

*Supplementary Material*

**A synthesis of functionalized 2-amino-3-cyano pyrroles from  
terminal alkynes, sulfonyl azides and phenacylmalononitriles**

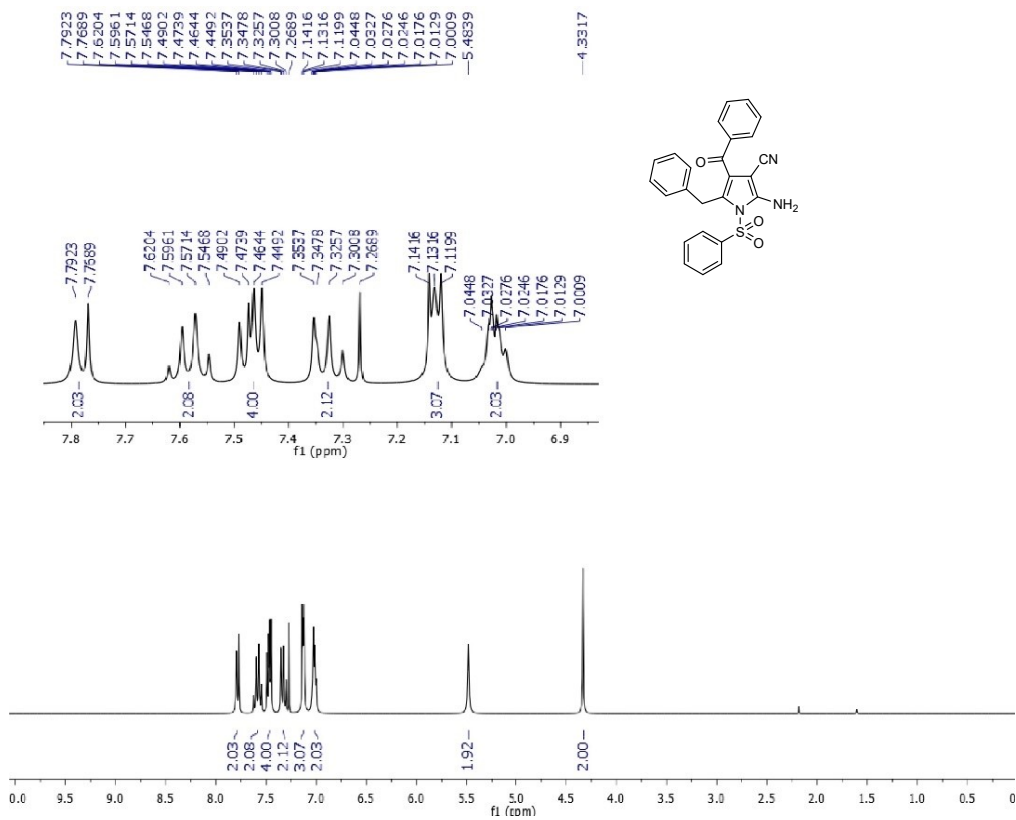
**Issa Yavari\*, Meysam Ghorbanzadeh and Somayeh Akbarzadeh**

Department of Chemistry, Tarbiat Modares University, PO Box 14115-175, Tehran, Iran

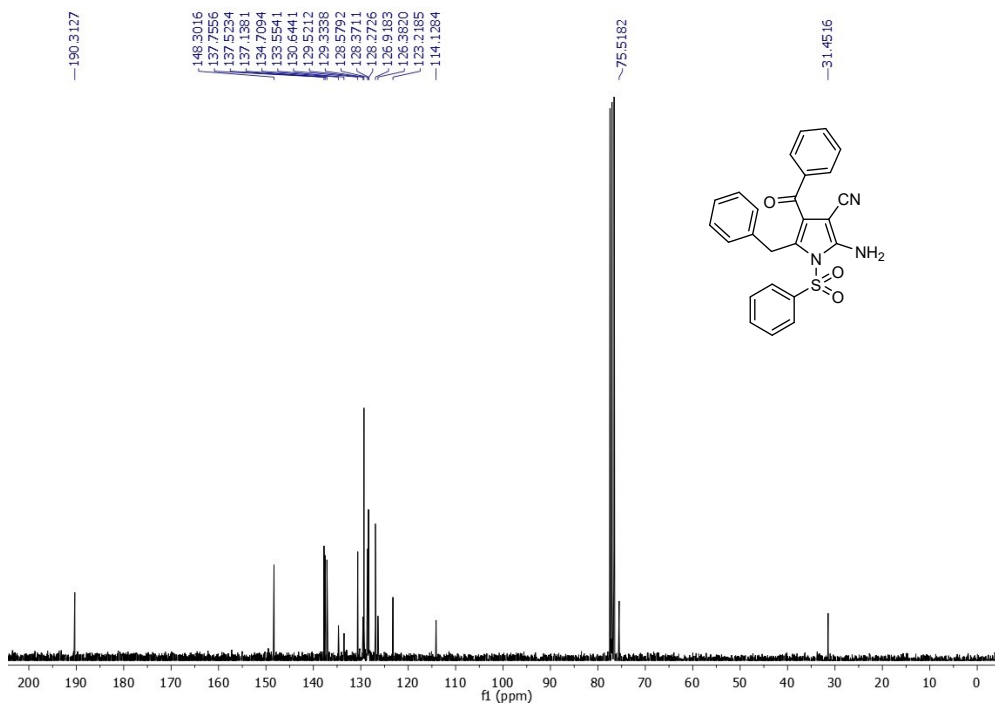
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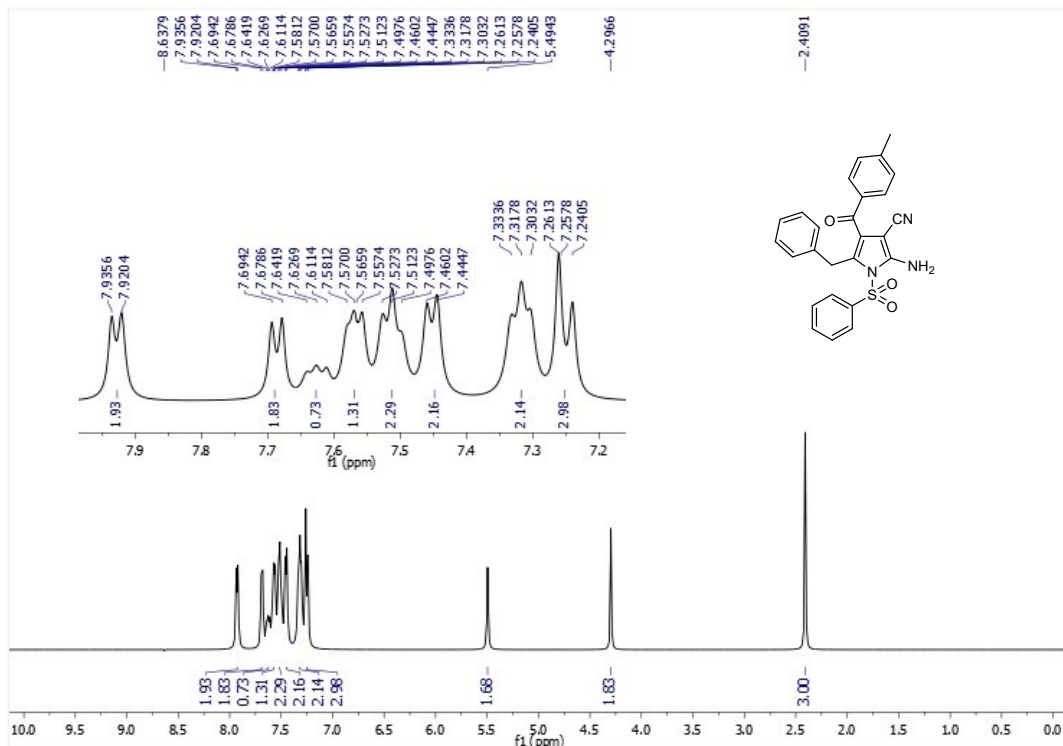
# NMR spectra of 2-amino-3-cyano pyrroles 4



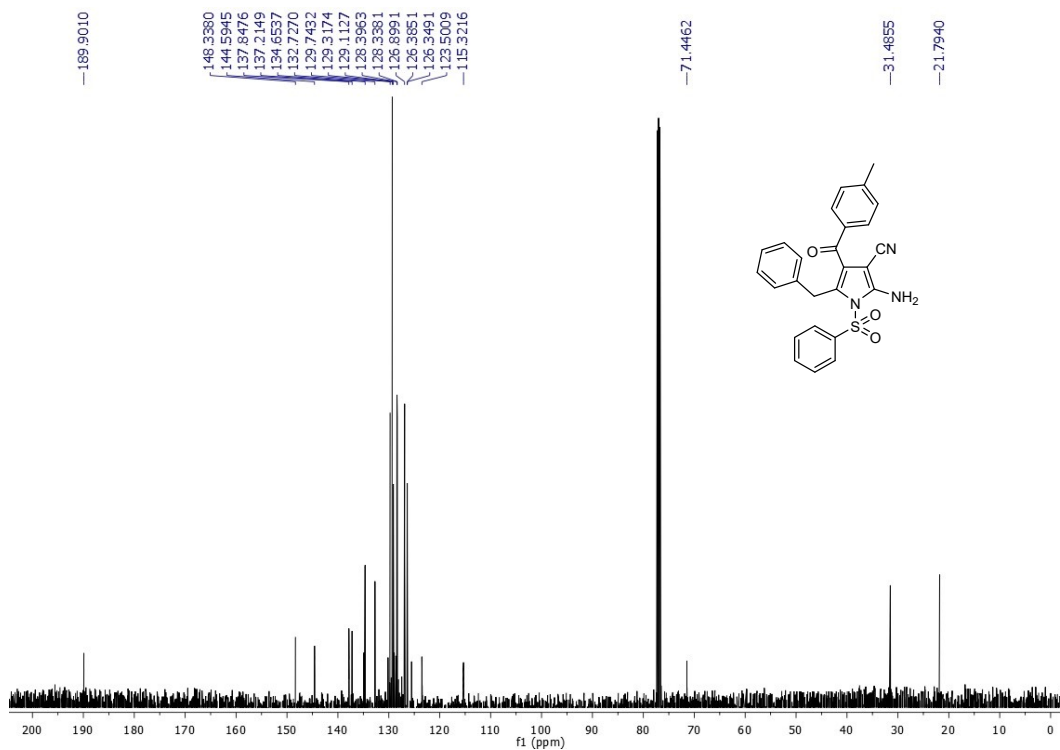
**<sup>1</sup>H NMR (300 MHz) of Compound 4a in CDCl<sub>3</sub>**



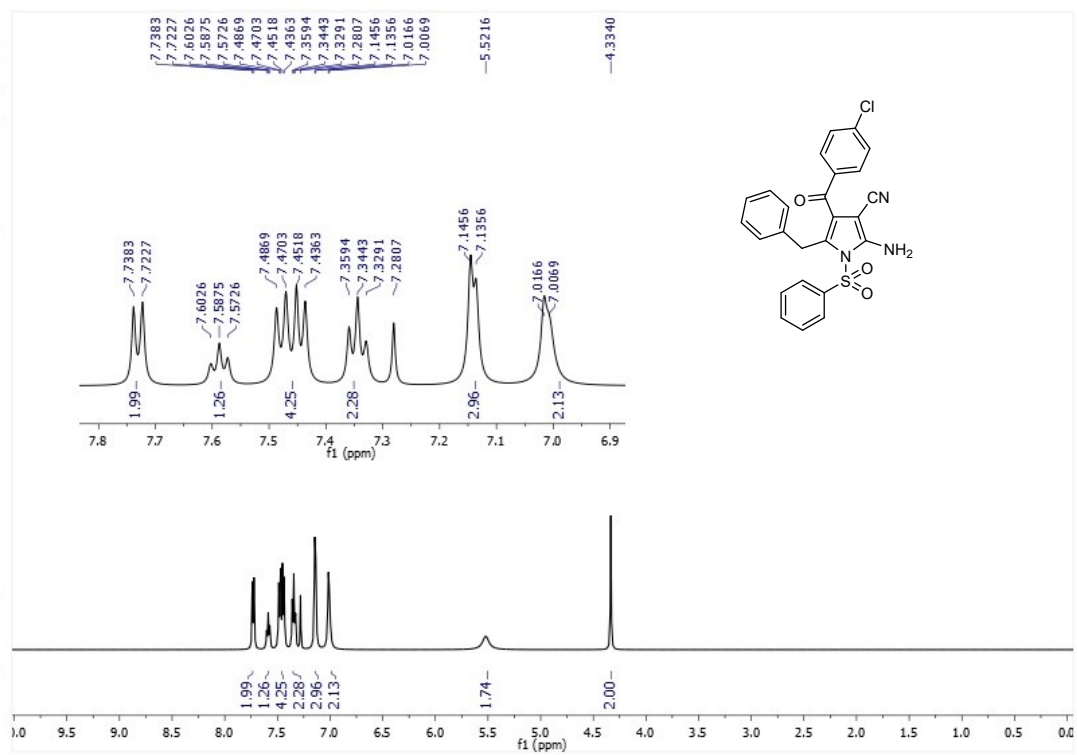
**<sup>13</sup>C NMR (75 MHz) of Compound 4a in CDCl<sub>3</sub>**



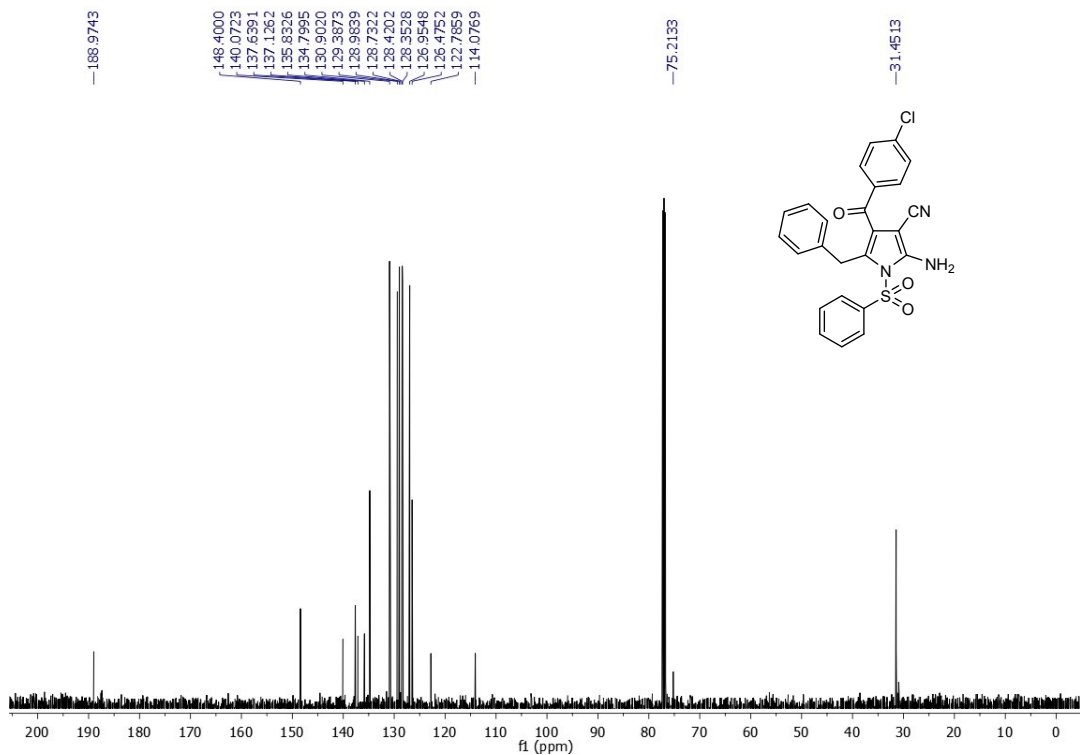
**<sup>1</sup>H NMR (500 MHz) of Compound 4b in CDCl<sub>3</sub>**



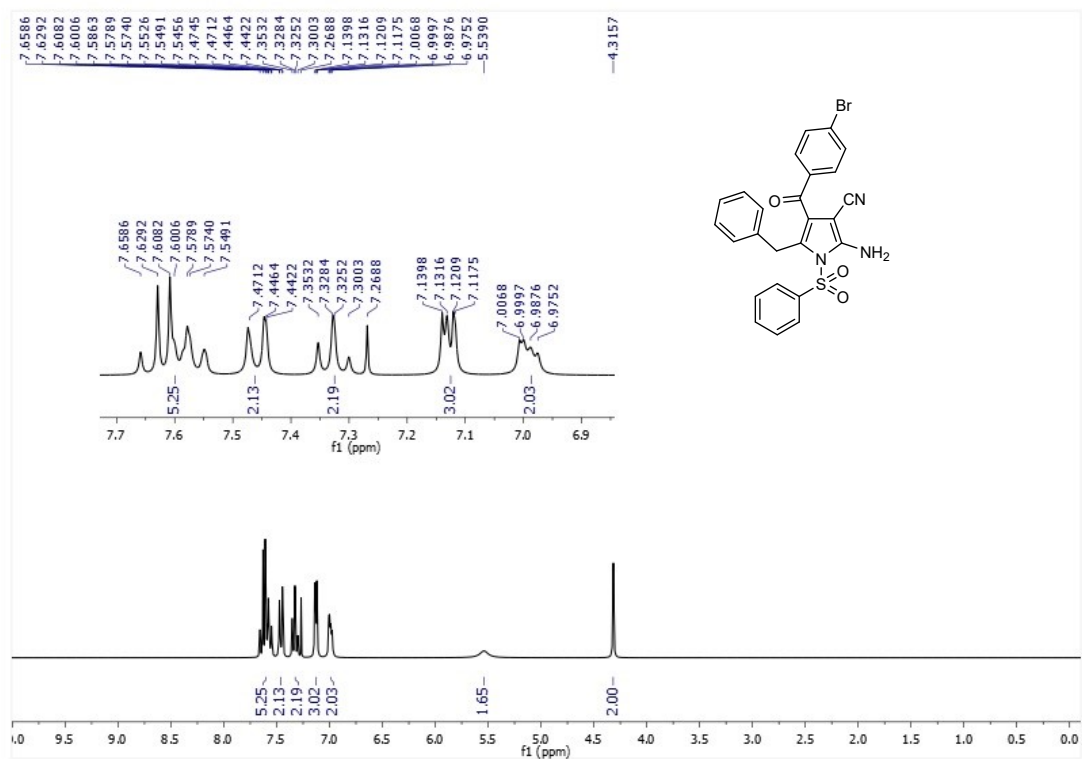
**<sup>13</sup>C NMR (126 MHz) of Compound 4b in CDCl<sub>3</sub>**



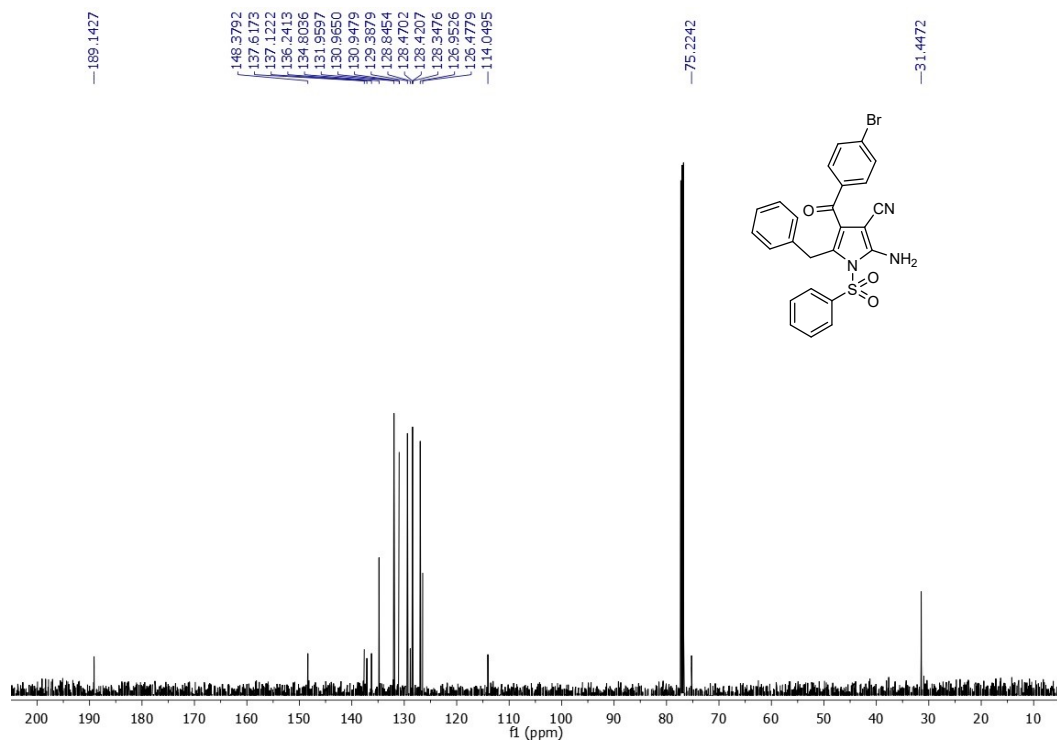
**<sup>1</sup>H NMR (500 MHz) of Compound 4c in CDCl<sub>3</sub>**



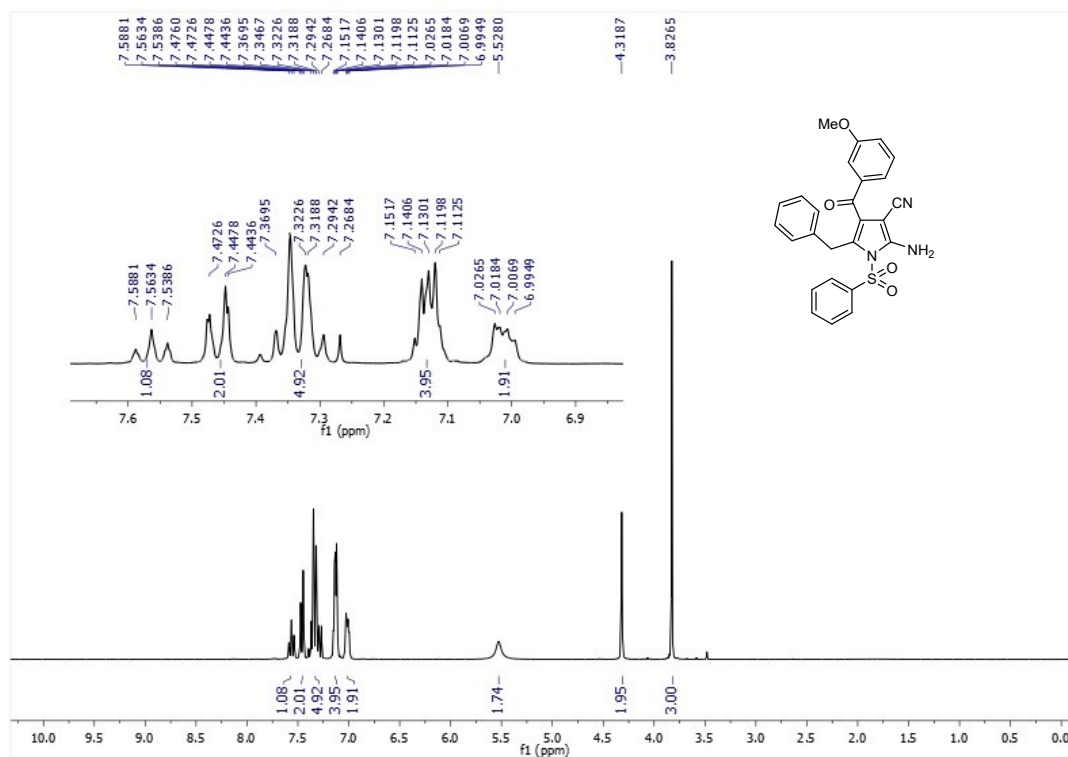
**<sup>13</sup>C NMR (126 MHz) of Compound 4c in CDCl<sub>3</sub>**



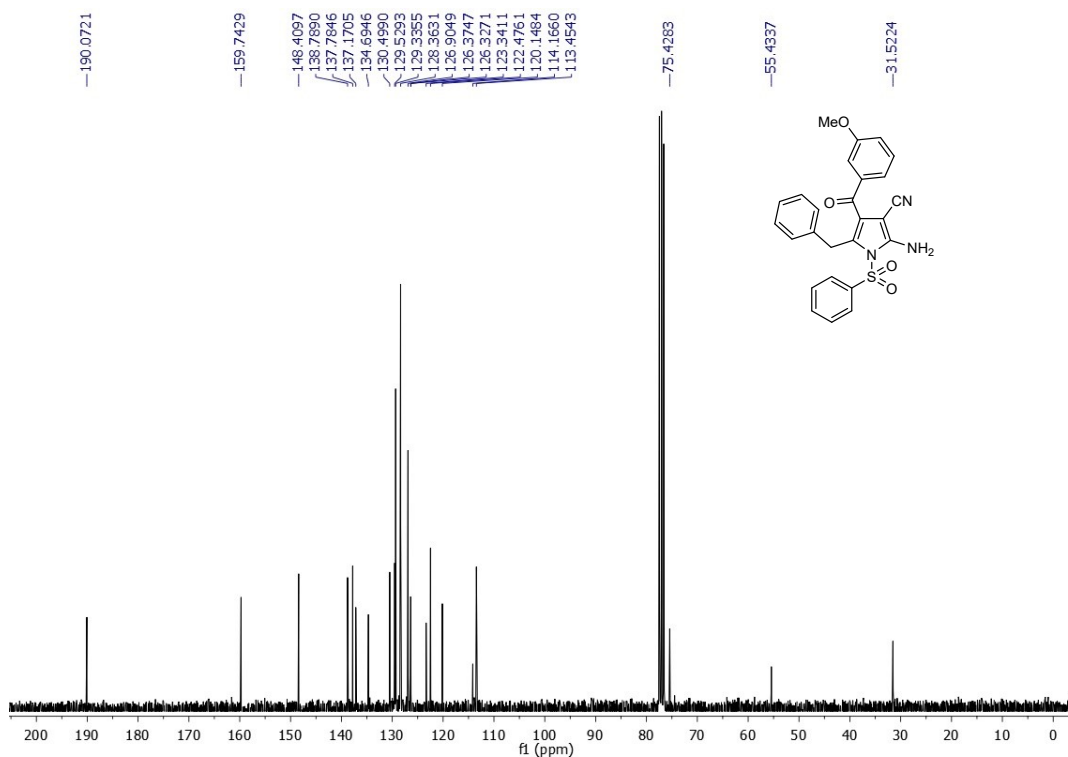
$^1\text{H}$  NMR (500 MHz) of Compound **4d** in  $\text{CDCl}_3$



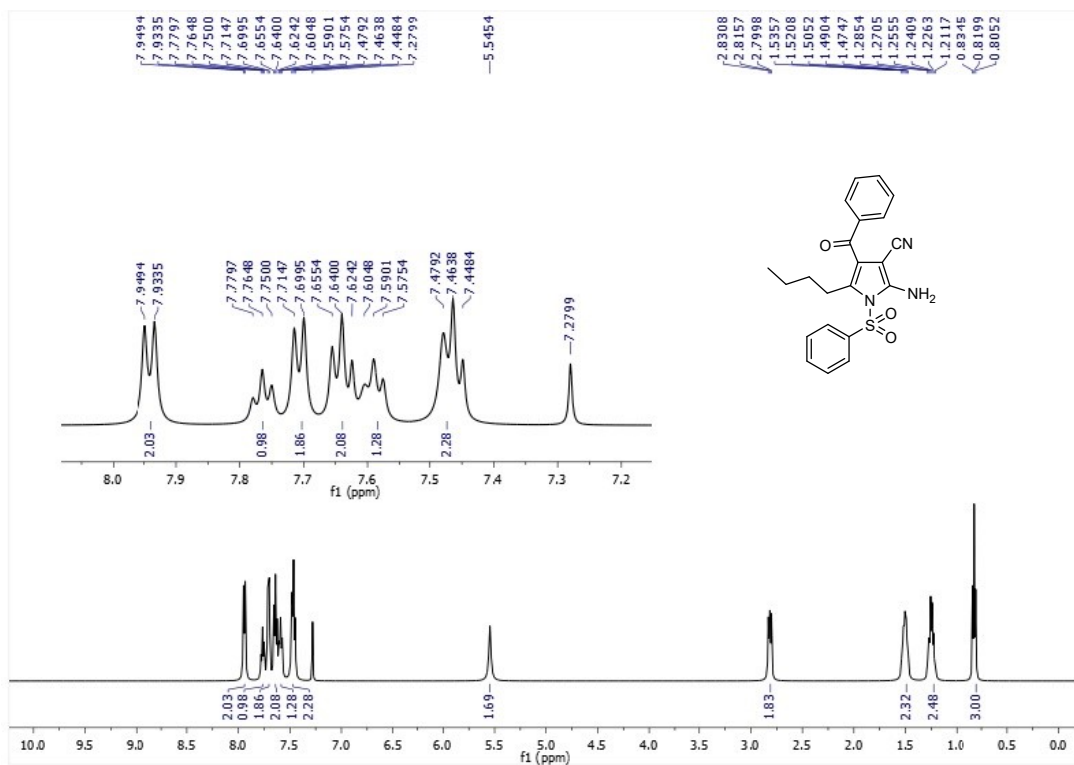
$^{13}\text{C}$  NMR (126 MHz) of Compound **4d** in  $\text{CDCl}_3$



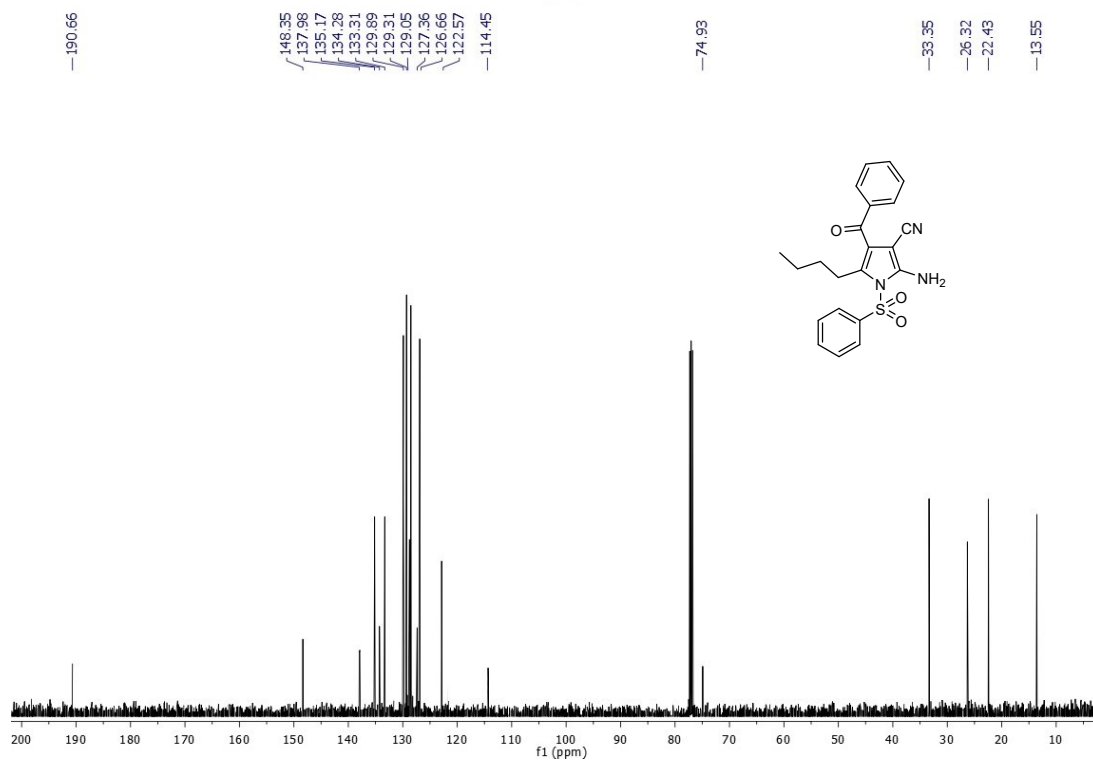
**<sup>1</sup>H NMR (300 MHz) of Compound 4e in CDCl<sub>3</sub>**



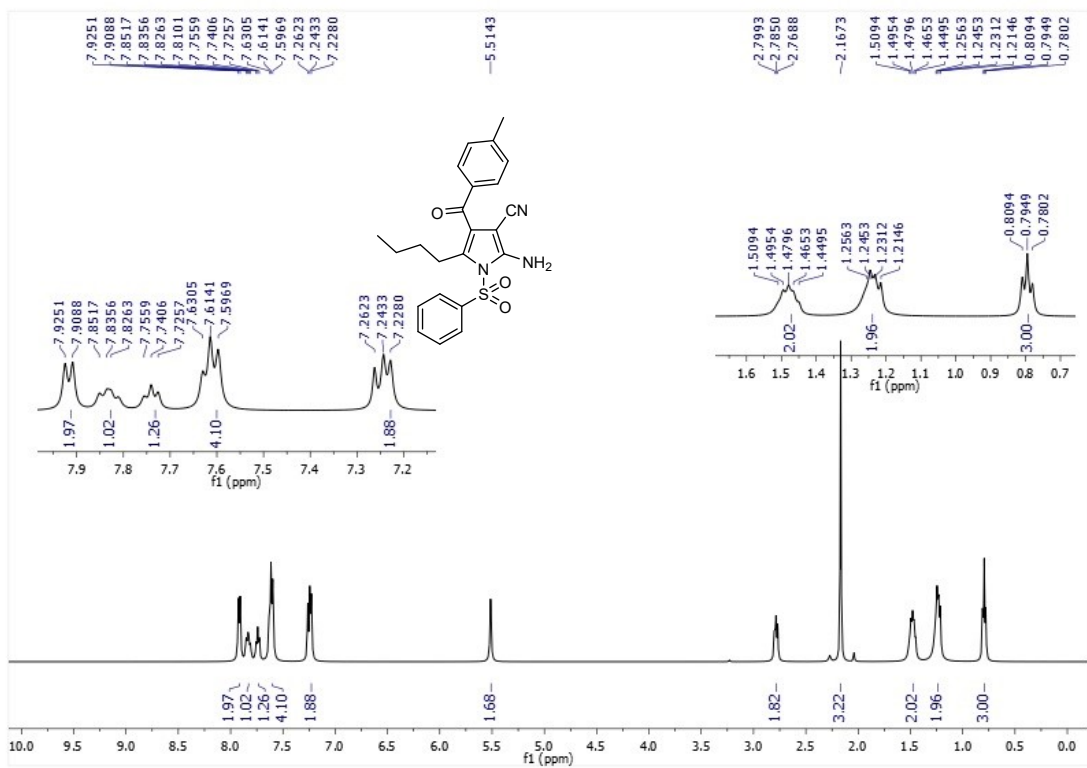
**<sup>13</sup>C NMR (75 MHz) of Compound 4e in CDCl<sub>3</sub>**



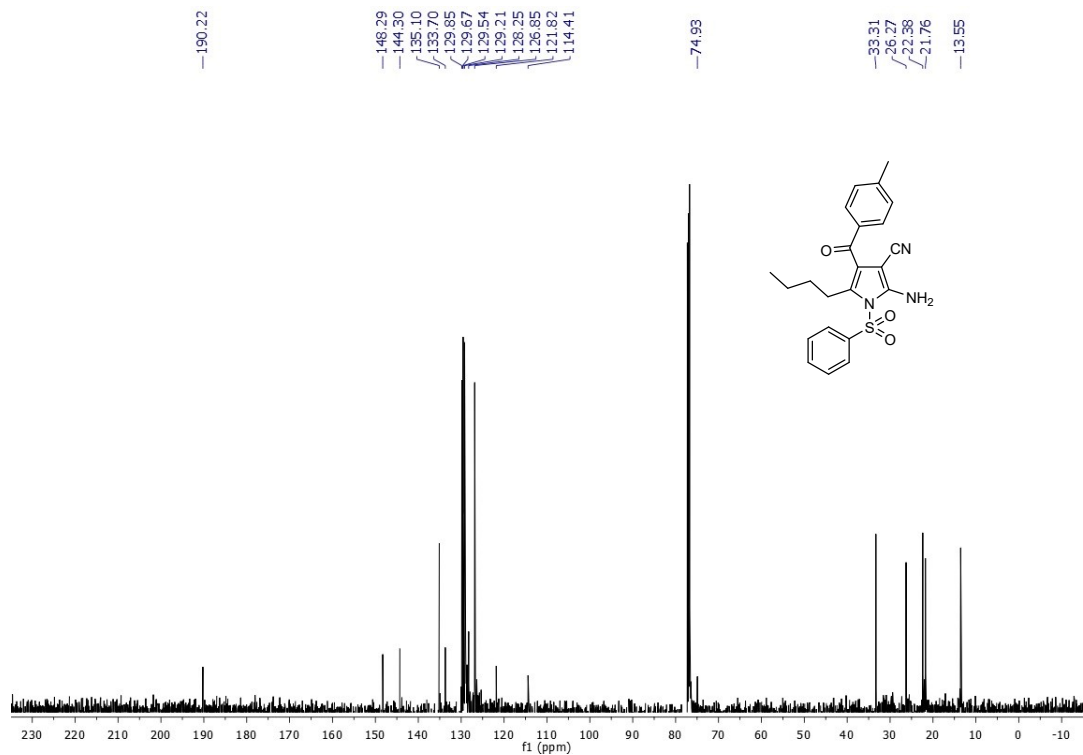
**<sup>1</sup>H NMR (500 MHz) of Compound 4f in CDCl<sub>3</sub>**



**<sup>13</sup>C NMR (126 MHz) of Compound 4f in CDCl<sub>3</sub>**

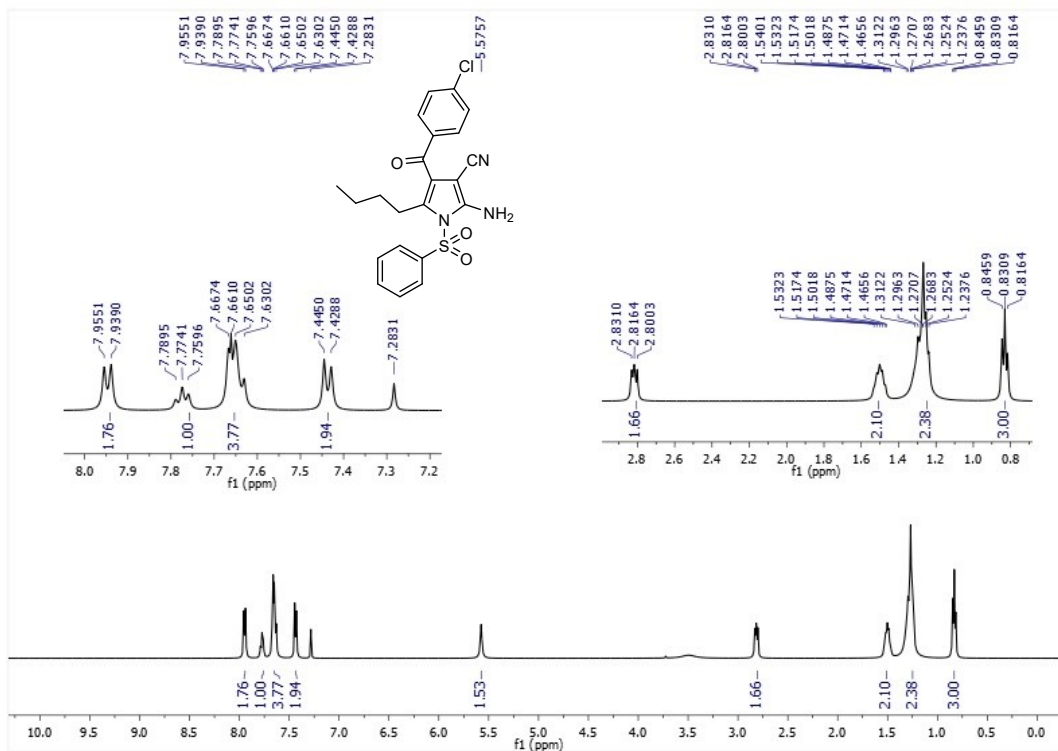


**<sup>1</sup>H NMR (500 MHz) of Compound 4g in CDCl<sub>3</sub>**

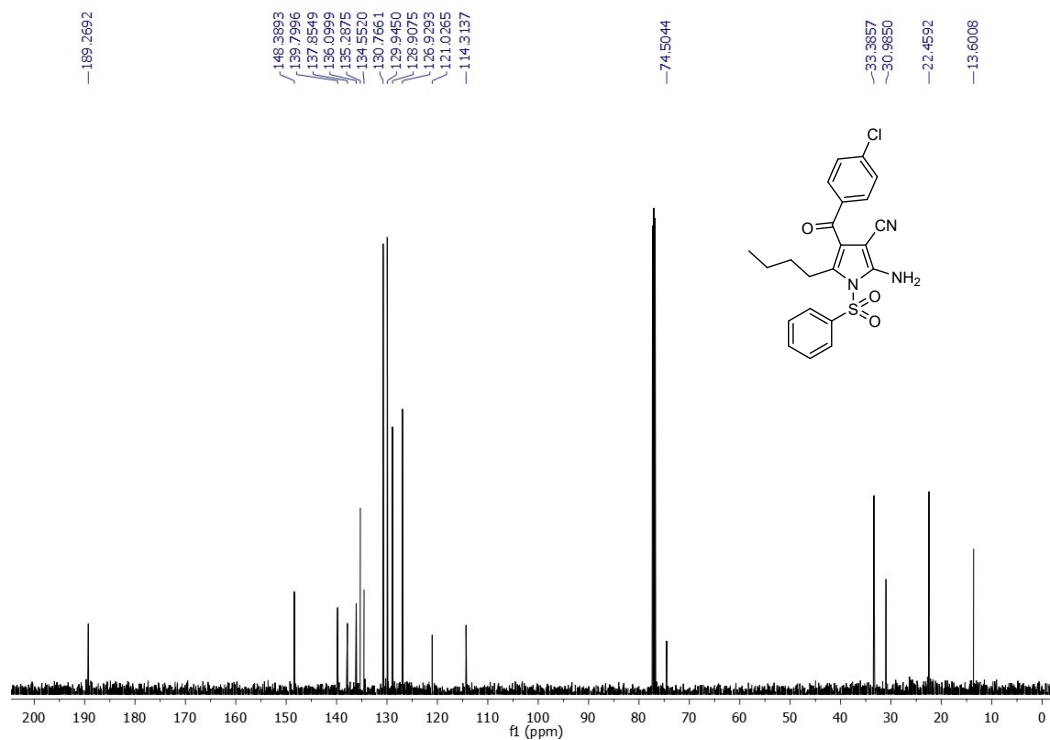


**<sup>13</sup>C NMR (126 MHz) of Compound 4g in CDCl<sub>3</sub>**

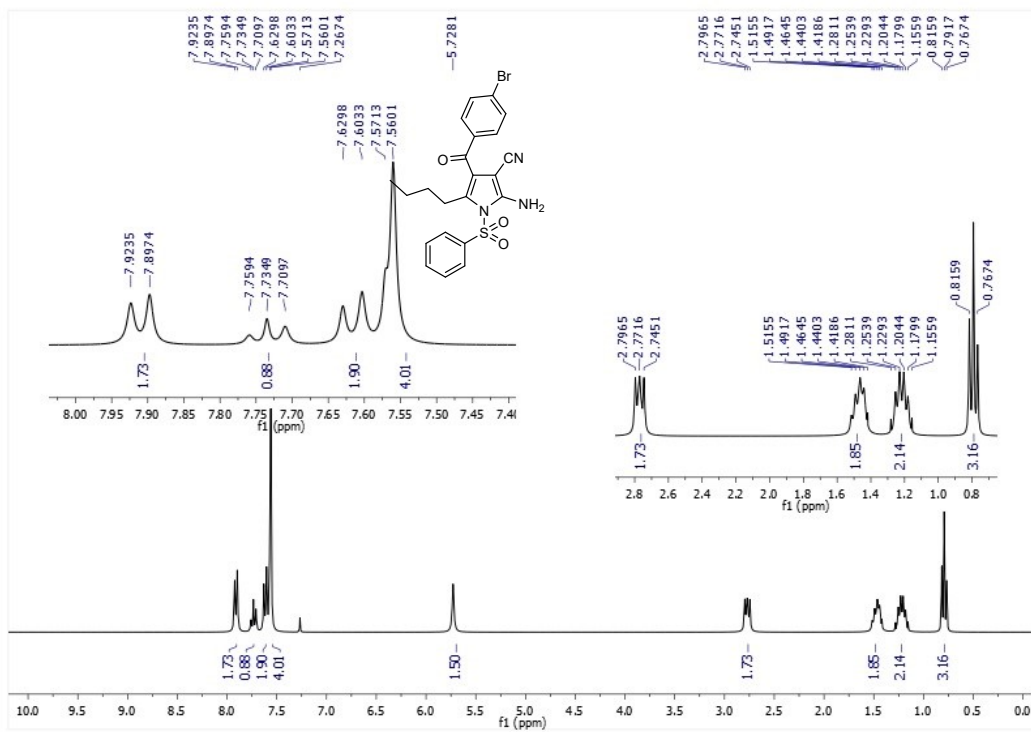




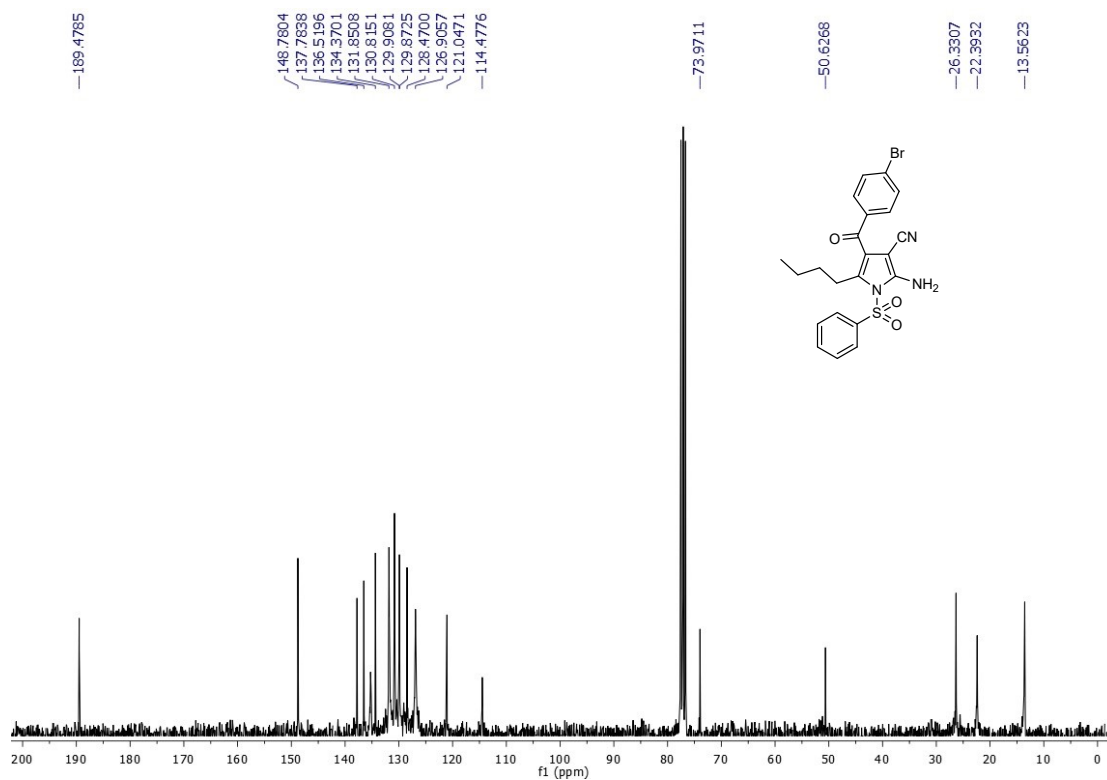
**<sup>1</sup>H NMR (500 MHz) of Compound 4h in CDCl<sub>3</sub>**



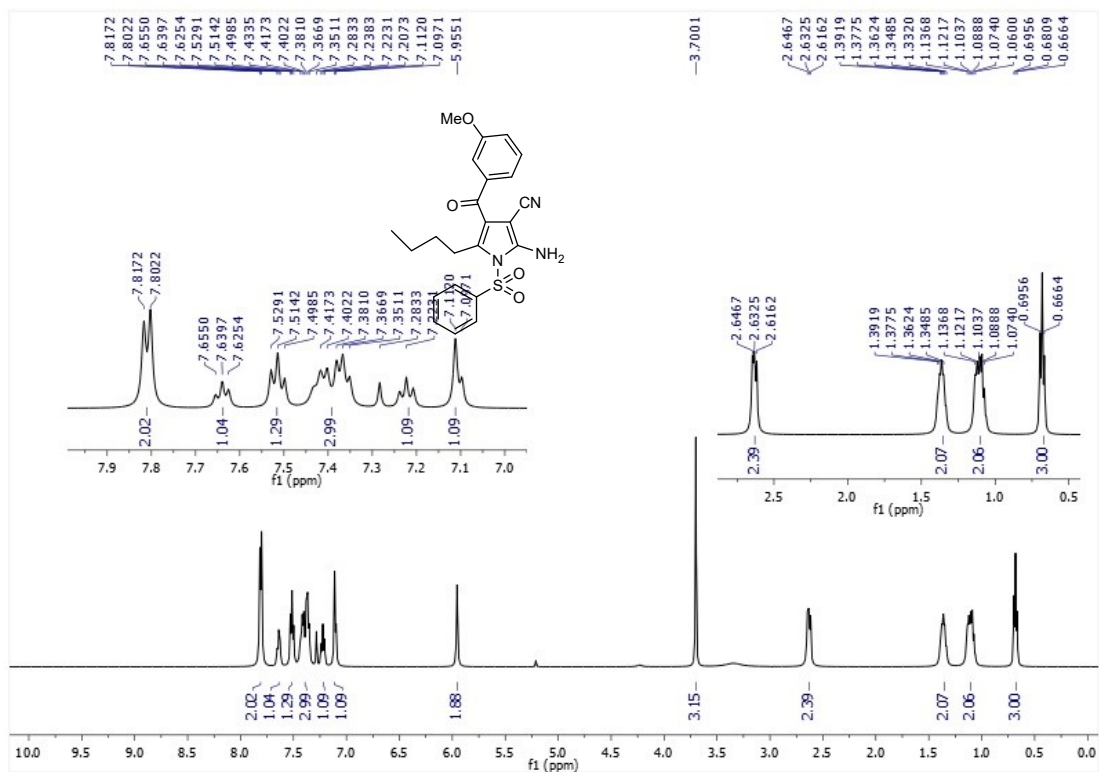
**<sup>13</sup>C NMR (126 MHz) of Compound 4h in CDCl<sub>3</sub>**



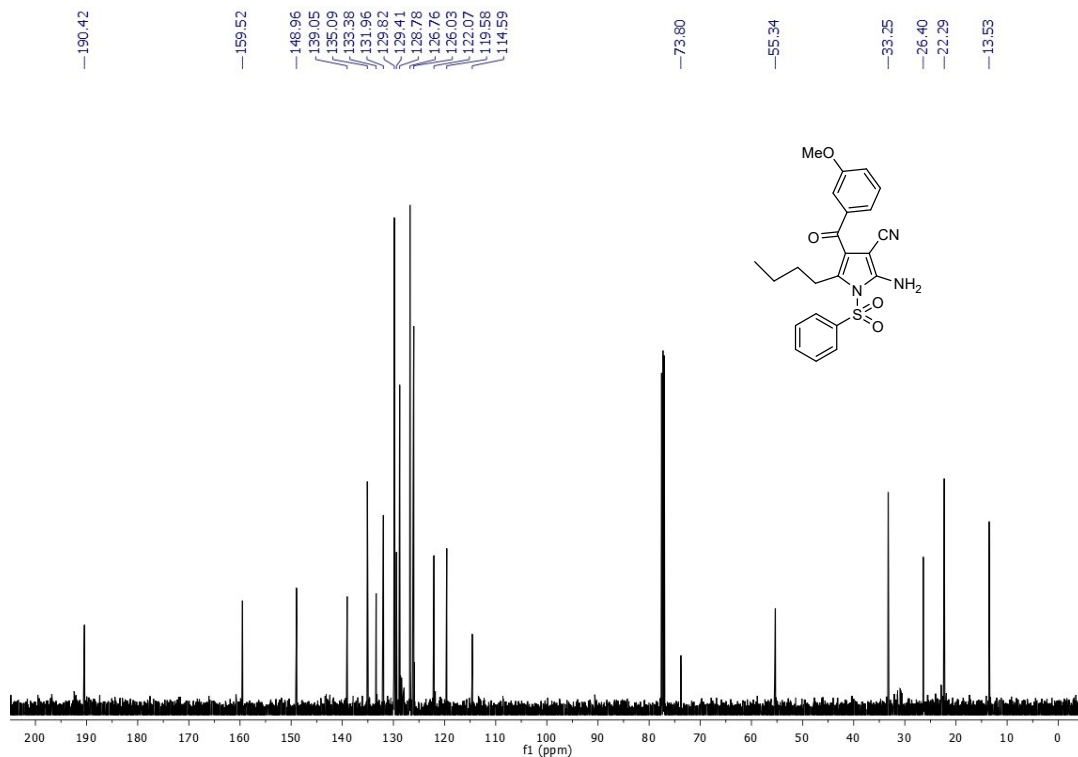
**<sup>1</sup>H NMR (300 MHz) of Compound 4i in CDCl<sub>3</sub>**



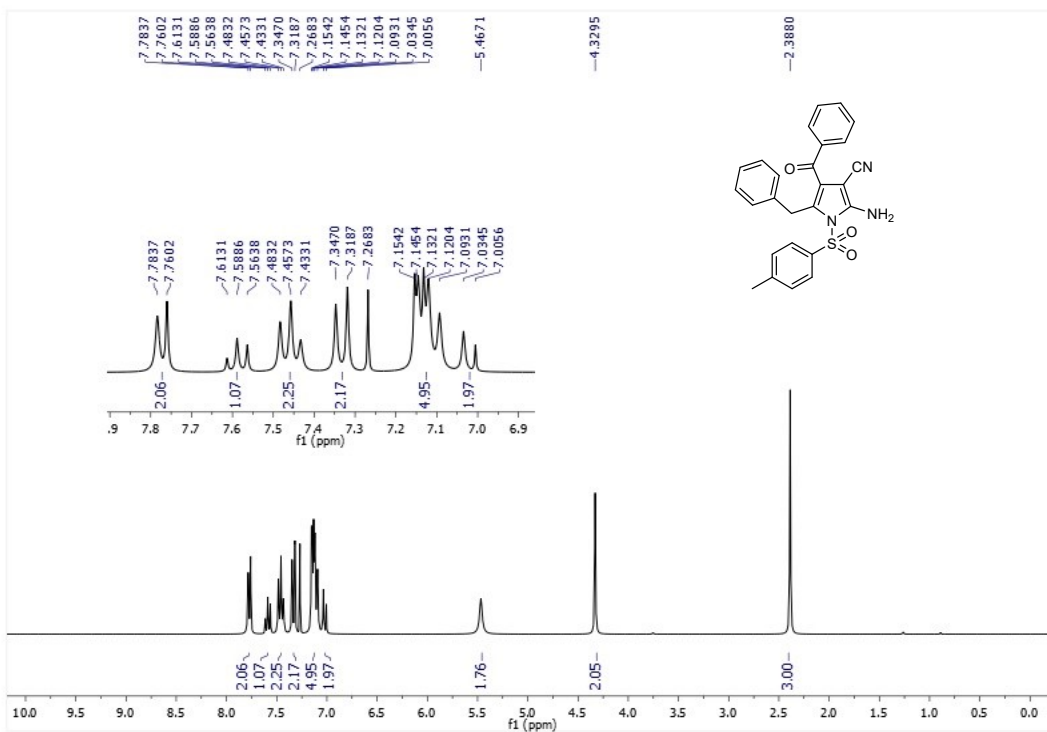
**<sup>13</sup>C NMR (75 MHz) of Compound 4i in CDCl<sub>3</sub>**



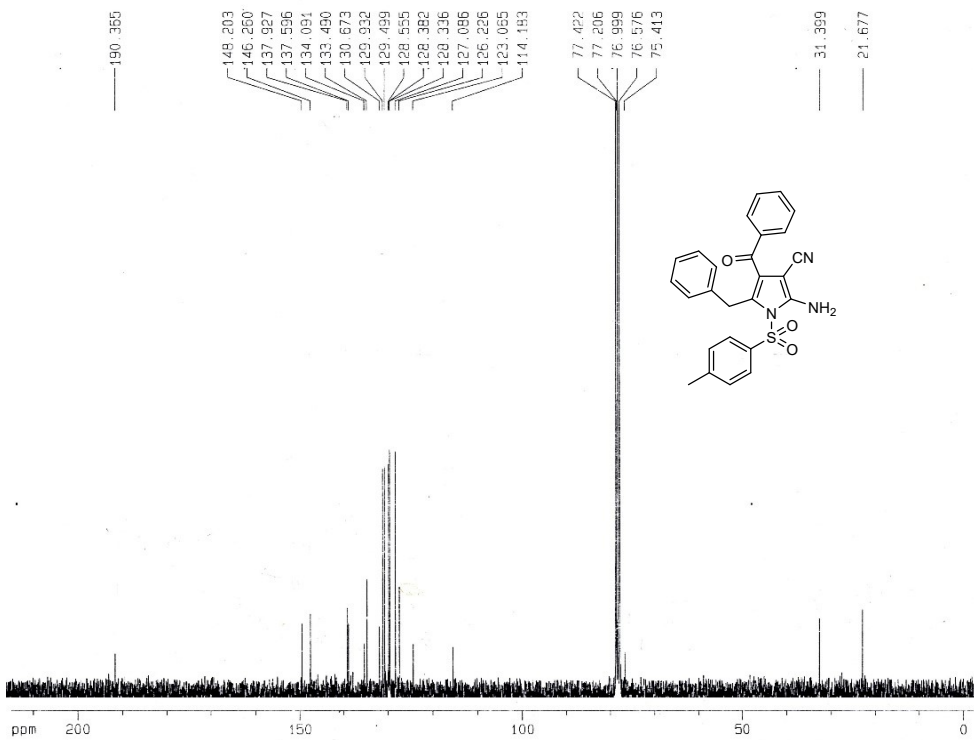
**<sup>1</sup>H NMR (500 MHz) of Compound 4j in CDCl<sub>3</sub>**



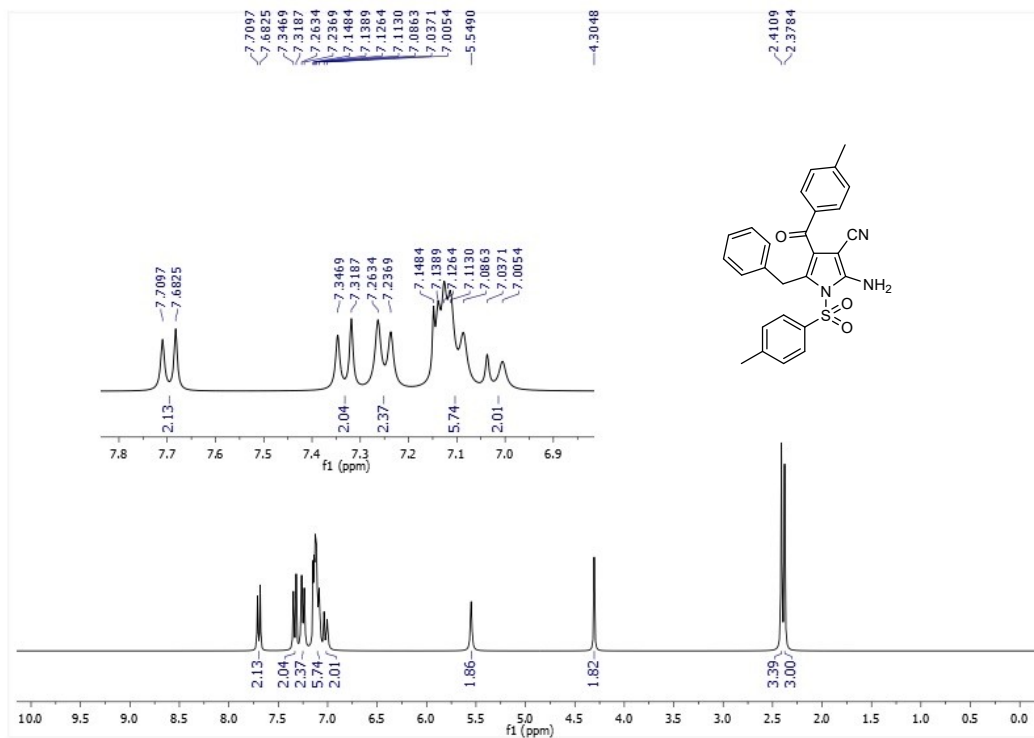
**<sup>13</sup>C NMR (126 MHz) of Compound 4j in CDCl<sub>3</sub>**



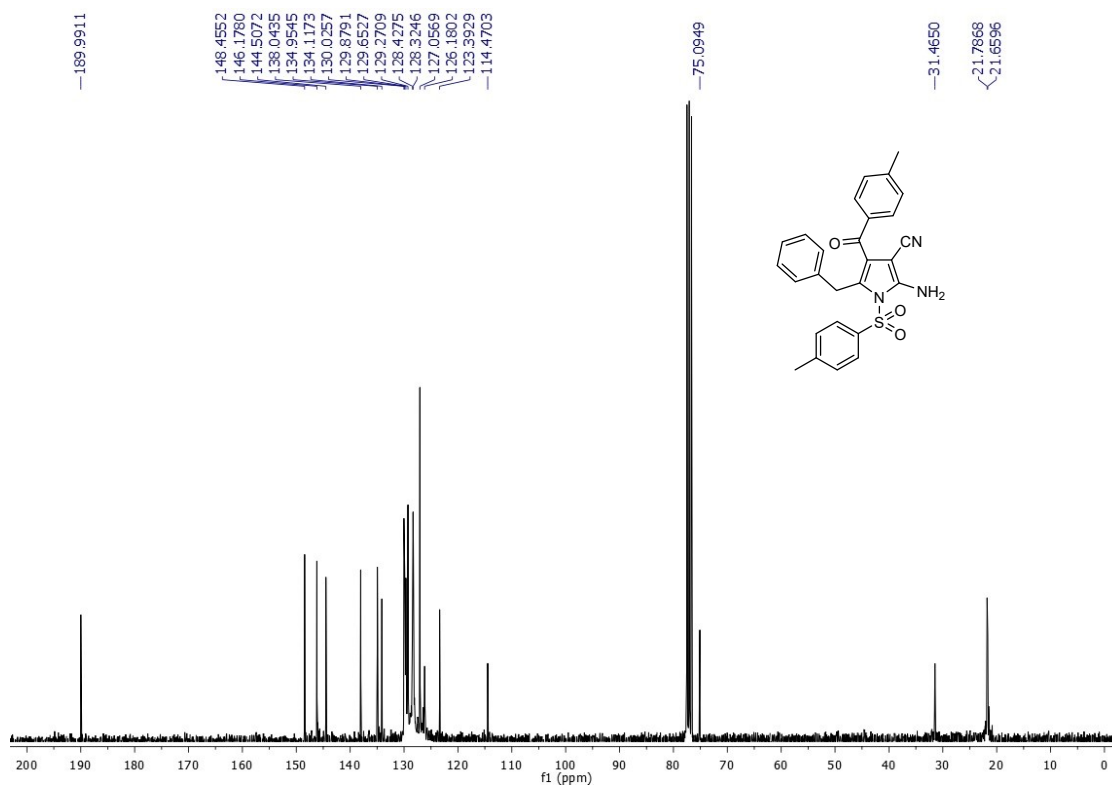
**<sup>1</sup>H NMR (300 MHz) of Compound 4k in CDCl<sub>3</sub>**



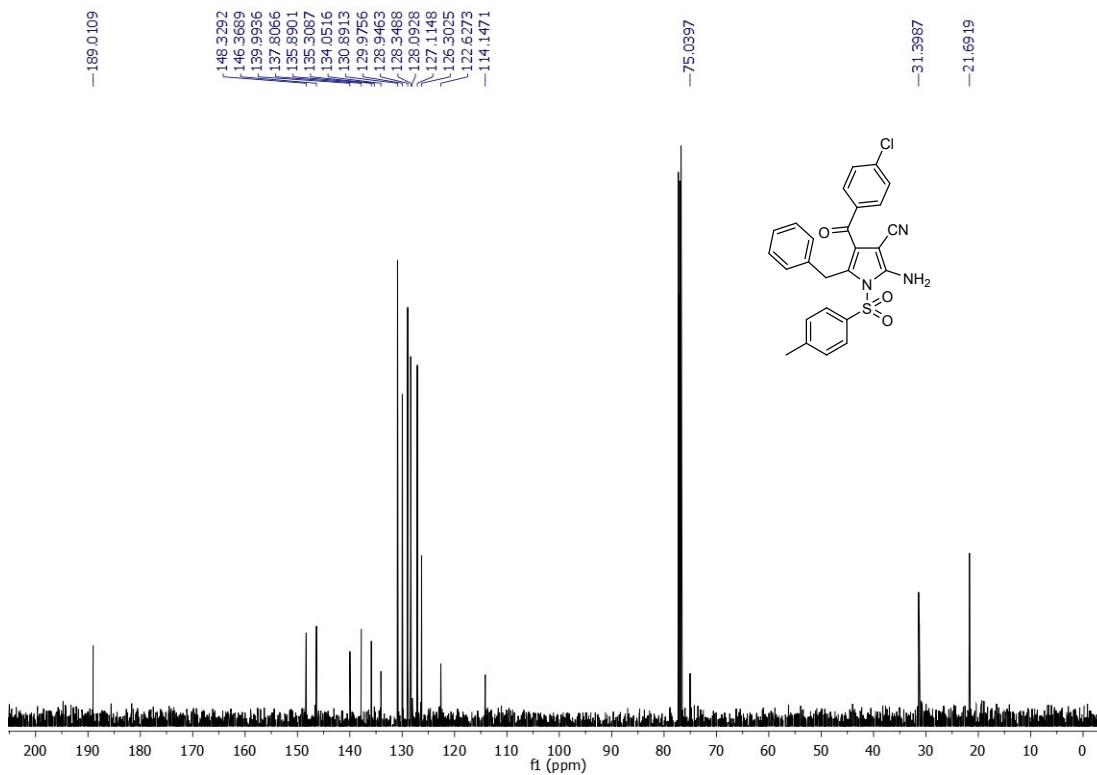
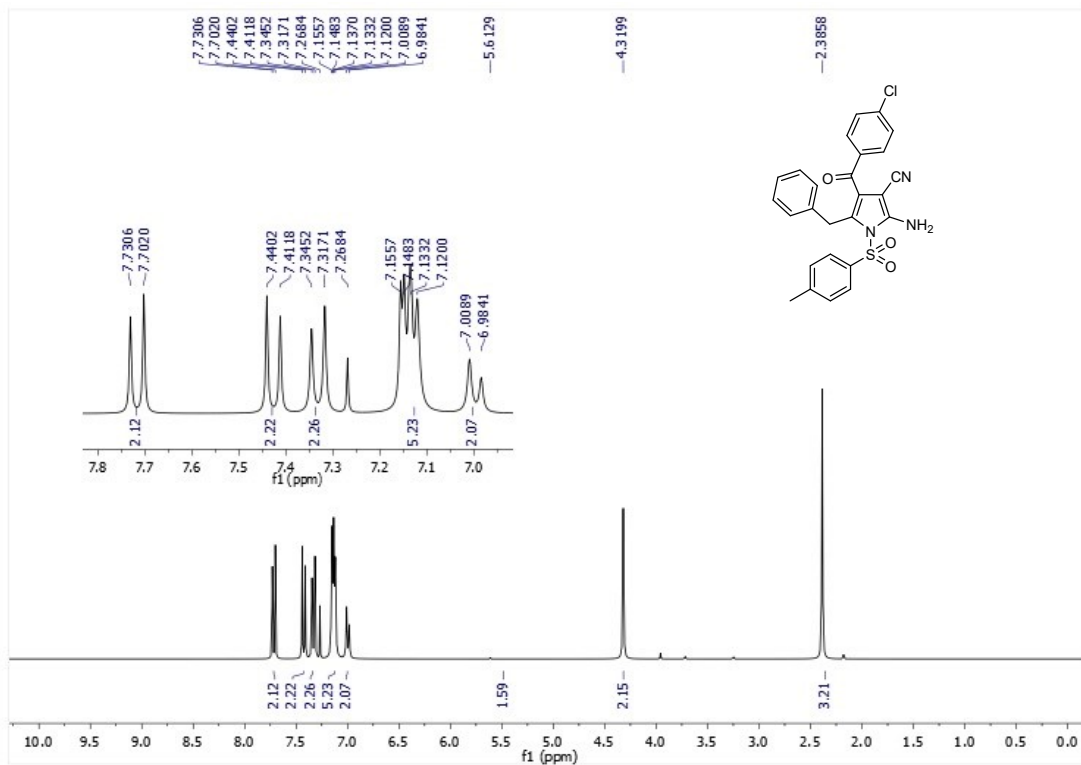
**<sup>13</sup>C NMR (75 MHz) of Compound 4k in CDCl<sub>3</sub>**

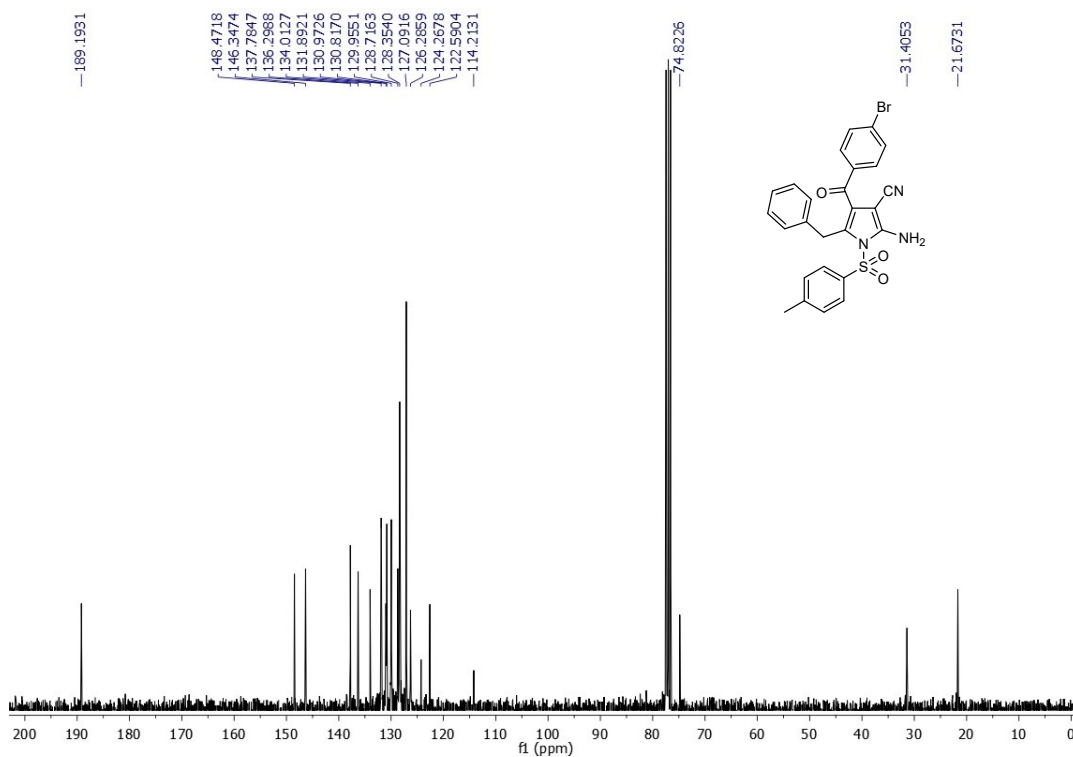
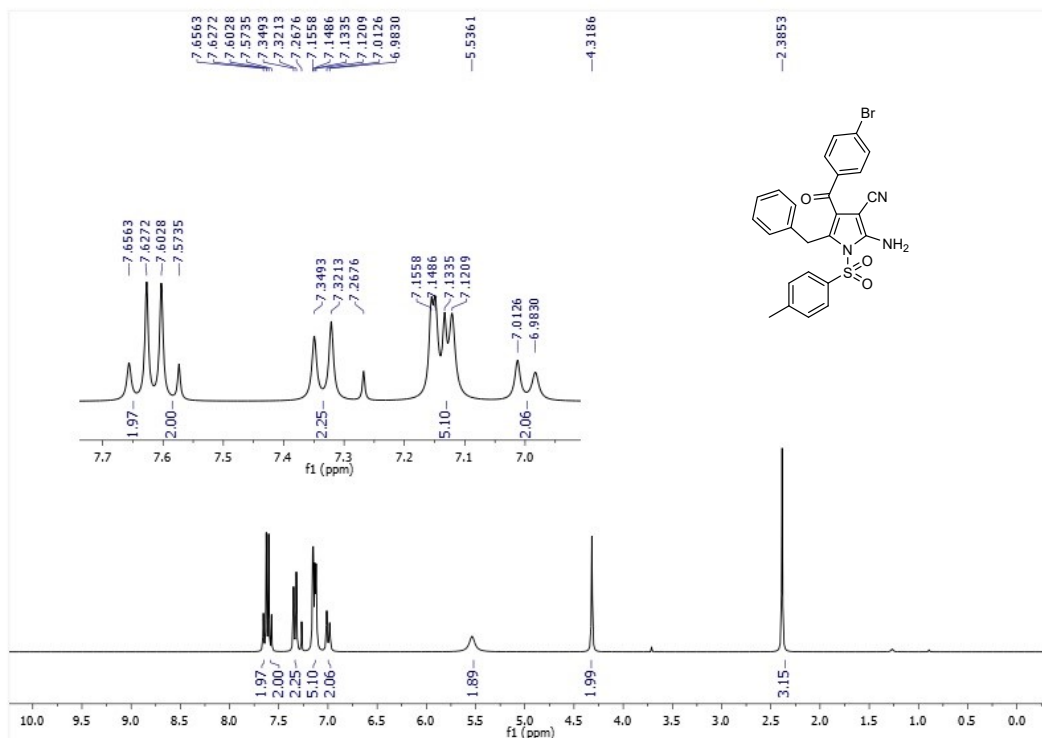


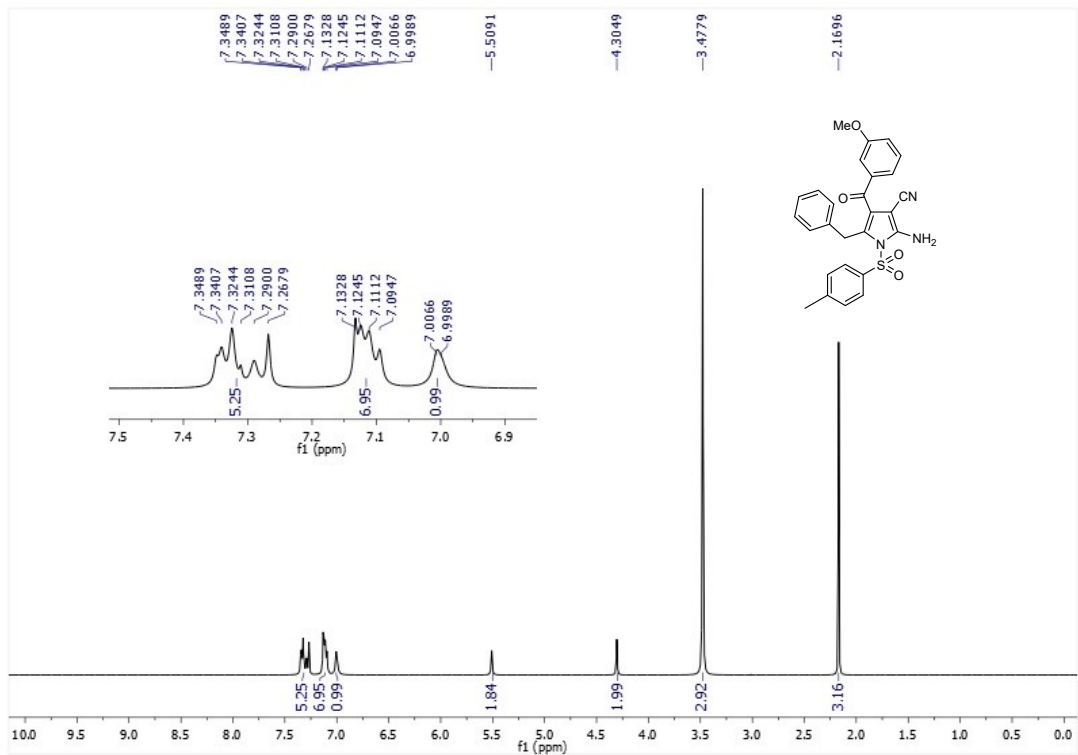
**<sup>1</sup>H NMR (300 MHz) of Compound 4I in CDCl<sub>3</sub>**



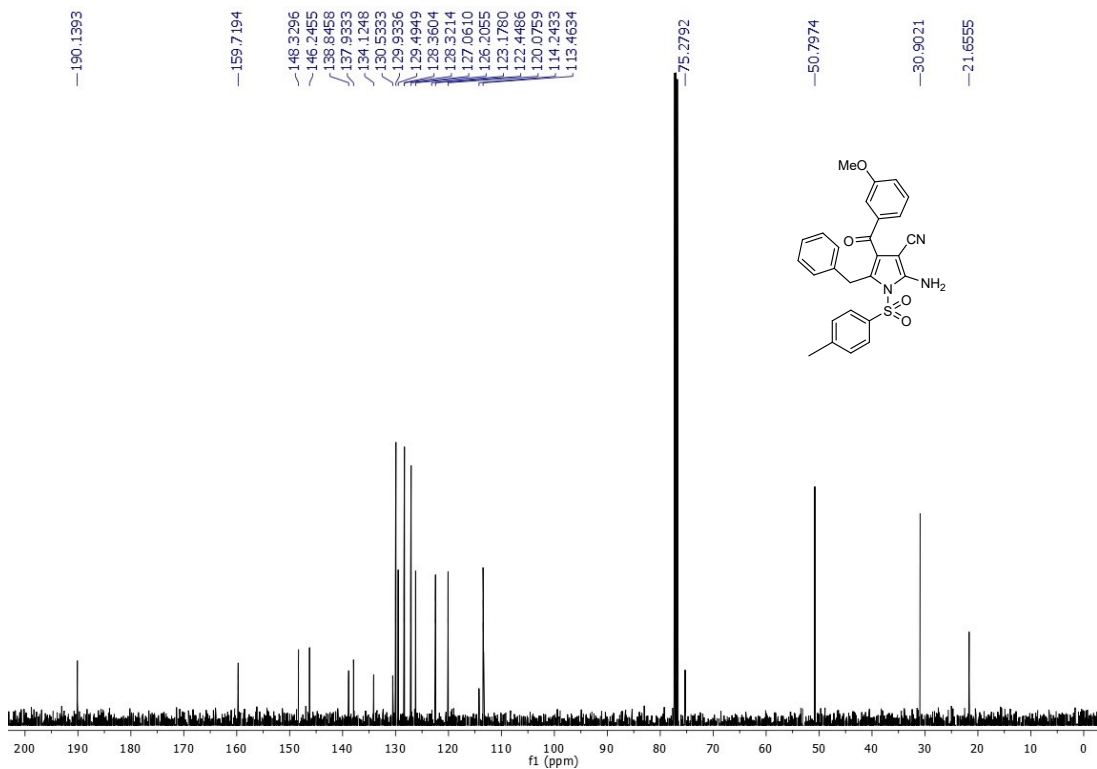
**<sup>13</sup>C NMR (75 MHz) of Compound 4I in CDCl<sub>3</sub>**





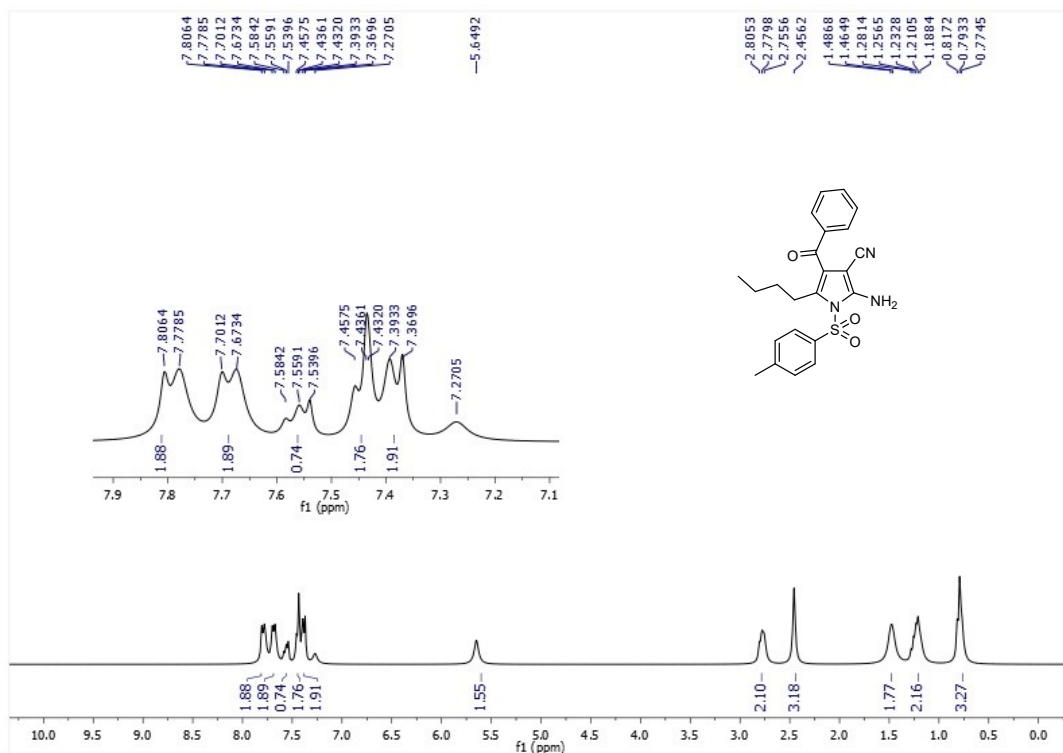


<sup>1</sup>H NMR (500 MHz) of Compound **40** in CDCl<sub>3</sub>

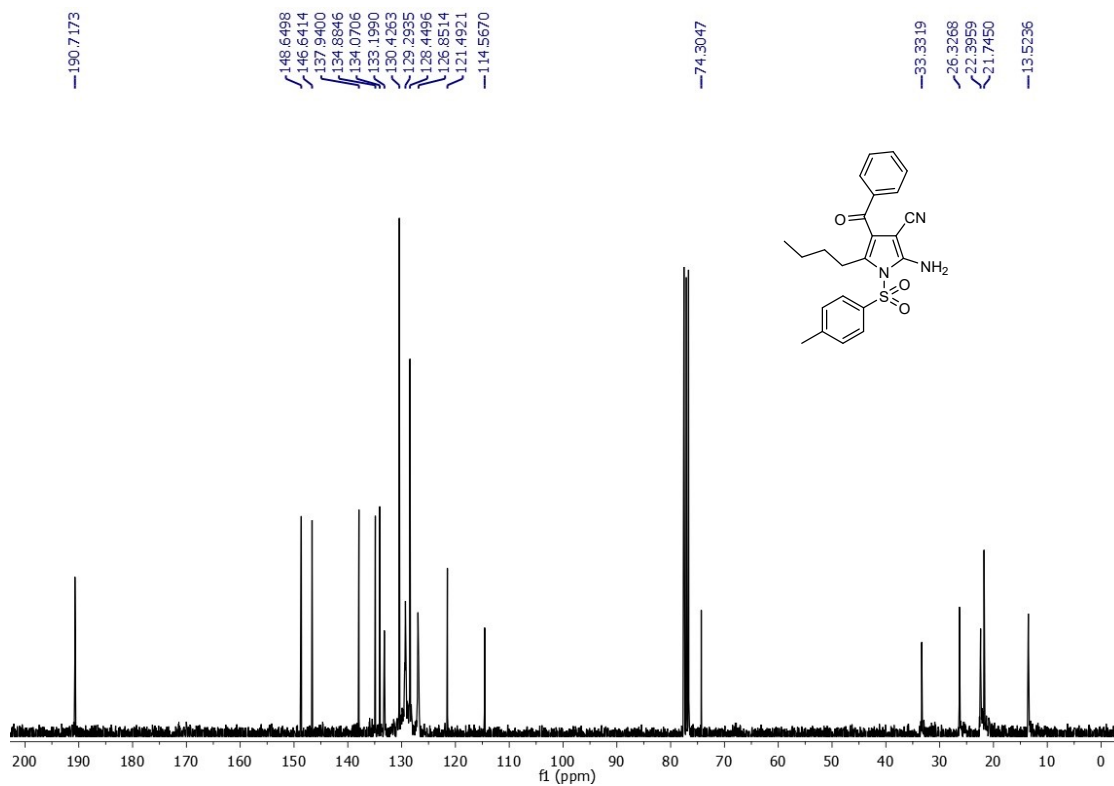


<sup>13</sup>C NMR (126 MHz) of Compound **40** in CDCl<sub>3</sub>

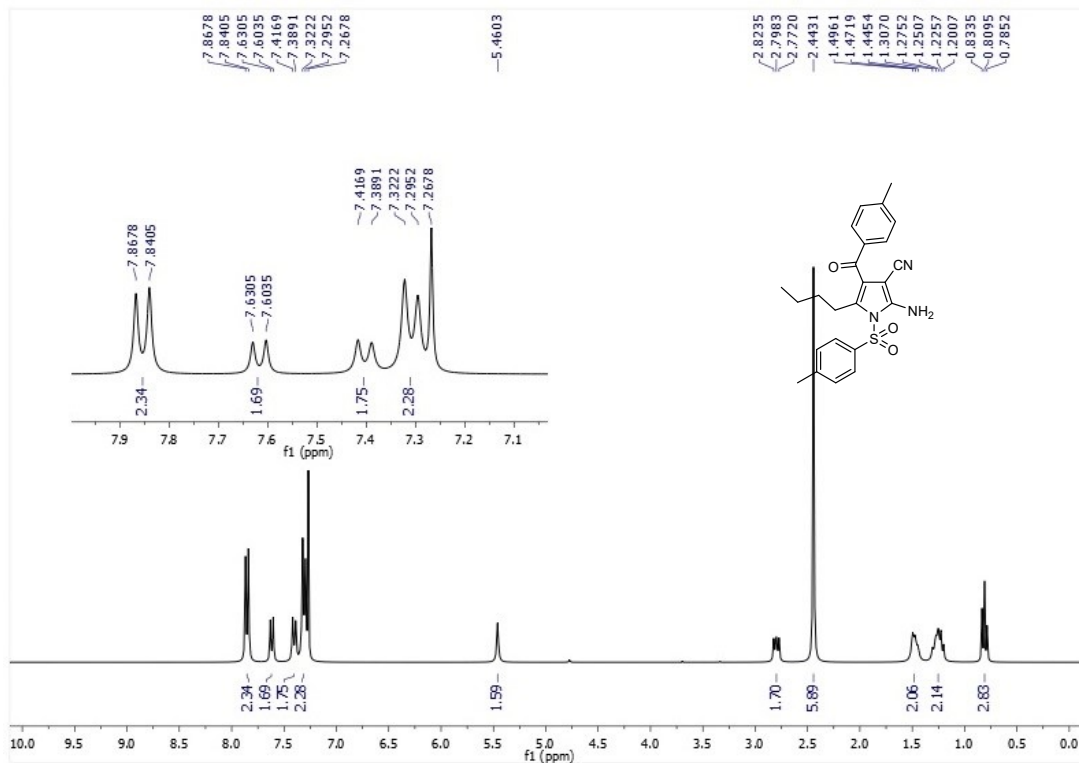




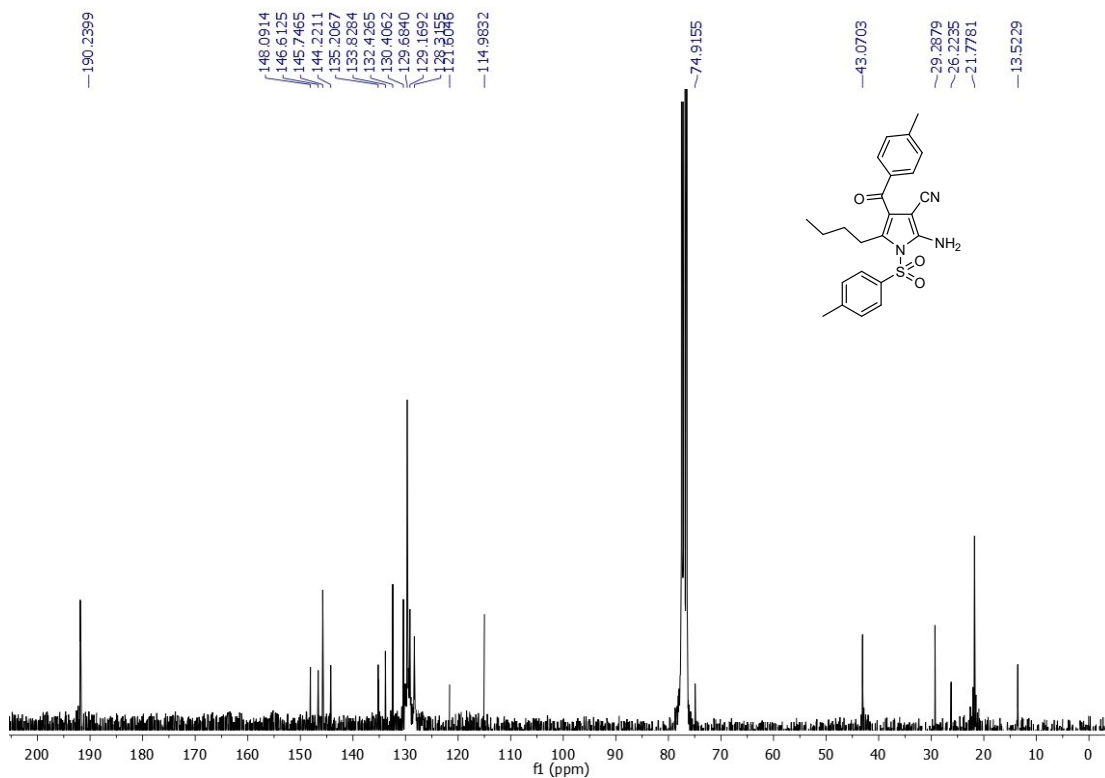
**<sup>1</sup>H NMR (300 MHz) of Compound 4p in CDCl<sub>3</sub>**



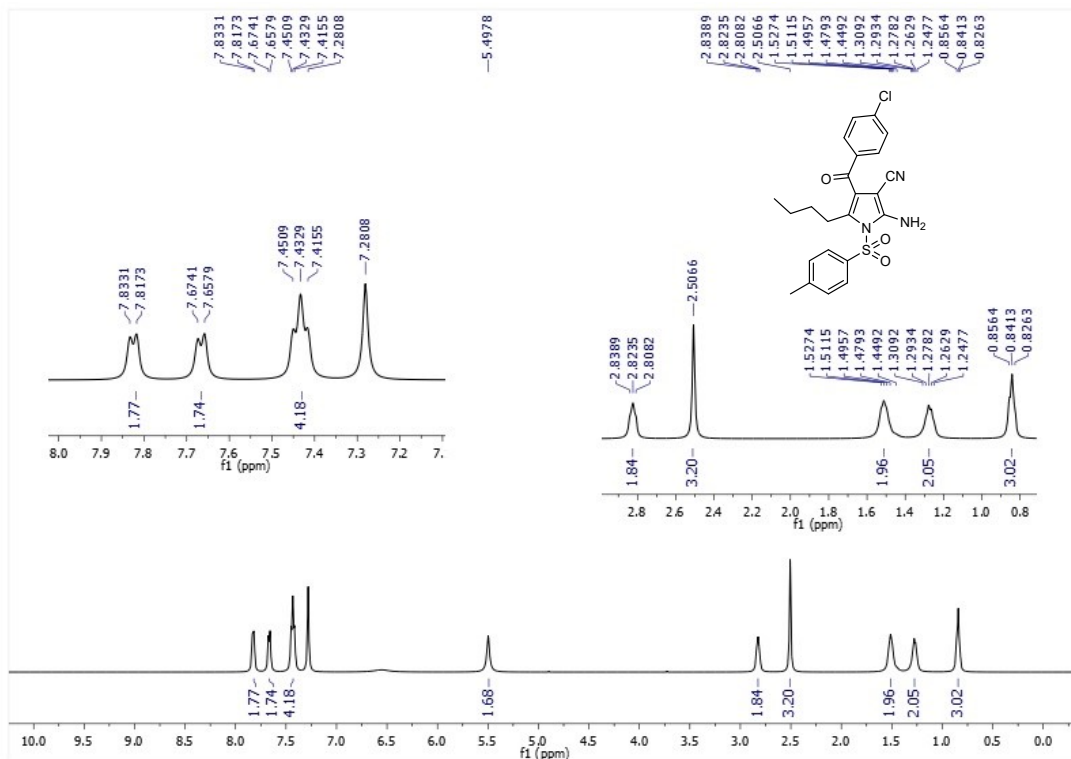
**<sup>13</sup>C NMR (75 MHz) of Compound 4p in CDCl<sub>3</sub>**



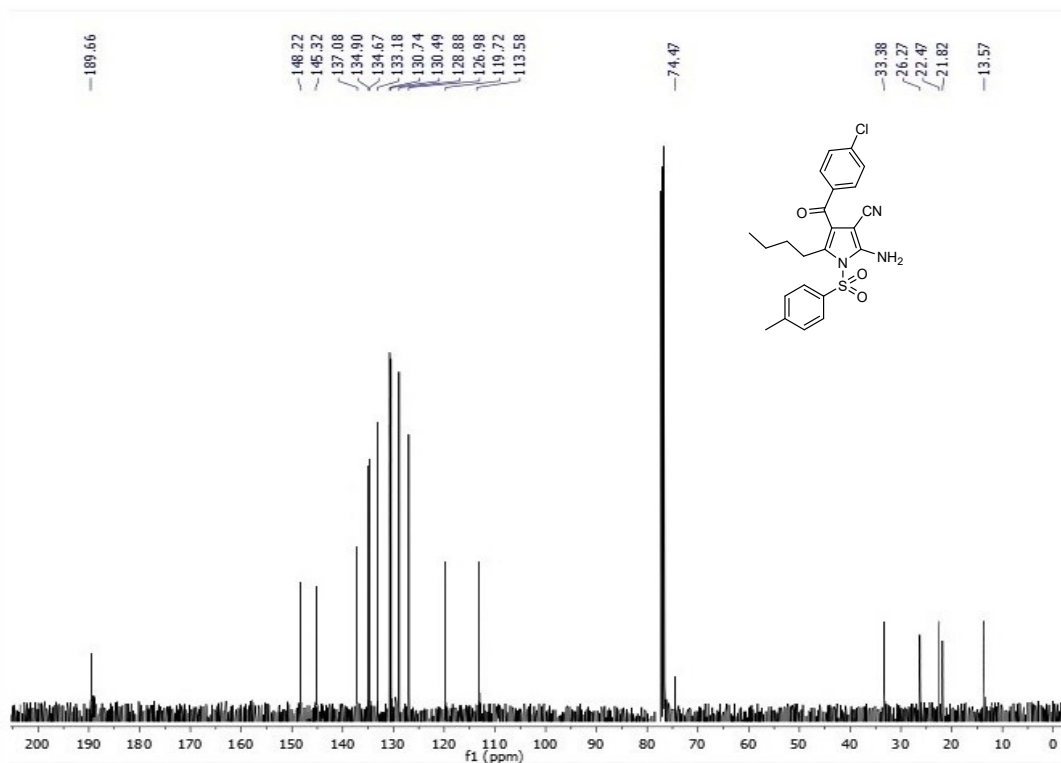
**<sup>1</sup>H NMR (300 MHz) of Compound 4q in CDCl<sub>3</sub>**



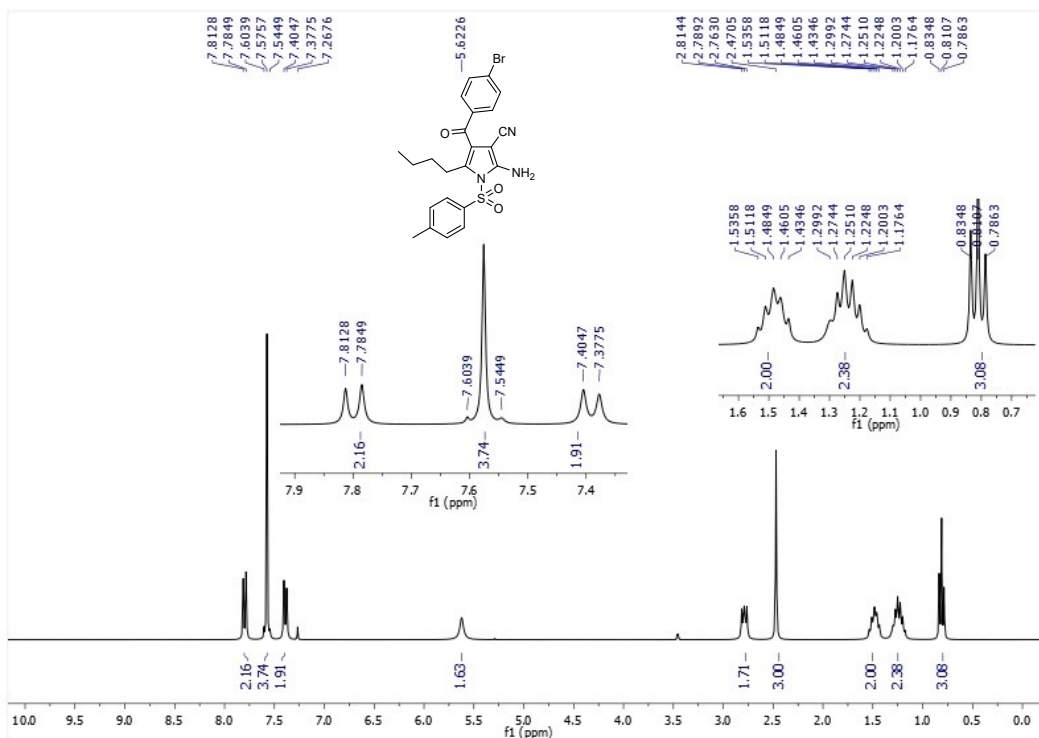
**<sup>13</sup>C NMR (75 MHz) of Compound 4q in CDCl<sub>3</sub>**



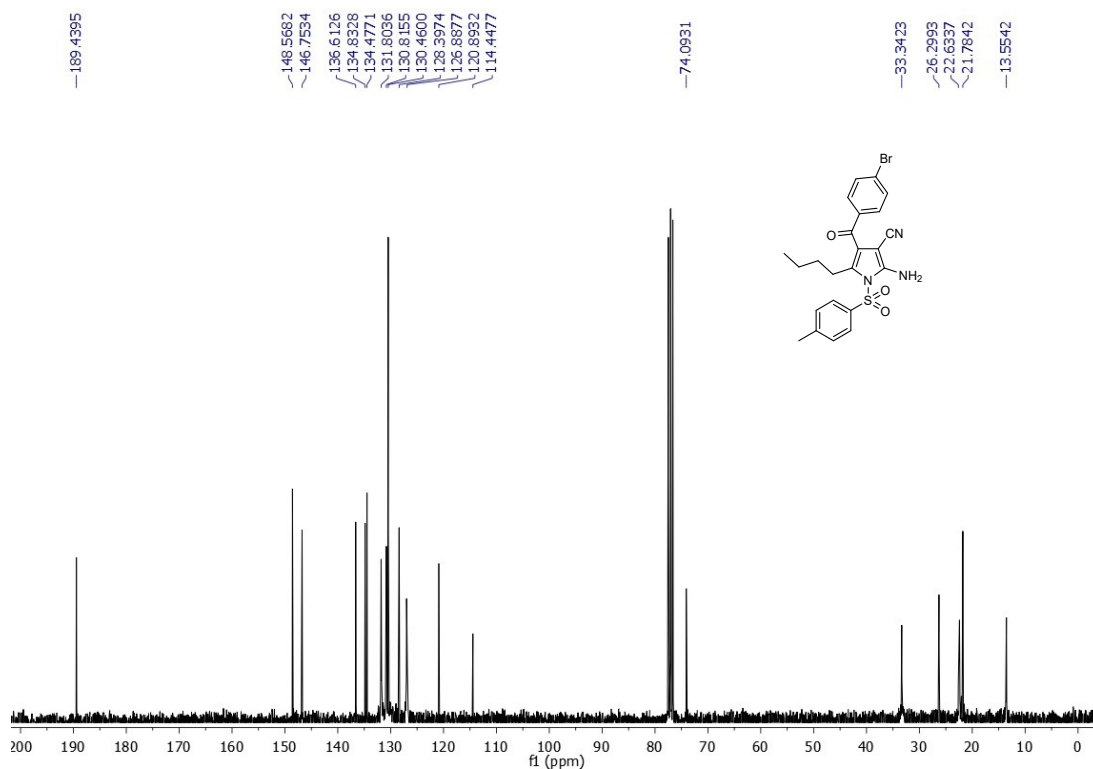
**<sup>1</sup>H NMR (500 MHz) of Compound 4r in CDCl<sub>3</sub>**



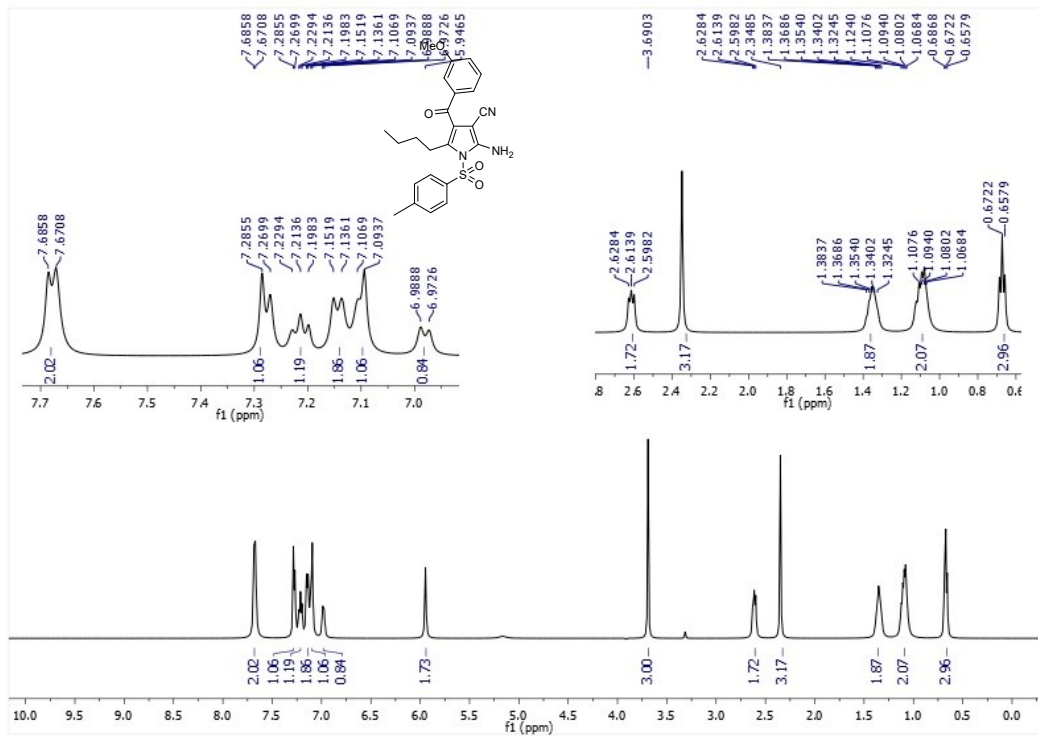
**<sup>13</sup>C NMR (126 MHz) of Compound 4r in CDCl<sub>3</sub>**



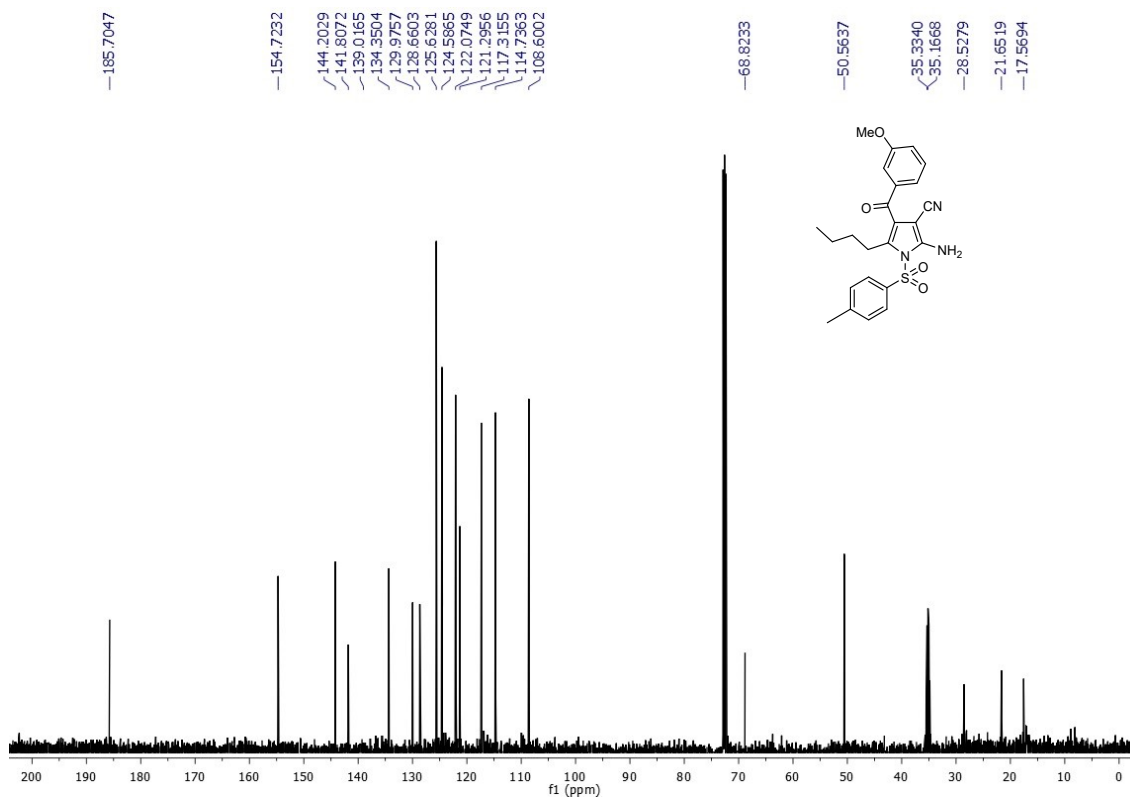
**<sup>1</sup>H NMR (300 MHz) of Compound 4s in CDCl<sub>3</sub>**



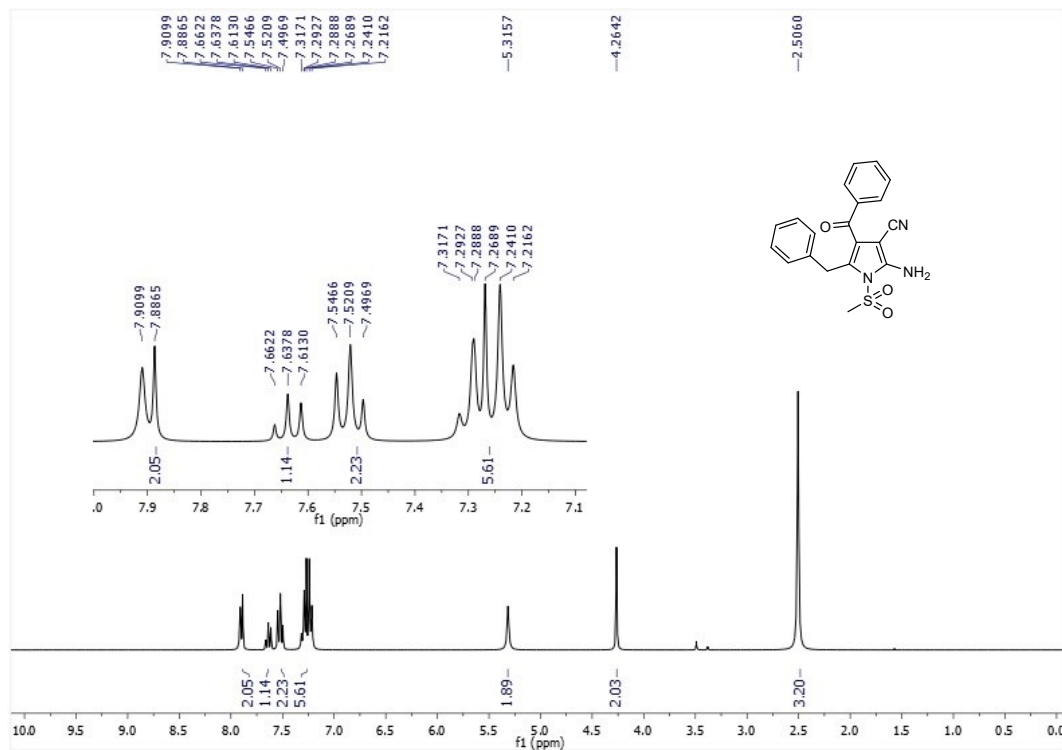
**<sup>13</sup>C NMR (75 MHz) of Compound 4s in CDCl<sub>3</sub>**



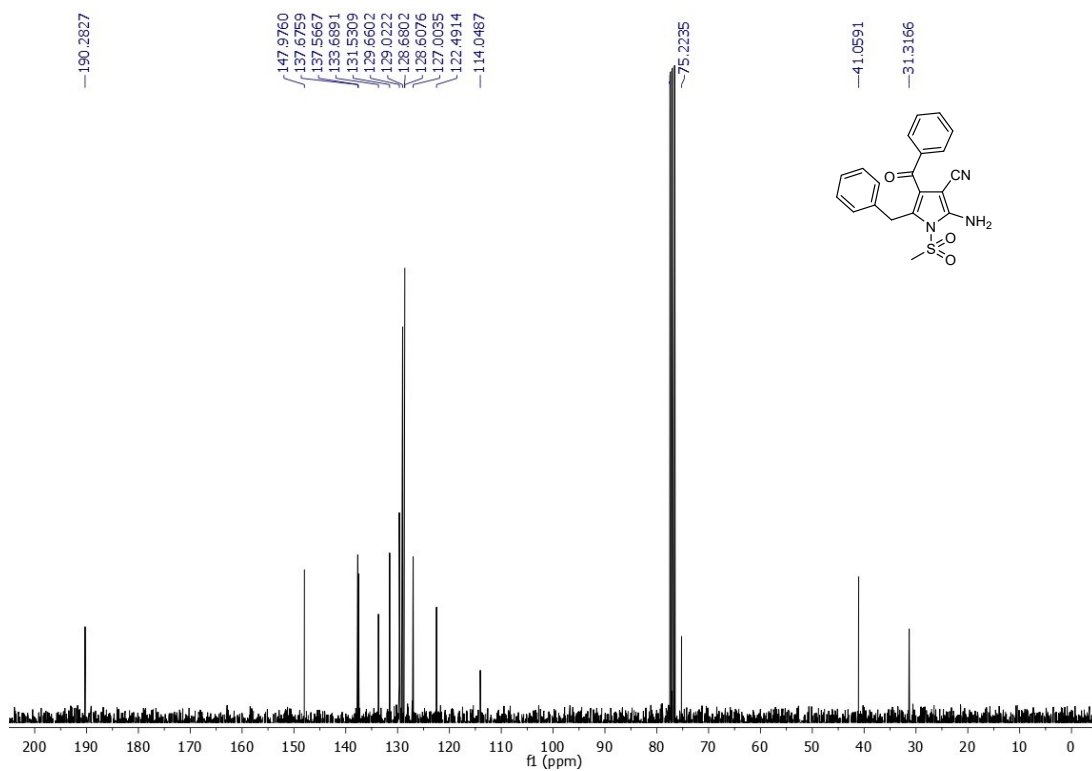
**<sup>1</sup>H NMR (500 MHz) of Compound 4t in CDCl<sub>3</sub>**



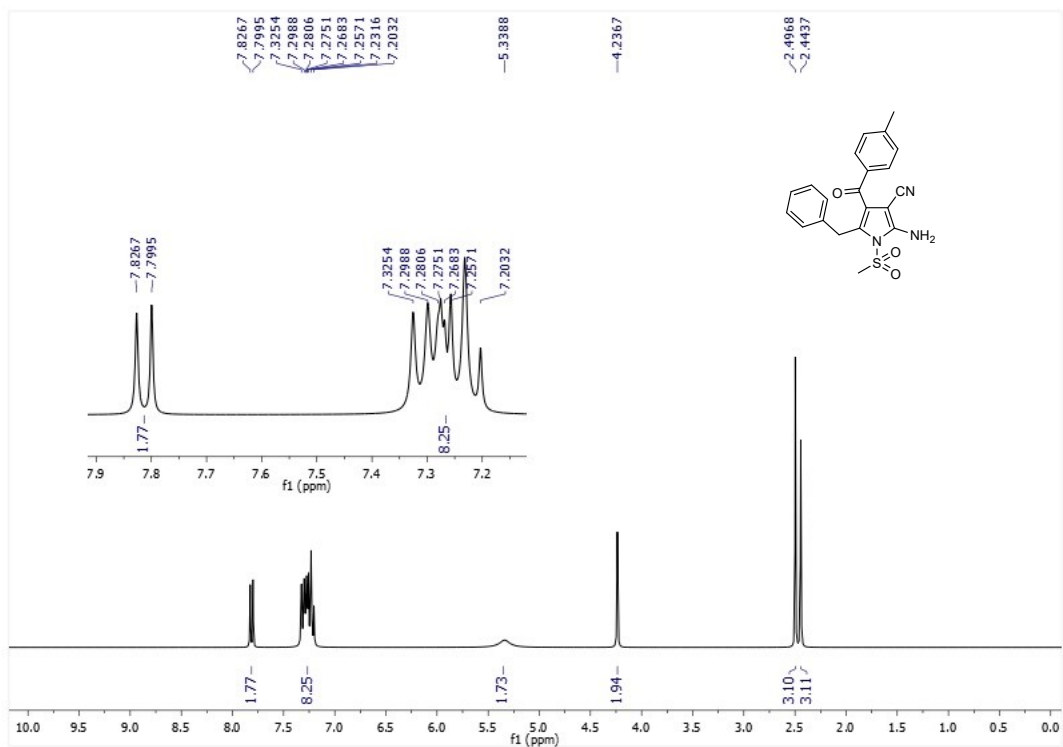
**<sup>13</sup>C NMR (126 MHz) of Compound 4t in CDCl<sub>3</sub>**



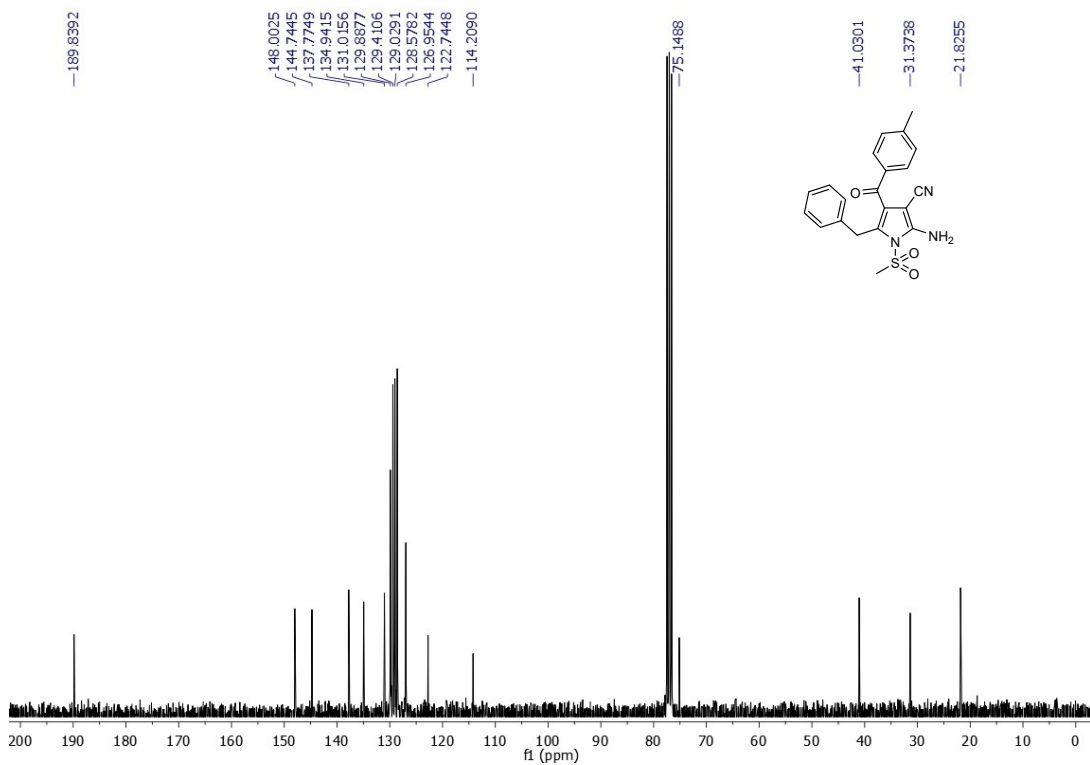
**<sup>1</sup>H NMR (300 MHz) of Compound **4u** in CDCl<sub>3</sub>**



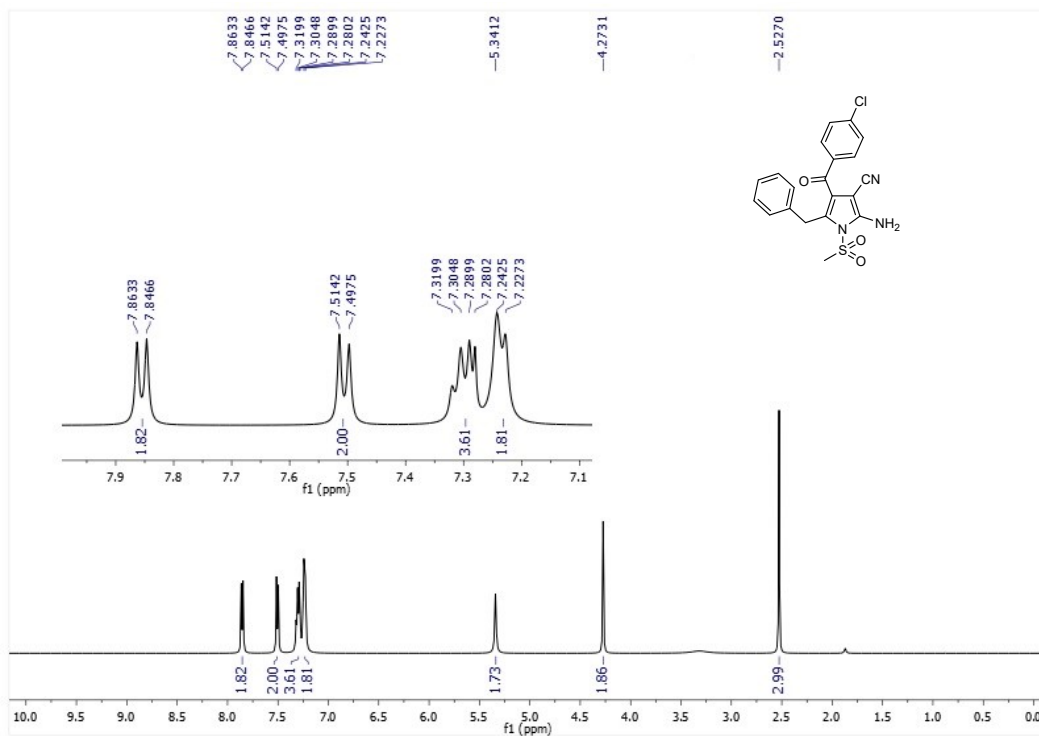
**<sup>13</sup>C NMR (75 MHz) of Compound **4u** in CDCl<sub>3</sub>**



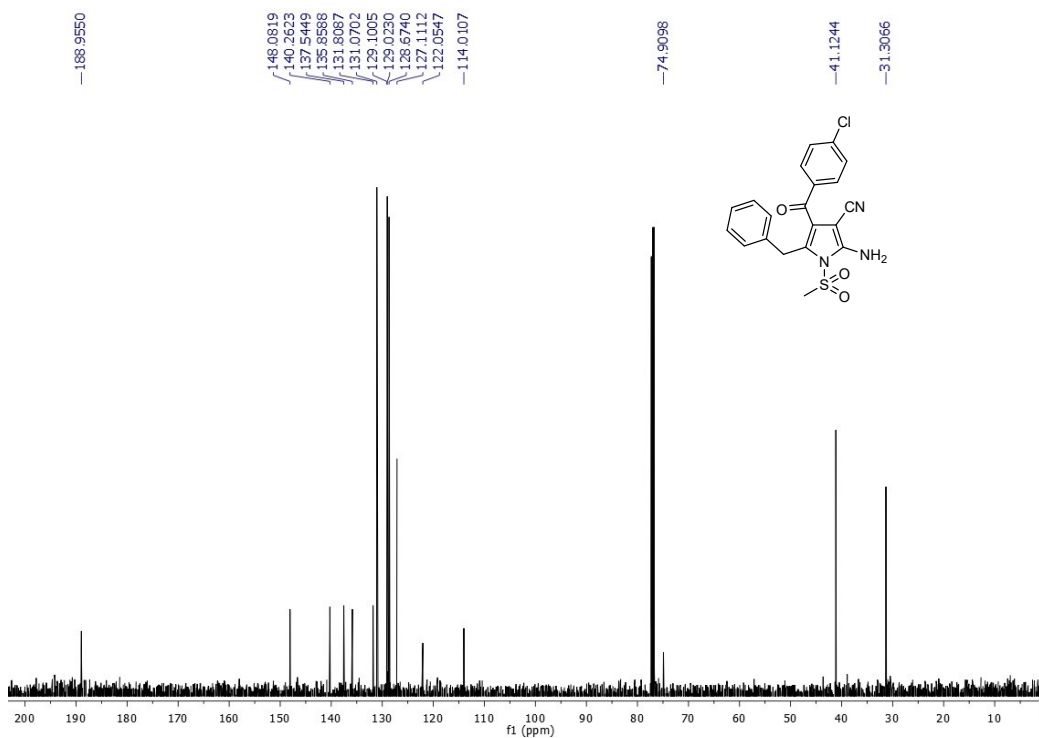
$^1\text{H NMR}$  (300 MHz) of Compound **4v** in  $\text{CDCl}_3$



$^{13}\text{C NMR}$  (75 MHz) of Compound **4v** in  $\text{CDCl}_3$

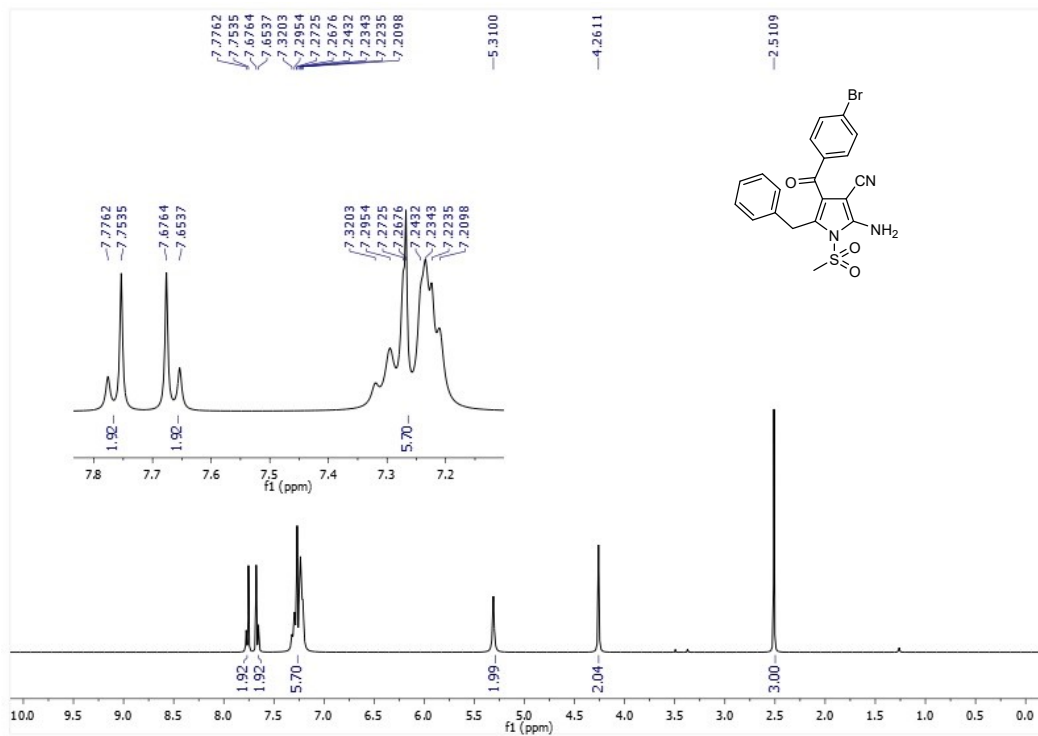


$^1\text{H}$  NMR (500 MHz) of Compound **4w** in  $\text{CDCl}_3$

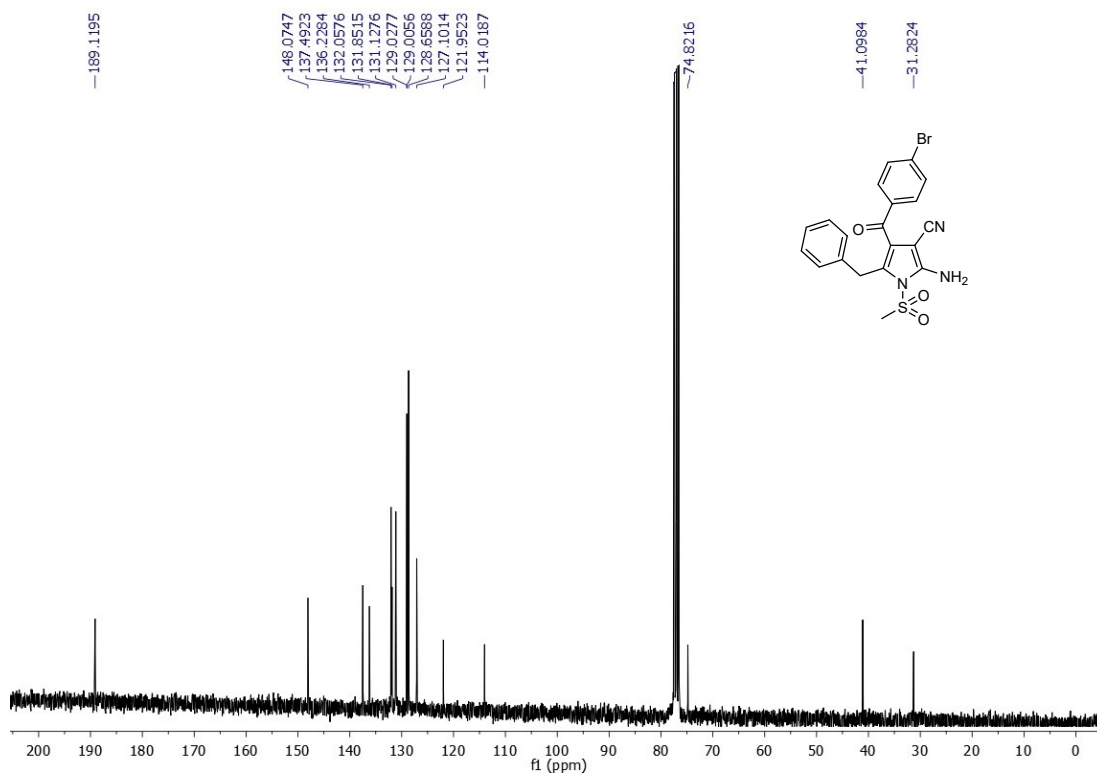


$^{13}\text{C}$  NMR (126 MHz) of Compound **4w** in  $\text{CDCl}_3$

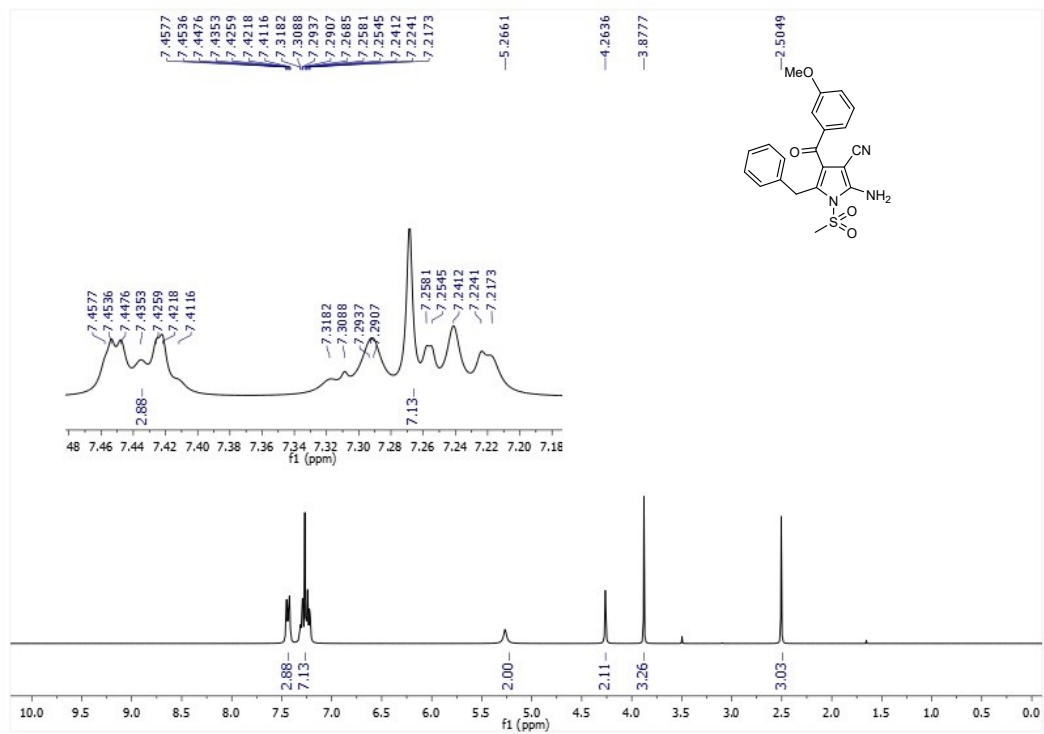




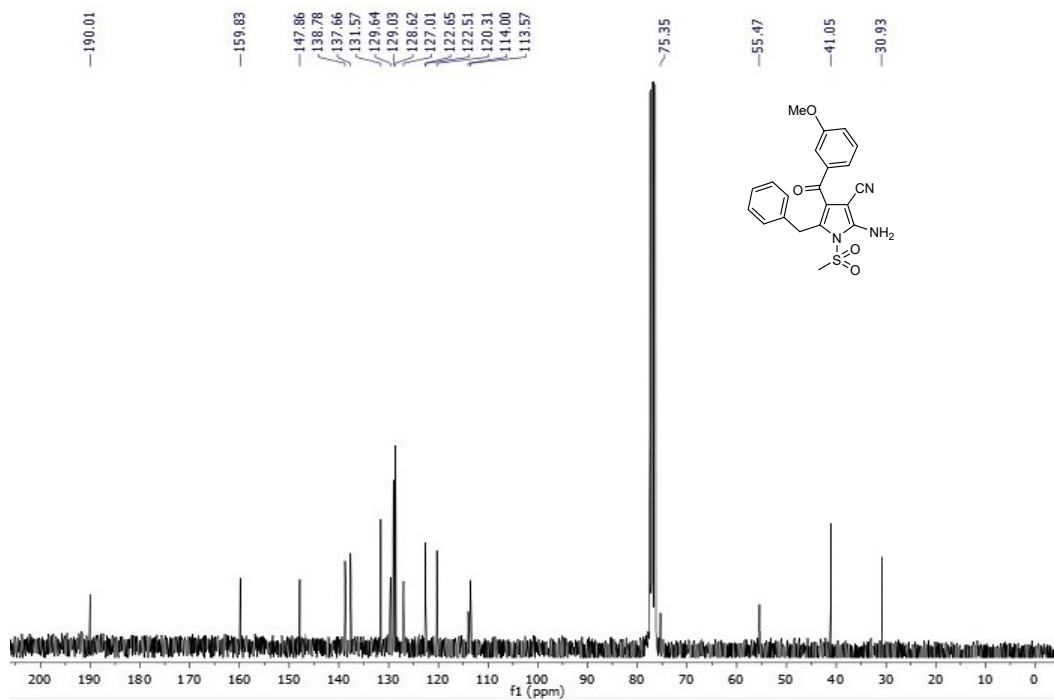
<sup>1</sup>H NMR (300 MHz) of Compound 4x in CDCl<sub>3</sub>



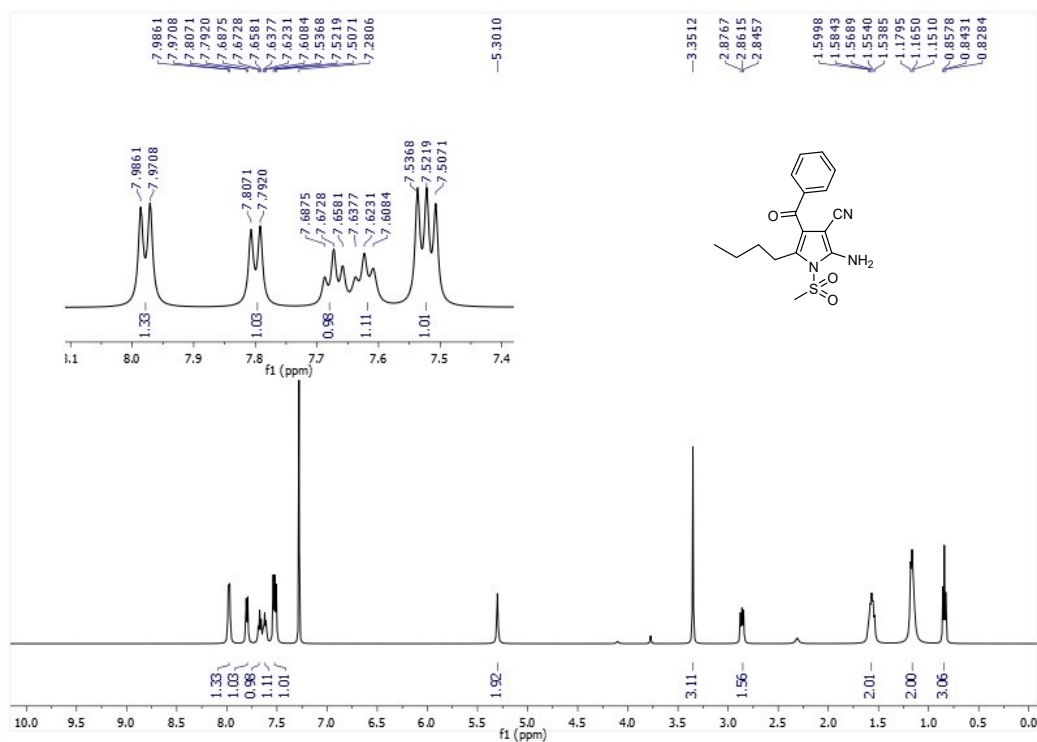
<sup>13</sup>C NMR (75 MHz) of Compound 4x in CDCl<sub>3</sub>



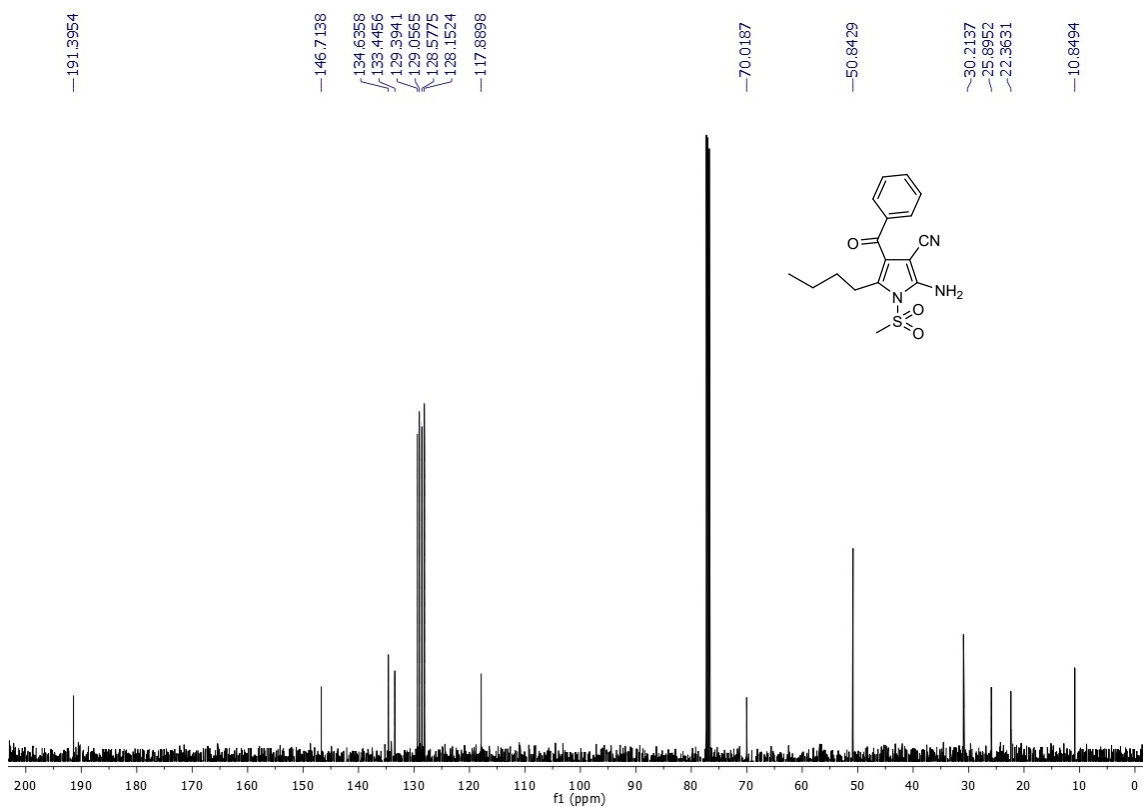
**<sup>1</sup>H NMR (300 MHz) of Compound 4y in CDCl<sub>3</sub>**



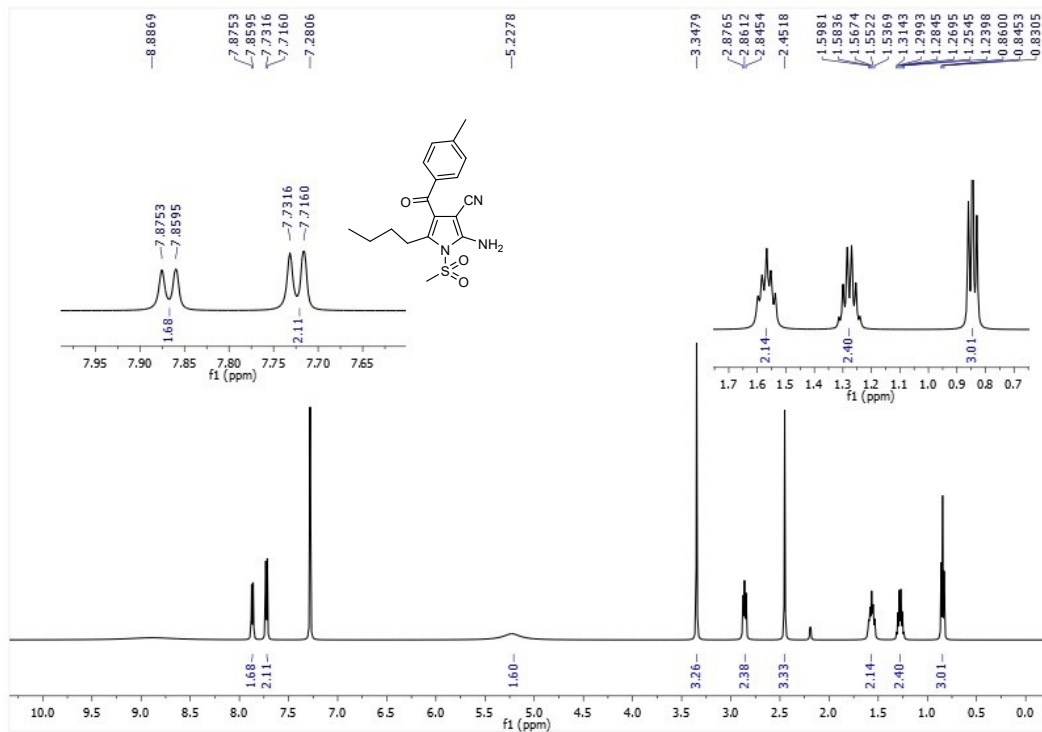
**<sup>13</sup>C NMR (75 MHz) of Compound 4y in CDCl<sub>3</sub>**



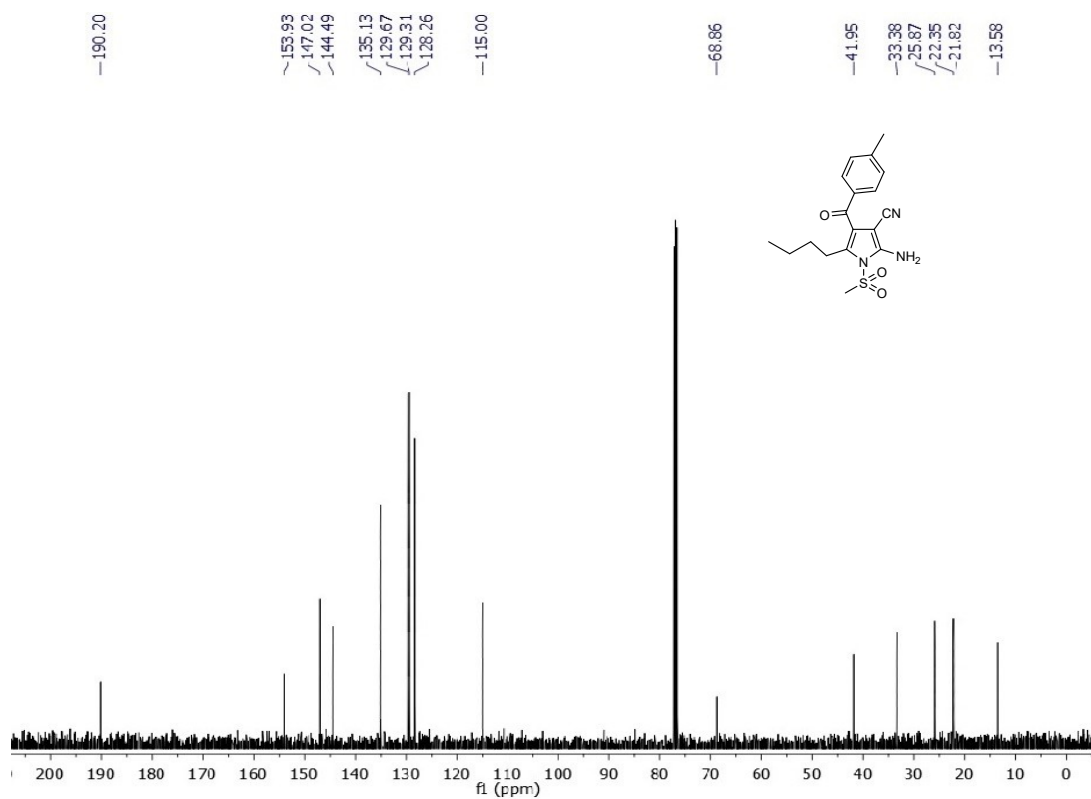
<sup>1</sup>H NMR (500 MHz) of Compound 4z in CDCl<sub>3</sub>



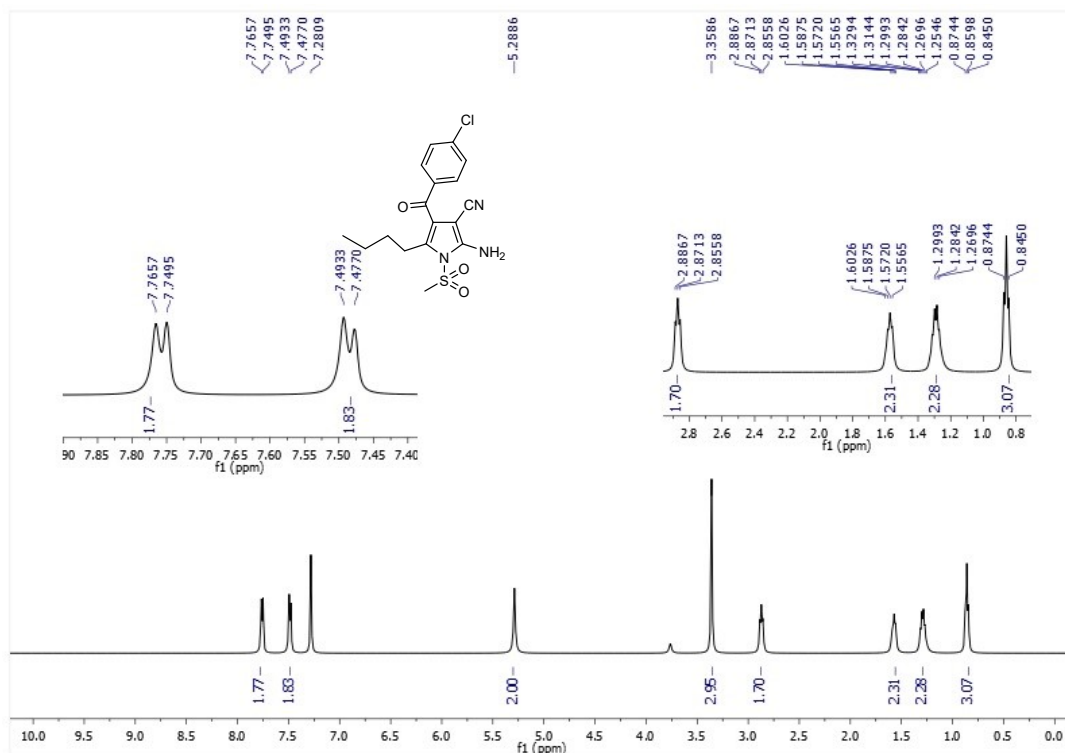
<sup>13</sup>C NMR (126 MHz) of Compound 4z in CDCl<sub>3</sub>



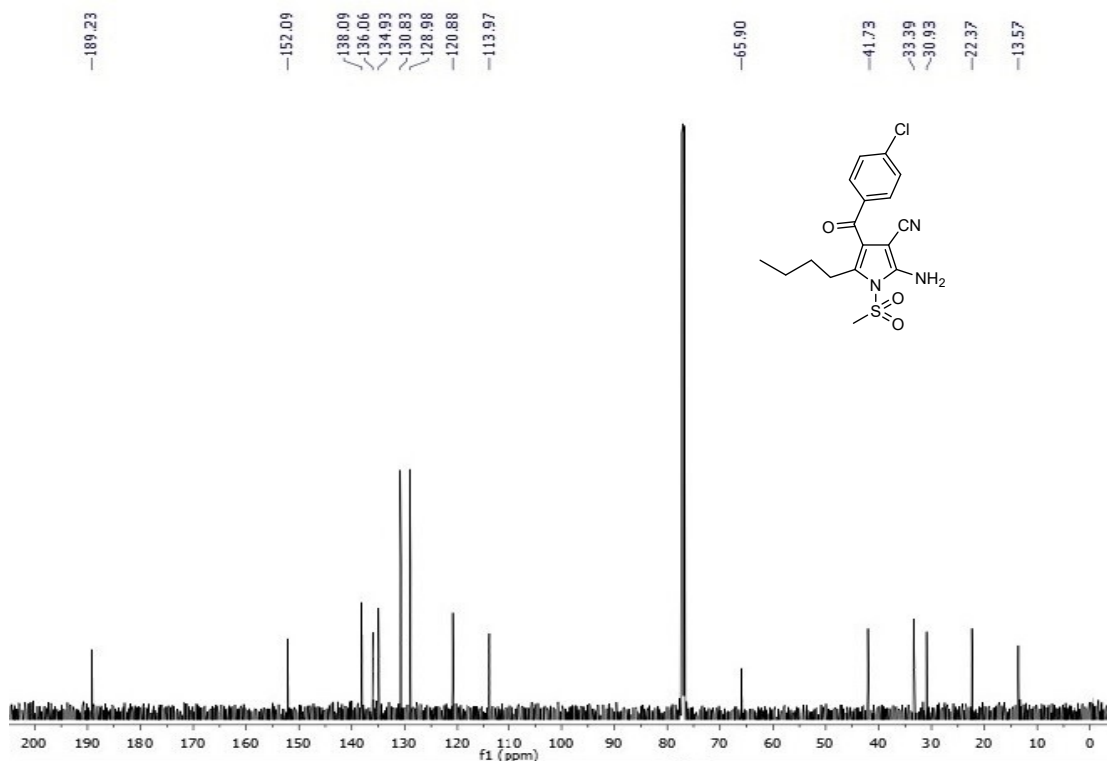
**<sup>1</sup>H NMR (500 MHz) of Compound 4aa in CDCl<sub>3</sub>**



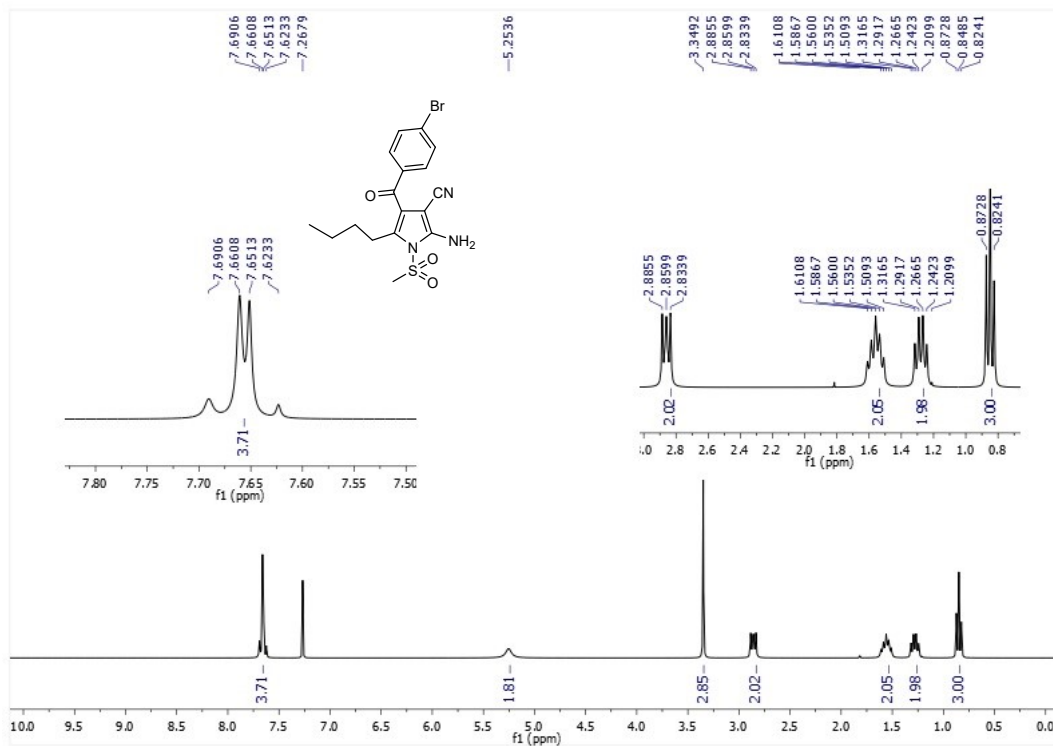
**<sup>13</sup>C NMR (126 MHz) of Compound 4aa in CDCl<sub>3</sub>**



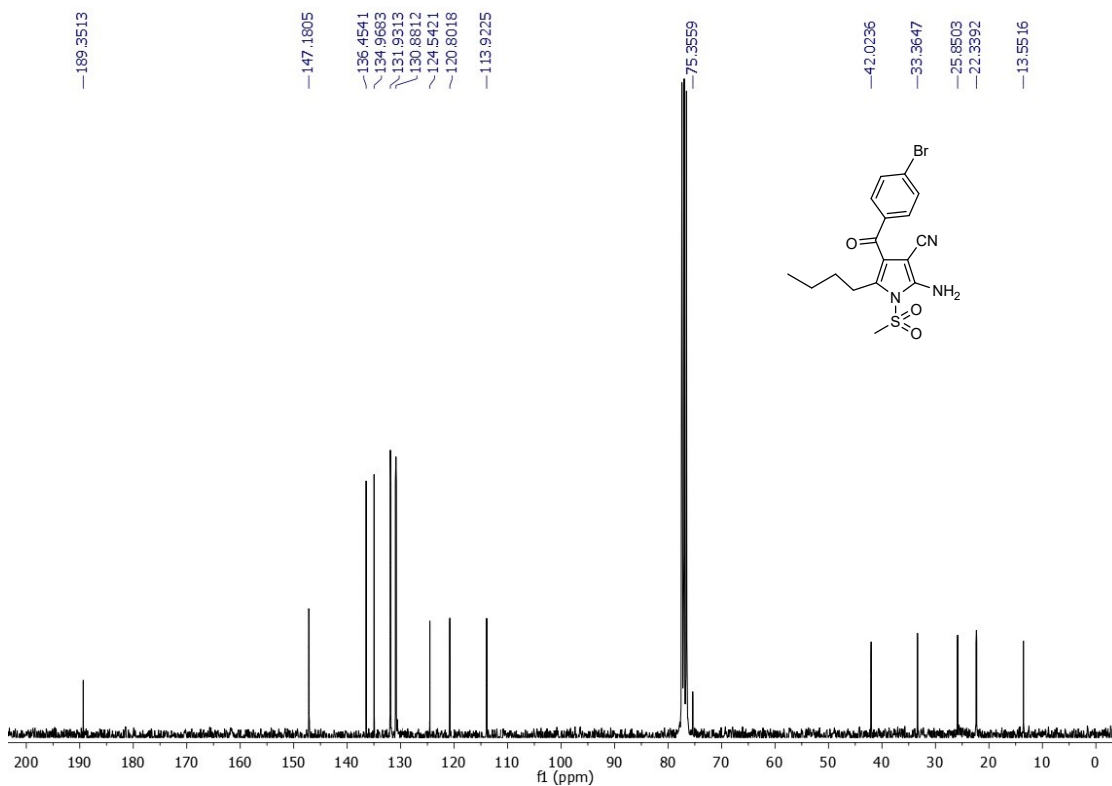
<sup>1</sup>H NMR (500 MHz) of Compound 4ab in CDCl<sub>3</sub>



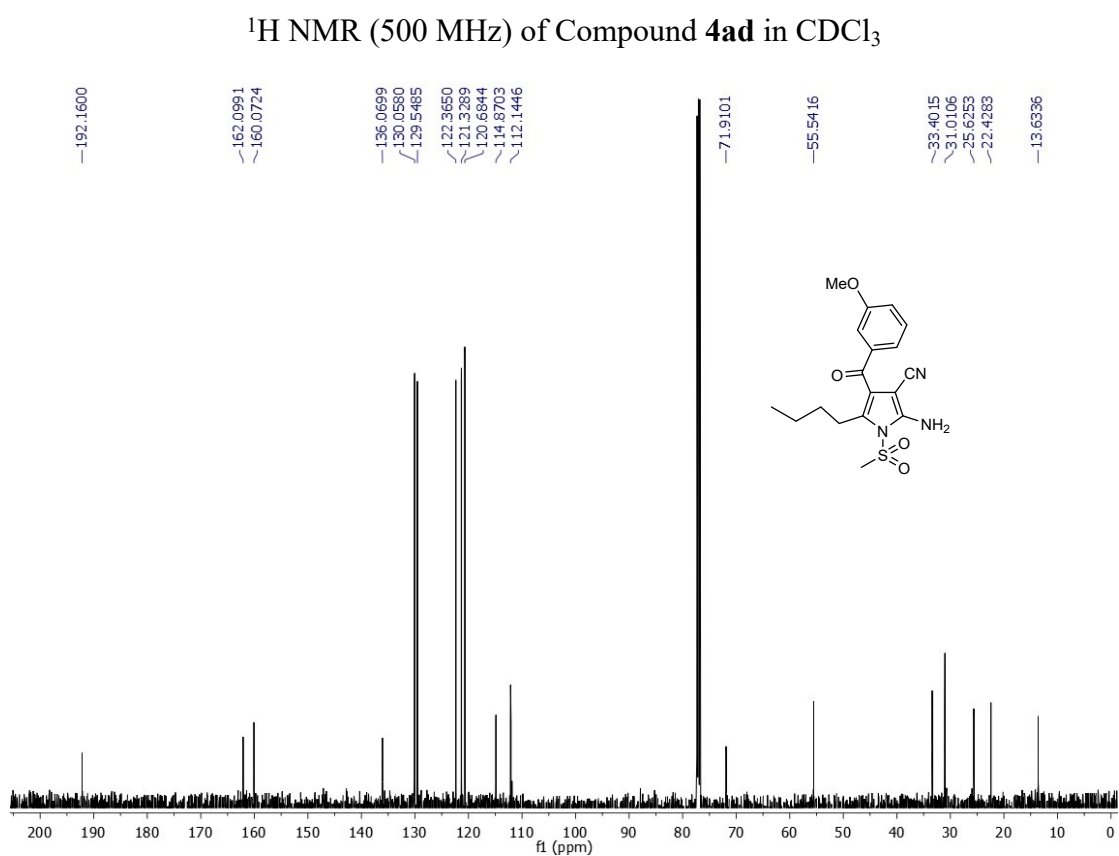
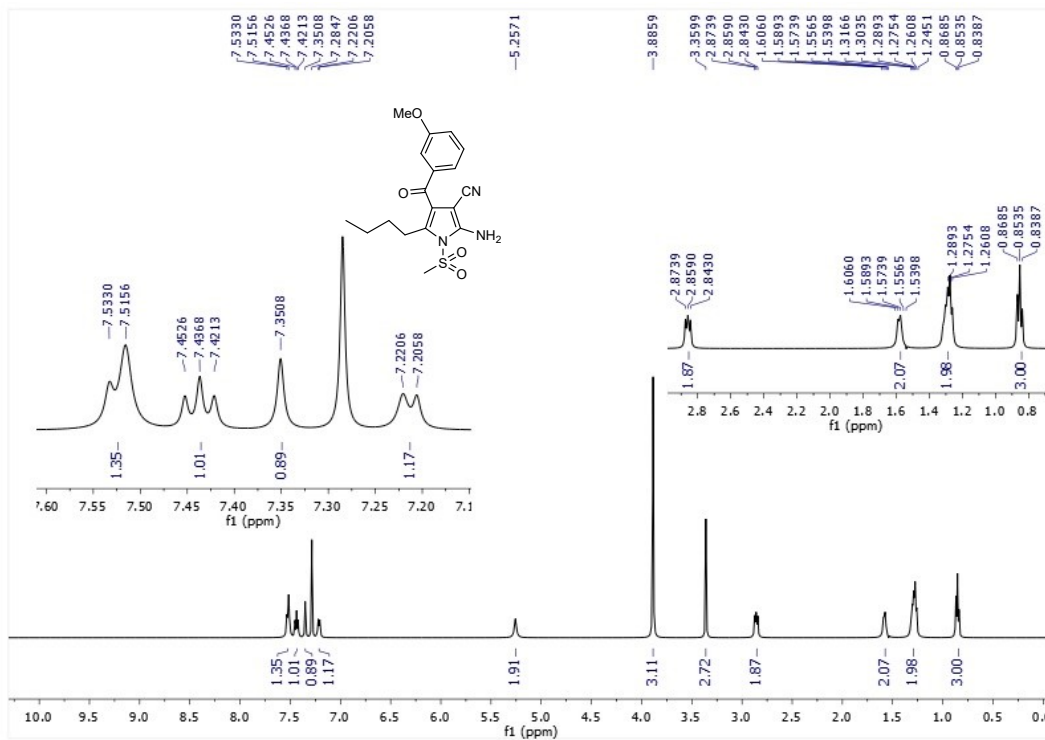
<sup>13</sup>C NMR (126 MHz) of Compound 4ab in CDCl<sub>3</sub>



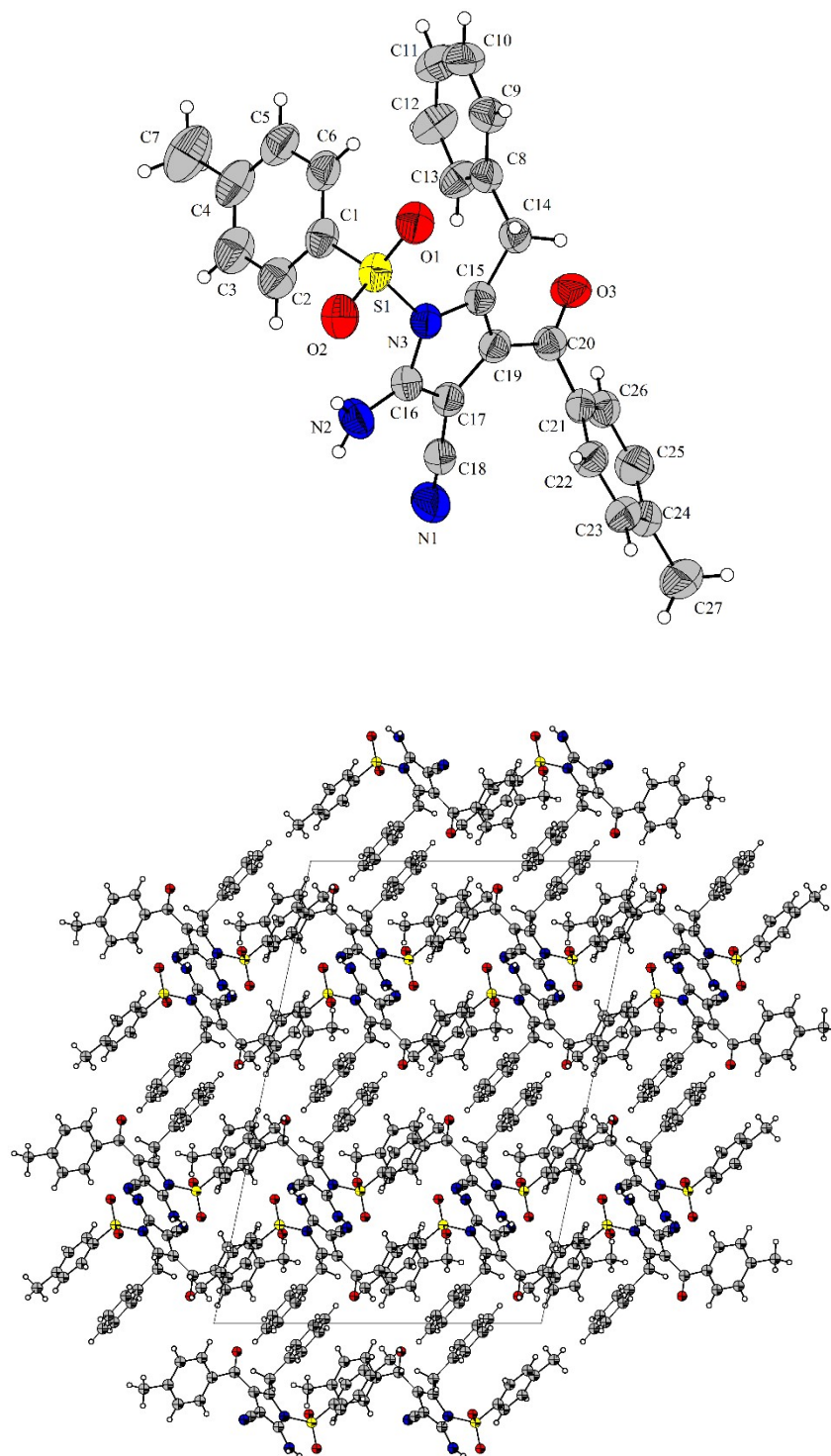
**<sup>1</sup>H NMR (300 MHz) of Compound 4ac in CDCl<sub>3</sub>**



**<sup>13</sup>C NMR (75 MHz) of Compound 4ac in CDCl<sub>3</sub>**



## X-ray crystal-structure determination of compound **41**



**Figure S1.** X-ray crystal-structure determination of compound **41**. The ellipsoid contour probability levels are 50%. CCDC 2132591 (**41**) contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* [www.ccdc.cam.ac.uk/getstructures](http://www.ccdc.cam.ac.uk/getstructures).



**Table S1.** Experimental details of Crystal data

<b>Chemical formula</b>	<b>C<sub>27</sub>H<sub>23</sub>N<sub>3</sub>O<sub>3</sub>S</b>
<i>Mr</i>	469.54
Crystal system, space group	Monoclinic, <i>I12/c1</i>
Temperature (K)	290
<i>a</i> , <i>b</i> , <i>c</i> (Å)	17.402 (4), 11.109 (2), 25.127 (10)Å
$\beta$ (°)	101.82 (3)
<i>V</i> (Å <sup>3</sup> )	4755 (2)
<i>Z</i>	4
Radiation type	Mo <i>K</i> $\alpha$
$\mu$ (mm <sup>-1</sup> )	0.17 mm <sup>-1</sup>
Crystal size (mm)	0.4 × 0.3 × 0.25 mm

**Data collection**

Diffractometer	MAR345
<i>h</i> , <i>k</i> , <i>l</i>	-13→13, -20→20, -19→20
<i>T</i> <sub>min</sub> , <i>T</i> <sub>max</sub>	0.969, 1.047
No. of measured, independent and observed [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )] reflections	13895, 4626, 4117
<i>R</i> <sub>int</sub>	0.098
$\theta$ <sub>max</sub> , $\theta$ <sub>min</sub>	25.0°, 2.1°

**Refinement**

<i>R</i> [ <i>F</i> <sup>2</sup> > 2 $\sigma$ ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.051, 0.132, 1.09
No. of reflections	4626
No. of parameters	318
No. of restraints	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho$ <sub>max</sub> , $\Delta\rho$ <sub>min</sub> (e Å <sup>-3</sup> )	0.24, -0.31

Computer programs: MAR345 dtb Program (1.24-4, 2013), Automar software package (3.3a, 2015), *SHELXT* 2018/2 (Sheldrick, 2018), *SHELXL2016/6* (Sheldrick, 2016), *DIAMOND* (Brandenburg, 1999), *PLATON* (2018).

## References

Sheldrick, G. M. (2015). *Acta Cryst. A* 71, 3-8.

Sheldrick, G. M. (2015). *Acta Cryst. C* 71, 3-8.