

Supporting Information

Synthesis of Triarylmethanes via Palladium-Catalyzed Suzuki Coupling of Trimethylammonium Salts and Arylboronic Acids

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1. Mechanistic study by monitoring the reaction with ESI-MS analysis

Figure 1 shows the ESI-MS spectrum of the reaction mixture of cross-coupling between 1,1-diphenylmethyl-trimethylammonium triflate with phenylboronic acid. The reaction mixture diluted by MeOH was injected to ESI-MS after reaction time of 0.5 h. Diphenylmethylium **A** (m/z 166), oxidative addition intermediate **B** (m/z 798) and **D** (m/z 1126), and transmetalation intermediate **C** (m/z 874) were detected.

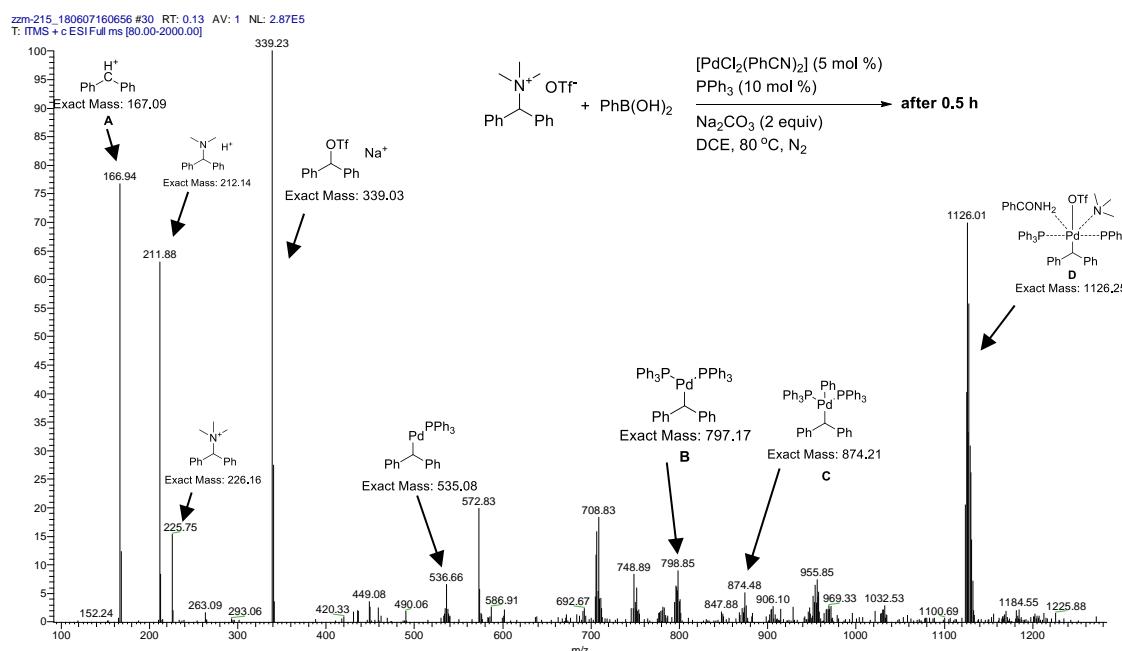


Figure 1

Figure 2 shows the ESI-MS spectrum of the reaction mixture of stoichiometric reaction of 1,1-diphenylmethyl-trimethylammonium triflate in the absence of phenylboronic acid. The reaction mixture diluted by MeOH was injected to ESI-MS after reaction time of 0.5 h. Diphenylmethylium **A** (m/z 166), oxidative addition intermediate **B** (m/z 795), **D** (m/z 1127) and **E** (m/z 749) were detected.

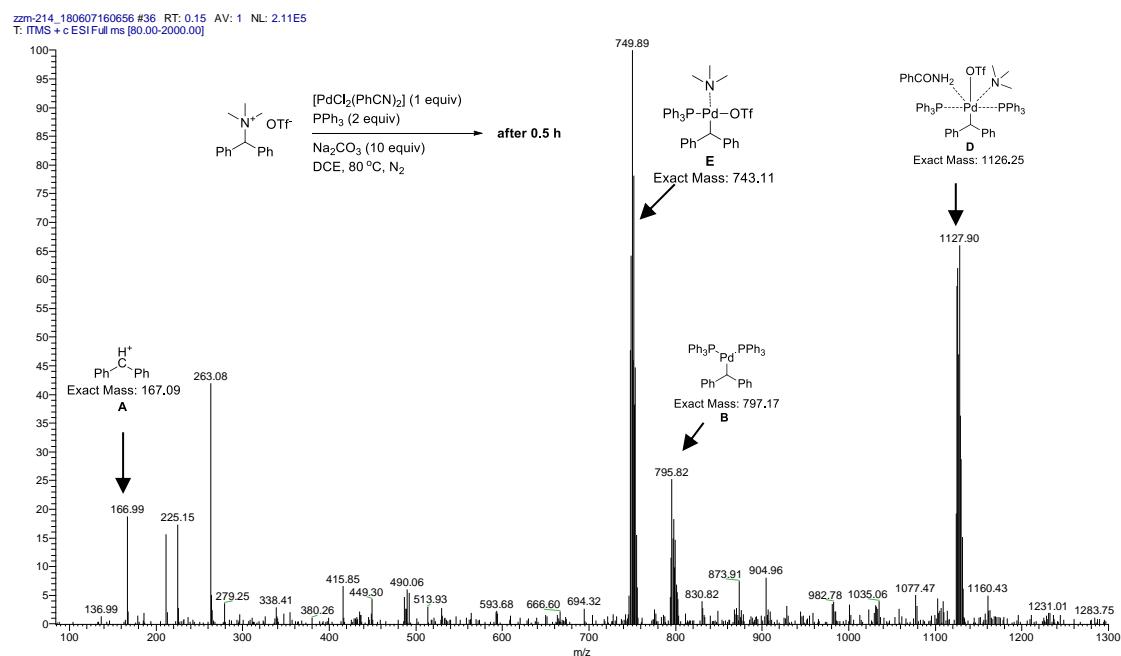
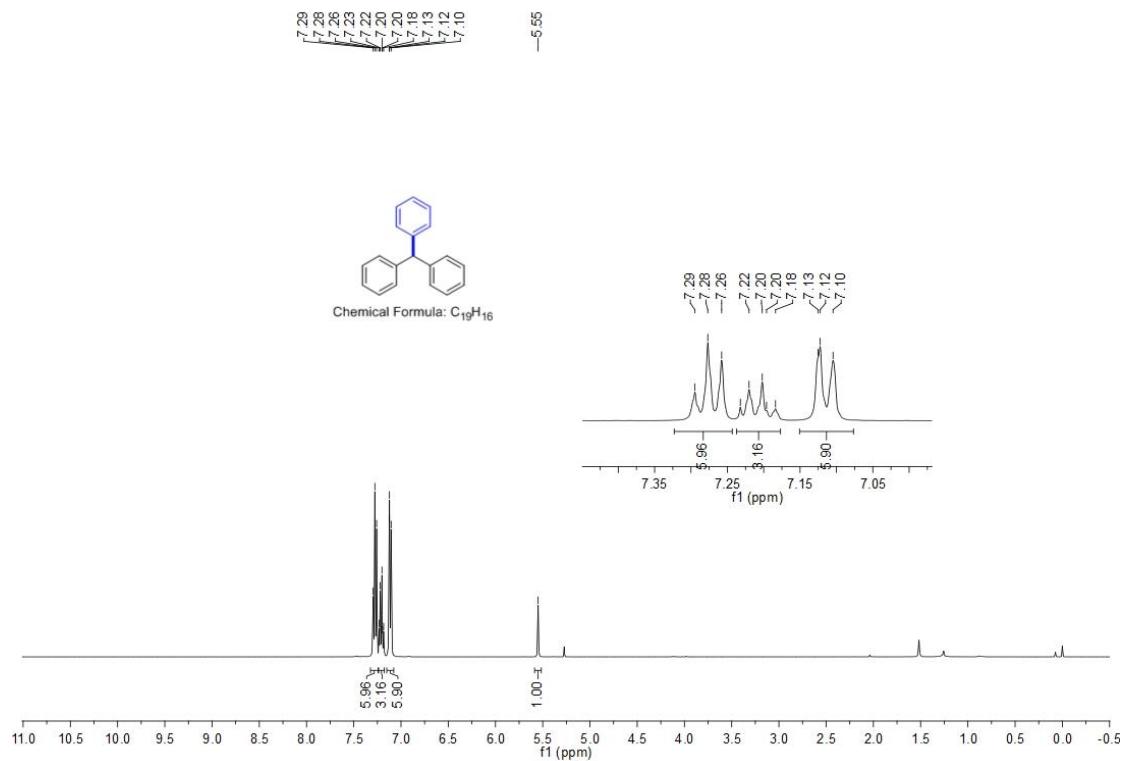
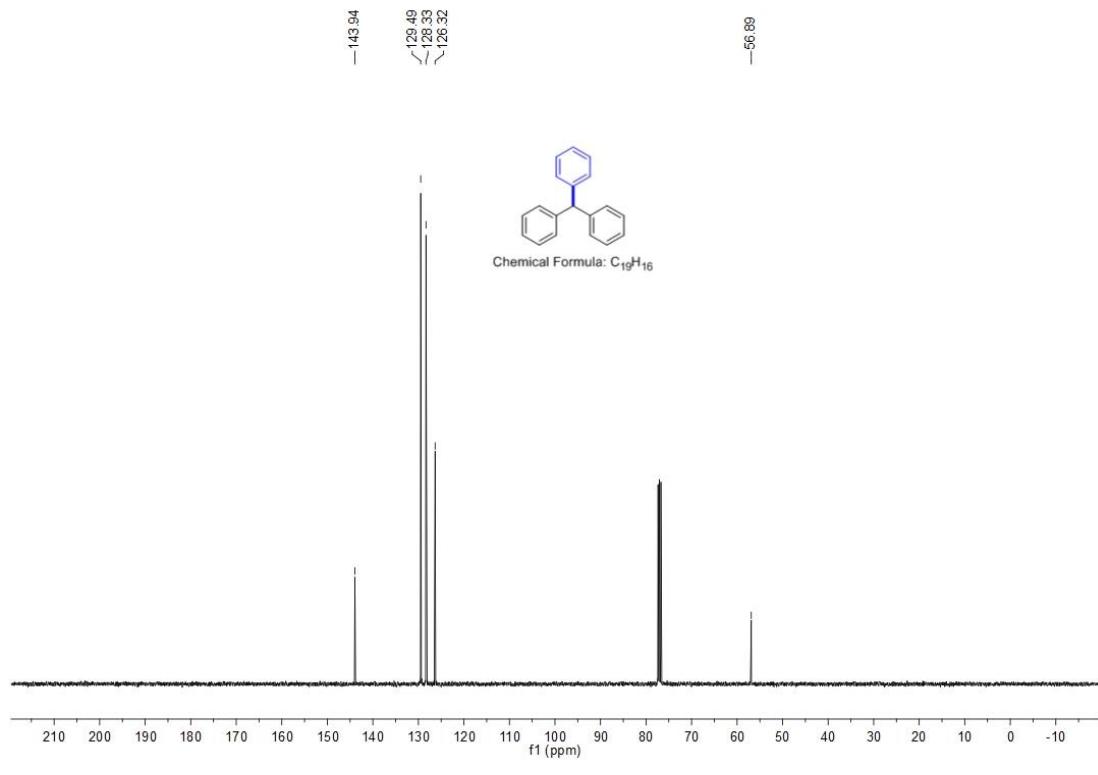


Figure 2

2. Copies of ^1H -NMR & ^{13}C - NMR Spectra



^1H NMR of **3a**



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

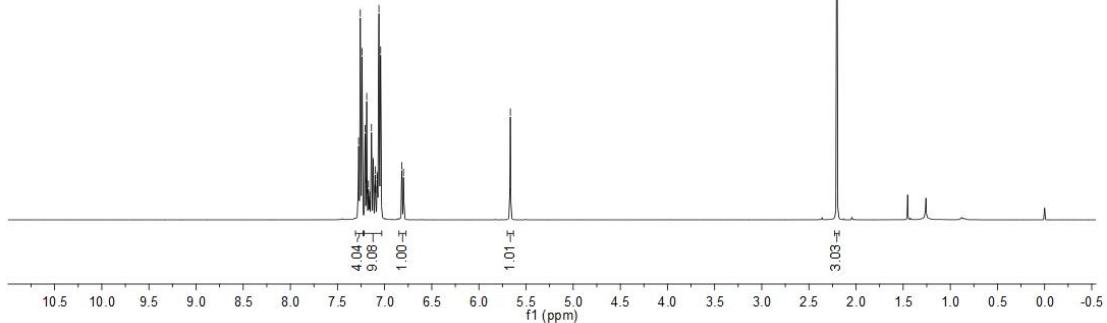
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7.24
7.21
7.20
7.19
7.18
7.17
7.16
7.16
7.16
7.14
7.14
7.12
7.12
7.10
7.10
7.09
7.08
7.08
7.06
7.04
6.82
6.80

-5.67

-2.20



Chemical Formula: C₂₀H₁₈



¹H NMR of 3b

143.48
142.41
129.68
129.52
128.35
128.44
126.44
126.30
125.82
136.67
130.47

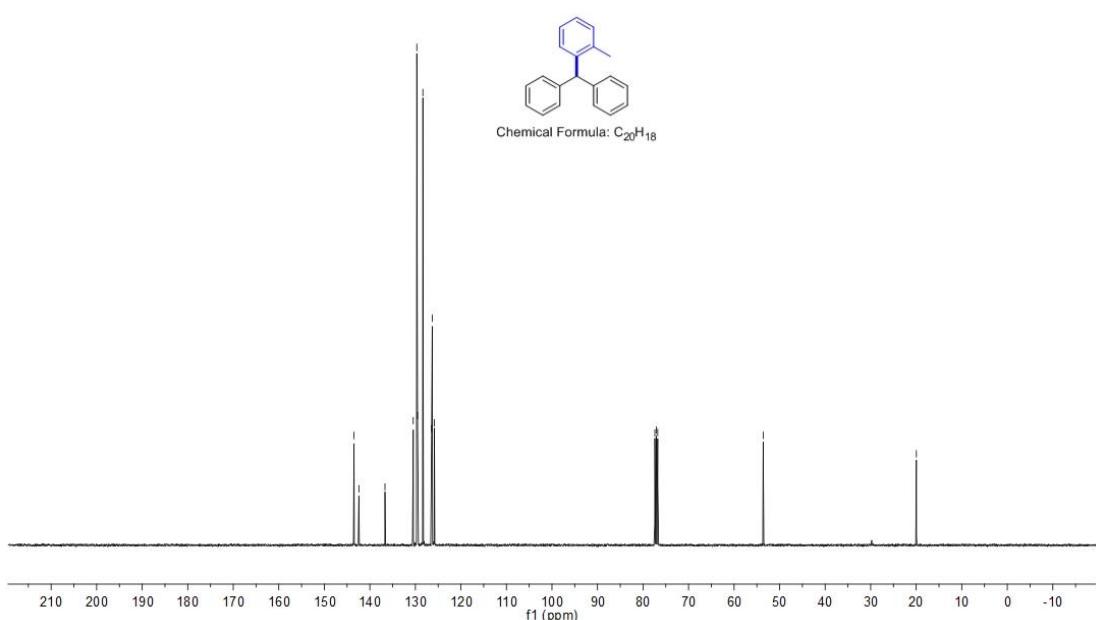
77.08
76.77

-53.61

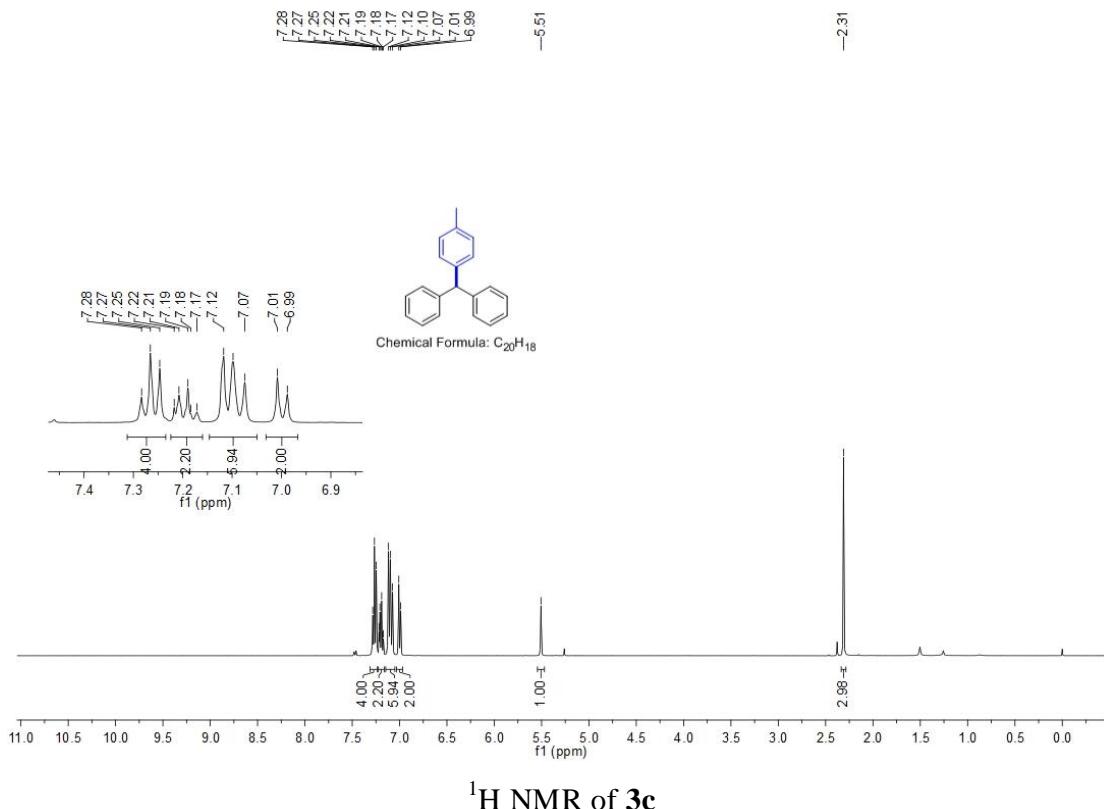
-19.96



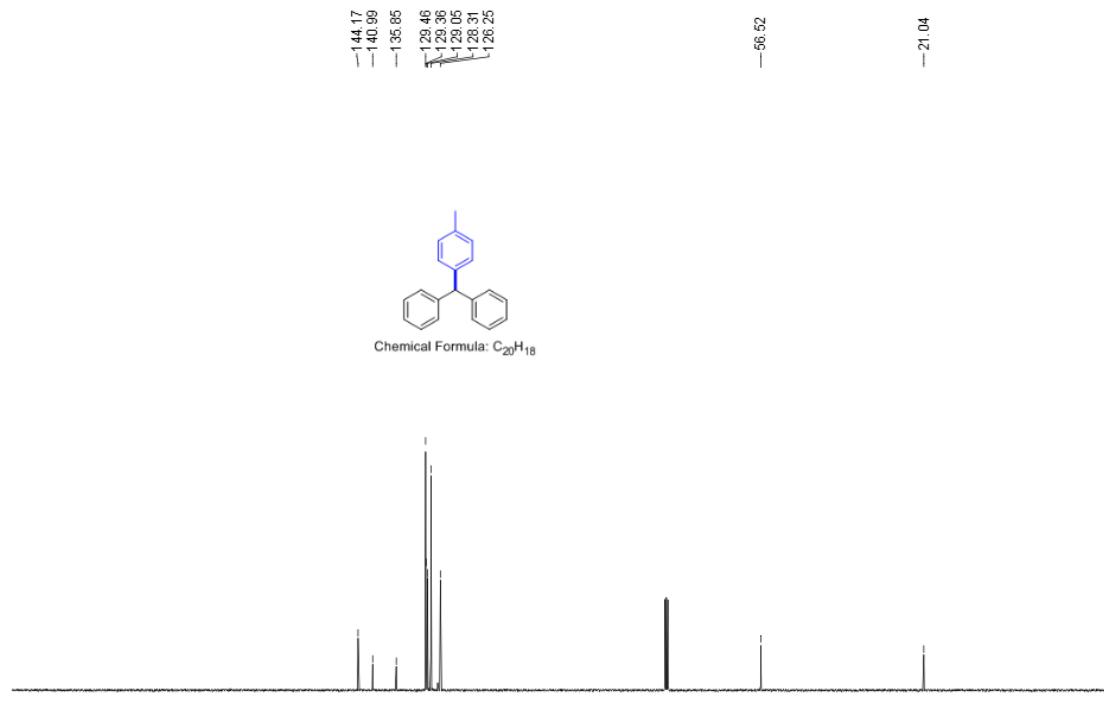
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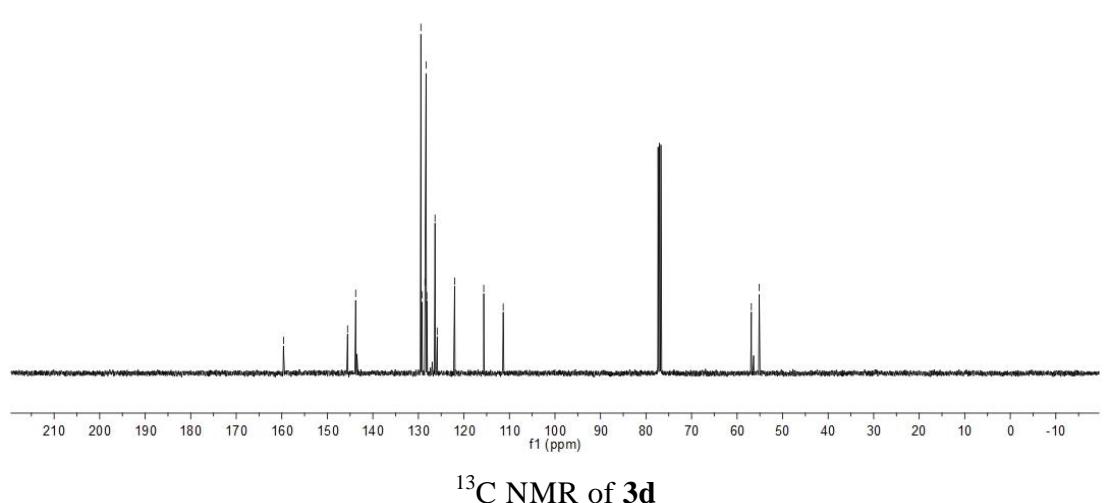
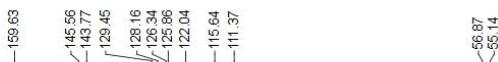
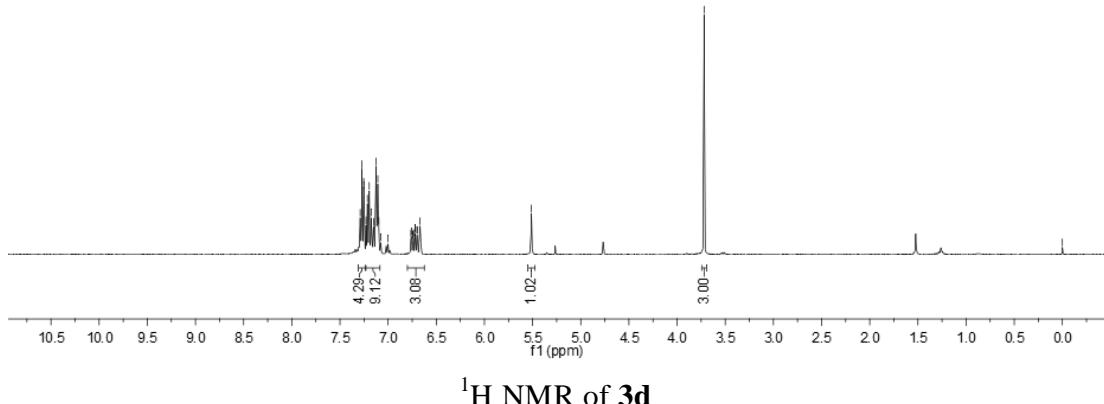
¹³C NMR of 3b

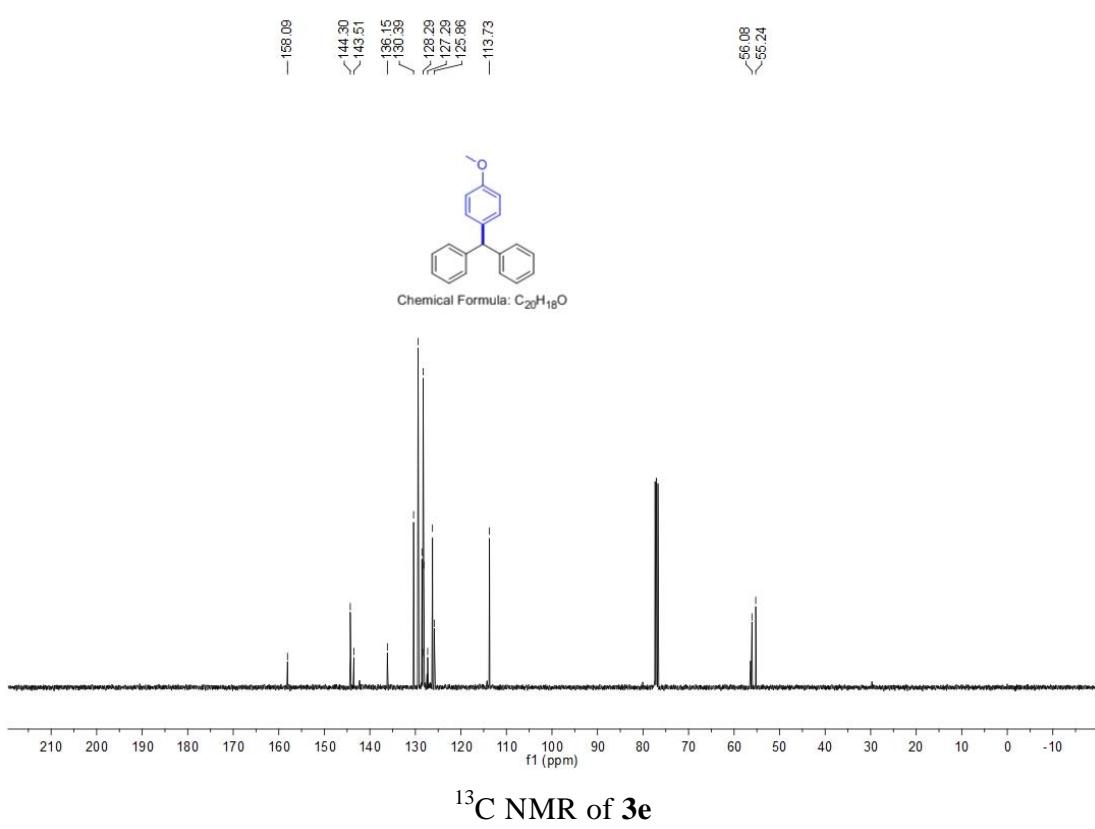
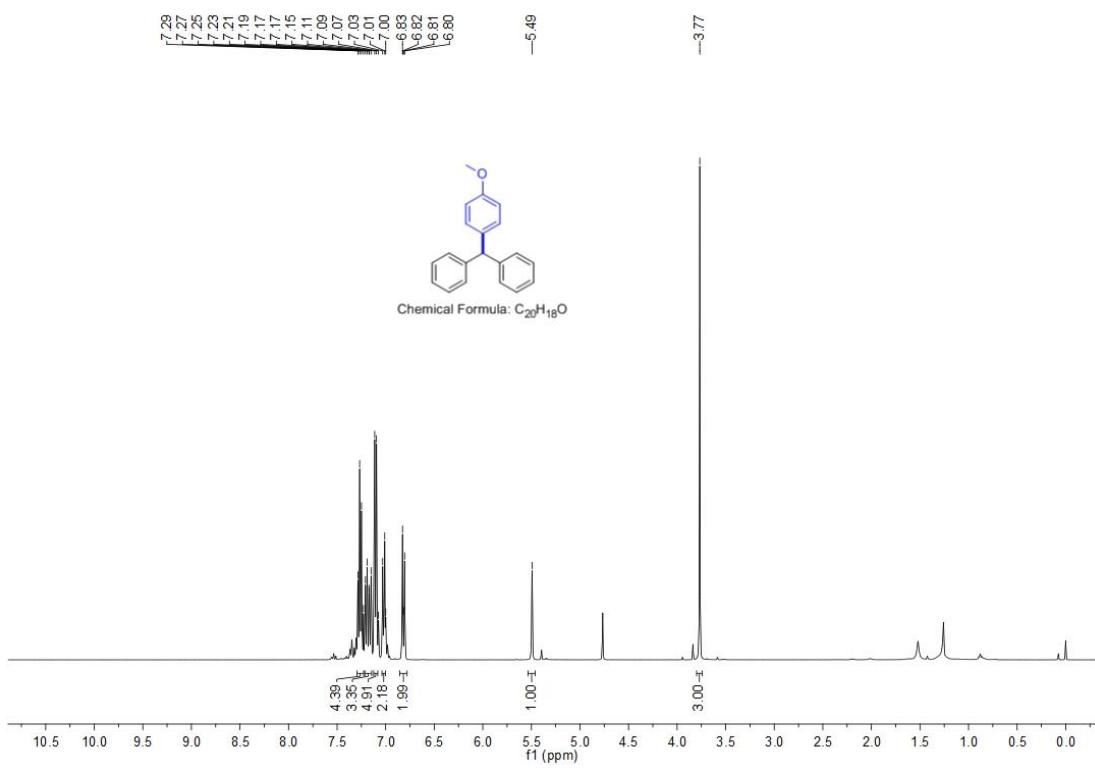


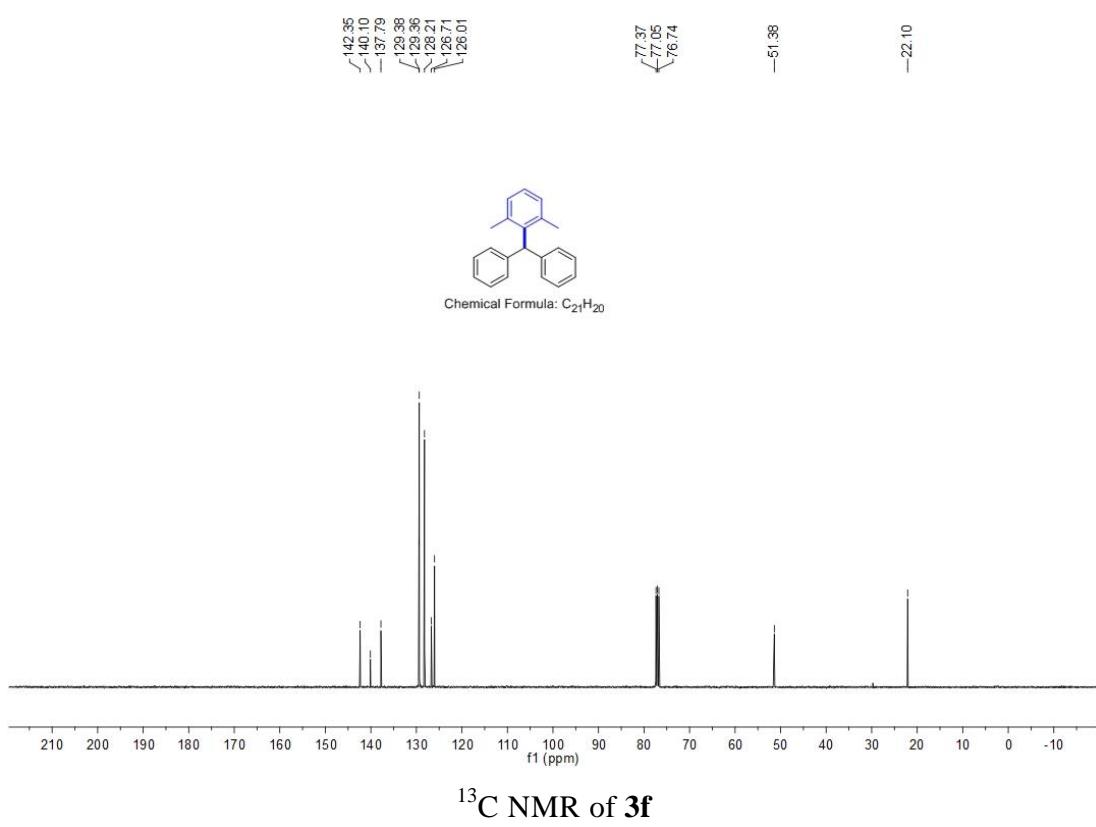
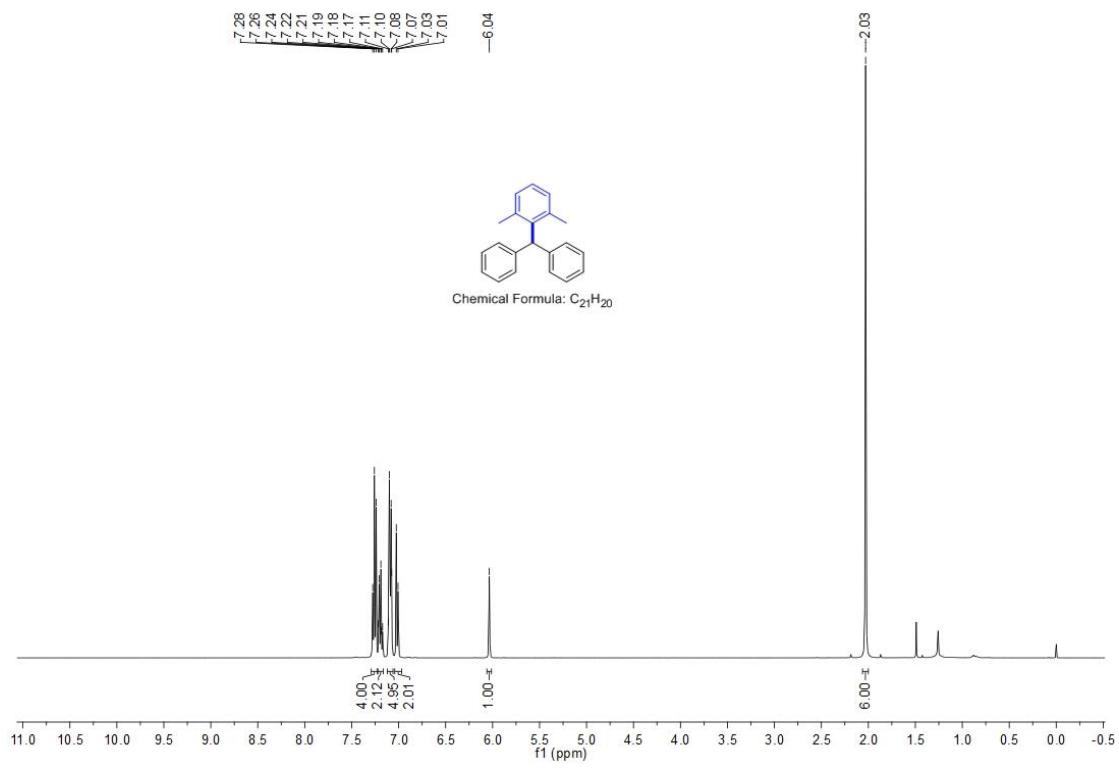
¹H NMR of 3c

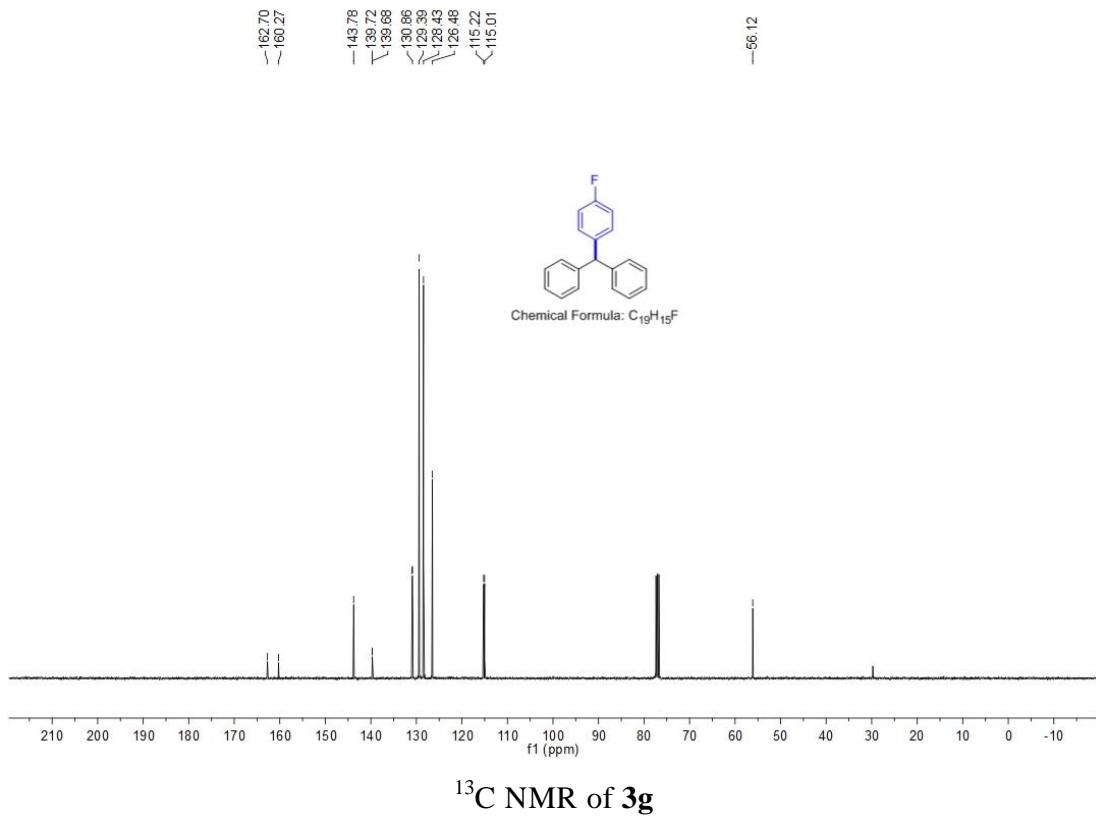
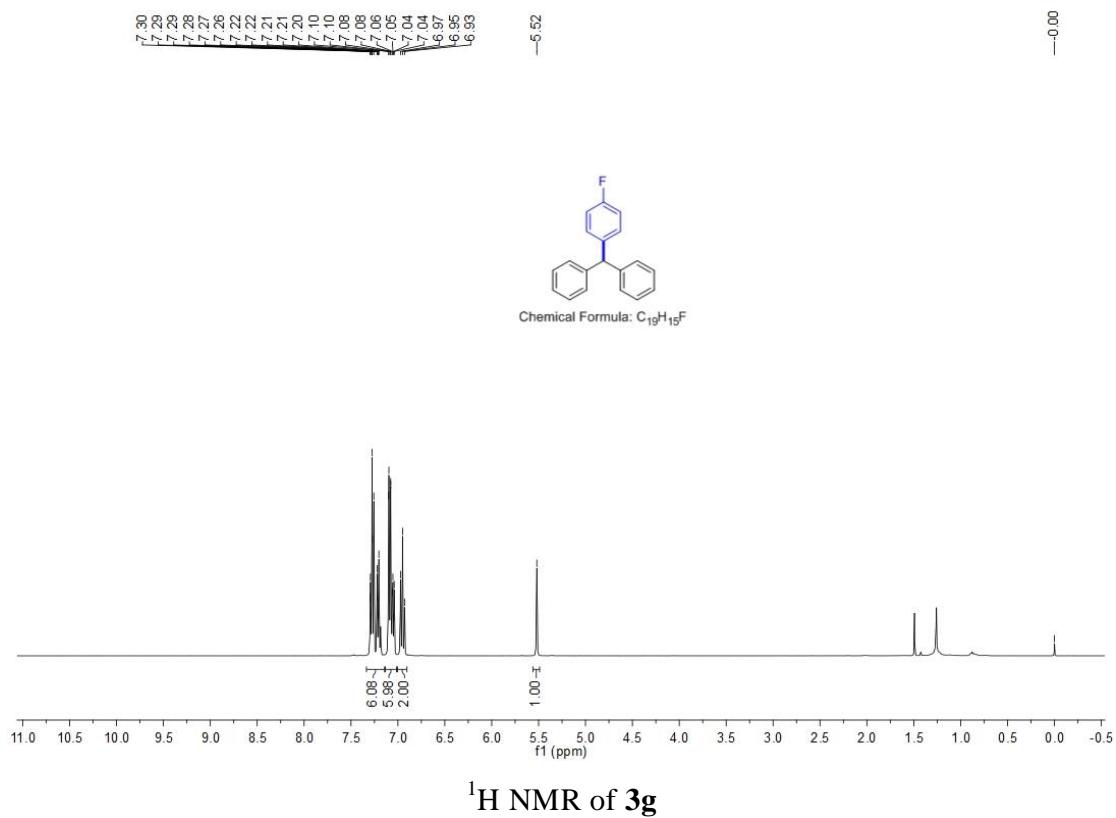


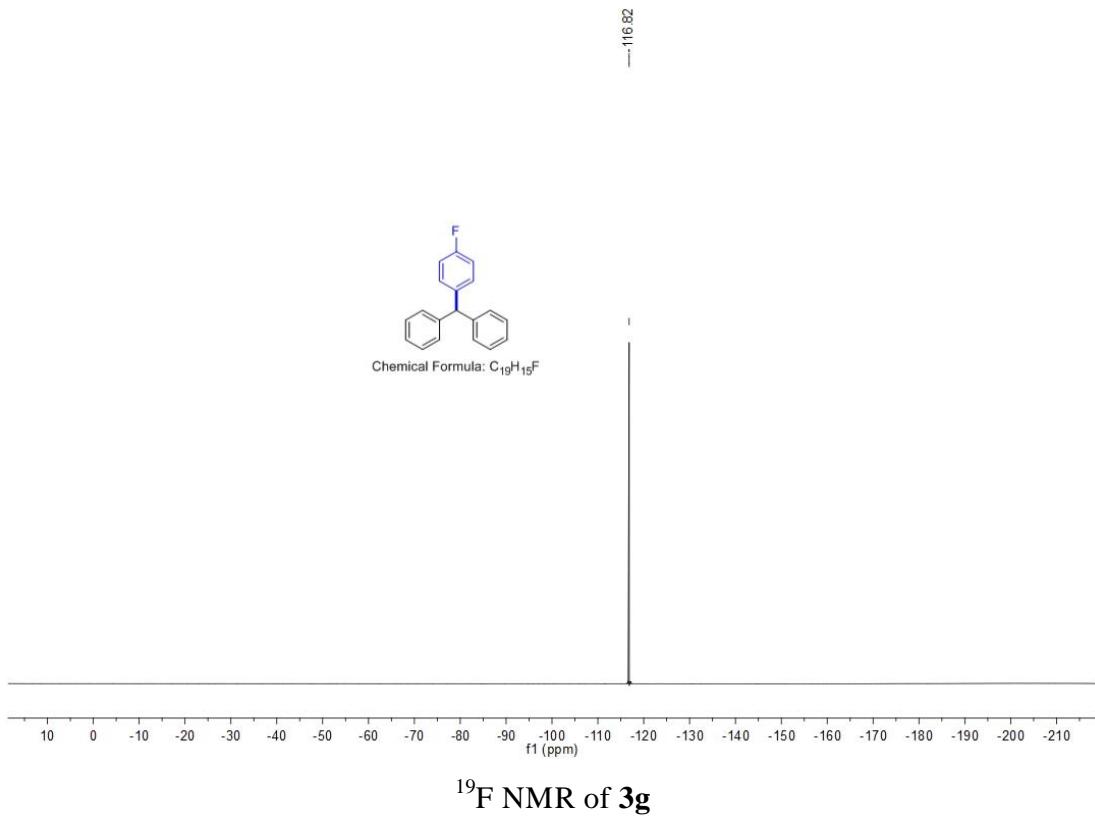
¹³C NMR of 3c

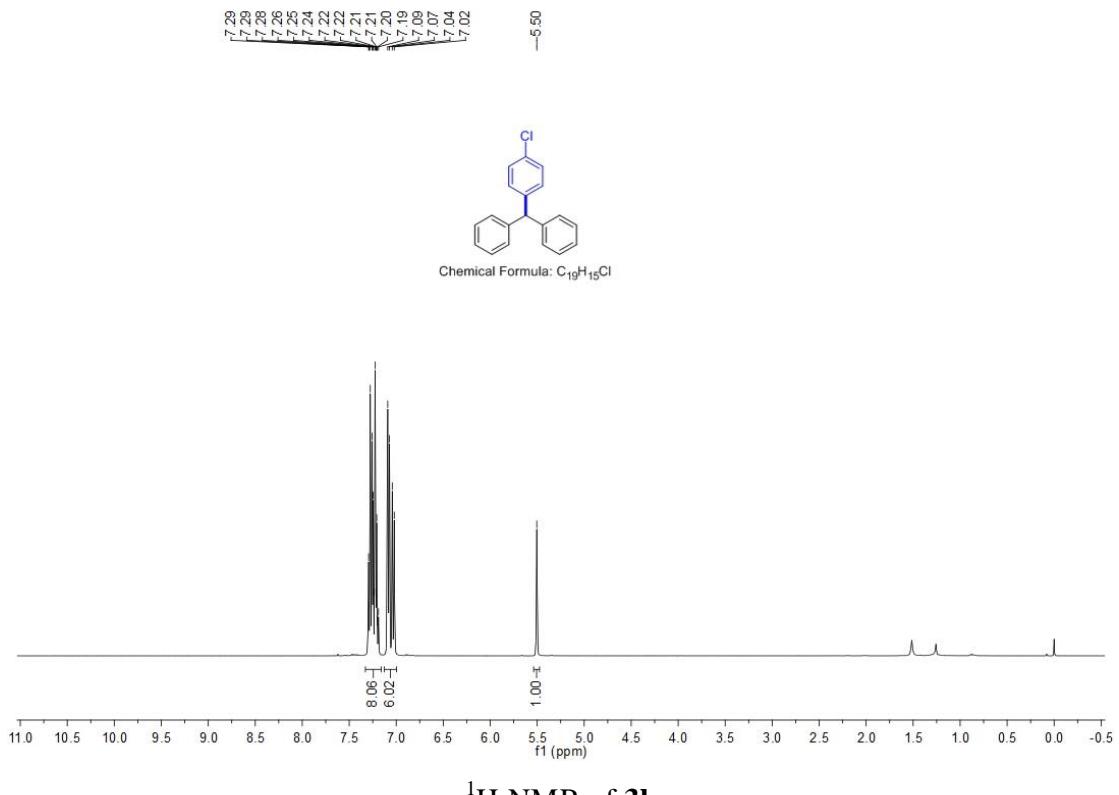




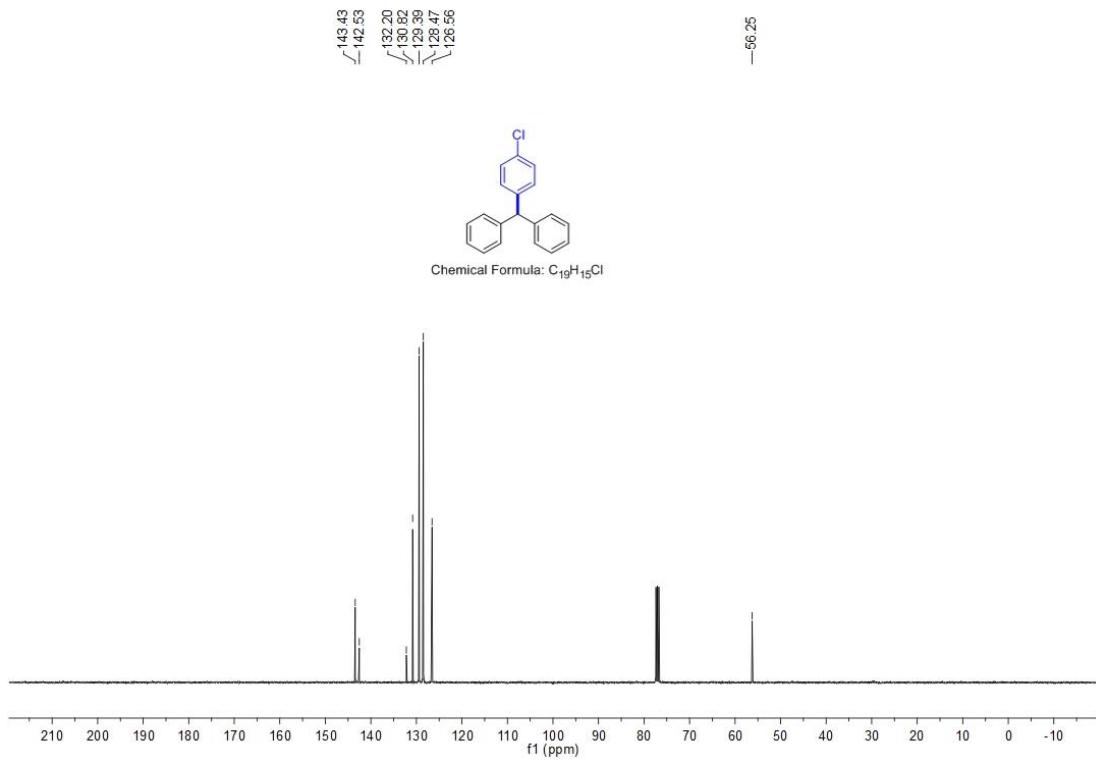




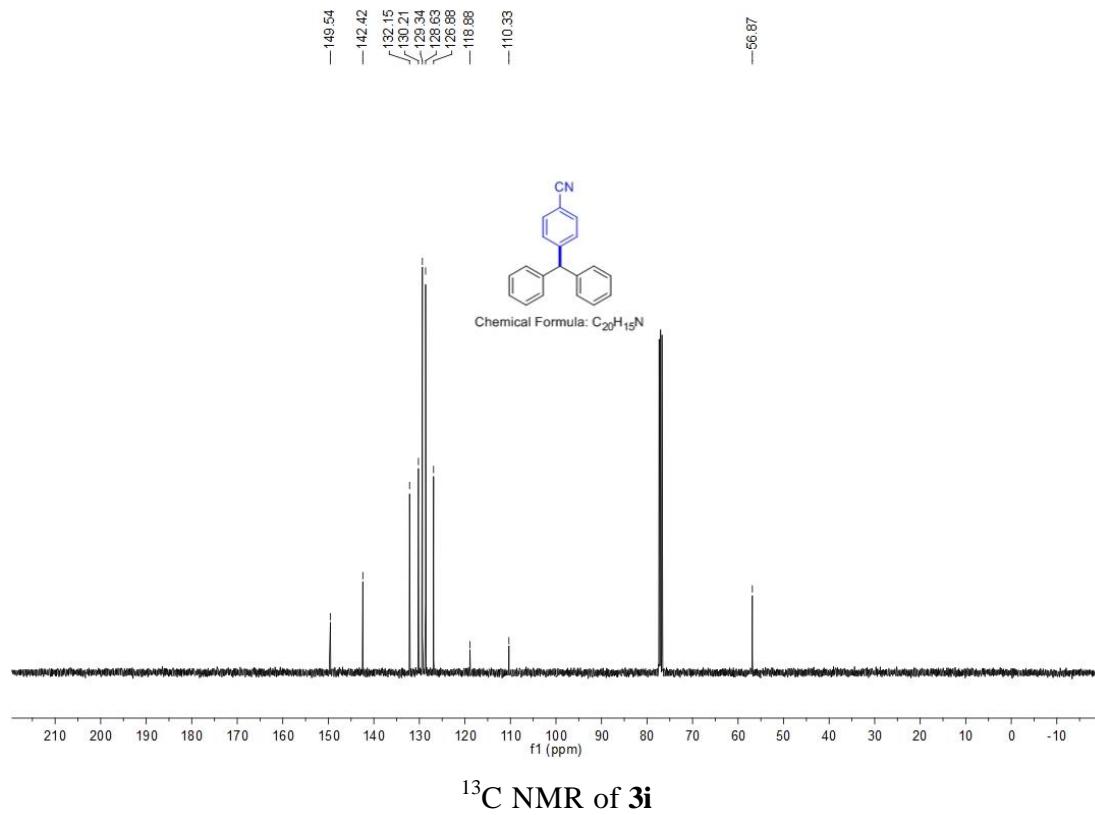
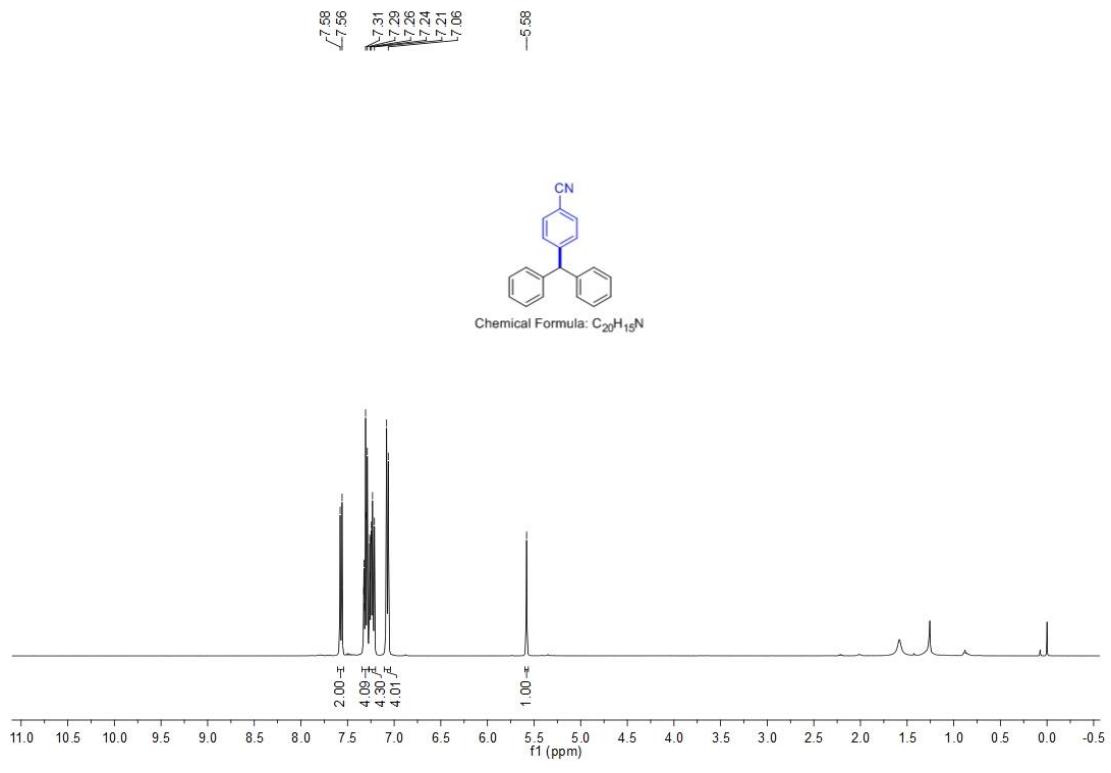




¹H NMR of 3h



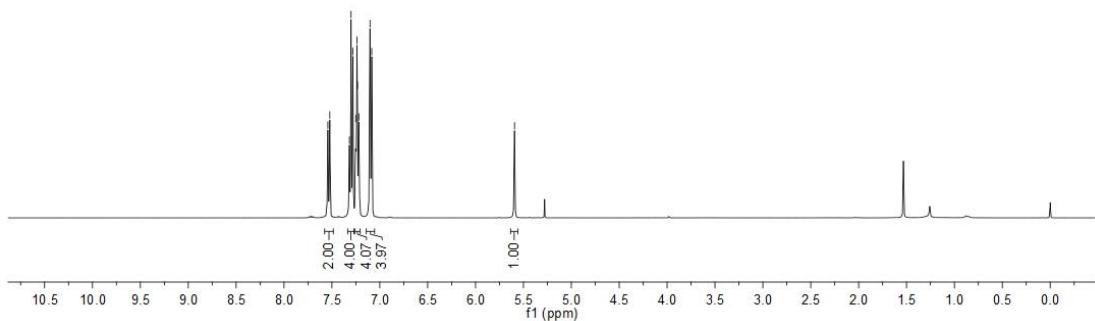
¹³C NMR of **3h**



7.54
7.52
7.30
7.24
7.23
7.22
7.19
7.08
-5.59



Chemical Formula: $\text{C}_{20}\text{H}_{15}\text{F}_3$

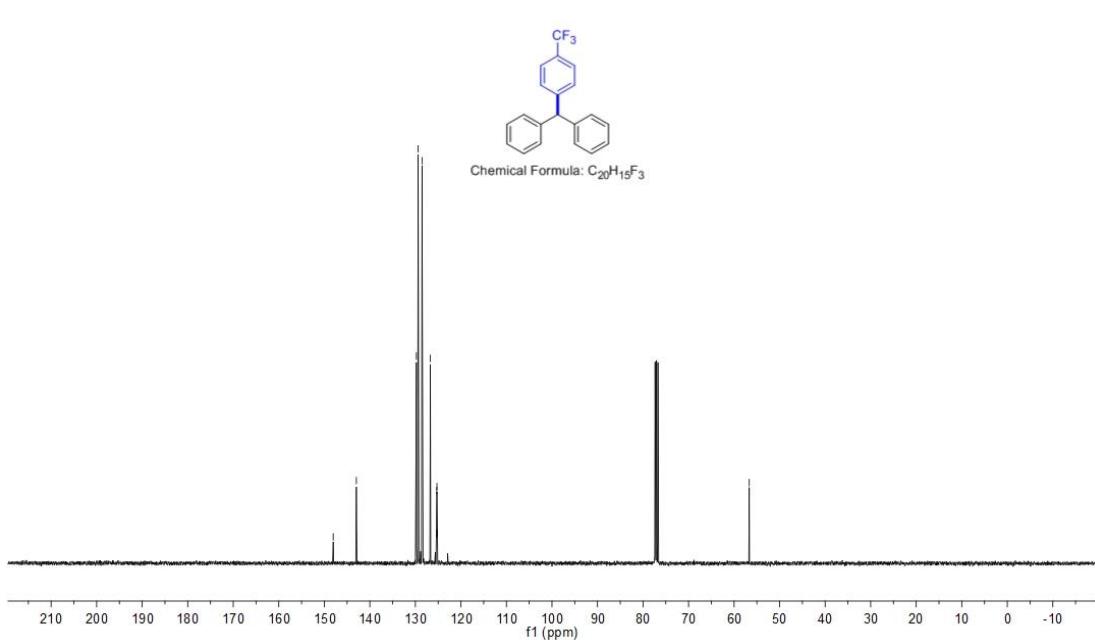


^1H NMR of **3j**

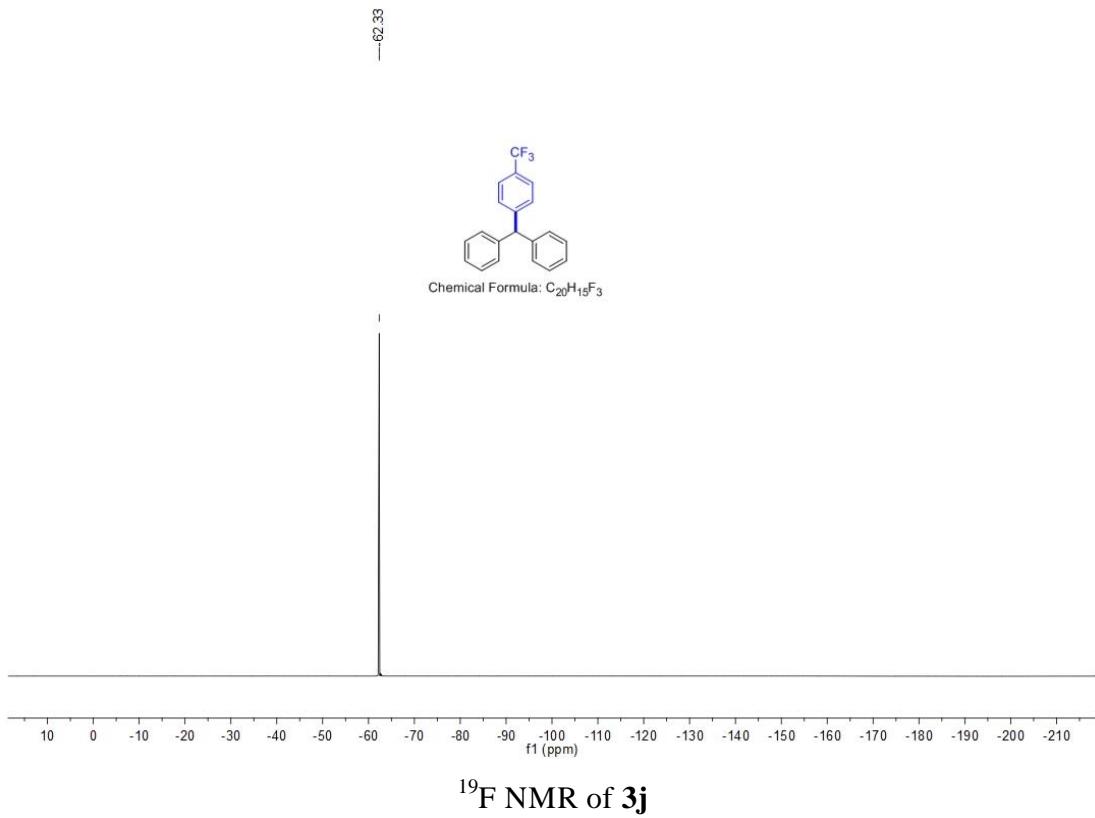
-148.04
-142.96
-129.78
-129.40
-128.54
-128.71
-125.33
-125.30
-125.26
-125.22
-56.67

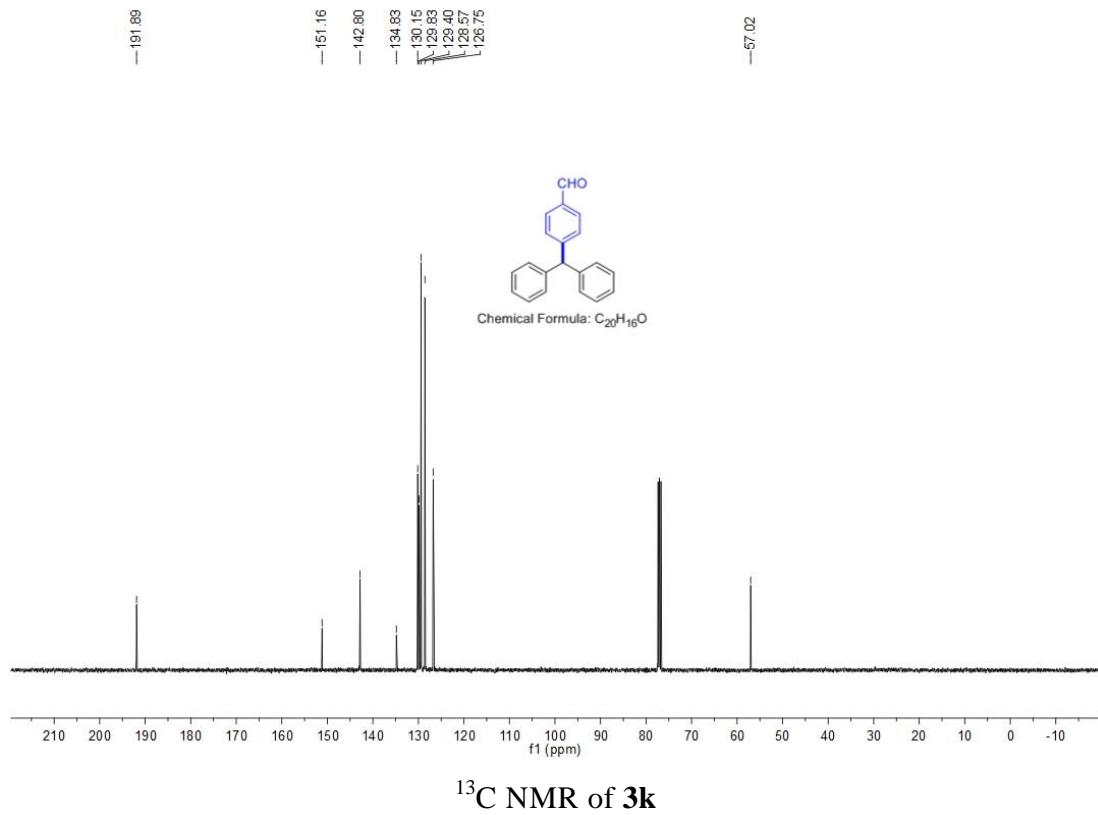
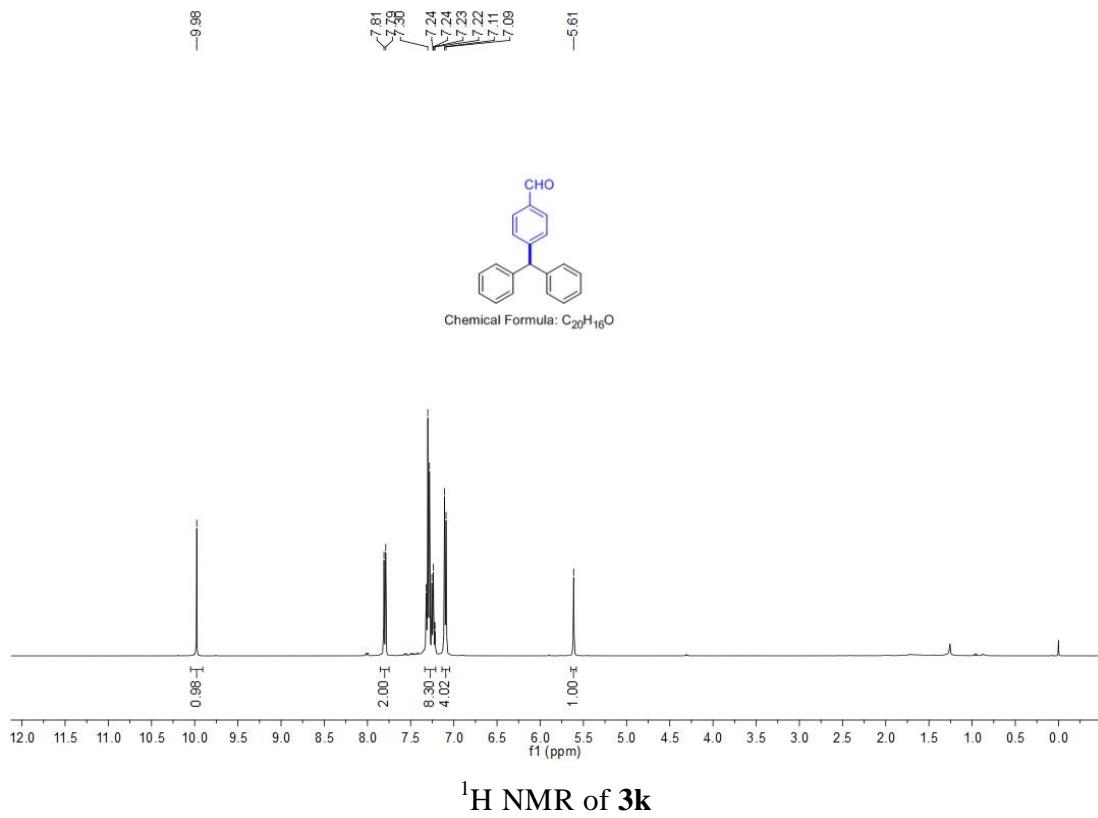


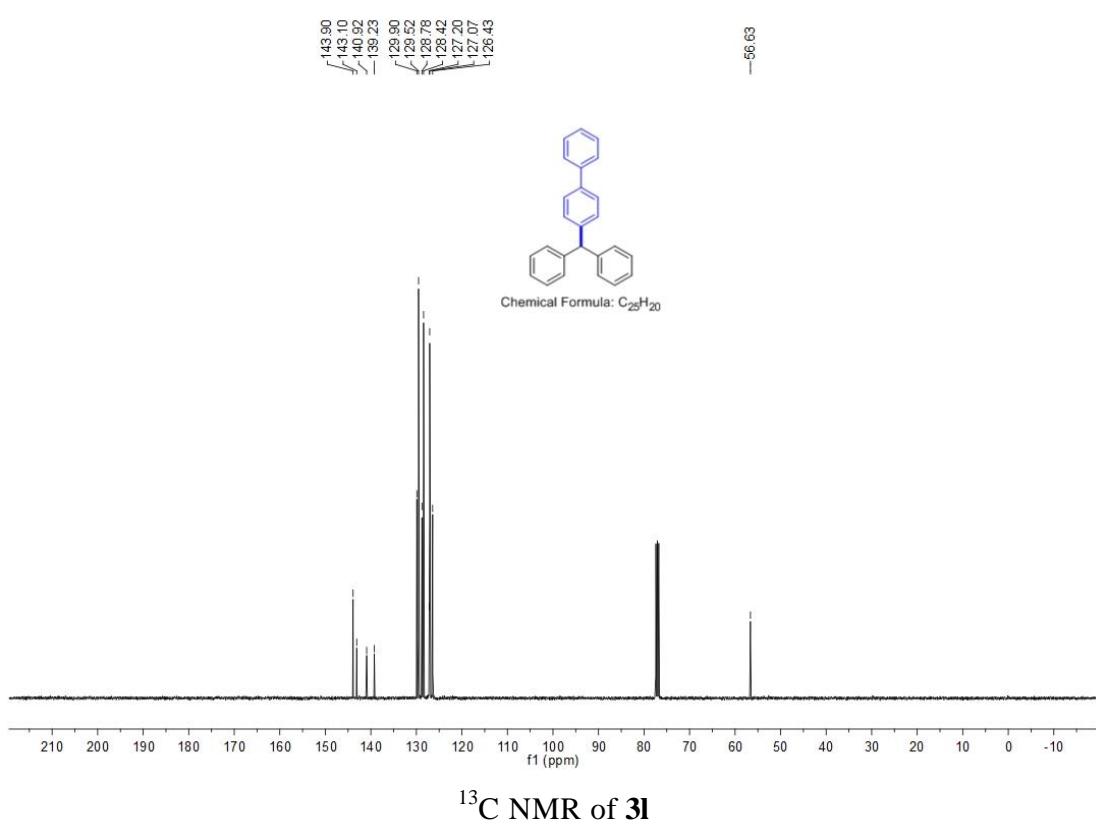
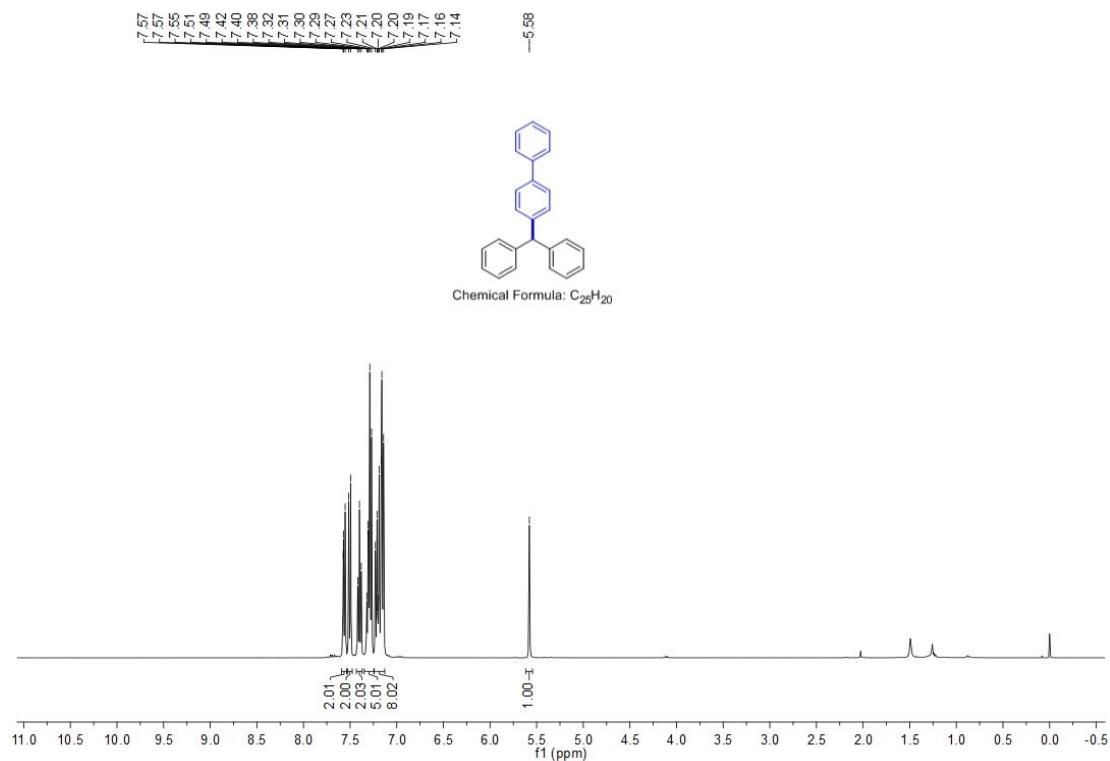
Chemical Formula: $\text{C}_{20}\text{H}_{15}\text{F}_3$

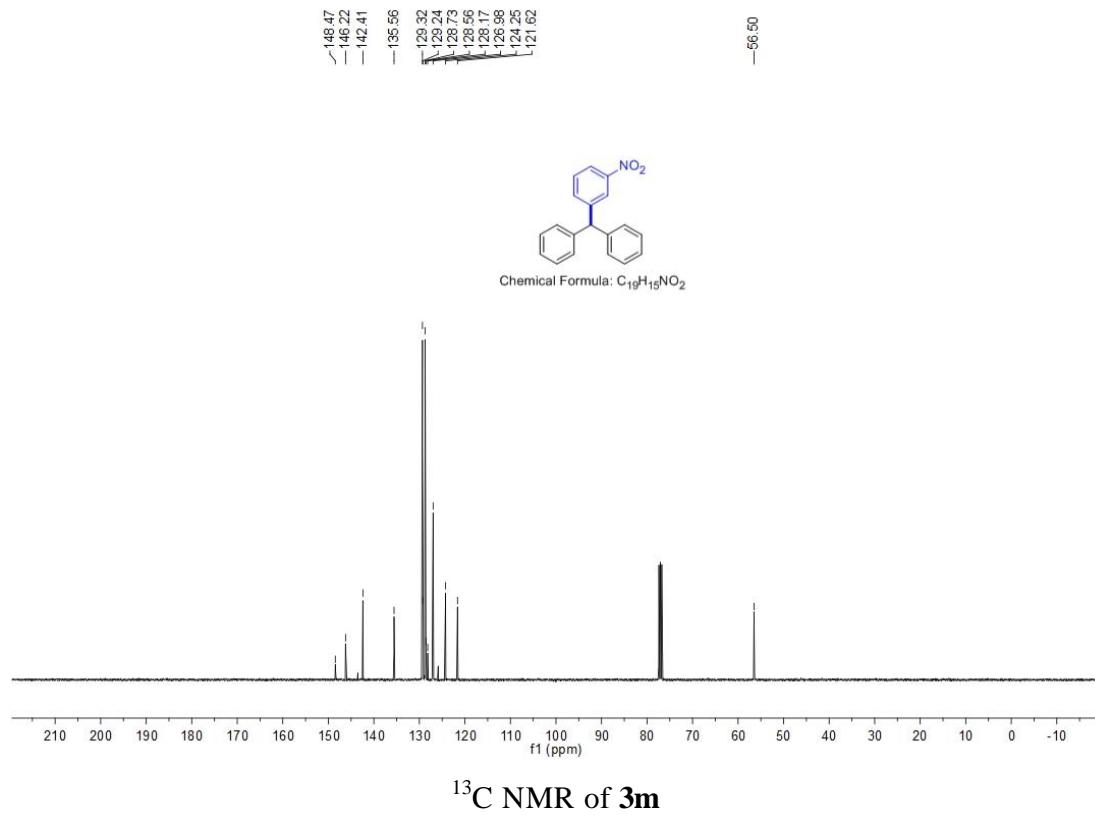
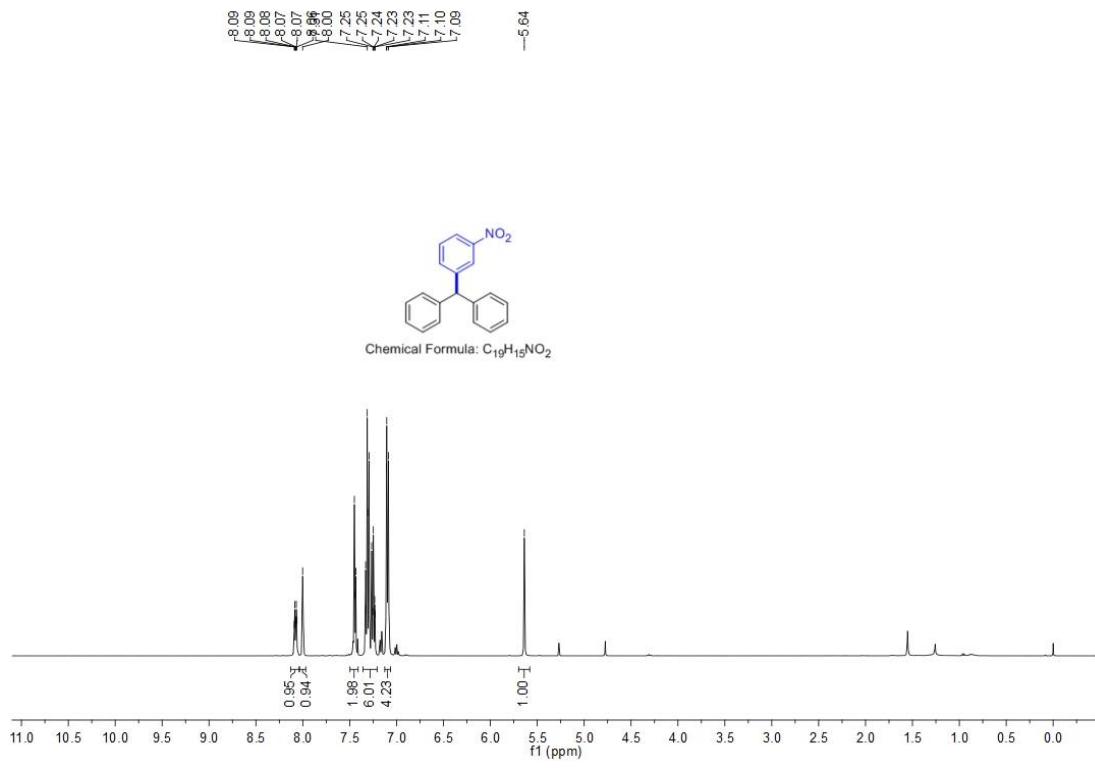


^{13}C NMR of **3j**

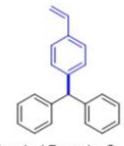




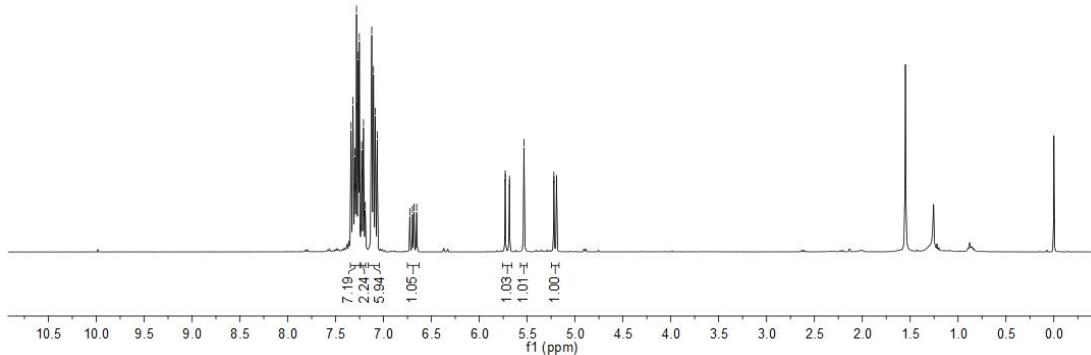




7.34
7.32
7.30
7.28
7.26
7.24
7.23
7.22
7.21
7.20
7.19
7.18
7.16
7.12
7.10
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5.73
5.69
5.68
5.53
5.22
5.19
5.19

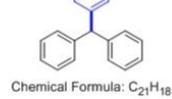


Chemical Formula: C₂₁H₁₈

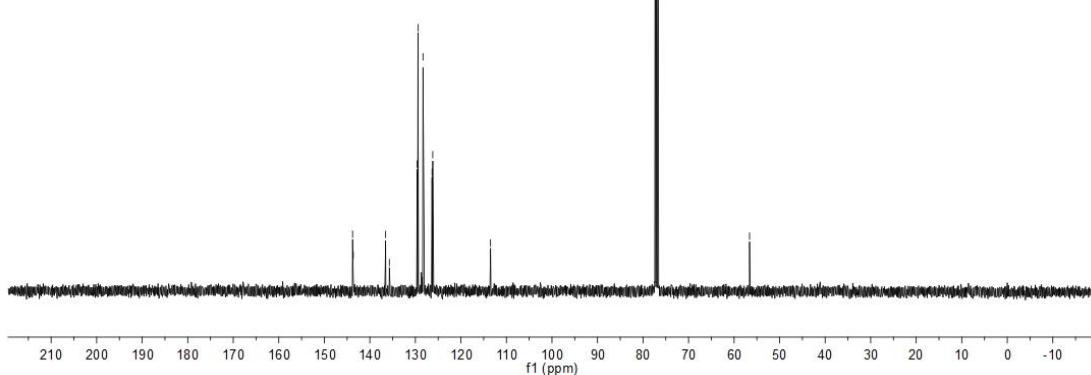


¹H NMR of 3n

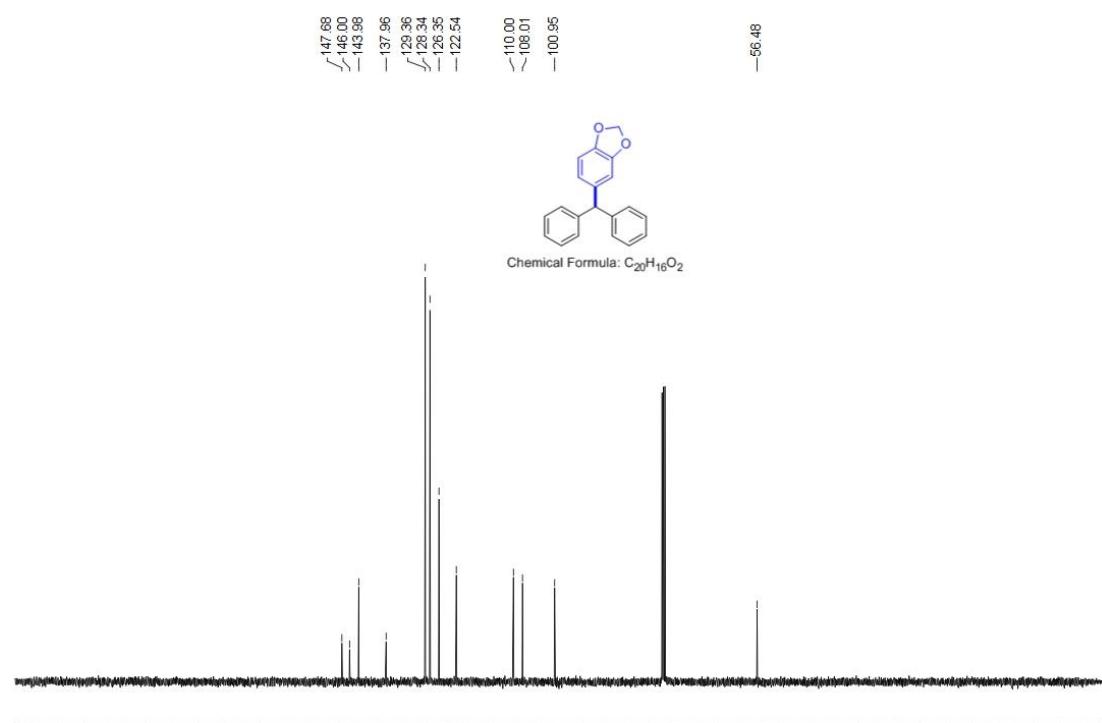
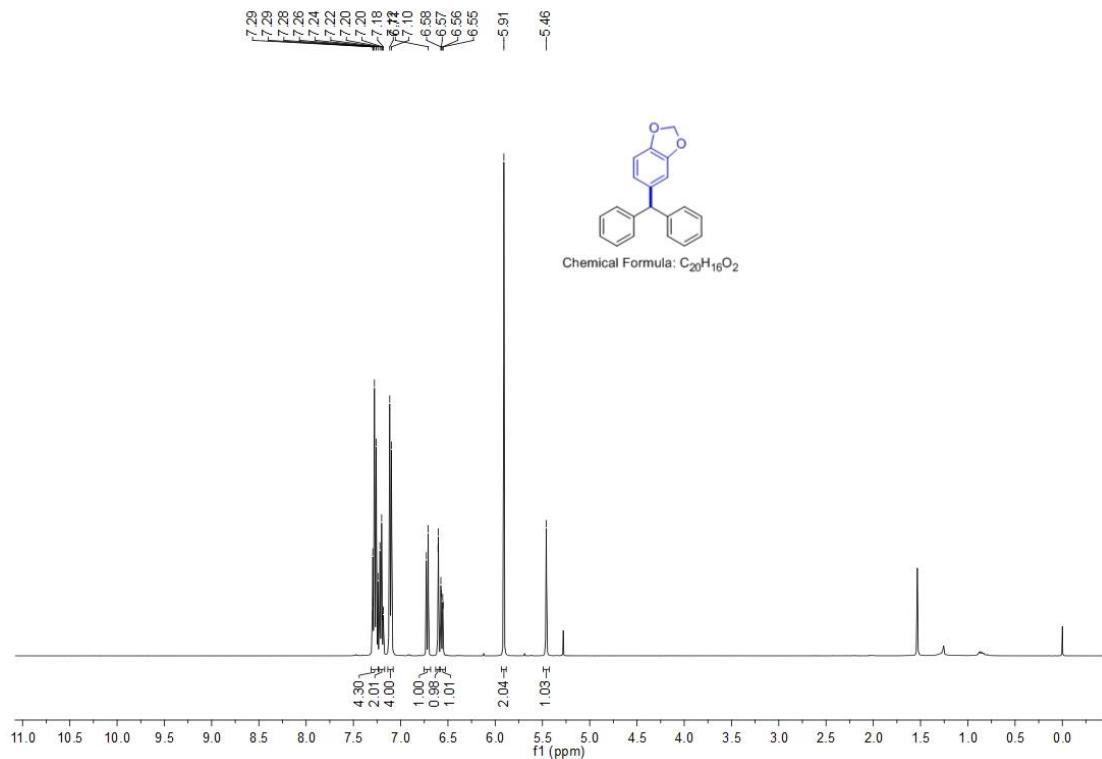
143.79
143.64
138.53
136.72
129.43
126.34
126.18
113.49
—56.60



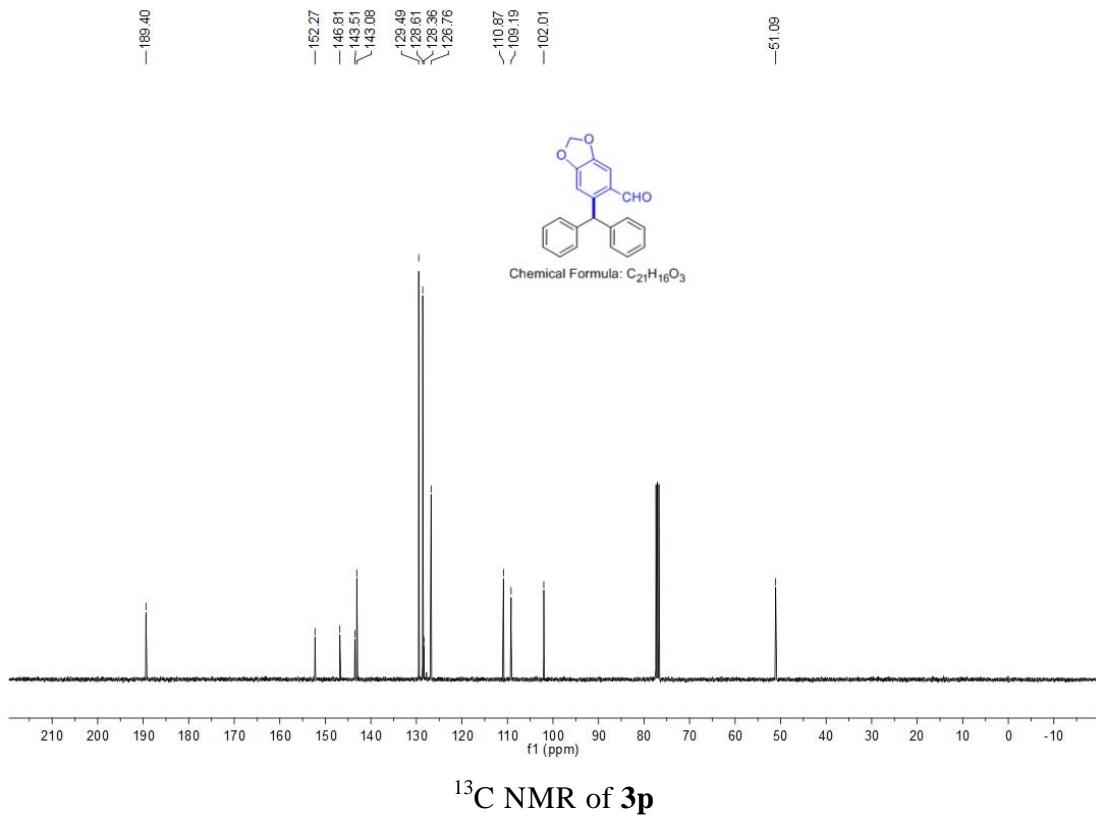
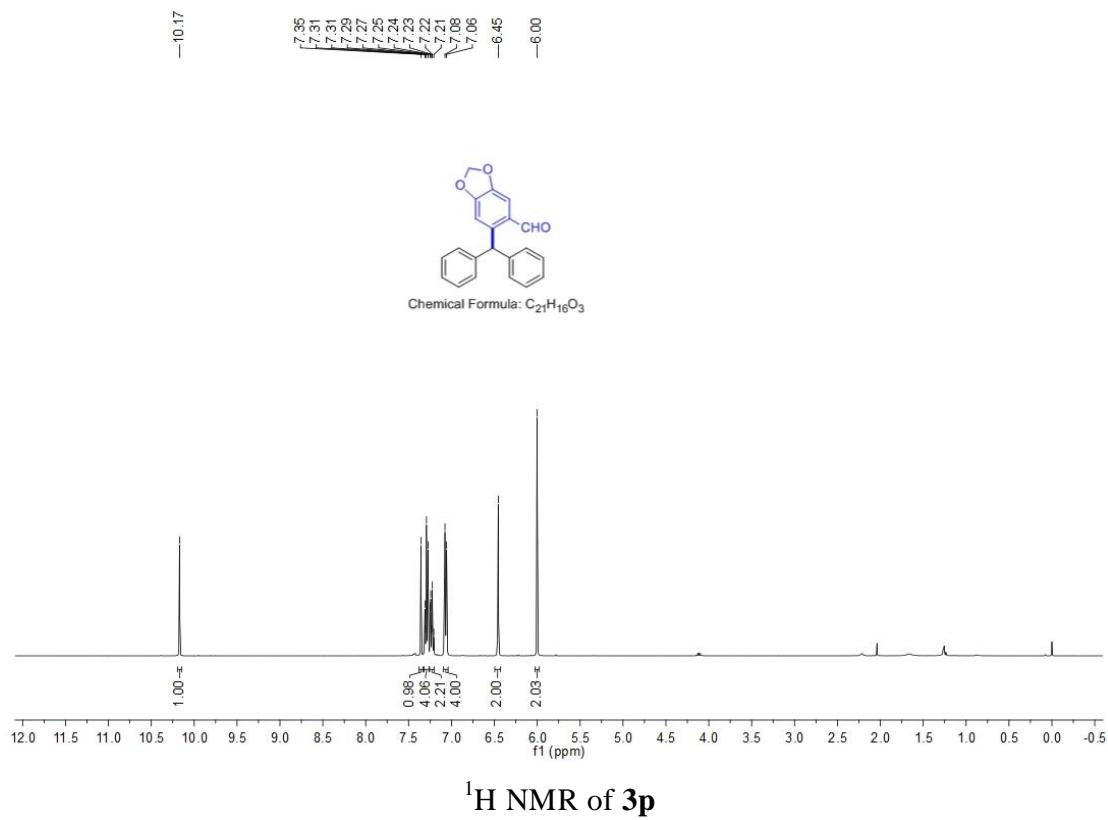
Chemical Formula: C₂₁H₁₈



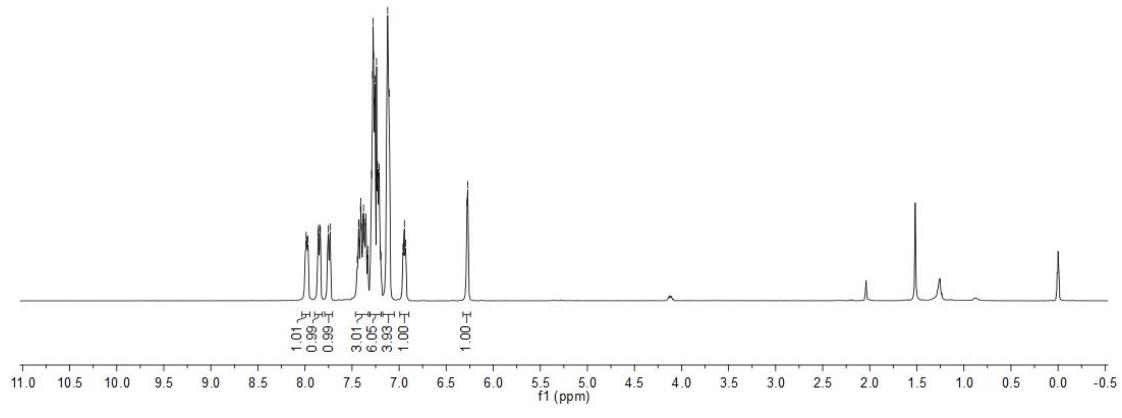
¹³C NMR of 3n



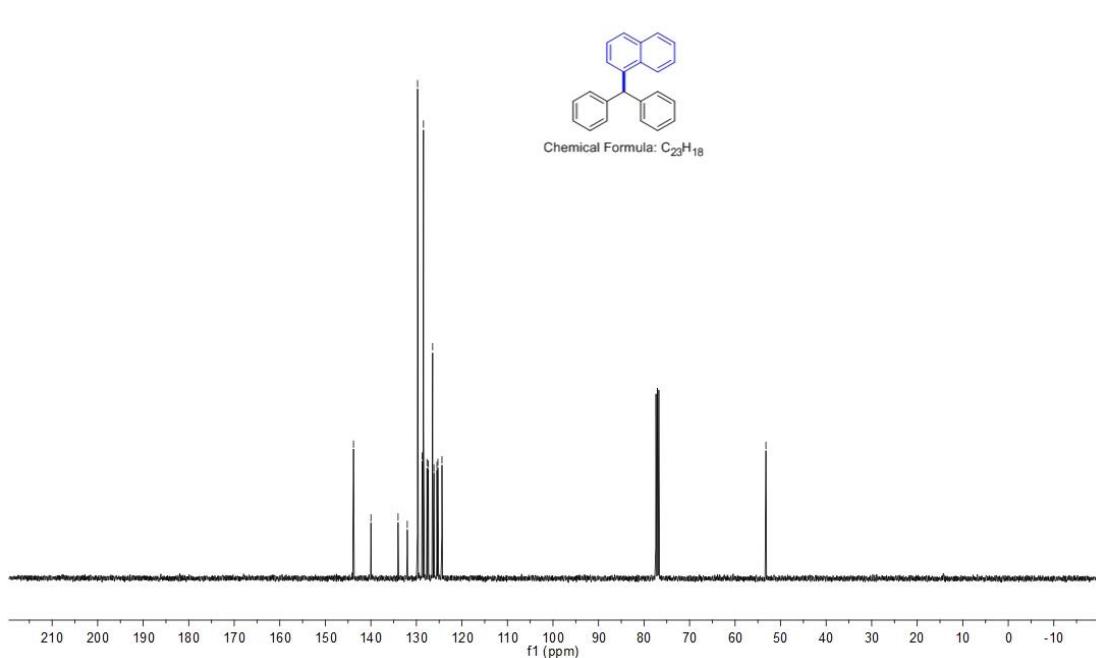
¹³C NMR of **3o**



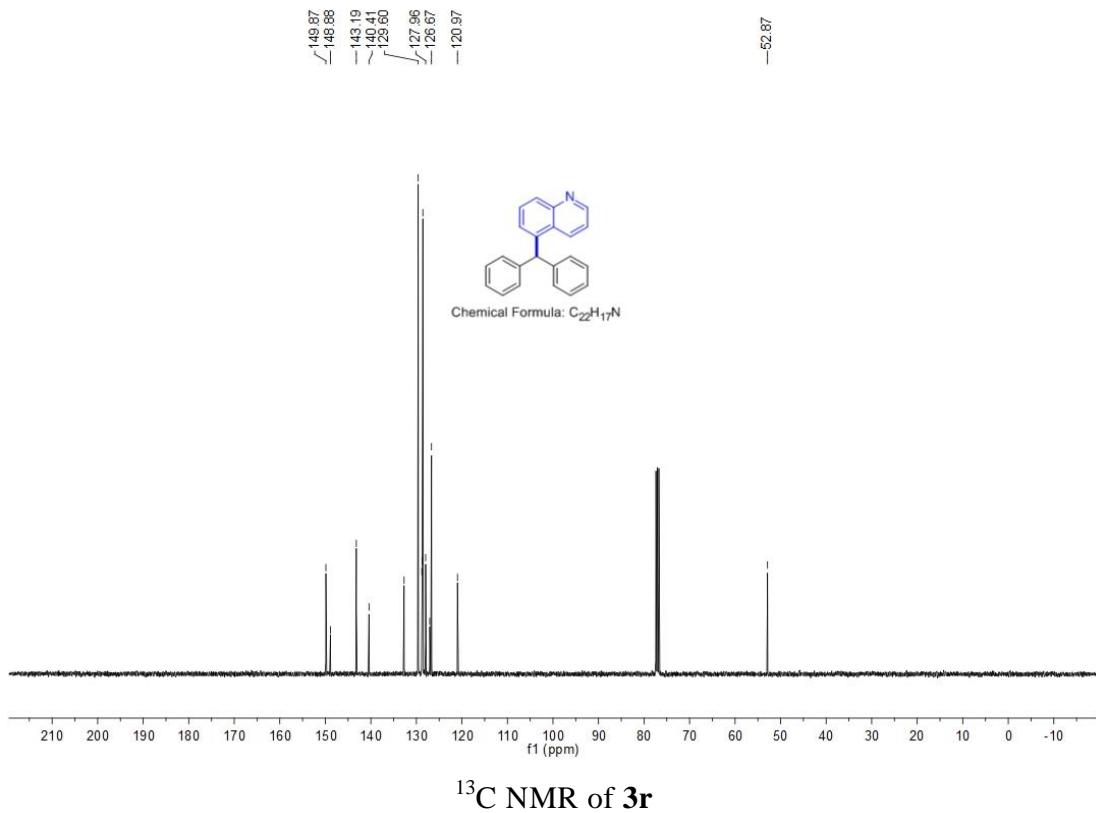
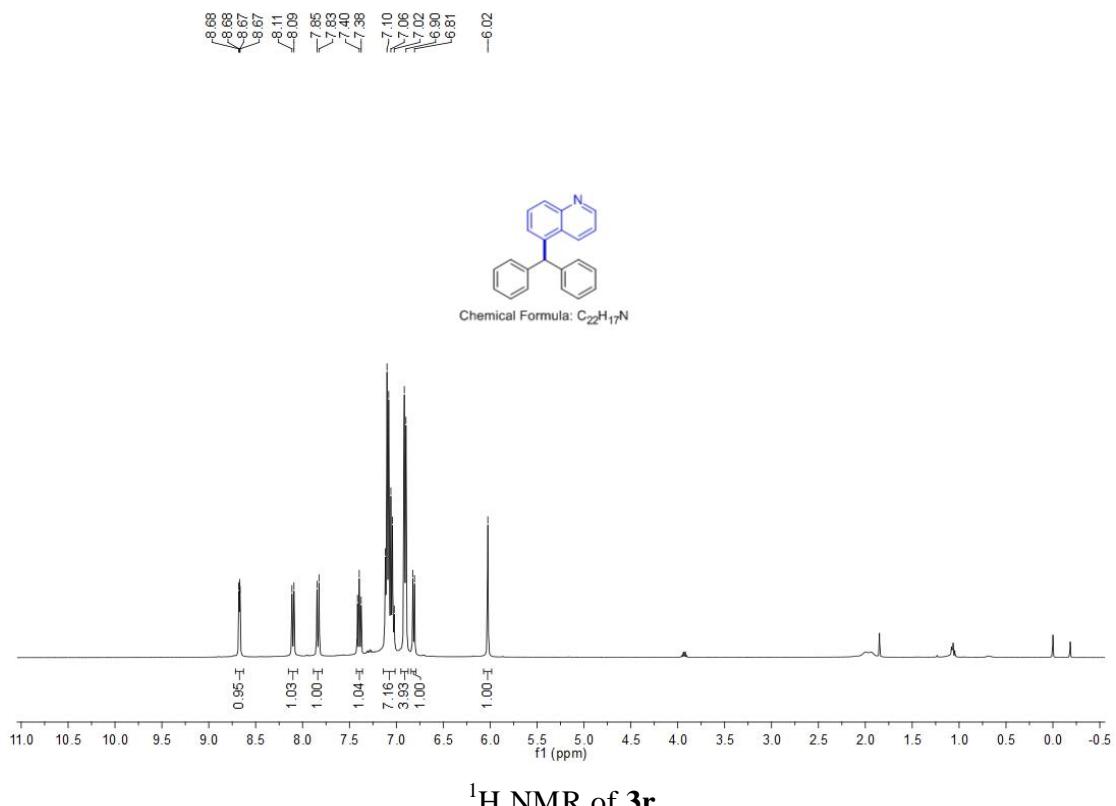
7.99
7.98
7.97
7.86
7.86
7.84
7.84
7.75
7.75

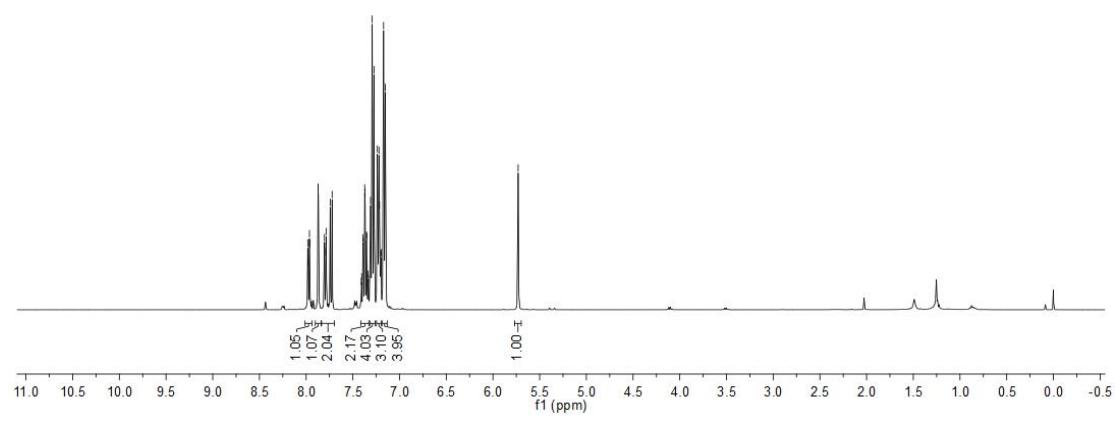


-143.81
-139.98
-134.02
-131.99
-129.73
-128.75
-128.44
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-127.37
-126.43
-126.14
-125.49
-125.27
-124.38
-53.23

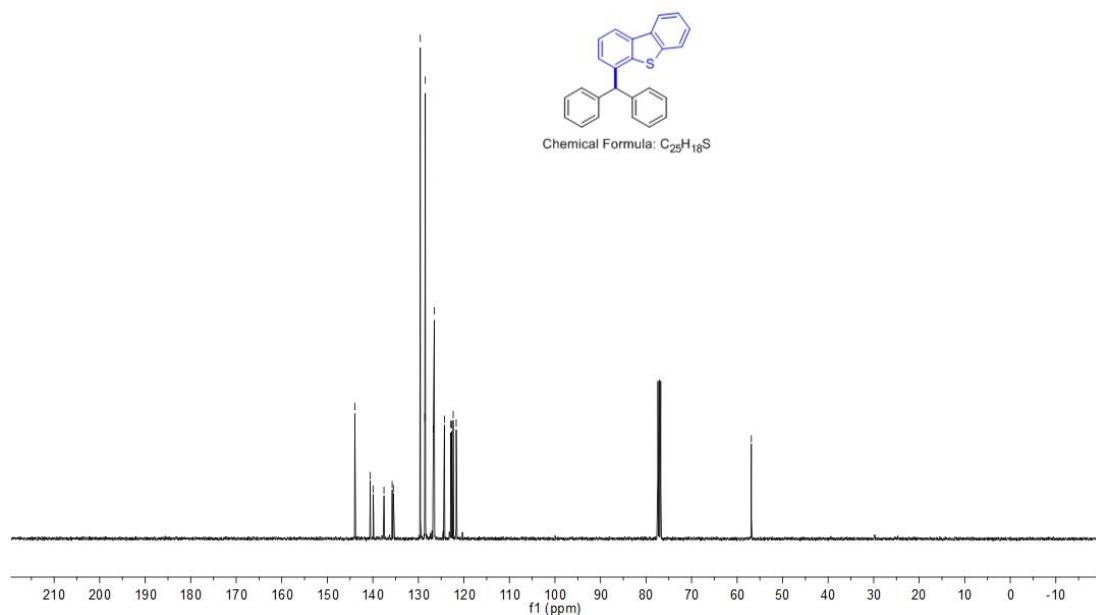
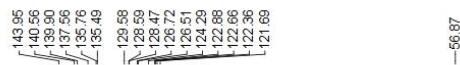


¹³C NMR of 3q





¹H NMR of **3s**

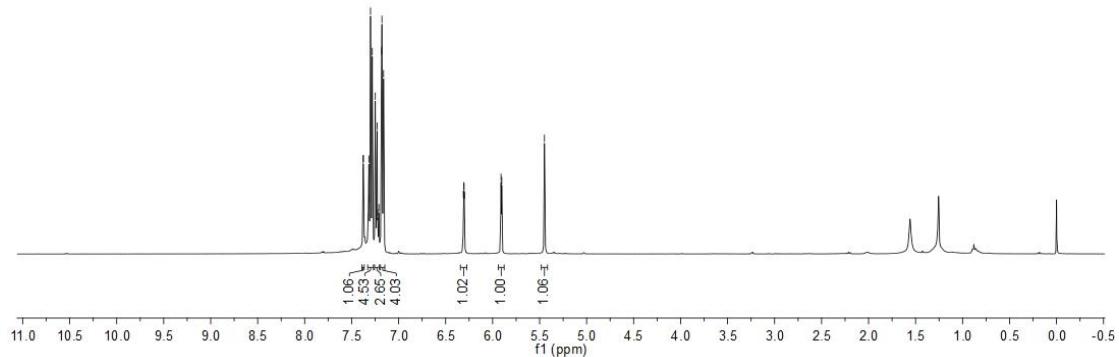


¹³C NMR of **3s**

7.38
7.33
7.32
7.31
7.30
7.28
7.23
7.22
7.21
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7.18
7.16
6.39
6.30
5.91
5.90
-5.45

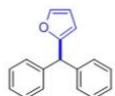


Chemical Formula: C₁₇H₁₄O

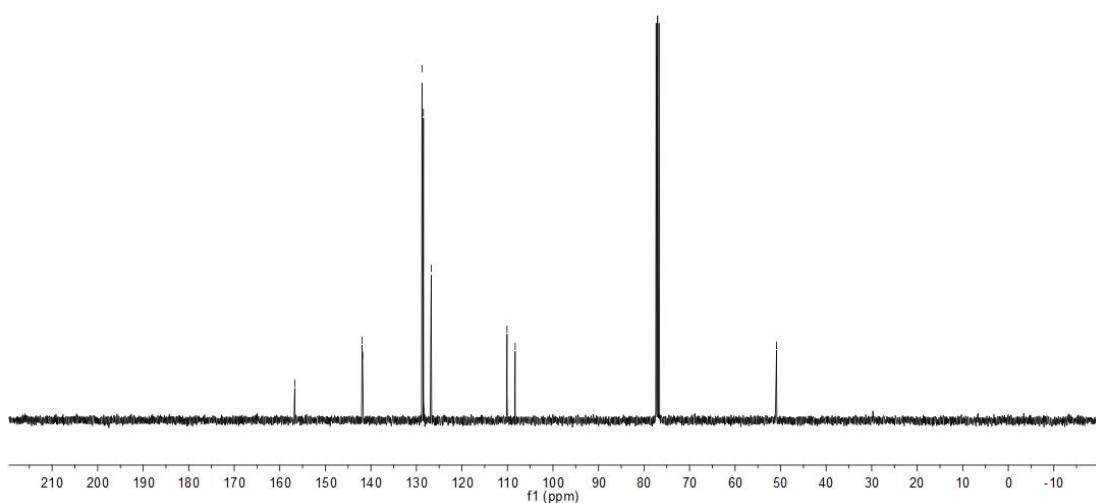


¹H NMR of 3t

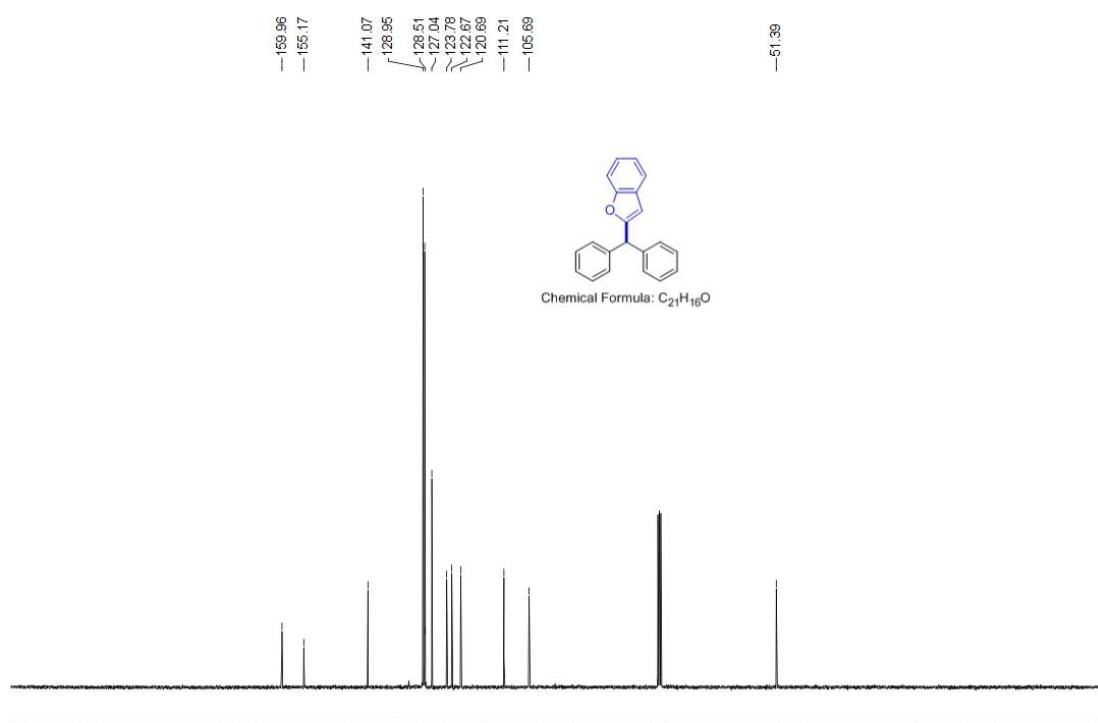
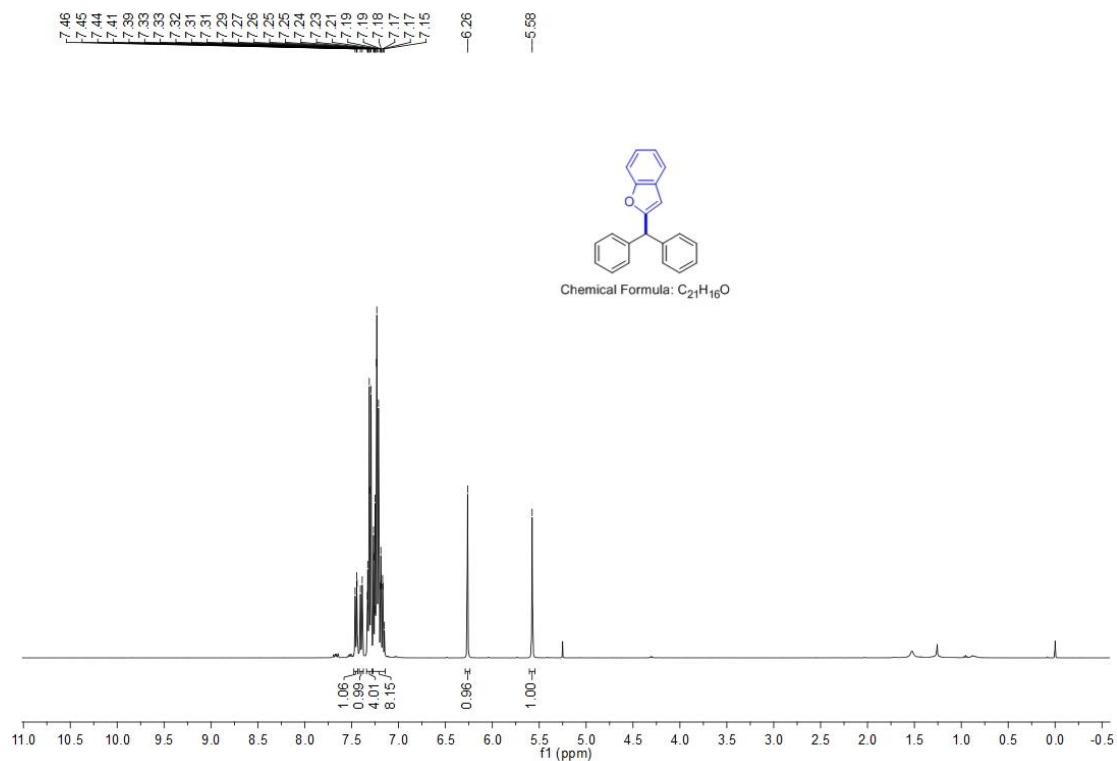
-156.72
<141.93
<141.82
128.76
<128.44
<129.75
110.09
<108.31
-50.91

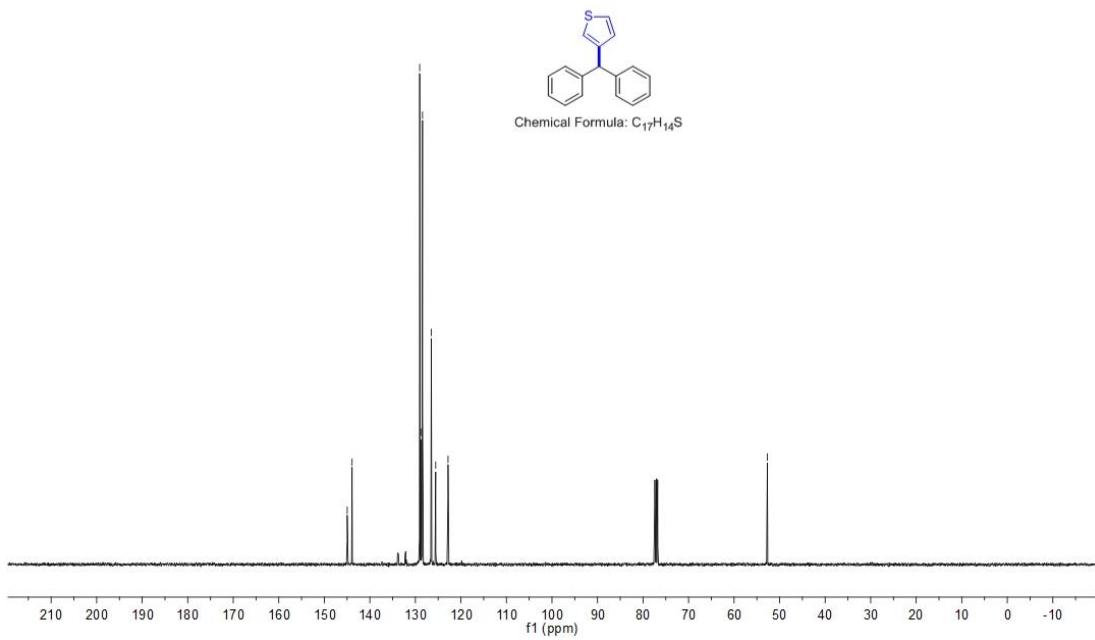
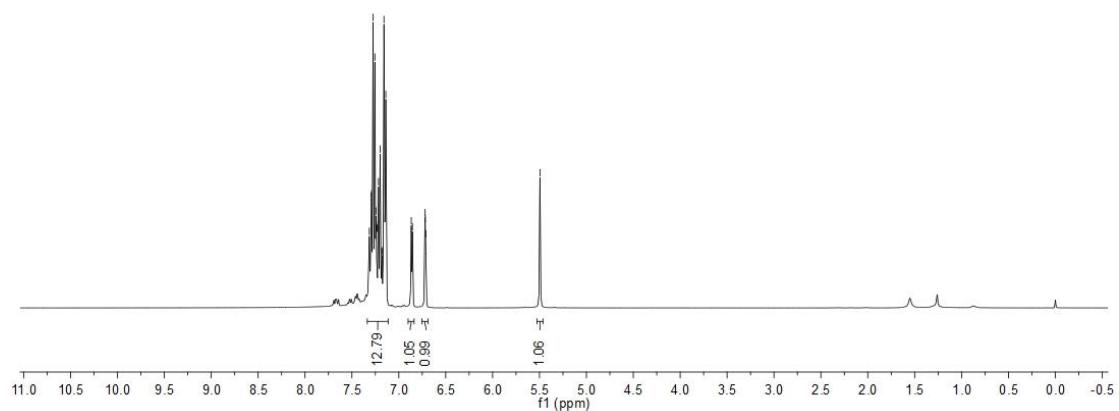
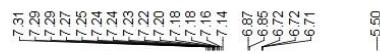


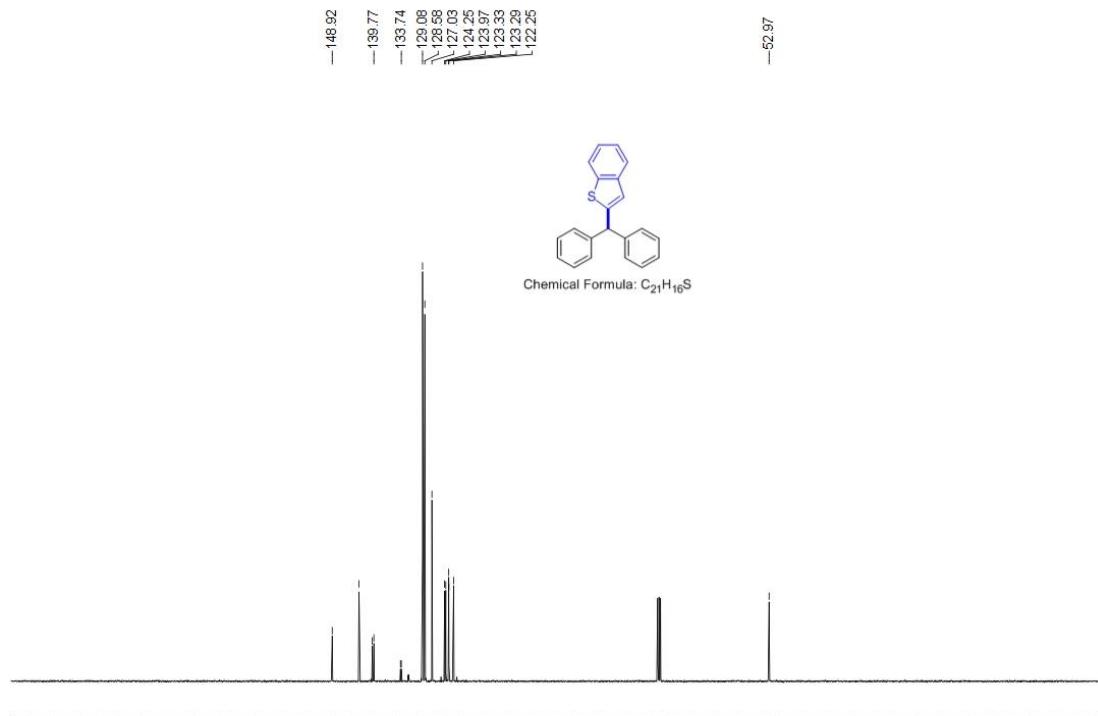
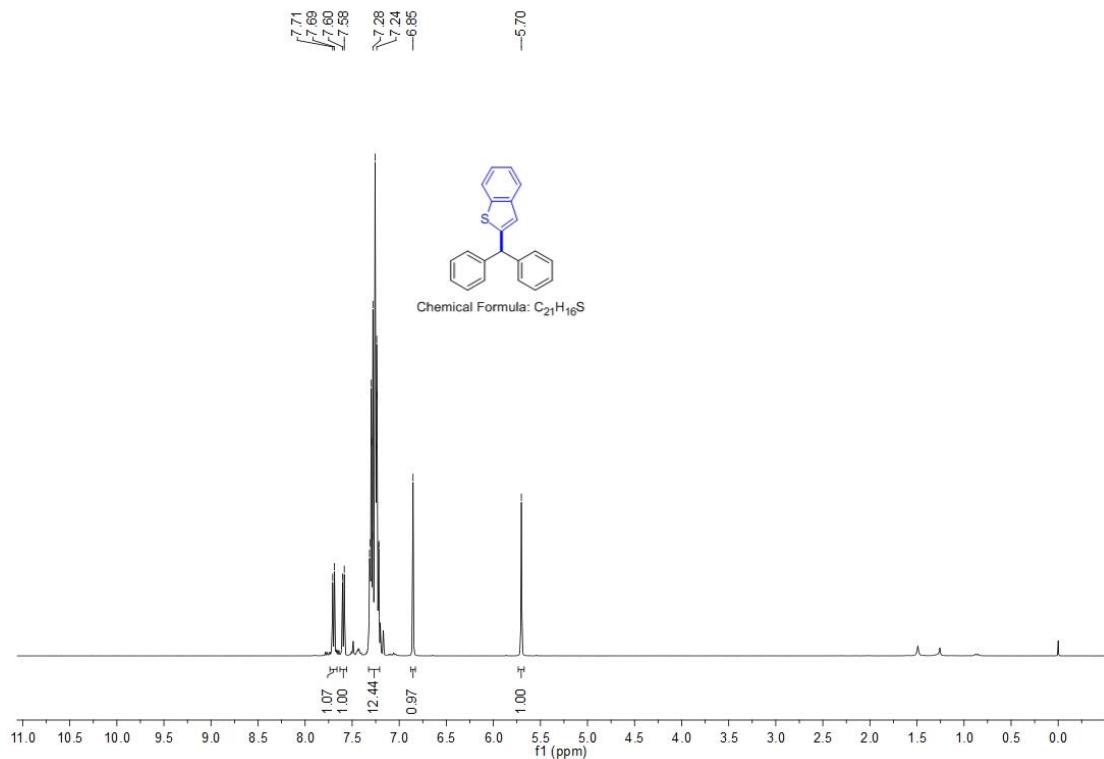
Chemical Formula: C₁₇H₁₄O



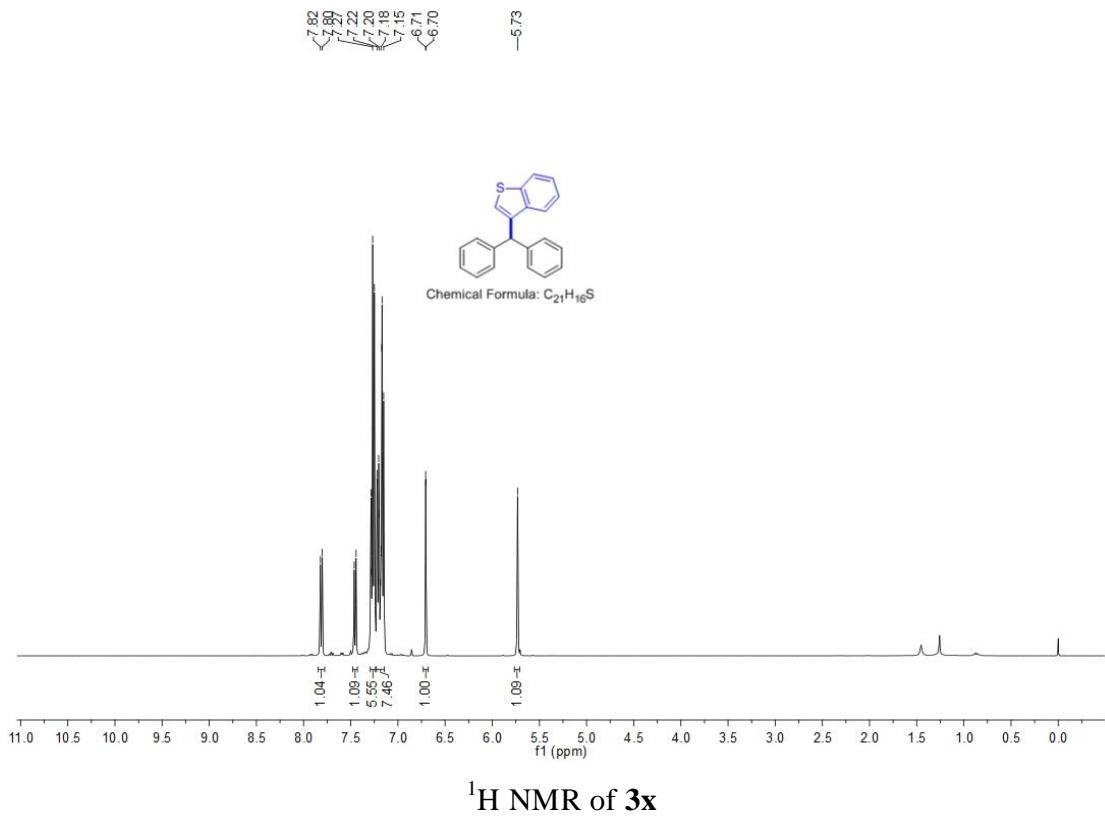
¹³C NMR of 3t



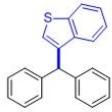
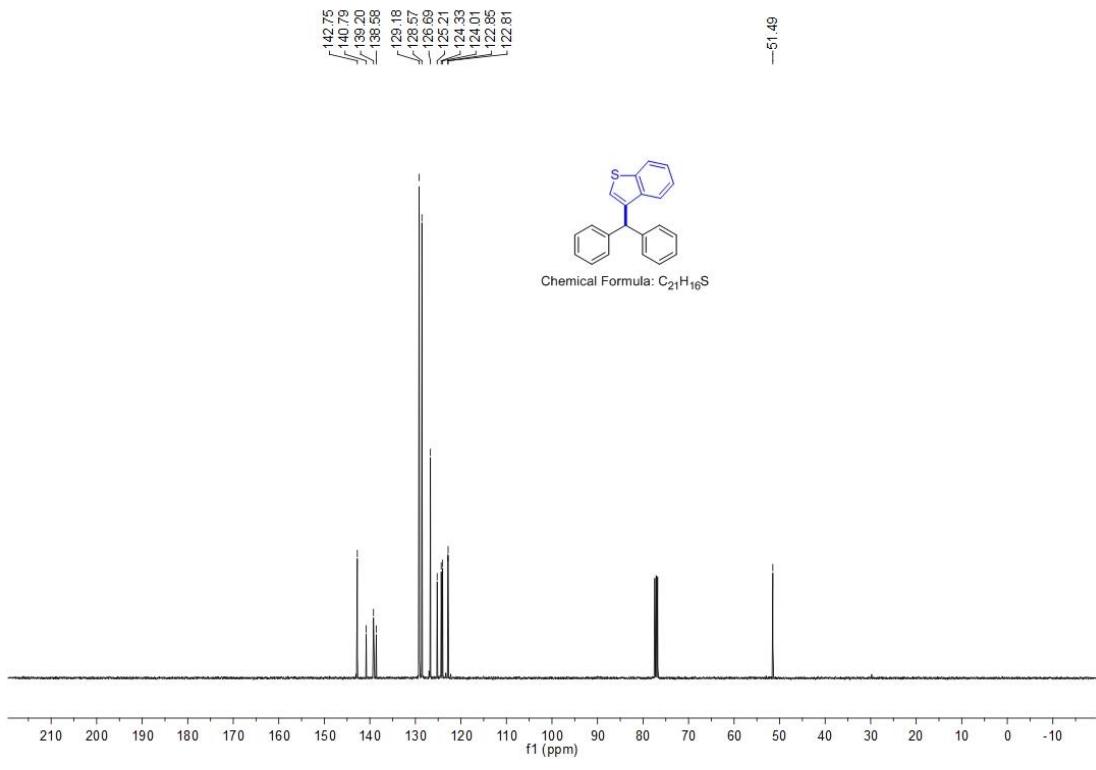




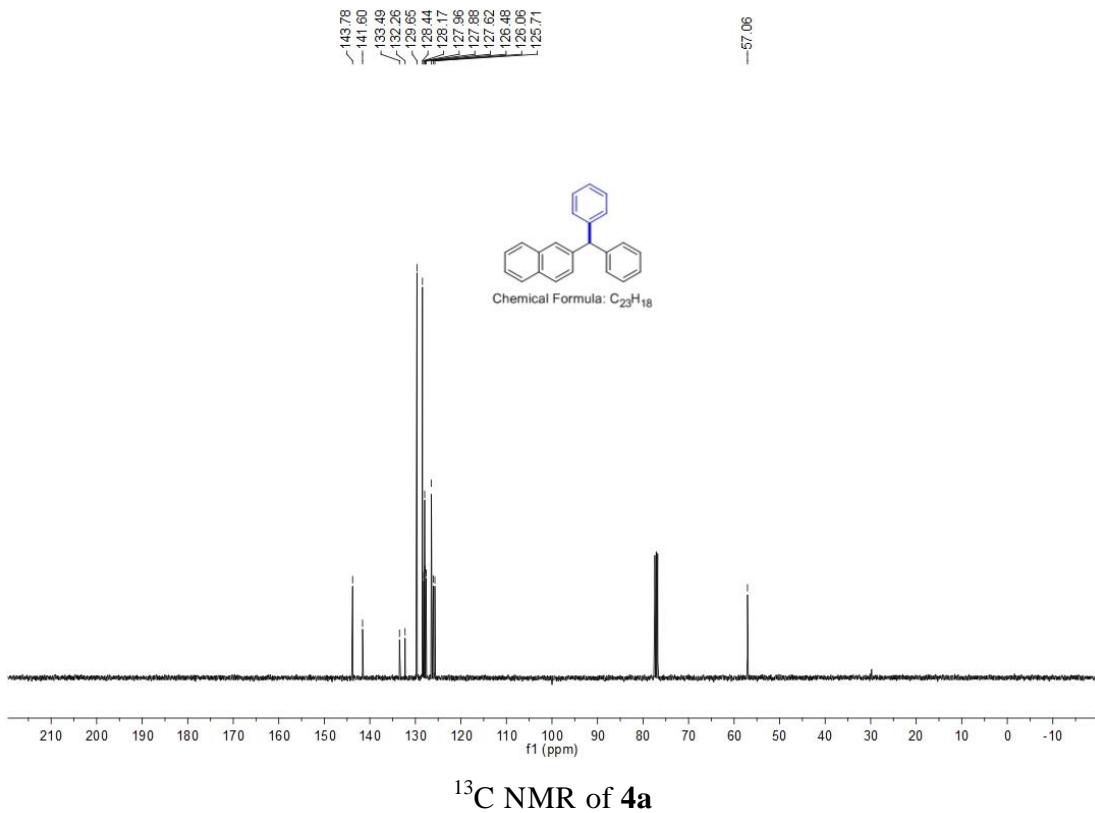
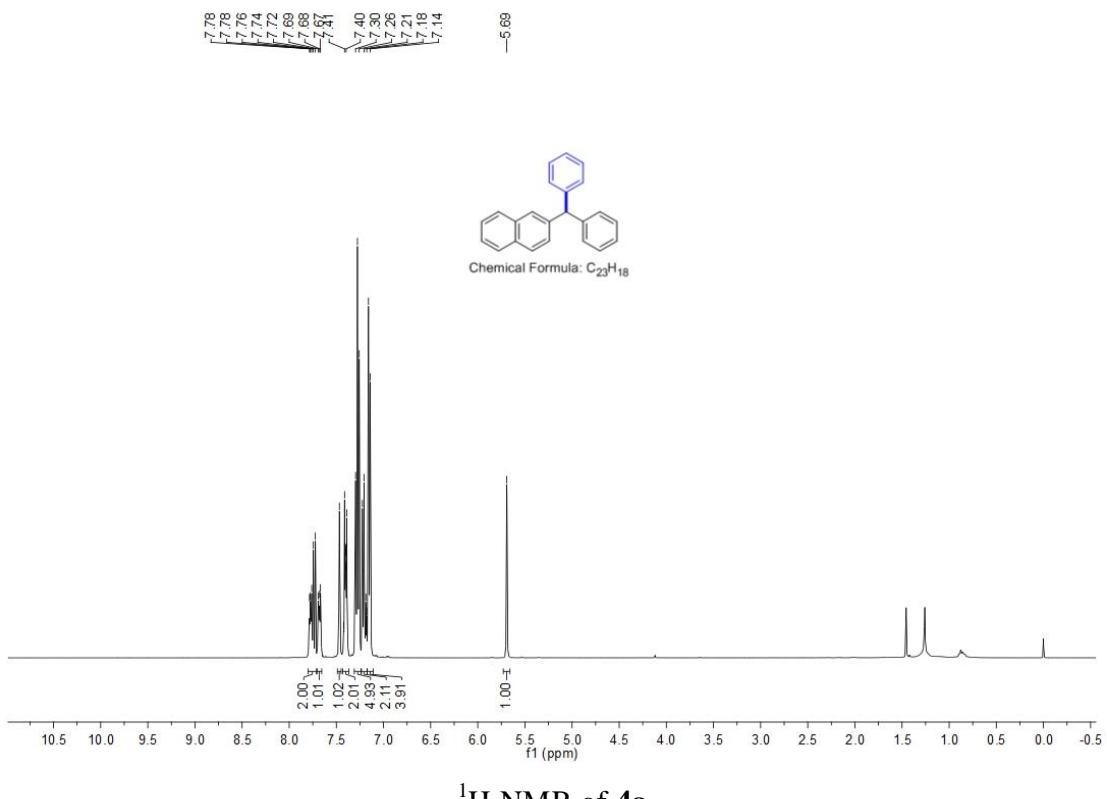
¹³C NMR of **3w**

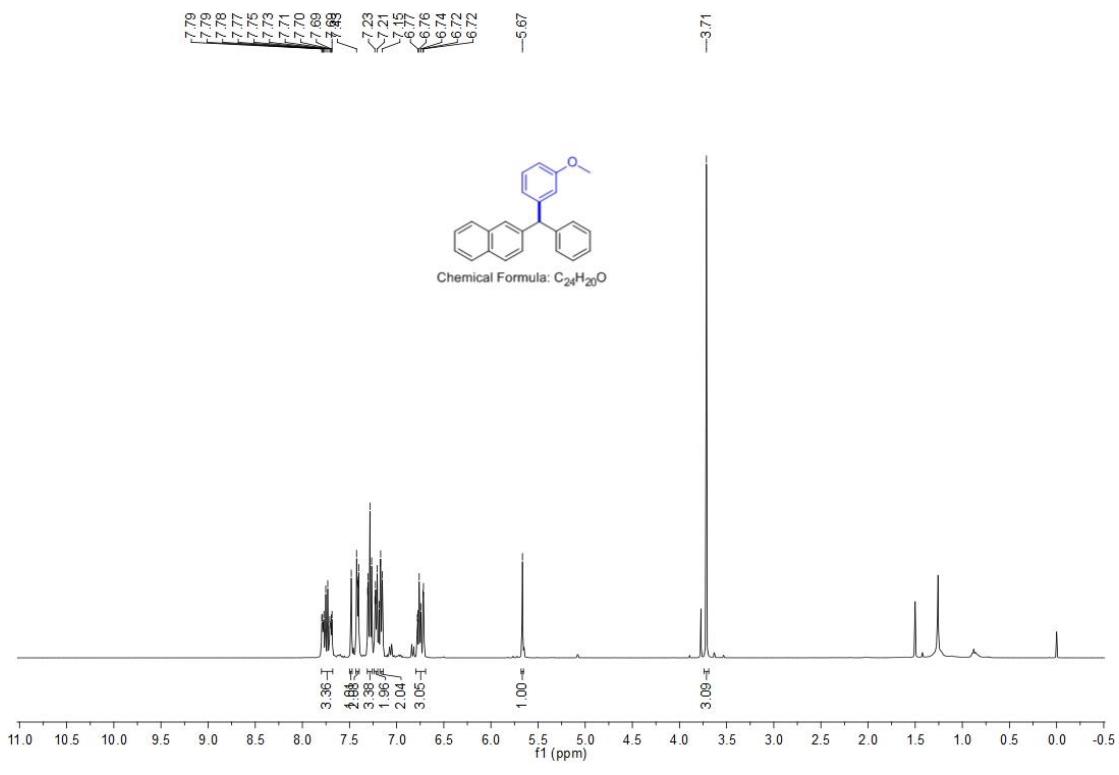


Chemical Formula: C₂₁H₁₆S

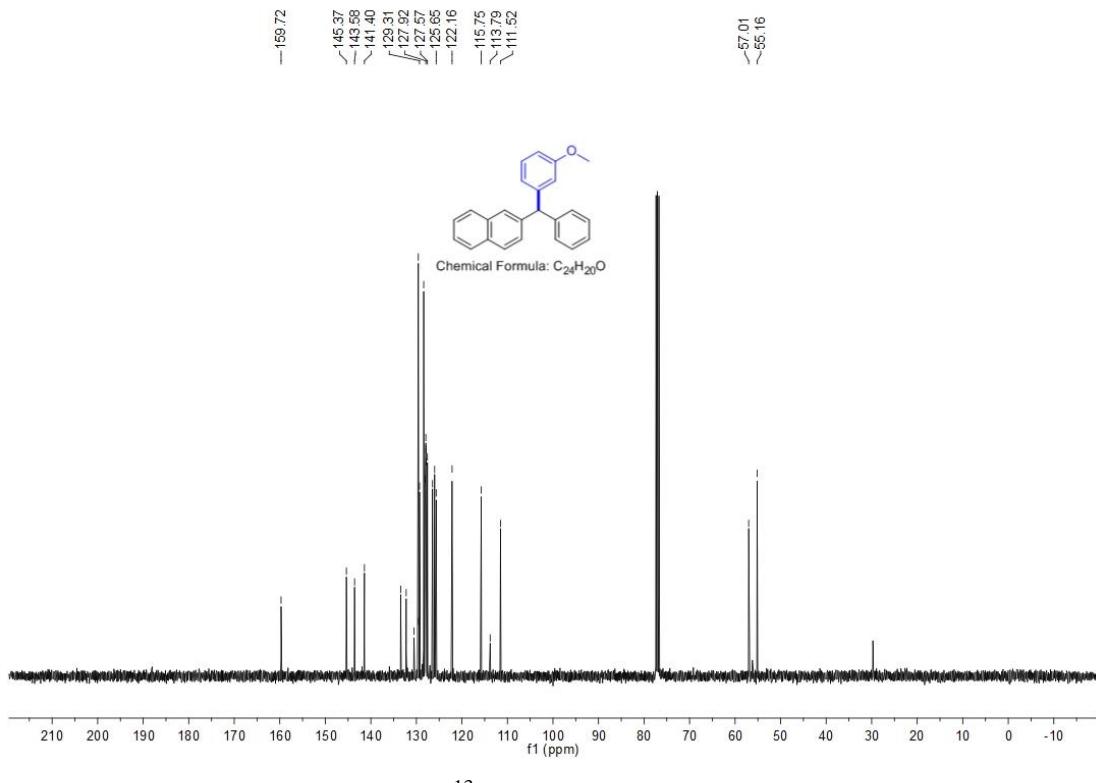


Chemical Formula: C₂₁H₁₆S

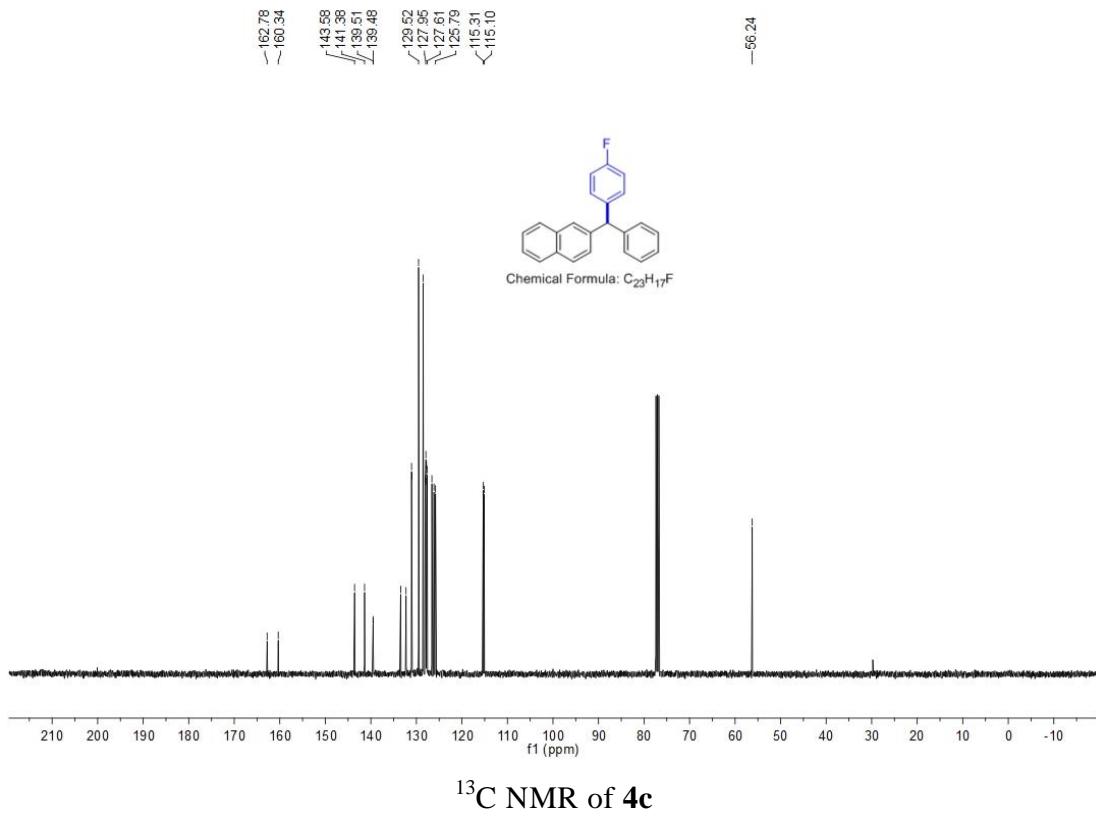
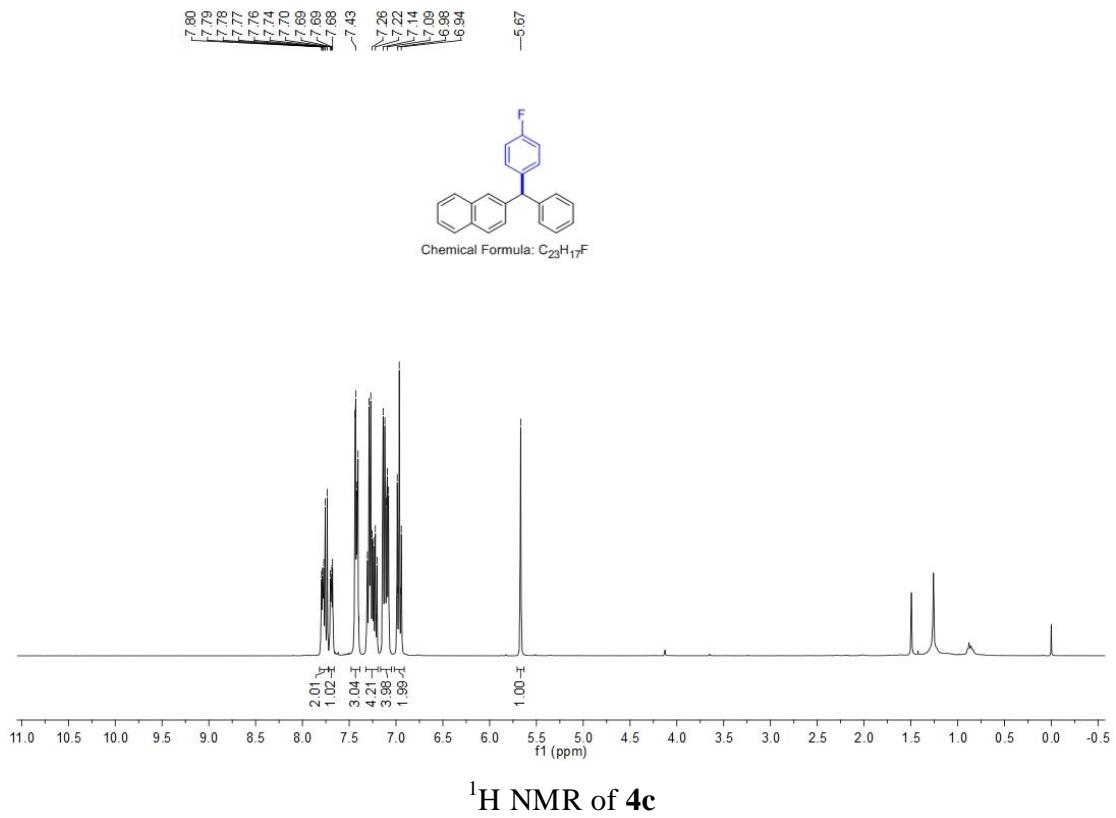


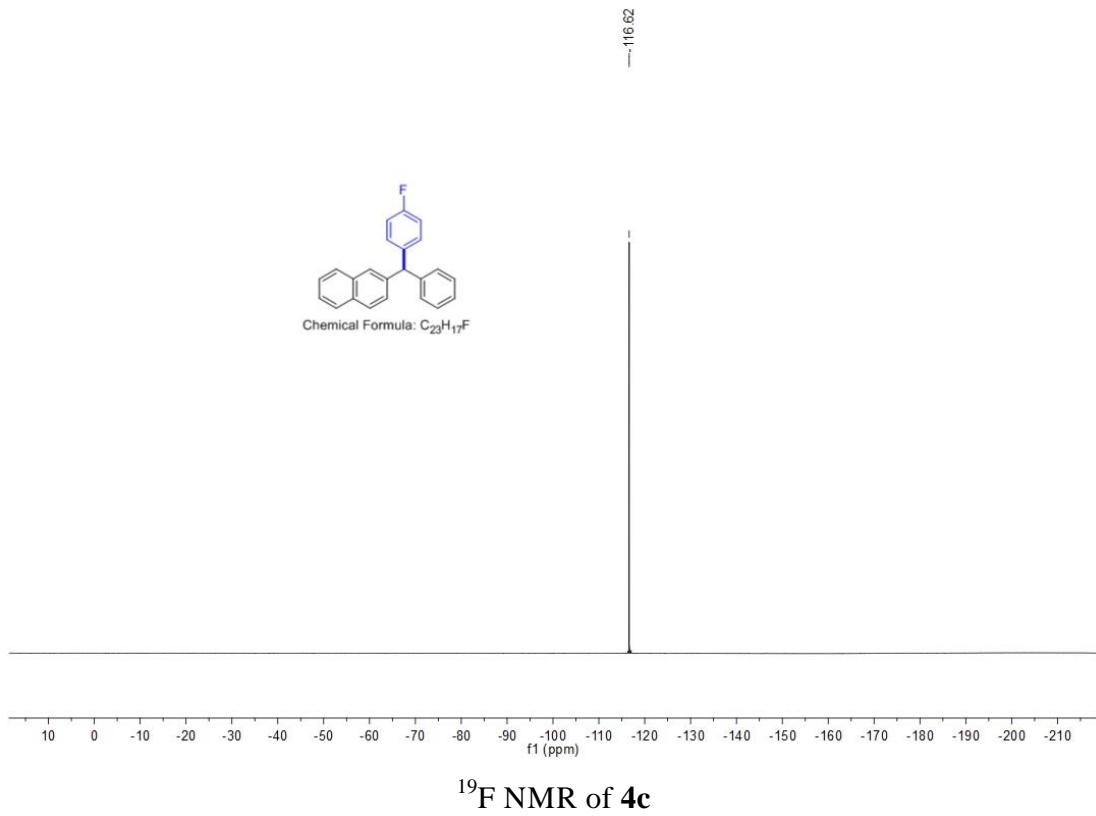


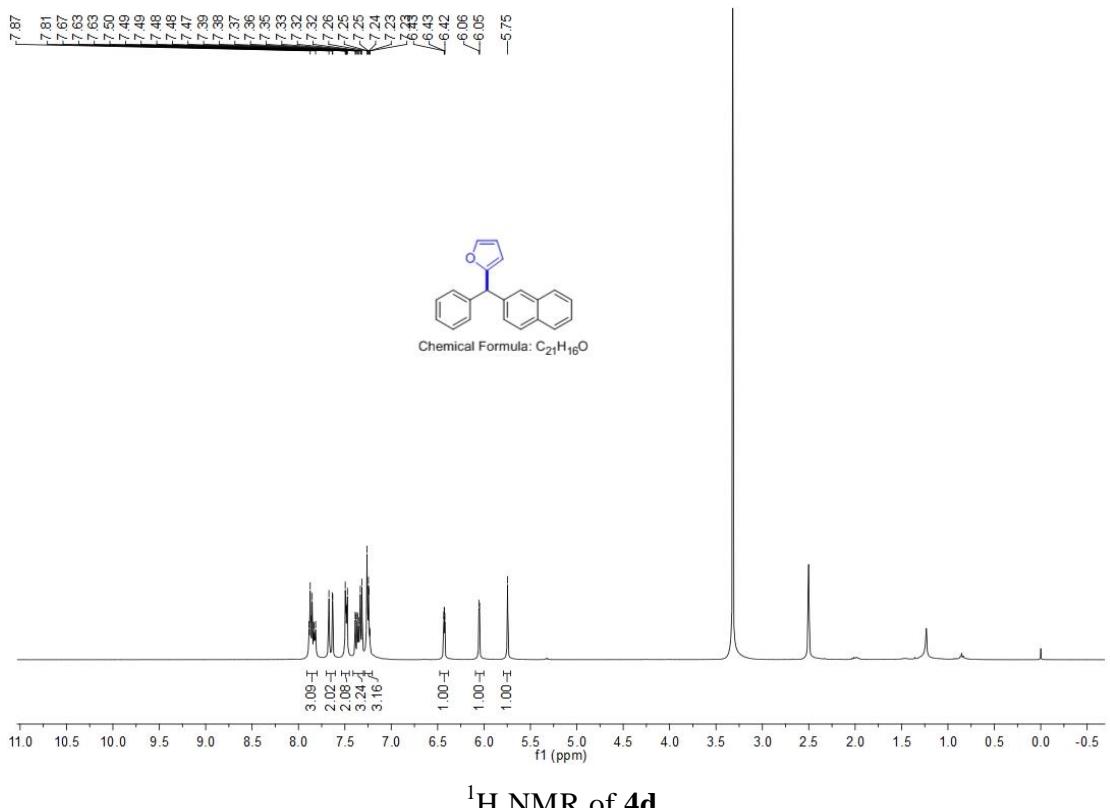
¹H NMR of **4b**



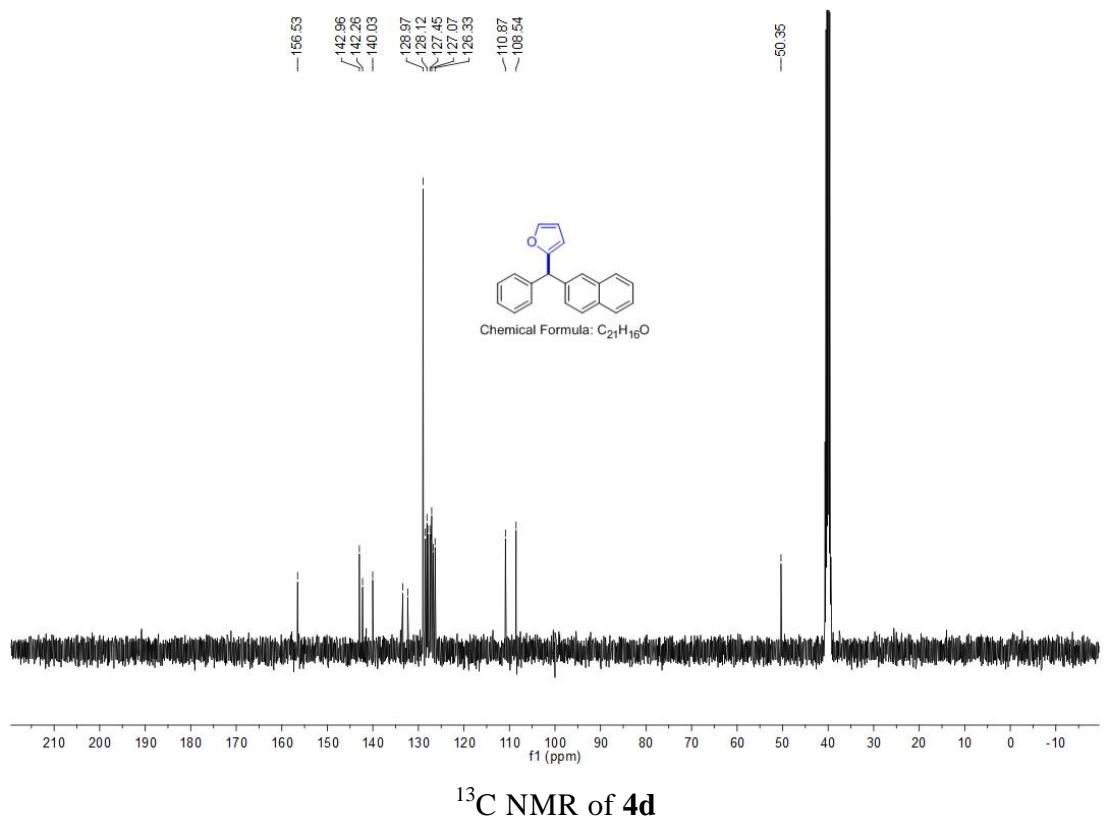
¹³C NMR of **4b**



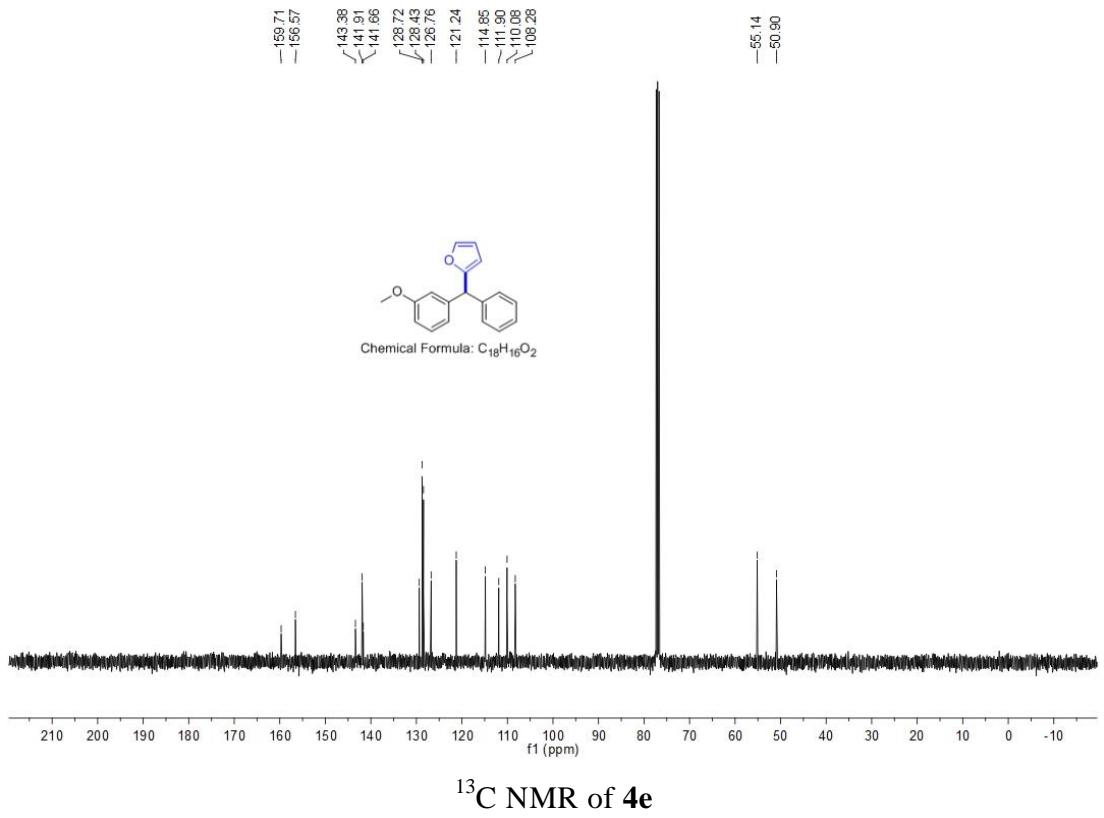
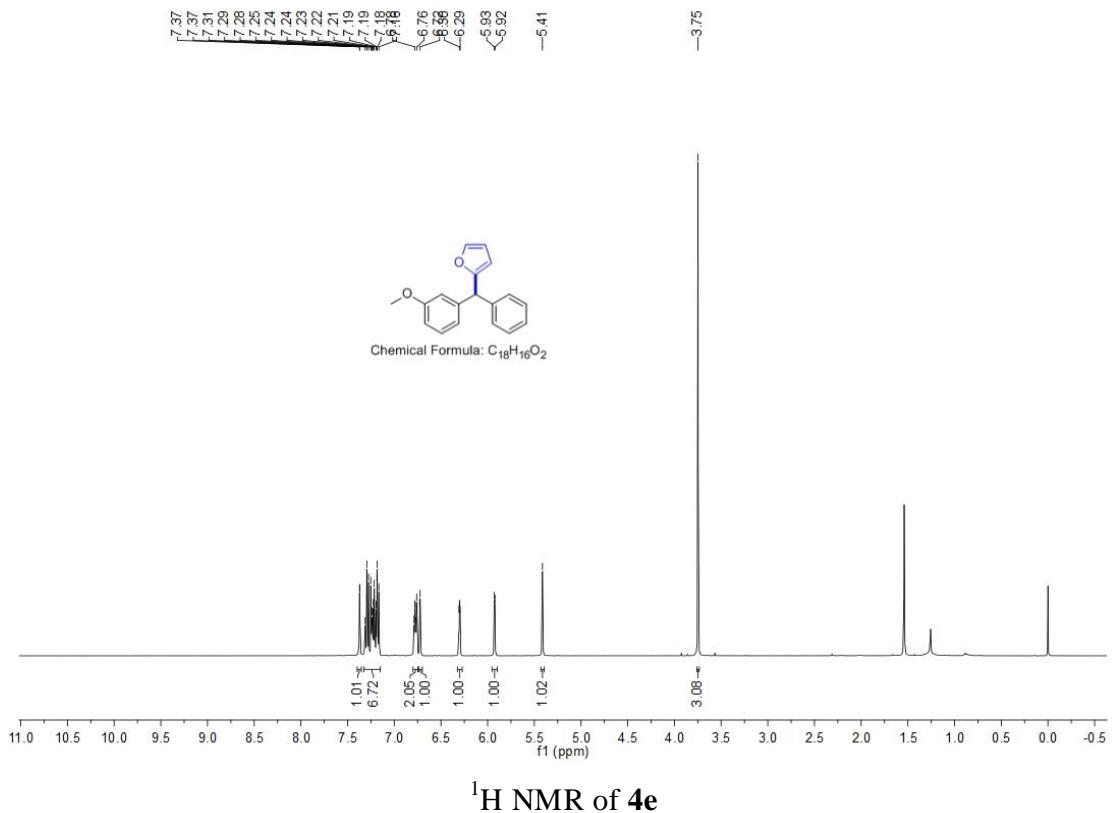


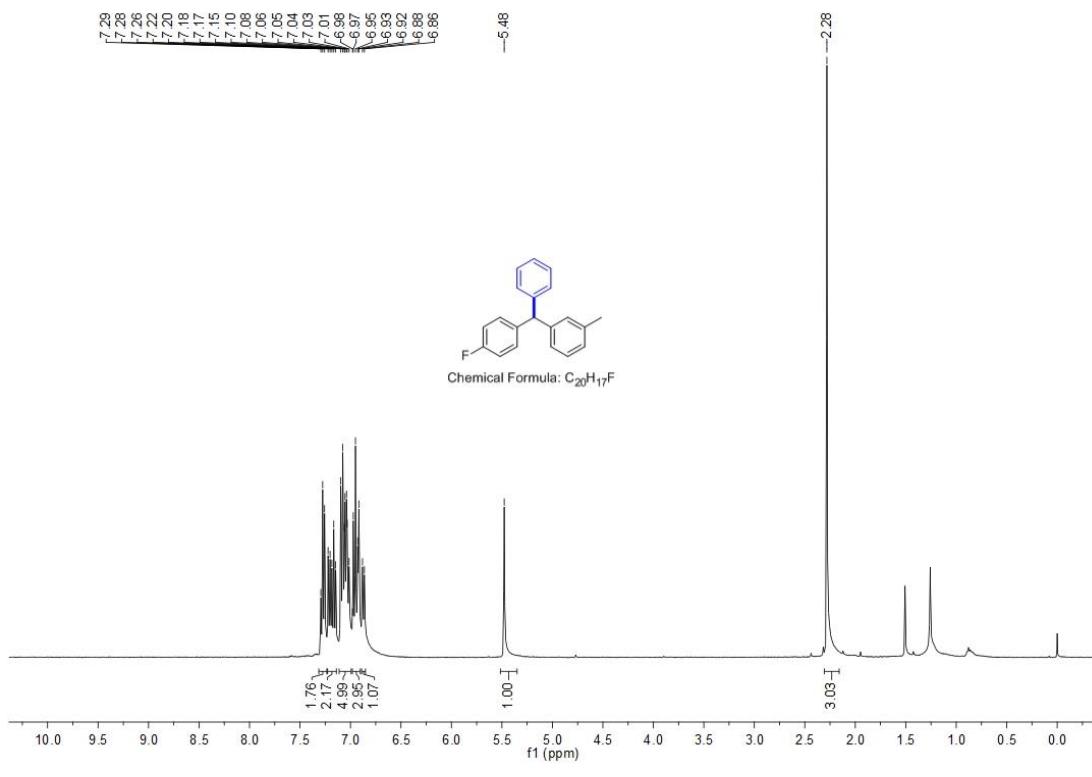


1H NMR of **4d**

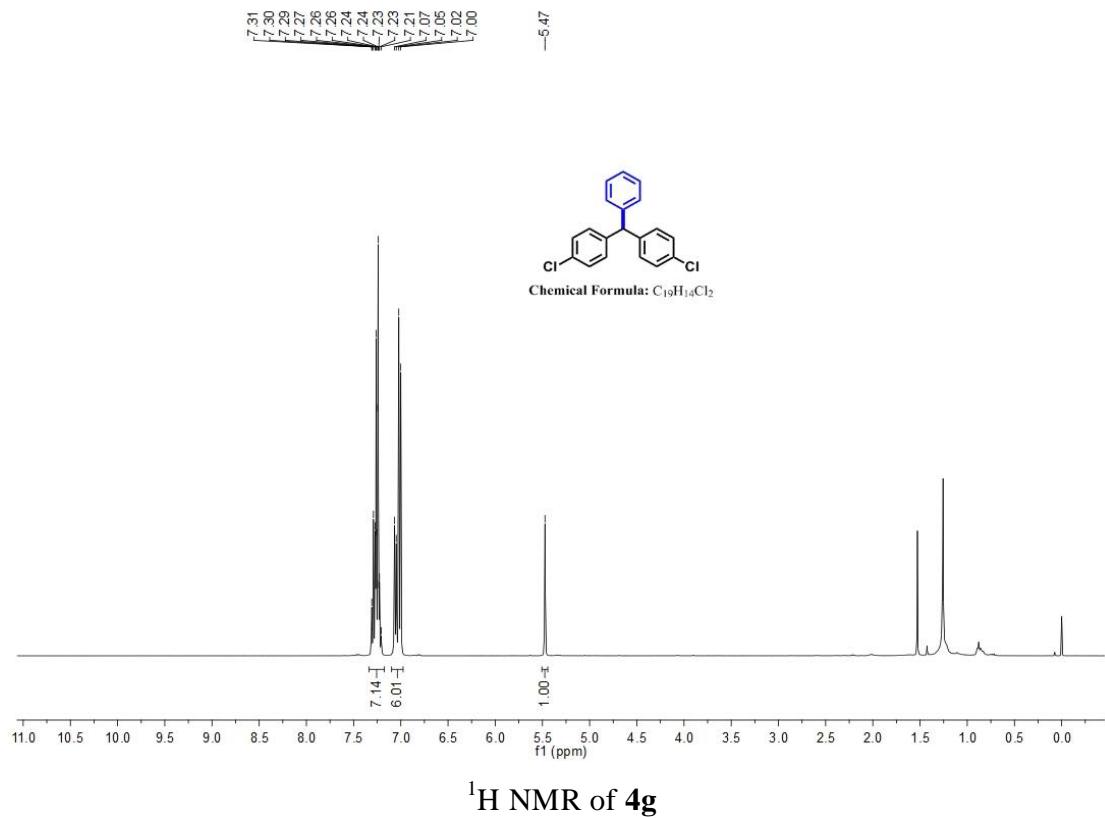


^{13}C NMR of **4d**





¹³C NMR of **4f**



Chemical Formula: C₁₉H₁₄Cl₂

