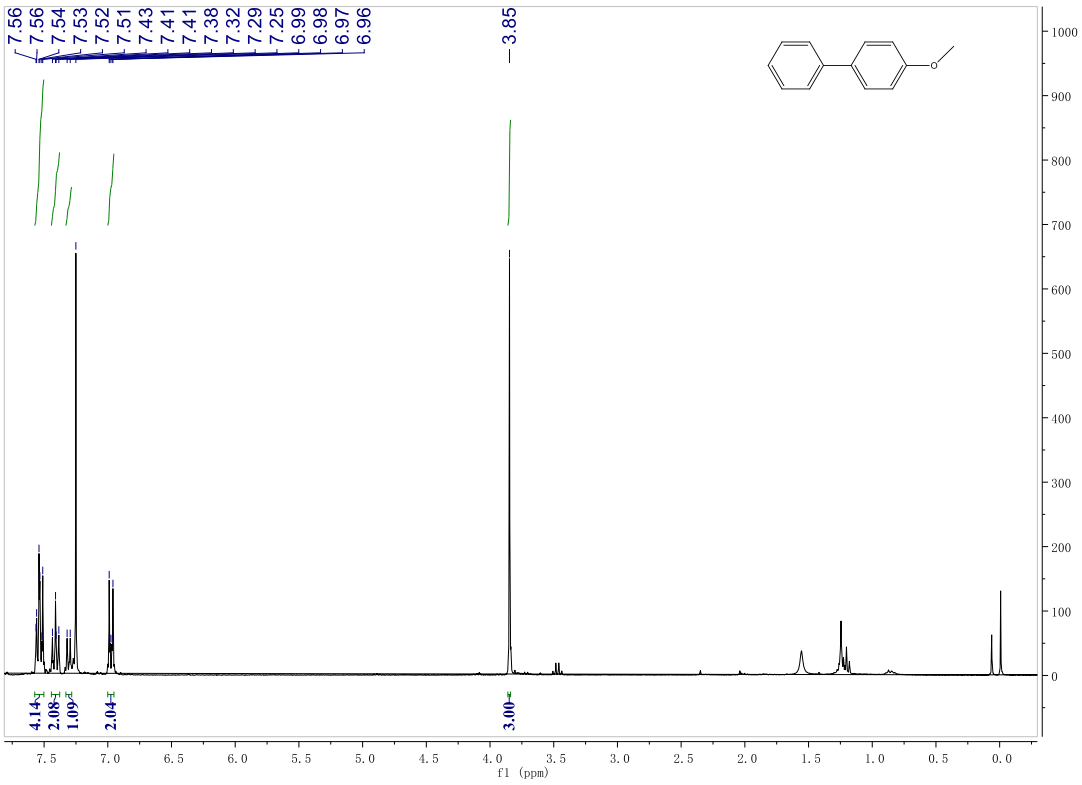
SIII ^{1}H and ^{13}C NMR spectra of coupling products

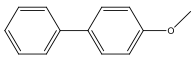


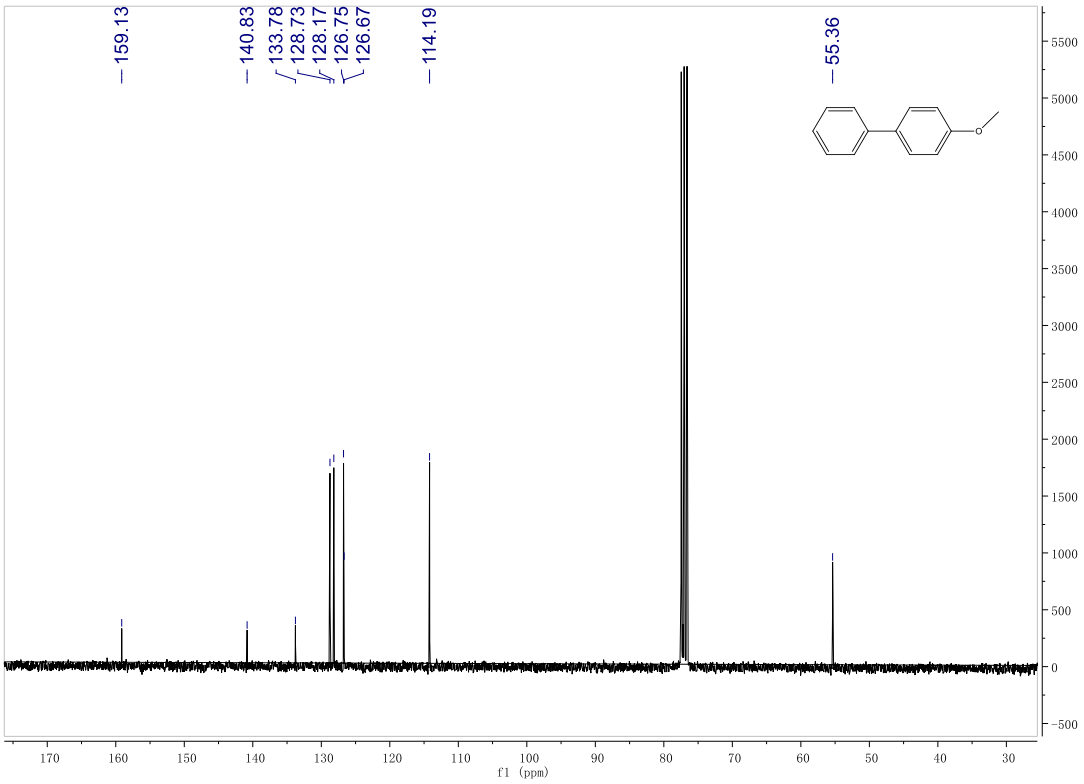
^{1}H NMR of compound 

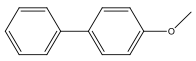


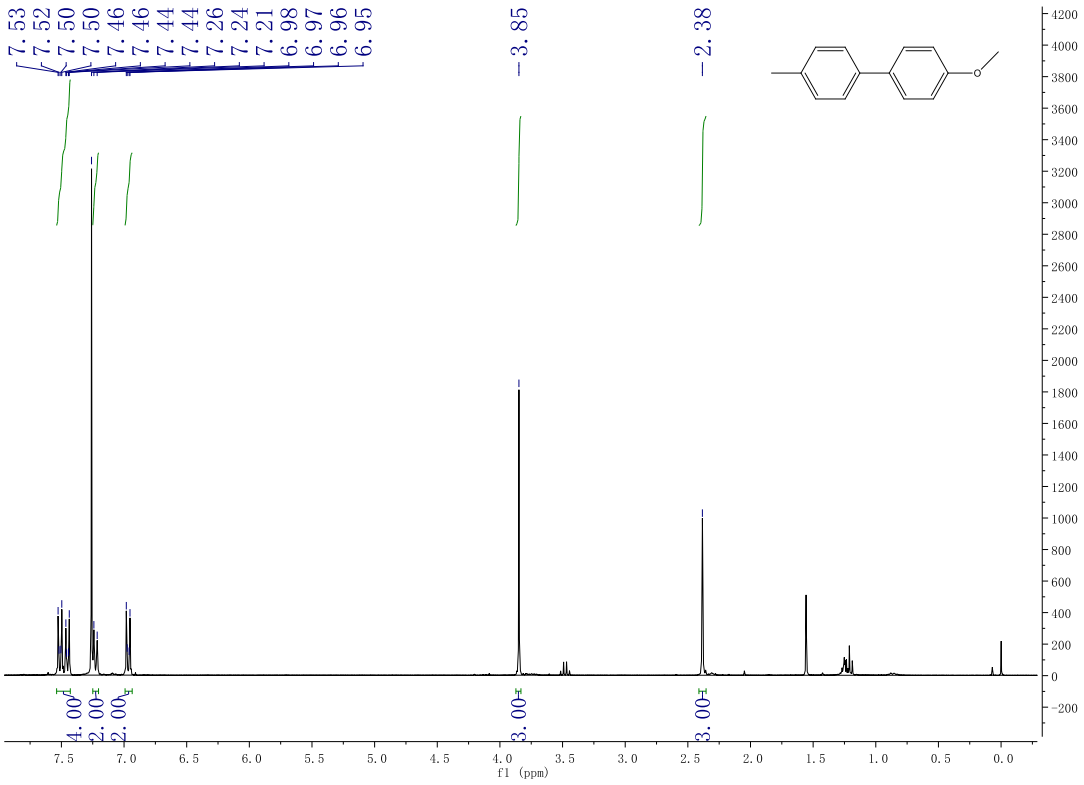
^{13}C NMR of compound 

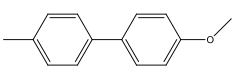


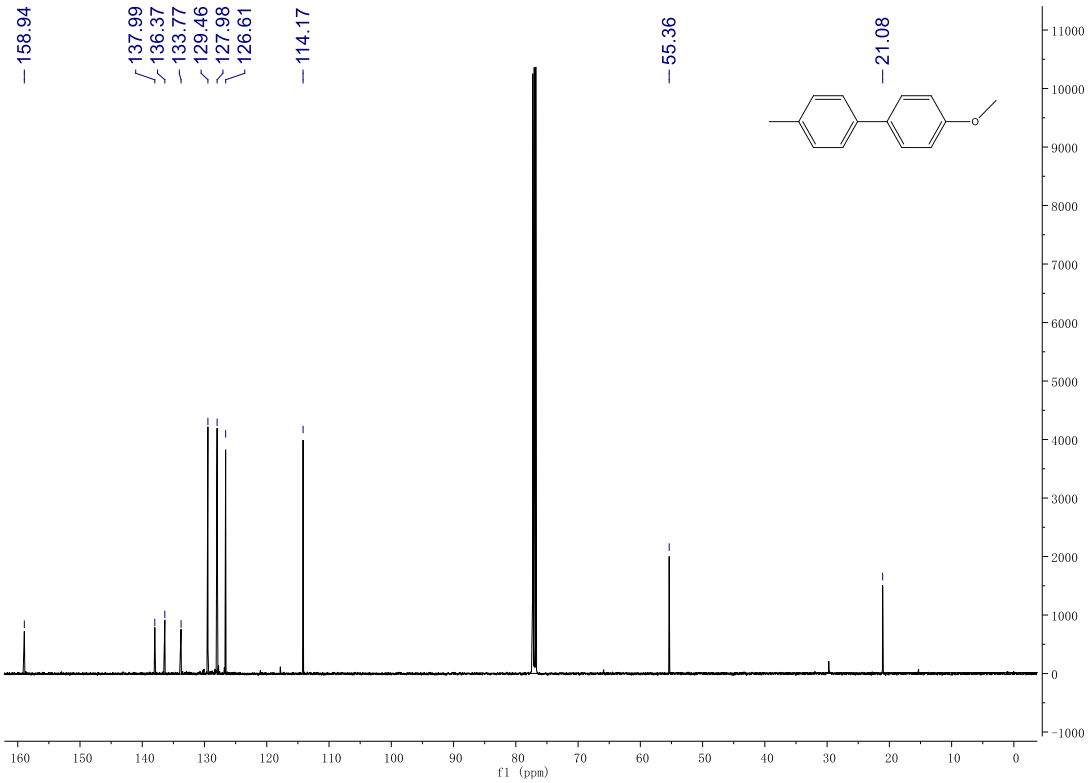
^{1}H NMR of compound 

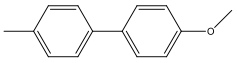


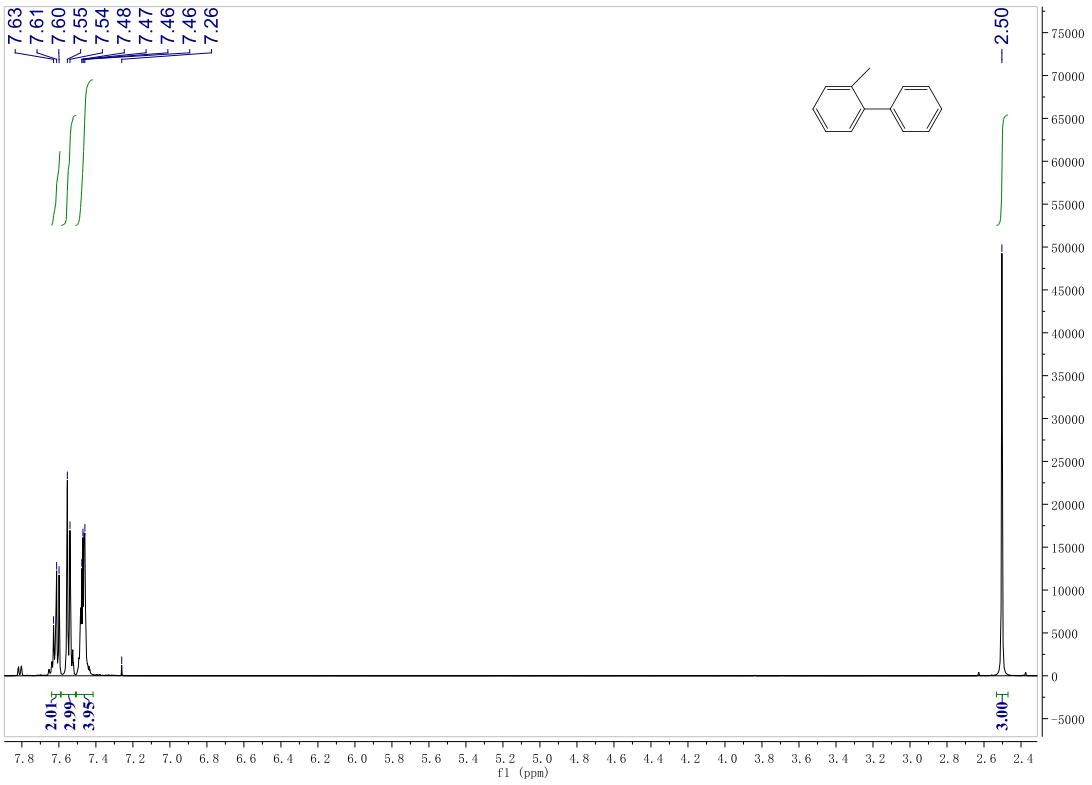
^{13}C NMR of compound 

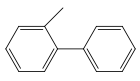


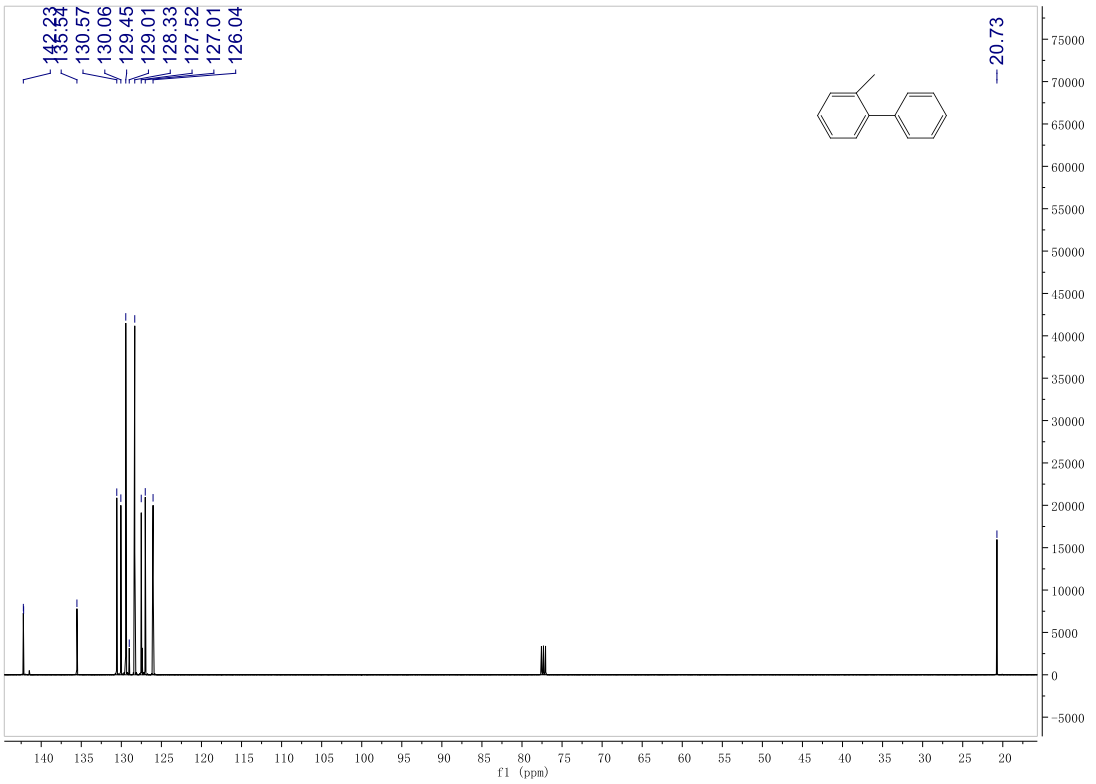
^{1}H NMR of compound 

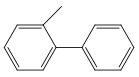


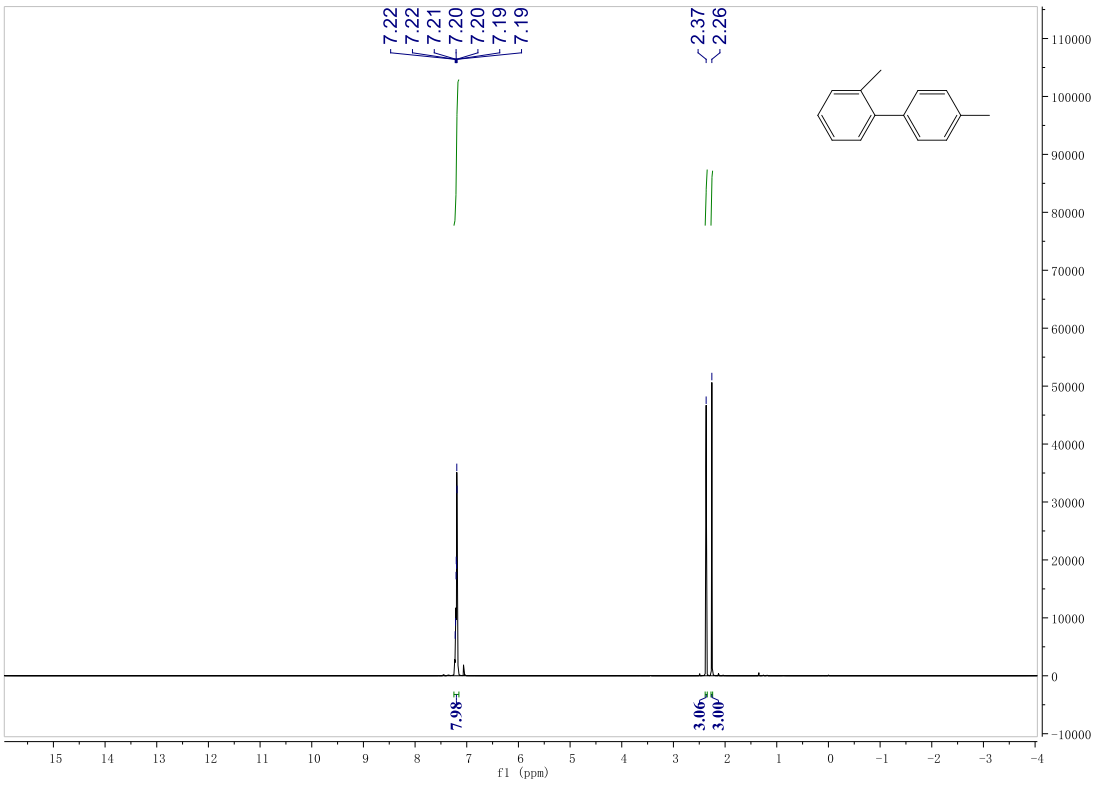
^{13}C NMR of compound 

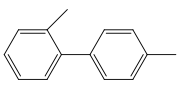


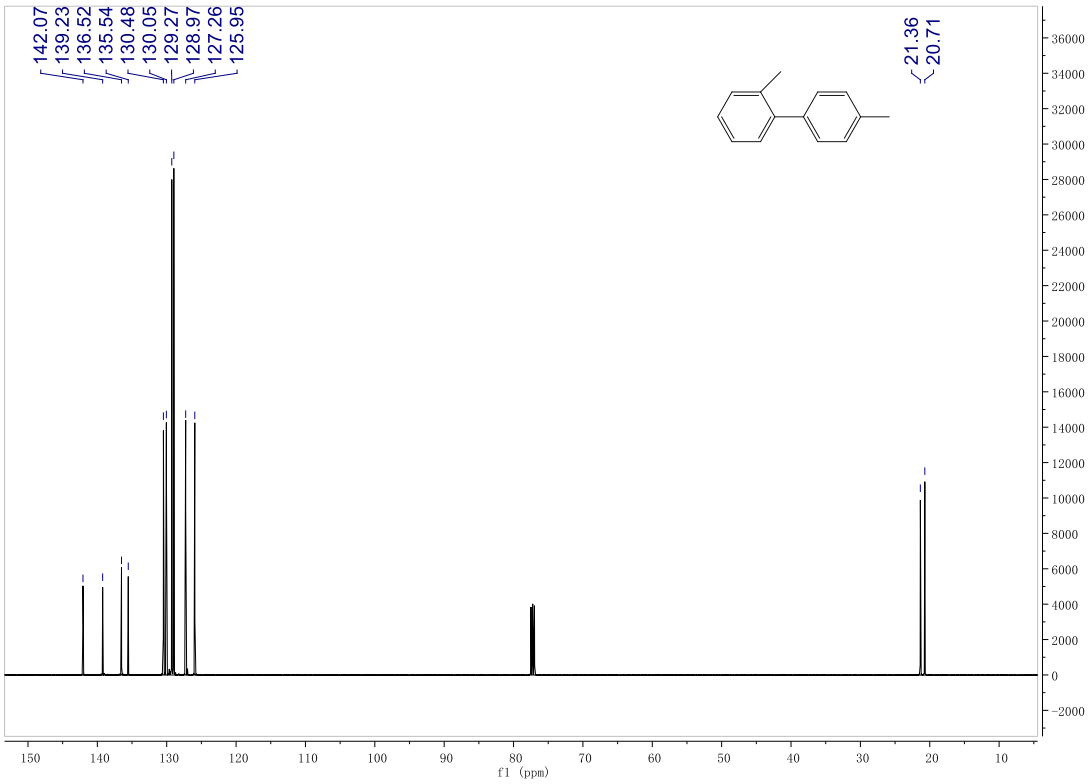
^{1}H NMR of compound 

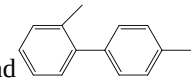


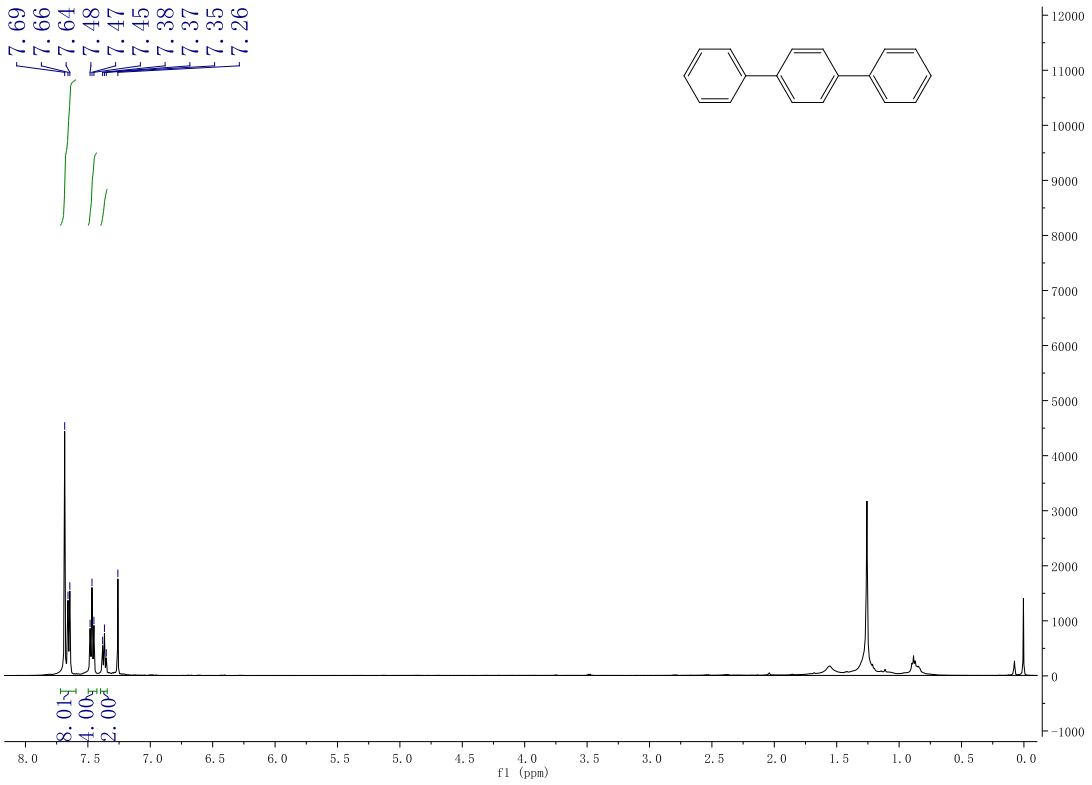
^{13}C NMR of compound 

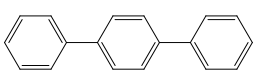


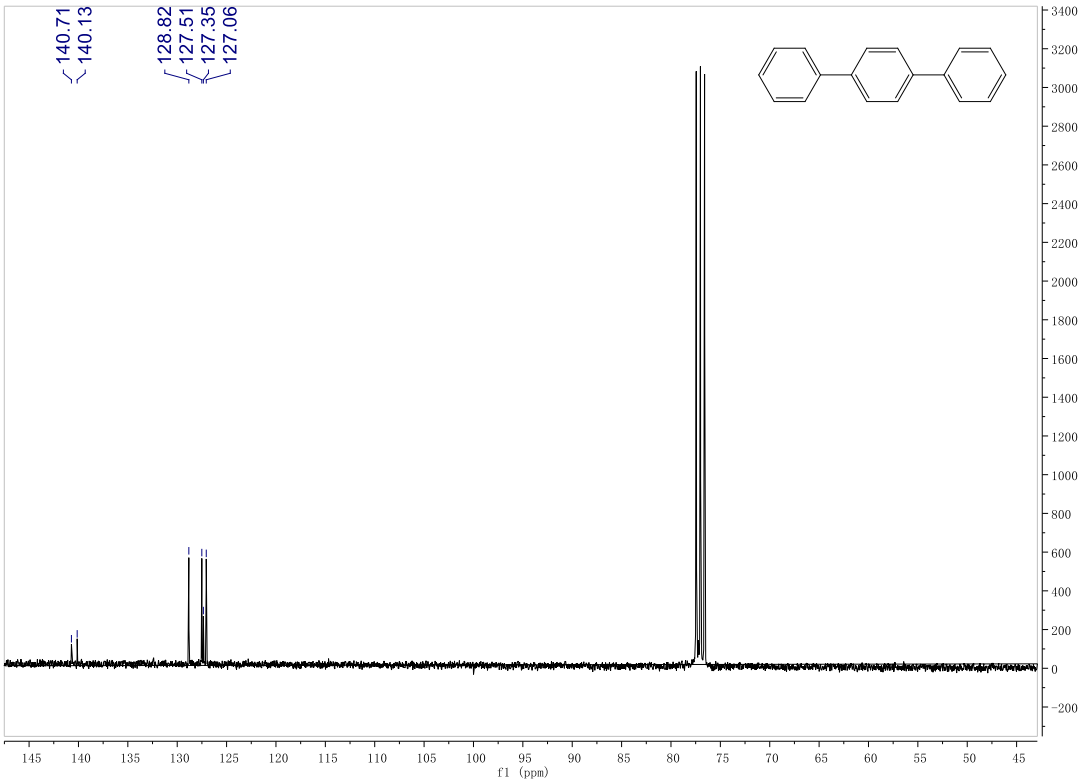
^{1}H NMR of compound 

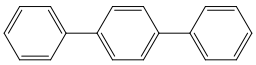


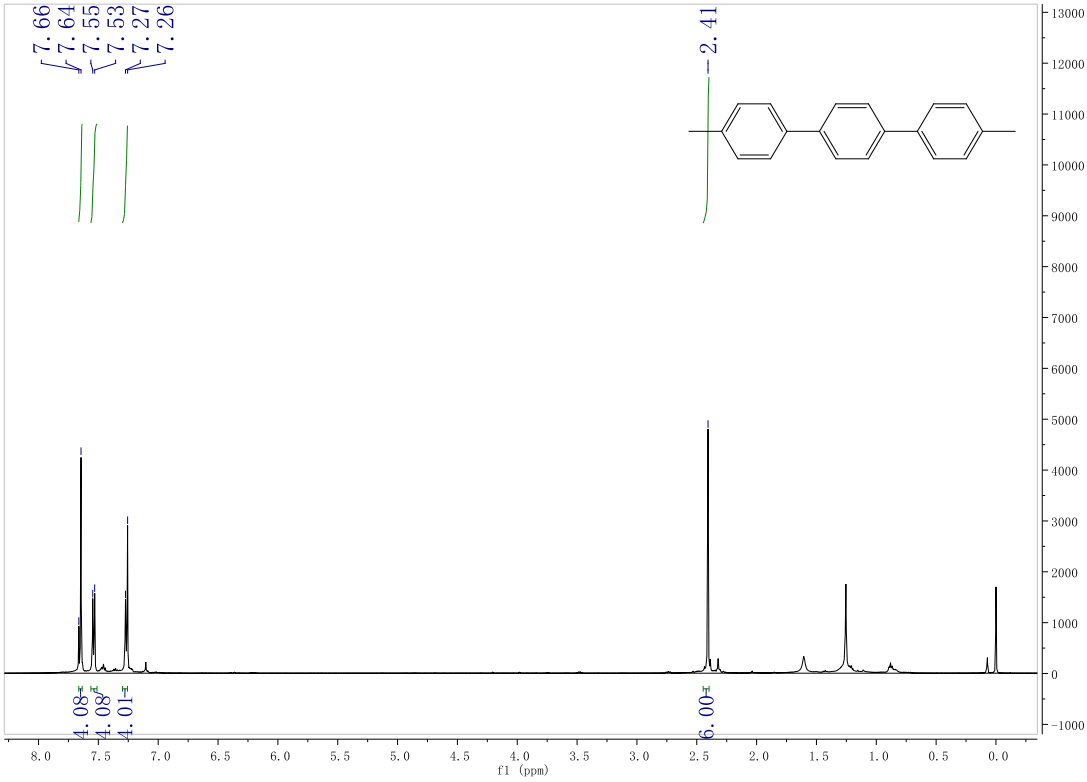
^{13}C NMR of compound 



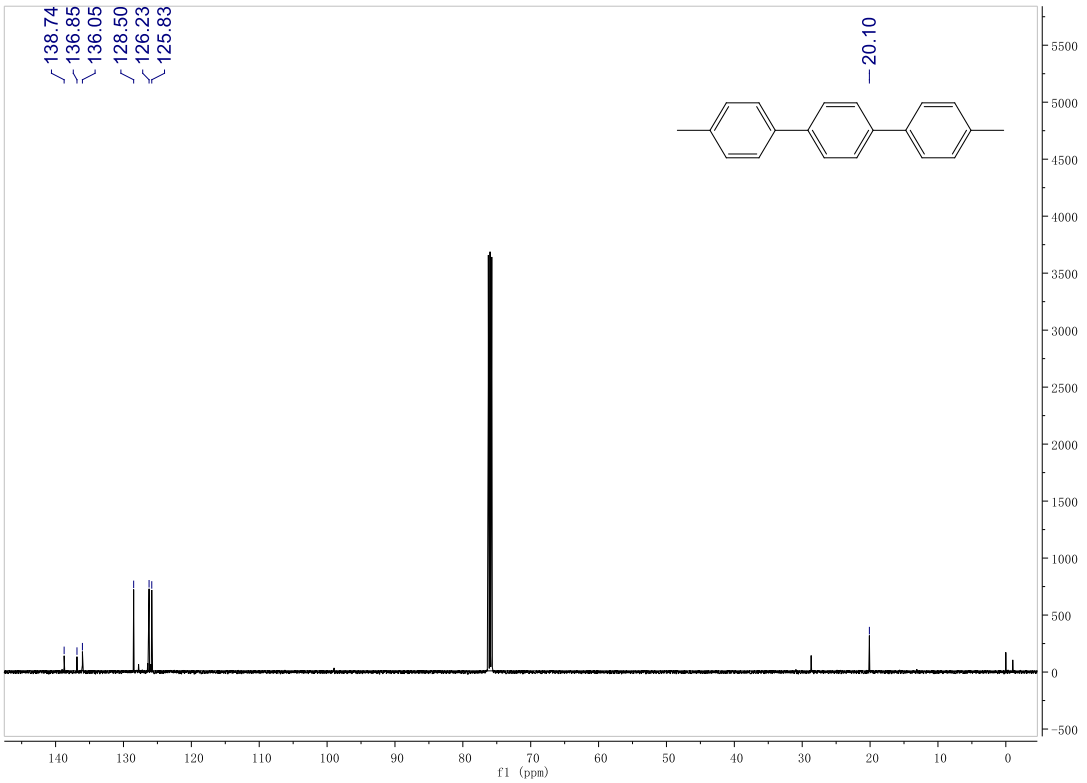
^{1}H NMR of compound 

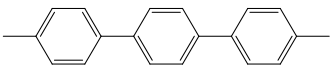


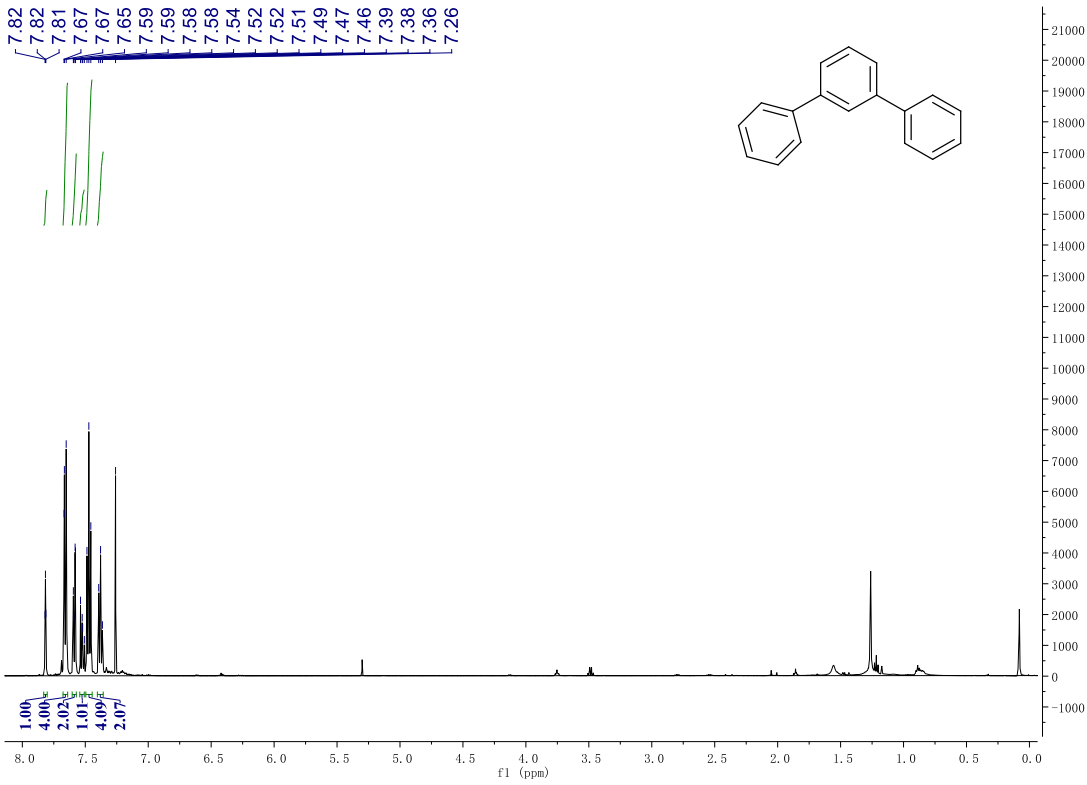
^{13}C NMR of compound 

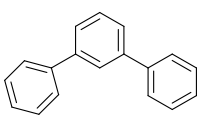


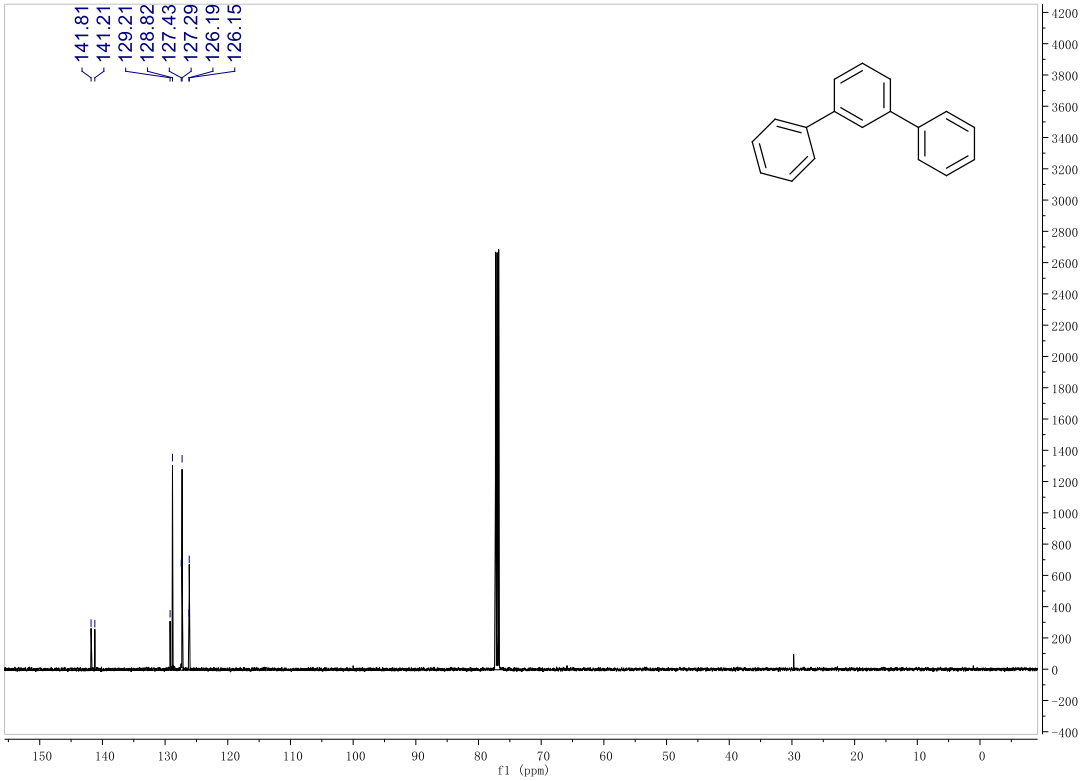
^{1}H NMR of compound 



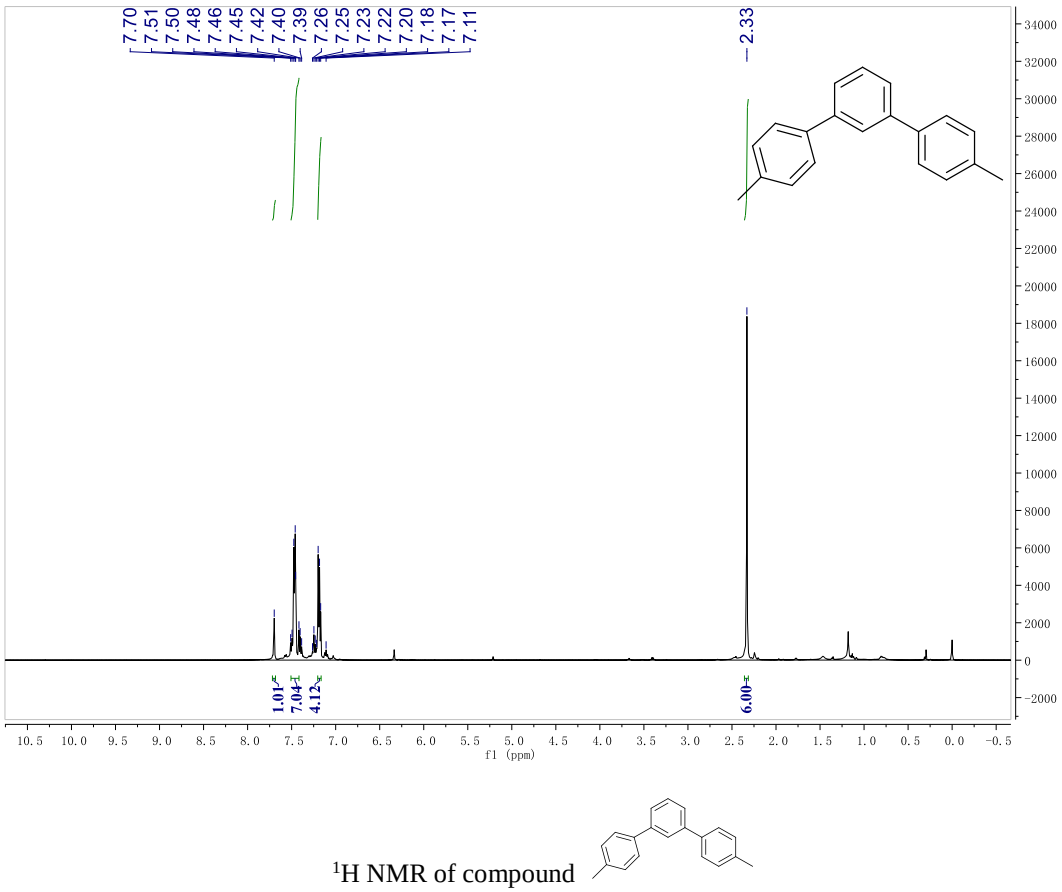
^{13}C NMR of compound 



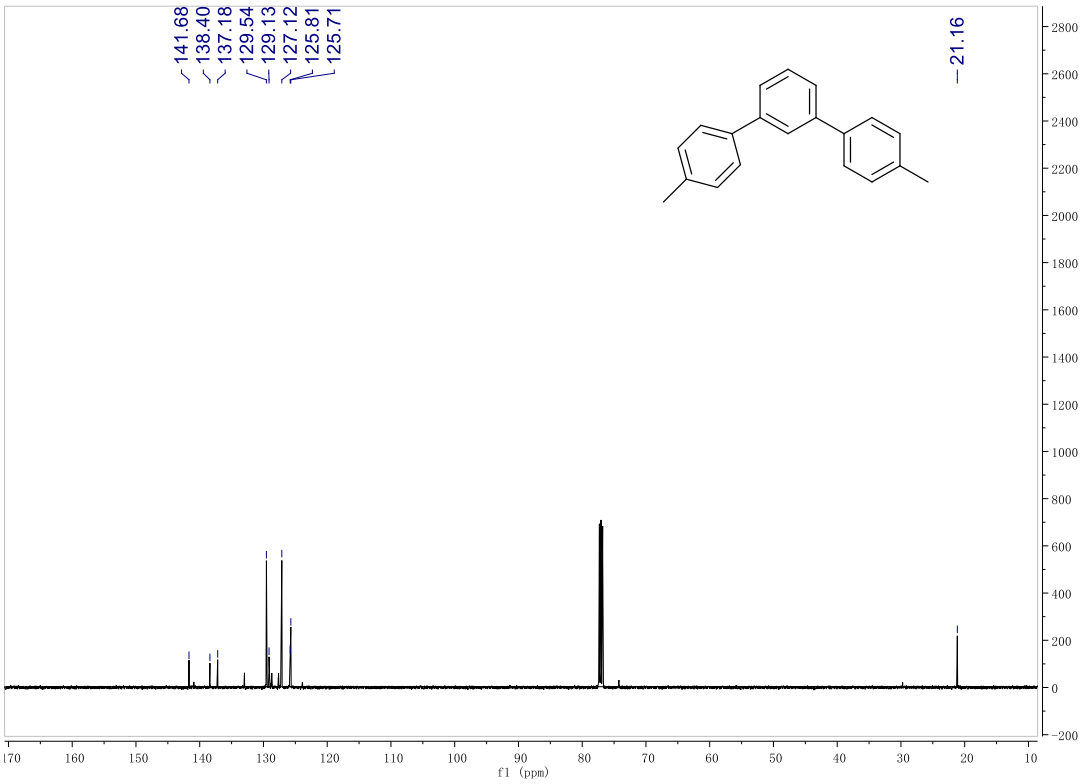
^{1}H NMR of compound 

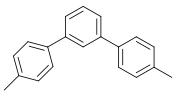


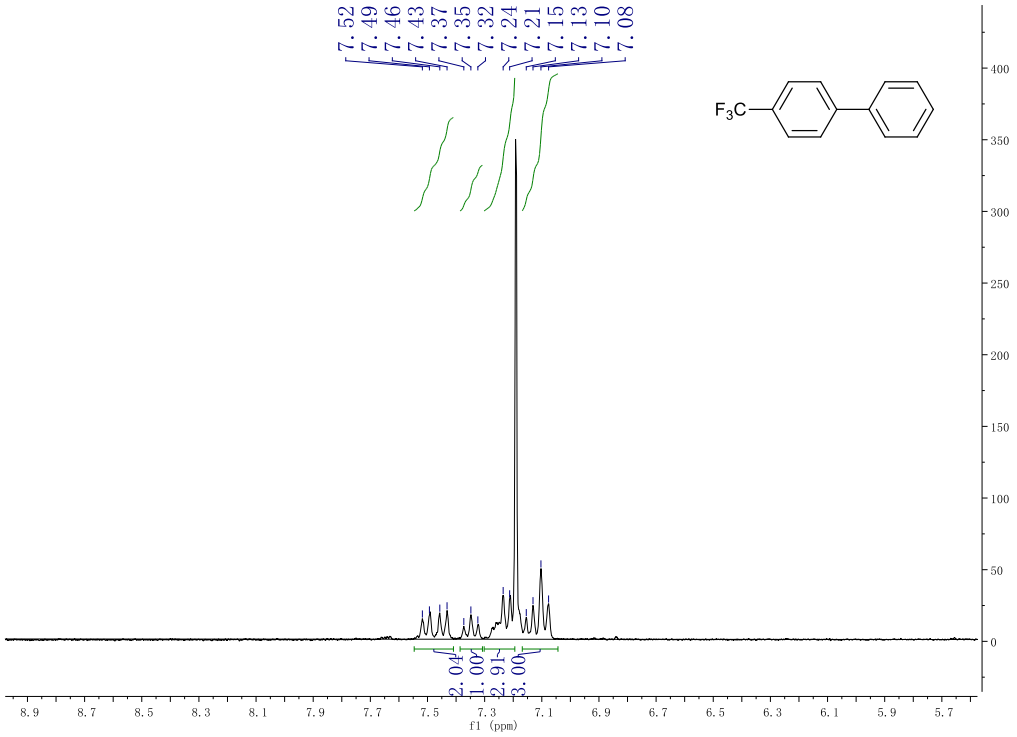
^{13}C NMR of compound

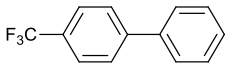


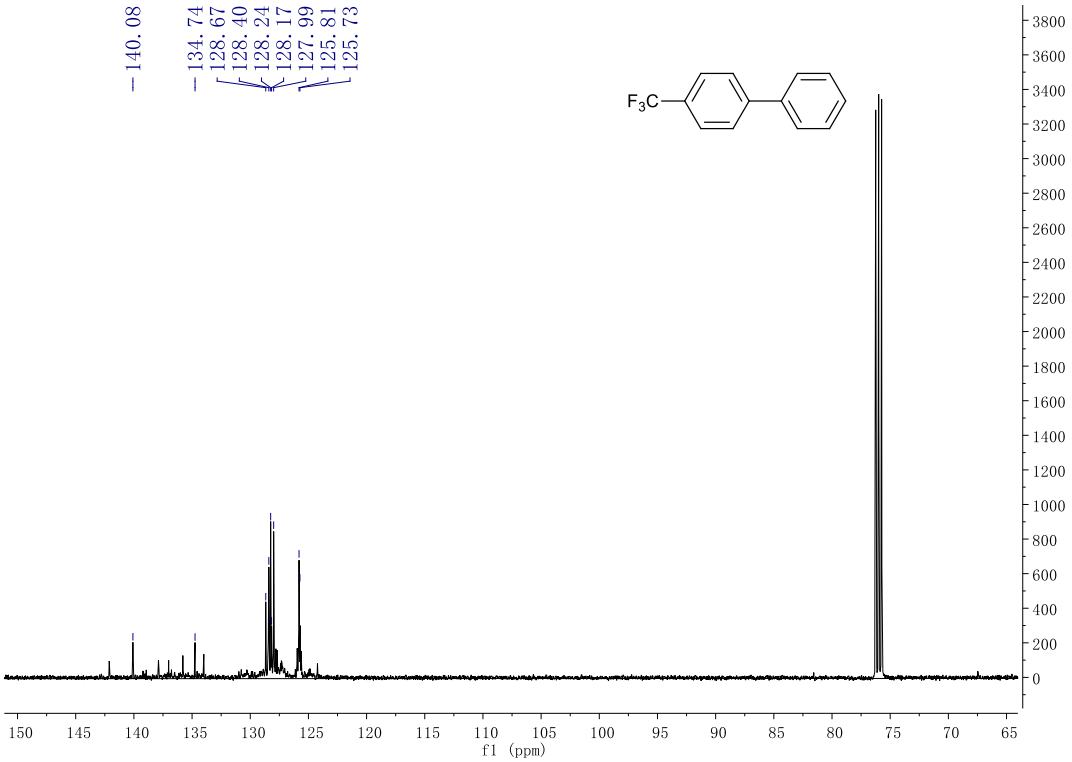
^{1}H NMR of compound

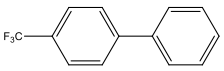


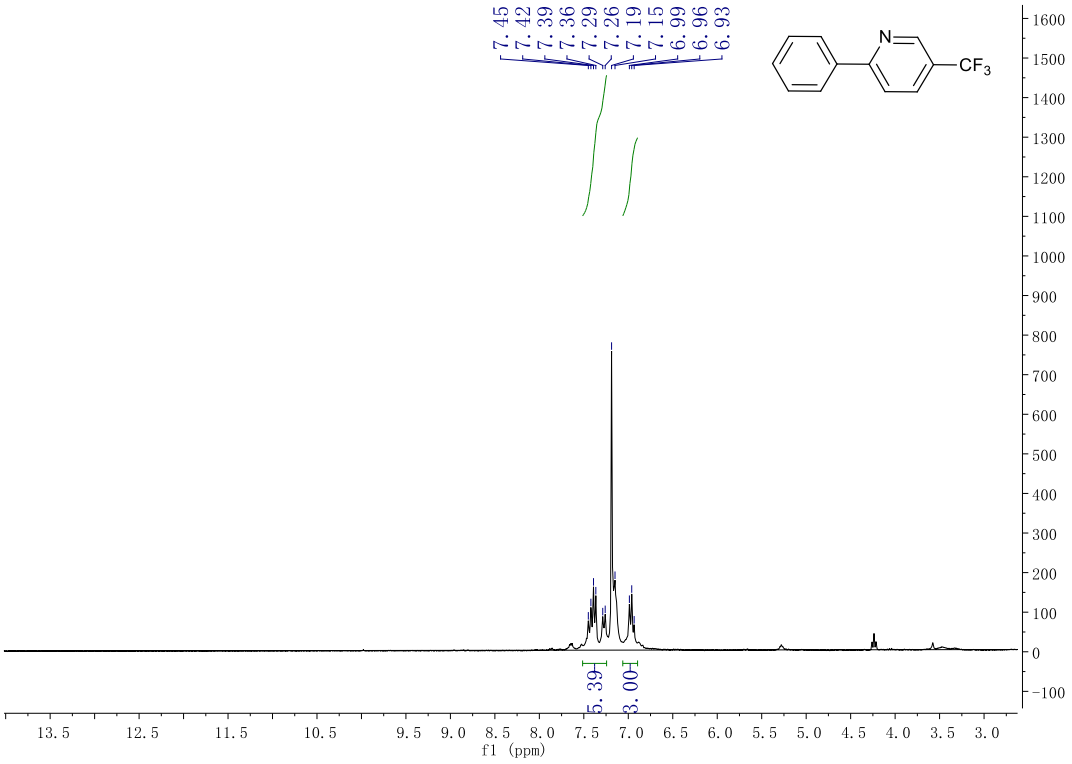
^{13}C NMR of compound 

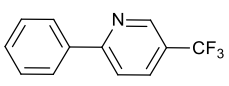


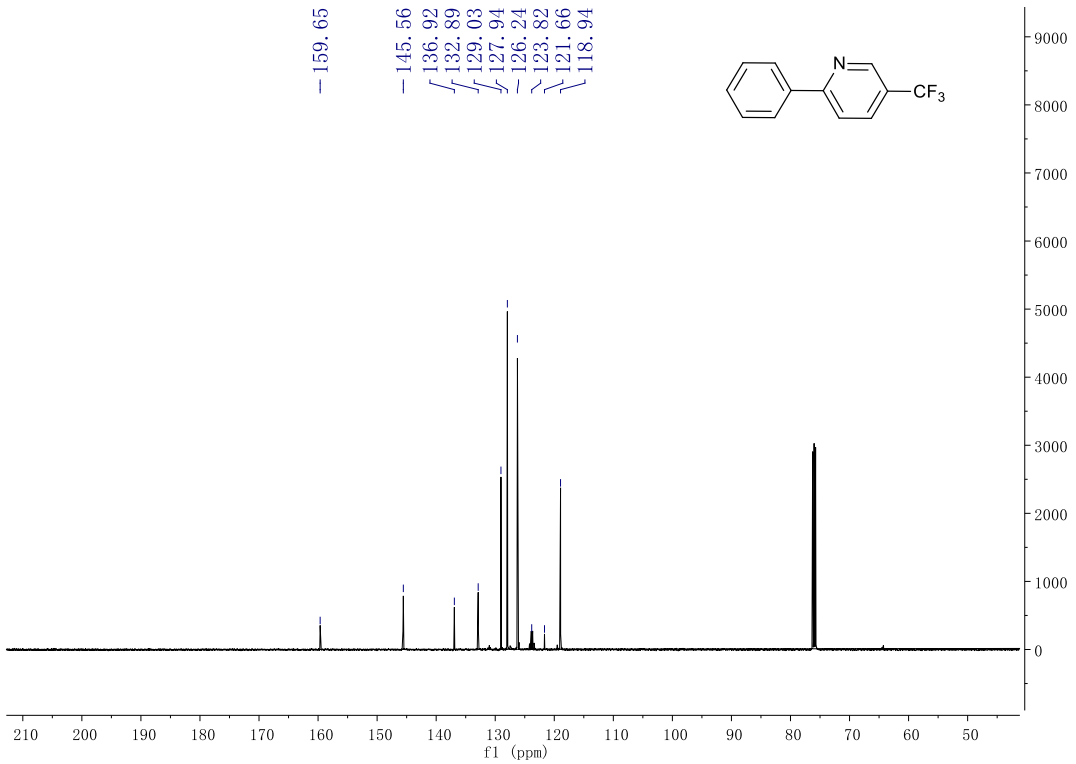
^{1}H NMR of compound 

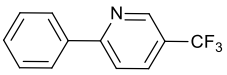


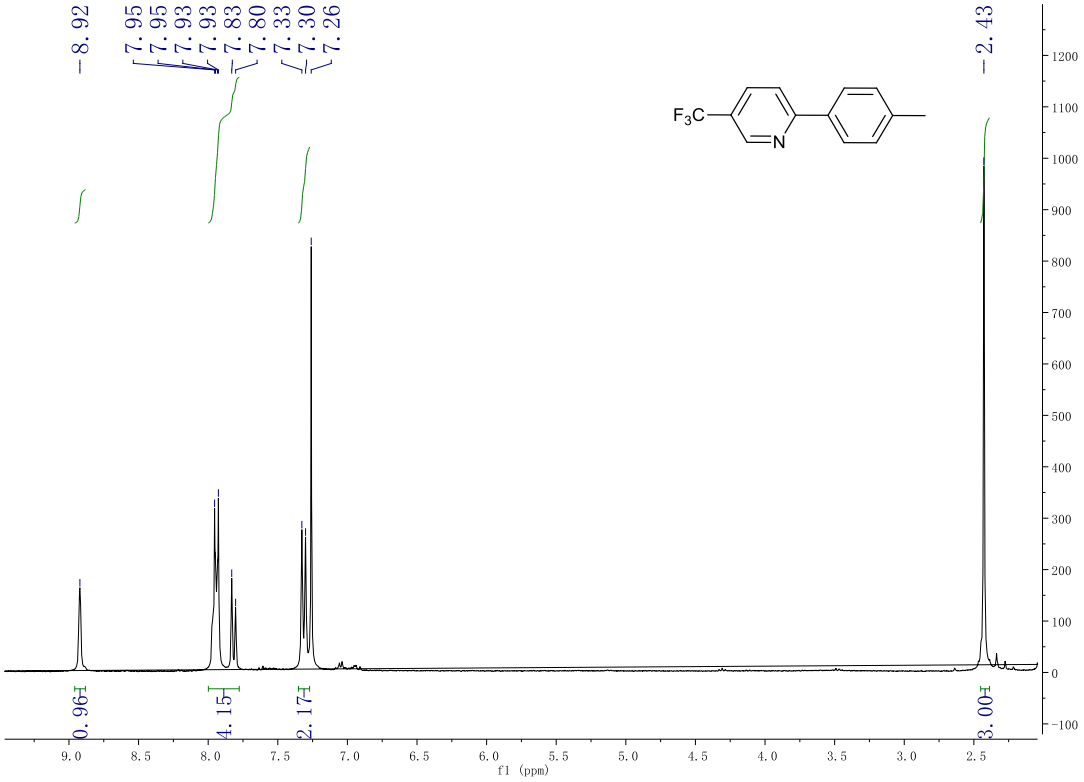
^{13}C NMR of compound 

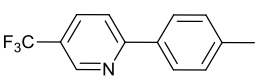


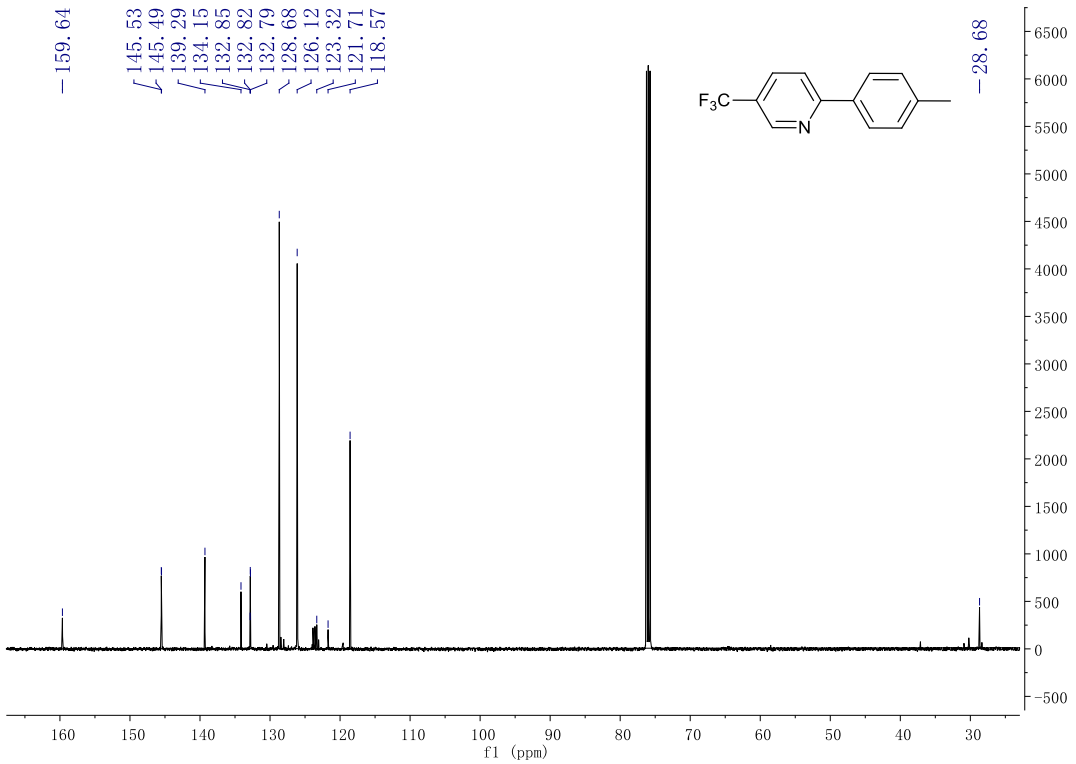
^{1}H NMR of compound 

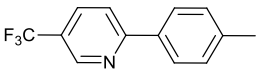


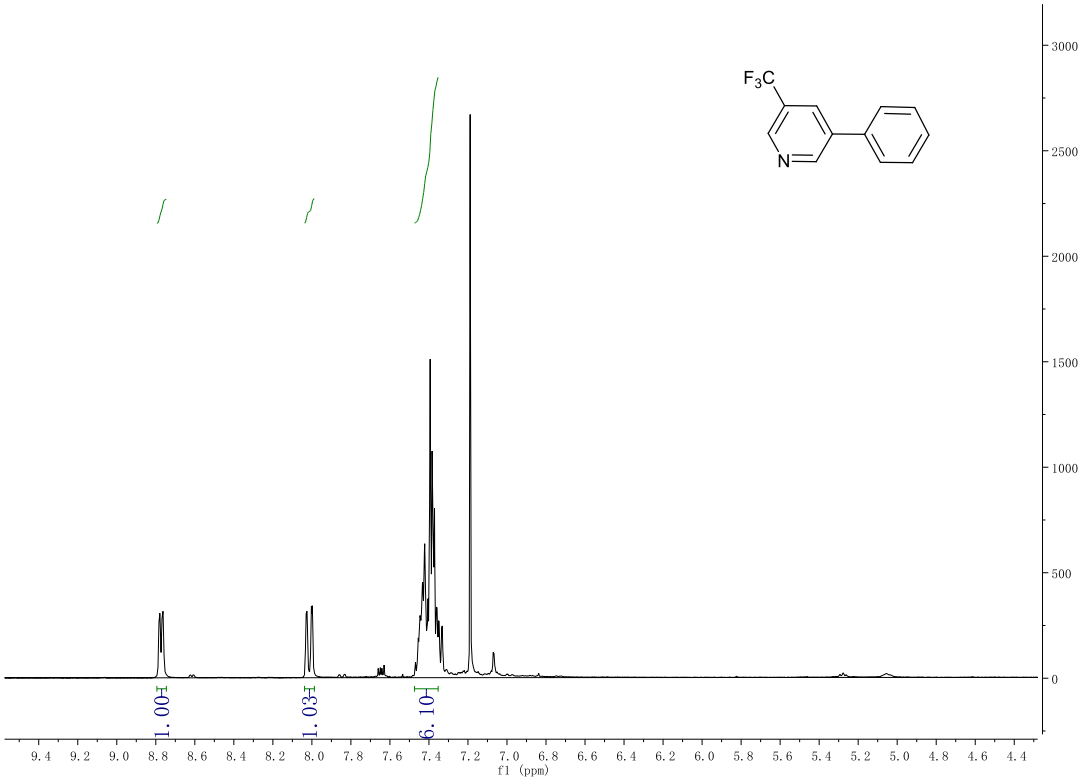
^{13}C NMR of compound 

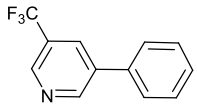


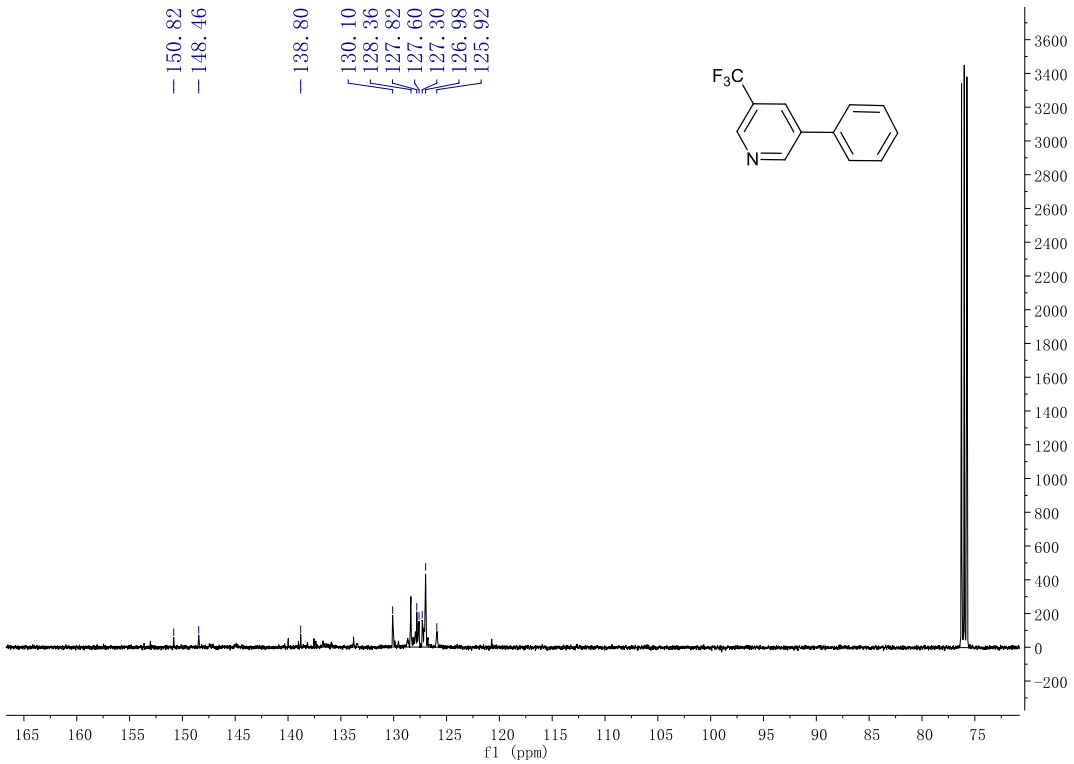
^{1}H NMR of compound 

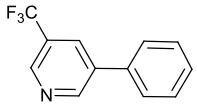


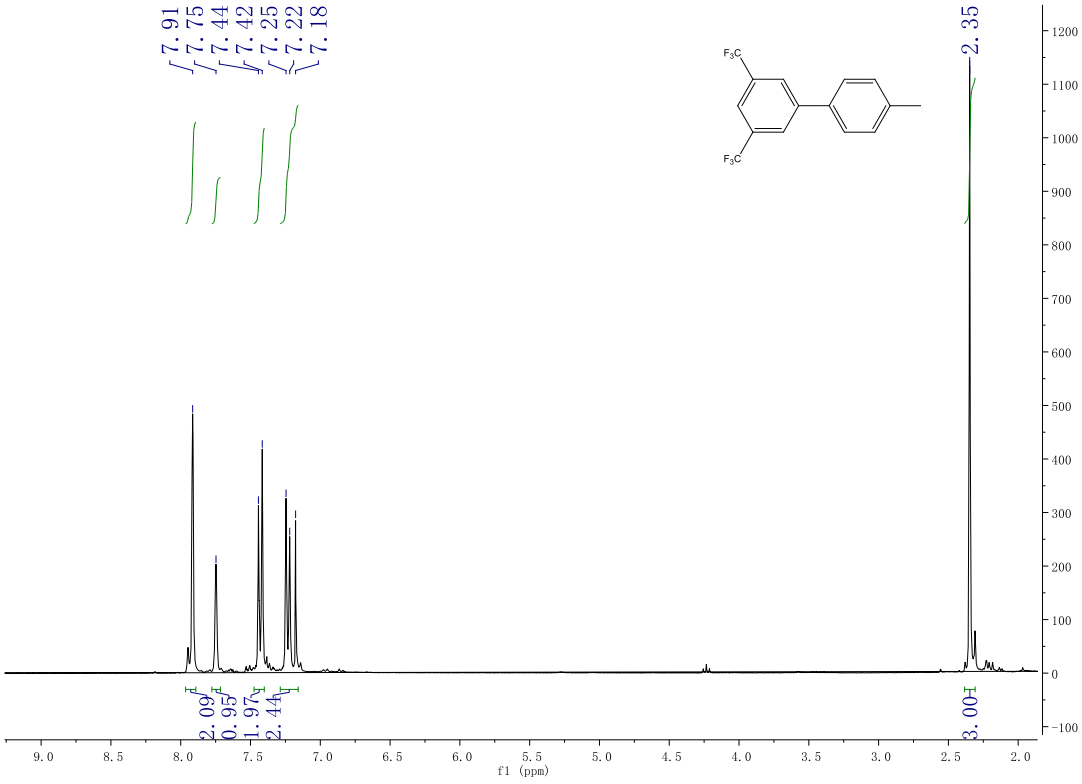
^{13}C NMR of compound 

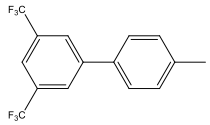


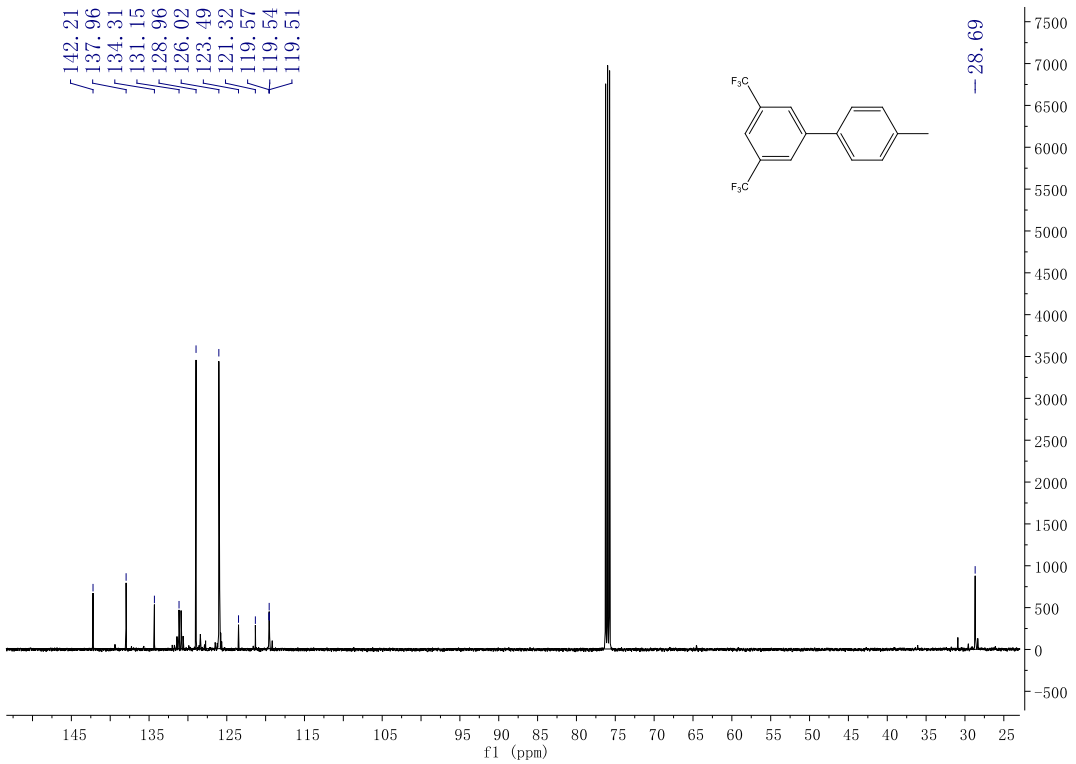
^{1}H NMR of compound 

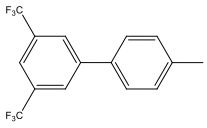


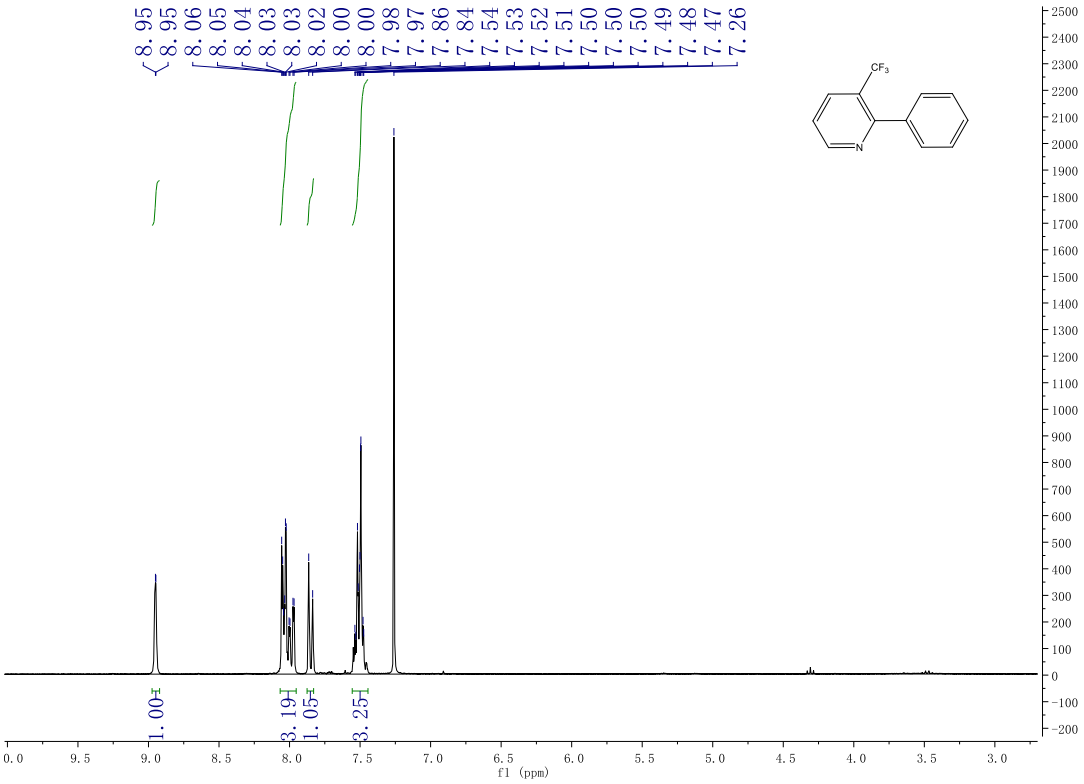
^{13}C NMR of compound 

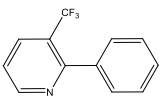


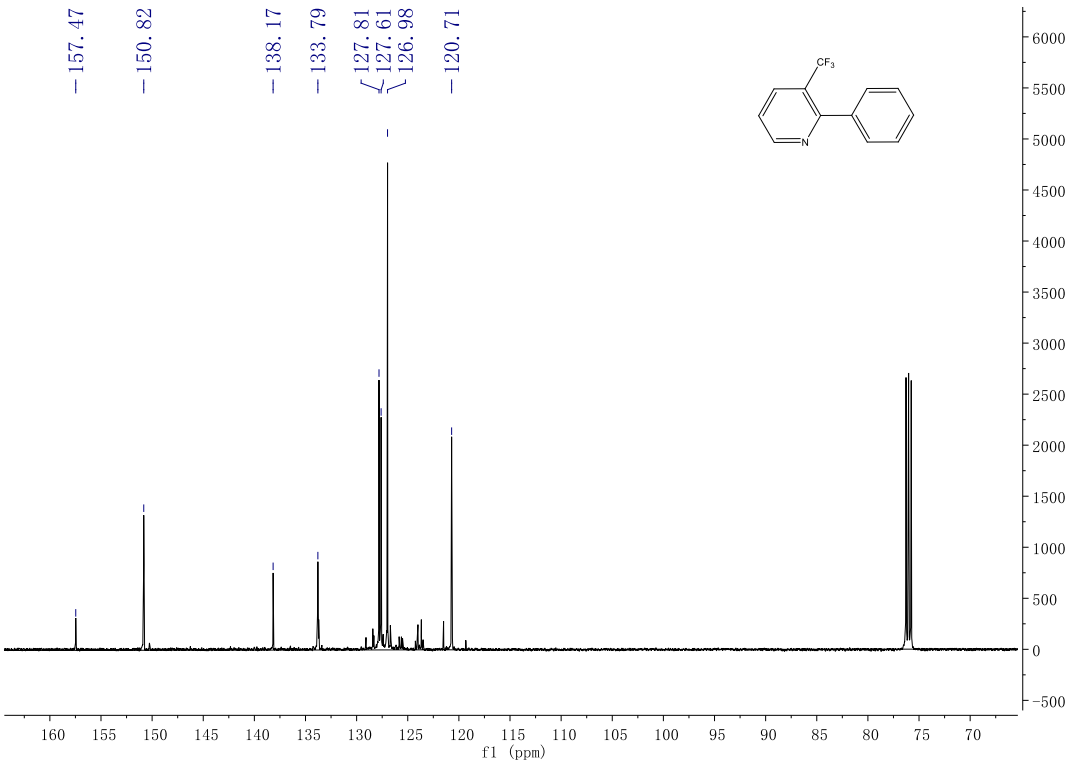
^{1}H NMR of compound 

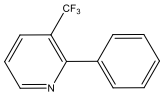


^{13}C NMR of compound 

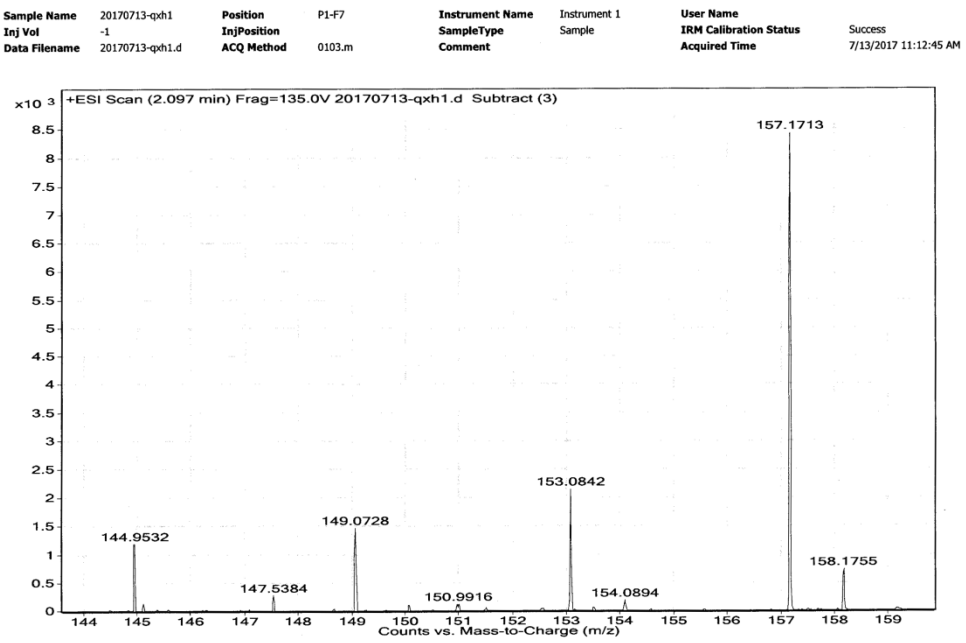


^{1}H NMR of compound 

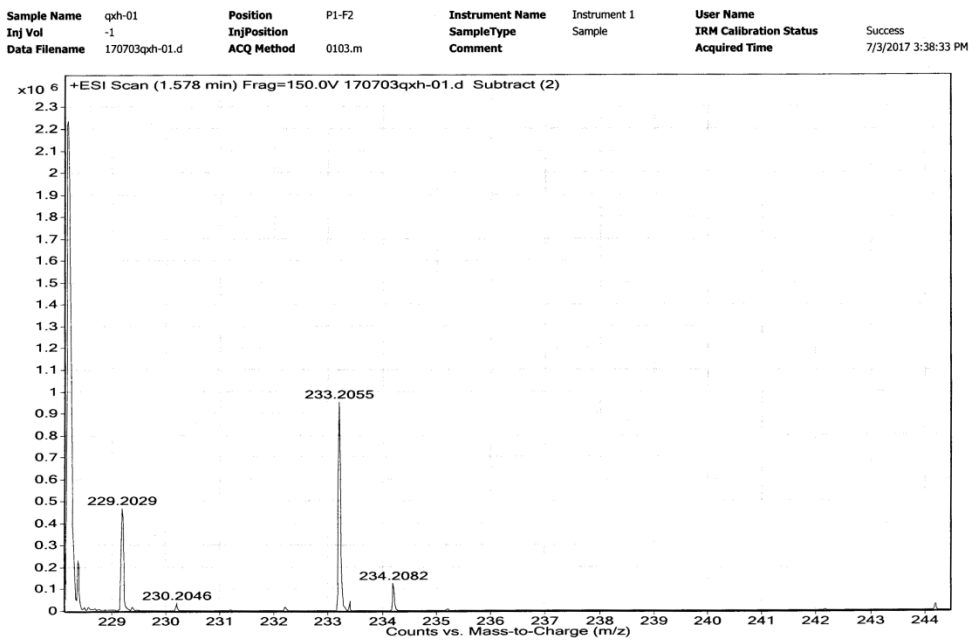


^{13}C NMR of compound 

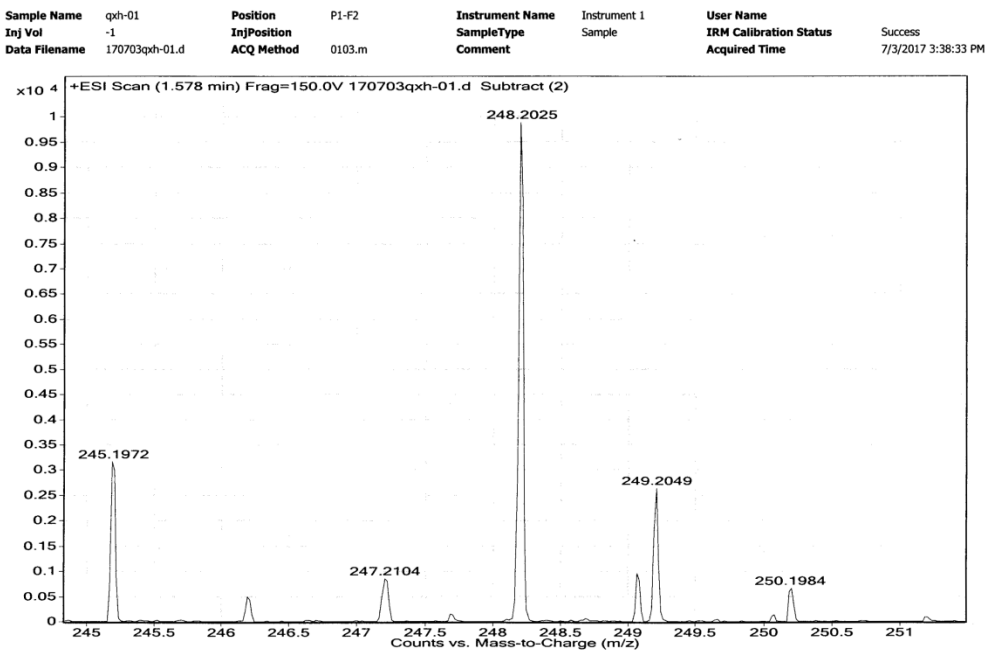
SIV MS of study on the catalytic reaction mechanism



MS of biphenyl



MS of the TEMPO capture product of phenyl radical



MS of the TEMPO capture product of 4-methyl-phenyl radical