Supporting Information

Pd Nanoparticles-Loaded Honeycomb-Structured Bionanocellulose as a Heterogeneous Catalyst for Heteroaryl Cross-Coupling Reaction

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1. GENERAL INFORMATION

The chemicals used in all the experiments were procured commercially and used without further purification. The progress of the reaction was monitored through thin layer chromatography on Merck Kieselgel Silica gel 60 F_{254} plates using short wave UV light (λ=254 nm). The products were purified by column chromatography using Silica gel 60-120 mesh. The identification of the purified products was carried out by NMR (^{1}H and ^{13}C) spectroscopy. The NMR spectrum were recorded on a 400 MHz JEOL NMR spectrophotometer (400 MHz for ^{1}H and 100 MHz for ^{13}C NMR spectroscopy). Chemical shifts for both ^{1}H (δ_H) and ^{13}C (δ_C) NMR are assigned in parts per million (ppm) using TMS (0 ppm) as the internal reference and $CDCl_3$ and DMSO-d_6 as solvent ($CDCl_3$: δ_H = 7.25 ppm and δ_C = 77.1 ppm; DMSO-d_6: δ_H = 2.5 ppm, DMSO-d_6 absorbed water = 3.3 ppm and δ_C = 40.0 ppm).

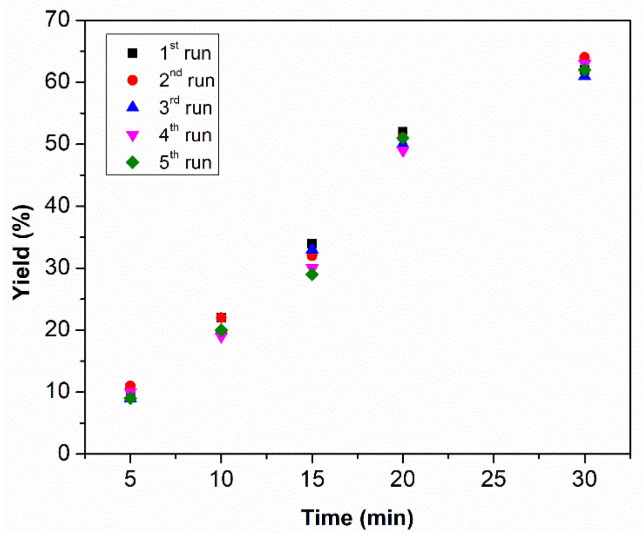


Figure S1: Effect of catalyst recycling on the yield in Suzuki-Miyaura reaction. Reactions were carried out with 4-bromoanisole (0.5 mmol), phenylboronic (0.6 mmol), PdNPs@NCmw (10 wt%), K_2CO_3 (1.5 mmol), EtOH:H_2O (1:1) (4 mL), rt (25 ºC), Yields were determined with GC using n-dodecane as internal standard.

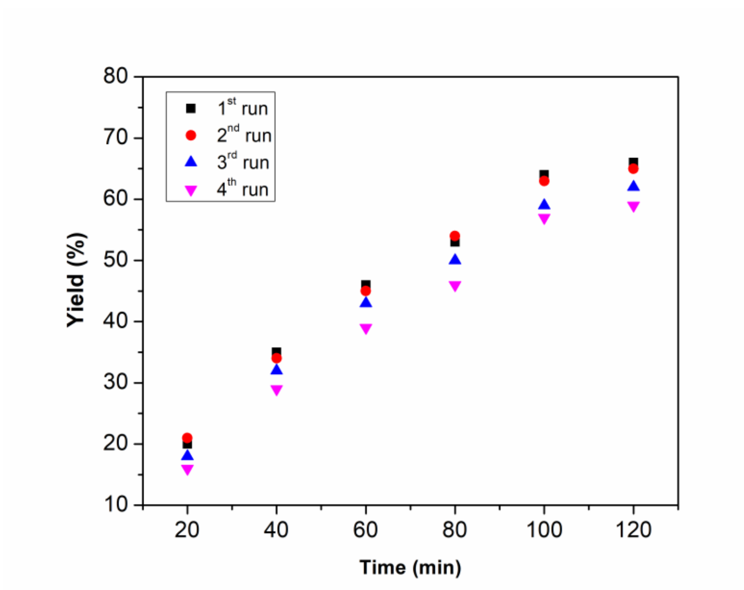


Figure S2: Effect of catalyst recycling on the yield in Sonogashira reaction. Reactions were carried out with 4-iodotoluene (0.5 mmol), phenylacetylene (0.75 mmol), PdNPs@NCmw (10 wt%), H_2O:EtOH (1:7, 4 mL) K_2CO_3 (1.5 mmol), reactions were carried out at 70 ºC, Yields were determined with GC using benzophenone as internal standard.

Copies of ^{1}H NMR and ^{13}C NMR spectrum of isolated products

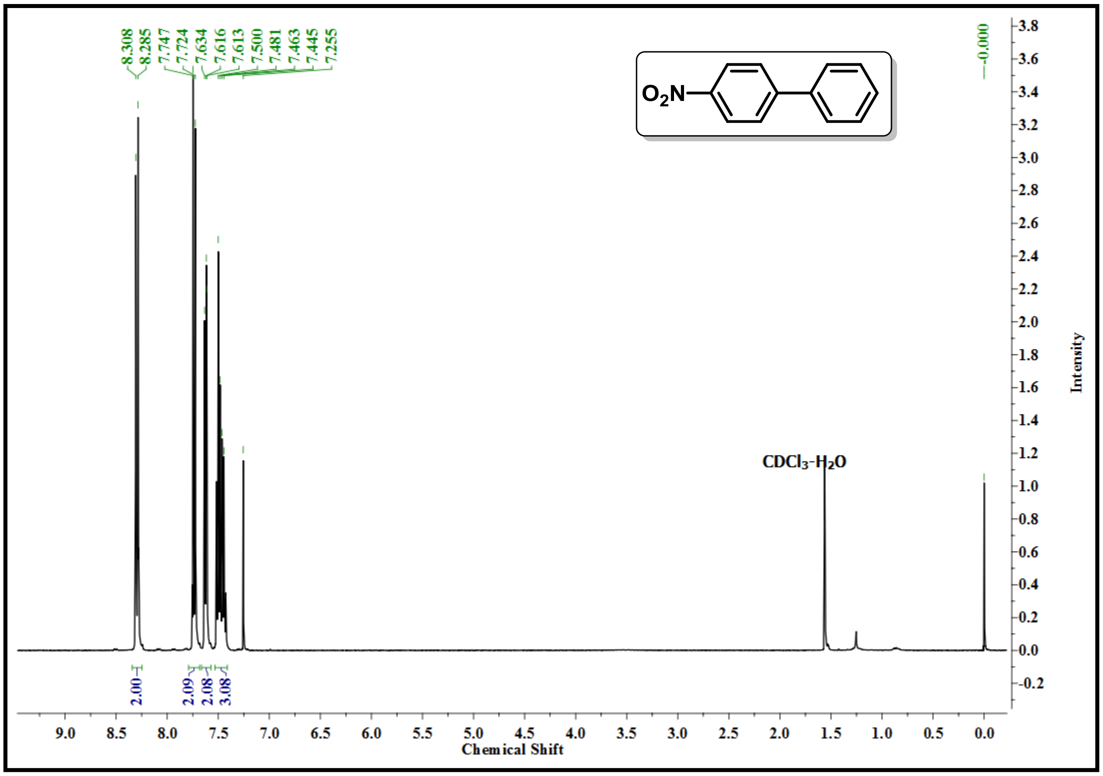


Figure S3 (^{1}H NMR of 3a)

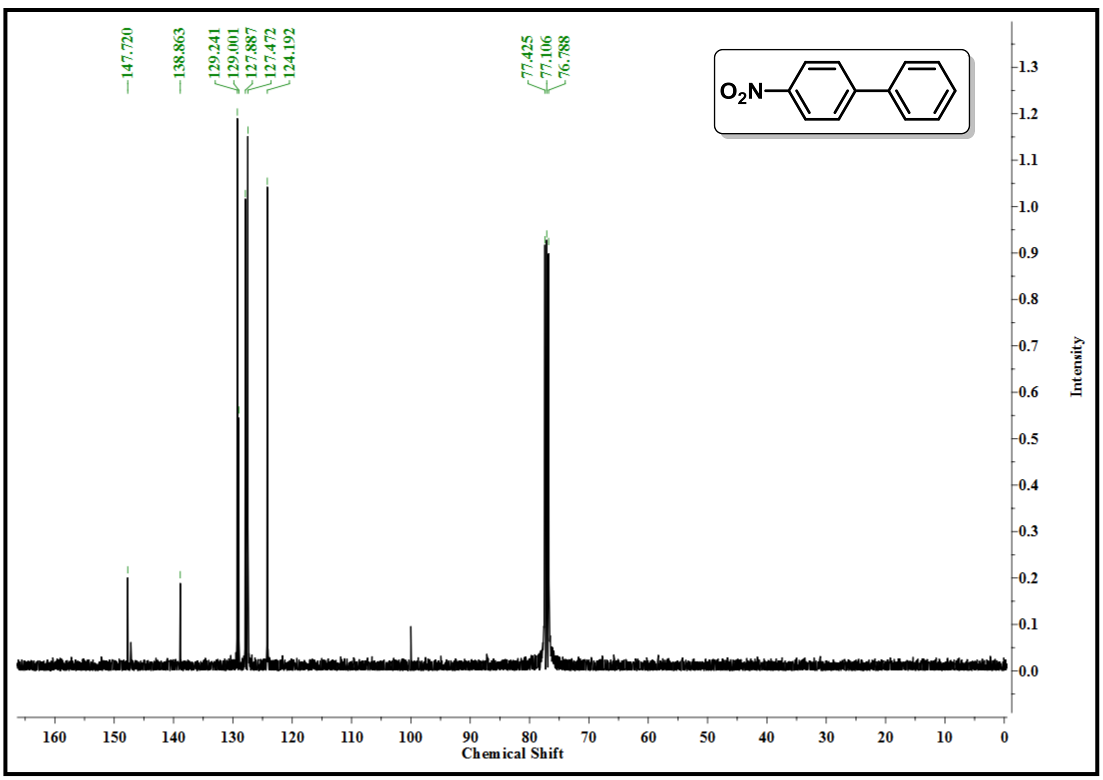


Figure S4 (^{13}C NMR of 3a)

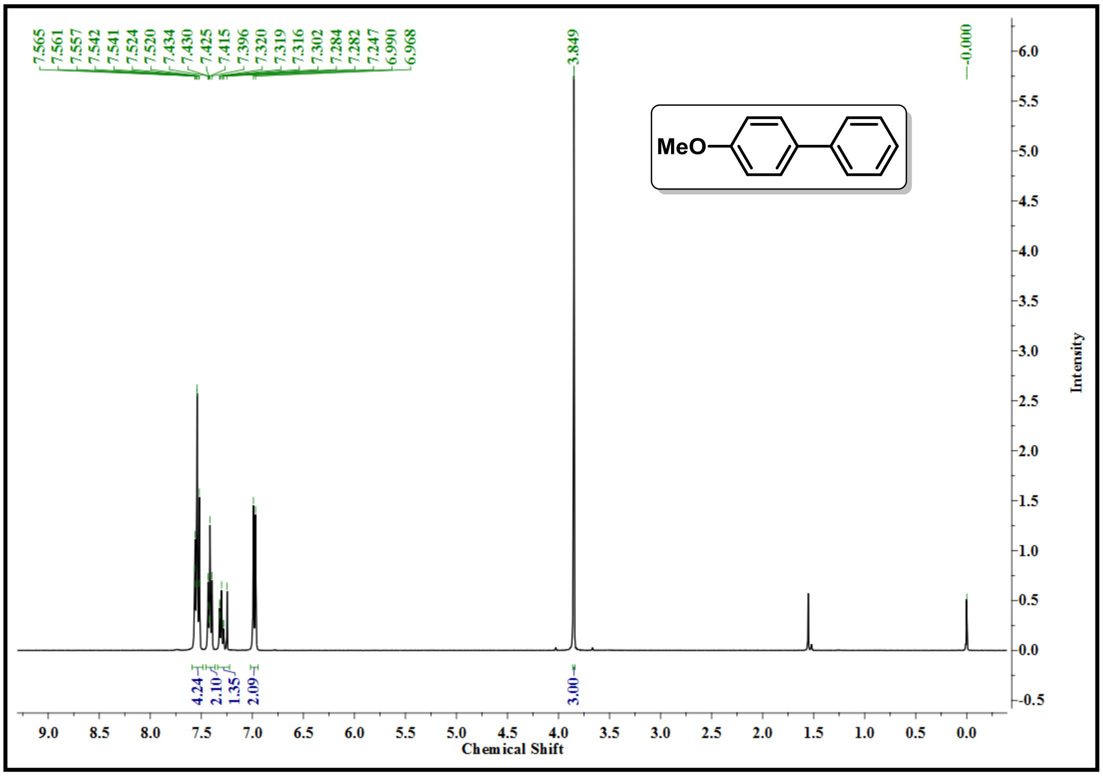


Figure S5 (^{1}H NMR of 3b)

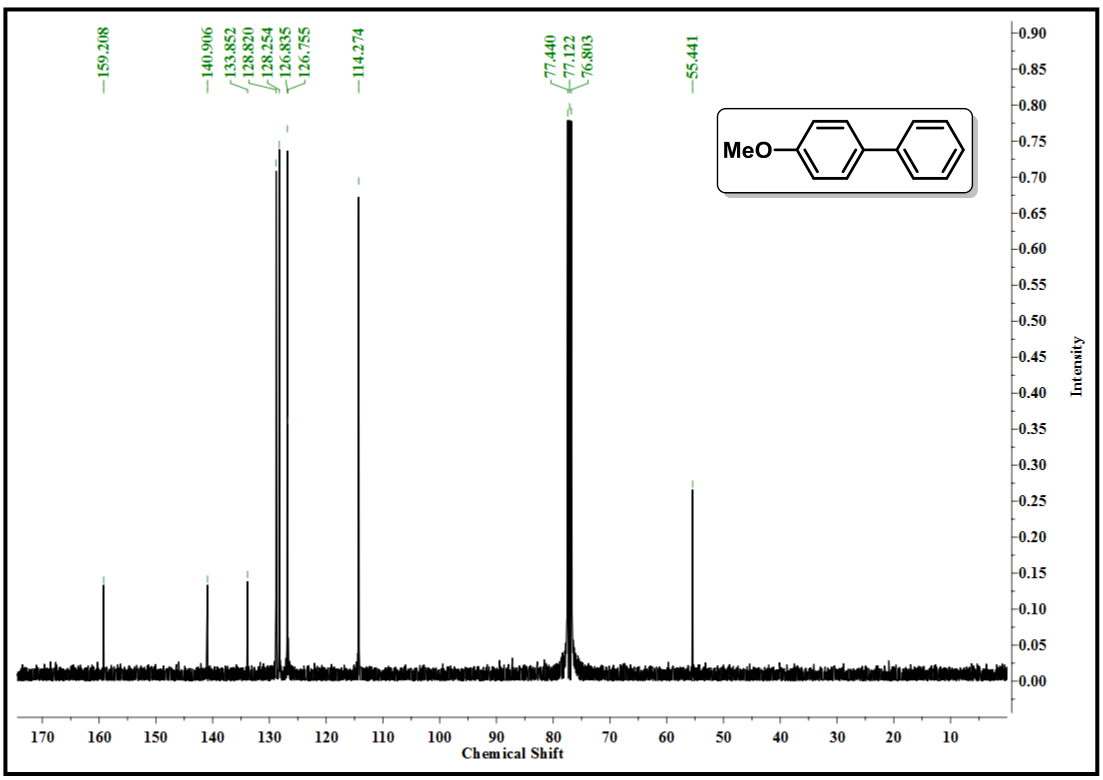
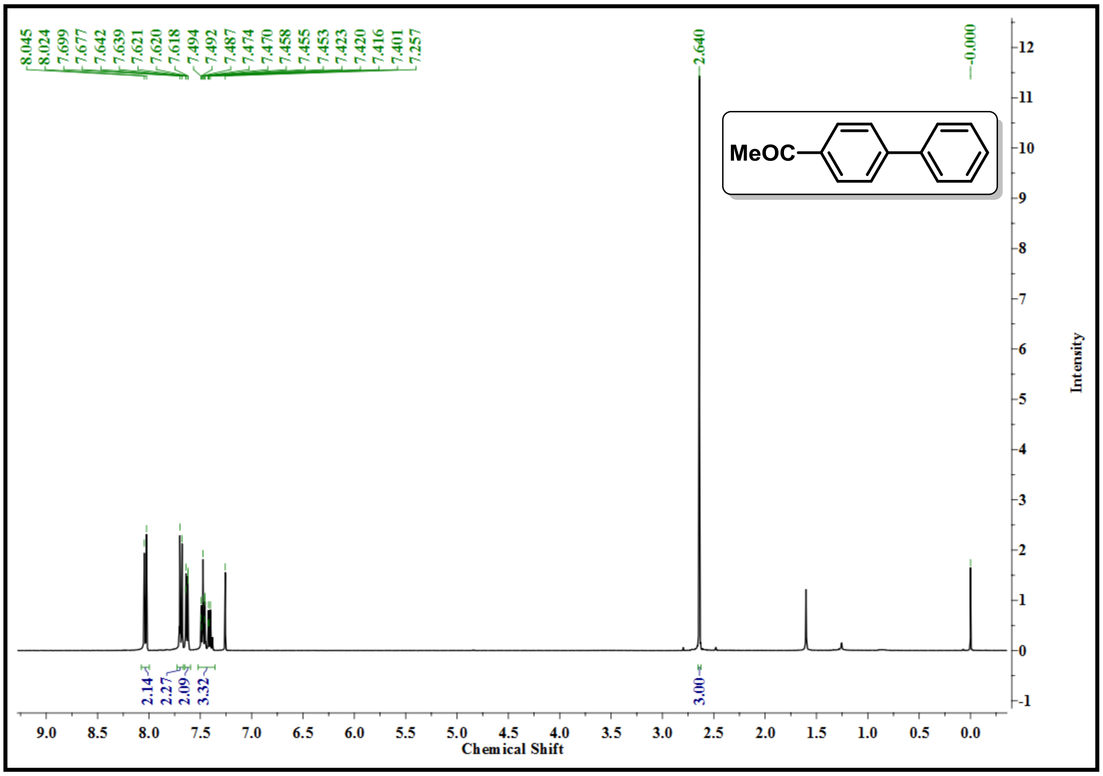


Figure S6 (^{13}C NMR of 3b)



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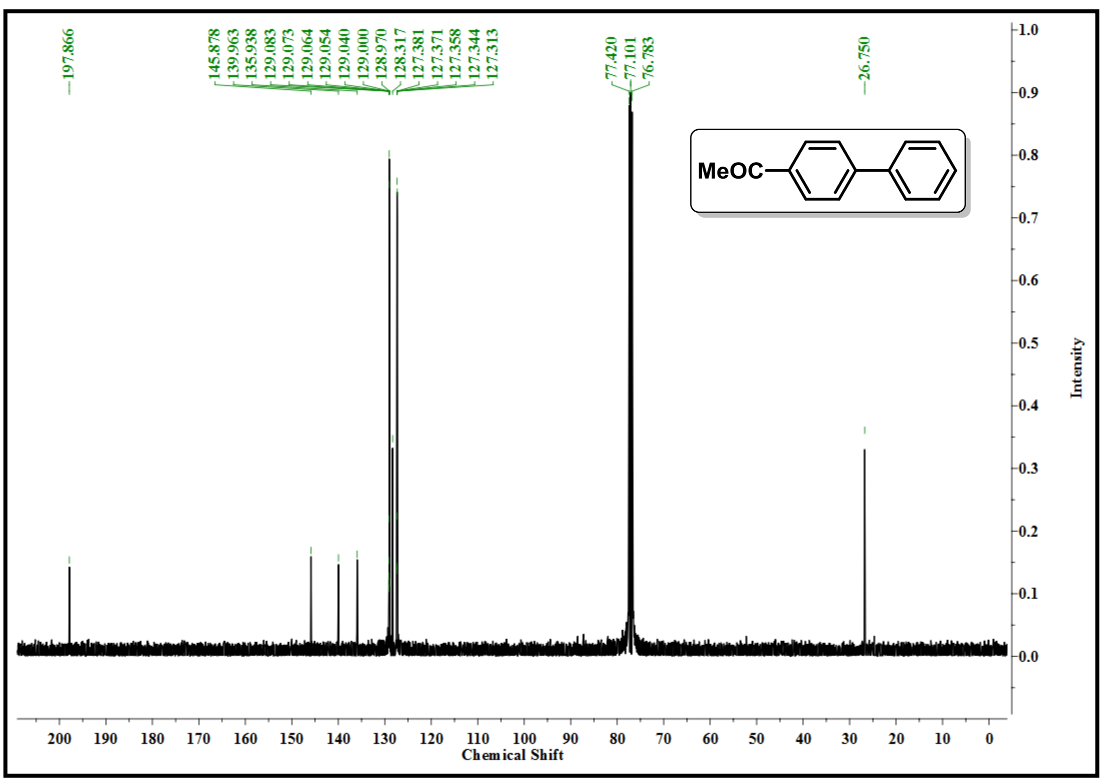
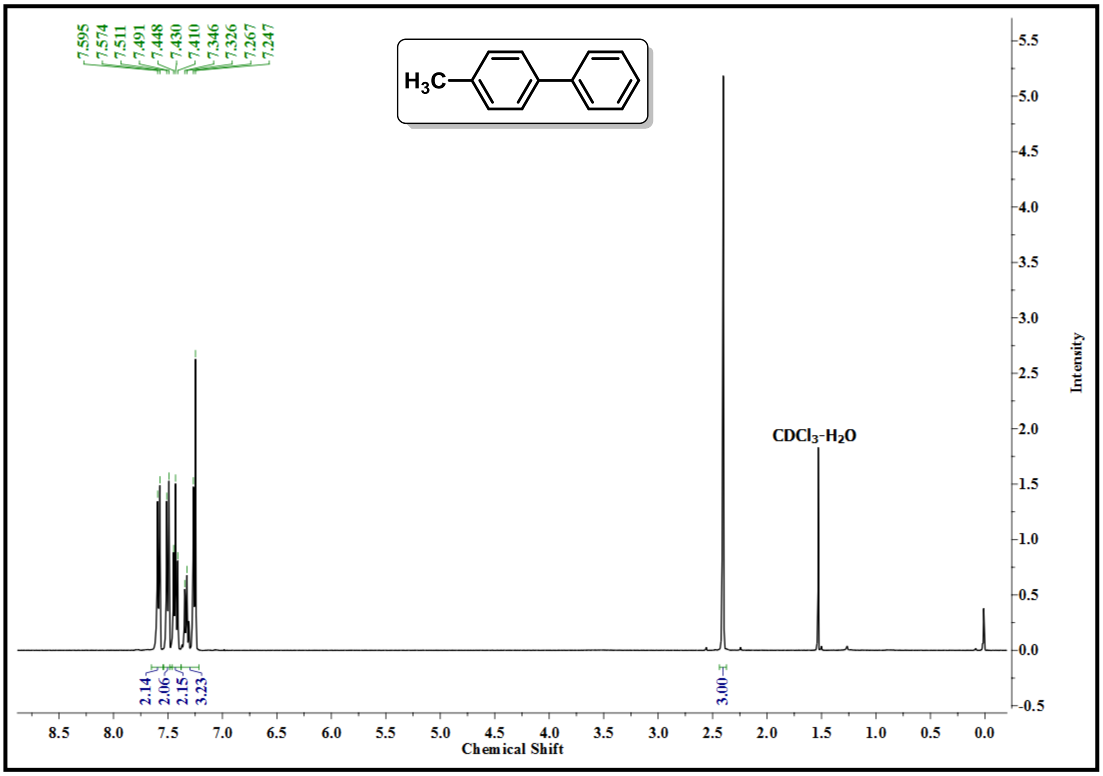


Figure S8 (^{13}C NMR of 3c)



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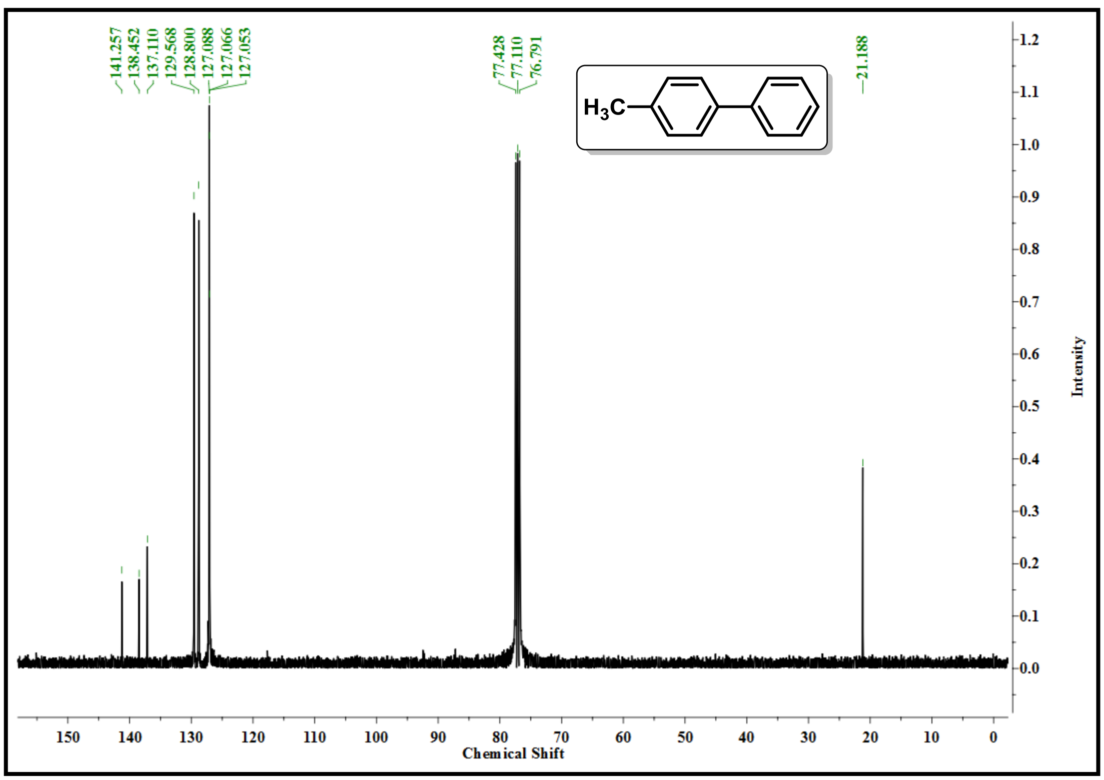

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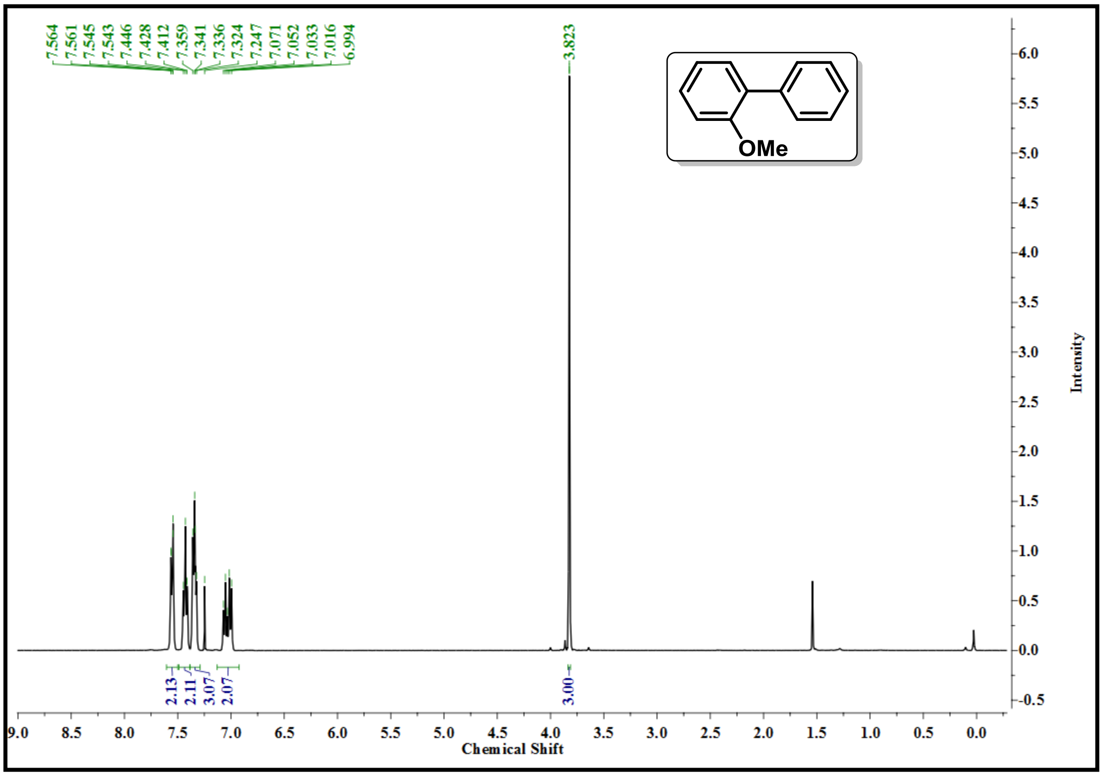

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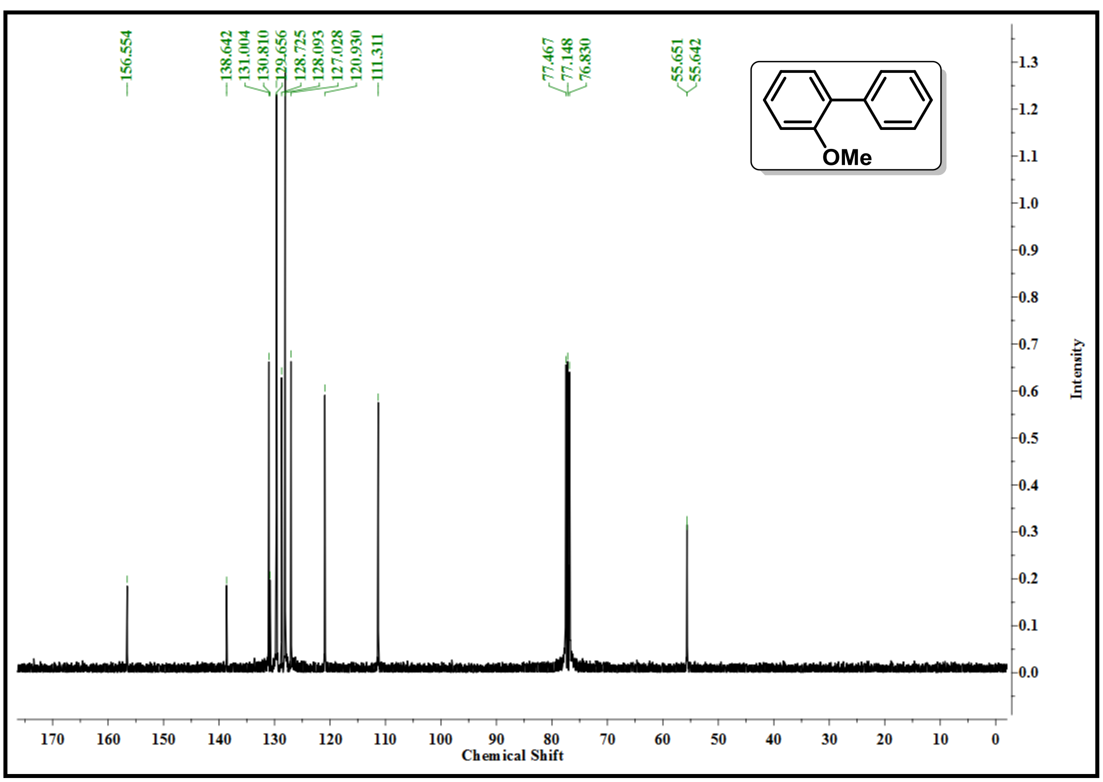

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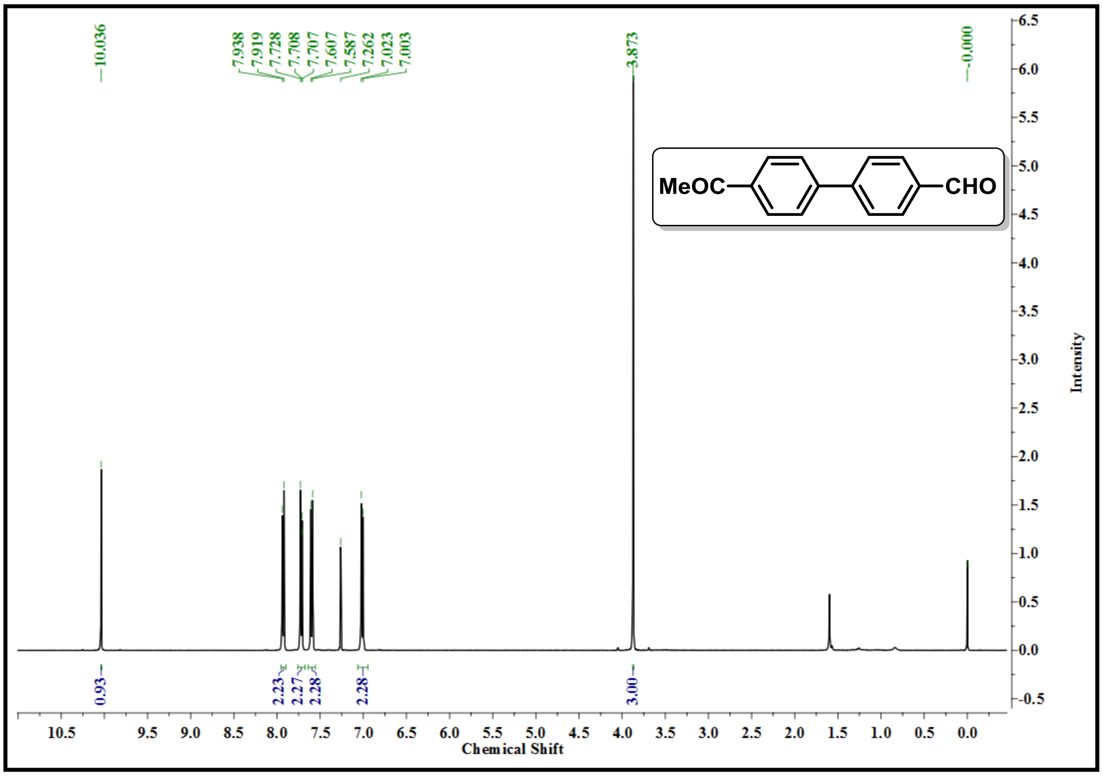
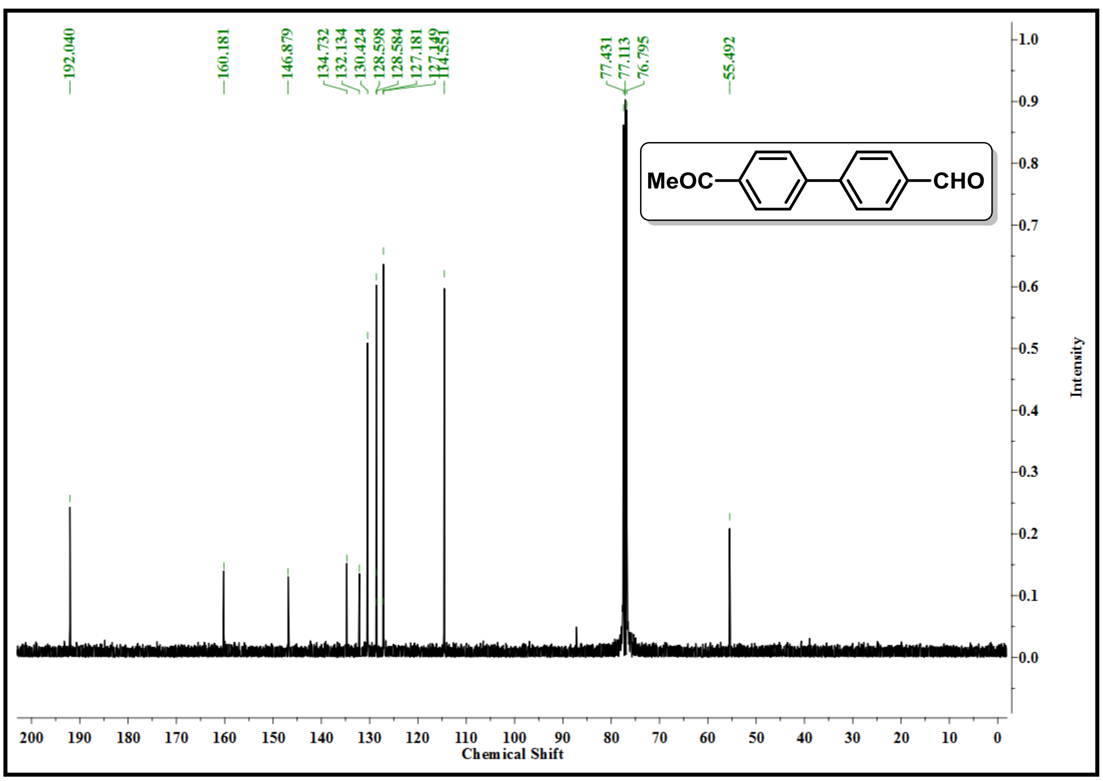


Figure S13 (^{1}H NMR of 3f)



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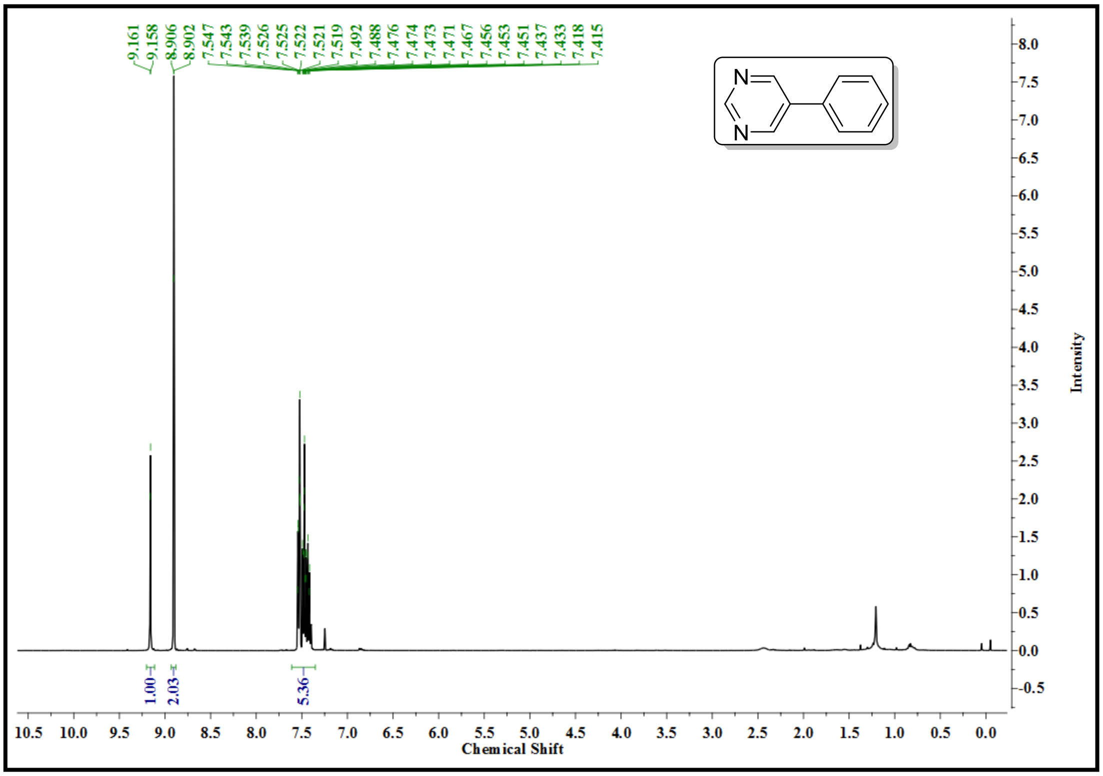

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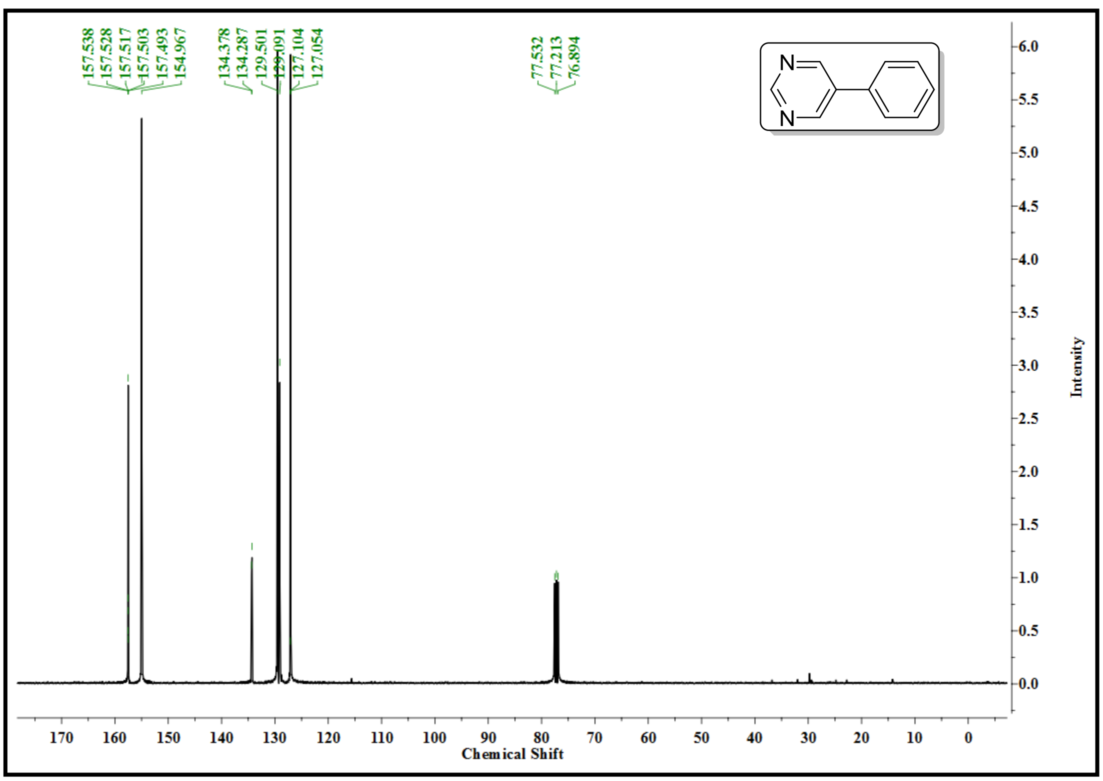

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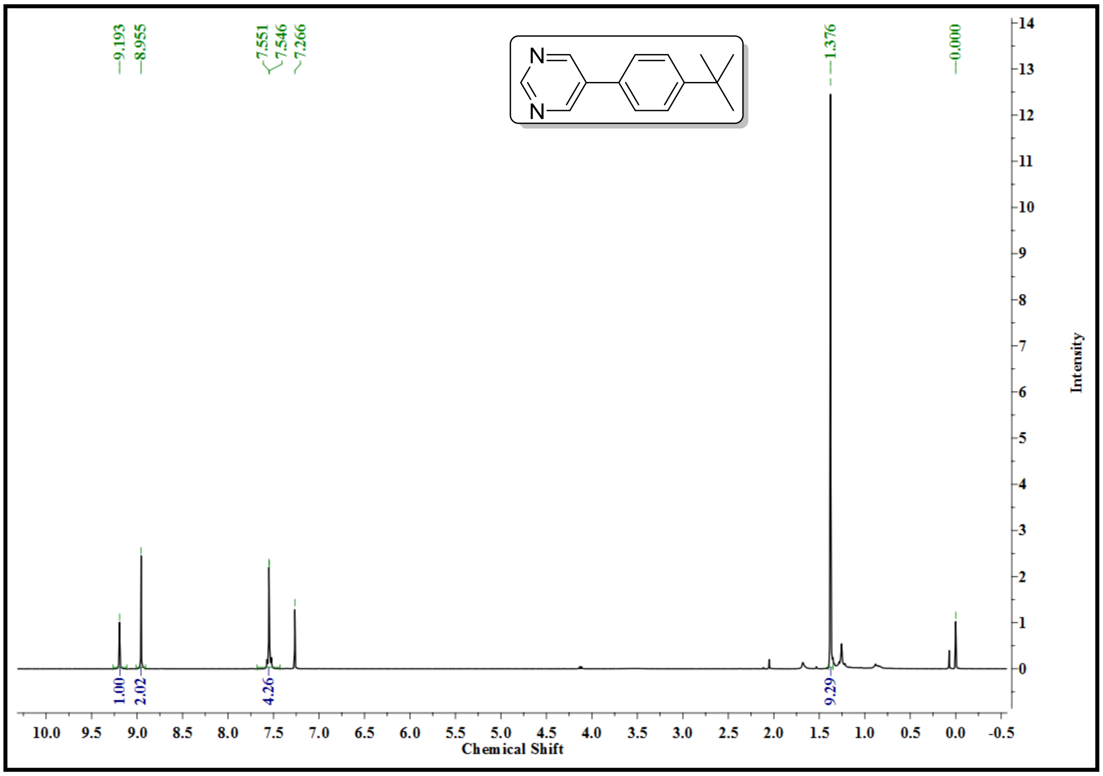

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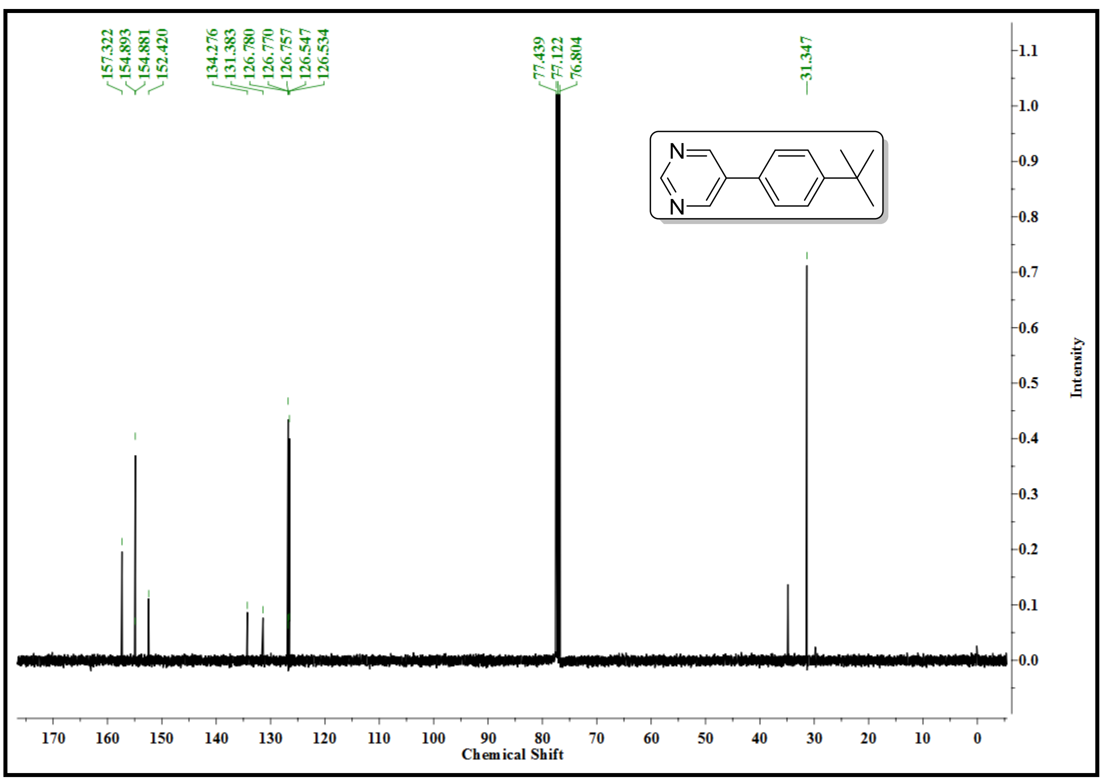

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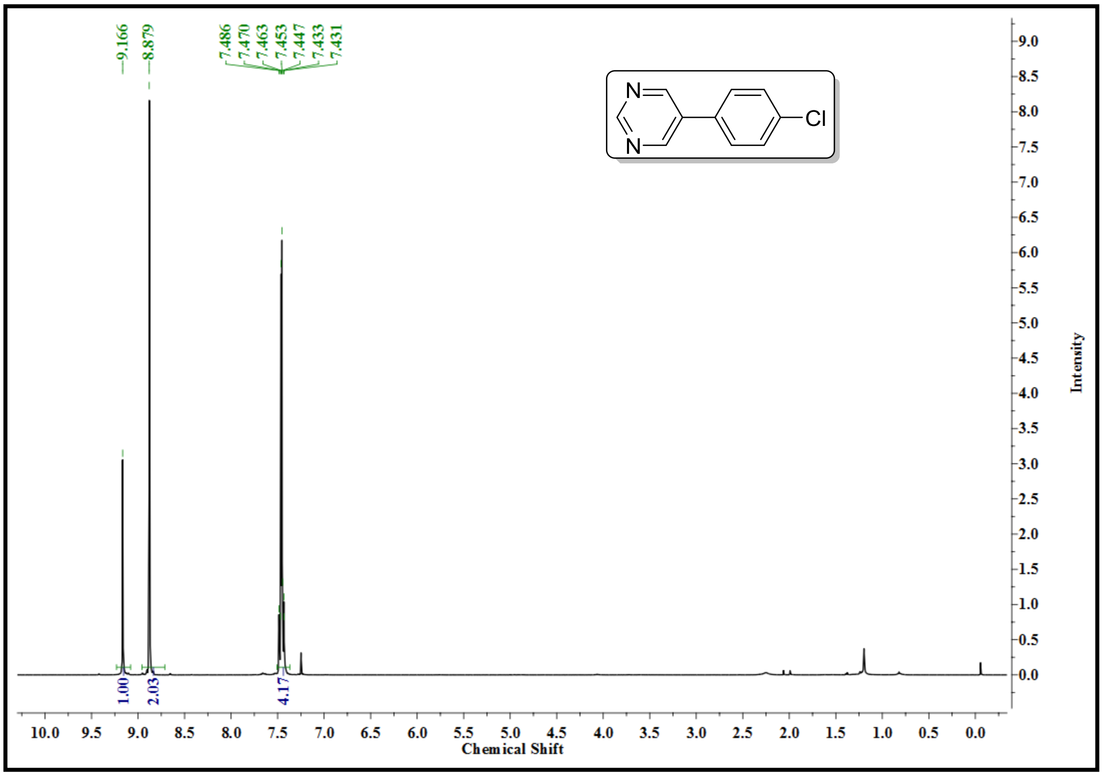

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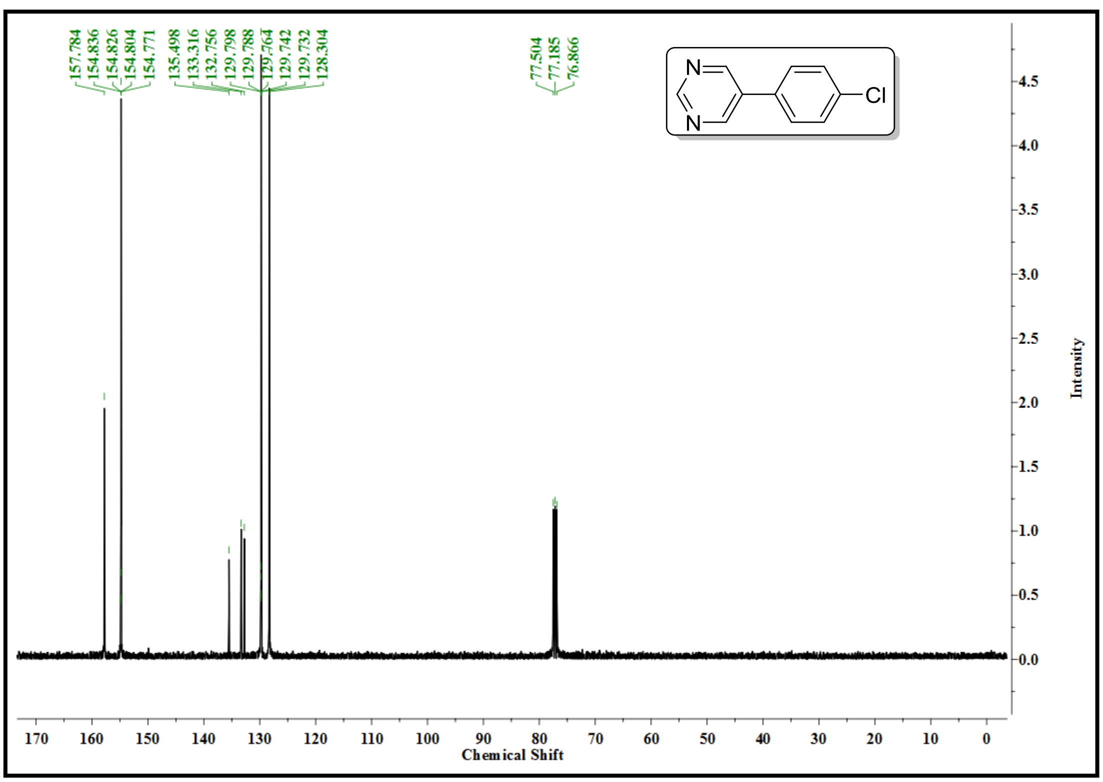

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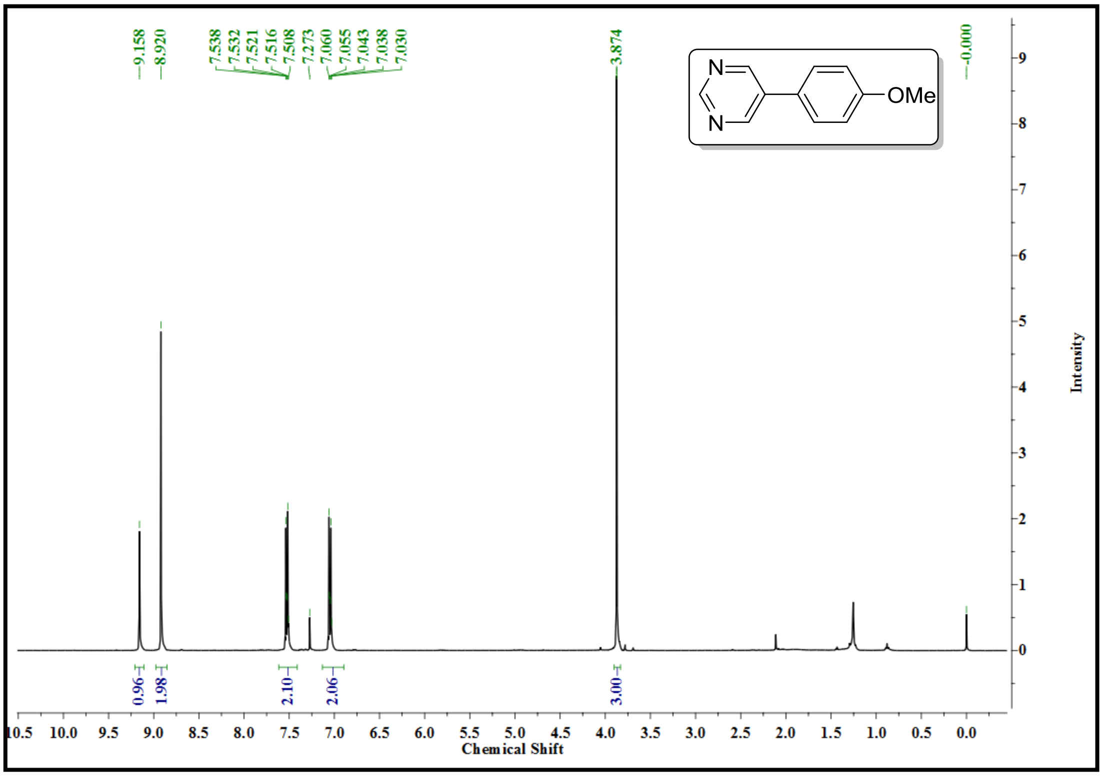

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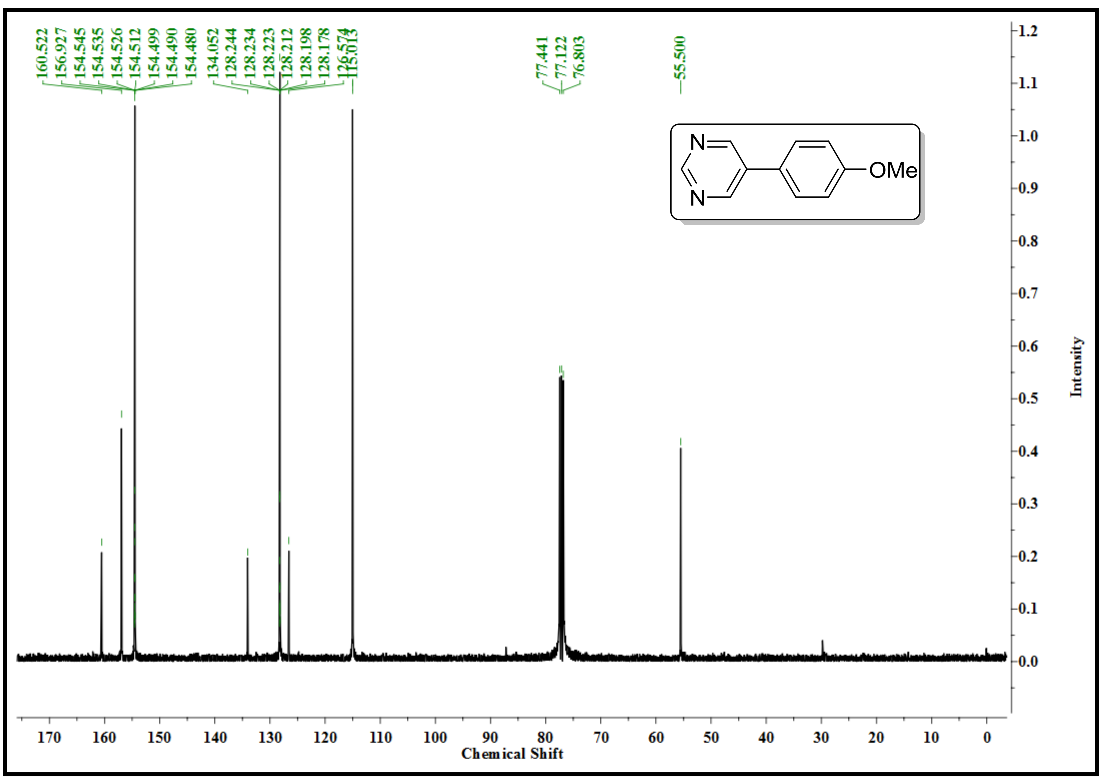

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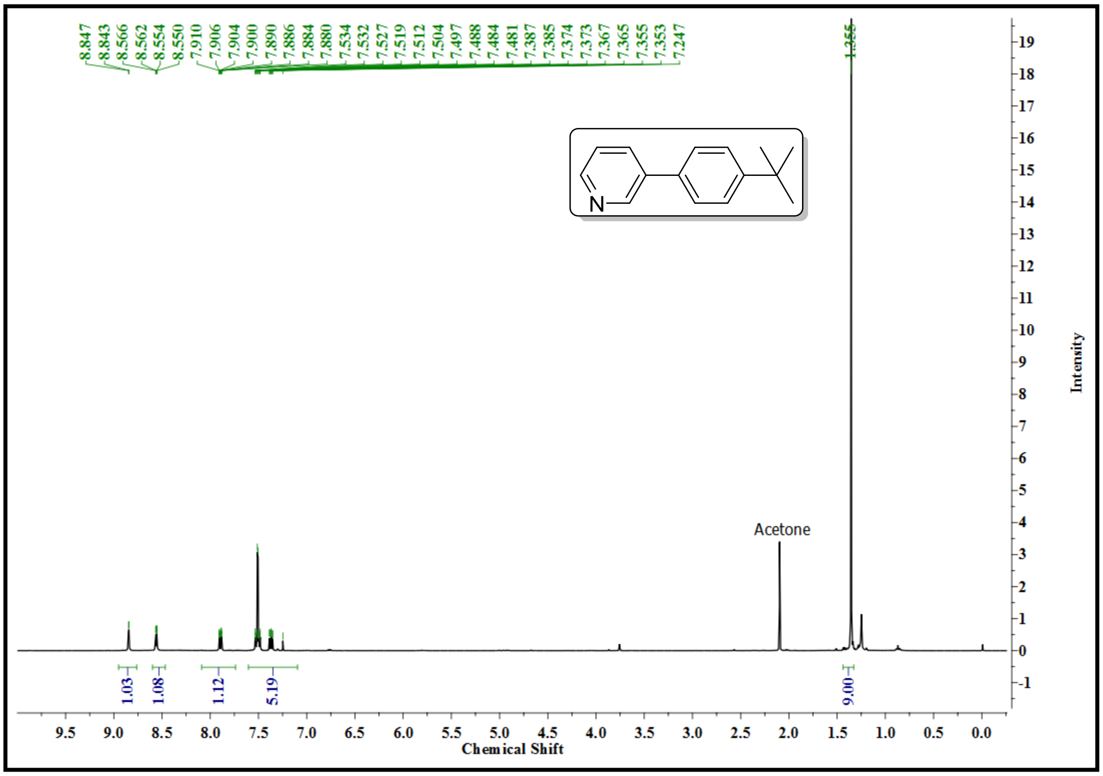

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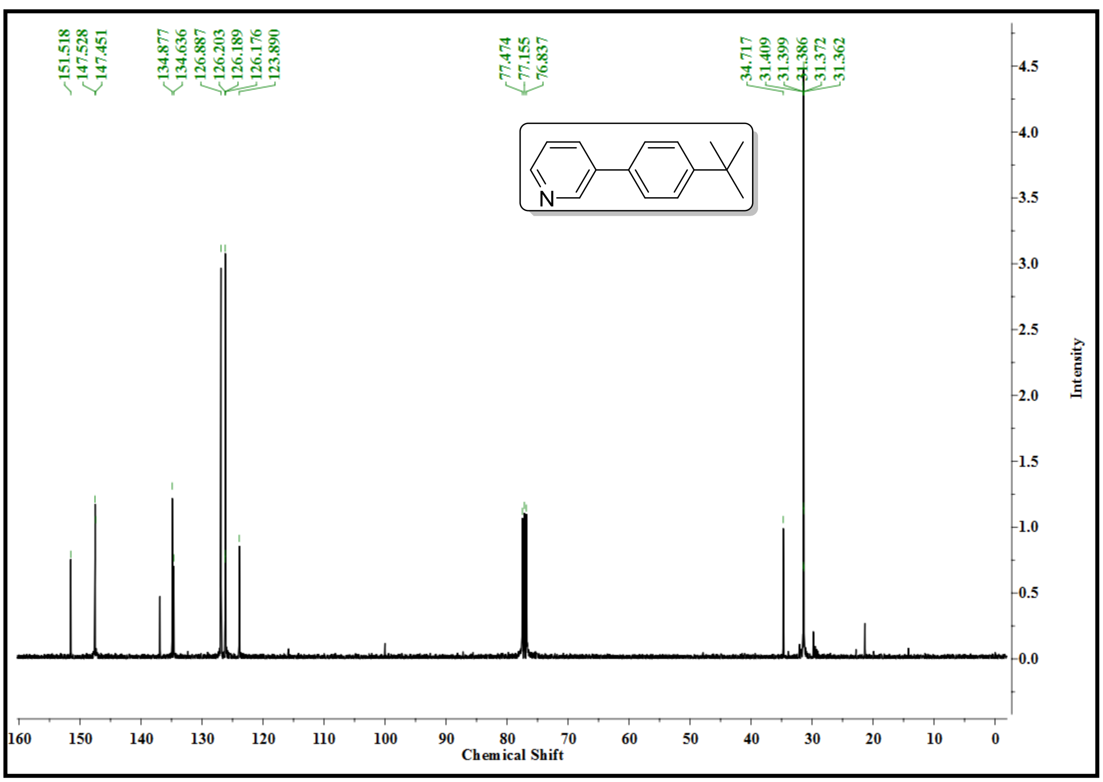

Figure S24 ([13]C NMR of 3k)

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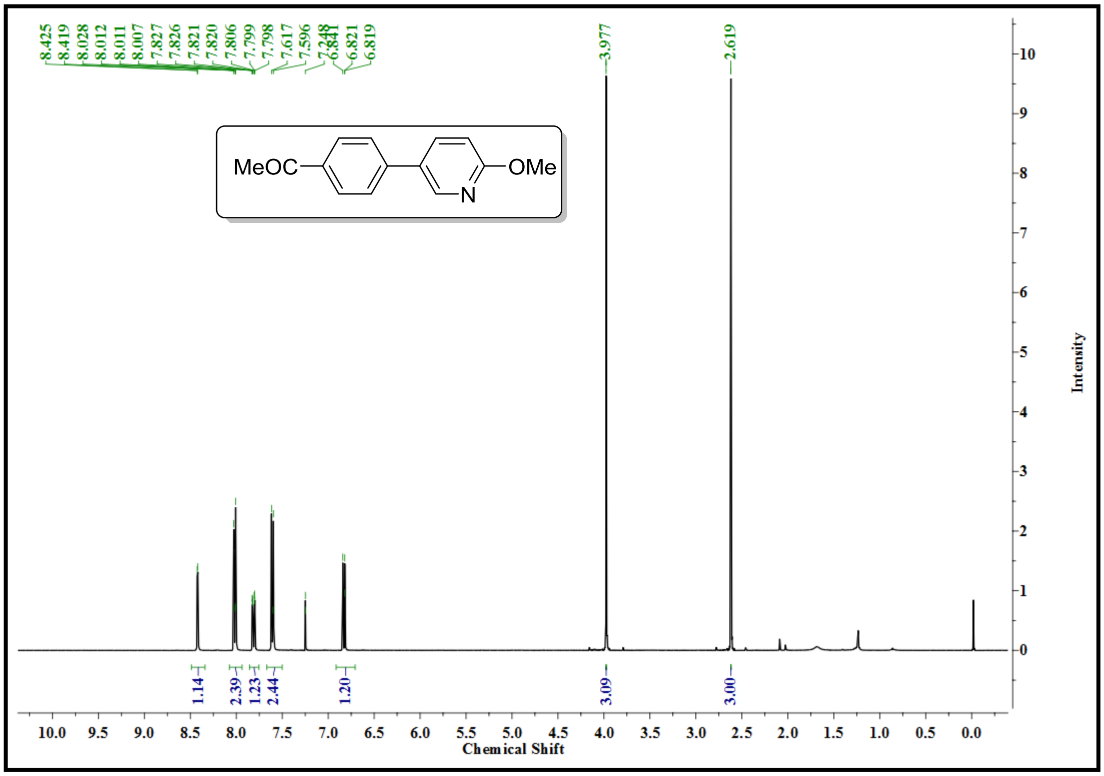

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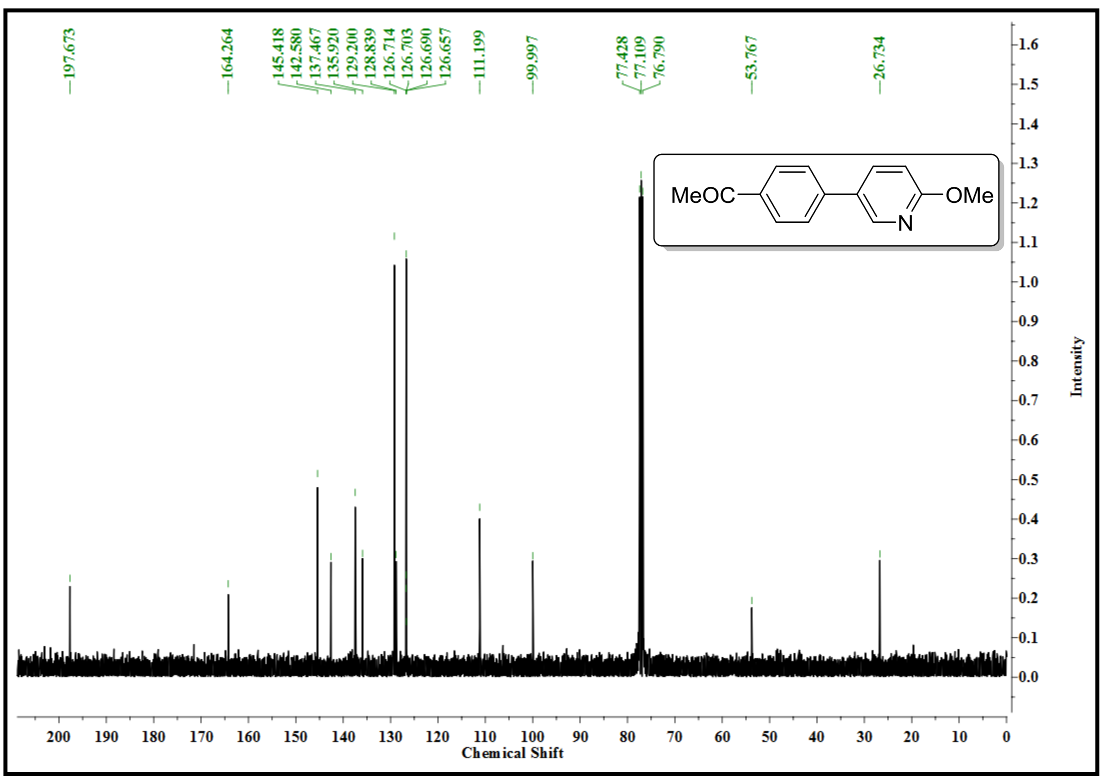

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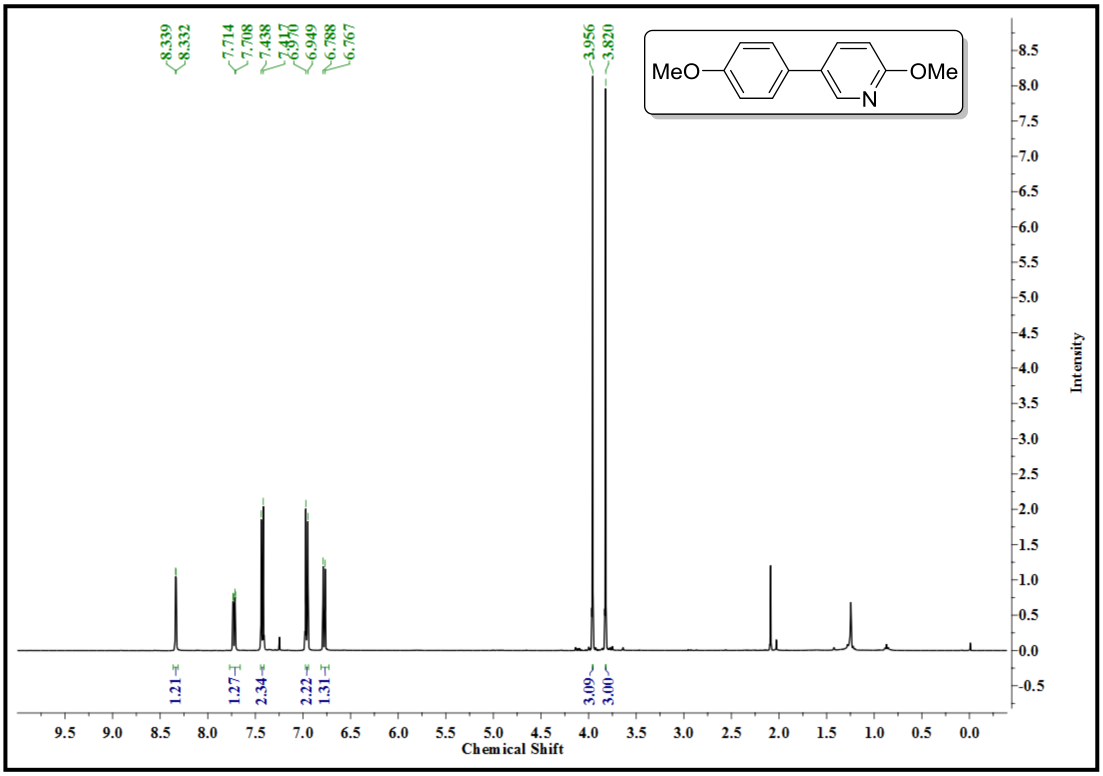
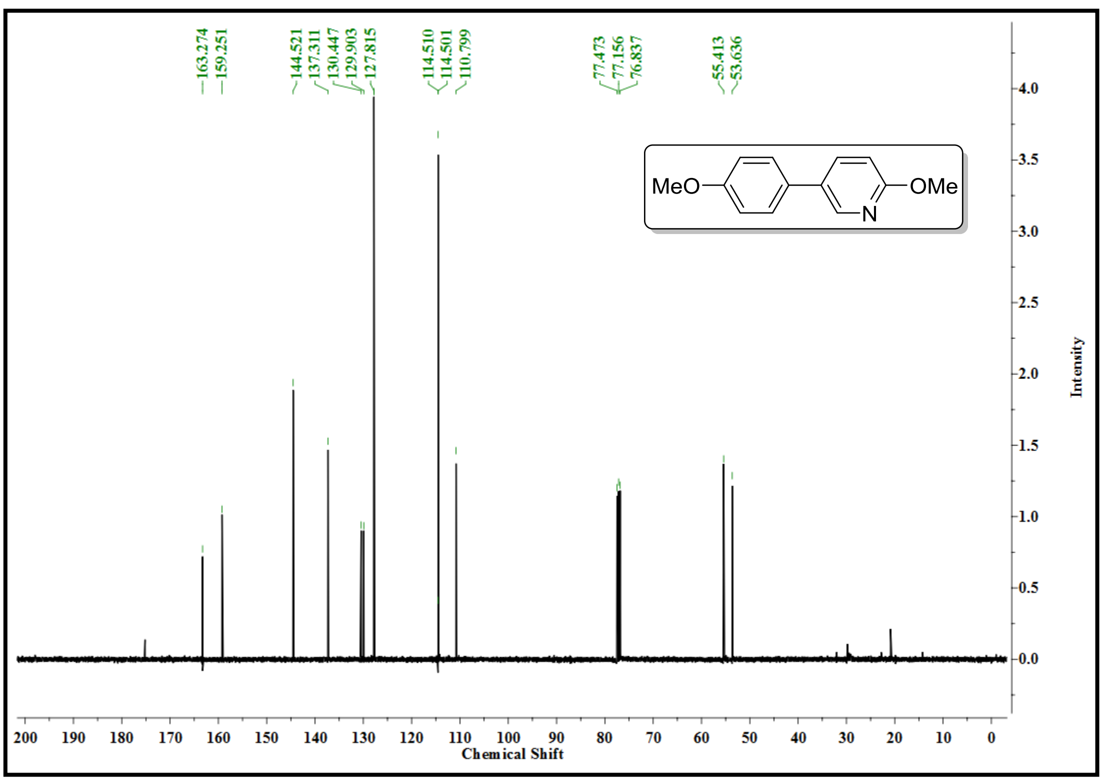


Figure S27 (^{1}H NMR of 3m)



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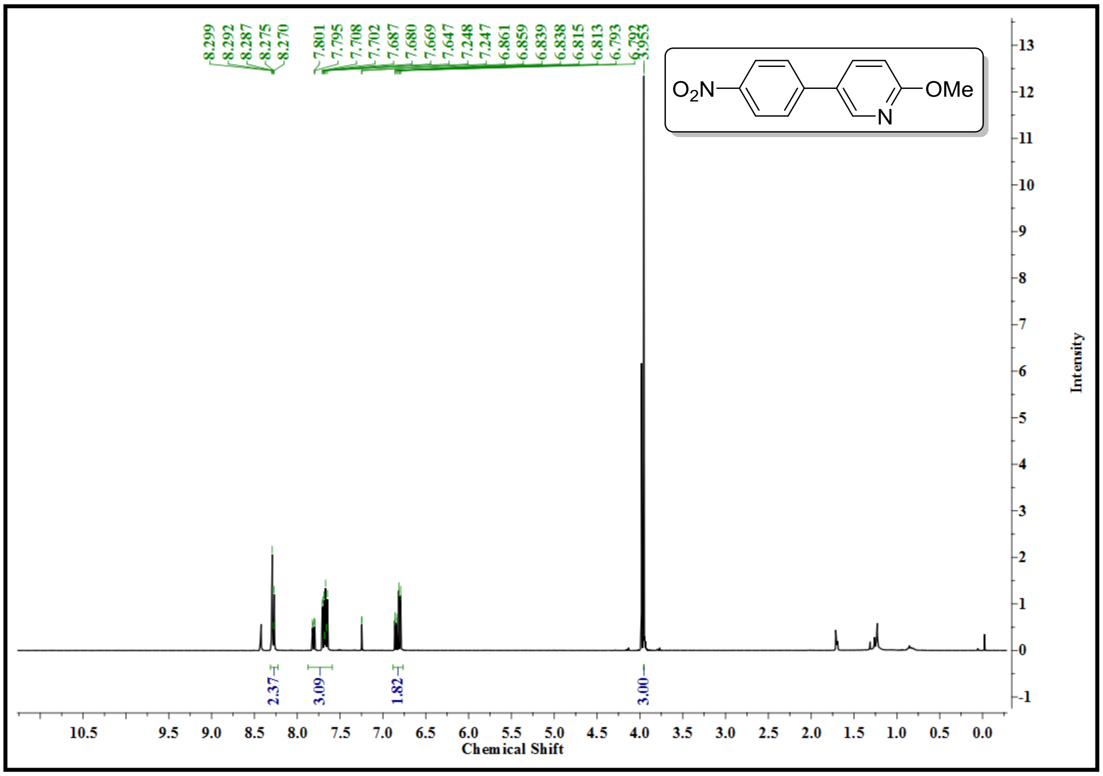

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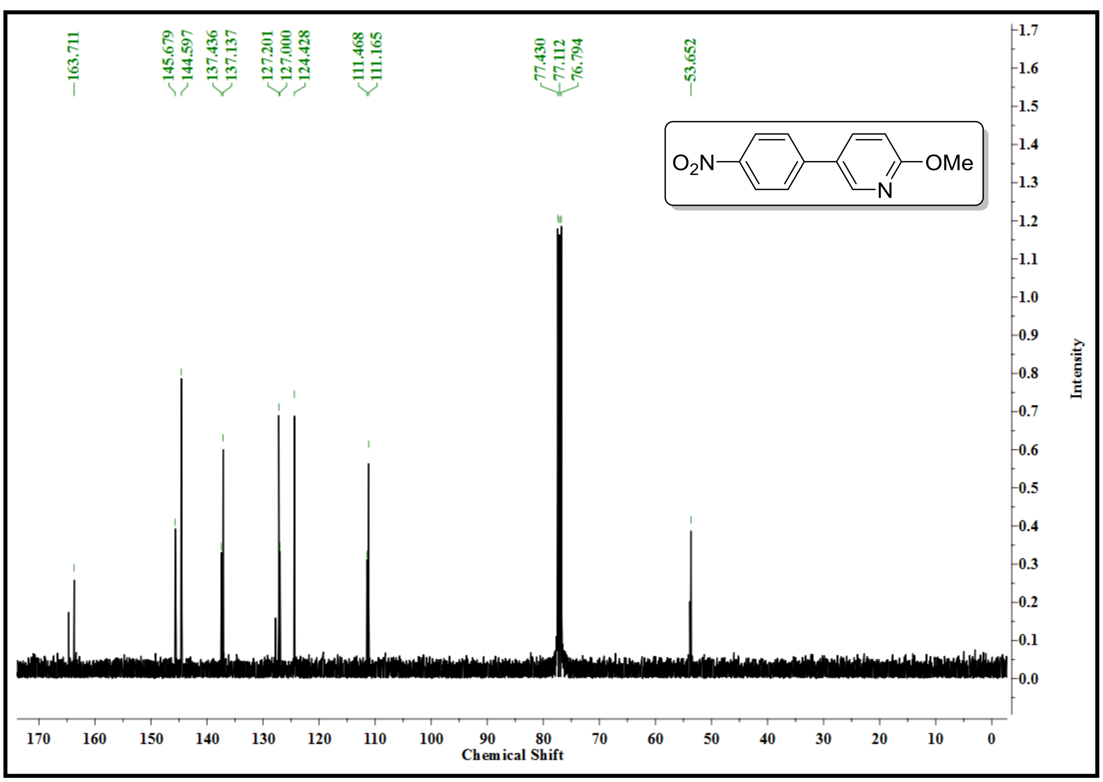

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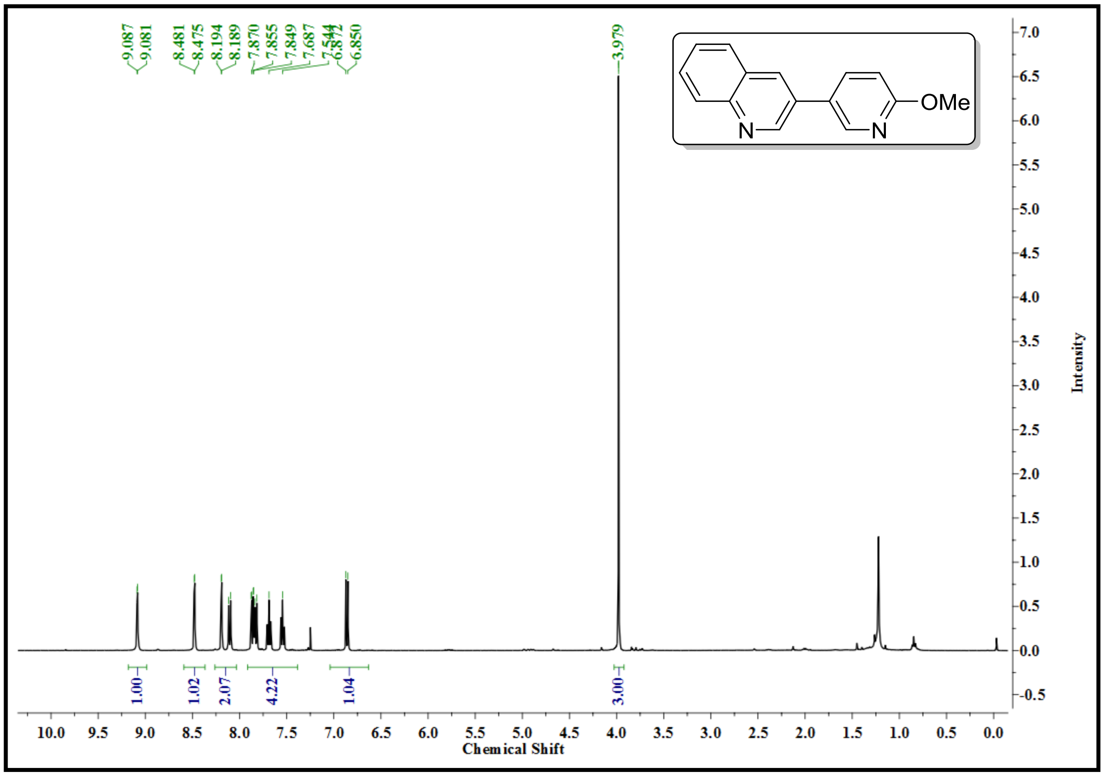


Figure S31 (^{1}H NMR of 3o)

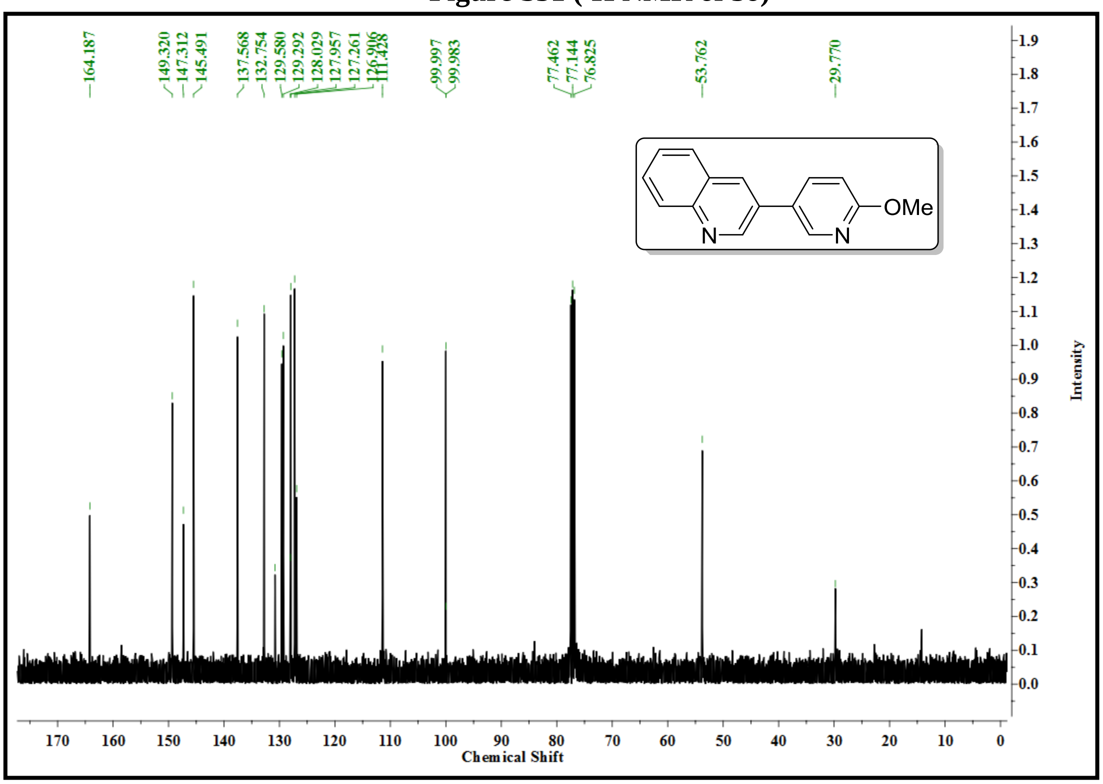


Figure S32 (^{13}C NMR of 3o)

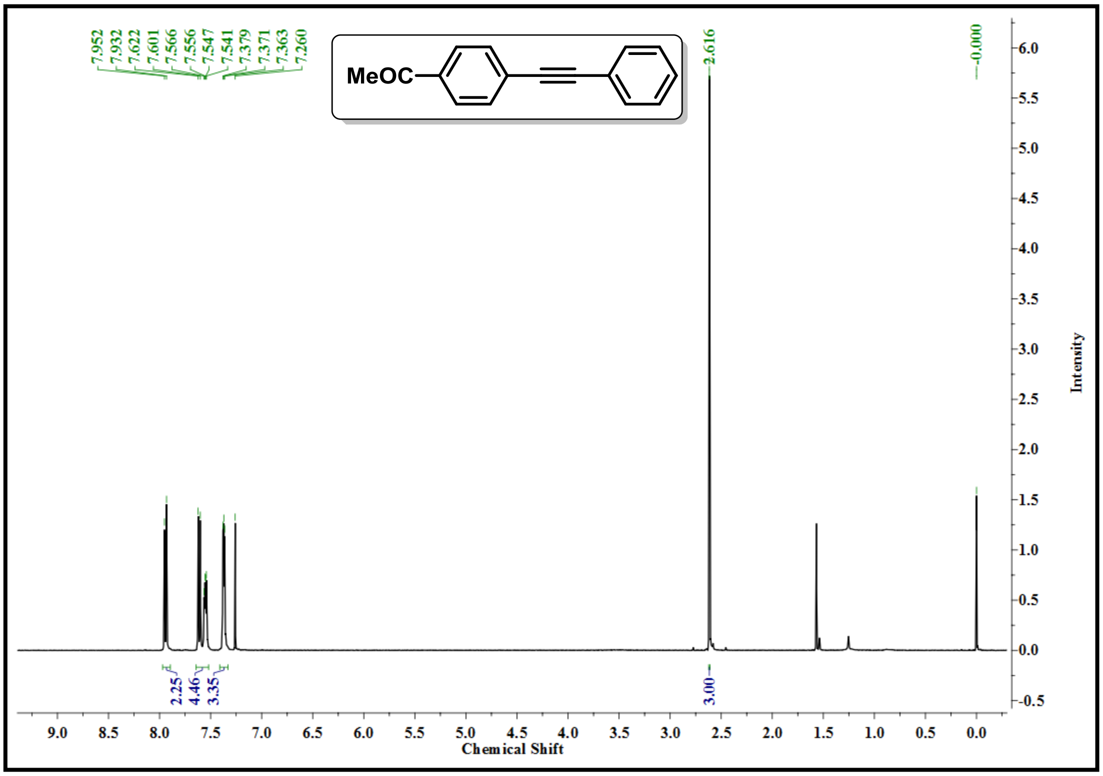


Figure S33 (^{1}H NMR of 6a)

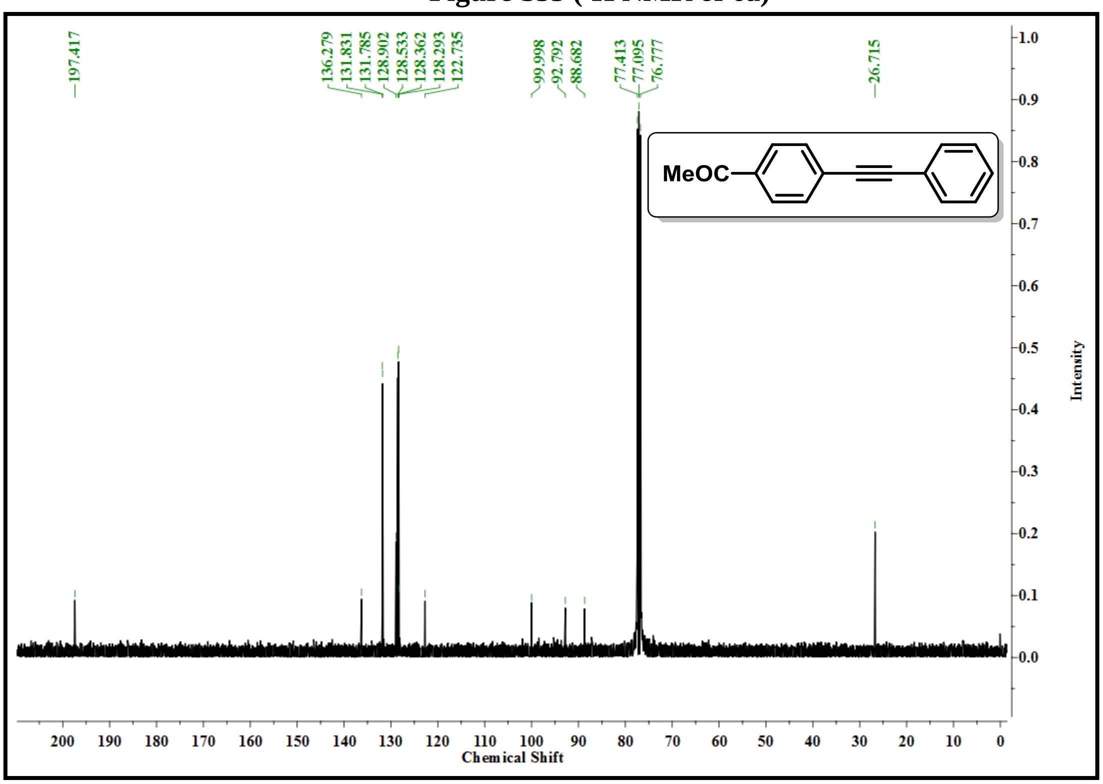


Figure S34 (^{13}C NMR of 6a)

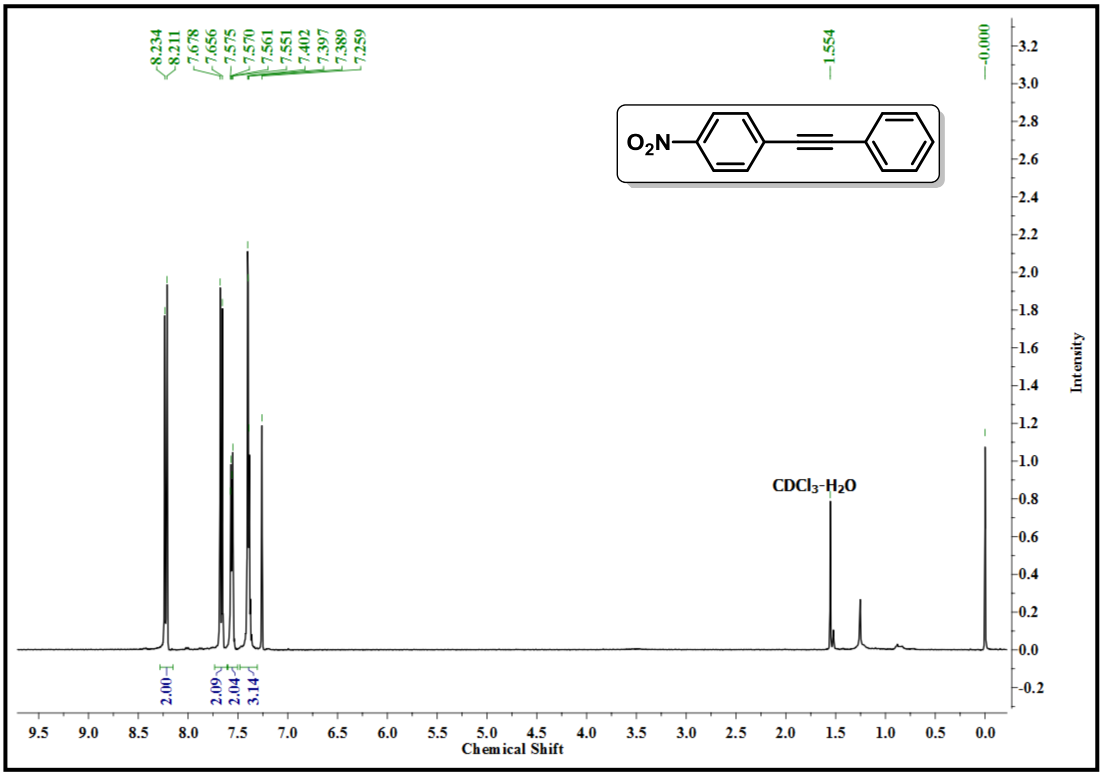
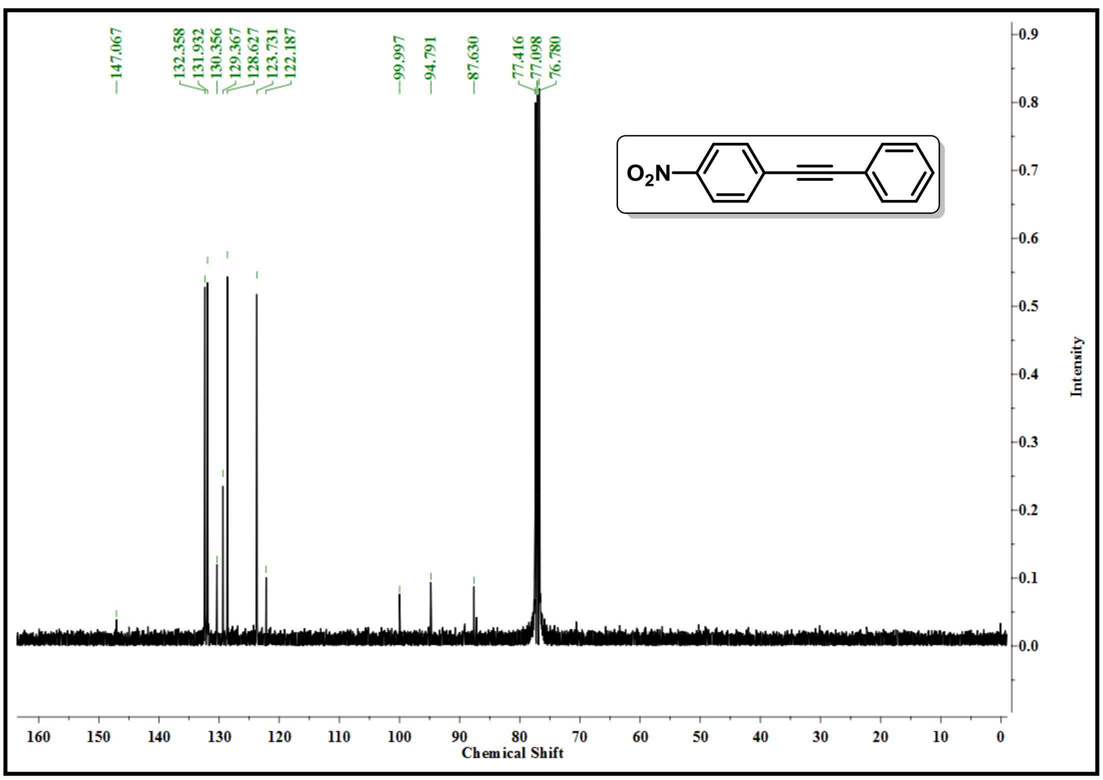


Figure S35 (^{1}H NMR of 6b)



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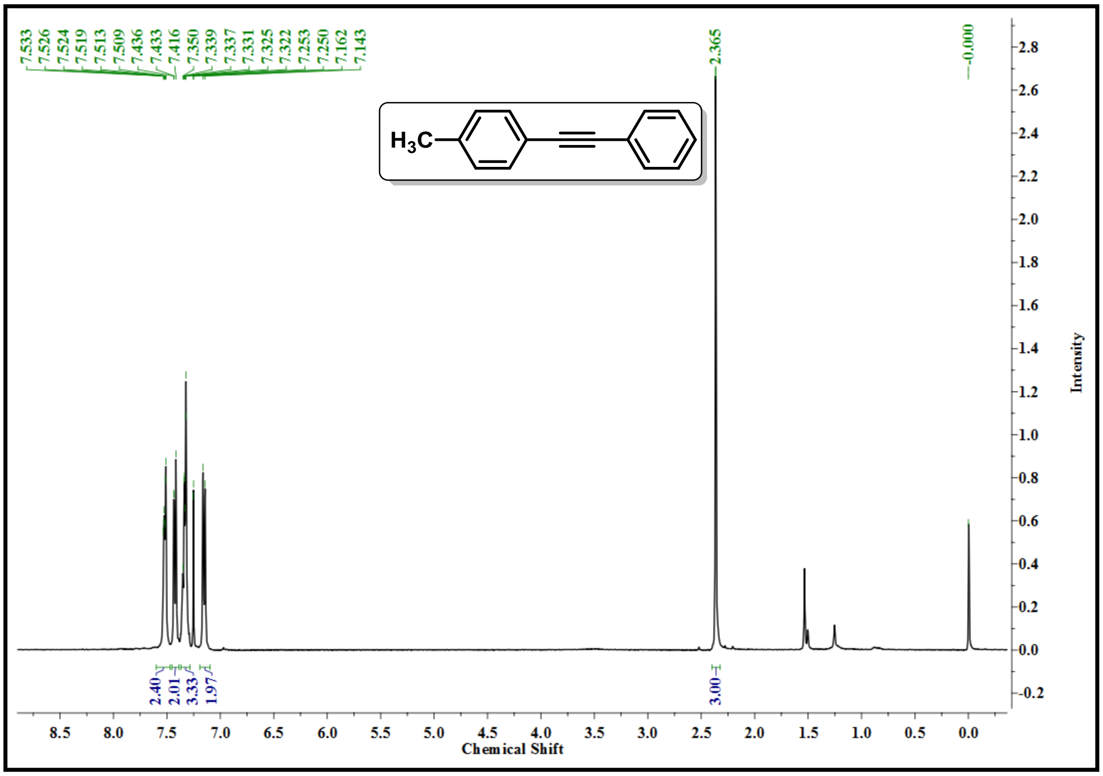


Figure S37 (^{1}H NMR of 6c)

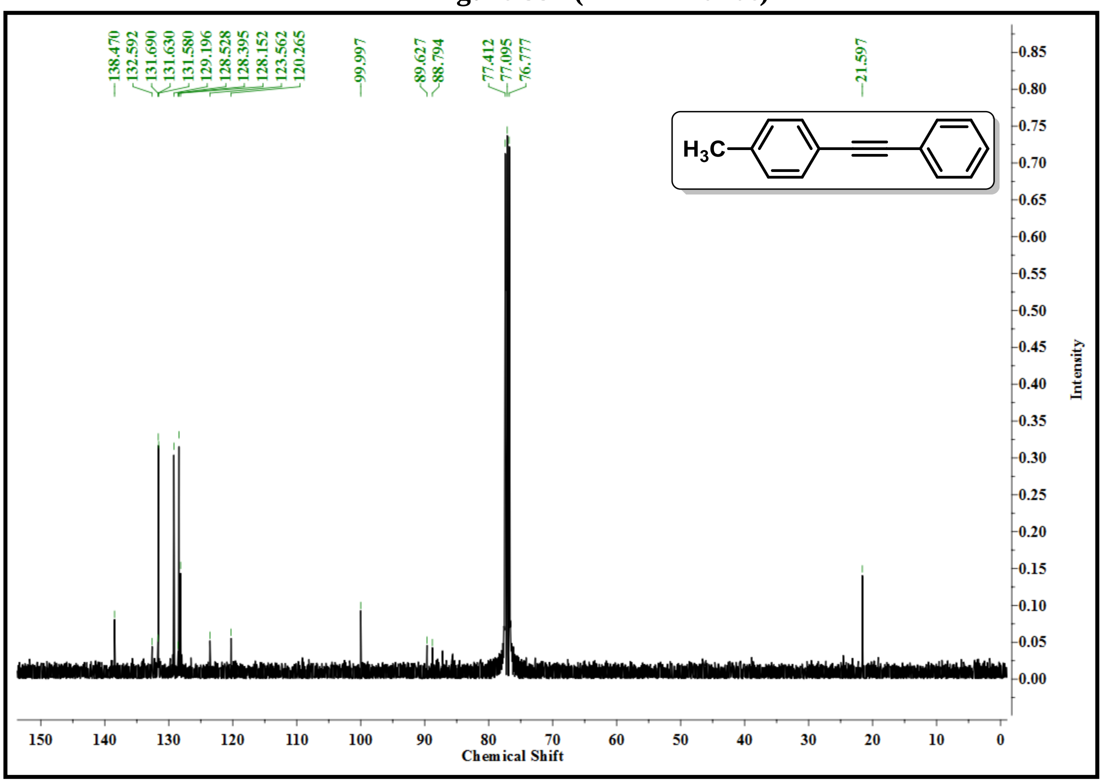
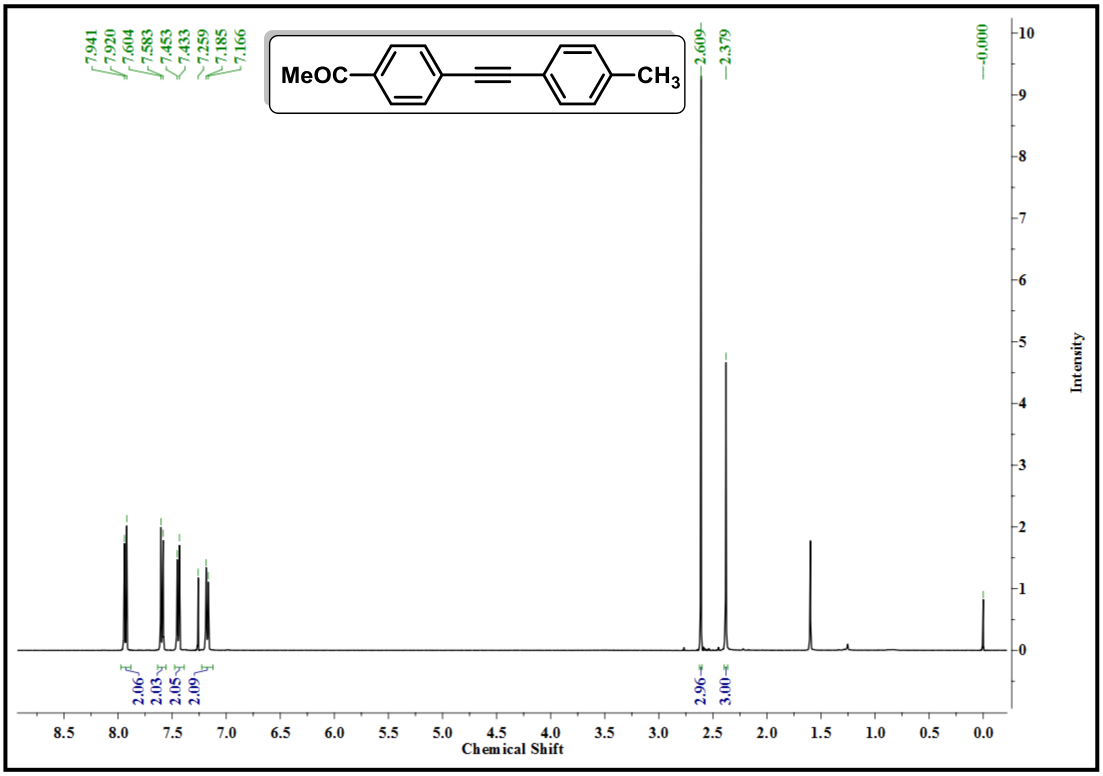


Figure S38 (^{13}C NMR of 6c)



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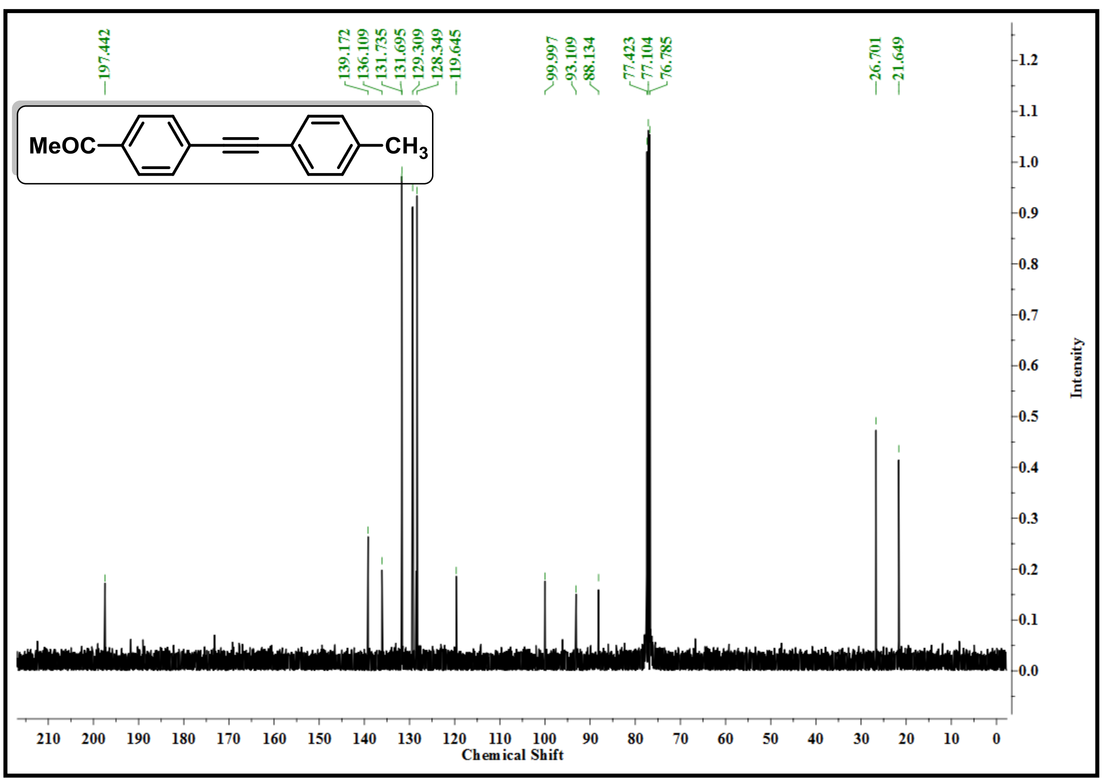

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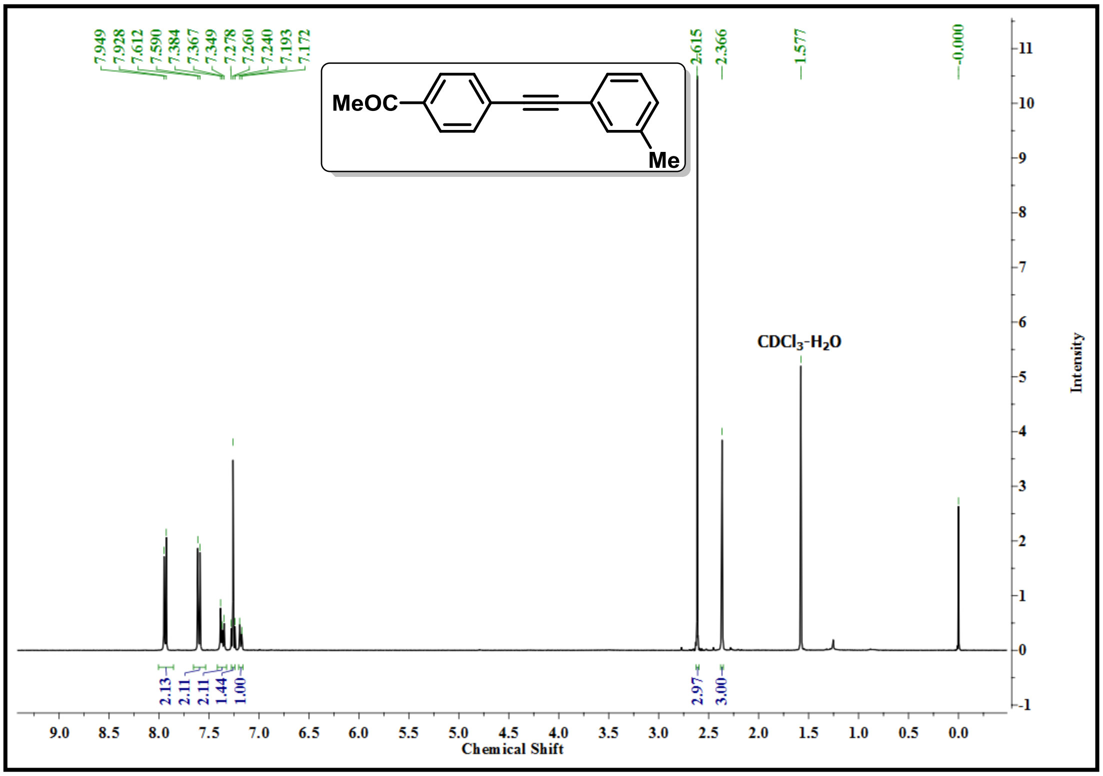

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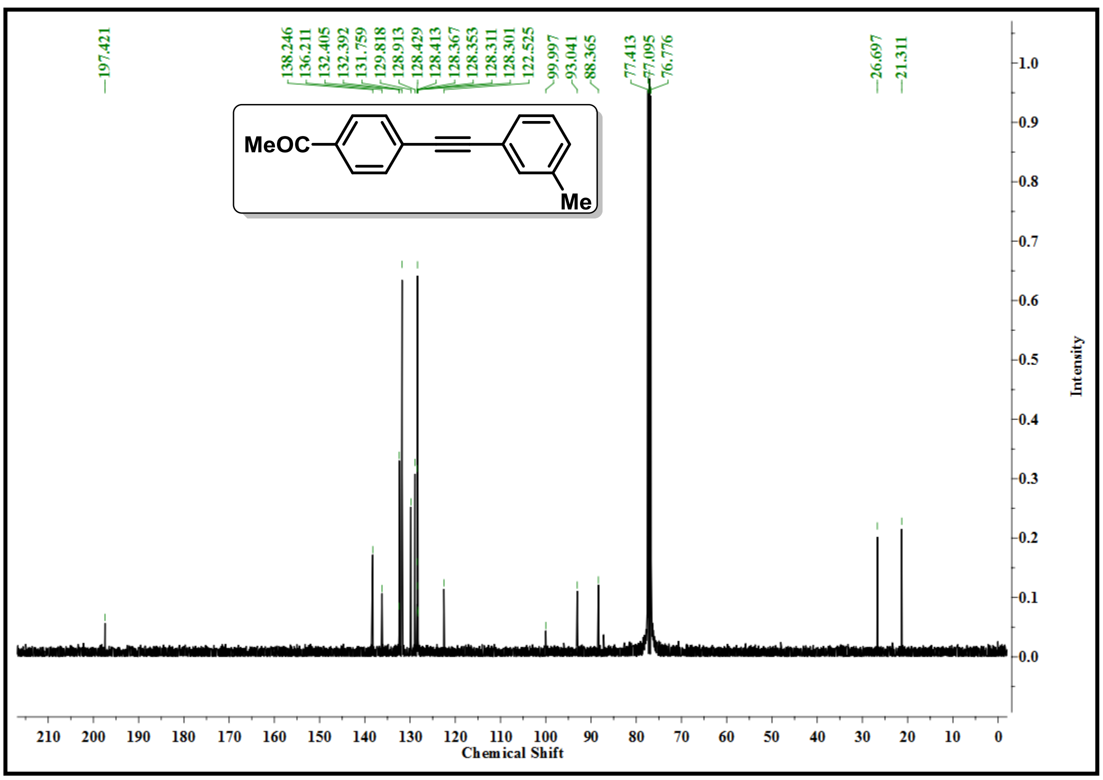

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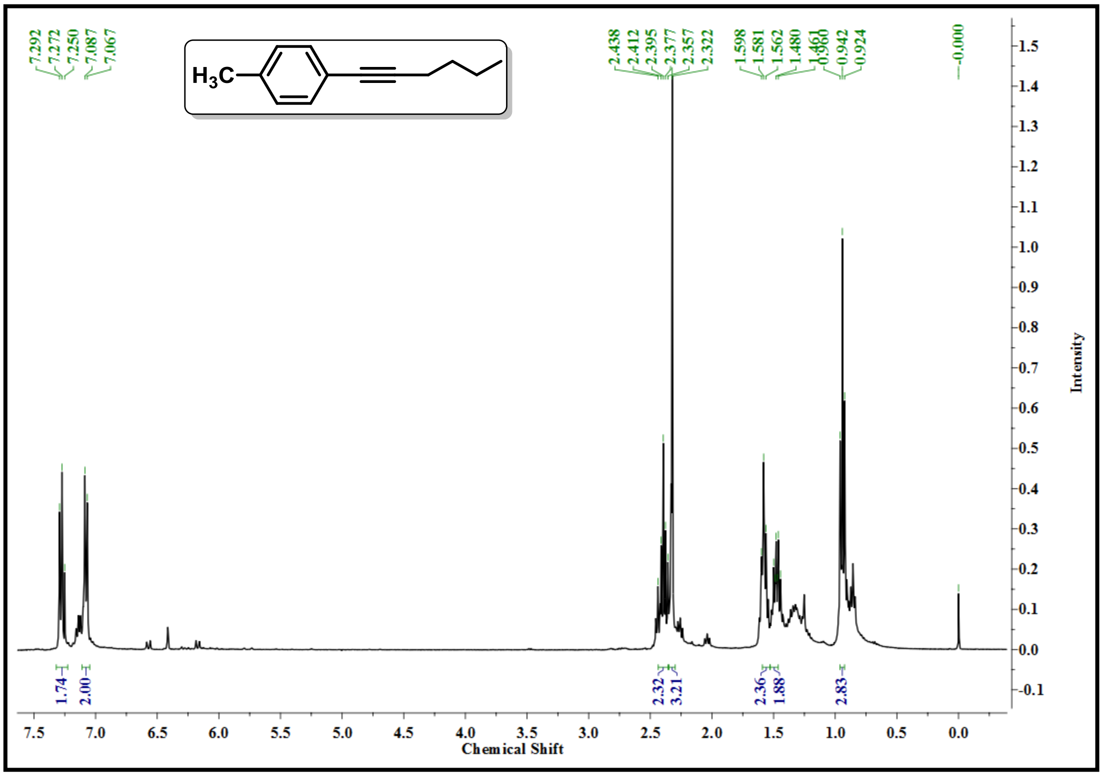

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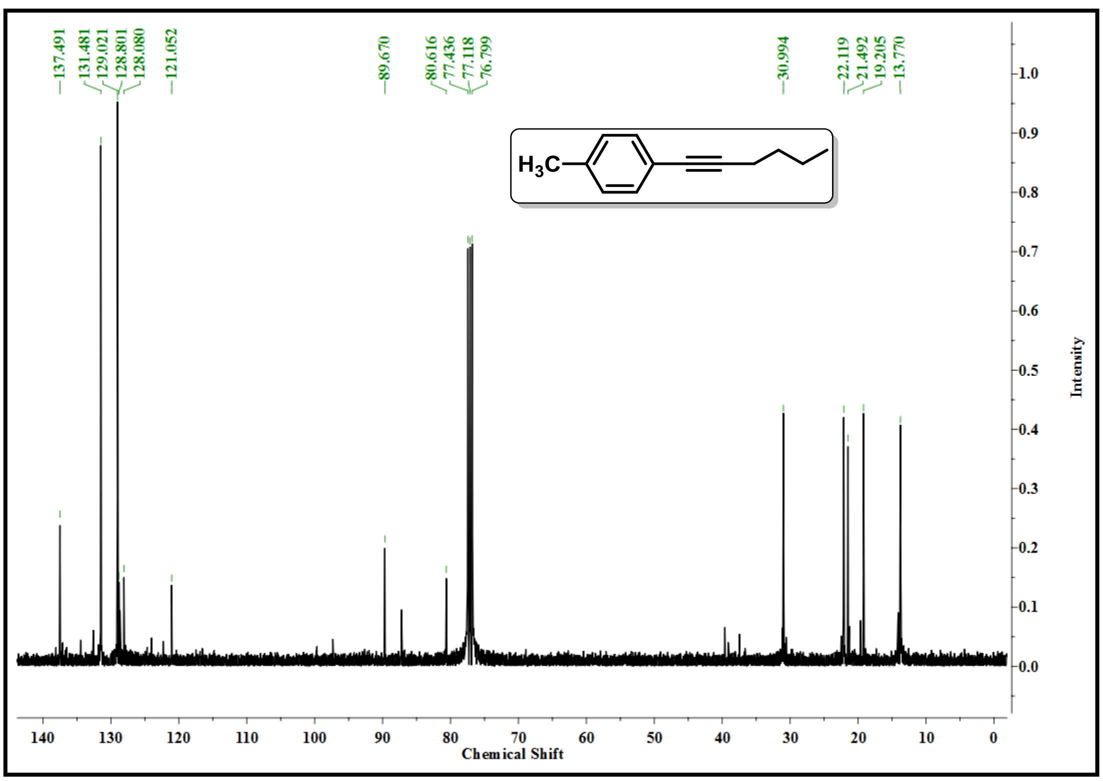

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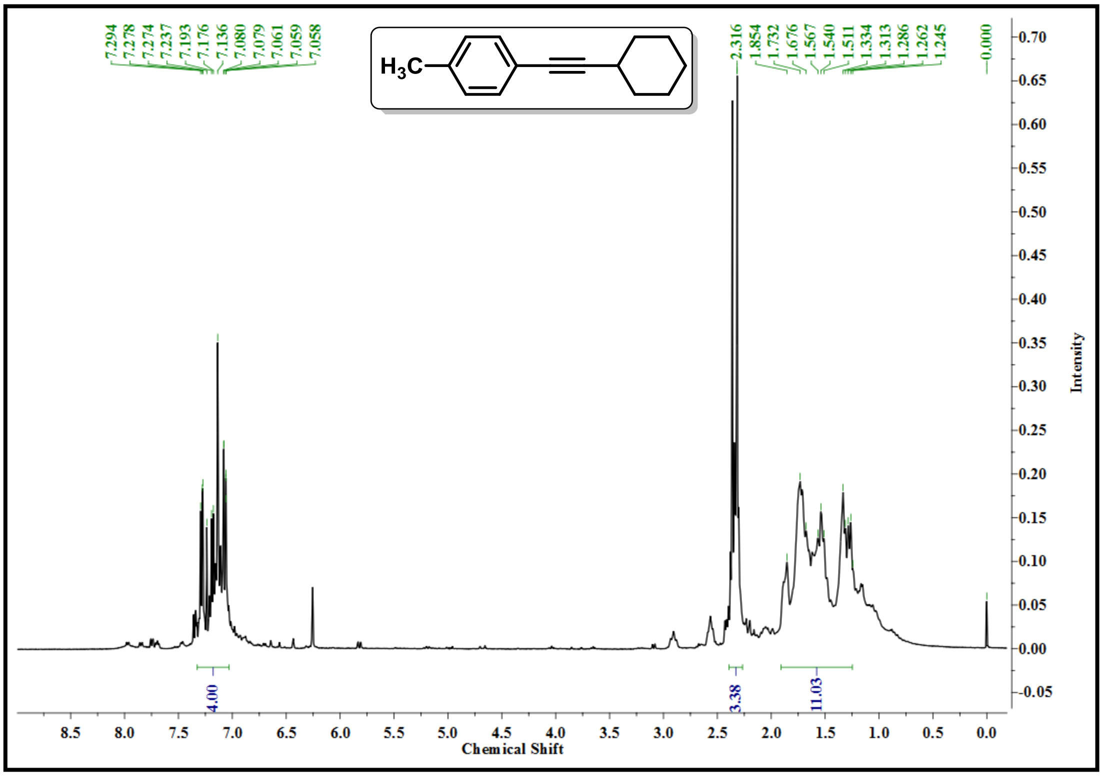
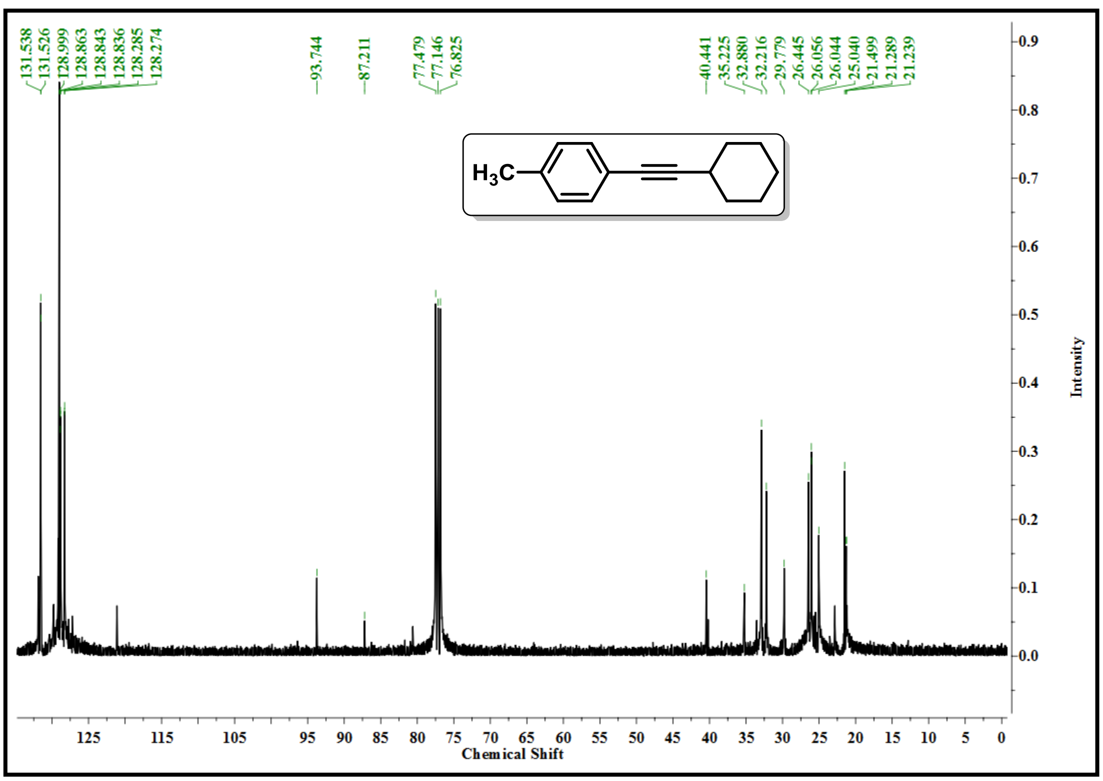


Figure S45 (^{1}H NMR of 6g)



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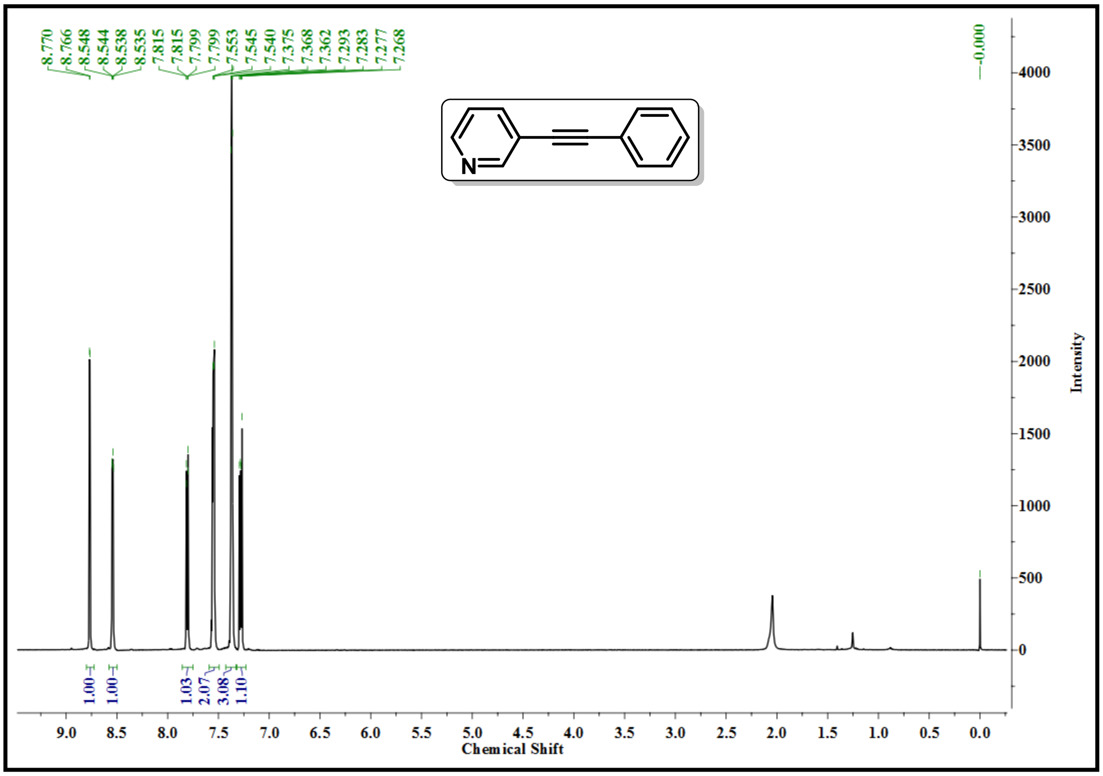

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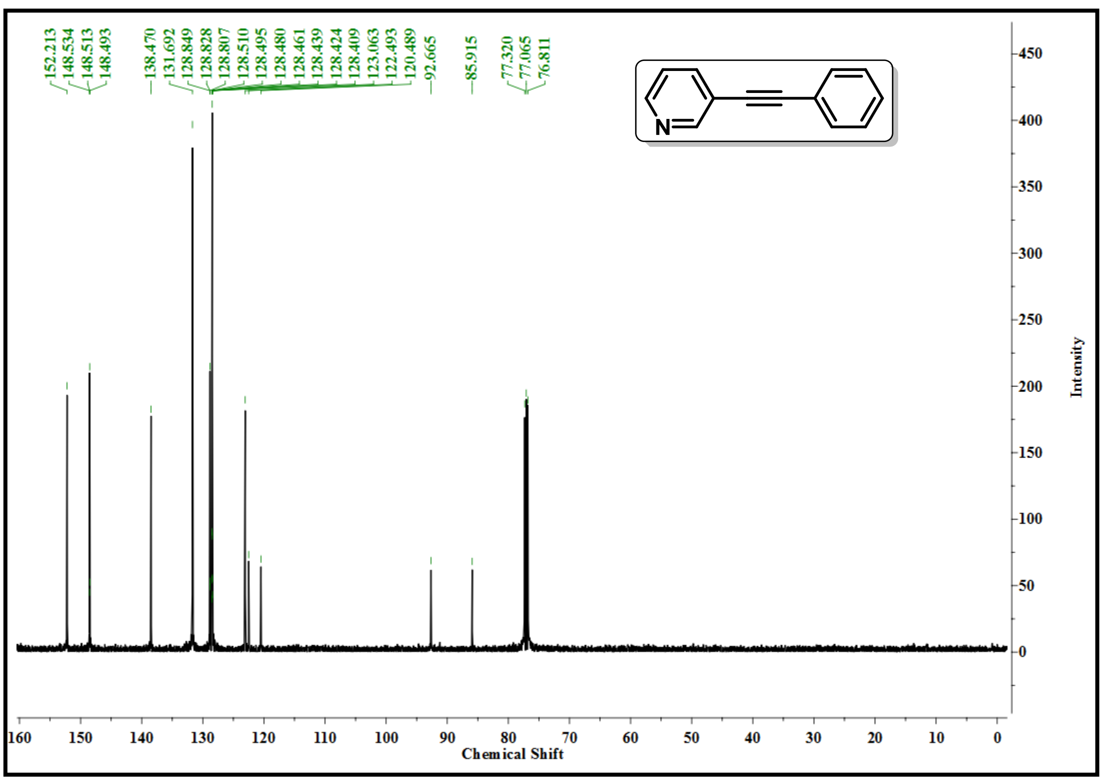

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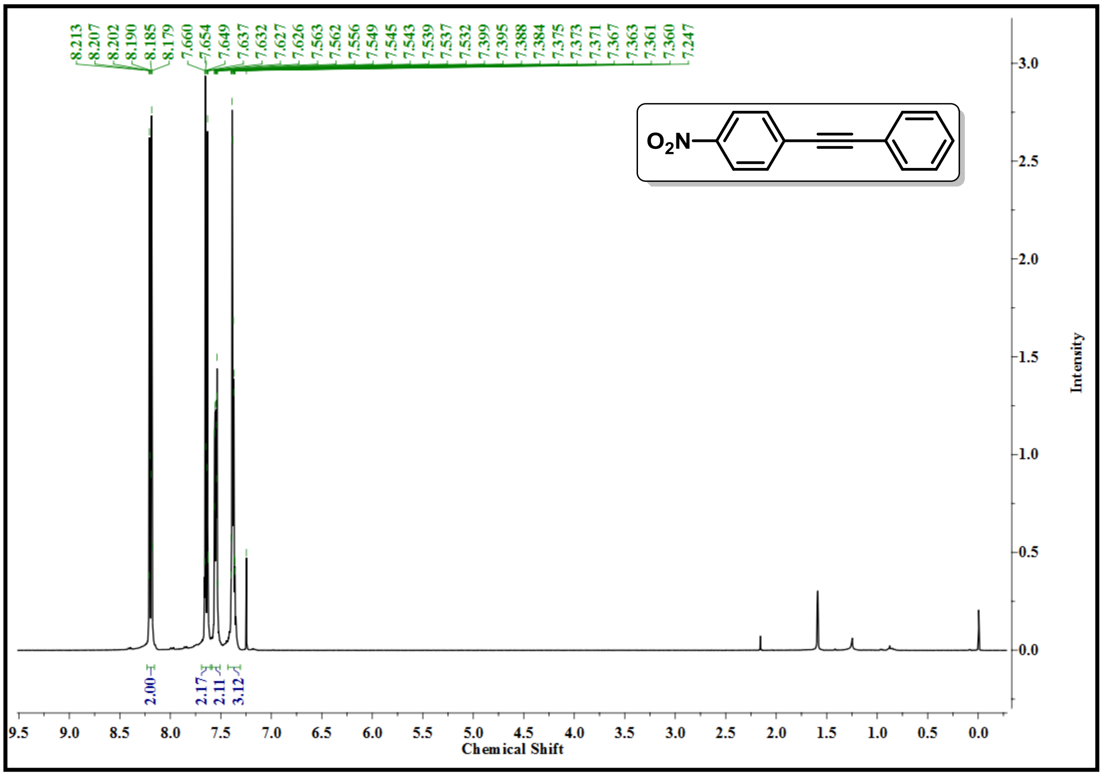
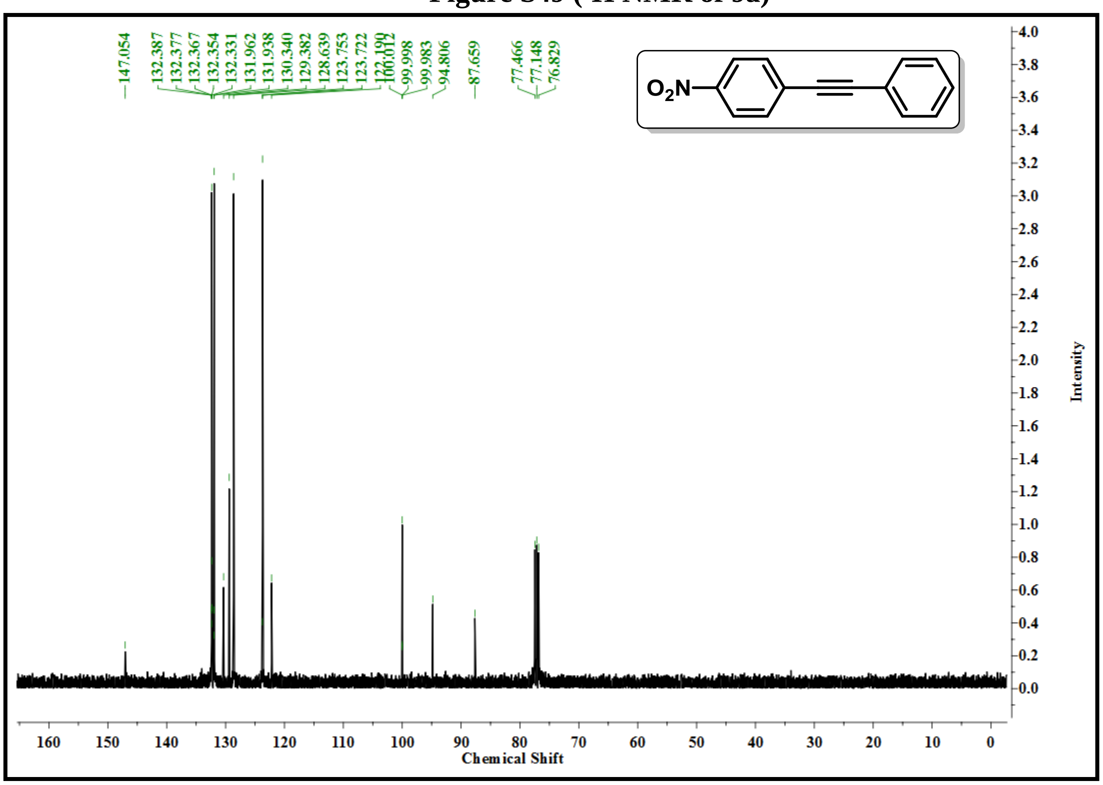


Figure S49 (^{1}H NMR of 9a)



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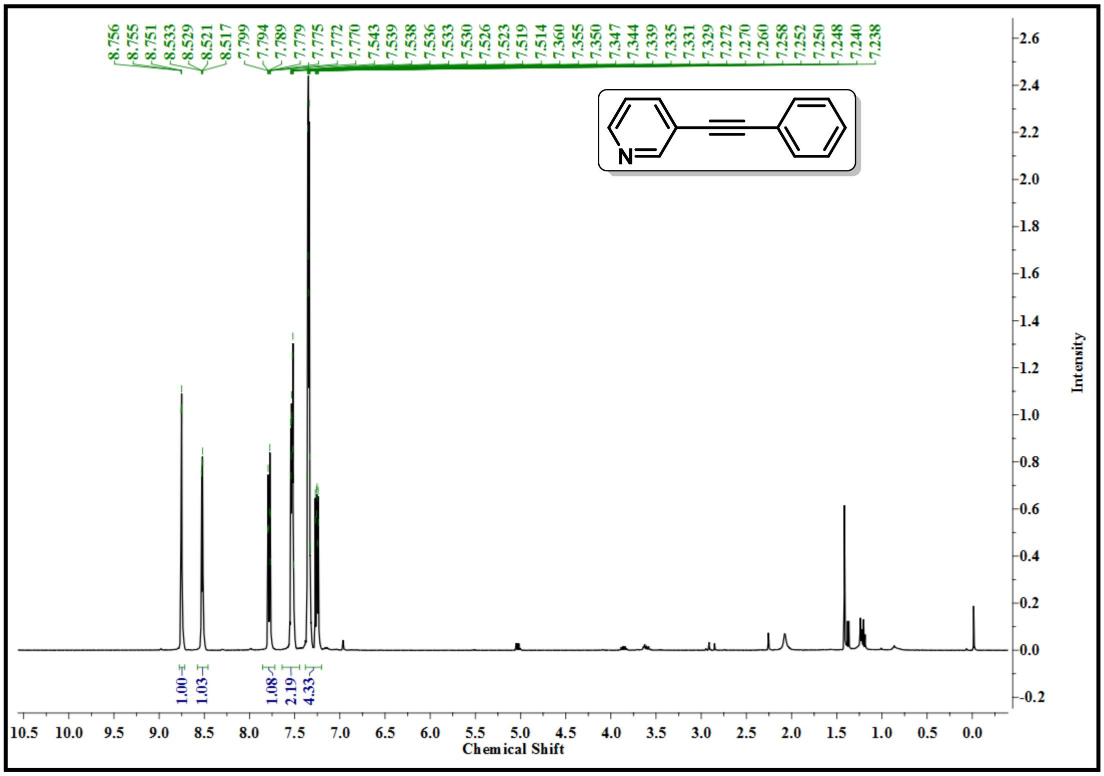

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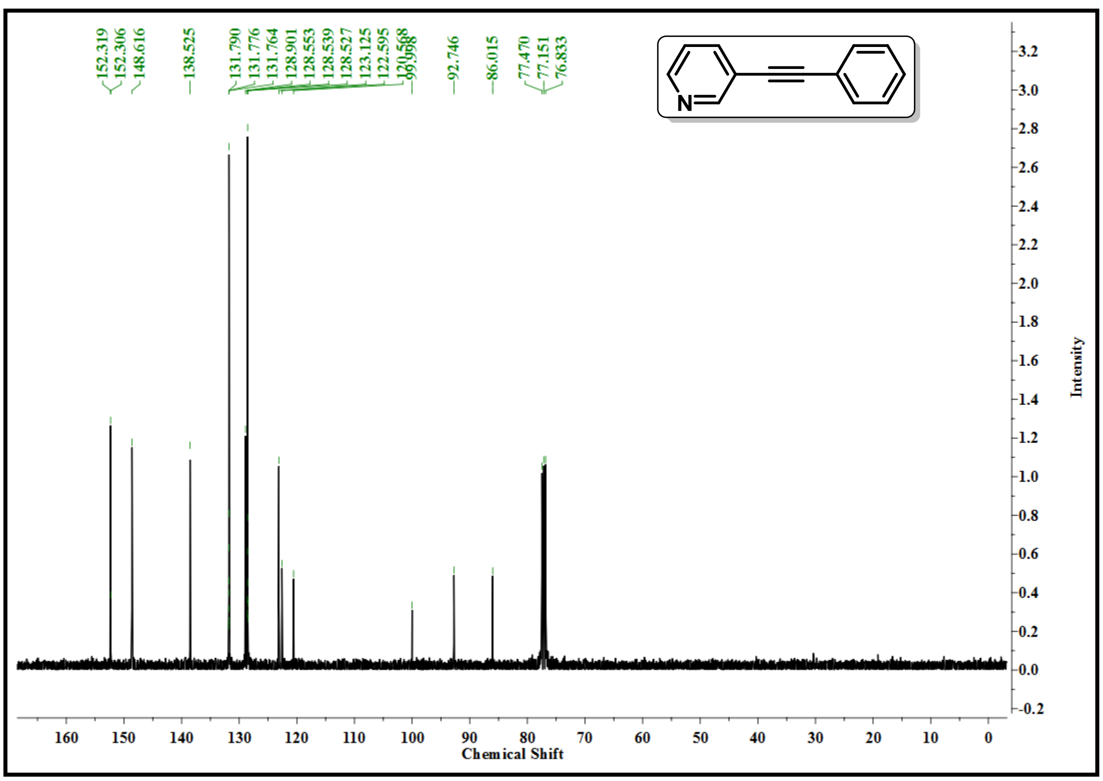

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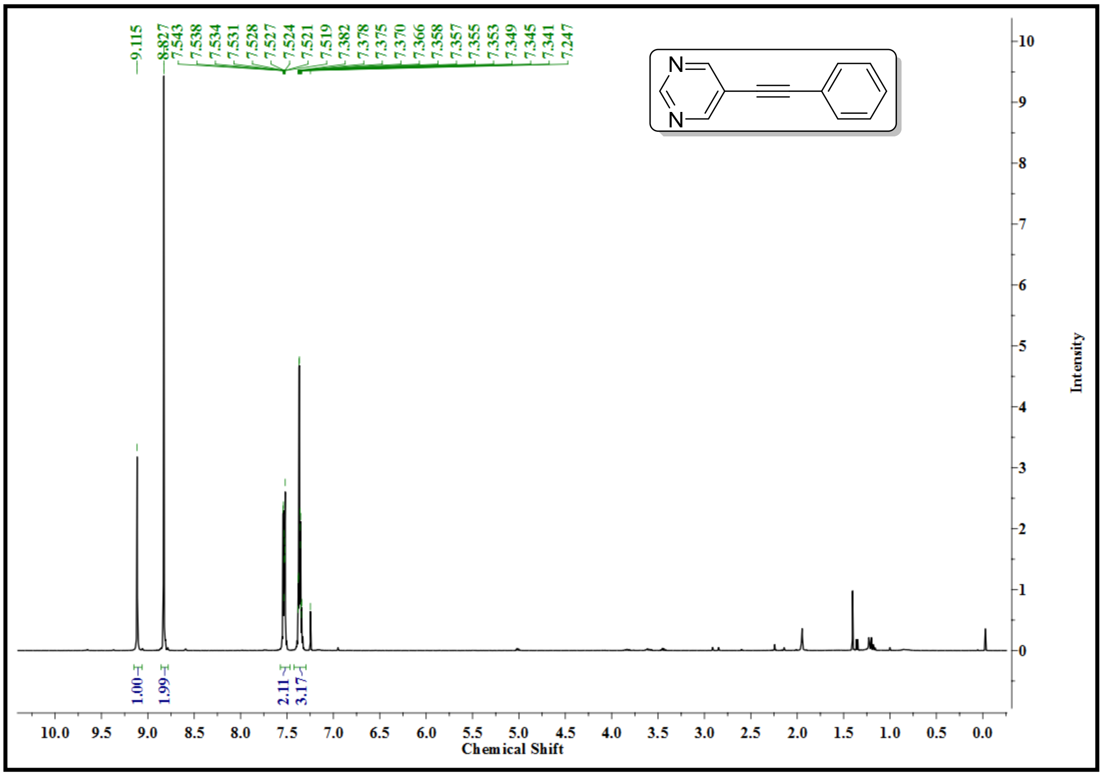

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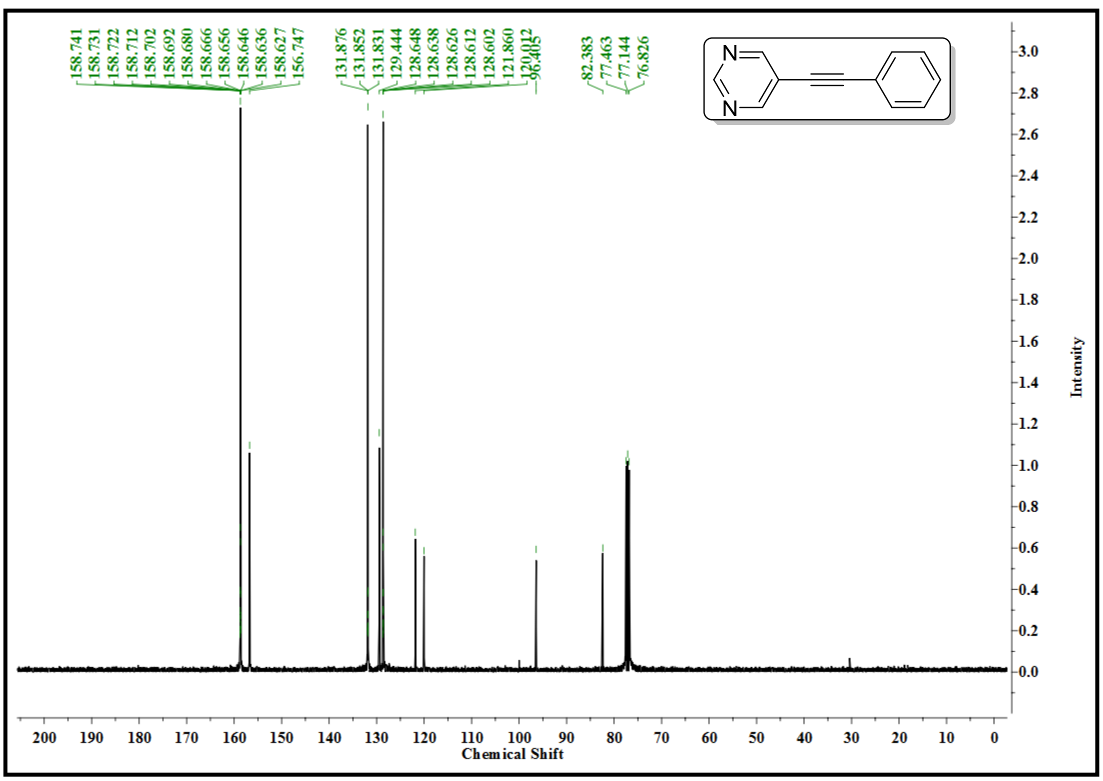

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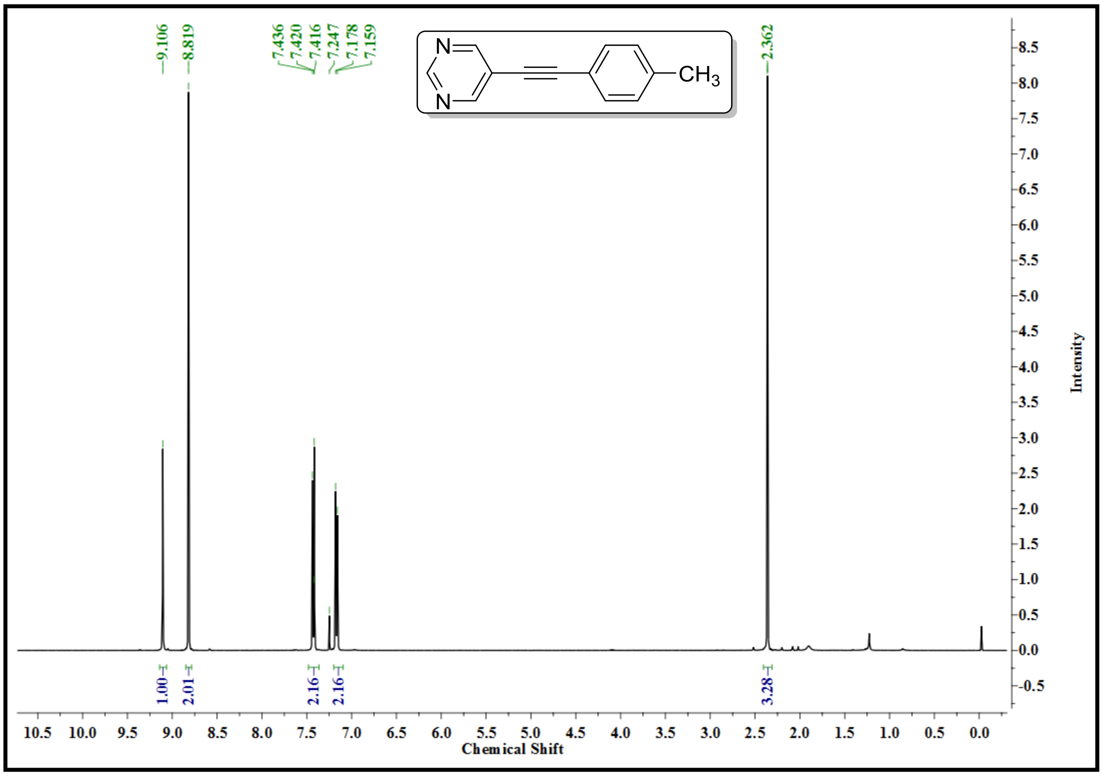

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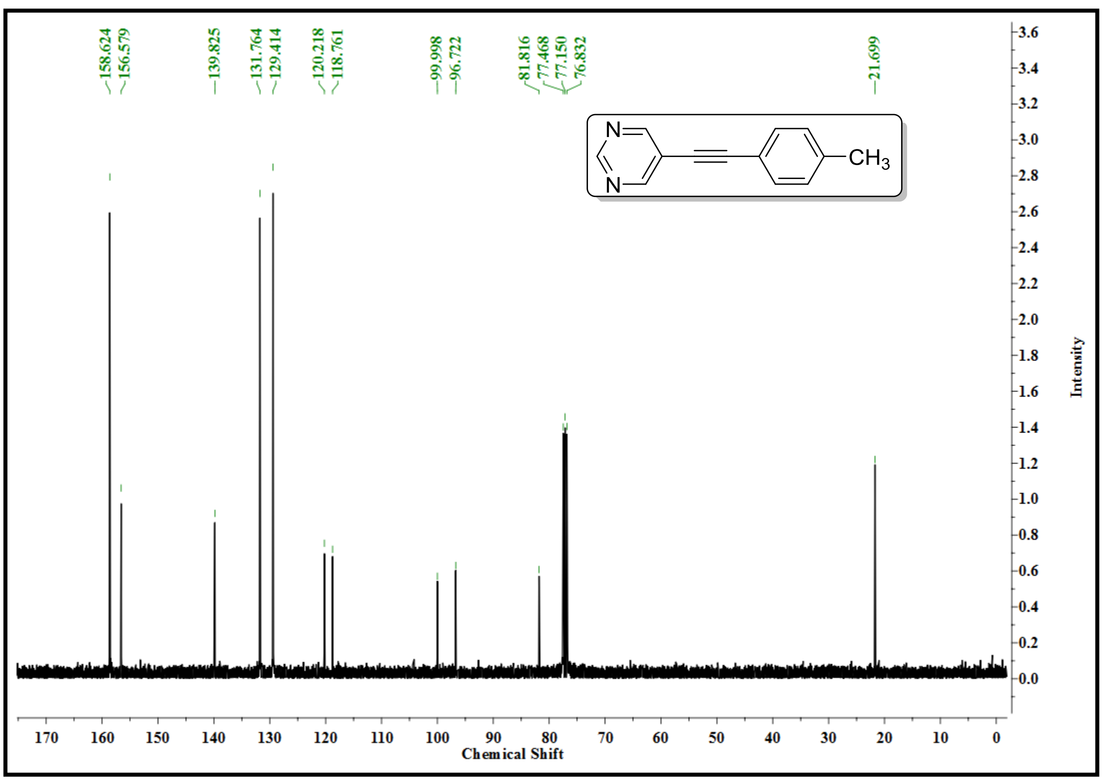

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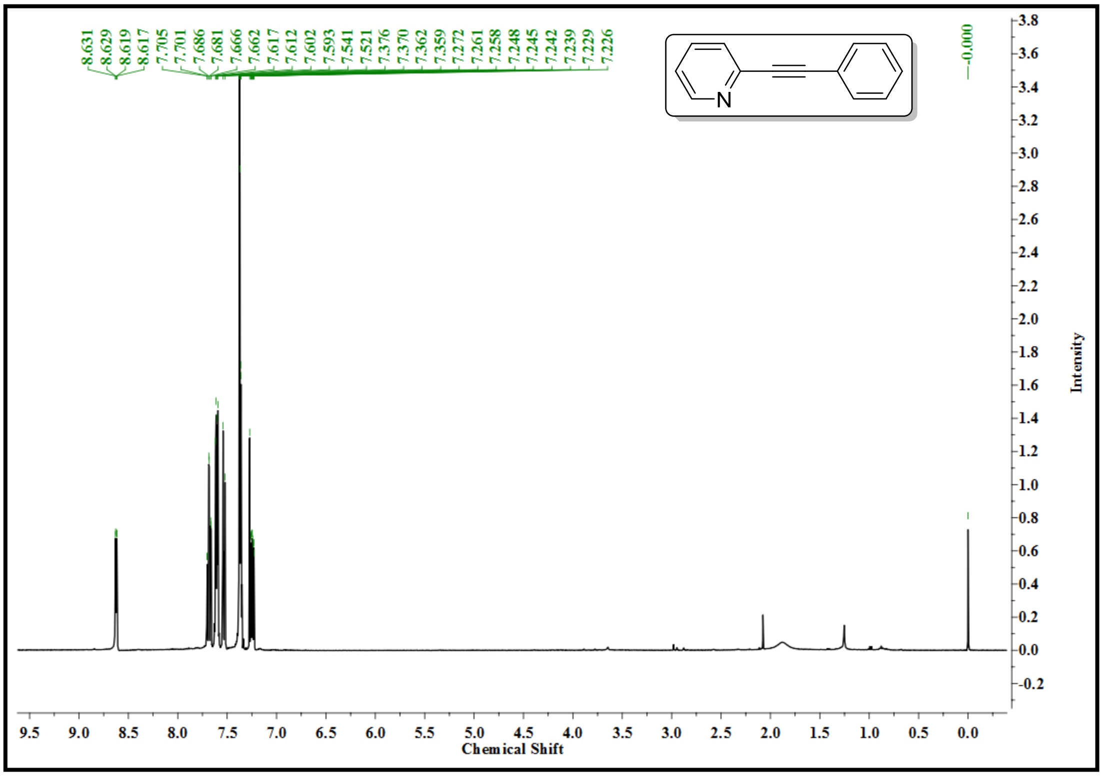

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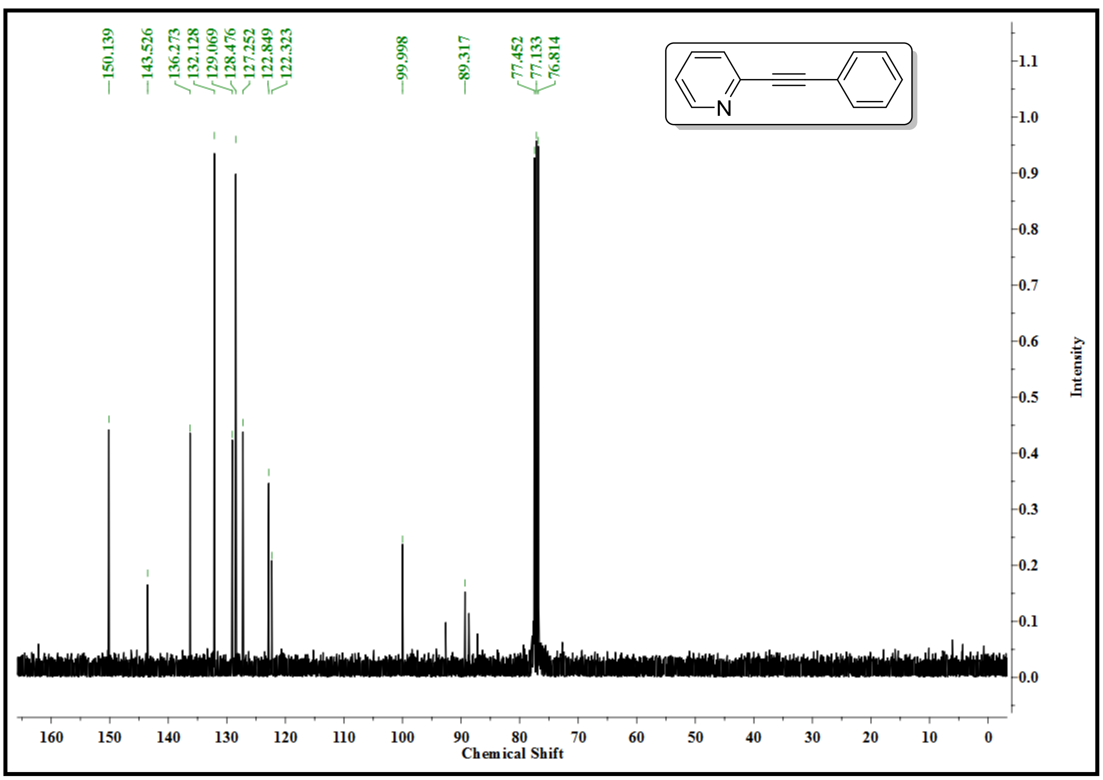

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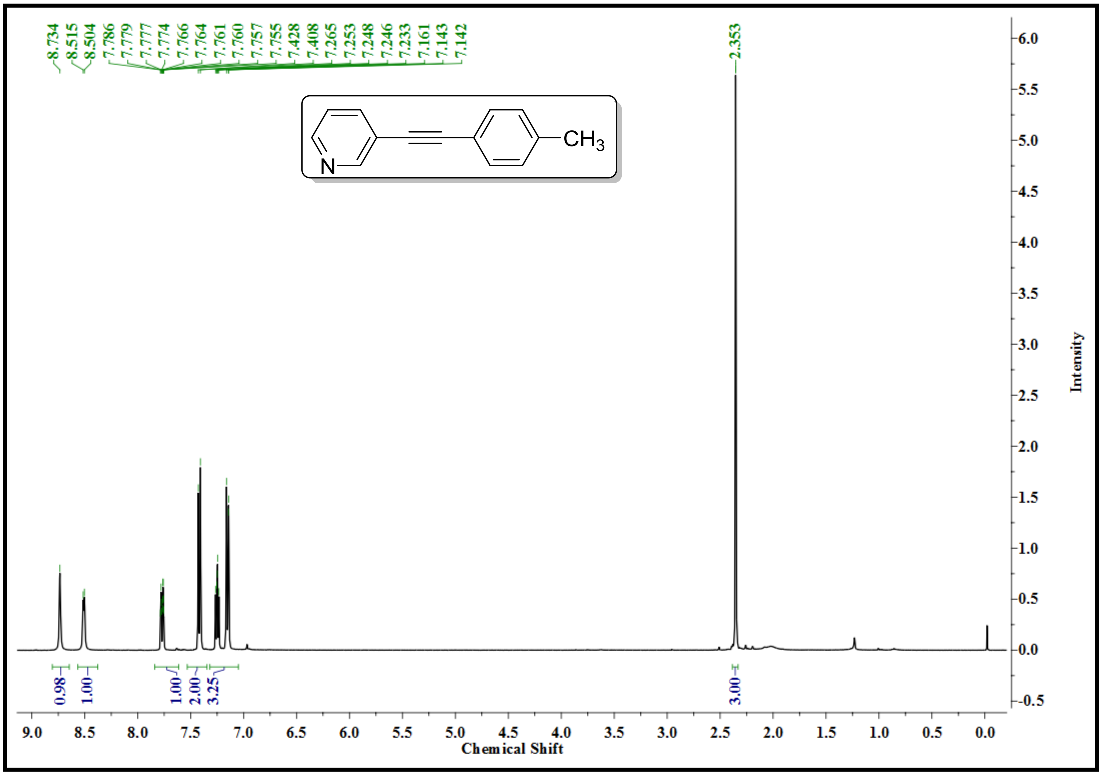

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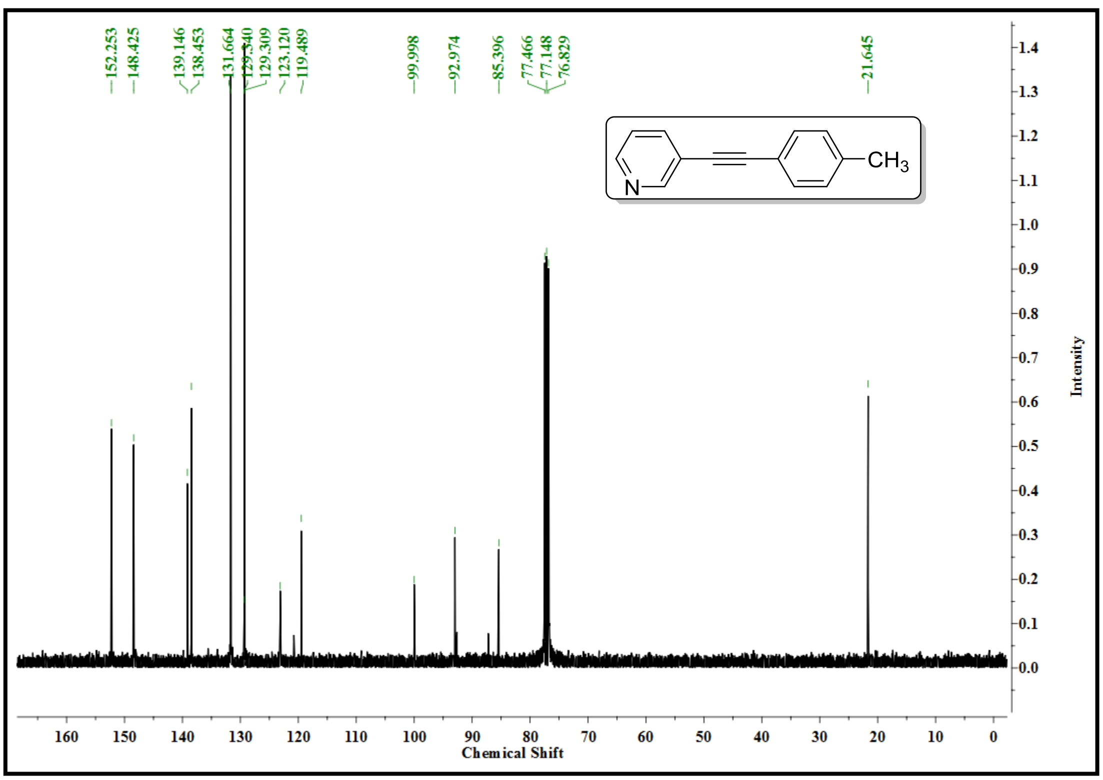

Figure S60 (^{13}C NMR of 9g)