

**Supporting information**  
for

**Direct C-H bond activation: Palladium-on-carbon as a reusable  
heterogeneous catalyst for C-2 arylation of indoles with arylboronic acids**

Prantika Bhattacharjee<sup>a</sup>, Purna K Boruah<sup>b,c</sup>, Manash R Das<sup>b,c</sup> and Utpal Bora<sup>a\*</sup>

<sup>a</sup>*Department of Chemical Sciences, Tezpur University, Napaam, Tezpur, Assam, India, Pin 784028*

<sup>b</sup>*Advanced Materials Group, Materials Sciences and Technology Division, CSIR-North East Institute of Science and  
Technology, Jorhat 785006, Assam, India*

<sup>c</sup>*Academy of Scientific and Innovative Research (AcSIR), CSIR-NEIST Campus, India*

*E-mail: [ubora@tezu.ernet.in](mailto:ubora@tezu.ernet.in); [utbora@yahoo.co.in](mailto:utbora@yahoo.co.in)*

**Contents**

1	<sup>1</sup> H and <sup>13</sup> C NMR spectra of all compounds	S2
2	References	S21

# 1. $^1\text{H}$ and $^{13}\text{C}$ NMR spectra of all compounds

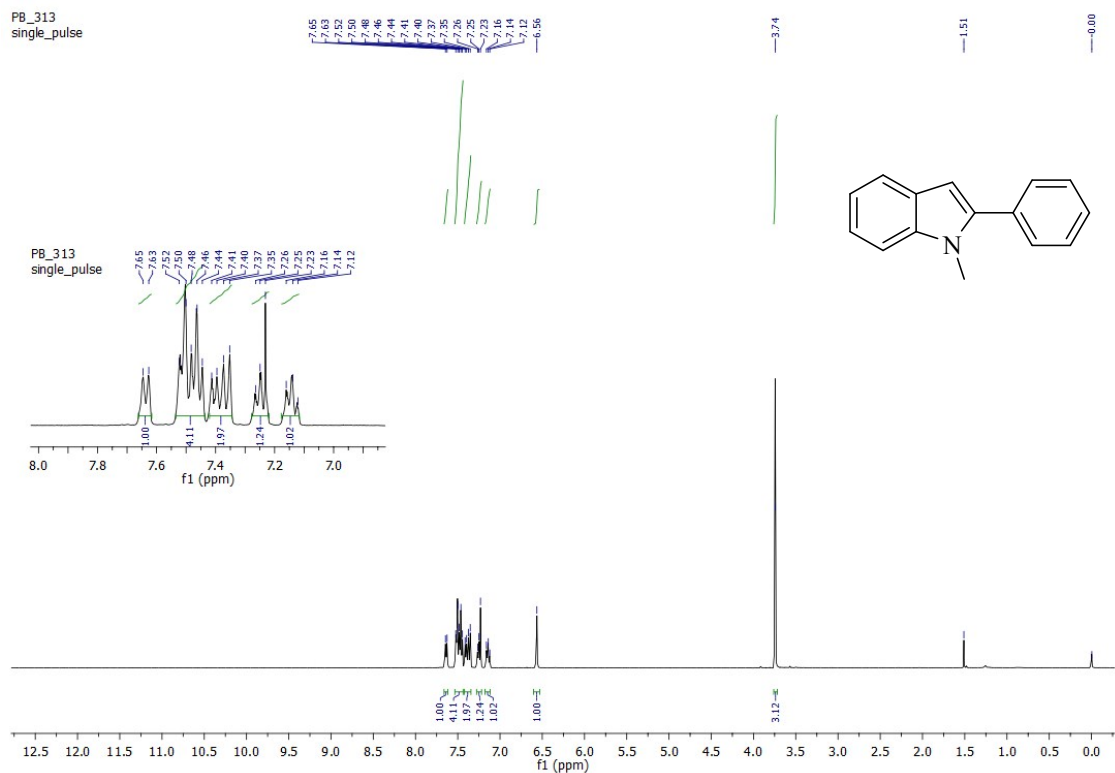


Figure 1. 400 MHz  $^1\text{H}$  NMR spectrum of  $3a^1$  in  $\text{CDCl}_3$

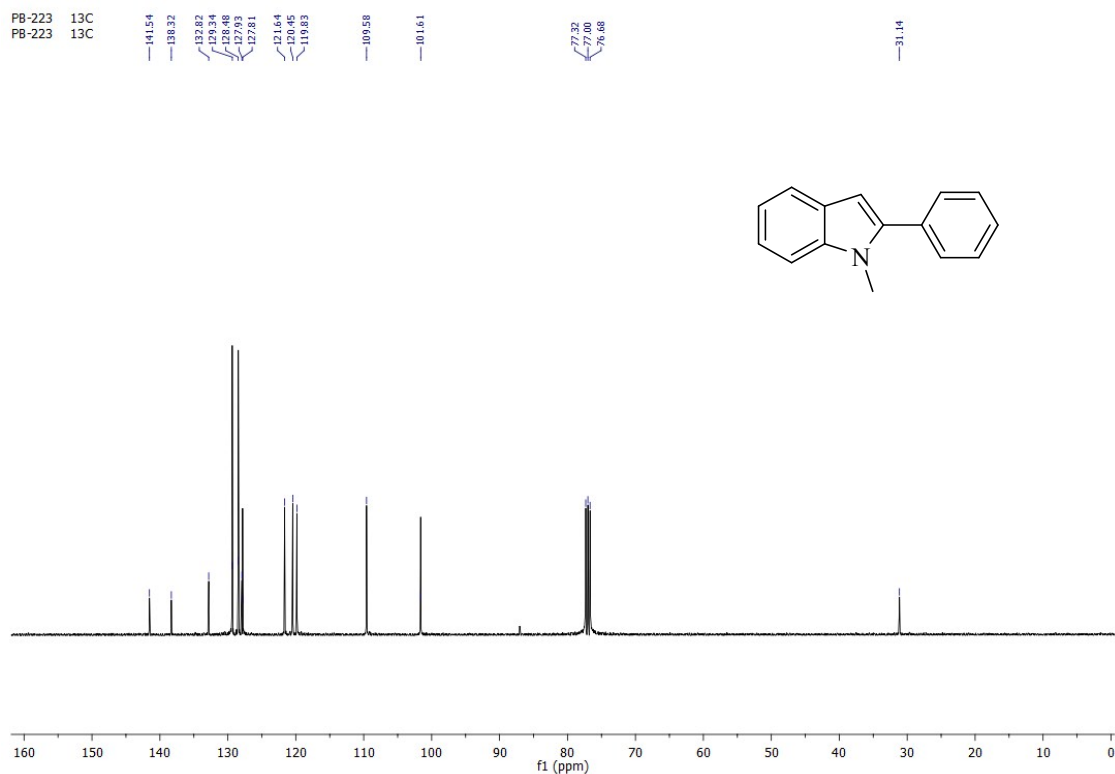
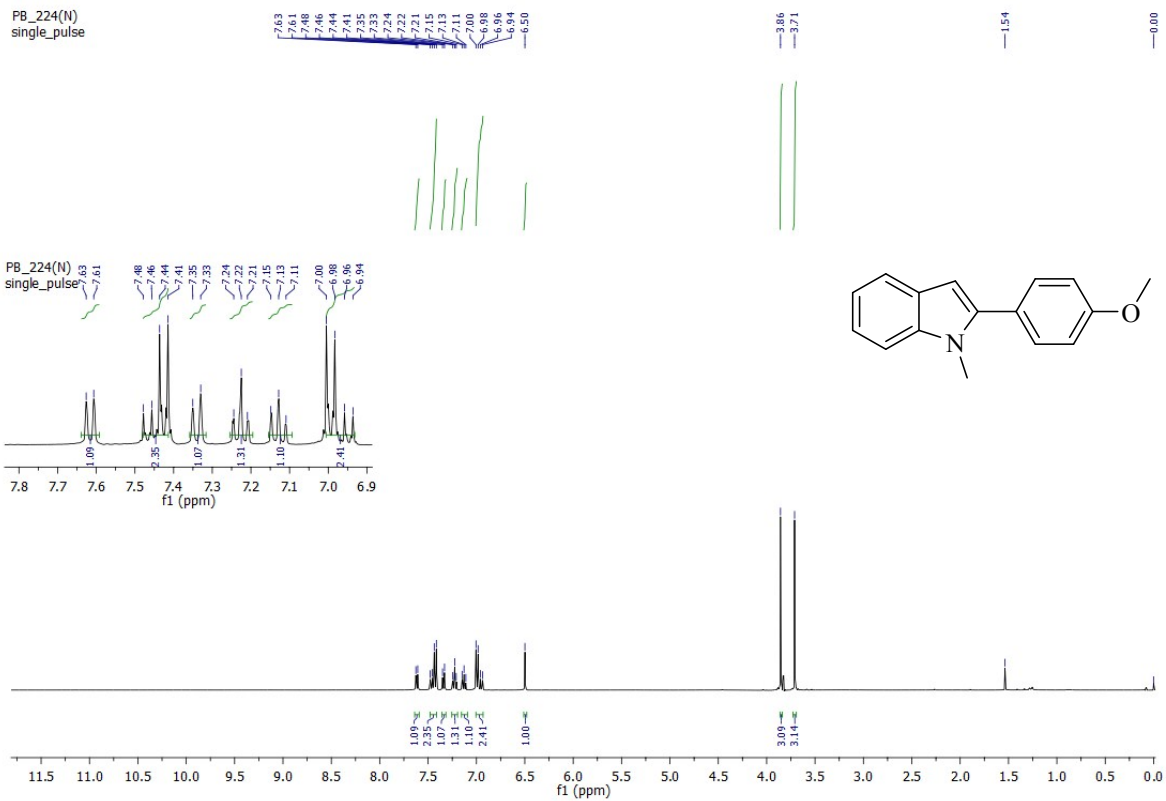
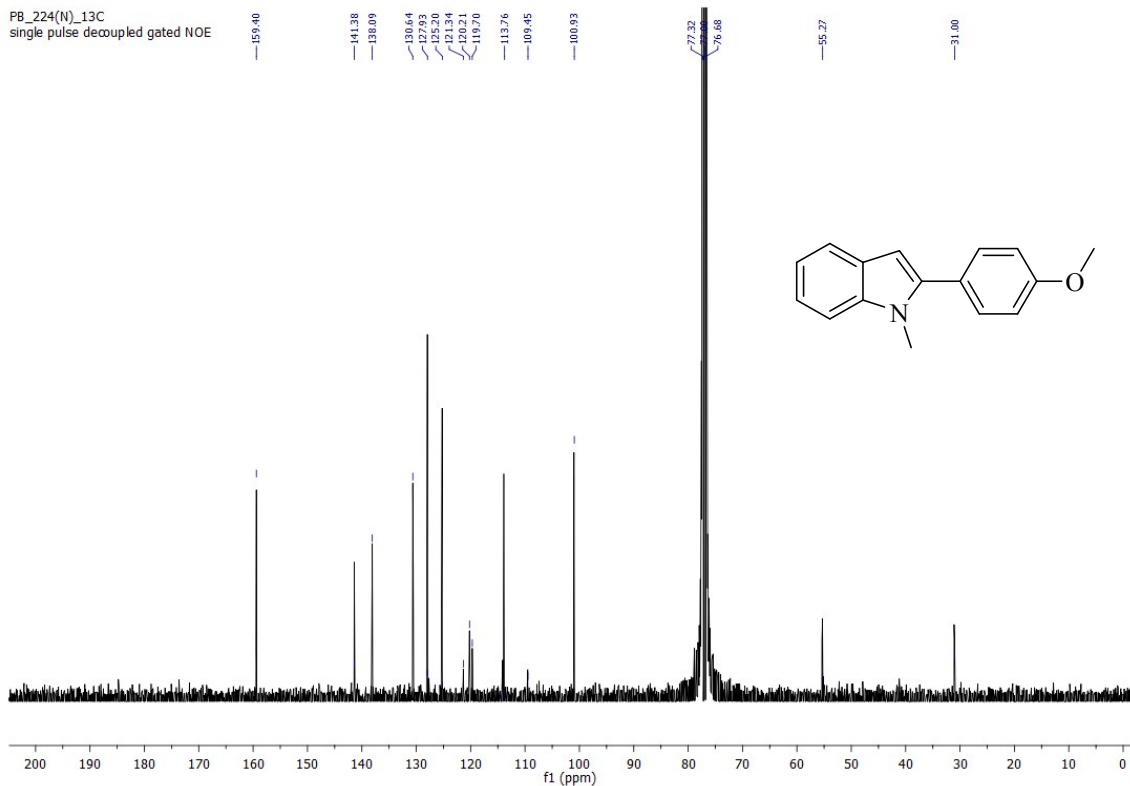


Figure 2. 100 MHz  $^{13}\text{C}$  NMR spectrum of  $3a$  in  $\text{CDCl}_3$



**Figure 3.** 400 MHz  $^1\text{H}$  NMR spectrum of **3b** in  $\text{CDCl}_3$



**Figure 4.** 100 MHz  $^{13}\text{C}$  NMR spectrum of **3b** in  $\text{CDCl}_3$

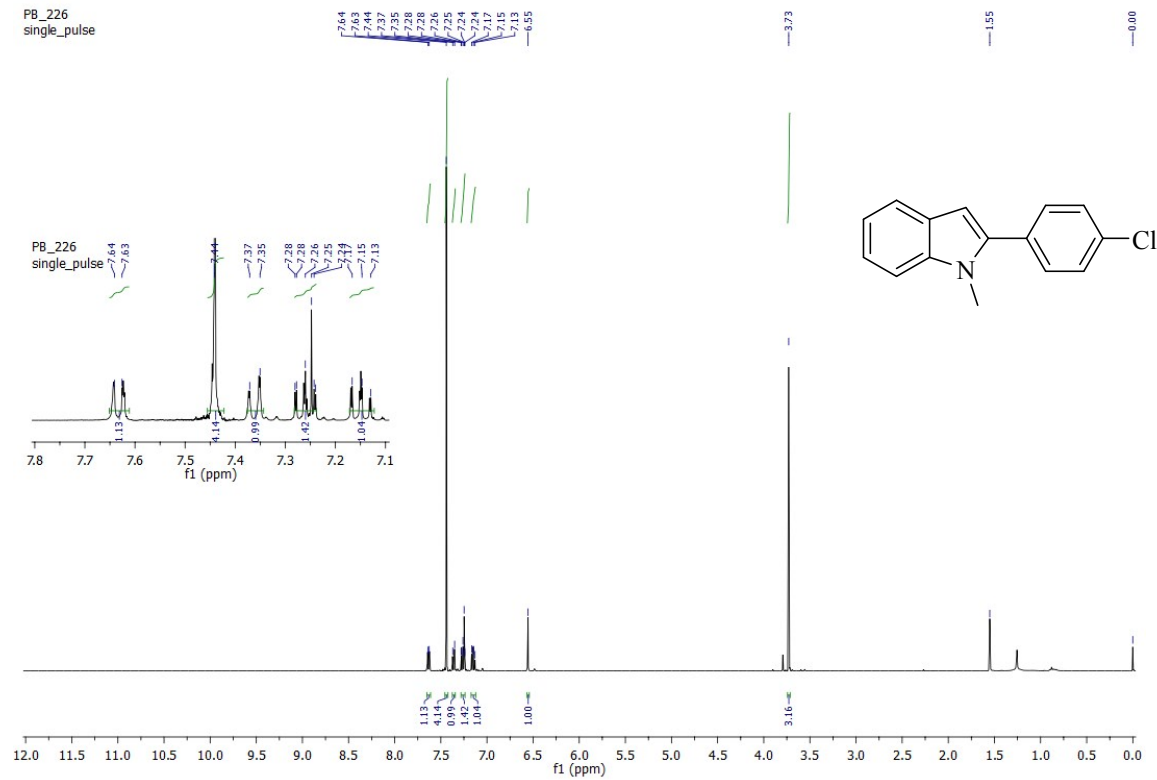


Figure 5. 400 MHz  $^1\text{H}$  NMR spectrum of **3c** in  $\text{CDCl}_3$

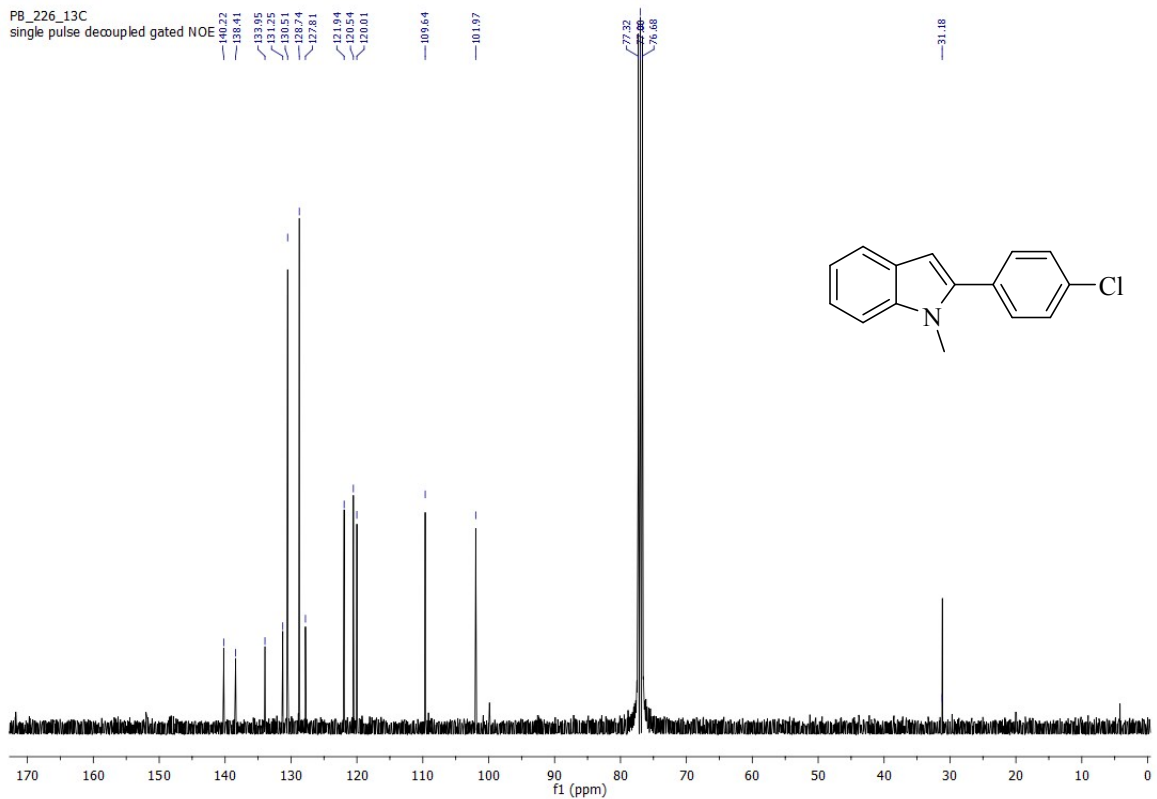
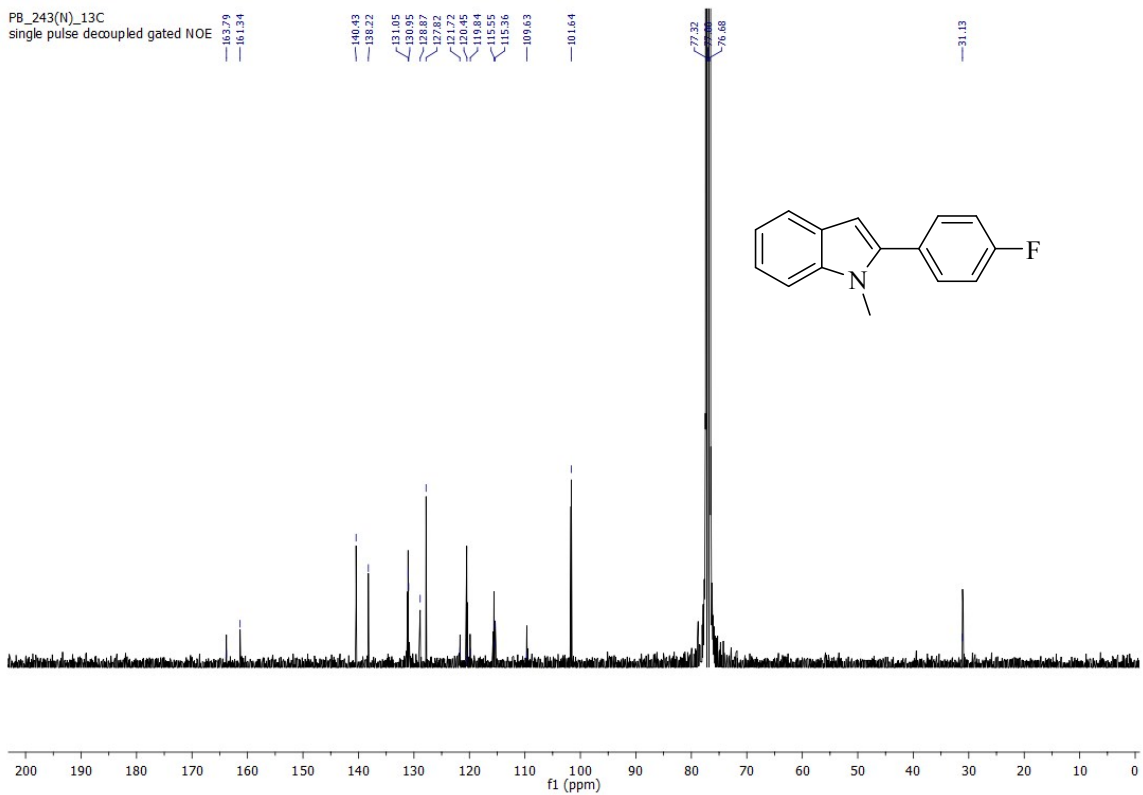
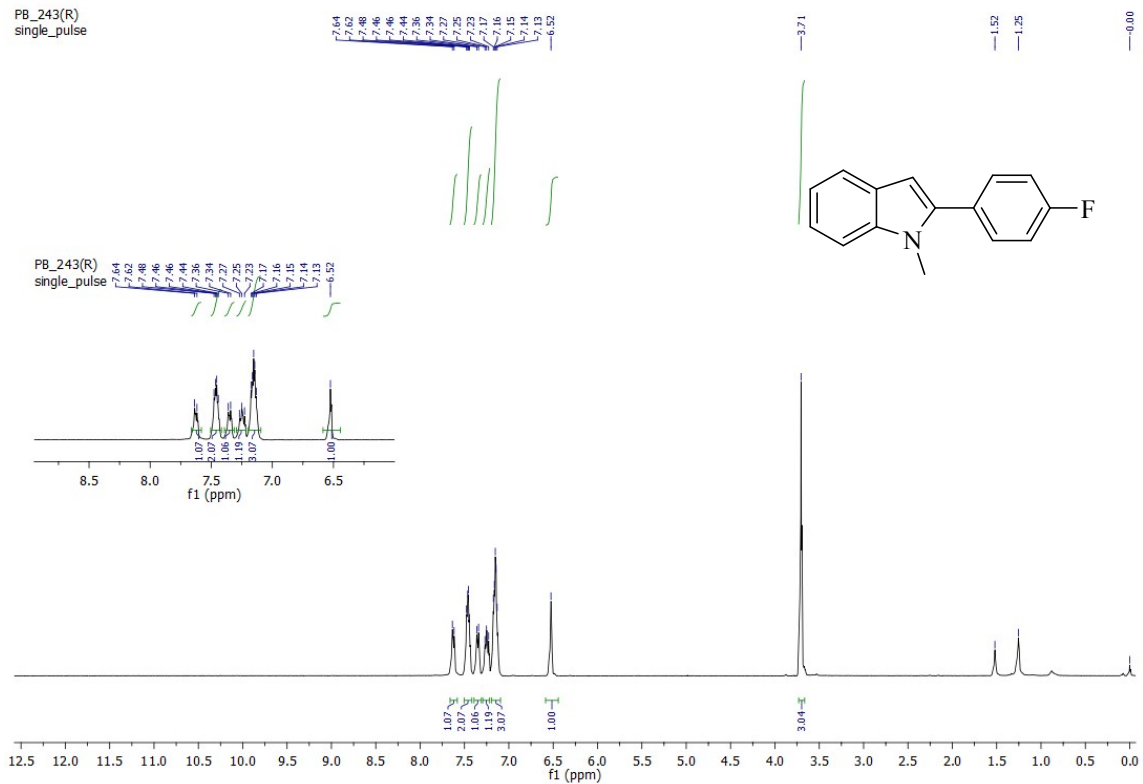


Figure 6. 100 MHz  $^{13}\text{C}$  NMR spectrum of **3c** in  $\text{CDCl}_3$



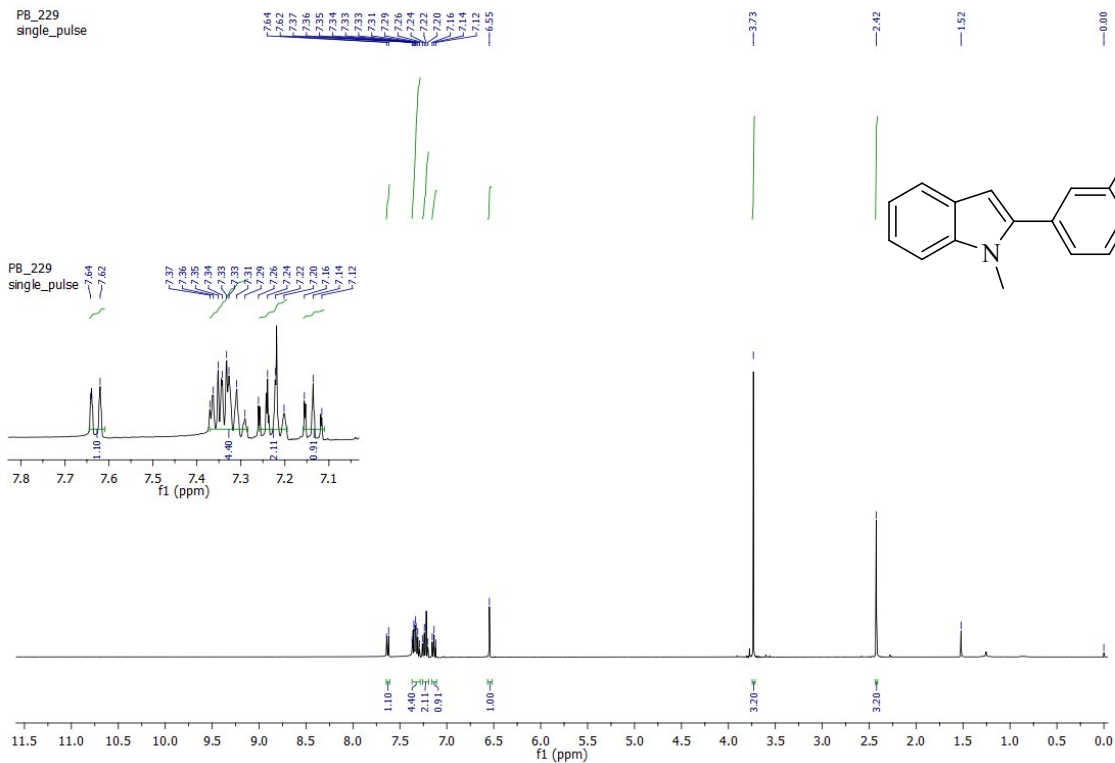


Figure 9. 400 MHz  $^1\text{H}$  NMR spectrum of  $3e^2$  in  $\text{CDCl}_3$

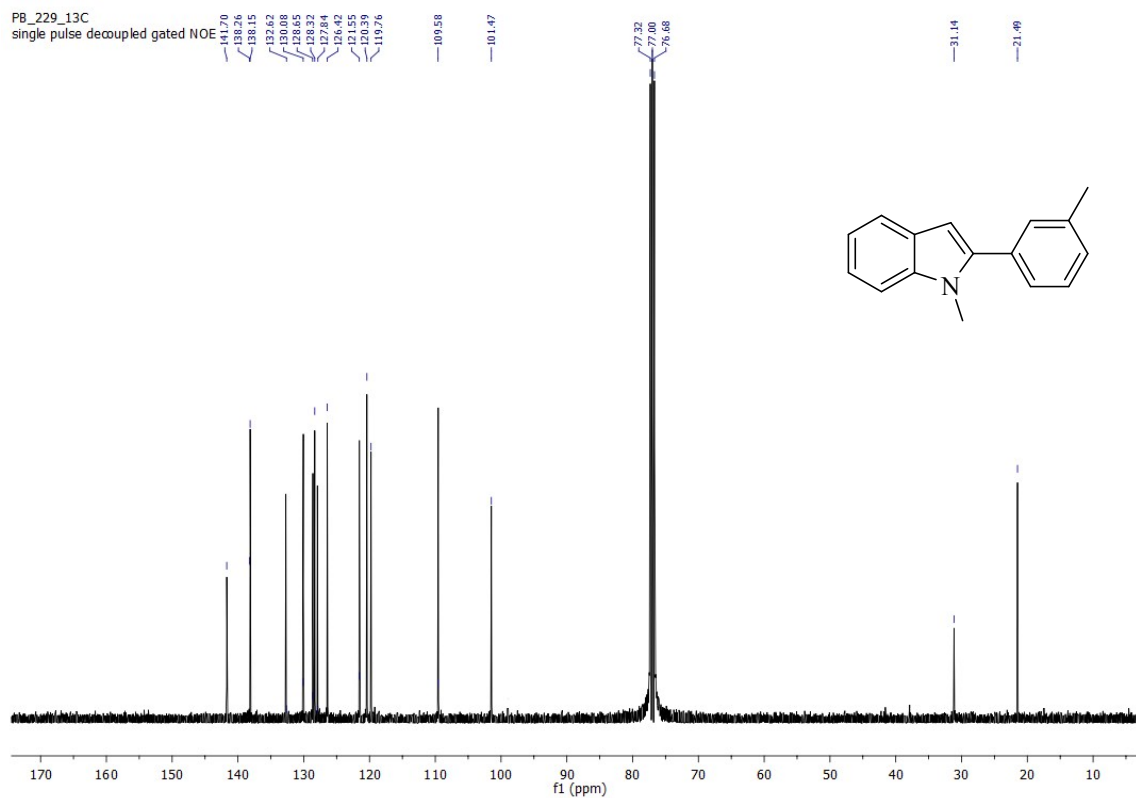
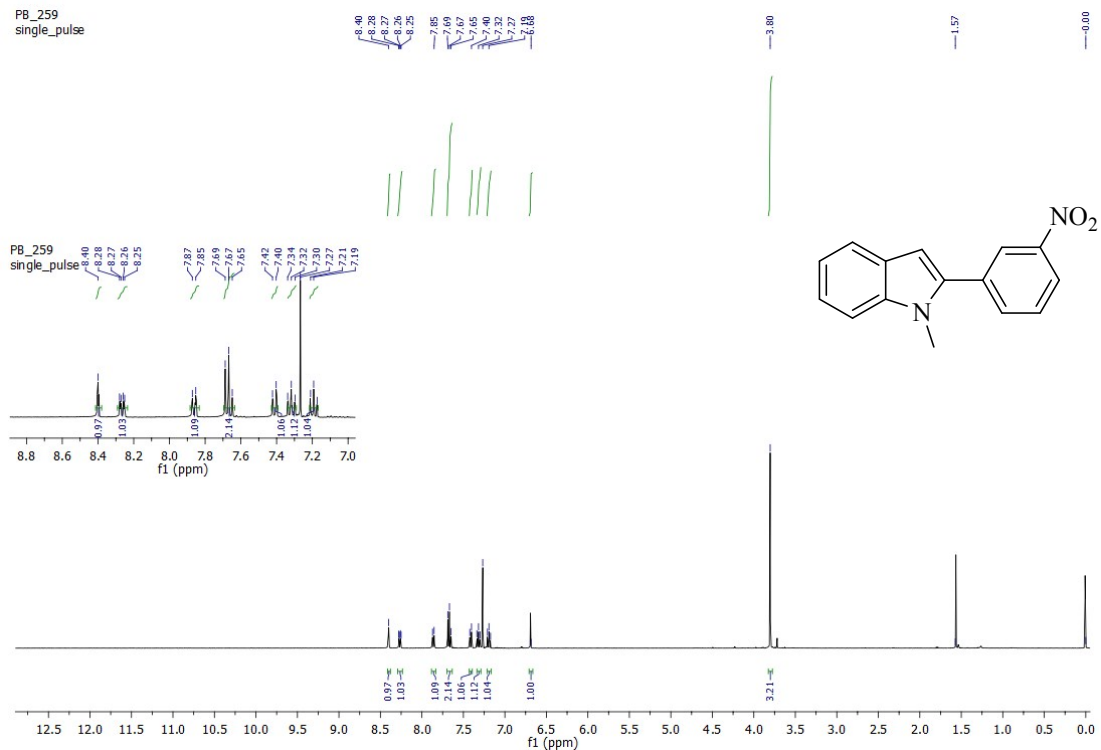
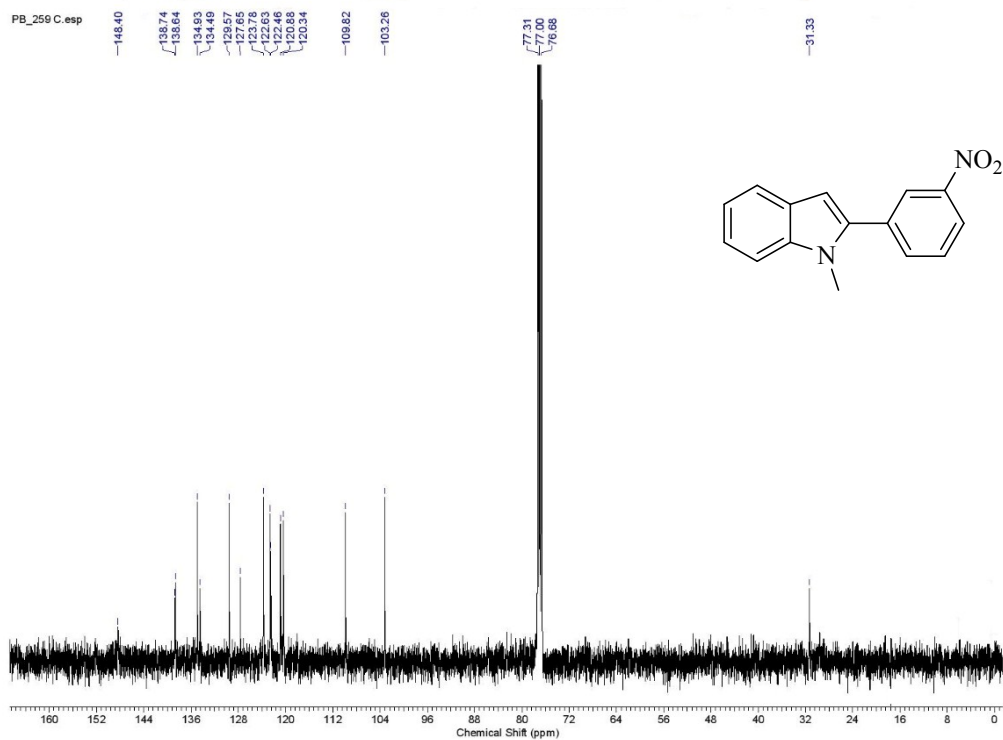


Figure 10. 100 MHz  $^{13}\text{C}$  NMR spectrum of  $3e$  in  $\text{CDCl}_3$



**Figure 11.** 400 MHz <sup>1</sup>H NMR spectrum of **3f** in CDCl<sub>3</sub>



**Figure 12.** 100 MHz <sup>13</sup>C NMR spectrum of **3f** in CDCl<sub>3</sub>

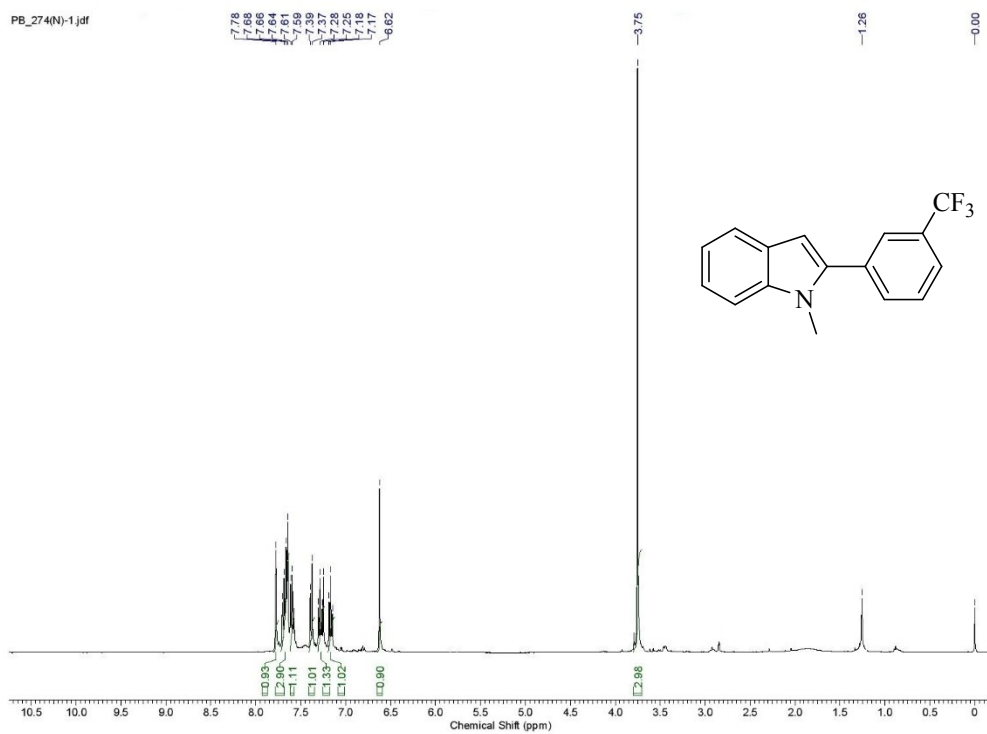


Figure 13. 400 MHz  $^1\text{H}$  NMR spectrum of **3g** in  $\text{CDCl}_3$

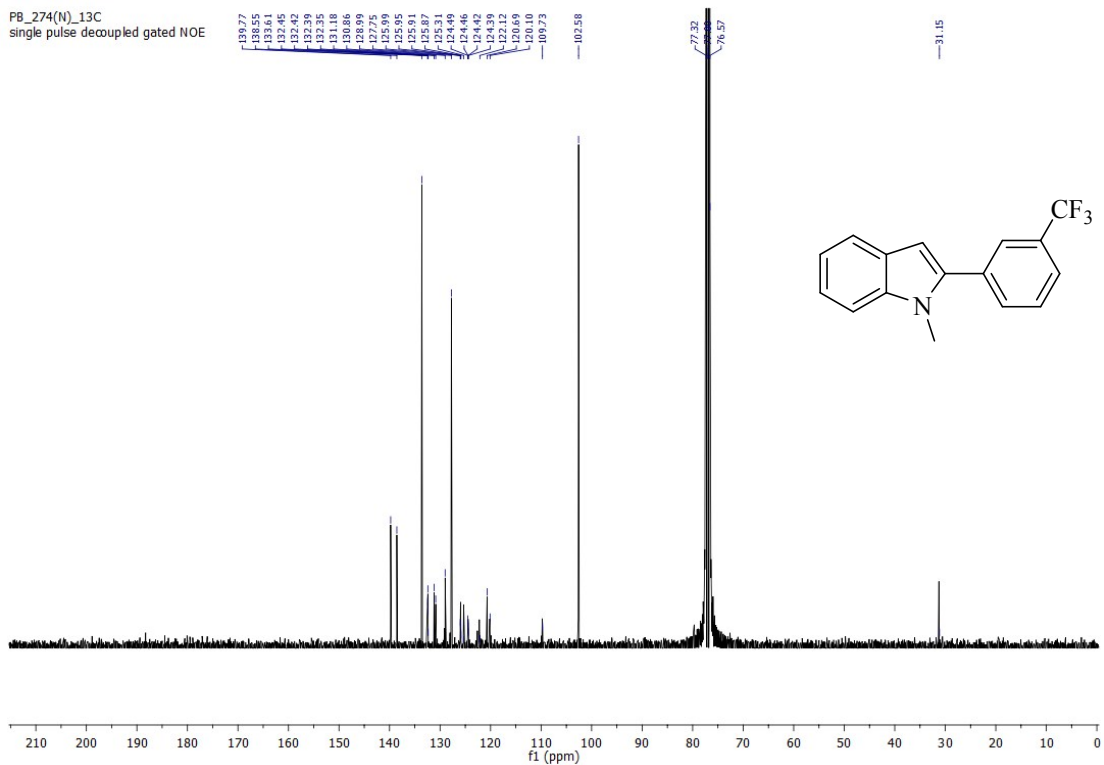
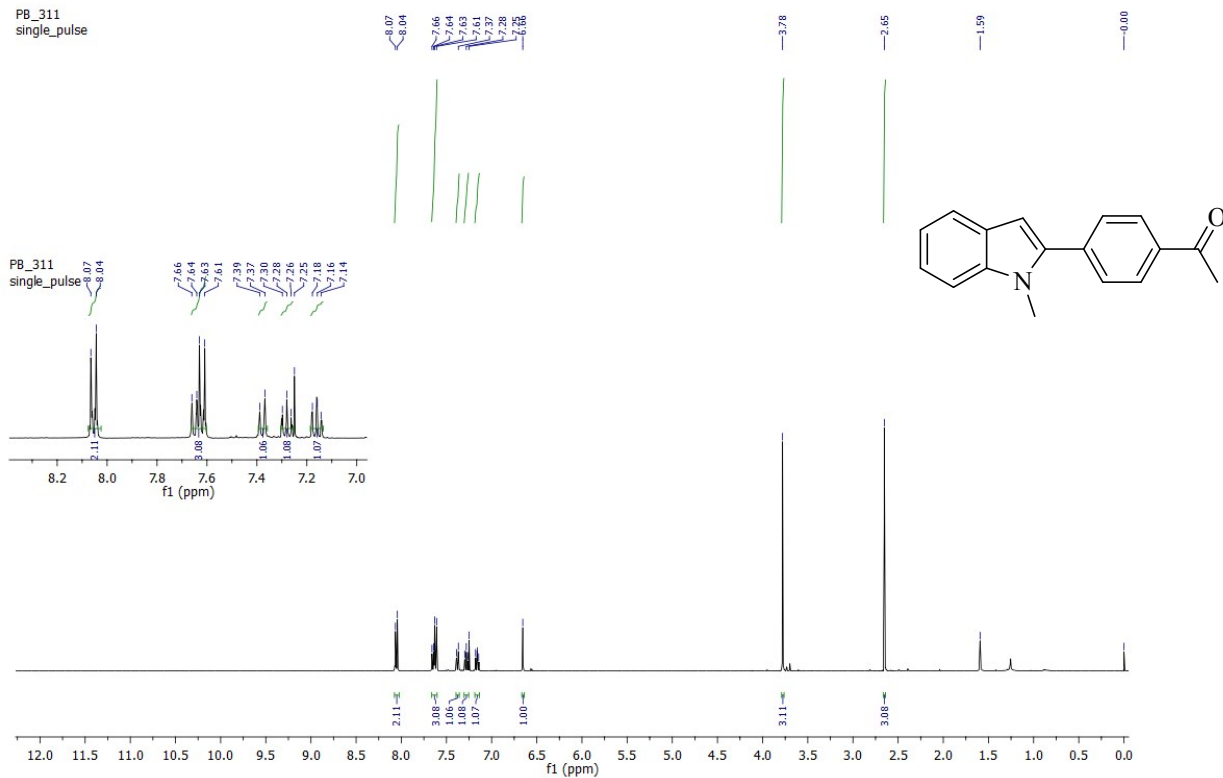
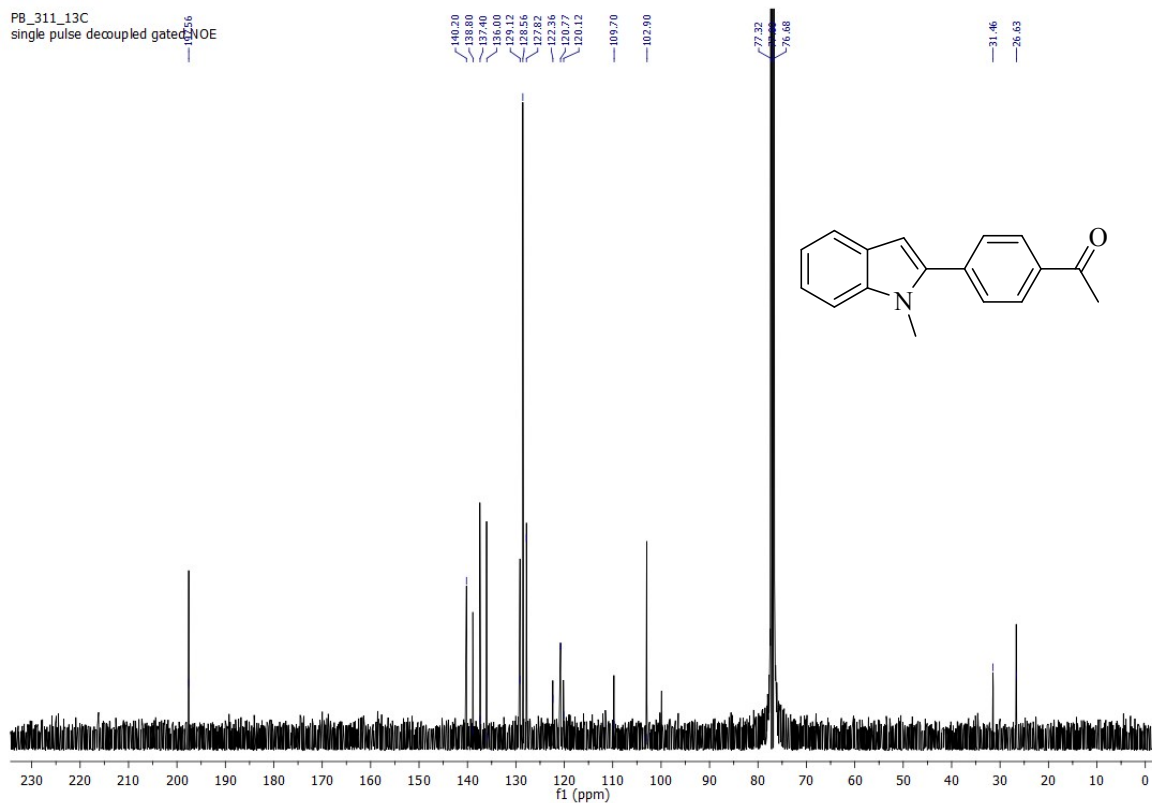


Figure 14. 100 MHz  $^{13}\text{C}$  NMR spectrum of **3g** in  $\text{CDCl}_3$

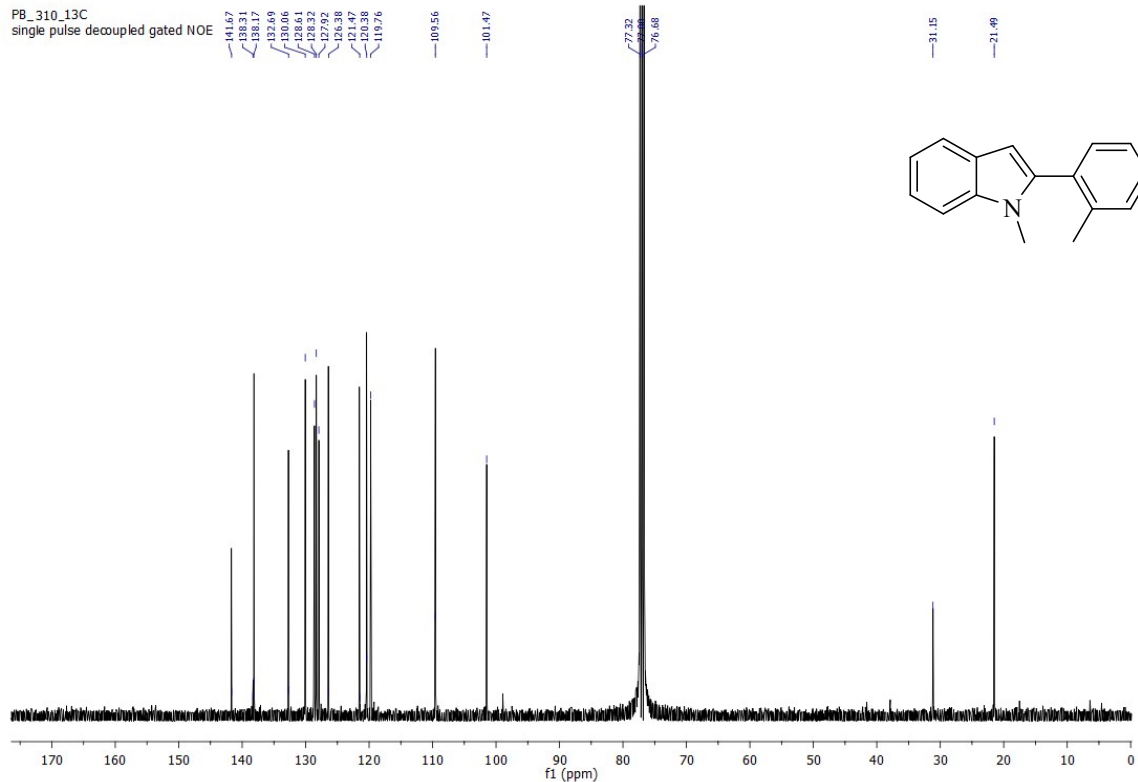
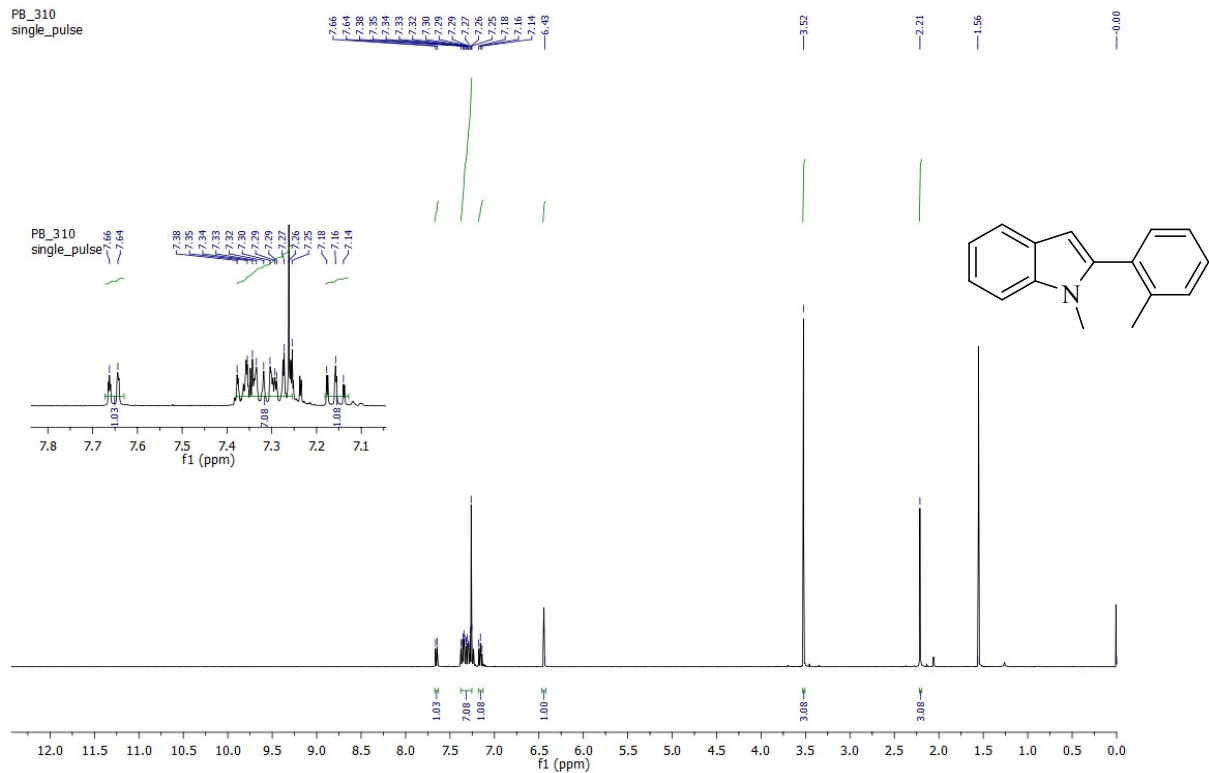




**Figure 15.** 400 MHz  $^1\text{H}$  NMR spectrum of **3h<sup>4</sup>** in  $\text{CDCl}_3$



**Figure 16.** 100 MHz  $^{13}\text{C}$  NMR spectrum of **3h** in  $\text{CDCl}_3$



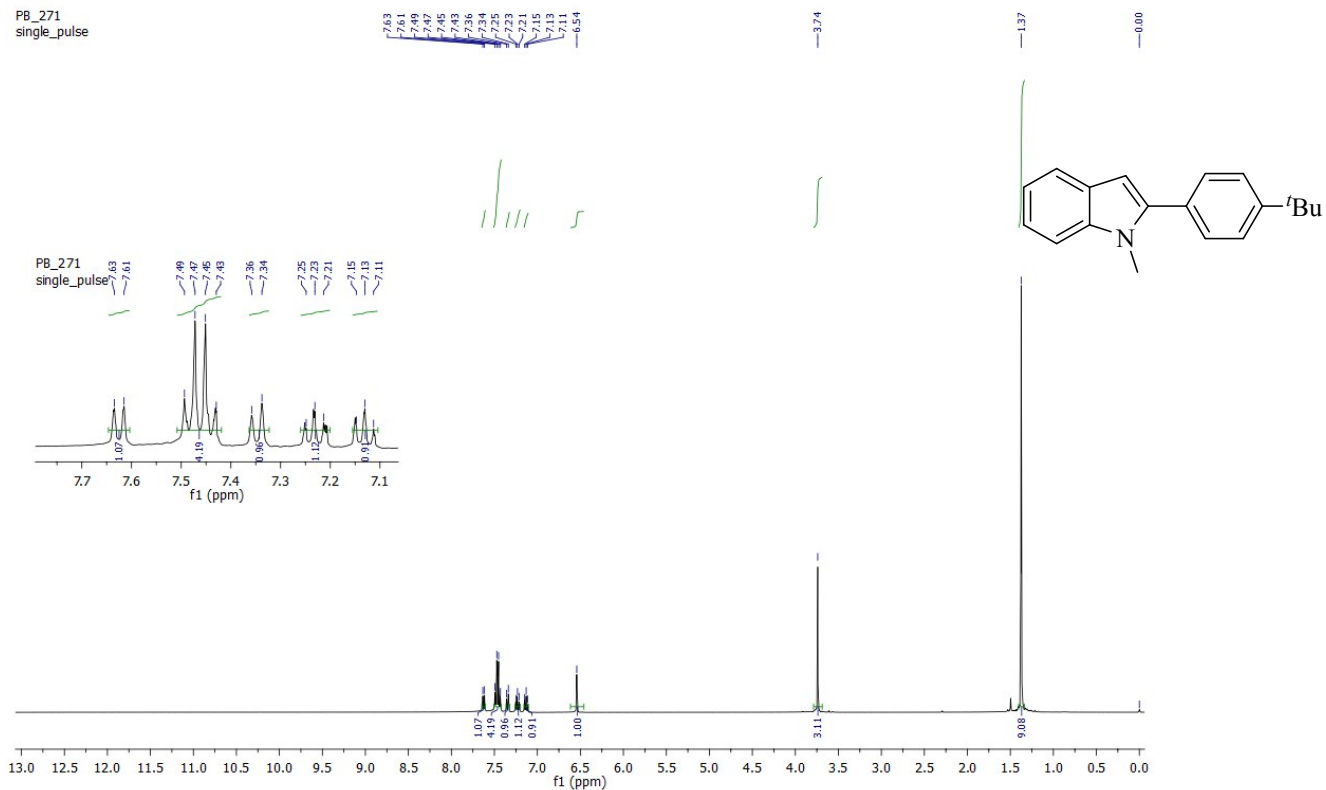


Figure 19. 400 MHz  $^1\text{H}$  NMR spectrum of **3j** in  $\text{CDCl}_3$

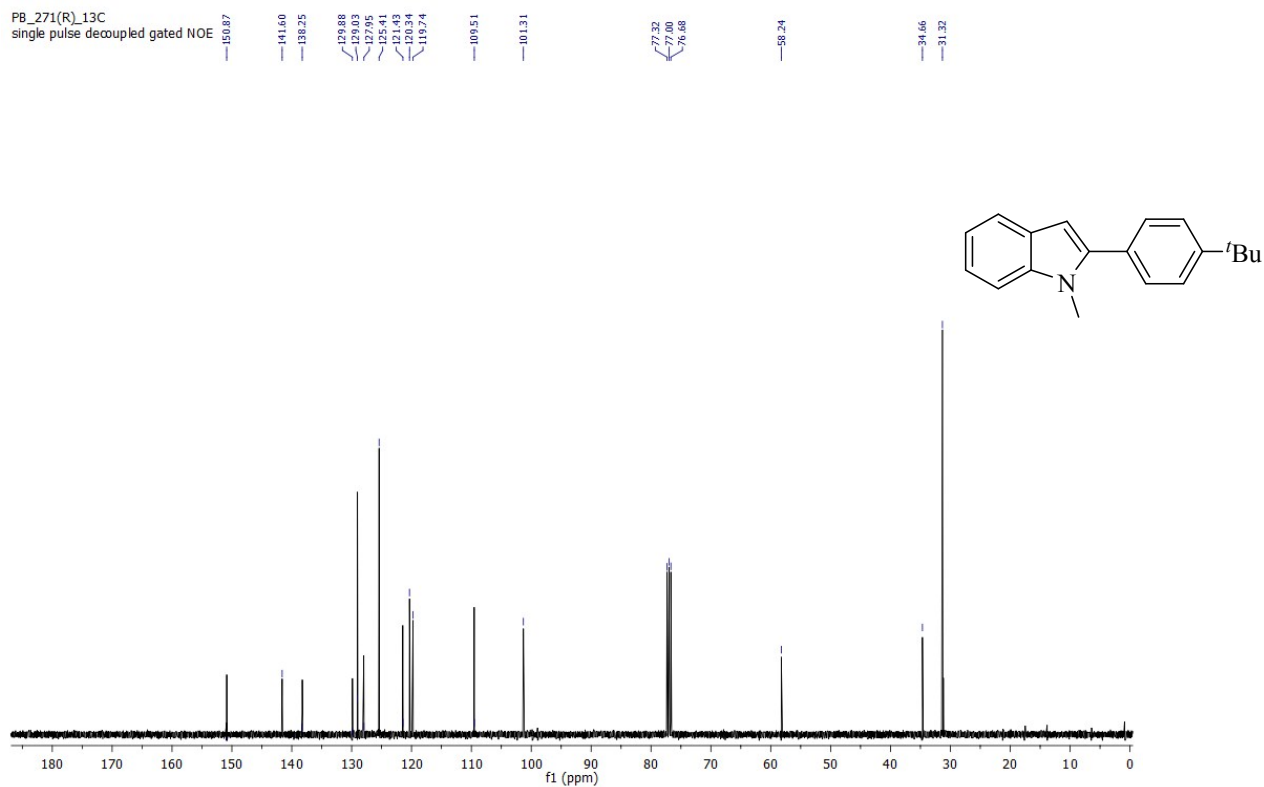
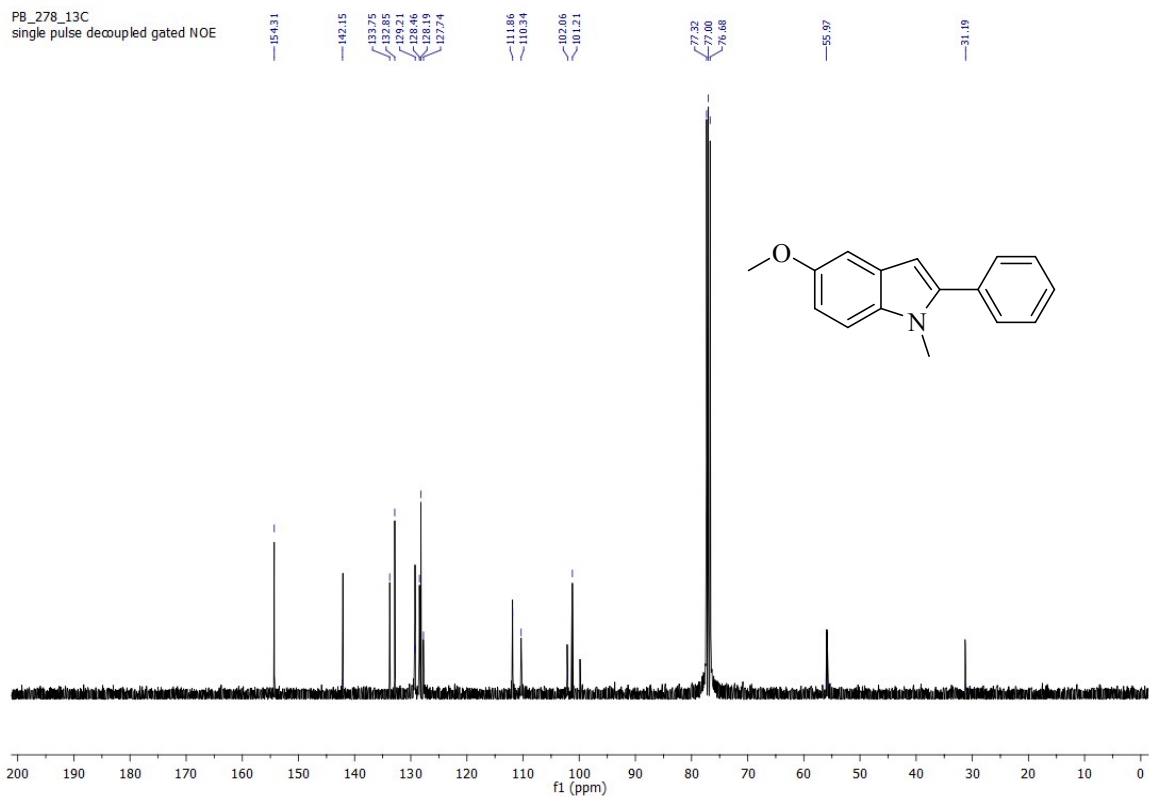
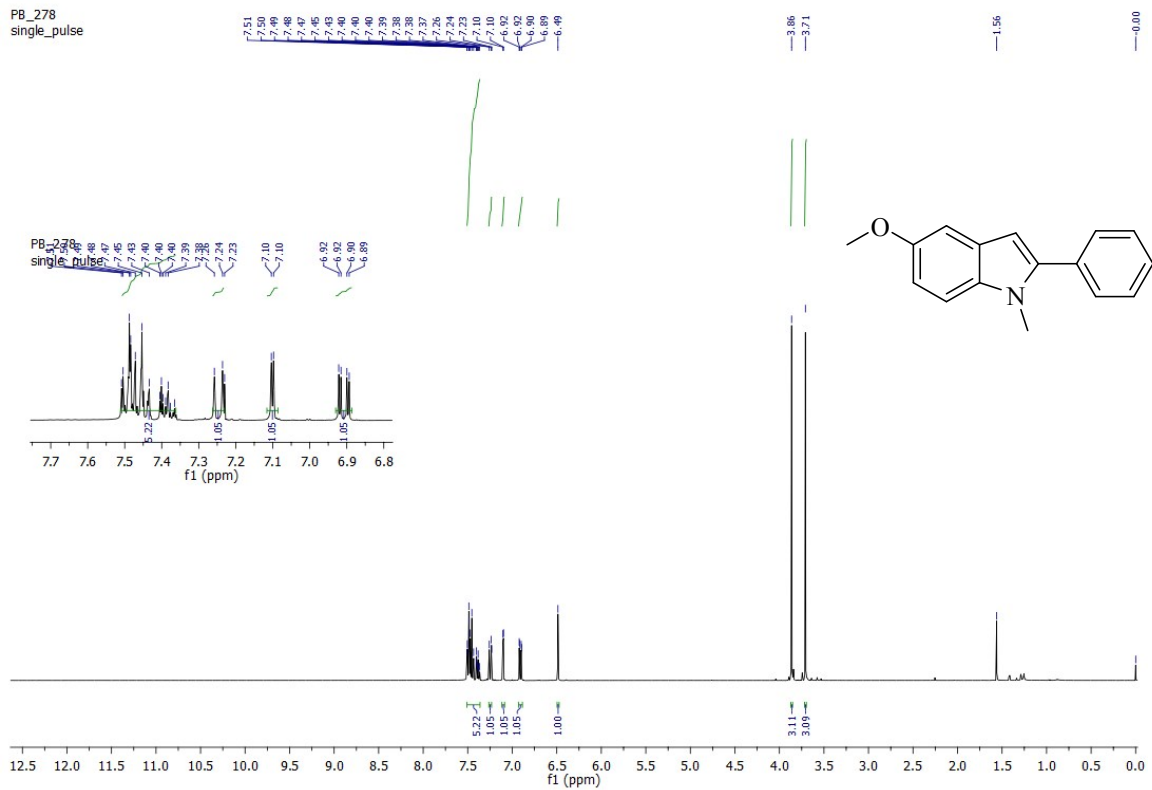


Figure 20. 100 MHz  $^{13}\text{C}$  NMR spectrum of **3j** in  $\text{CDCl}_3$



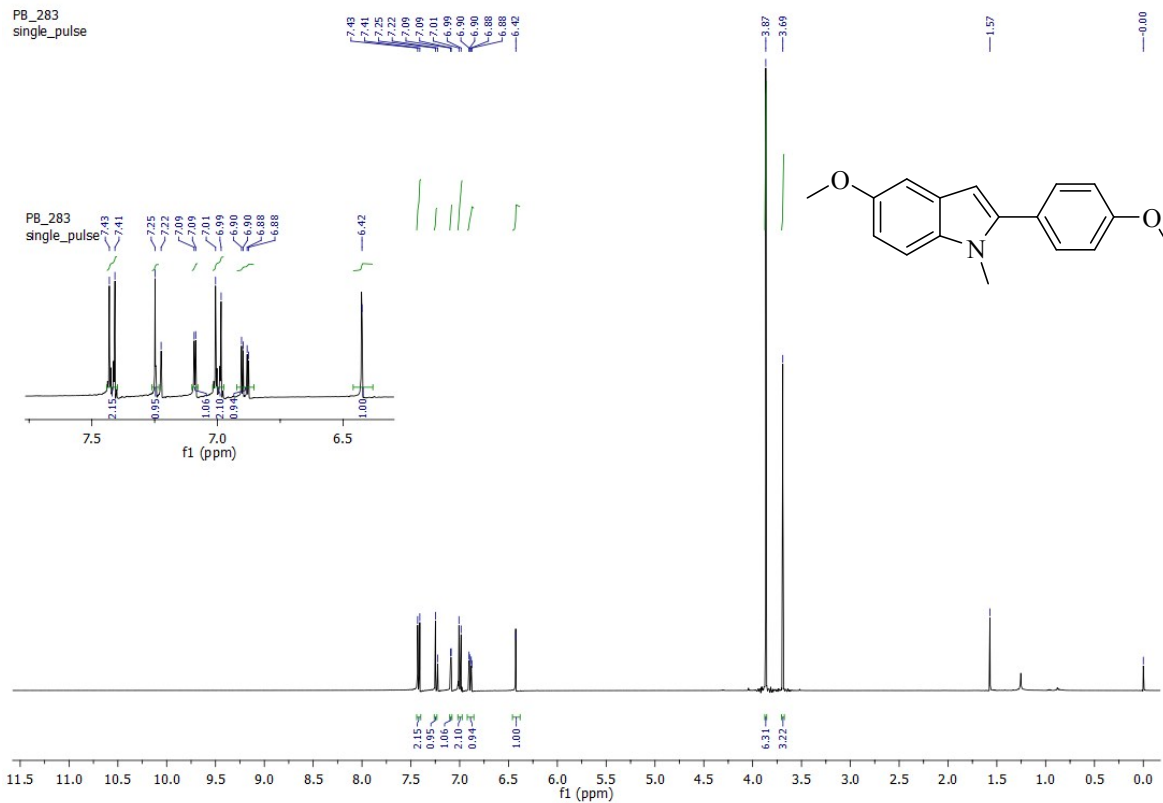


Figure 23. 400 MHz  $^1\text{H}$  NMR spectrum of **3I** in  $\text{CDCl}_3$

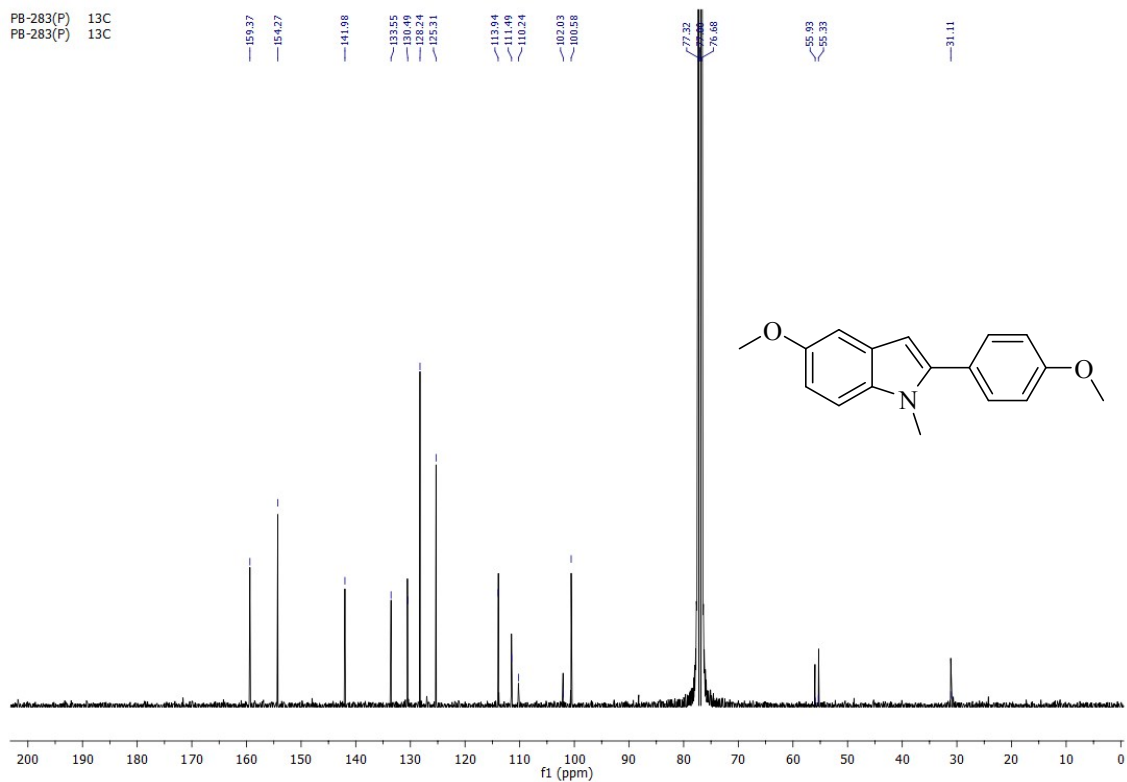
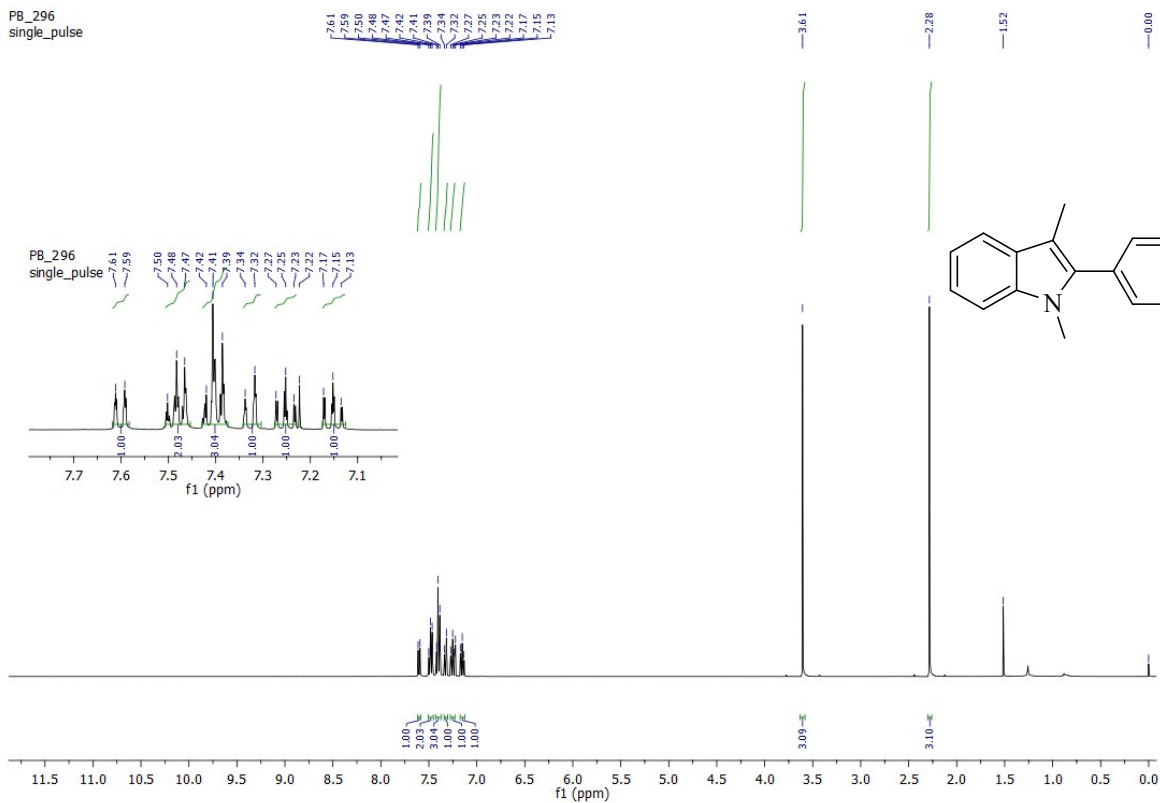
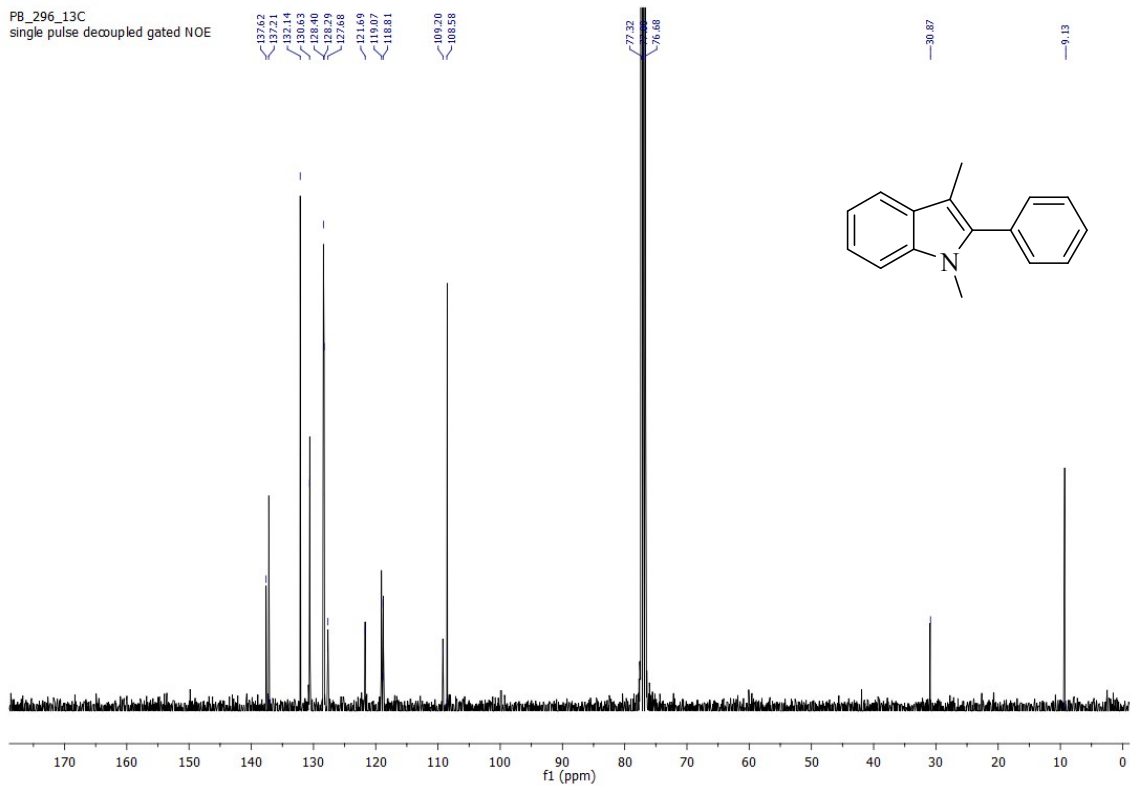


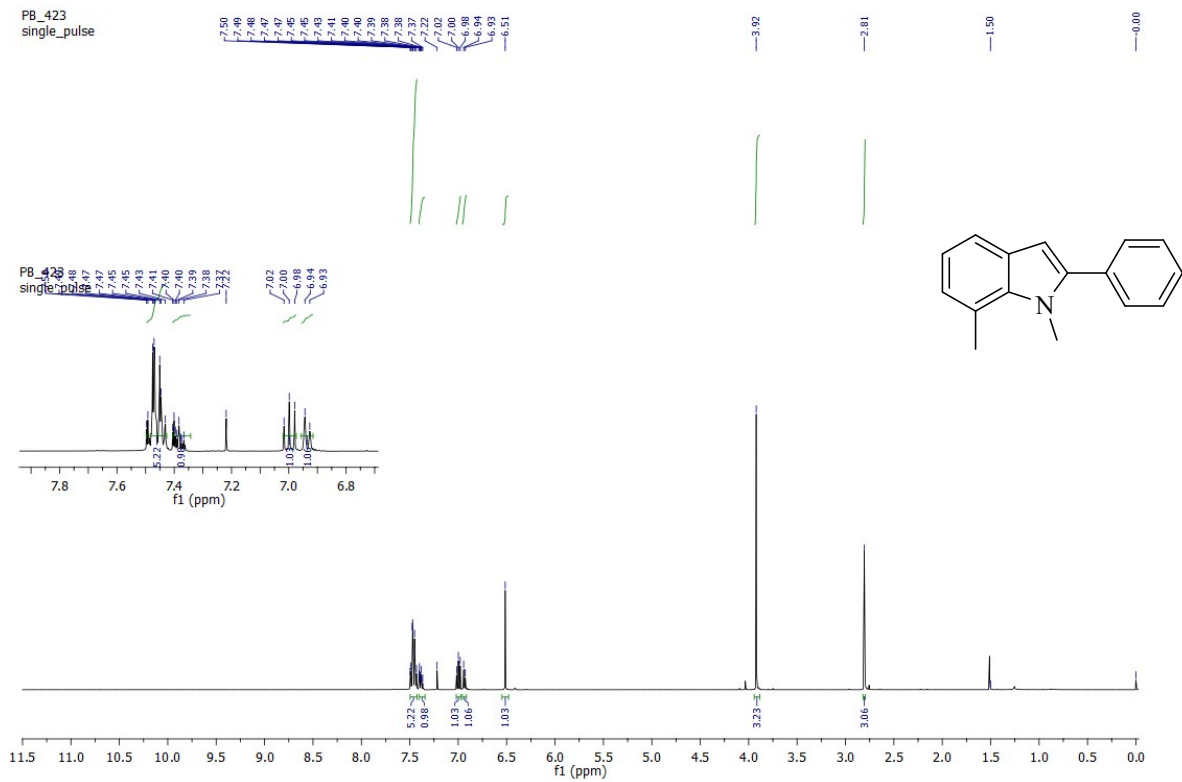
Figure 24. 100 MHz  $^{13}\text{C}$  NMR spectrum of **3I** in  $\text{CDCl}_3$



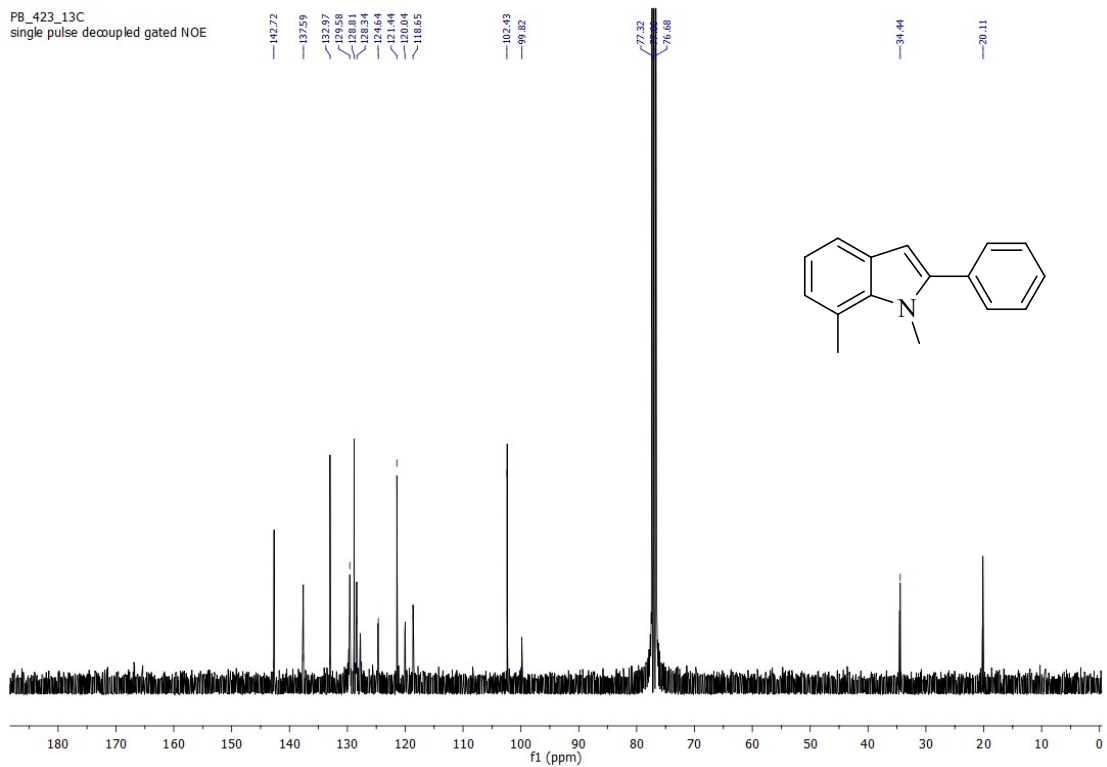
**Figure 25.** 400 MHz  $^1\text{H}$  NMR spectrum of **3m<sup>1</sup>** in  $\text{CDCl}_3$



**Figure 26.** 100 MHz  $^{13}\text{C}$  NMR spectrum of **3m** in  $\text{CDCl}_3$



**Figure 27.** 400 MHz <sup>1</sup>H NMR spectrum of **3n**<sup>1</sup> in CDCl<sub>3</sub>



**Figure 28.** 100 MHz <sup>13</sup>C NMR spectrum of **3n** in CDCl<sub>3</sub>

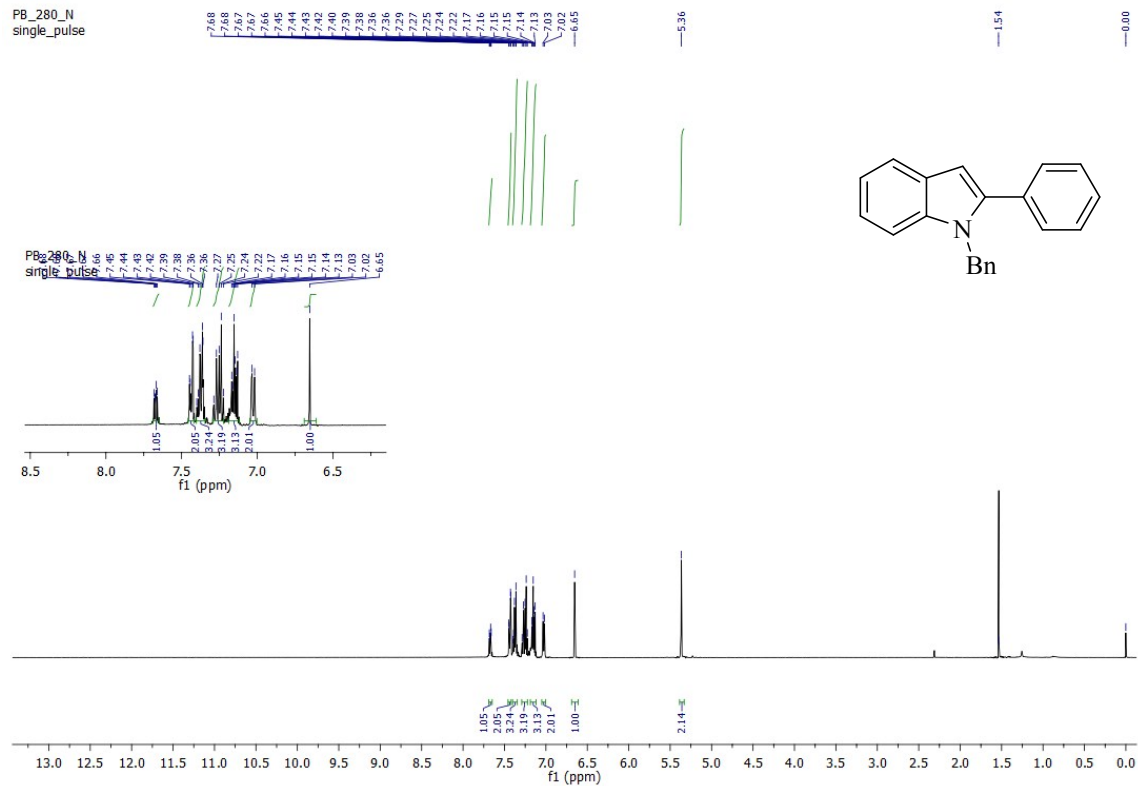


Figure 29. 400 MHz  $^1\text{H}$  NMR spectrum of **3o**<sup>1</sup> in  $\text{CDCl}_3$

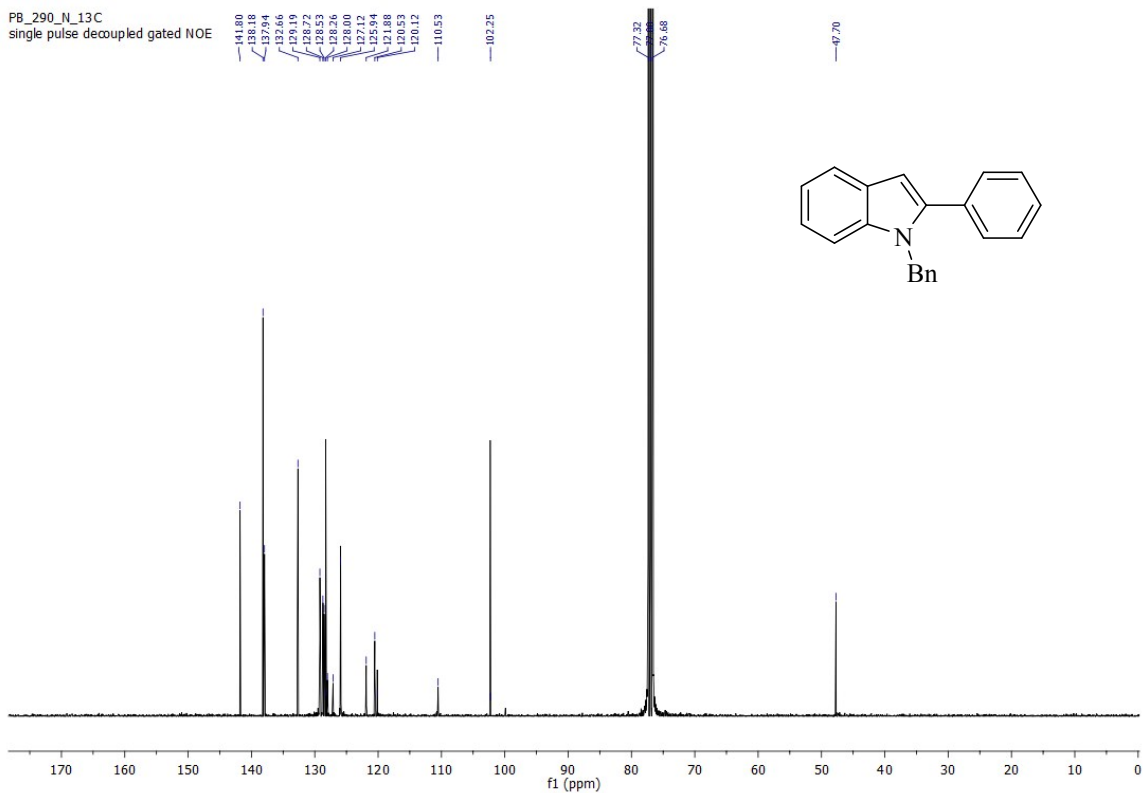
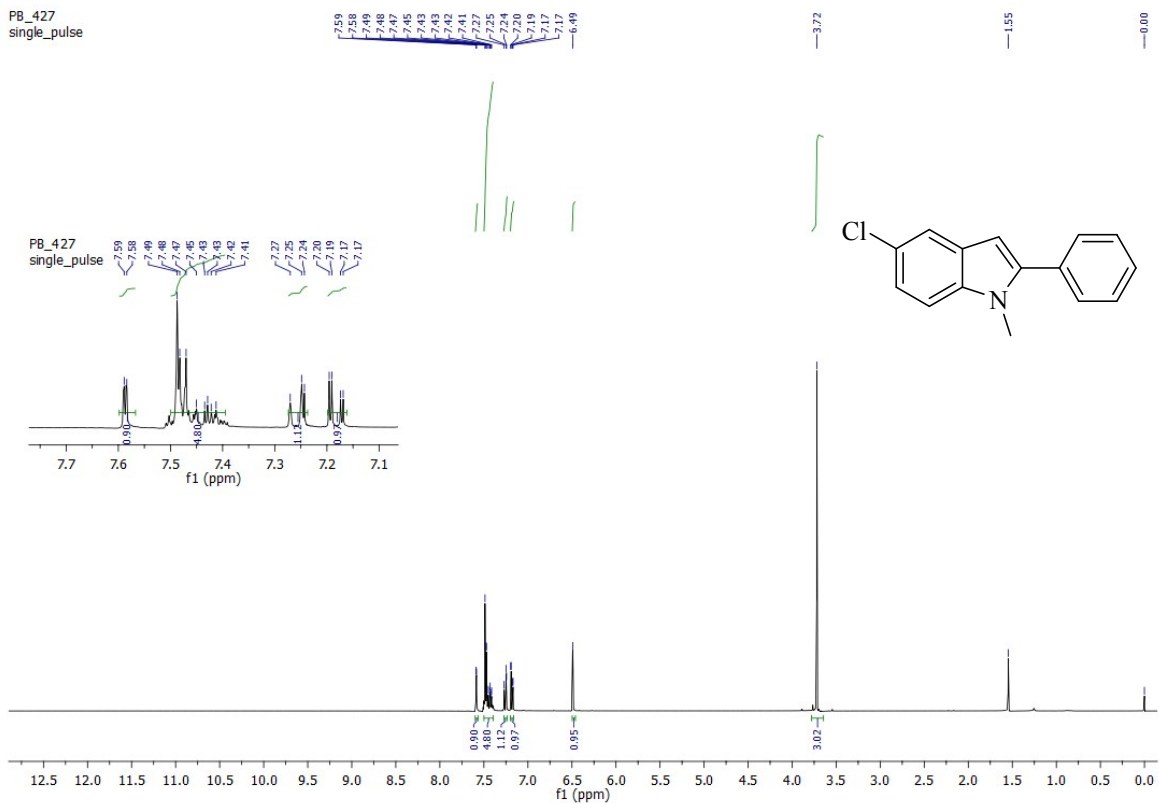
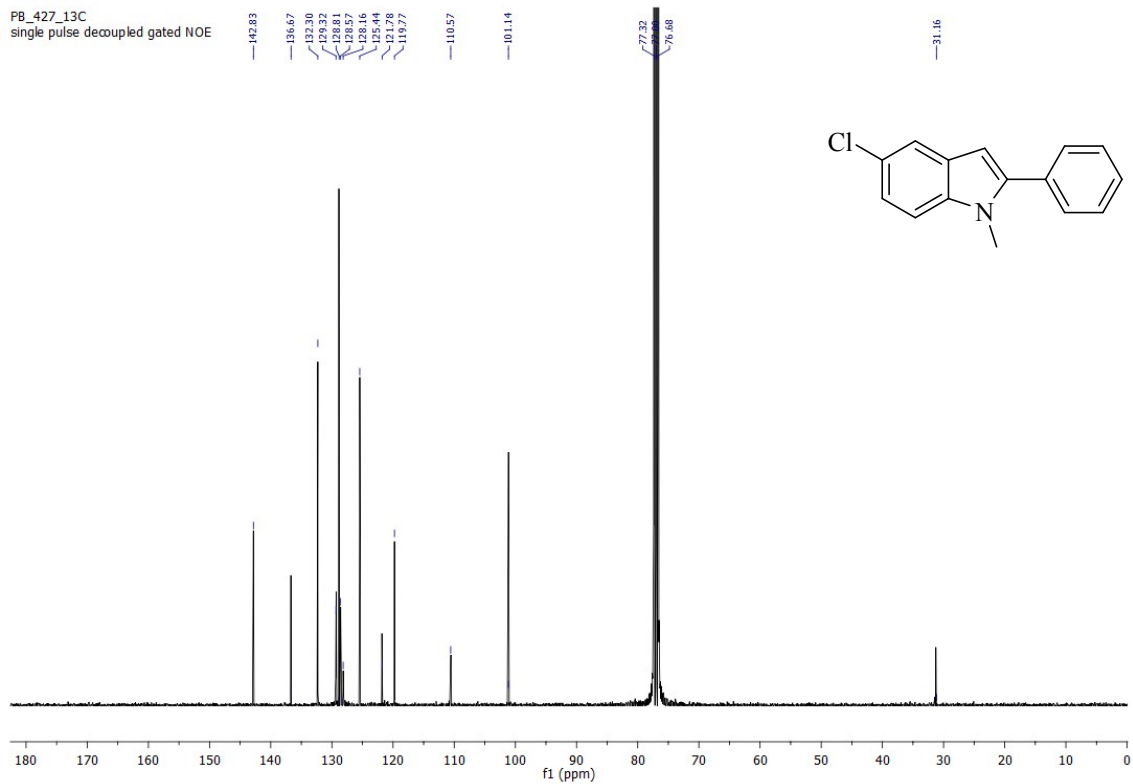


Figure 30. 100 MHz  $^{13}\text{C}$  NMR spectrum of **3o** in  $\text{CDCl}_3$





**Figure 31.** 400 MHz  $^1\text{H}$  NMR spectrum of **3p<sup>6</sup>** in  $\text{CDCl}_3$



**Figure 32.** 100 MHz  $^{13}\text{C}$  NMR spectrum of **3p** in  $\text{CDCl}_3$

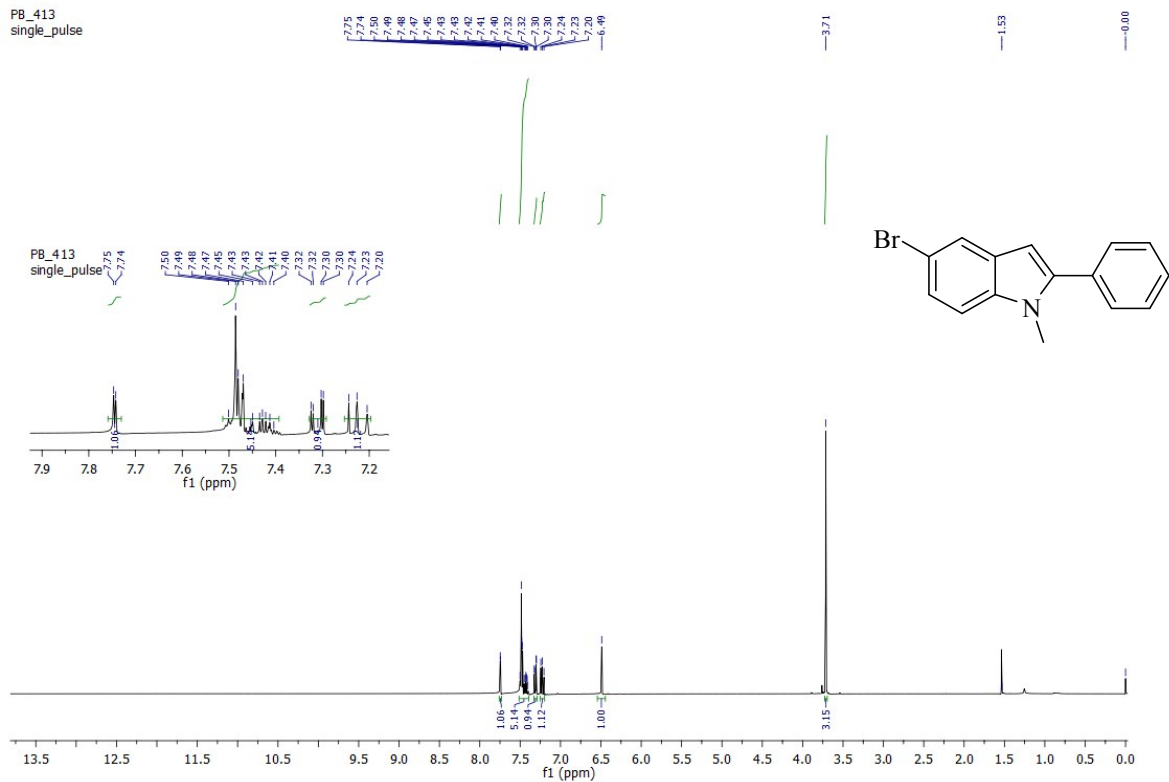


Figure 33. 400 MHz  $^1\text{H}$  NMR spectrum of **3q**<sup>7</sup> in  $\text{CDCl}_3$

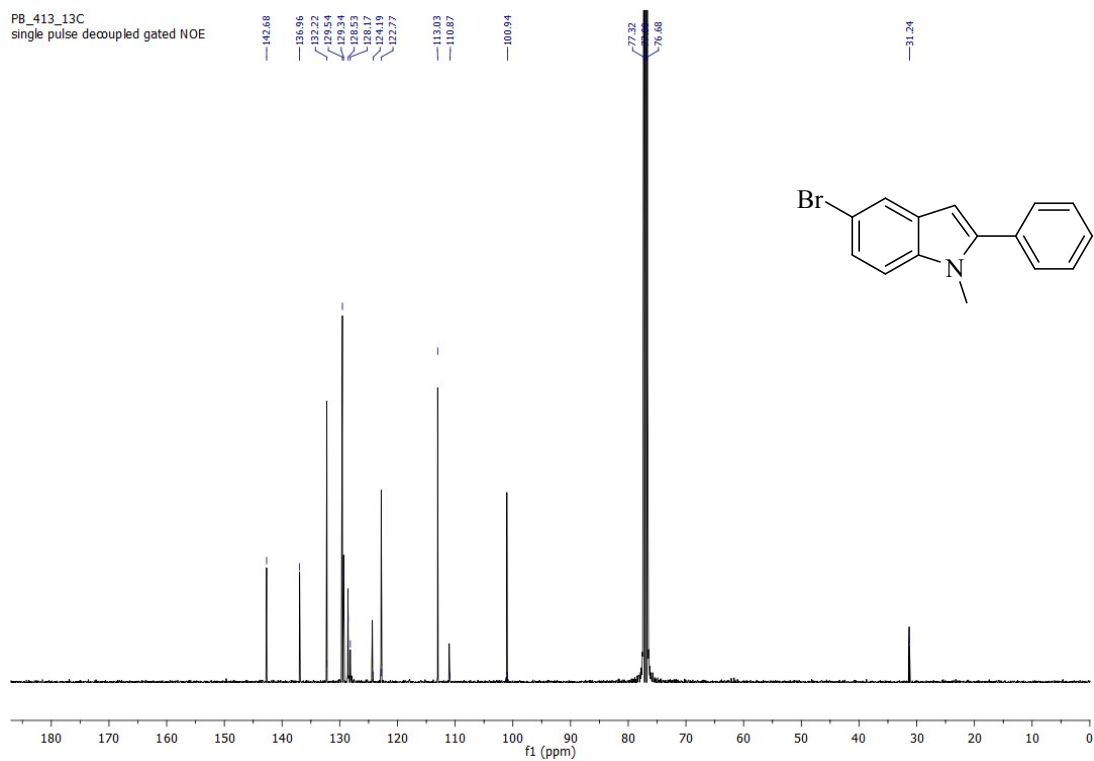
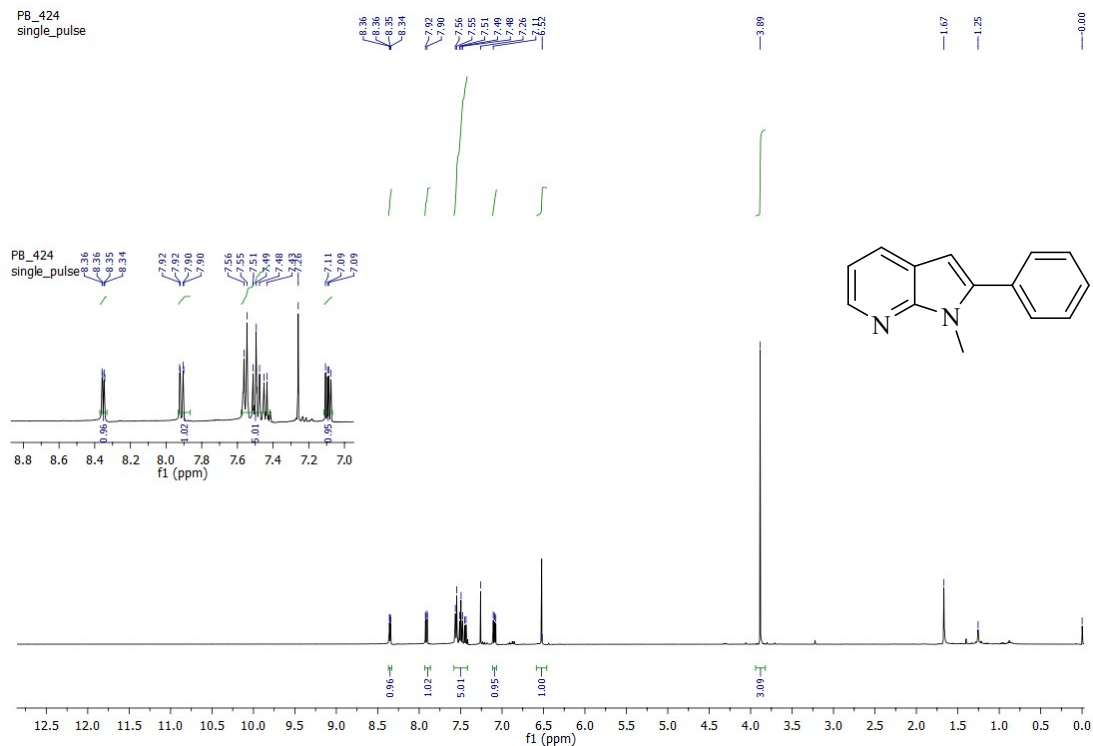
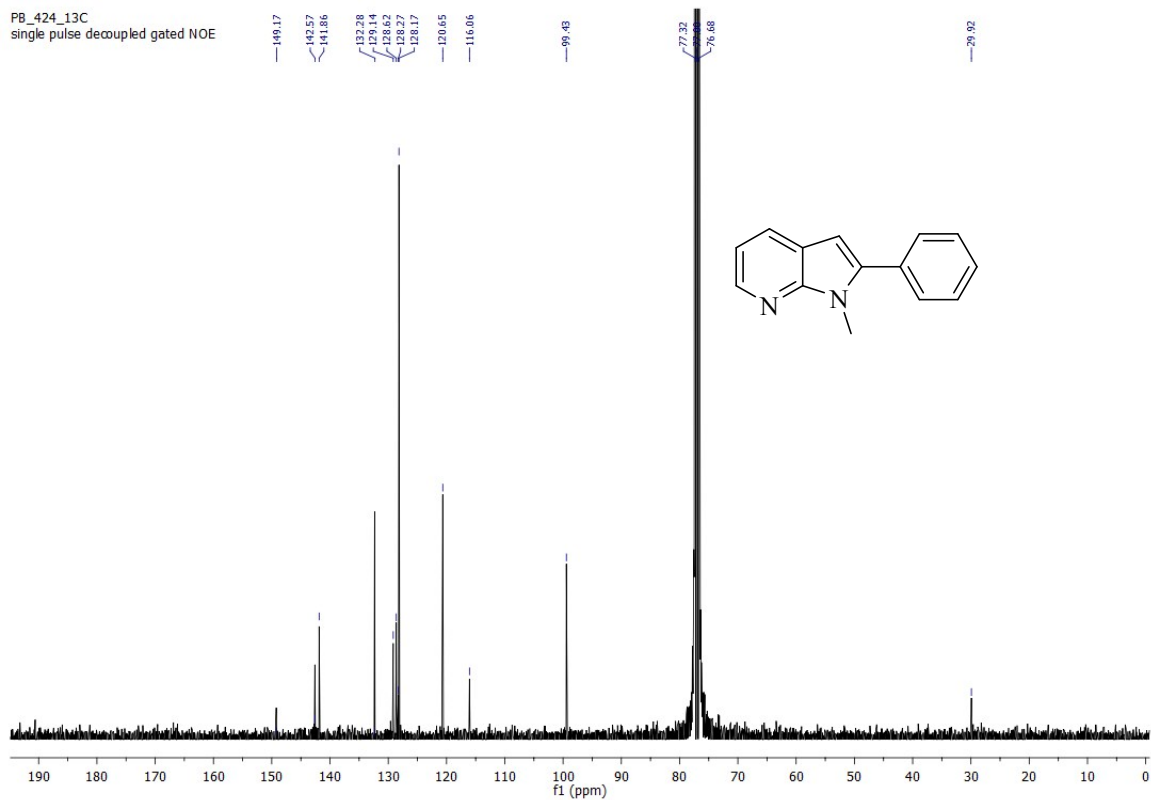


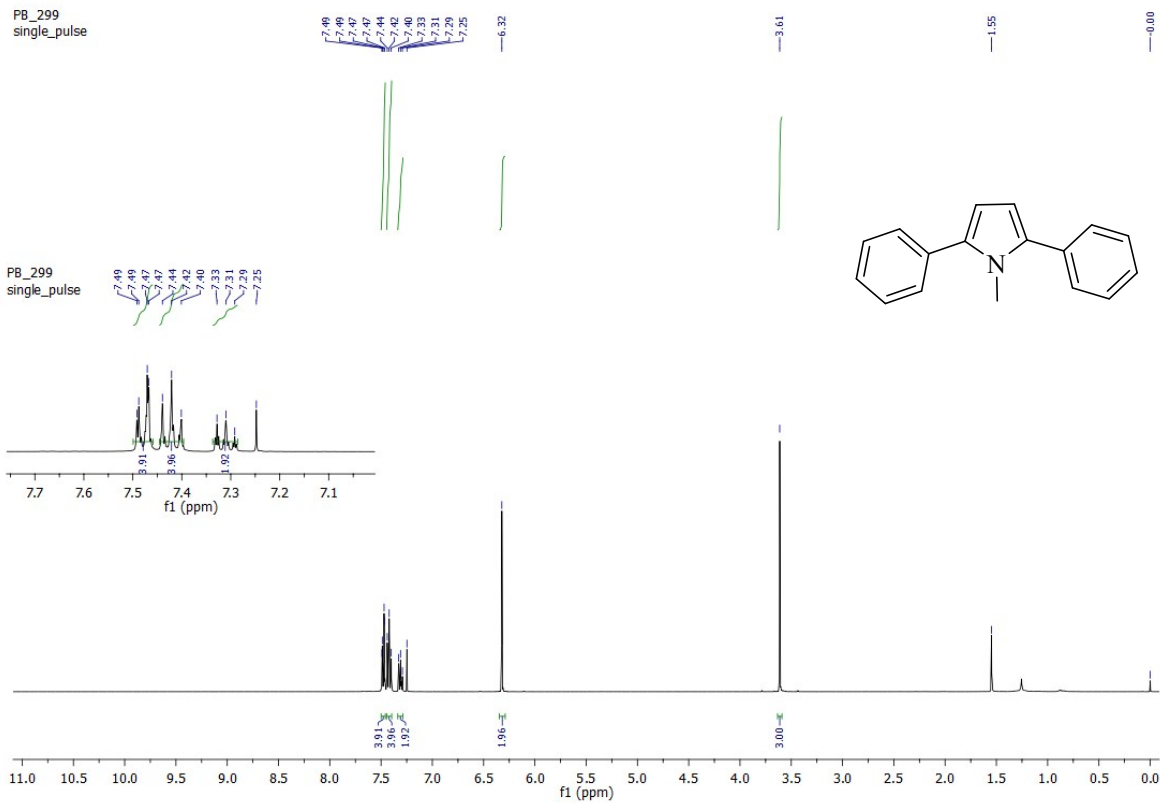
Figure 34. 100 MHz  $^{13}\text{C}$  NMR spectrum of **3q** in  $\text{CDCl}_3$



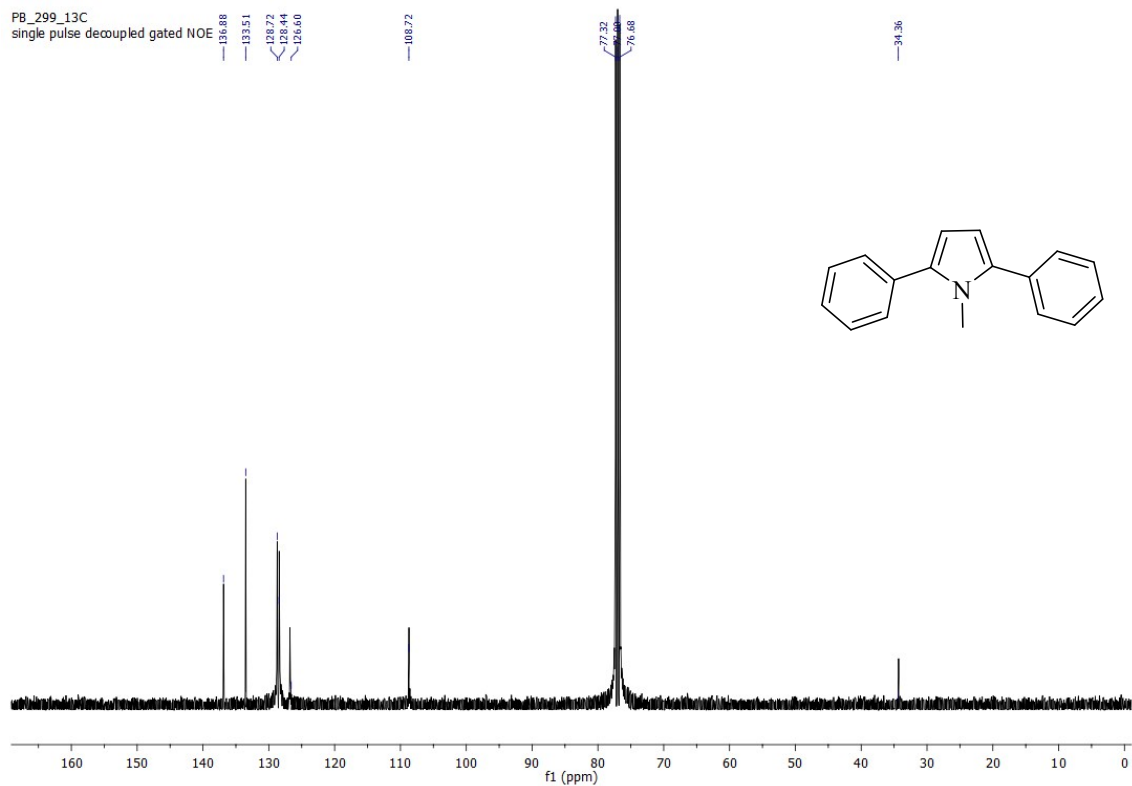
**Figure 35.** 400 MHz  $^1\text{H}$  NMR spectrum of  $3\text{r}^2$  in  $\text{CDCl}_3$



**Figure 36.** 100 MHz  $^{13}\text{C}$  NMR spectrum of  $3\text{r}$  in  $\text{CDCl}_3$



**Figure 37.** 400 MHz  $^1\text{H}$  NMR spectrum of **3s**<sup>8</sup> in  $\text{CDCl}_3$



**Figure 38.** 100 MHz  $^{13}\text{C}$  NMR spectrum of **3s** in  $\text{CDCl}_3$

## 2. References:

1. Z. Liang, B. Yao and Y. Zhang, *Org. Lett.*, 2010, **12**, 3185-3187.
2. Y. Huang, T. Ma, P. Huang, D. Wu, Z. Lin and R. Cao, *ChemCatChem*, 2013, **5**, 1877–1883.
3. P. Ni, J. Tan, W. Zhao, H. Huang, F. Xiao and G. J. Deng, *Org. Lett.*, 2019, **21**, 3518–3522.
4. Y. Son, S. Lee, H. S. Kim, M. S. Eom, M. S. Han and S. Lee, *Adv. Synth. Catal.*, 2018, **360**, 3916-3923.
5. E. Von Angerer, J. Prekajac and J. Strohmeier, *J. Med. Chem.*, 1984, **27**, 1439-1447.
6. S. Yang, C. Sun, Z. Fang, B. Li, Y. Li and Z. Shi, *Angew. Chem.*, 2008, **120**, 1495–1498.
7. D. Das, Z. T. Bhutia, A. Chatterjee and M. Banerjee, *J. Org. Chem.*, 2019, **84**, 10764–10774.
8. B. S. Cho, H. J. Bae and Y. K. Chung, *J. Org. Chem.*, 2015, **80**, 5302–5307.