



## Supporting Information

for

### **Cyanothioacetamides as a synthetic platform for the synthesis of aminopyrazole derivatives**

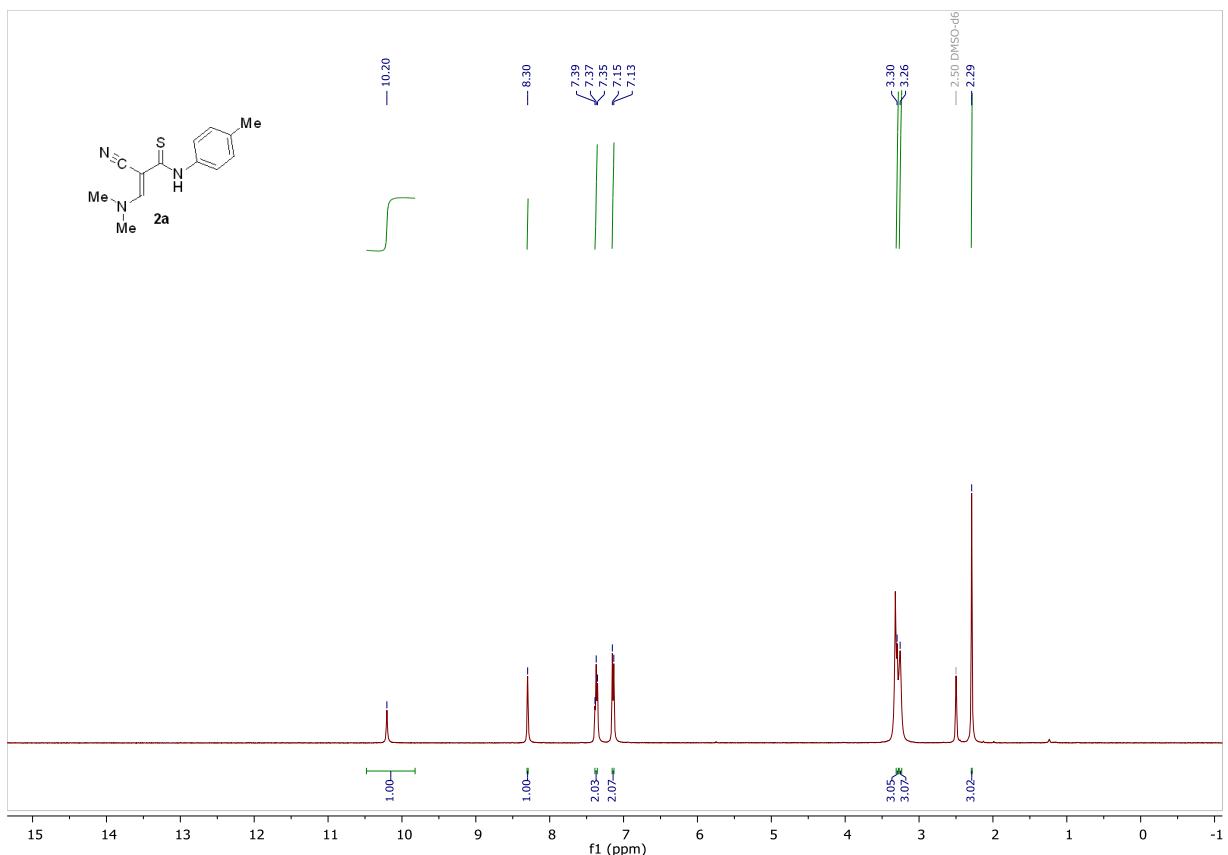
Valeriy O. Filimonov, Alexandra I. Topchiy, Vladimir G. Ilkin, Tetyana V. Beryozkina and Vasiliy A. Bakulev

*Beilstein J. Org. Chem.* **2023**, *19*, 1191–1197. doi:10.3762/bjoc.19.87

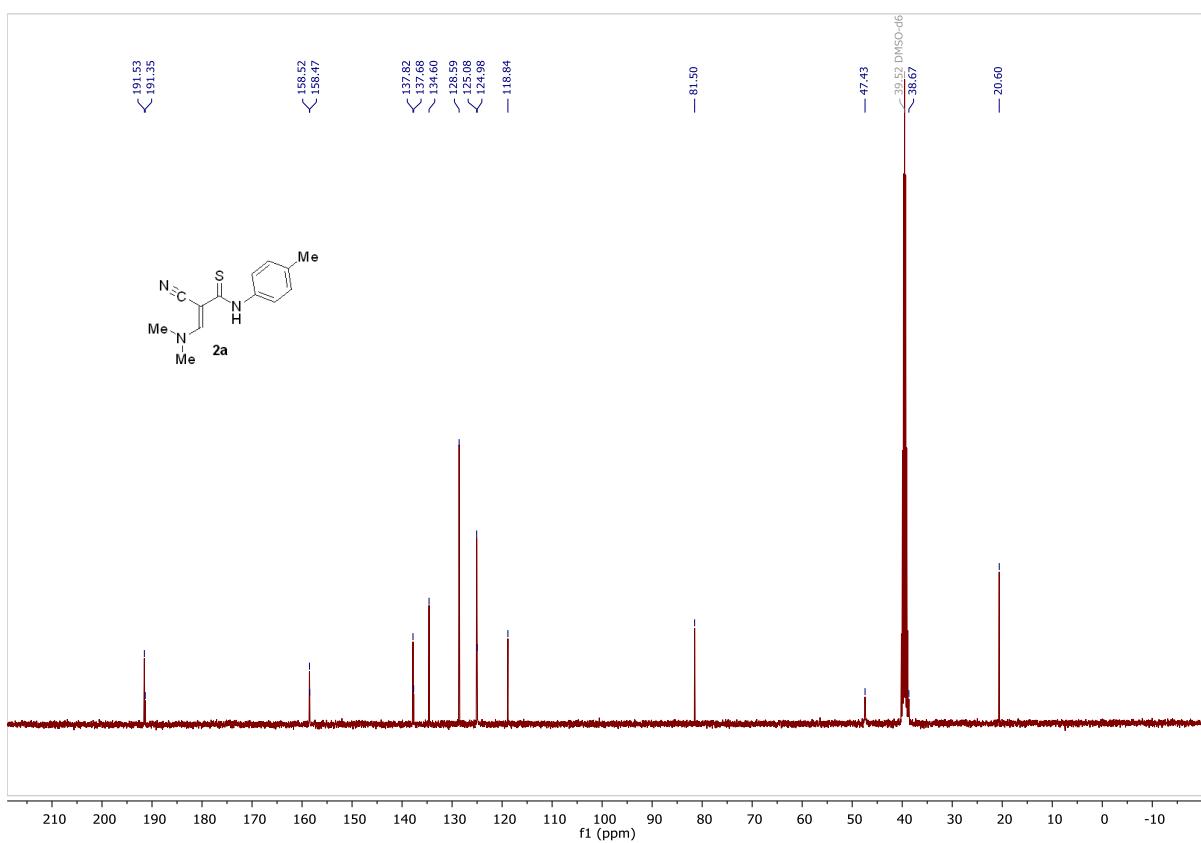
### **Copies of NMR spectra of all new compounds**

**NMR spectra of compounds 2a,e, 4a–c, 5a–e, 6a–f, 7a–k**

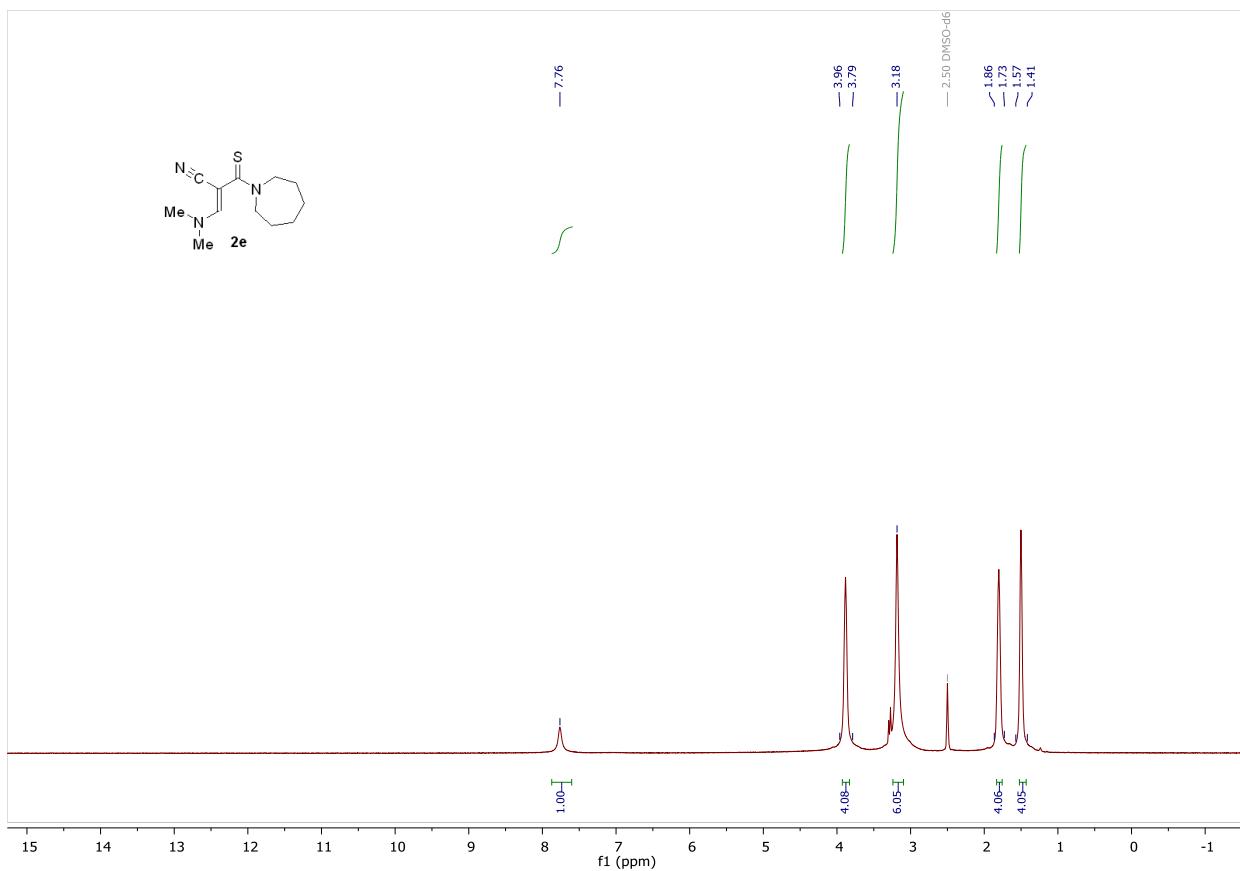
**Figure S1.**  $^1\text{H}$  NMR spectrum (DMSO- $d_6$ ) of **2a**.



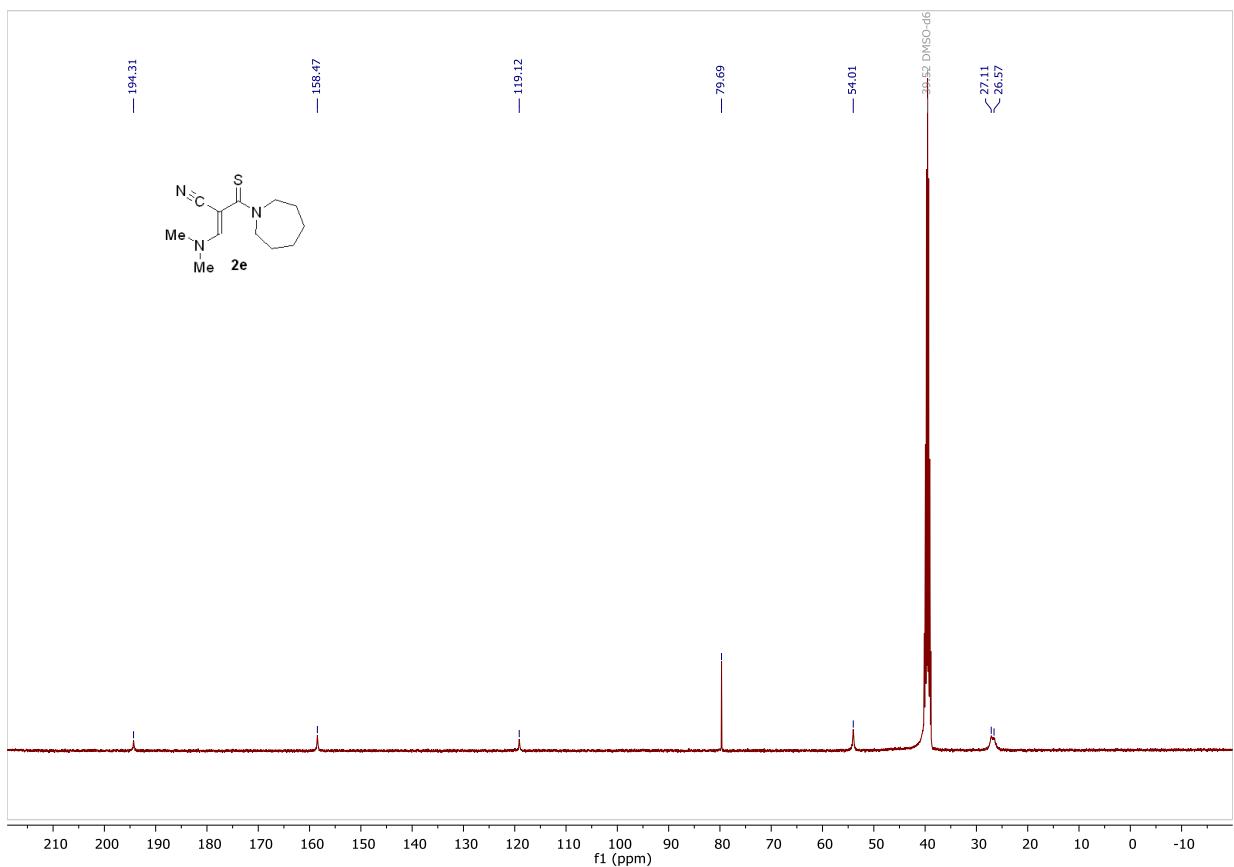
**Figure S2.**  $^{13}\text{C}$  NMR spectrum (DMSO- $d_6$ ) of **2a**.



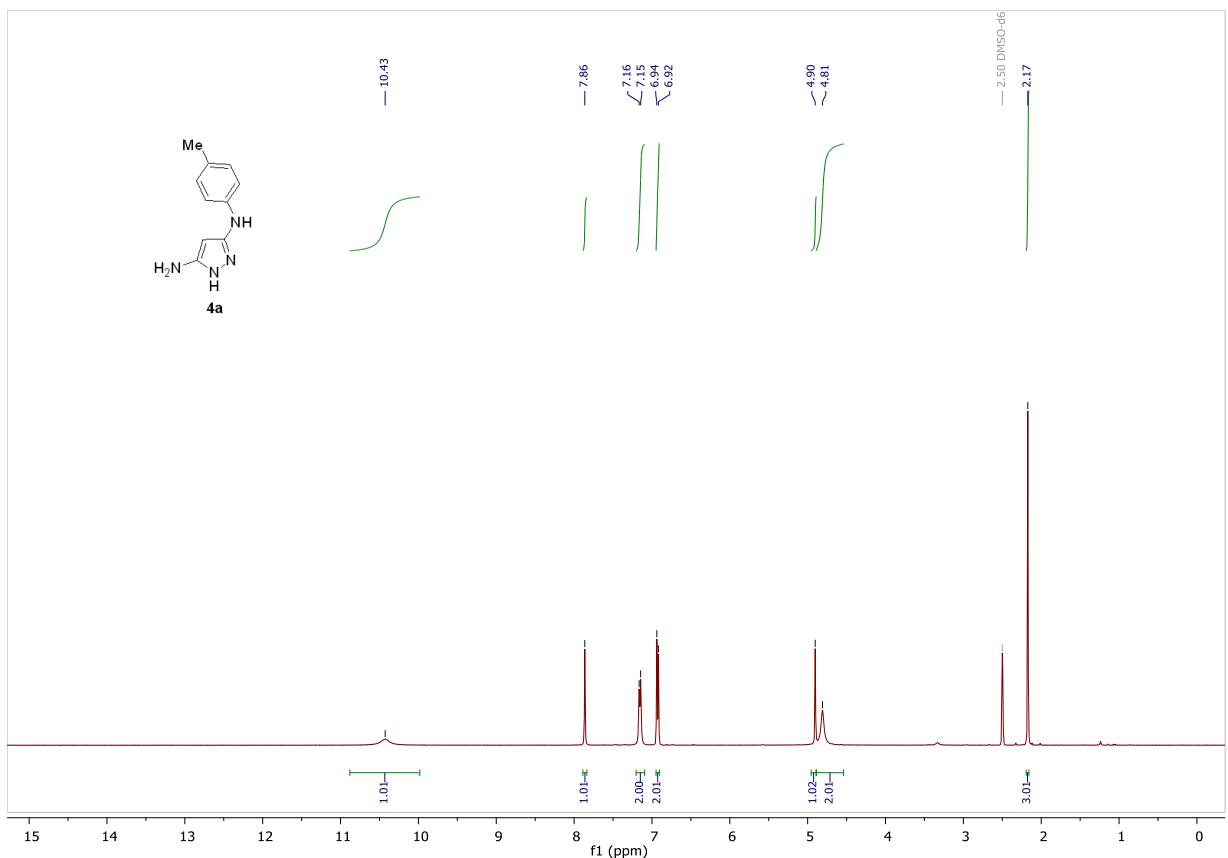
**Figure S3.**  $^1\text{H}$  NMR spectrum (DMSO- $d_6$ ) of **2e**.



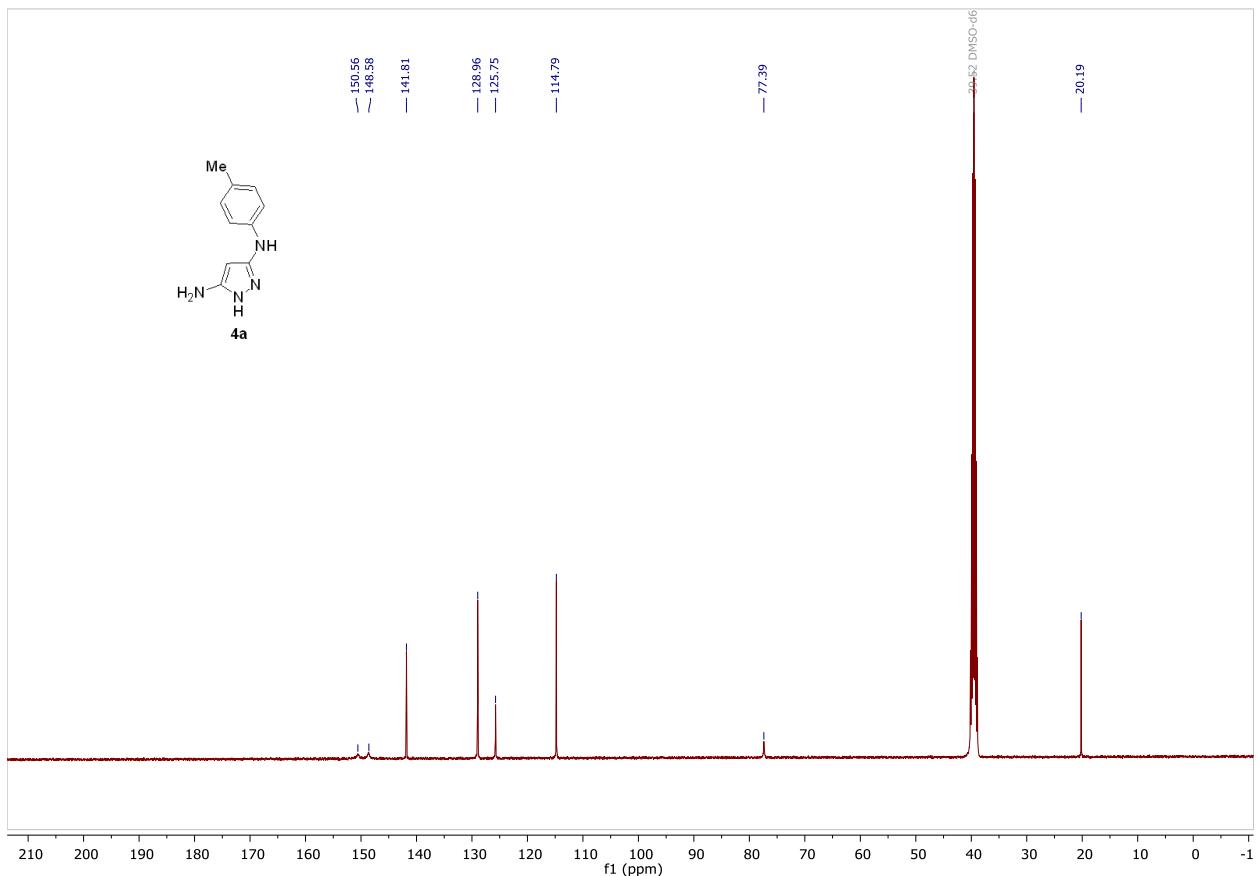
**Figure S4.**  $^{13}\text{C}$  NMR spectrum (DMSO- $d_6$ ) of **2e**.



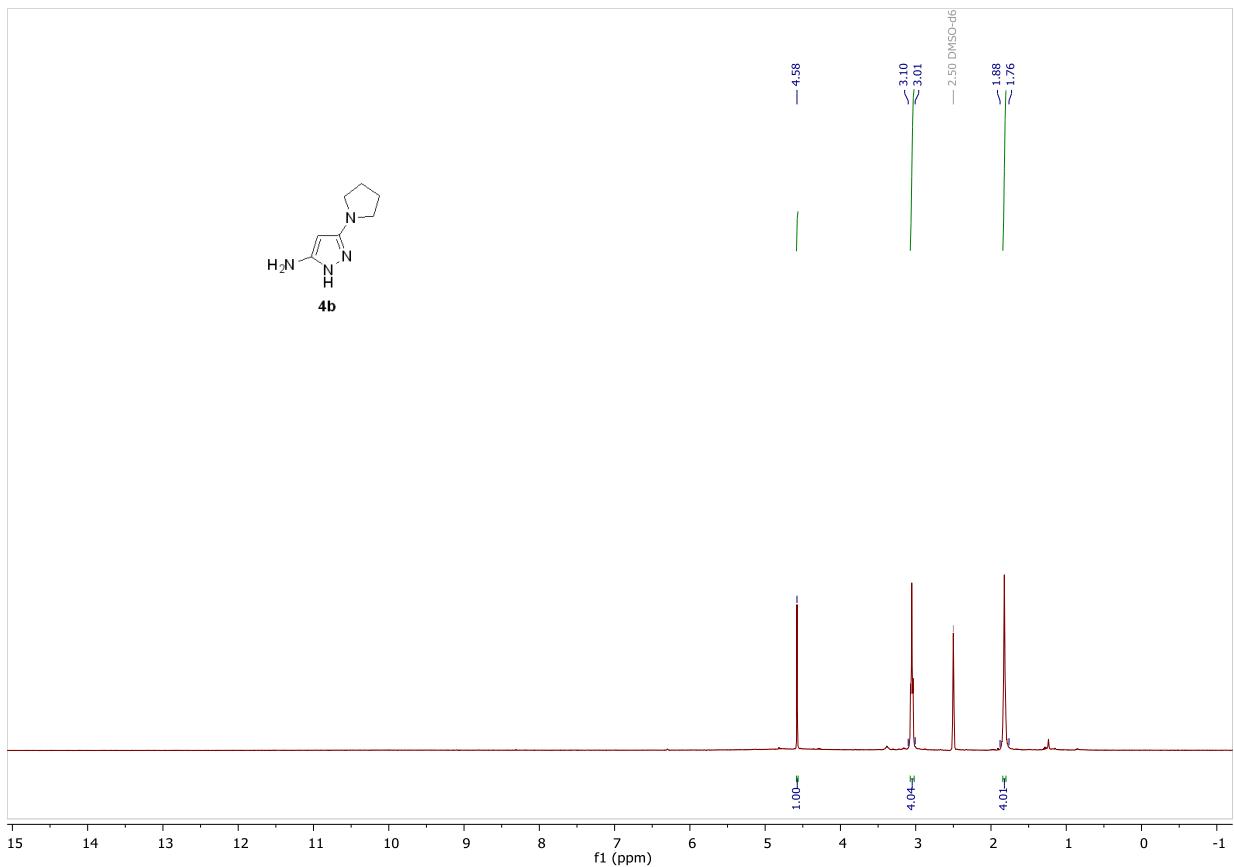
**Figure S5.**  $^1\text{H}$  NMR spectrum (DMSO- $d_6$ ) of **4a**.



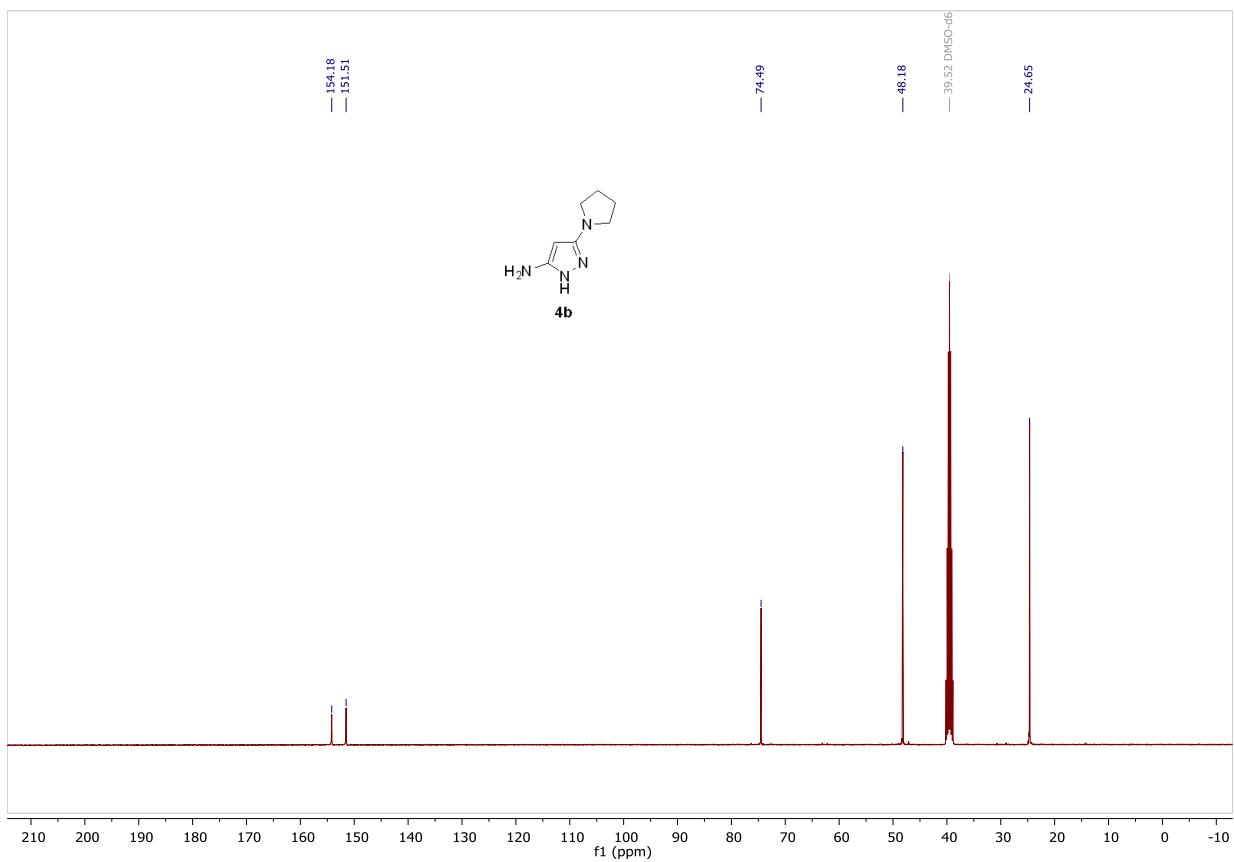
**Figure S6.**  $^{13}\text{C}$  NMR spectrum (DMSO- $d_6$ ) of **4a**.



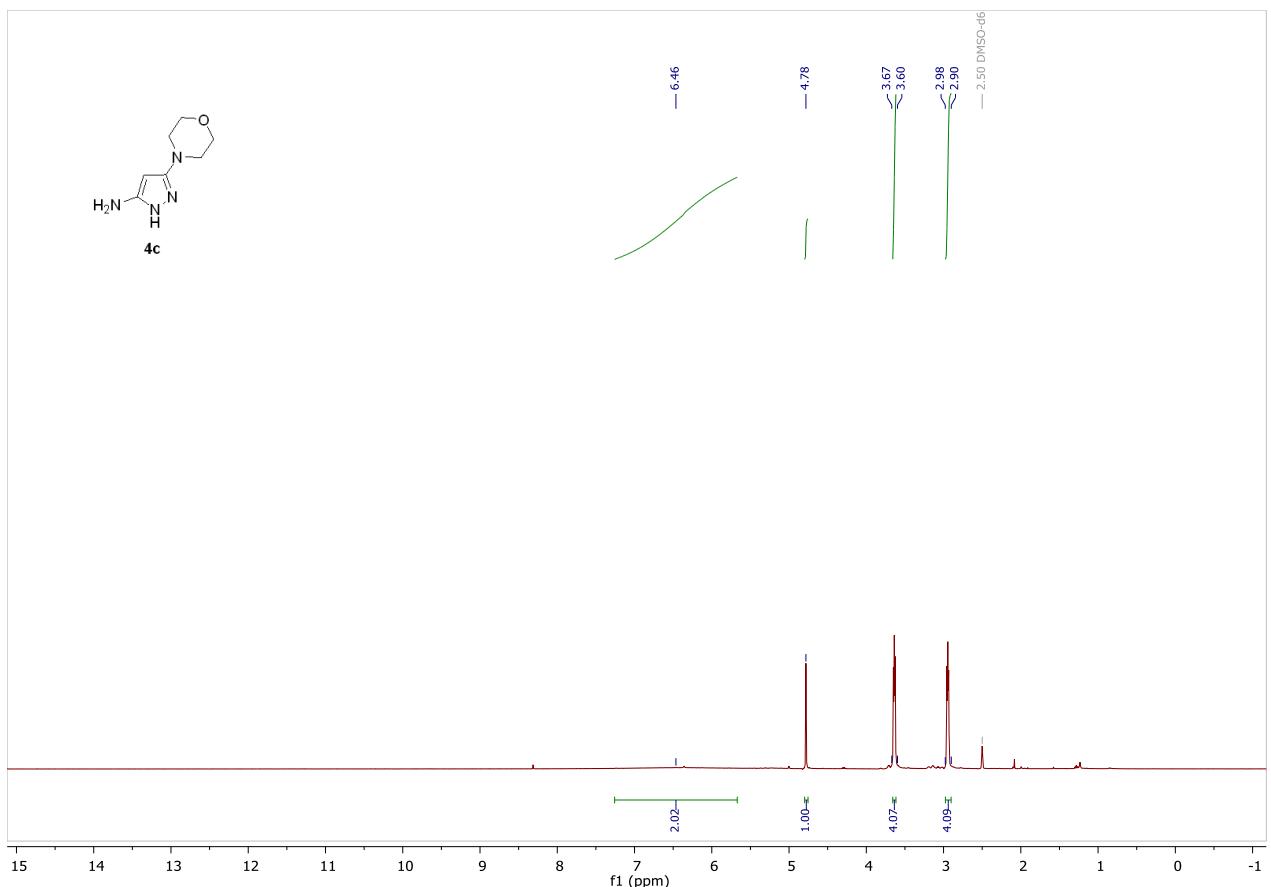
**Figure S7.**  $^1\text{H}$  NMR spectrum (DMSO- $d_6$ ) of **4b**.



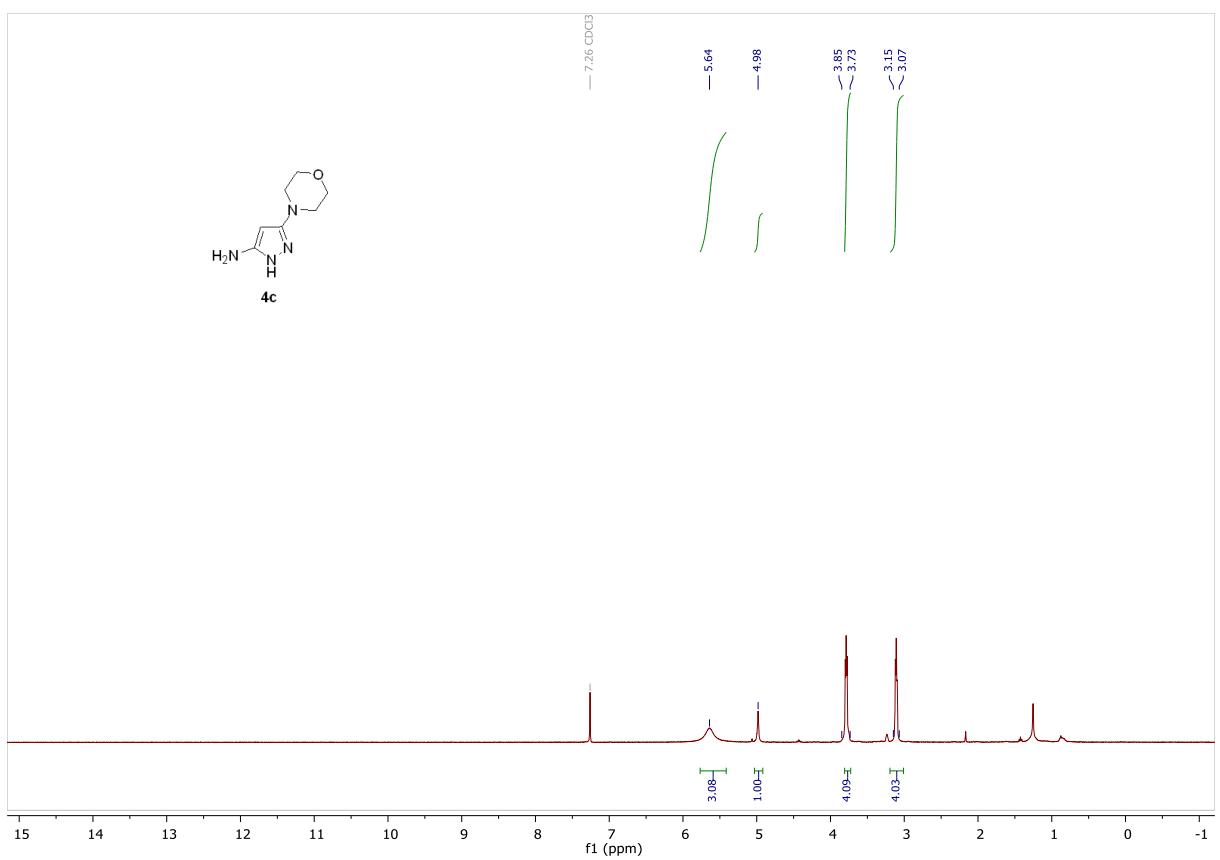
**Figure S8.**  $^{13}\text{C}$  NMR spectrum (DMSO- $d_6$ ) of **4b**.



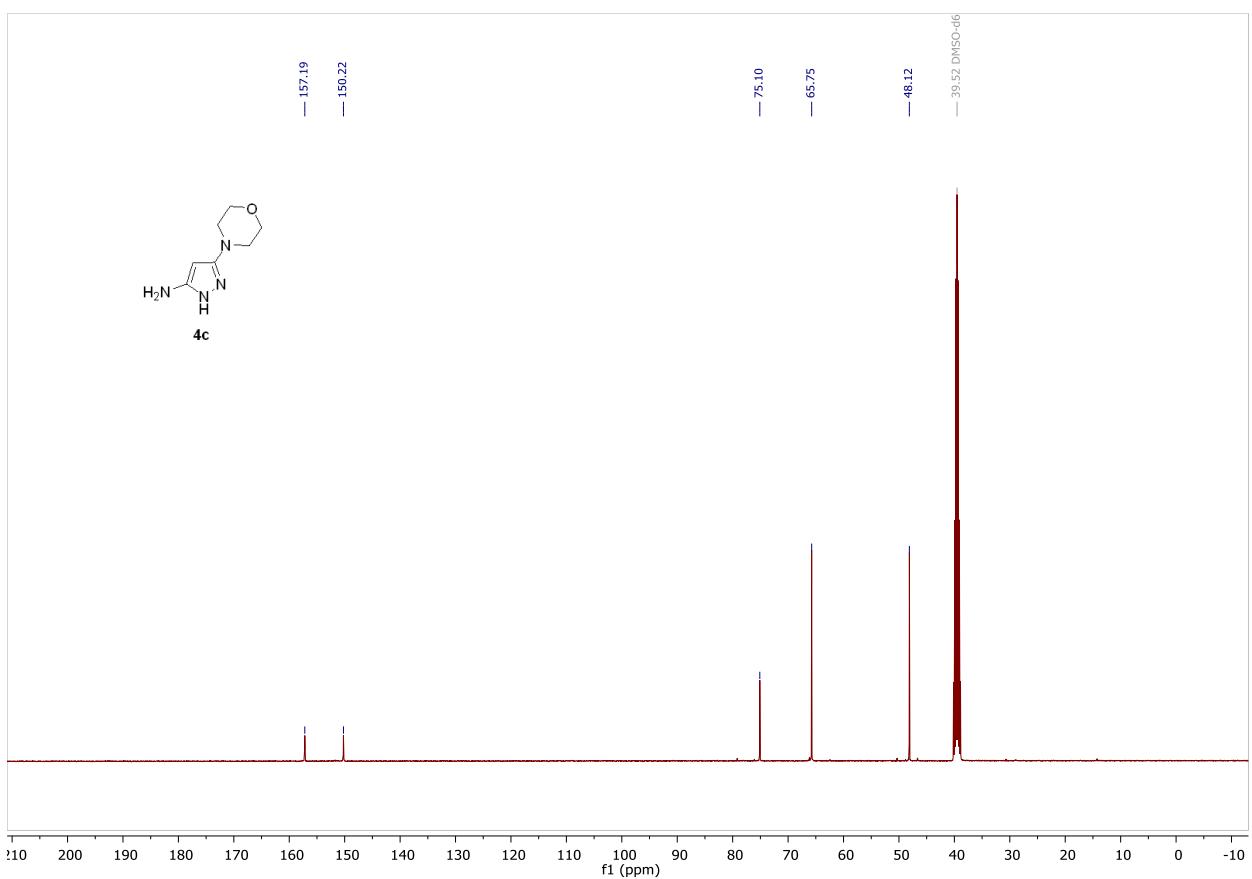
**Figure S9.**  $^1\text{H}$  NMR spectrum ( $\text{DMSO}-d_6$ ) of **4c**.



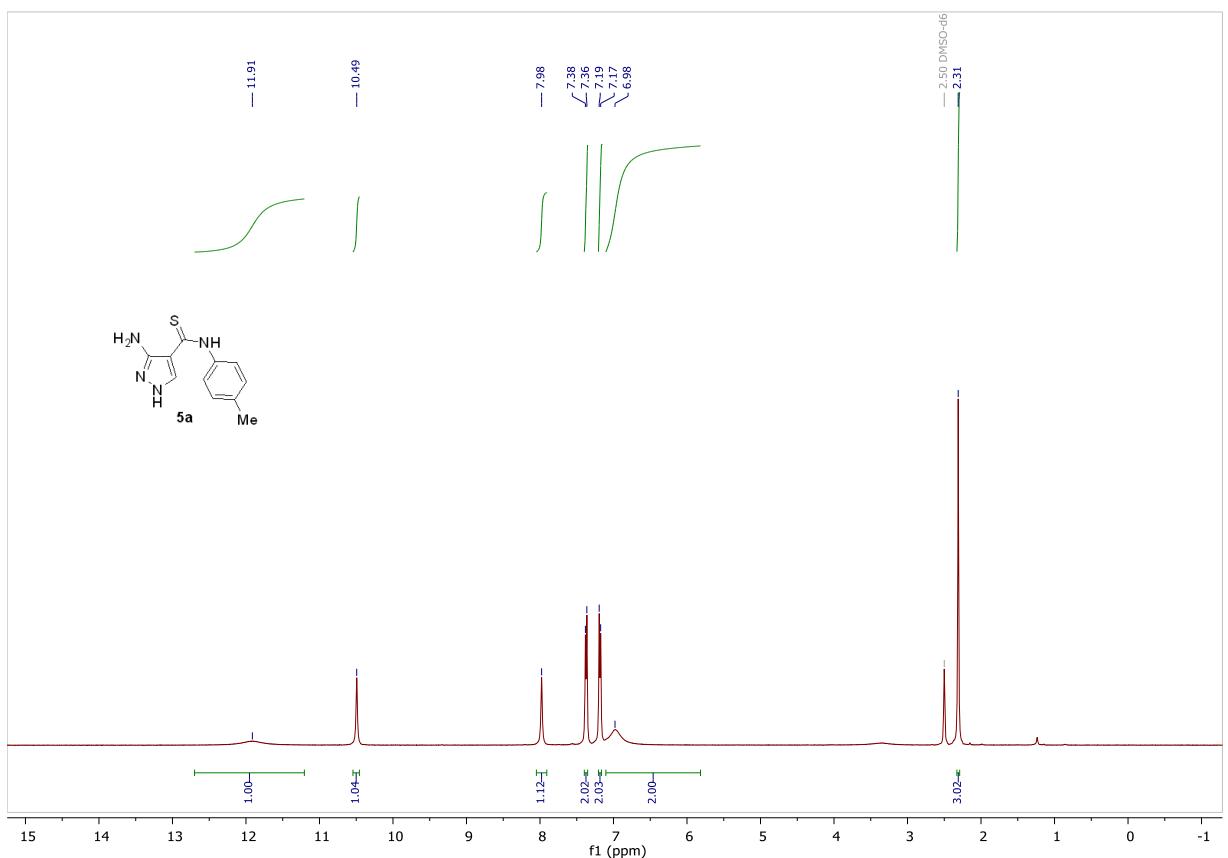
**Figure S10.**  $^1\text{H}$  NMR spectrum ( $\text{CDCl}_3$ ) of **4c**.



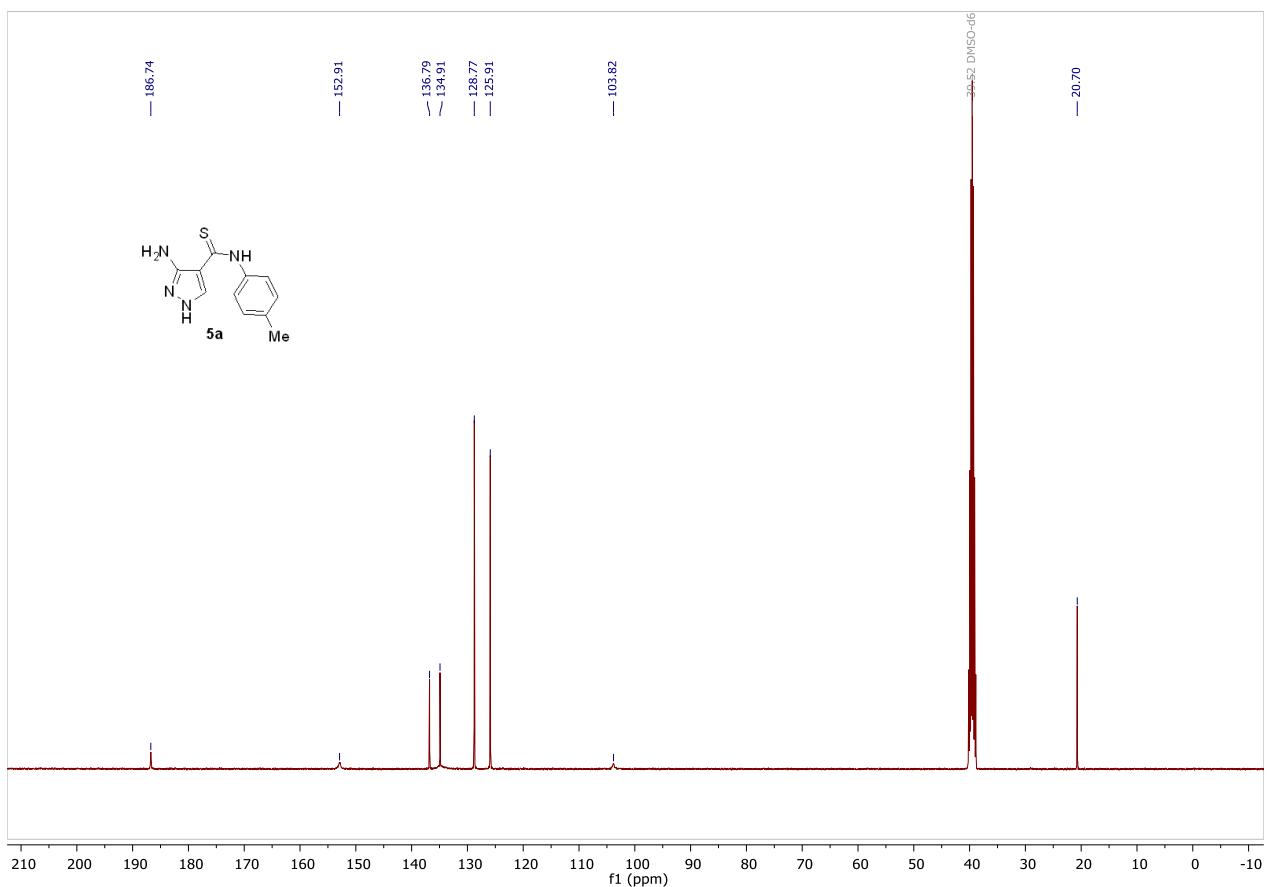
**Figure S11.**  $^{13}\text{C}$  NMR spectrum (DMSO- $d_6$ ) of **4c**.



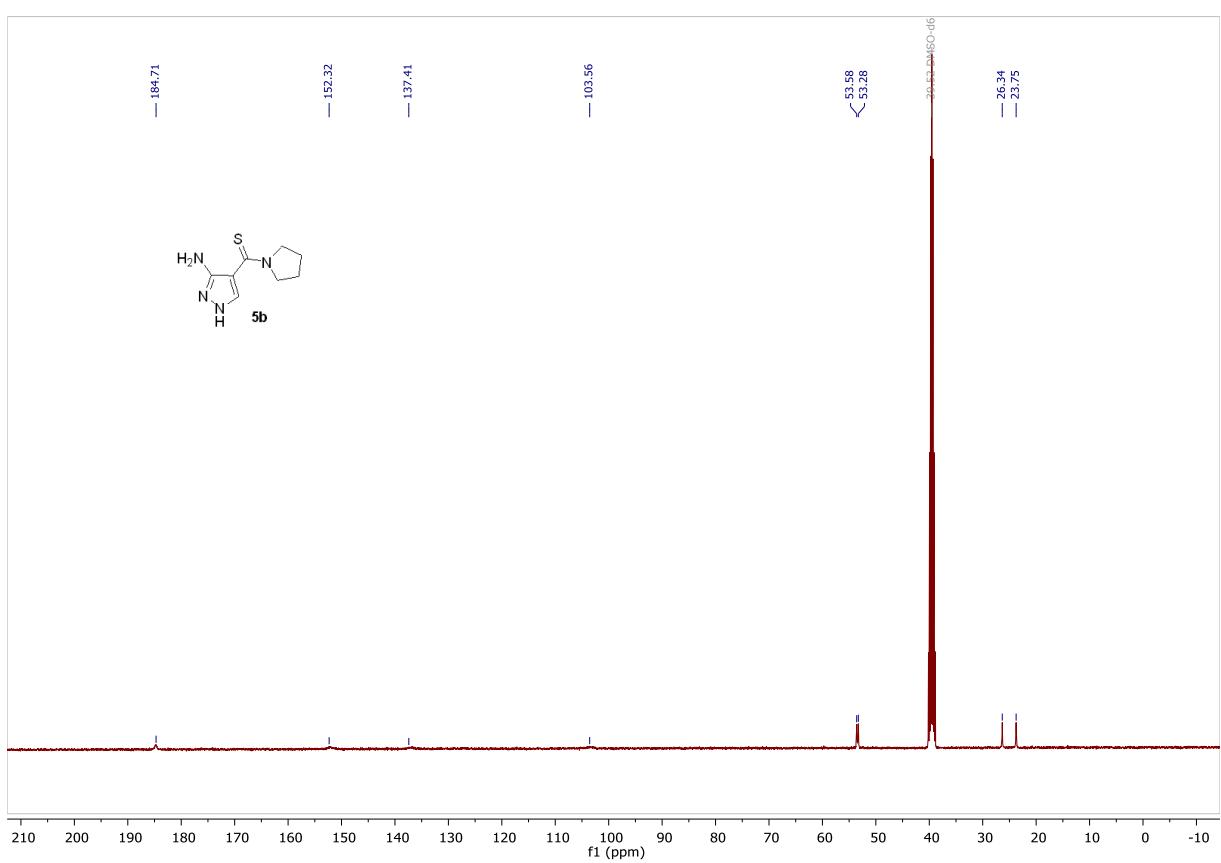
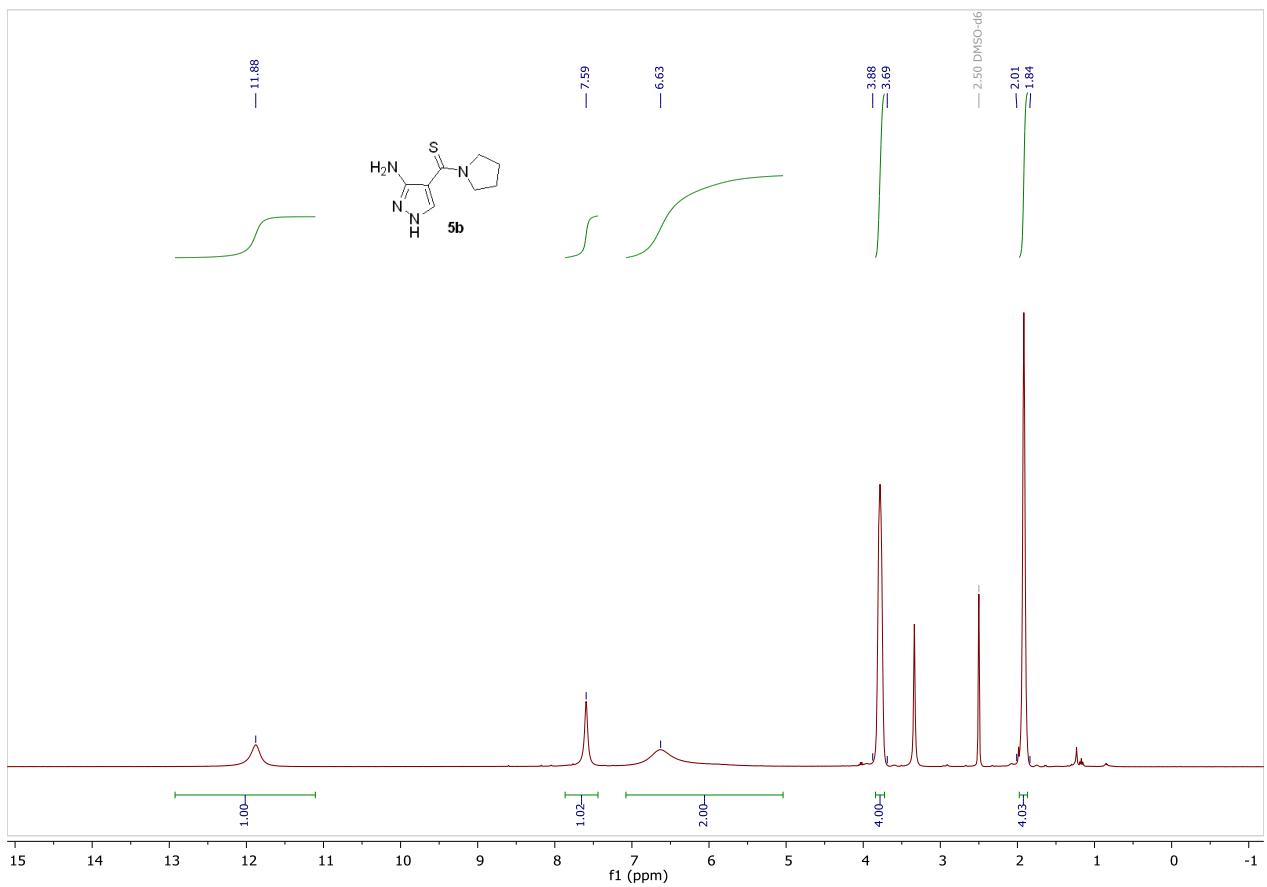
**Figure S12.**  $^1\text{H}$  NMR spectrum (DMSO- $d_6$ ) of **5a**.



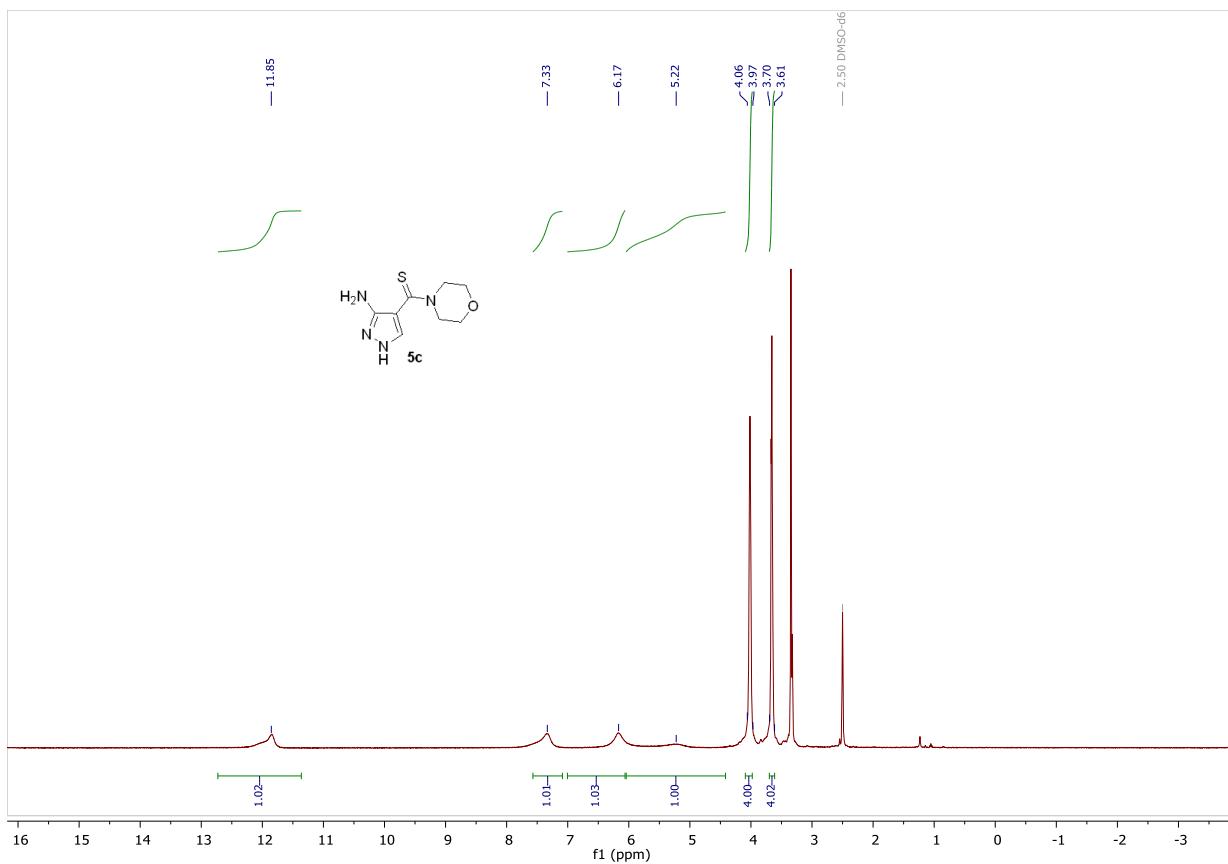
**Figure S13.**  $^{13}\text{C}$  NMR spectrum (DMSO- $d_6$ ) of **5a**.



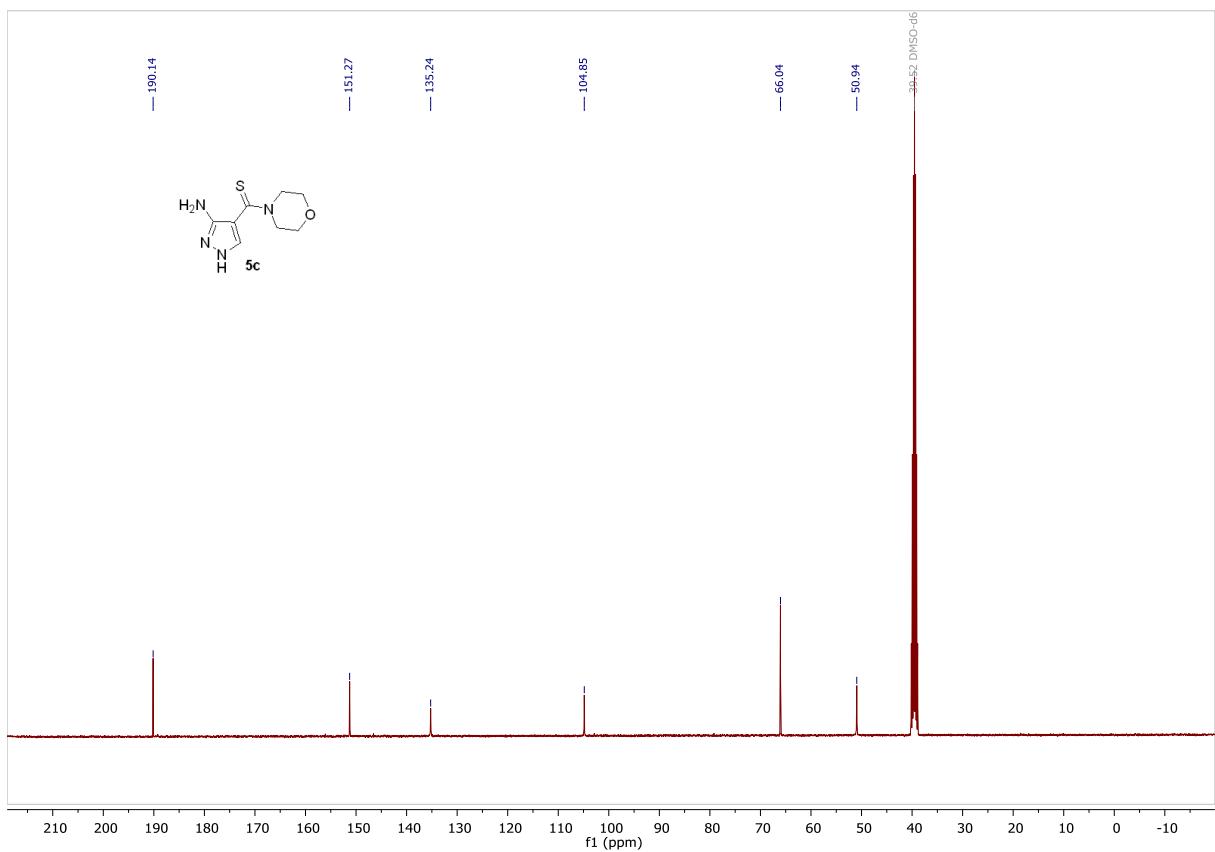
**Figure S14.**  $^1\text{H}$  NMR spectrum (DMSO- $d_6$ ) of **5b**.



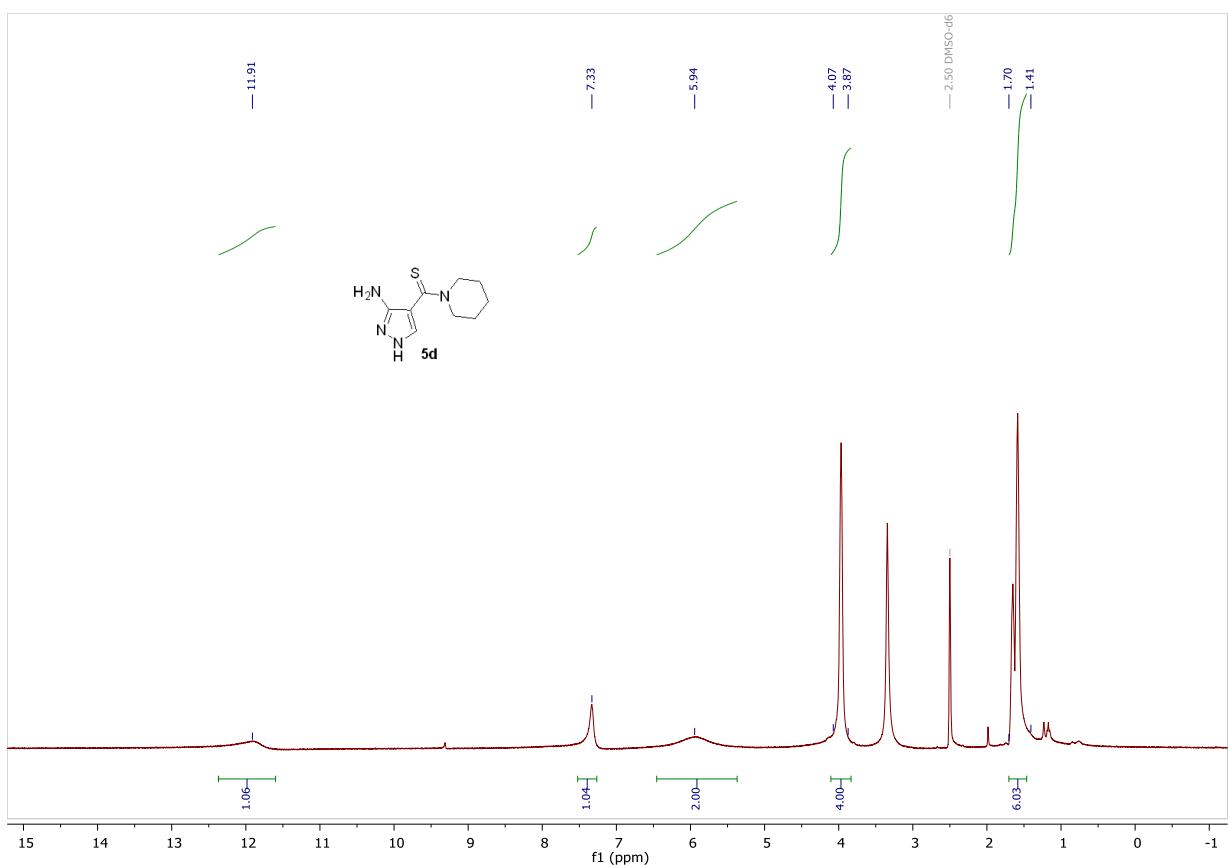
**Figure S16.**  $^1\text{H}$  NMR spectrum (DMSO- $d_6$ ) of **5c**.



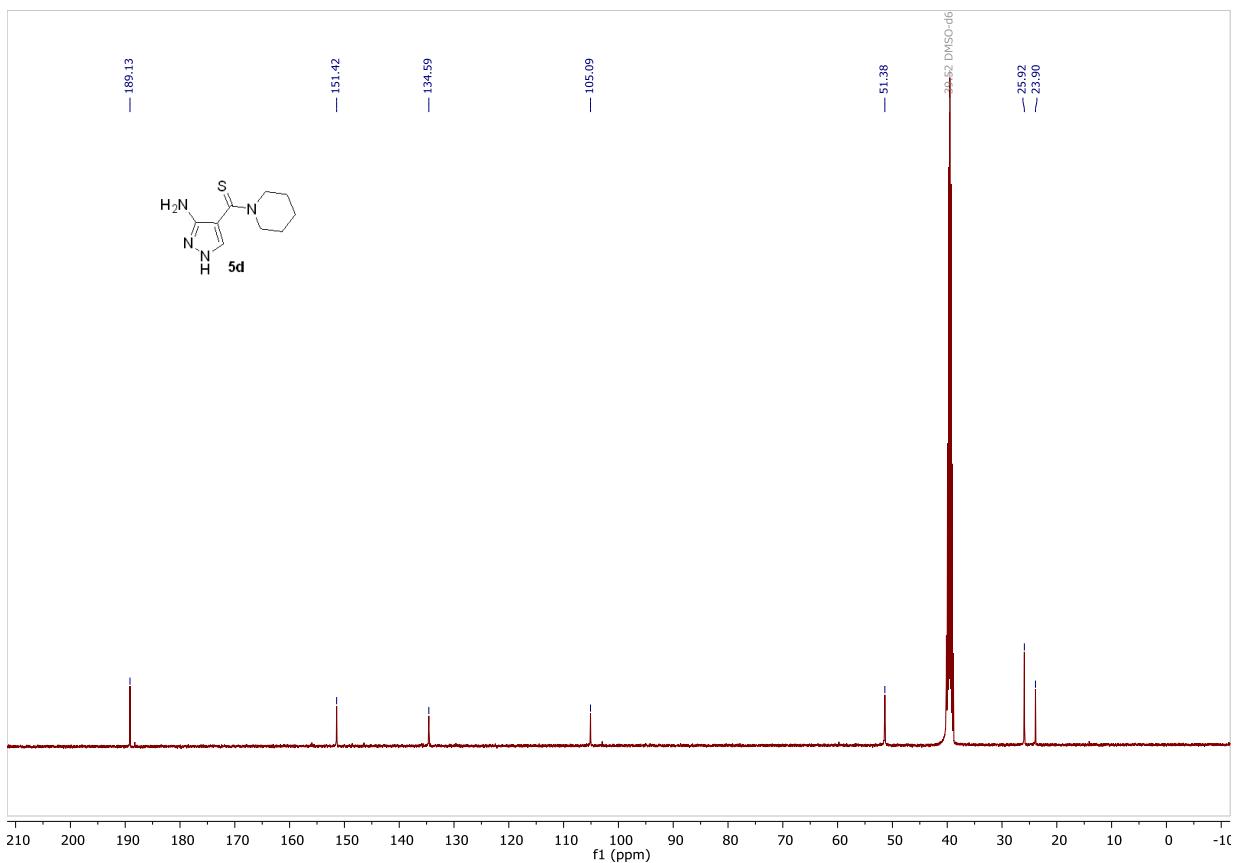
**Figure S17.**  $^{13}\text{C}$  NMR spectrum (DMSO- $d_6$ ) of **5c**.



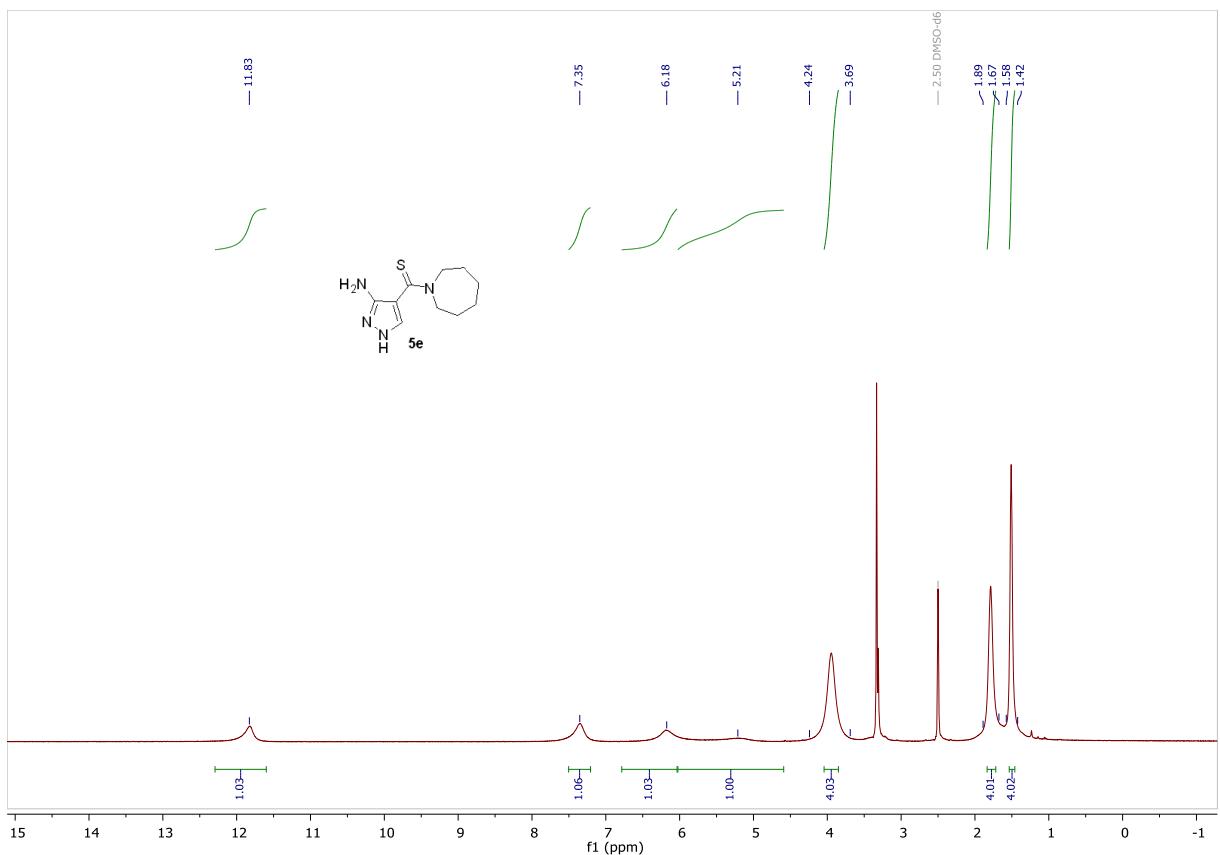
**Figure S18.**  $^1\text{H}$  NMR spectrum (DMSO- $d_6$ ) of **5d**.



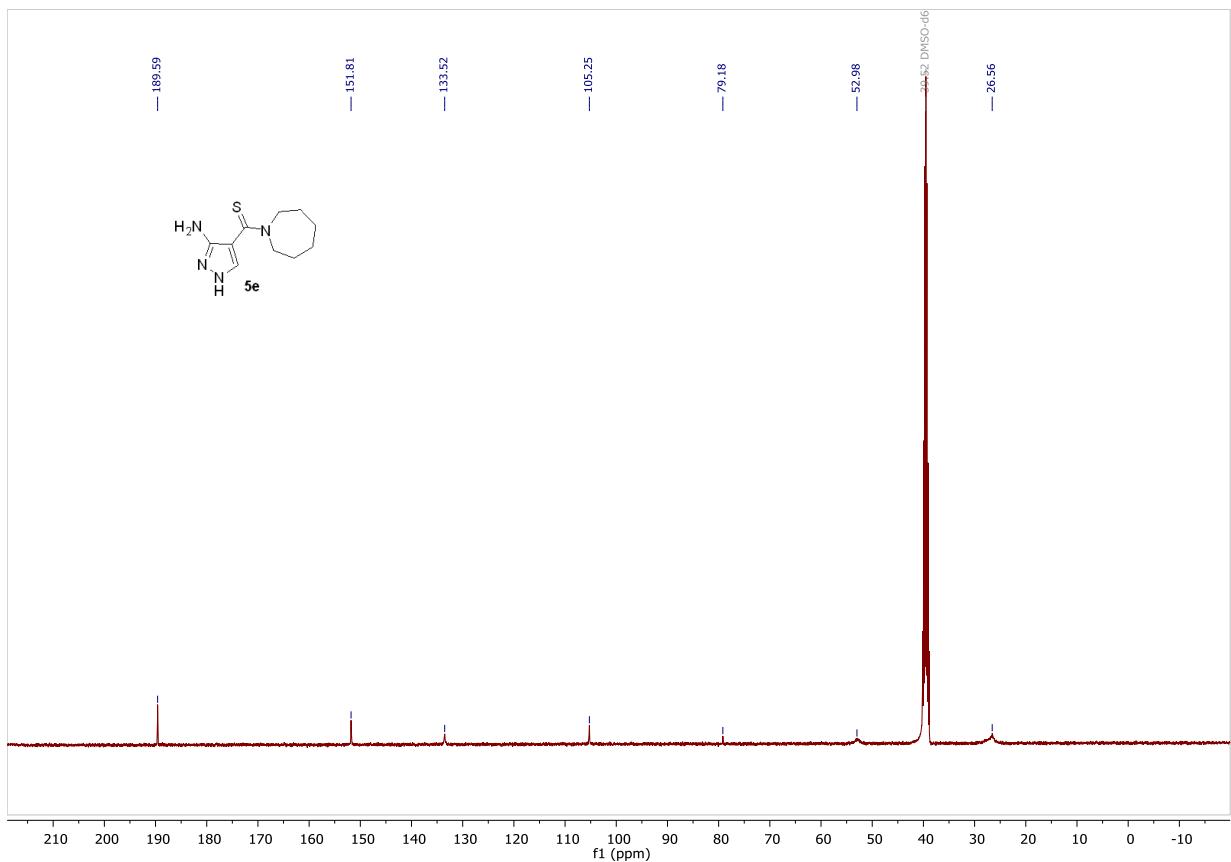
**Figure S19.**  $^{13}\text{C}$  NMR spectrum (DMSO- $d_6$ ) of **5d**.



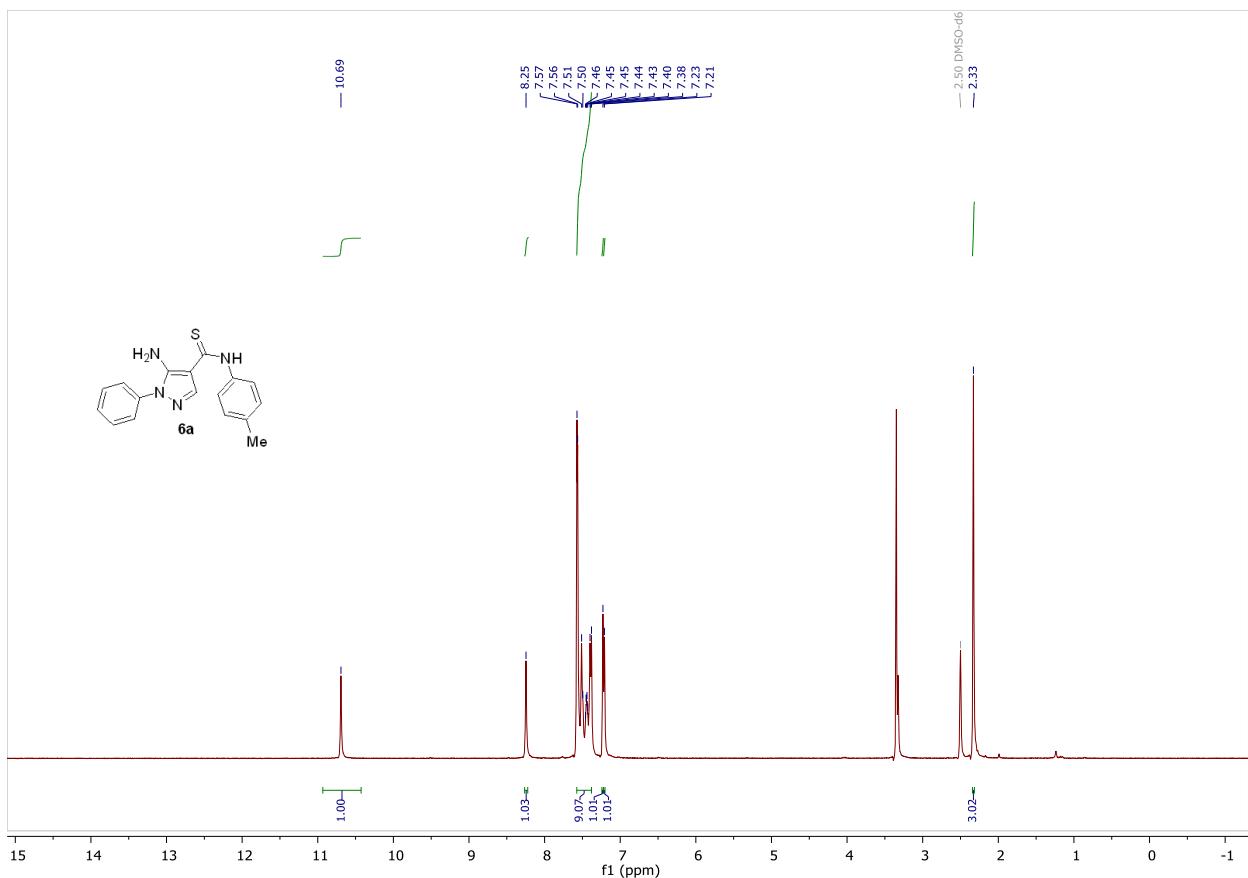
**Figure S20.**  $^1\text{H}$  NMR spectrum (DMSO- $d_6$ ) of **5e**.



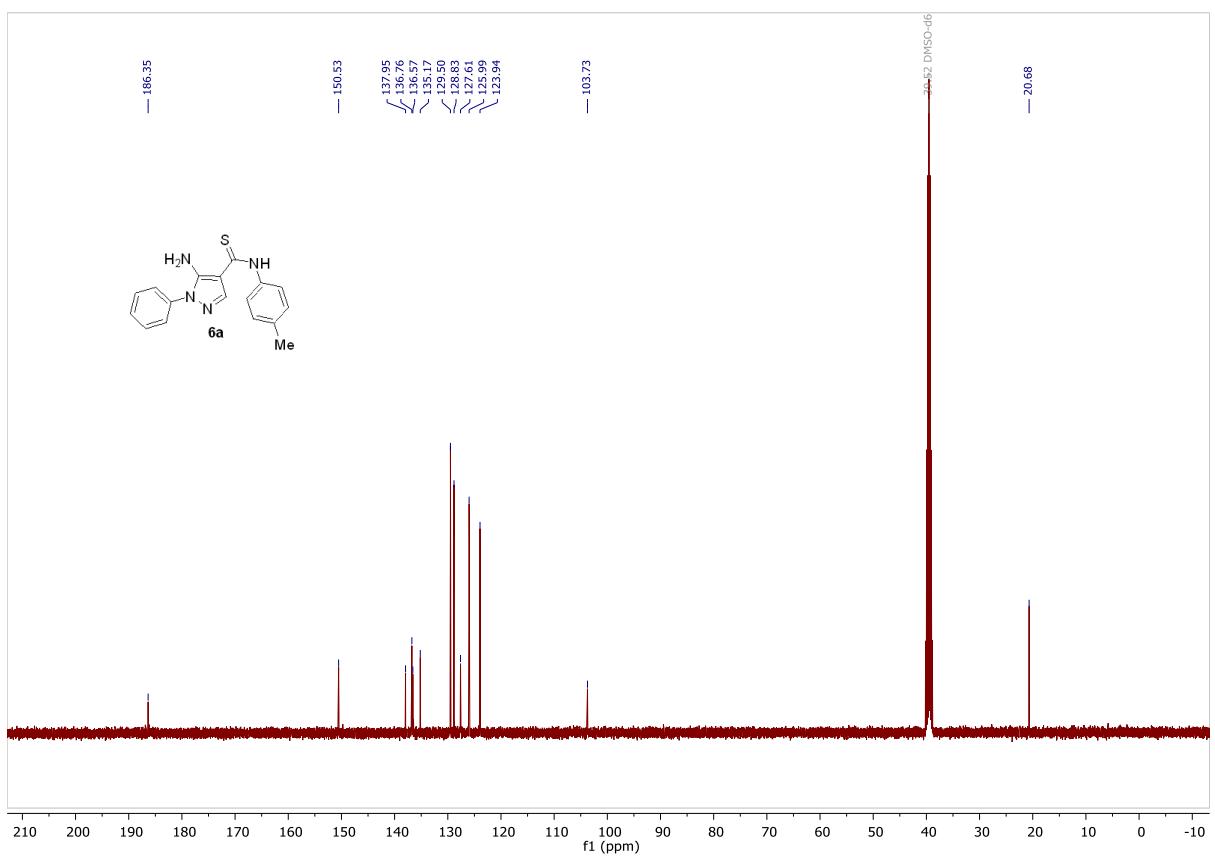
**Figure S21.**  $^{13}\text{C}$  NMR spectrum (DMSO- $d_6$ ) of **5e**.



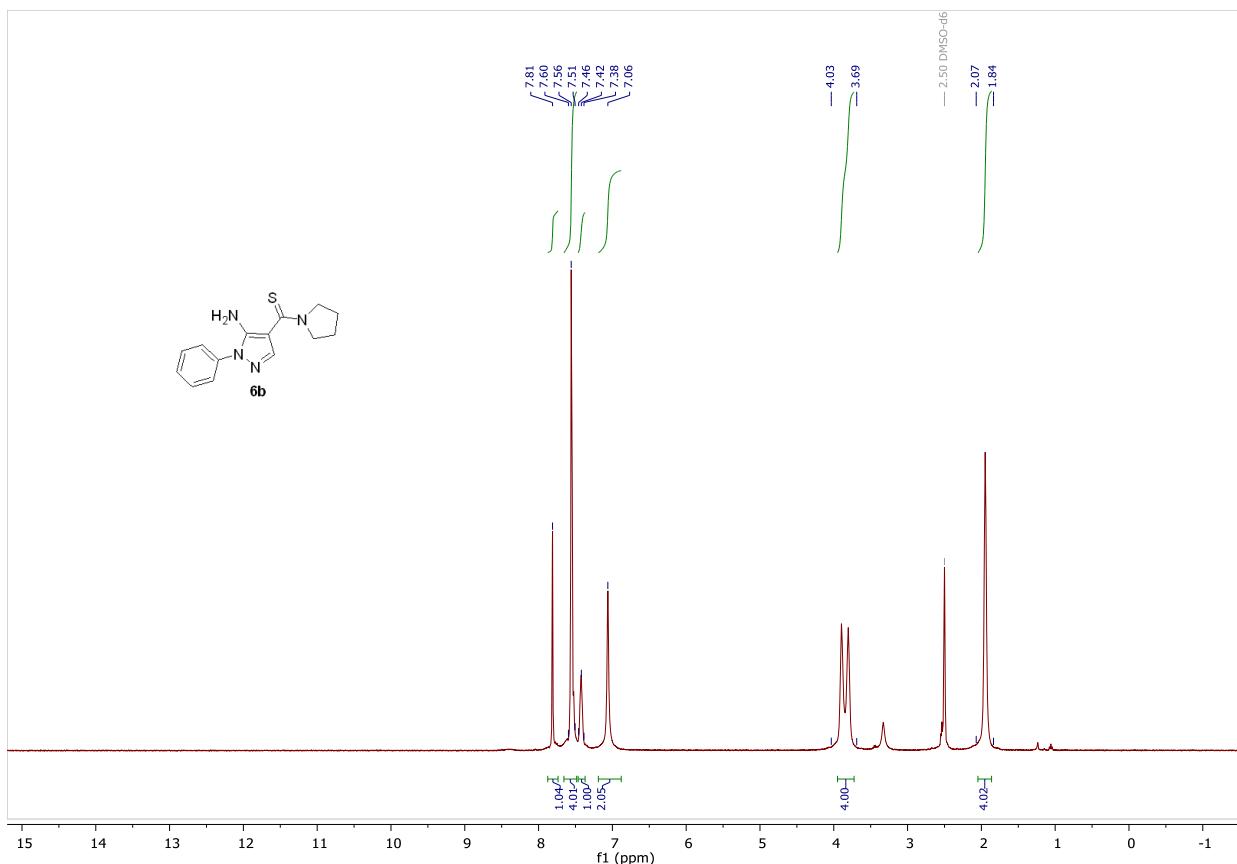
**Figure S22.**  $^1\text{H}$  NMR spectrum (DMSO- $d_6$ ) of **6a**.



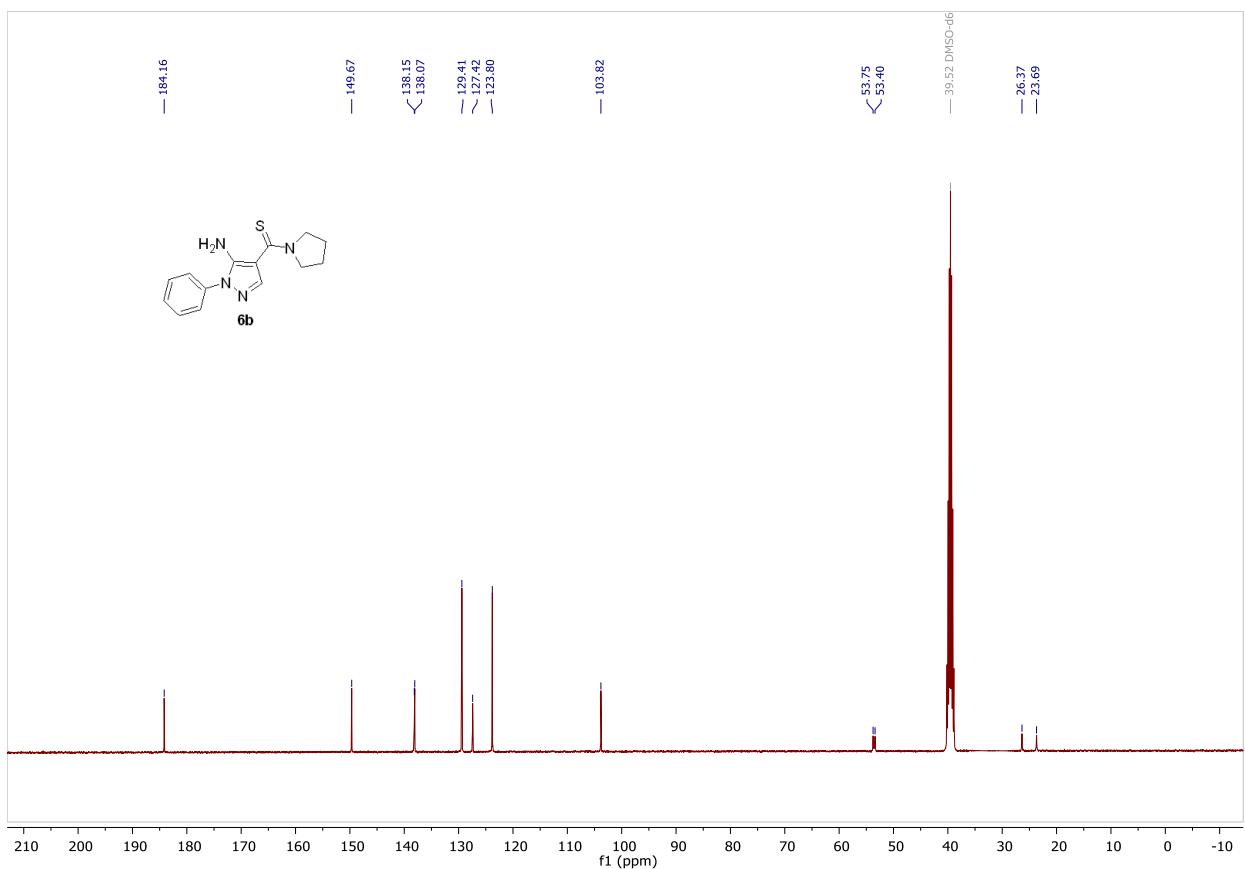
**Figure S23.**  $^{13}\text{C}$  NMR spectrum (DMSO- $d_6$ ) of **6a**.



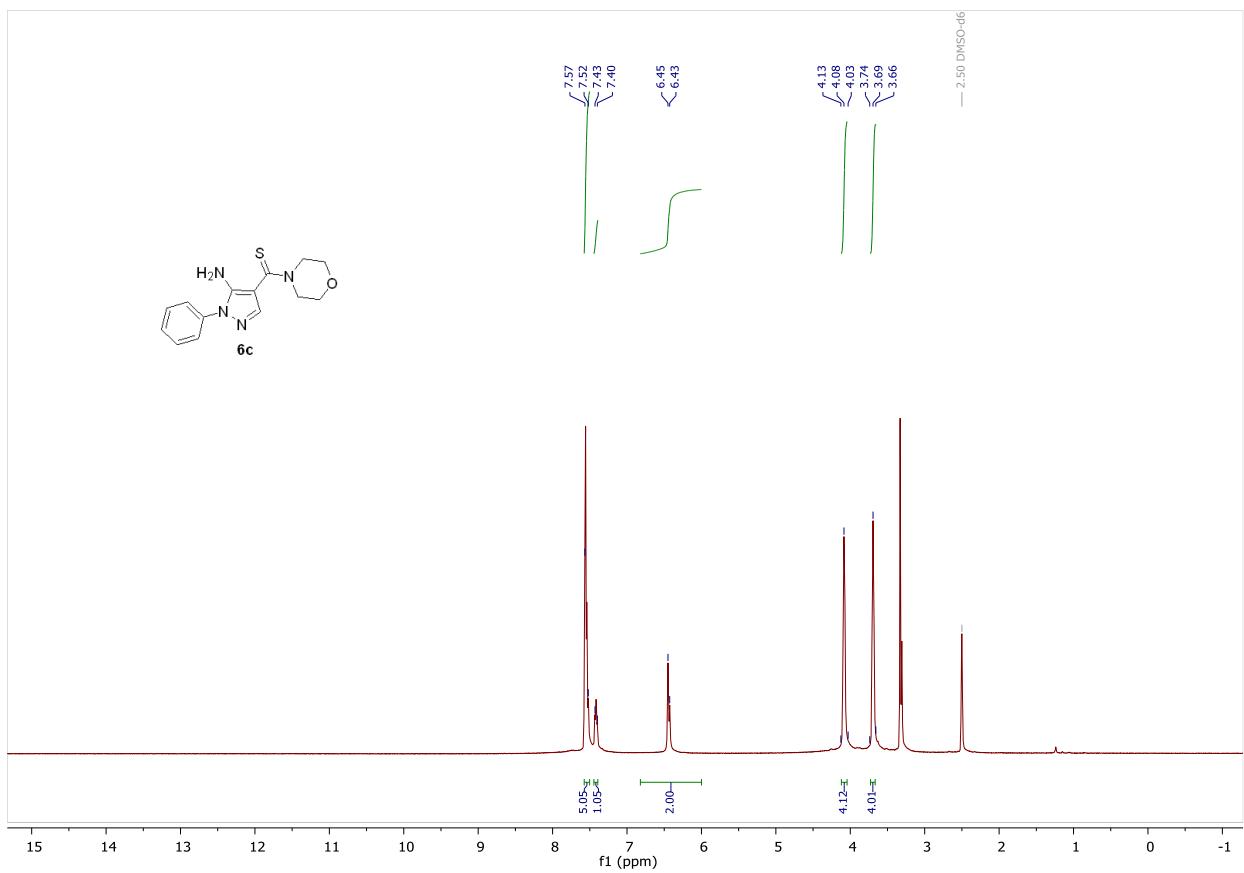
**Figure S24.**  $^1\text{H}$  NMR spectrum (DMSO- $d_6$ ) of **6b**.



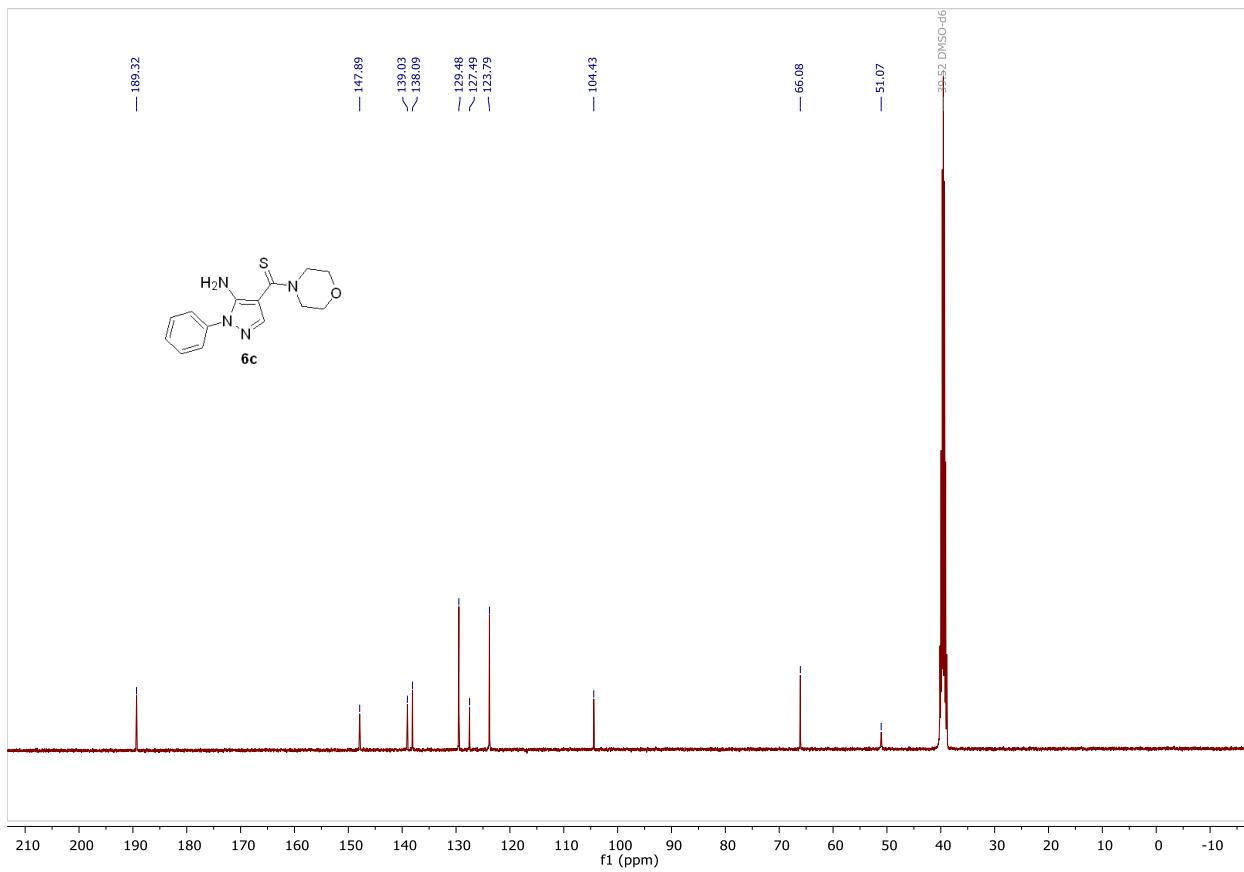
**Figure S25.**  $^{13}\text{C}$  NMR spectrum (DMSO- $d_6$ ) of **6b**.



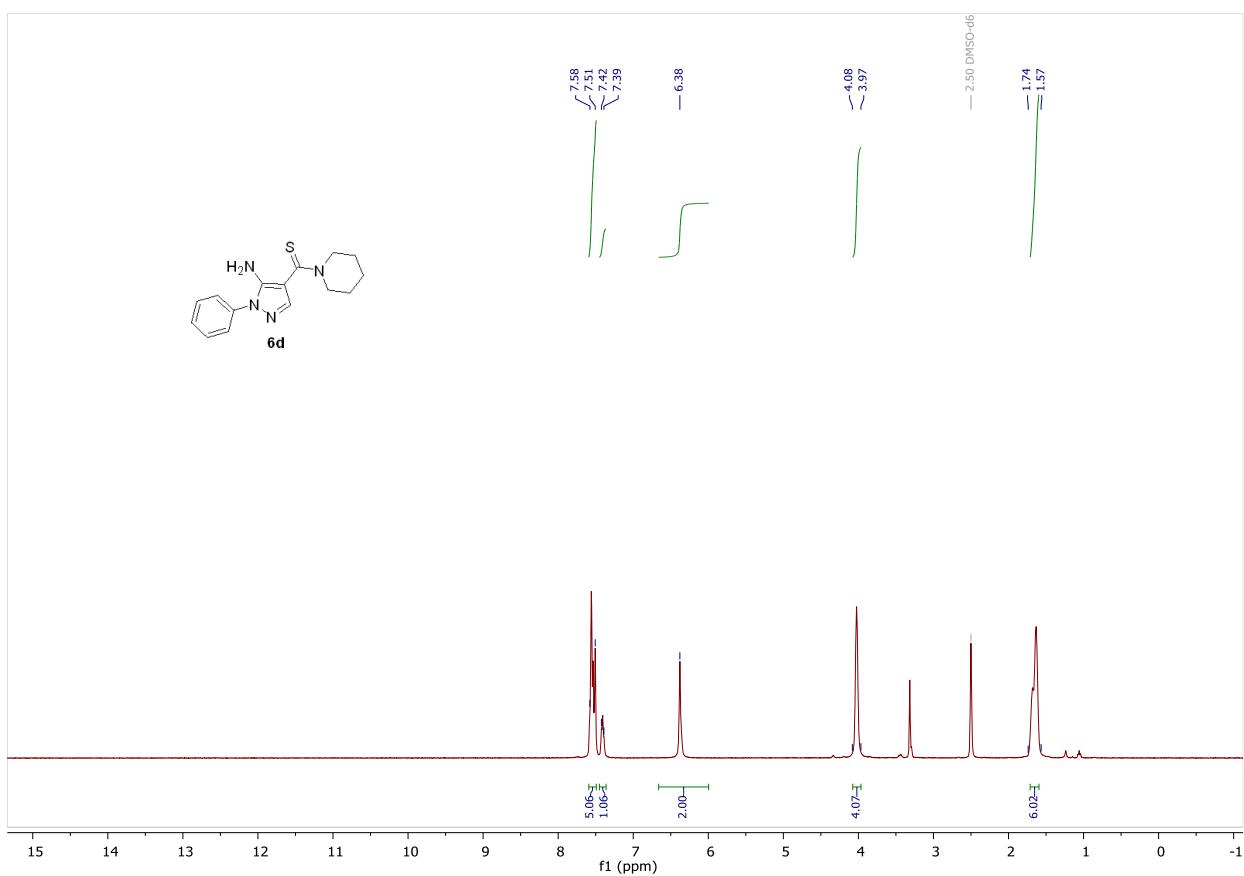
**Figure S26.**  $^1\text{H}$  NMR spectrum (DMSO- $d_6$ ) of **6c**.



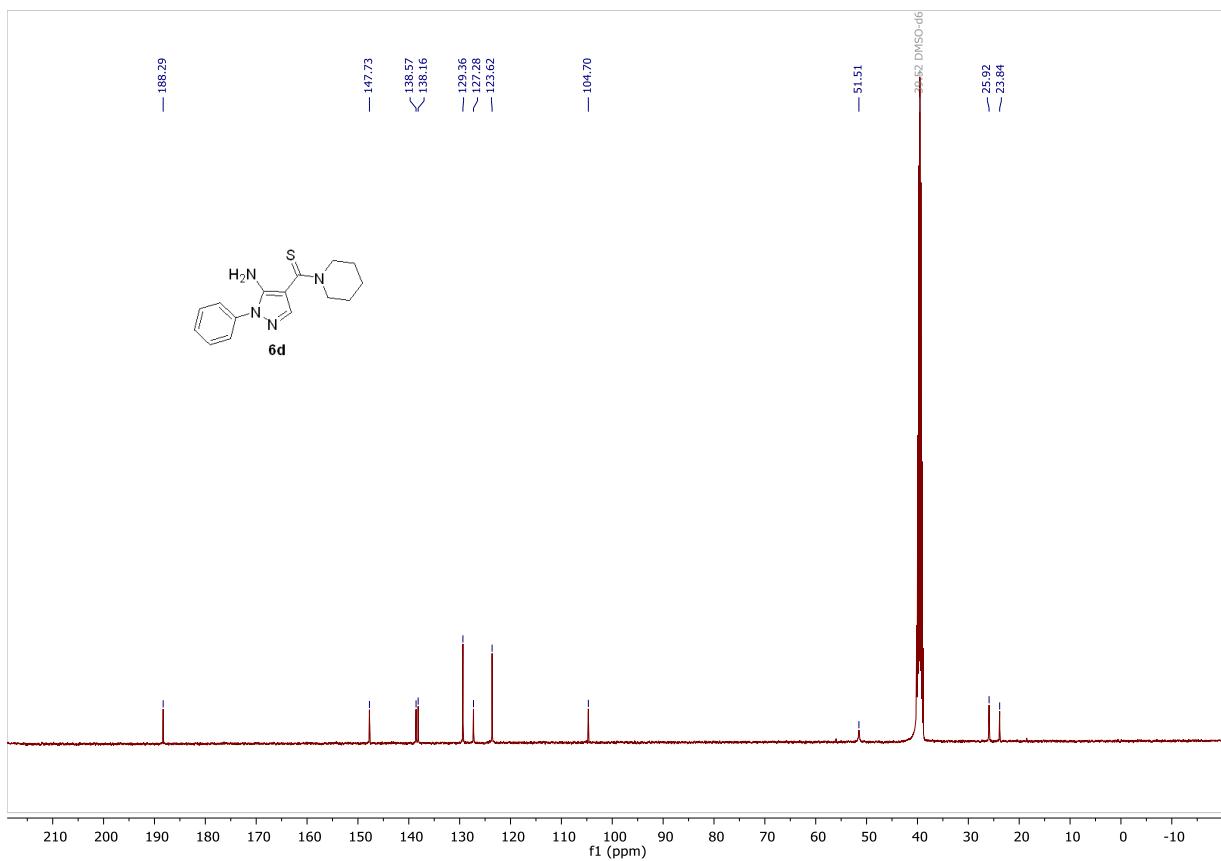
**Figure S27.**  $^{13}\text{C}$  NMR spectrum (DMSO- $d_6$ ) of **6c**.



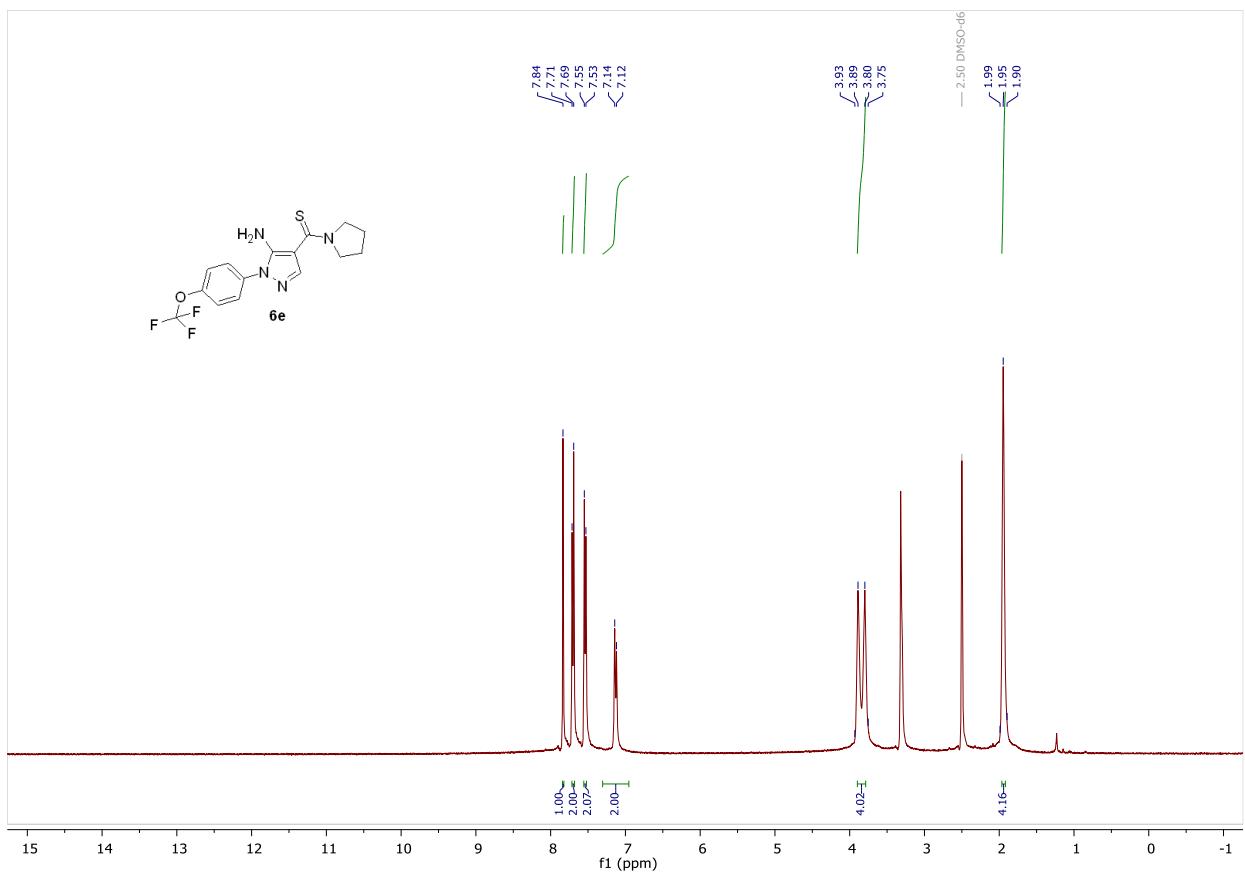
**Figure S28.**  $^1\text{H}$  NMR spectrum (DMSO- $d_6$ ) of **6d**.



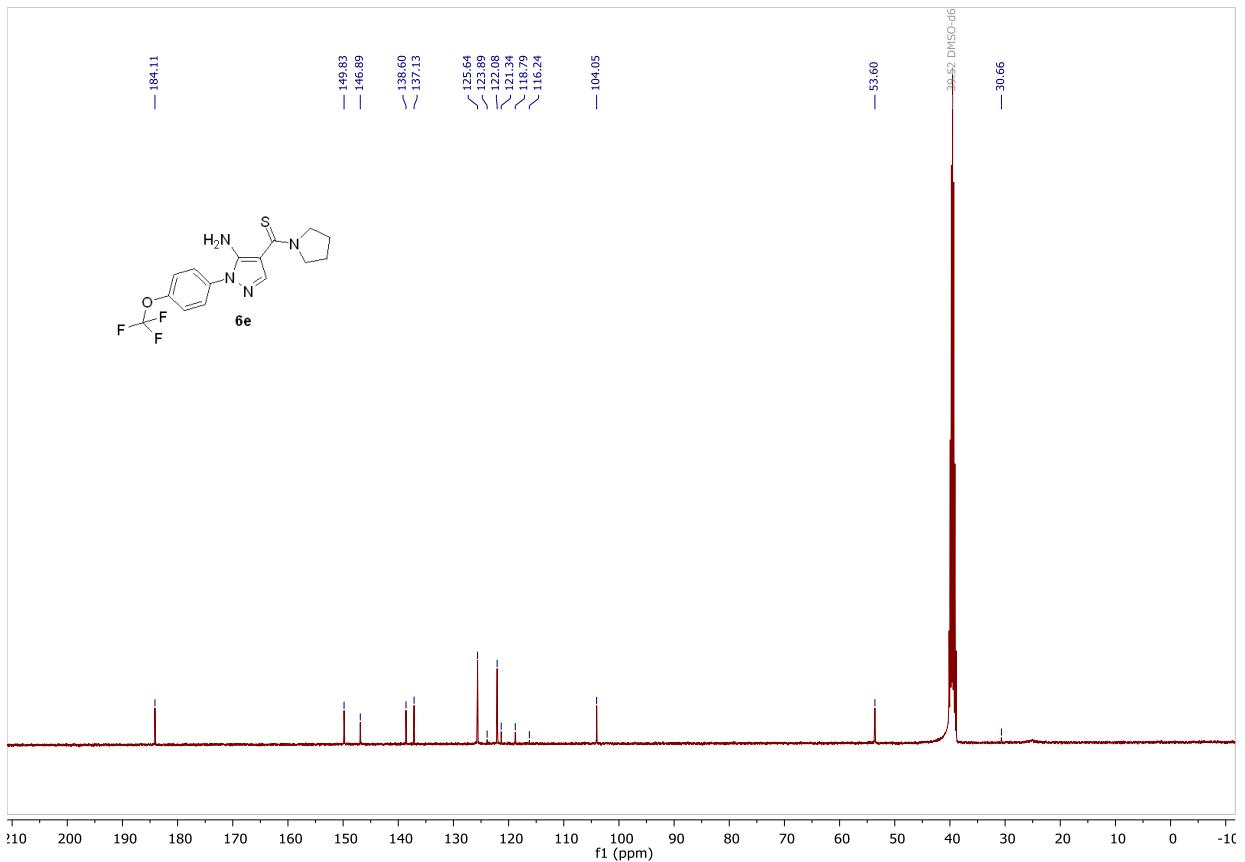
**Figure S29.**  $^{13}\text{C}$  NMR spectrum (DMSO- $d_6$ ) of **6d**.



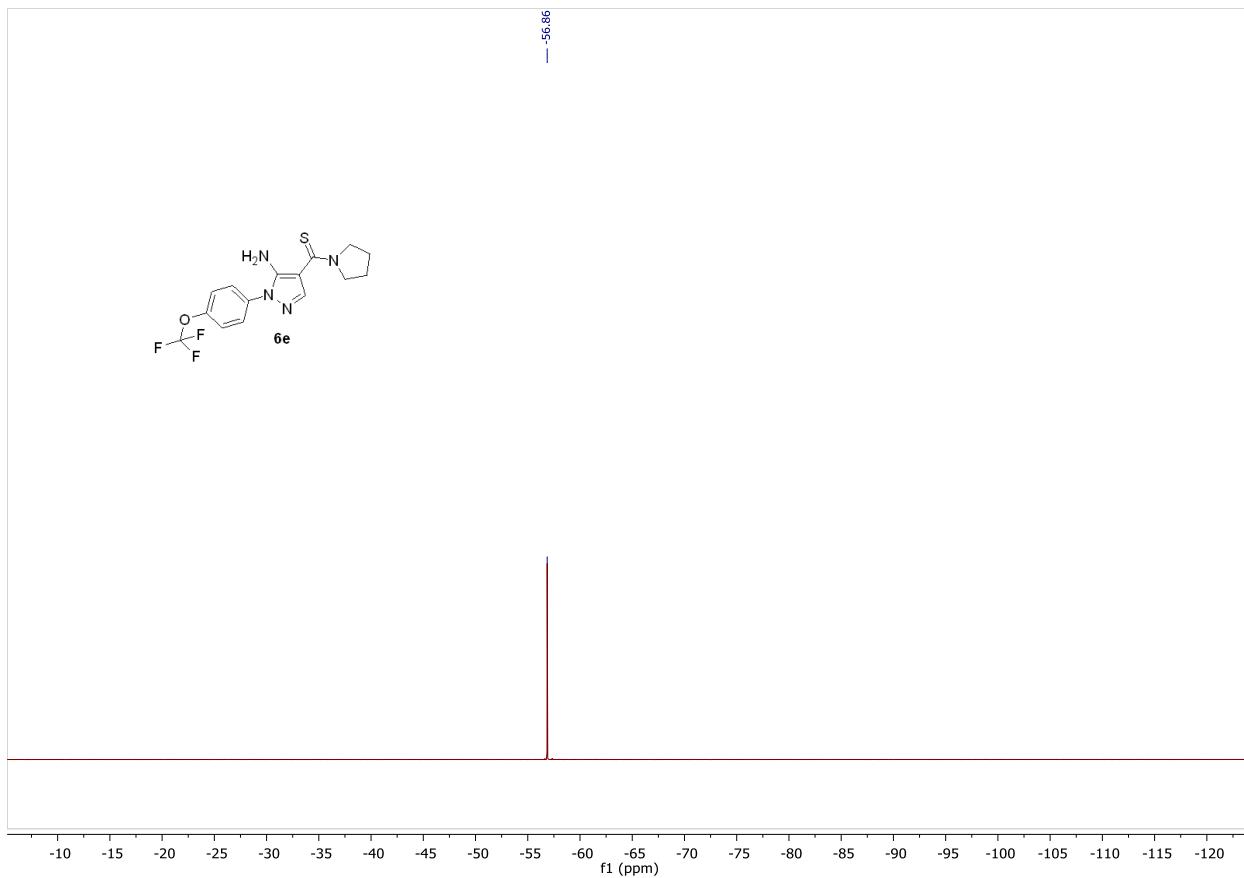
**Figure S30.**  $^1\text{H}$  NMR spectrum (DMSO- $d_6$ ) of **6e**.



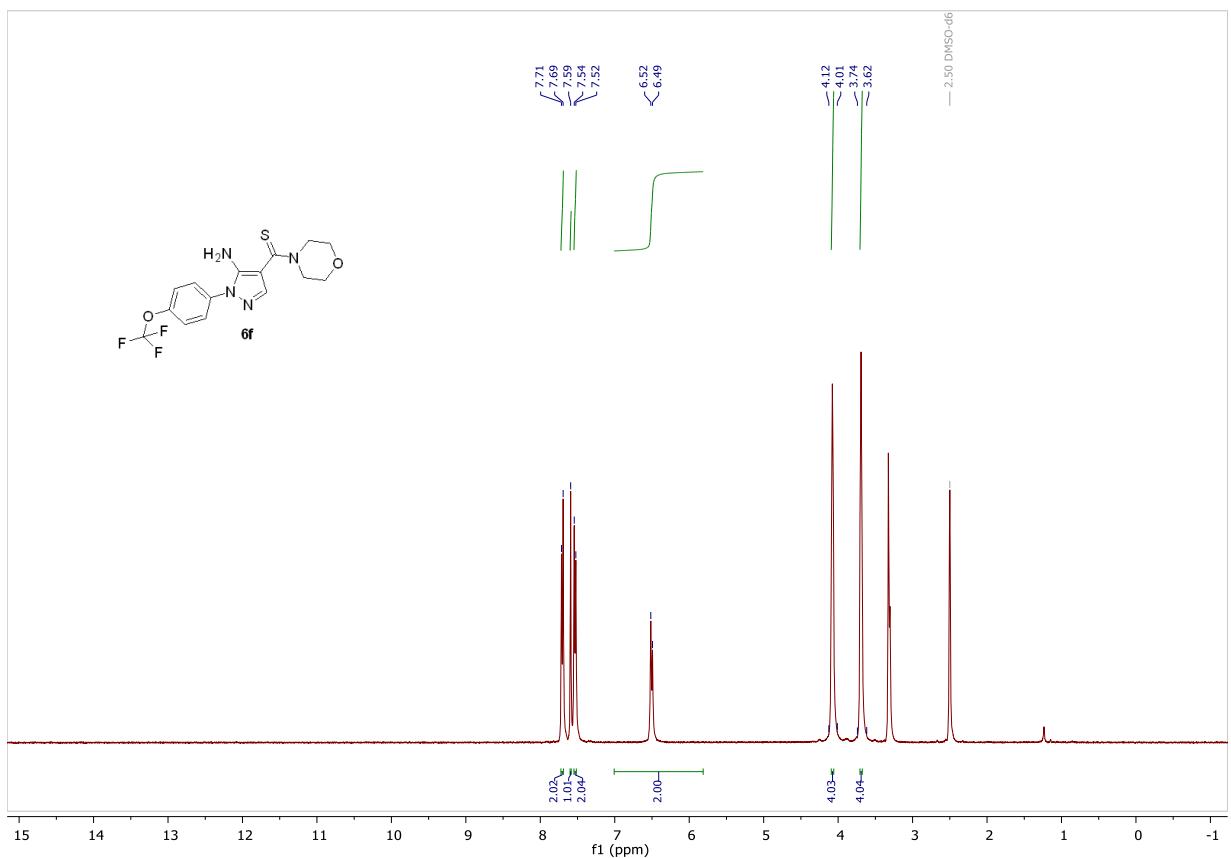
**Figure S31.**  $^{13}\text{C}$  NMR spectrum (DMSO- $d_6$ ) of **6e**.



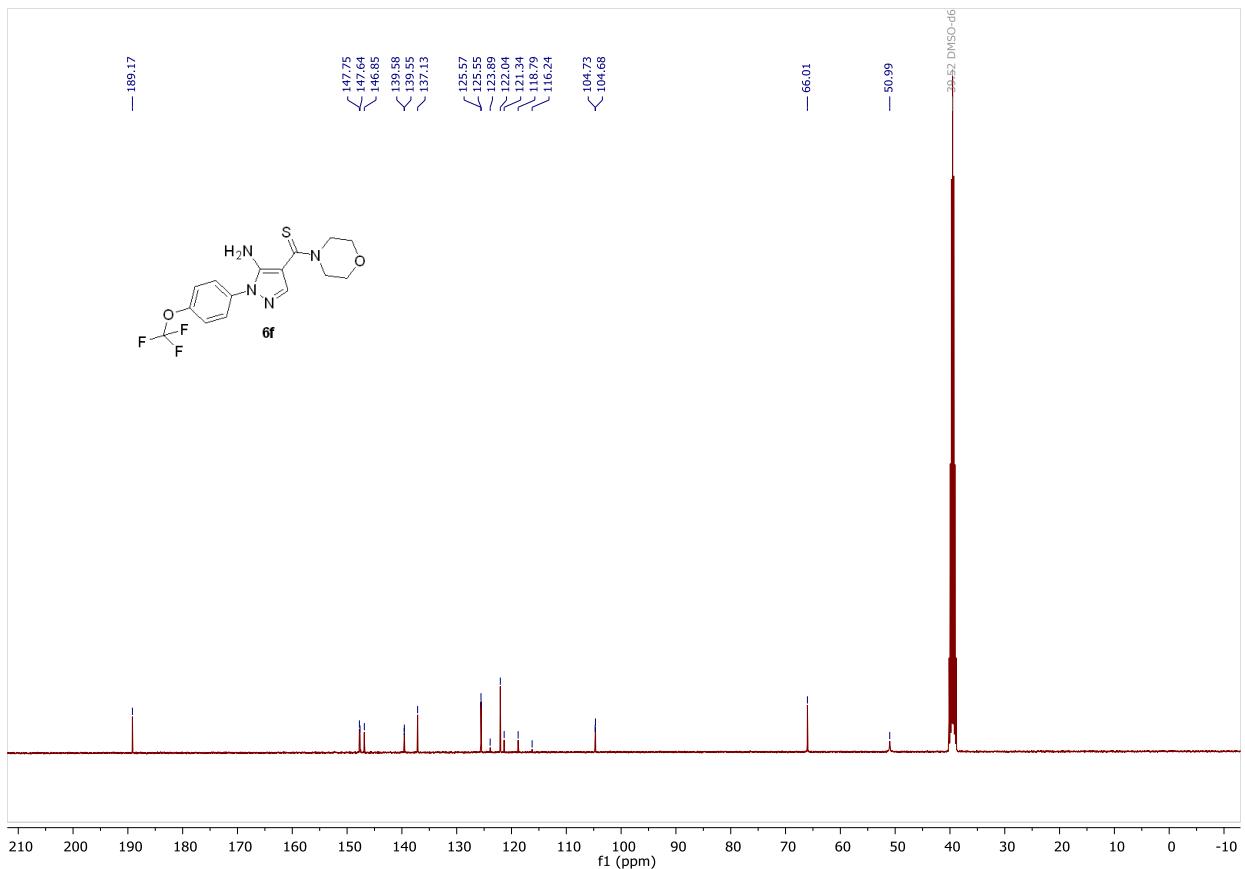
**Figure S32.**  $^{19}\text{F}$  NMR spectrum (DMSO- $d_6$ ) of **6e**.



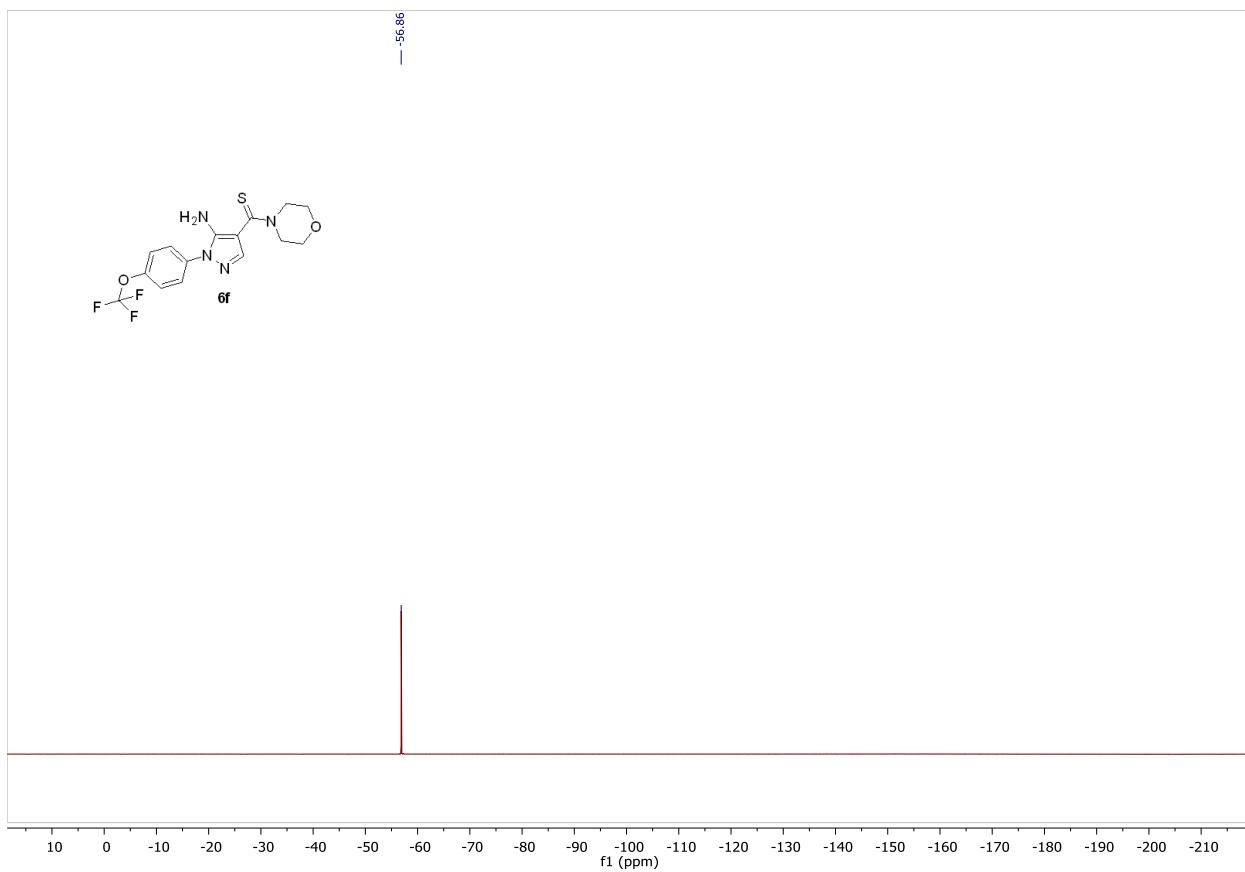
**Figure S33.**  $^1\text{H}$  NMR spectrum (DMSO- $d_6$ ) of **6f**.



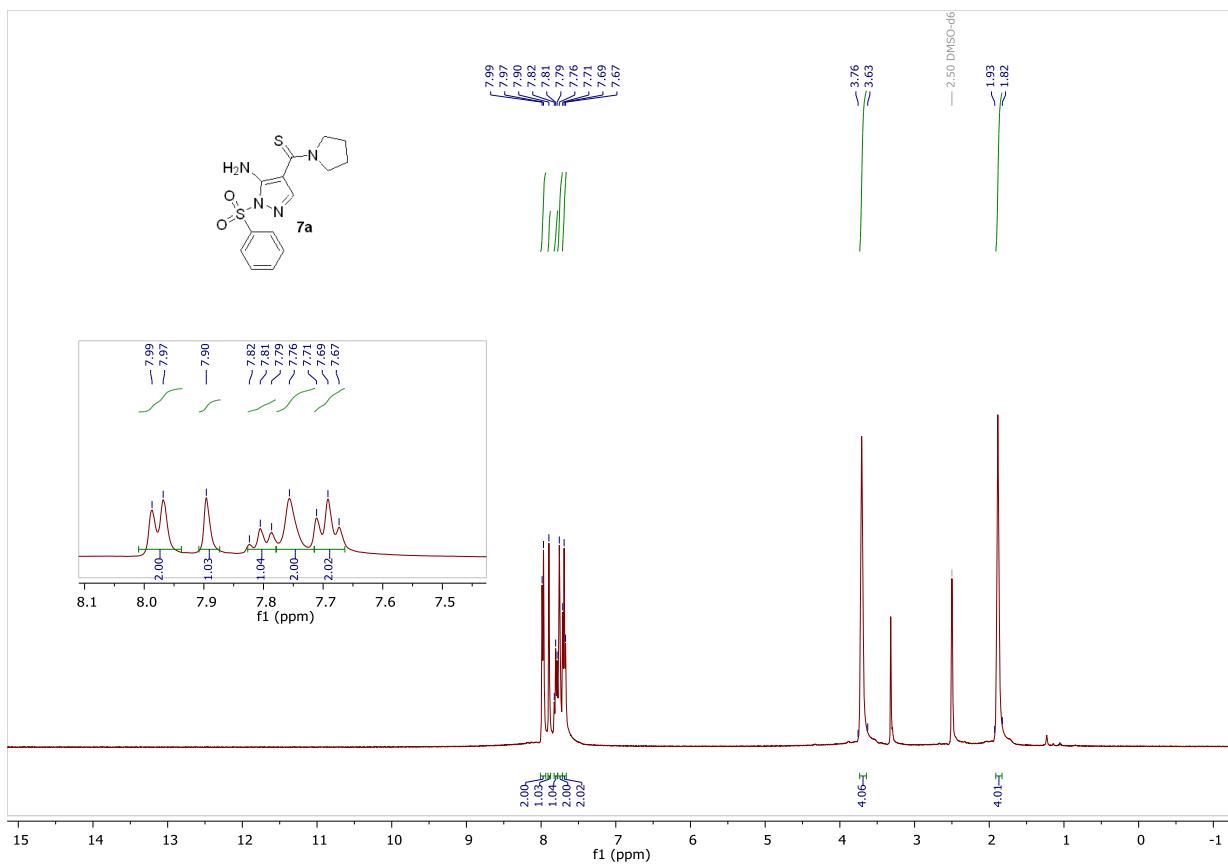
**Figure S34.**  $^{13}\text{C}$  NMR spectrum (DMSO- $d_6$ ) of **6f**.



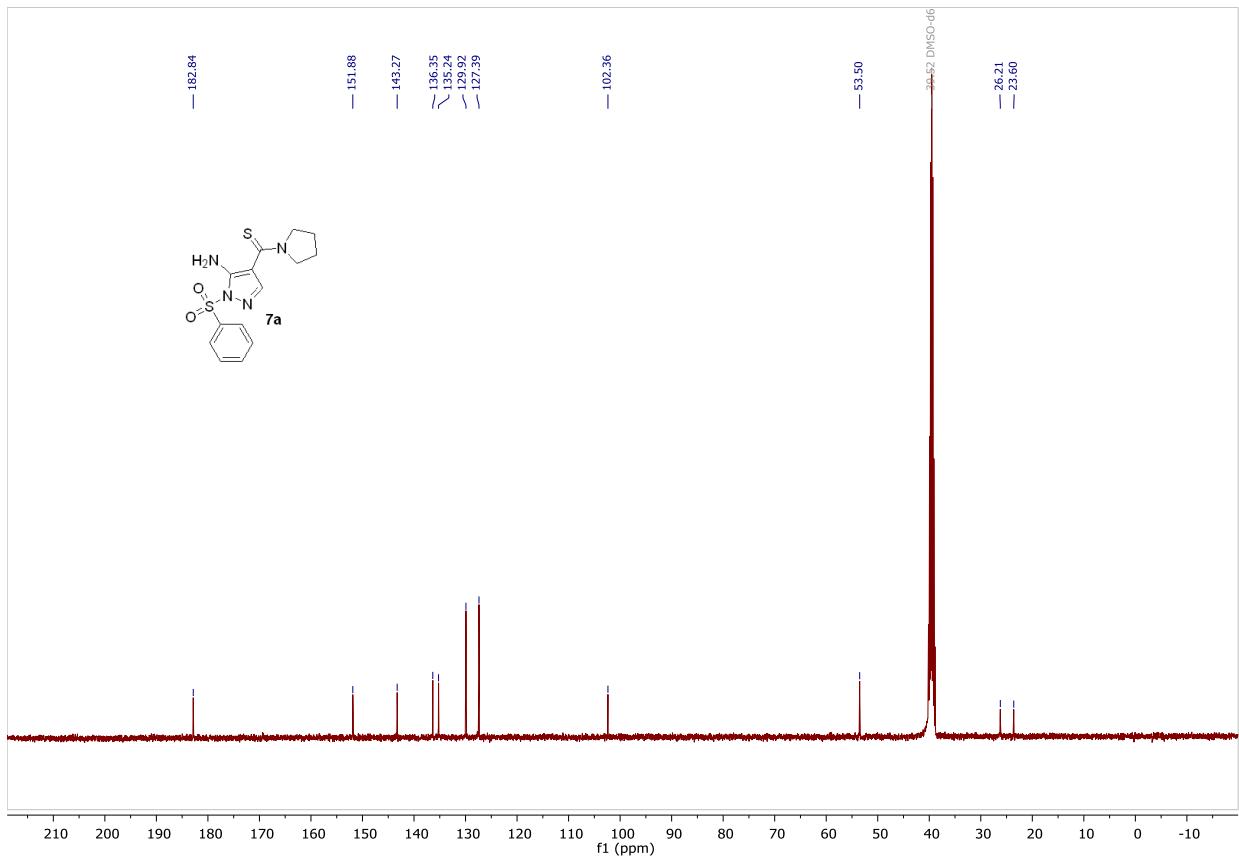
**Figure S35.**  $^{19}\text{F}$  NMR spectrum (DMSO- $d_6$ ) of **6f**.



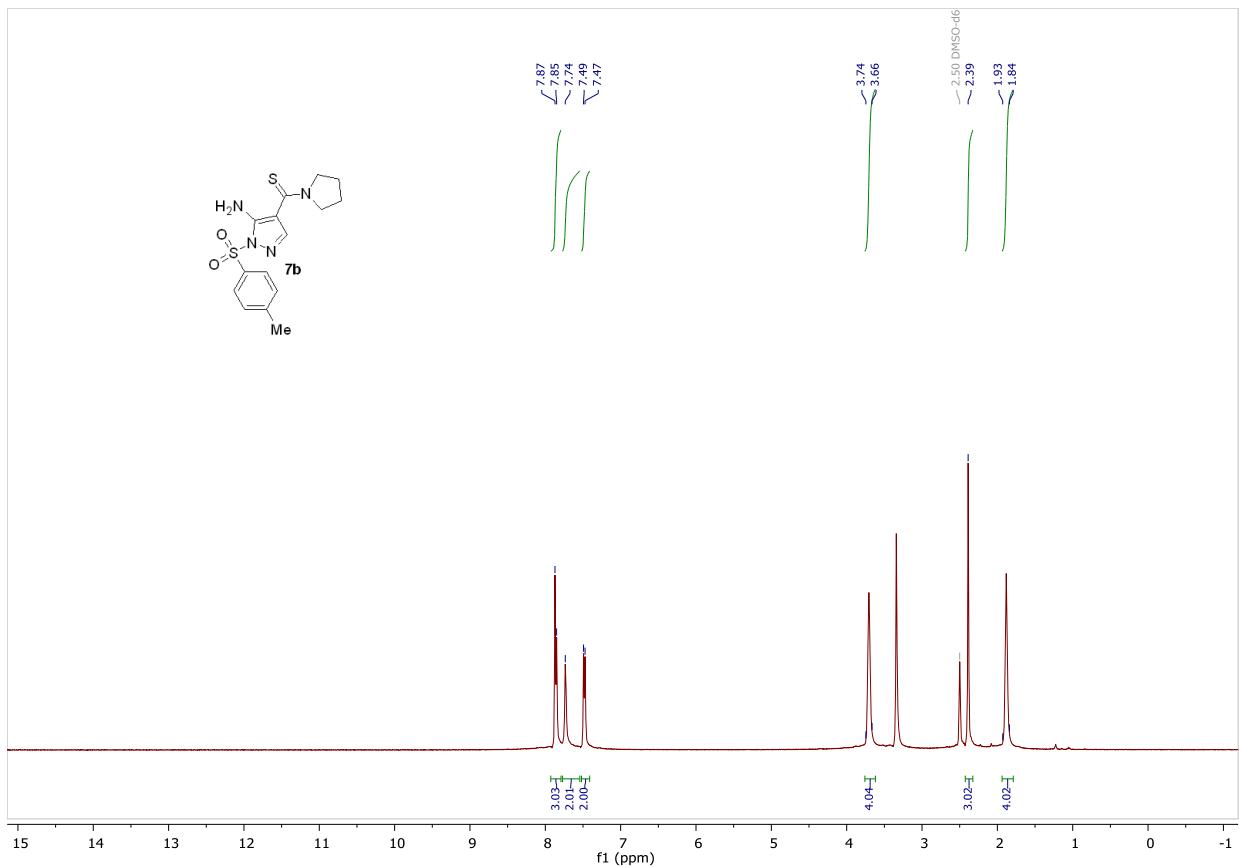
**Figure S36.**  $^1\text{H}$  NMR spectrum (DMSO- $d_6$ ) of **7a**.



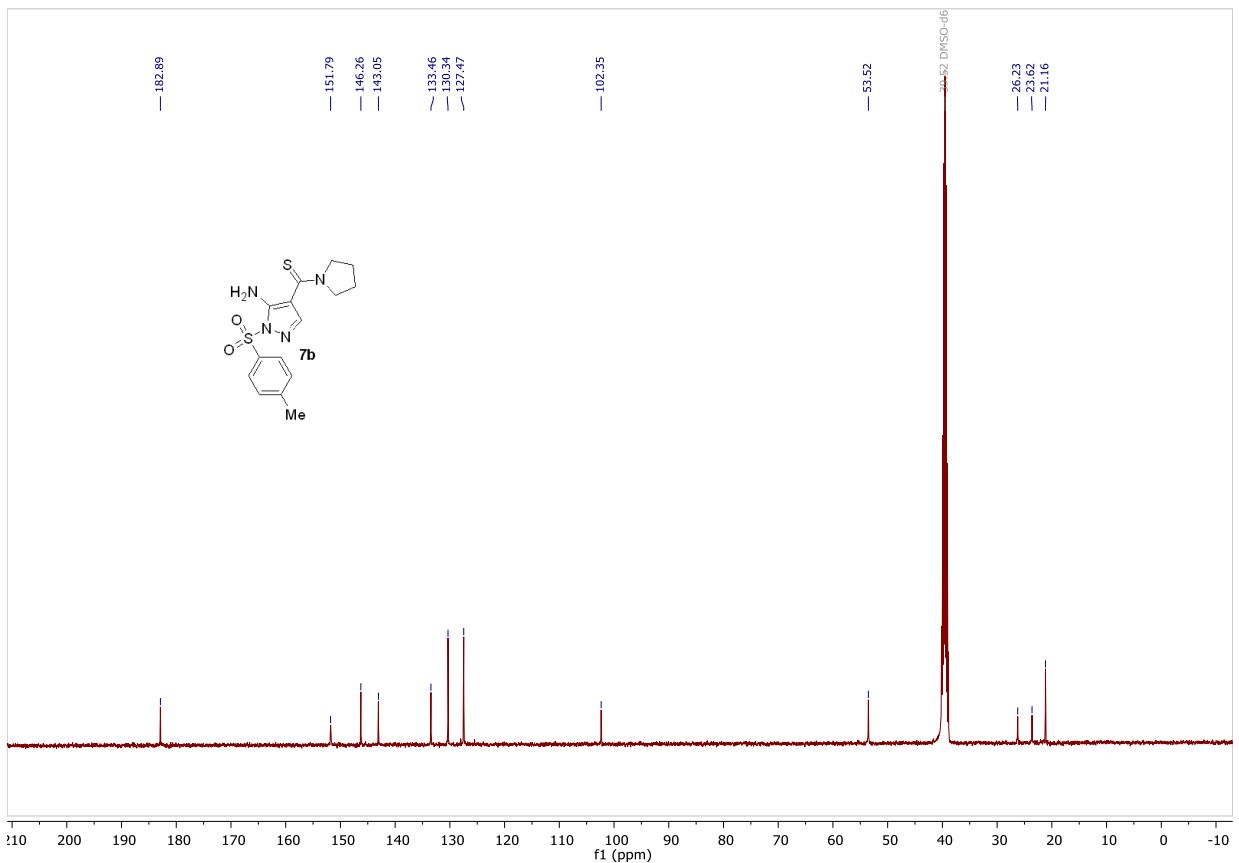
**Figure S37.**  $^{13}\text{C}$  NMR spectrum (DMSO- $d_6$ ) of **7a**.



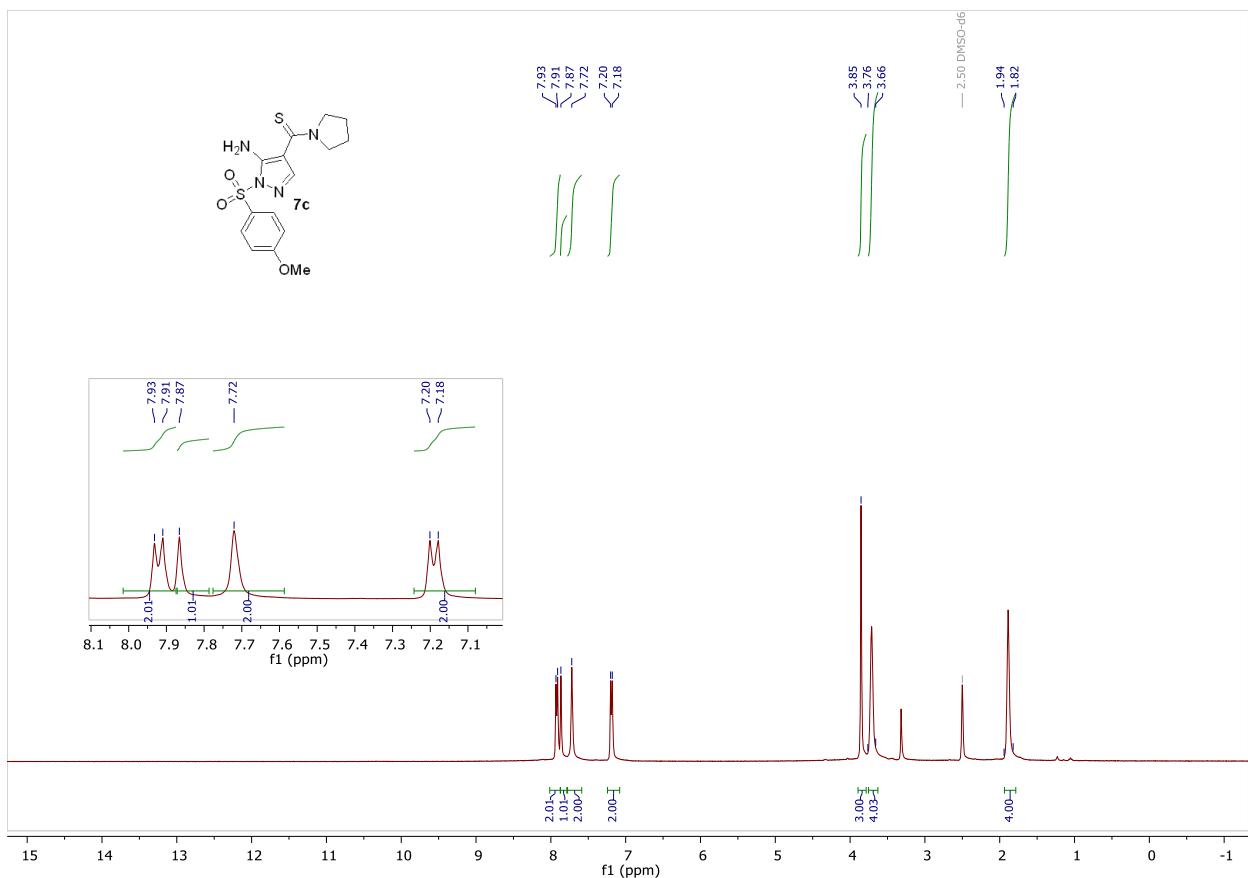
**Figure S38.**  $^1\text{H}$  NMR spectrum (DMSO- $d_6$ ) of **7b**.



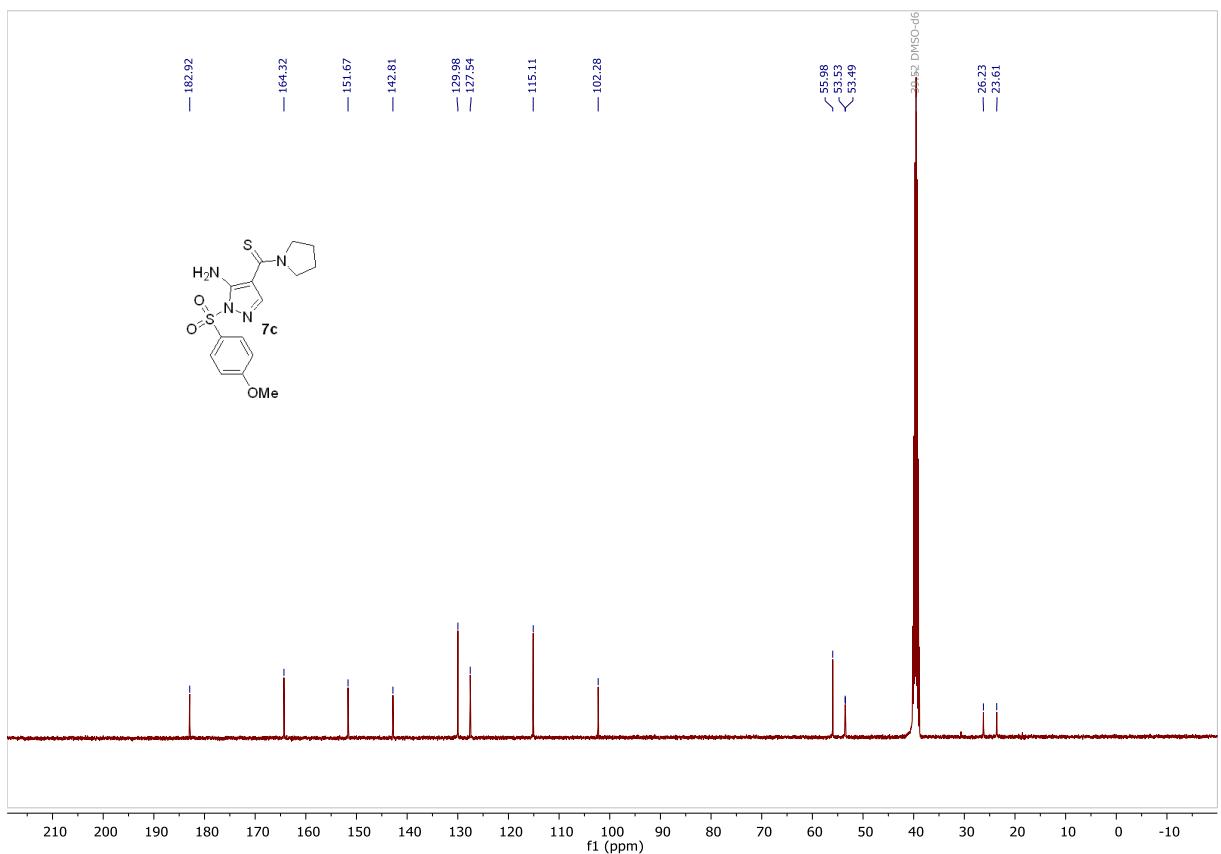
**Figure S39.**  $^{13}\text{C}$  NMR spectrum (DMSO- $d_6$ ) of **7b**.



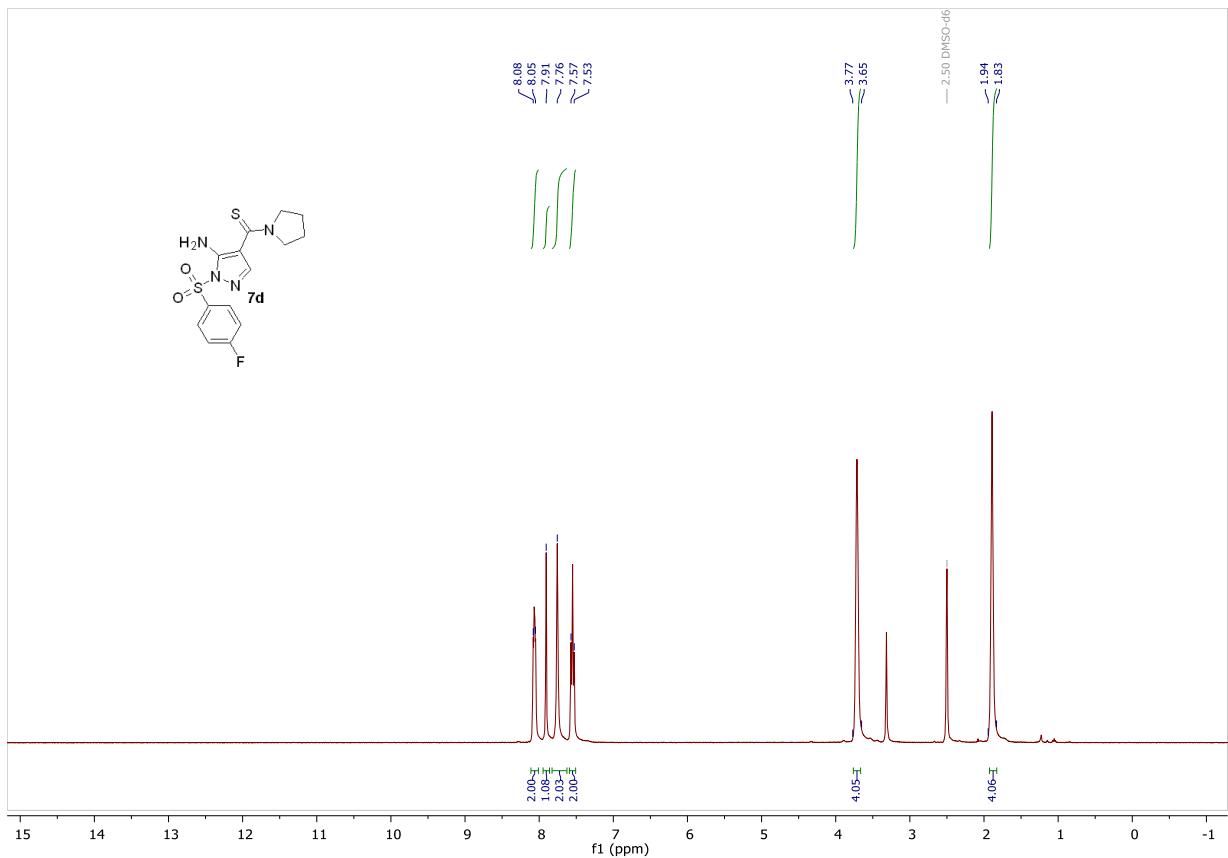
**Figure S40.**  $^1\text{H}$  NMR spectrum (DMSO- $d_6$ ) of **7c**.



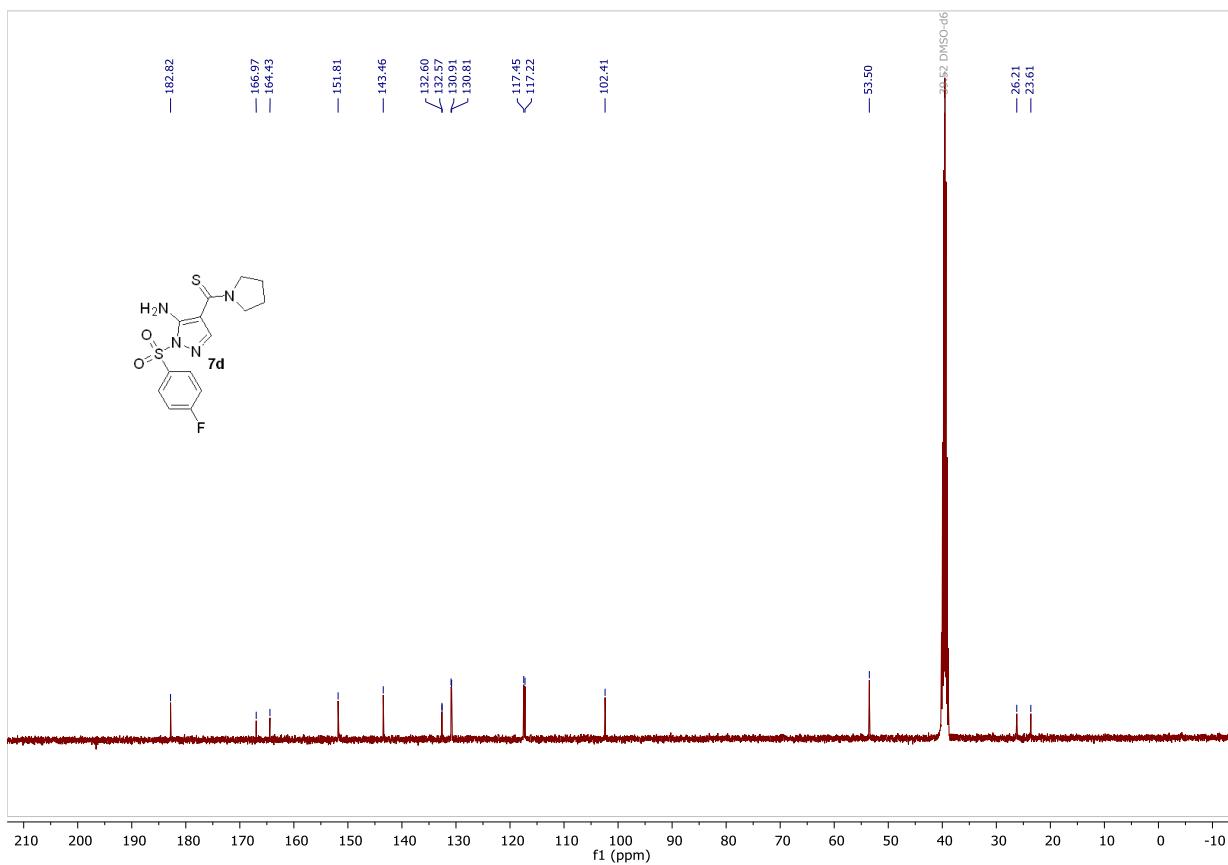
**Figure S41.**  $^{13}\text{C}$  NMR spectrum (DMSO- $d_6$ ) of **7c**.



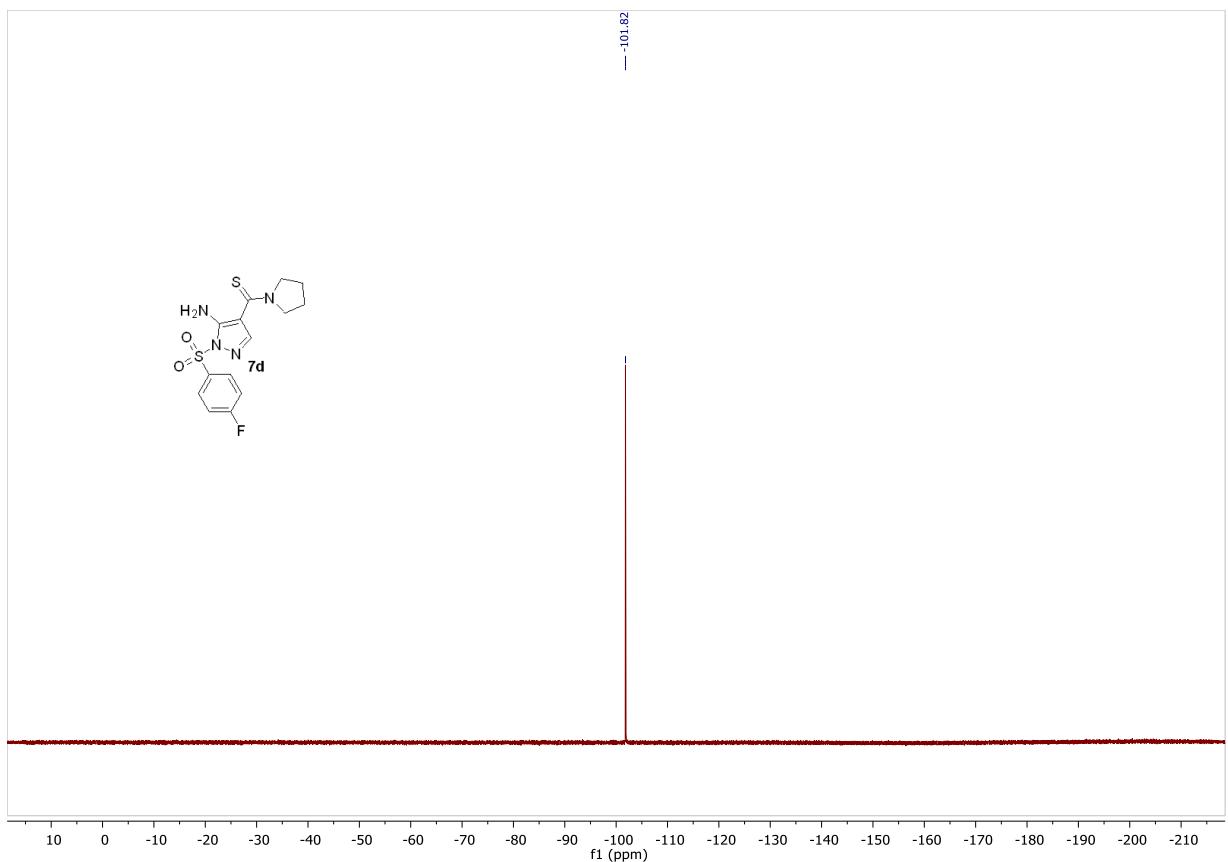
**Figure S42.**  $^1\text{H}$  NMR spectrum (DMSO- $d_6$ ) of **7d**.



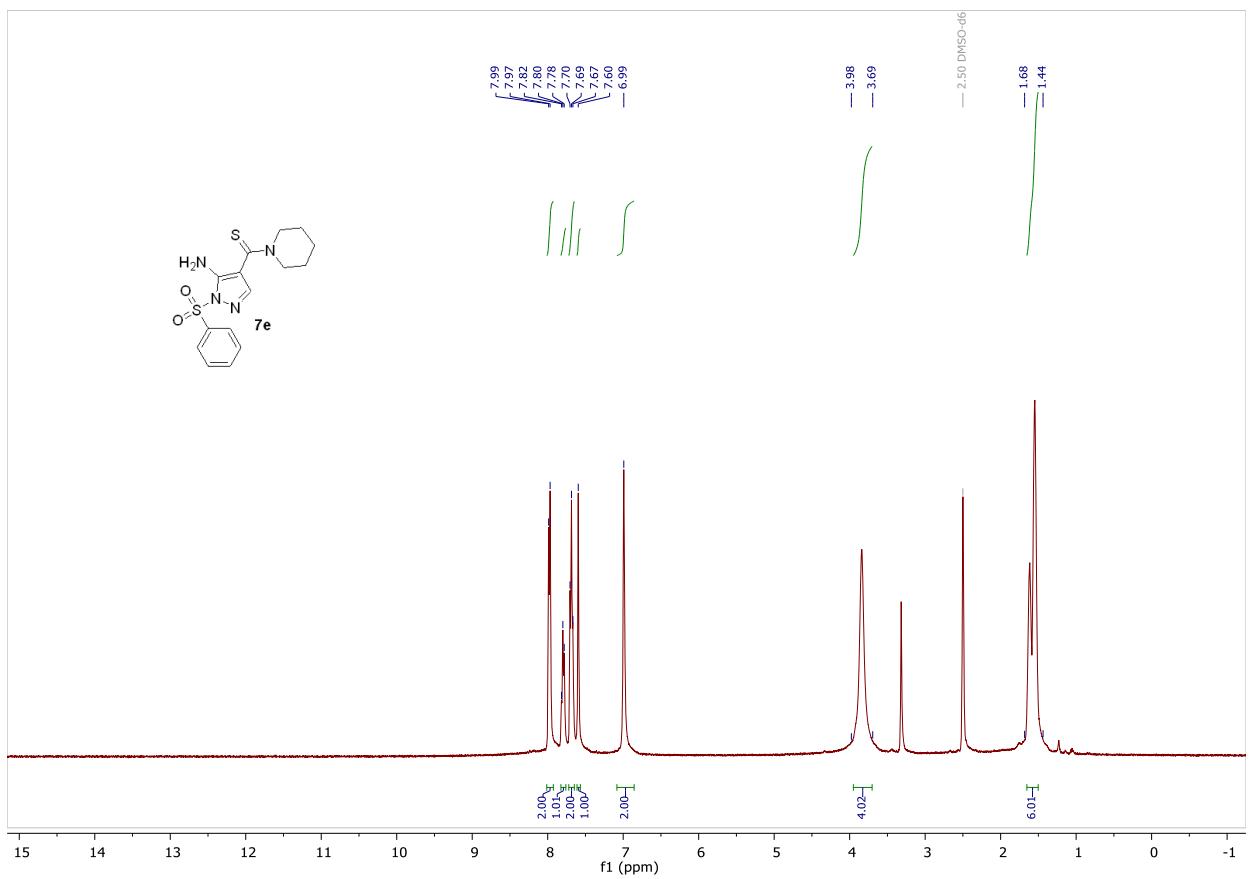
**Figure S43.**  $^{13}\text{C}$  NMR spectrum (DMSO- $d_6$ ) of **7d**.



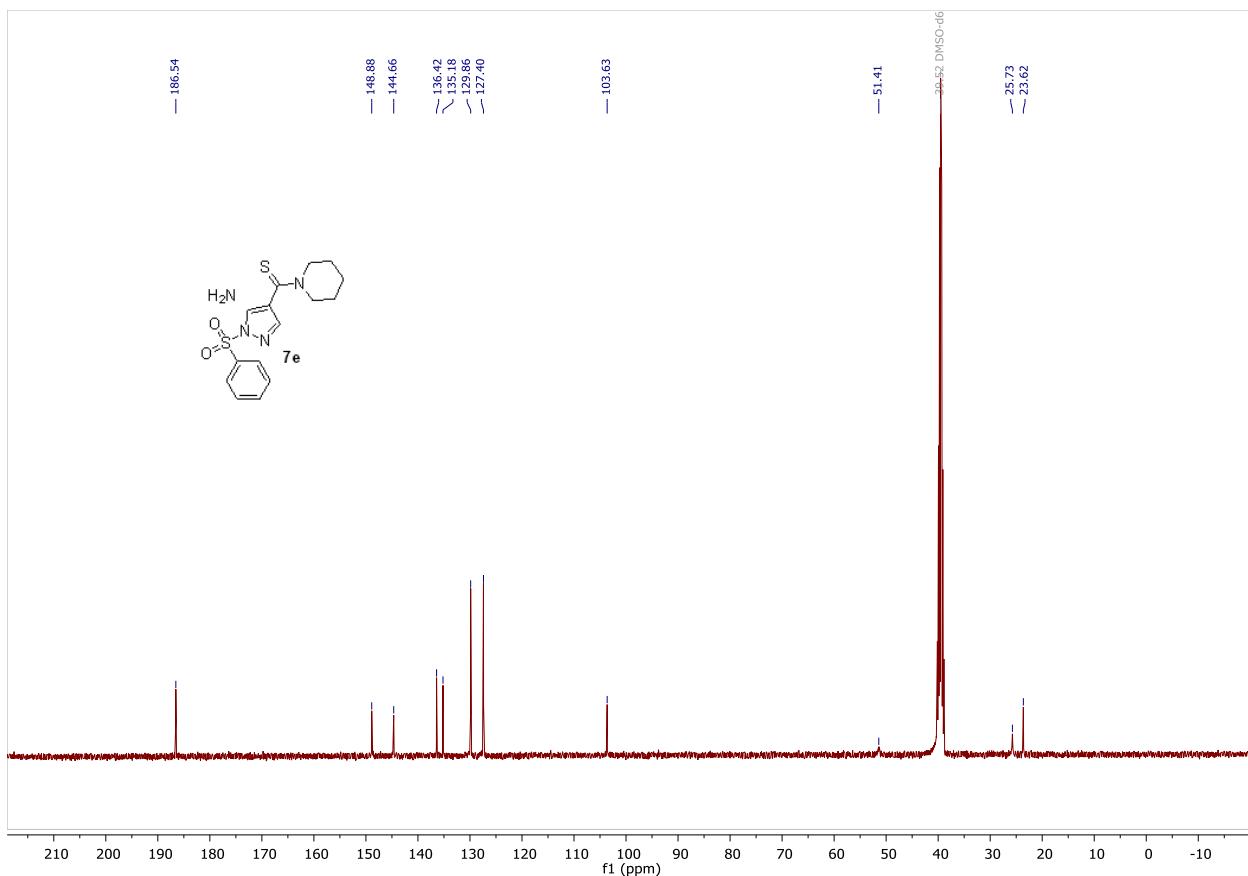
**Figure S44.**  $^{19}\text{F}$  NMR spectrum (DMSO- $d_6$ ) of **7d**.



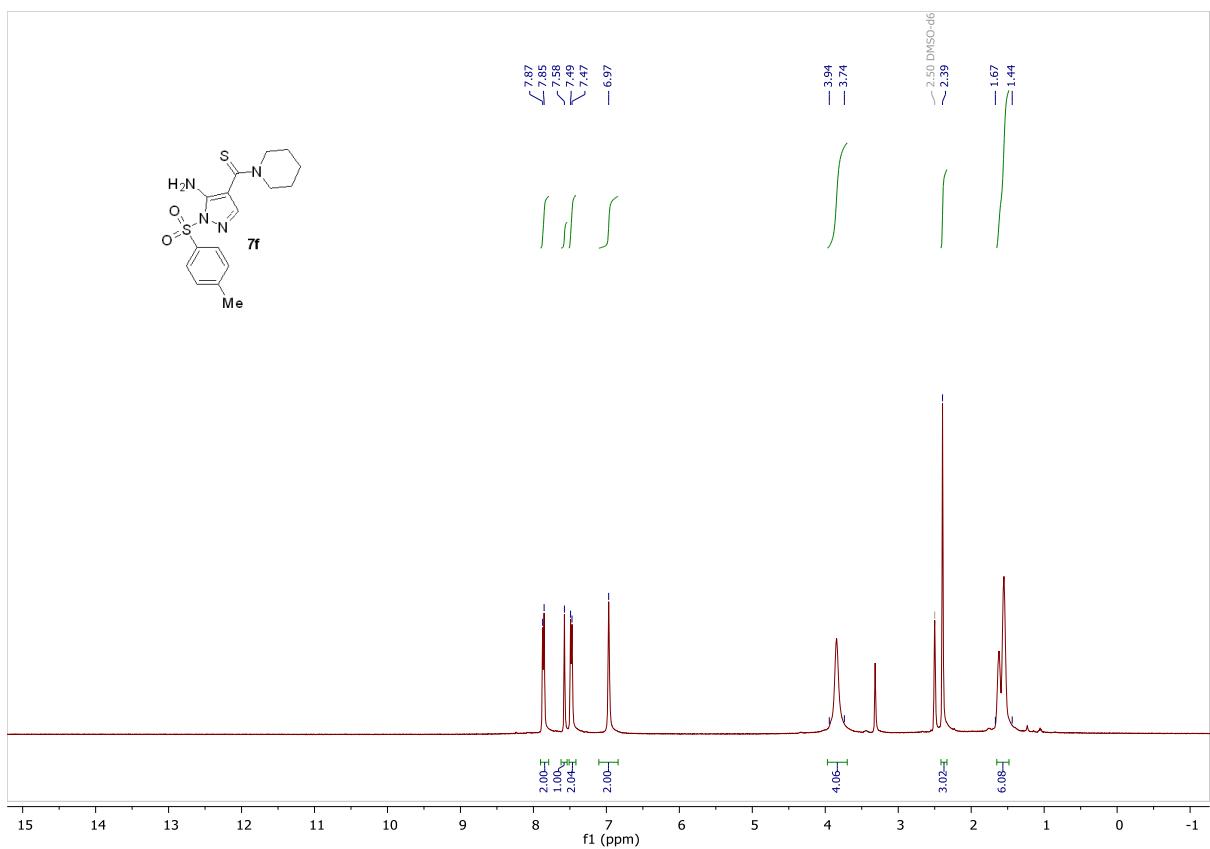
**Figure S45.**  $^1\text{H}$  NMR spectrum (DMSO- $d_6$ ) of **7e**.



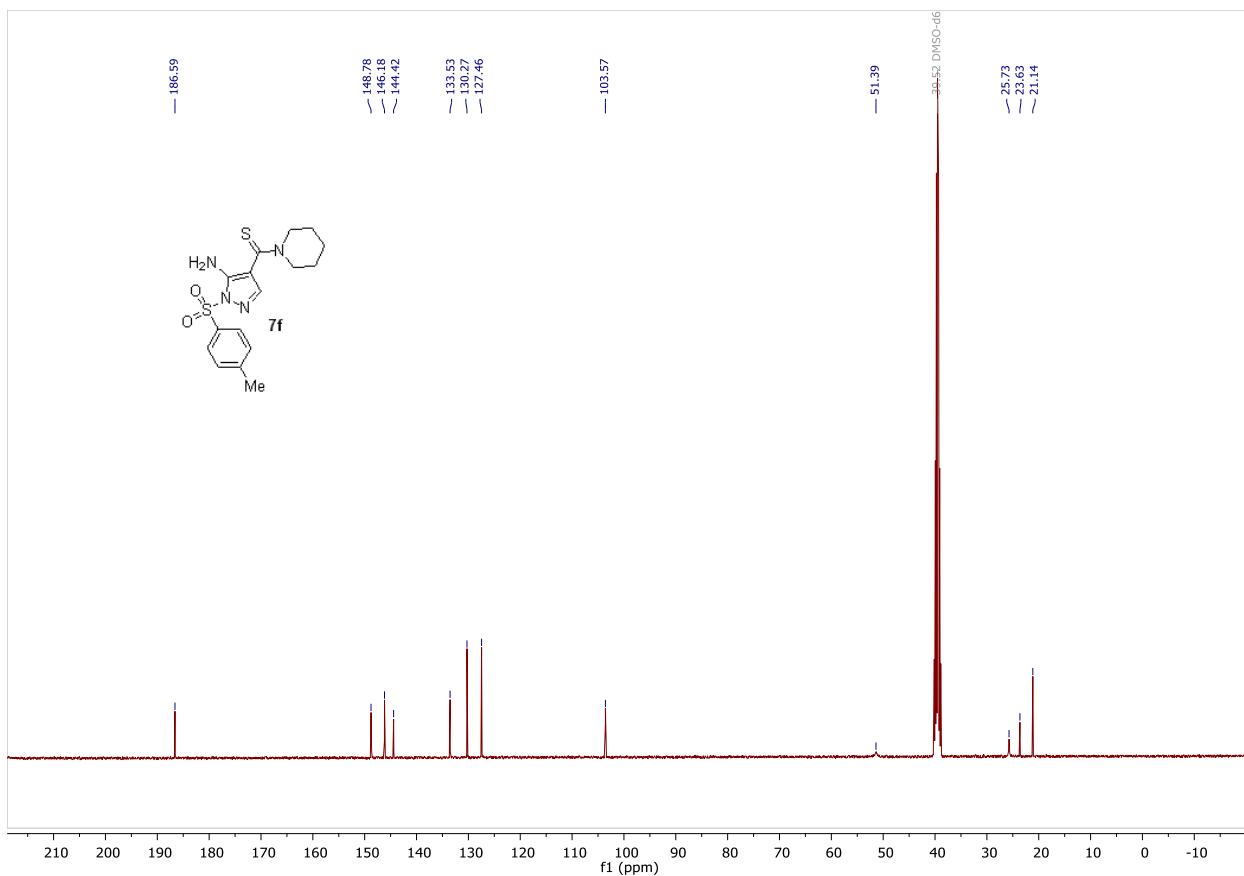
**Figure S46.**  $^{13}\text{C}$  NMR spectrum (DMSO- $d_6$ ) of **7e**.



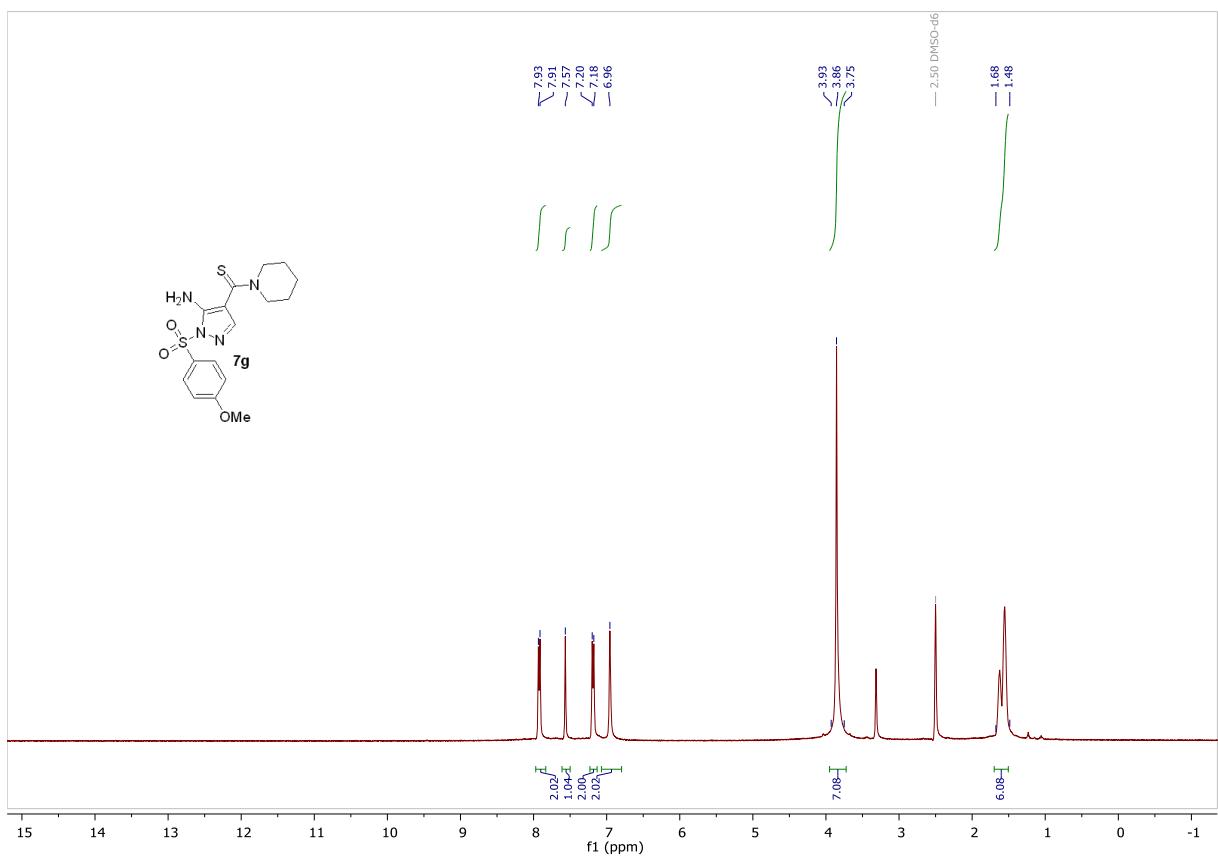
**Figure S47.**  $^1\text{H}$  NMR spectrum (DMSO- $d_6$ ) of **7f**.



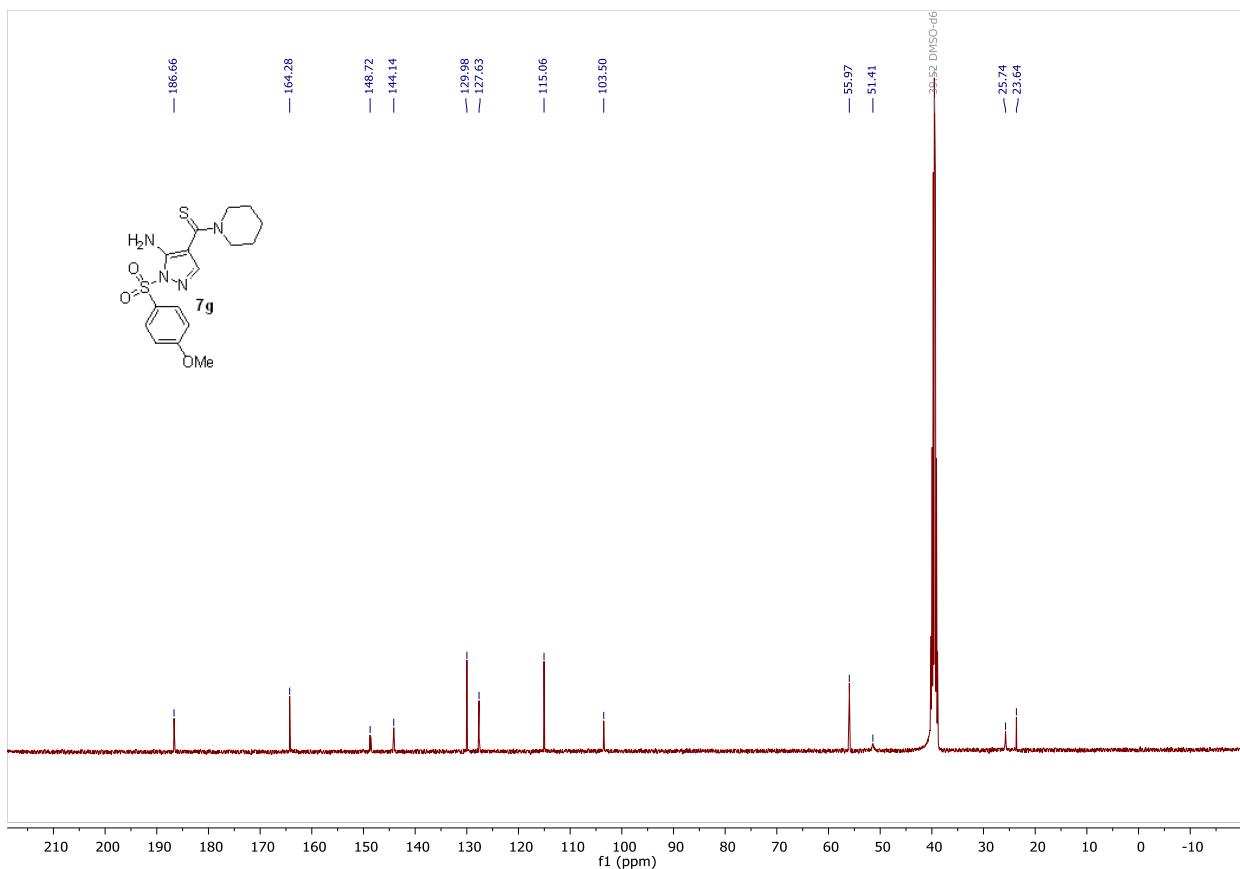
**Figure S48.**  $^{13}\text{C}$  NMR spectrum (DMSO- $d_6$ ) of **7f**.



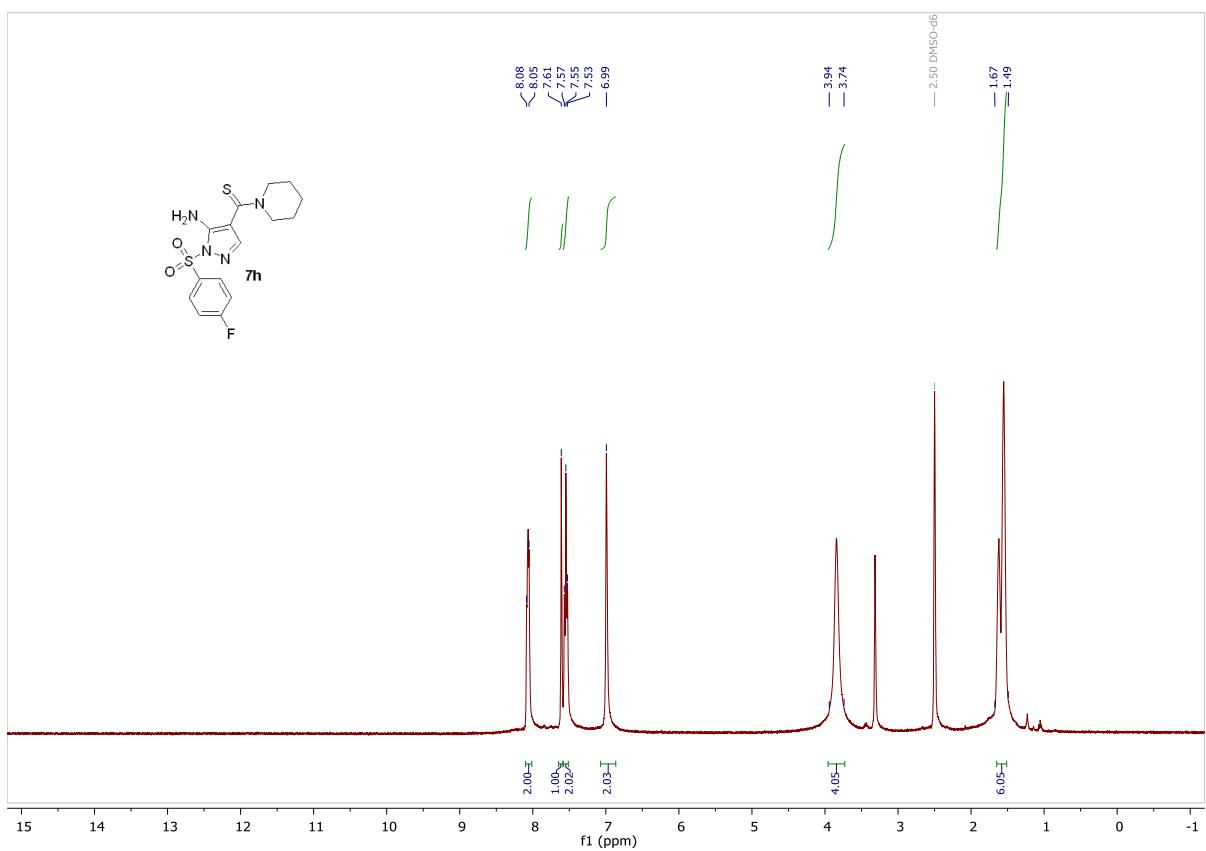
**Figure S49.**  $^1\text{H}$  NMR spectrum (DMSO- $d_6$ ) of **7g**.



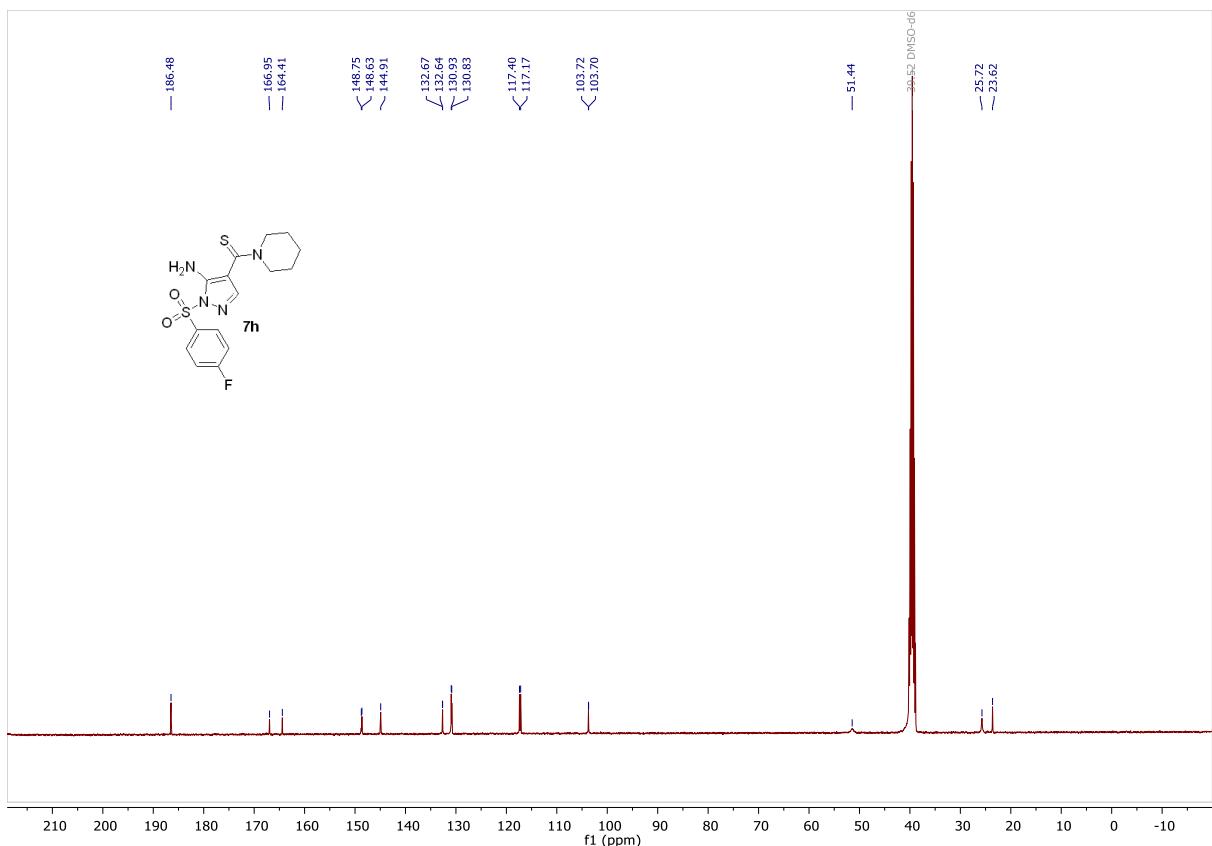
**Figure S50.**  $^{13}\text{C}$  NMR spectrum (DMSO- $d_6$ ) of **7g**.



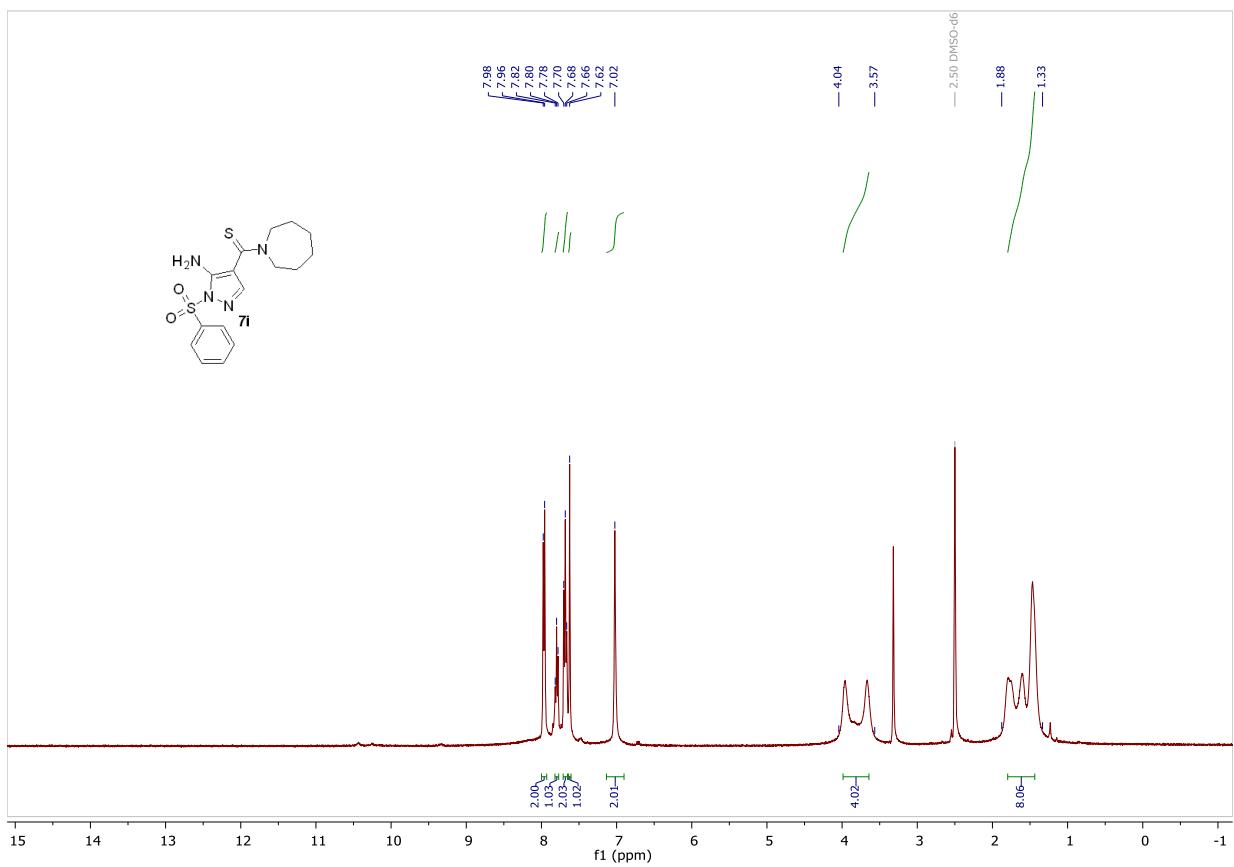
**Figure S51.**  $^1\text{H}$  NMR spectrum (DMSO- $d_6$ ) of **7h**.



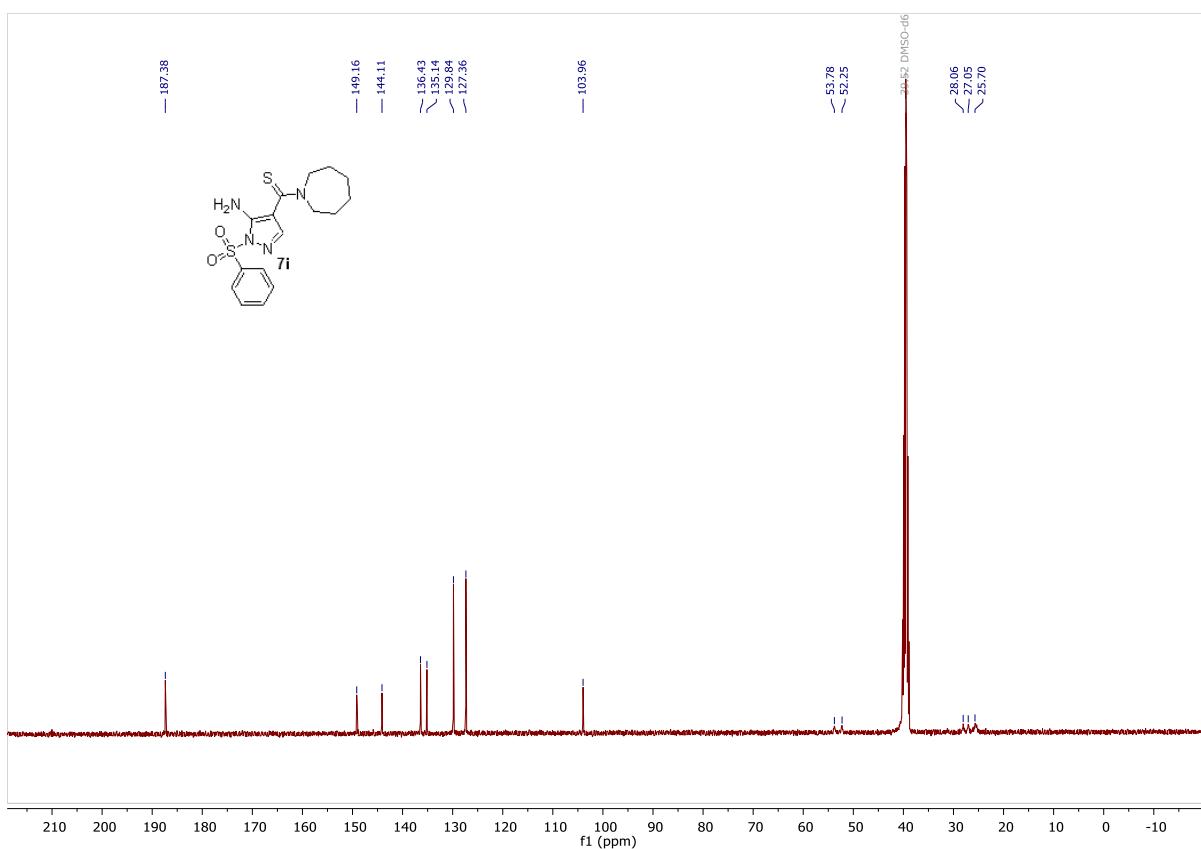
**Figure S52.**  $^{13}\text{C}$  NMR spectrum (DMSO- $d_6$ ) of **7h**.



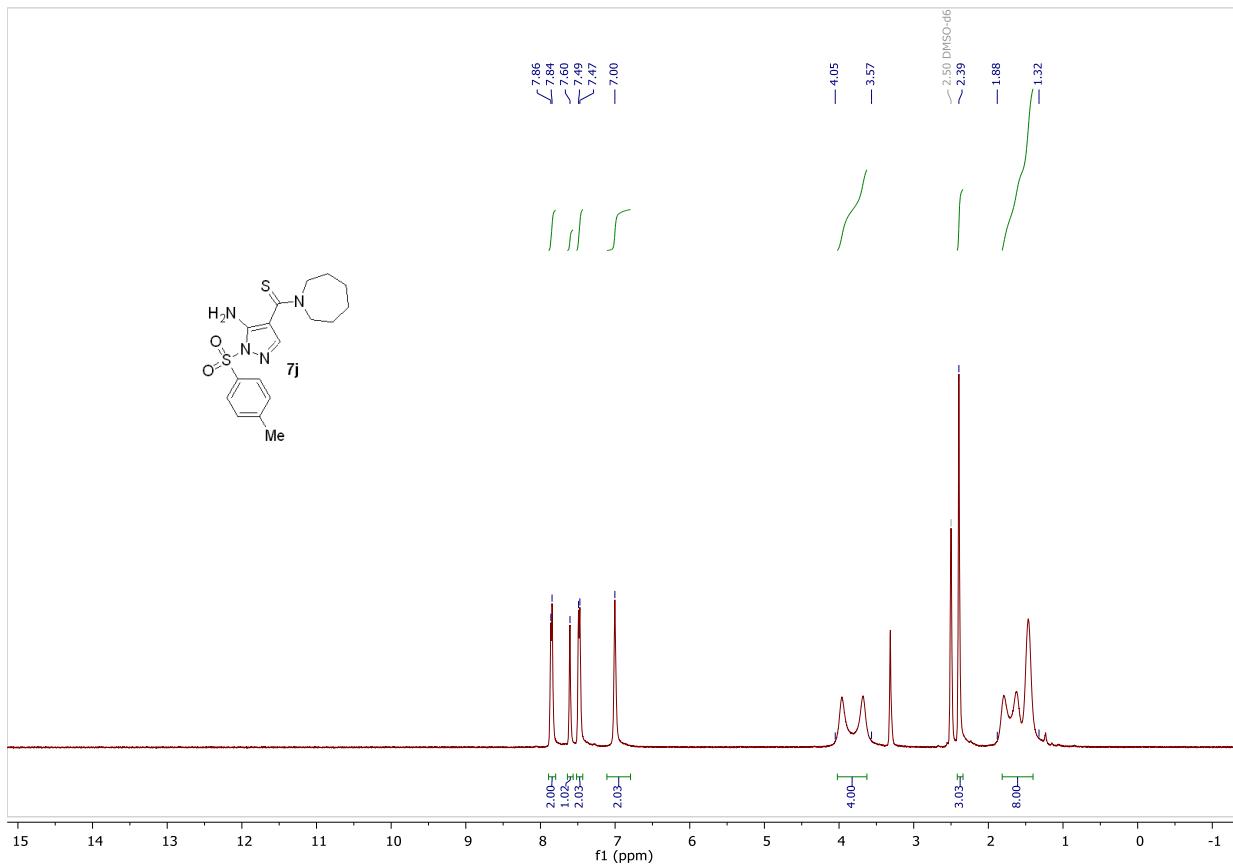
**Figure S53.**  $^1\text{H}$  NMR spectrum (DMSO- $d_6$ ) of **7i**.



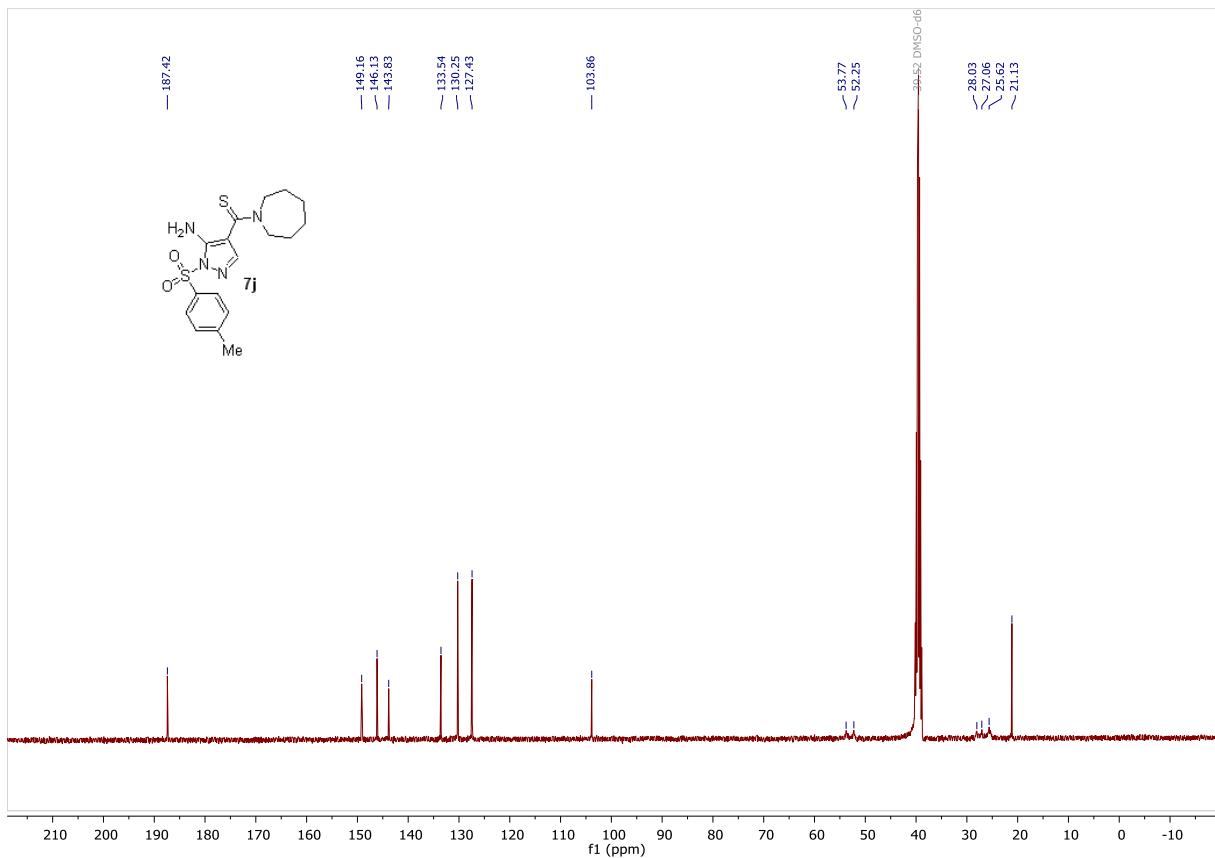
**Figure S54.**  $^{13}\text{C}$  NMR spectrum (DMSO- $d_6$ ) of **7i**.



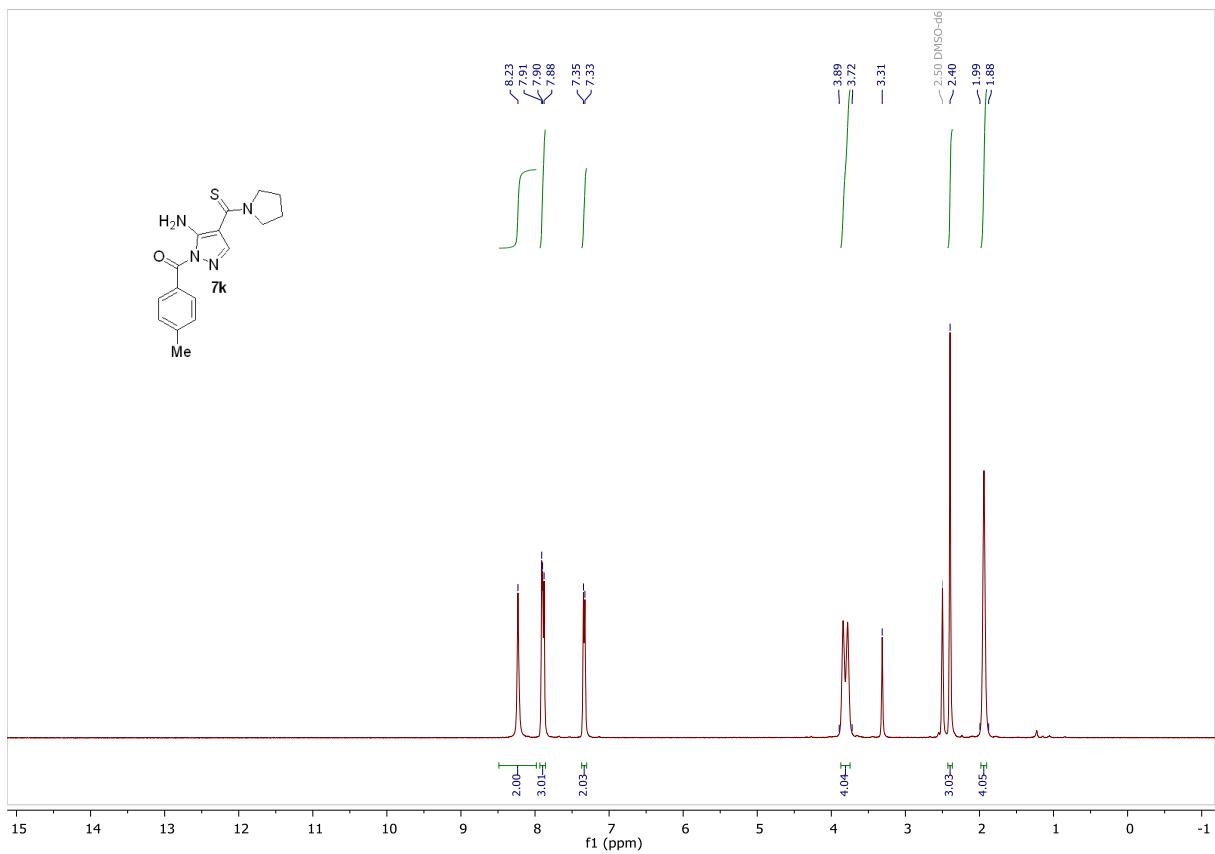
**Figure S55.**  $^1\text{H}$  NMR spectrum (DMSO- $d_6$ ) of **7j**.



**Figure S56.**  $^{13}\text{C}$  NMR spectrum (DMSO- $d_6$ ) of **7j**.



**Figure S57.**  $^1\text{H}$  NMR spectrum (DMSO- $d_6$ ) of **7k**.



**Figure S58.**  $^{13}\text{C}$  NMR spectrum (DMSO- $d_6$ ) of **7k**.

