

*Supporting Information for*

**Rhodium-Catalyzed Redox-Neutral Coupling of  
Phenidones with Alkynes**

Zhoulong Fan,<sup>a,b,+</sup> Heng Lu,<sup>c,+</sup> Wei Li,<sup>a</sup> Kaijun Geng,<sup>a,b</sup> and Ao Zhang<sup>\*a,b,c</sup>

<sup>a</sup> CAS Key Laboratory of Receptor Research, and the State Key Laboratory of Drug Research,  
Shanghai Institute of Materia Medica (SIMM), Chinese Academy of Sciences, Shanghai 201203,  
China.

E-mail: aozhang@simm.ac.cn

<sup>b</sup> University of Chinese Academy of Sciences, Beijing 100049, China

<sup>c</sup> ShanghaiTech University, Shanghai 201210, China

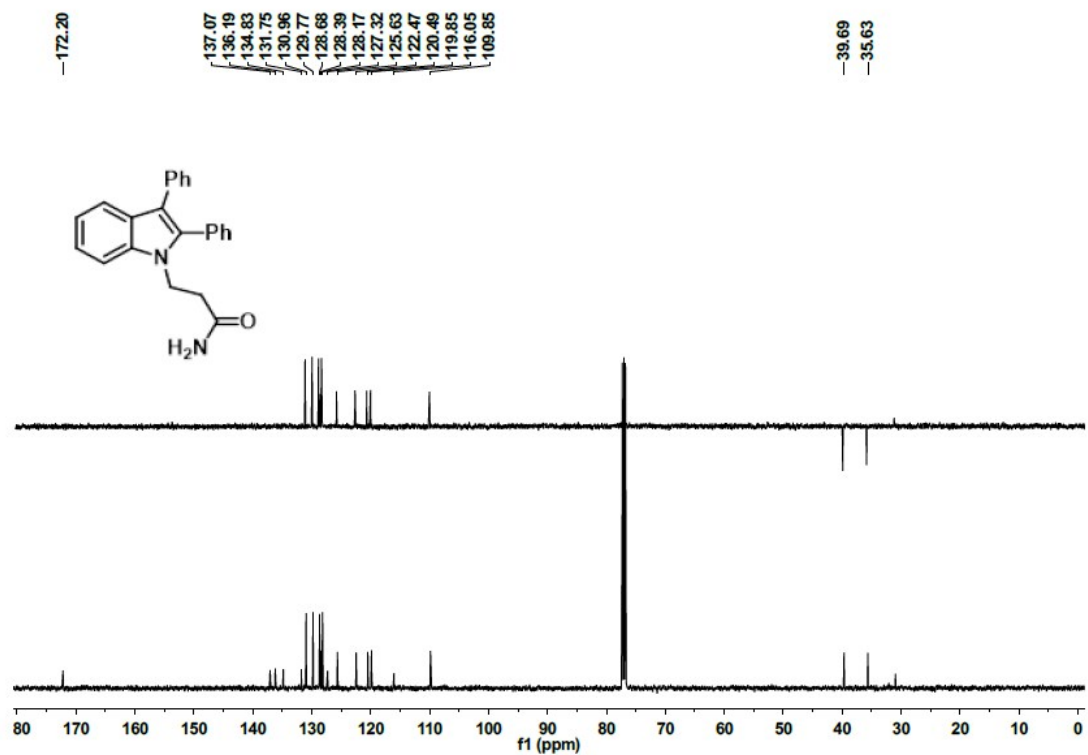
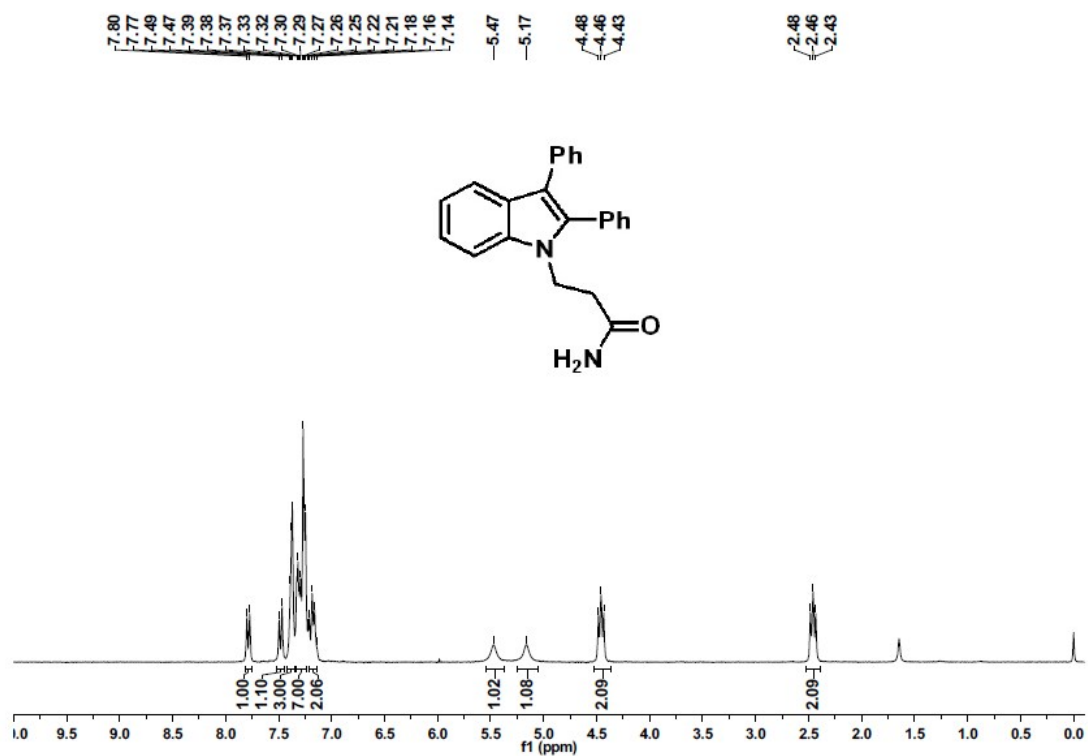
<sup>+</sup> These two authors contributed equally to this work

## Table of Contents

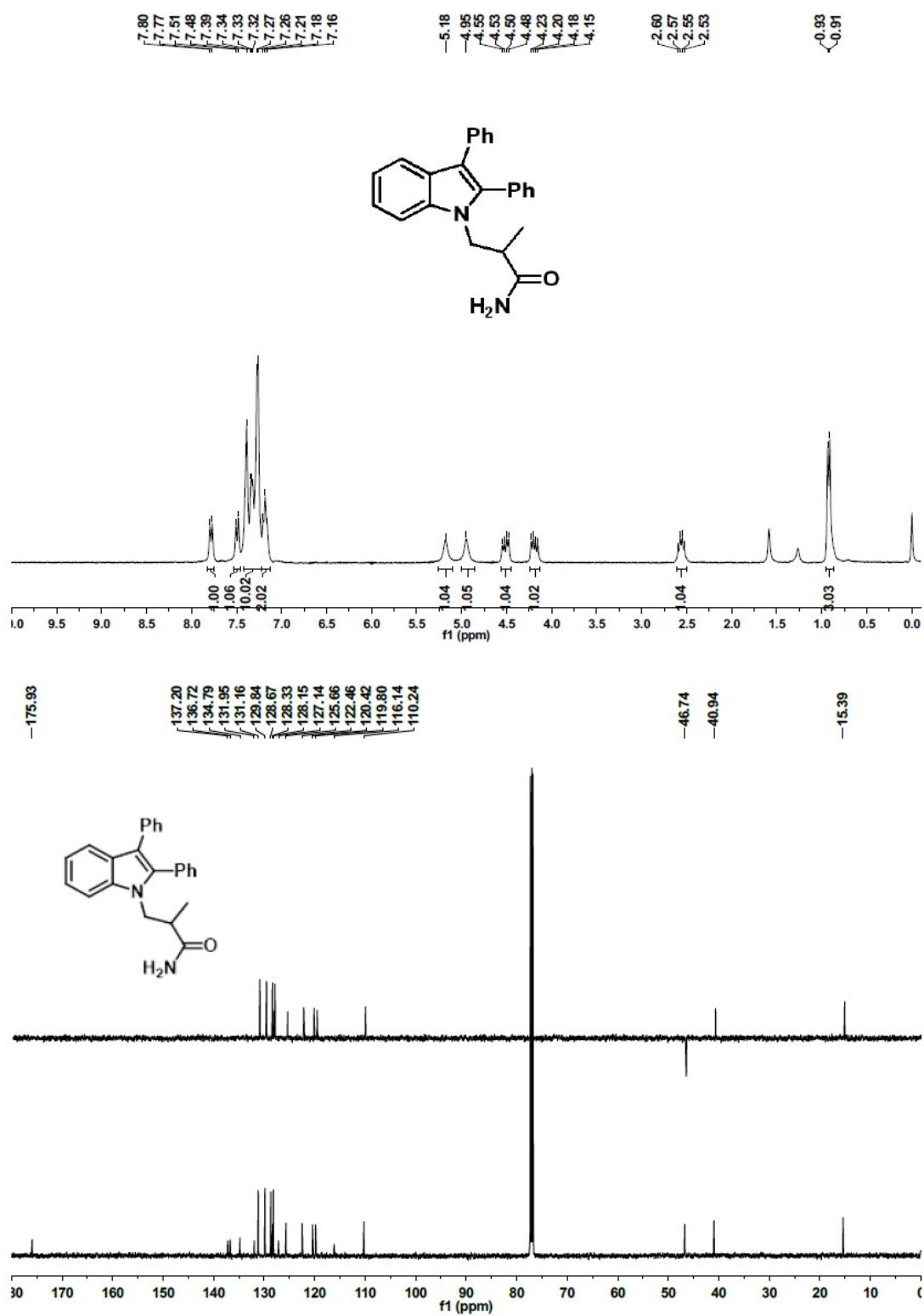
<b>1. Copies of NMR spectra data</b> -----	S1
<b>2. X-ray structure of compound 3a</b> -----	S35

# 1. Copies of NMR spectra data

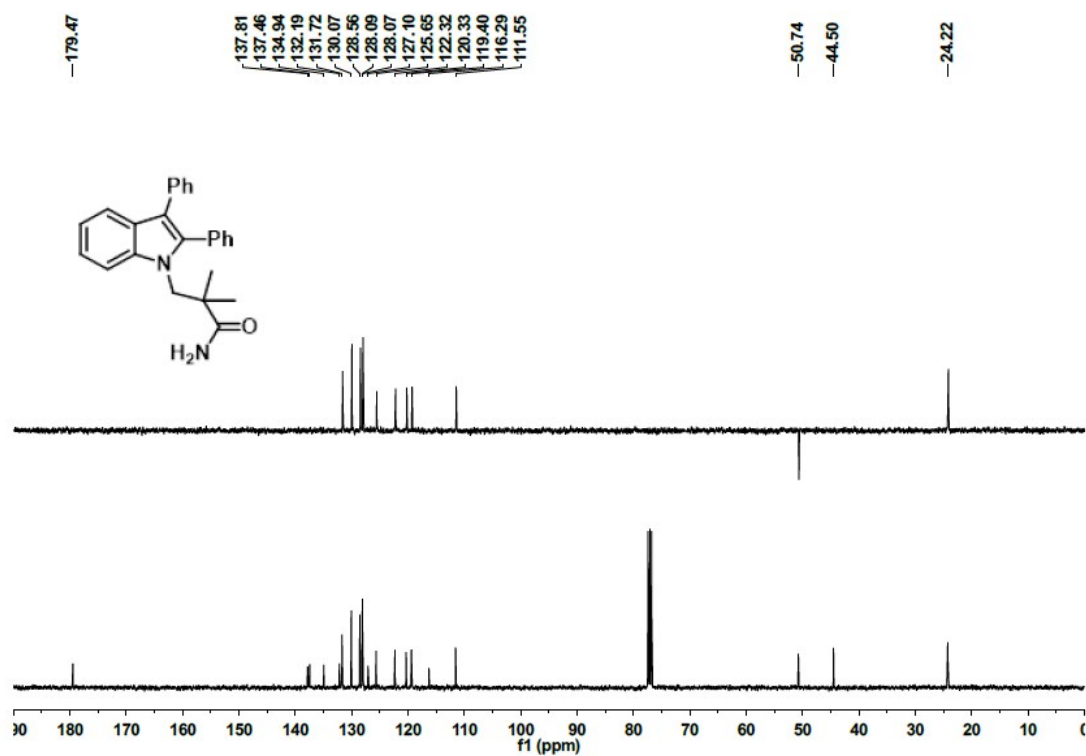
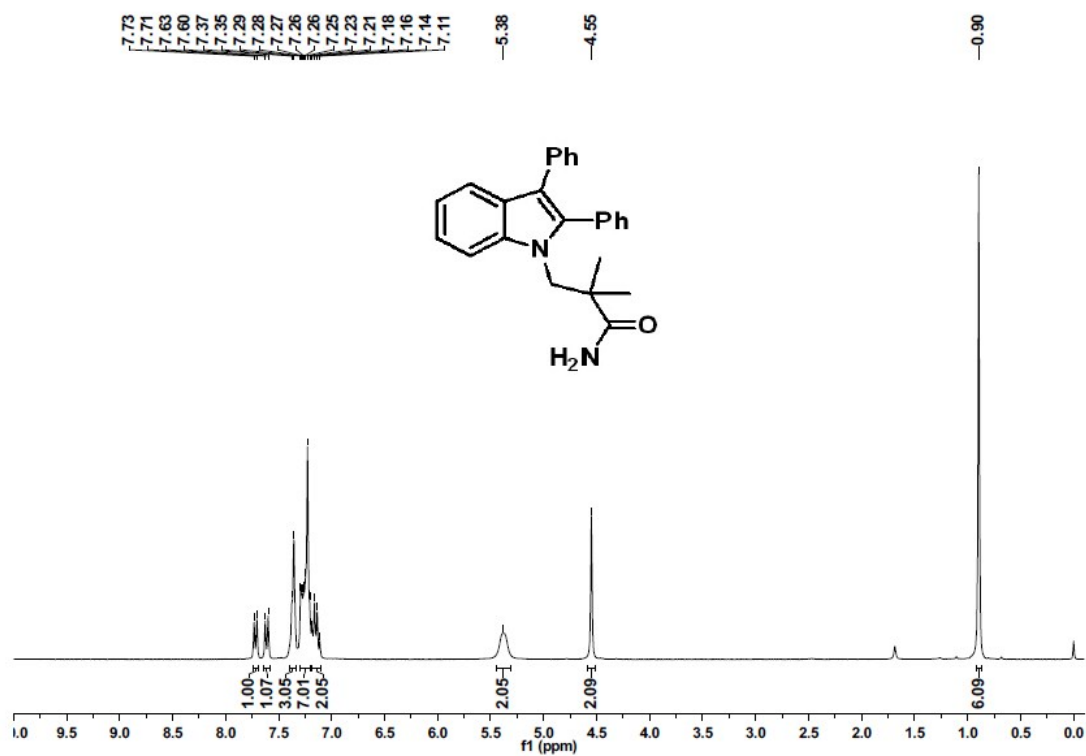
## $^1\text{H}$ and $^{13}\text{C}$ NMR spectra of compound 3a



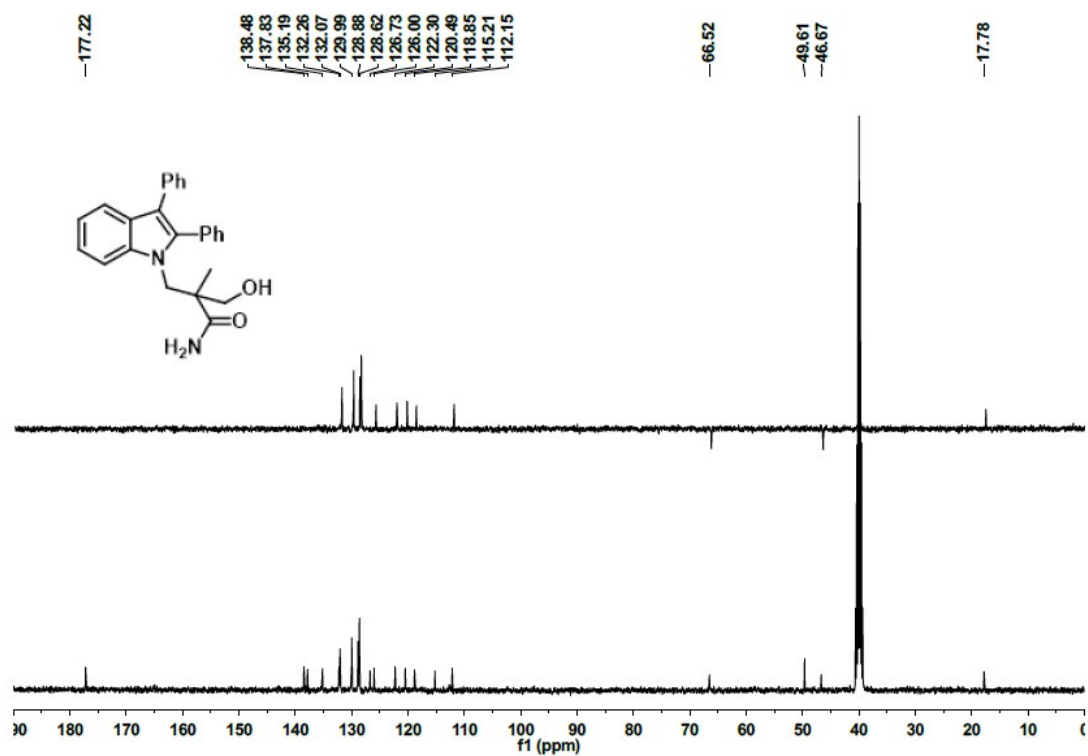
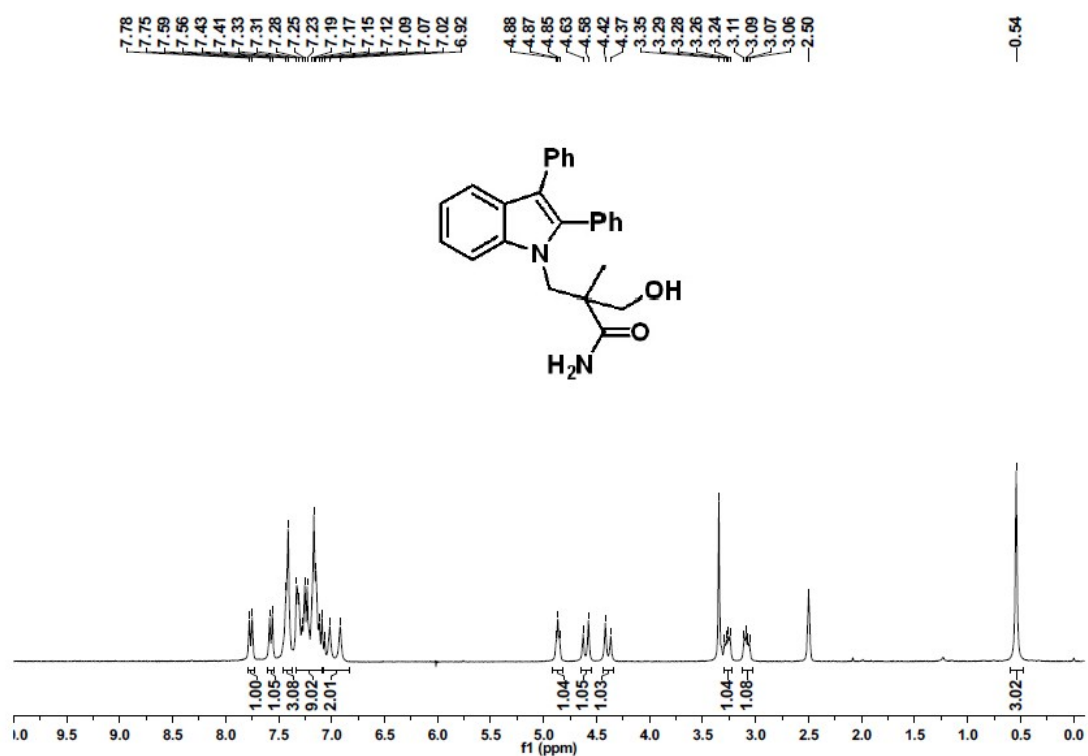
### $^1\text{H}$ and $^{13}\text{C}$ NMR spectra of compound 3b



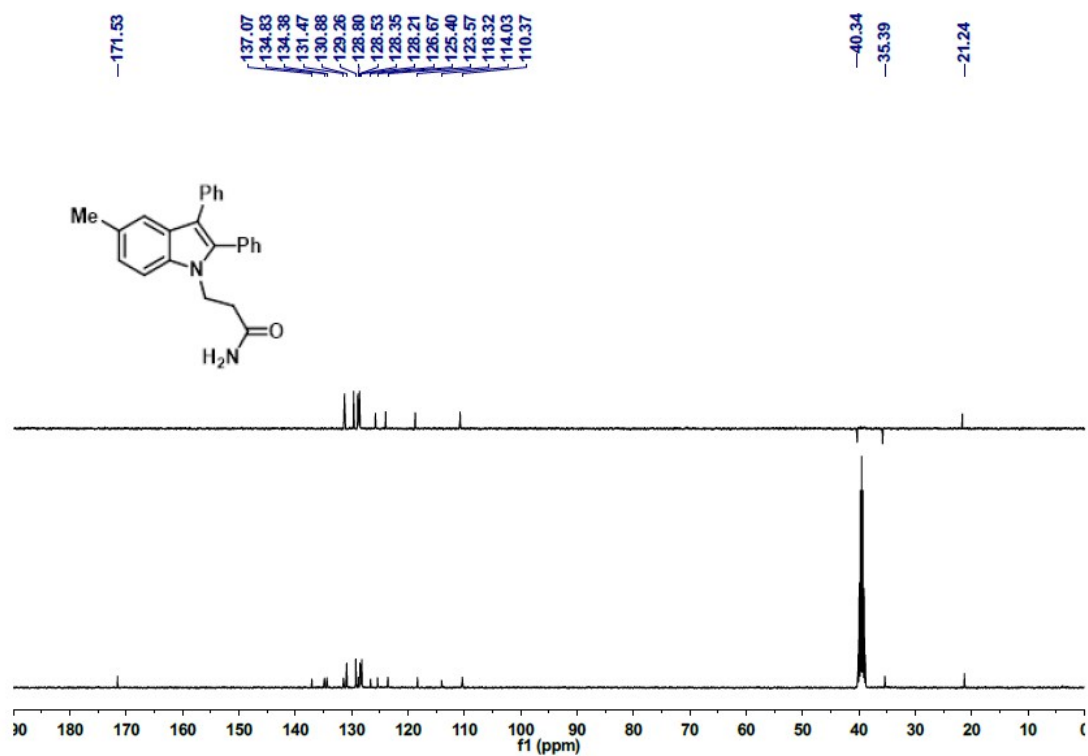
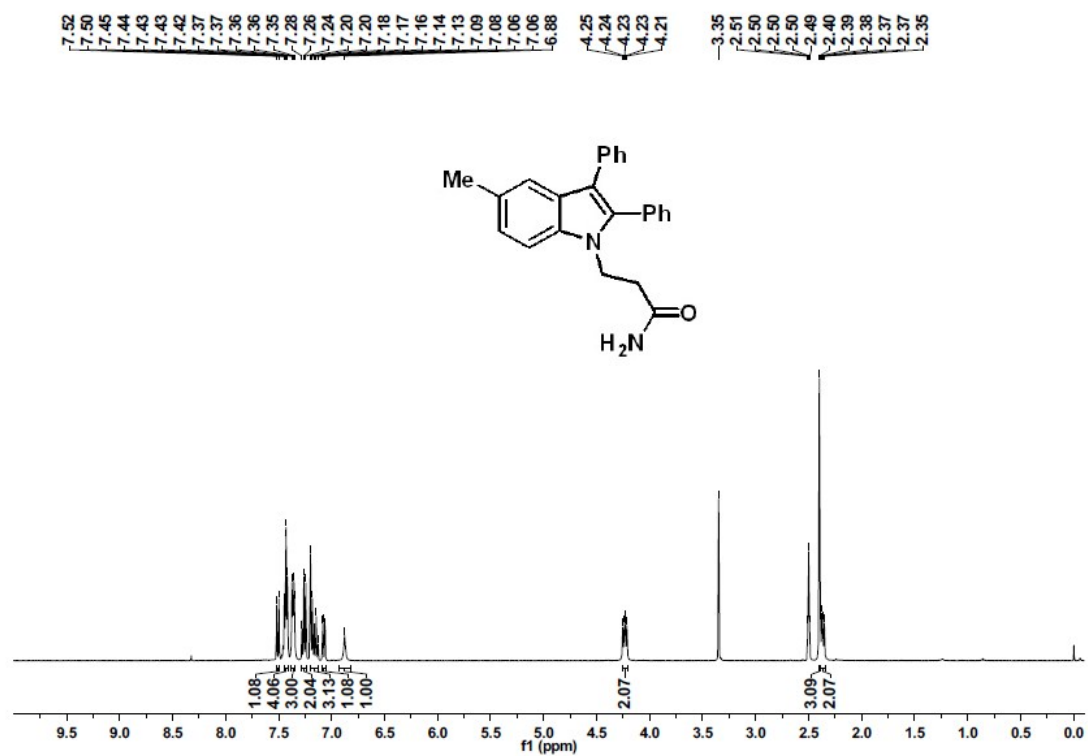
# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 3c



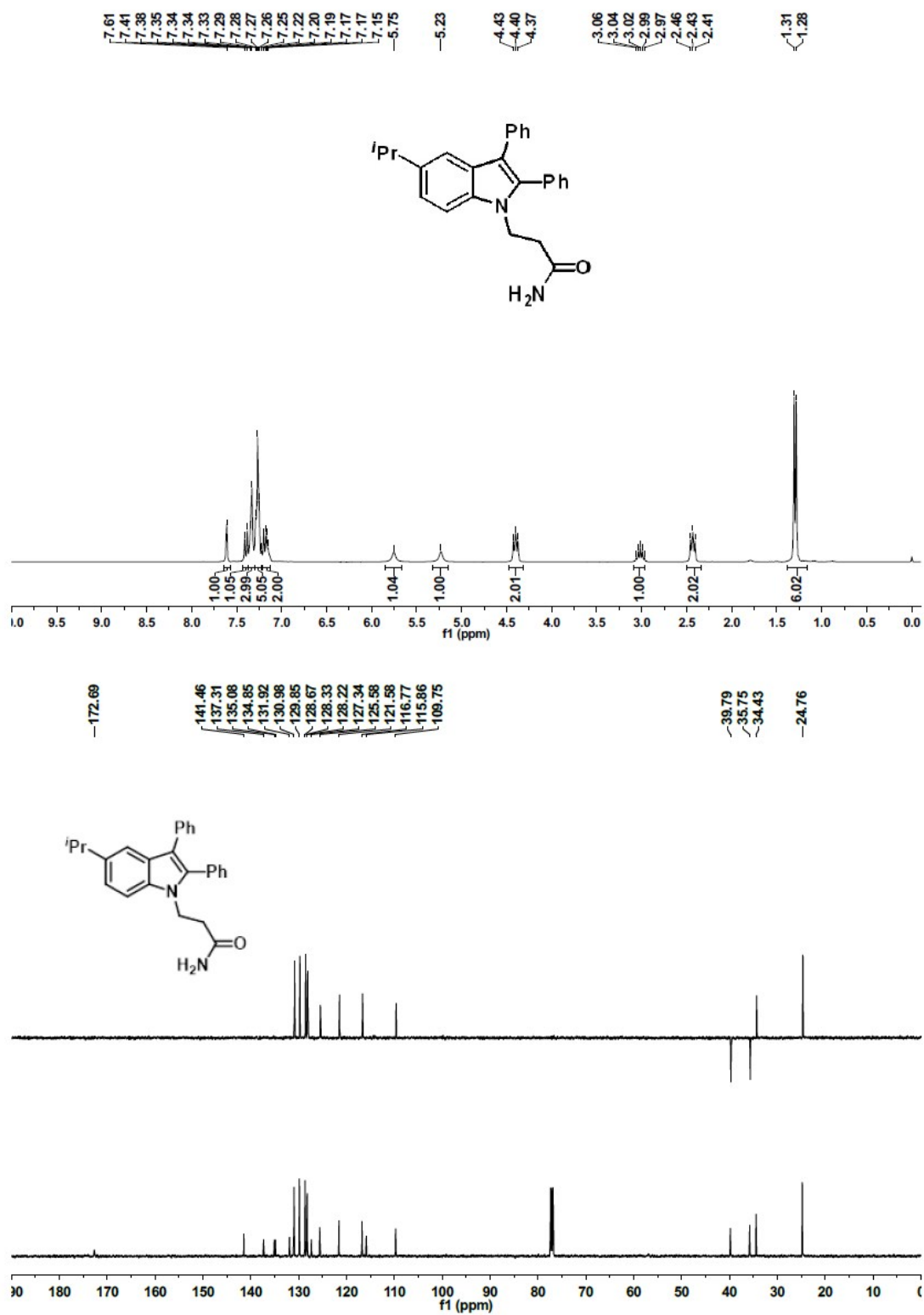
# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 3d



<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 3e

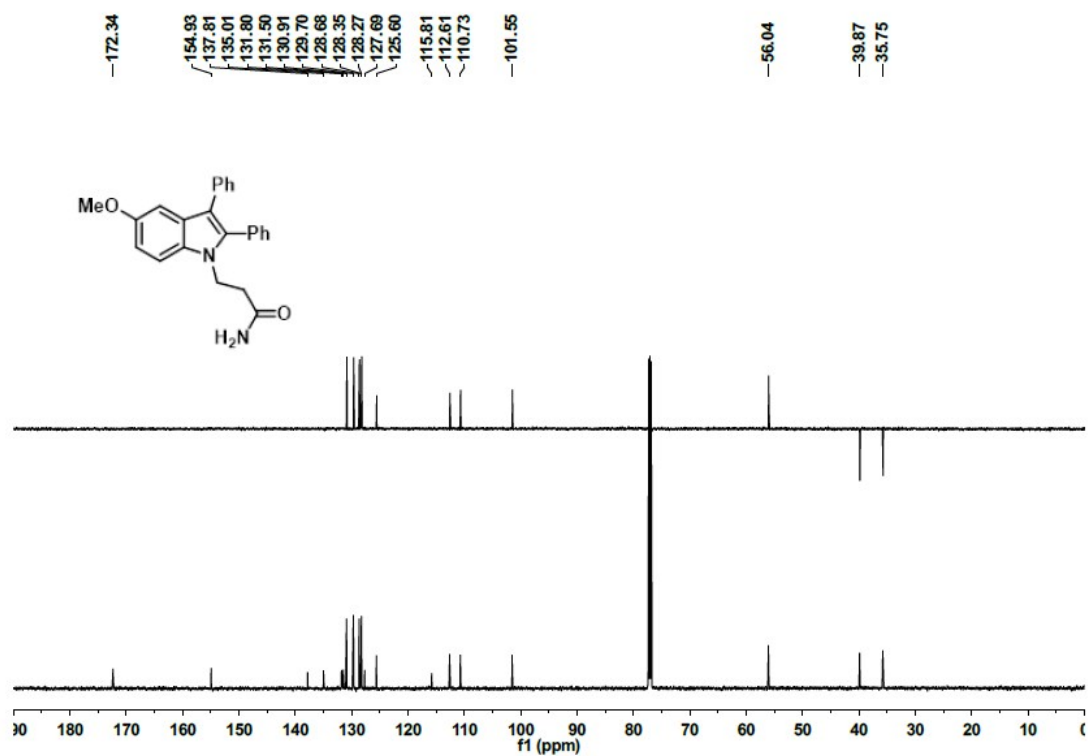
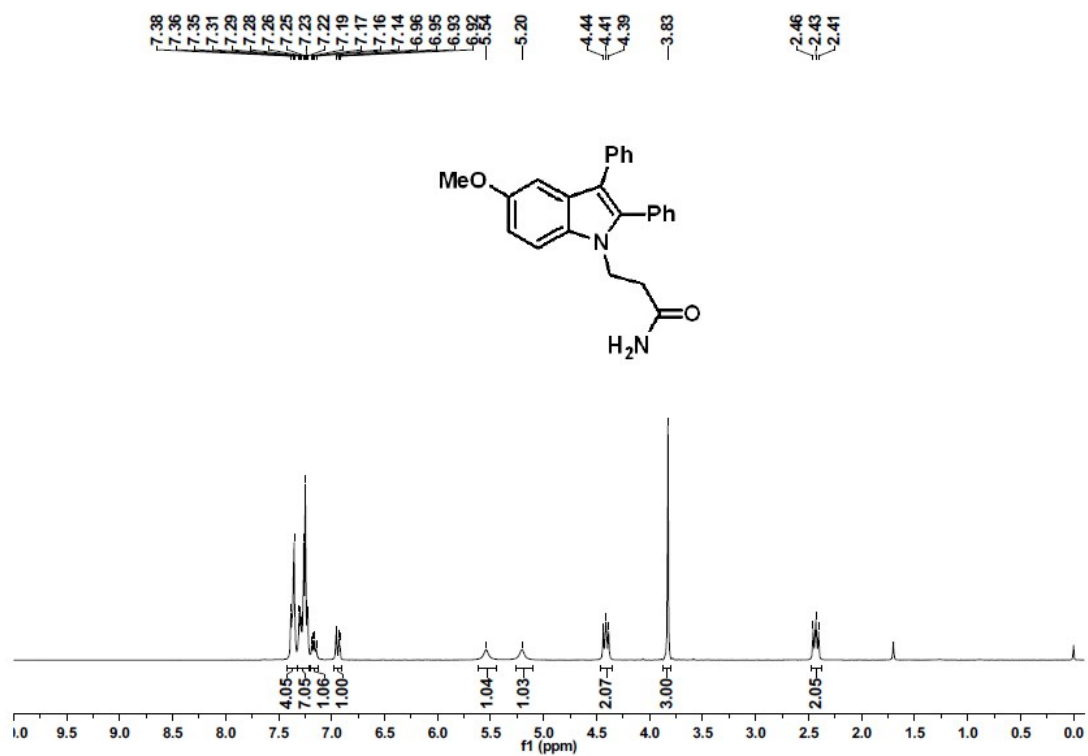


# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 3f

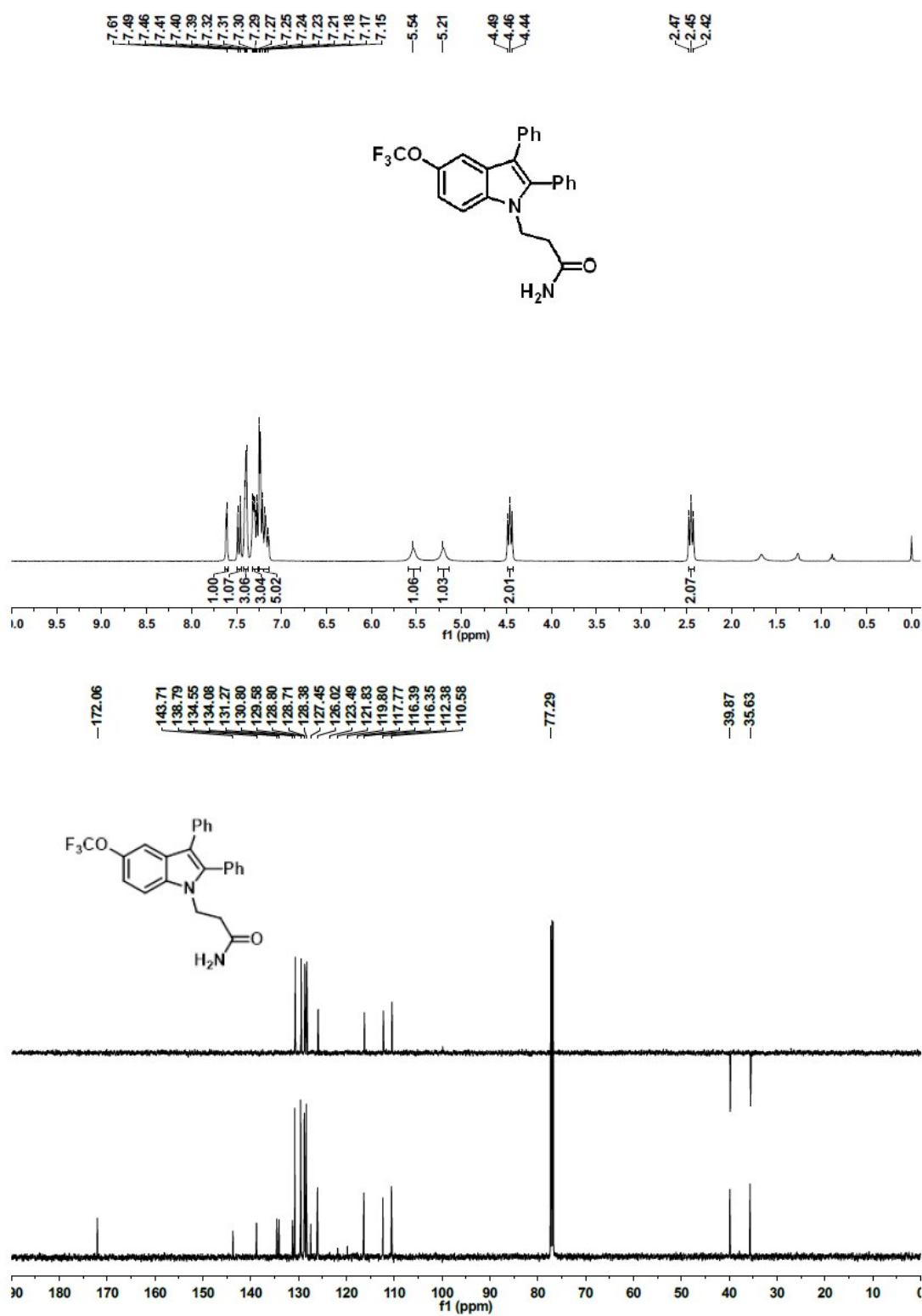




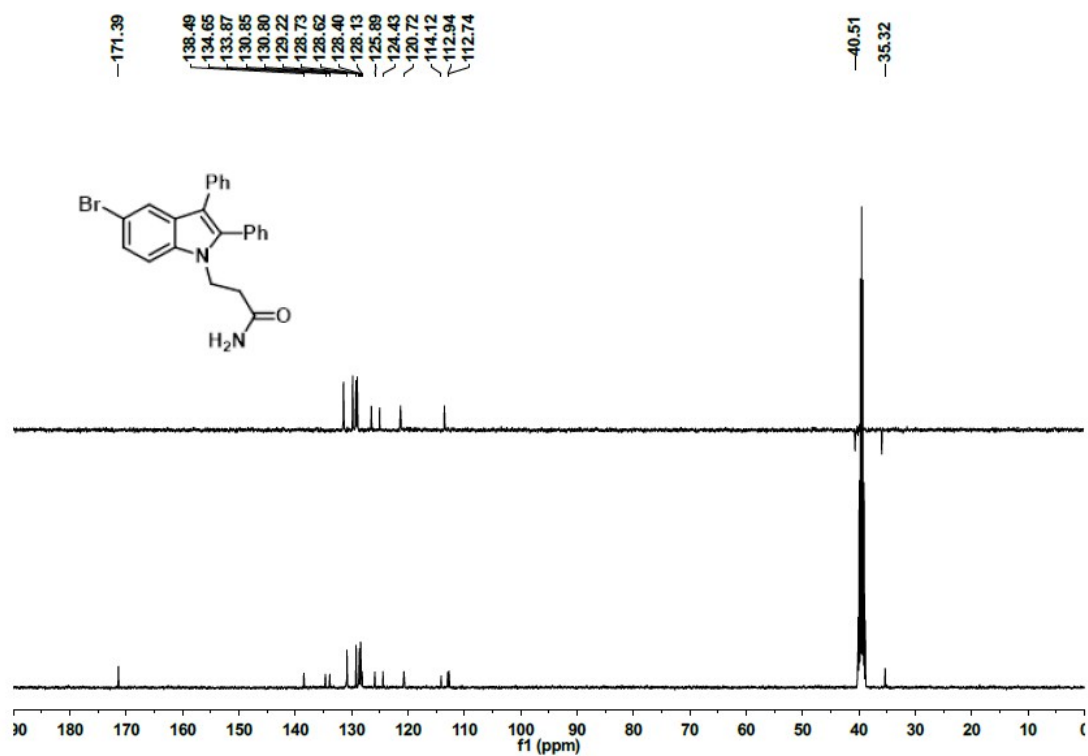
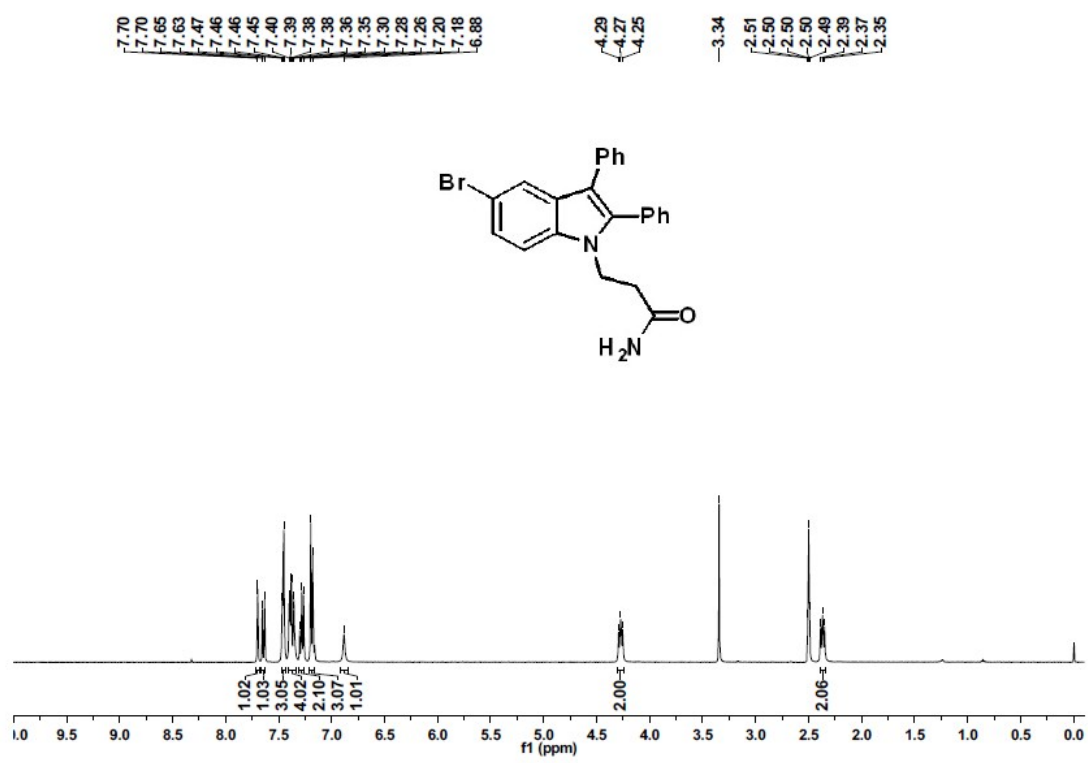
# $^1\text{H}$ and $^{13}\text{C}$ NMR spectra of compound 3g



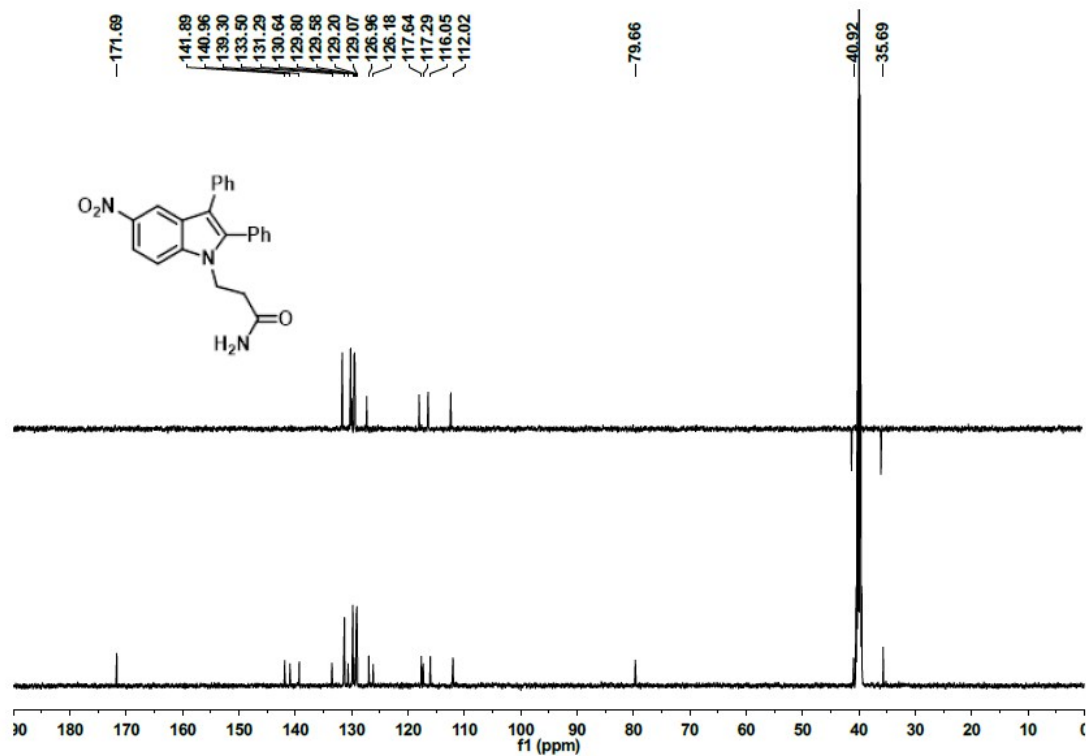
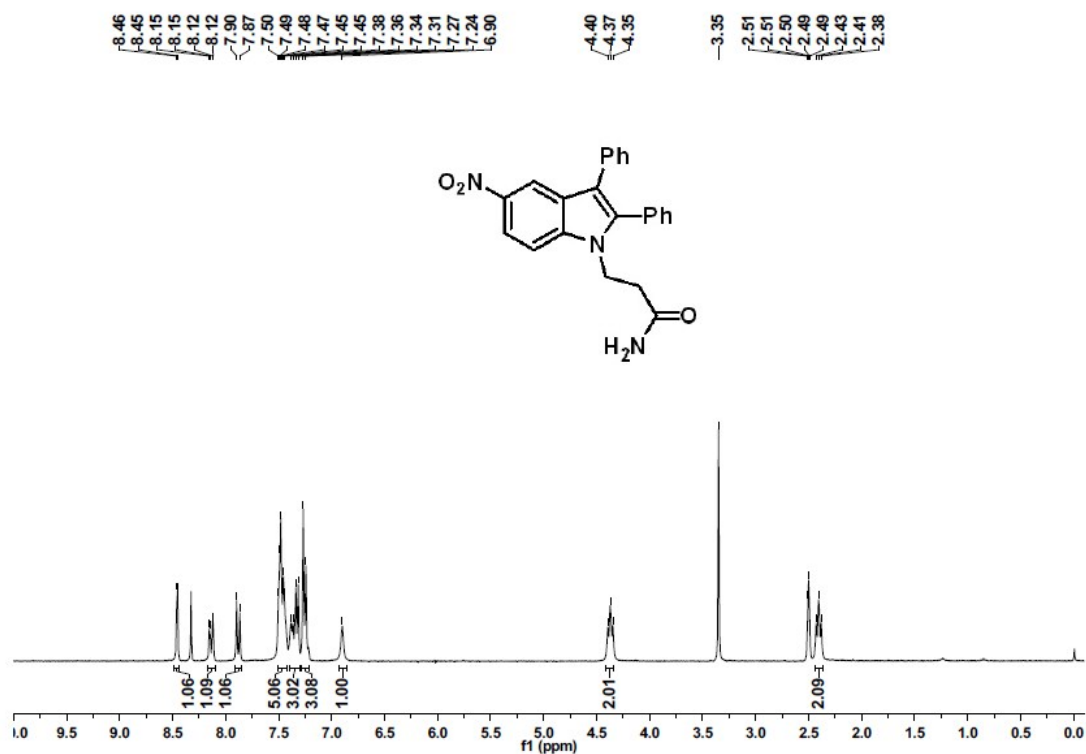
# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 3h



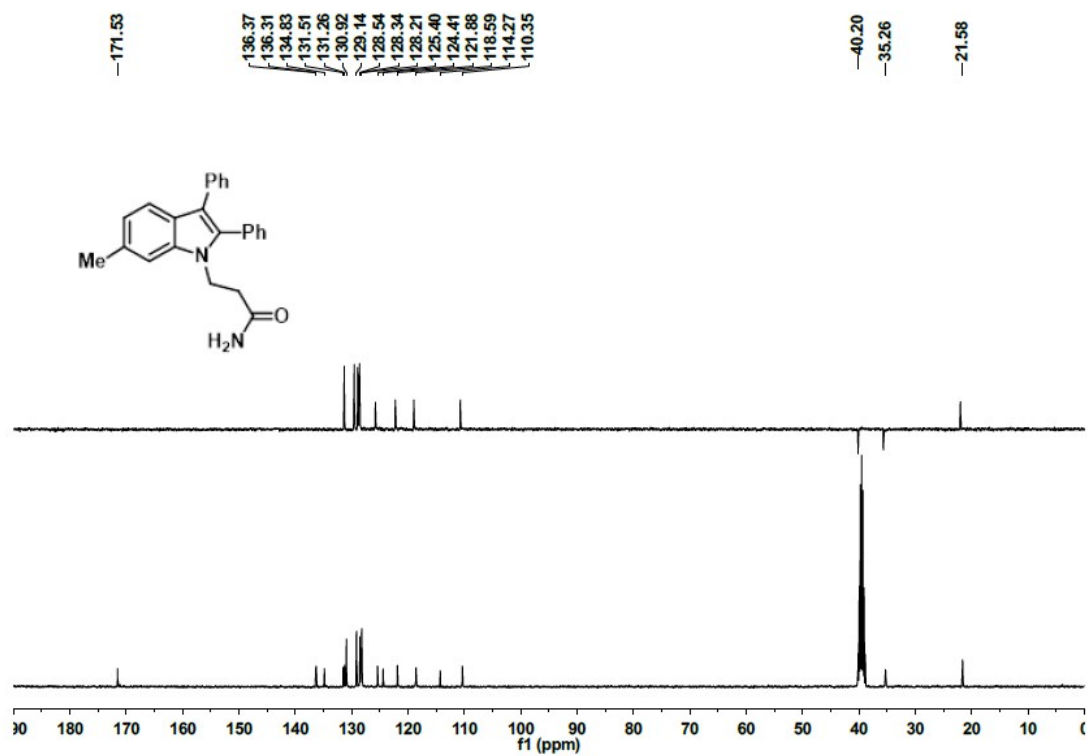
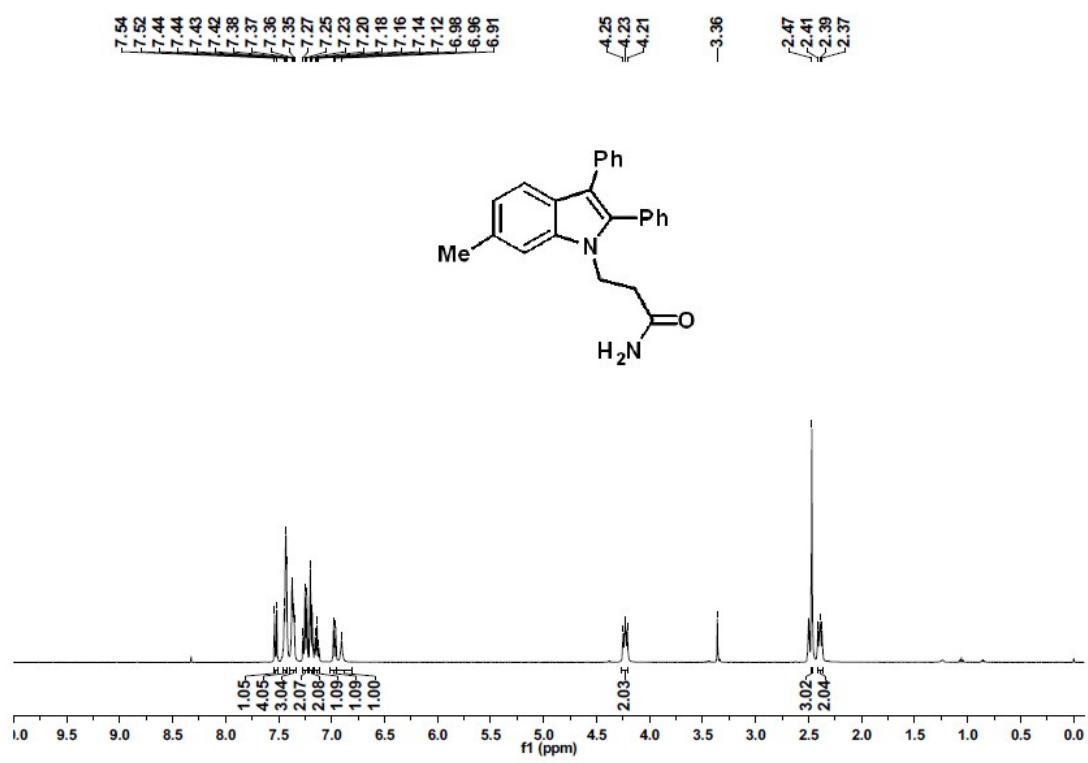
# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 3i



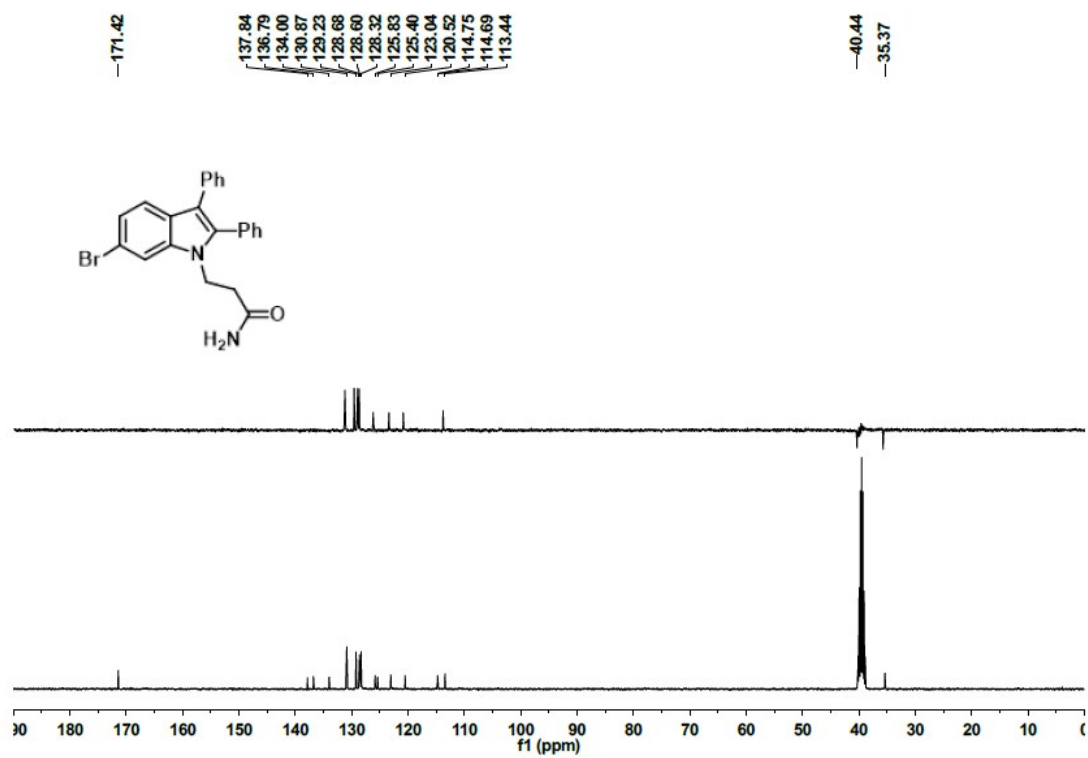
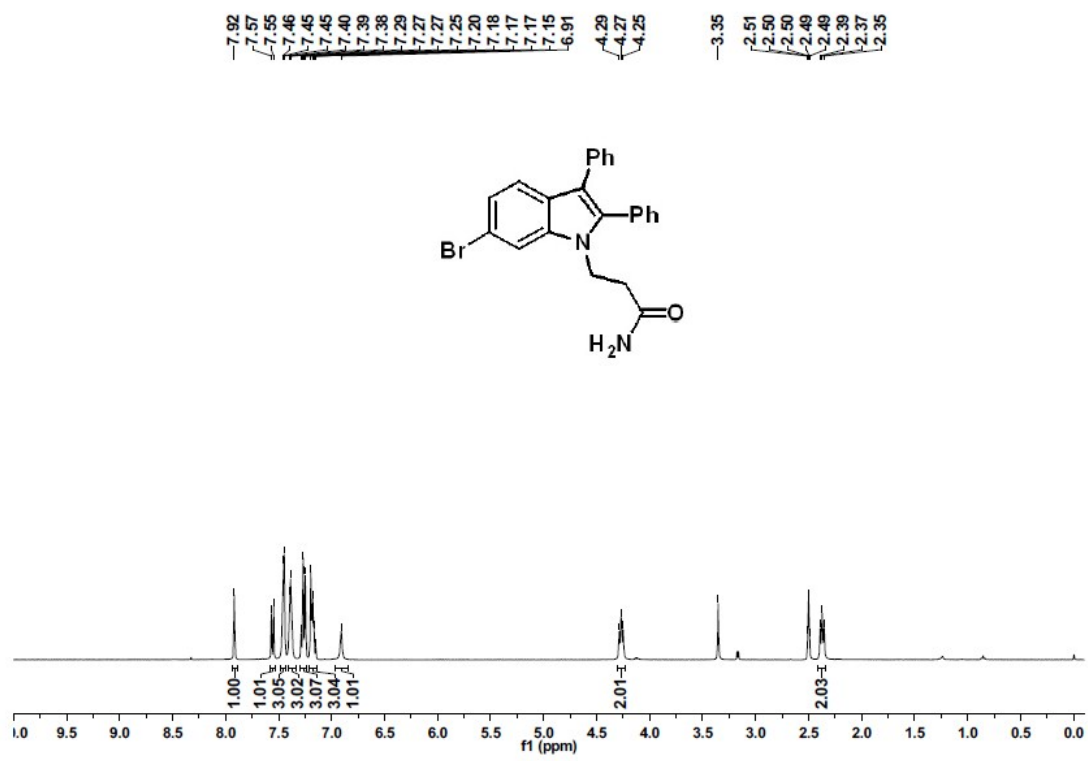
# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 3j



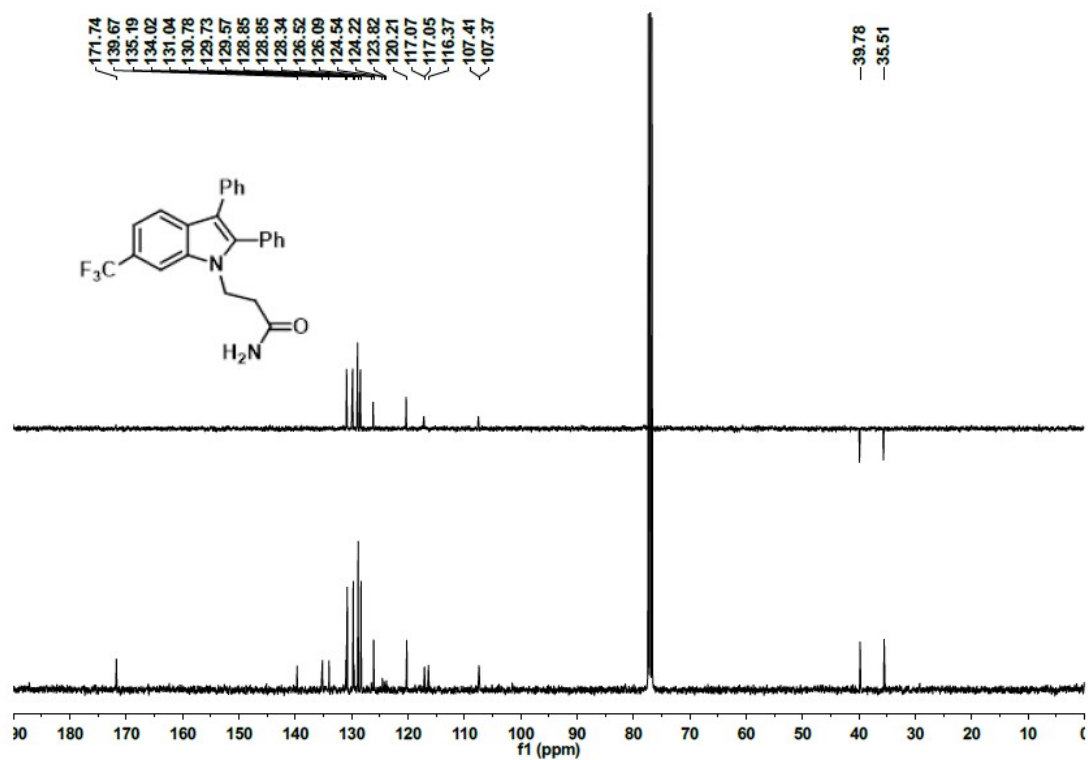
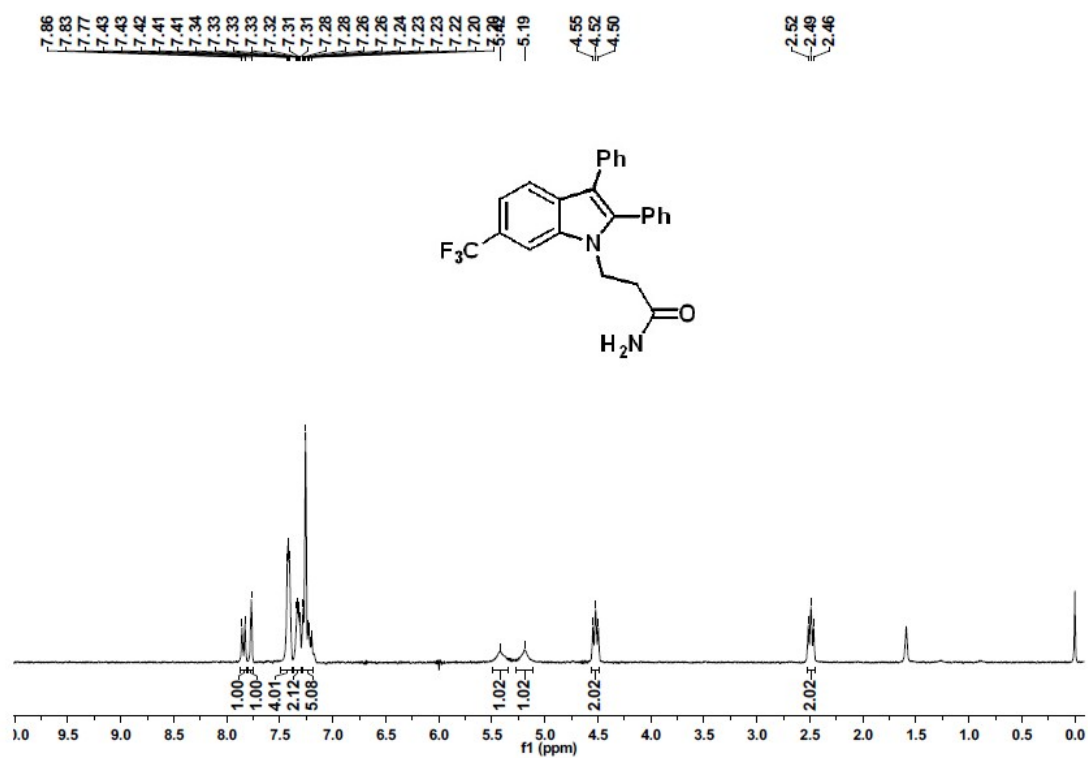
# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 3k



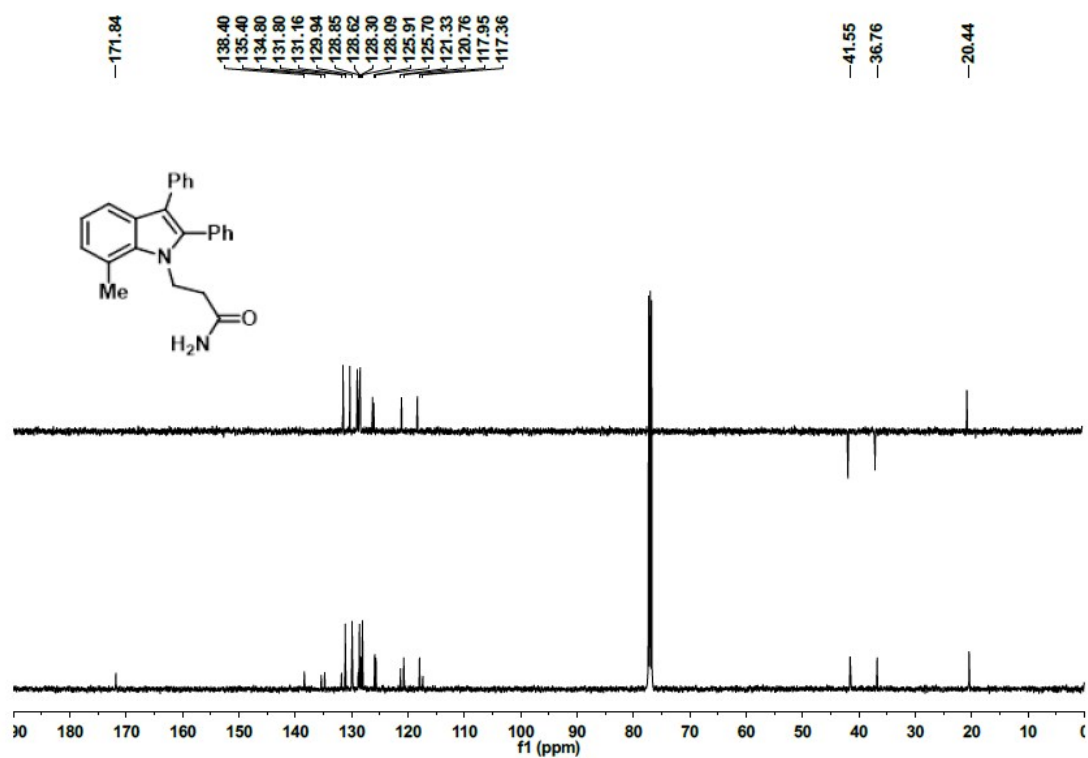
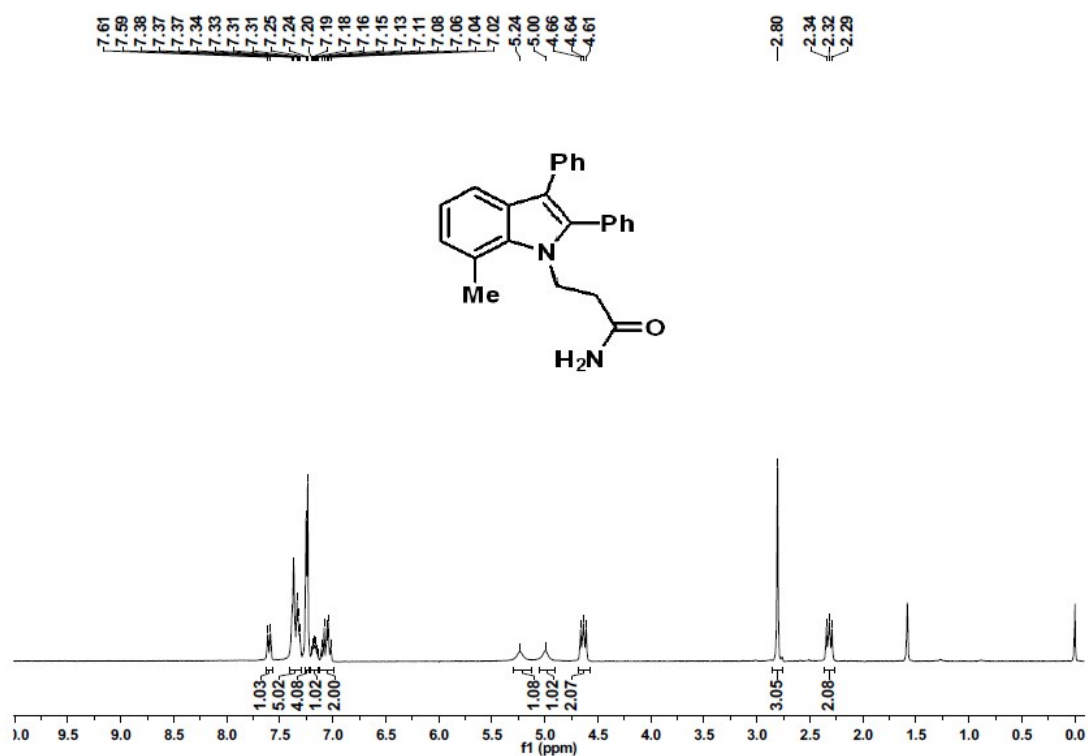
# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 3I



# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 3m

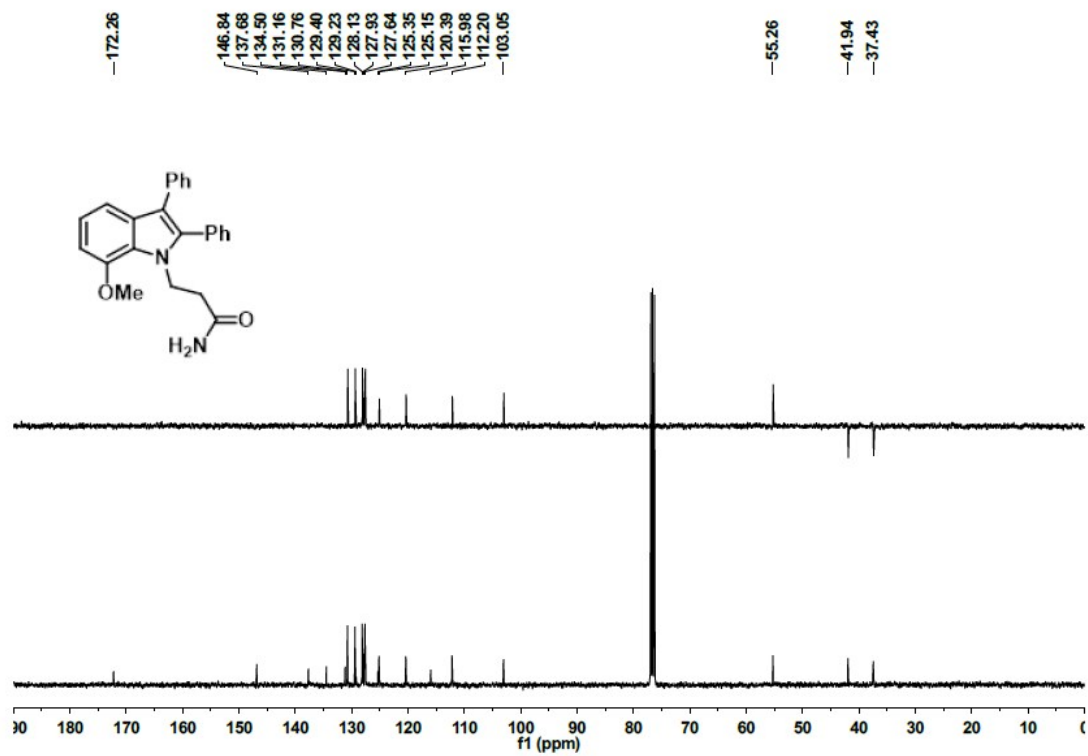
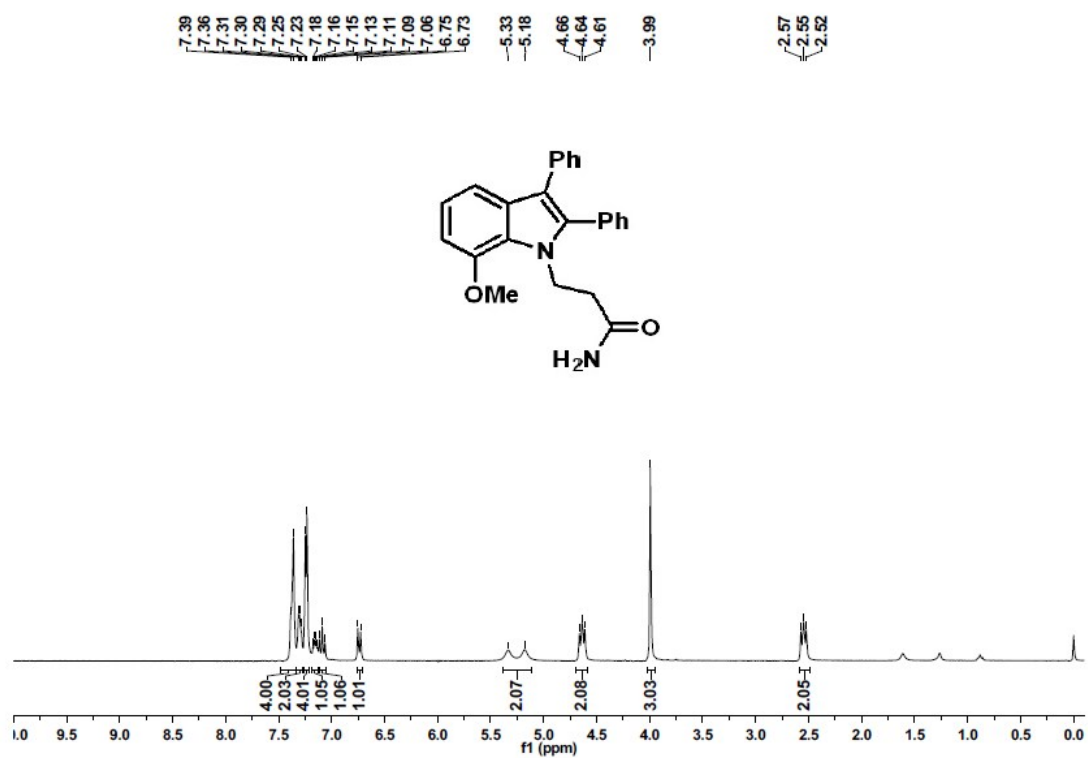


### <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 3n

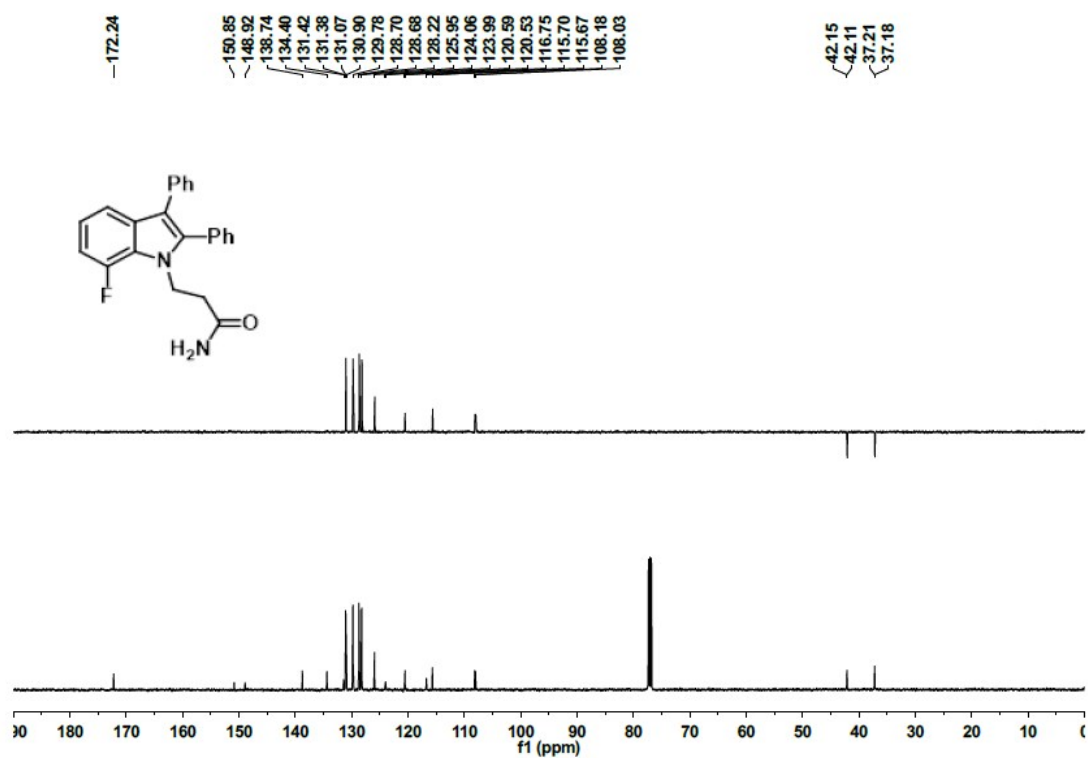
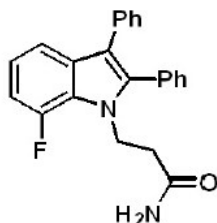
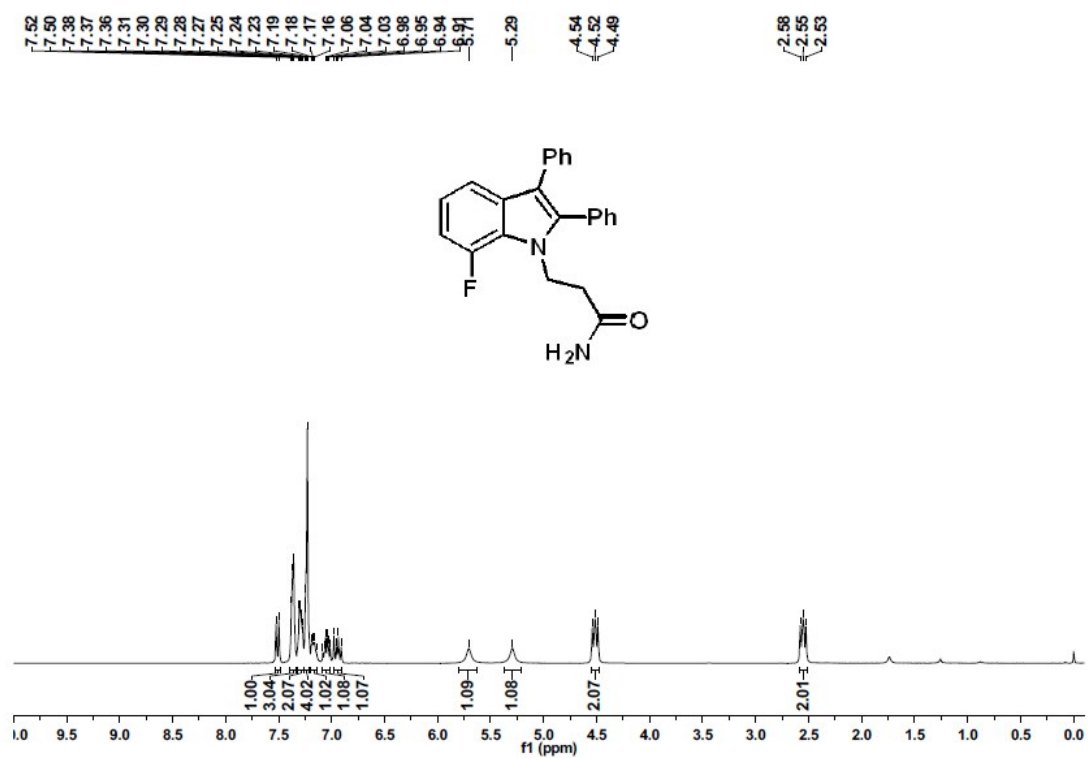




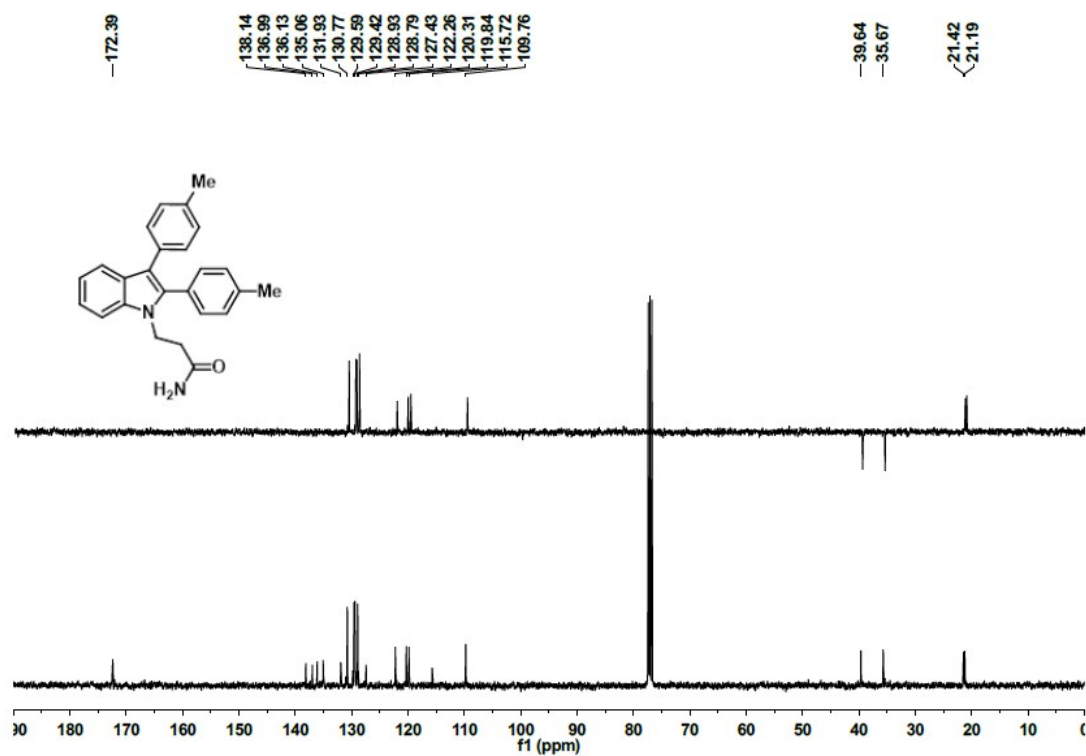
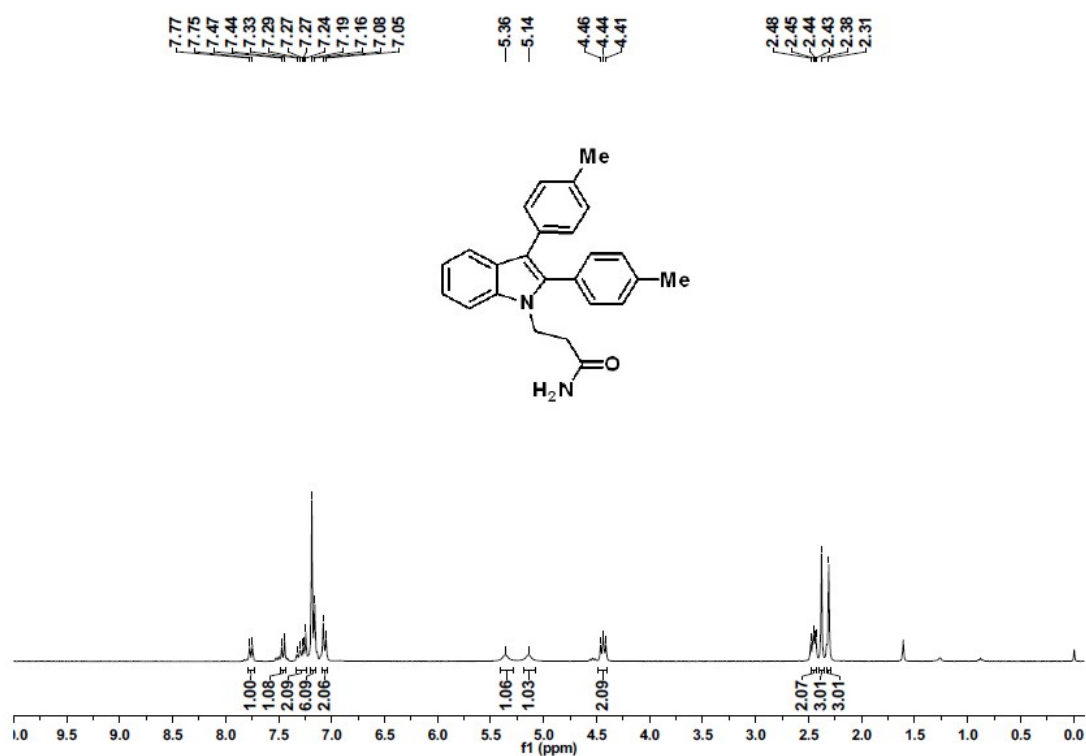
# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 3o



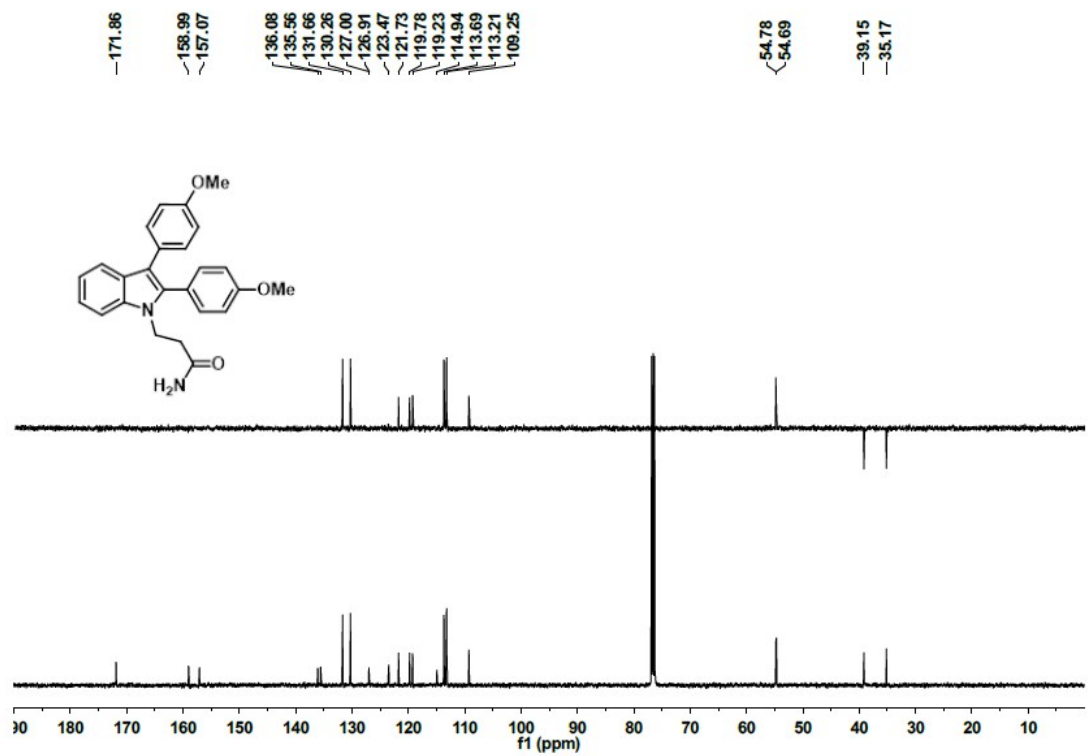
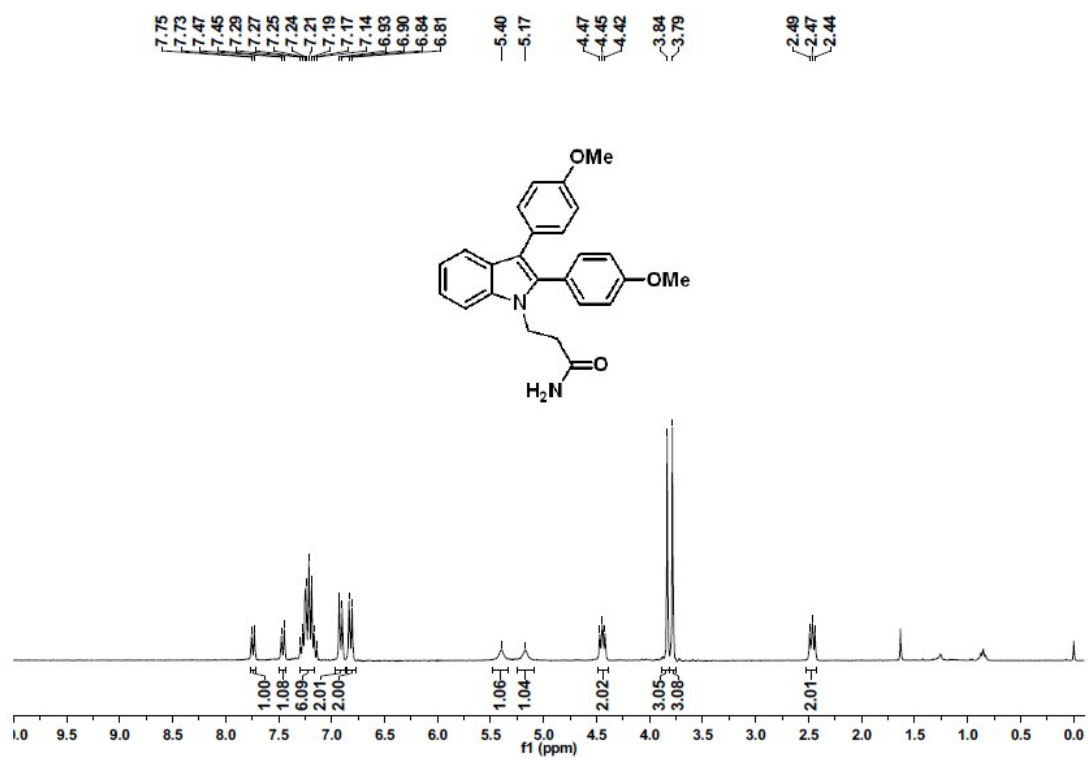
**$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of compound 3p**



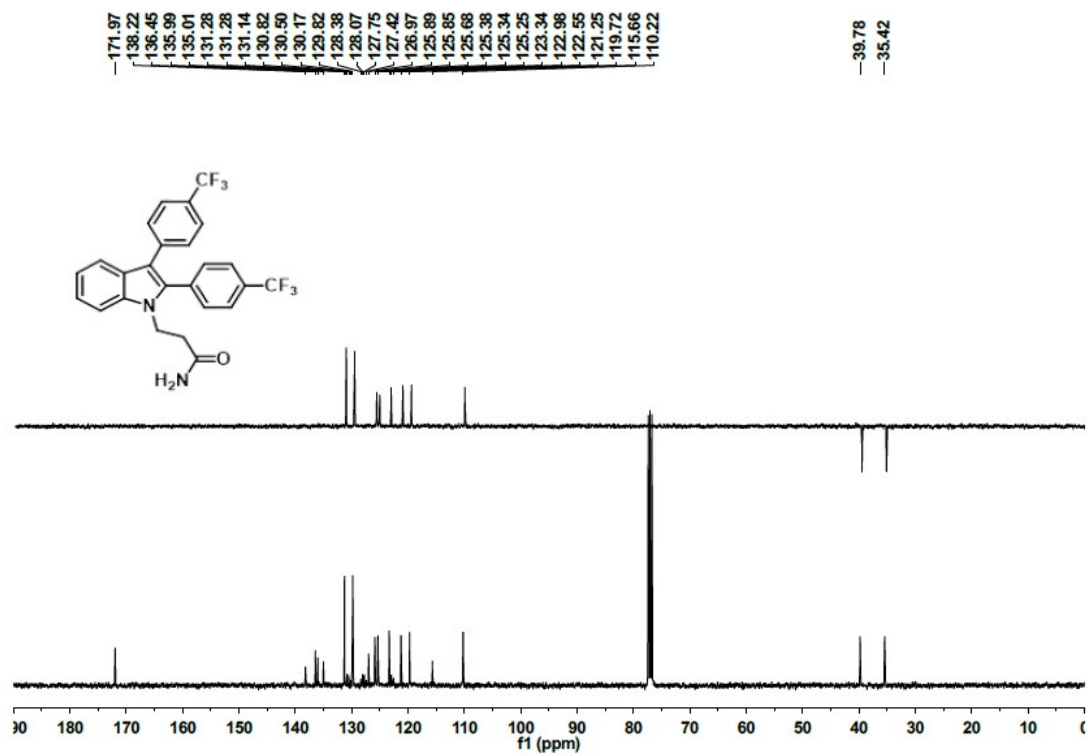
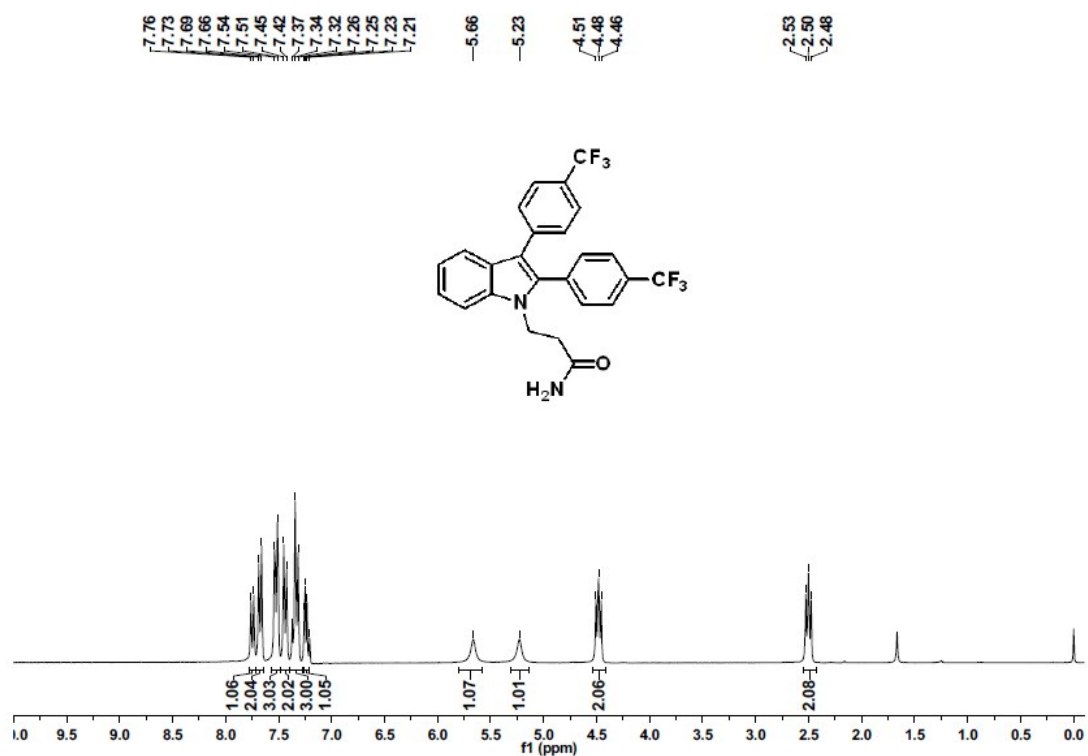
# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 3q



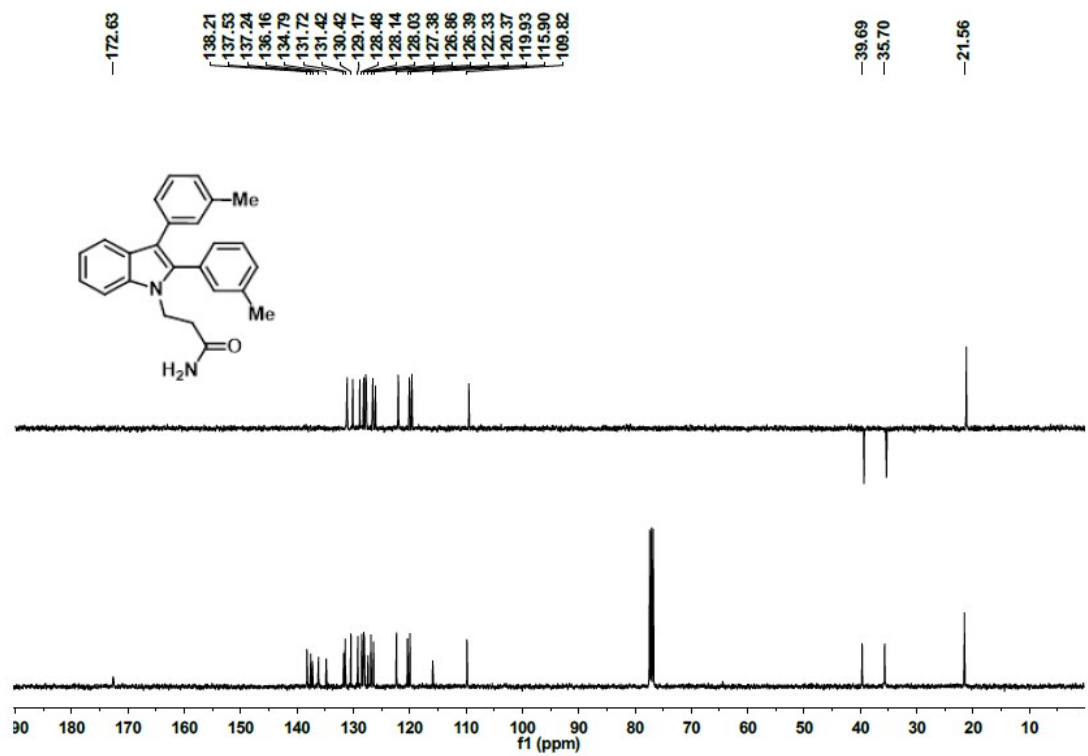
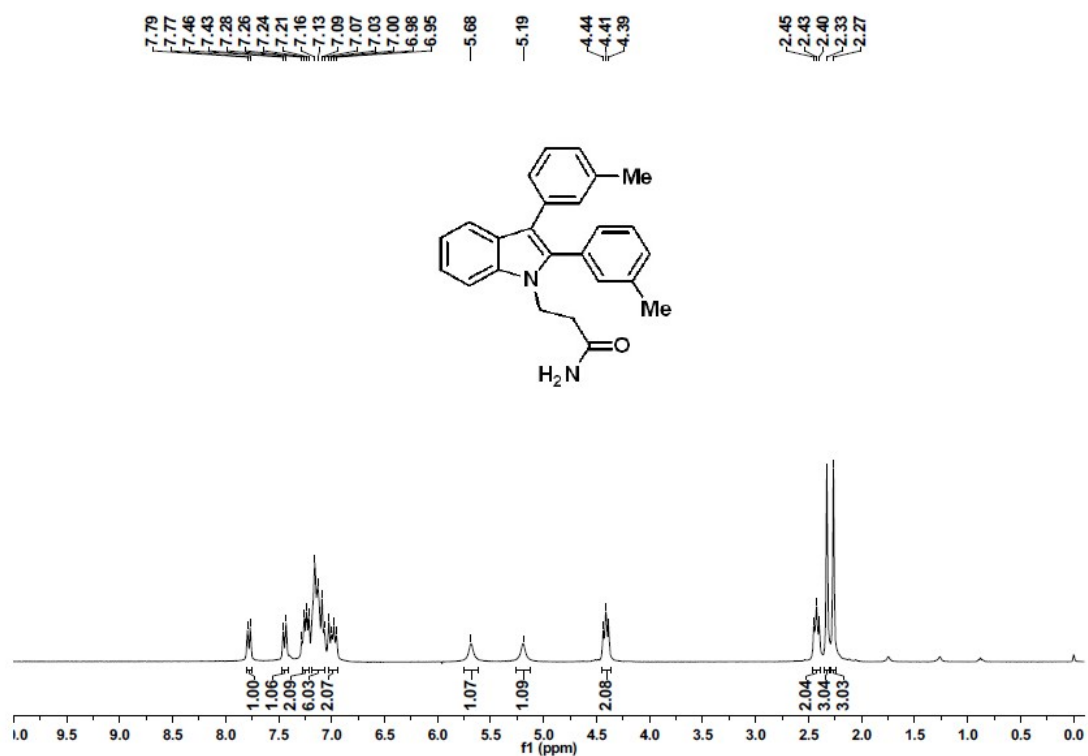
### <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 3r



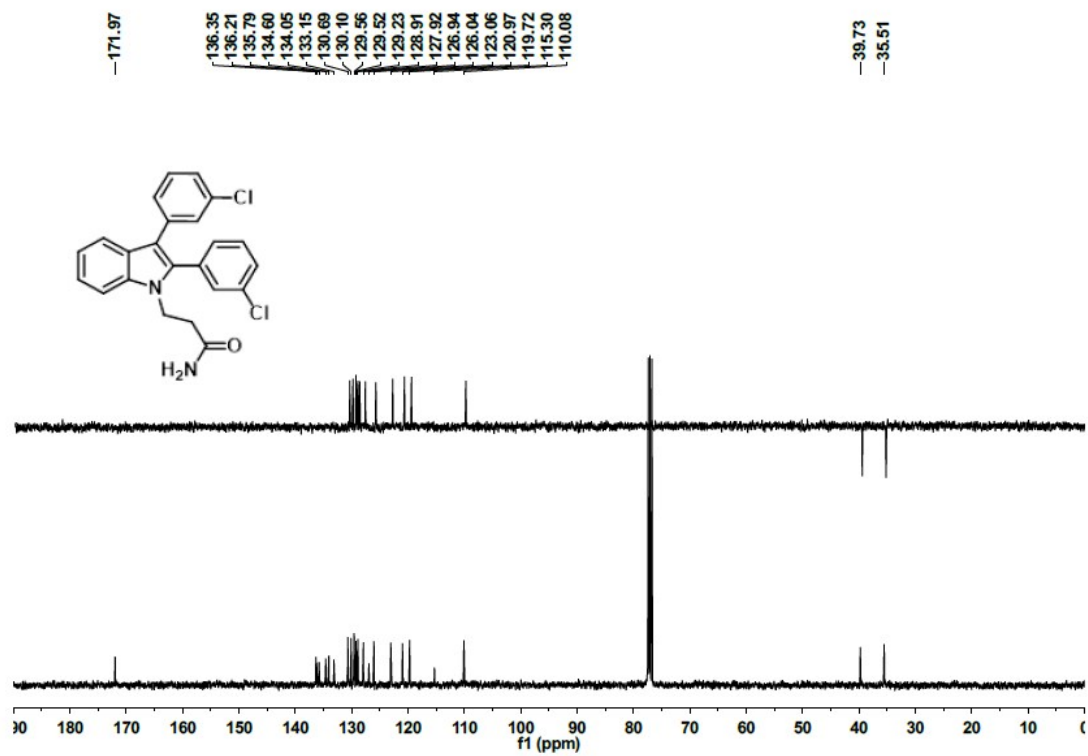
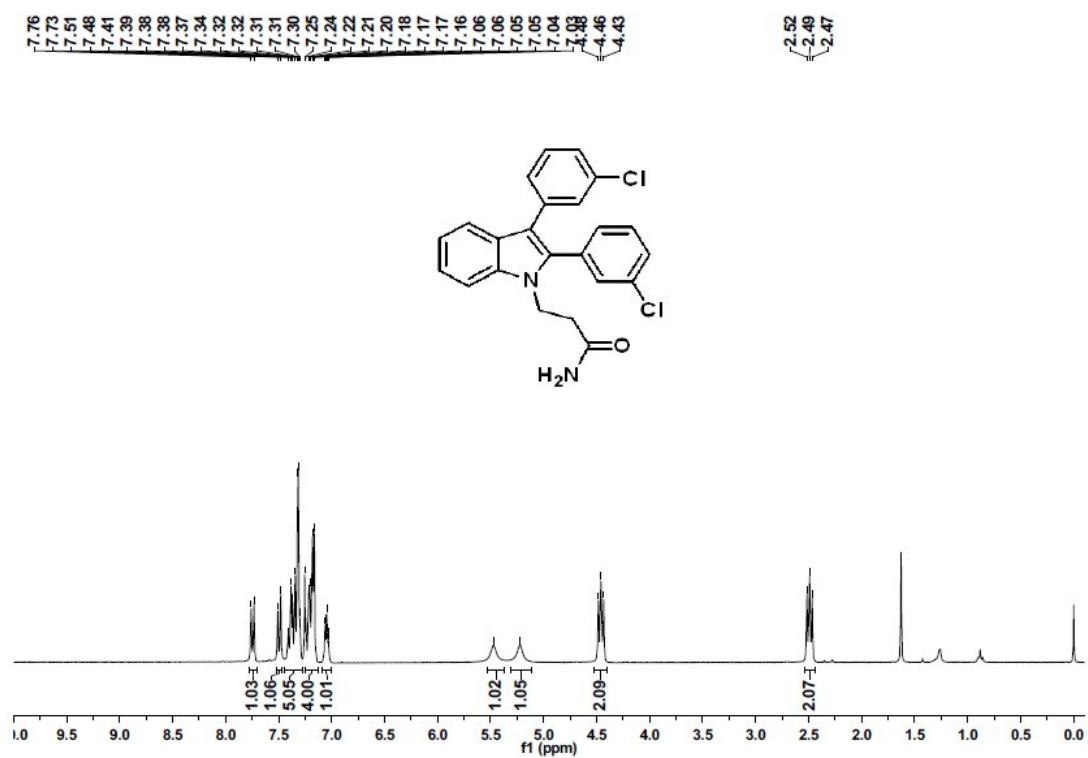
# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 3s



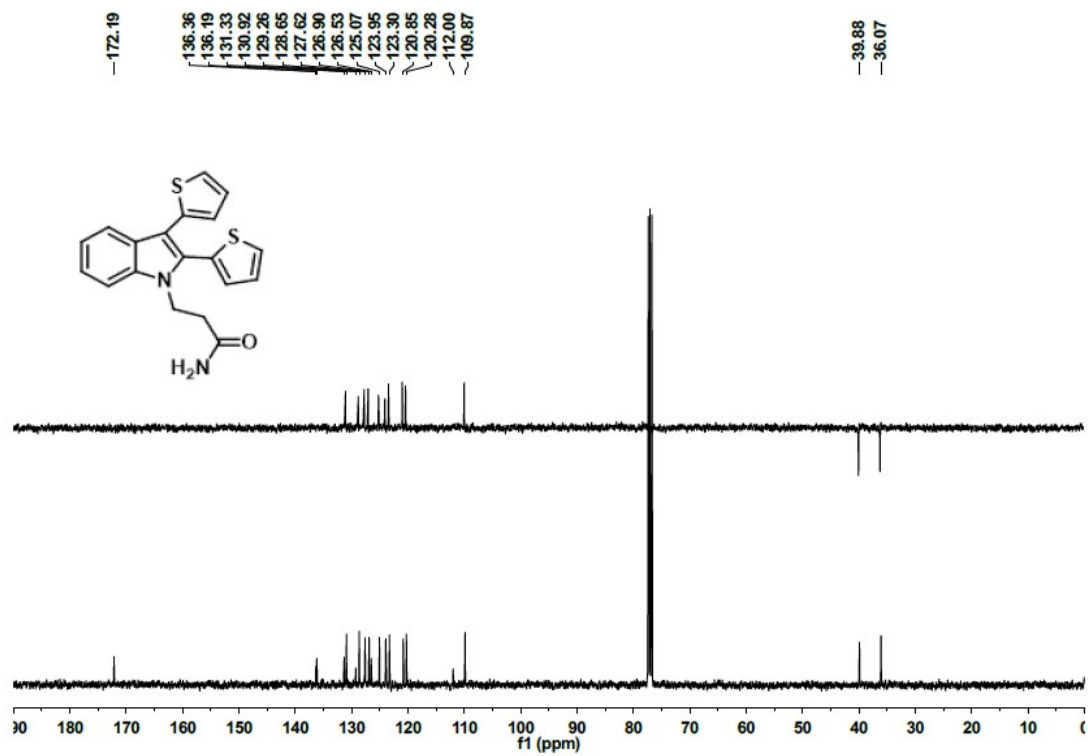
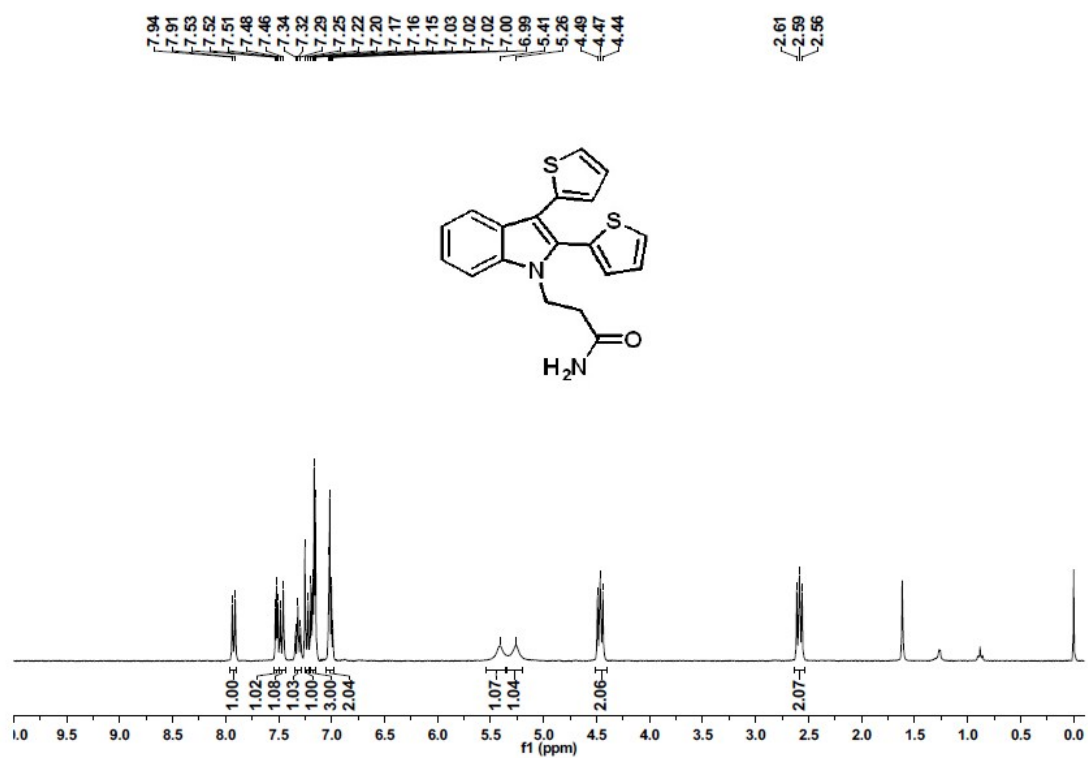
# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 3t



**<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 3u**

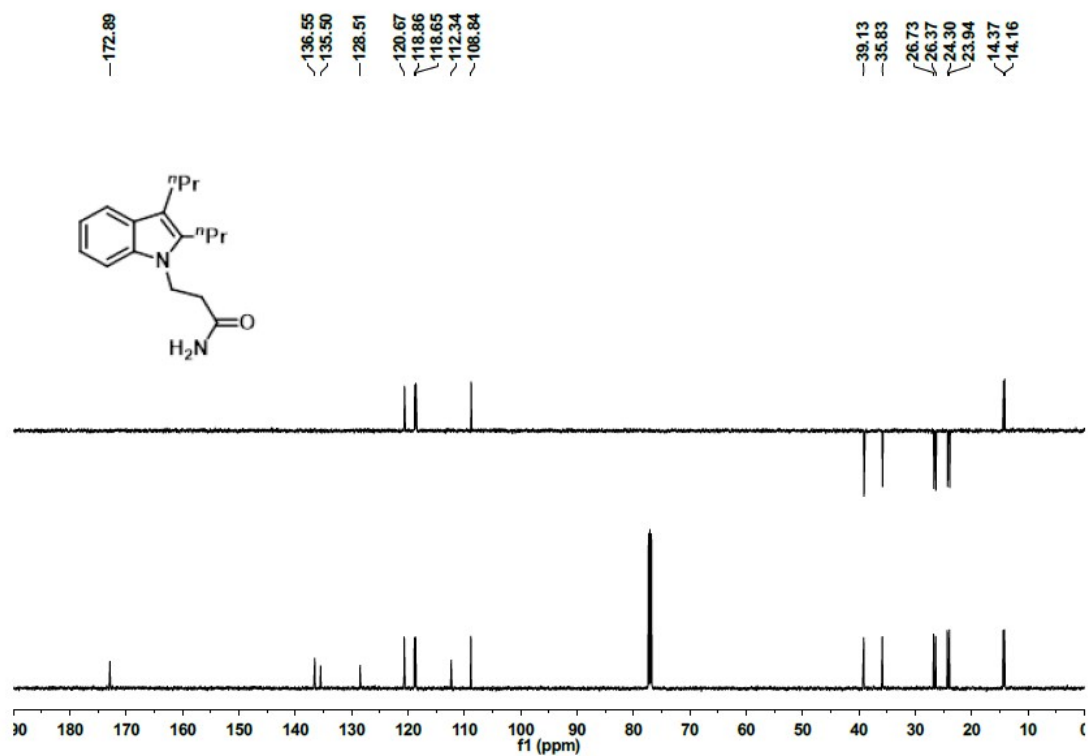
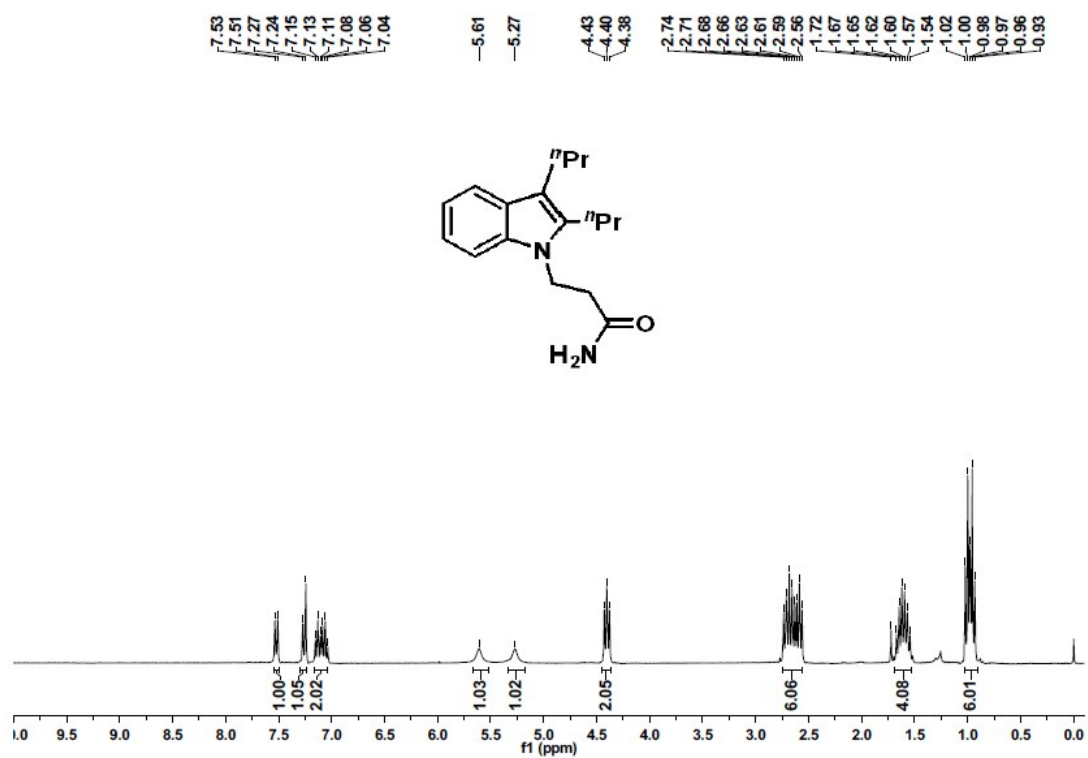


# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 3v

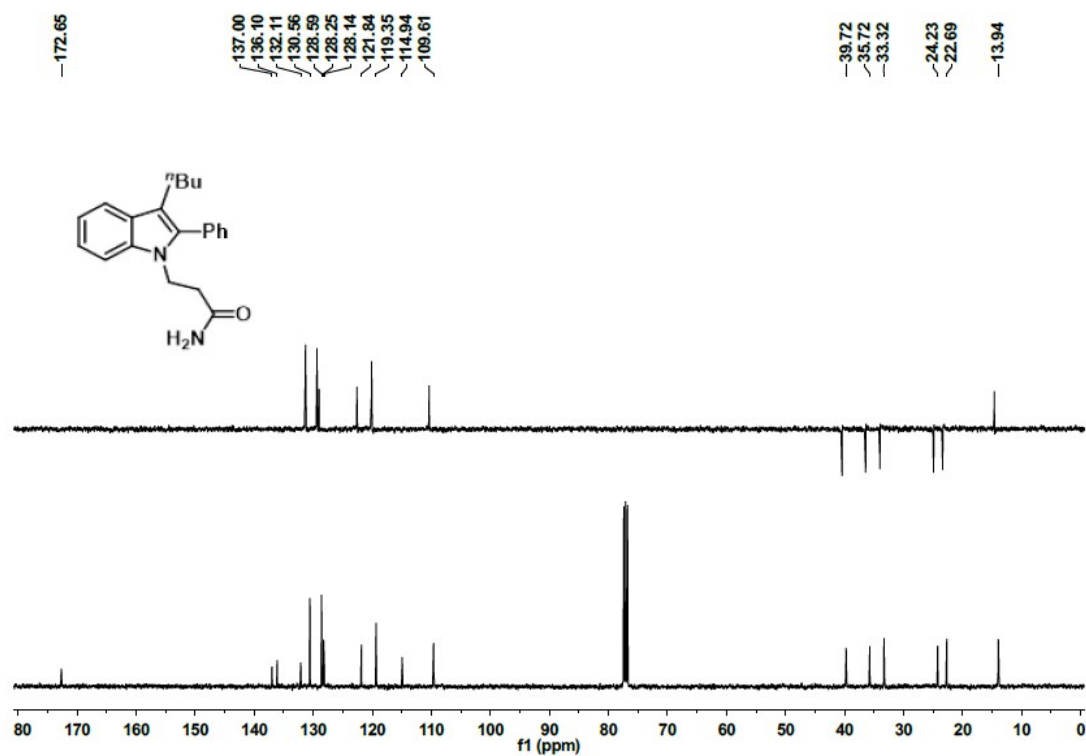
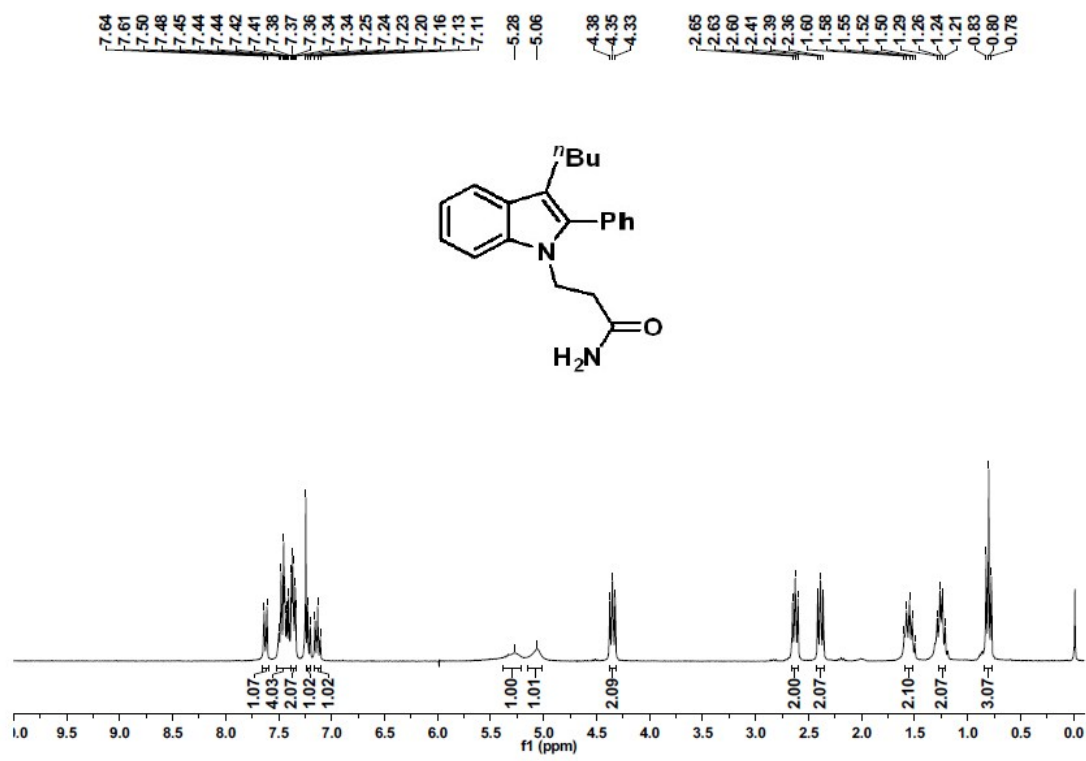




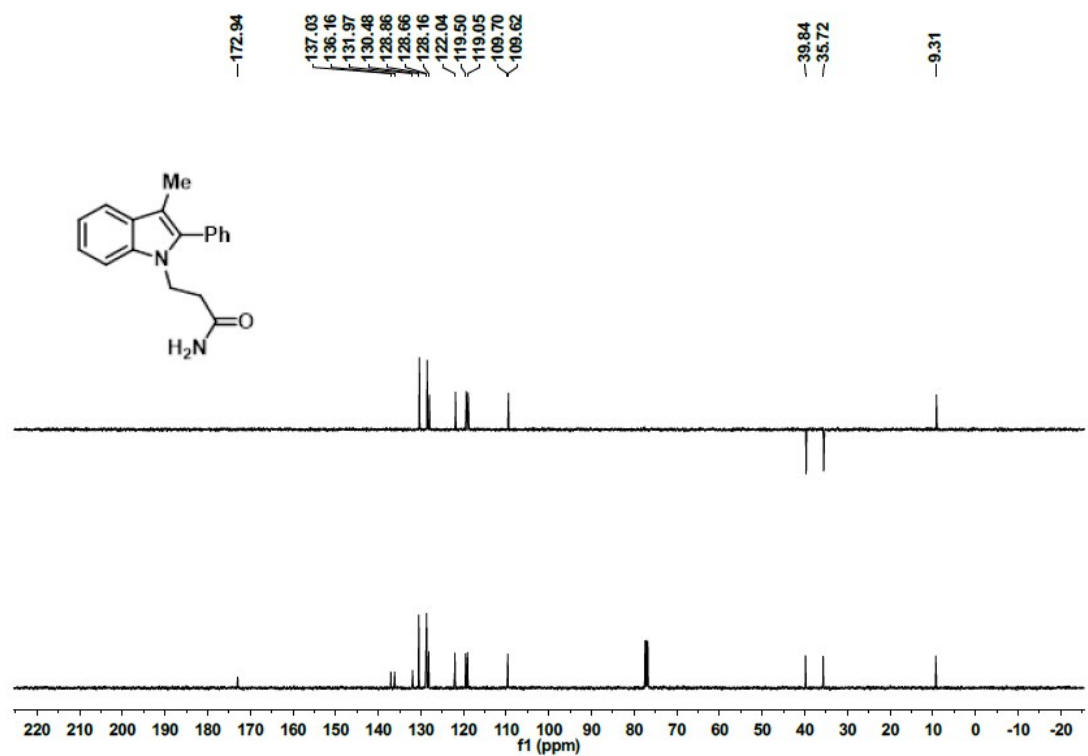
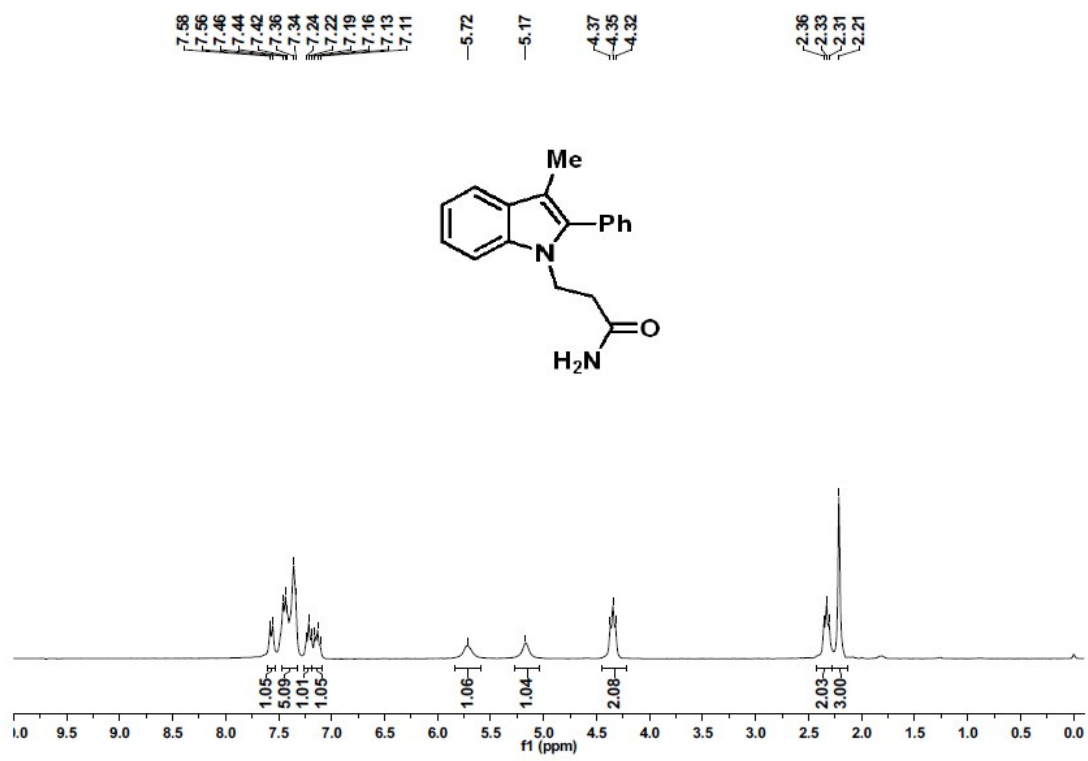
**<sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 3w**



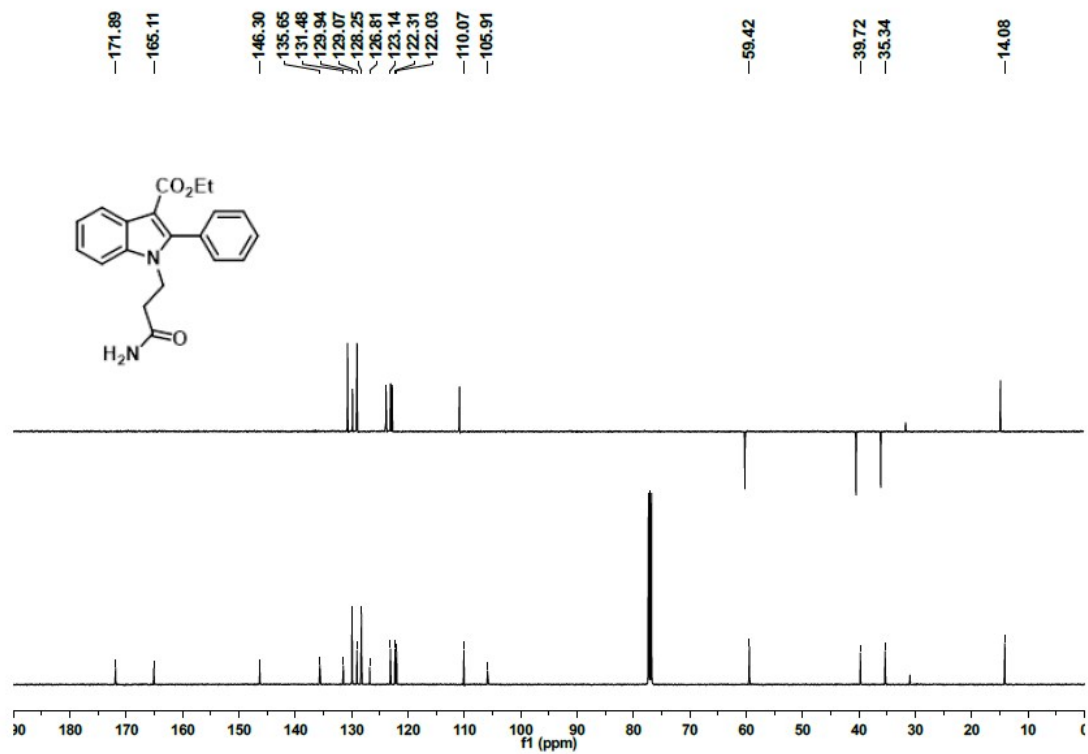
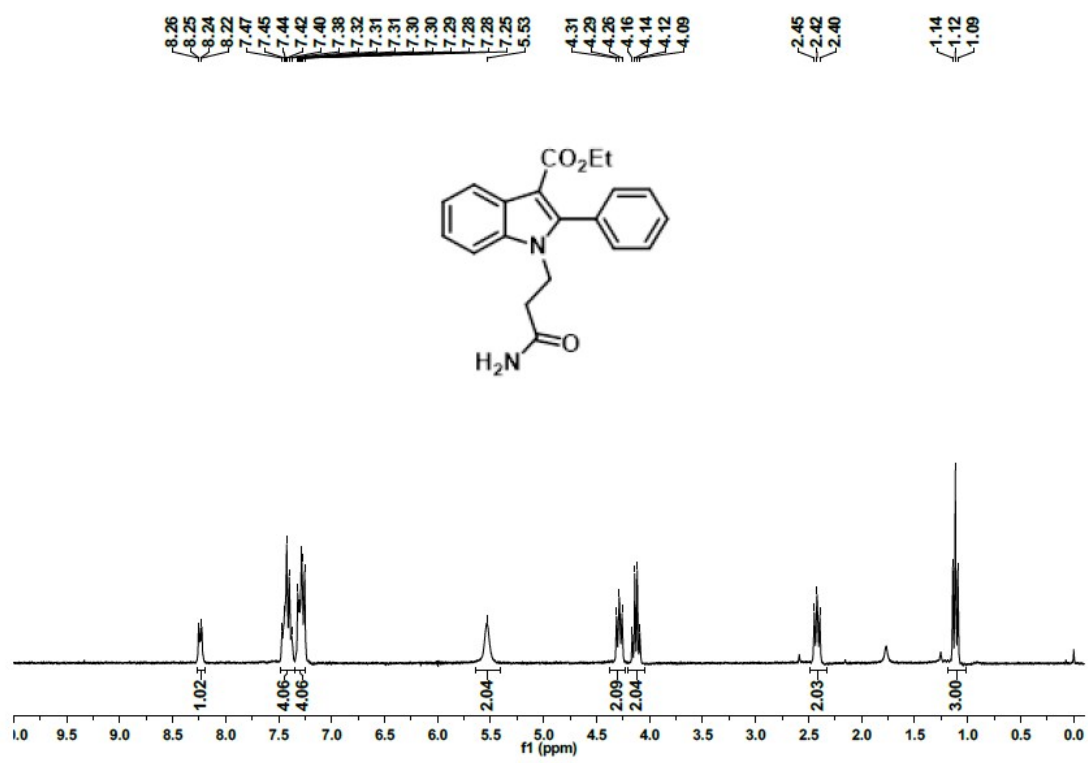
# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 3x



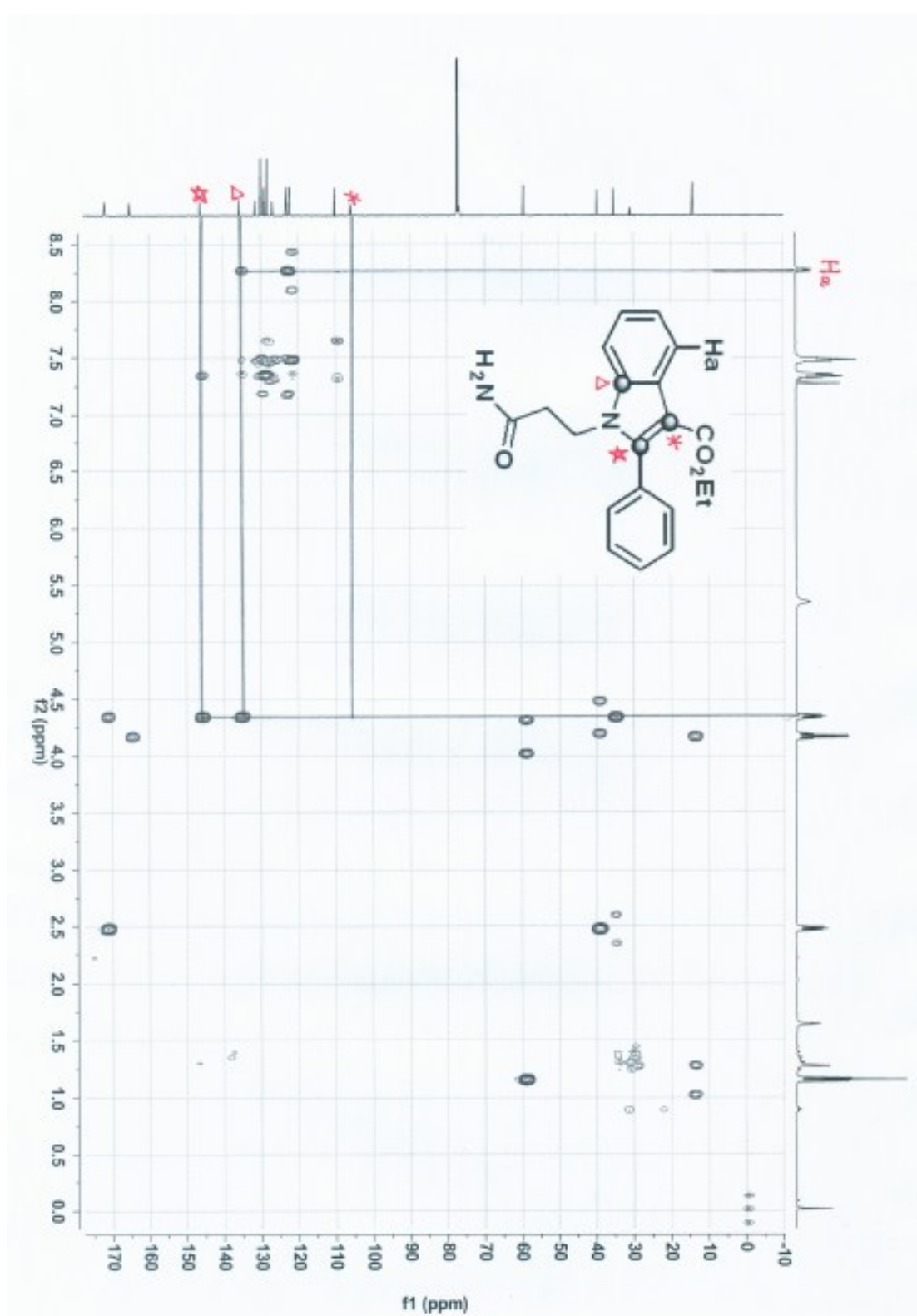
### <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 3y



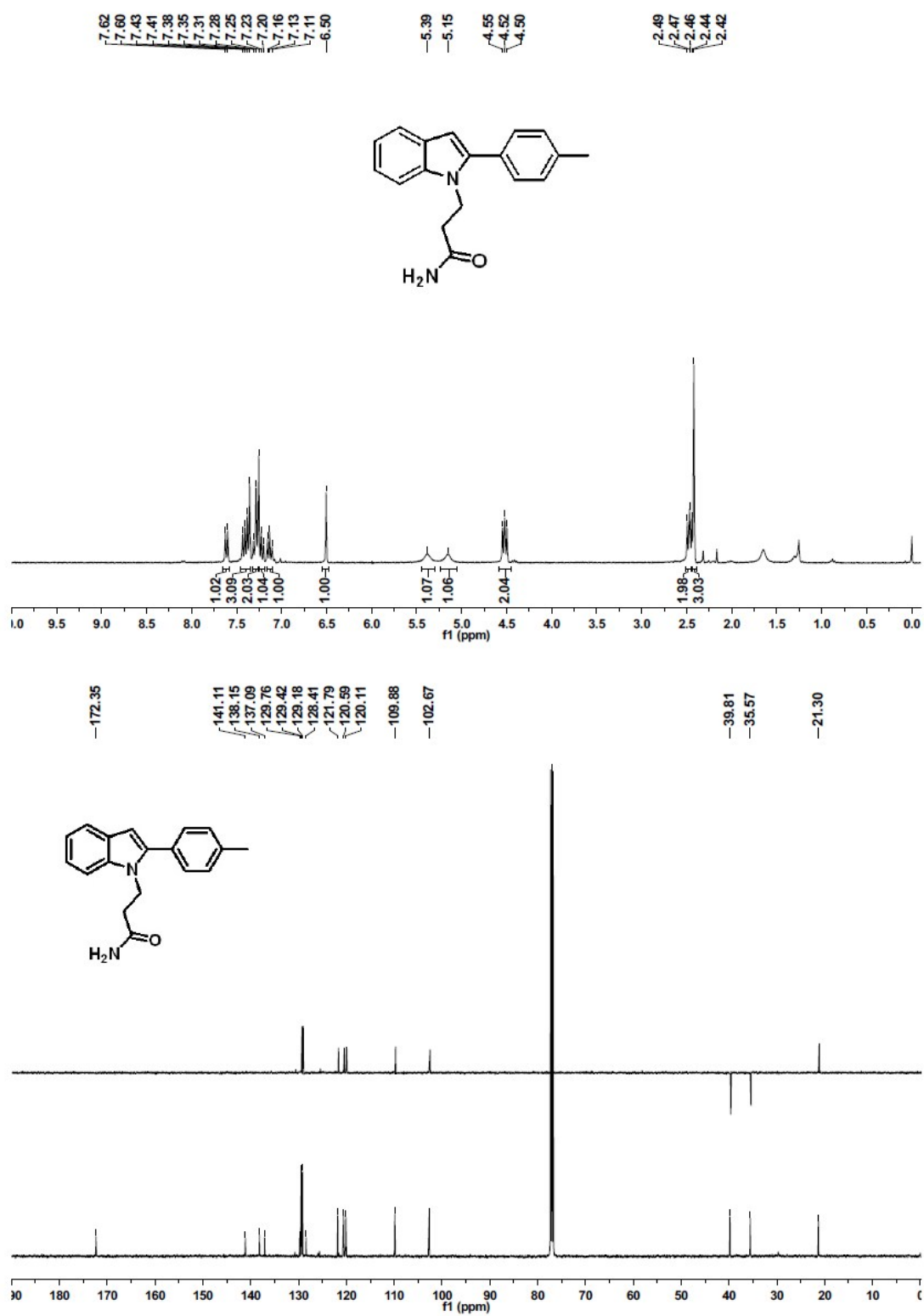
# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 3z



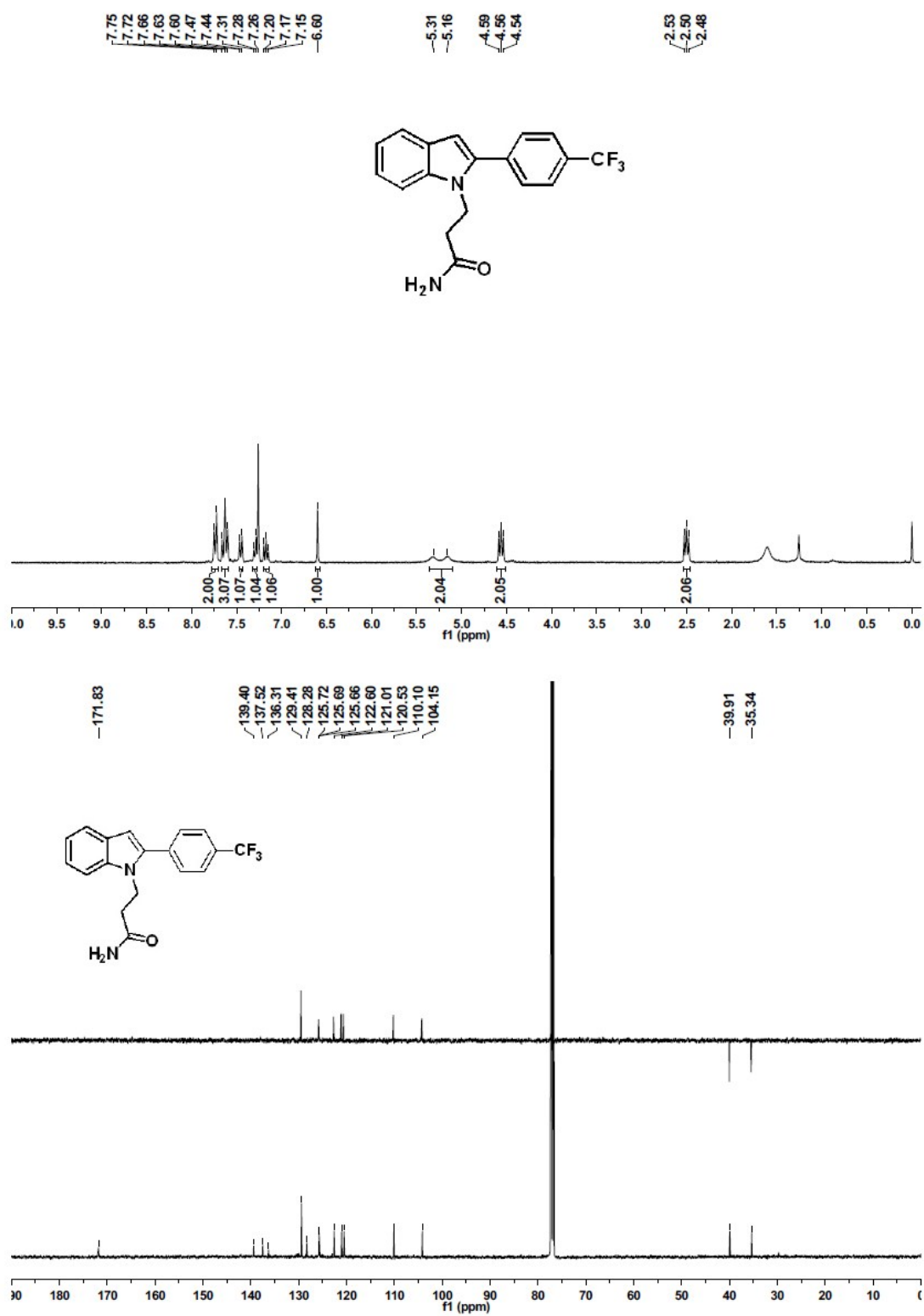
### HMBC of compound 3z



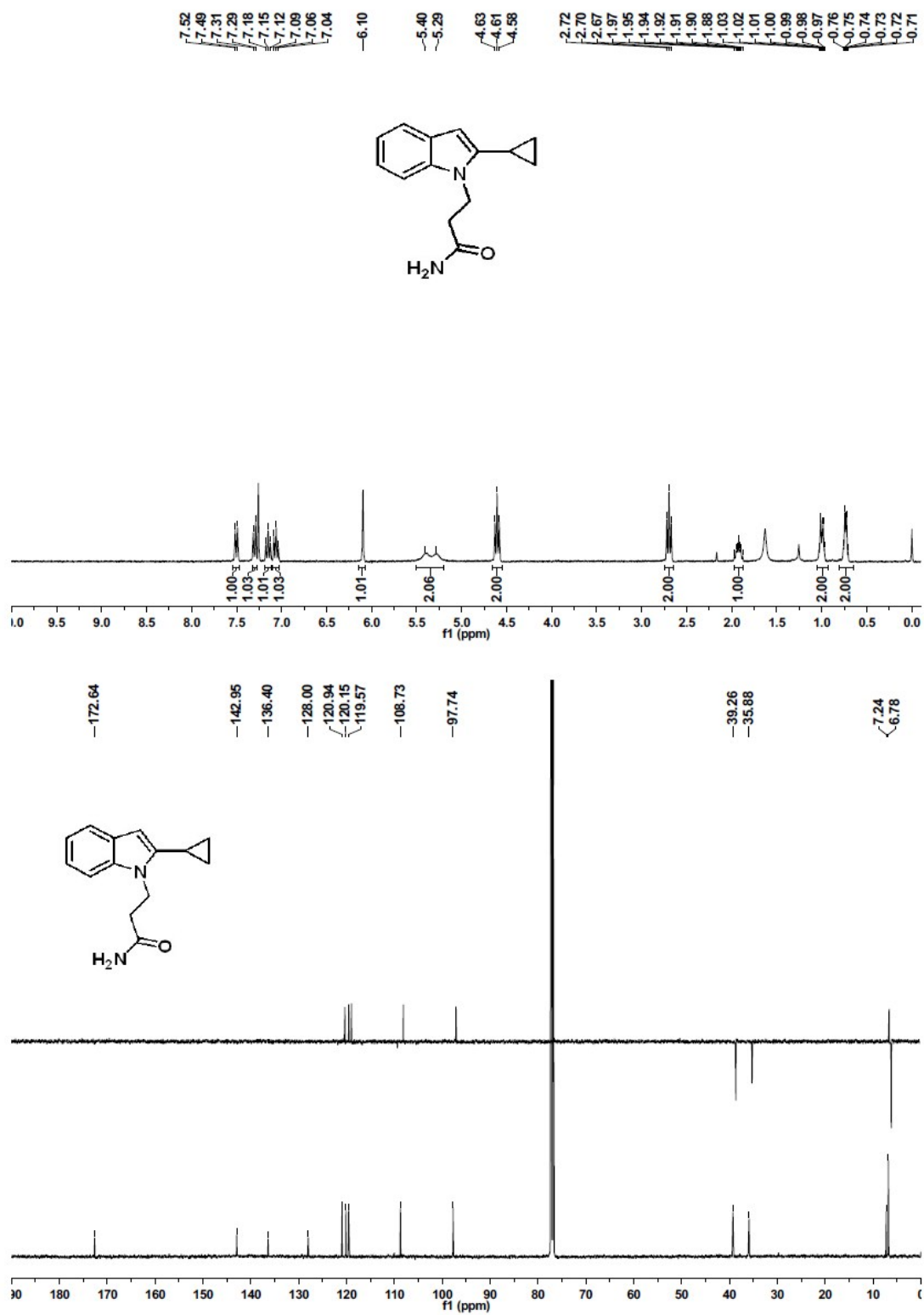
# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 3aa



# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 3ab

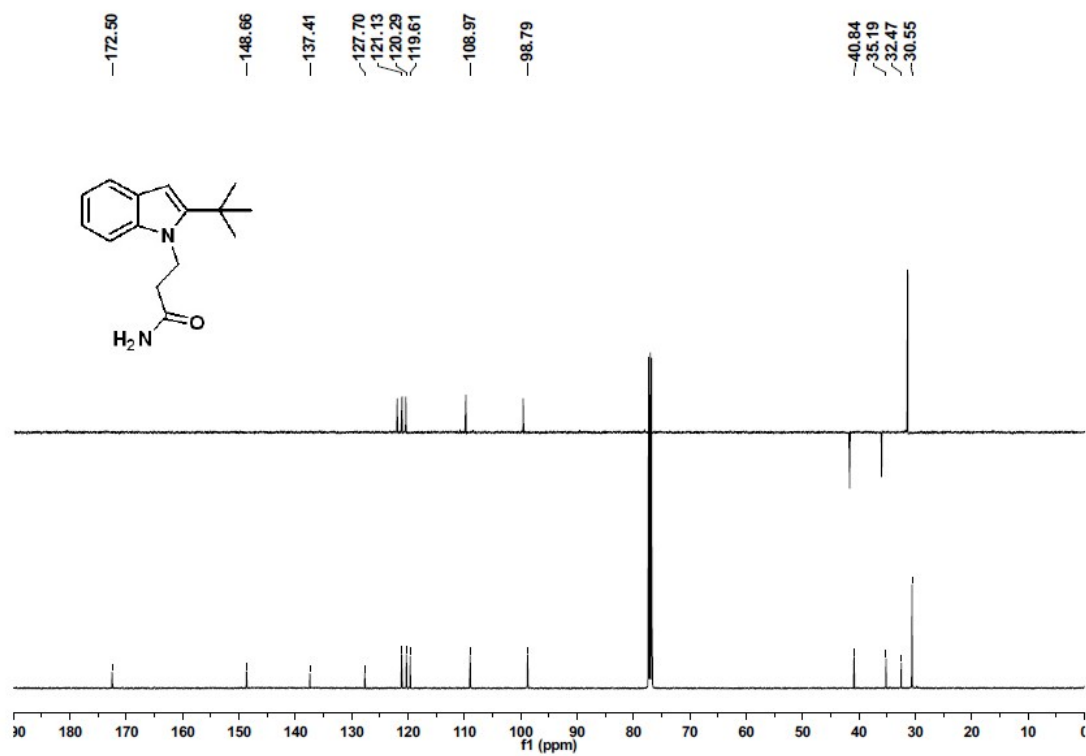
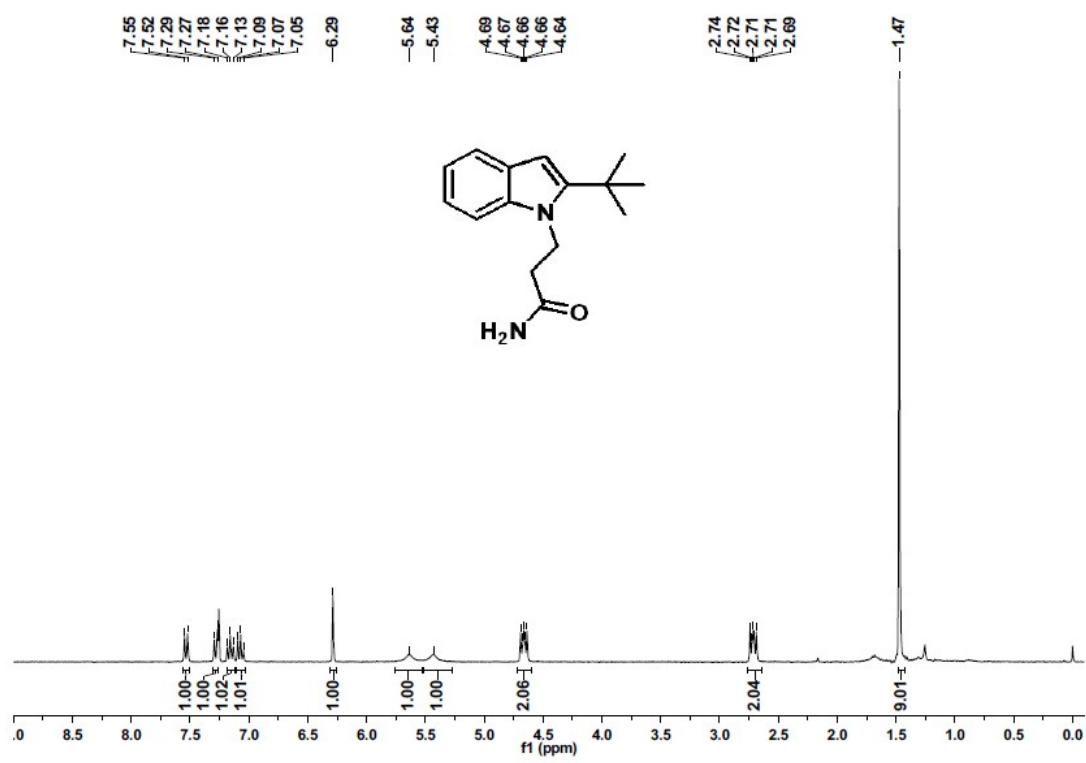


### $^1\text{H}$ and $^{13}\text{C}$ NMR spectra of compound 3ac

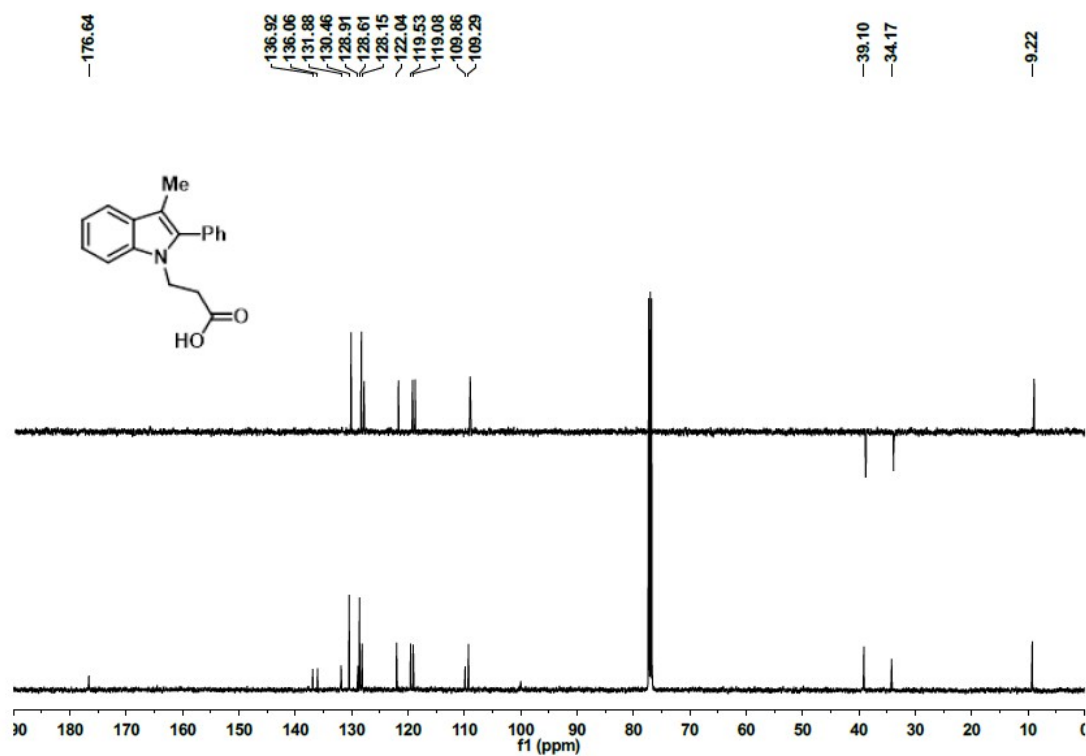
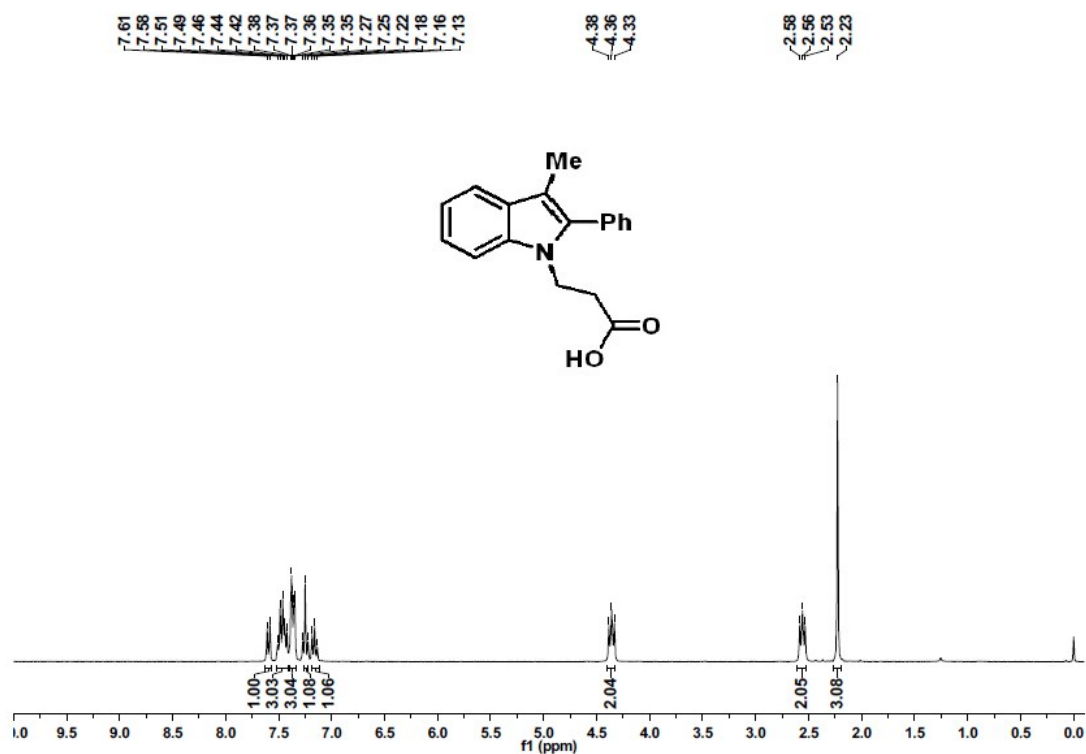




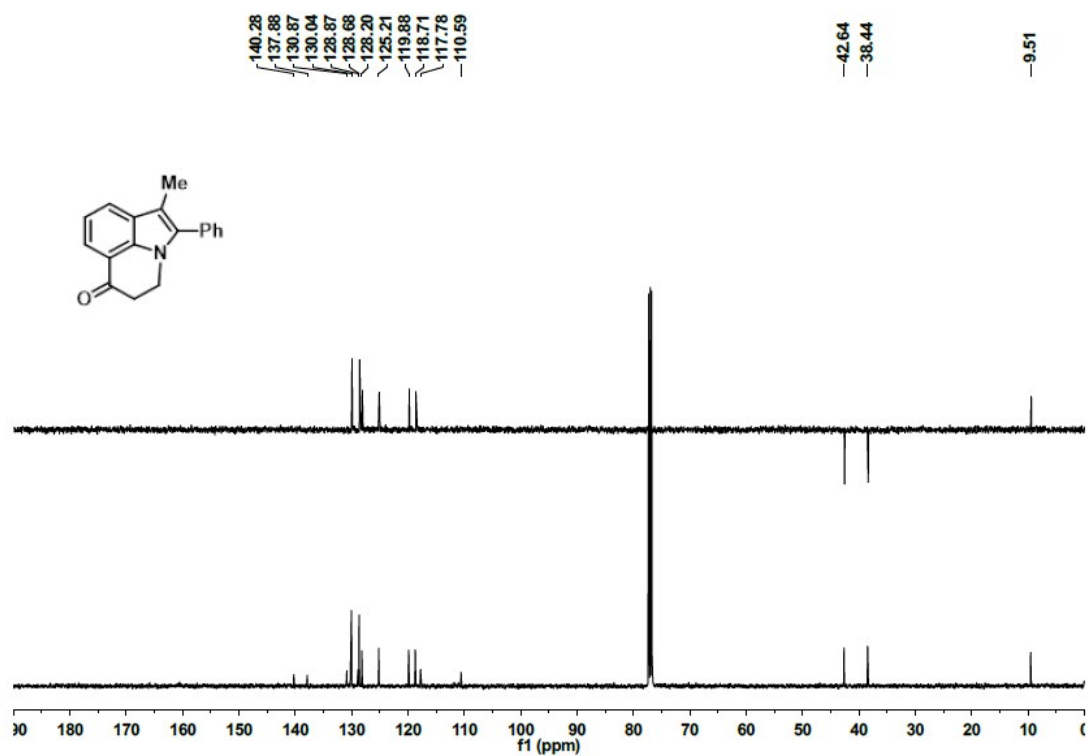
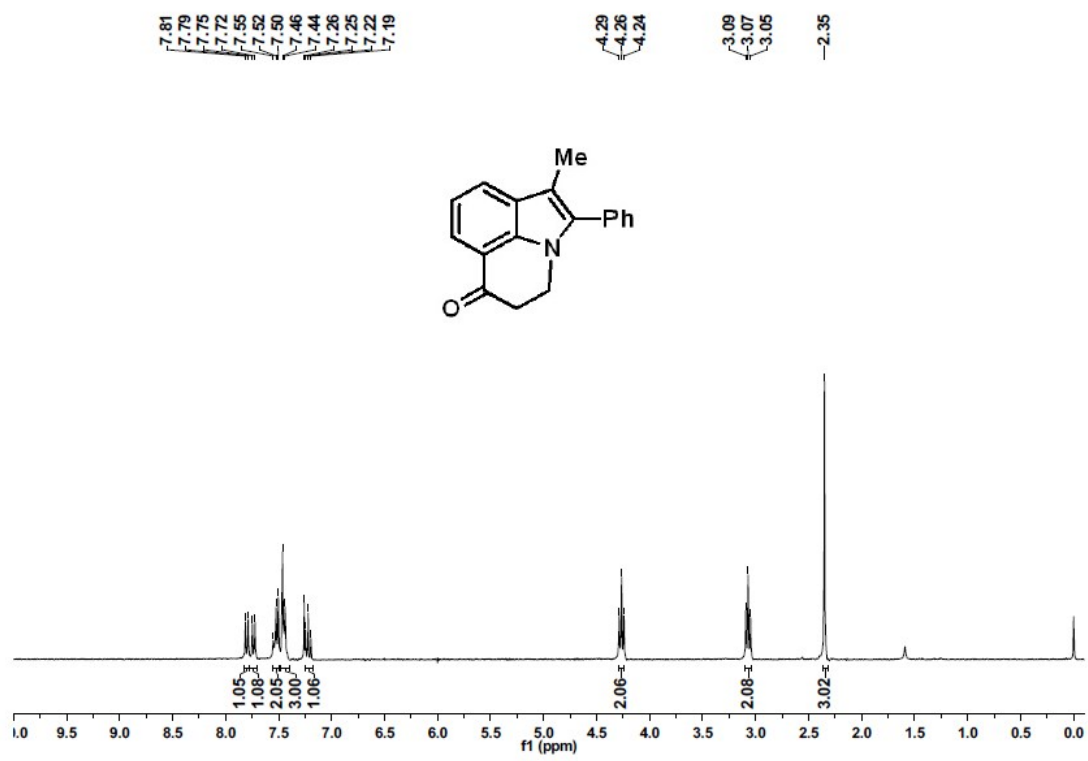
# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 3ad



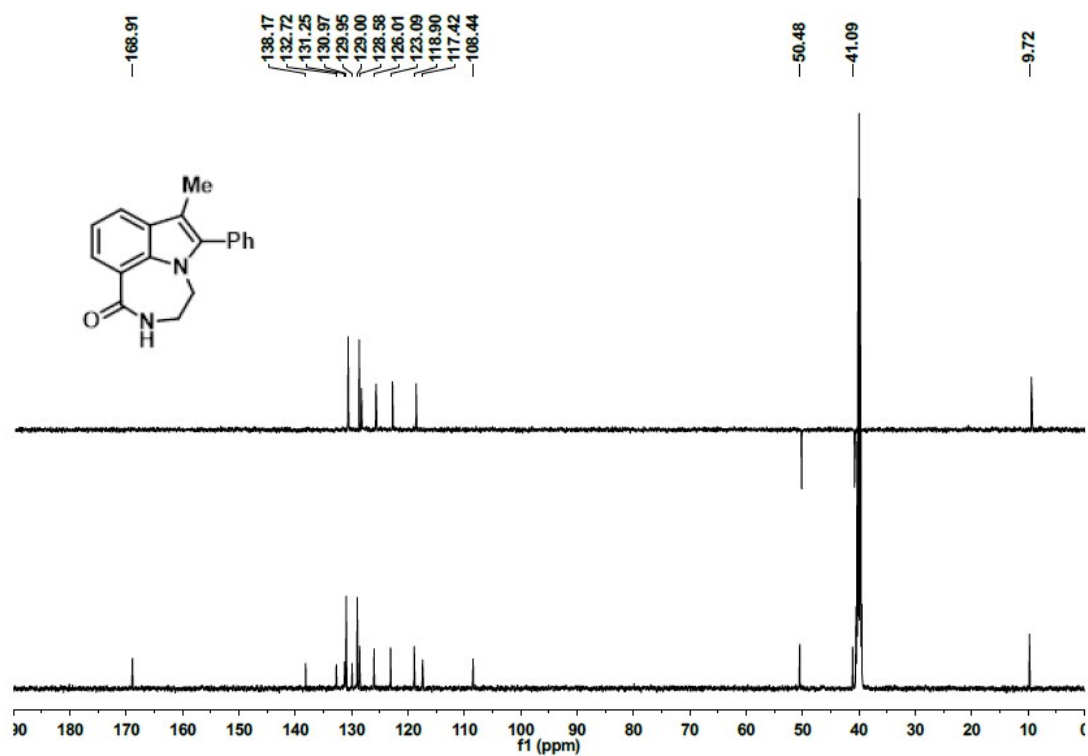
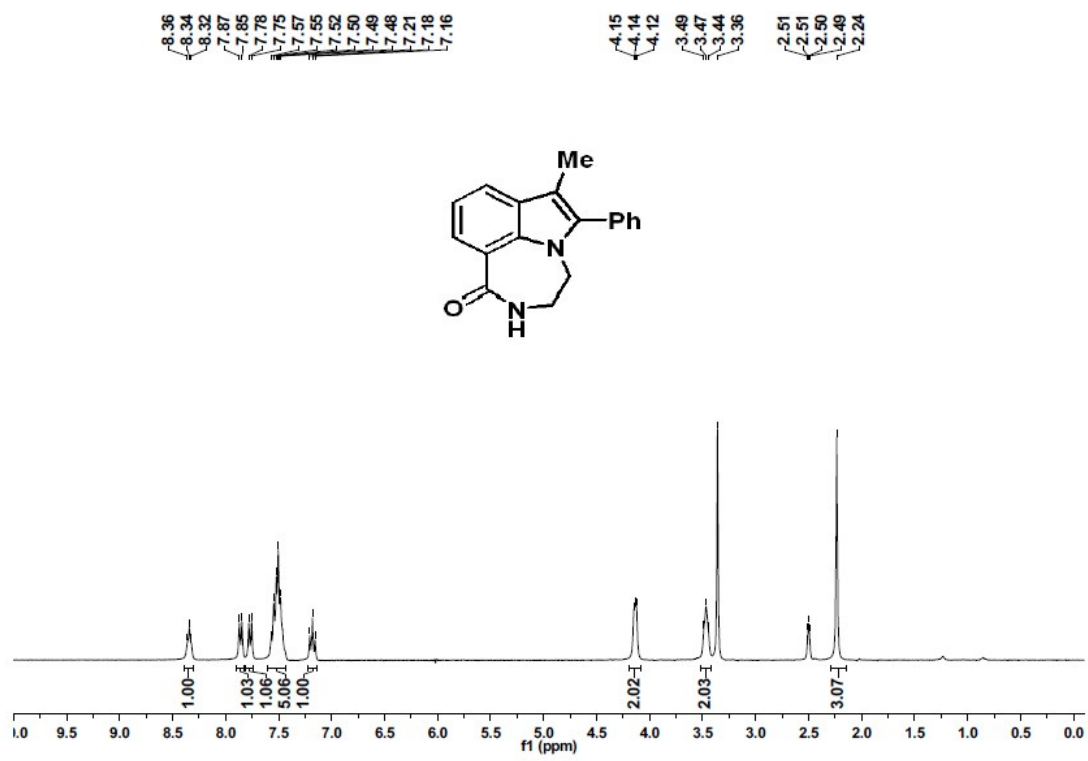
# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 4



# <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound 5



# $^1\text{H}$ and $^{13}\text{C}$ NMR spectra of compound 6



## 2. X-ray structure of compound 3a

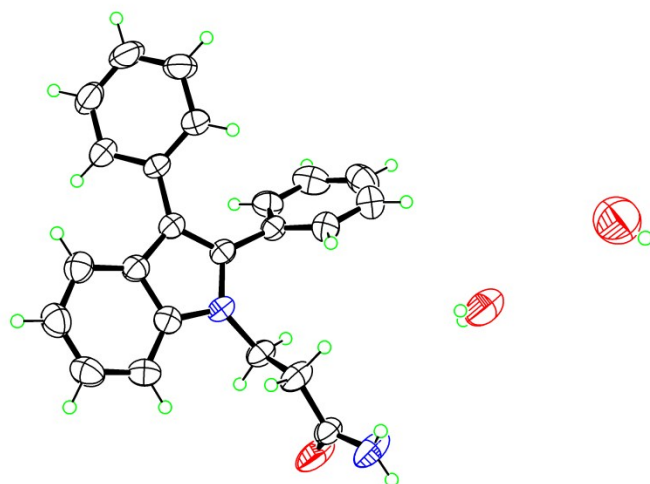


Figure S1. Ortep representation of compound 3a

Table S1. Sample and crystal data for compound 3a

CCDC	1540588
Chemical formula	$C_{23}H_{20}N_2O_{2.50}$
Formula weight	364.41
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal size	0.050 x 0.080 x 0.100 mm
Crystal system	monoclinic
Space group	$C 1 2/c 1$
Unit cell dimensions	$a = 24.0516(14)$ Å $\alpha = 90^\circ$ $b = 8.6236(5)$ Å $\beta = 106.207(3)^\circ$ $c = 20.5558(10)$ Å $\gamma = 90^\circ$
Volume	$4094.1(4)$ Å <sup>3</sup>
Z	8
Density (calculated)	1.182 Mg/cm <sup>3</sup>
Absorption coefficient	0.078 mm <sup>-1</sup>
F(000)	1536

Table S2. Data collection and structure refinement for compound 3a

---

<b>Theta range for data collection</b>	1.76 to 25.00°
<b>Index ranges</b>	-25<=h<=28, -10<=k<=10, -24<=l<=24
<b>Reflections collected</b>	15097
<b>Independent reflections</b>	3602 [R(int) = 0.0283]
<b>Coverage of independent reflections</b>	99.9%
<b>Absorption correction</b>	multi-scan
<b>Structure solution technique</b>	direct methods
<b>Structure solution program</b>	SHELXS-97 (Sheldrick, 2008)
<b>Refinement method</b>	Full-matrix least-squares on F <sup>2</sup>
<b>Refinement program</b>	SHELXL-97 (Sheldrick, 2008)
<b>Function minimized</b>	$\Sigma w(F_o^2 - F_c^2)^2$
<b>Data / restraints / parameters</b>	3602 / 8 / 258
<b>Goodness-of-fit on F<sup>2</sup></b>	1.751
<b><math>\Delta/\sigma_{\max}</math></b>	2.988
<b>Final R indices</b>	2662 data; I>2 $\sigma$ (I) R1 = 0.1179, wR2 = 0.3808 all data R1 = 0.1386, wR2 = 0.4087
<b>Weighting scheme</b>	w=1/[ $\sigma^2(F_o^2)+(0.2000P)^2+0.0000P$ ] where P=(F <sub>o</sub> <sup>2</sup> +2F <sub>c</sub> <sup>2</sup> )/3
<b>Extinction coefficient</b>	0.0110(30)
<b>Largest diff. peak and hole</b>	1.808 and -0.506 eÅ <sup>-3</sup>
<b>R.M.S. deviation from mean</b>	0.131 eÅ <sup>-3</sup>

---