Electronic Supplementary Material (ESI) for RSC Advances.


# In situ generated and stabilized Pd nanoparticles by $N^2$,$N^4$,$N^6$-tridodecyl-1,3,5-triazine-2,4,6-triamine (TDTAT) as reactive and efficient catalyst for Suzuki-Miyaura reaction in water

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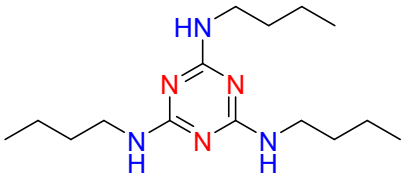
## Outline

1. **Spectral data for synthesized compounds**
2. **Copies of $^1$HNMR and $^{13}$CNMR for all synthesized compounds**

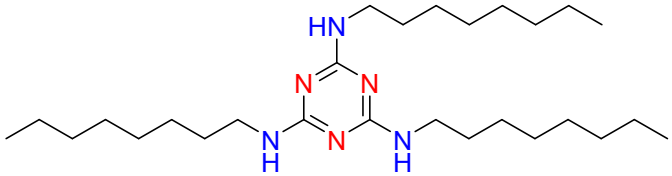
## 1. Spectral data for synthesized compounds

### 1.1 $N^2$,$N^4$,$N^6$-Tributyl-1,3,5-triazine-2,4,6-triamine



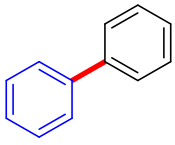
$^1$H NMR (250 MHz, $CDCl_3$): δ (ppm) = 0.97 (t, *J* = 5 Hz, 9H), 1.27-1.40 (m, 6H), 1.53-1.63 (m, 6H), 3.31-3.45 (m, 6H), 5.42 (t, *J* = 50 Hz, 3H). $^{13}$C NMR (62.5 MHz, $CDCl_3$): 14.1, 22.2, 29.7, 41.4, 163.5. Anal. Calcd. for $C_{15}H_{30}N_6$: C, 61.19; H, 10.27; N, 28.54. Found: C, 61.10; H, 10.22; N, 28.46.

### 1.2 $N^2$,$N^4$,$N^6$-Trioctyl-1,3,5-triazine-2,4,6-triamine



$^1$H NMR (250 MHz, $CDCl_3$): δ (ppm) = 0.97 (t, *J* = 5 Hz, 9H), 1.33 (brs, 30H), 1.61-1.72 (m, 6H), 3.32-3.46 (m, 6H), 5.42 (t, *J* = 50 Hz, 3H). $^{13}$C NMR (62.5 MHz, $CDCl_3$): 14.1, 22.6, 26.9, 28.9, 29., 29.6, 31.8, 41.4, 163.4. Anal. Calcd. for $C_{27}H_{54}N_6$: C, 70.08; H, 11.76; N, 18.16. Found: C, 70.01; H, 11.65; N, 18.07.

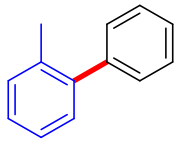
### 1.3. 1,1'-biphenyl (3a)



**3a**

$^1$H NMR (250 MHz, $CDCl_3$): δ (ppm) = 7.53-7.68 (m, 6H), 7.81-7.85 (m, 4H). $^{13}$C NMR (62.5 MHz, $CDCl_3$): 127.4, 127.5, 129.0, 141.5.

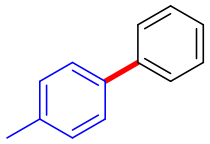
### 1.4. 2-methyl-1,1'-biphenyl (3b)



**3b**

$^{1}$H NMR (250 MHz, $CDCl_3$): δ (ppm) = 2.24 (s, 3H), 7.19-7.39 (m, 9H). $^{13}$C NMR (62.5 MHz, $CDCl_3$): 20.4, 125.7, 126.7, 127.2, 128.1, 129.1, 129.7, 130.2, 135.2, 141.9, 142.0.

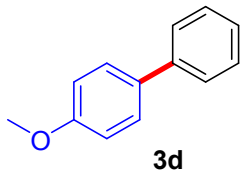
### 1.5. 4-methyl-1,1'-biphenyl (3c)



**3c**

$^{1}$H NMR (250 MHz, $CDCl_3$): δ (ppm) = 2.39 (s, 3H), 7.25 (d, *J* = 5 Hz, 2H), 7.32-7.62 (m, 7H). $^{13}$C NMR (62.5 MHz, $CDCl_3$): 21.1, 127.0, 127.1, 128.7, 129.5, 137.1, 138.3, 141.1.

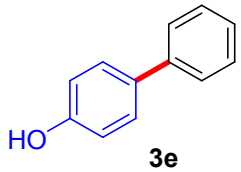
### 1.6. 4-methoxy-1,1'-biphenyl (3d)




**3d**

$^{1}$H NMR (250 MHz, $CDCl_3$): δ (ppm) = 3.79 (s, 3H), 6.95 (d, *J* = 9 Hz, 2H), 7.24-7.31 (m, 1H), 7.39 (t, *J* = 7.5 Hz, 2H), 7.47-7.55 (m, 4H). $^{13}$C NMR (62.5 MHz, $CDCl_3$): 55.2, 114.2, 126.5, 127.3, 128.2, 128.8, 133.7, 140.8, 159.2.

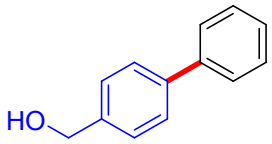
### 1.7. [1,1'-biphenyl]-4-ol (3e)




**3e**

$^{1}$H NMR (250 MHz, DMSO-$d_6$): δ (ppm) = 6.84-6.87 (m, 2H), 7.23-7.52 (m, 7H), 9.56 (s, 1H). $^{13}$C NMR (62.5 MHz, DMSO-$d_6$): 115.6, 125.9, 126.3, 127.7, 128.7, 130.9, 140.1, 157.0.

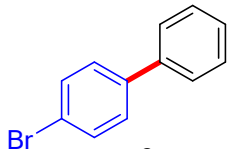
### 1.8. [1,1'-biphenyl]-4-ylmethanol (3f)




**3f**

$^{1}$H NMR (250 MHz, $CDCl_3$): δ (ppm) = 1.93 (s, 1H), 4.73 (s, 2H), 7.32-7.49 (m, 5H), 7.58-7.63 (m, 4H). $^{13}$C NMR (62.5 MHz, $CDCl_3$): 65.1, 127.1, 127.3, 127.5, 128.8, 139.9, 140.6, 140.8.

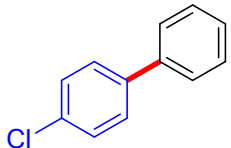
### 1.9. 4-bromo-1,1'-biphenyl (3g)




**3g**

$^{1}$H NMR (250 MHz, $CDCl_3$): δ (ppm) = 7.38-7.62 (m, 9H). $^{13}$C NMR (62.5 MHz, $CDCl_3$): 121.6, 127.0, 127.7, 128.8, 128.9, 131.9, 140.0, 140.1.

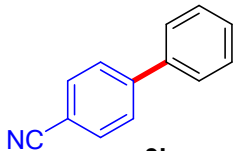
### 1.10. 4-chloro-1,1'-biphenyl (3h)




**3h**

$^{1}$H NMR (250 MHz, $CDCl_3$): δ (ppm) = 7.36-7.69 (m, 9H). $^{13}$C NMR (62.5 MHz, $CDCl_3$): 126.6, 127.7, 128.4, 128.8, 128.9, 132.3, 136.2, 139.6.

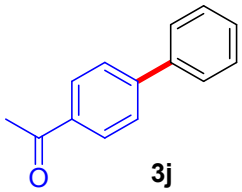
### 1.11. [1,1'-biphenyl]-4-carbonitrile (3i)




**3i**

$^{1}$H NMR (250 MHz, $CDCl_3$): δ (ppm) = 7.29-7.65 (m, 9H). $^{13}$C NMR (62.5 MHz, $CDCl_3$): 110.9, 119.0, 127.2, 127.7, 128.7, 129.1, 132.6, 139.1, 145.6.

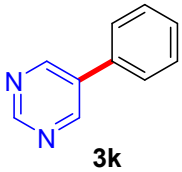
### 1.12. 1-([1,1'-biphenyl]-4-yl)ethan-1-one (3j)



**3j**

$^{1}$H NMR (250 MHz, $CDCl_3$): δ (ppm) = 2.63 (s, 3H), 7.40-7.51 (m, 3H), 7.61-7.71 (m, 4H), 8.03 (d, $J$ = 8.25 Hz, 2H). $^{13}$C NMR (62.5 MHz, $CDCl_3$): 26.7, 127.2, 127.3, 128.2, 128.9, 129.0, 135.8, 139.8, 145.8, 197.7.

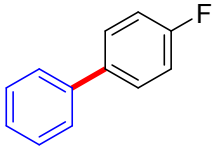
### 1.13. 5-phenylpyrimidine (3k)



**3k**

$^{1}$H NMR (250 MHz, $CDCl_3$): δ (ppm) = 7.45-7.60 (m, 5H), 8.95 (s, 2H), 9.21 (s, 1H). $^{13}$C NMR (62.5 MHz, $CDCl_3$): 127.0, 129.0, 129.2, 134.2, 134.3, 154.8, 157.4.

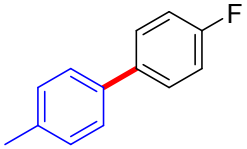
### 1.14. 4-fluoro-1,1'-biphenyl (3l)



**3l**

$^{1}$H NMR (250 MHz, $CDCl_3$): δ (ppm) = 7.25 (t, $J$ = 8.75 Hz, 2H), 7.45-7.69 (m, 7H). $^{13}$C NMR (62.5 MHz, $CDCl_3$): 115.7 (d, $^{2}J_{CF}$ = 21.25 Hz), 127.1, 127.4, 128.8 (d, $^{3}J_{CF}$ = 7.94 Hz), 129.0, 137.46 (d, $^{4}J_{CF}$ = 3.19 Hz), 140.4, 162.6 ($^{1}J_{CF}$ = 244.62 Hz).

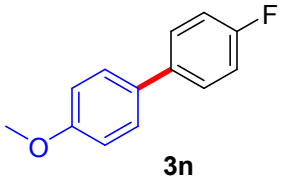
### 1.15. 4-fluoro-4'-methyl-1,1'-biphenyl (3m)



**3m**

$^{1}$H NMR (250 MHz, $CDCl_3$): δ (ppm) = 2.51 (s, 3H), 7.22 (t, *J* = 8.75 Hz, 2H), 7.35 (d, *J* = 8 Hz, 2H), 7.55 (d, *J* = 8.25 Hz, 2H), 7.60-7.66 (m, 2H). $^{13}$C NMR (62.5 MHz, $CDCl_3$): 21.1, 115.6 (d, $^{2}J_{CF}$ = 21.19 Hz), 127.0, 128.6 (d, $^{3}J_{CF}$ = 7.94 Hz), 129.7, 137.1, 137.4 (d, $^{4}J_{CF}$ = 3.19 Hz), 137.5, 162.4 ($^{1}J_{CF}$ = 244.31 Hz).

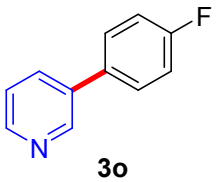
### 1.16. 4-fluoro-4'-methoxy-1,1'-biphenyl (3n)




**3n**

$^{1}$H NMR (250 MHz, $CDCl_3$): δ (ppm) = 3.89 (s, 3H), 7.03 (d, *J* = 8.75 Hz, 2H), 7.16 (t, *J* = 8.75 Hz, 2H), 7.51-7.58 (m, 4H). $^{13}$C NMR (62.5 MHz, $CDCl_3$): 55.3, 114.3, 115.6 (d, $^{2}J_{CF}$ = 21.25 Hz), 128.1, 128.2 (d, $^{3}J_{CF}$ = 7.87 Hz), 132.8, 137.0 (d, $^{4}J_{CF}$ = 3.25 Hz), 159.2, 162.4 ($^{1}J_{CF}$ = 243.87 Hz).

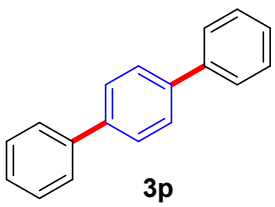
### 1.17. 3-(4-fluorophenyl)pyridine (3o)




**3o**

$^{1}$H NMR (250 MHz, $CDCl_3$): δ (ppm) = 6.97-7.04 (m, 2H), 7.17-7.22 (m, 1H), 7.35-7.41 (m, 2H), 7.64-7.69 (m, 1H), 8.45 (d, *J* = 4.75 Hz, 1H), 8.66 (s, 1H). $^{13}$C NMR (62.5 MHz, $CDCl_3$): 116.0 (d, $^{2}J_{CF}$ = 21.5 Hz), 123.5, 128.7 (d, $^{3}J_{CF}$ = 8.19 Hz), 133.8 (d, $^{4}J_{CF}$ = 3.31 Hz), 134.1, 135.6,147.9, 148.3, 162.8 ($^{1}J_{CF}$ = 246.25 Hz).

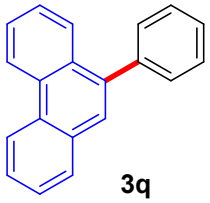
### 1.18. 1,1':4',1''-terphenyl (3p)



**3p**

$^{1}$H NMR (250 MHz, $CDCl_3$): δ (ppm) = 7.35-7.49 (m, 10H), 7.55-7.57 (m, 4H). $^{13}$C NMR (62.5 MHz, $CDCl_3$): 126.9, 127.6, 128.7, 128.9, 138.5, 140.1.

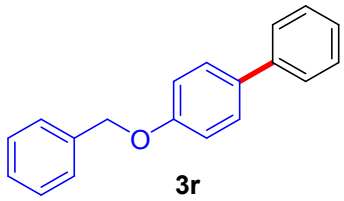
**1.19. 9-phenylphenanthrene (3q)**



**3q**

$^{1}$H NMR (250 MHz, $CDCl_3$): δ (ppm) = 7.49-7.73 (m, 10H), 7.91-7.99 (m, 2H), 8.74-8.83 (m, 2H). $^{13}$C NMR (62.5 MHz, $CDCl_3$): 122.6, 122.9, 126.4, 126.5, 126.6, 126.9, 127.0, 127.4, 127.5, 128.3, 128.7, 130.0, 130.1, 130.6, 131.1, 131.6, 138.8, 140.8.

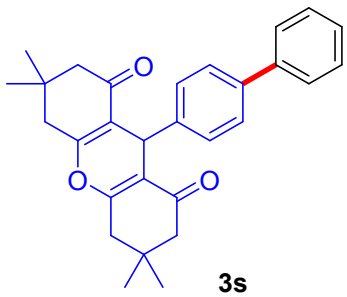
**1.20. 4-(benzyloxy)-1,1'-biphenyl (3r)**




**3r**

$^{1}$H NMR (250 MHz, $CDCl_3$): δ (ppm) = 5.13 (s, 2H), 7.02 (d, *J* = 9.25 Hz, 2H), 7.21-7.27 (m, 6H), 7.45-7.58 (m, 4H), 7.69 (d, *J* = 9.25 Hz, 2H). $^{13}$C NMR (62.5 MHz, $CDCl_3$): 70.3, 117.0, 127.5, 127.8, 128.2, 128.4, 128.7, 128.9, 129.4, 132.6, 136.8, 140.0, 158.1.

**1.21. 9-([1,1'-biphenyl]-4-yl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (3s)**

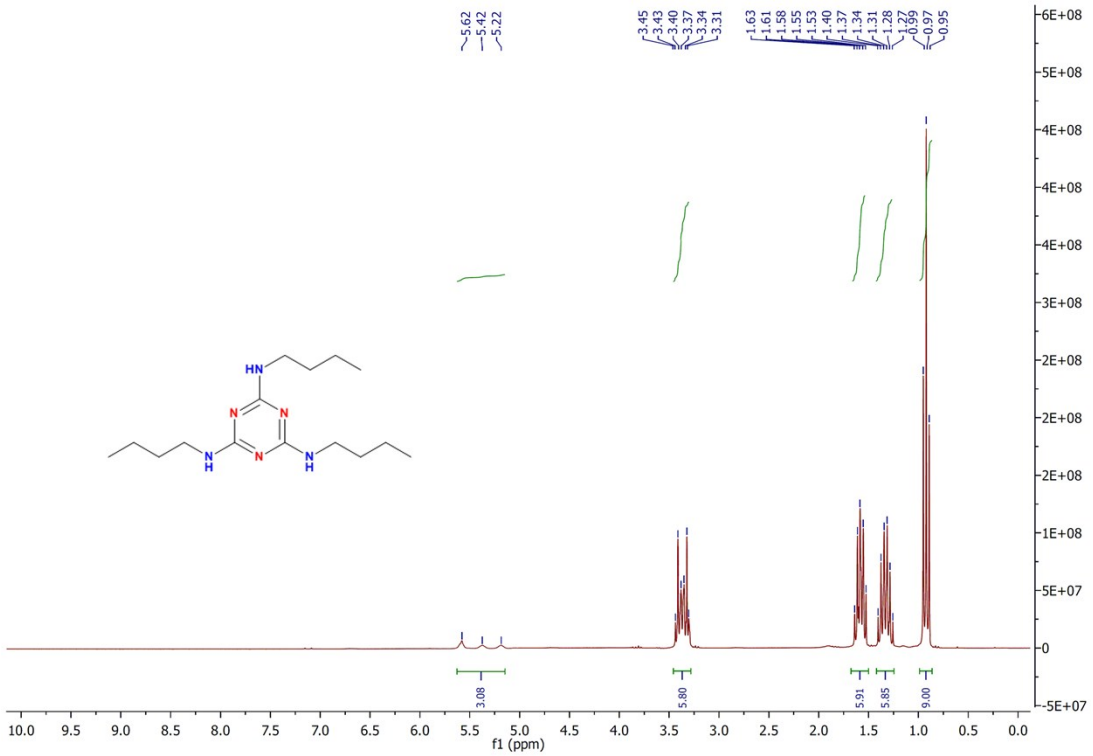


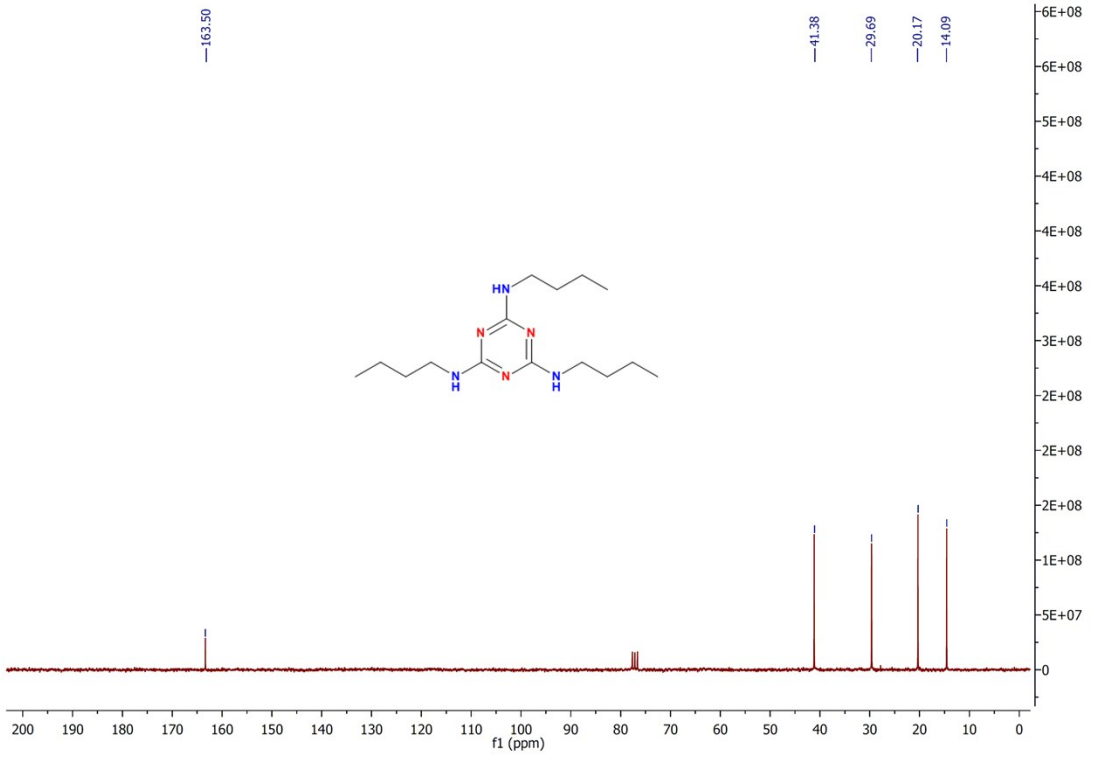

**3s**

$^{1}$H NMR (250 MHz, $CDCl_3$): δ (ppm) = 1.07 (s, 12H), 2.18 (s, 4H), 2.44 (s, 4H), 4.39 (s, 1H), 7.37-7.44 (m, 9H). $^{13}$C NMR (62.5 MHz, $CDCl_3$): 29.2, 31.5, 32.2, 40.8, 50.6, 115.1, 127.0, 127.1, 128.6, 129.4, 130.2, 138.6, 140.4, 141.1, 162.5, 196.3.

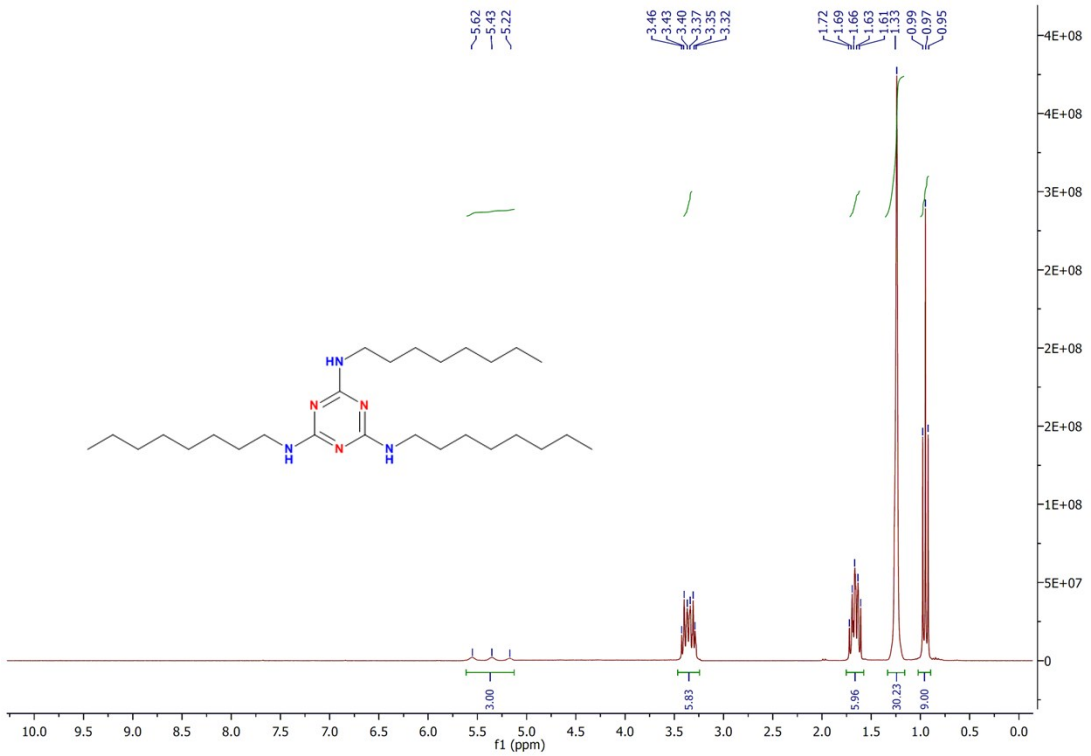
## 2. Copies of $^{1}H$, $^{13}C$ NMR for all synthesized compounds

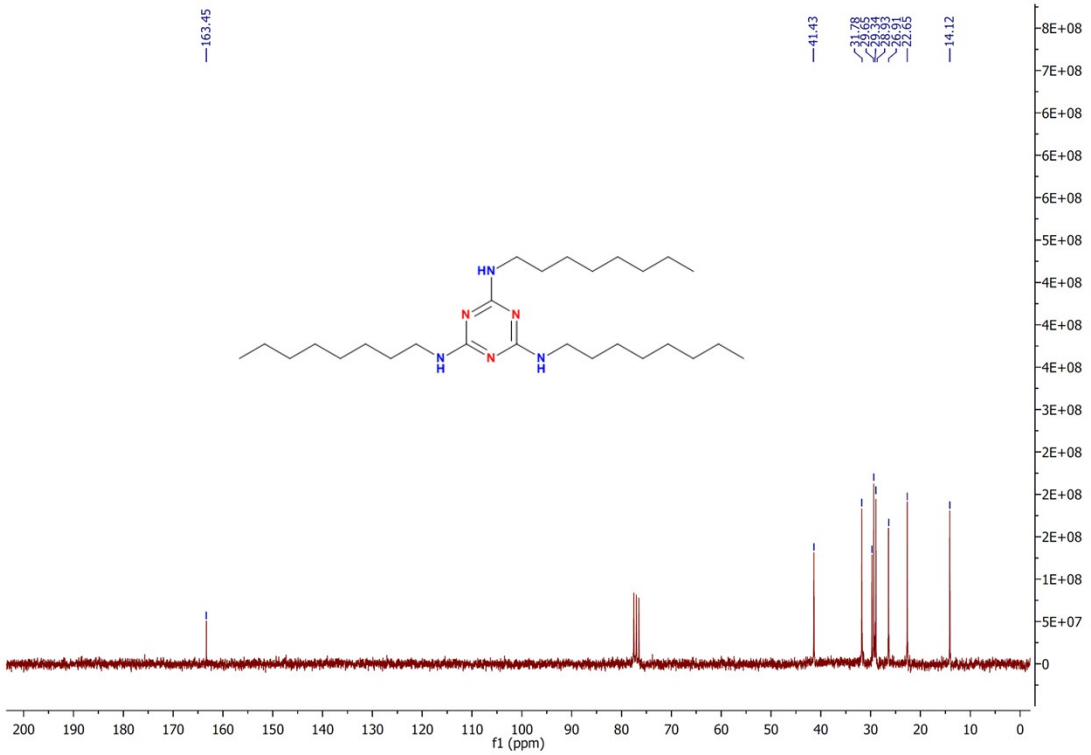
### 2.1. *N*$^{2}$,*N*$^{4}$,*N*$^{6}$-Tributyl-1,3,5-triazine-2,4,6-triamine



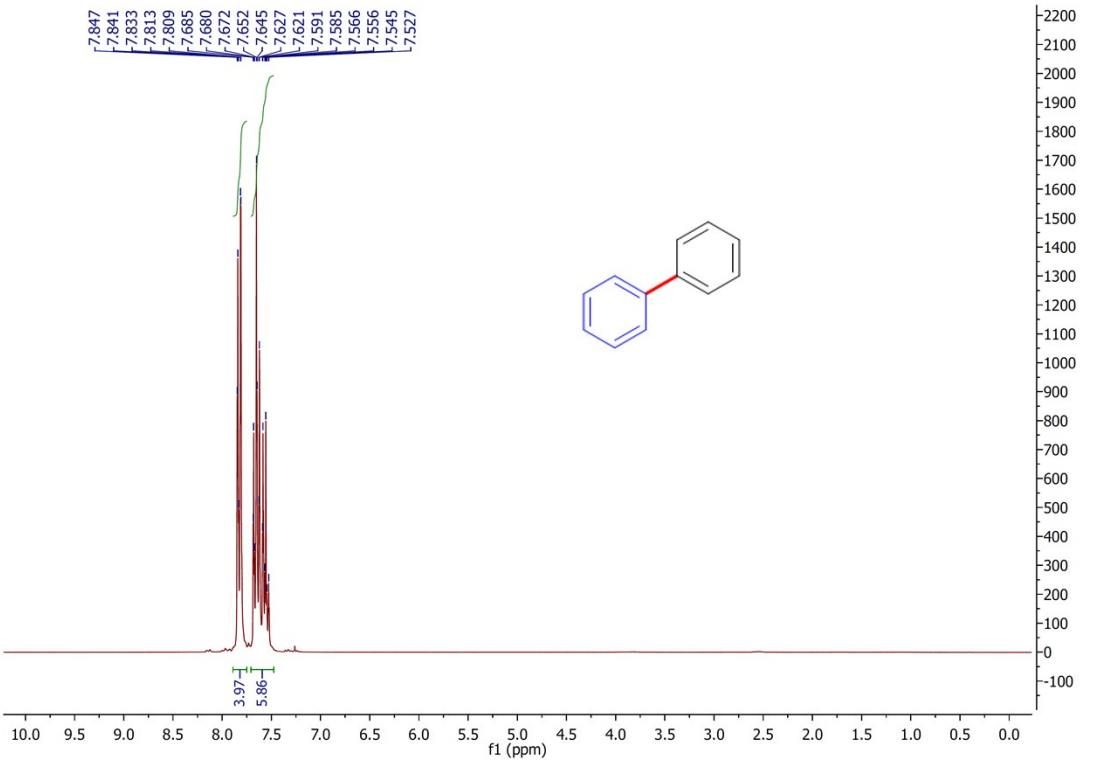



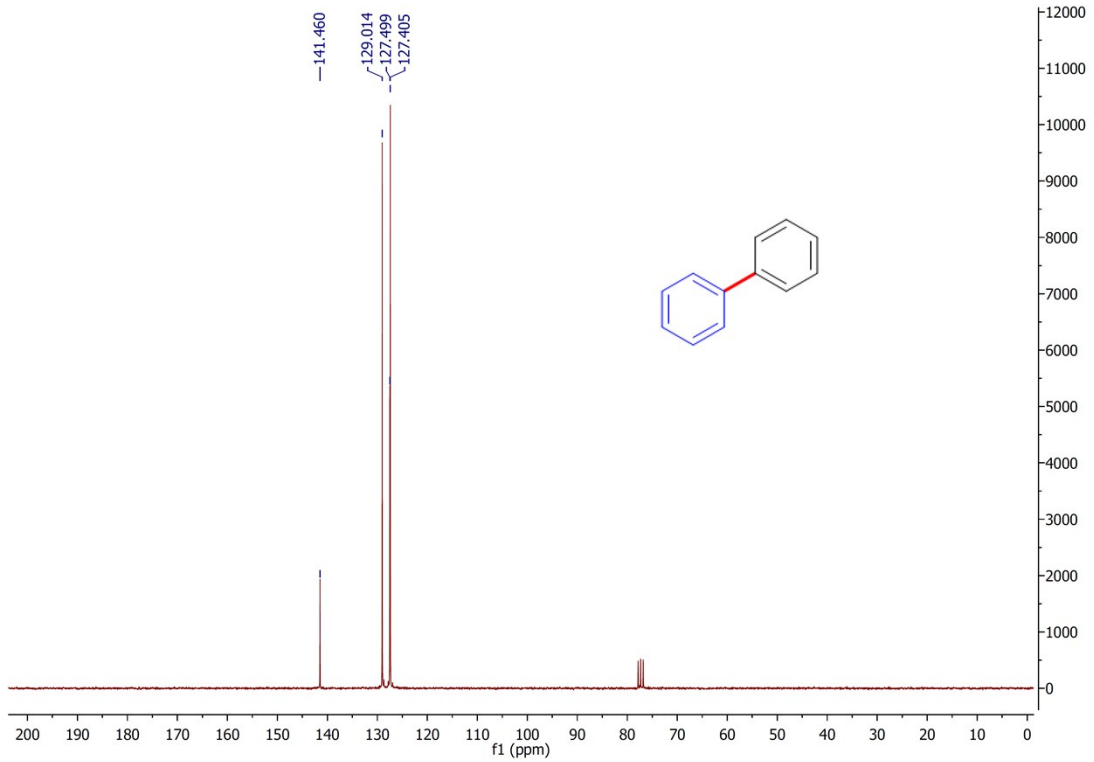
## 2.2. $N^2,N^4,N^6$-Trioctyl-1,3,5-triazine-2,4,6-triamine



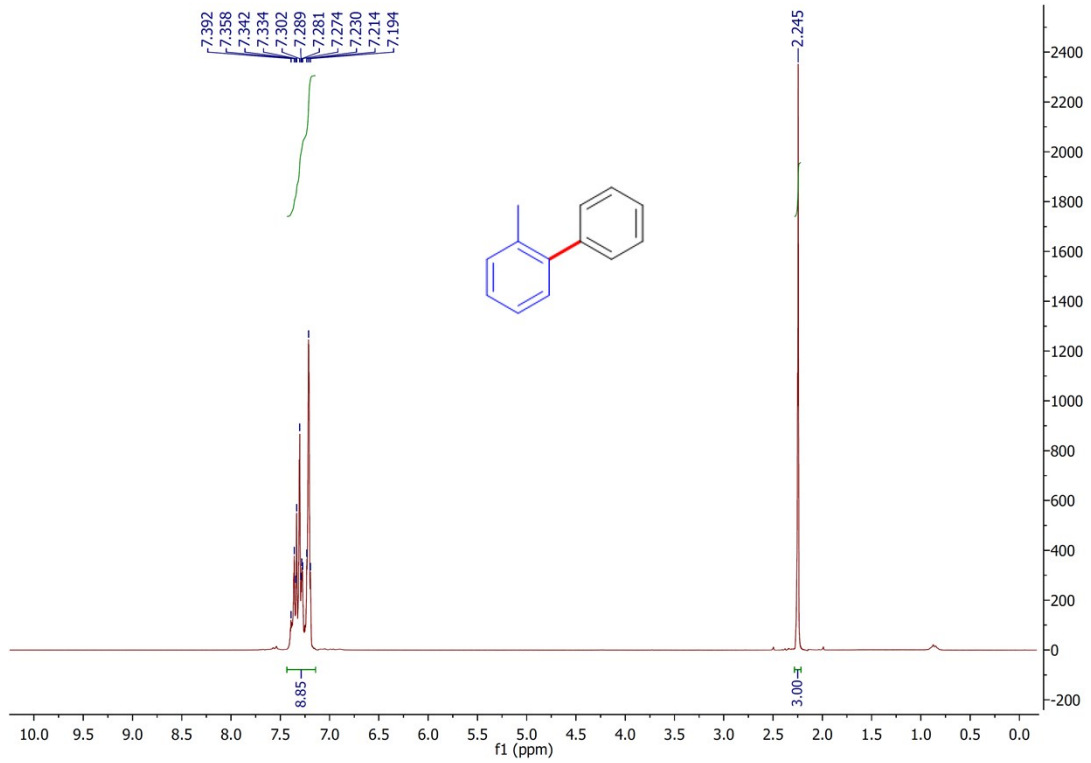



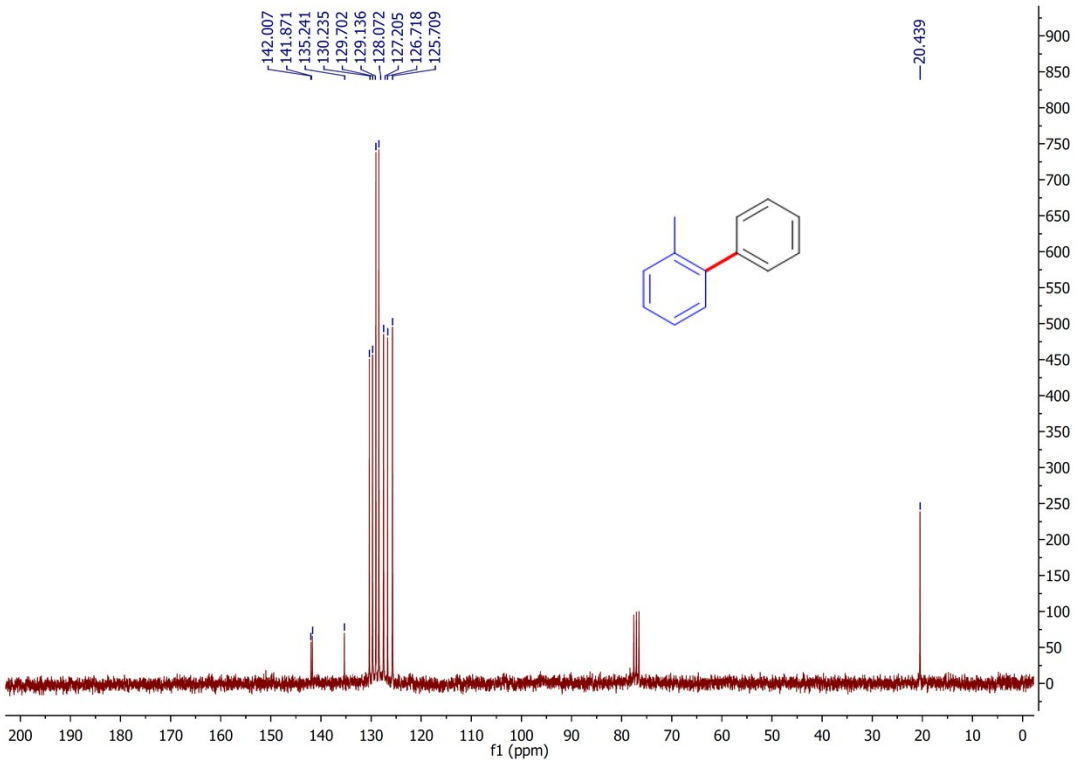
## 2.3. 1,1'-biphenyl (3a)



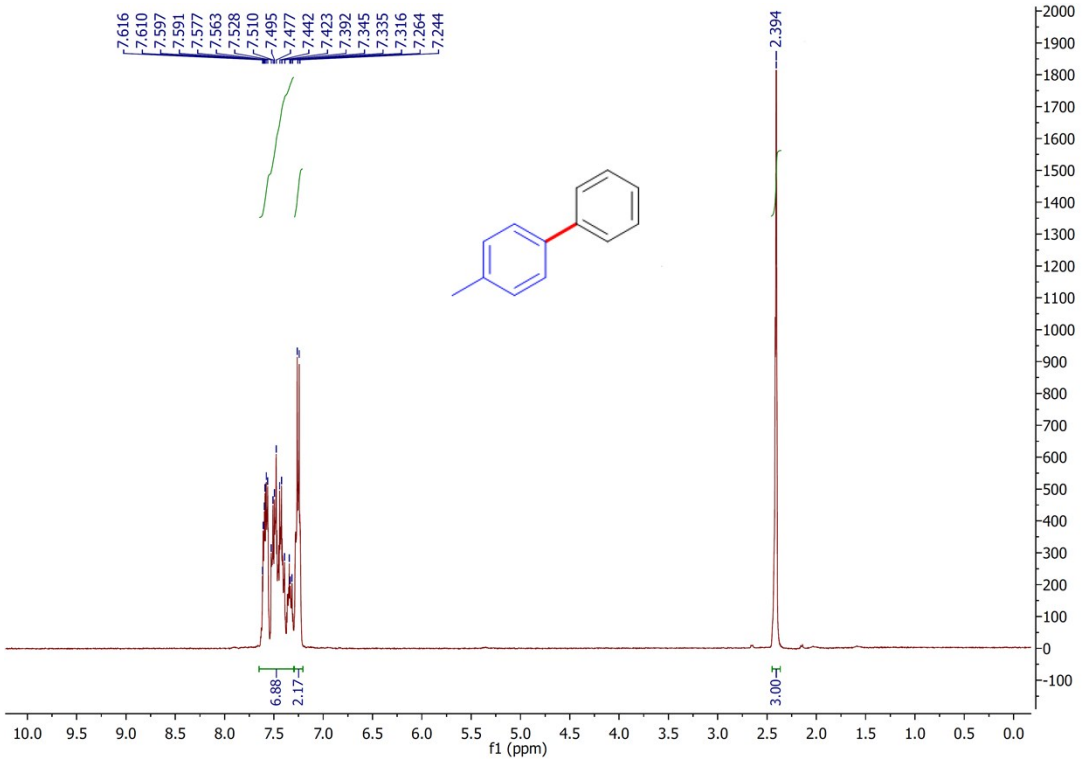



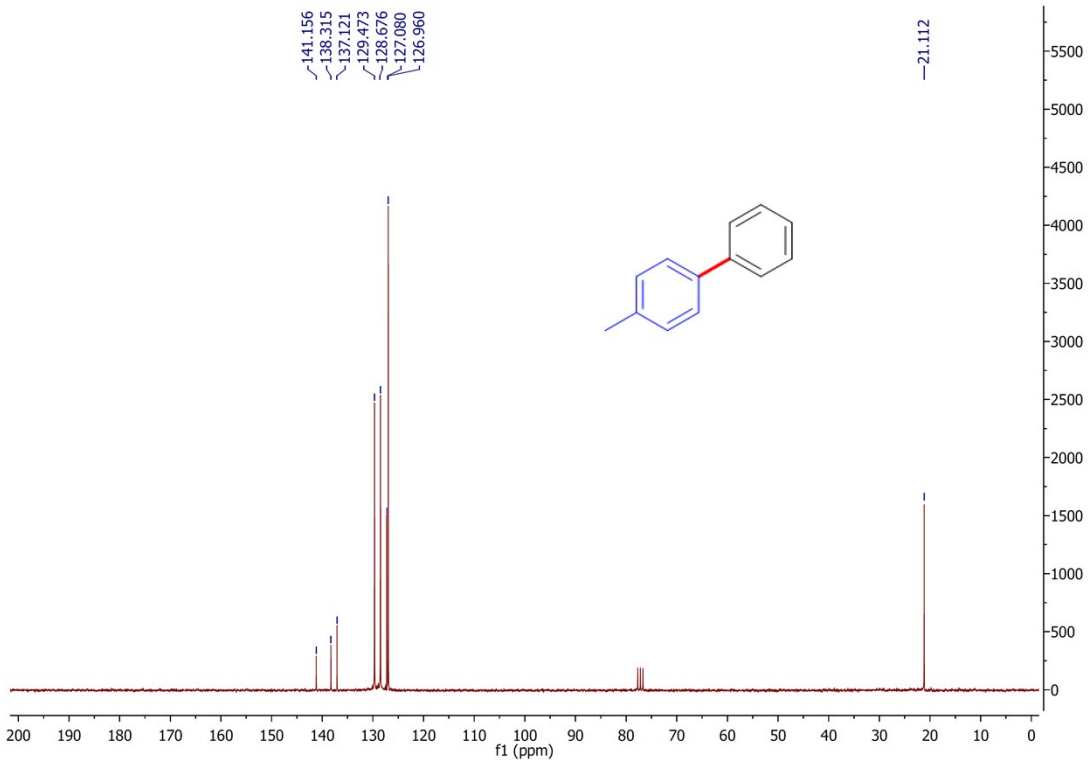
## 2.4. 2-methyl-1,1'-biphenyl (3b)



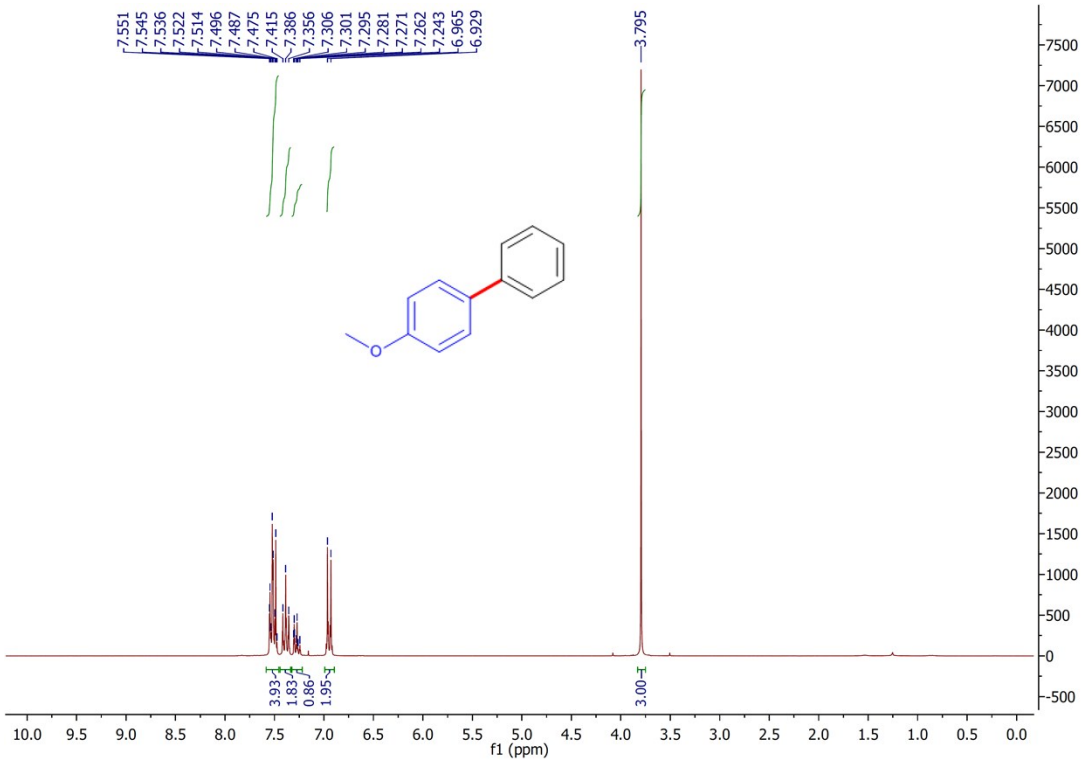



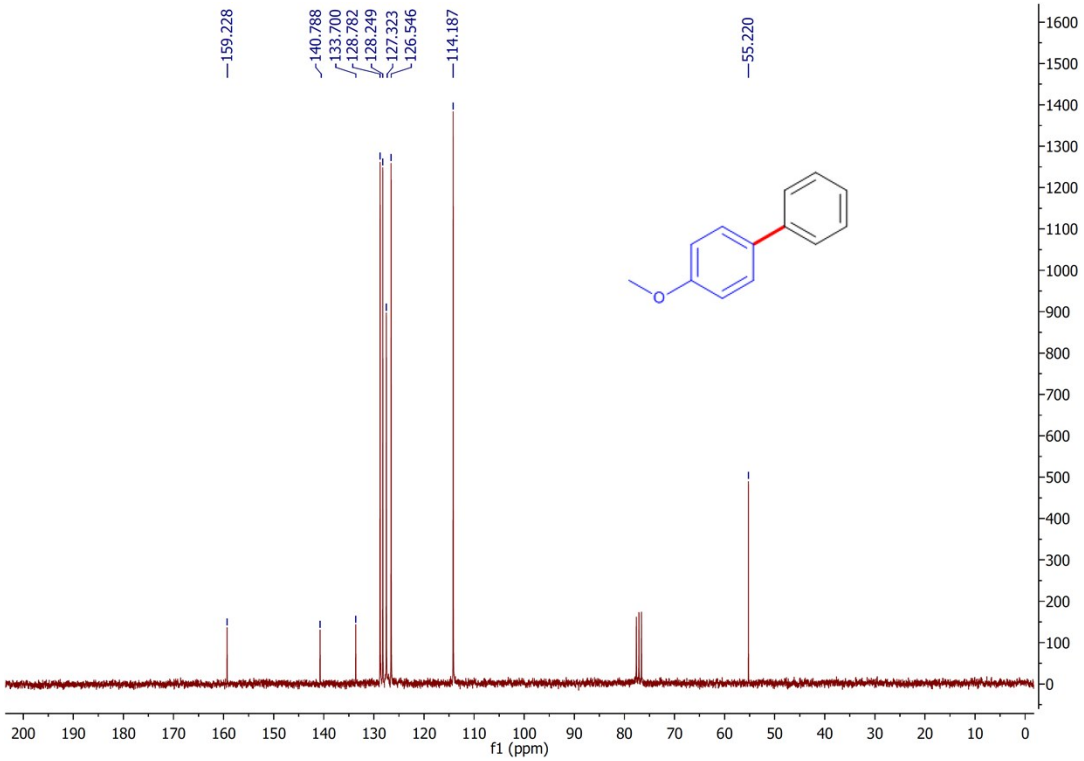
## 2.5. 4-methyl-1,1'-biphenyl (3c)



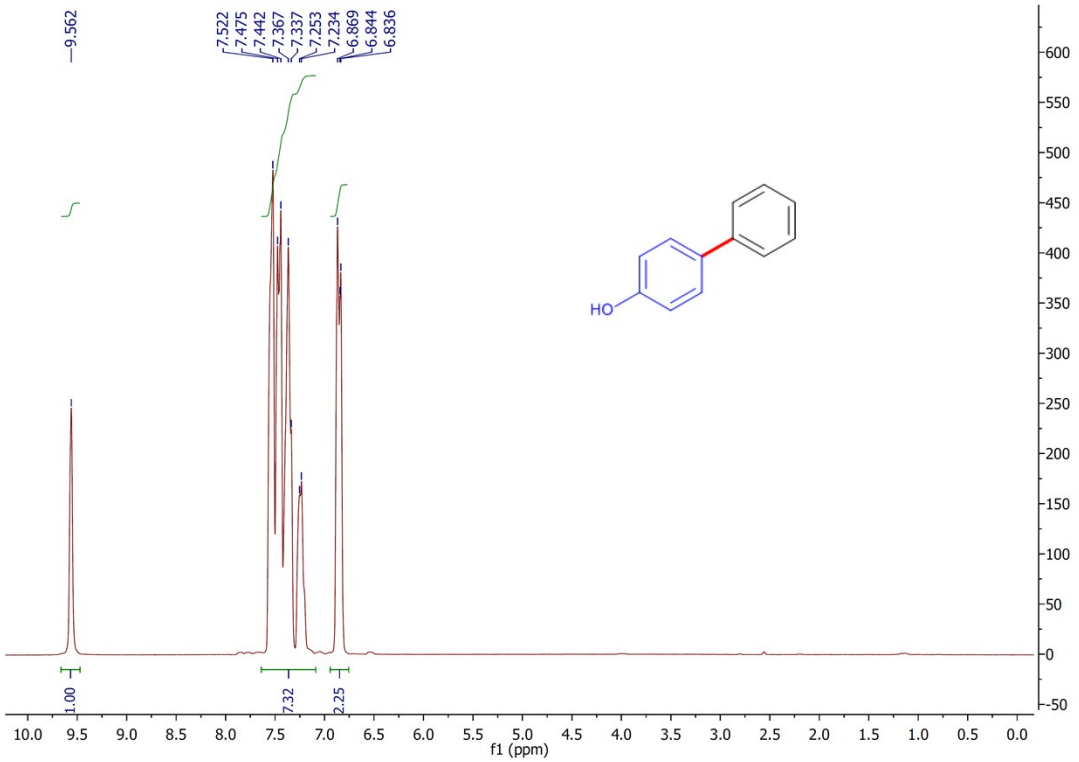



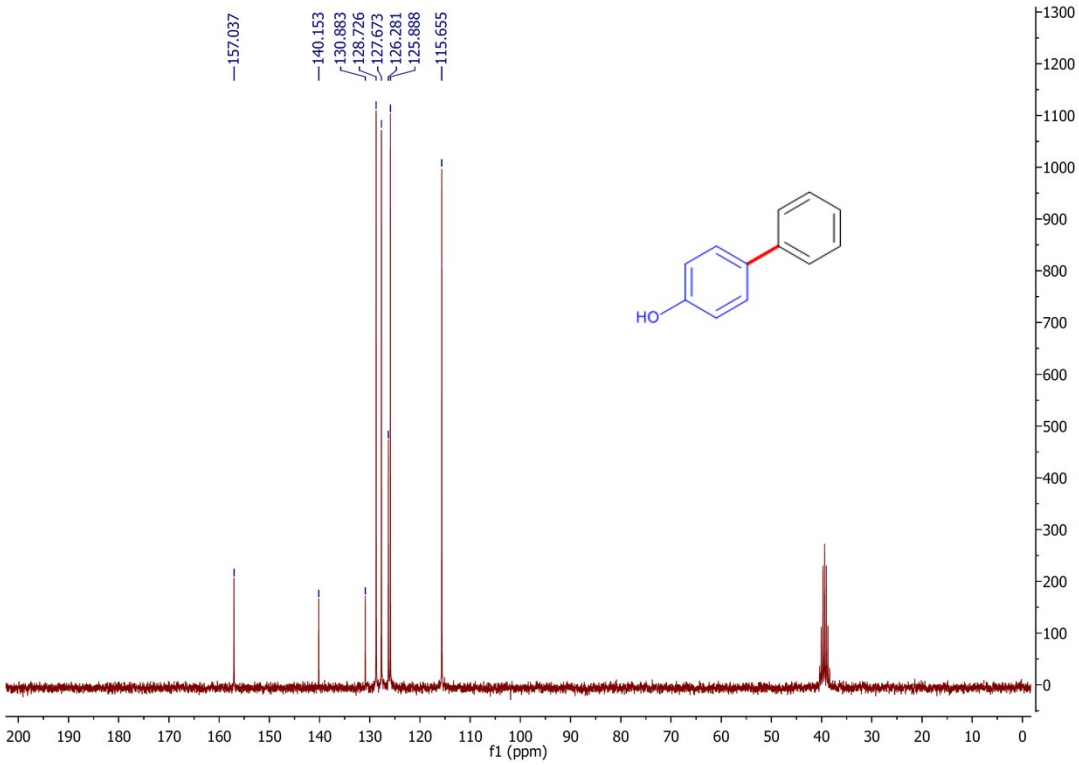
## 2.6. 4-methoxy-1,1'-biphenyl (3d)



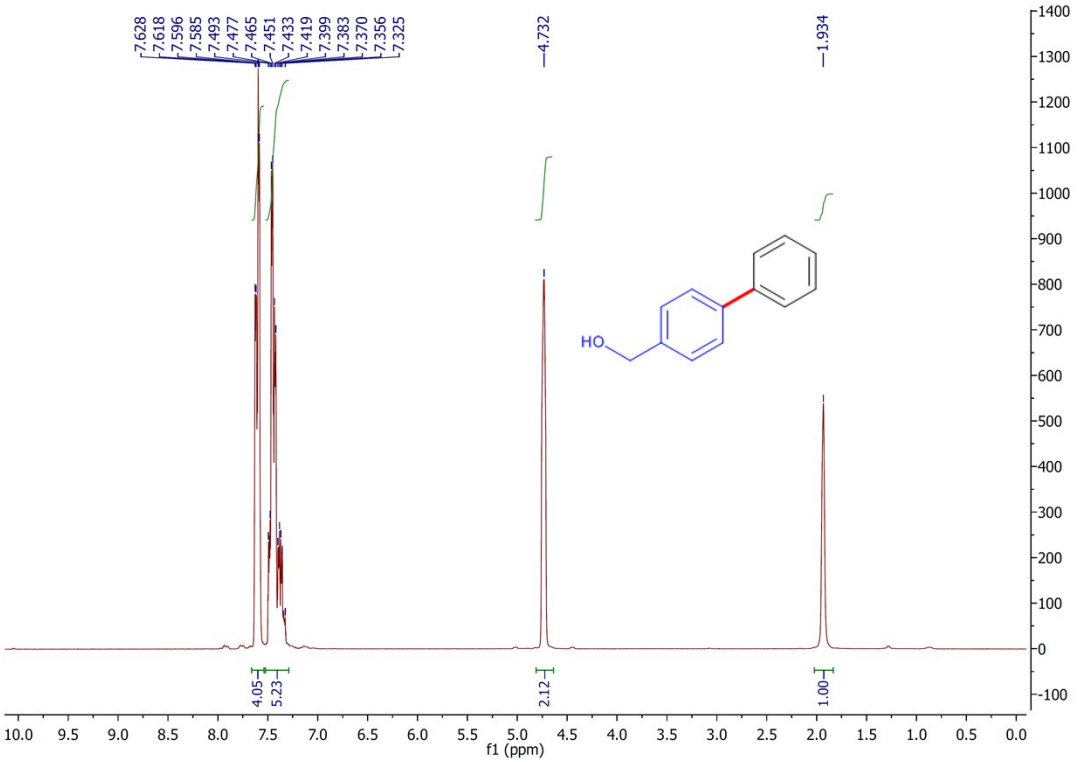



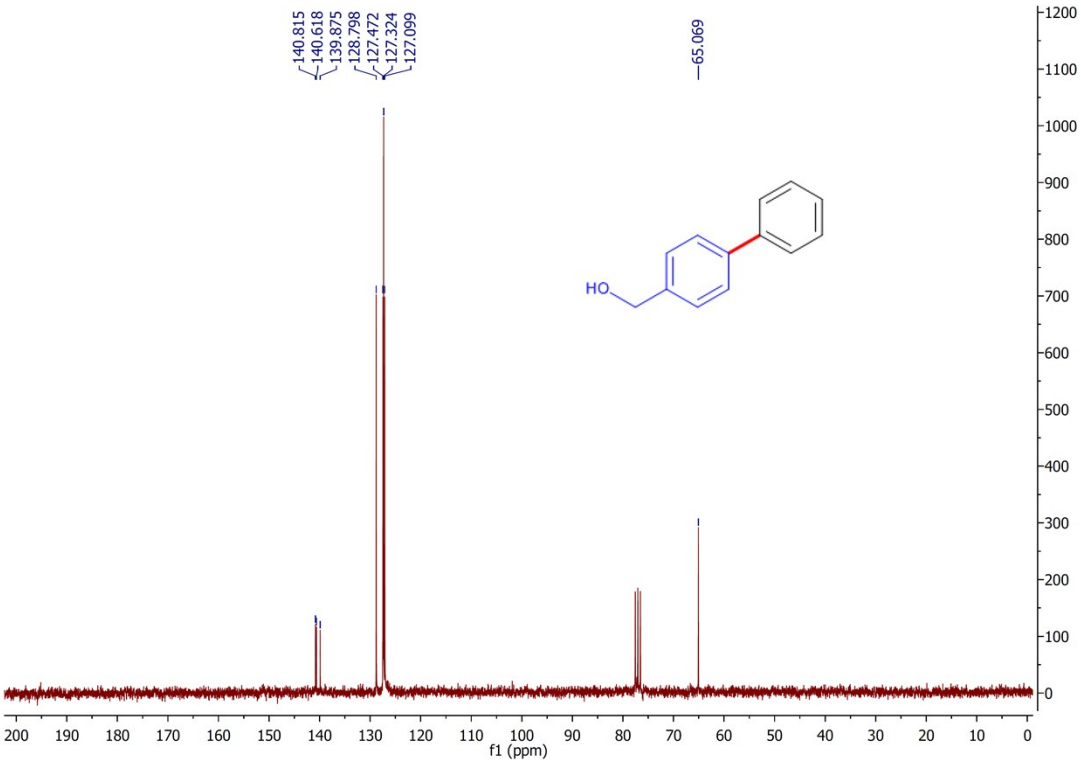
## 2.7. [1,1'-biphenyl]-4-ol (3e)



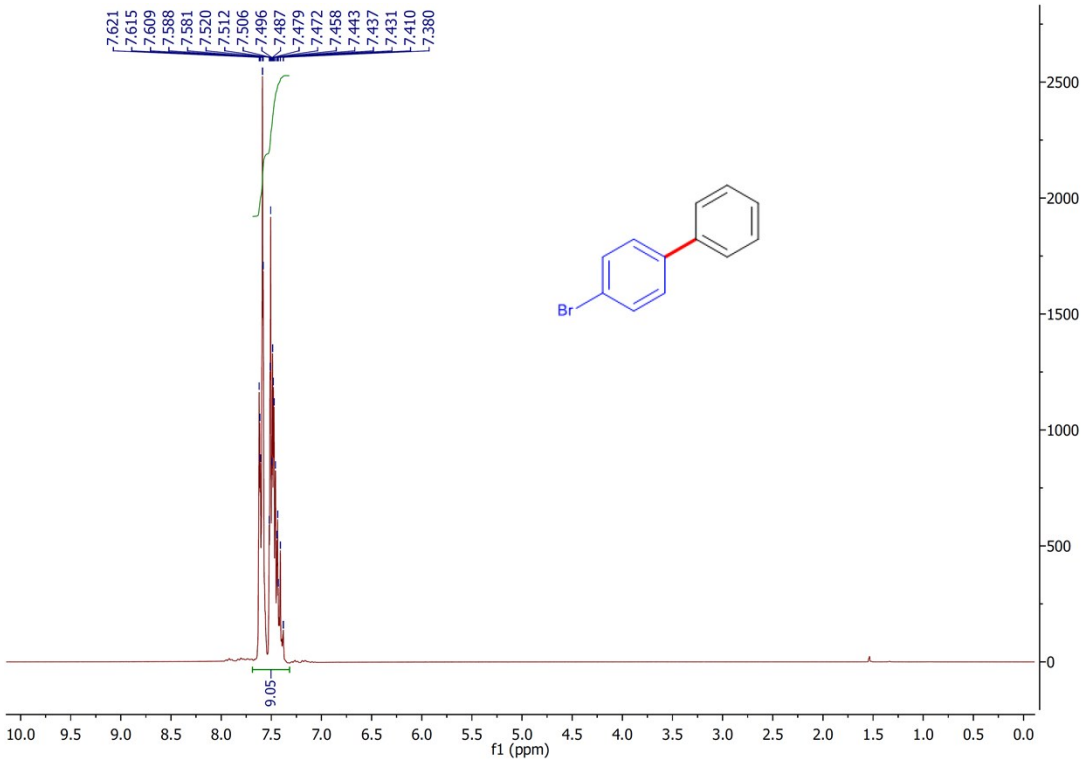



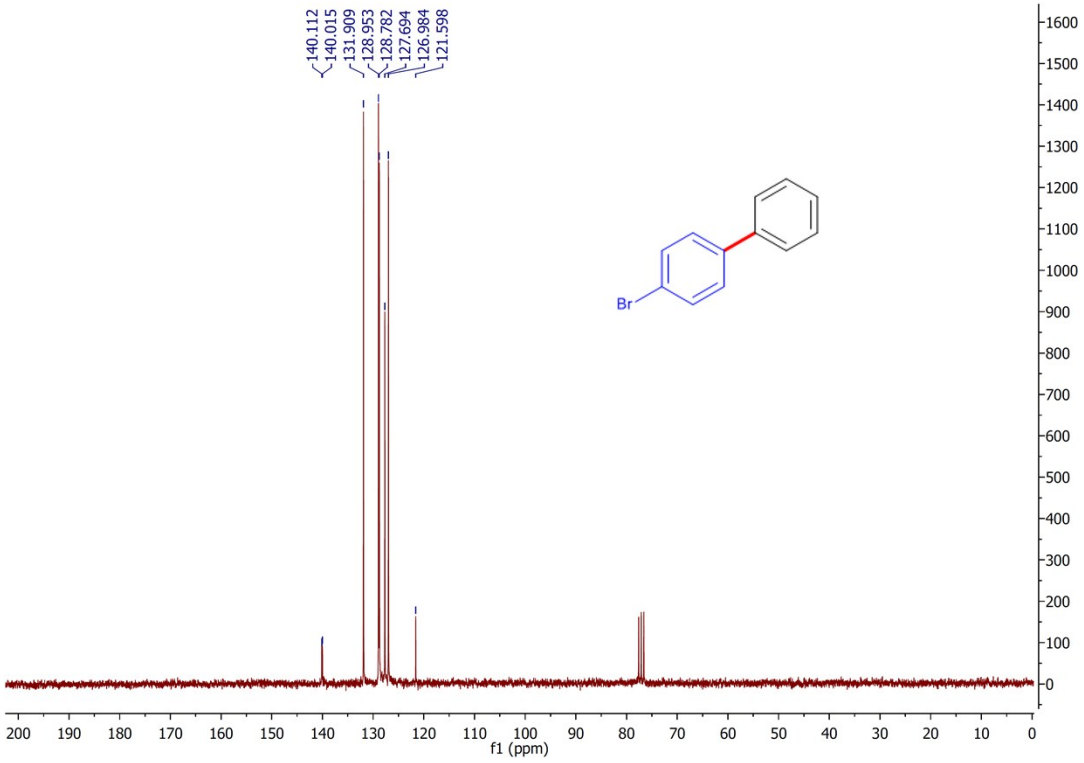
## 2.8. [1,1'-biphenyl]-4-ylmethanol (3f)



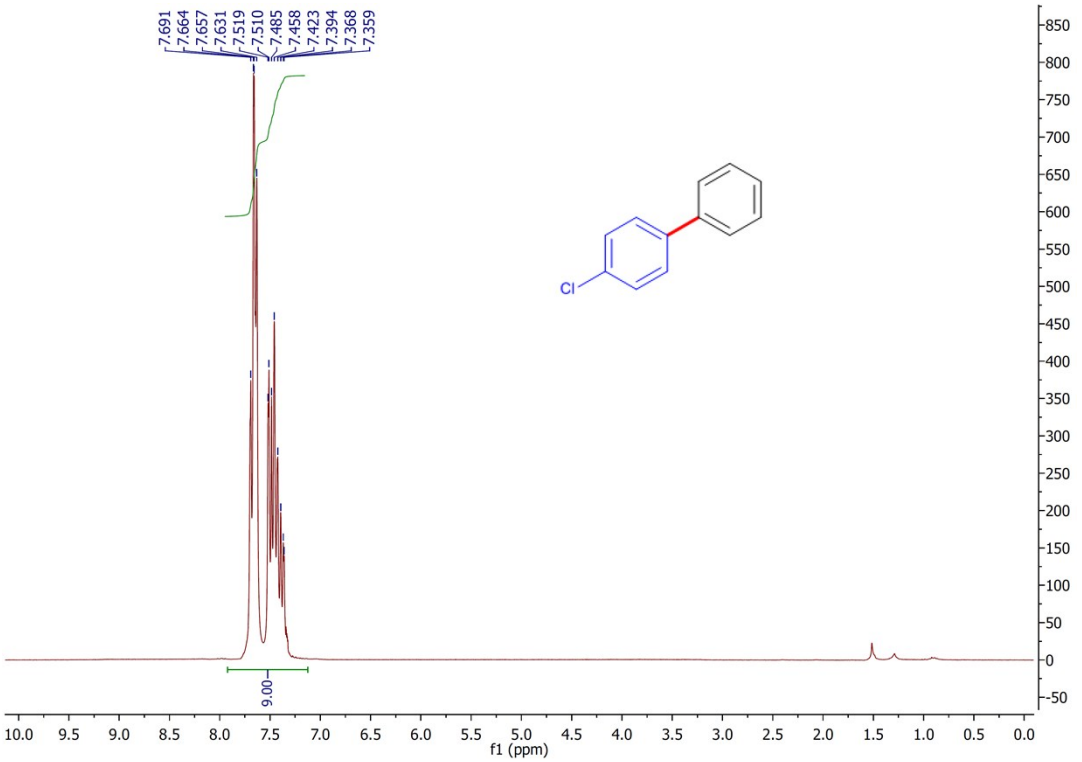



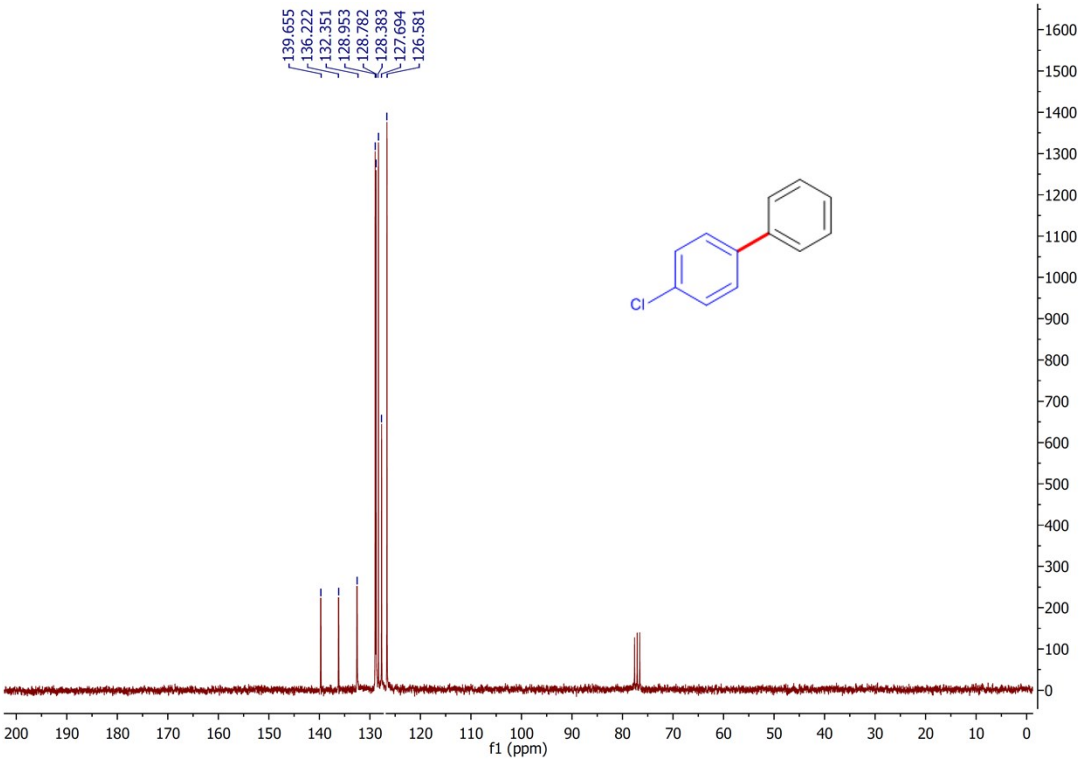
## 2.9. 4-bromo-1,1'-biphenyl (3g)



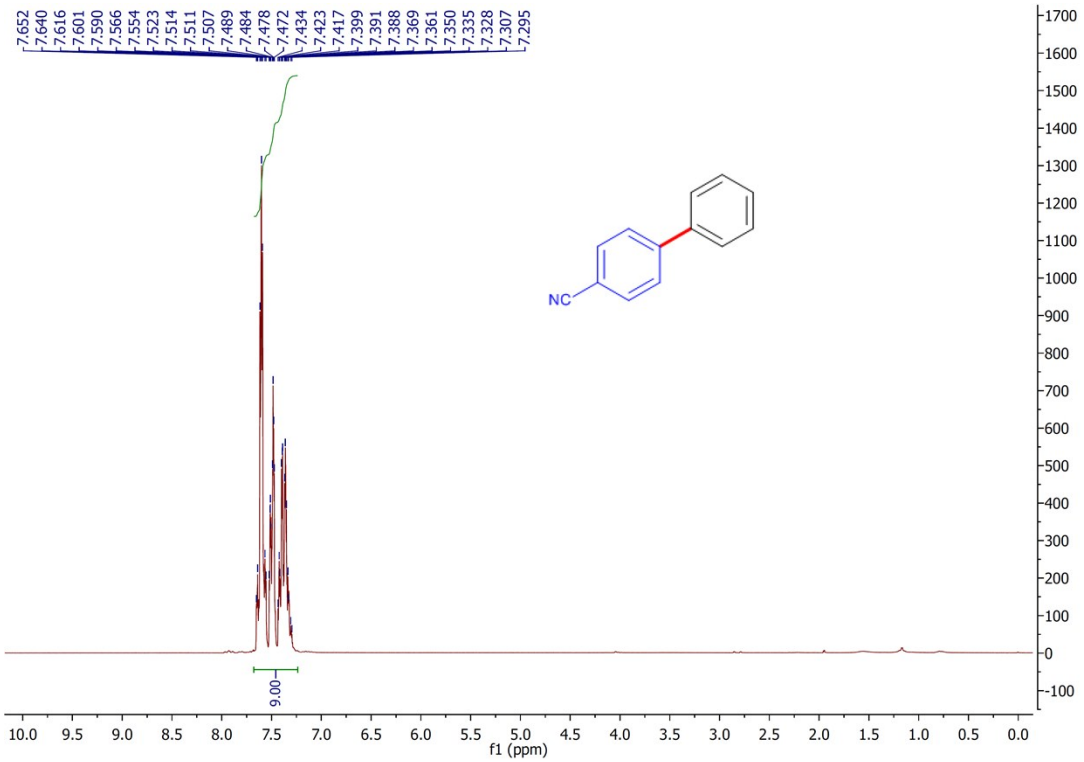



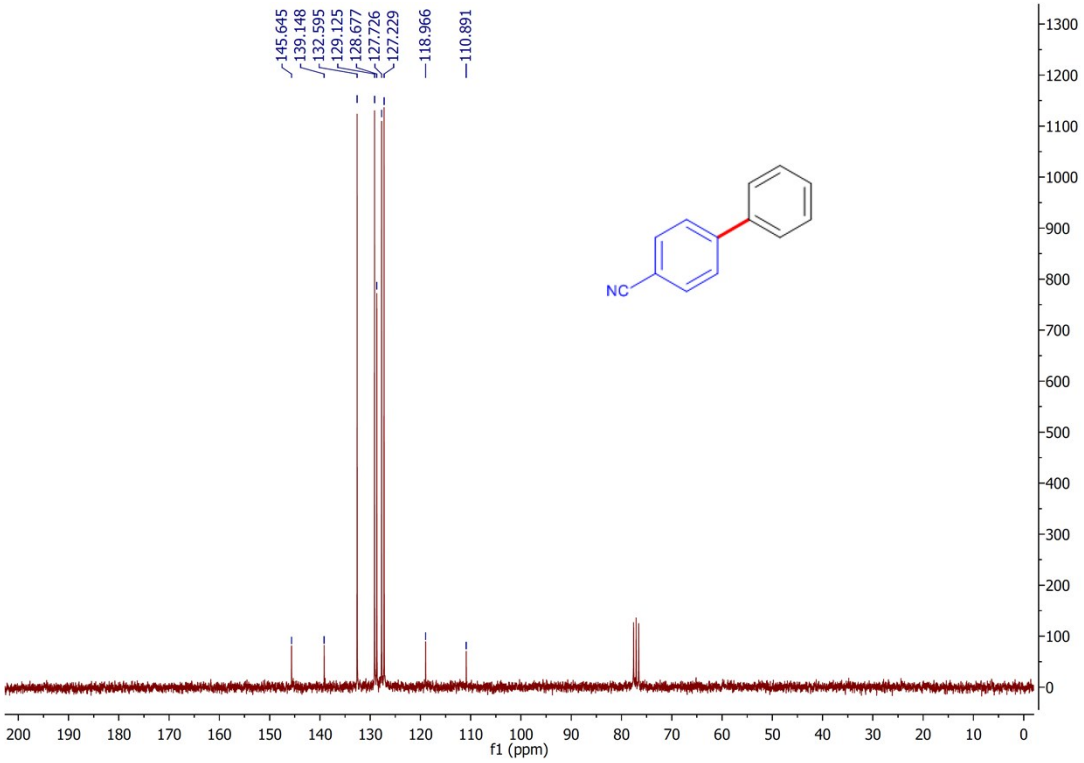
## 2.10. 4-chloro-1,1'-biphenyl (3h)



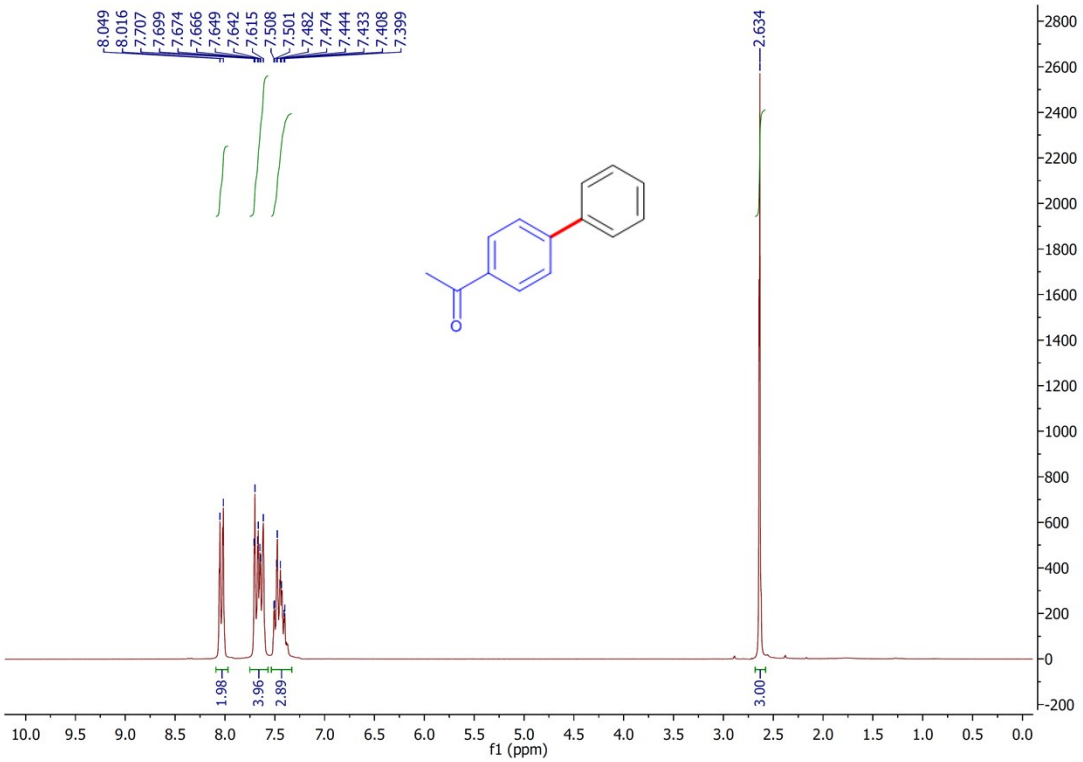



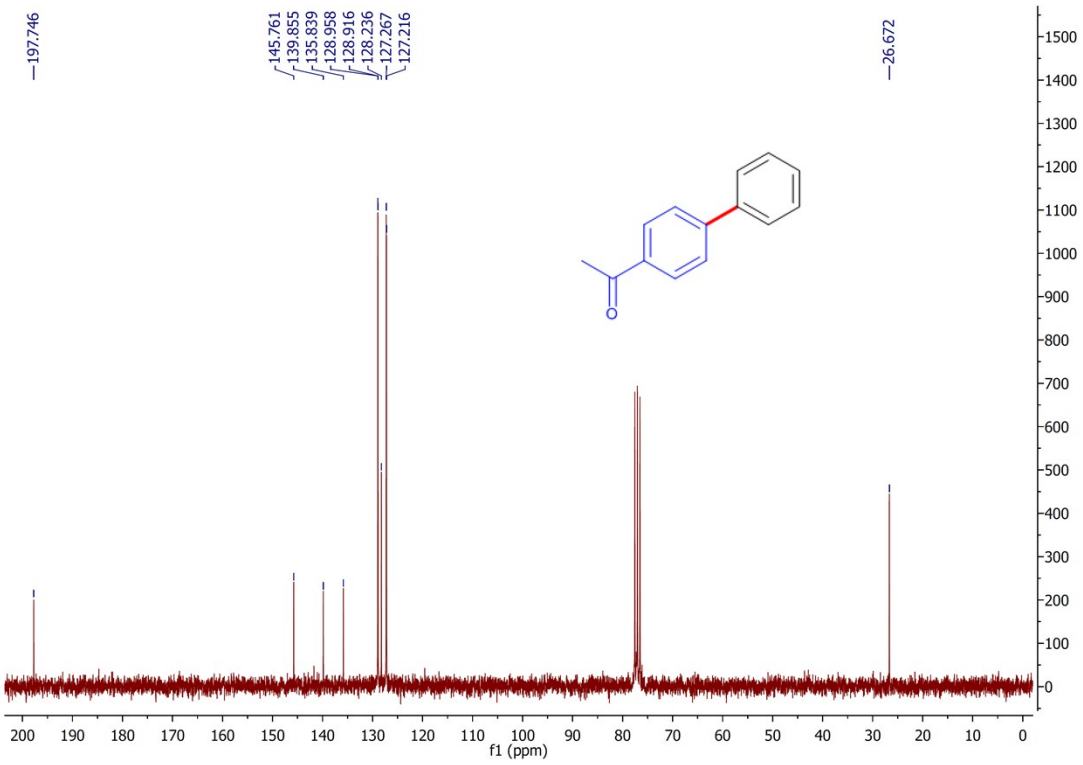
## 2.11. [1,1'-biphenyl]-4-carbonitrile (3i)



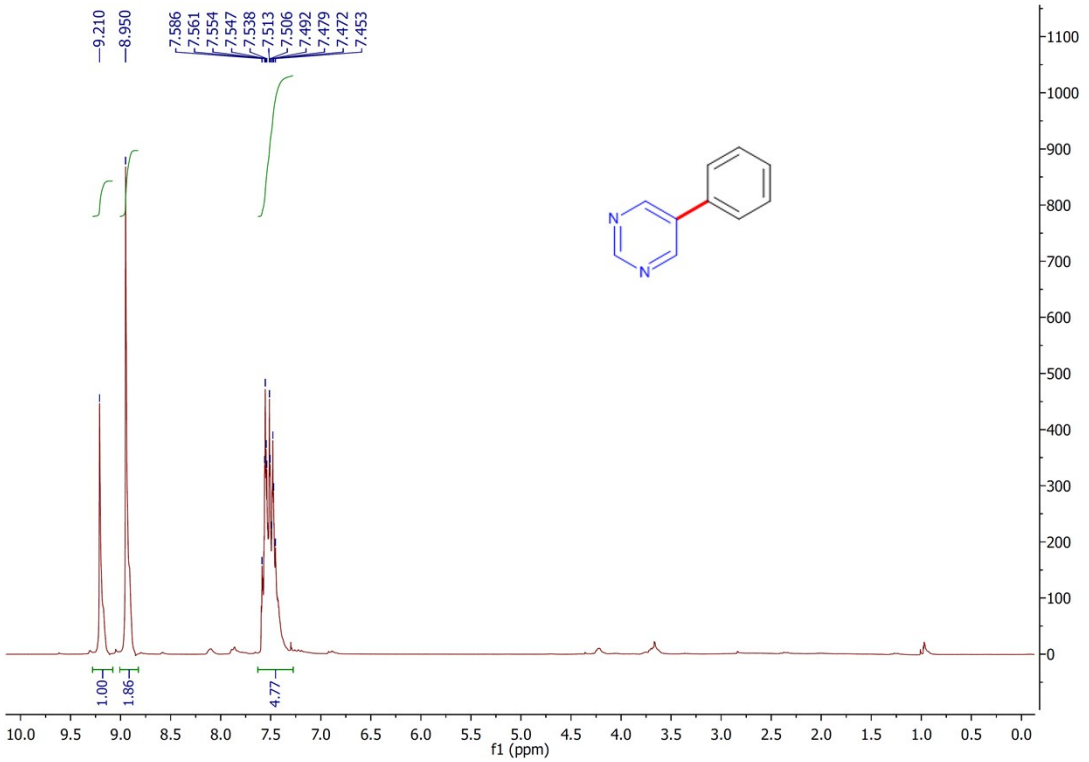



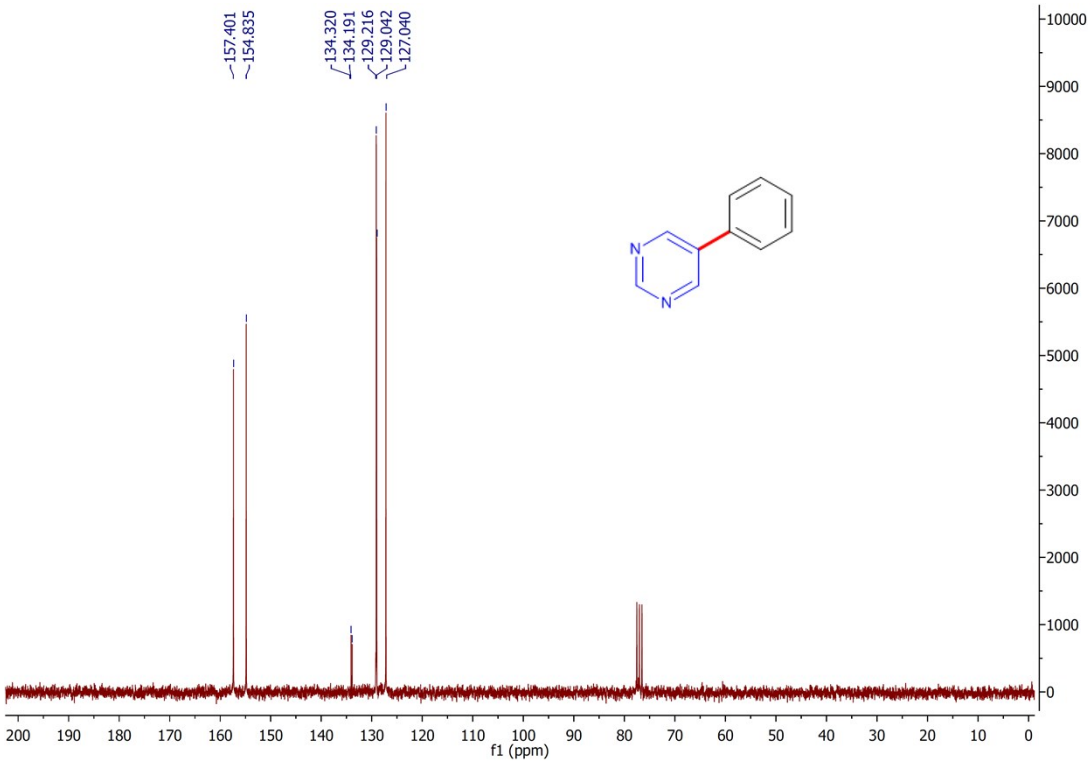
## 2.12. 1-([1,1'-biphenyl]-4-yl)ethan-1-one (3j)



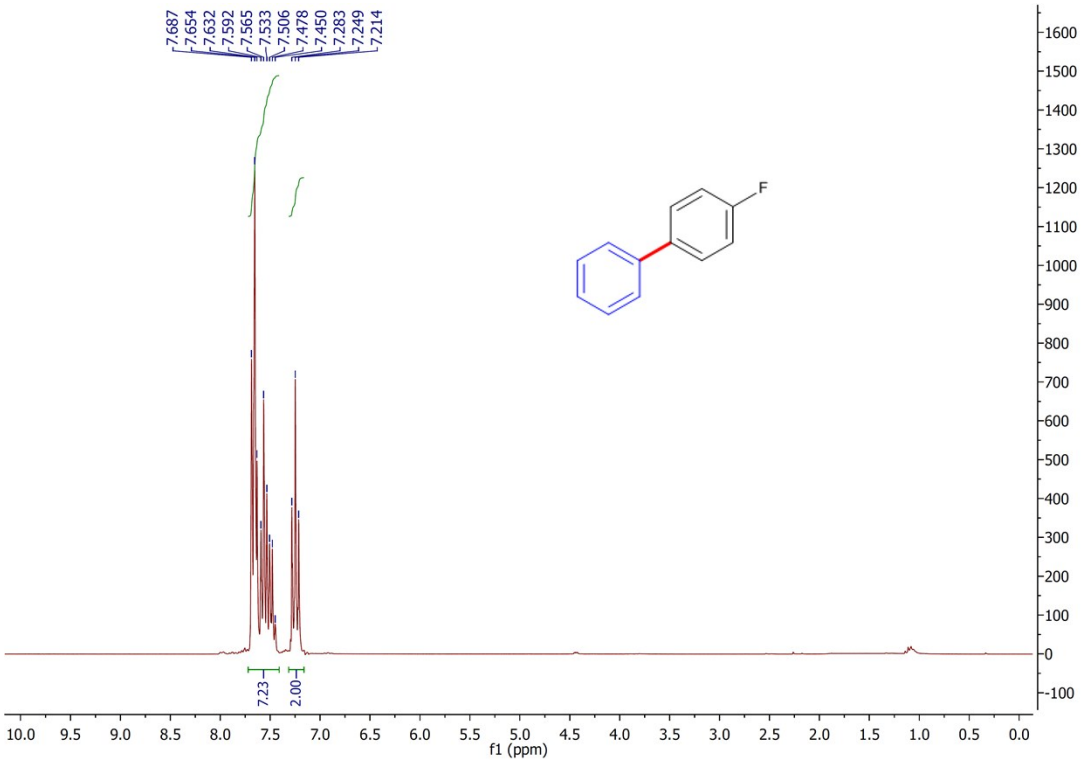



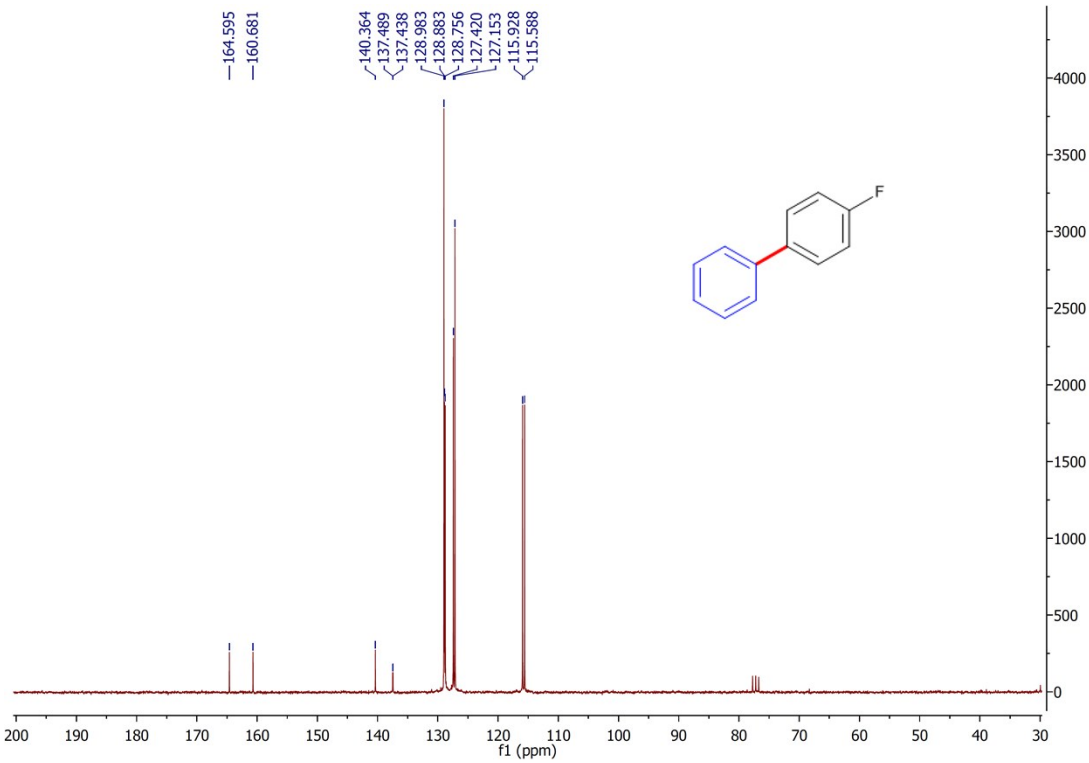
## 2.13. 5-phenylpyrimidine (3k)



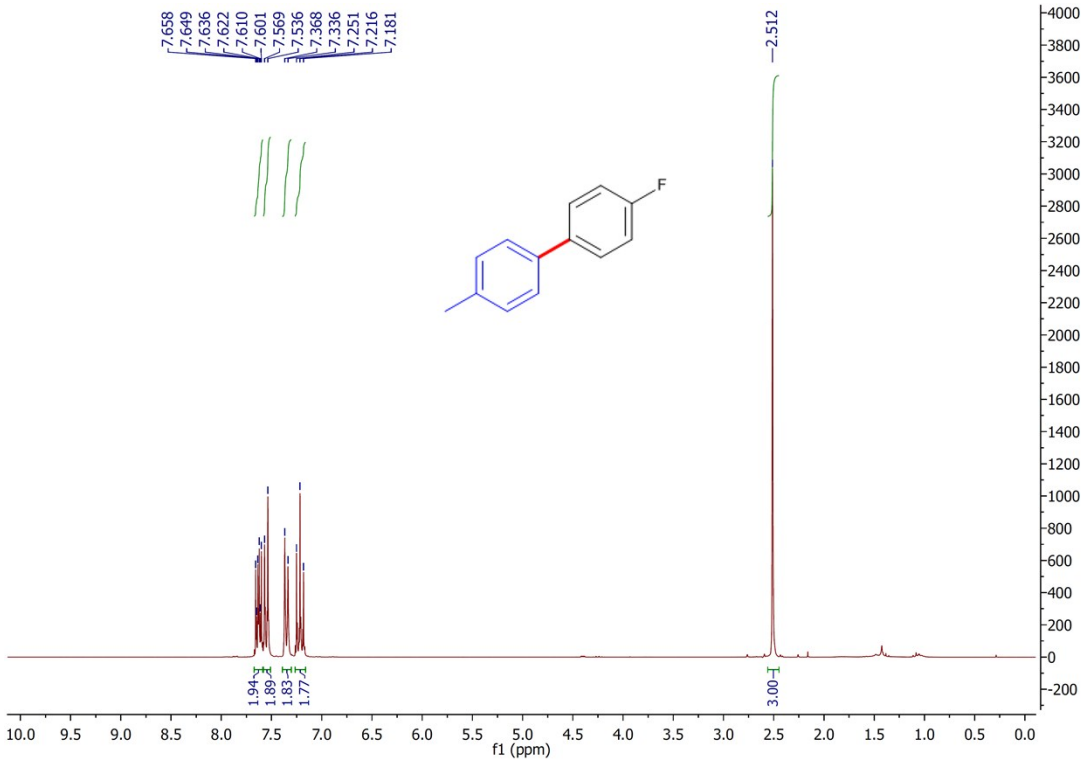



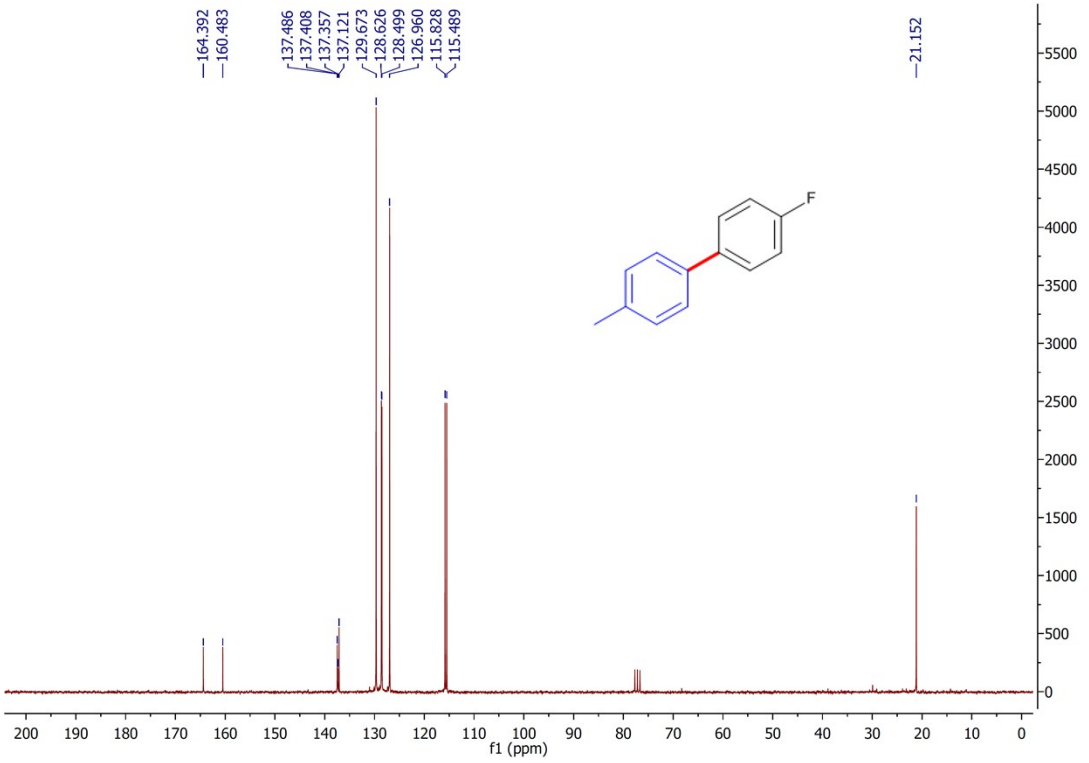
## 2.14. 4-fluoro-1,1'-biphenyl (3l)



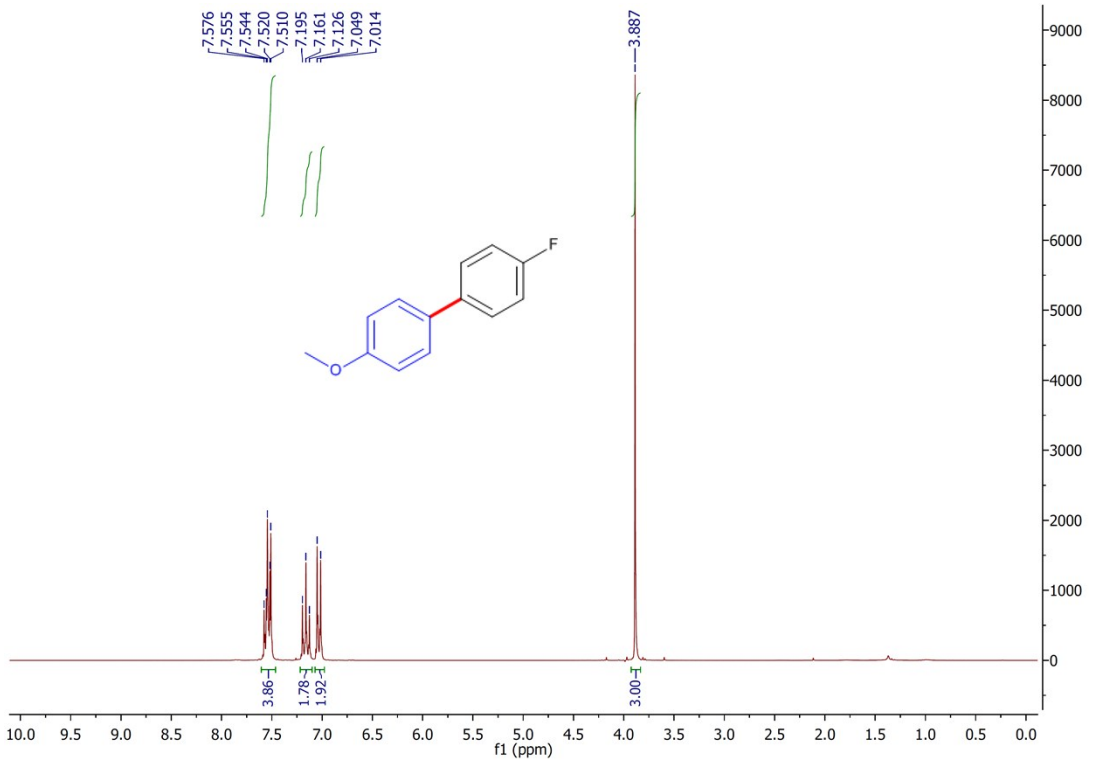



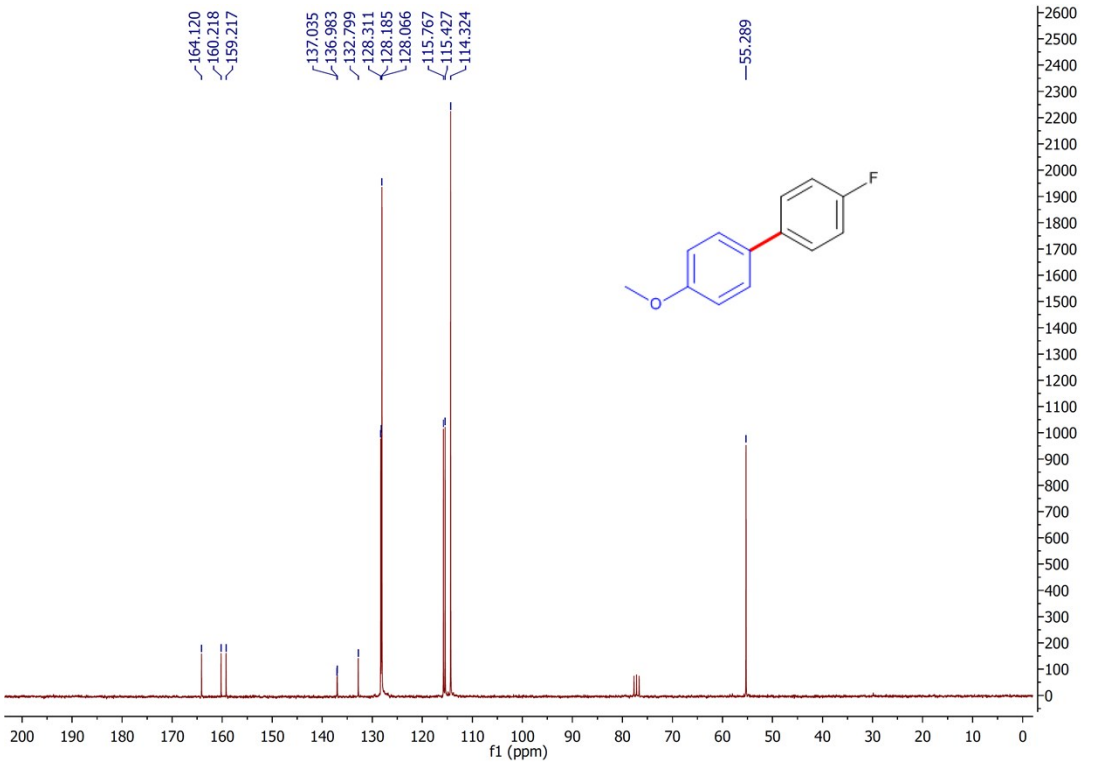
## 2.15. 4-fluoro-4'-methyl-1,1'-biphenyl (3m)



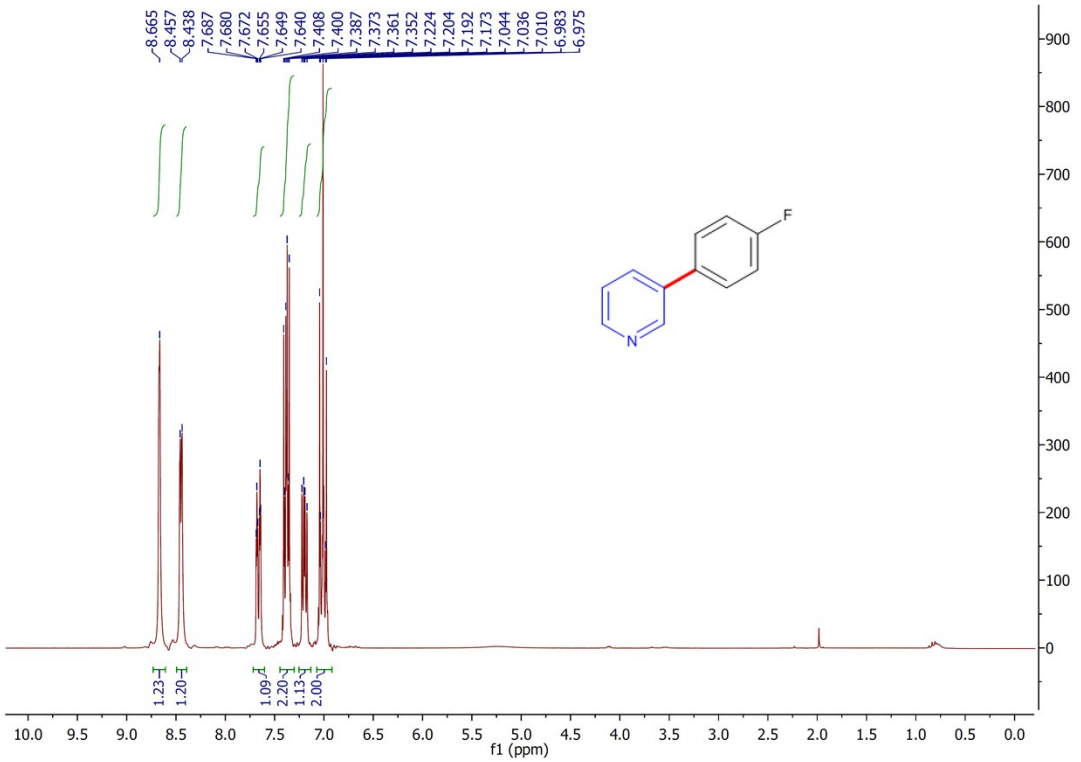



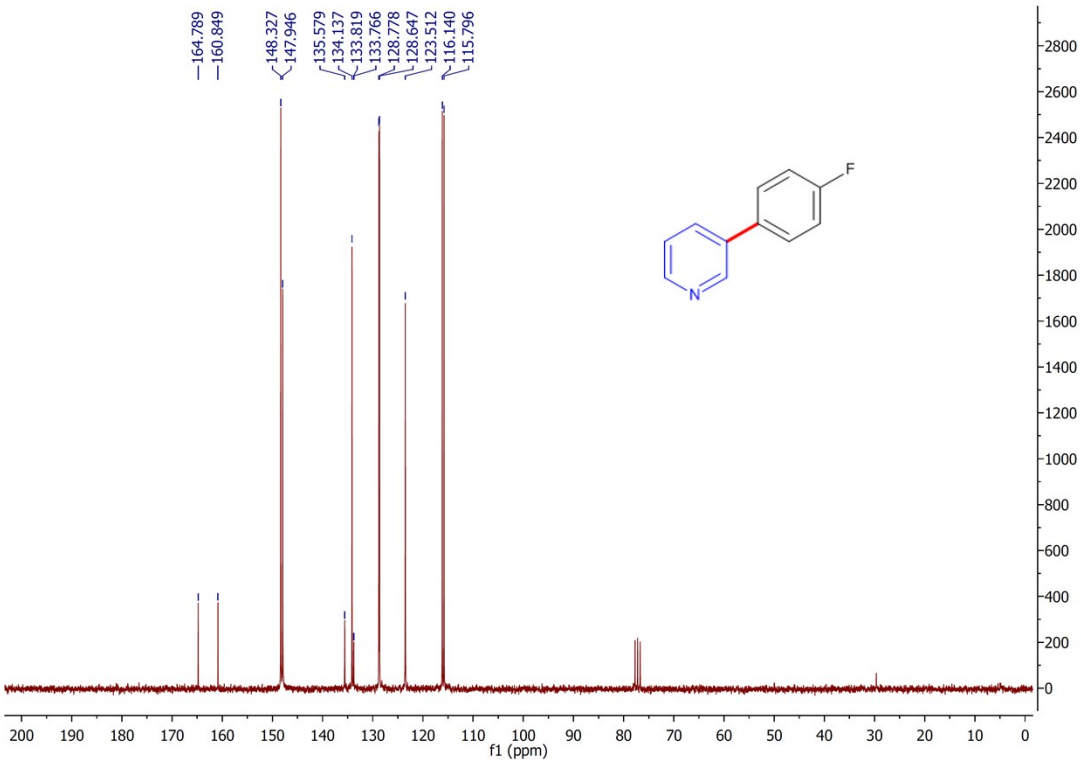
## 2.16. 4-fluoro-4'-methoxy-1,1'-biphenyl (3n)



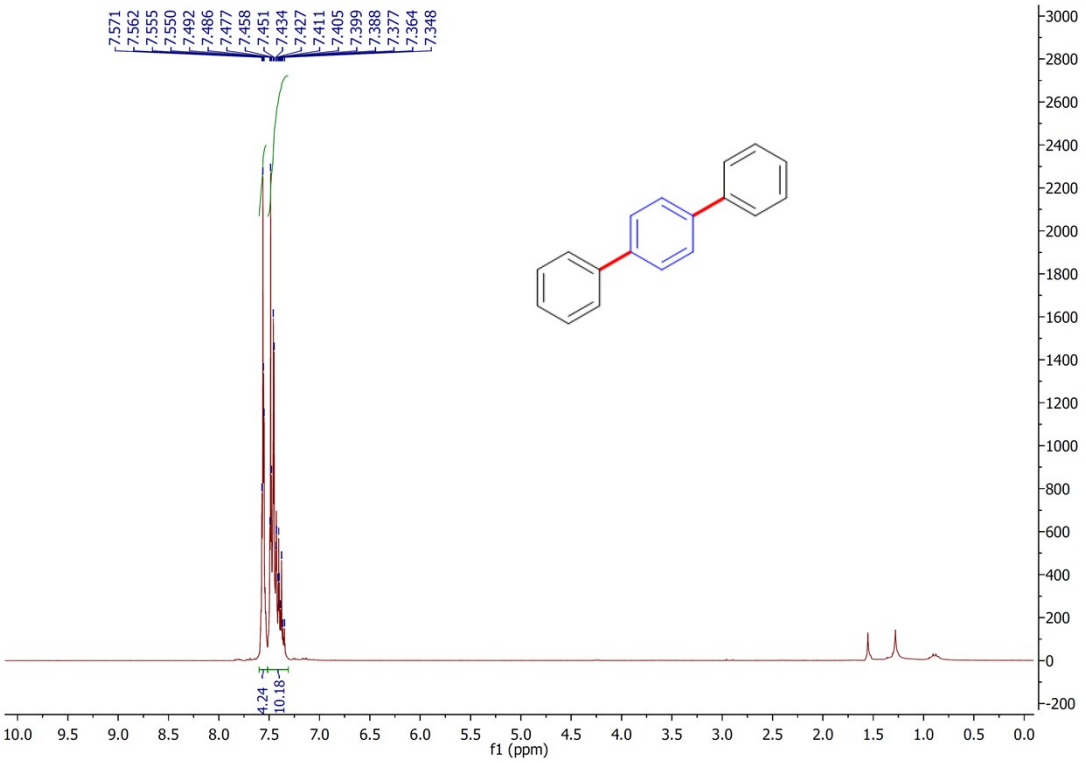



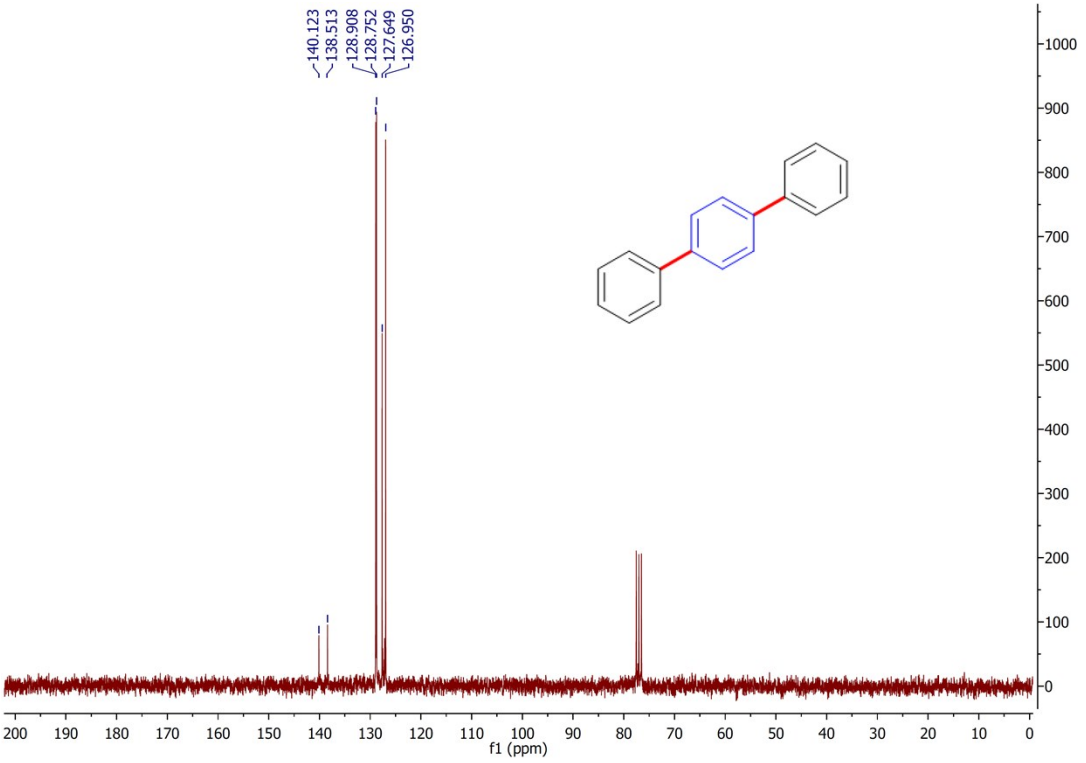
## 2.17. 3-(4-fluorophenyl)pyridine (3o)



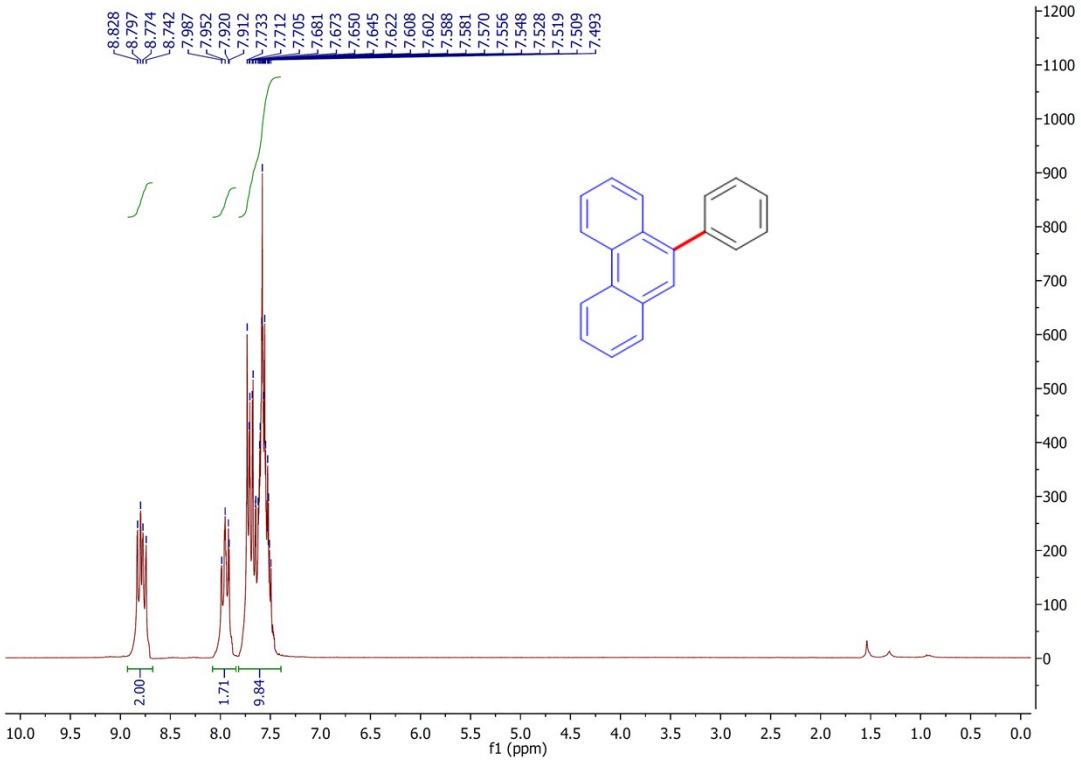



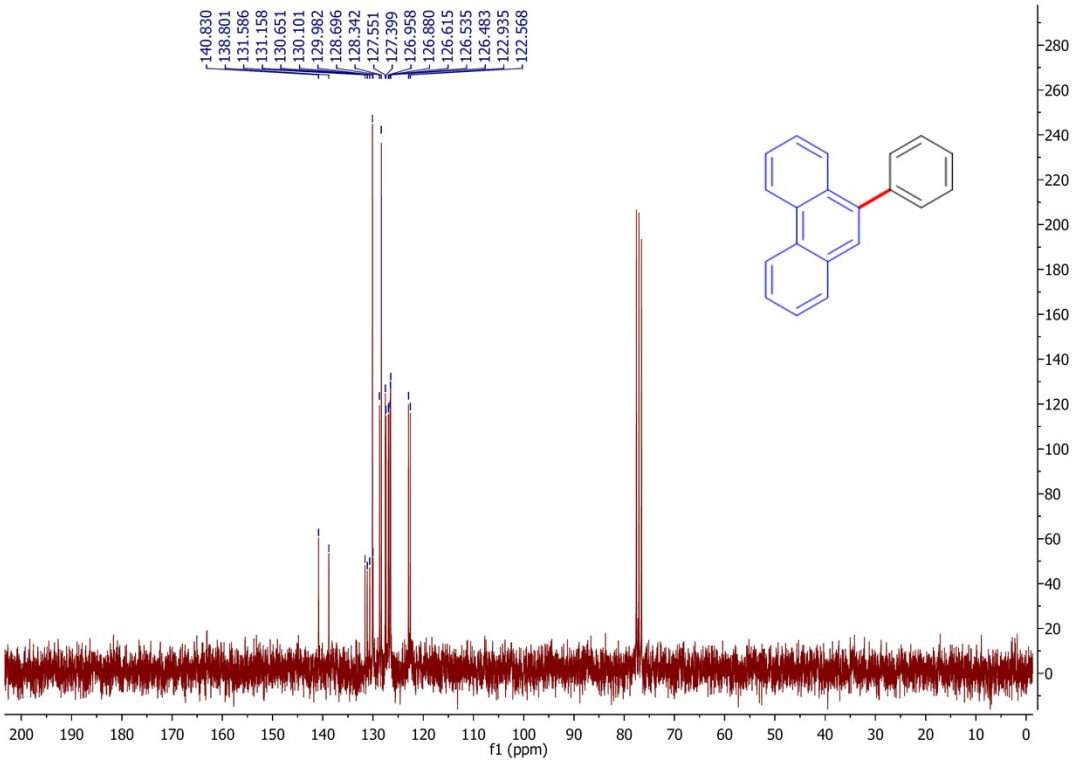
## 2.18. 1,1':4',1''-terphenyl (3p)



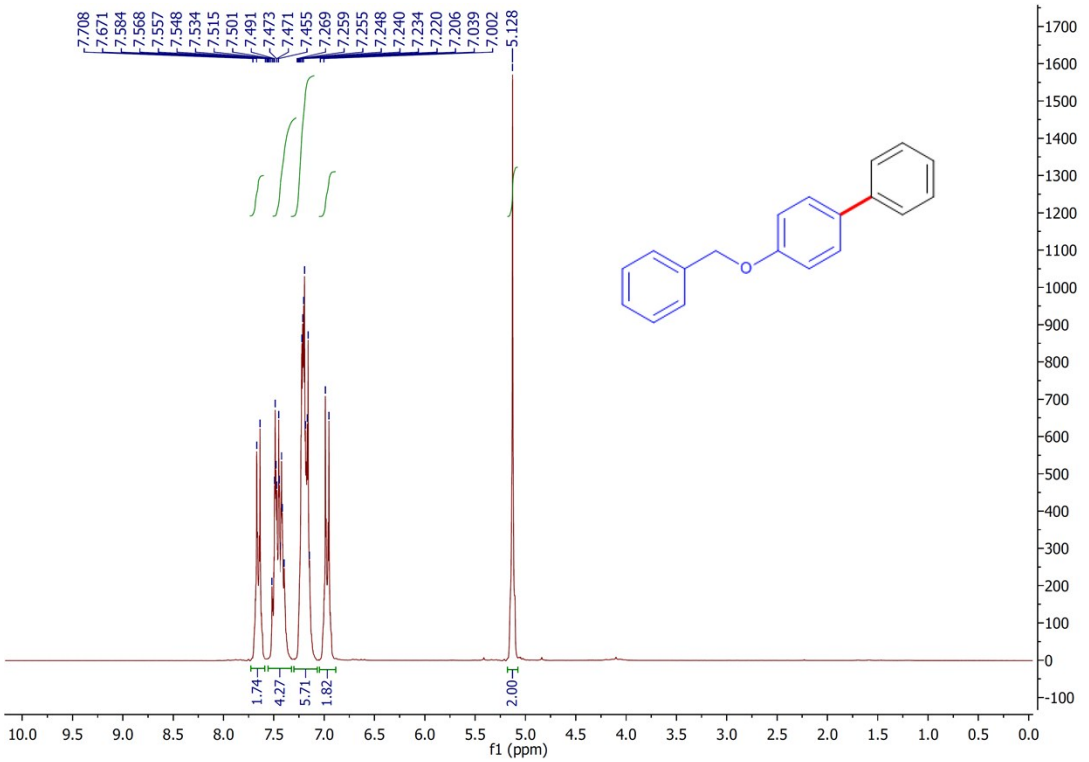



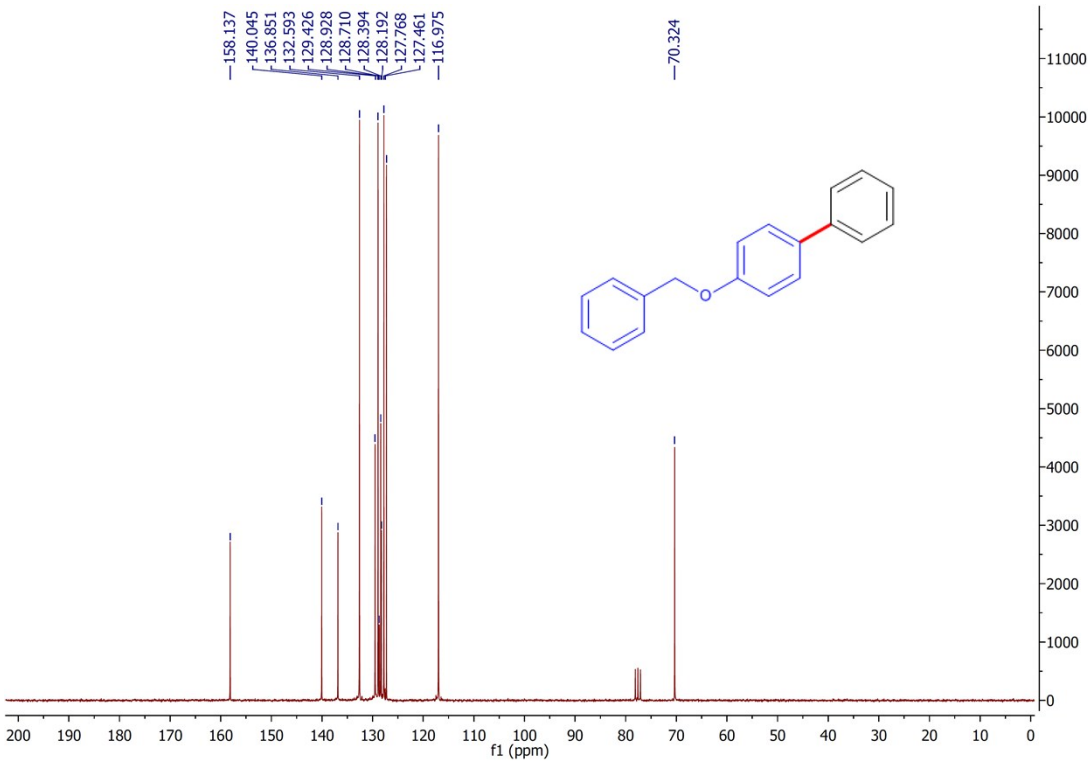
## 2.19. 9-phenylphenanthrene (3q)



## 2.20. 4-(benzyloxy)-1,1'-biphenyl (3r)



**2.21. 9-([1,1'-biphenyl]-4-yl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (3s)**