New Journal of Chemistry

Synthesis and catalytic application of [PPP]-pincer iron, nickel and cobalt complexes for hydrosilylation of aldehydes and ketones

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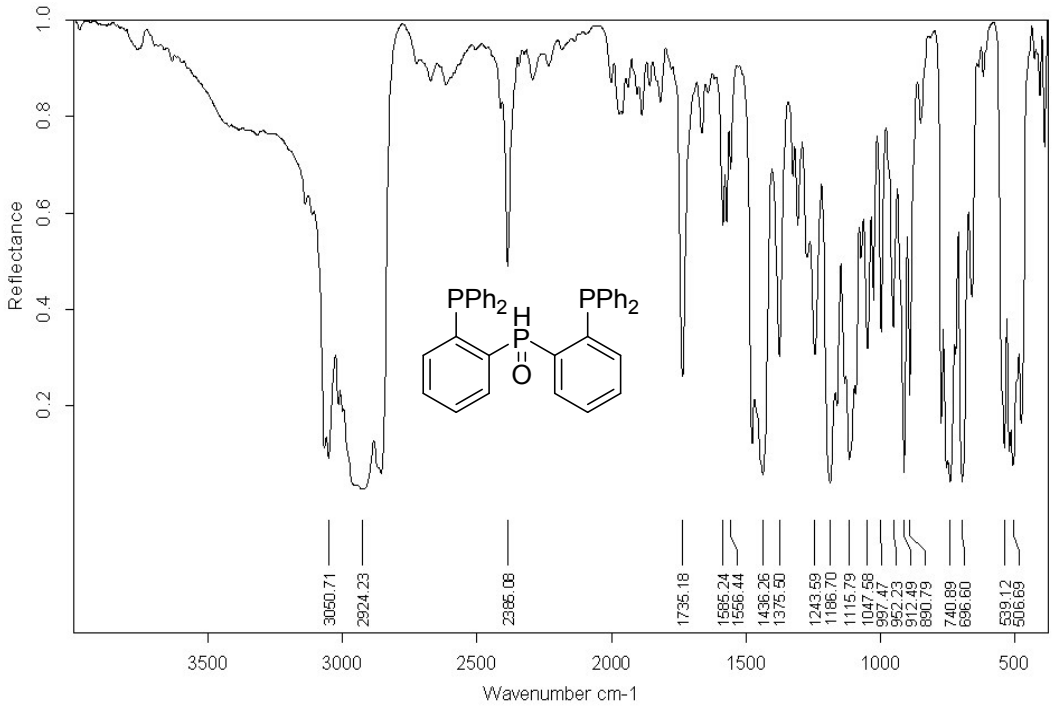
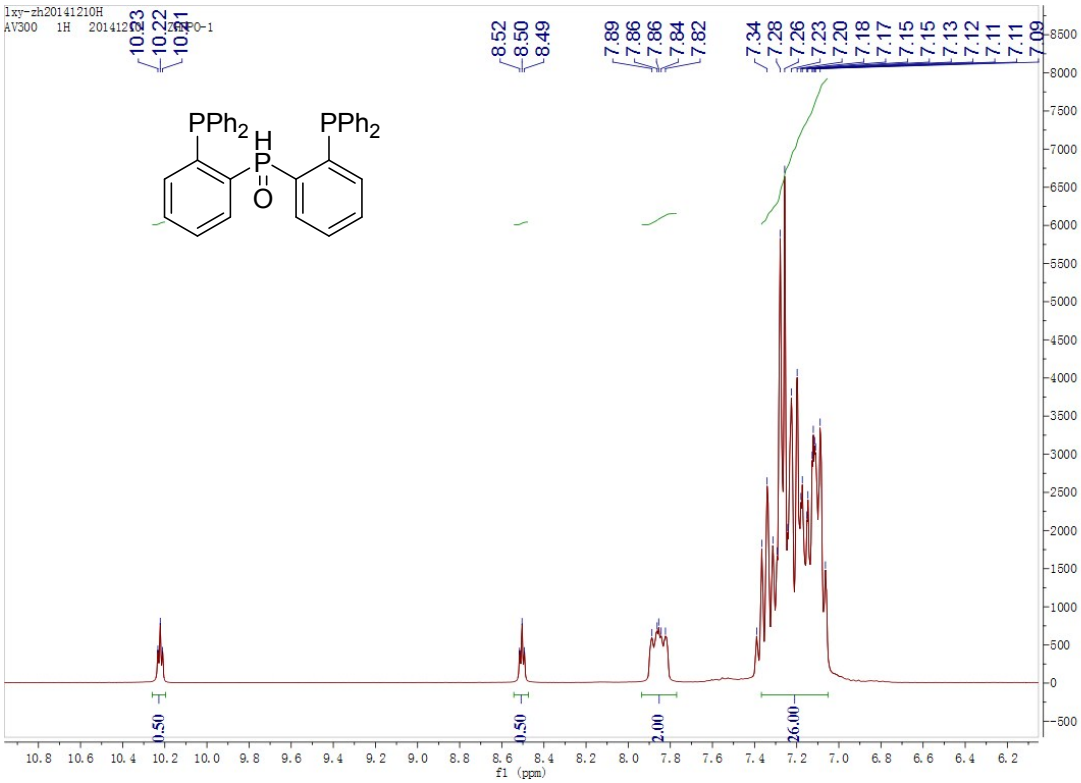
SI Crystallographic Data for Complexes 2, 3 and 4

	2	**3**	**4**
formula	$C_{50}H_{63}FeO_3P_5$	$C_{43}H_{48}NiO_2P_4$	$C_{50}H_{62}CoO_3P_5$
M_z	922.70	779.40	924.77
crystal system	Triclinic	Monoclinic	Triclinic
space group	P1	$P2_1/c$	P1
a [Å]	11.509(3)	14.5424(6)	11.4187(4)
b [Å]	11.656(3)	14.4087(8)	11.7446(4)
c [Å]	19.386(5)	19.0352(8)	18.9017(4)
α [°]	99.039(2)	90.00	98.822(2)
β [°]	103.741(2)	97.876(3)	103.269(3)
γ [°]	108.331(2)	90.00	106.982(3)
V [Å^3]	2321.0(10)	3951.0(3)	2292.52(12)
T [K]	293(2)	180(2)	100.01(10)
Z	2	4	2
μ[mm^{-1}]	0.539	0.688	4.907
total reflns	30652	10559	23807
unique reflns	10669	455	7949
R_{int}	0.0187	0.0388	0.0759
R_1[I>2σ(I)]	0.0426	0.0364	R_1 = 0.0651
wR(F^2)[I>2σ(I)]	0.1053	0.0892	0.1618
R_1(all data)	0.0524	0.0557	0.0738
wR(F^2)(all data)	0.1125	0.1026	0.1689
GOF on F^2	1.032	1.070	0.995

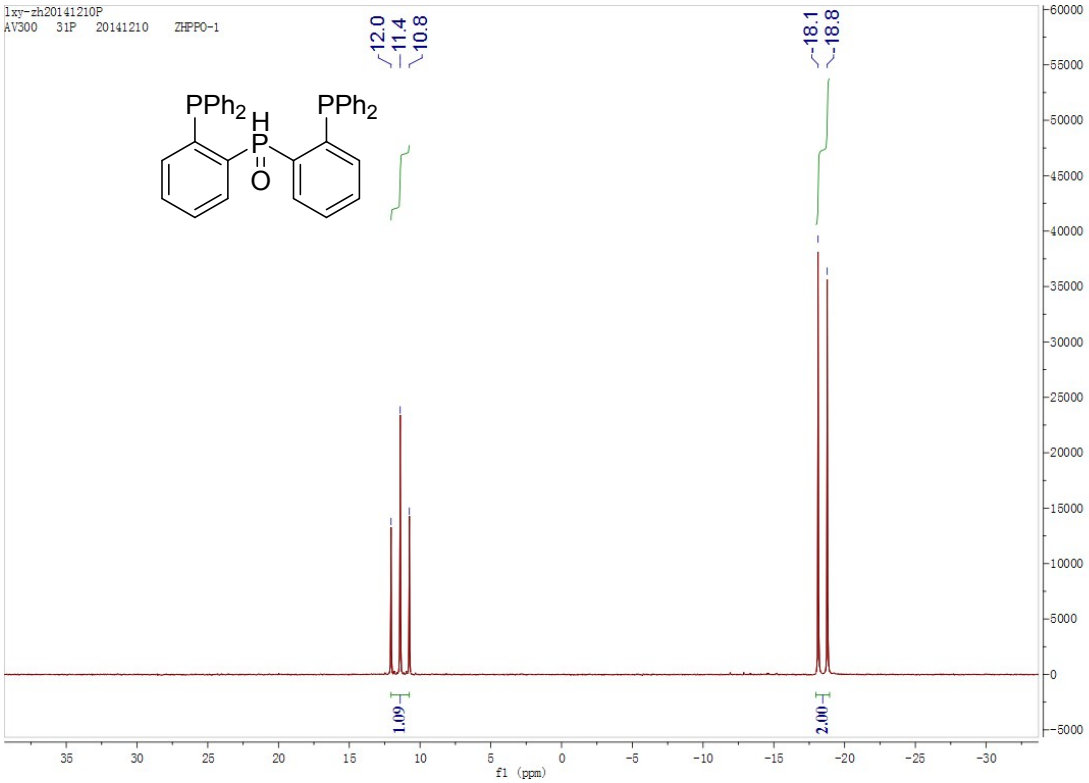
SII IR, ^{1}H NMR, ^{31}P NMR and ^{13}C NMR Spectra of Compounds 1 - 4



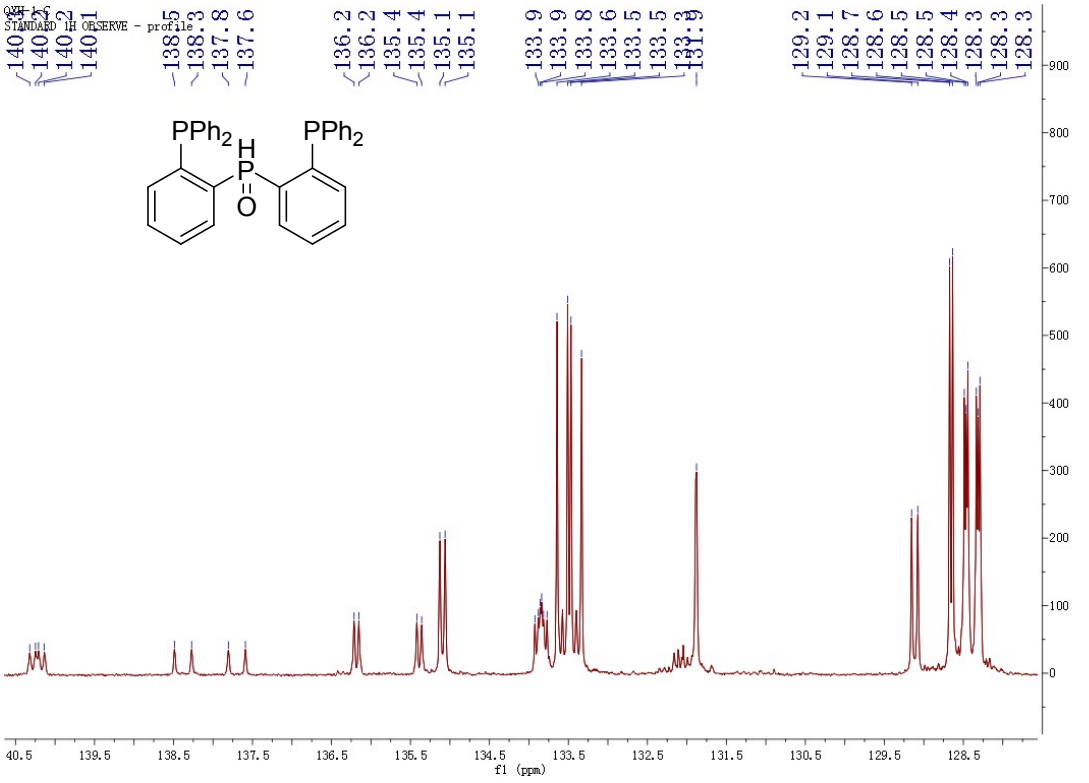
IR spectrum of ligand **1**



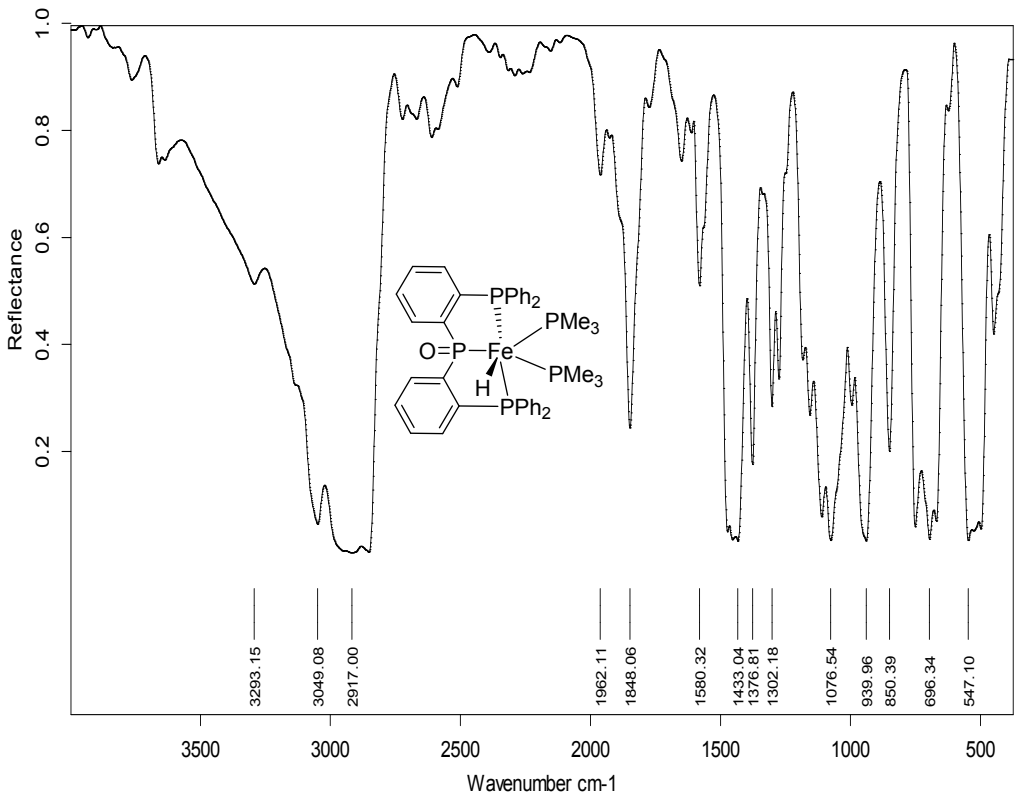
^{1}H NMR spectrum of ligand **1**



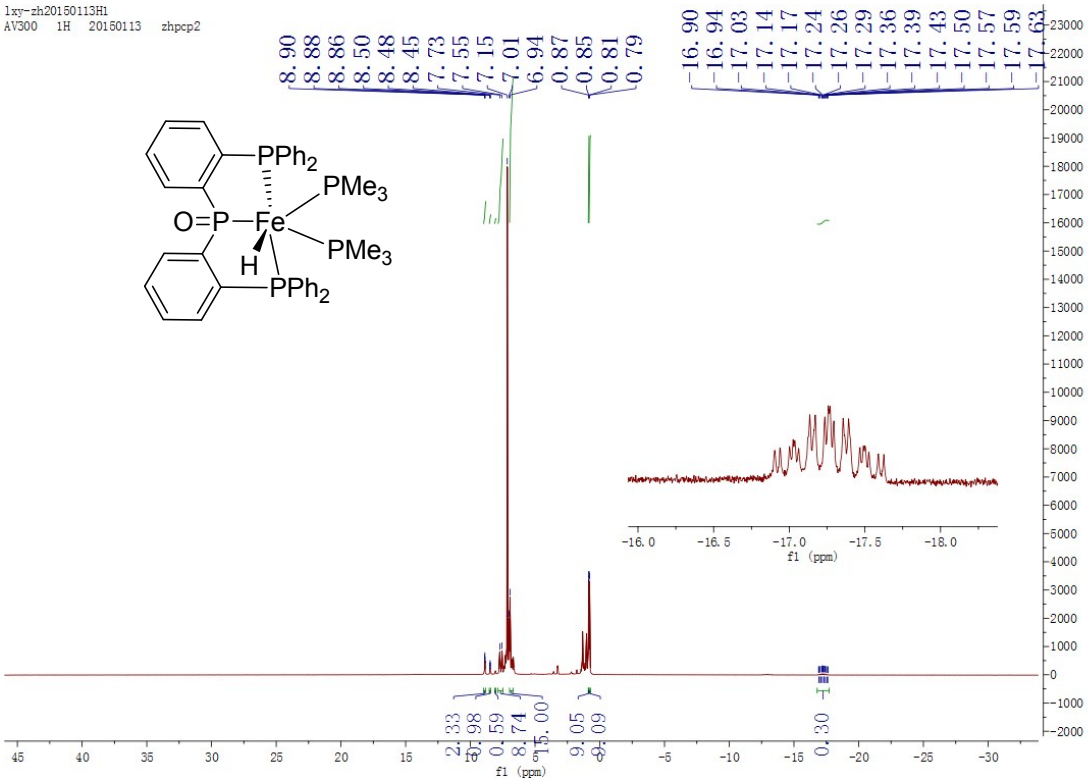
^{31}P NMR spectrum of ligand **1**



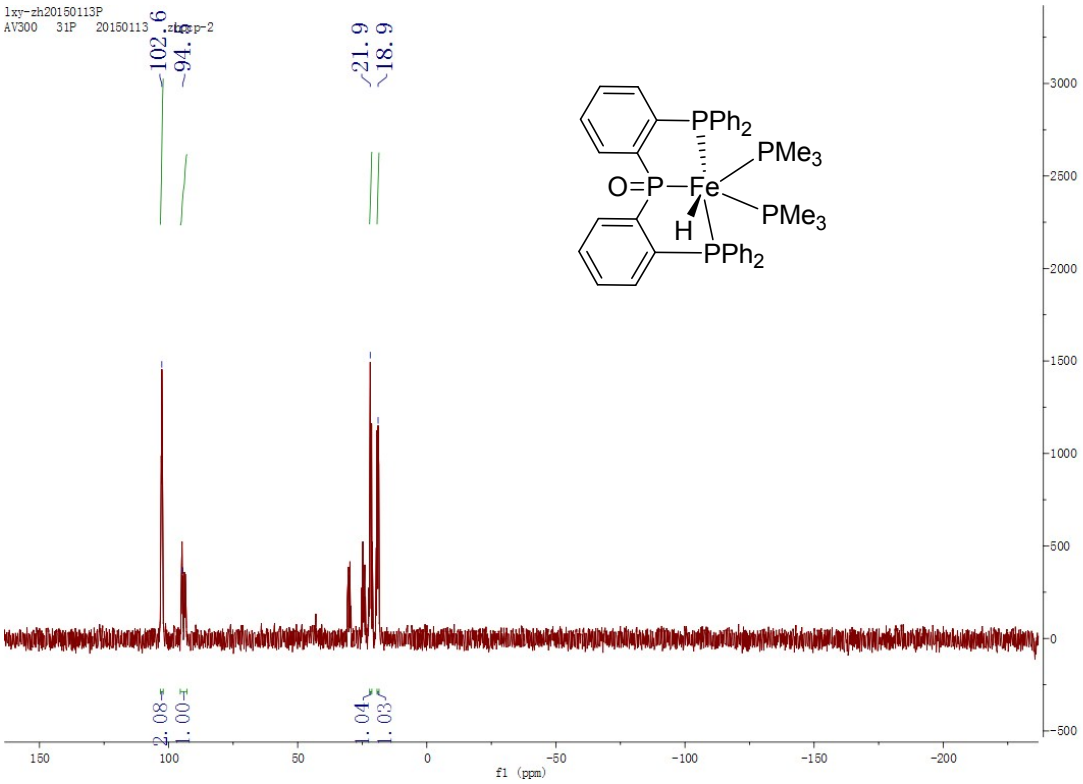
^{13}C NMR spectrum of ligand **1**



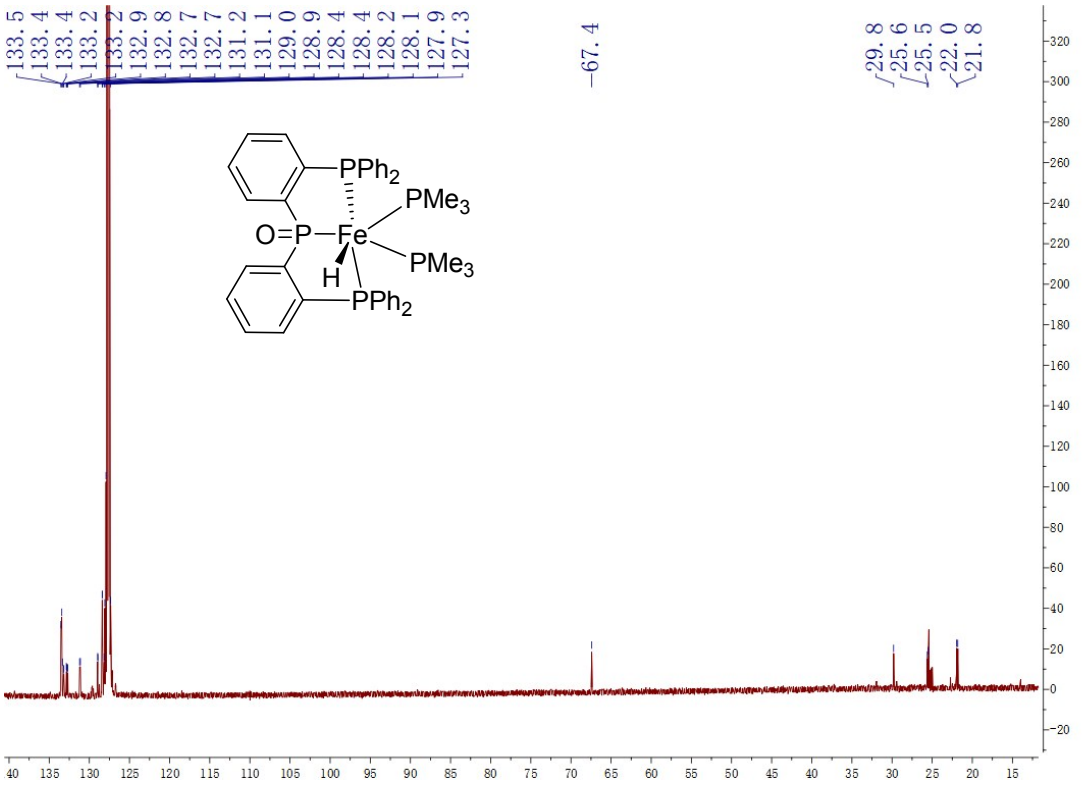
IR spectrum of complex **2**



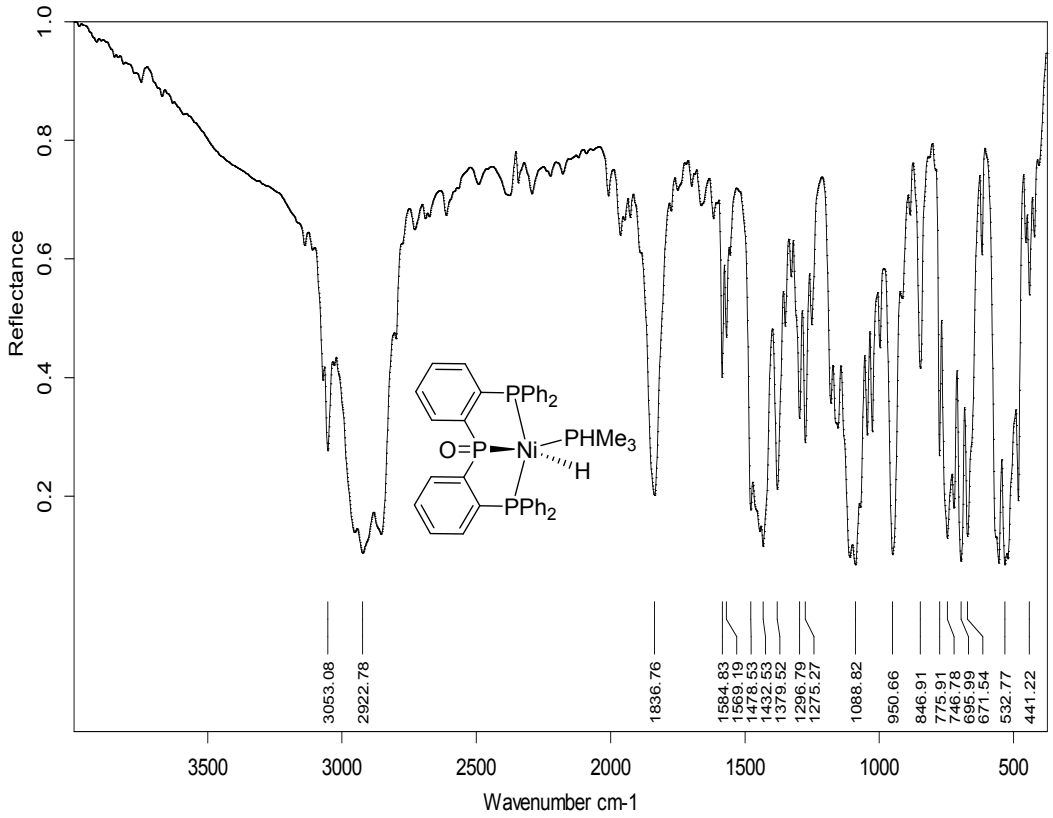
^{1}H NMR spectrum of complex **2**



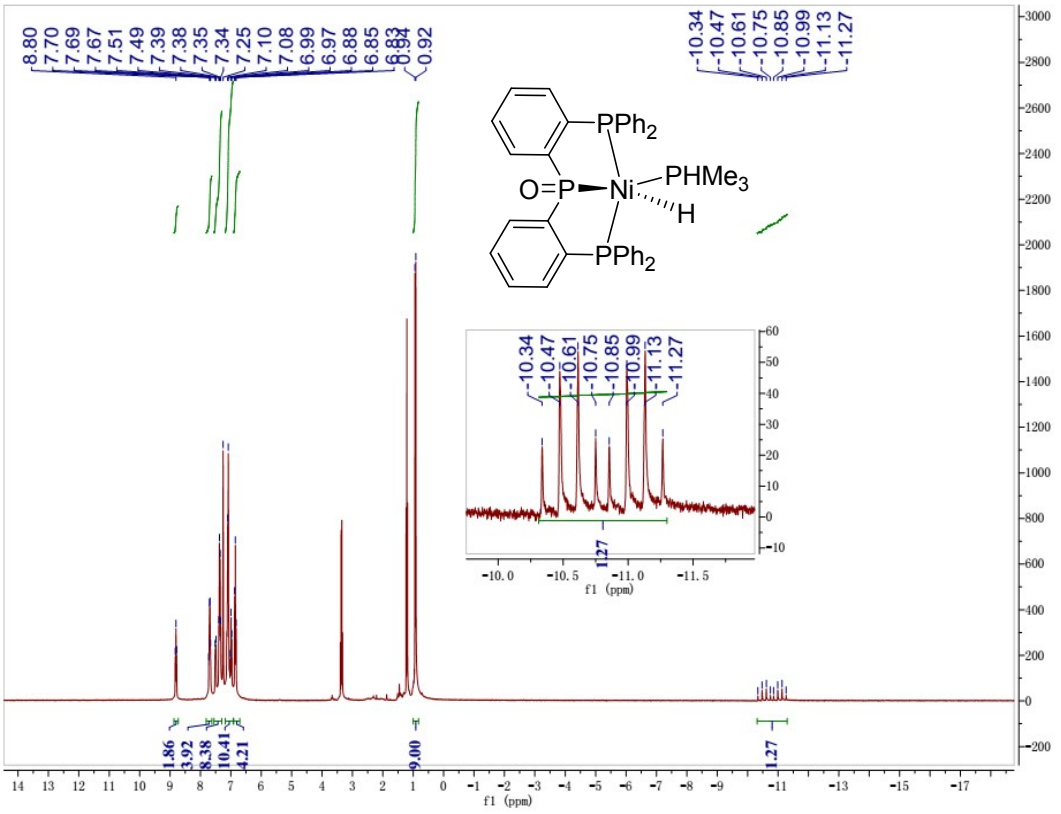
^{31}P NMR spectrum of complex **2**



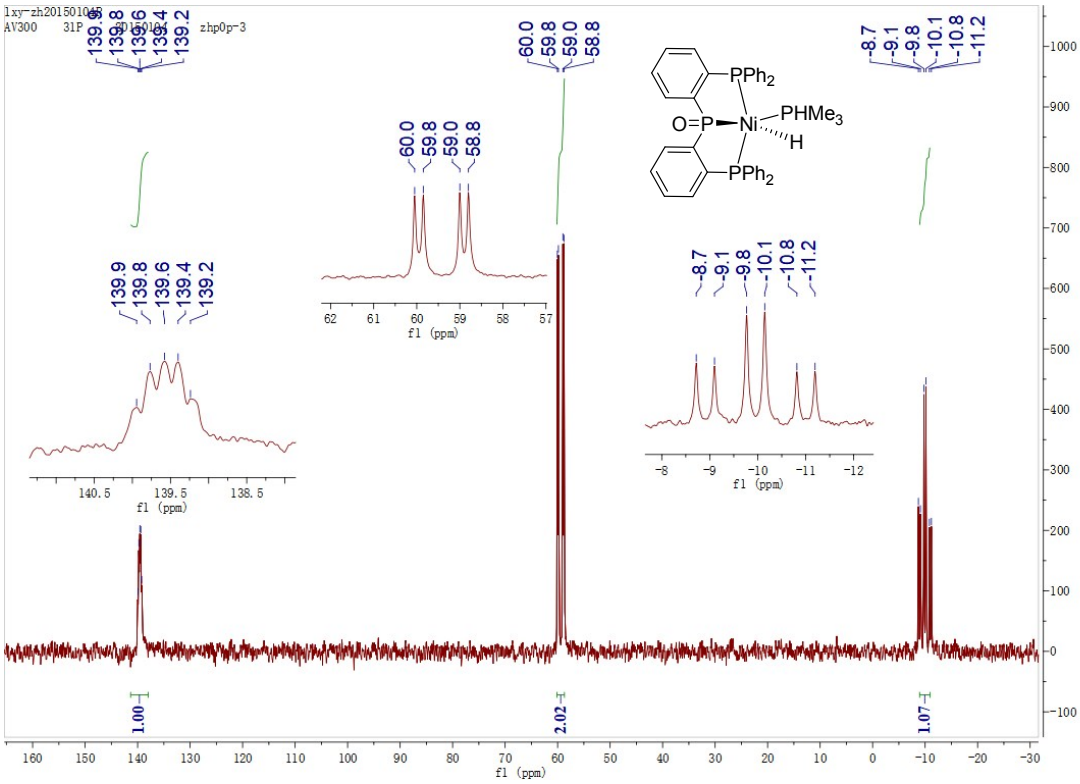
^{13}C NMR spectrum of complex **2**



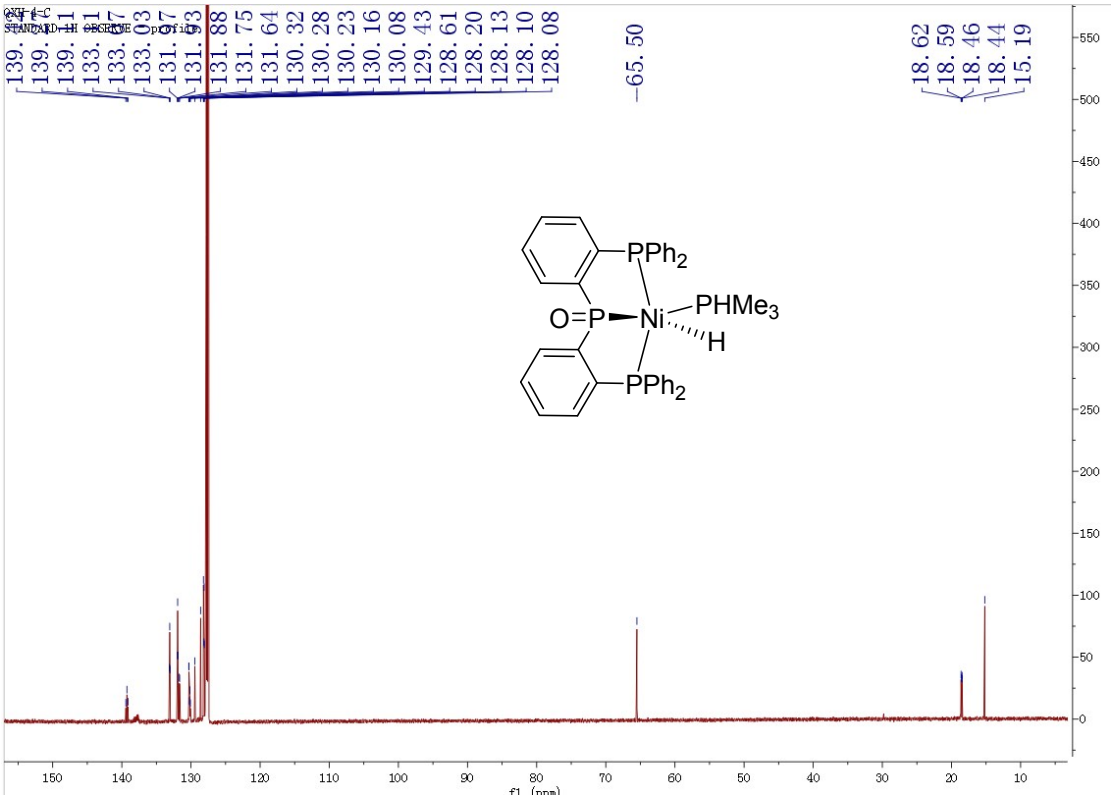
IR spectrum of complex **3**



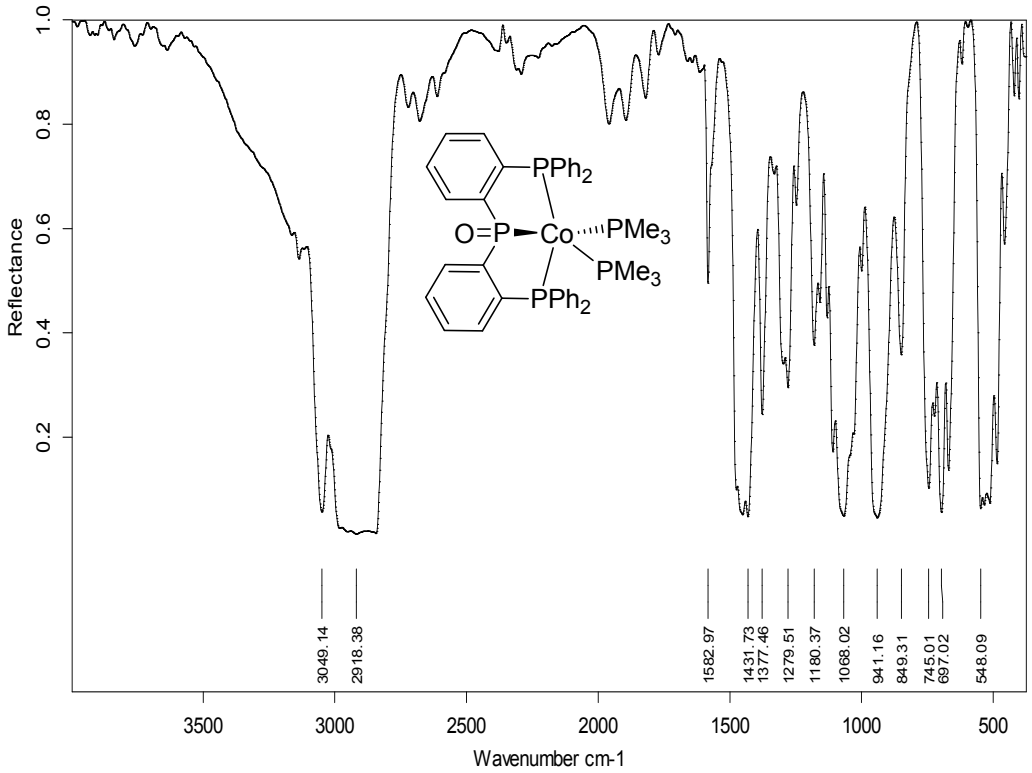
^{1}H NMR spectrum of complex **3**



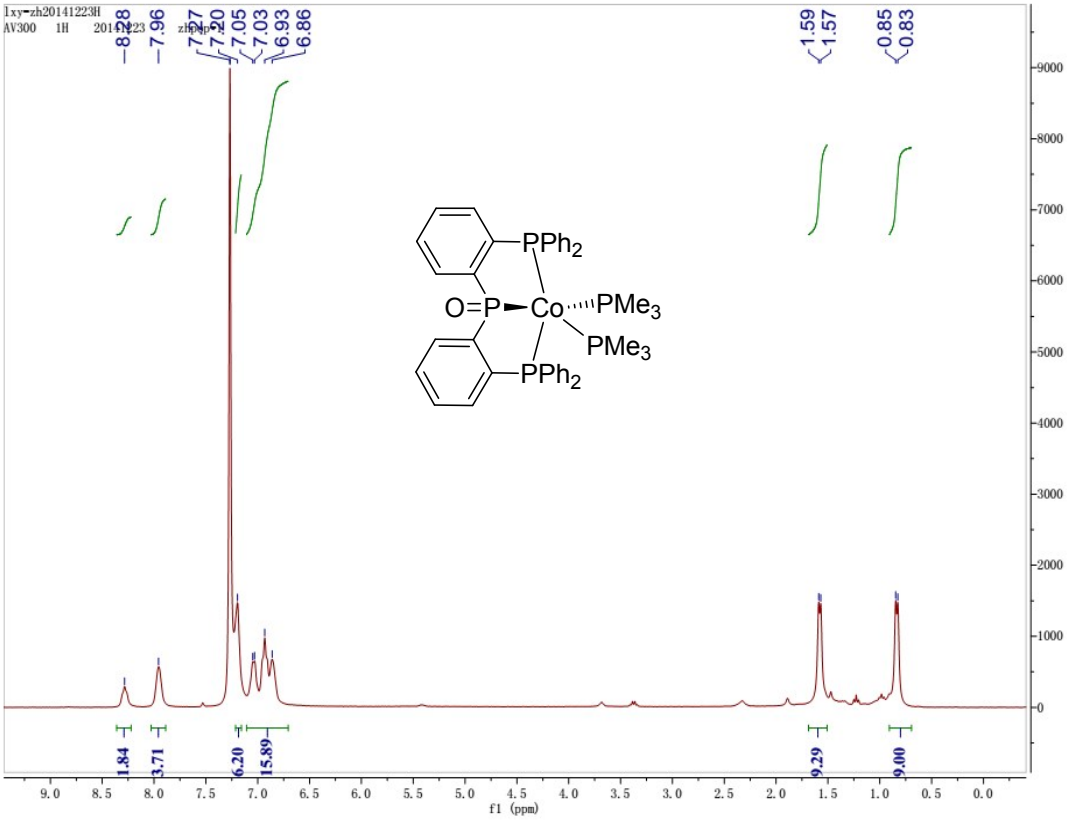
^{31}P NMR spectrum of complex **3**



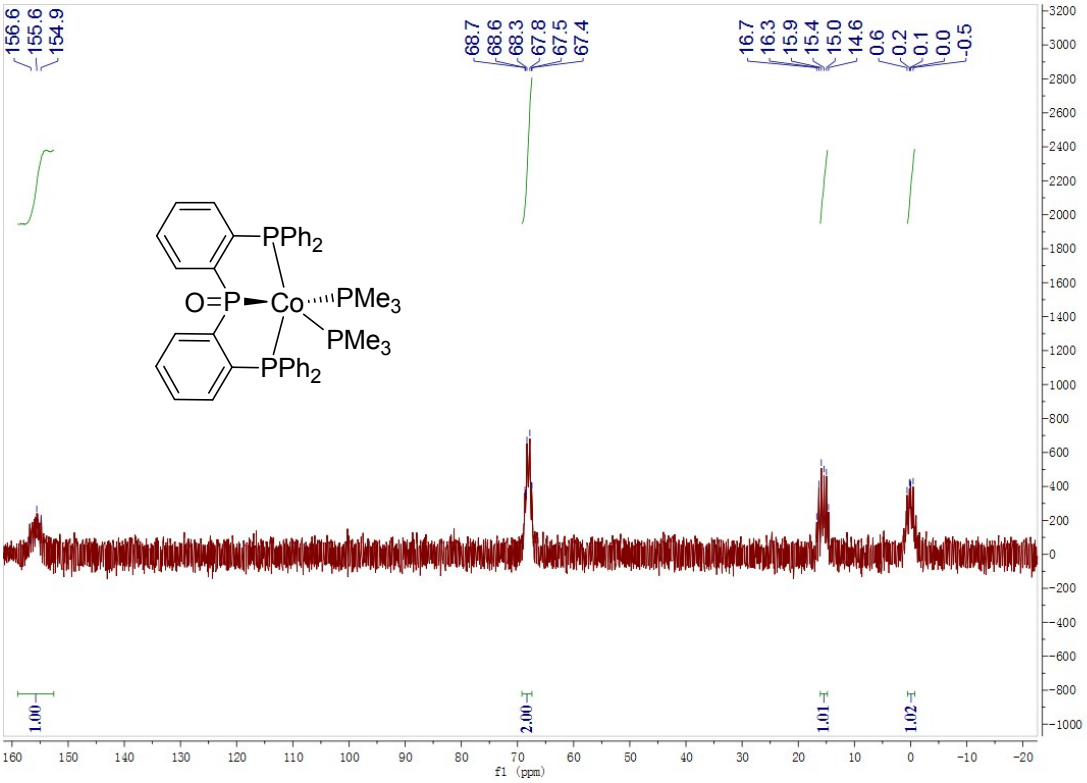
^{13}C NMR spectrum of complex **3**



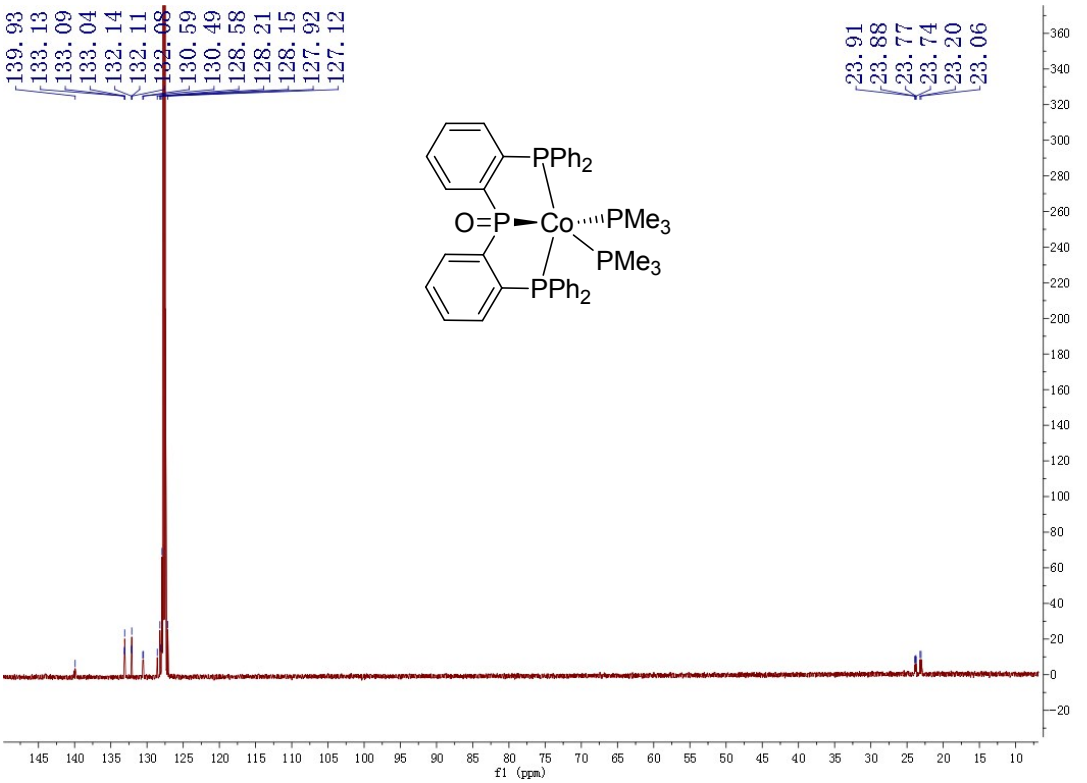
IR spectrum of complex **4**



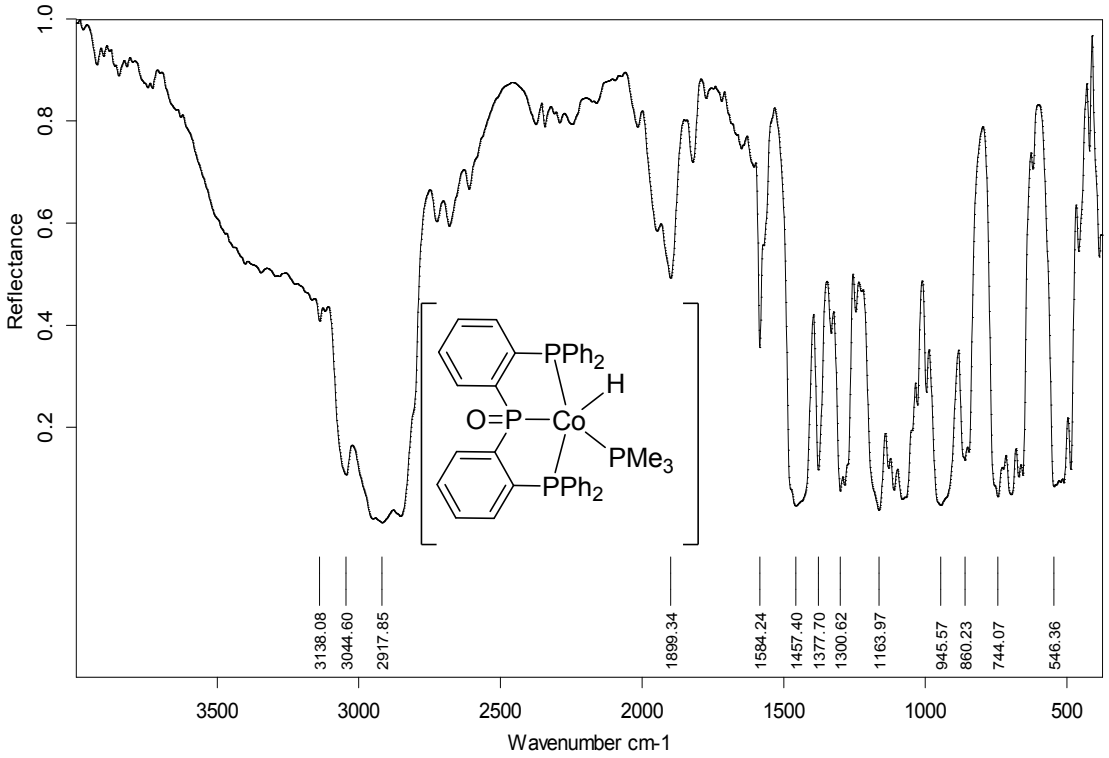
^{1}H NMR spectrum of complex **4**



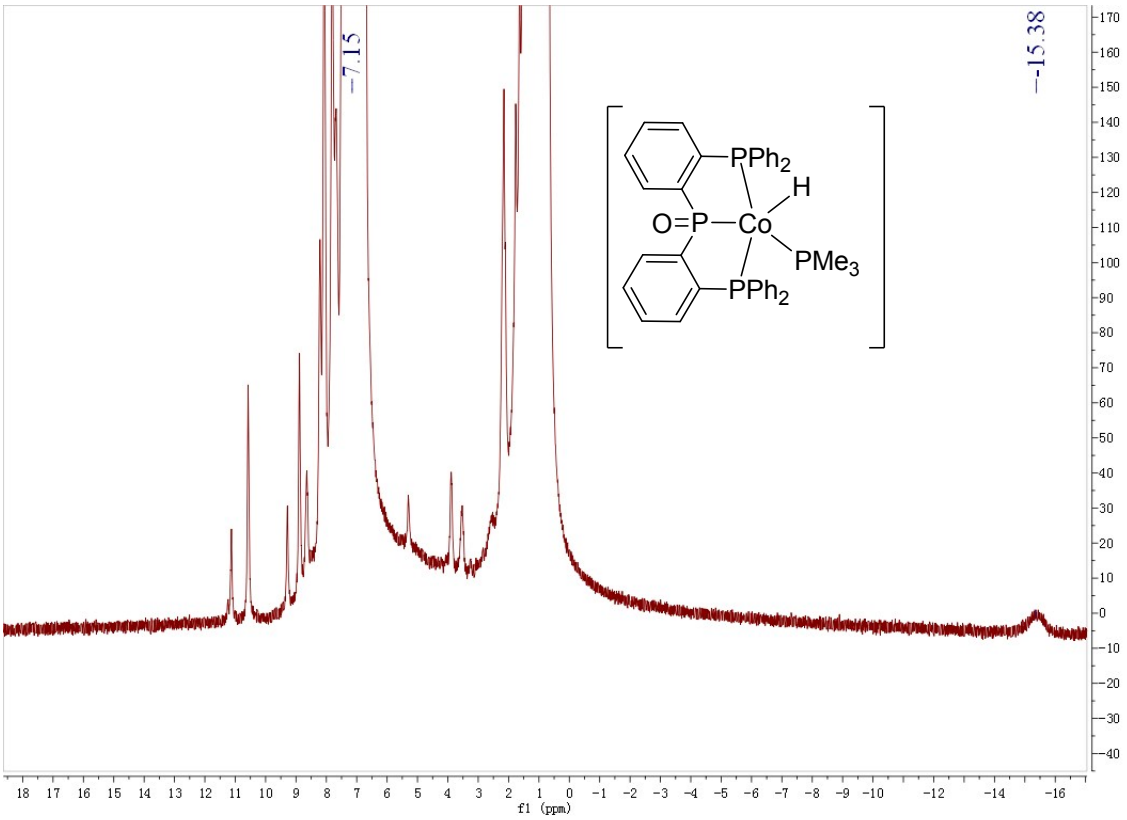
^{31}P NMR spectrum of complex **4**



^{13}C NMR spectrum of complex **4**

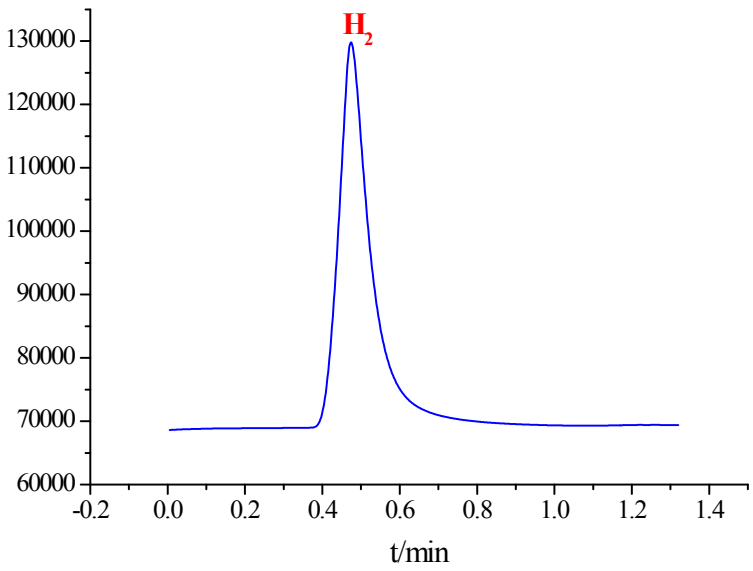


IR spectrum of complex **4a**



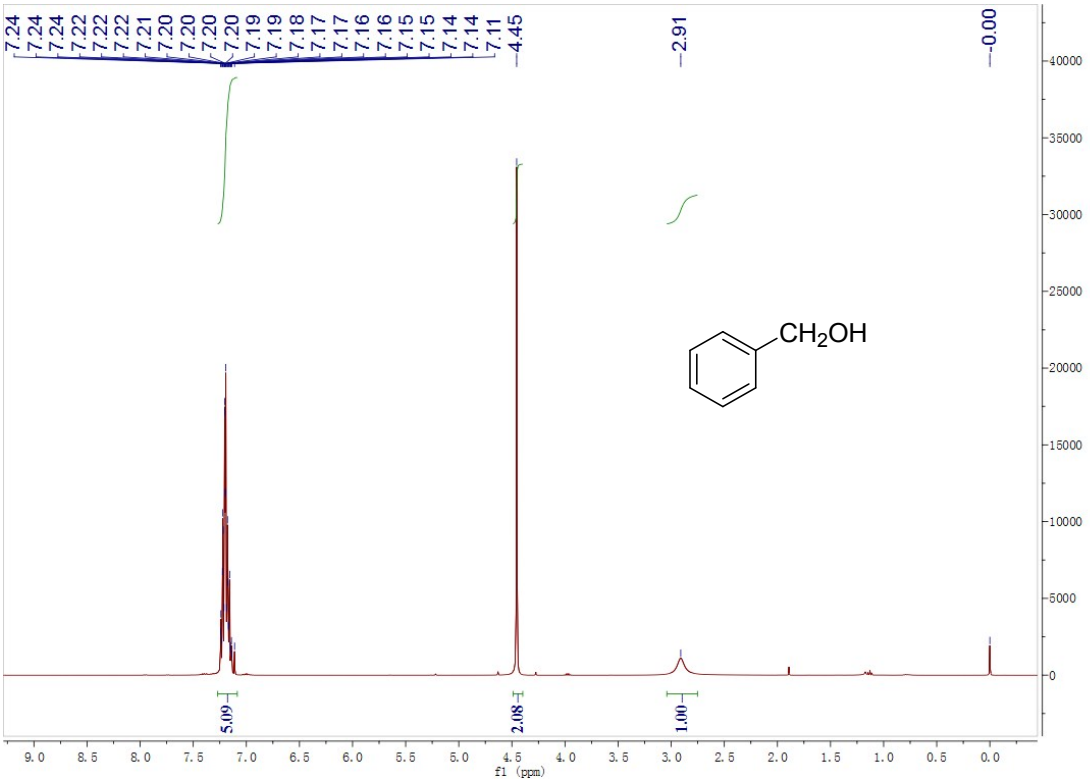
^{1}H NMR spectrum of complex **4a**

SIII

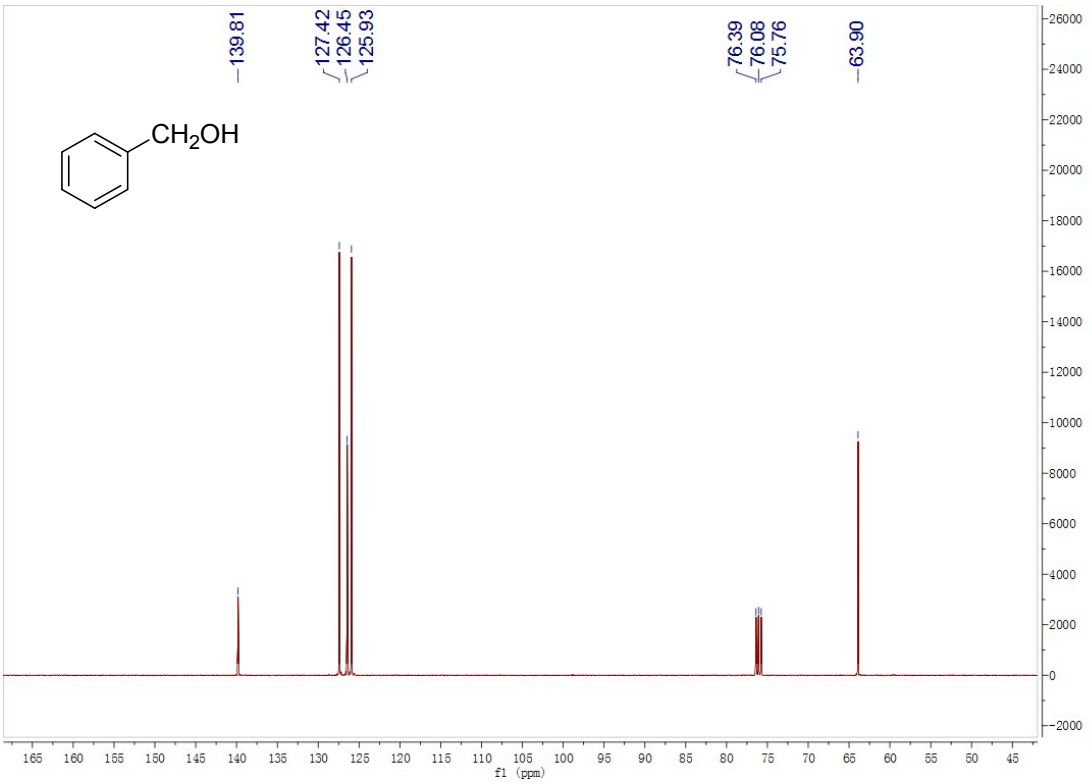


The release of H_2 from reaction of $Co(PMe_3)_4$ with **1** by GC.

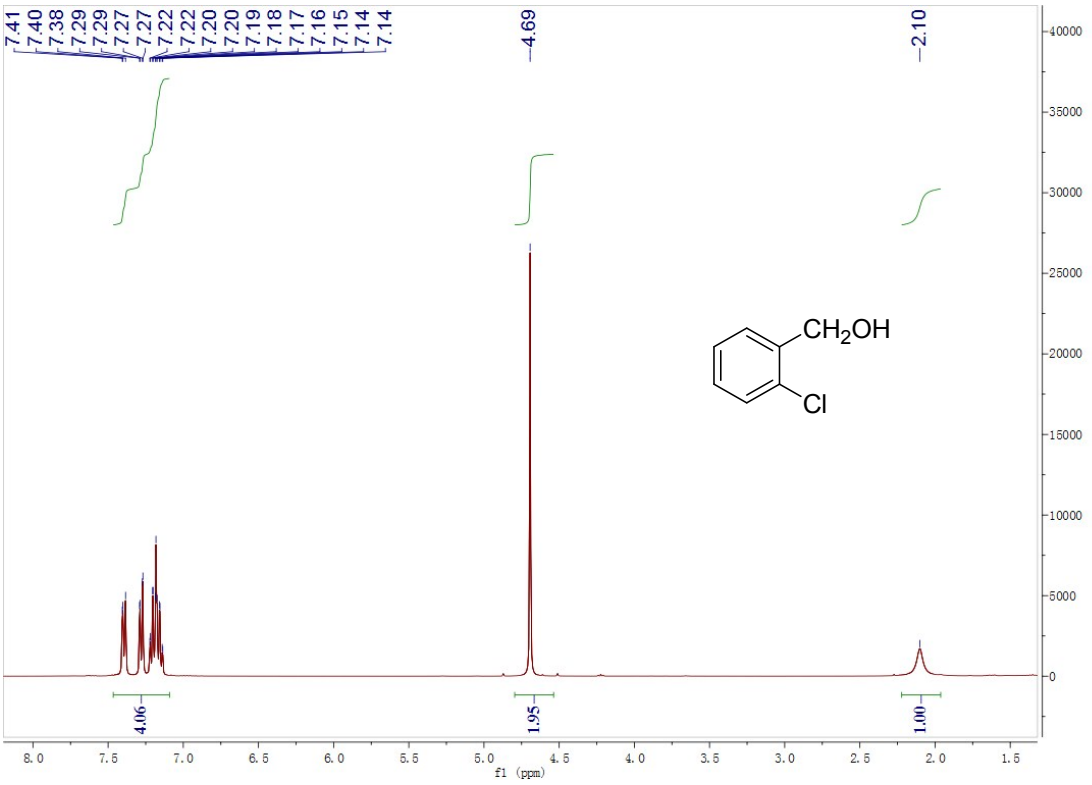
SIV ^{1}H and ^{13}C NMR Spectra of the Hydrosilylation Reduction Products



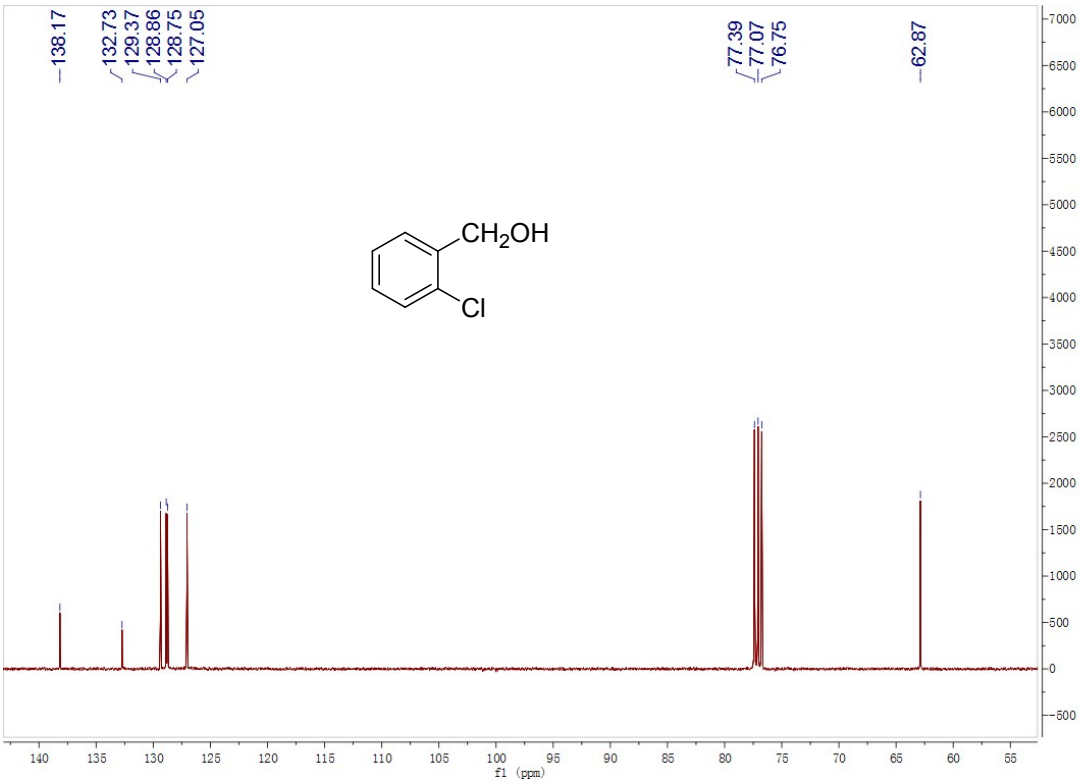
^{1}H NMR of compound **6a**



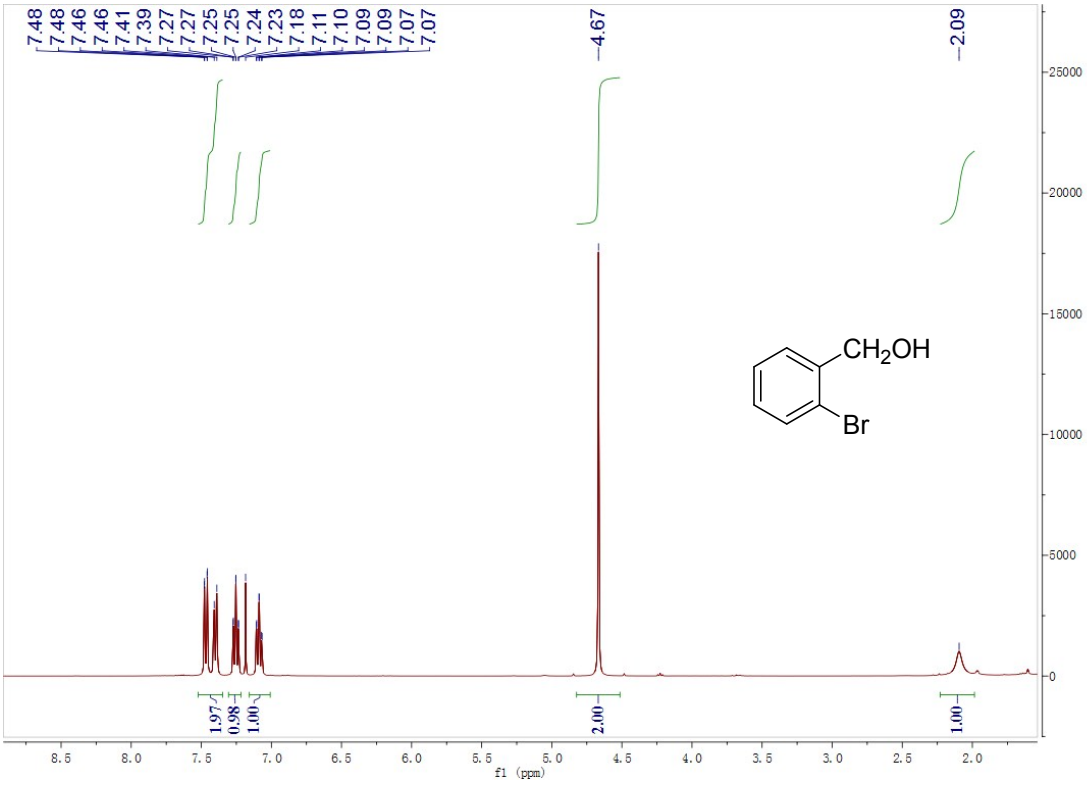
^{13}C NMR of compound **6a**



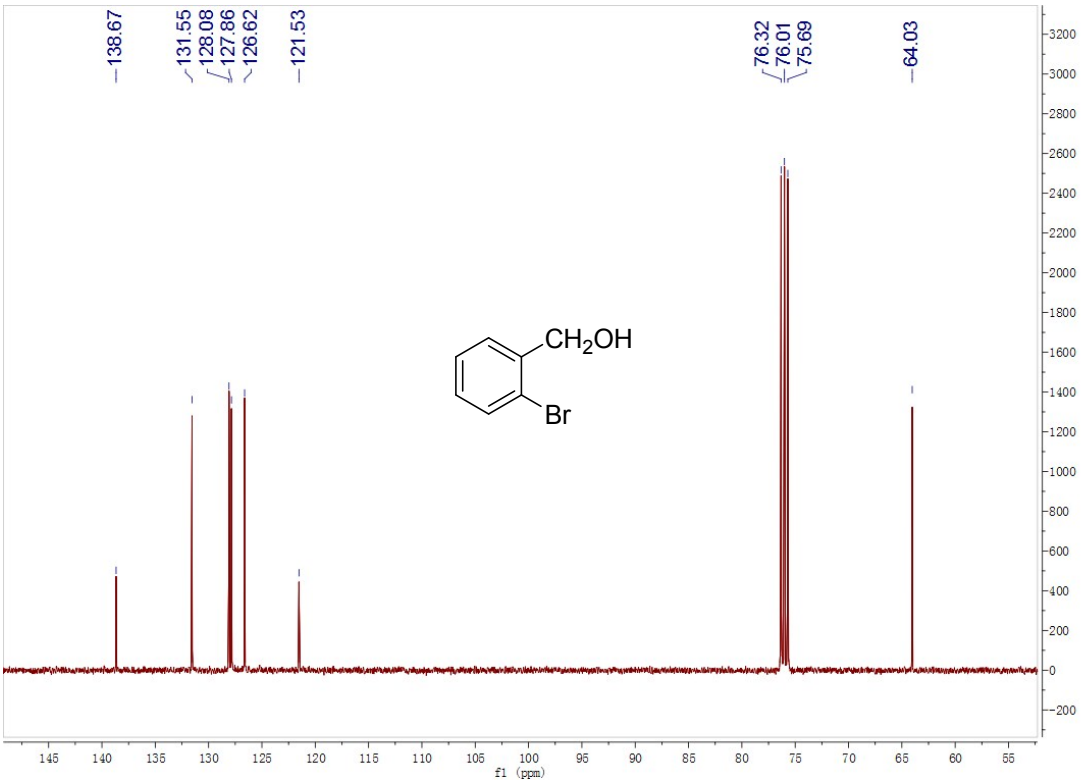
^{1}H NMR of compound **6b**



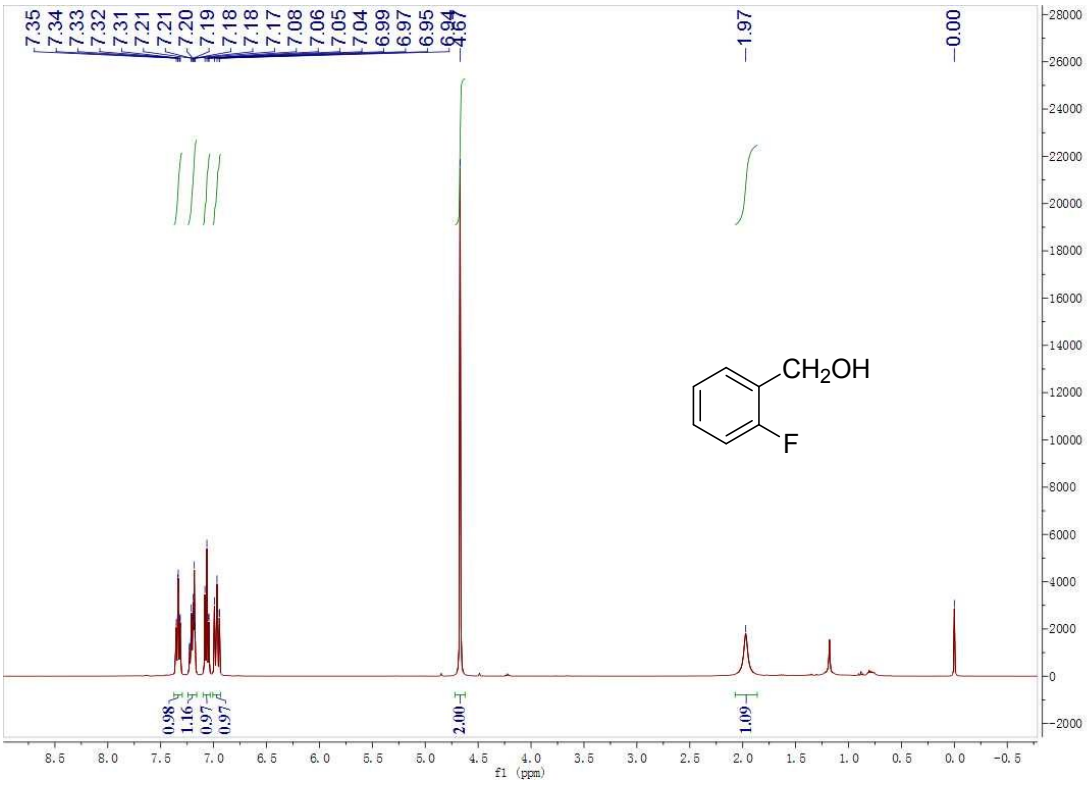
^{13}C NMR of compound **6b**



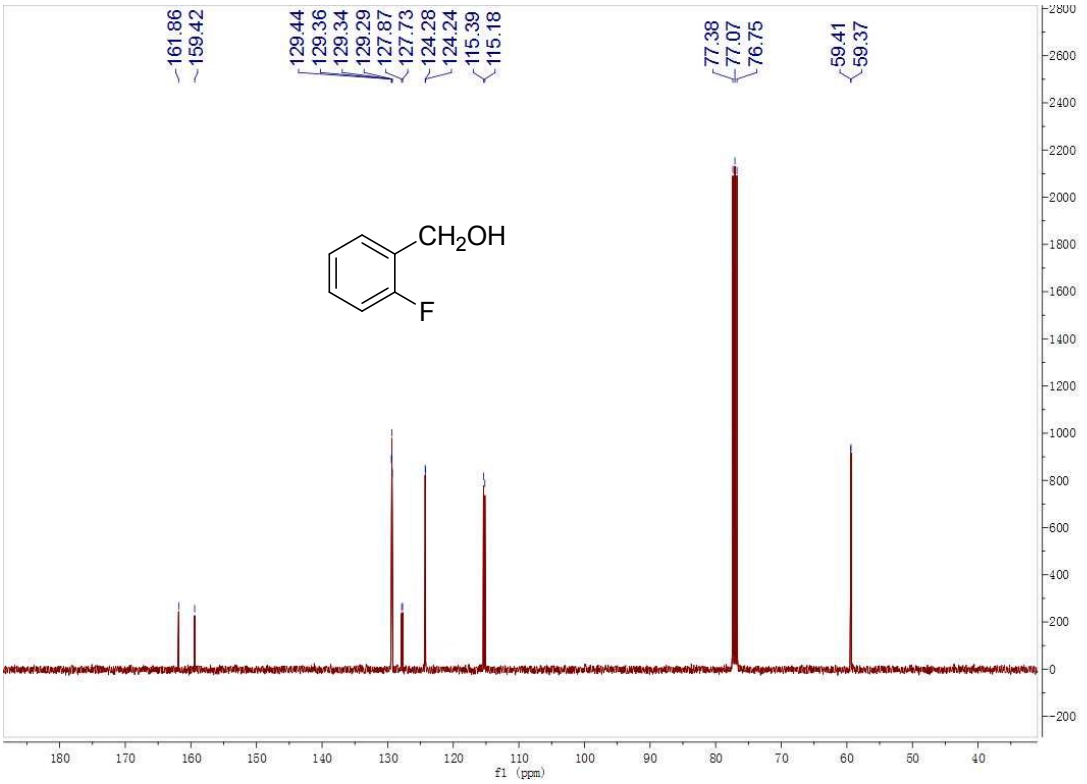
^{1}H NMR of compound **6c**



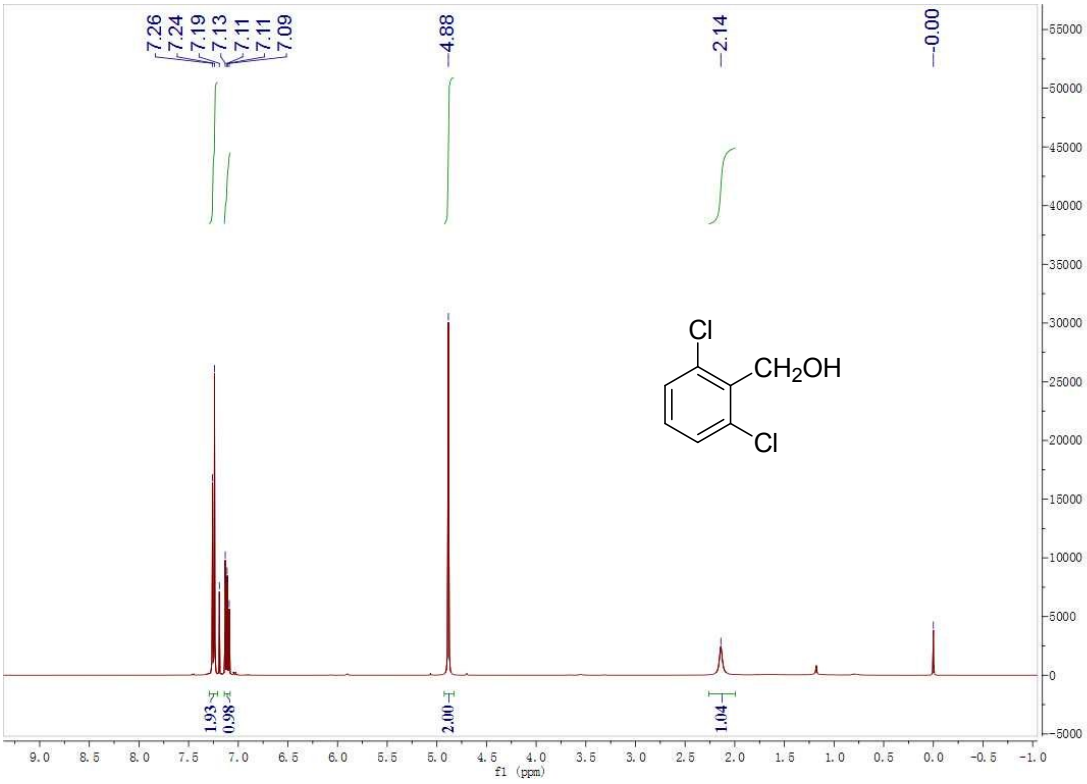
^{13}C NMR of compound **6c**



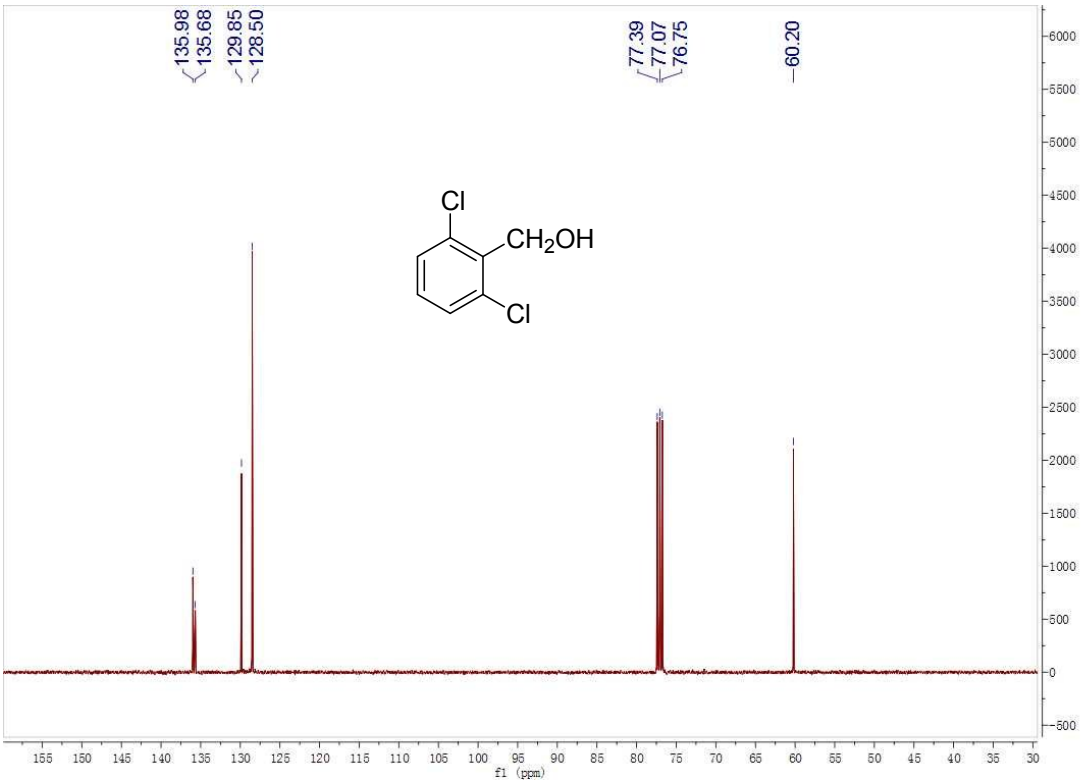
^{1}H NMR of compound **6d**



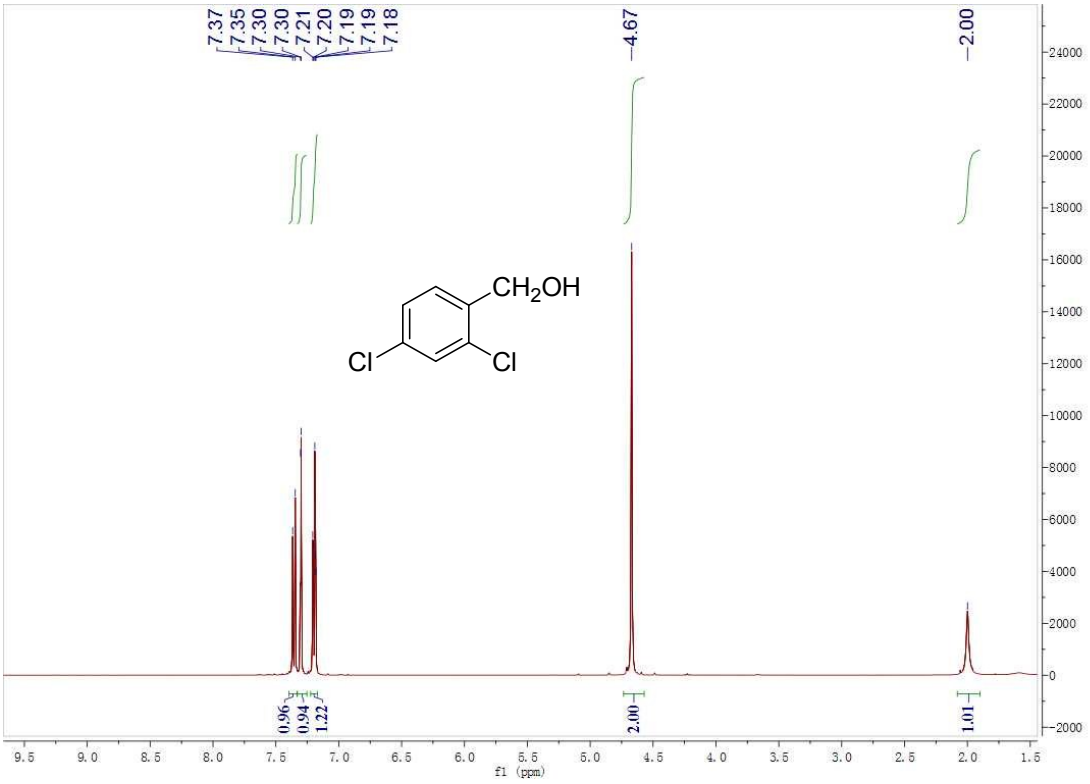
^{13}C NMR of compound **6d**



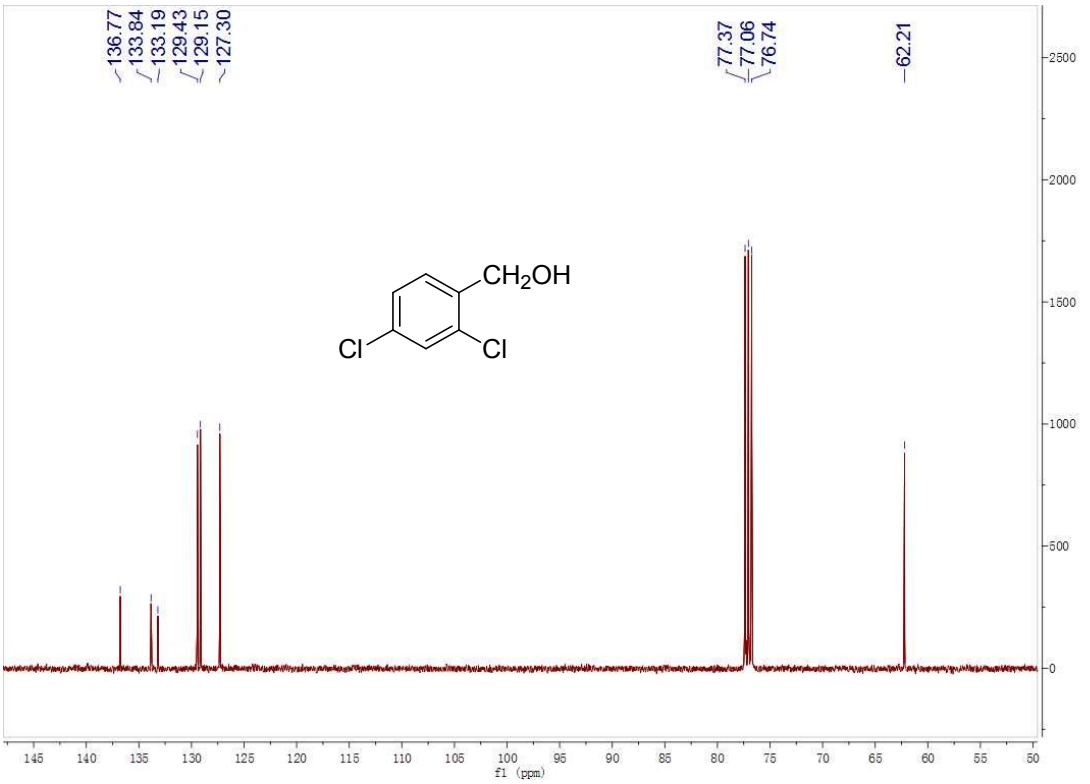
^{1}H NMR of compound **6e**



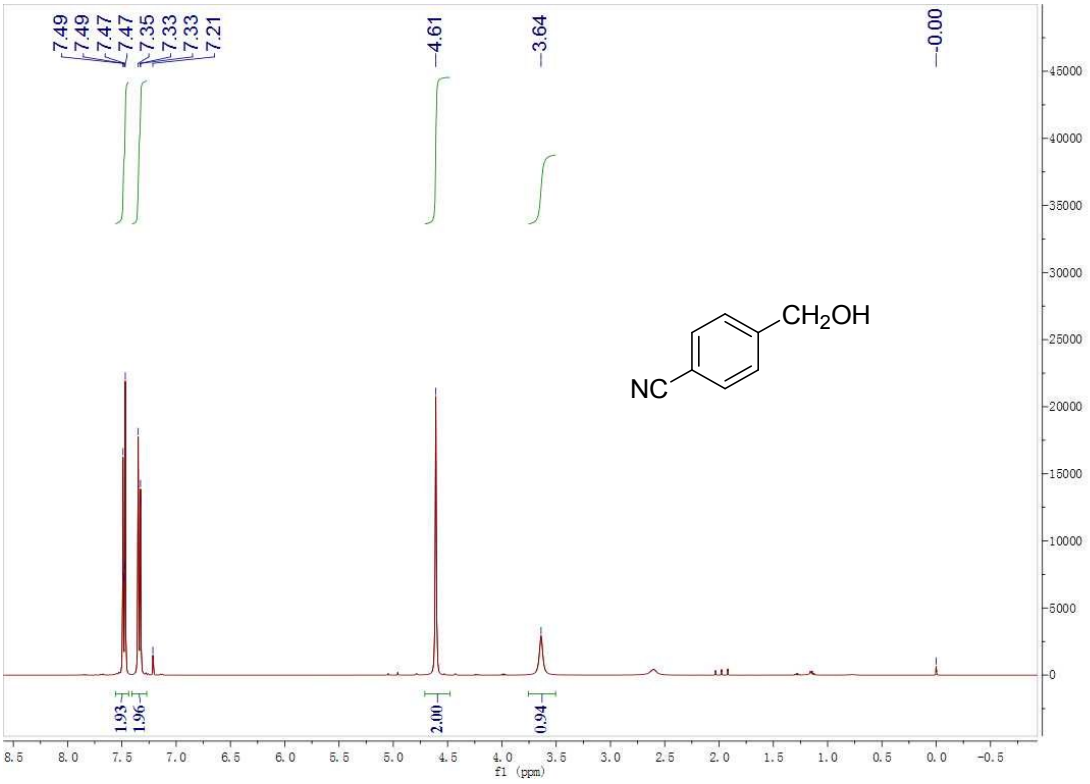
^{13}C NMR of compound **6e**



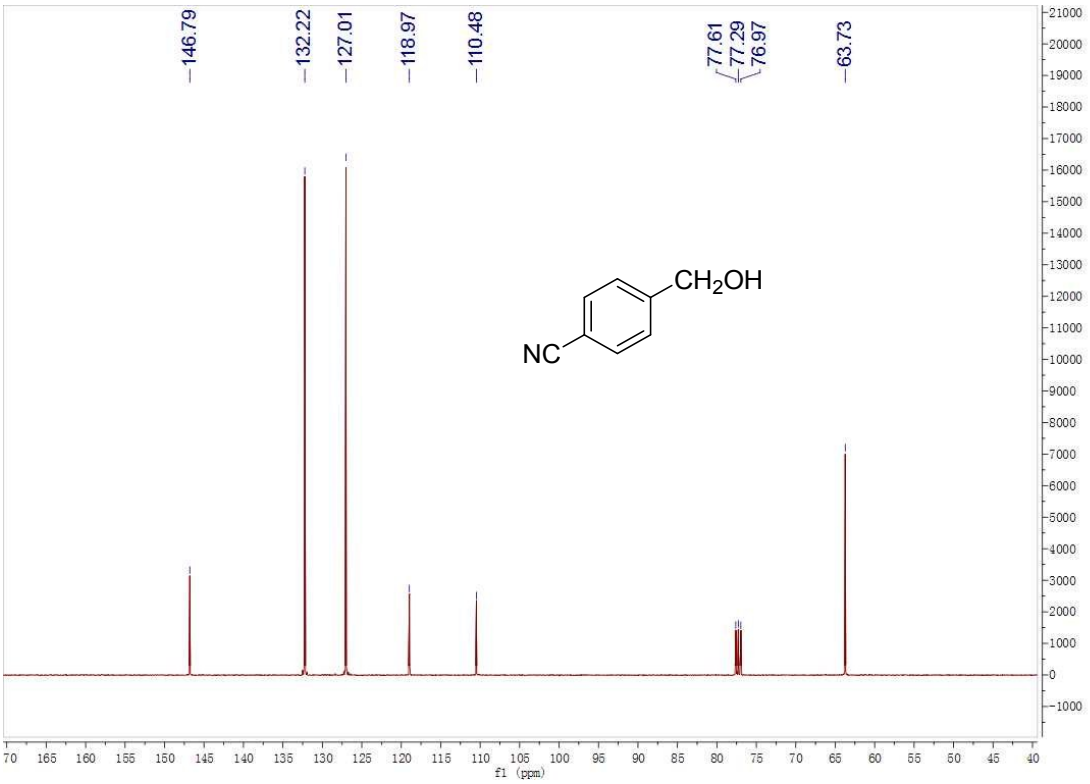
^{1}H NMR of compound **6f**



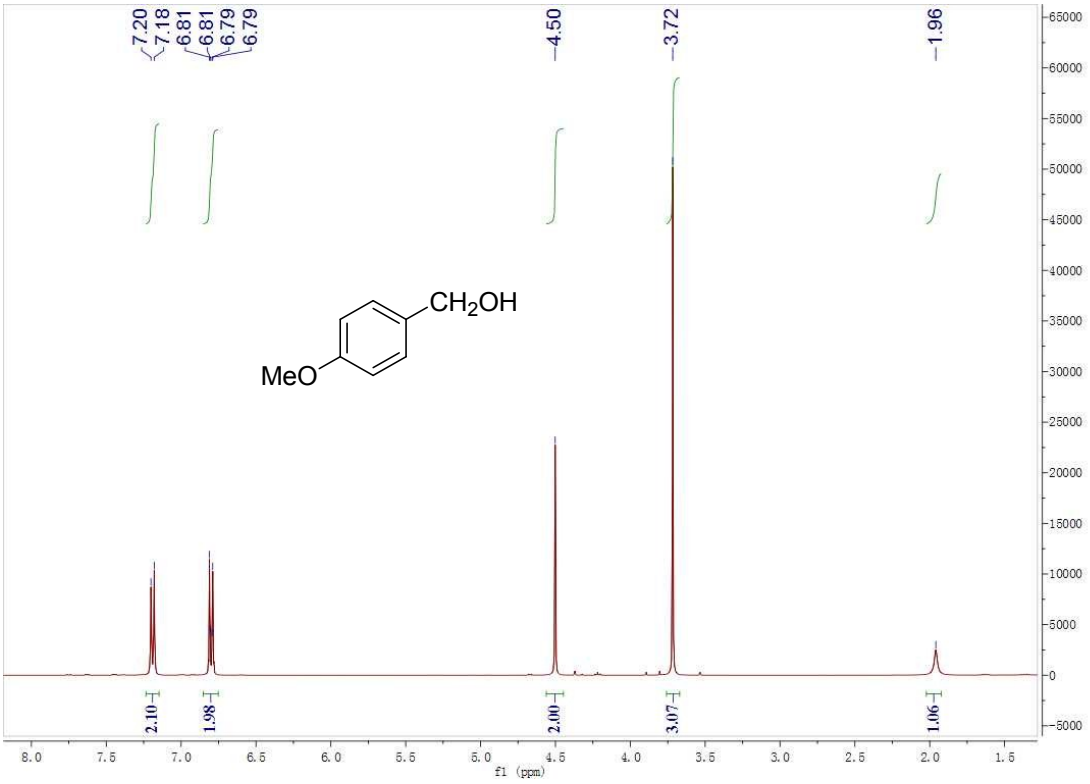
^{13}C NMR of compound **6f**



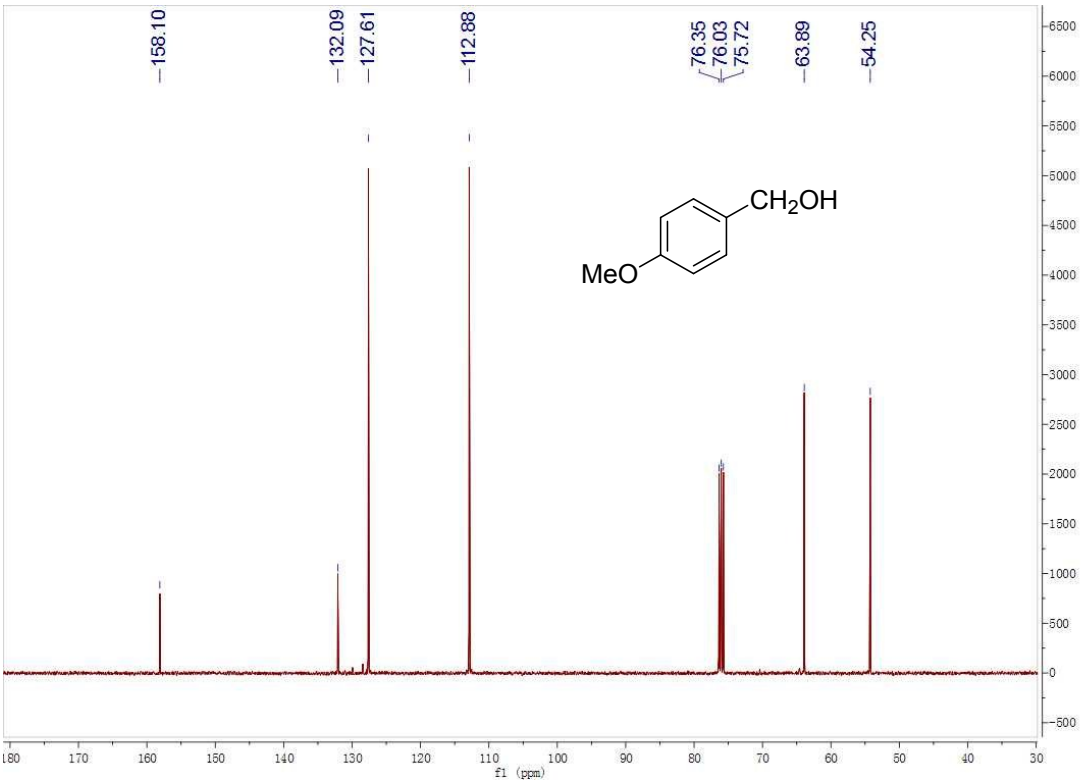
^{1}H NMR of compound **6g**



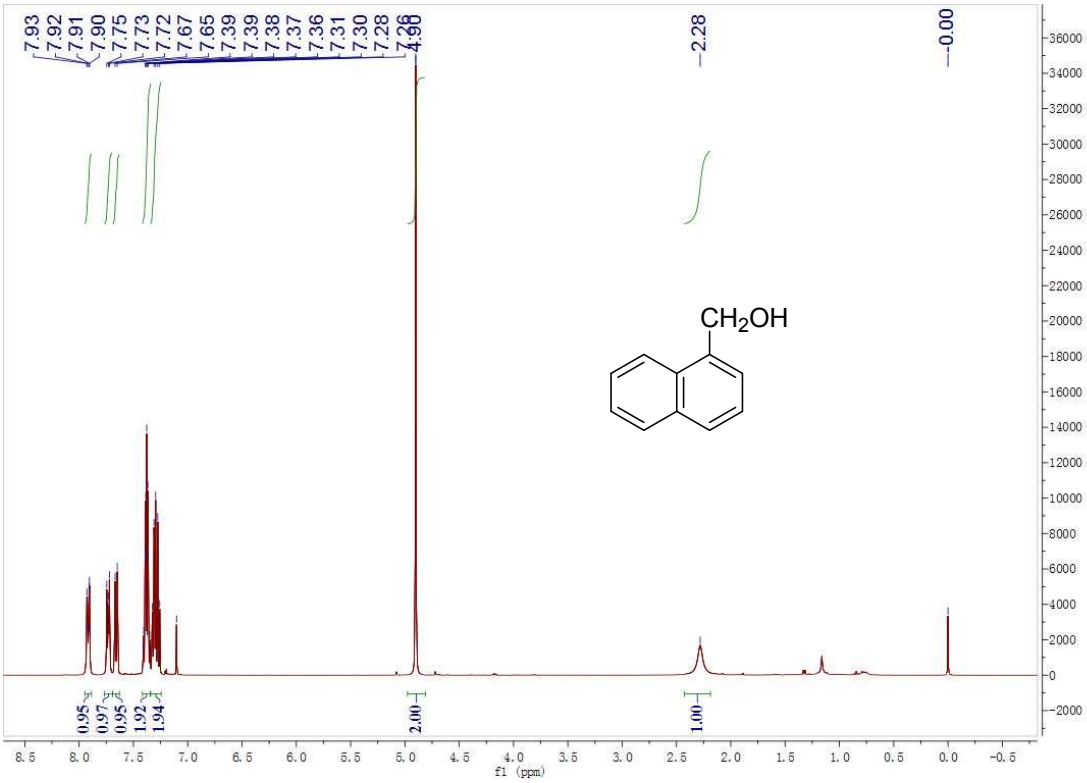
^{13}C NMR of compound **6g**



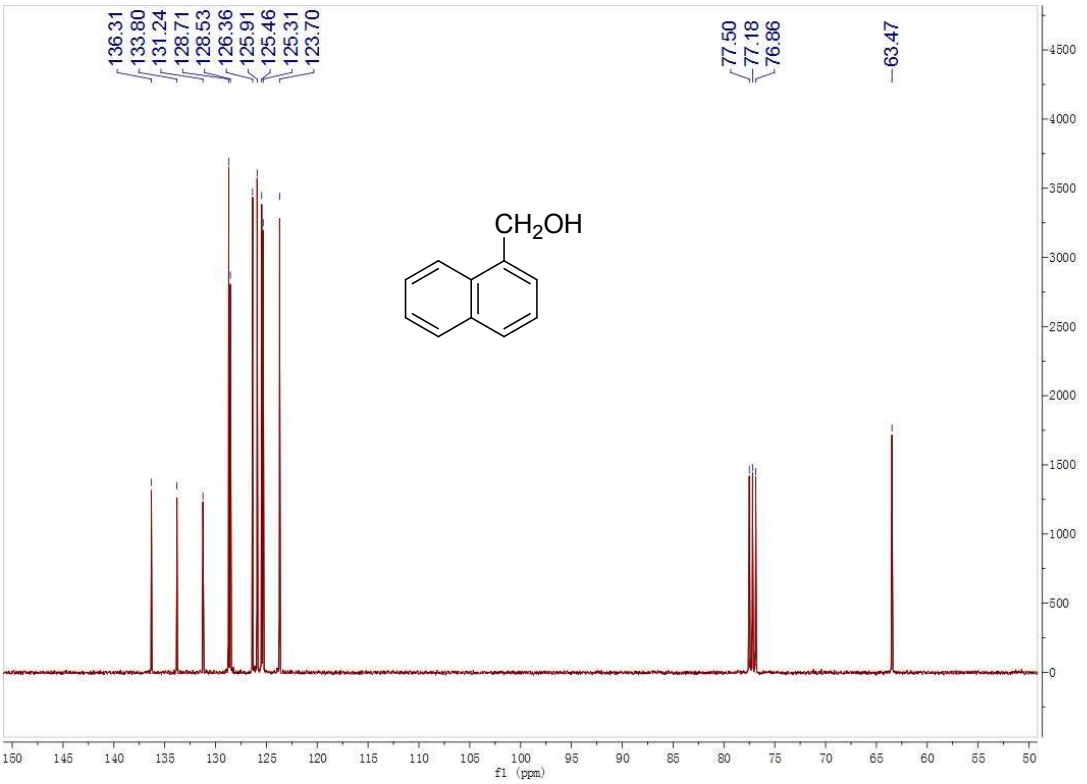
^{1}H NMR of compound **6h**



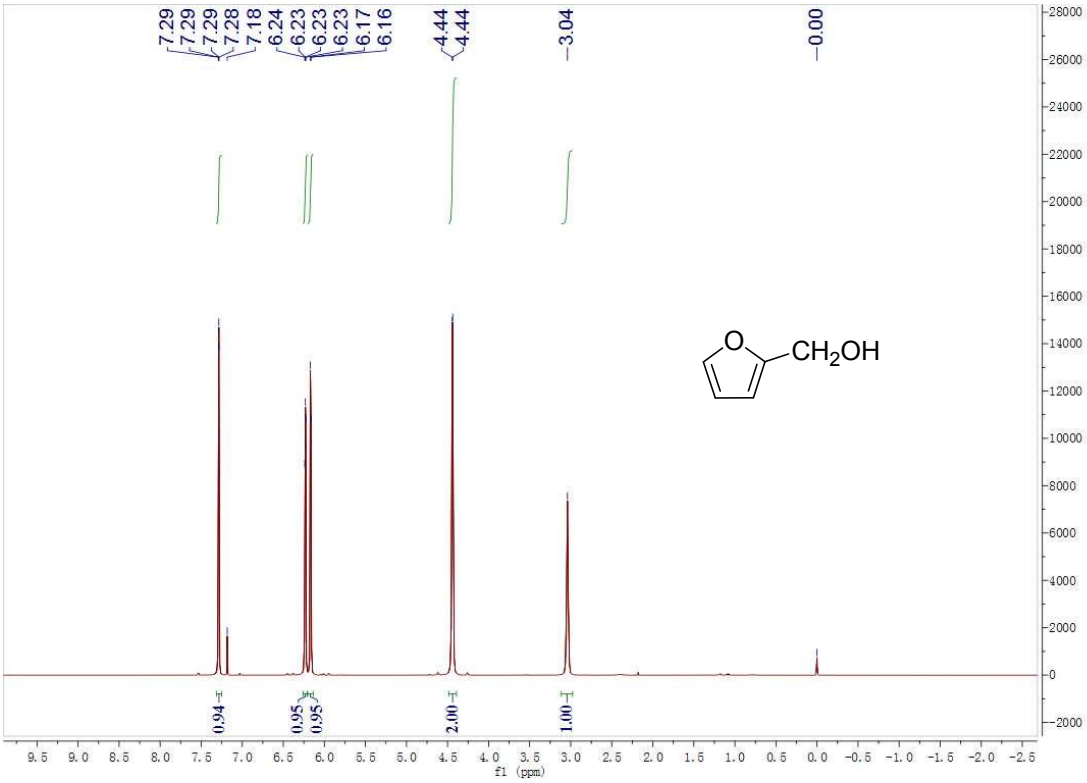
^{13}C NMR of compound **6h**



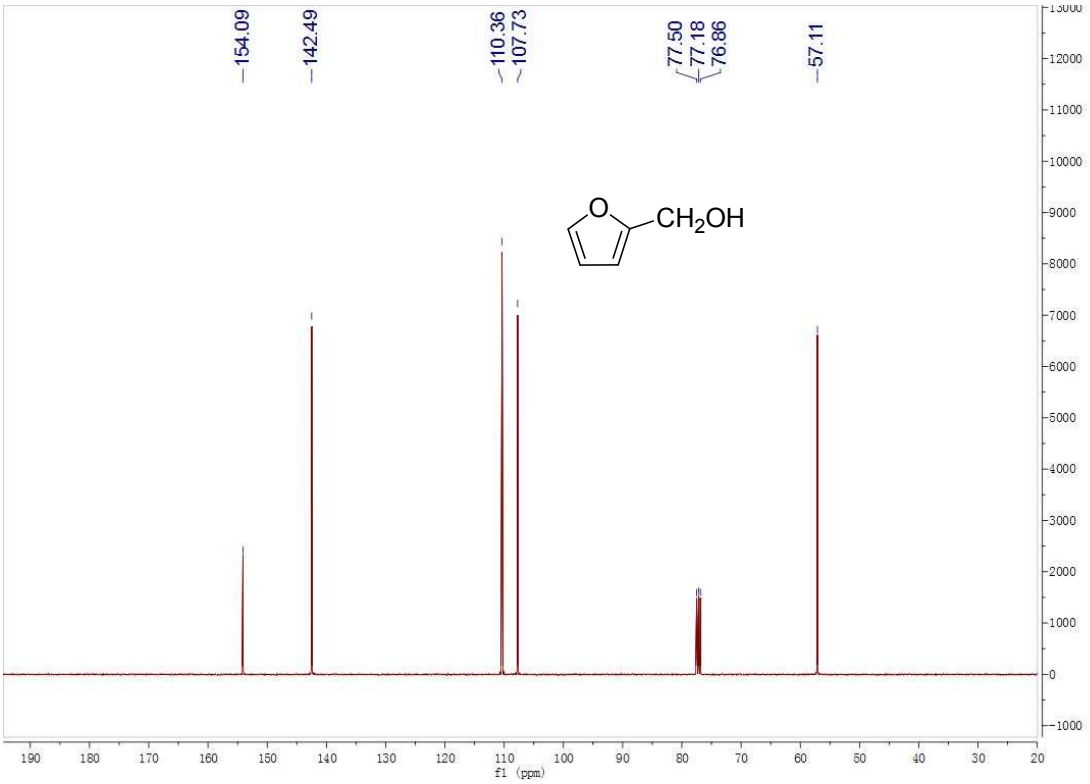
^{1}H NMR of compound **6i**



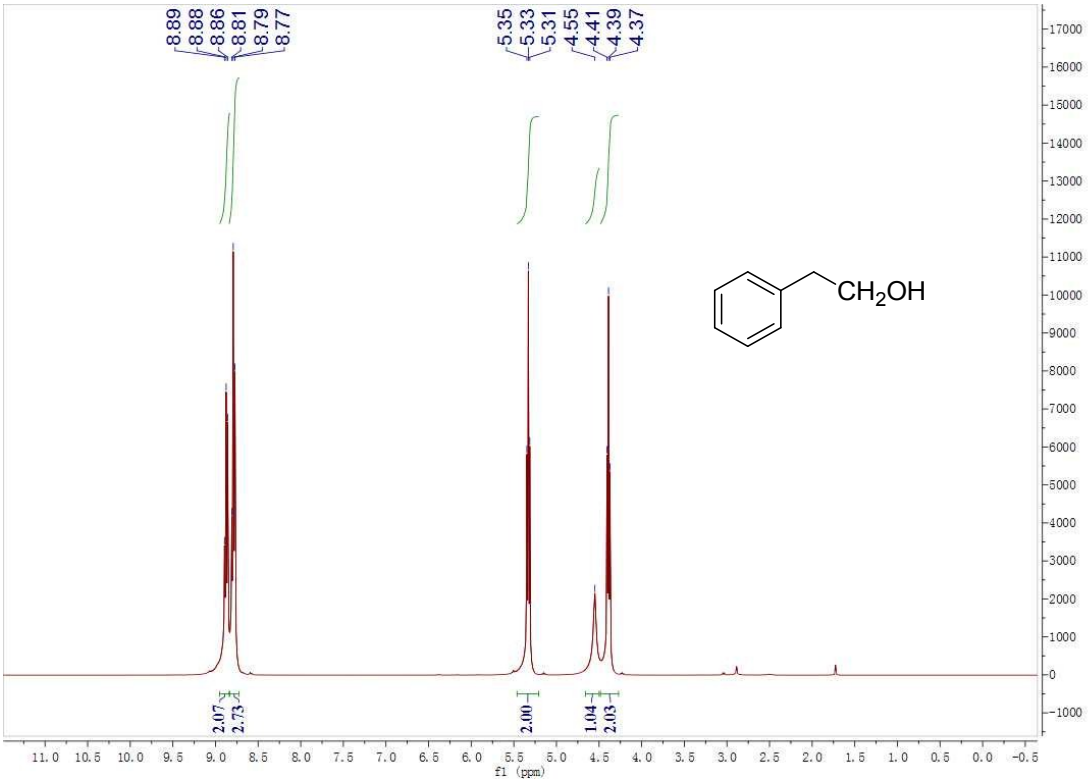
^{13}C NMR of compound **6i**



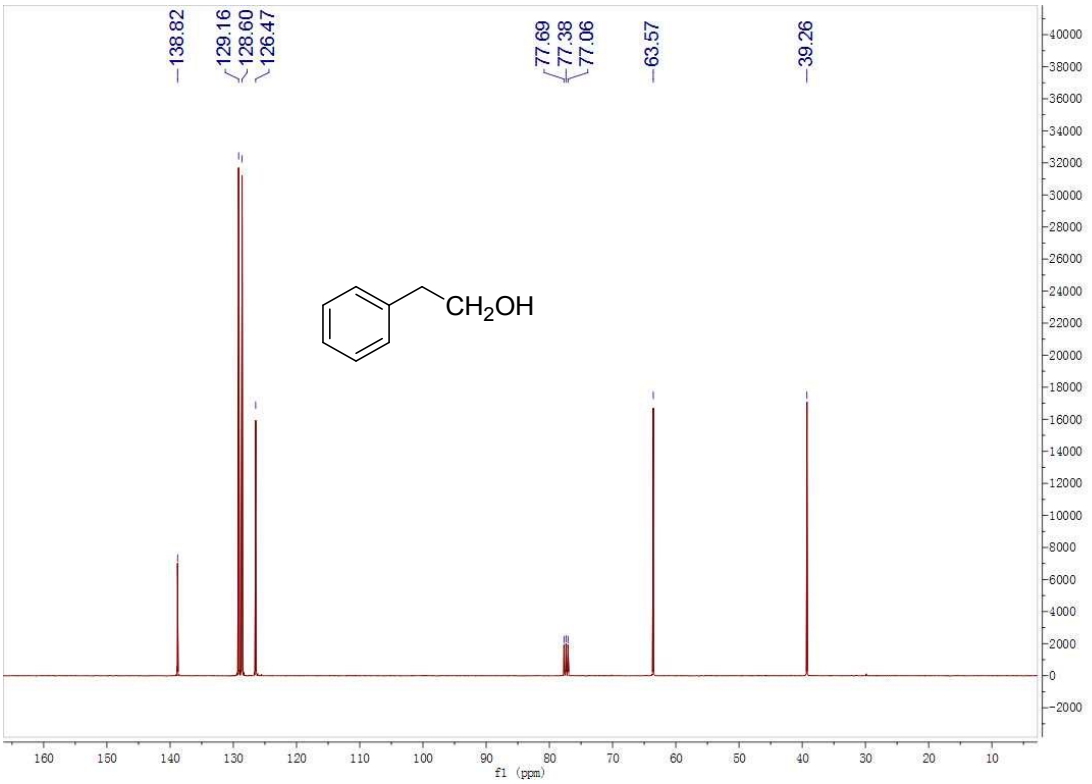
^{1}H NMR of compound **6j**



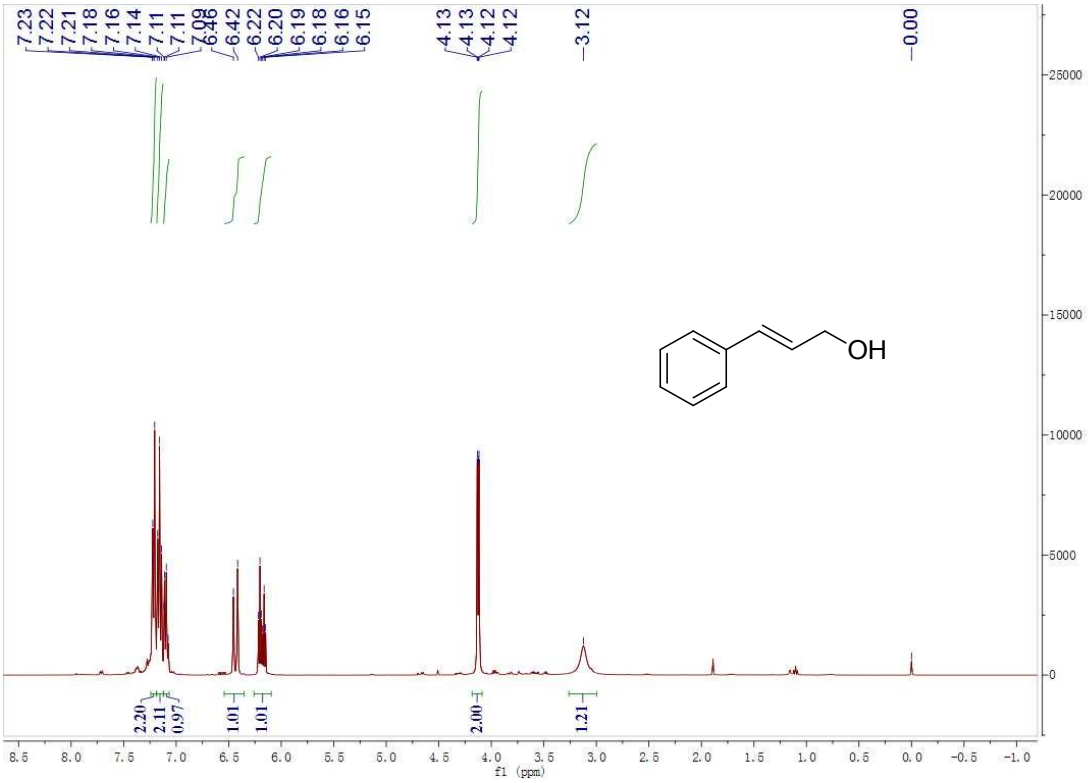
^{13}C NMR of compound **6j**



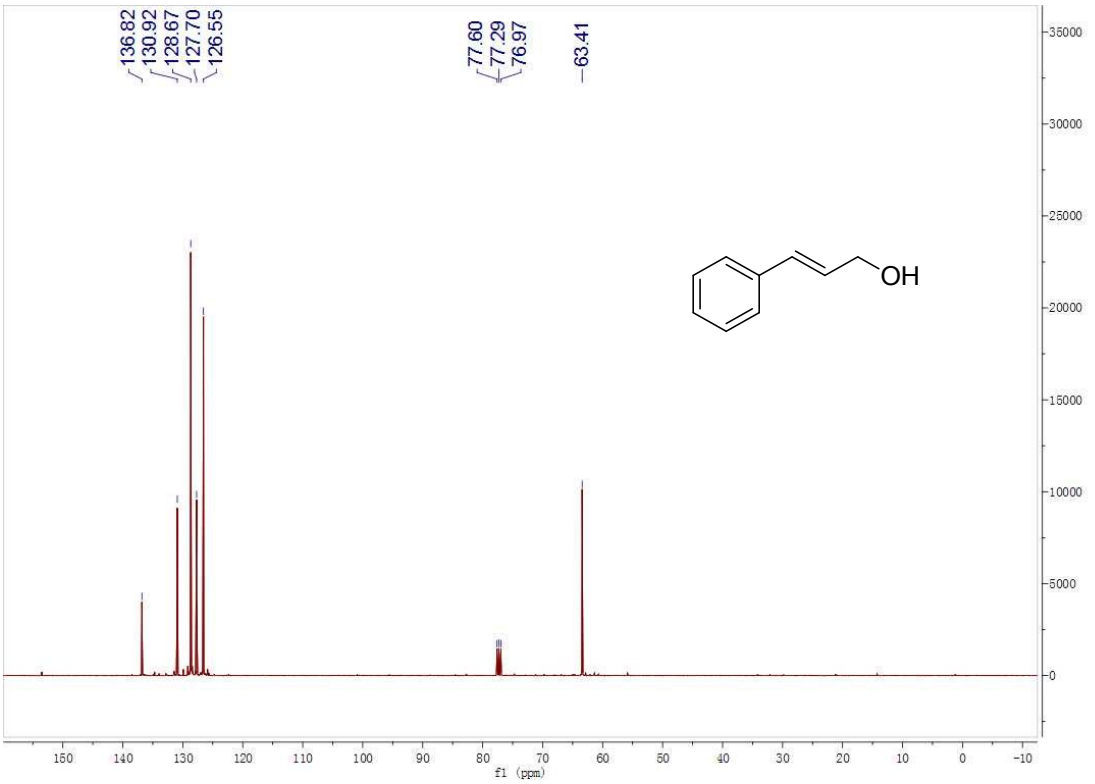
^{1}H NMR of compound **6k**



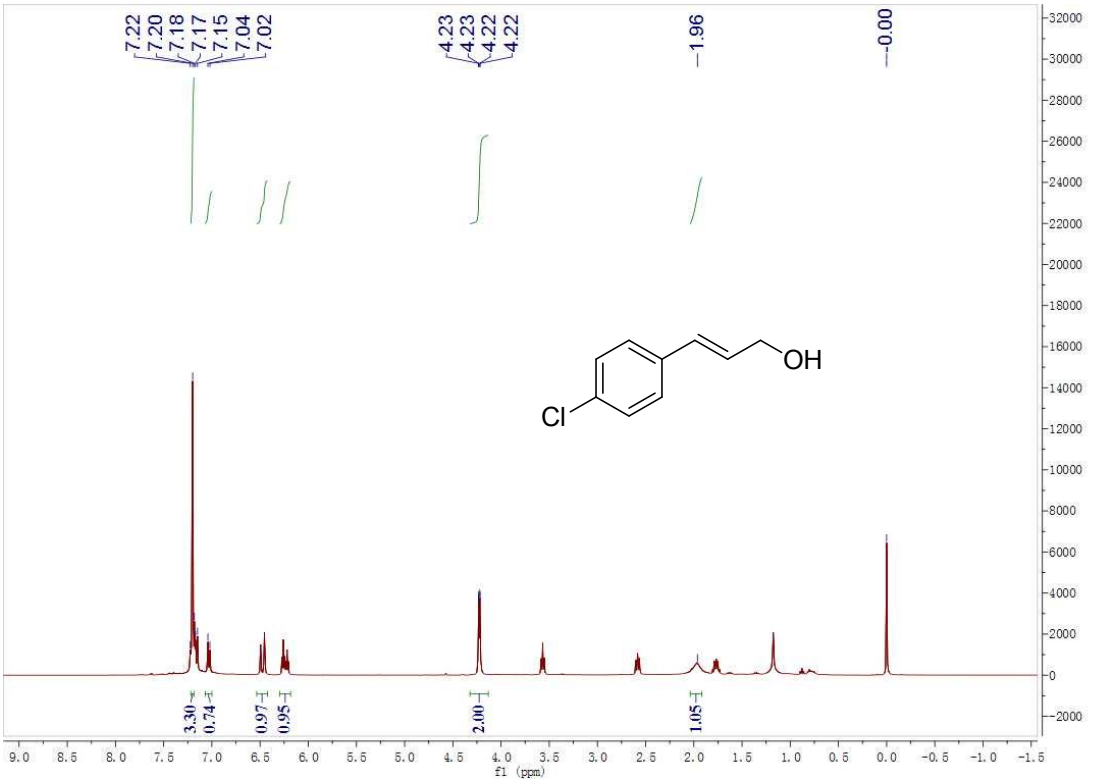
^{13}C NMR of compound **6k**



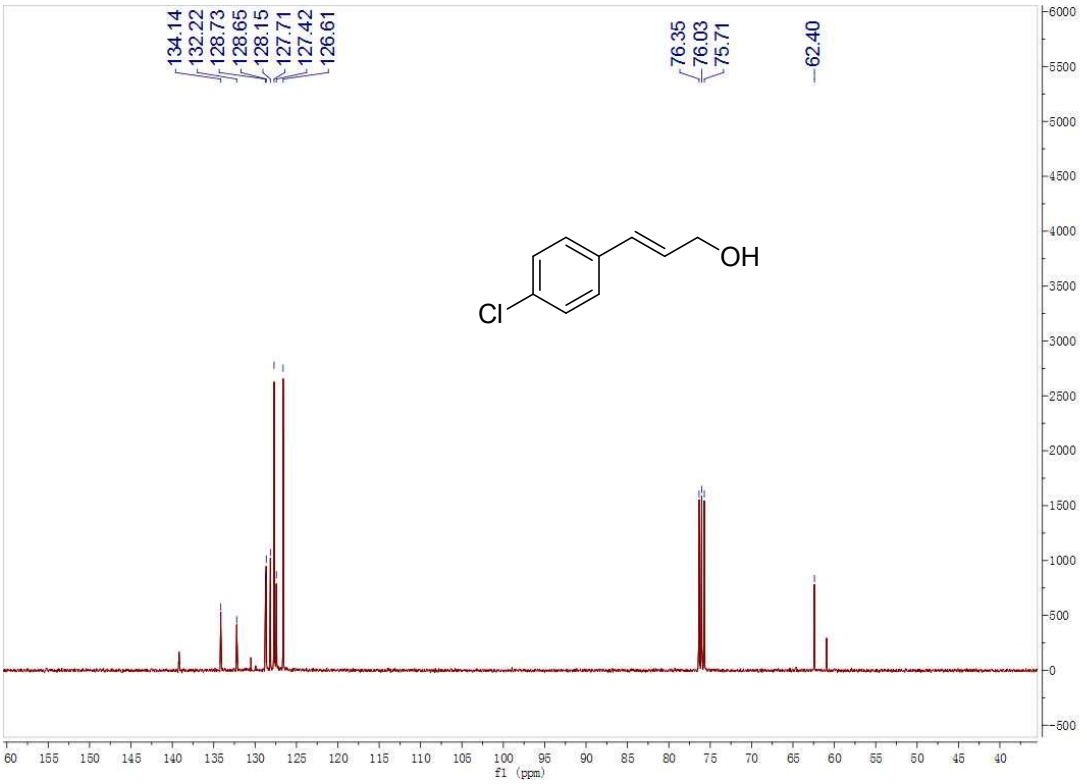
^{1}H NMR of compound **6l**



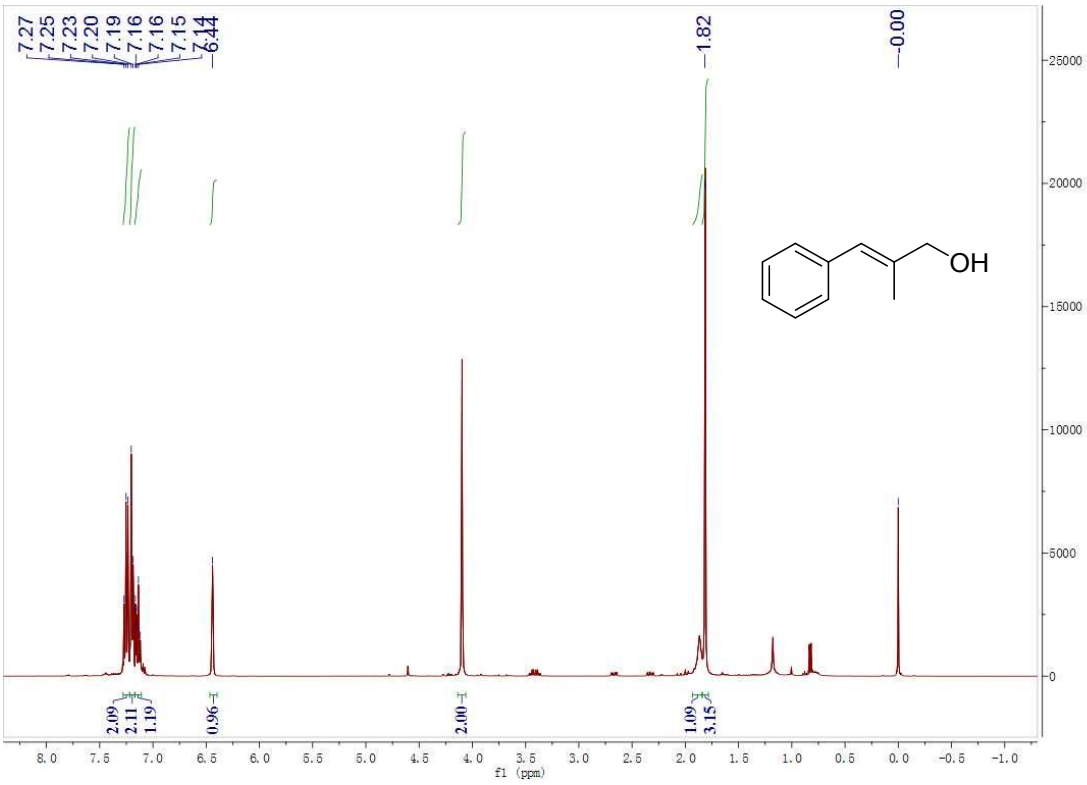
^{13}C NMR of compound **6l**



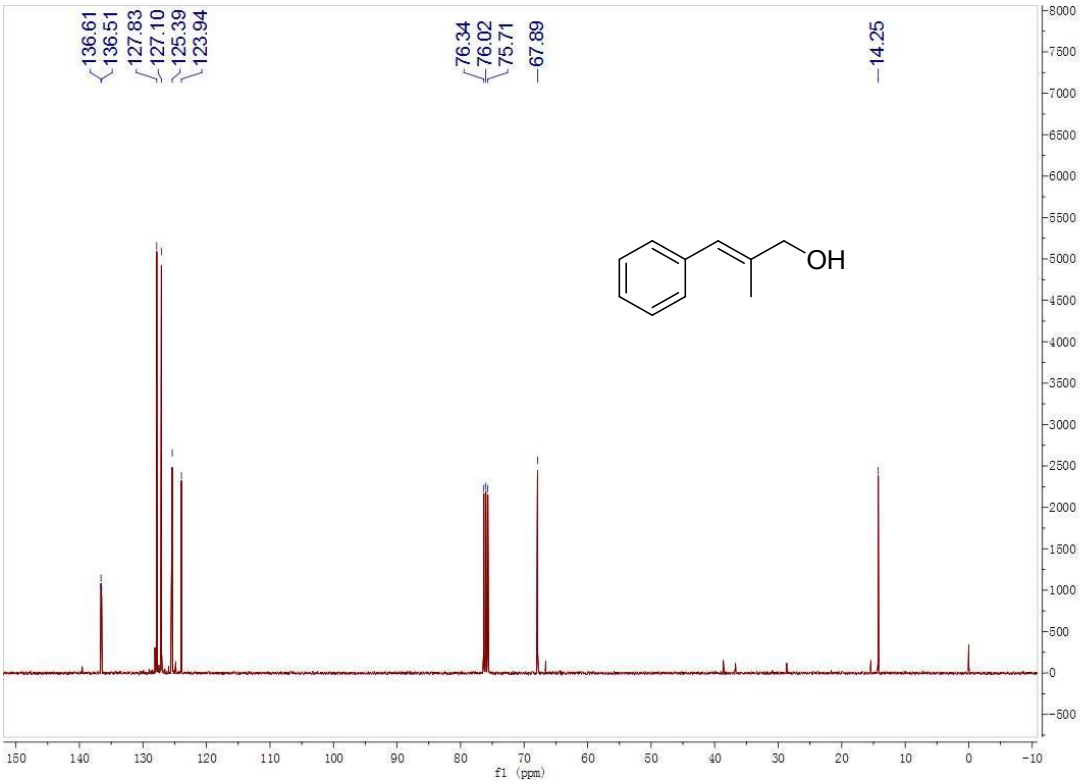
^{1}H NMR of compound **6m**



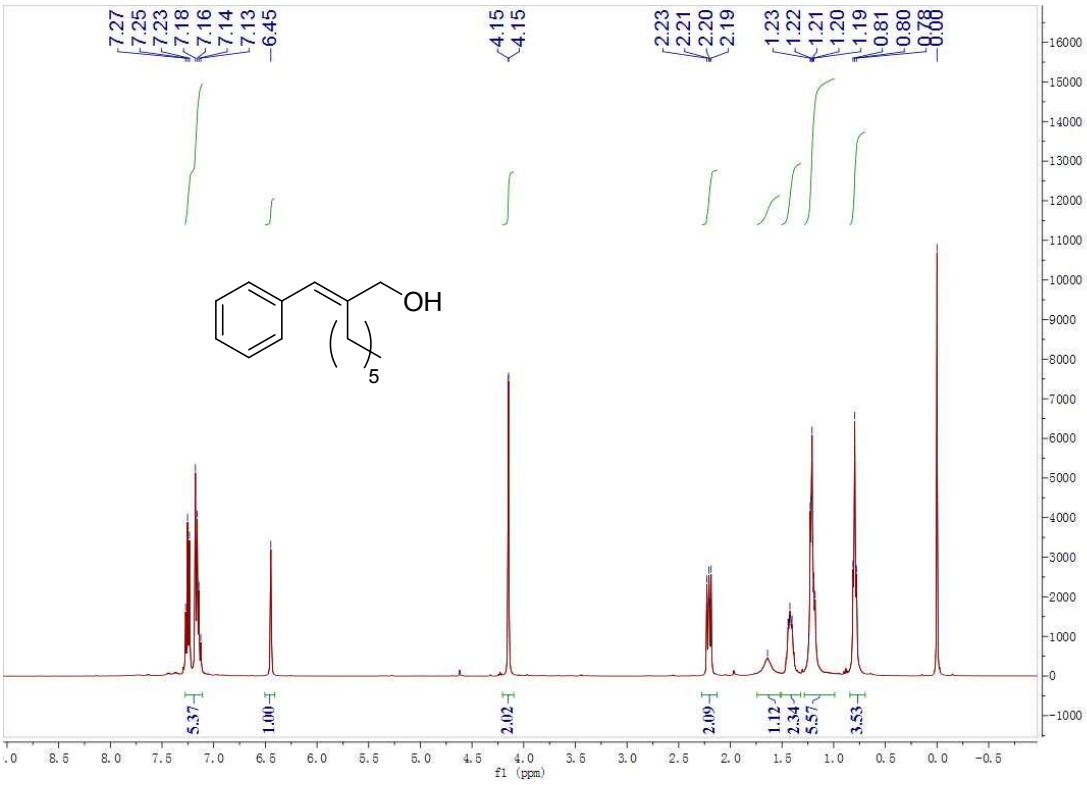
^{13}C NMR of compound **6m**



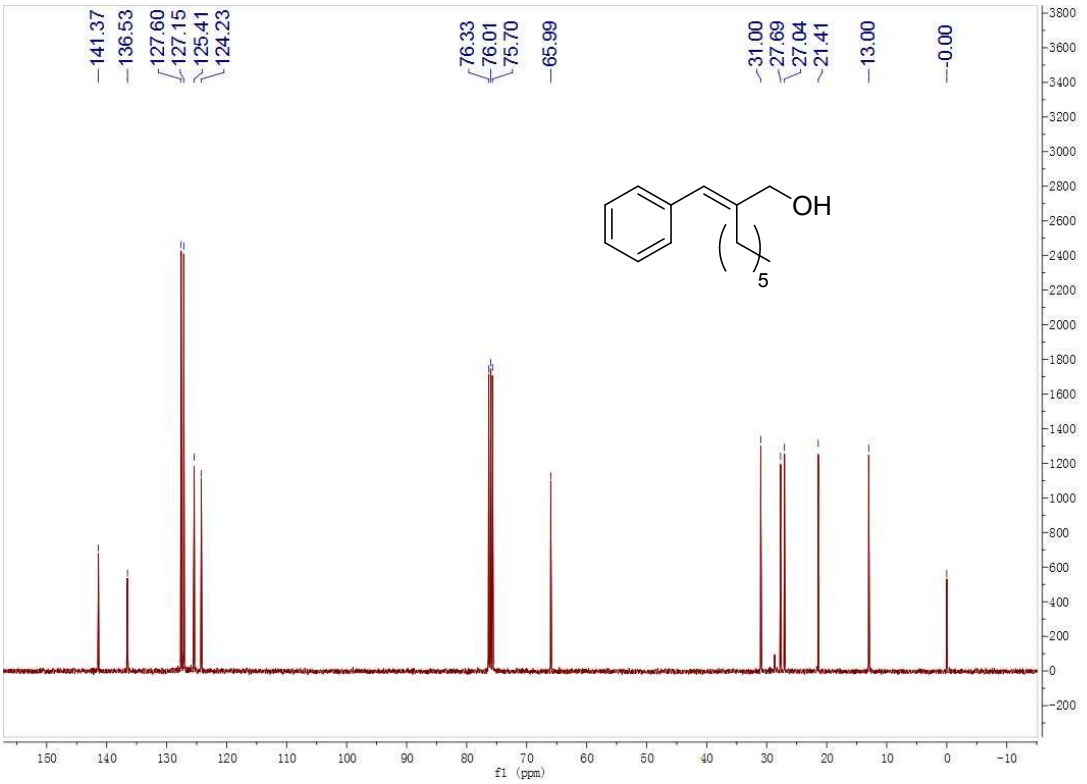
^{1}H NMR of compound **6n**



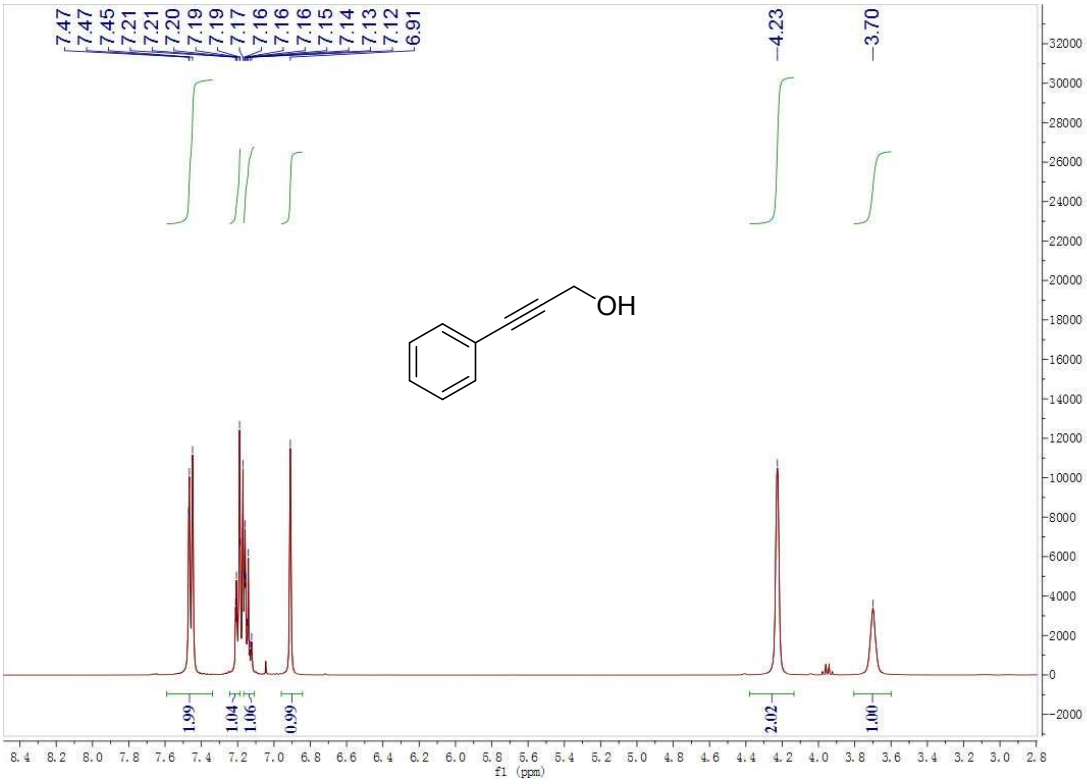
^{13}C NMR of compound **6n**



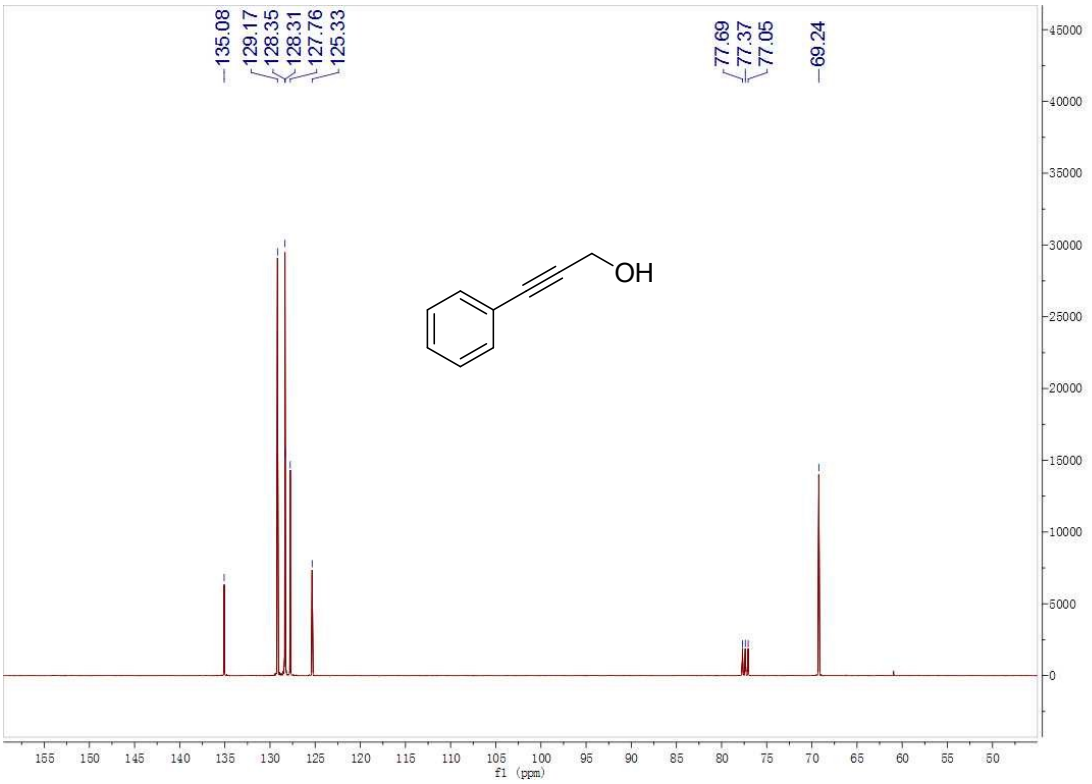
^{1}H NMR of compound **6o**



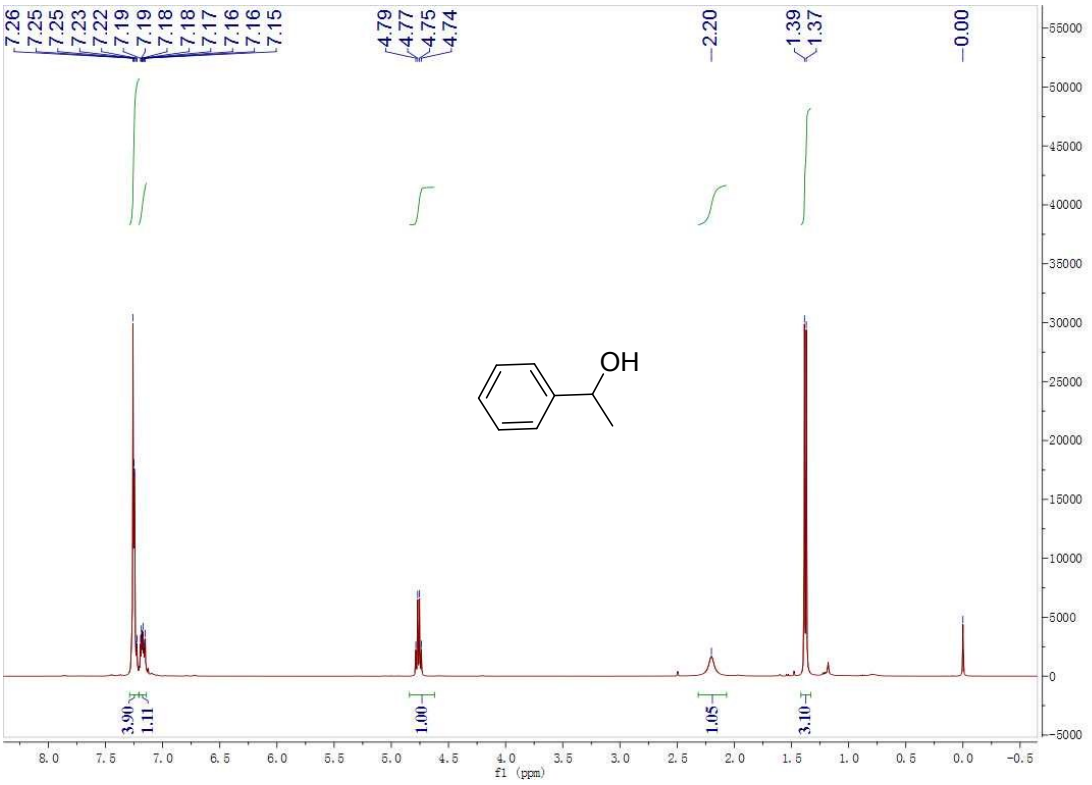
^{13}C NMR of compound **6o**



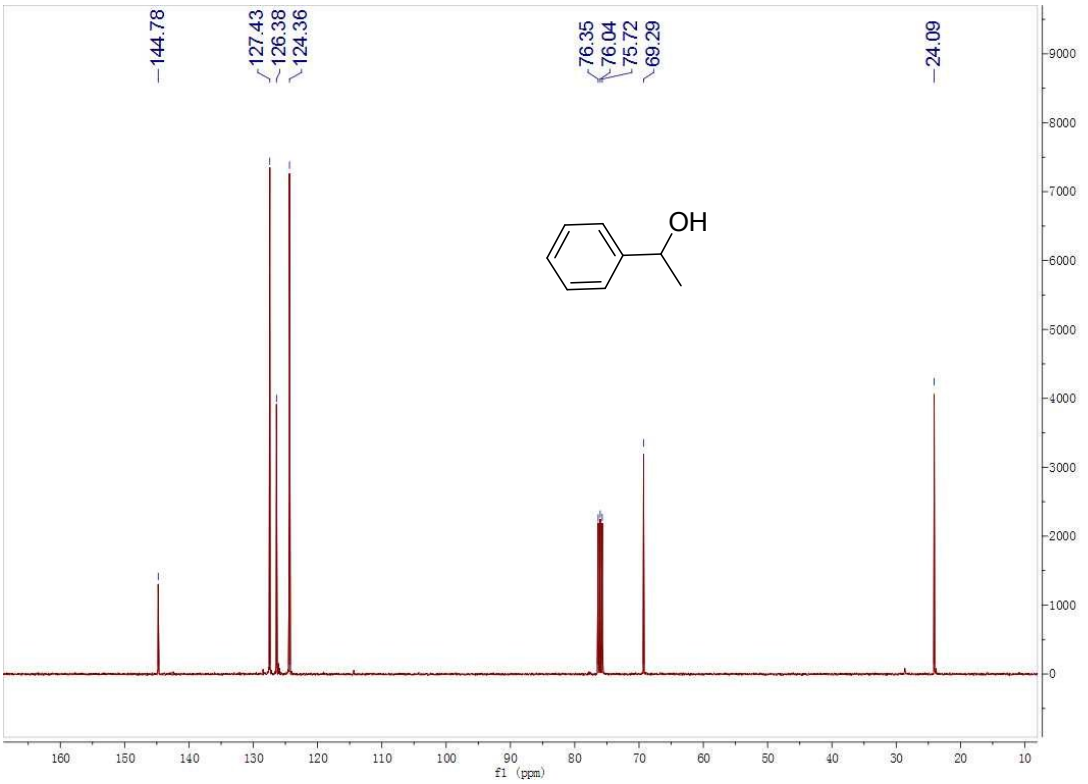
^{1}H NMR of compound **6p**



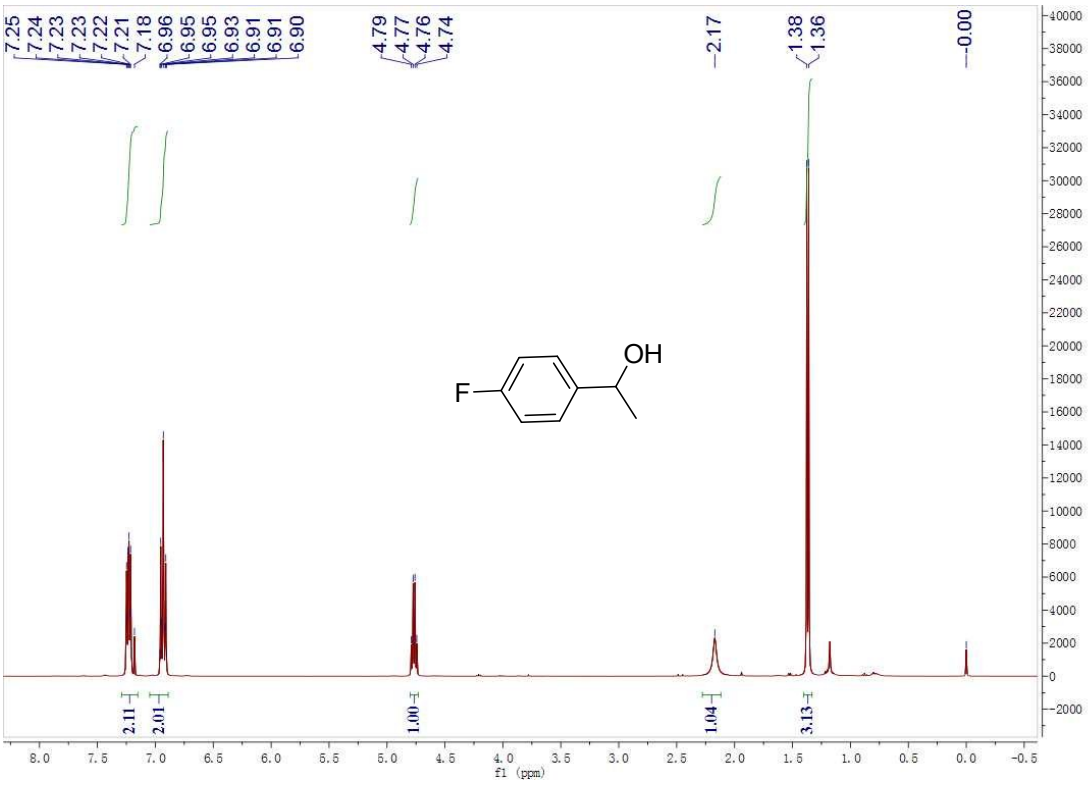
^{13}C NMR of compound **6p**



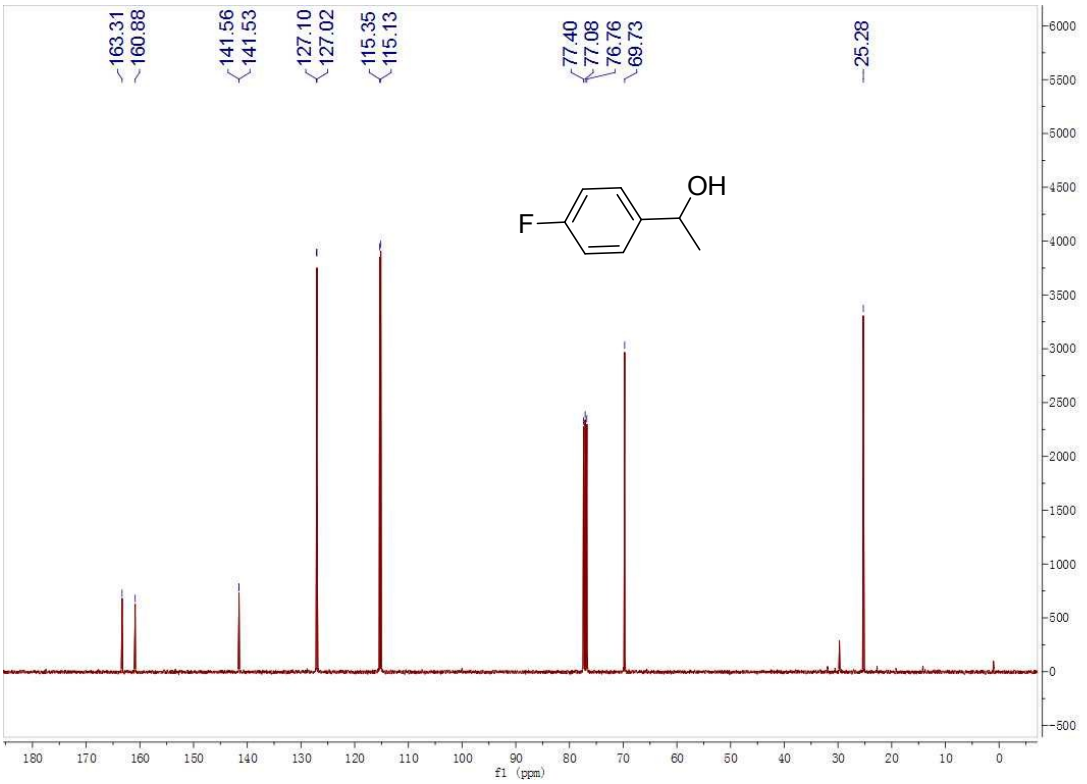
^{1}H NMR of compound **8a**



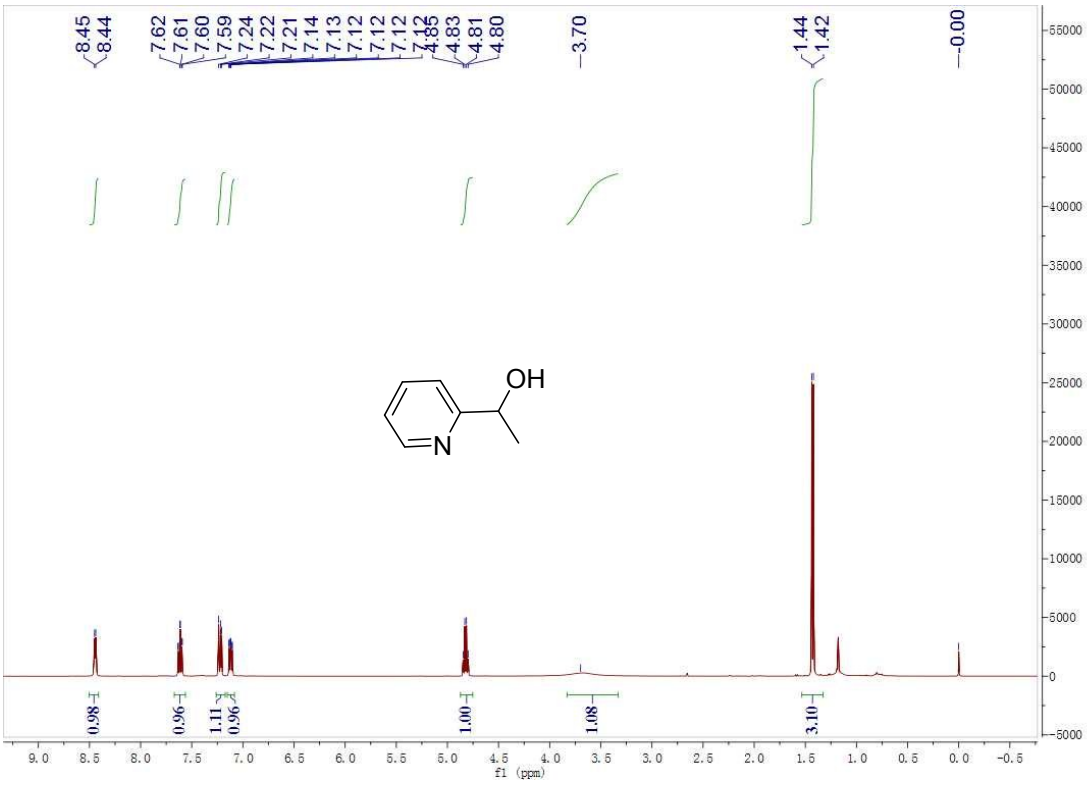
^{13}C NMR of compound **8a**



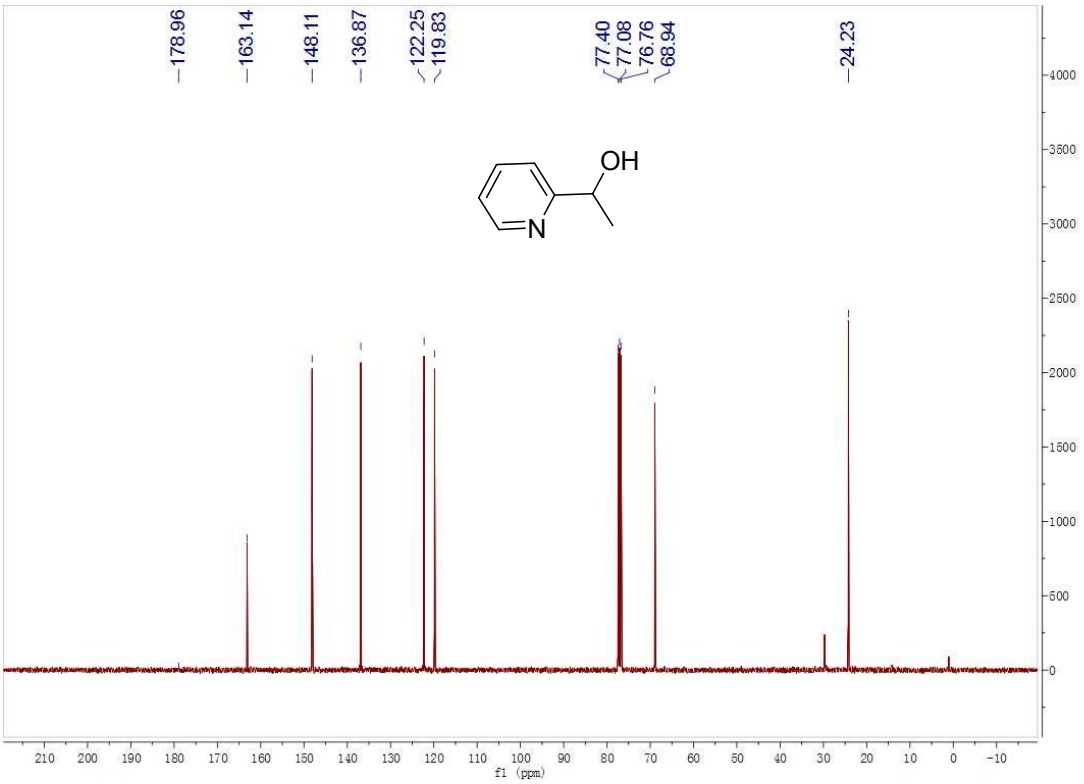
^{1}H NMR of compound **8b**



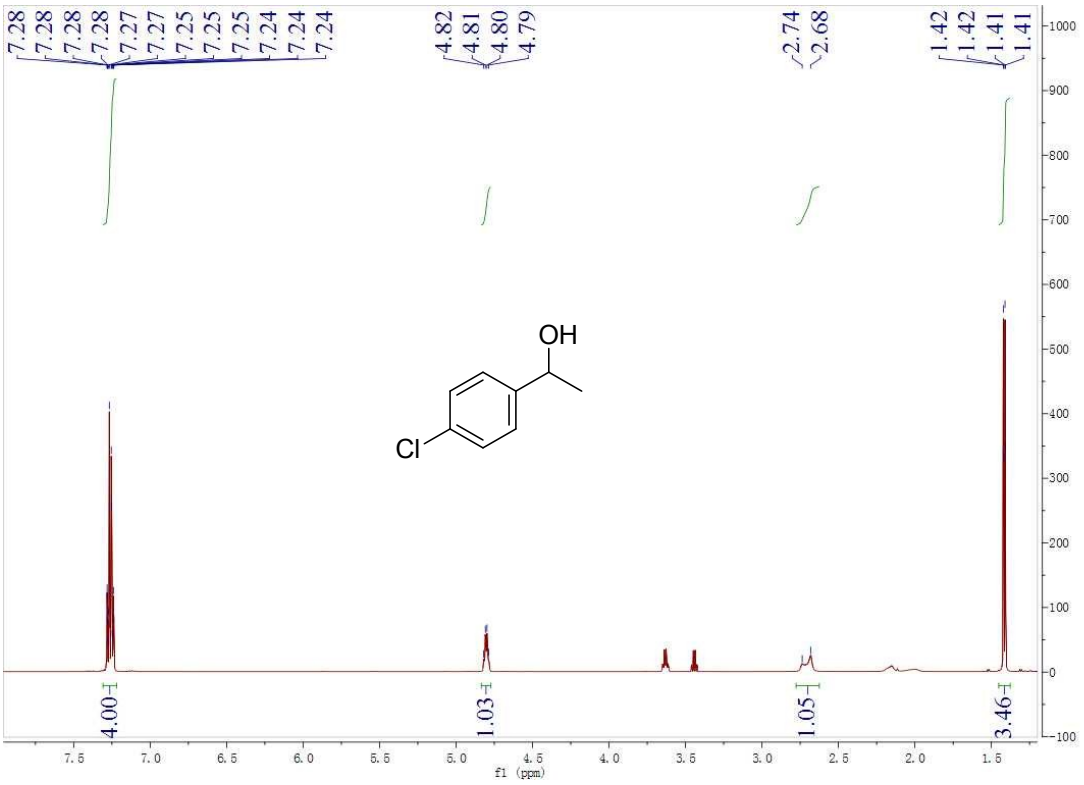
^{13}C NMR of compound **8b**



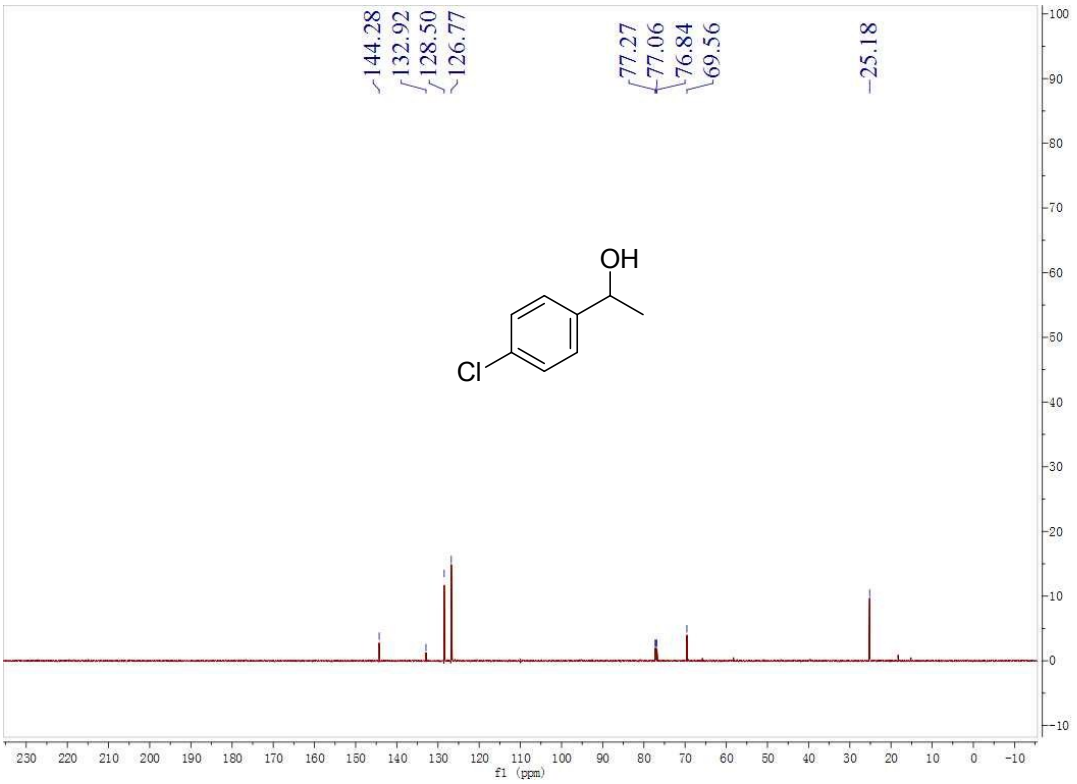
^{1}H NMR of compound **8c**



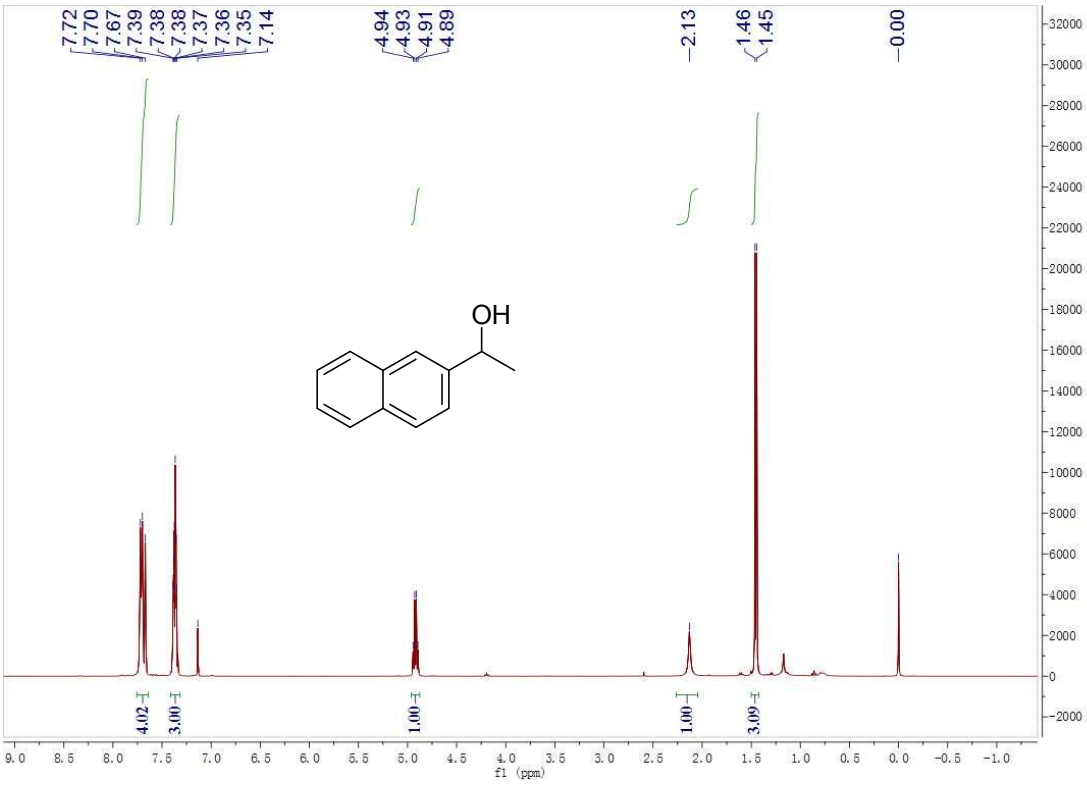
^{13}C NMR of compound **8c**



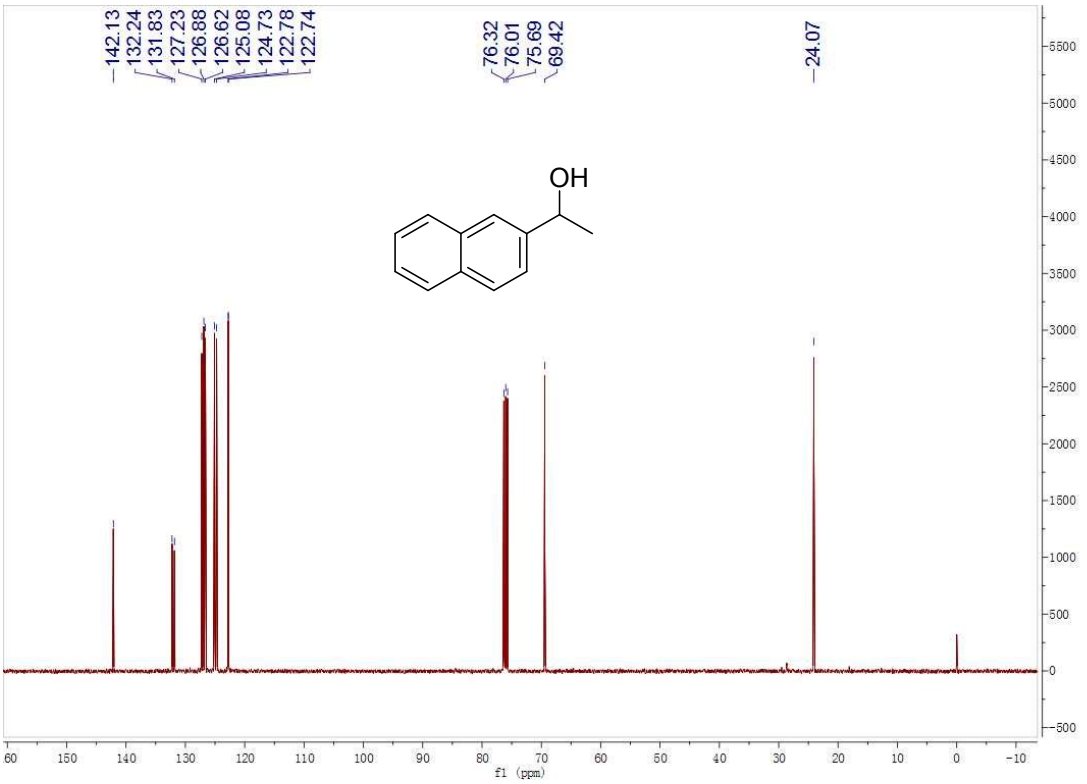
^{1}H NMR of compound **8d**



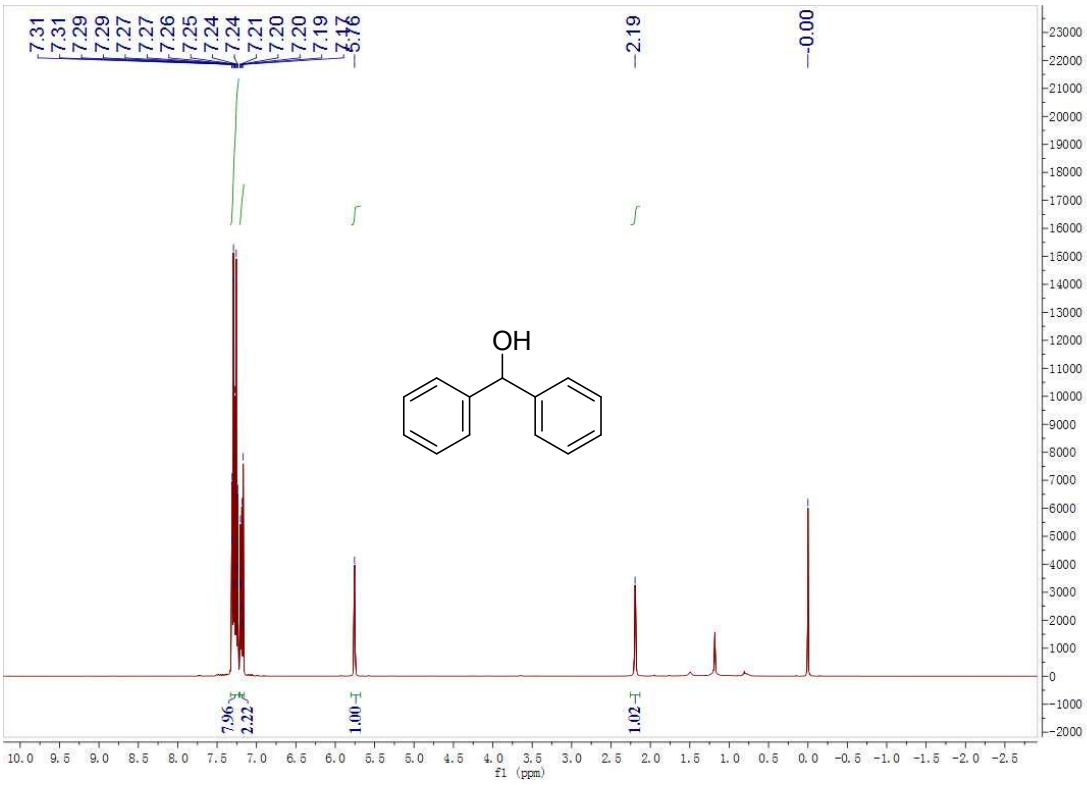
^{13}C NMR of compound **8d**



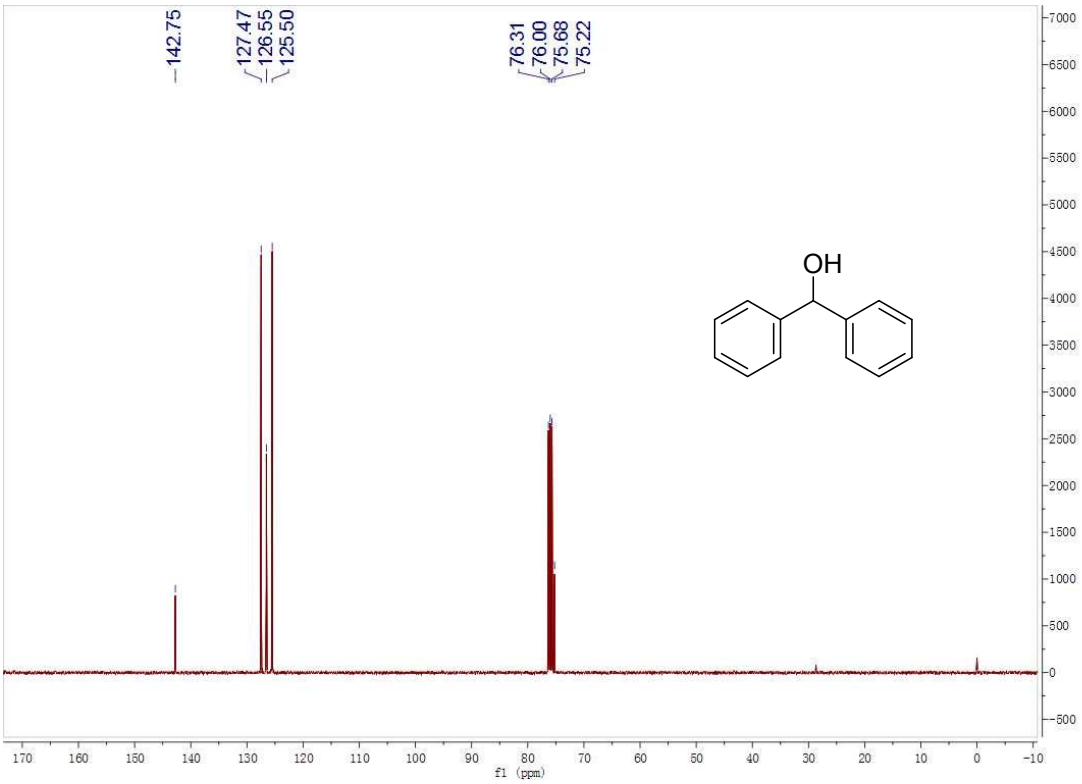
^{1}H NMR of compound **8e**



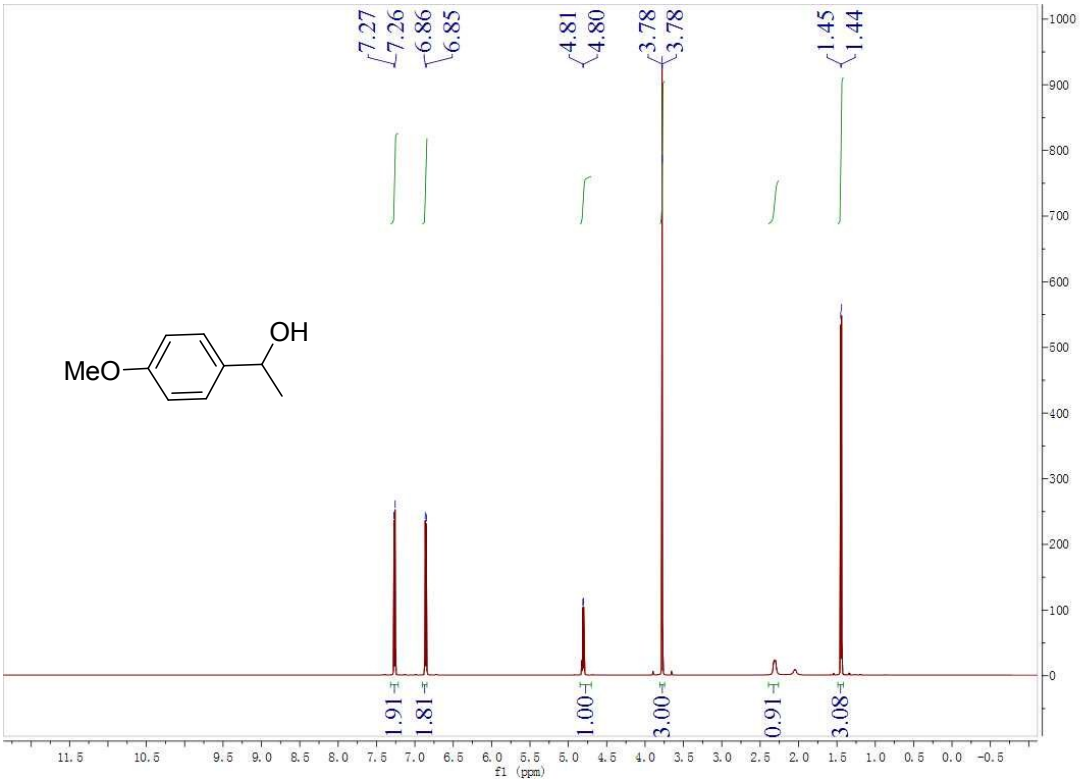
^{13}C NMR of compound **8e**



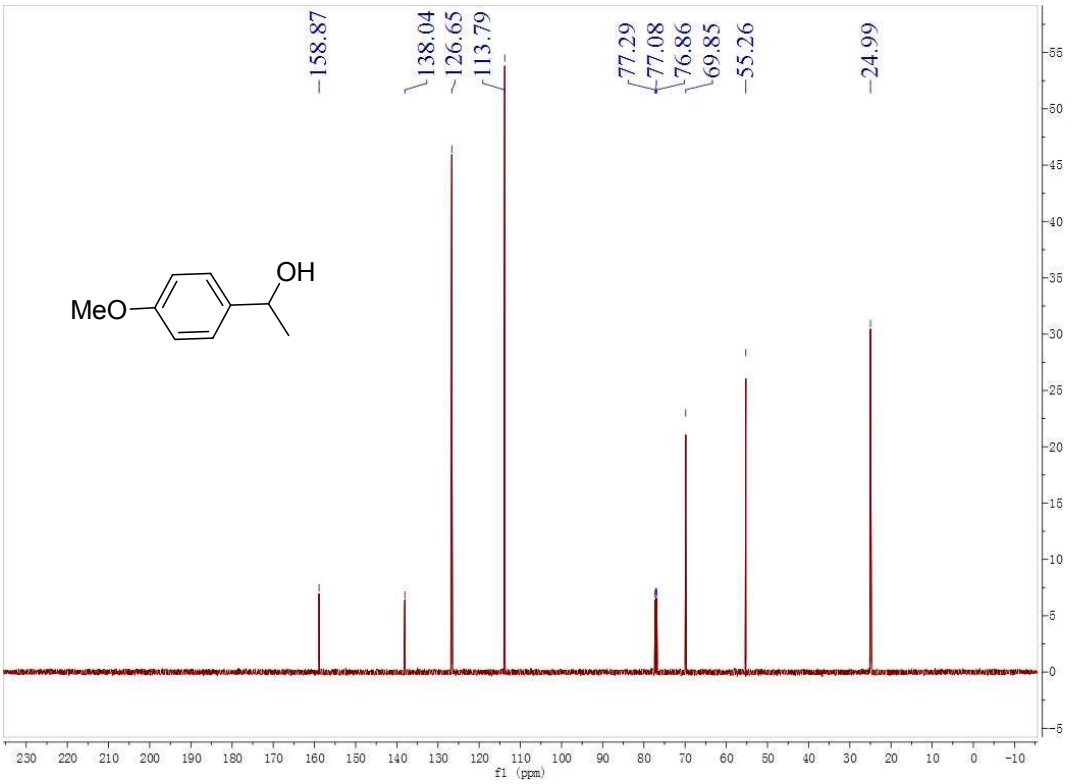
^{1}H NMR of compound **8f**



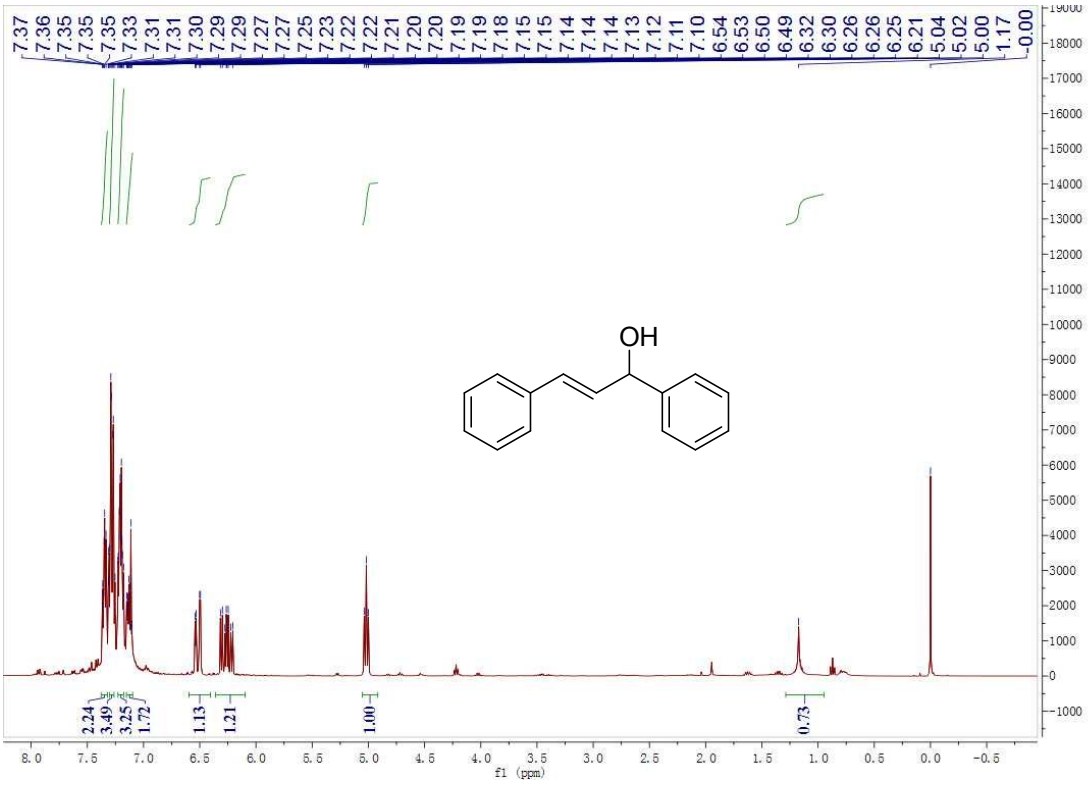
^{13}C NMR of compound **8f**



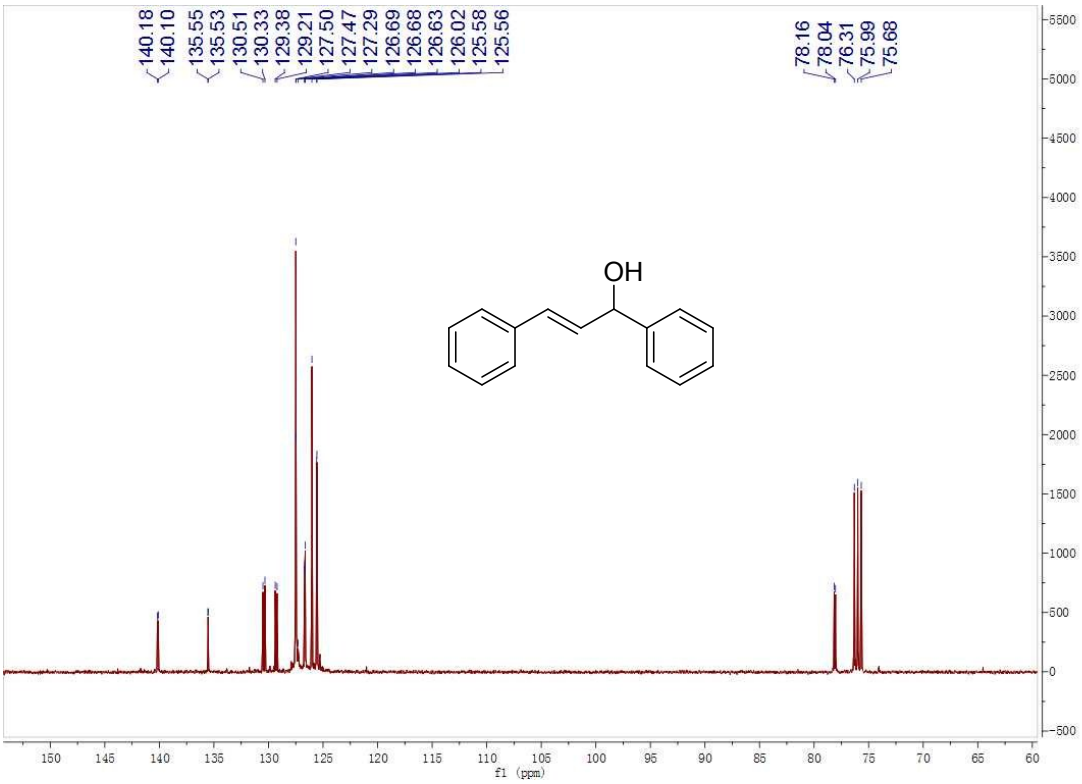
^{1}H NMR of compound **8g**



^{13}C NMR of compound **8g**



^{1}H NMR of compound **8h**



^{13}C NMR of compound **8h**