

## Supporting Information

### **Boron Lewis Acid Catalysis Enables the Direct Cyanation of Benzyl Alcohols by means of Isonitrile as Cyanide Source**

**Tong-Tong Xu, Jin-Lan Zhou, Guang-Yuan Cong, Jiang-Yi-Hui Sheng,  
Shi-Qi Wang, Yating Ma, and Jian-Jun Feng\***

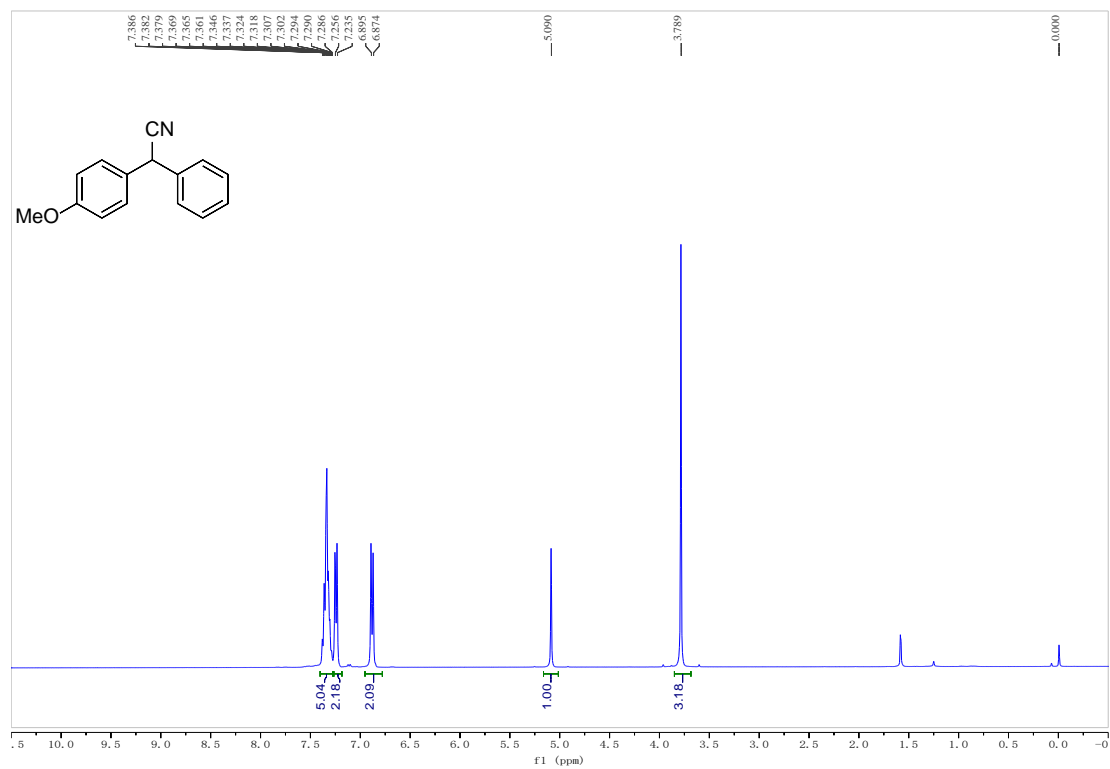
*State Key Laboratory of Chemo/Biosensing and Chemometrics, Advanced Catalytic Engineering Research Center of the Ministry of Education, College of Chemistry and Chemical Engineering, Hunan University, Changsha, Hunan 410082, P. R. China*

*jianjunfeng@hnu.edu.cn*

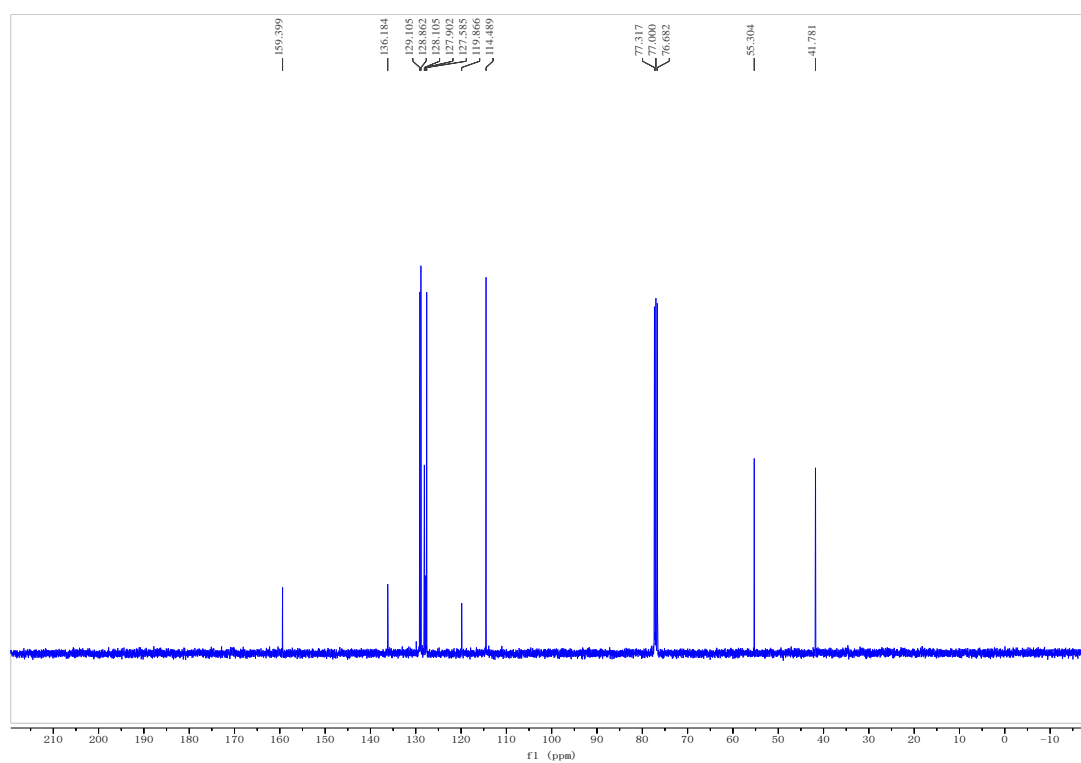
## NMR Spectra

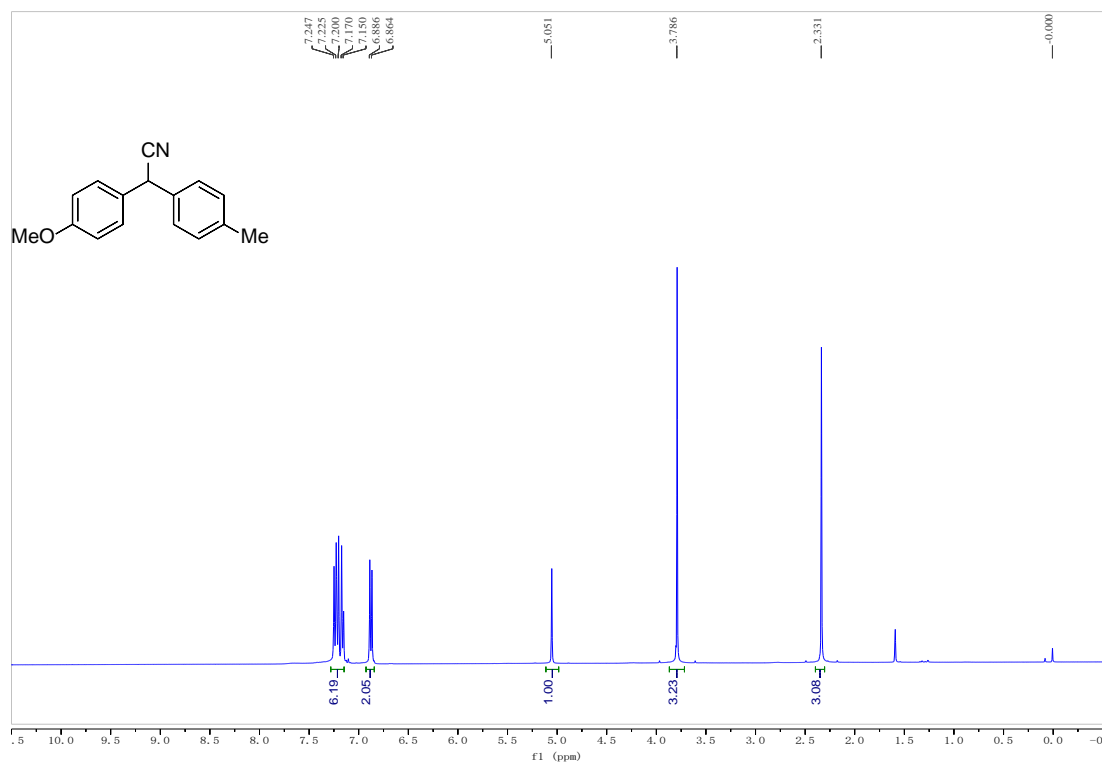
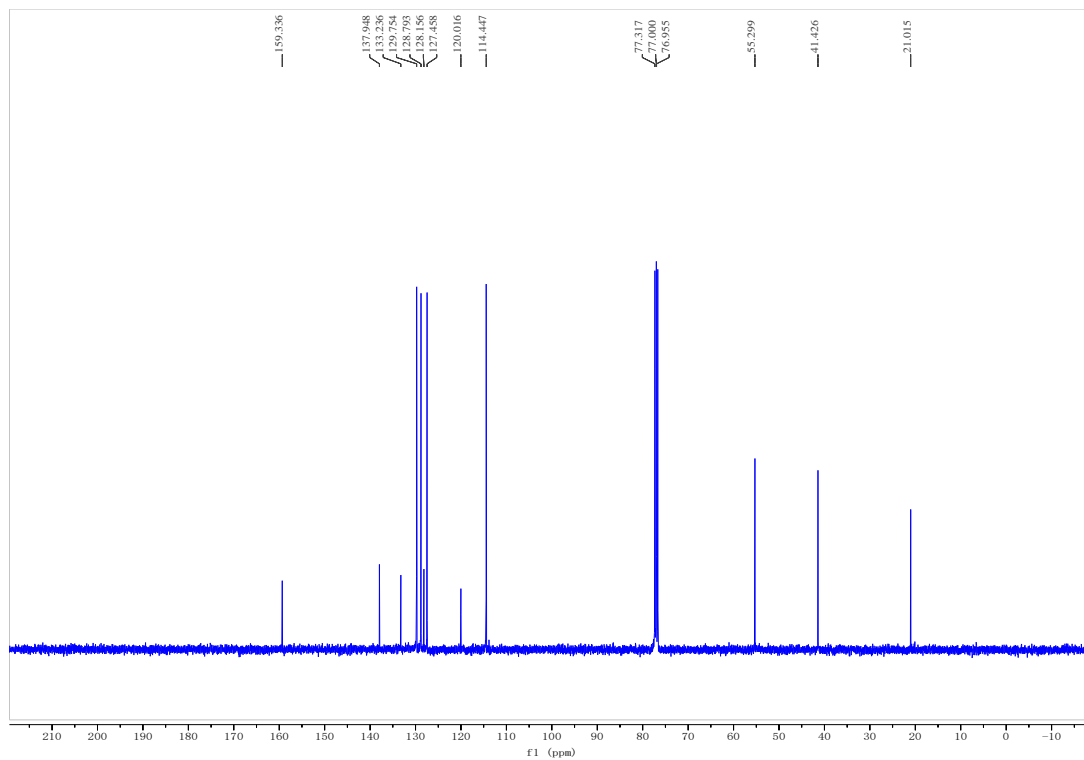
### $^1\text{H}$ and $^{13}\text{C}$ NMR Spectra for Compound 3a:

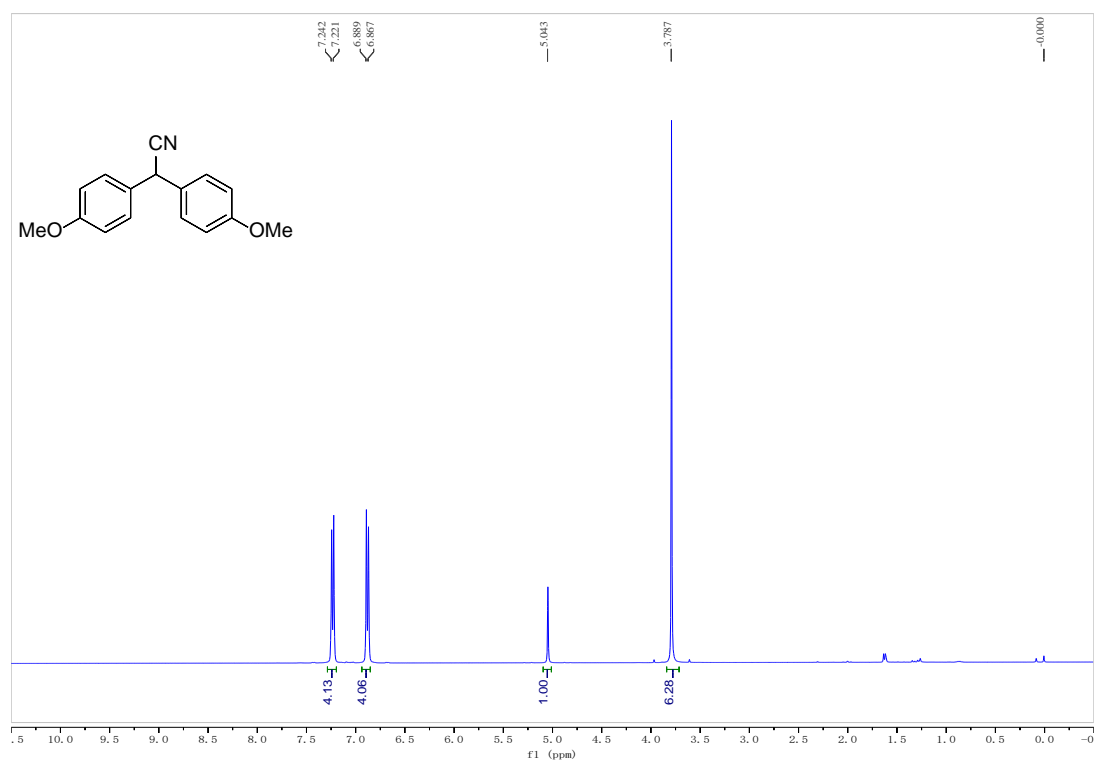
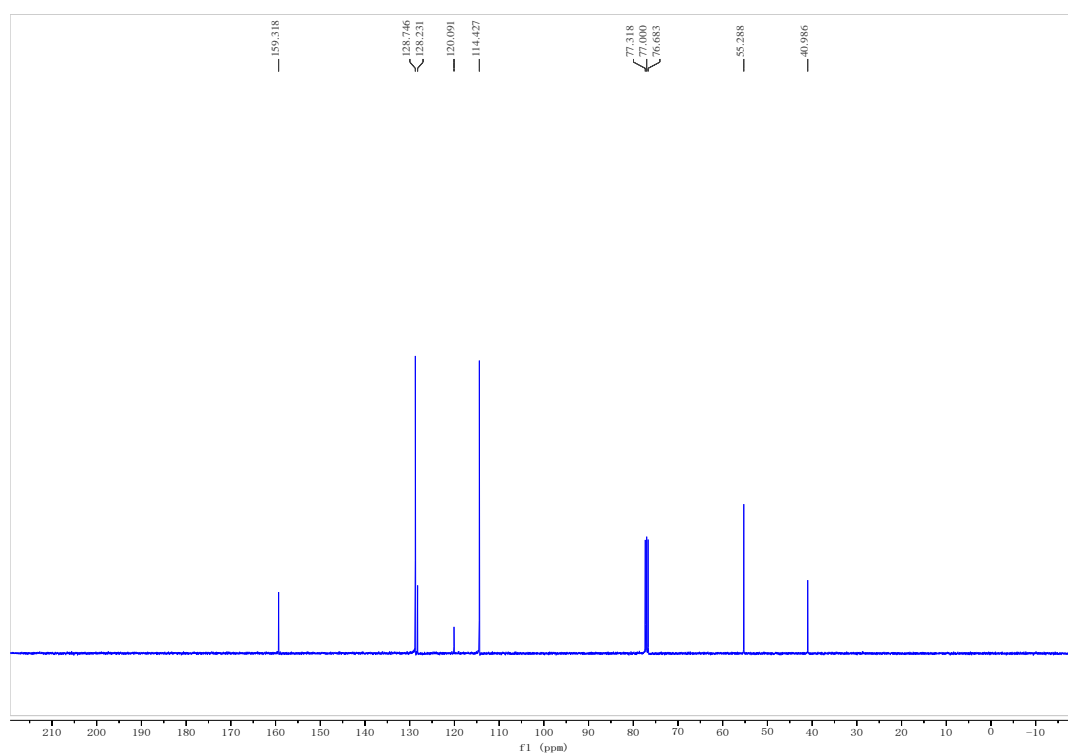
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

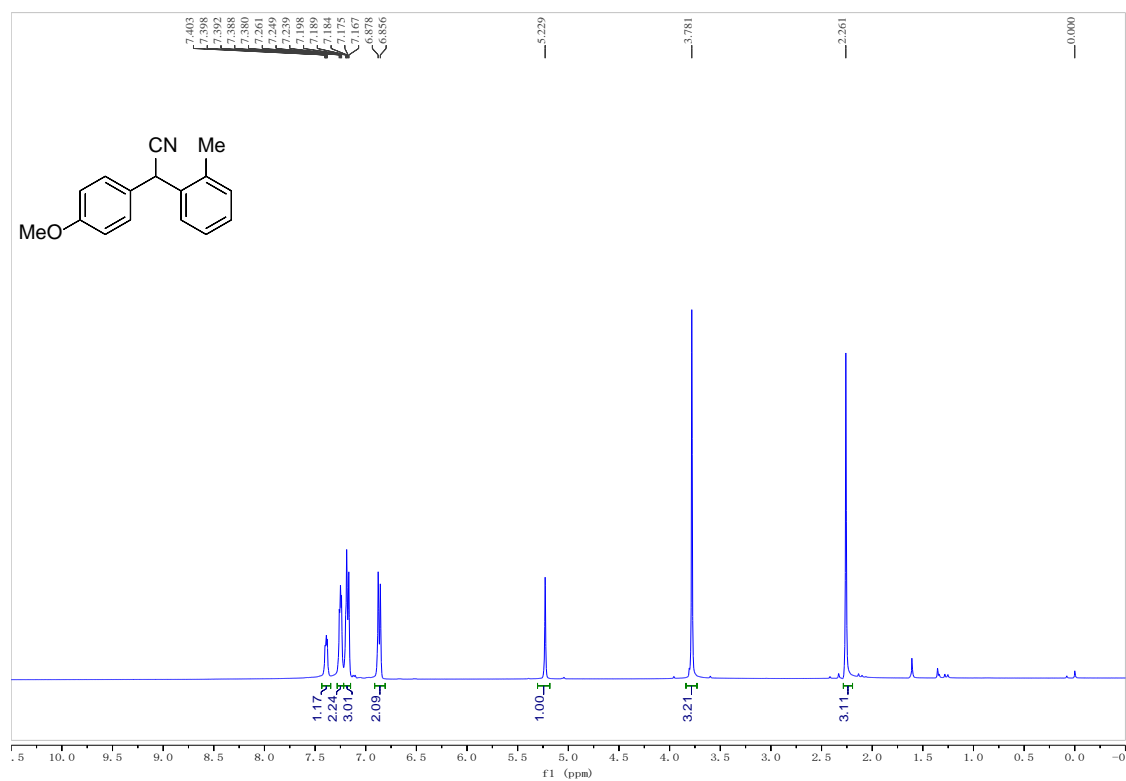
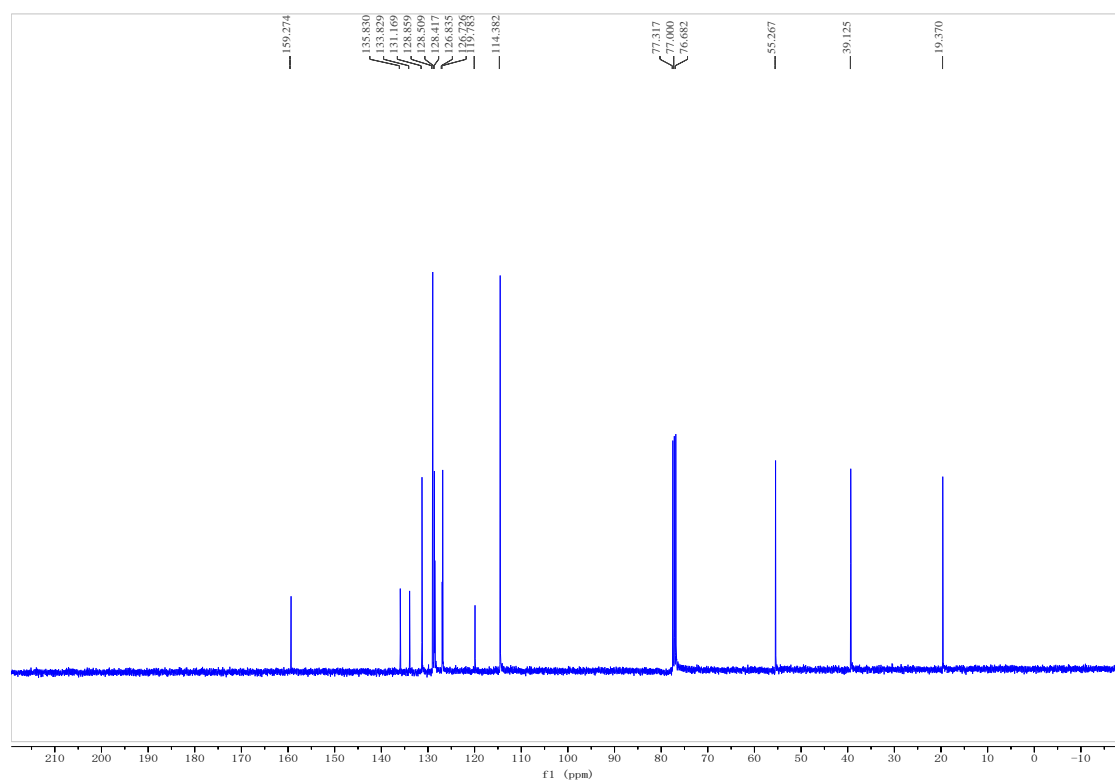


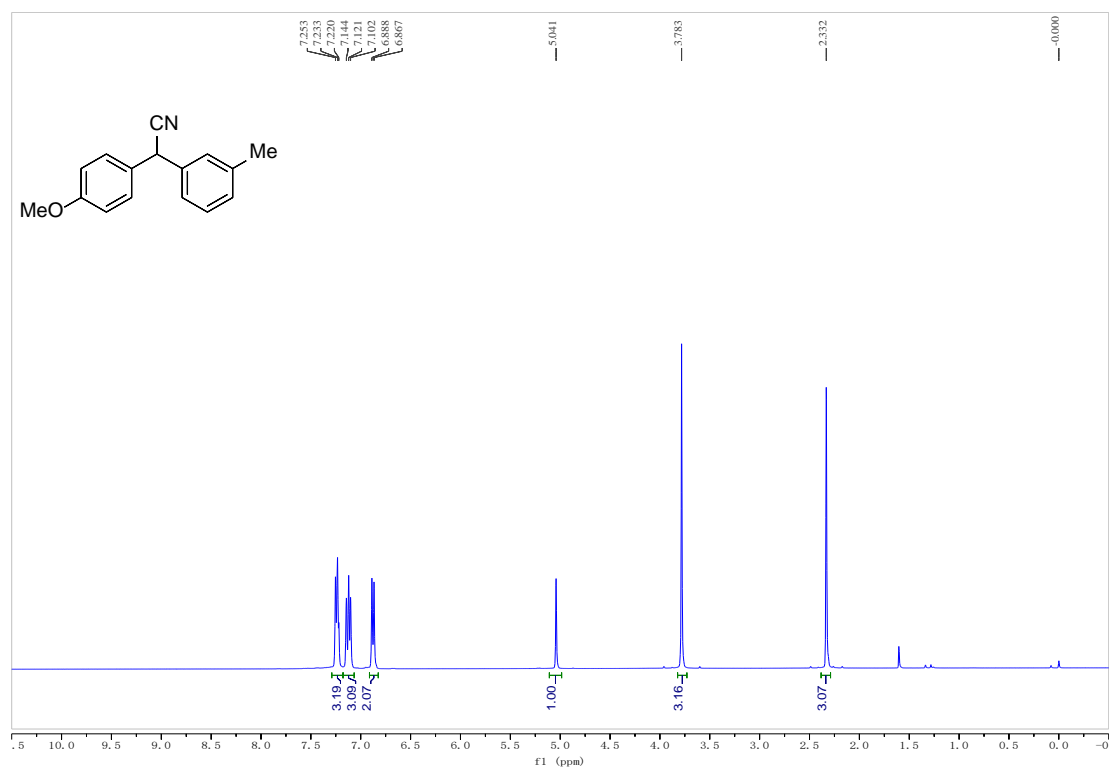
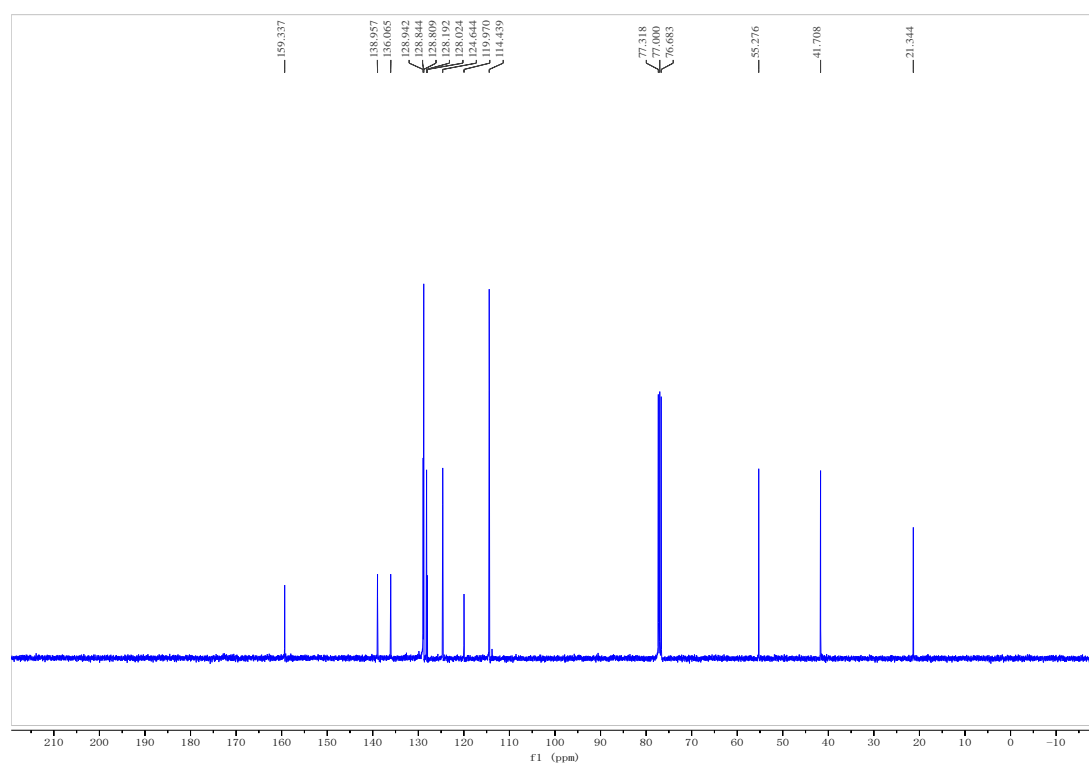
$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

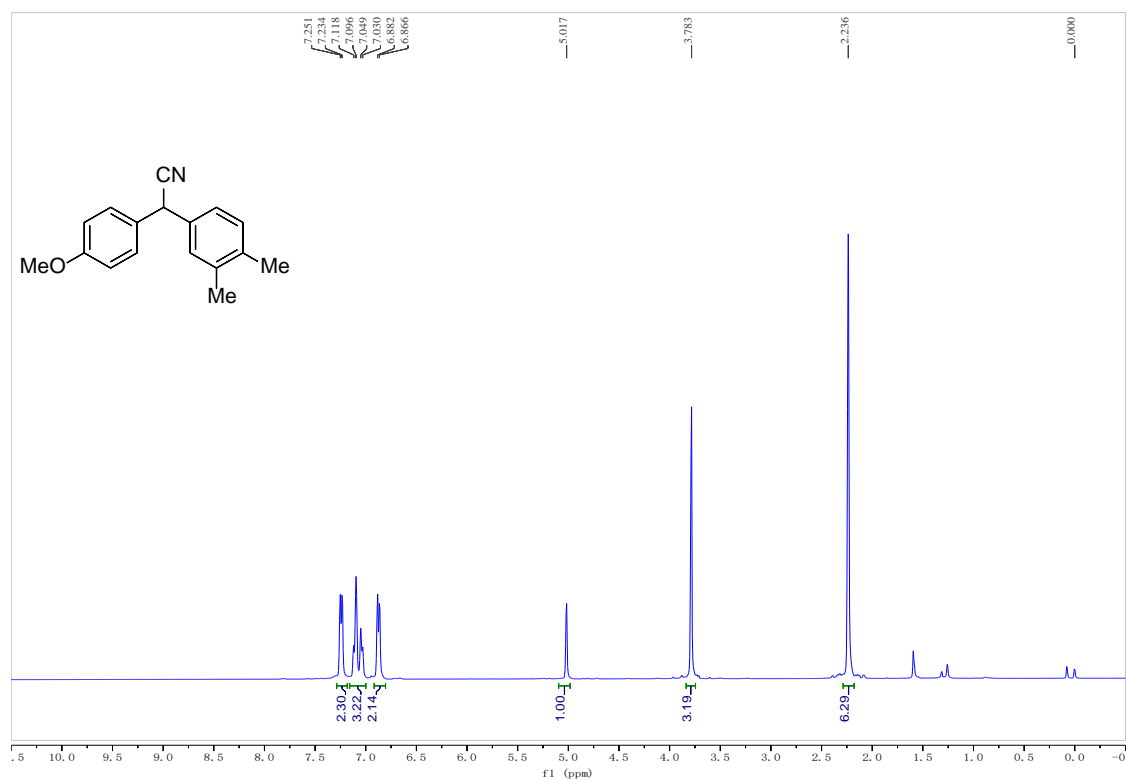
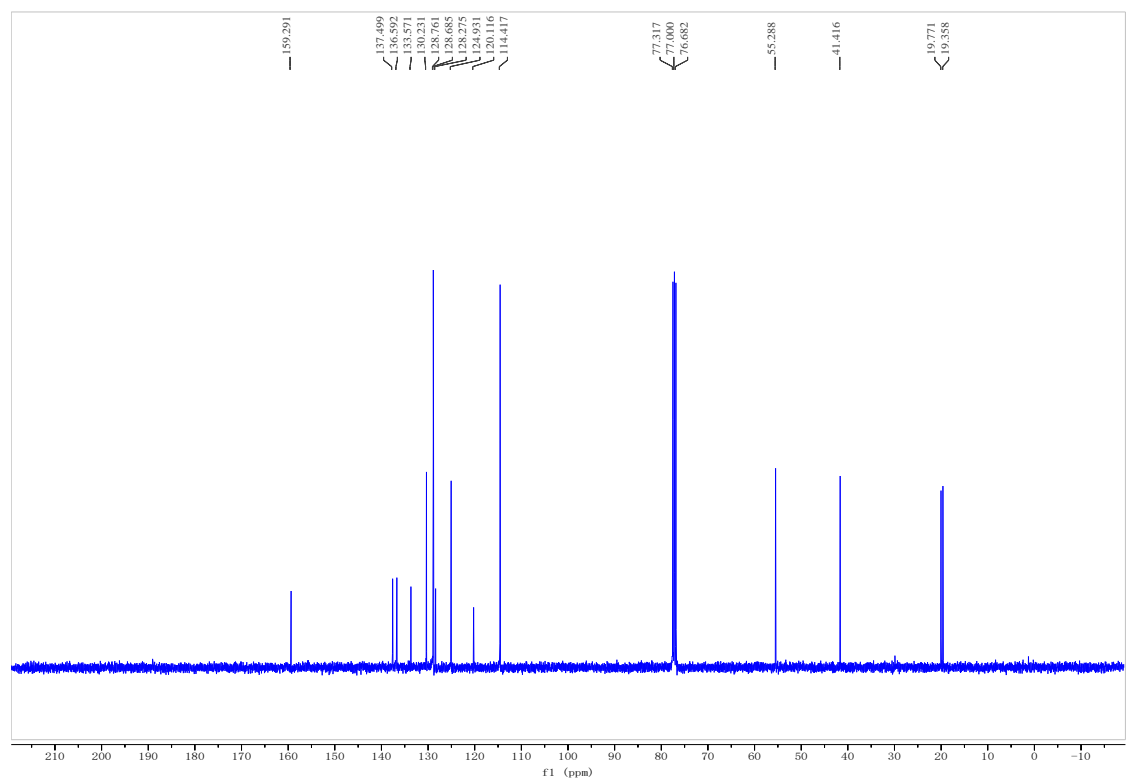


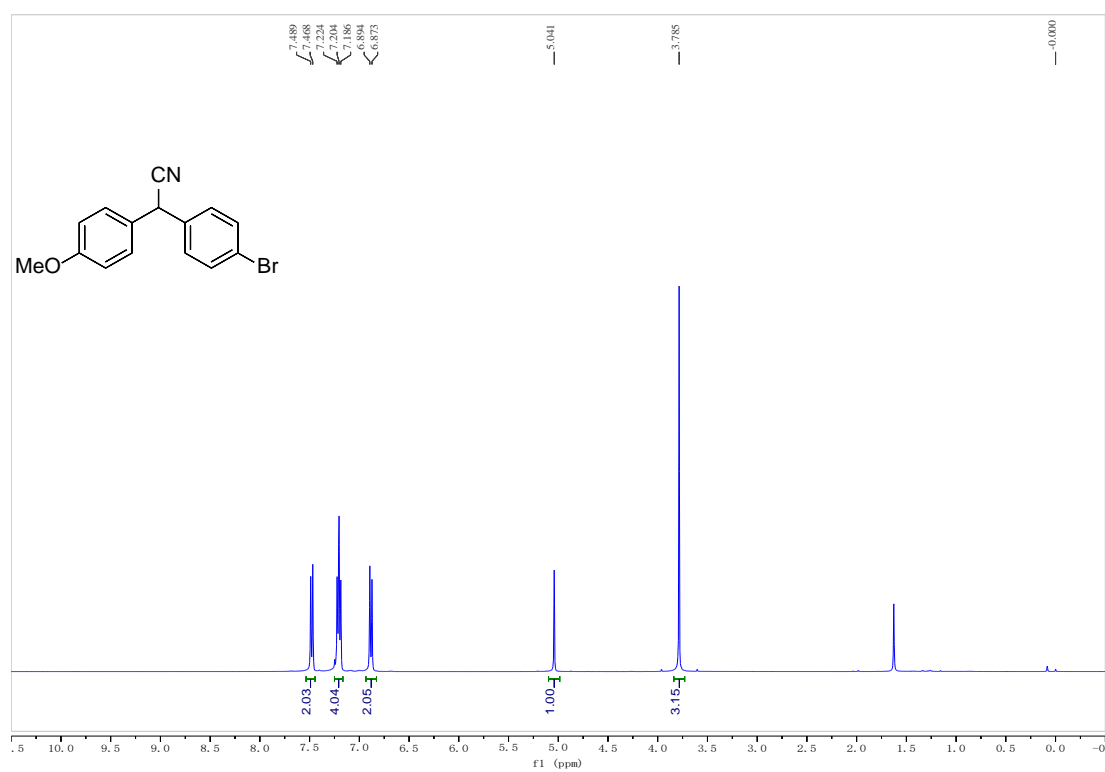
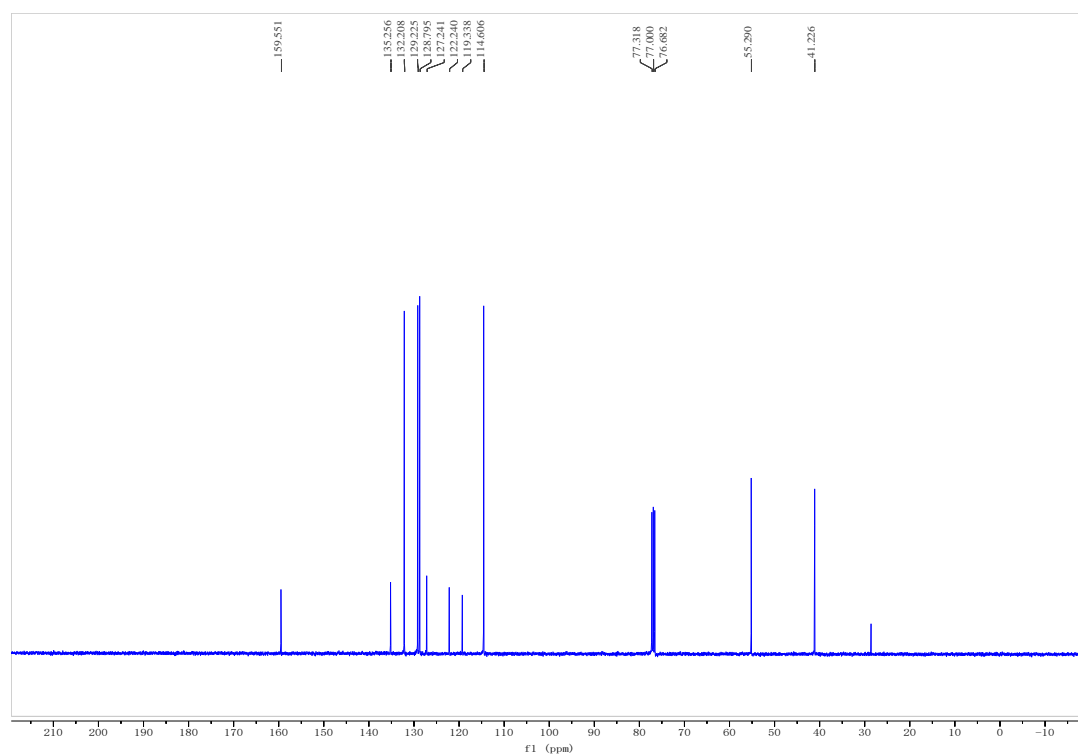
**$^1\text{H}$  and  $^{13}\text{C}$  NMR Spectra for Compound 3b:** $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

**$^1\text{H}$  and  $^{13}\text{C}$  NMR Spectra for Compound 3c:** $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

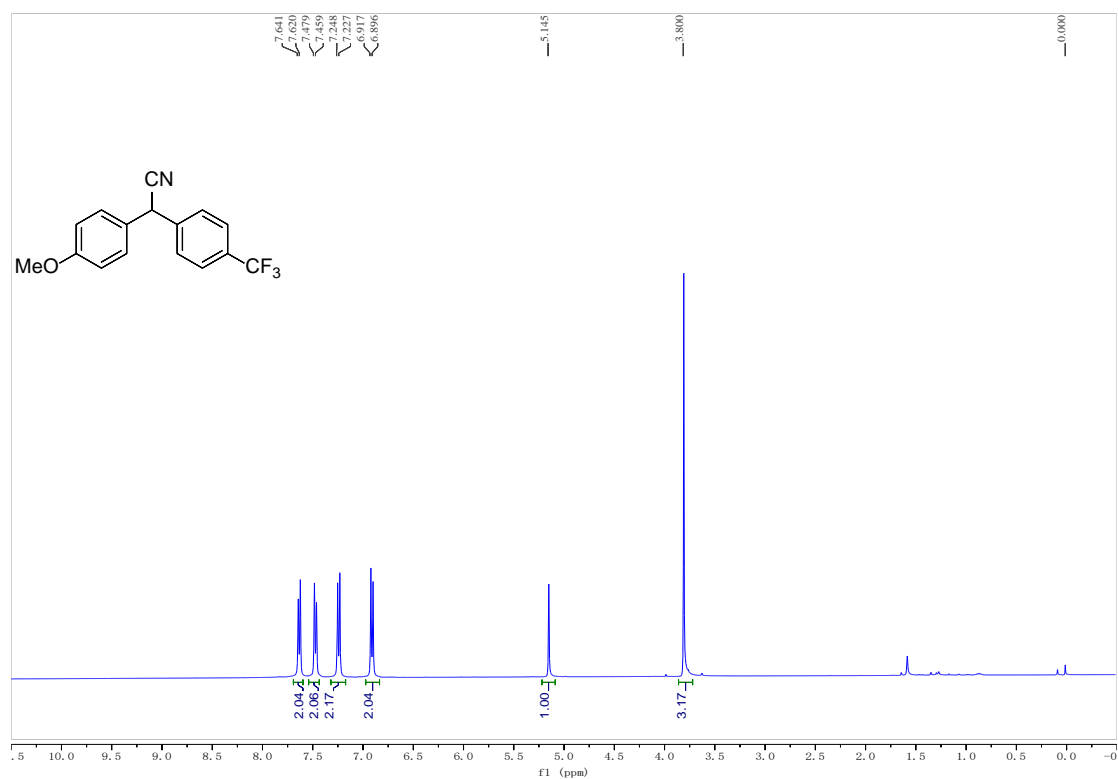
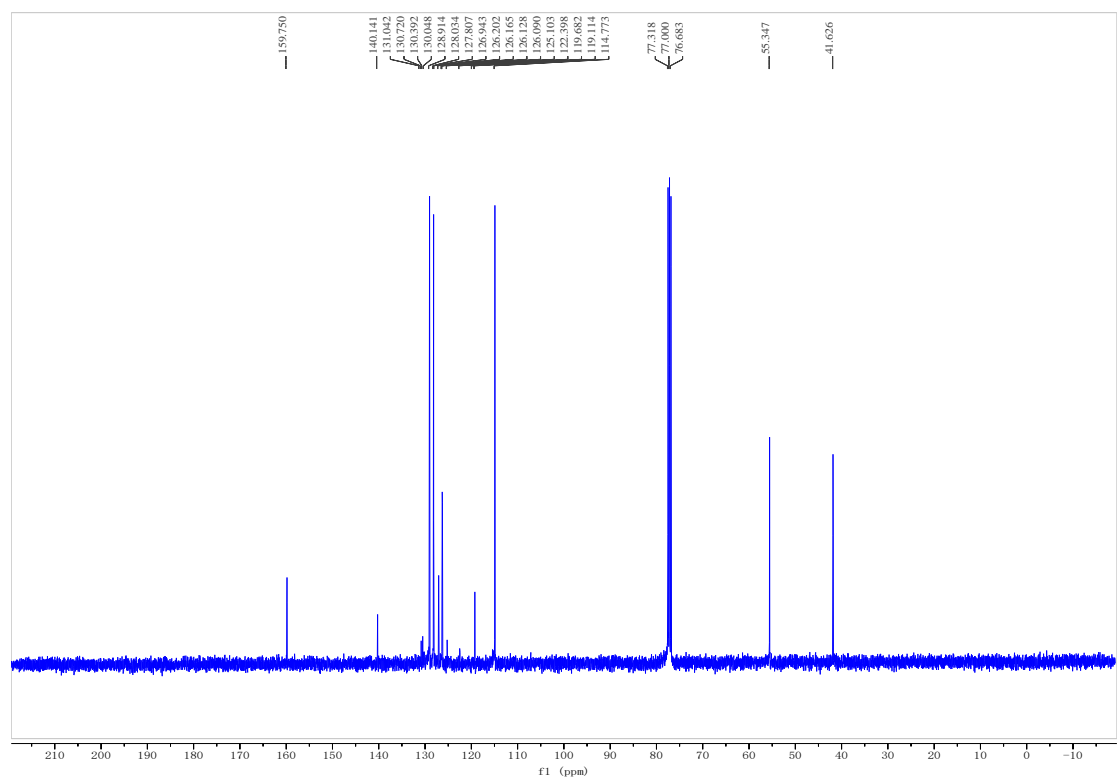
**$^1\text{H}$  and  $^{13}\text{C}$  NMR Spectra for Compound 3d:** $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

**$^1\text{H}$  and  $^{13}\text{C}$  NMR Spectra for Compound 3e:** $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

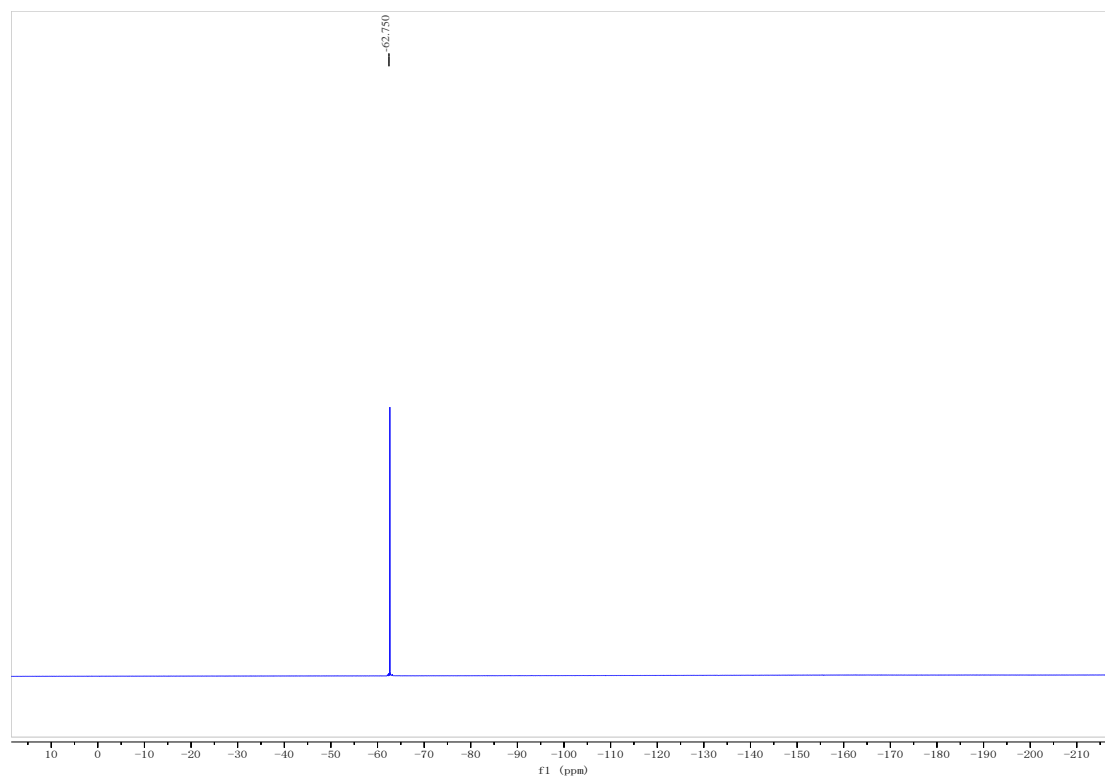
**$^1\text{H}$  and  $^{13}\text{C}$  NMR Spectra for Compound 3f:** $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

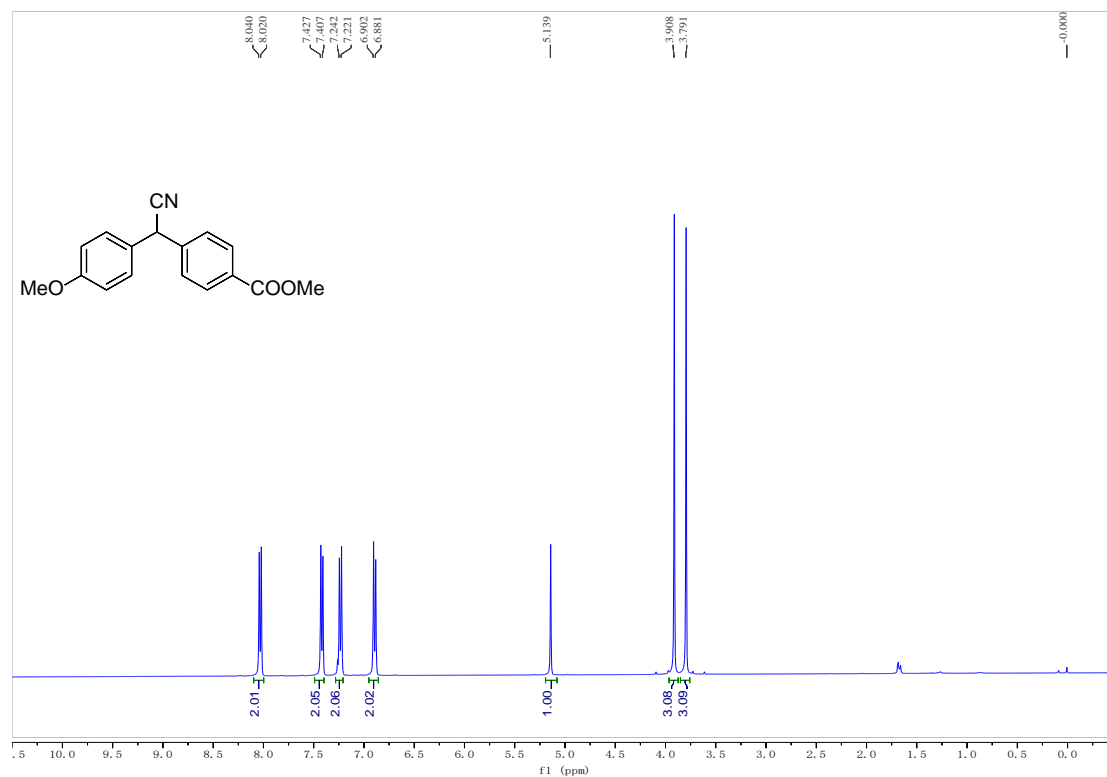
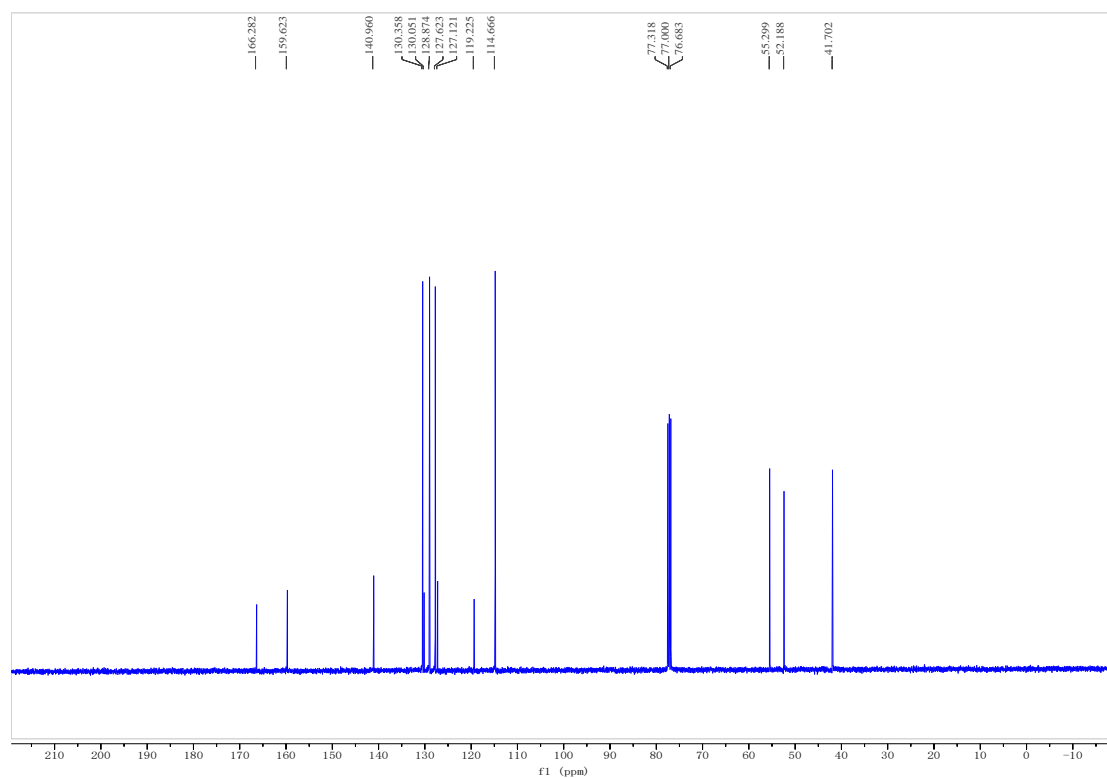
**$^1\text{H}$  and  $^{13}\text{C}$  NMR Spectra for Compound 3g:** $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

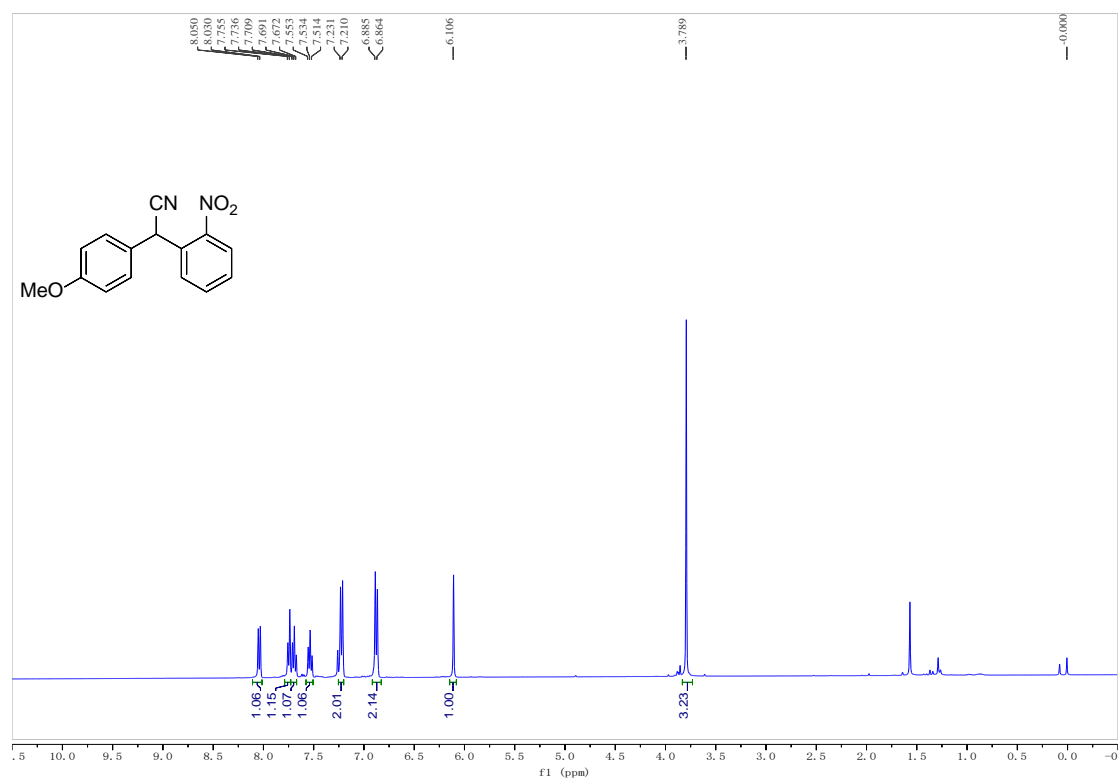
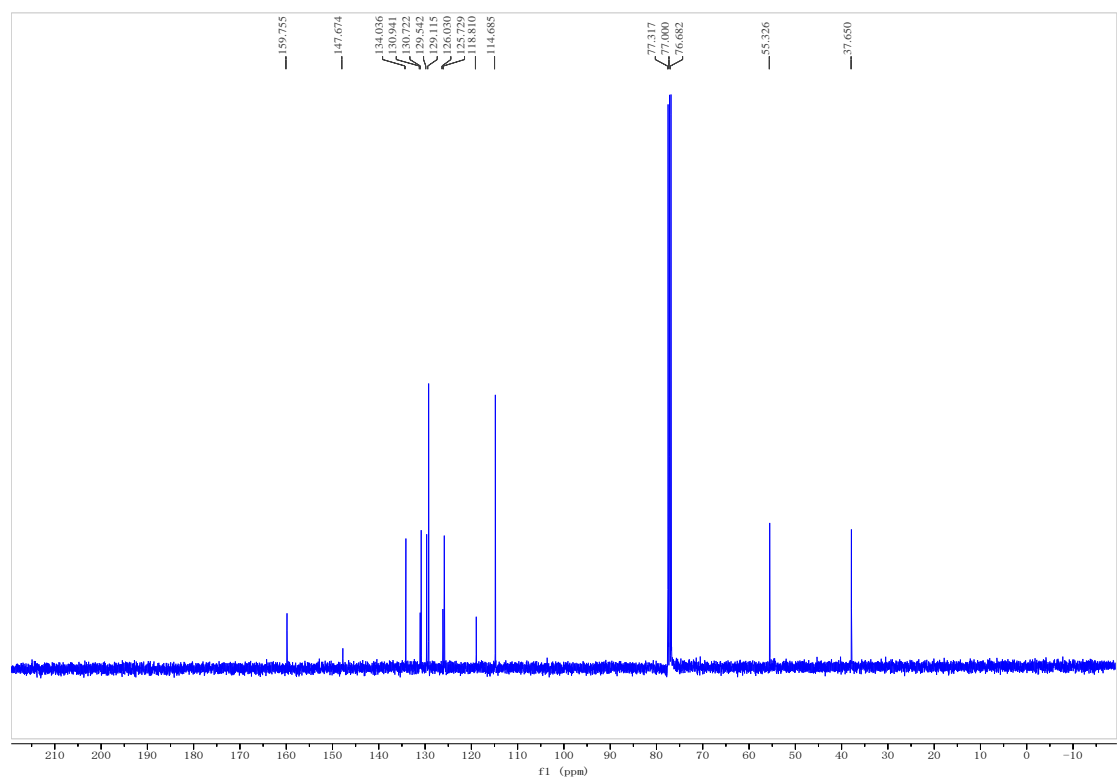


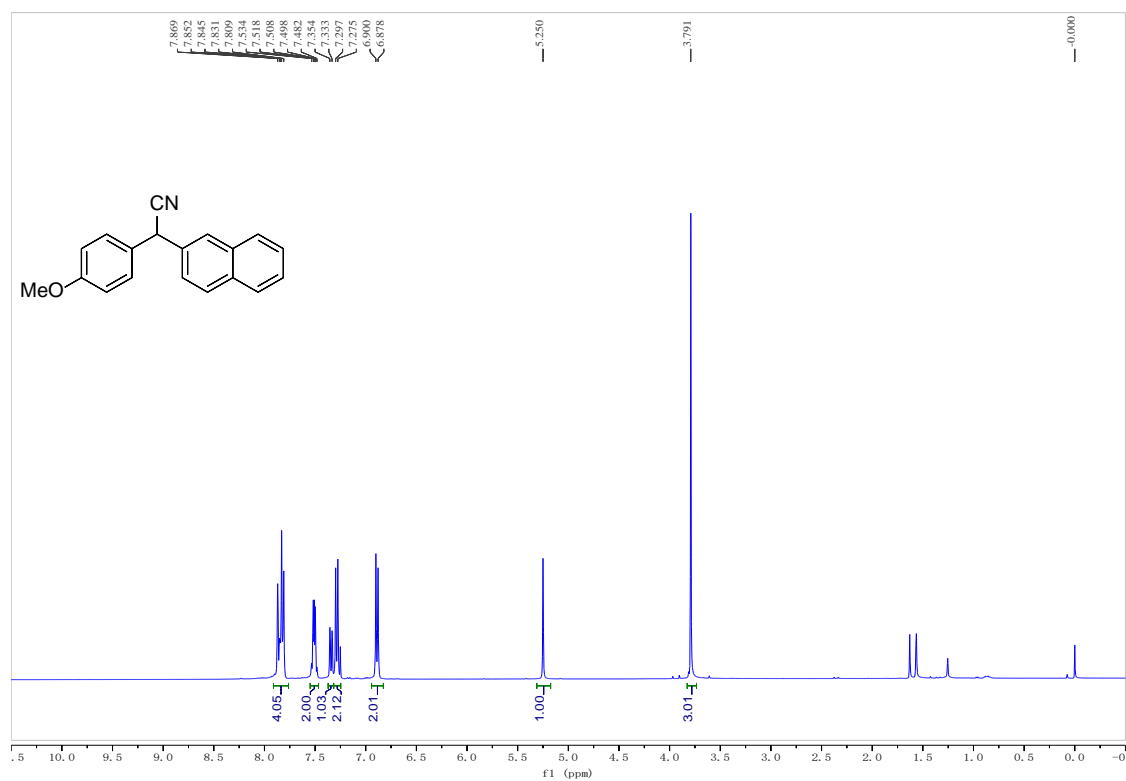
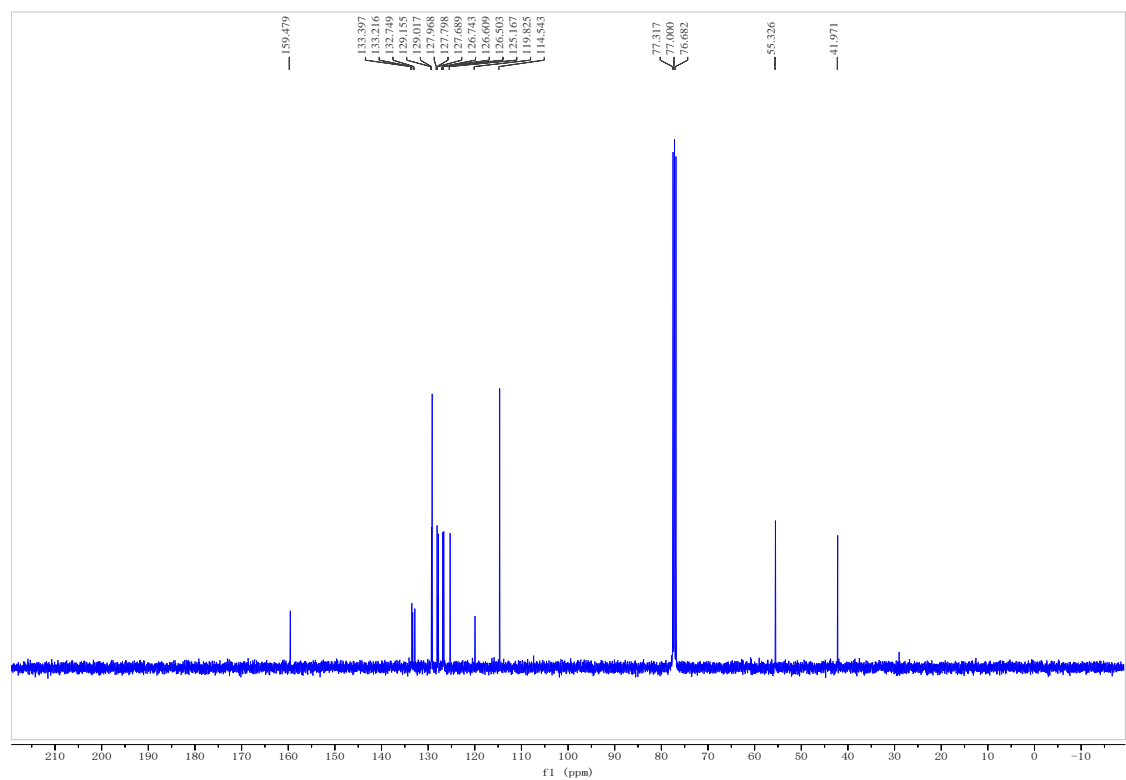
**$^1\text{H}$ ,  $^{13}\text{C}$  and  $^{19}\text{F}$  NMR Spectra for Compound 3h:** $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

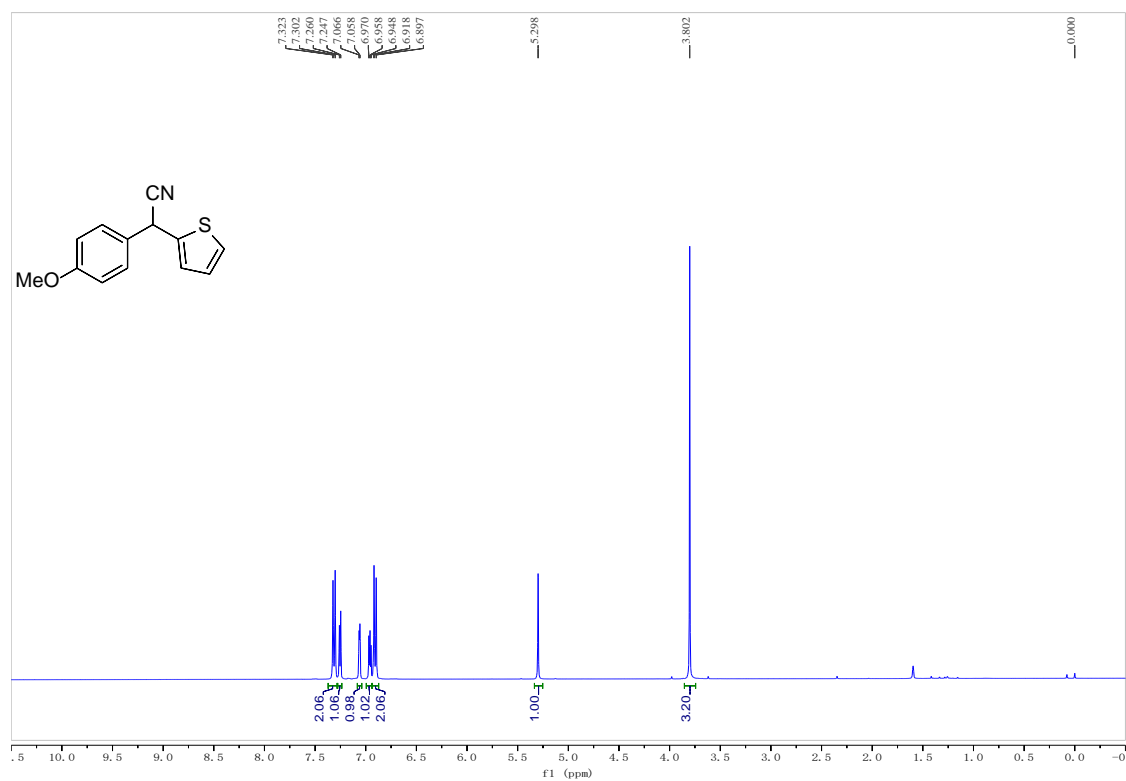
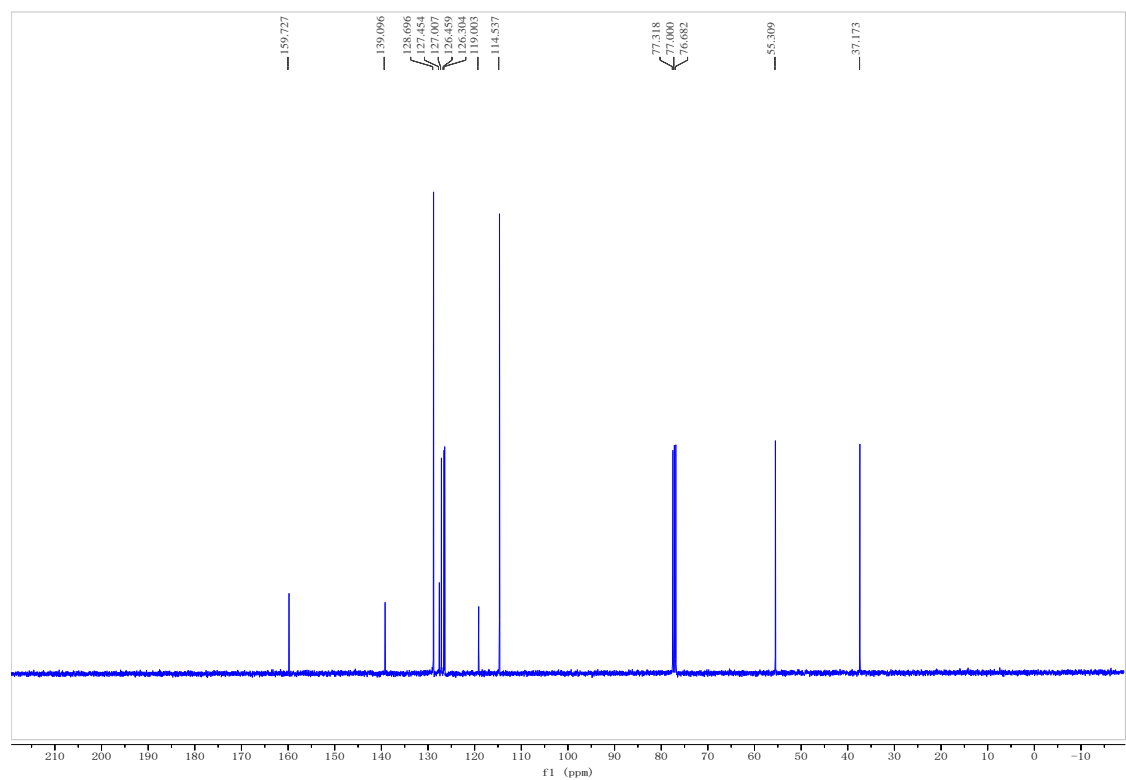
$^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )

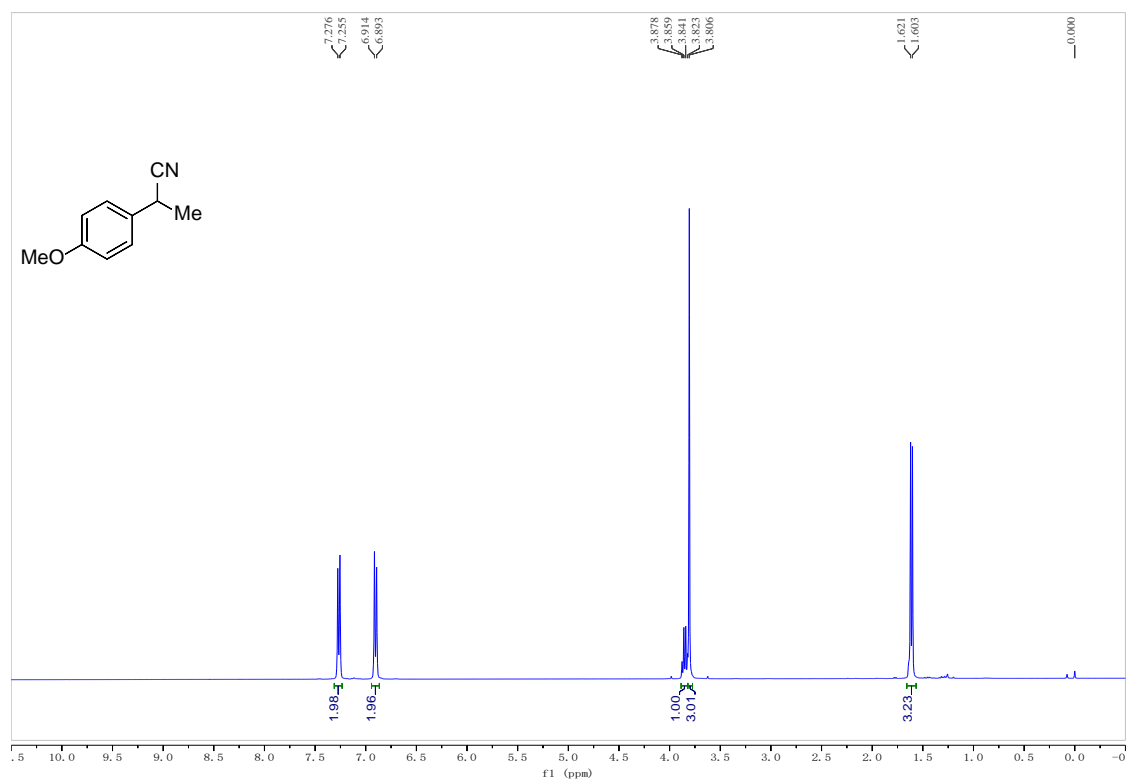
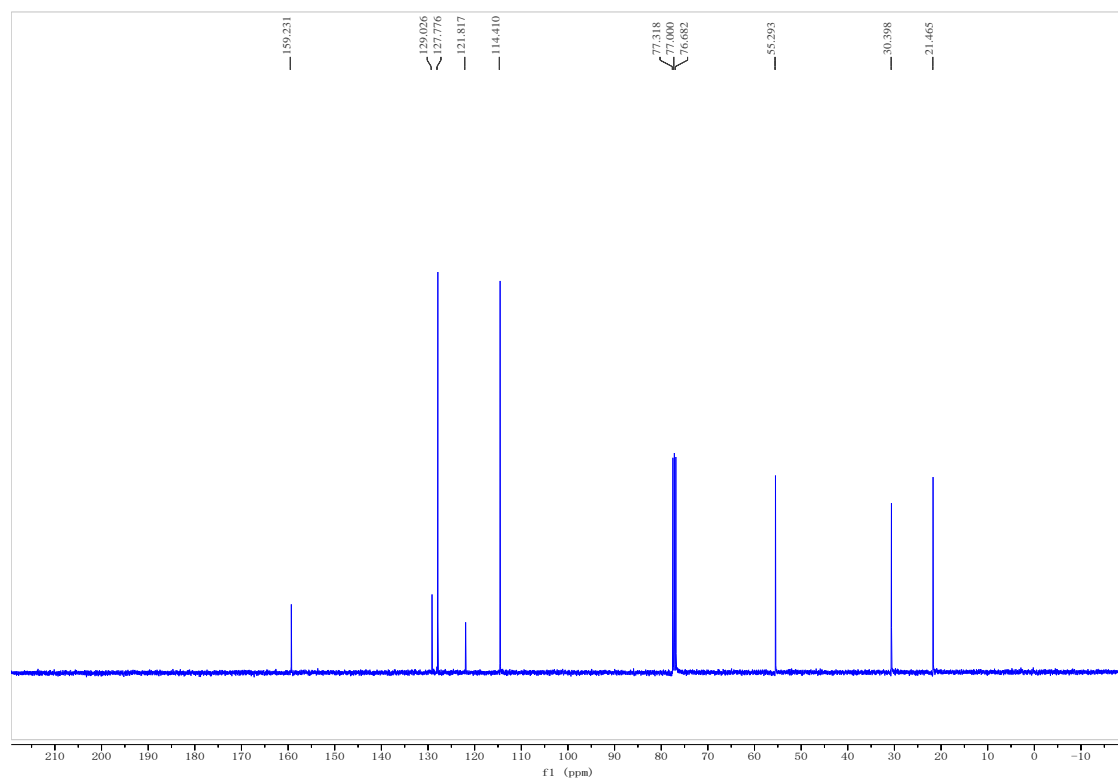


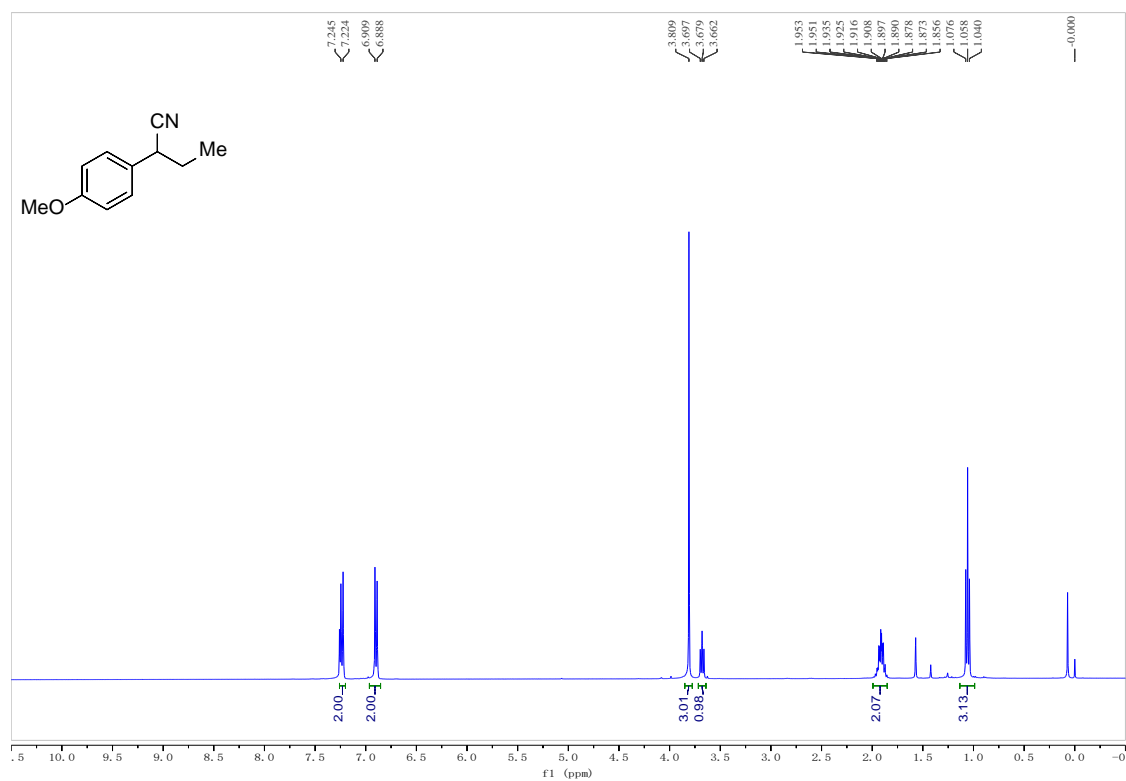
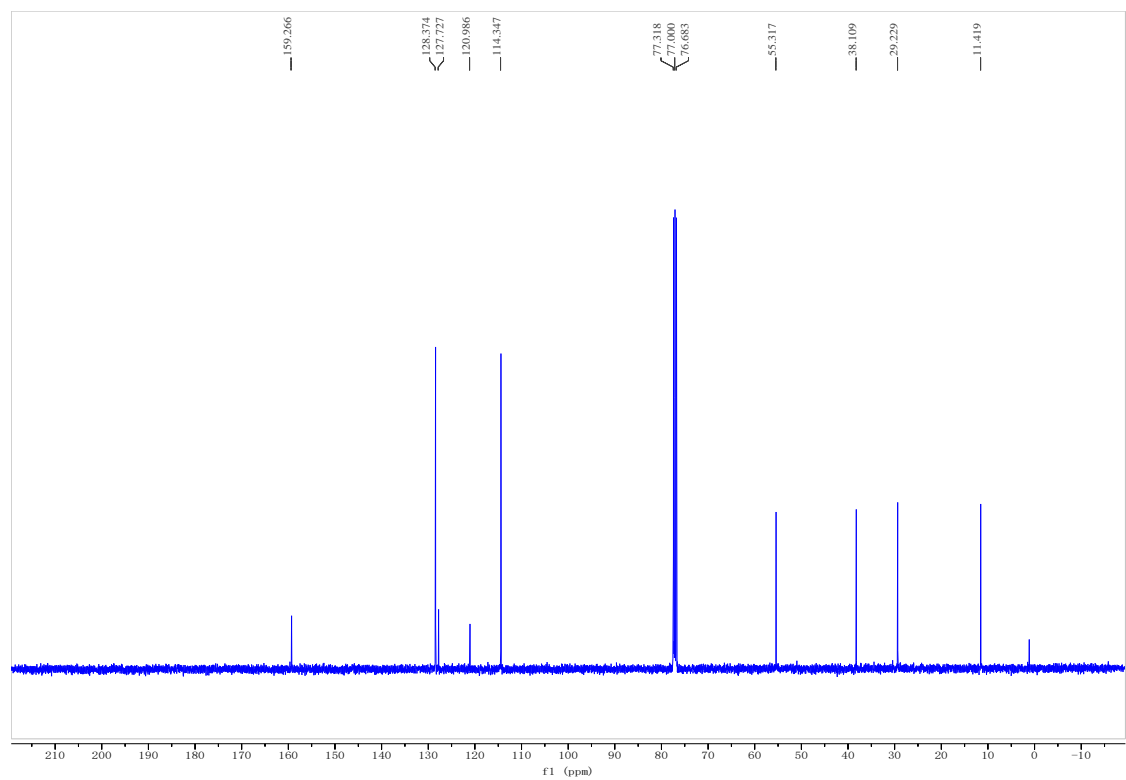
**$^1\text{H}$  and  $^{13}\text{C}$  NMR Spectra for Compound 3i:** $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

**$^1\text{H}$  and  $^{13}\text{C}$  NMR Spectra for Compound 3j:** $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

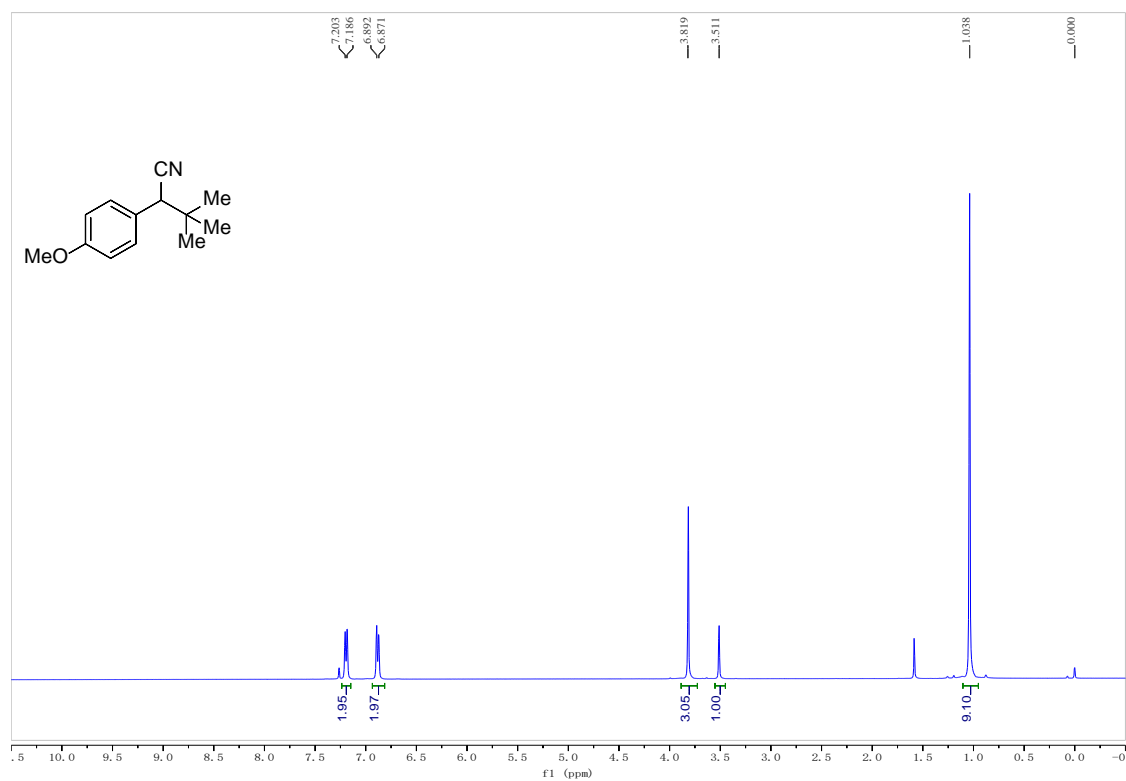
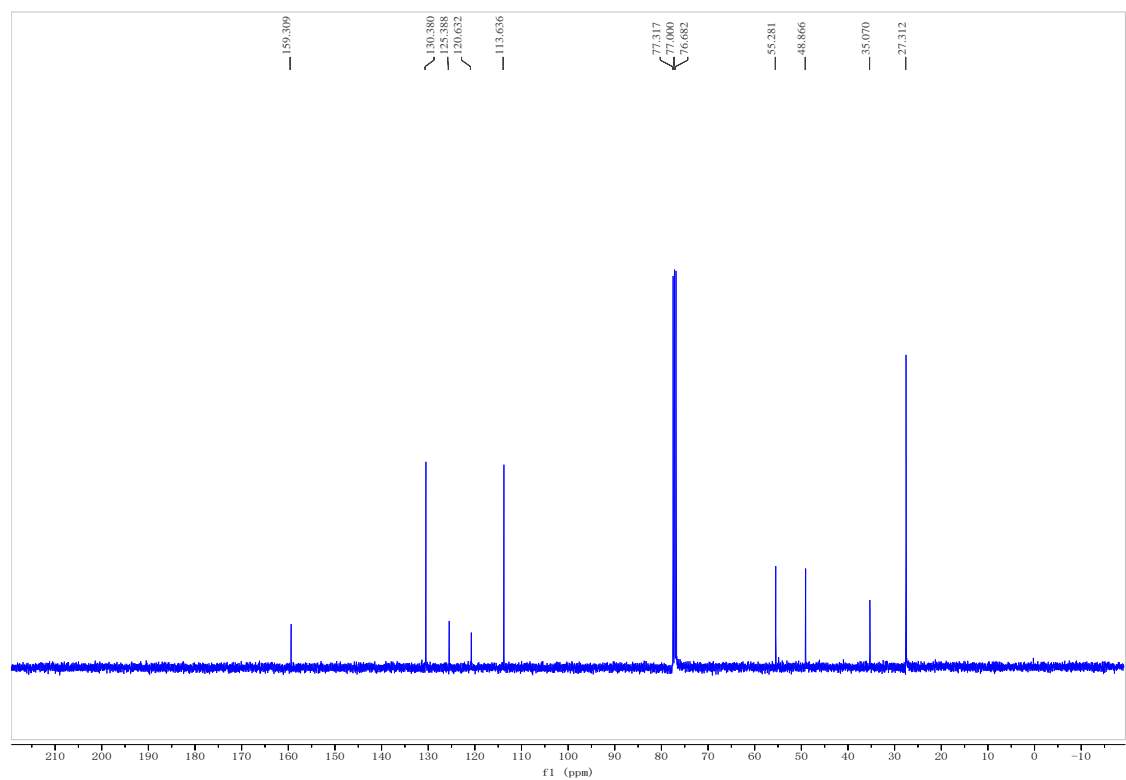
**$^1\text{H}$  and  $^{13}\text{C}$  NMR Spectra for Compound 3k:** $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

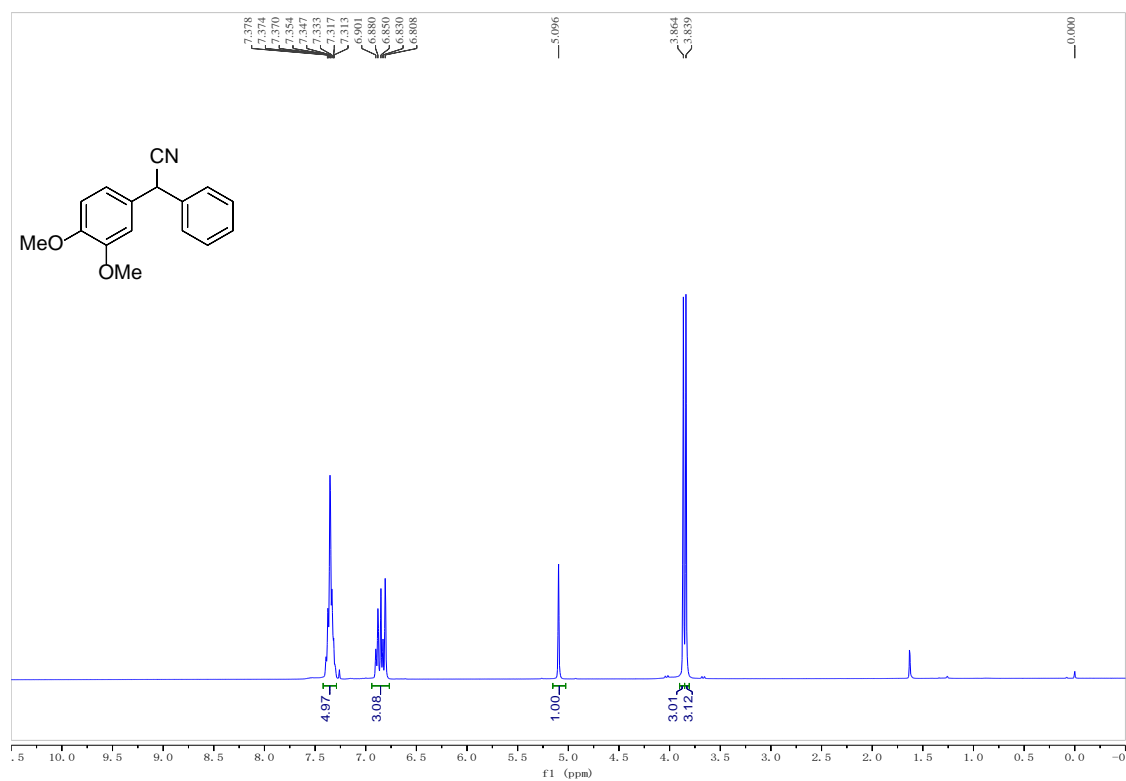
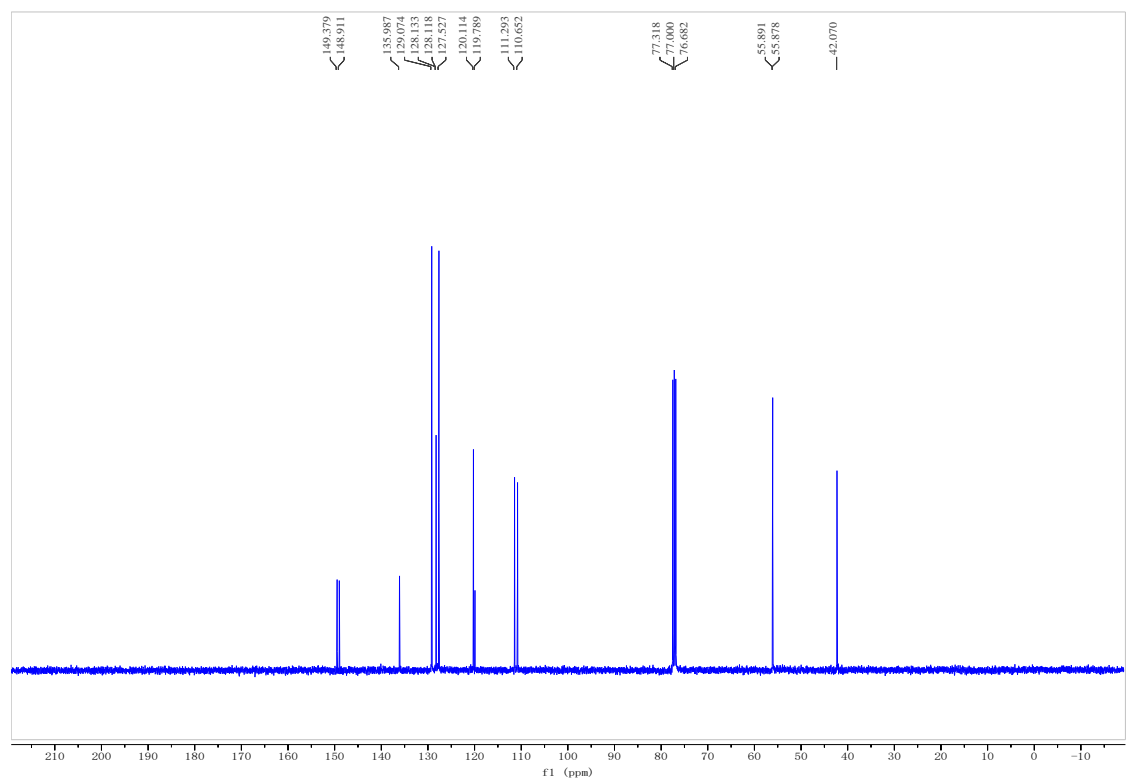
**$^1\text{H}$  and  $^{13}\text{C}$  NMR Spectra for Compound 3l:** $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

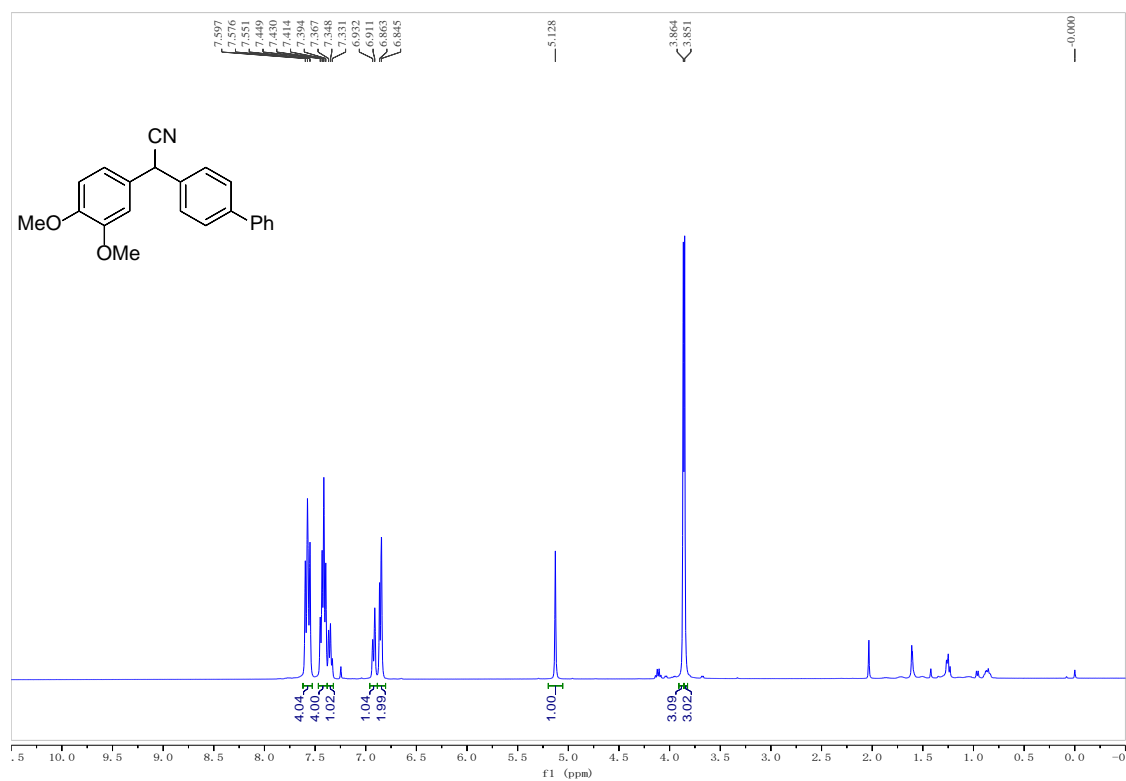
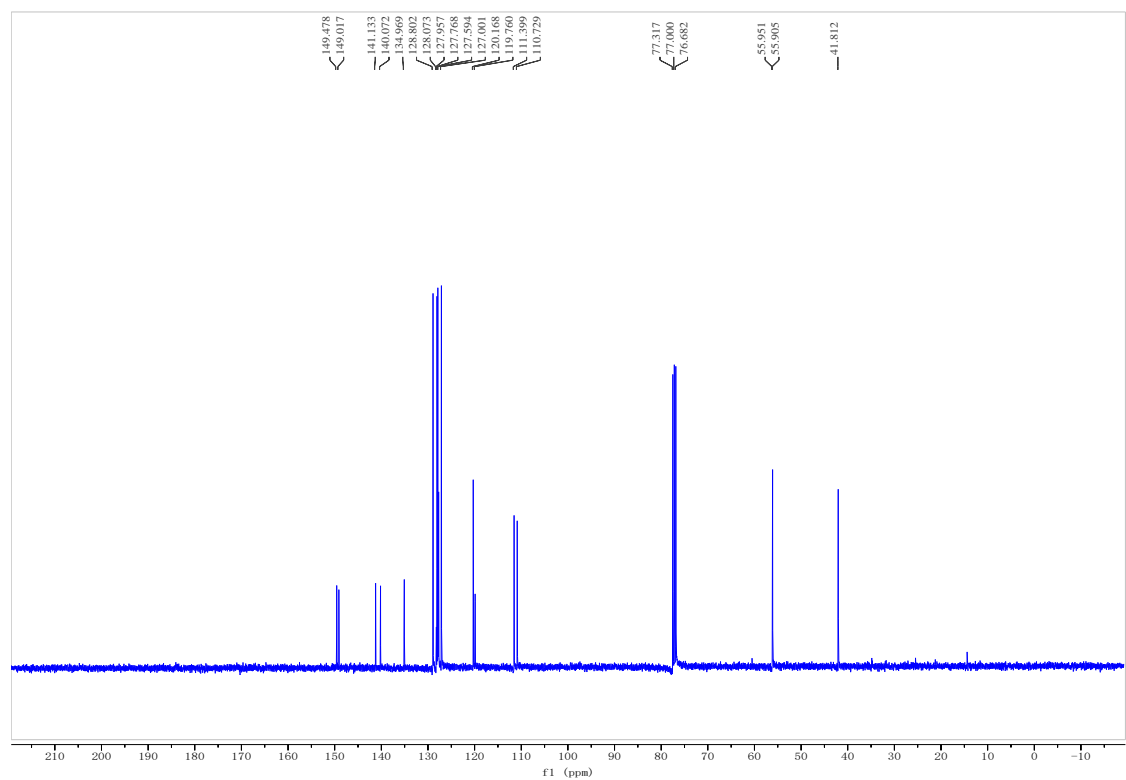
**$^1\text{H}$  and  $^{13}\text{C}$  NMR Spectra for Compound 3m:** $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

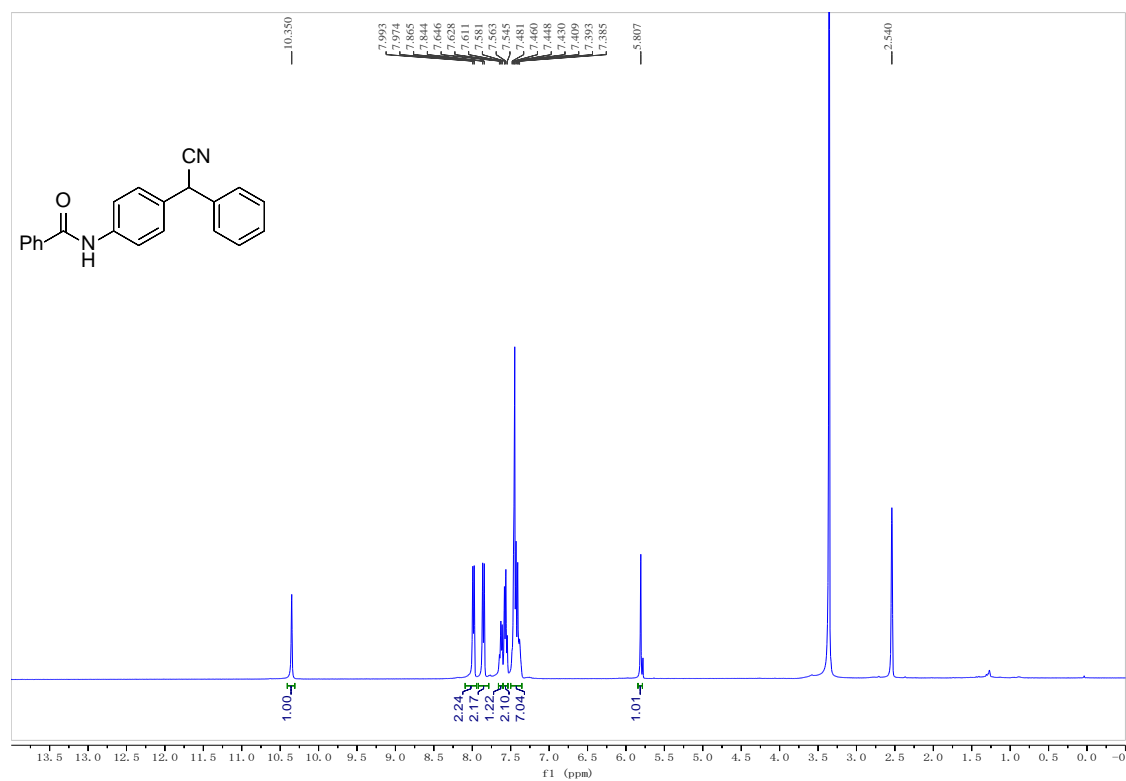
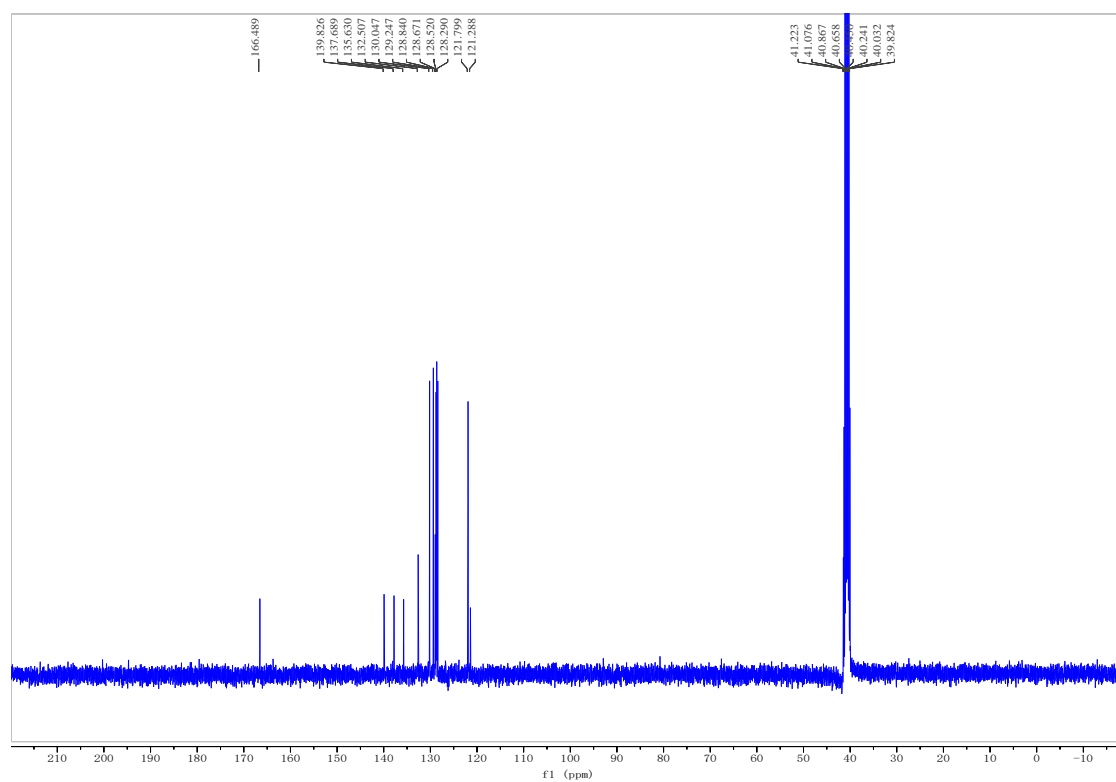
**$^1\text{H}$  and  $^{13}\text{C}$  NMR Spectra for Compound 3n:** $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

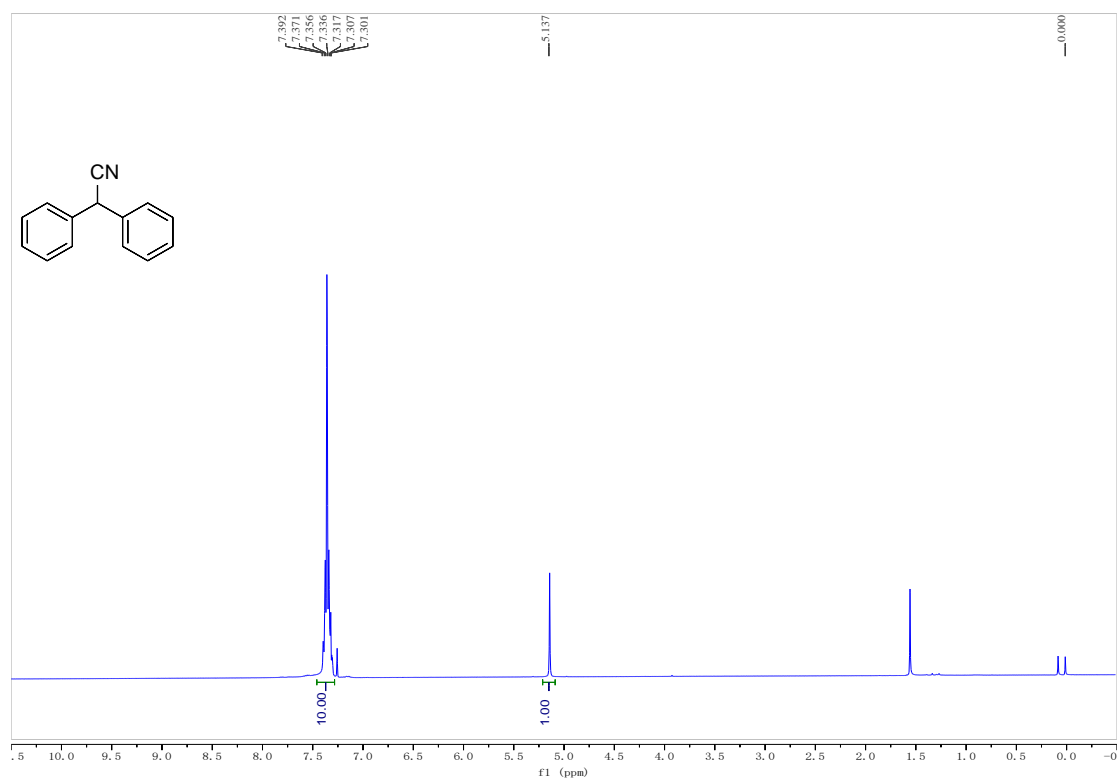
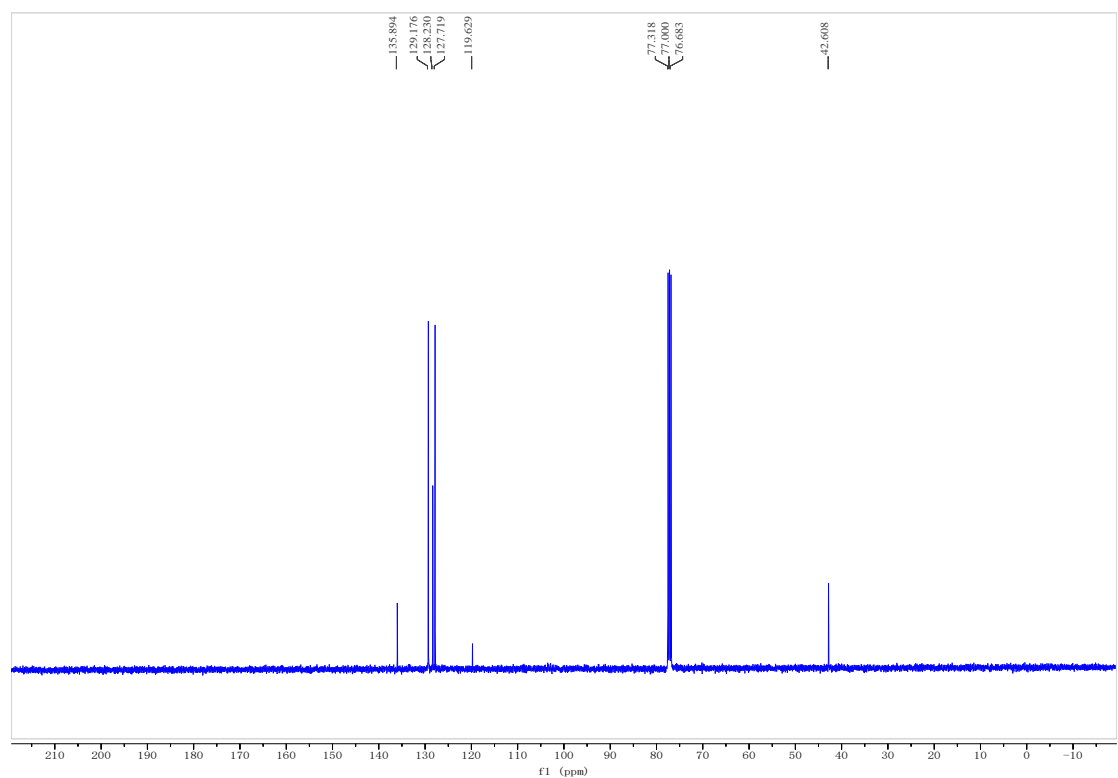


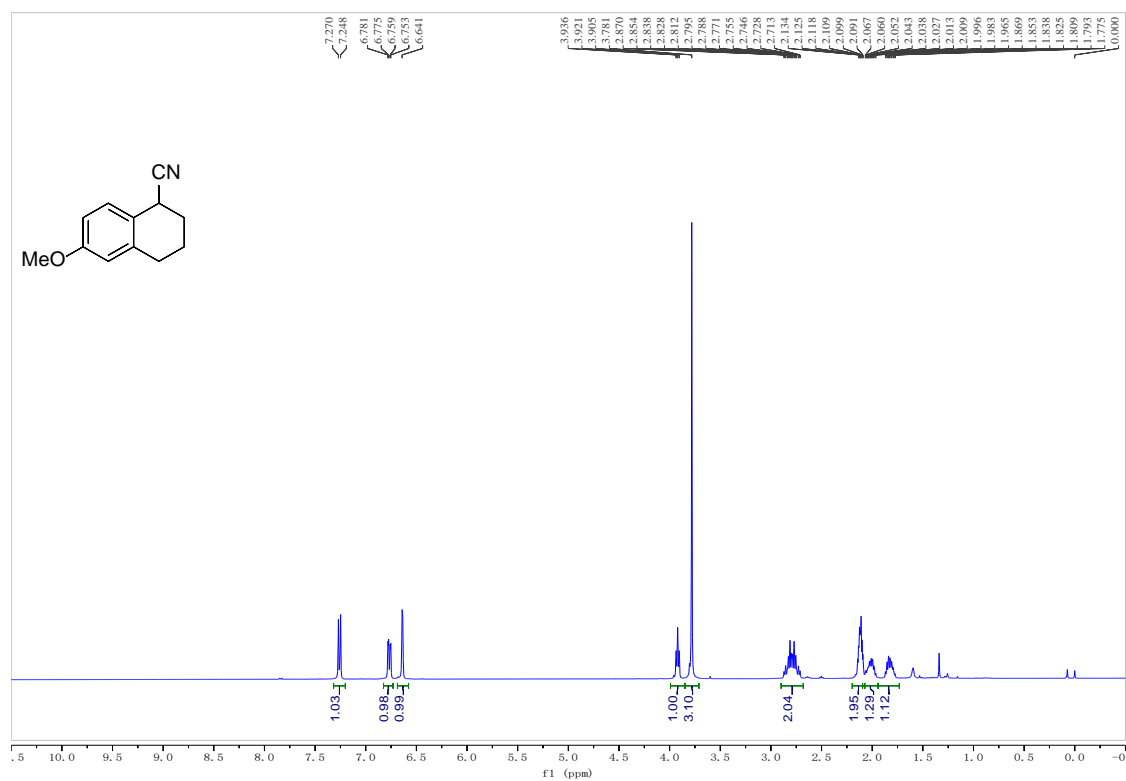
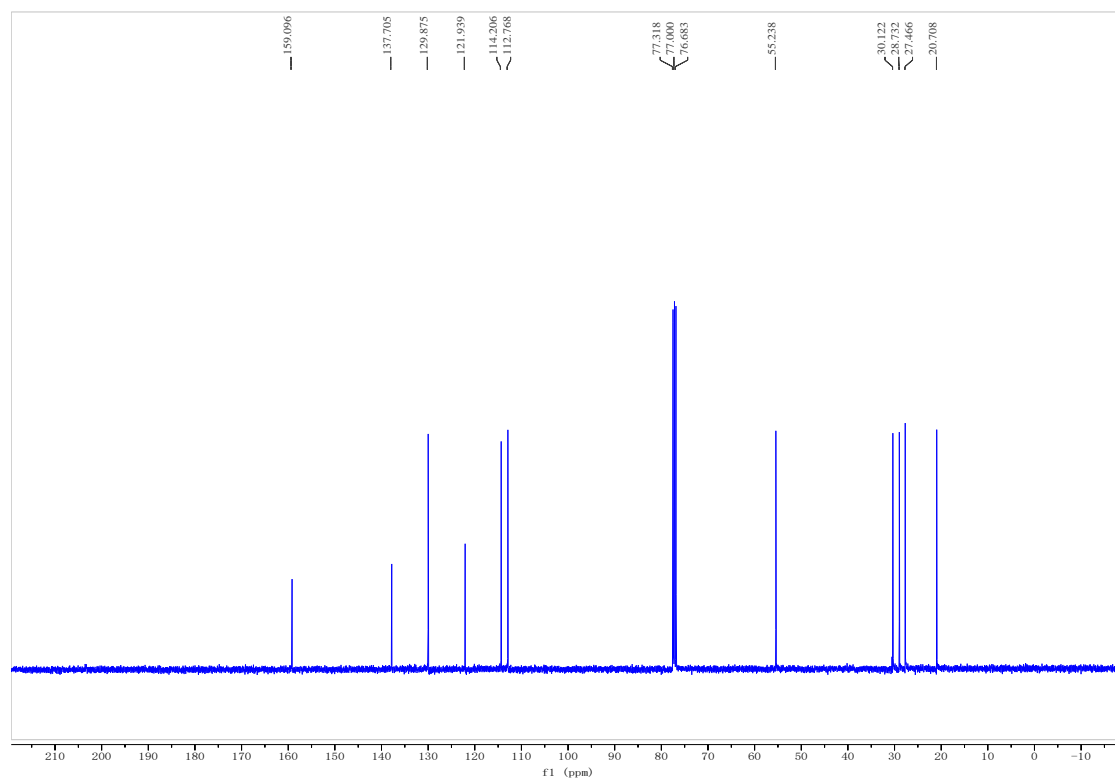
**$^1\text{H}$  and  $^{13}\text{C}$  NMR Spectra for Compound 3o:** $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

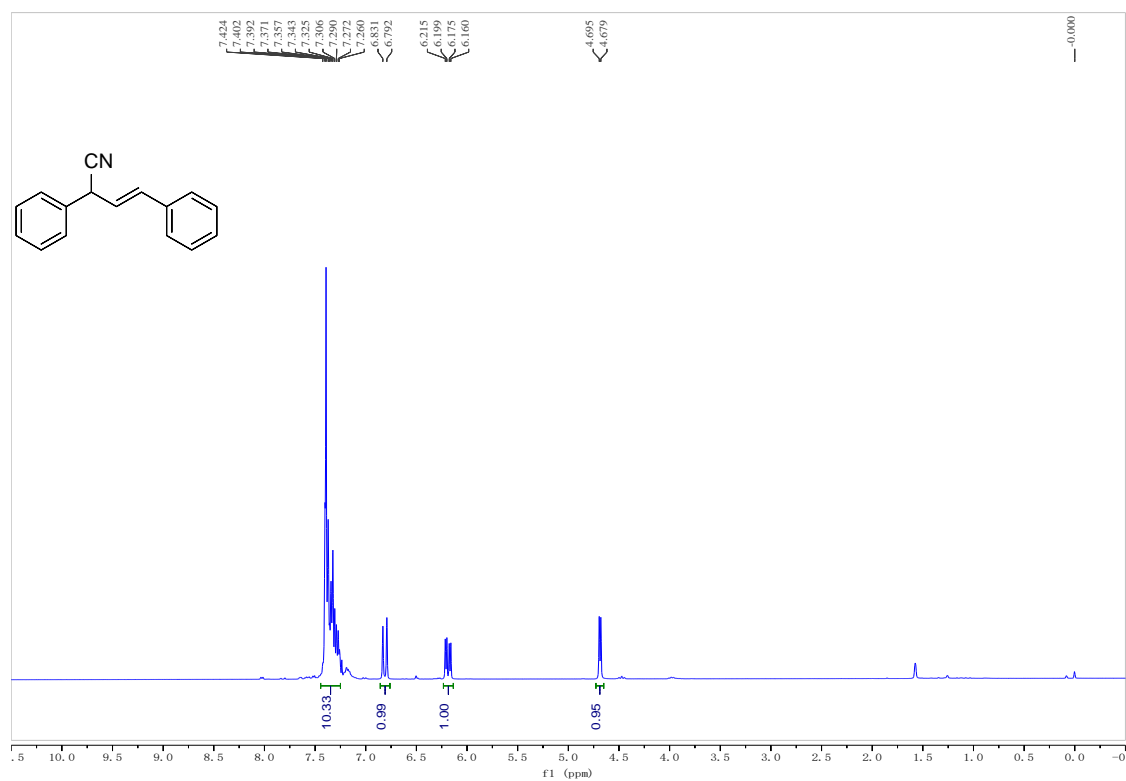
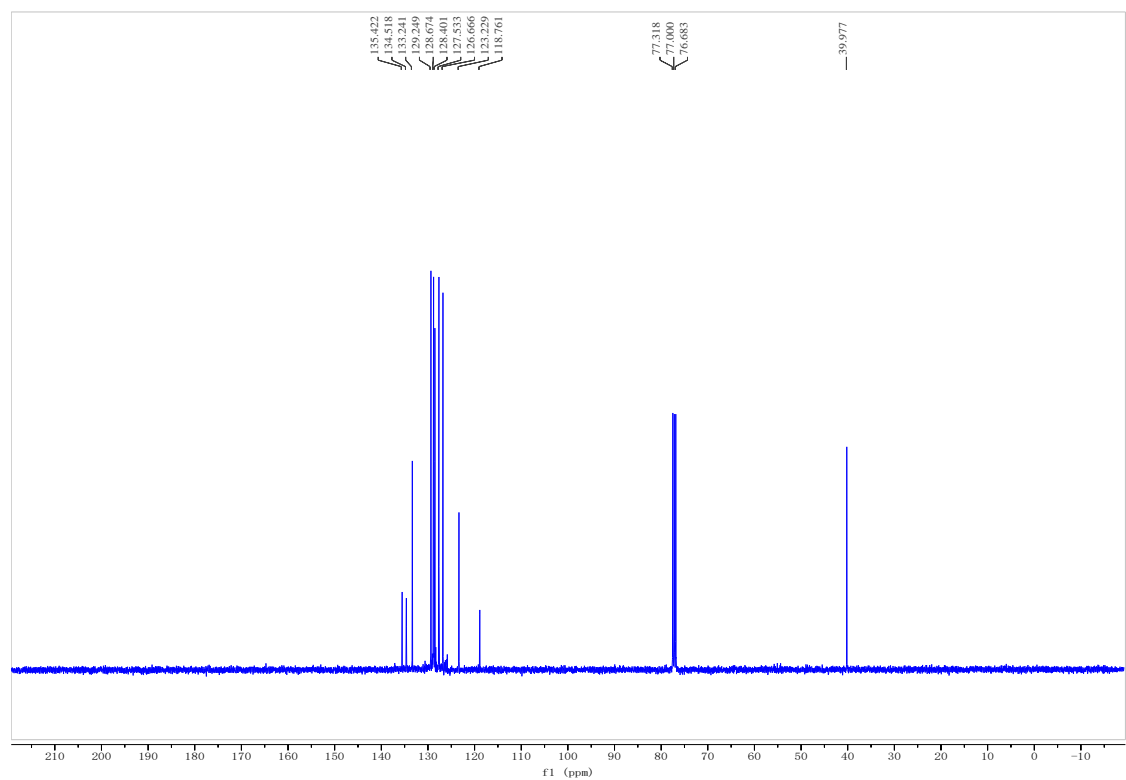
**$^1\text{H}$  and  $^{13}\text{C}$  NMR Spectra for Compound 3p:** $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

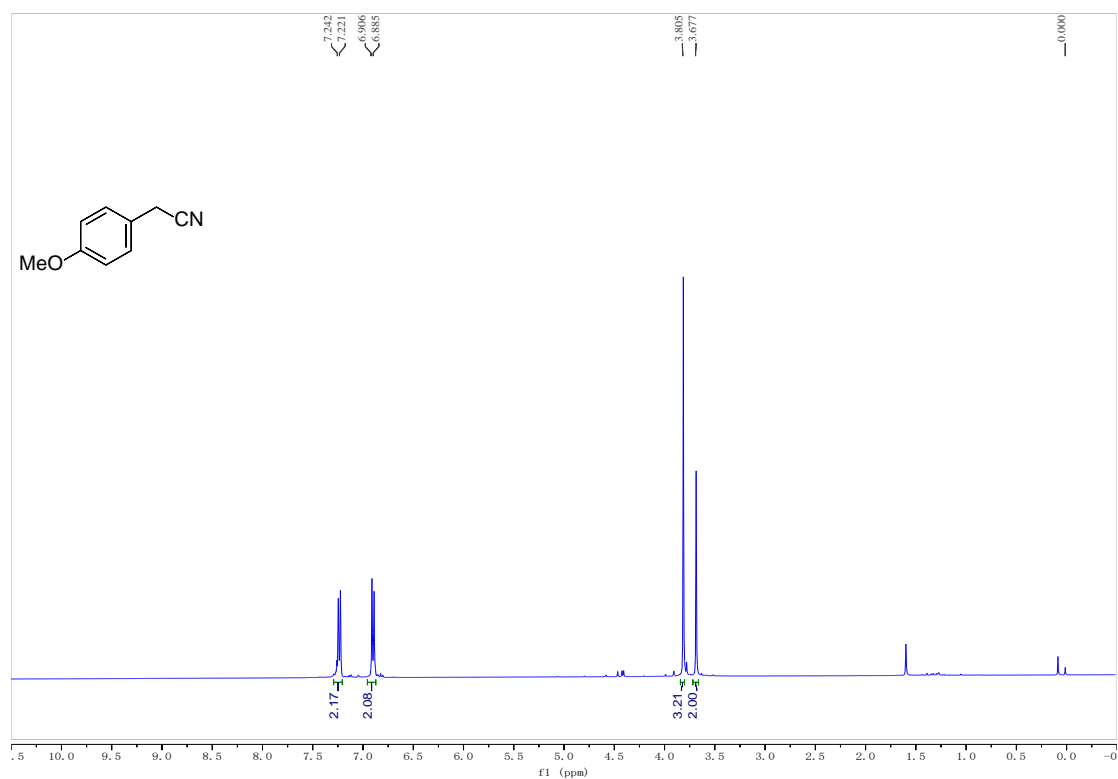
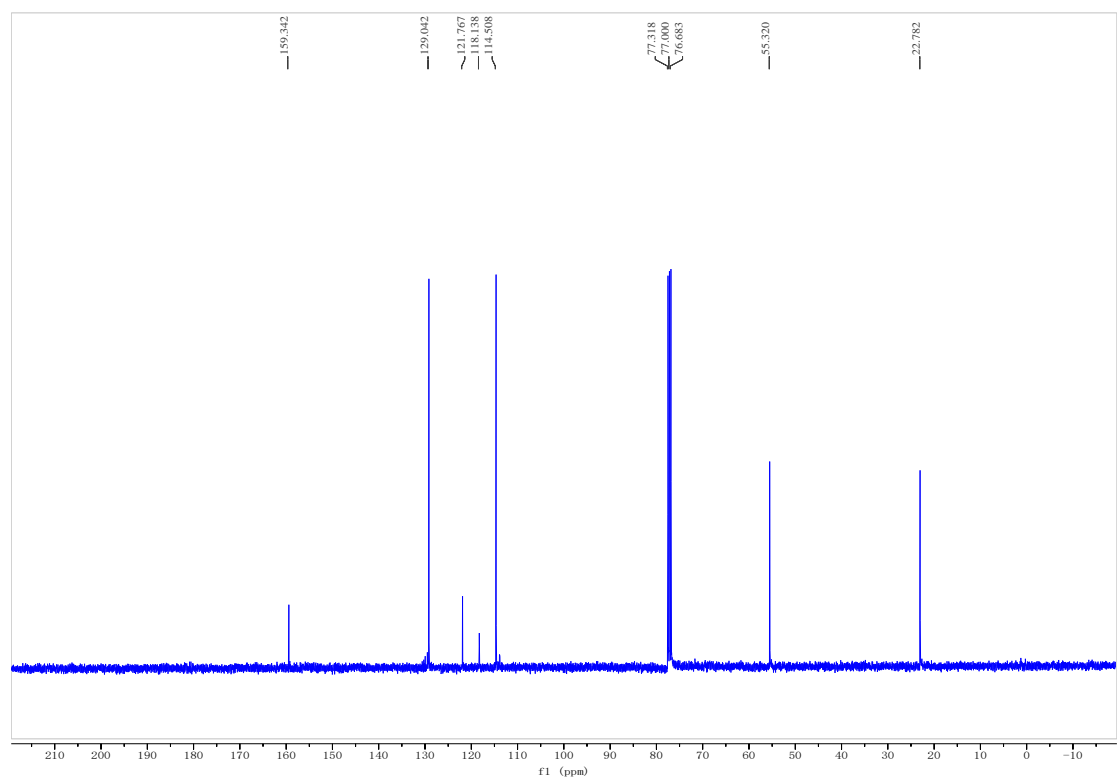
**$^1\text{H}$  and  $^{13}\text{C}$  NMR Spectra for Compound 3q:** $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

**$^1\text{H}$  and  $^{13}\text{C}$  NMR Spectra for Compound 3r:** $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ ) $^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ )

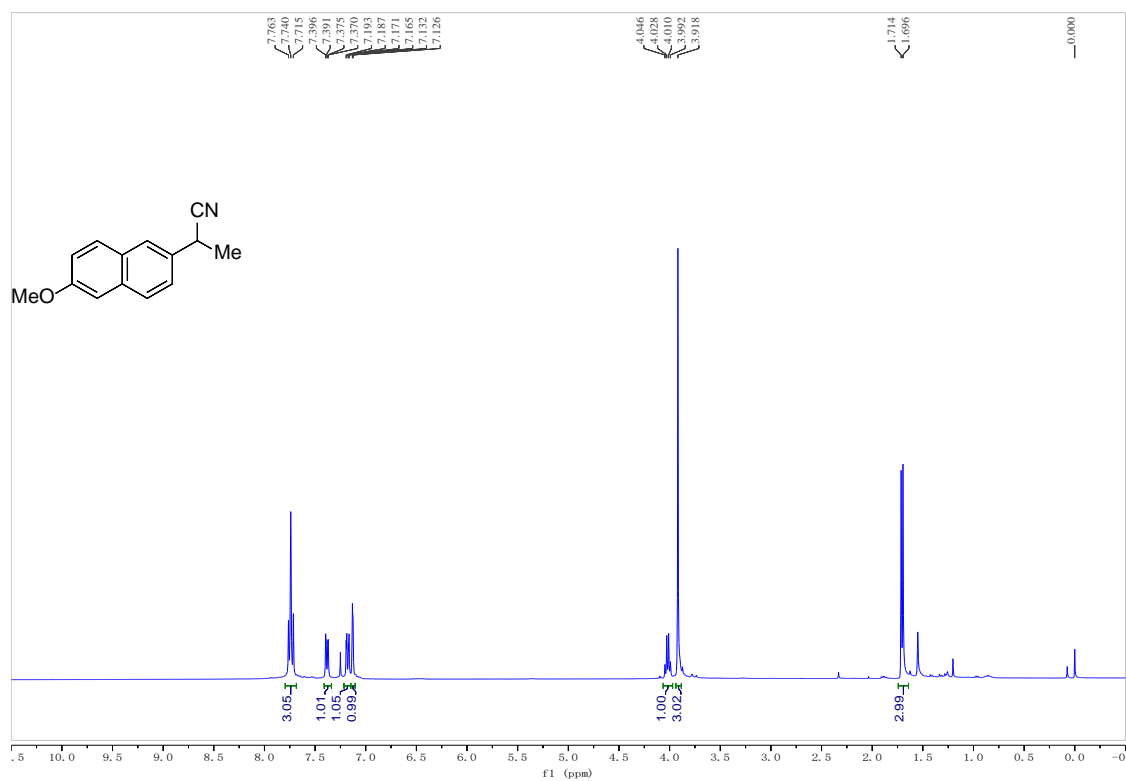
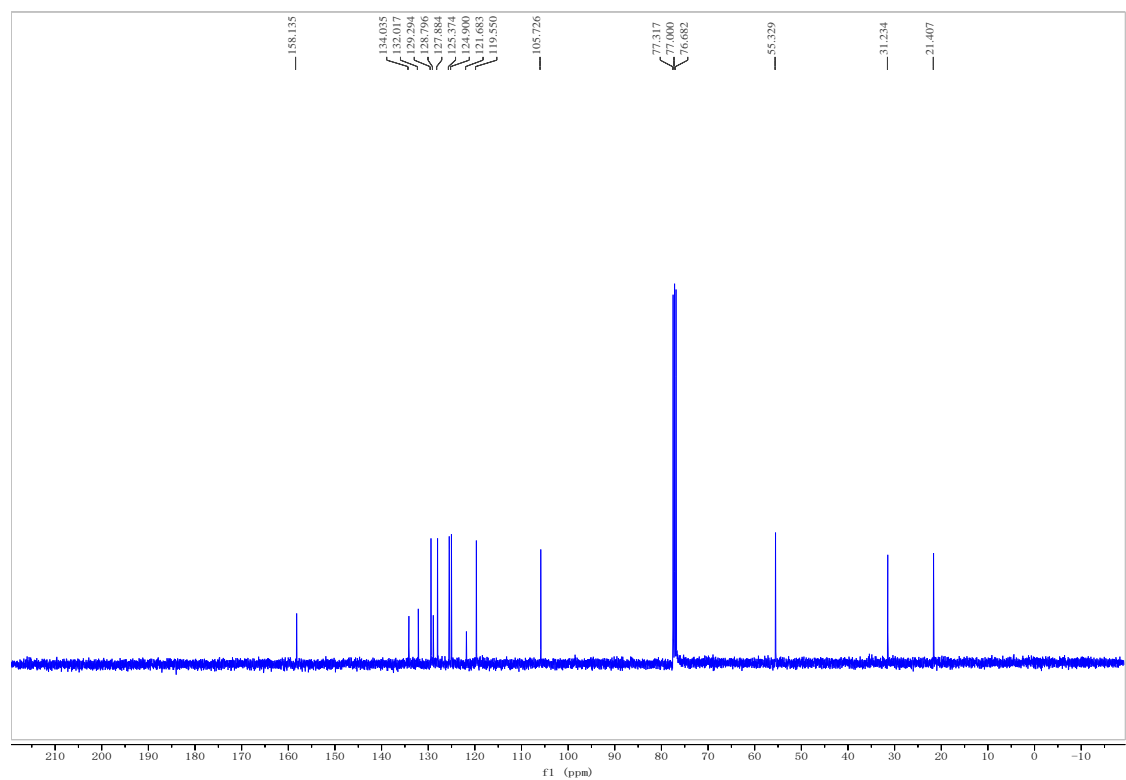
**$^1\text{H}$  and  $^{13}\text{C}$  NMR Spectra for Compound 3s:** $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

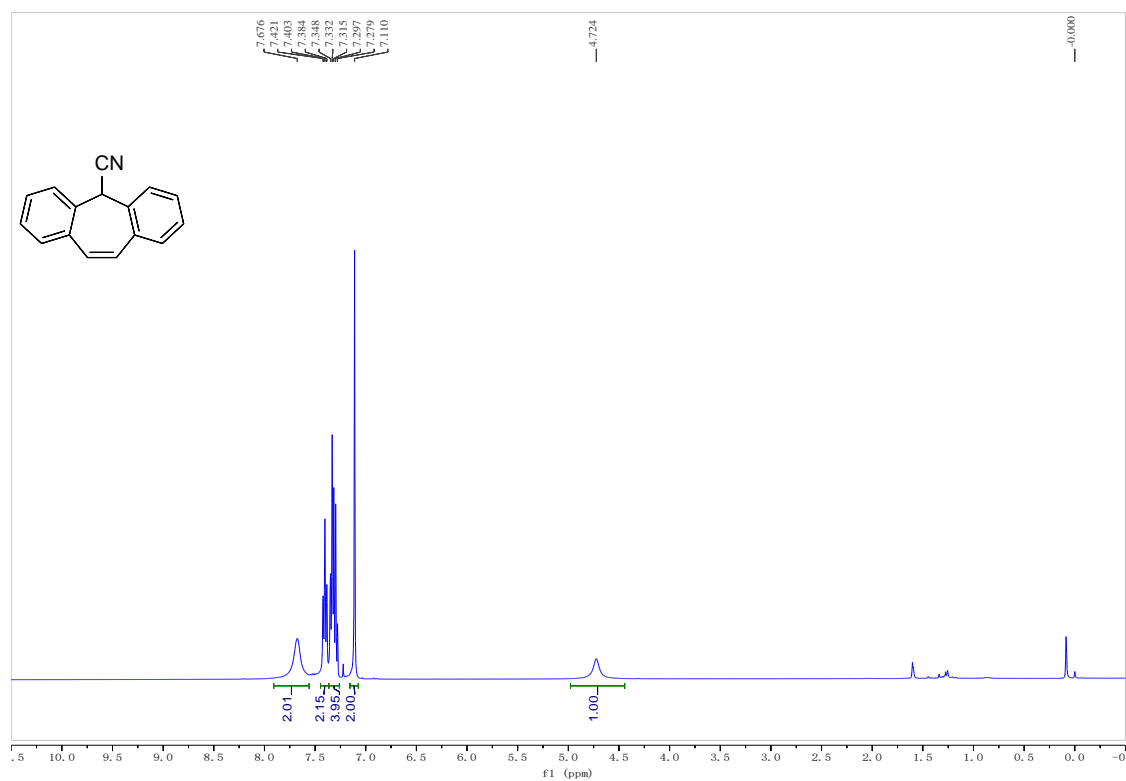
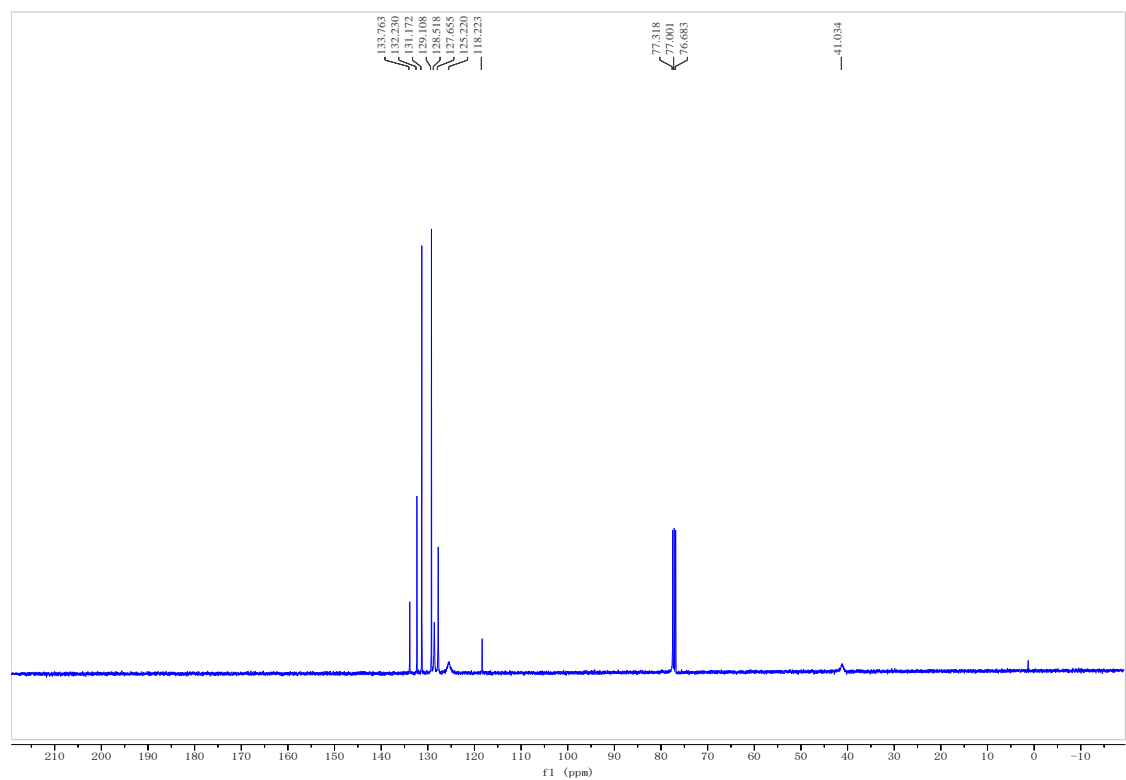
**$^1\text{H}$  and  $^{13}\text{C}$  NMR Spectra for Compound 3t:** $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

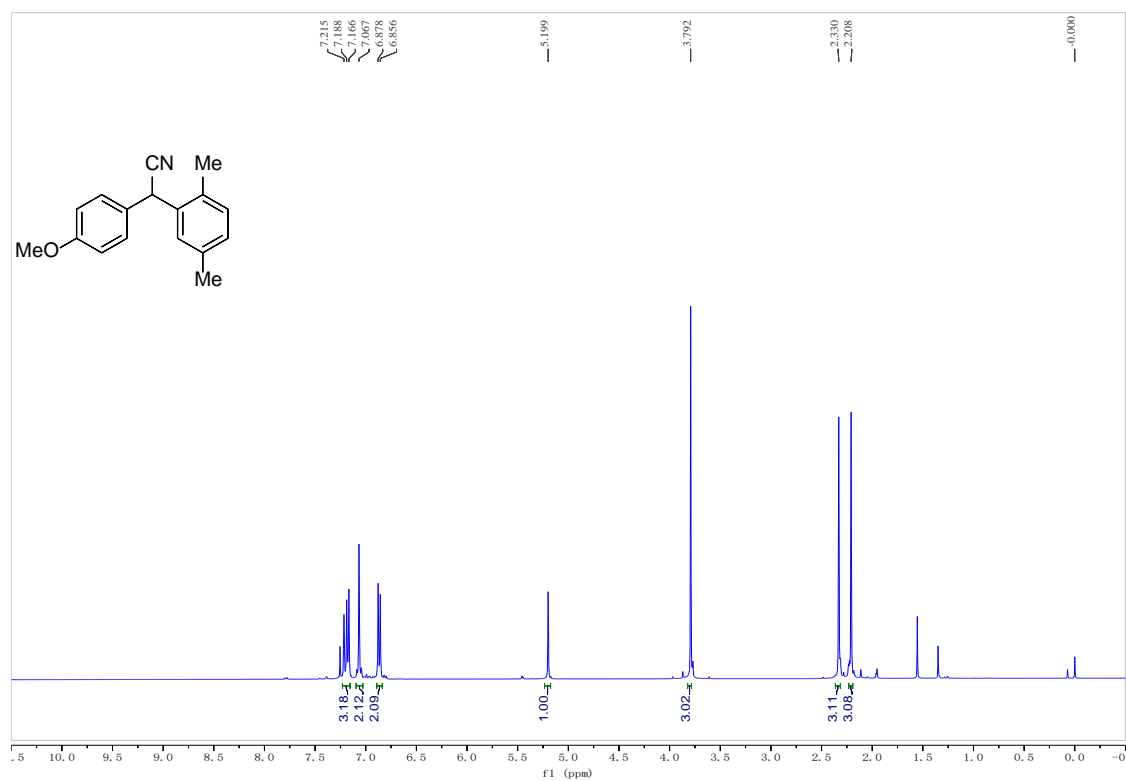
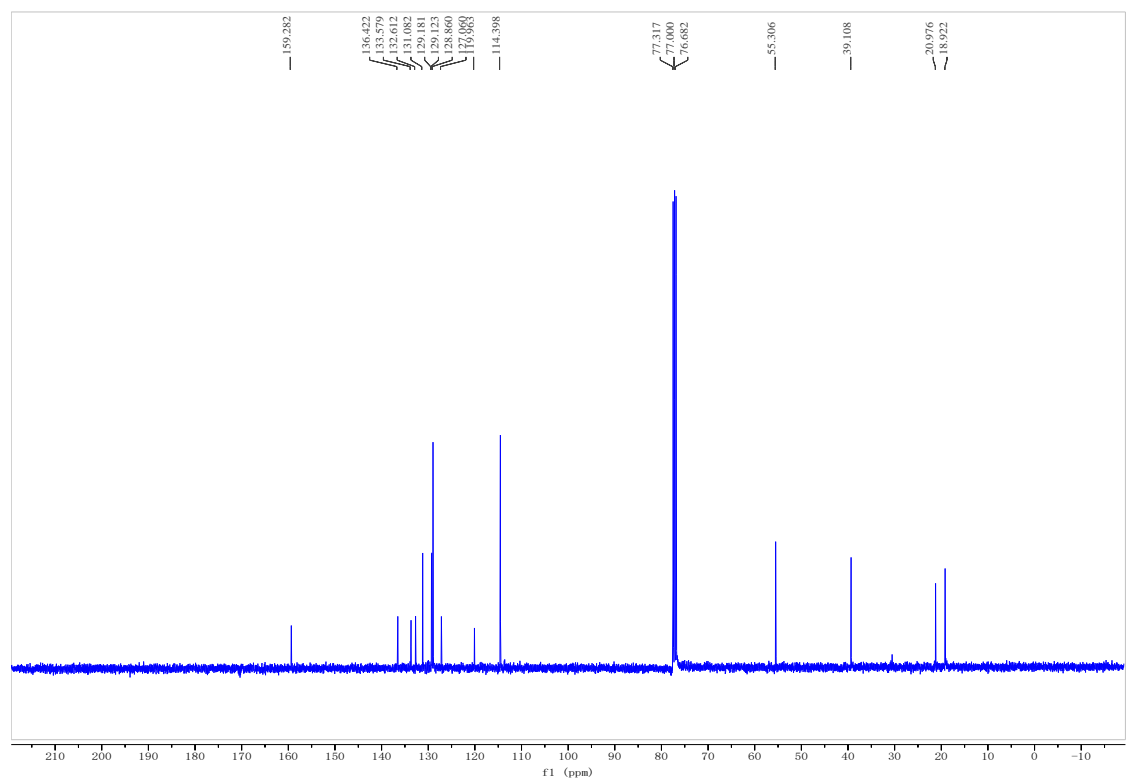
**$^1\text{H}$  and  $^{13}\text{C}$  NMR Spectra for Compound 3u:** $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

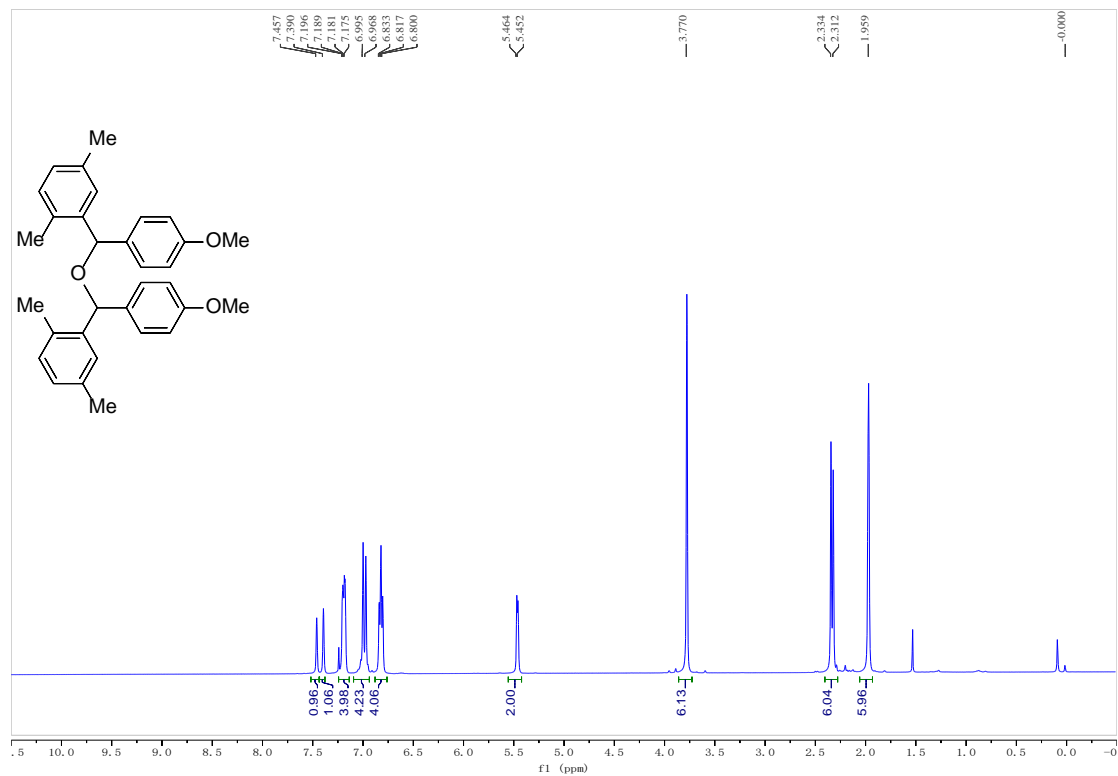
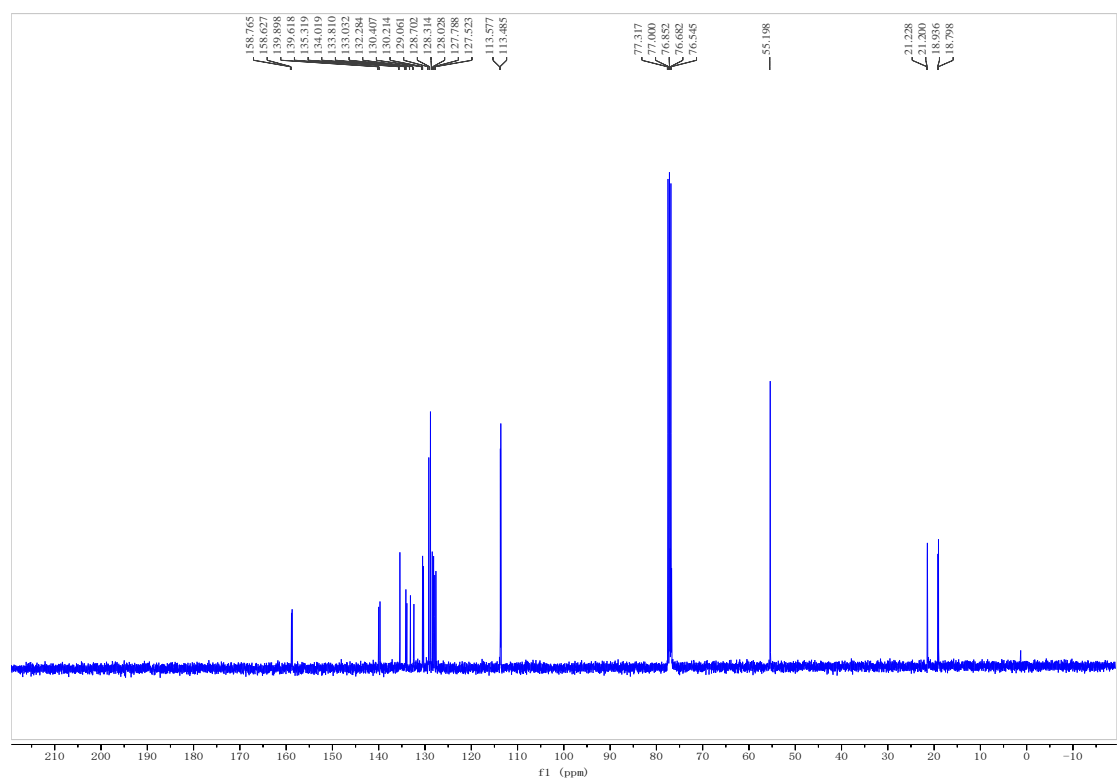
**$^1\text{H}$  and  $^{13}\text{C}$  NMR Spectra for Compound 3v:** $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

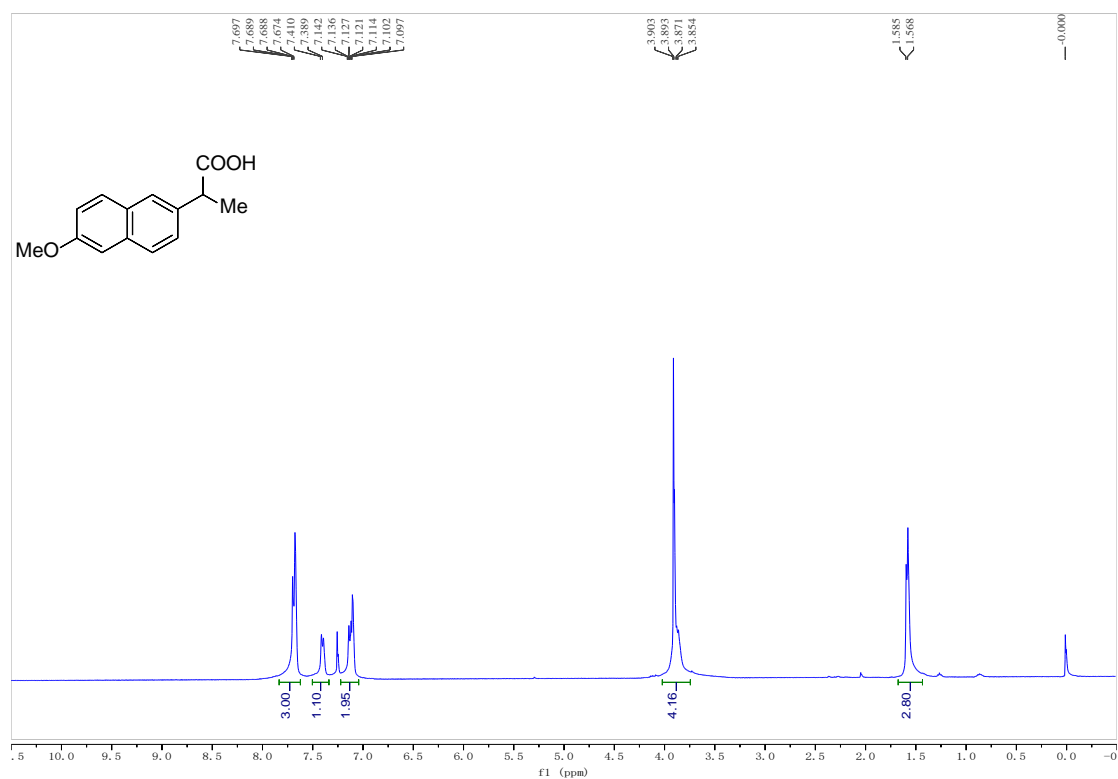
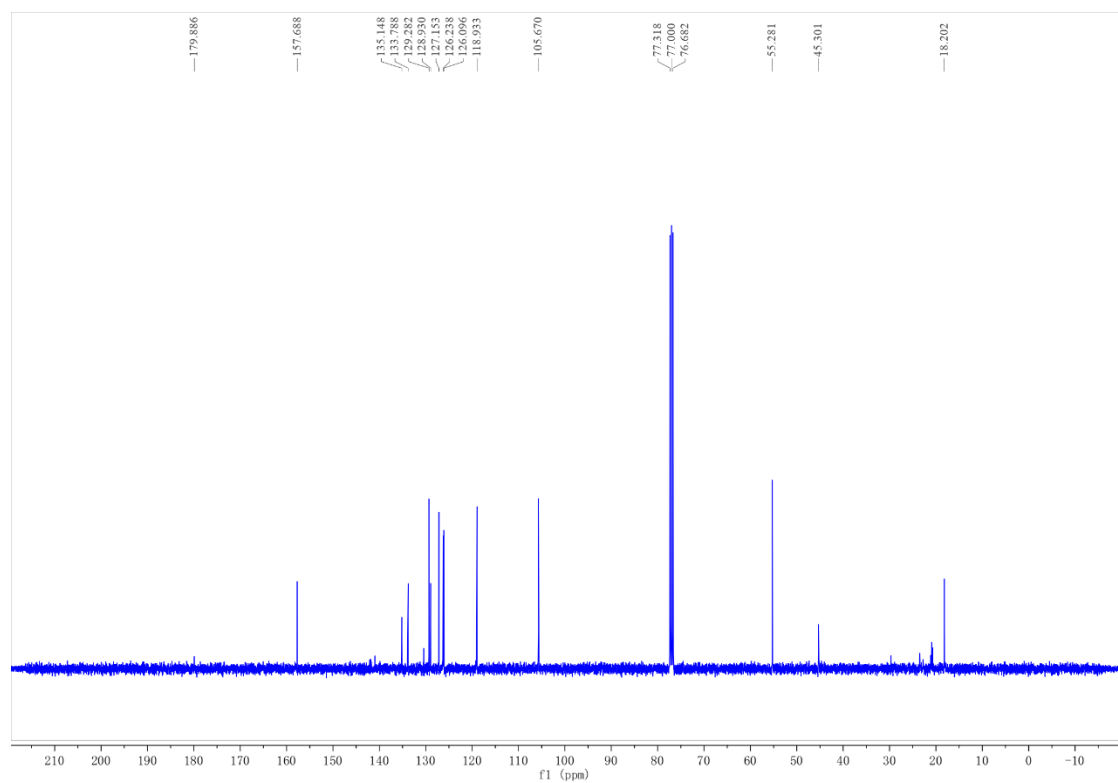


**$^1\text{H}$  and  $^{13}\text{C}$  NMR Spectra for Compound 3w:** $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

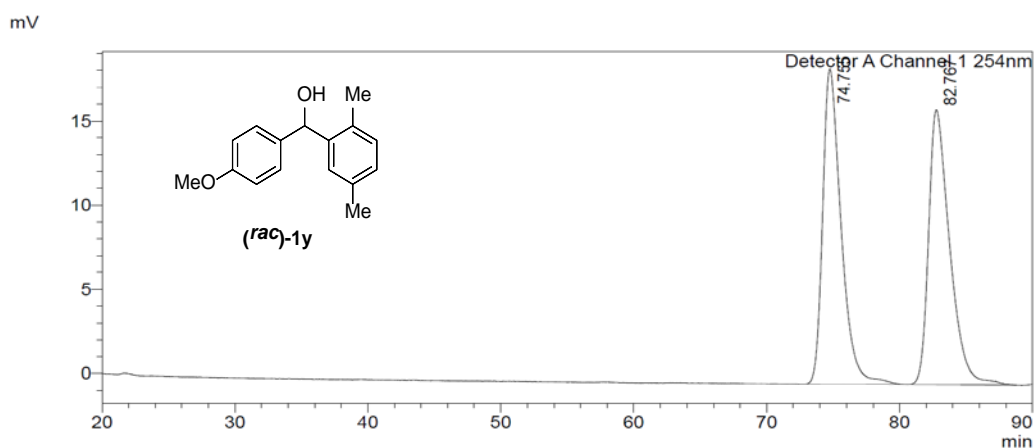
**$^1\text{H}$  and  $^{13}\text{C}$  NMR Spectra for Compound 3x:** $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

**$^1\text{H}$  and  $^{13}\text{C}$  NMR Spectra for Compound 3y:** $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

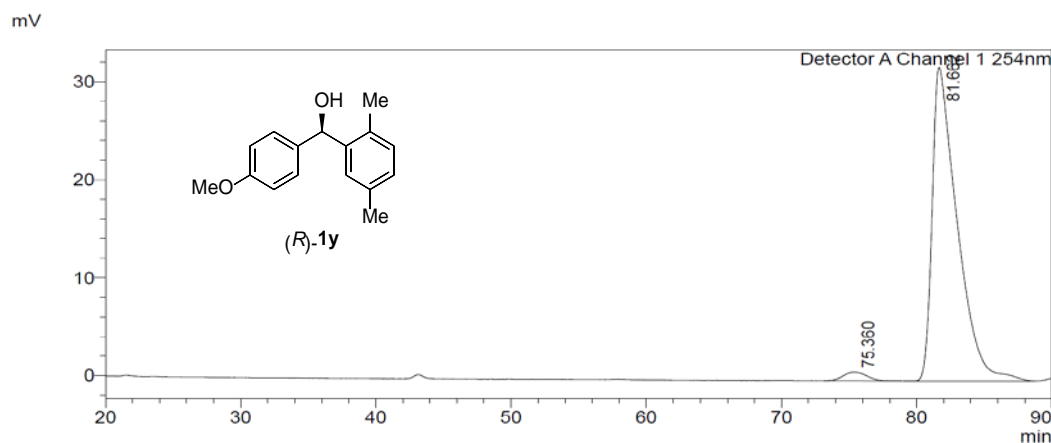
**$^1\text{H}$  and  $^{13}\text{C}$  NMR Spectra for Compound 4y:** $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

**$^1\text{H}$  and  $^{13}\text{C}$  NMR Spectra for Naproxen:** $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

## HPLC spectra:

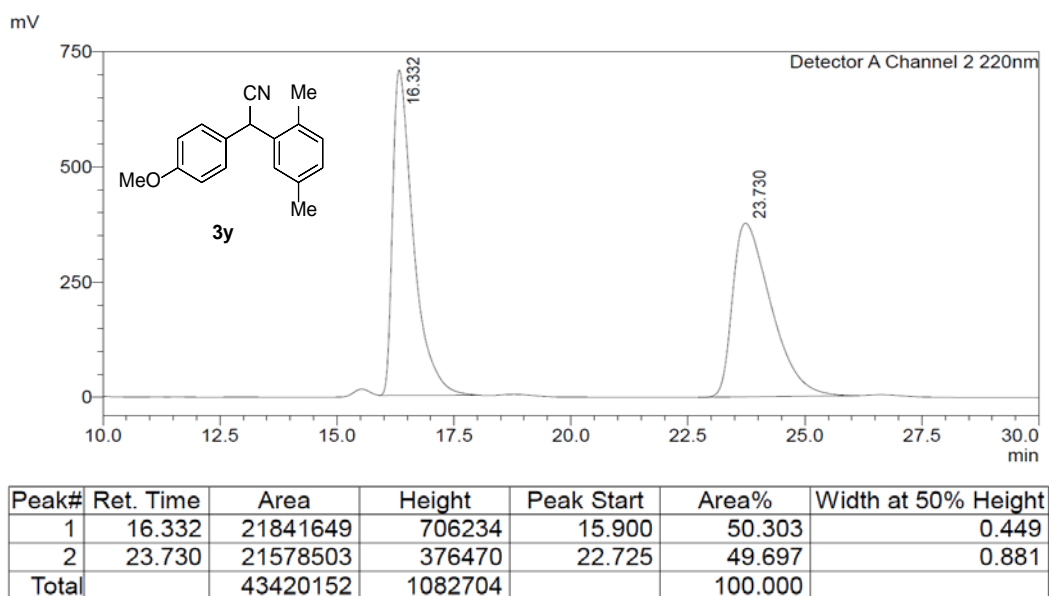
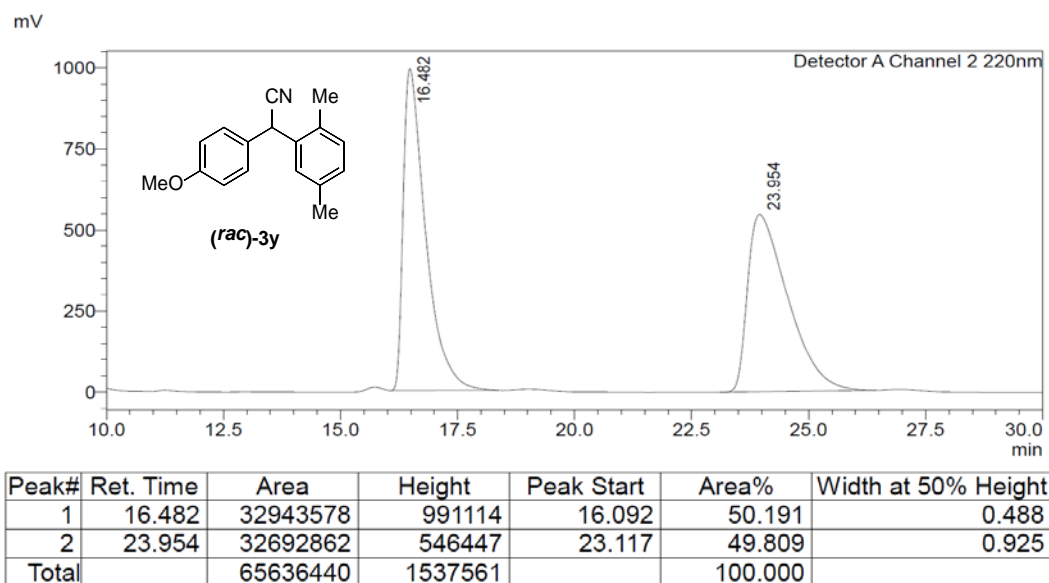


Peak#	Ret. Time	Area	Height	Peak Start	Area%	Width at 50% Height
1	74.755	1807604	18687	70.250	50.017	1.427
2	82.767	1806407	16312	80.508	49.983	1.644
Total		3614011	34999		100.000	

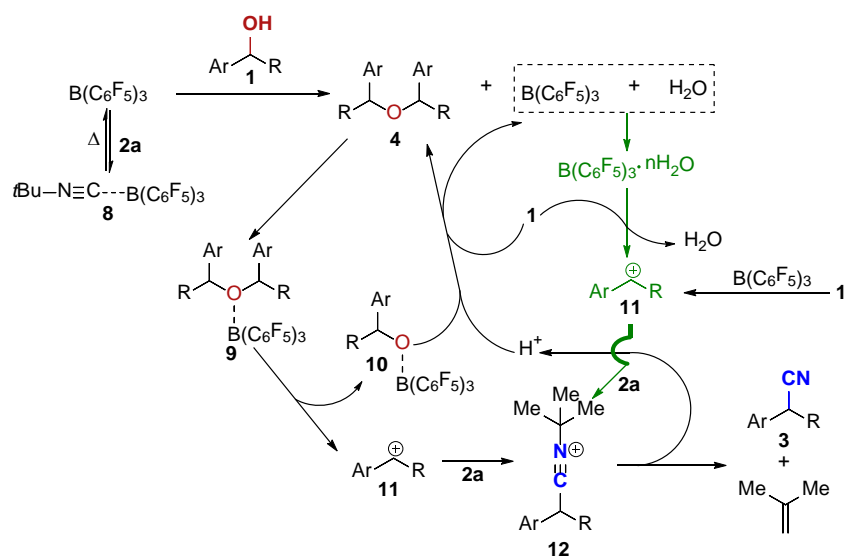


Peak#	Ret. Time	Area	Height	Peak Start	Area%	Width at 50% Height
1	75.360	105570	869	73.150	2.501	1.947
2	81.662	4115868	32019	78.992	97.499	1.905
Total		4221439	32888		100.000	

95% ee of (*R*)-**1y** was determined by HPLC: OJ-H Column, 5/95 *i*PrOH/hexane, 0.5 mL/min, 254 nm, 35 °C; retention time = 75.36 min (minor), 81.66 min (major).



0% ee of **3y** was determined by HPLC: AS-H Column, 5/95 *i*PrOH/hexane, 0.8 mL/min, 220 nm, 35 °C; retention time = 16.33 min (minor), 23.73 min (major)).

**Other Pathways for the Direct Cyanation of Benzyl Alcohols:****Scheme S1.** Proposed mechanism.