

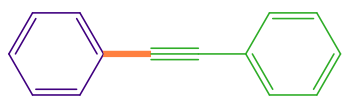
Supplementary Materials

A novel, efficient and magnetically recyclable Cu-Ni bimetallic alloy Nanoparticle as a highly active bifunctional catalyst for Pd-free Sonogashira and C–N cross-coupling reactions: A combined theoretical and experimental study

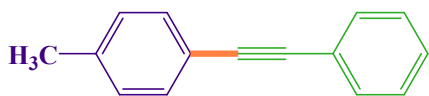
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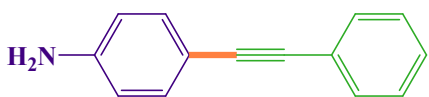
¹H NMR and ¹³C NMR characterization data of the sonogashira products:



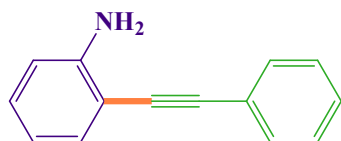
Colorless solid. ¹H-NMR (300 MHz, CDCl₃) δ: 7.21-7.26 (m, 6H), 7.49-7.51 (m, 4H) ppm; ¹³C-NMR (75 MHz, CDCl₃) δ: 89.6, 123.1, 128.4, 129.4, 131.5 ppm.



White solid. ¹H-NMR (300 MHz, CDCl₃) δ: 2.21 (s, 3H), 7.15 (d, 2H, *J* = 8.4 Hz), 7.17-7.40 (m, 7H) ppm; ¹³C-NMR (75 MHz, CDCl₃) δ: 21.6, 88.6, 89.5, 120.1, 123.4, 128.2, 128.1, 129.3, 131.4, 131.6, 138.5 ppm.



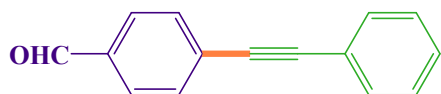
Yellow oil. ¹H-NMR (300 MHz, CDCl₃) δ: 3.61 (s, 2H), 6.53 (s, 2H), 7.24-7.42 (m, 7H) ppm; ¹³C-NMR (75 MHz, CDCl₃) δ: 87.1, 90.3, 112.4, 114.6, 123.8, 127.6, 128.2, 131.2, 132.7, 146.8 ppm.



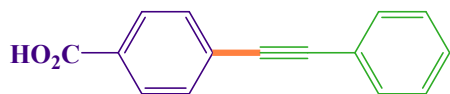
Yellowish-brown solid. ^1H NMR (300 MHz, CDCl_3) δ : 7.51-7.65 (m, 2H), 7.20-7.46 (m, 4H), 7.10-7.21 (m, 1H), 6.74-6.89 (m, 2H), 5.00 (br. s., 2H) ppm; ^{13}C NMR (75 MHz, CDCl_3) δ : 145.5, 131.8, 131.3, 129.5, 128.1, 127.7, 122.9, 118.7, 115.0, 108.7, 94.9, 85.3 ppm.



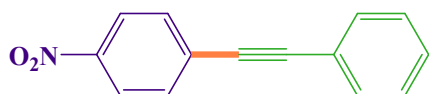
Yellow pale oil. ^1H NMR (300 MHz, CDCl_3) δ : 3.76 (s, 2H), 7.35-7.45 (m, 6H), 7.49-7.52 (m, 4H) ppm; ^{13}C NMR (75 MHz, CDCl_3) δ : 74.1, 81.6, 121.7, 128.6, 128.7, 129.2, 132.5 ppm.



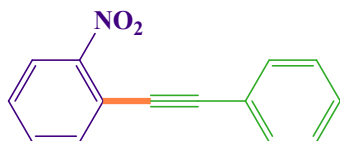
Brown oil. ^1H NMR (300 MHz, CDCl_3) δ : 7.30-7.36 (m, 7H), 7.52-7.59 (m, 1H), 7.80-7.89 (m, 1H), 10.58 (s, 1H) ppm; ^{13}C NMR (75 MHz, CDCl_3) δ : 126.5, 127.5, 128.0, 129.6, 129.8, 129.9, 130.8, 133.5, 135.1, 135.6, 190.0 ppm.



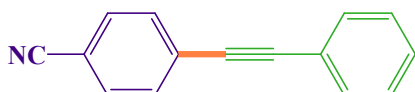
Brown solid. ^1H NMR (300 MHz, $\text{DMSO}-d_6$) δ : 7.50-7.53 (m, 3H), 7.73-8.01 (m, 6H), 12.89 (s, 1H) ppm; ^{13}C NMR (75 MHz, $\text{DMSO}-d_6$) δ : 127.2, 127.6, 129.1, 129.5, 130.0, 130.6, 140.2, 145.3, 167.8 ppm.



White solid. ^1H -NMR (300 MHz, CDCl_3) δ : 7.37-7.41 (m, 3H), 7.53-7.57 (m, 2H), 7.67 (d, 2H, $J=12.5$ Hz), 8.21 (d, 2H, $J=7.5$ Hz) ppm; ^{13}C -NMR (75 MHz, CDCl_3) δ : 87.4, 94.6, 122.0, 123.5, 128.6, 129.1, 130.2, 131.7, 132.2, 146.8 ppm.

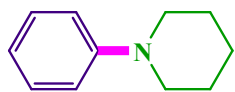


Orange oil. ¹H NMR (300 MHz, CDCl₃) δ: 7.39-7.45 (m, 5H), 7.60-7.62 (m, 4H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ: 74.1, 82.3, 121.5, 128.4, 129.4, 132.8 ppm.

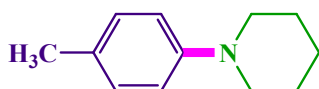


Pale yellow solid. ¹H-NMR (300 MHz, CDCl₃) δ: 7.26-7.29 (m, 3H), 7.43-7.53 (m, 6H) ppm; ¹³C-NMR (75 MHz, CDCl₃) δ: 87.6, 93.7, 111.3, 118.5, 122.1, 128.2, 128.6, 129.1, 131.8, 132.03, 132.07 ppm.

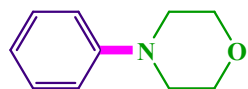
¹H NMR and ¹³C NMR spectral data for C-N coupling products:



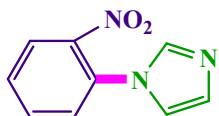
Yellow oil. ¹H NMR (300 MHz, CDCl₃) δ: 7.12-7.20 (m, 2H), 6.89 (d, 2H, *J* = 8.3 Hz), 6.80 (tt, 1H, *J* = 7.5, 1.4 Hz), 3.05-3.14 (m, 4H), 1.60-1.75 (m, 4H), 1.49-1.60 (m, 2H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ: 152.0, 129.2, 119.6, 116.7, 50.5, 25.7, 24.2 ppm.



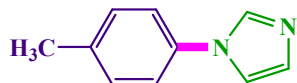
Yellow oil. ¹H NMR (300 MHz, CDCl₃) δ: 6.92-7.01 (m, 2H), 6.74-6.90 (m, 2H), 2.89-3.13 (m, 4H), 2.30 (s, 3H), 1.71 (tt, 4H, *J* = 7.4, 5.0 Hz), 1.48-1.55 (m, 2H) ppm; ¹³C NMR (75 MHz, CDCl₃) δ: 150.2, 129.7, 128.9, 116.6, 51.0, 25.7, 24.4, 20.6 ppm.



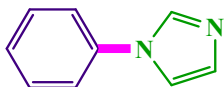
Purple solid. ¹H NMR (300 MHz, CDCl₃) δ: 7.21-7.36 (m, 2H), 6.78-6.89 (m, 3H), 3.79 (t, 4H, *J* = 4.9 Hz), 3.18 (t, 4H, *J* = 4.9 Hz) ppm; ¹³C NMR (75 MHz, CDCl₃) δ: 152.3, 129.5, 120.4, 116.7, 67.3, 50.2 ppm.



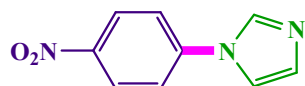
Pale yellow solid. ^1H NMR (300 MHz, CDCl_3) δ : 8.11 (dd, 1H, J = 8.40 Hz, 1.55 Hz), 7.80 (dt, 1H, J = 7.65 Hz, 1.55 Hz), 7.69-7.74 (m, 2H), 7.45-7.51 (m, 1H), 7.19 (s, 1H), 7.09 (s, 1H) ppm; ^{13}C NMR (75 MHz, CDCl_3) δ : 145.5, 137.3, 133.8, 130.3, 130.8, 129.7, 128.9, 125.4, 120.8 ppm.



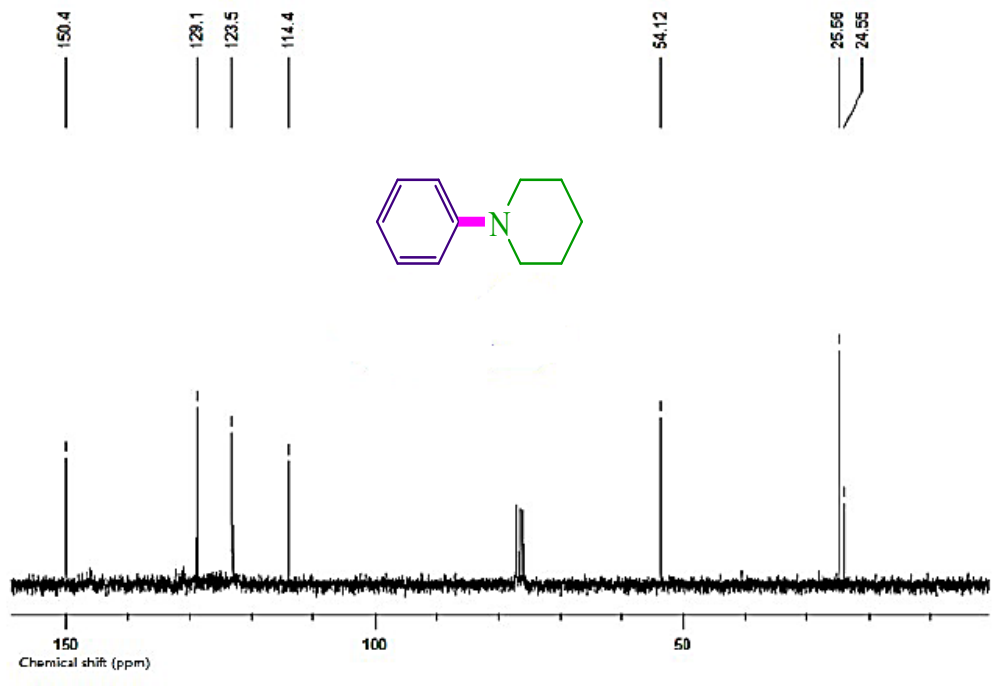
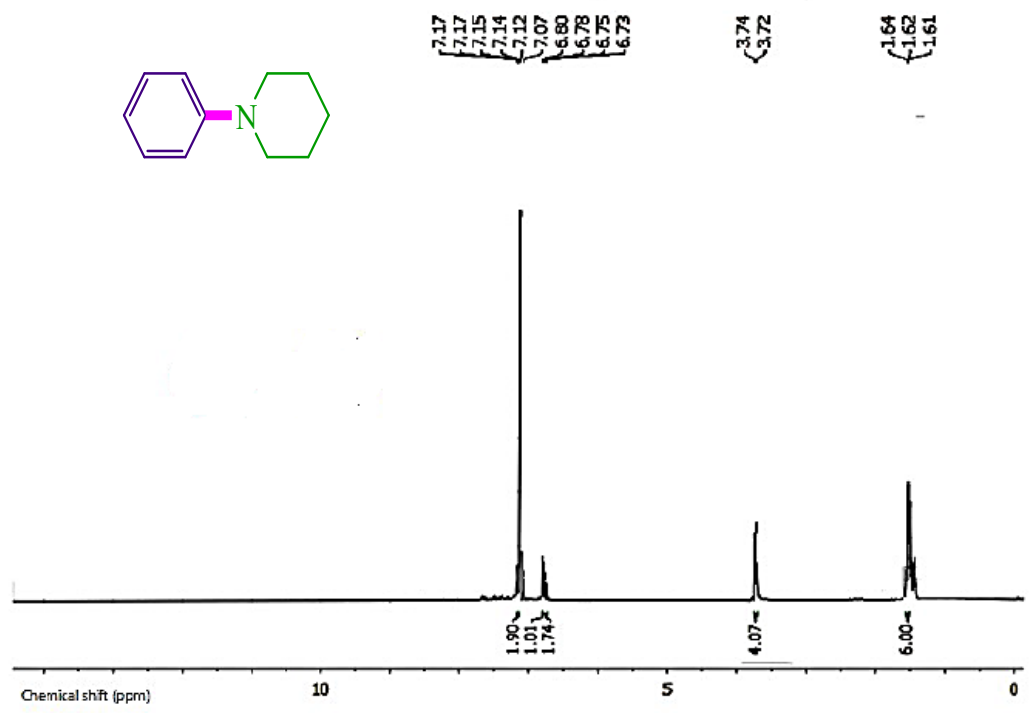
Yellow oil. ^1H NMR (300 MHz, CDCl_3) δ : 7.79 (s, 1H), 7.30 (s, 4H), 7.26 (s, 1H), 7.21 (s, 1H), 2.38 (s, 3H) ppm; ^{13}C NMR (75 MHz, CDCl_3) δ : 137.5, 135.6, 135, 130.2, 130.0, 121.6, 118.8, 21.2 ppm.

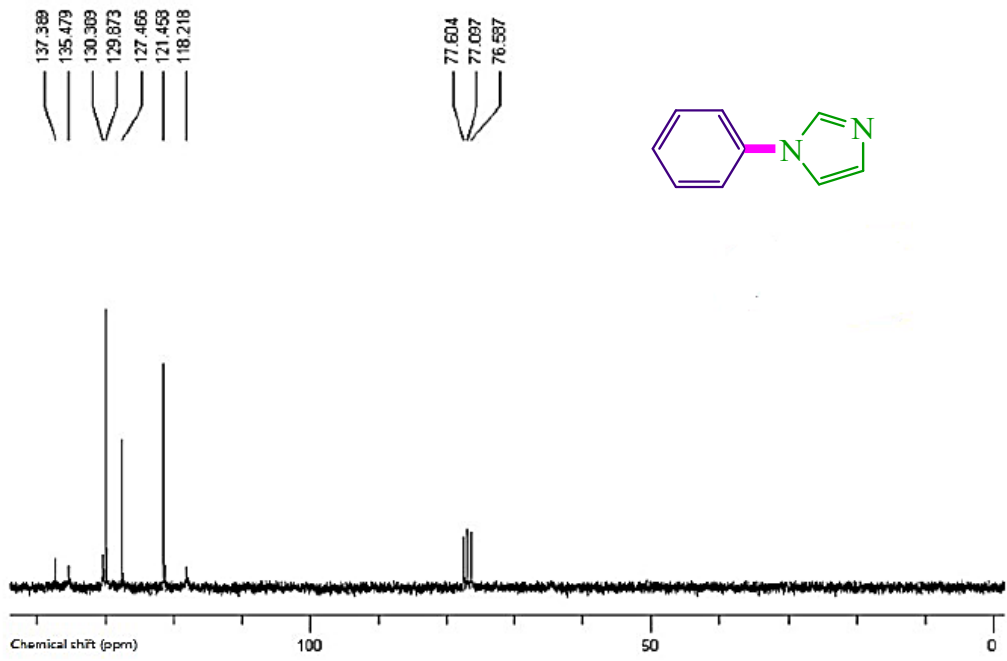
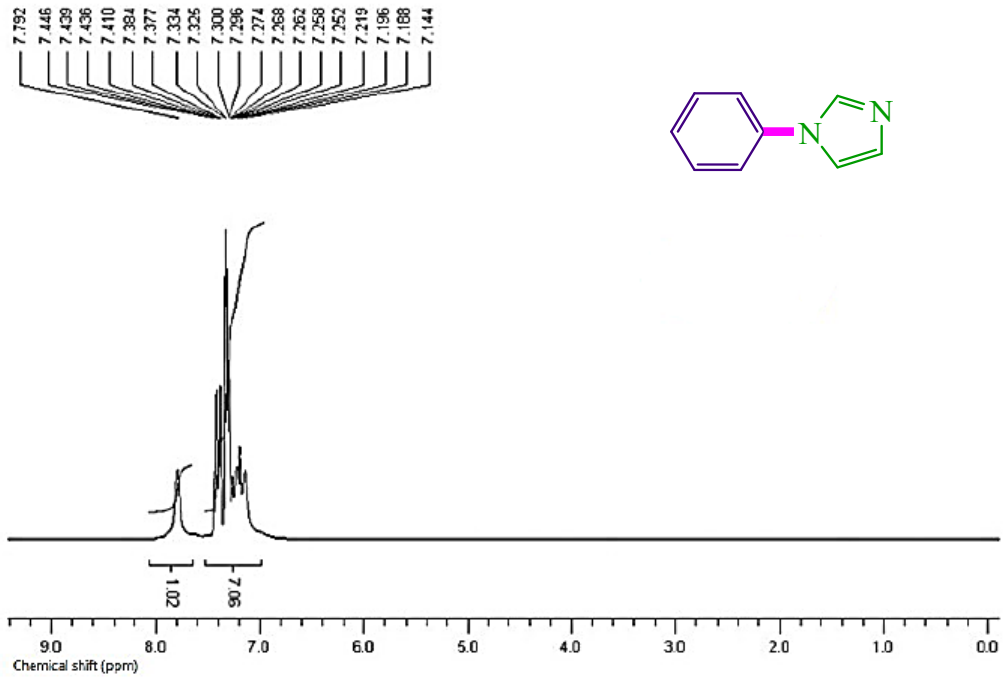


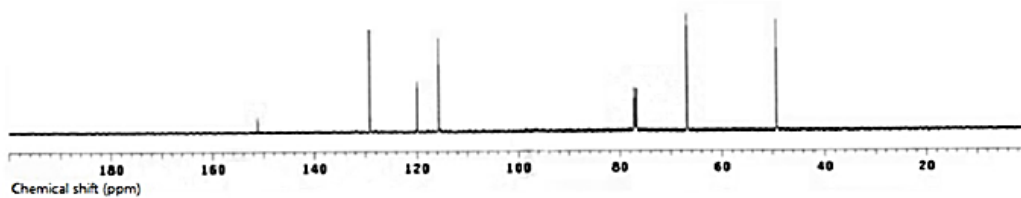
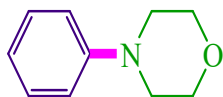
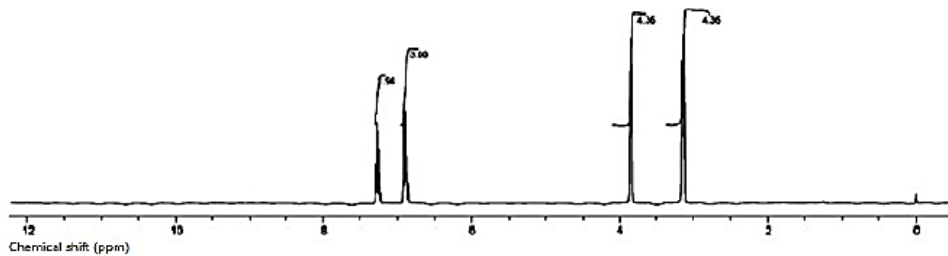
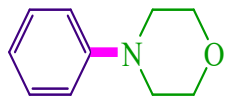
Yellow oil. ^1H NMR (300 MHz, CDCl_3) δ : 7.88 (s, 1H), 7.40-7.50 (m, 2H), 7.28-7.41 (m, 3H), 7.25 (s, 1H), 7.21 (s, 1H) ppm; ^{13}C NMR (75 MHz, CDCl_3) δ : 137.1, 135.3, 130.8, 29.7, 127.5, 121.3, 118.1 ppm.

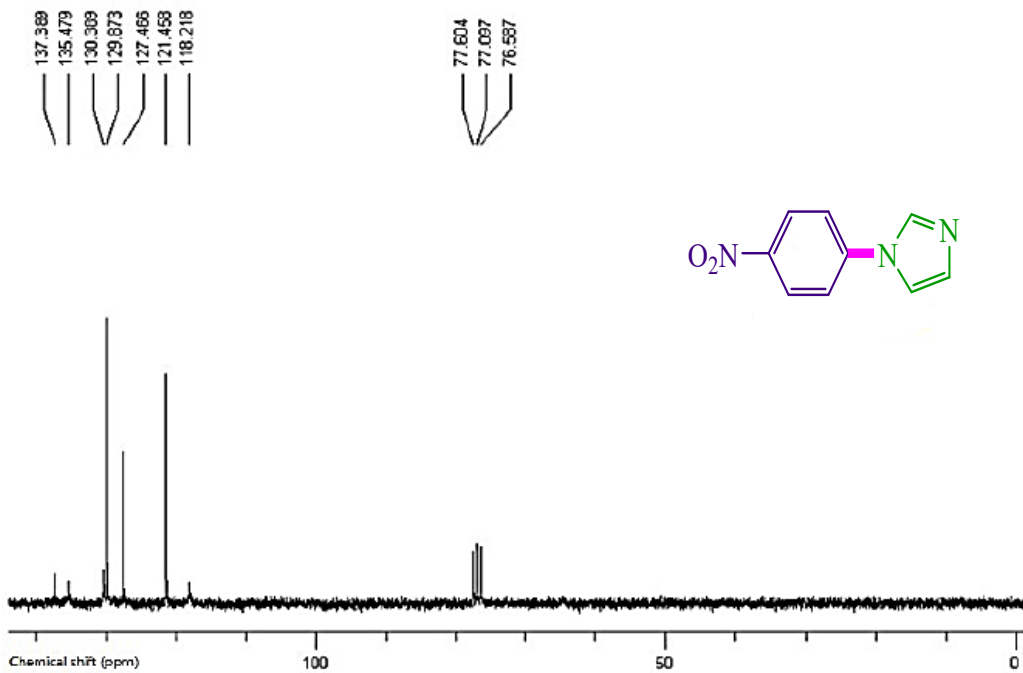
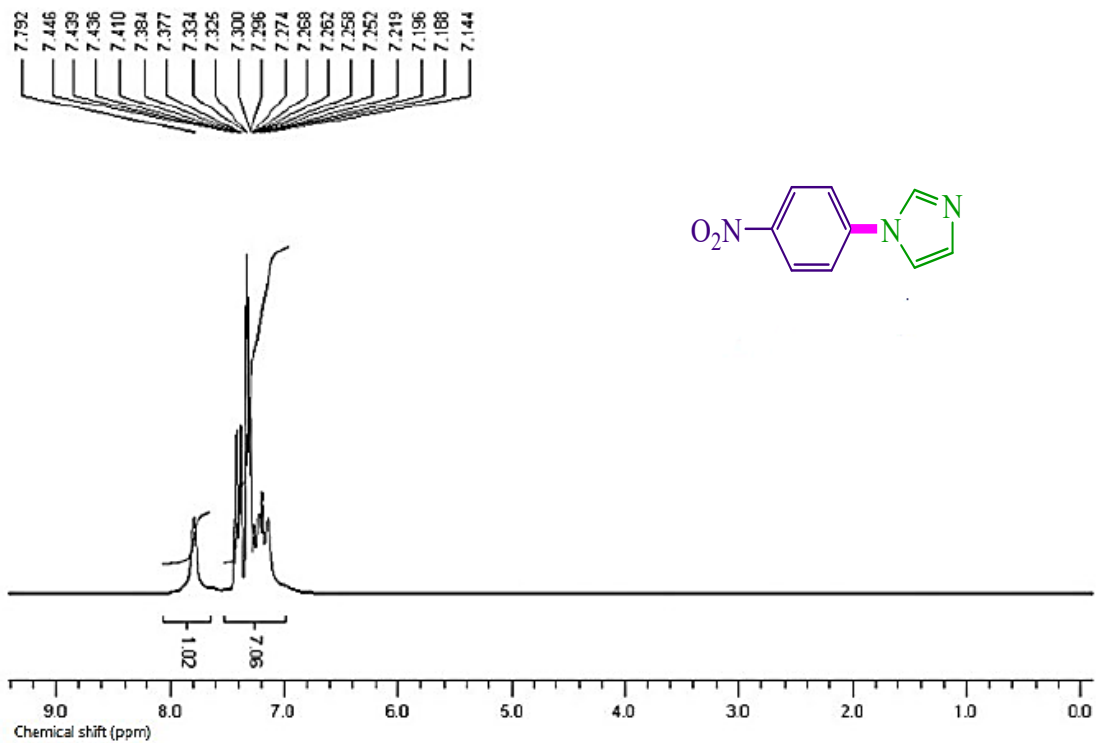


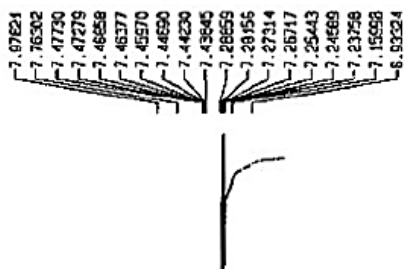
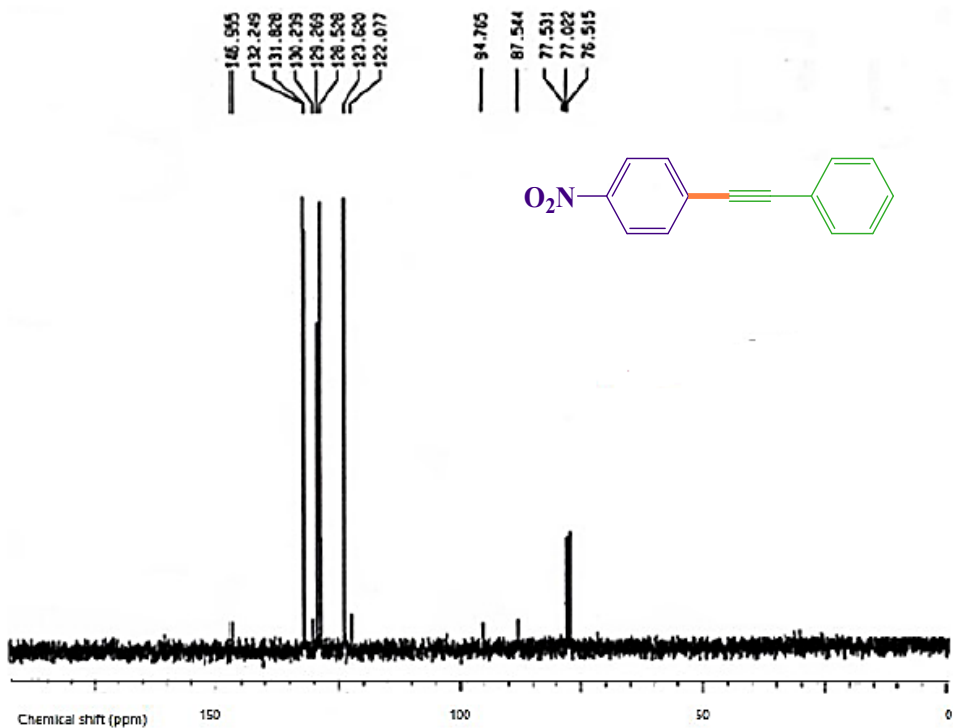
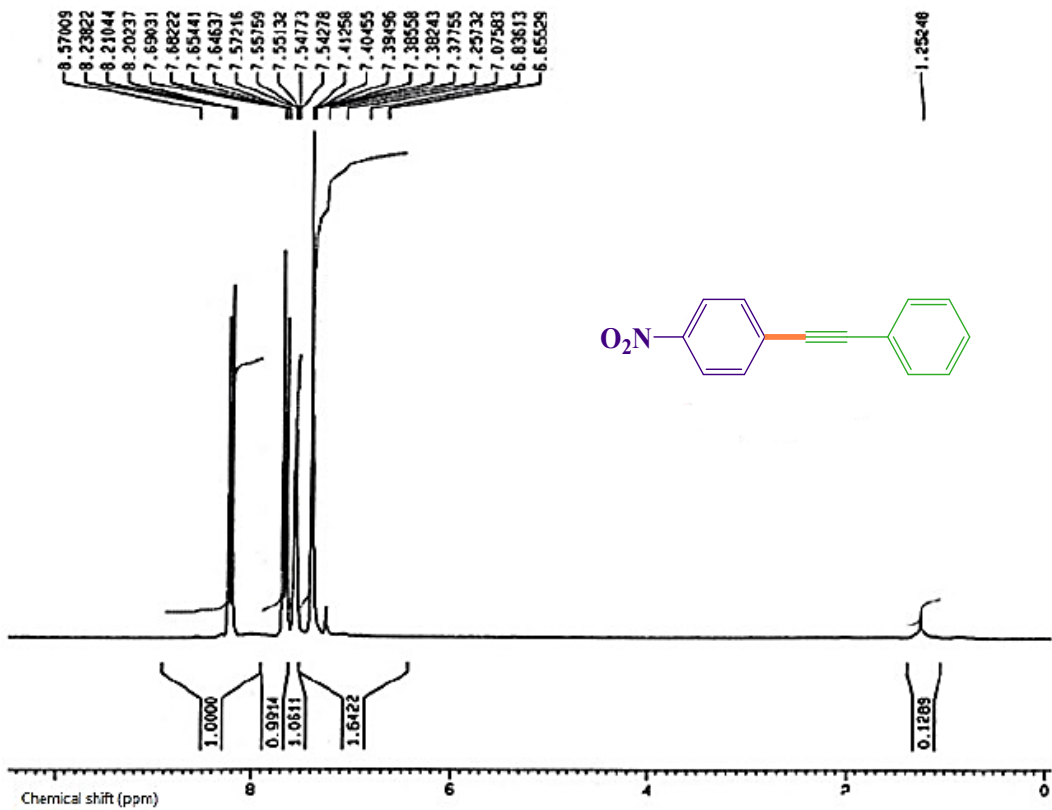
Pale yellow solid. ^1H NMR (300 MHz, CDCl_3) δ : 8.41 (d, 2H, J = 9.19 Hz), 8.10 (s, 1H), 7.62 (d, 2H, J = 9.19 Hz), 7.39 (s, 1H), 7.32 (s, 1H) ppm; ^{13}C NMR (75 MHz, CDCl_3) δ : 146.2, 142.1, 135.7, 131.8, 125.8, 121.3, 117.6 ppm.

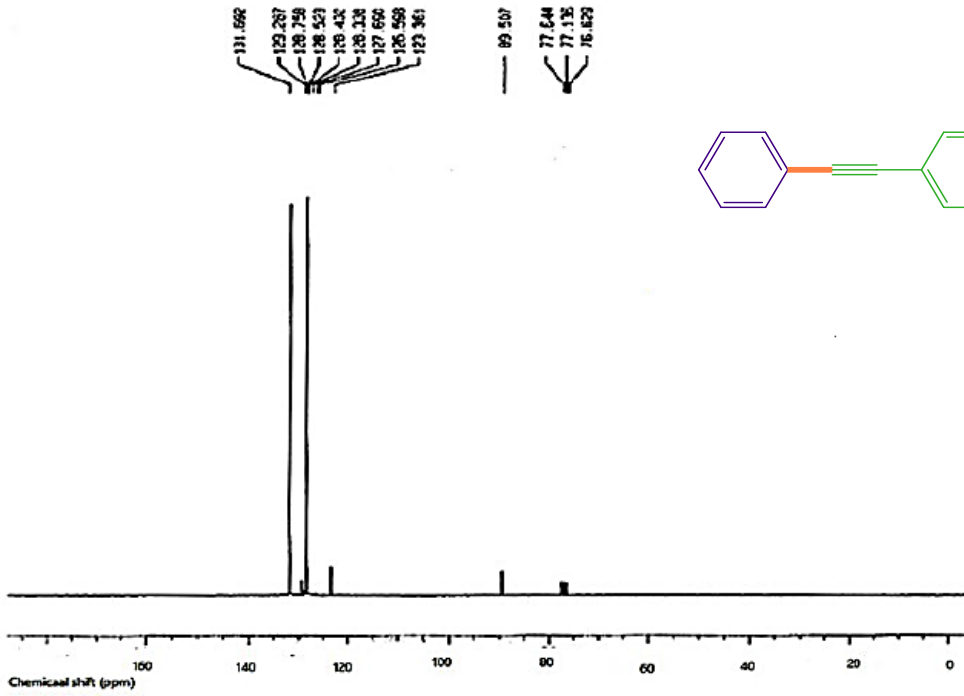
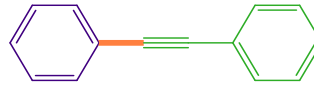


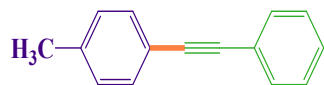












136.37
131.64
131.61
129.13
128.32
126.08
123.49
120.20

89.57
89.73

77.85
77.84
76.83

51.59

