

Transfer Hydrogenation of Aldehydes Catalyzed by Silyl Hydrido Iron Complexes Bearing a [PSiP] Pincer Ligand

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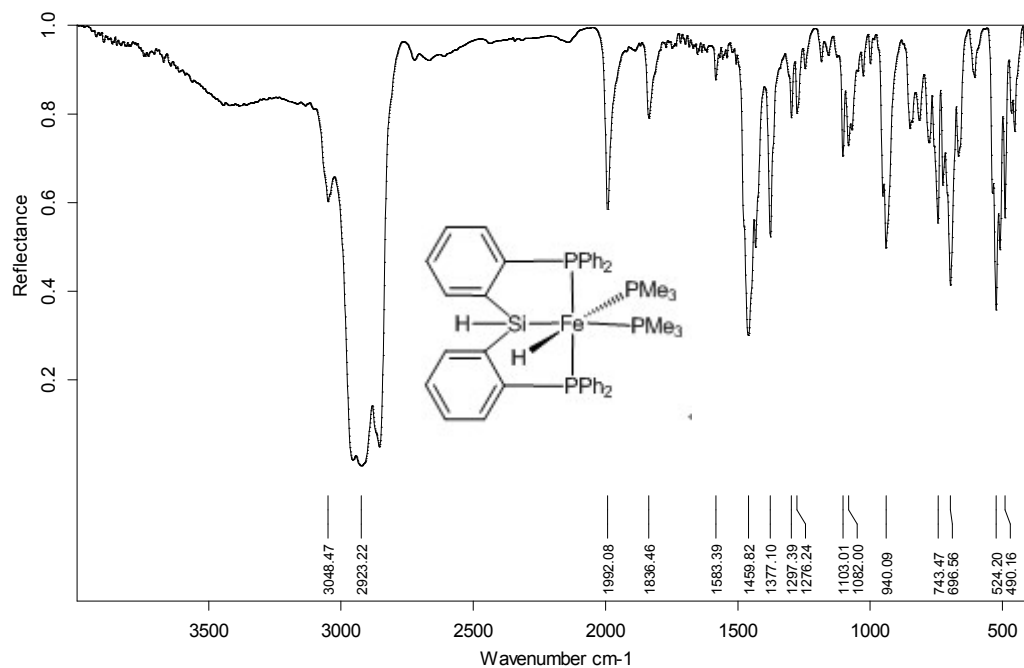
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1 Table S1 Crystallographic Data for complexes 3 and 7

Complex	3	7
Formula	C ₄₂ H ₄₈ FeP ₄ Si	C ₂₈ H ₄₉ FeOP ₃ Si
Mz	760.62	578.52
crystal system	monoclinic	monoclinic
space group	P2 ₁ /c	P2 ₁ /n
a [Å]	11.7181(7)	13.5670(5)
b [Å]	18.9232(6)	16.7800(5)
c [Å]	35.1134(2)	13.9927(5)
α[°]	90	90
β[°]	91.084(4)	106.554(3)
γ[°]	90	90
V [Å ³]	7784.8(6)	3053.46(2)
T [K]	200.15	153.15
Z	8	4
μ[mm ⁻¹]	5.169	0.709
total reflns	26696	15439
unique reflns	11341	5786
R _{int}	0.0446	0.0385
R1[I>2σ(I)]	0.0515	0.0352
wR(F ²)[I>2σ(I)]	0.1312	0.0877
R1(all data)	0.0710	0.0498
wR(F ²) (all data)	0.1419	0.0924
GOF on F ²	1.029	0.973

2 IR, ^1H NMR, ^{31}P NMR, ^{13}C NMR and ^{29}Si NMR spectrum of complexes **3**, **6** and **7**

IR spectrum of complex **3**



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Fig. S1 IR spectrum of complex **3**.

^1H NMR of complex **3**

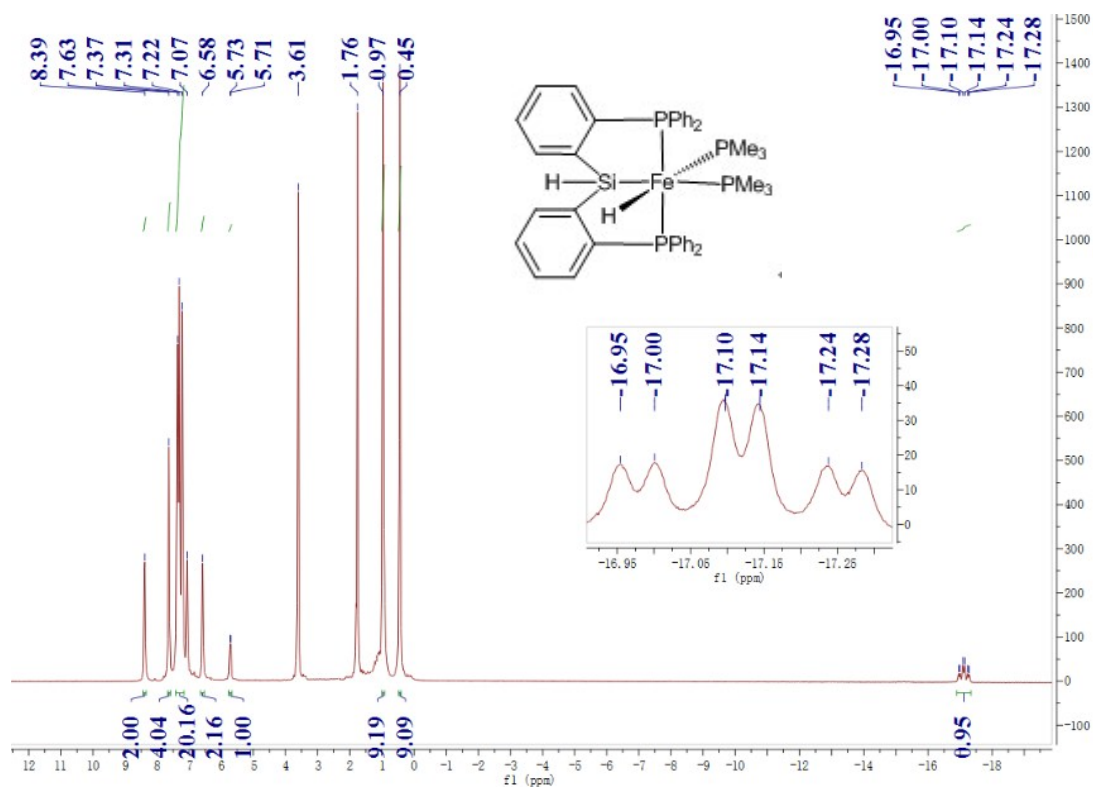


Fig. S2 ^1H NMR of complex **3** at -40°C

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

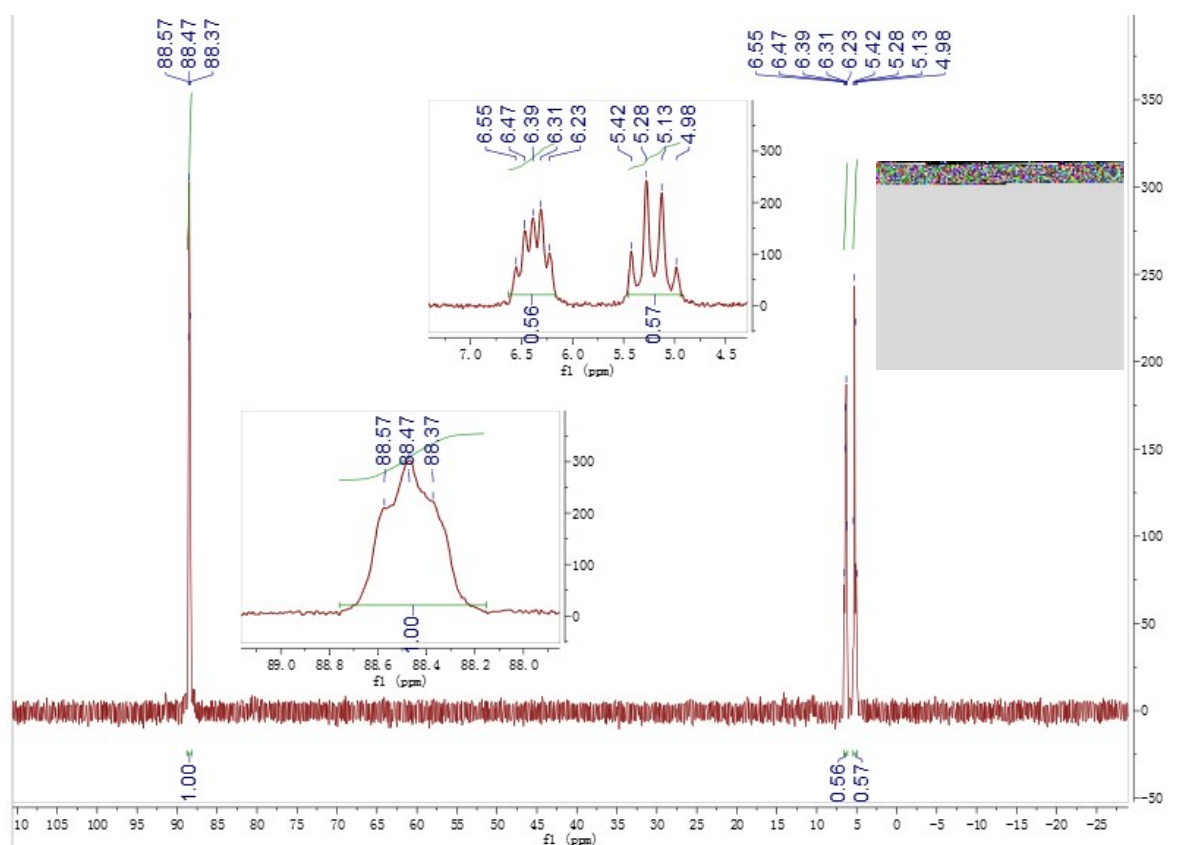


Fig. S3 ^{31}P NMR of complex **3** at -40°C

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

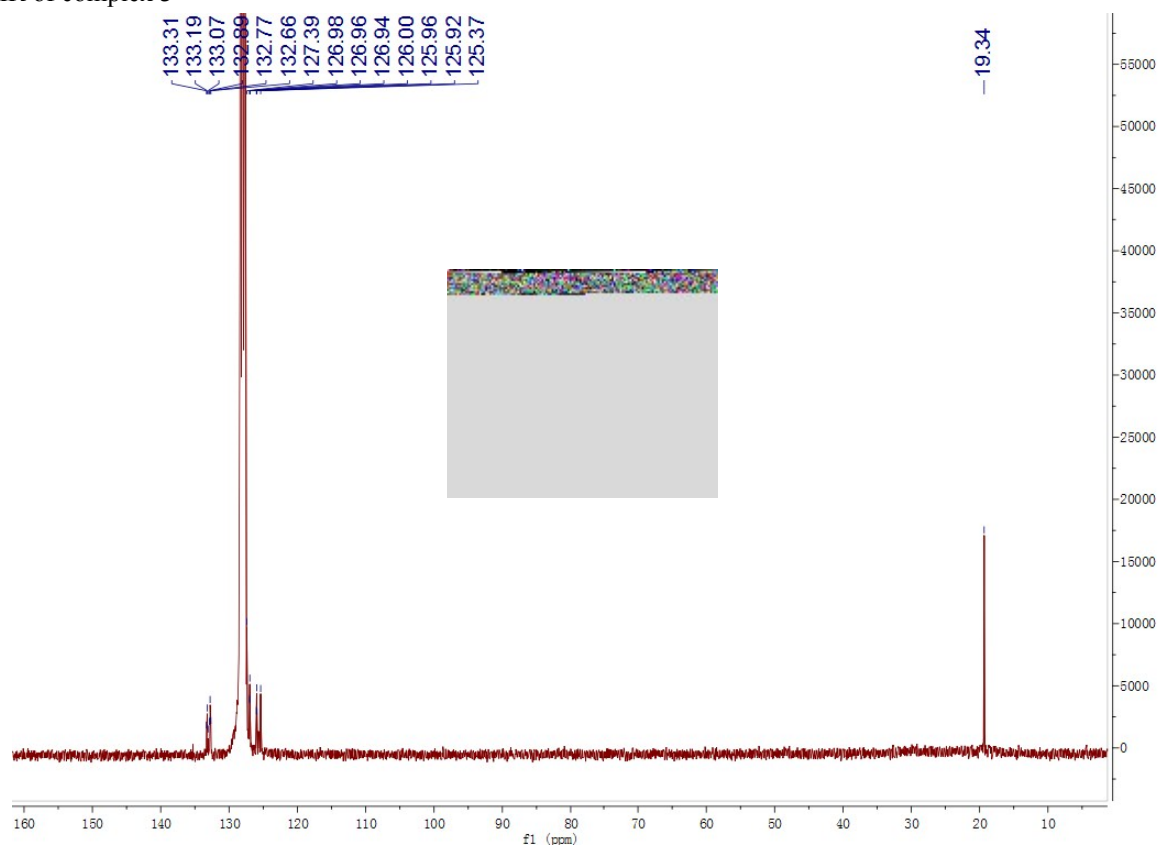


Fig. S4 ^{13}C NMR of complex **3**.

^{29}Si NMR of complex **3**

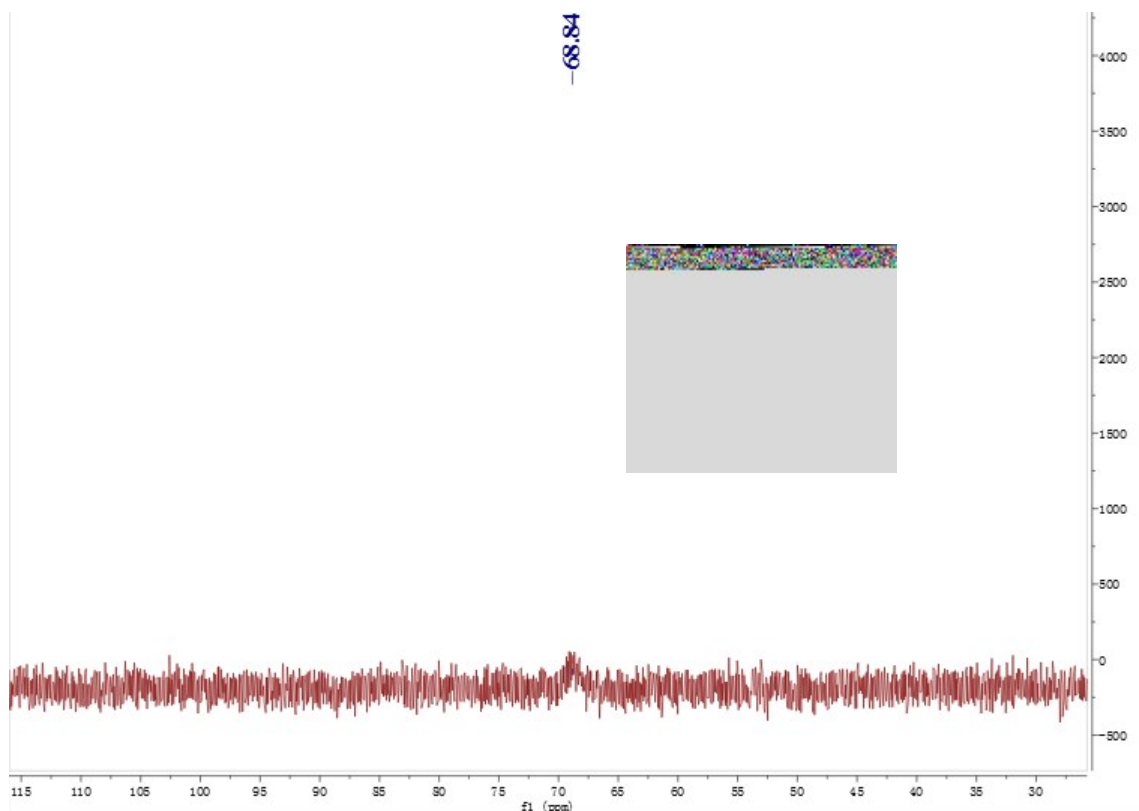
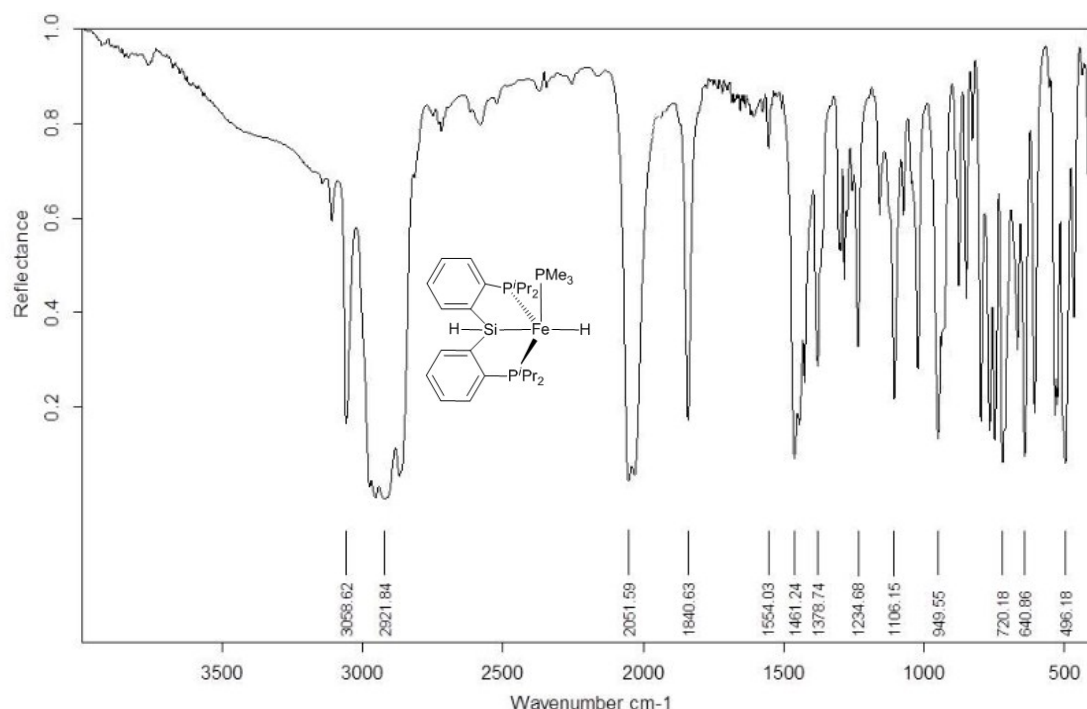


Fig. S5 ^{29}Si NMR of complex **3**.

IR spectrum of complex **6**



D:\张鹏\PSiP (二异丙基磷基) 与零价铁 THF 常温反应. 乙醚中析出浅黄色晶体 20160120.0

Sample description

Instrument type and

20/01/2016

Fig. S6 IR spectrum of complex **6**.

^1H NMR of complex **6**

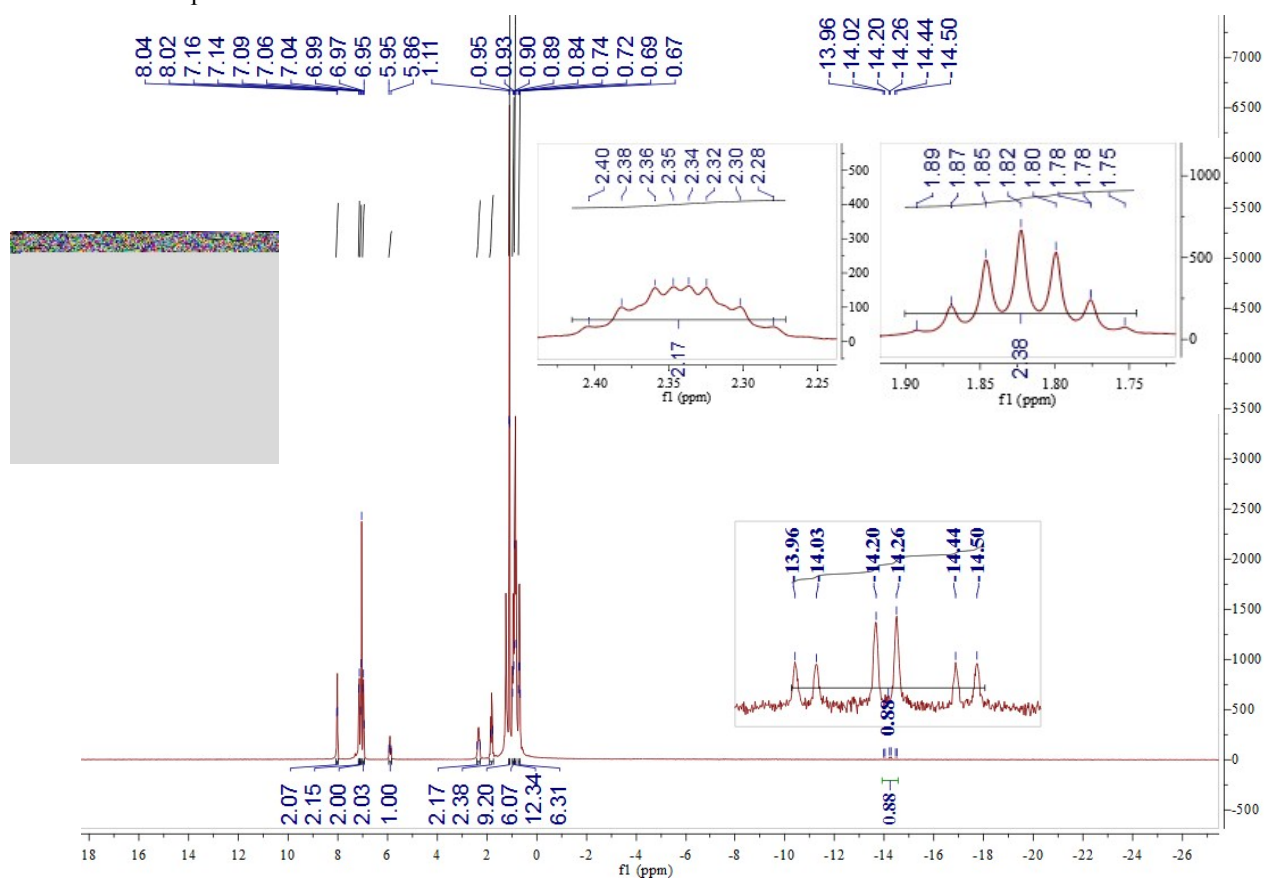


Fig. S7 ^1H NMR of complex **6**.

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

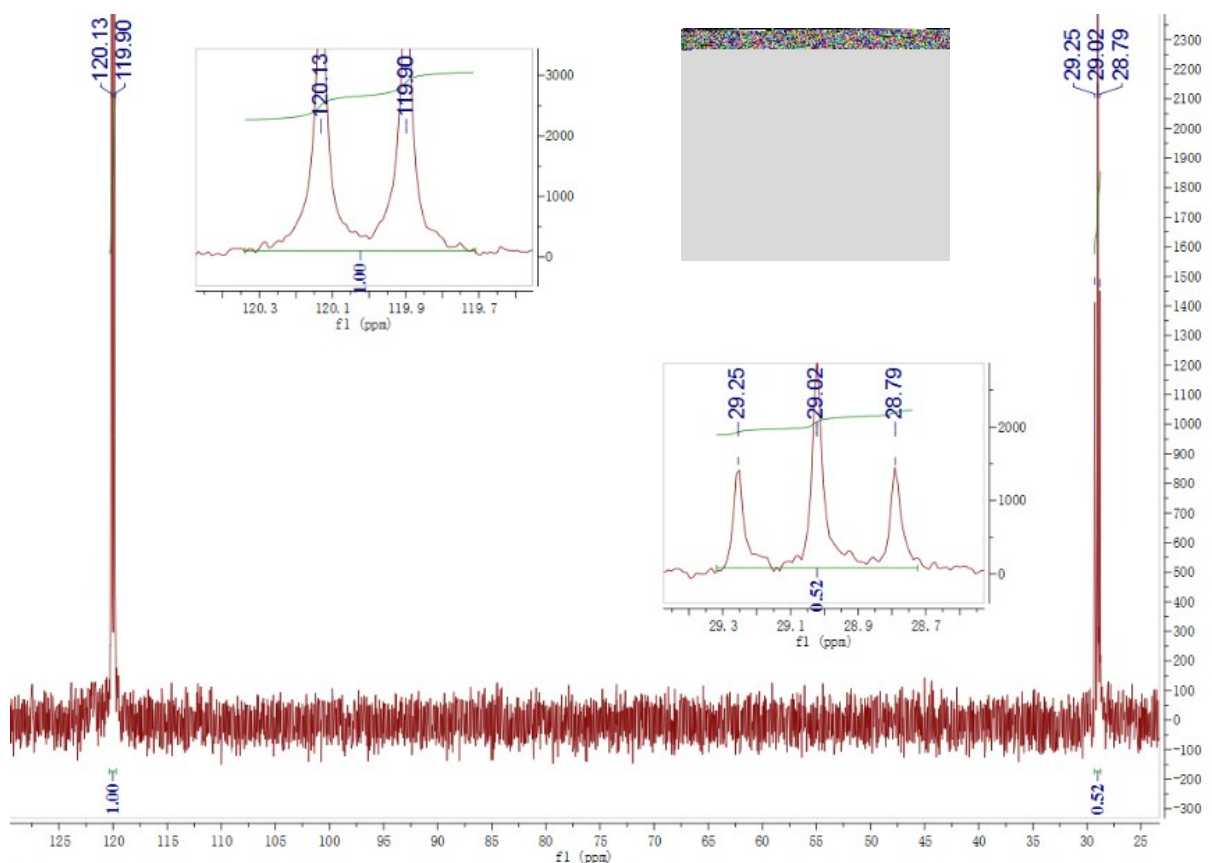


Fig. S8 ^{31}P NMR of complex **6**.

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

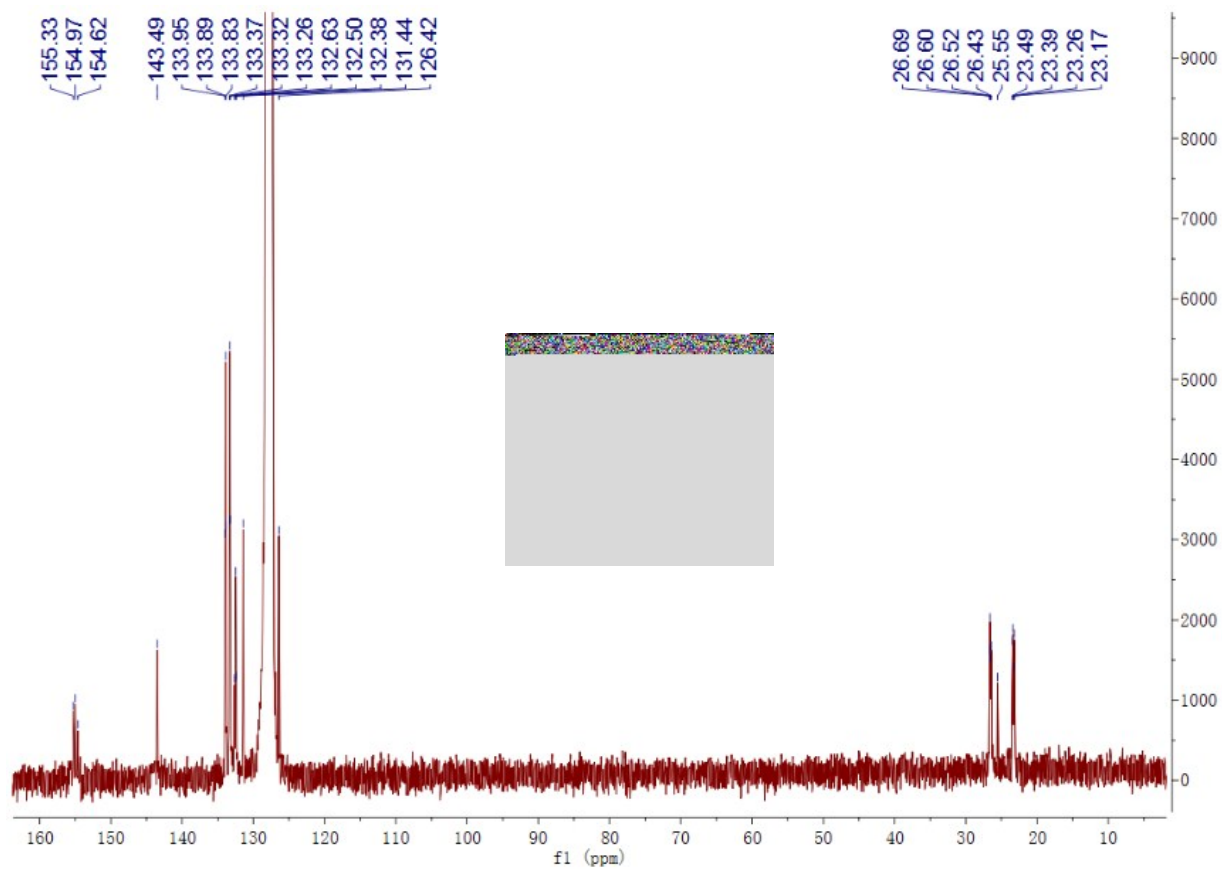


Fig. S9 ^{13}C NMR of complex **6**.

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

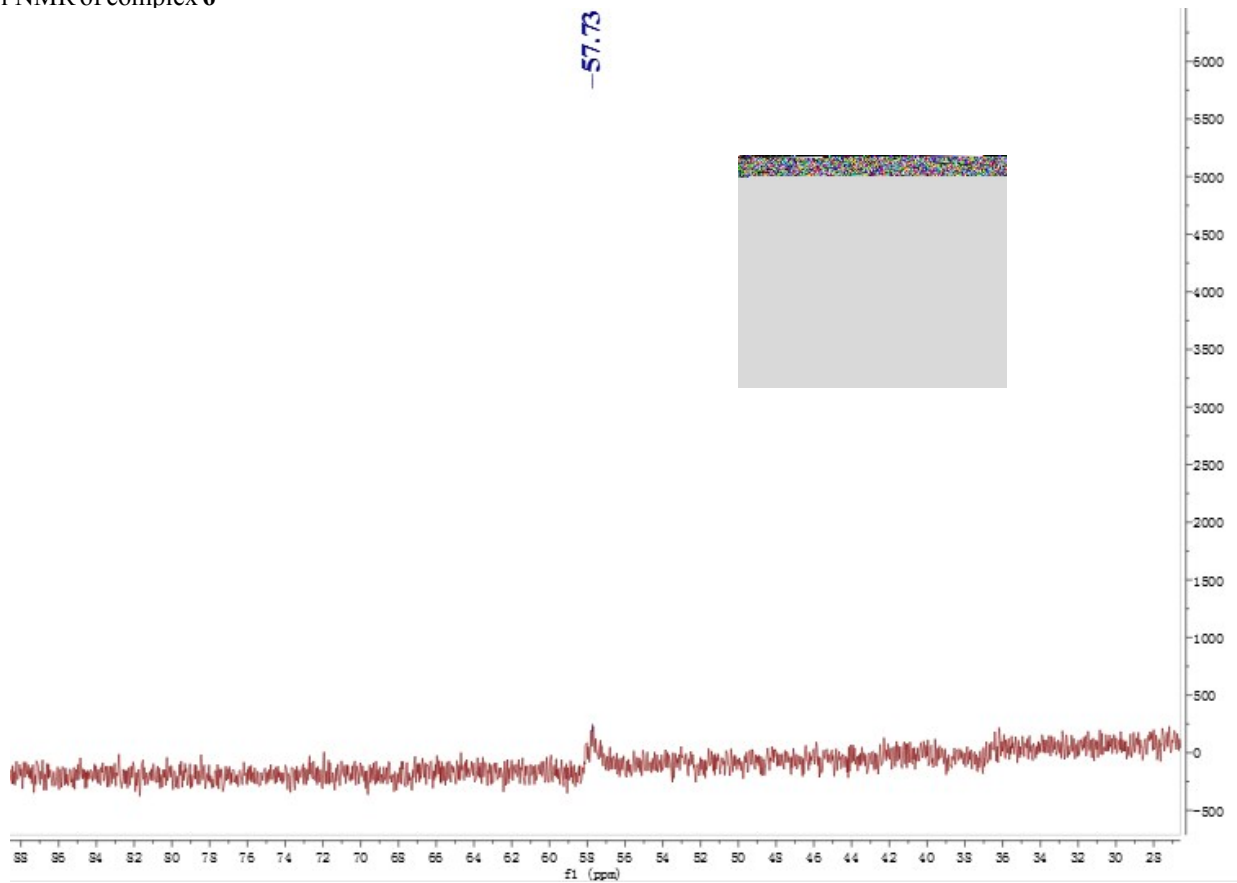
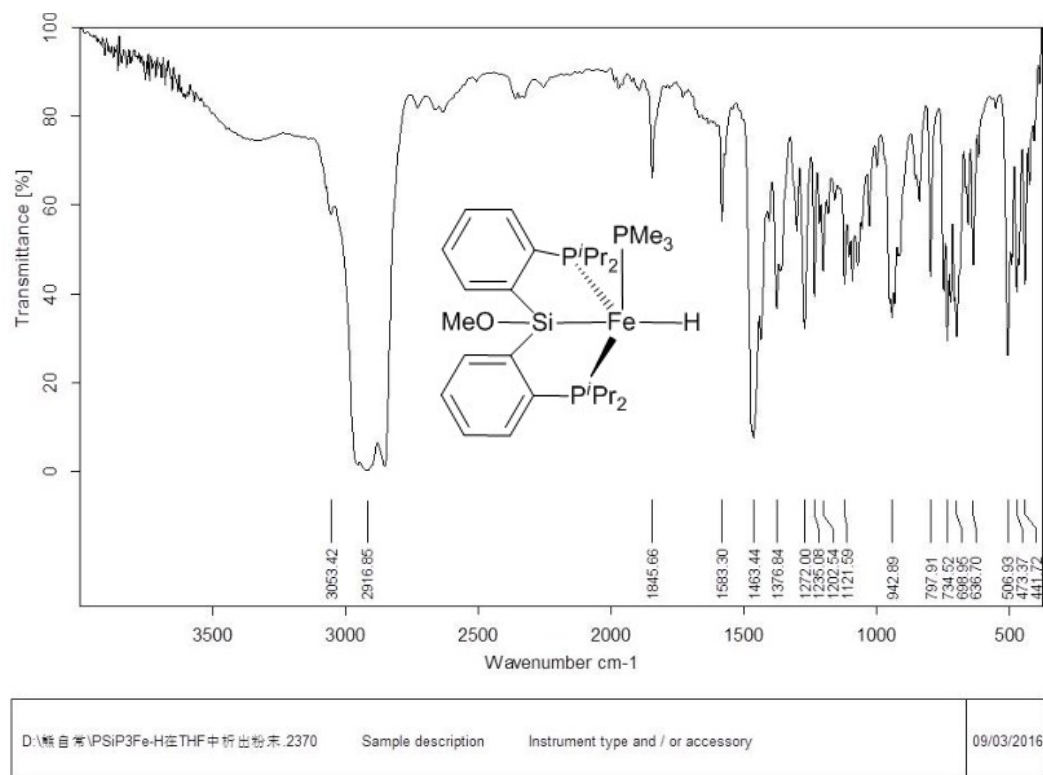


Fig. S10 ^{29}Si NMR of complex **6**.

IR spectrum of complex 7



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Fig. S11 IR spectrum of complex 7.

¹H NMR of complex 7

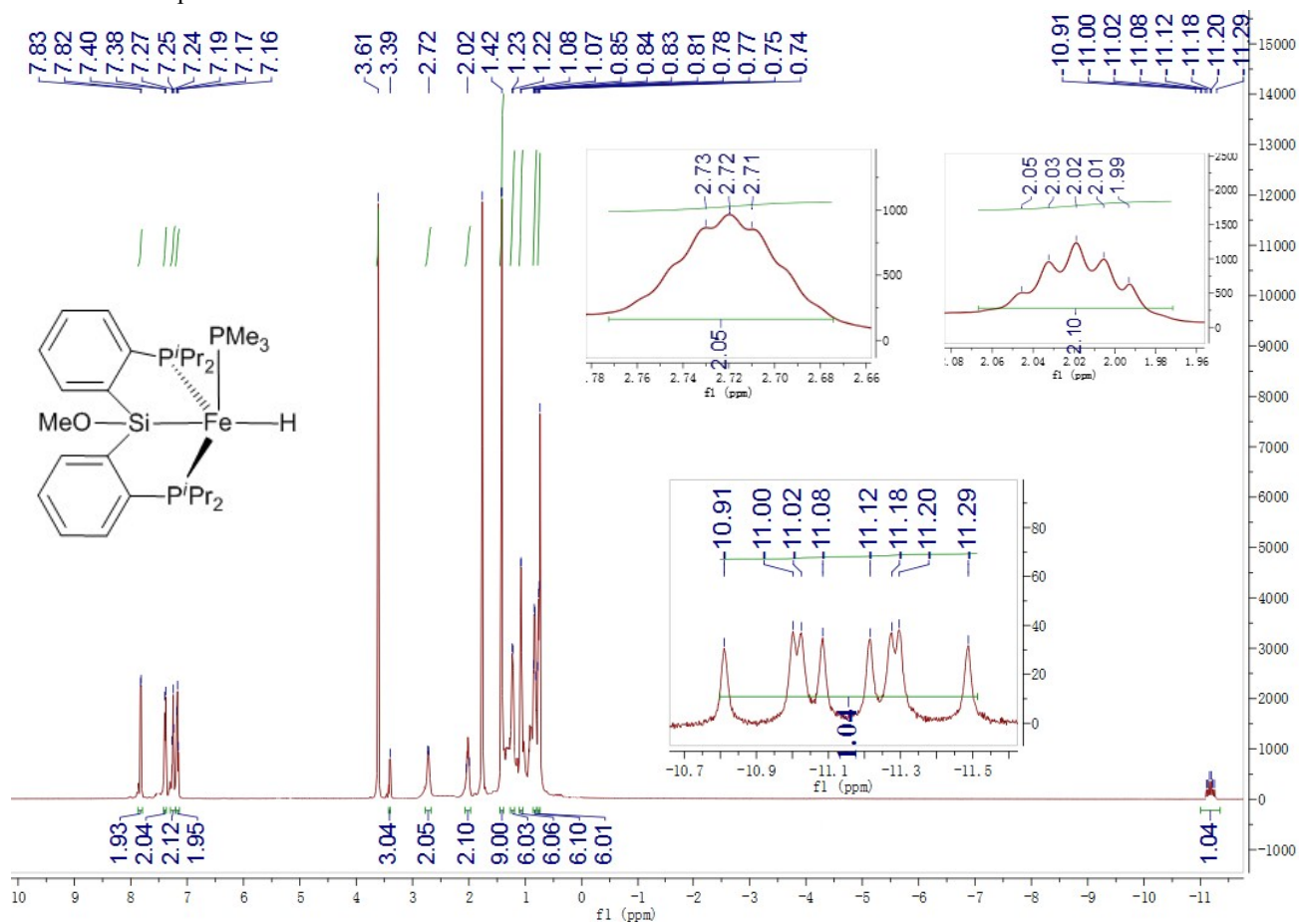


Fig. S12 ¹H NMR of complex 7 at -40°C

^{31}P NMR of complex 7

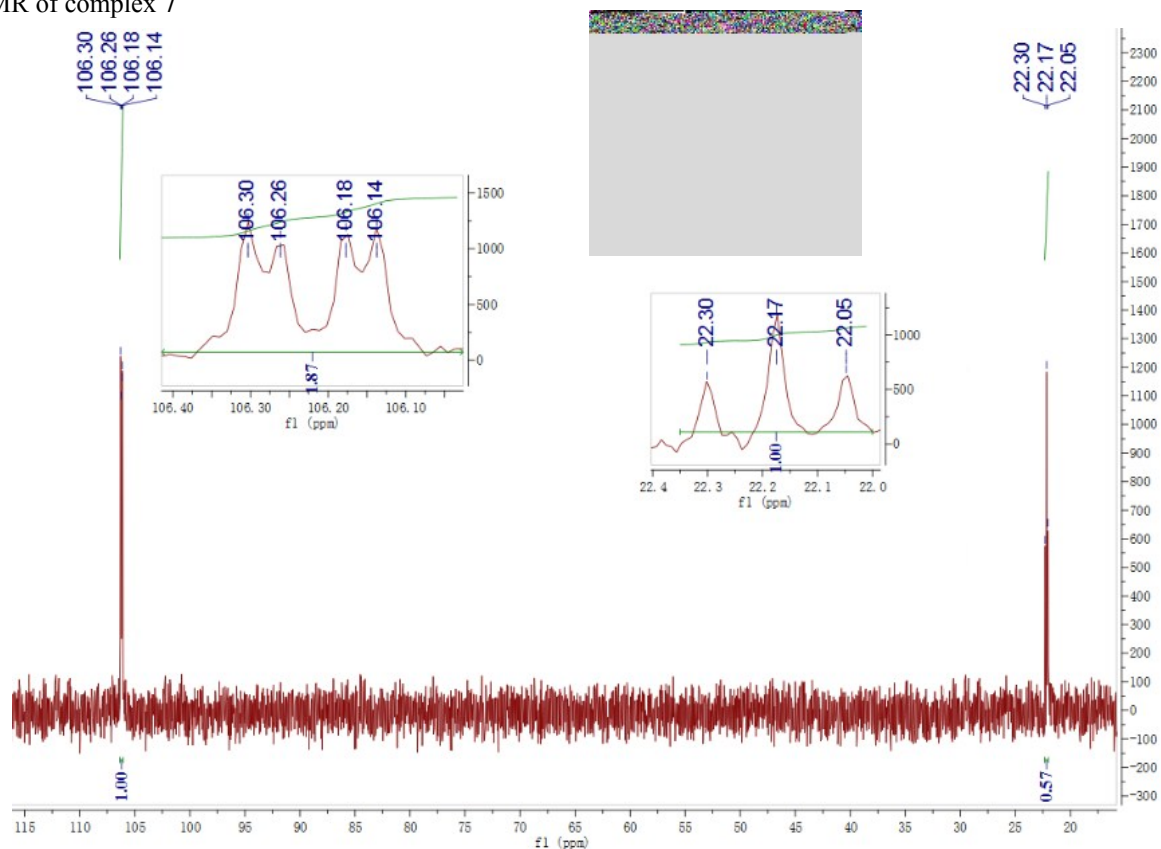


Fig. S13 ^{31}P NMR of complex 7.

^{13}C NMR of complex 7

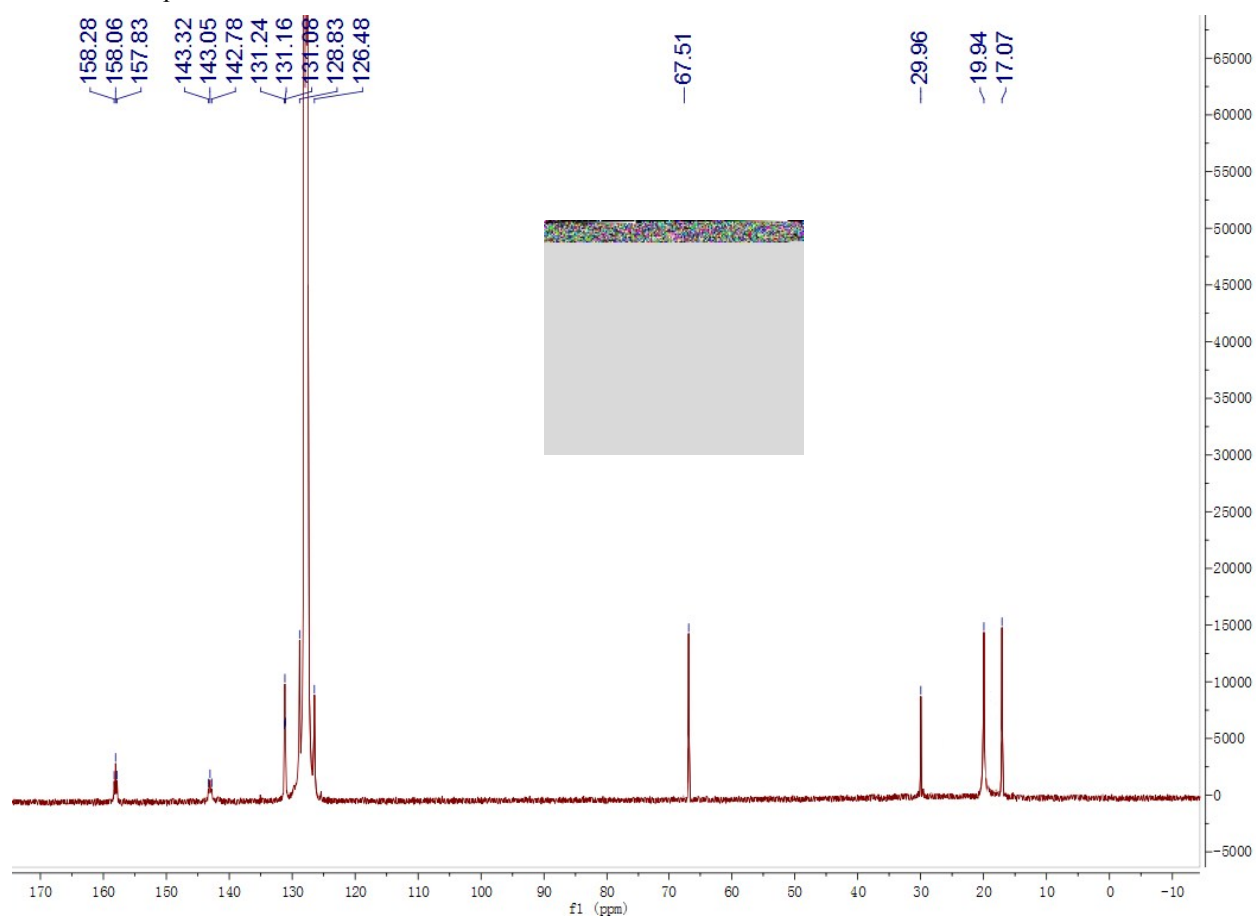


Fig. S14 ^{13}C NMR of complex 7.

^{29}Si NMR of complex 7

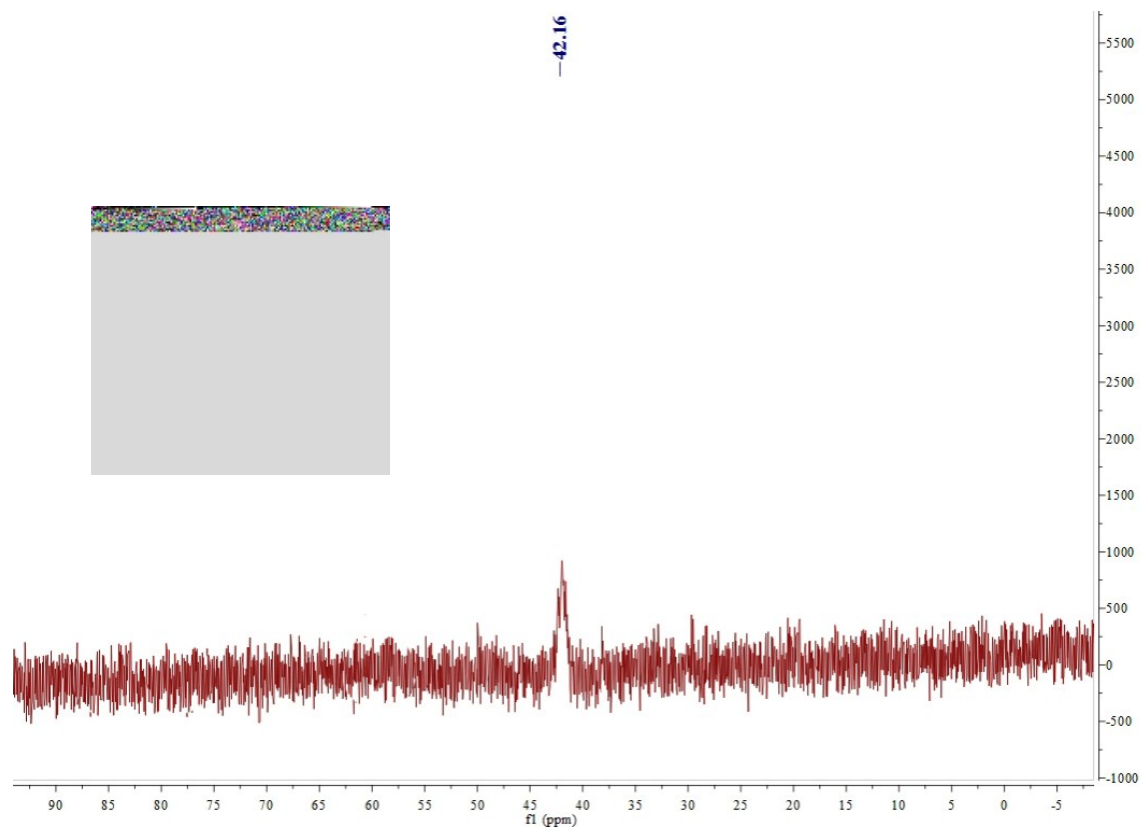
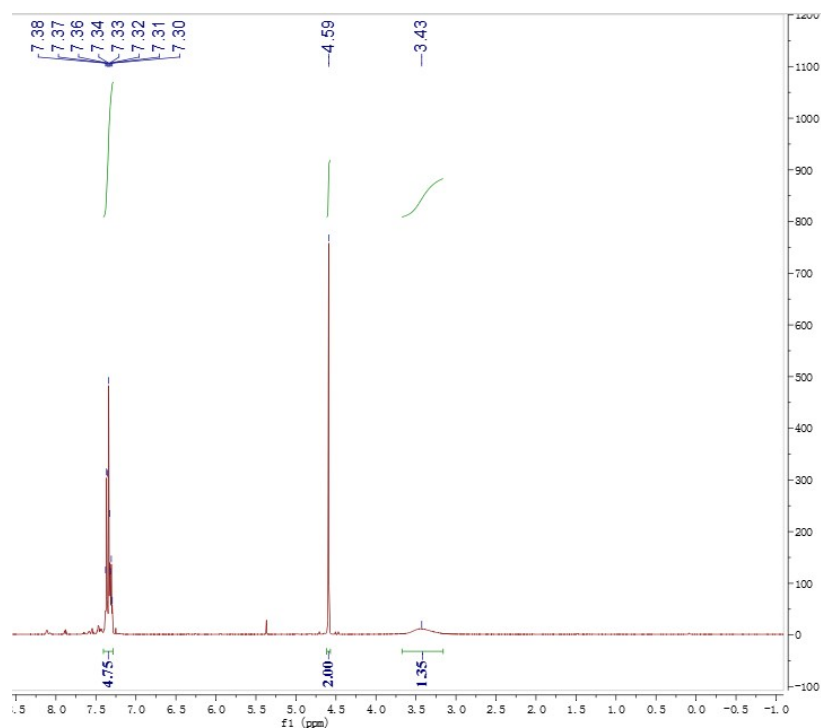


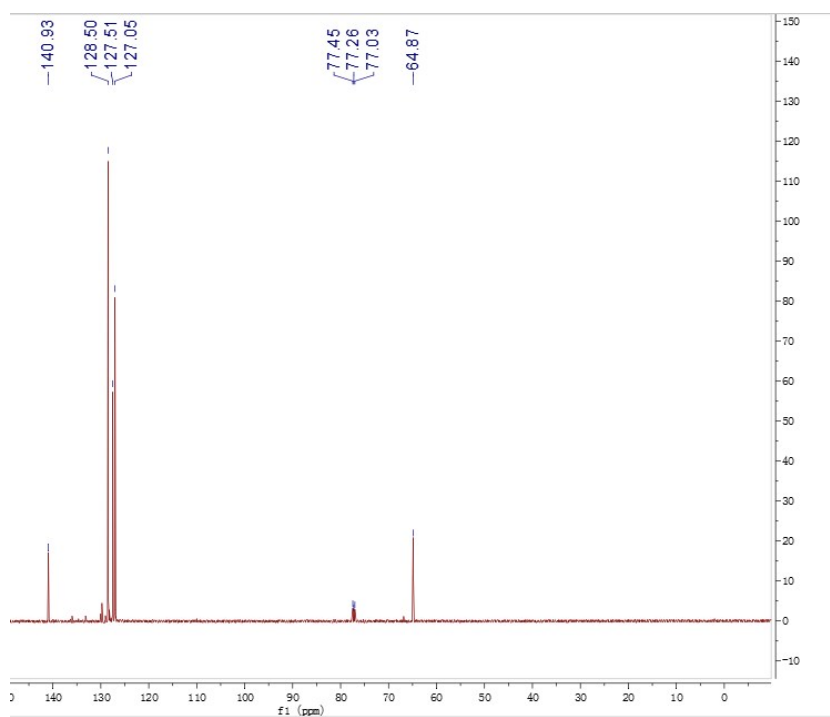
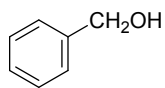
Fig. S15 ^{29}Si NMR of complex 7.

3 NMR spectra of the catalytic products

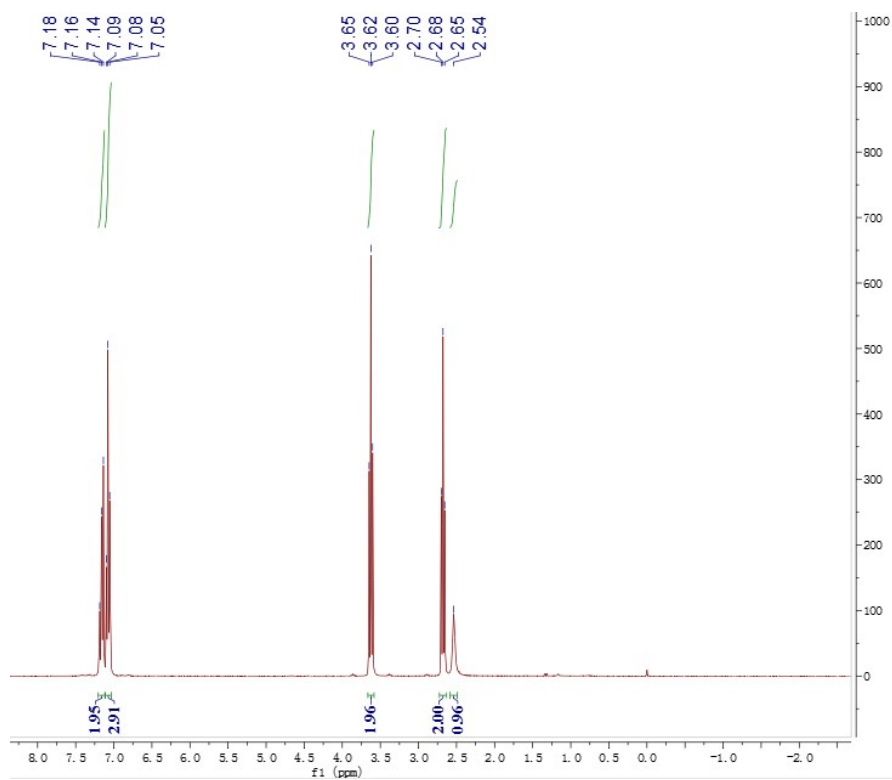
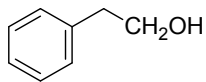
^1H NMR of compound c1ccccc1CO



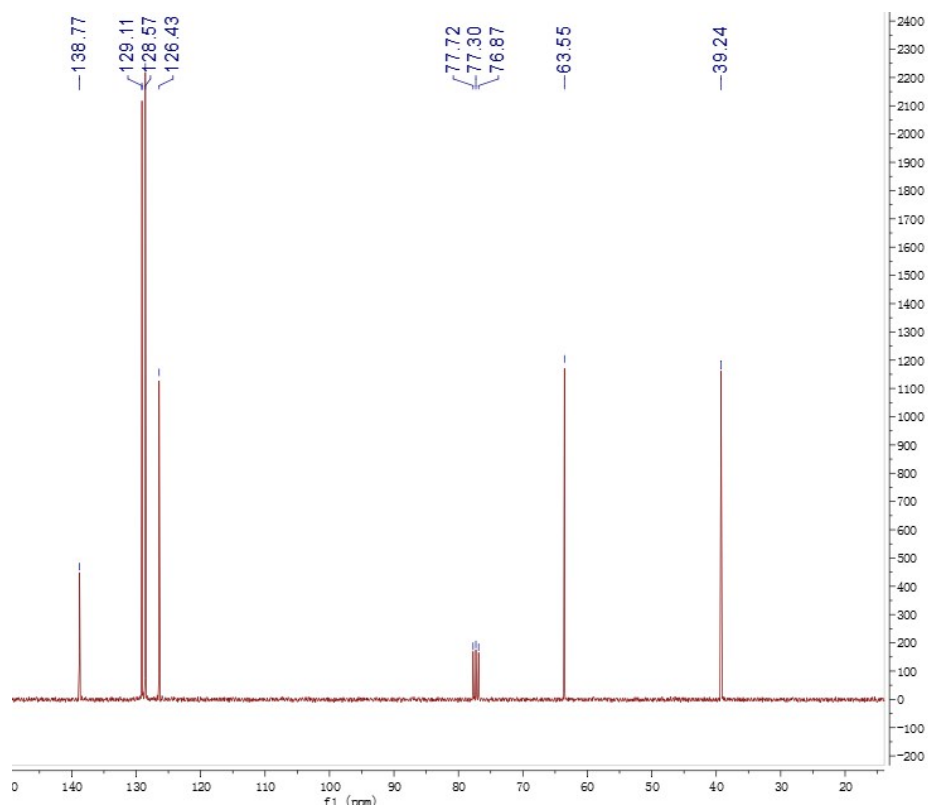
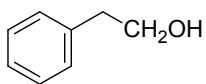
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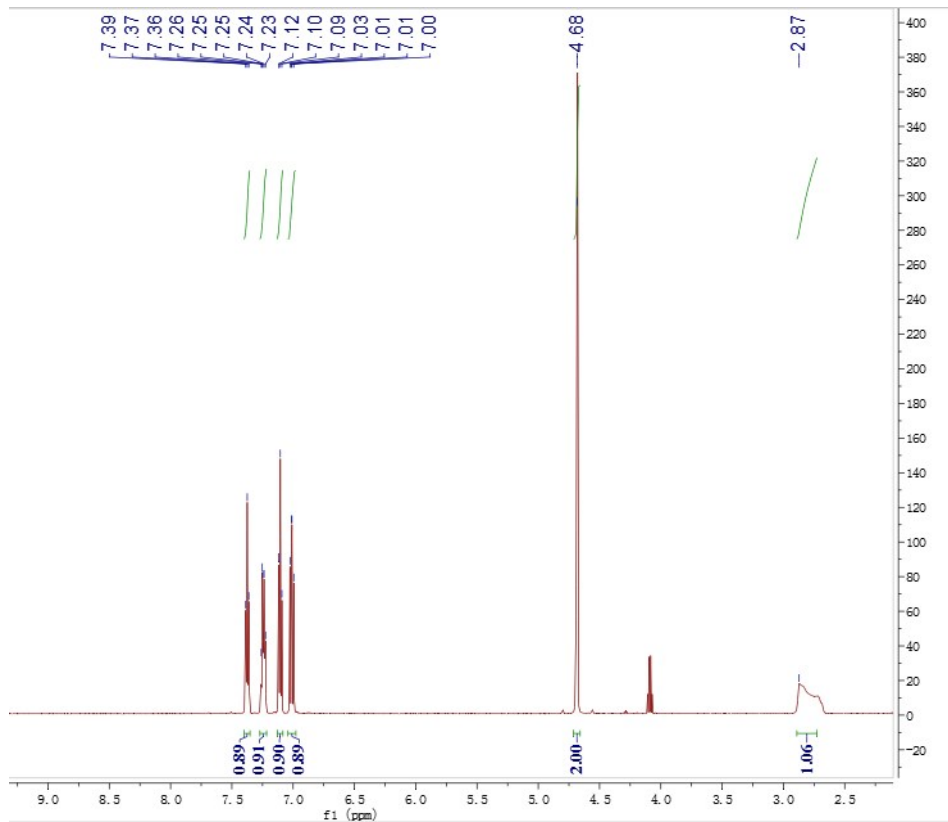
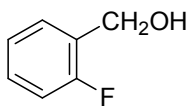
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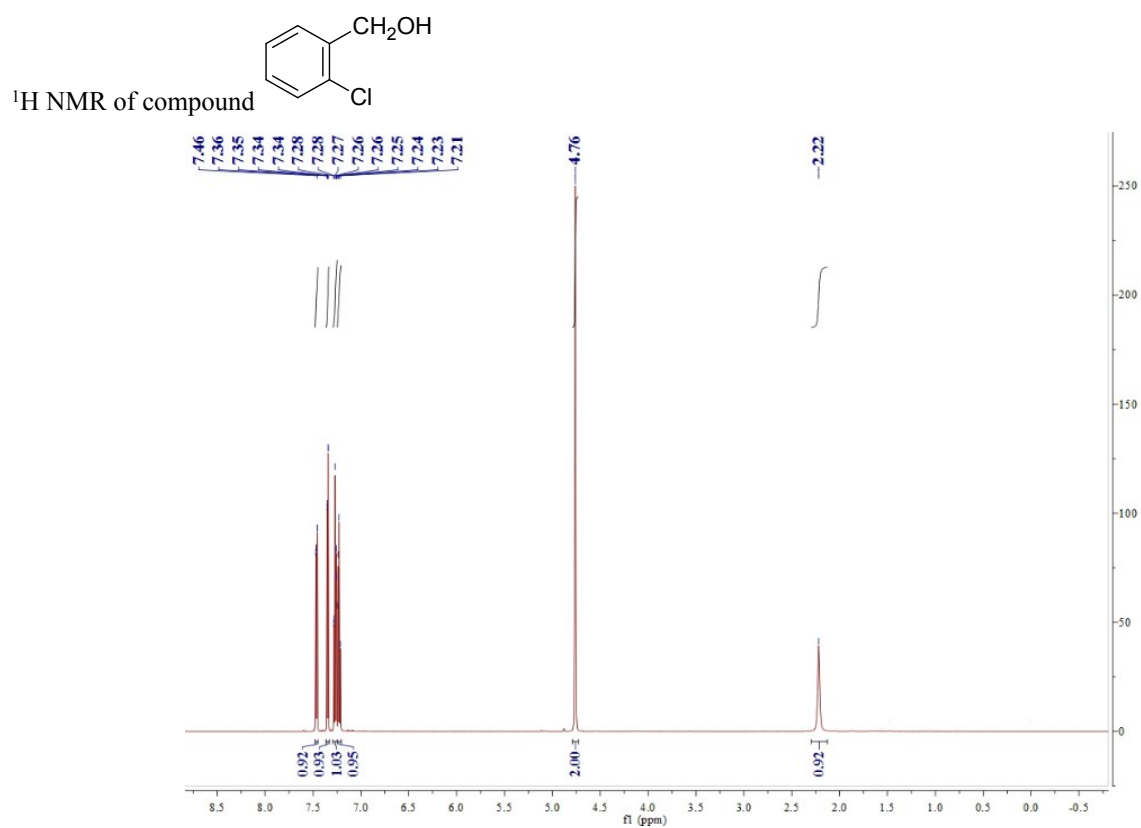
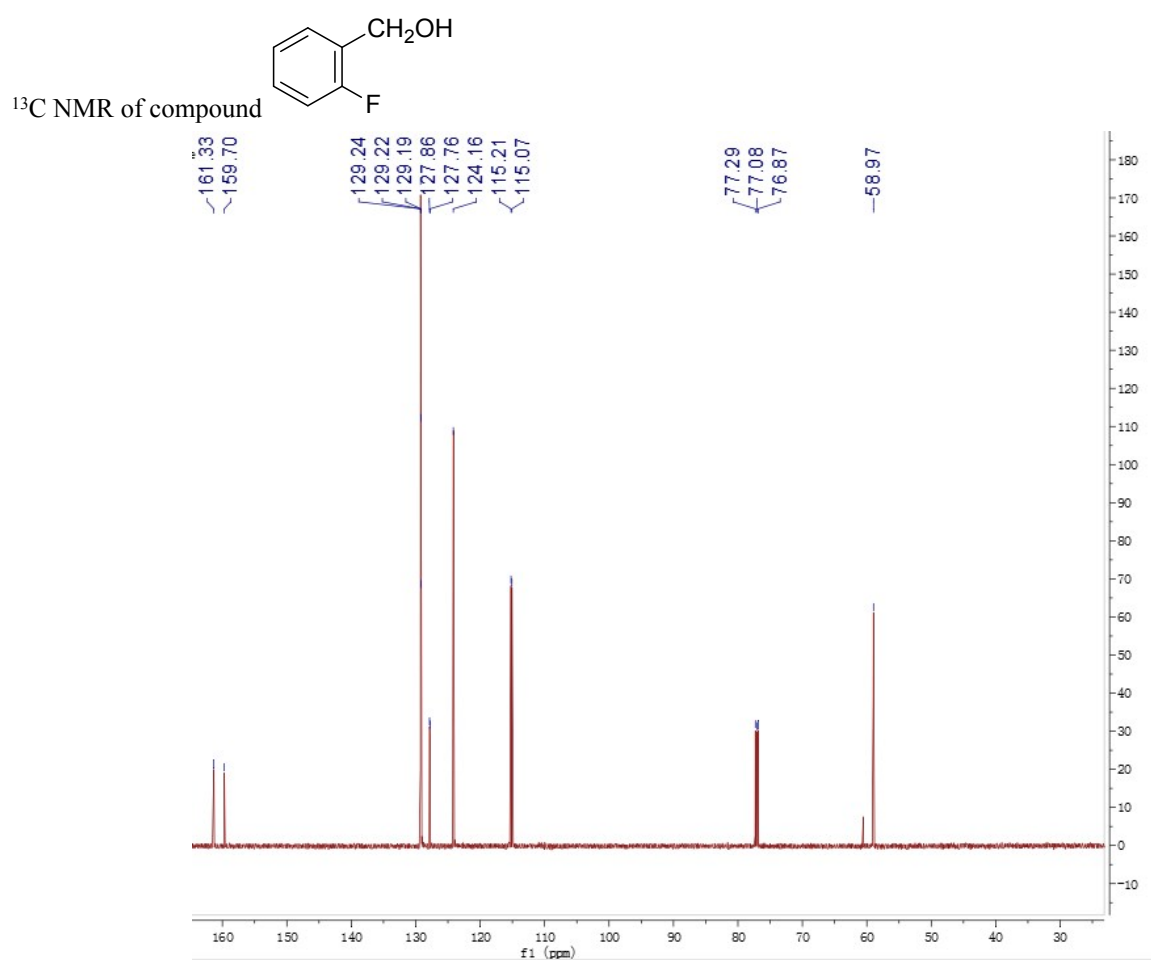


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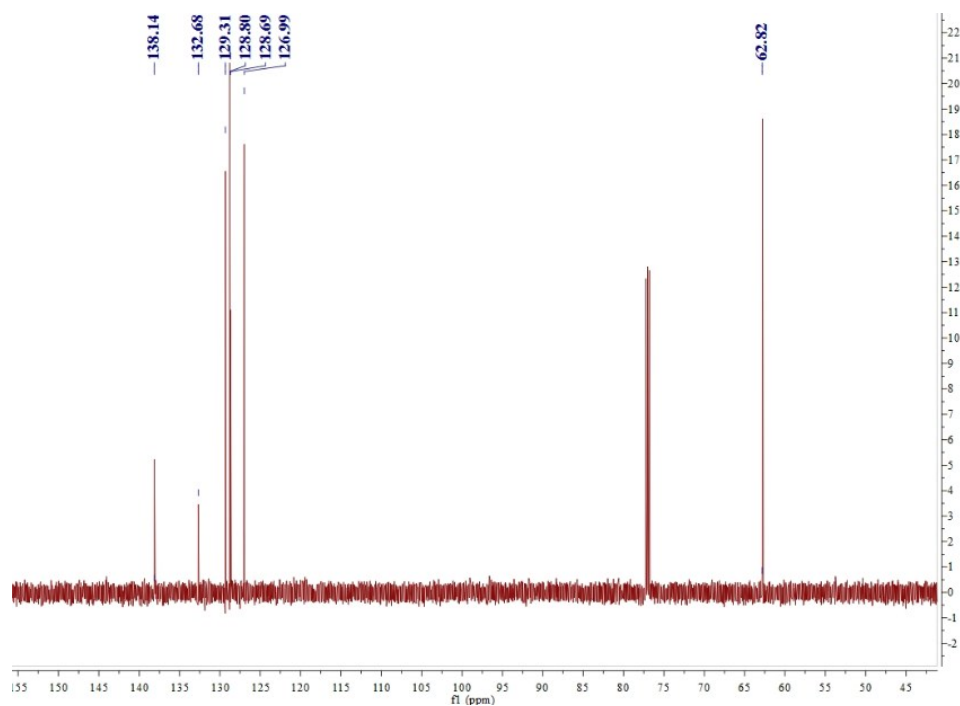
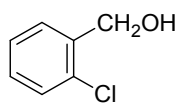


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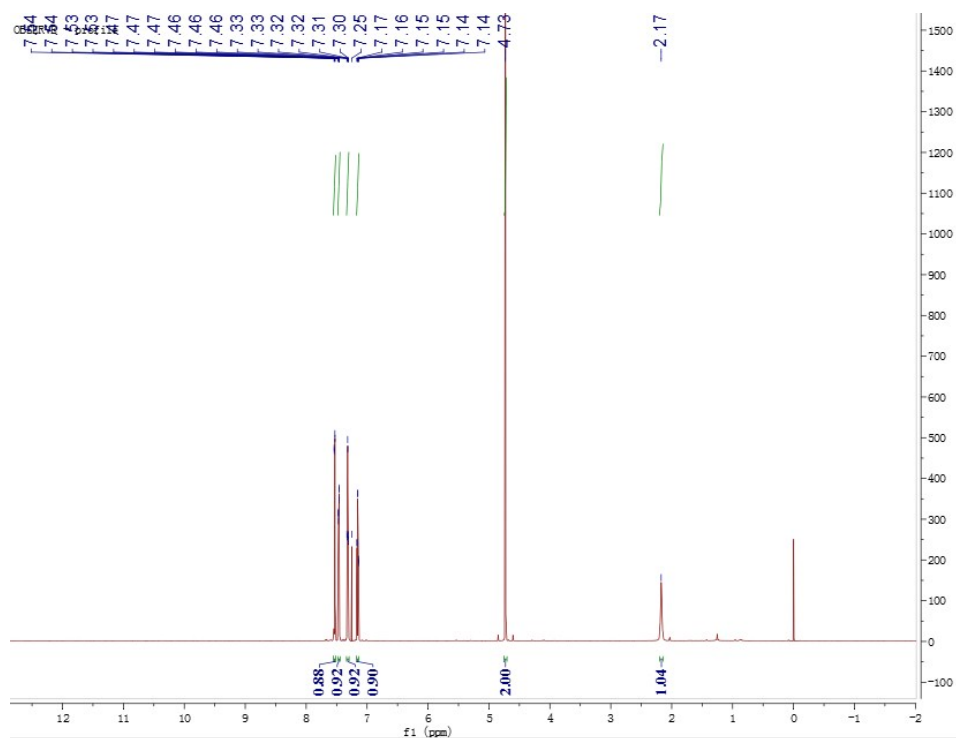
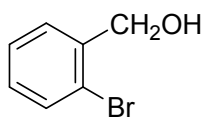




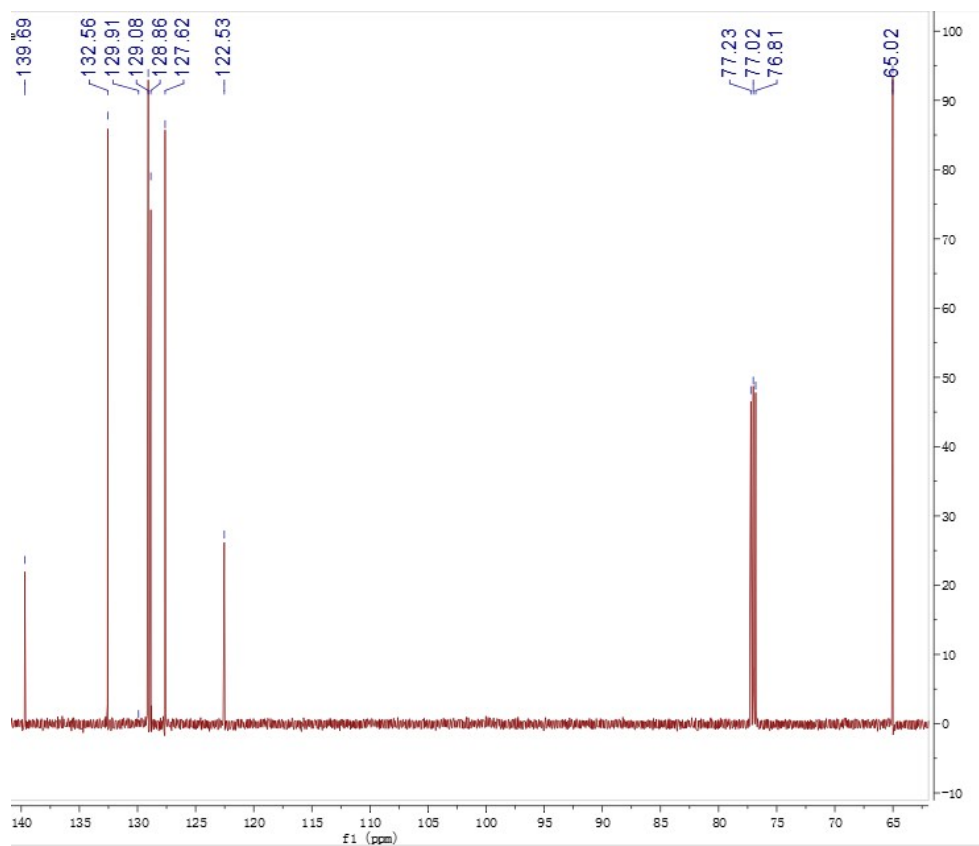
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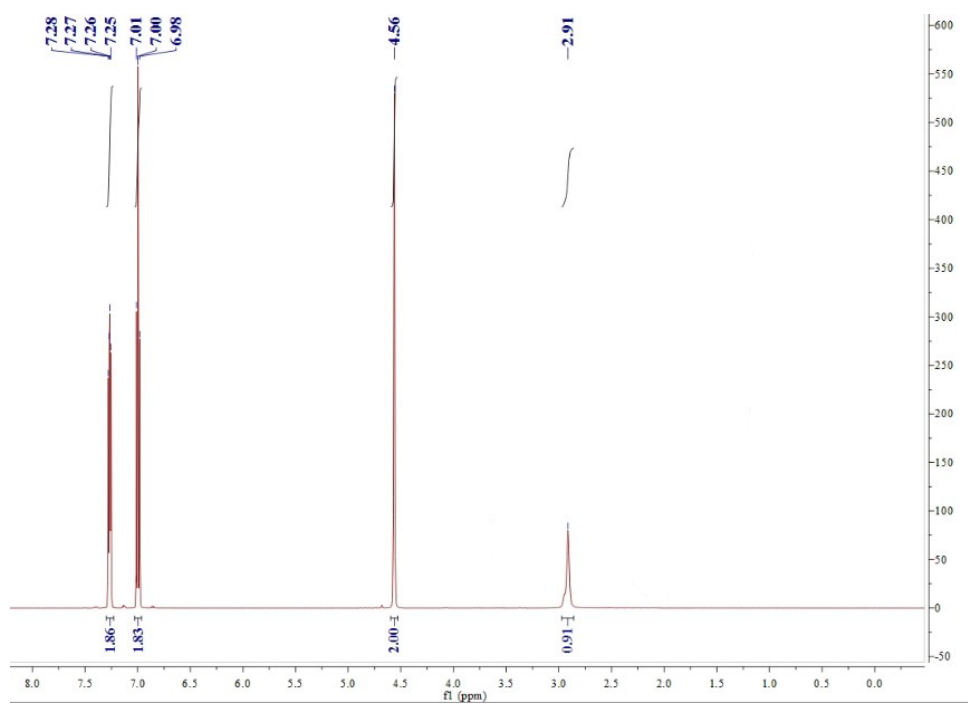
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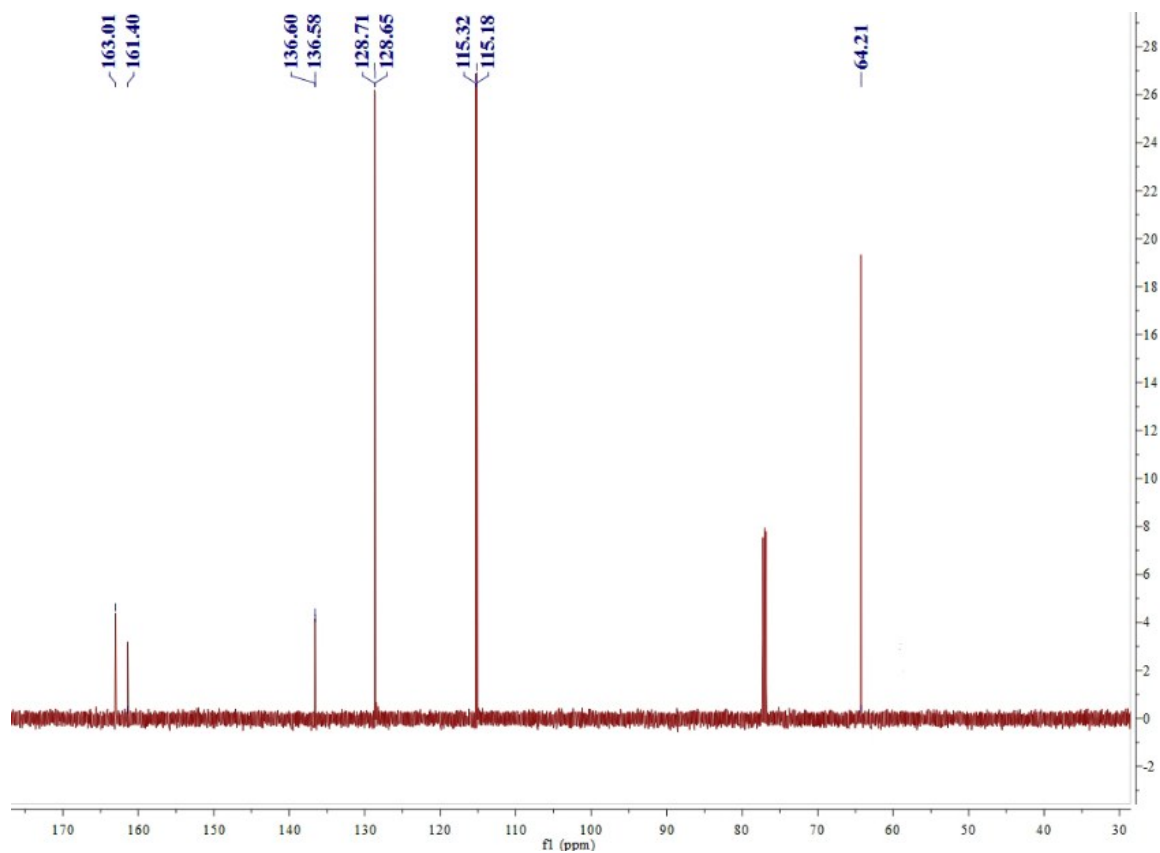
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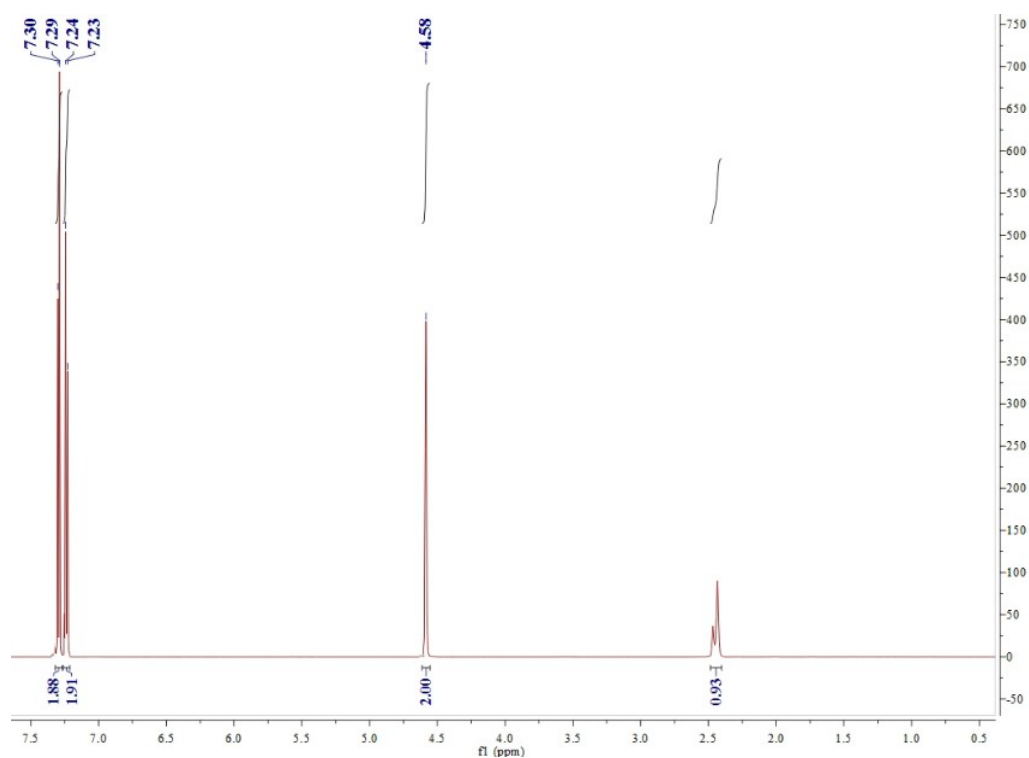
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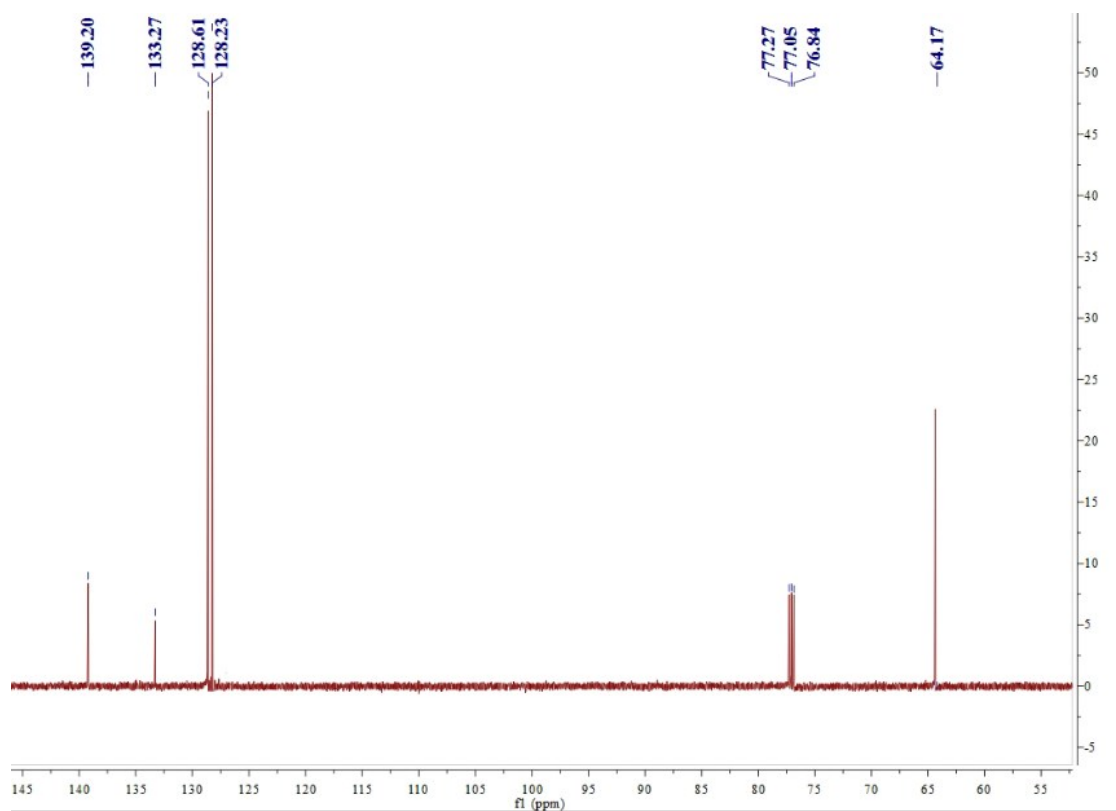
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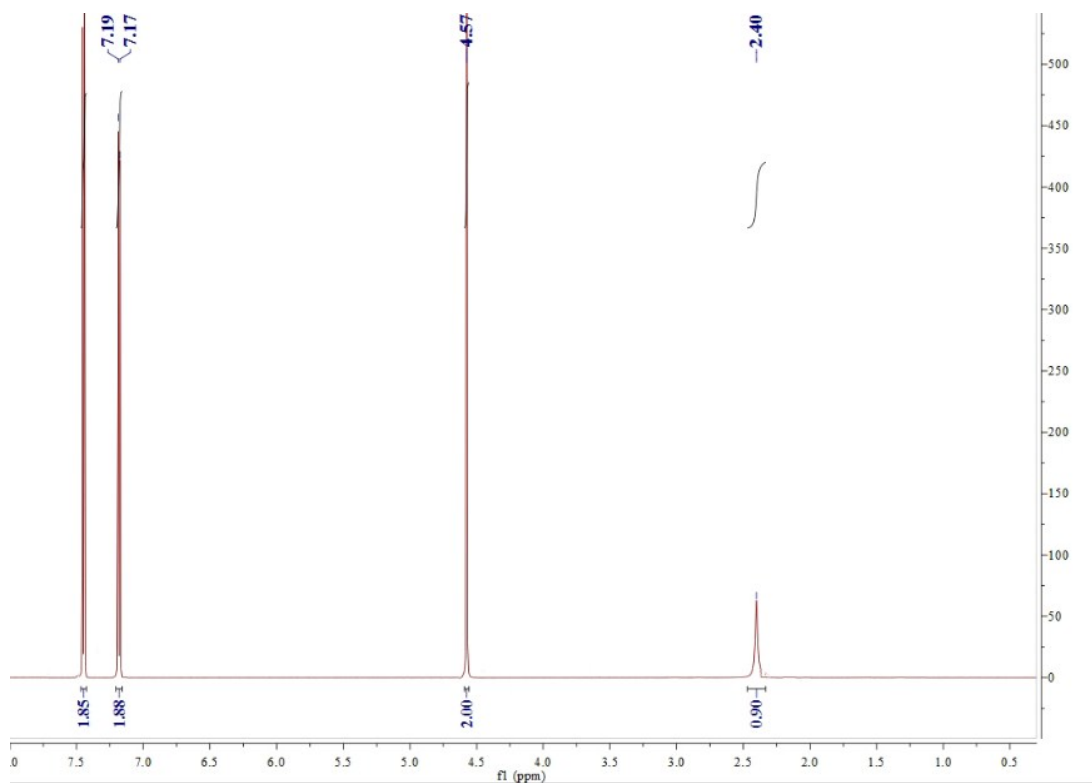
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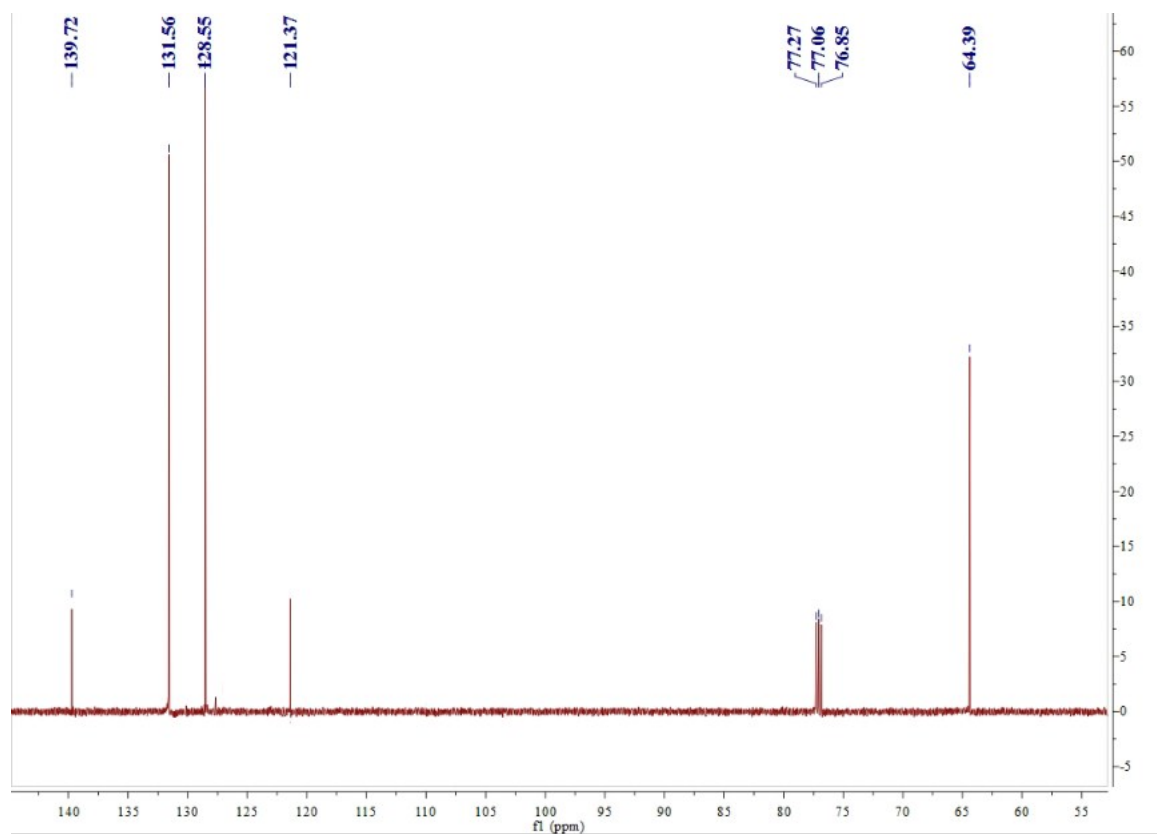
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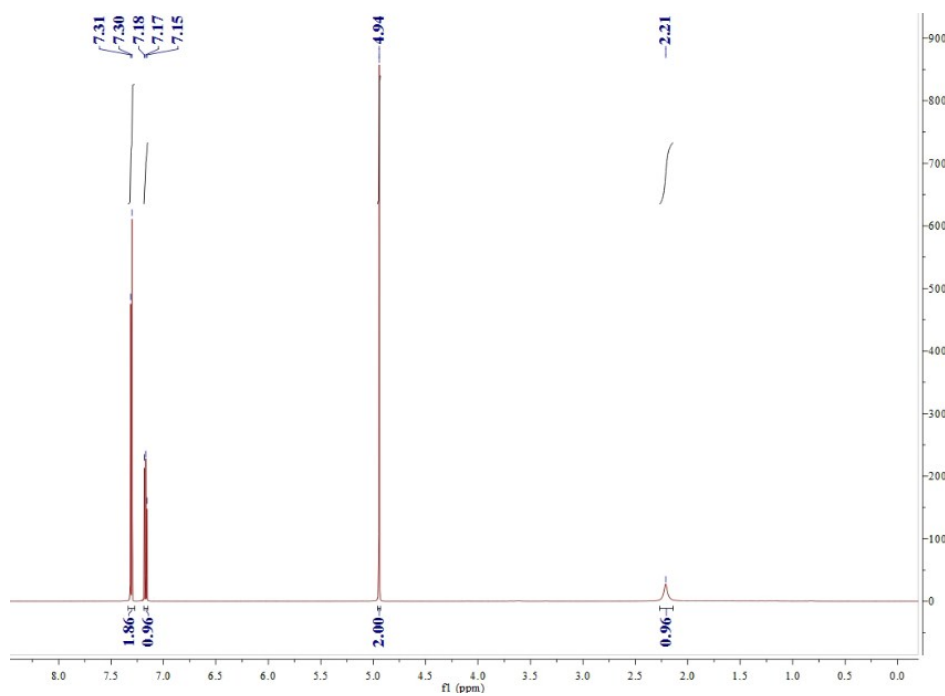
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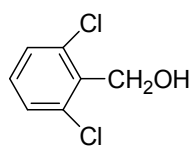


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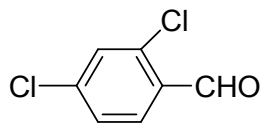
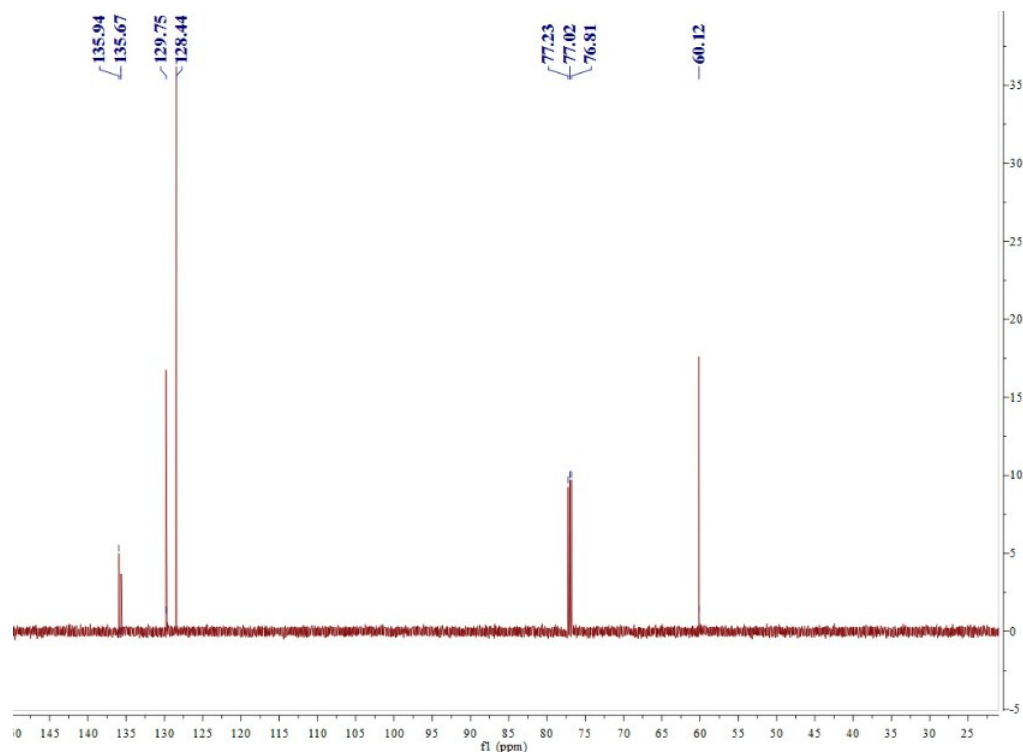


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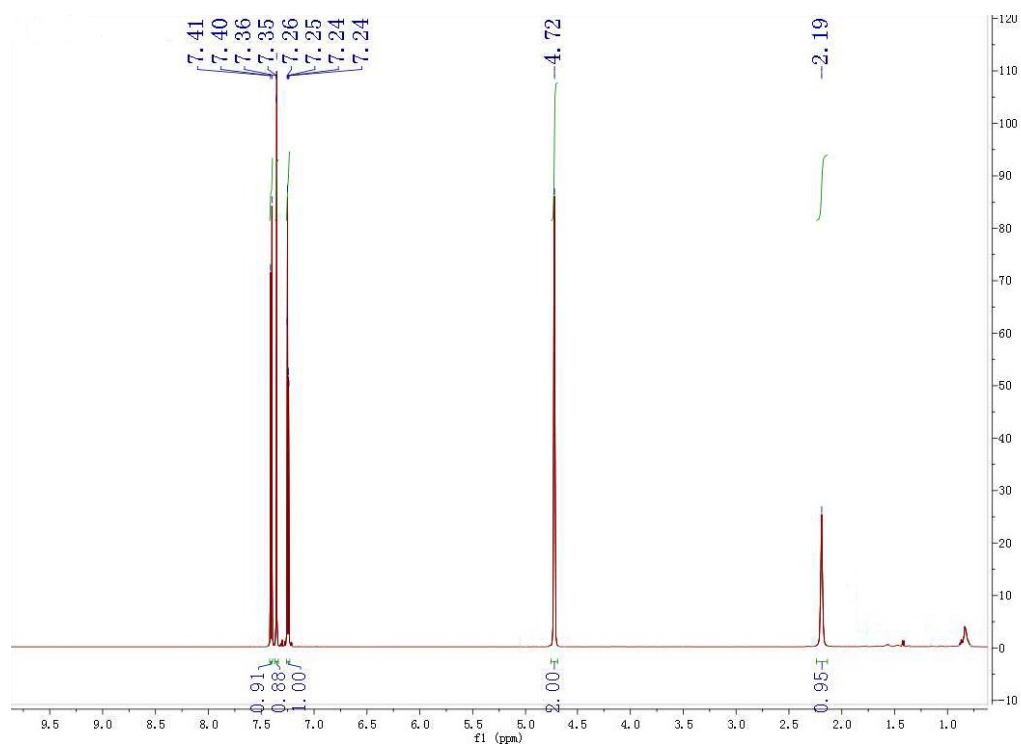


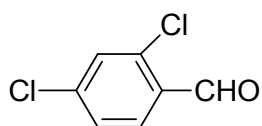


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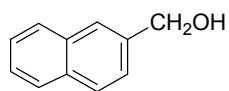
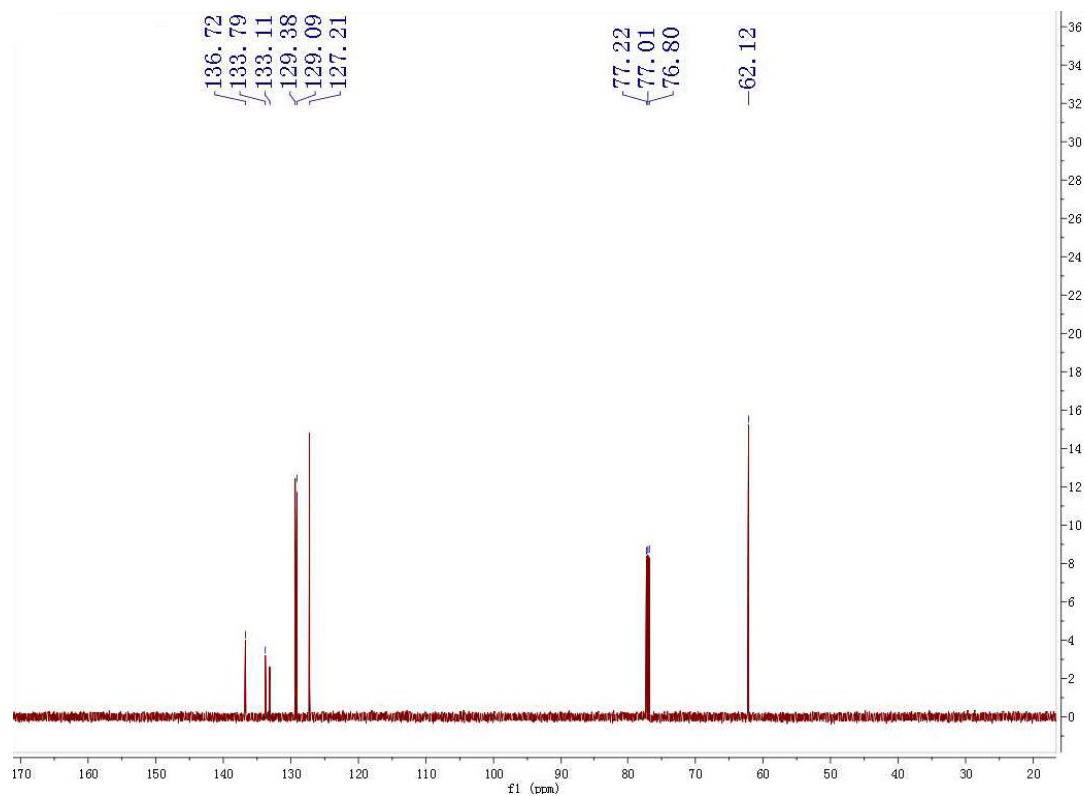


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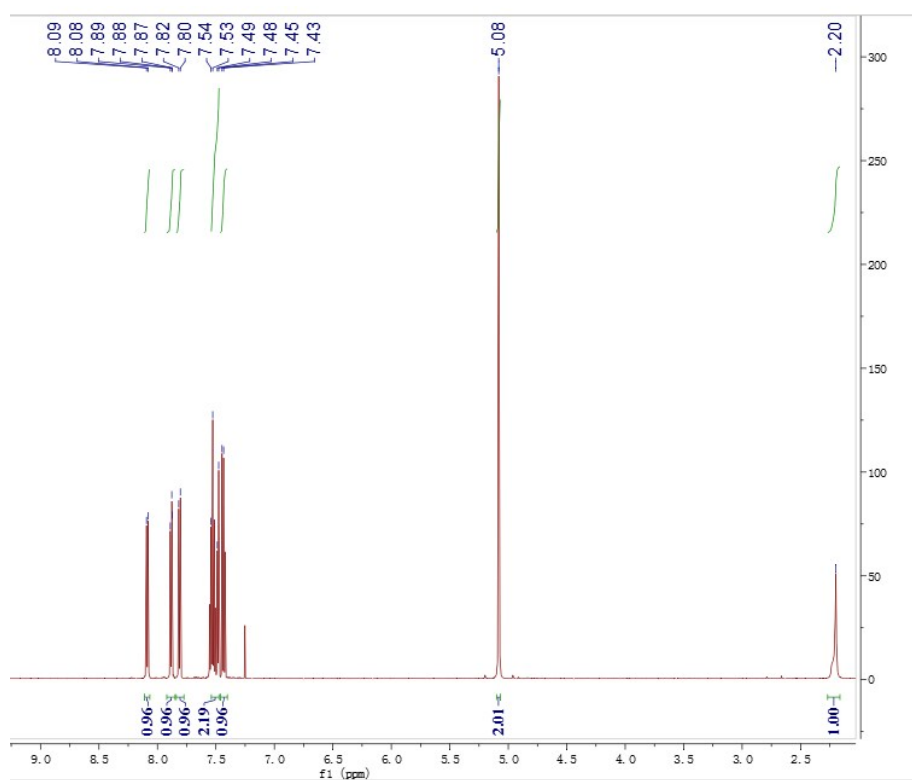




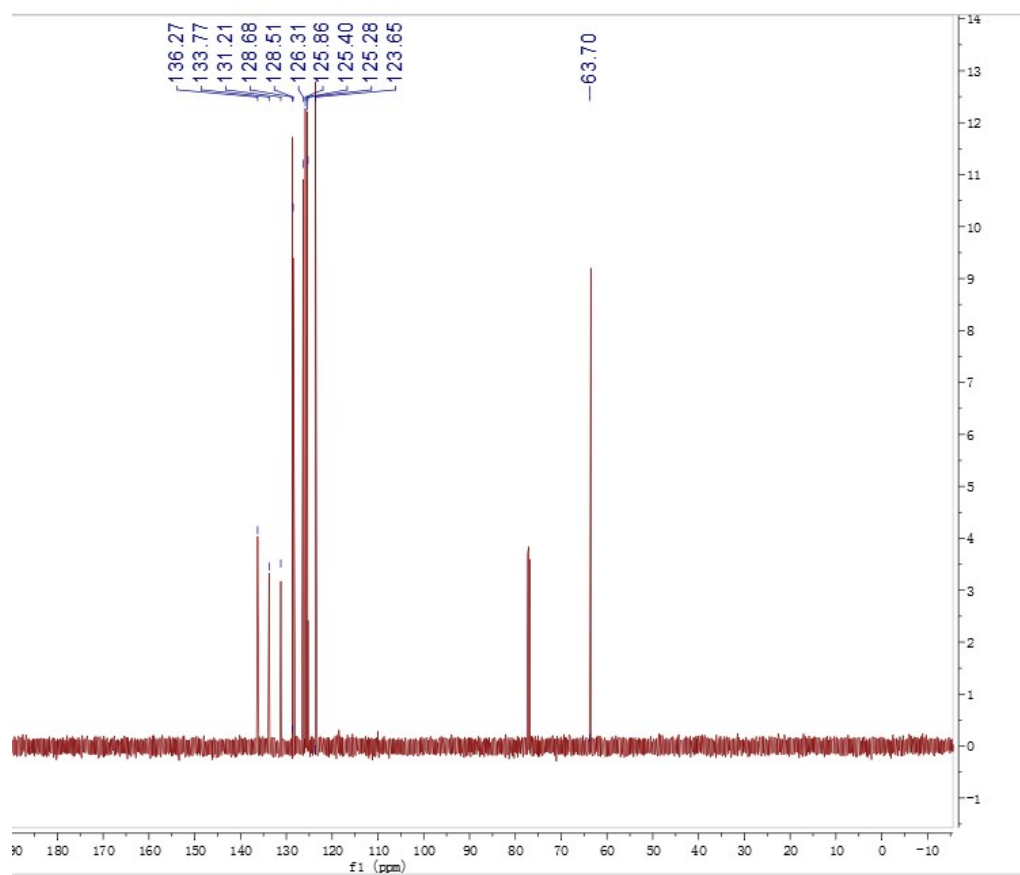
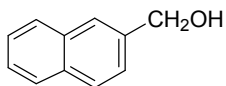
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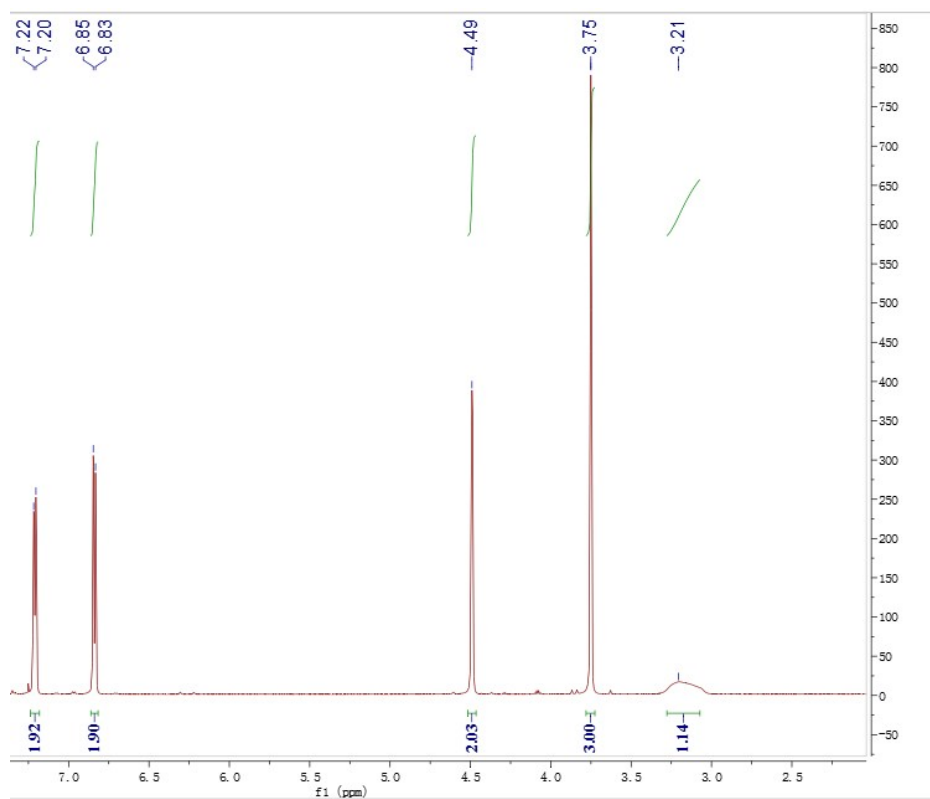
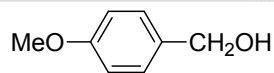
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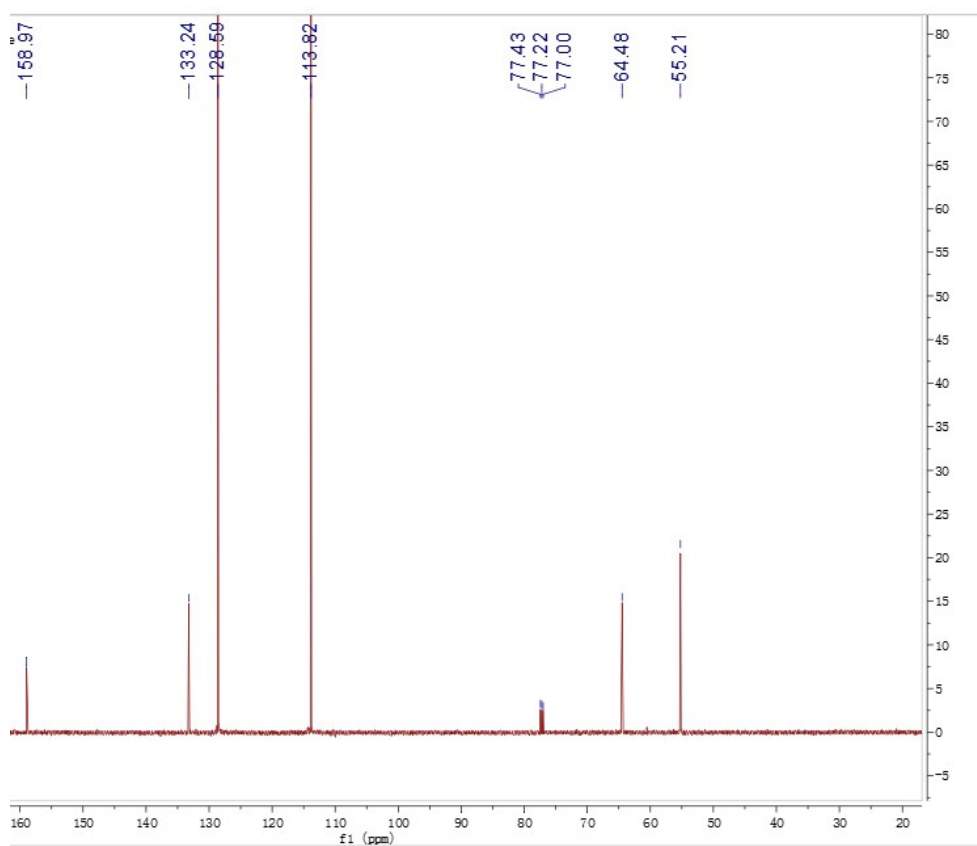
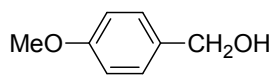
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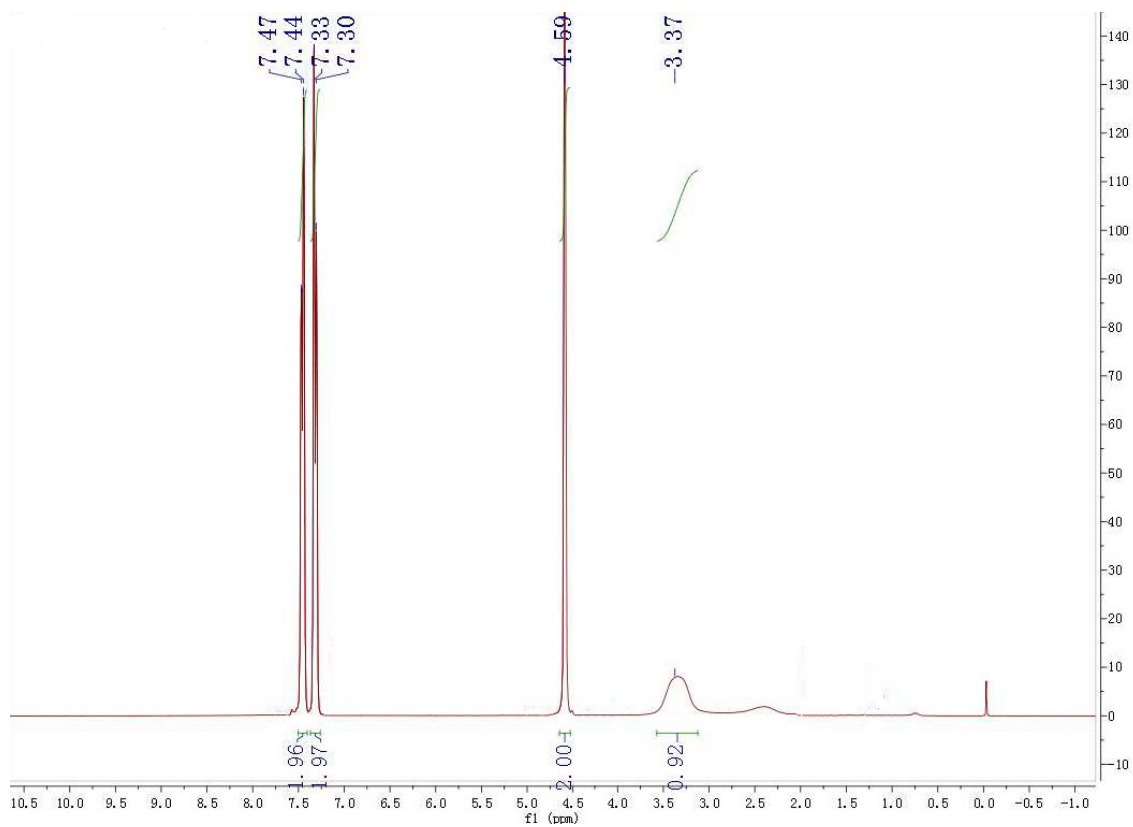
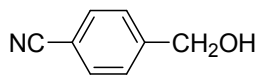
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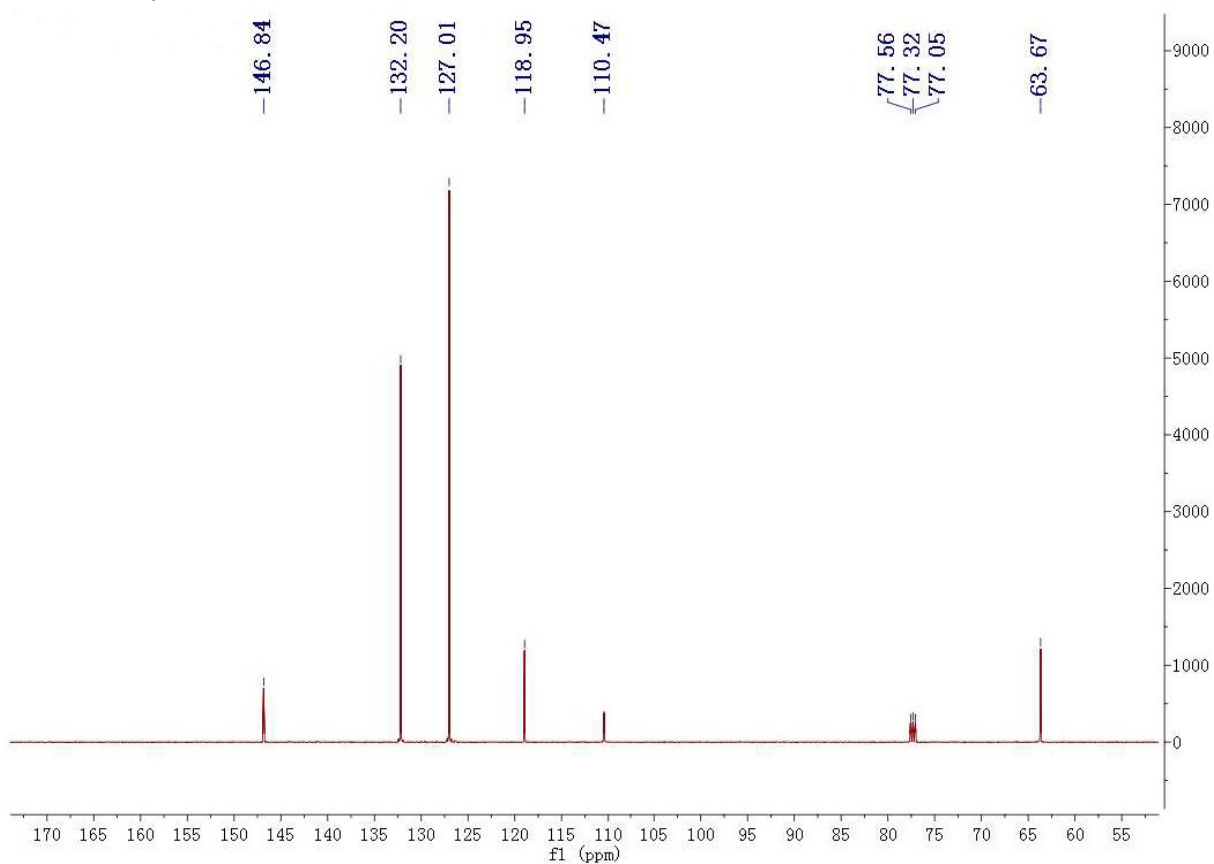
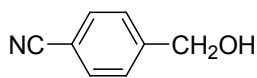
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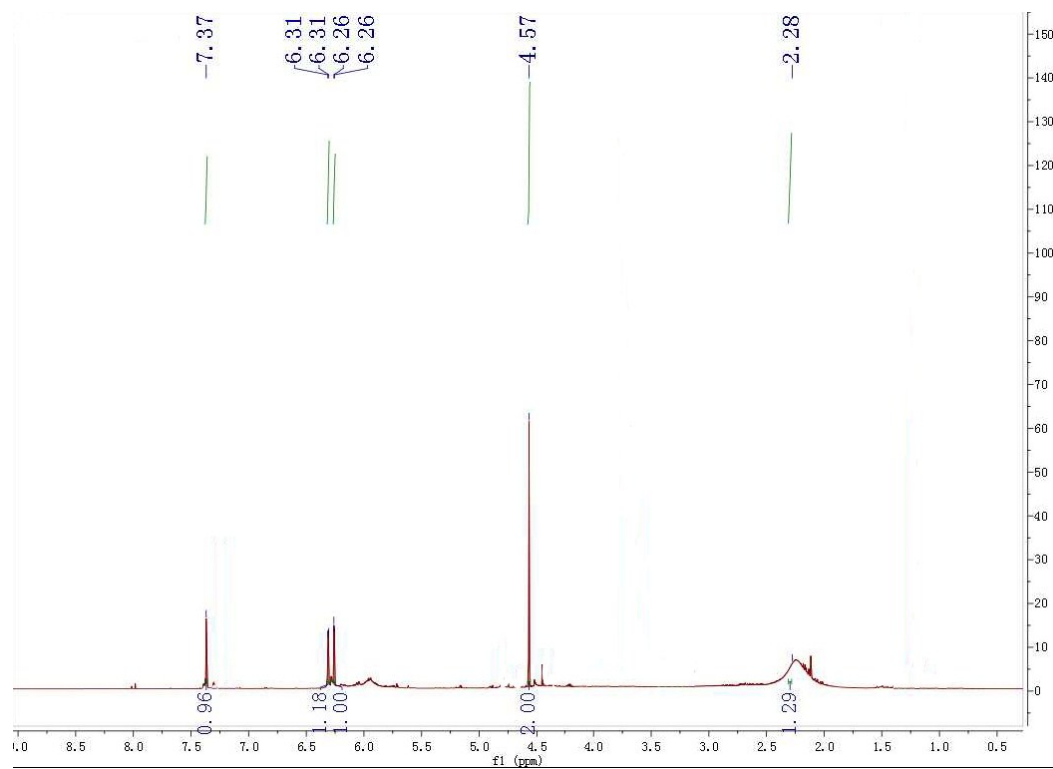
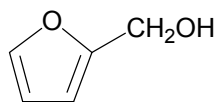
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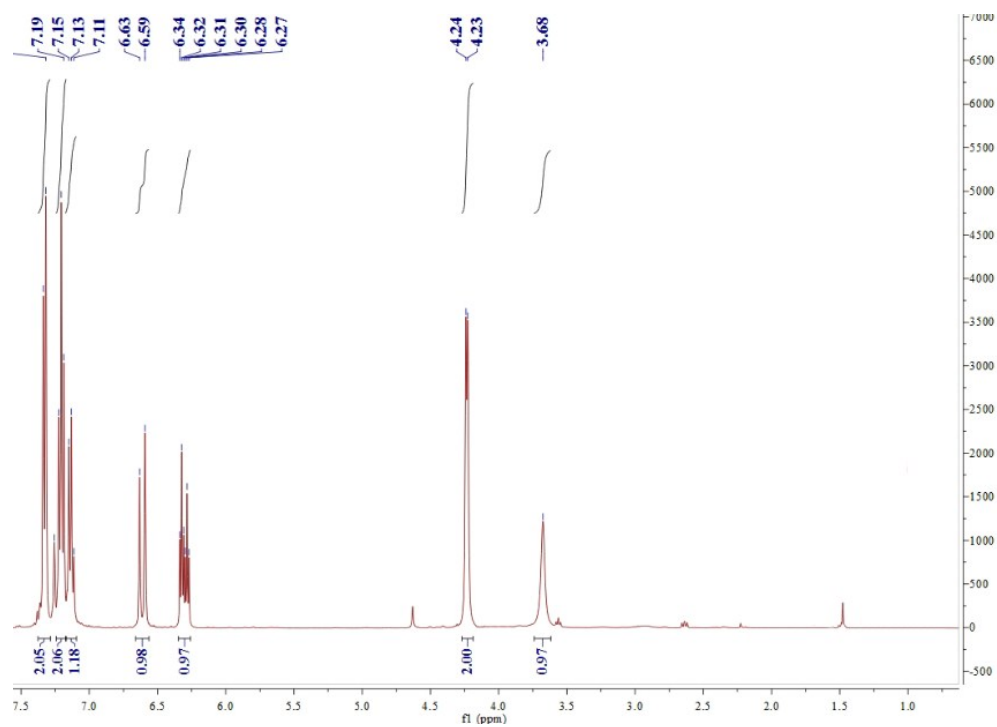
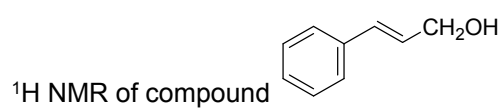
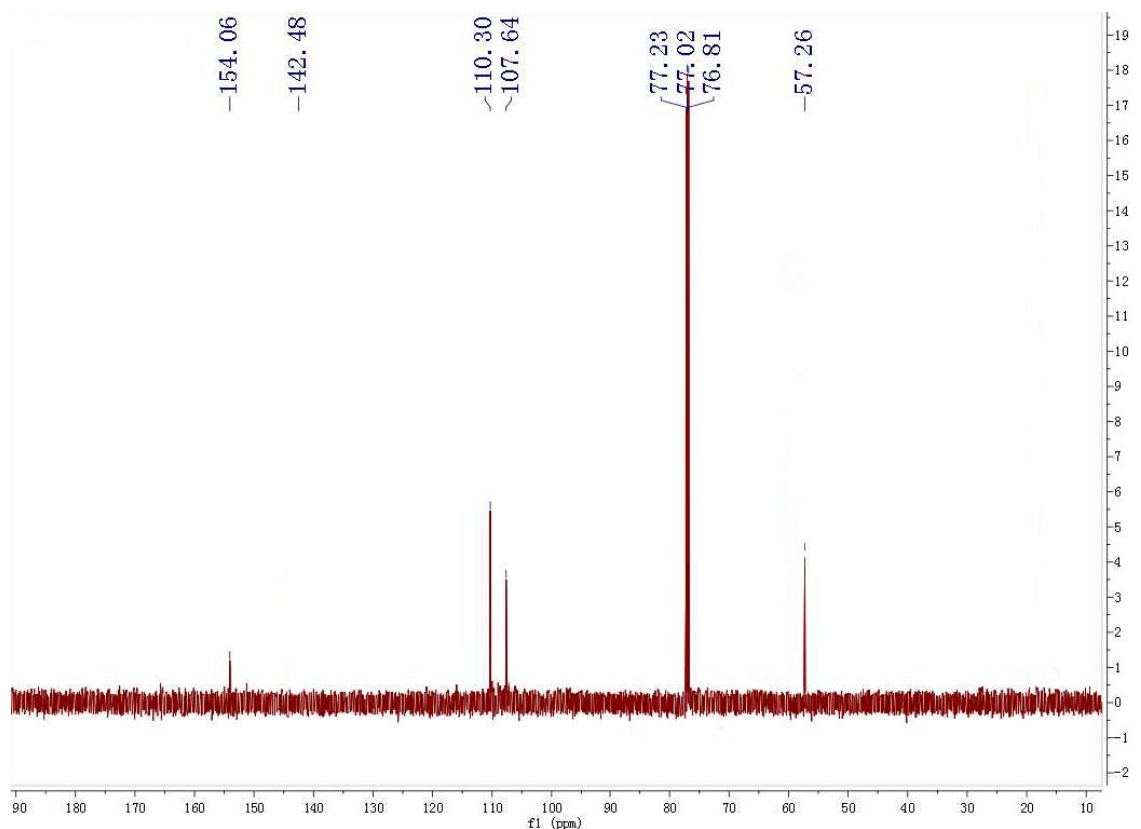
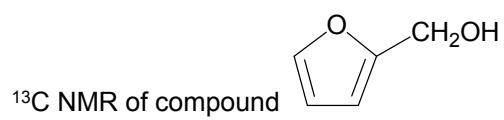


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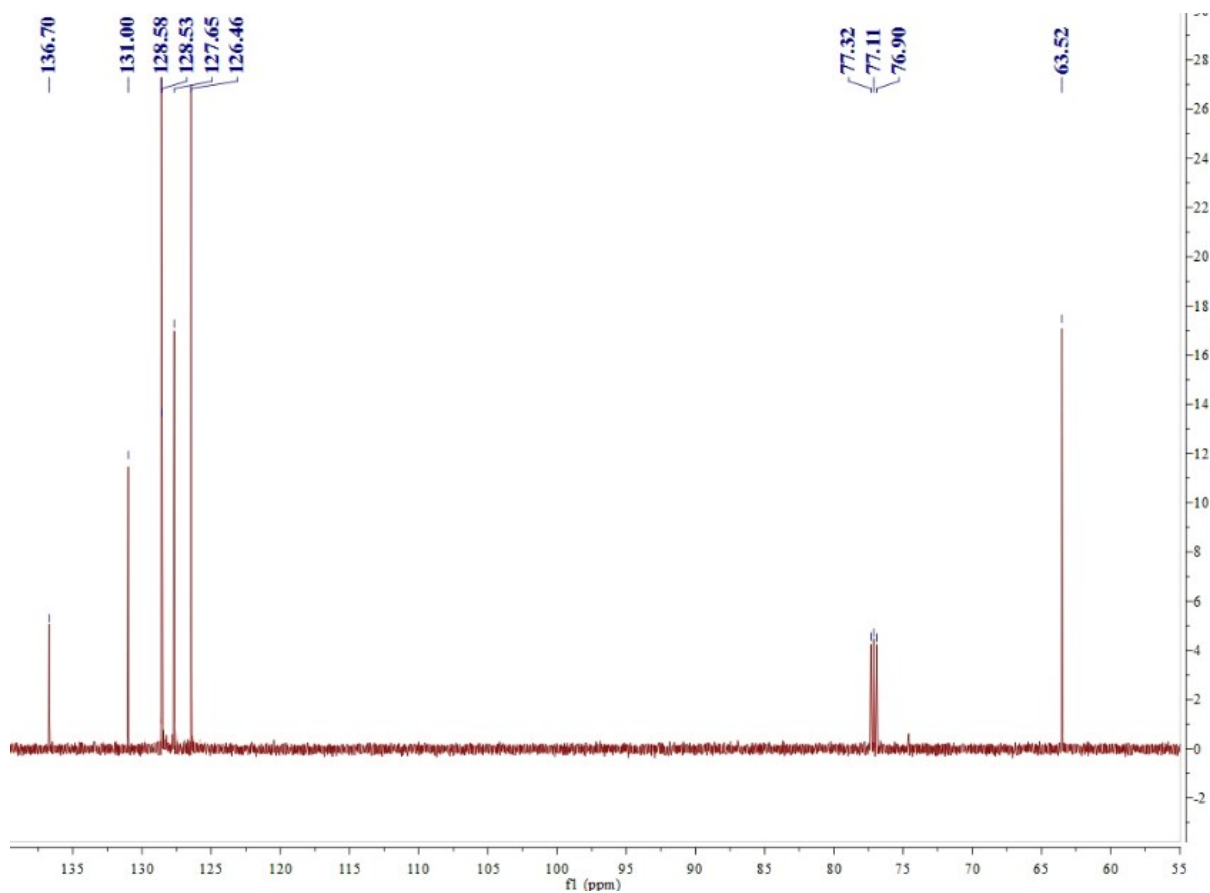


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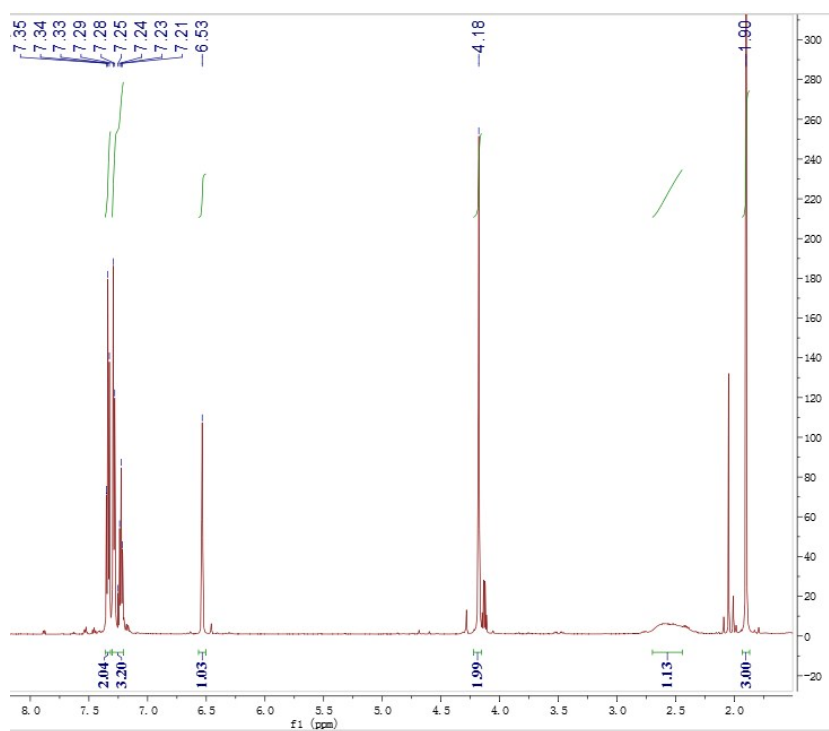




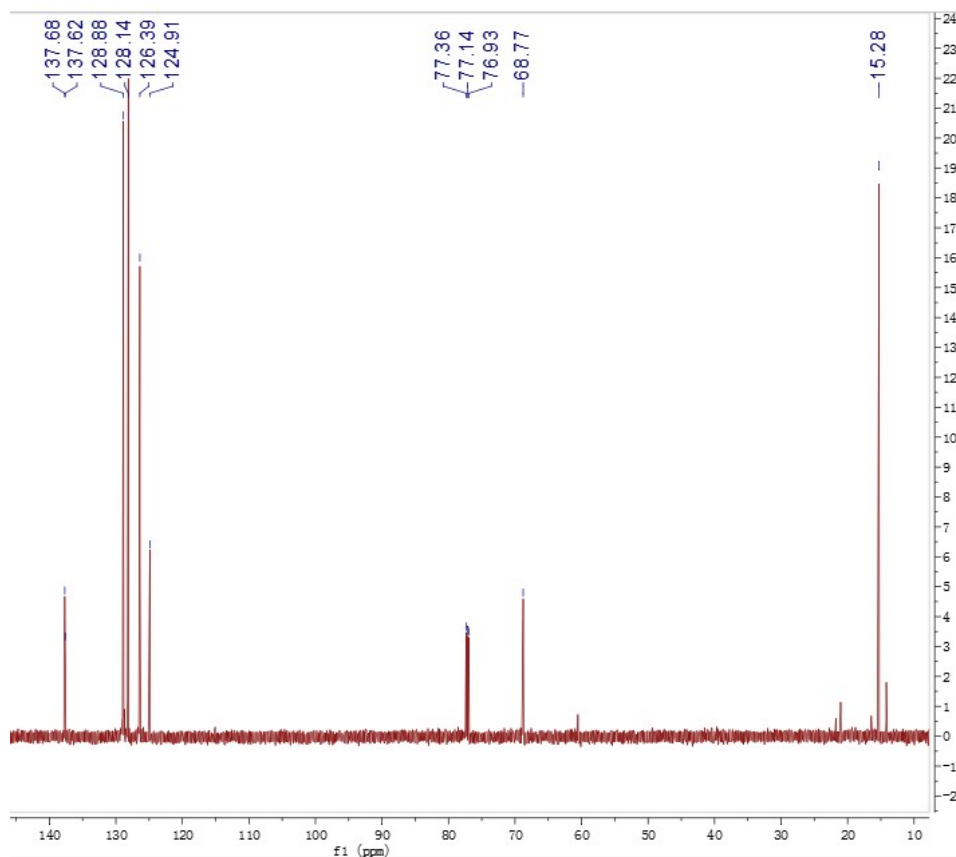
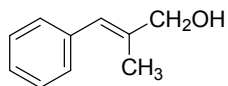
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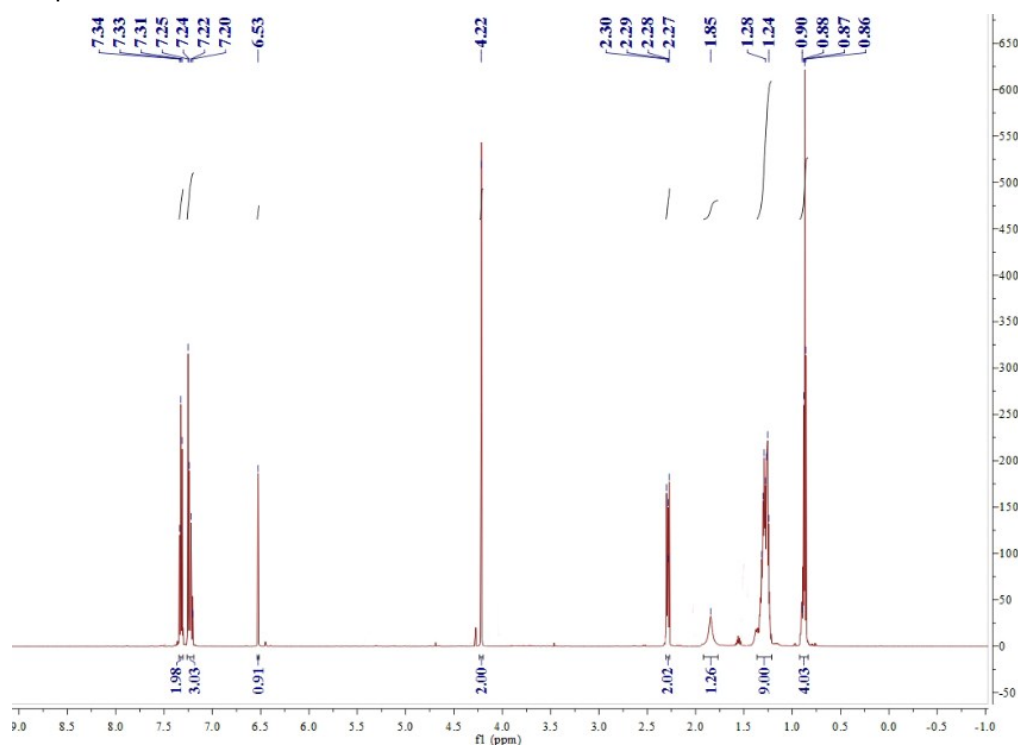
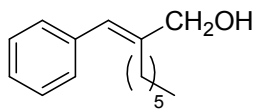
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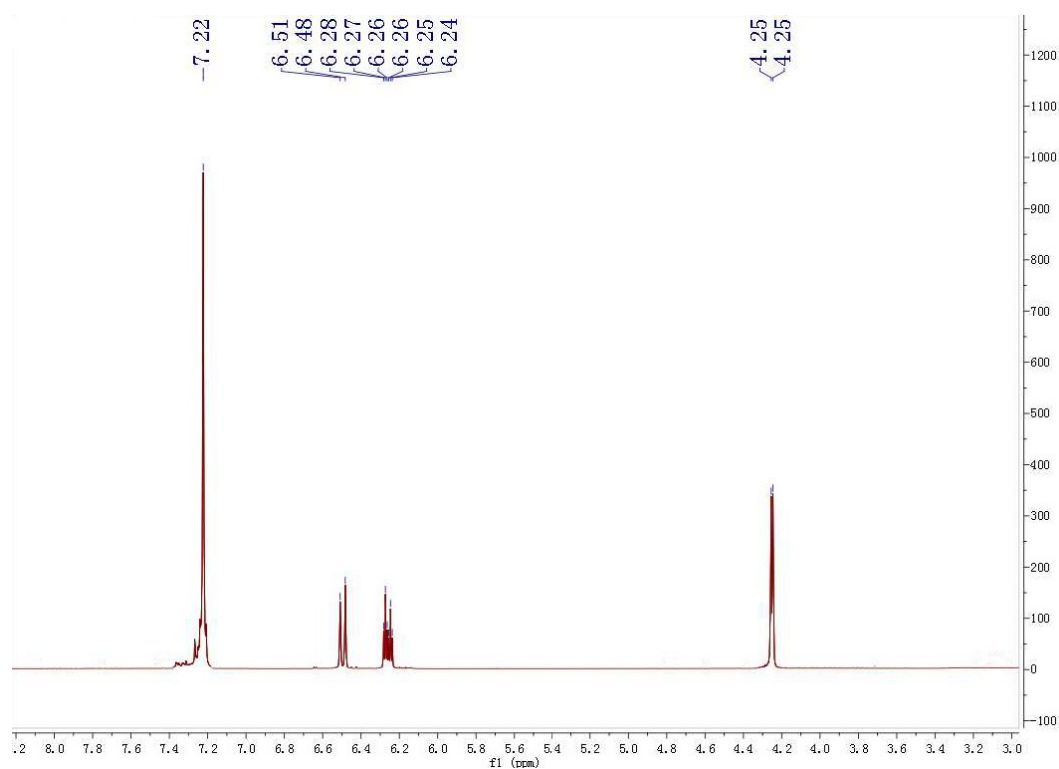
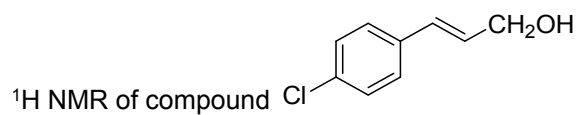
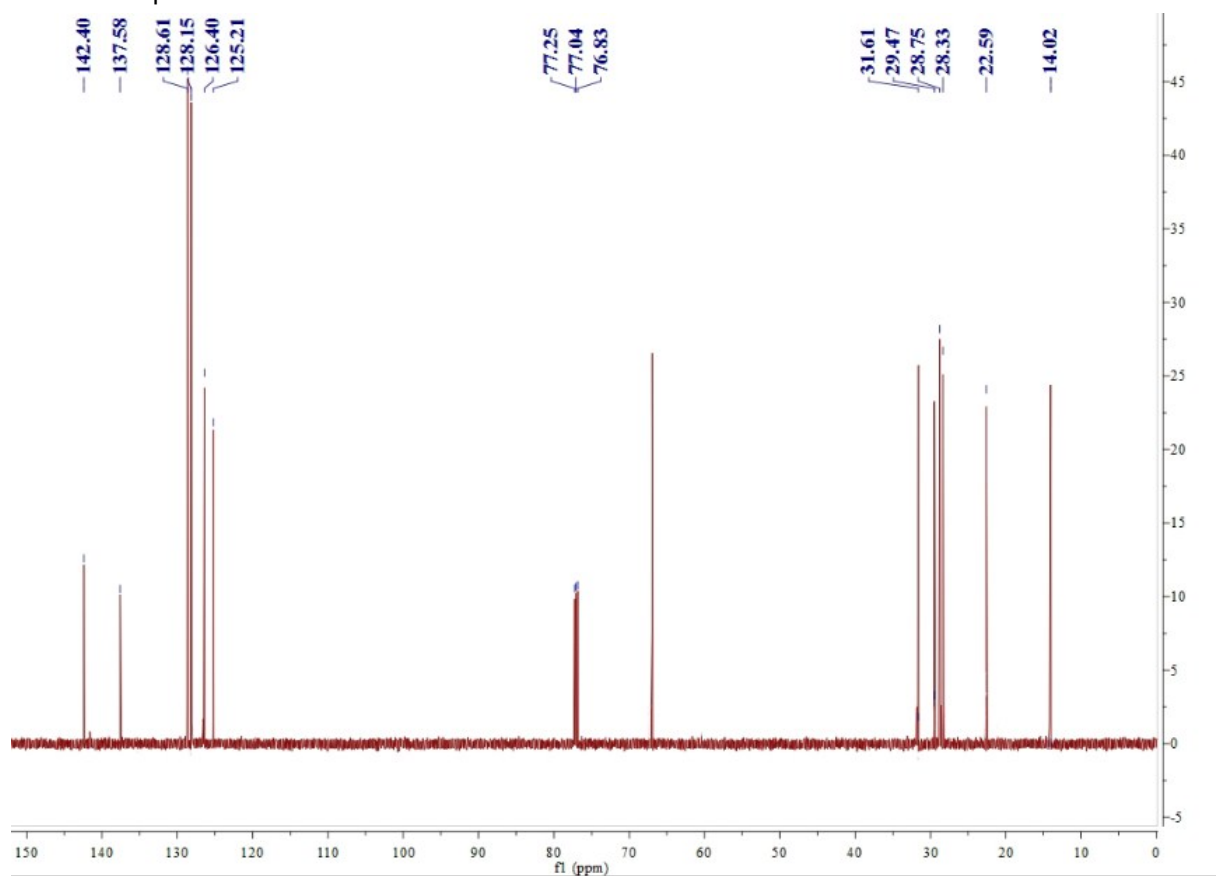
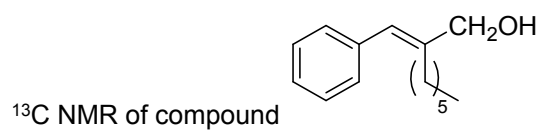


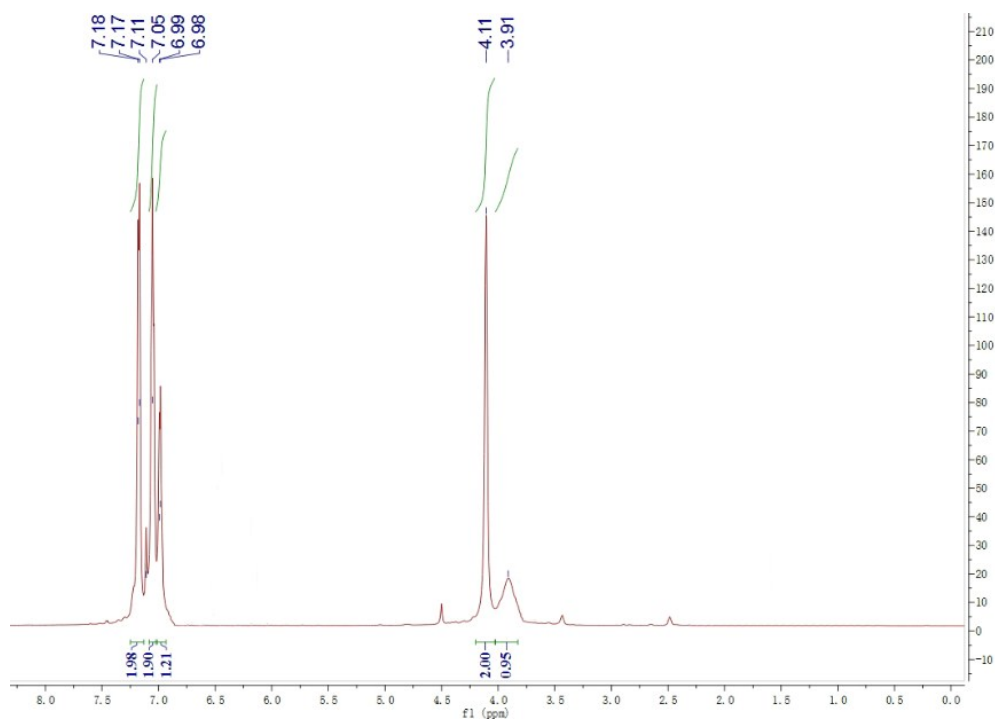
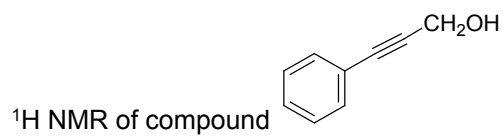
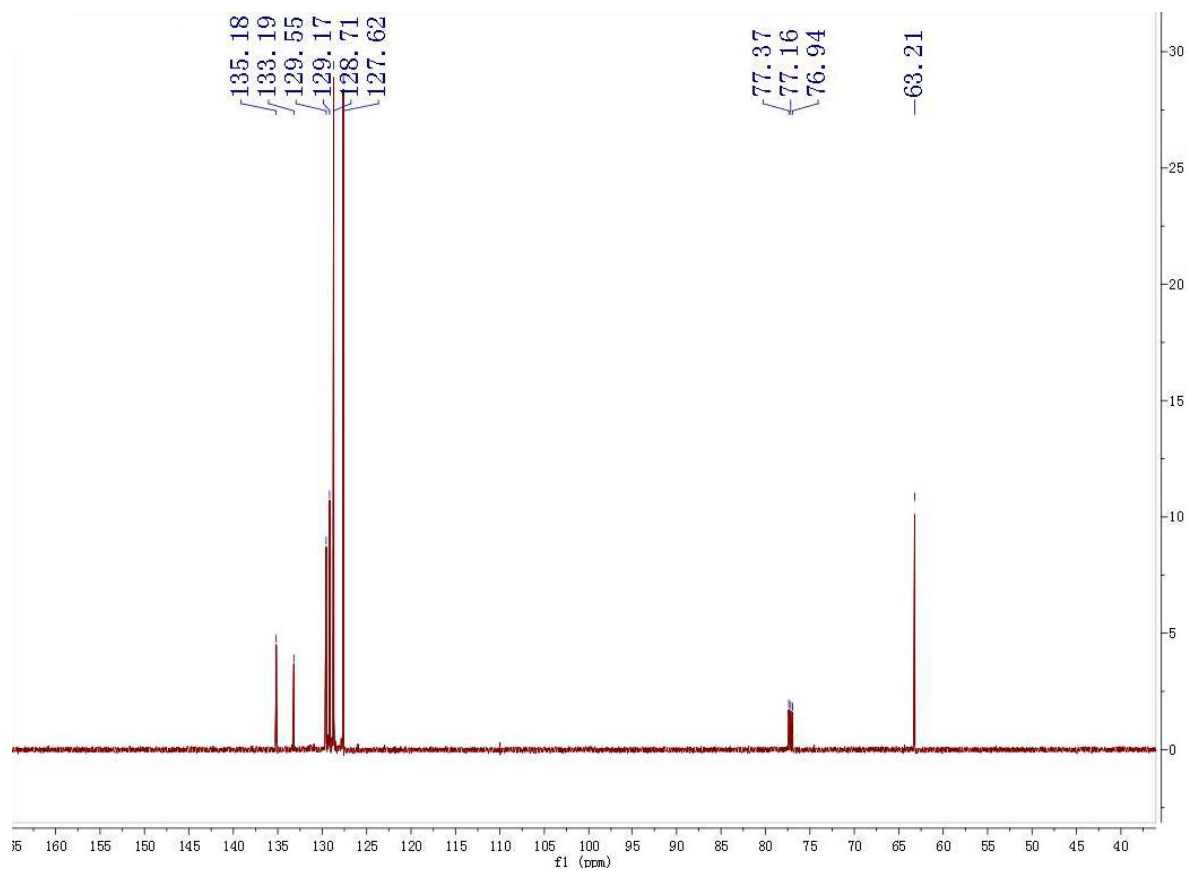
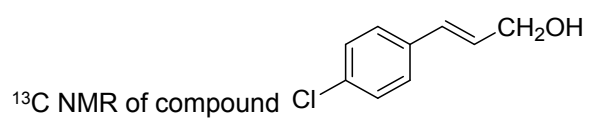
¹³C NMR of compound



¹H NMR of compound







¹³C NMR of compound

