Supporting information

Phosphinite-Functionalized Silica and Hexagonal Mesoporous Silica Containing Palladium Nanoparticles in Heck Coupling Reaction: Synthesis, Characterization, and Catalytic Activity

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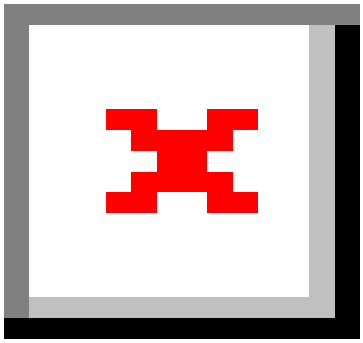
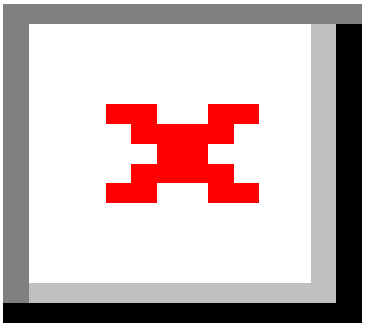
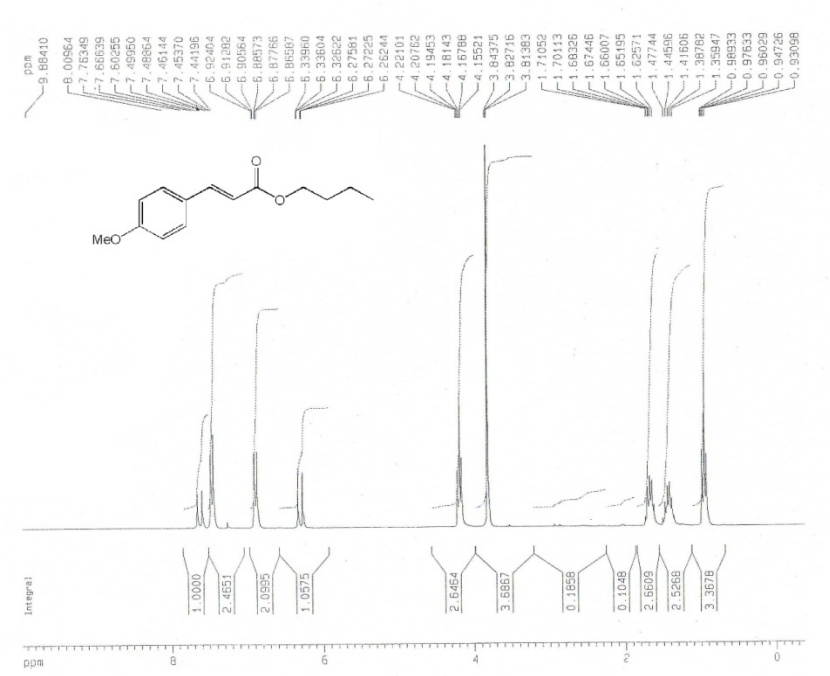
Representative ^{1}H-NMR, ^{13}C-NMR data and physical data.

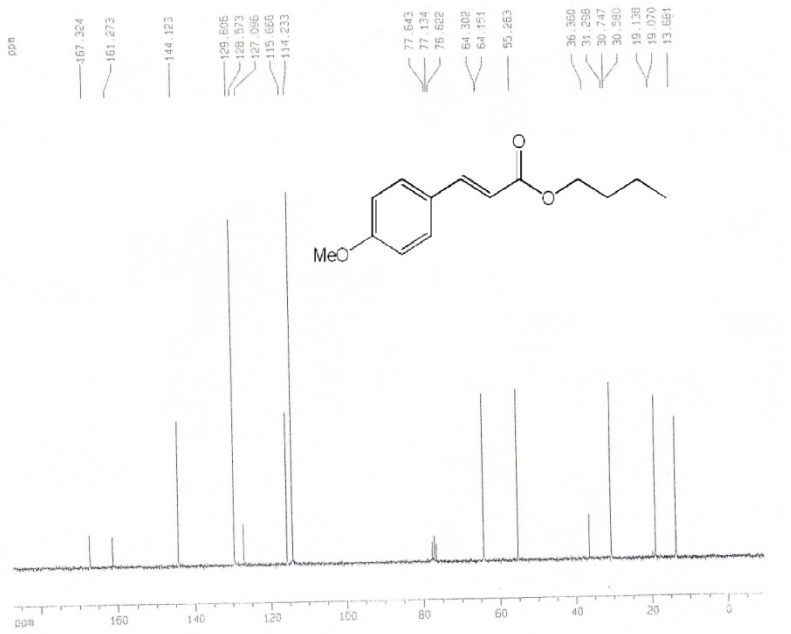
1) 3-phenyl acrylic acid butyl ester: ^{1}H-NMR (250 MHz, $CDCl_3$): δ 7.80 (d, 1H, J = 16 Hz), 7.41-7.62 (m, 2H), 7.17-7.29 (m, 3H), 6.32 (d, 1H, J = 16 Hz), 4.12 (t, 2H, J = 6.8 Hz), 1.54-1.69 (m, 2H, J = 7.3 Hz), 1.17-1.42 (m, 2H, J = 7.3 Hz), 0.87 (t, 3H, J = 7.3 Hz) ppm; ^{13}C-NMR (60 MHz, $CDCl_3$): δ 167.1, 144.5, 134.4, 130.2, 129.8, 128.1, 118.2, 64.3, 30.7, 19.1 13.7 ppm, Yellow solid m.p. 44-45 ºC [1-3].





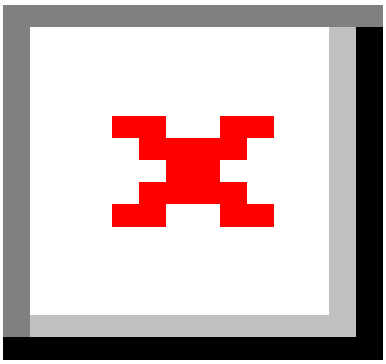
2) 3-(4-methoxy-phenyl)-acrylic acid butyl ester: ^{1}H-NMR (250 MHz, $CDCl_3$): δ 0.93-0.98 (t, J= 7.5 Hz, 3H), 1.38-1.47 (m, 2H), 1.62-1.71 (m, 2H), 3.82 (s, 3H), 4.21 (t, J= 6.7 Hz, 2H), 6.32 (d, J=16.0, 1H), 6.68-6.92 (m, 2H), 7.45-7.49 (m, 2H), 7.76 (d, J= 16.0, 1H) ppm; ^{13}C-NMR (60 MHz, $CDCl_3$): δ 167.3, 162.4, 144.1, 129.6, 127.0, 115.6, 114.2, 64.2, 55.2, 30.7, 19.1, 13.6 ppm [1-3].

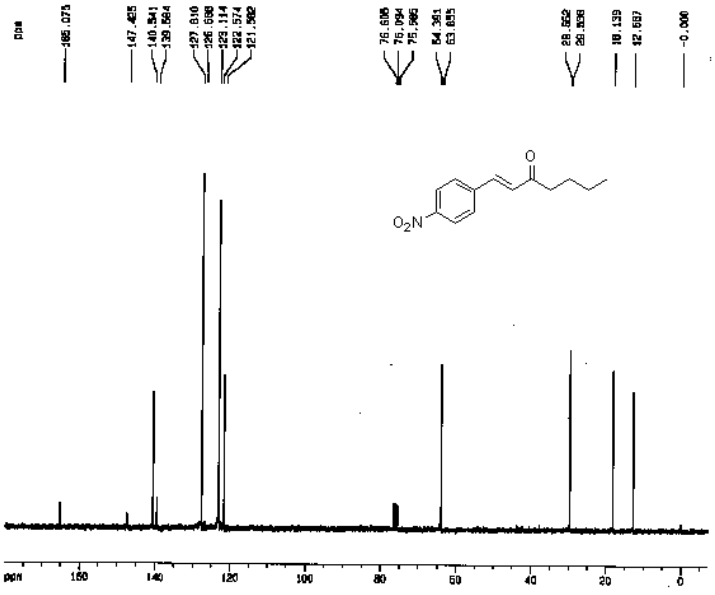




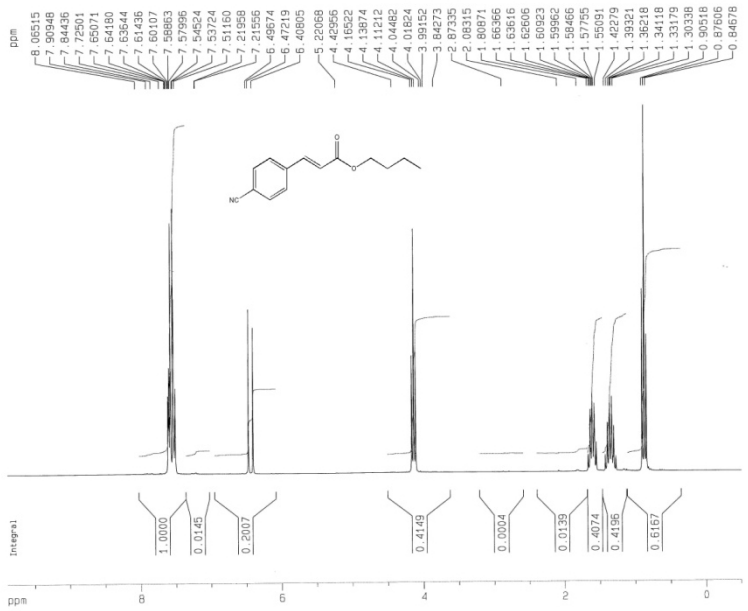
3) 3-(4-nitro-phenyl)-acrylic acid butyl ester: ^{1}H-NMR (250 MHz, $CDCl_3$): δ 8.20 (d, 2H, J = 8.7 Hz), 7.63-7.70 (m, 3H), 6.53 (d, 1H, J = 15.5 Hz), 4.17 (t, 2H, J = 7 Hz), 1.63-1.69 (m, 2H, J = 7.8 Hz), 1.36-1.45 (m, 2H, J = 7.5 Hz), 0.93 (t, 3H, J =

7.5 Hz) ppm; ^{13}C-NMR (60 MHz, $CDCl_3$): δ 184.0, 166.5, 155.5, 138.7, 133.5, 129.5, 123.3, 87.7, 54.4, 28.8, 15.5 ppm, Yellow solid (mp: 62-64 ºC)[1-3].

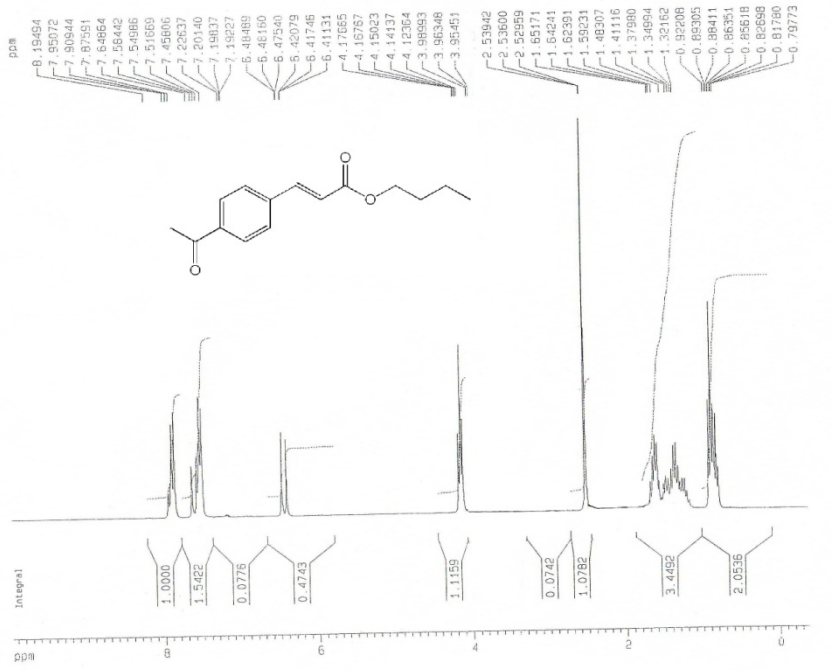




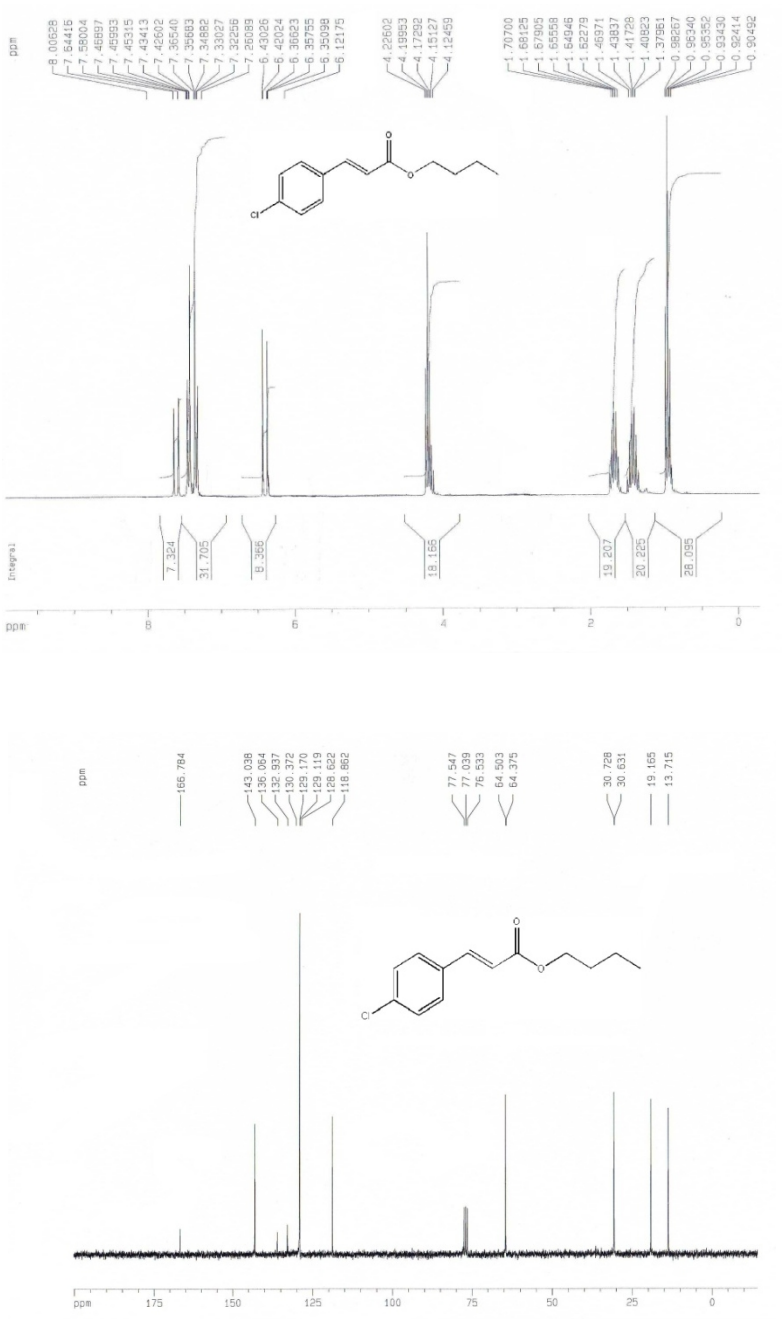
4) 3-(4-cyano-phenyl)-acrylic acid butyl ester :^{1}H-NMR (250 MHz, $CDCl_3$): δ 7.51–7.60 (m, 5H), 6.47 (d, 1H), 4.01 (t, 2H), 1.55-1.66 (m, 2H), 1.30-1.39 (m, 2H, J = 7.3 Hz), 0.84-0.90 (t, 3H, J = 7.3 Hz) ppm; ^{13}C-NMR (60 MHz, $CDCl_3$): δ 166.14, 142.0, 138.6, 132.5, 128.7, 121.8, 118.3, 113.2, 64.7, 30.6, 19.1, 13.6 ppm, white solid m.p. 43-44 ºC [1-3].



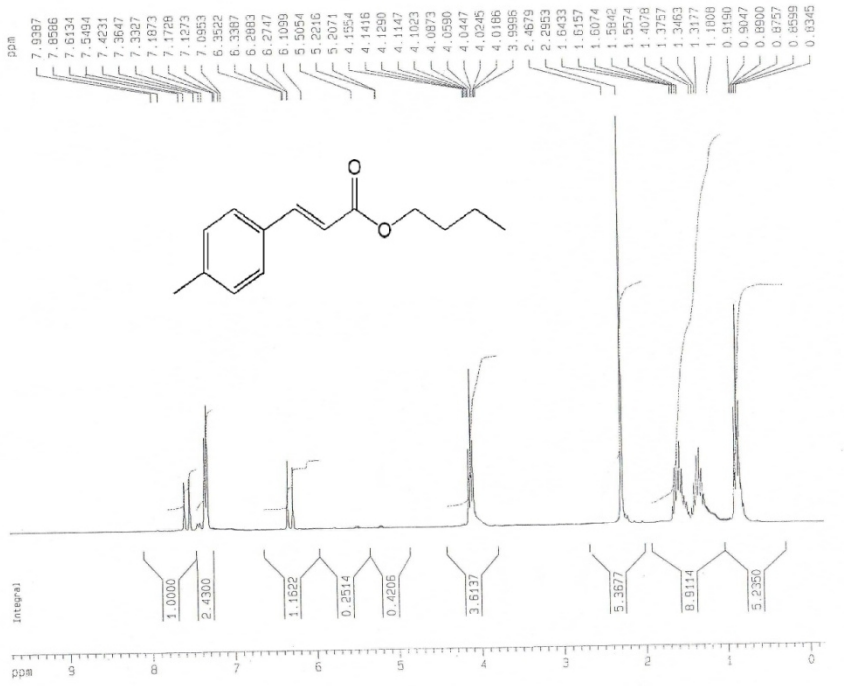
5) 3-(4-acetyl-phenyl)-acrylic acid butyl ester: ^{1}H-NMR (250 MHz, $CDCl_3$): δ 7.87-7.95 (d, 1H), 7.45-7.87 (m, 4H), 6.47 (d, 2H), 4.15 (m, 2H), 2.53 (S, 3H), 1.59-1.65 (m, 2H), 1.32-1.48 (m, 2H), 0.86-0.92 (m, 3H) ppm; ^{13}C-NMR (60 MHz, $CDCl_3$): δ 195.5, 172.5, 155.0, 146.5, 141.5, 132.6, 130.8, 125.5, 88.3, 45.0, 33.4, 23.4, 16.0 ppm, pale yellow liquid[1].



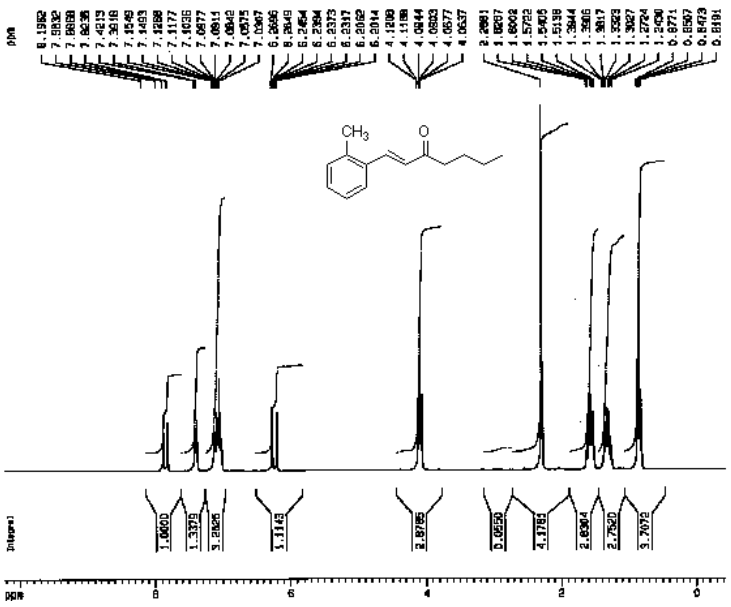
6) 3-(4-chloro-phenyl)-acrylic acid butyl ester: ^{1}H-NMR (250 MHz, $CDCl_3$): 7.60 (d, 1H),7.58-7.64 (m, 2H), 7.26-7.36 (m, 2H), 6.42 (d, 1H), 4.17 (t, 2H), 1.62-1.70 (m, 2H), 1.37-1.46 (m, 2H), δ 0.95 (t, J= 7.4 Hz, 3H) ppm; ^{13}C-NMR (60 MHz, $CDCl_3$): δ 166.7, 143.0, 136.0, 132.9, 129.1, 118.8, 64.4, 30.6, 19.1, 13.7 ppm[1, 3].



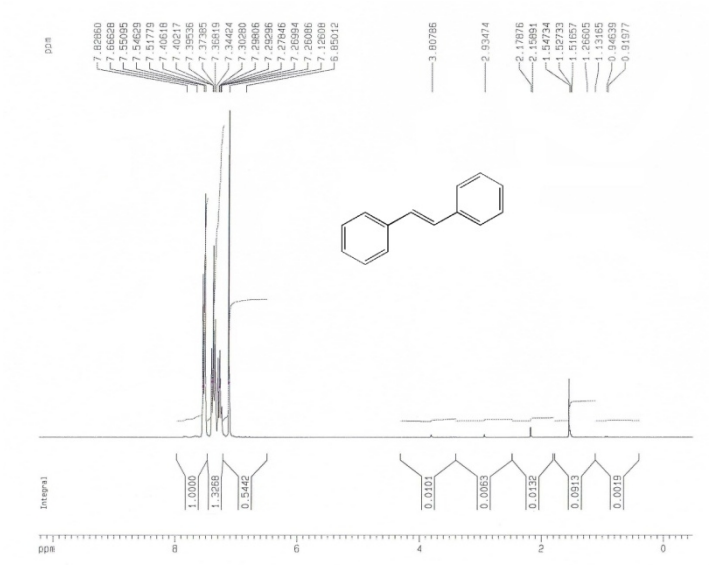
7) 3-(4-methyl-phenyl)-acrylic acid butyl ester: ^{1}H-NMR (250 MHz, $CDCl_3$): δ 7.87 (d, 1H), 7.55 (d, 2H), 7.25 (d, 2H), 6.30 (d, 1H), 4.90 (t, 2H), 2.29 (s, 3H), 1.60 (m, 2H), 1.34 (m, 2H), 0.88 (t, 3H) ppm; ^{13}C-NMR (60 MHz, $CDCl_3$): δ 175.5, 150.6, 144.5, 130.0, 129.0, 128.5, 119.0, 70.5, 41.3, 25.7, 17.5, 13.0 ppm, pale yellow liquid[1-3].

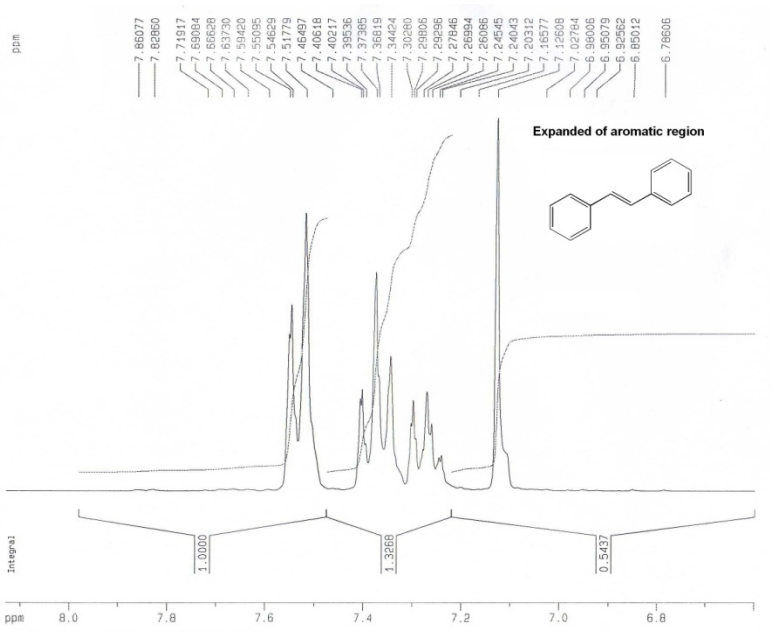


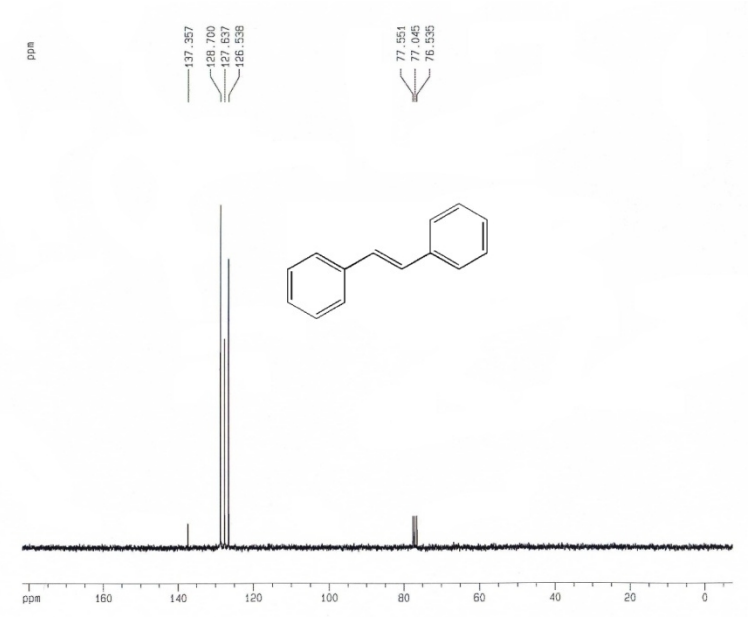
8) 3-(2-methyl-phenyl)-acrylic acid butyl ester: ^{1}H-NMR (250 MHz, $CDCl_3$): δ 8.03 (d, 1H), 7.60 (d, 1H), 6.94-7.31 (m, 3H), 6.15 (d, 1H), 4.0 (t, 2H), 2.2 (s, 3H), 1.44-1.51 (m, 2H) 1.17-1.26 (m, 2H), 0.75-0.78 (t, 3H), ppm; ^{13}C-NMR (60 MHz, $CDCl_3$): δ 167.1, 142.2, 137.5, 133.43, 130.7,129.9 126.7, 119, 64.4, 30.7, 19.7, 19.2, 13.7 ppm, pale yellow liquid[1-3].



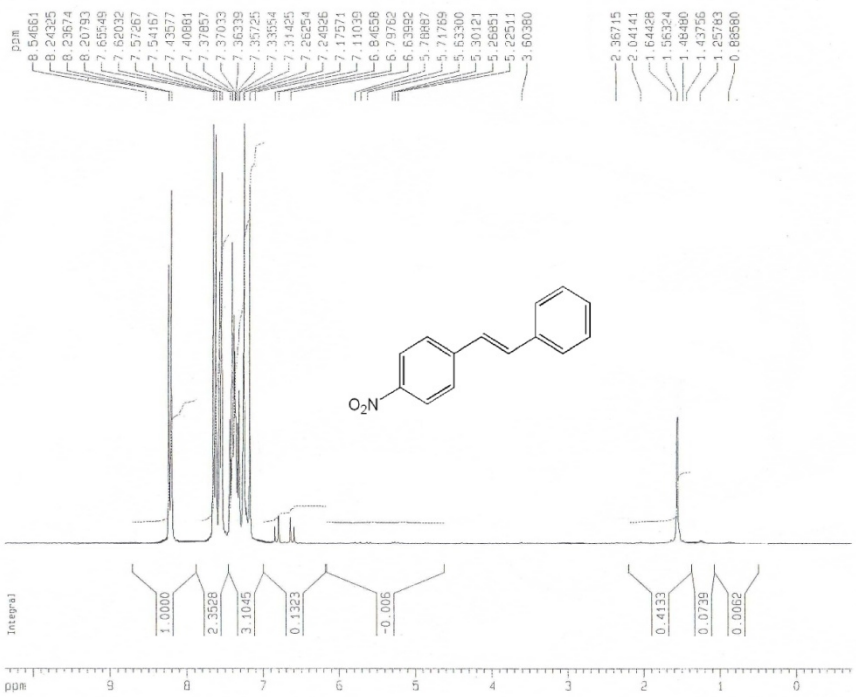
9) (E)-stilben: ^{1}H-NMR (250 MHz, $CDCl_3$): δ 7.55 (d, 4H, J = 7.5 Hz), 7.36 (t, 4H, J = 7.5 Hz), 7.30 (t, 2H, J = 7.5 Hz), 7.26 (s, 2H) ppm; ^{13}C-NMR (60 MHz, $CDCl_3$): δ 137.3, 128.7, 127.6, 126.5 ppm, white solid, m.p 123-125 ºC[1-3].







10)(E)-1-nitro-4-styryl-benzene: ^{1}H-NMR (250 MHz, $CDCl_3$): δ 8.23 (d, 2H, J = 9.3 Hz), 7.54 (d, 2H, J = 9.3 Hz), 7.36 (d, 2H, J = 7.3 Hz), 7.11-7.33 (m, 3H), 6.84 (d, 1H, J = 16 Hz), 6.63 (d, 1H, J = 16.5 Hz) ppm; ^{13}C-NMR (60 MHz, $CDCl_3$): δ 143.8, 136.1, 133.3, 129.6, 127.0, 126.8, 126.2, 124.1 ppm, white solid, m.p. 155–157^{o} C[1-3].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7.11039
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1.56324
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1.25783
0.88580
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Integral
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3.1045
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3
2
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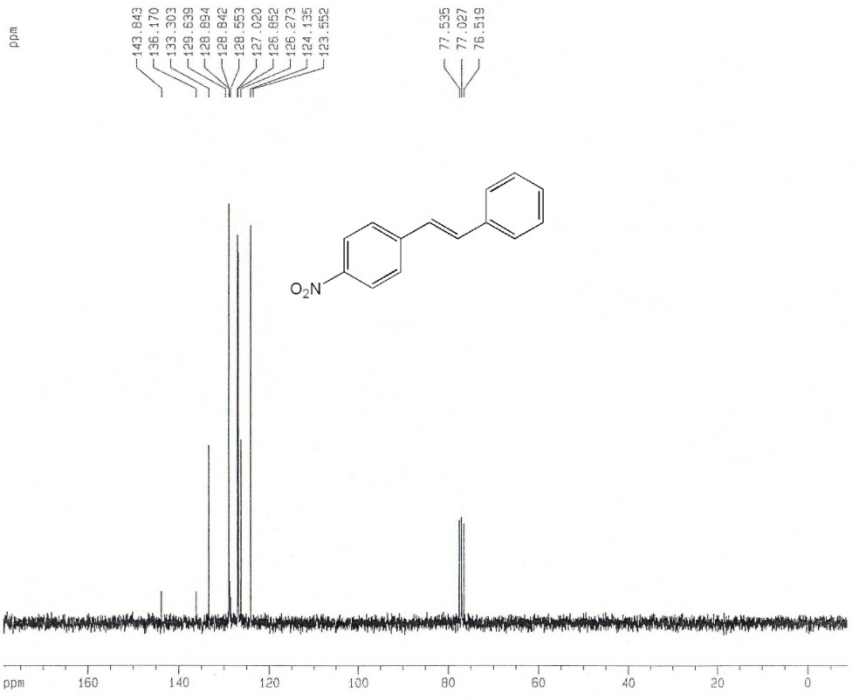
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133.303
129.639
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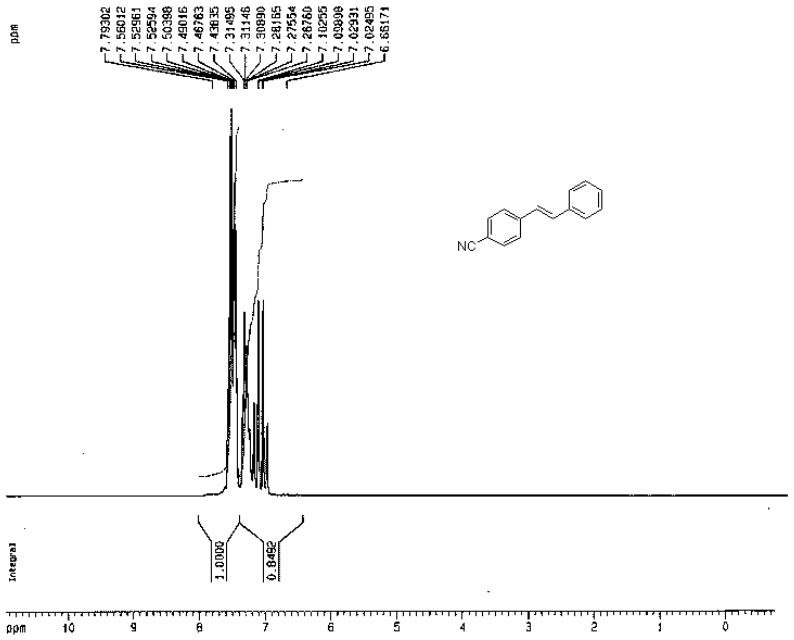
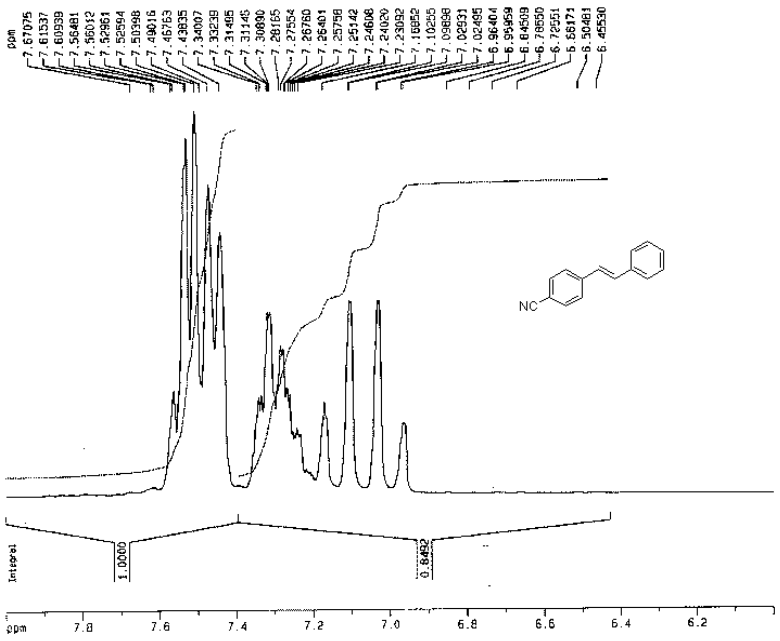
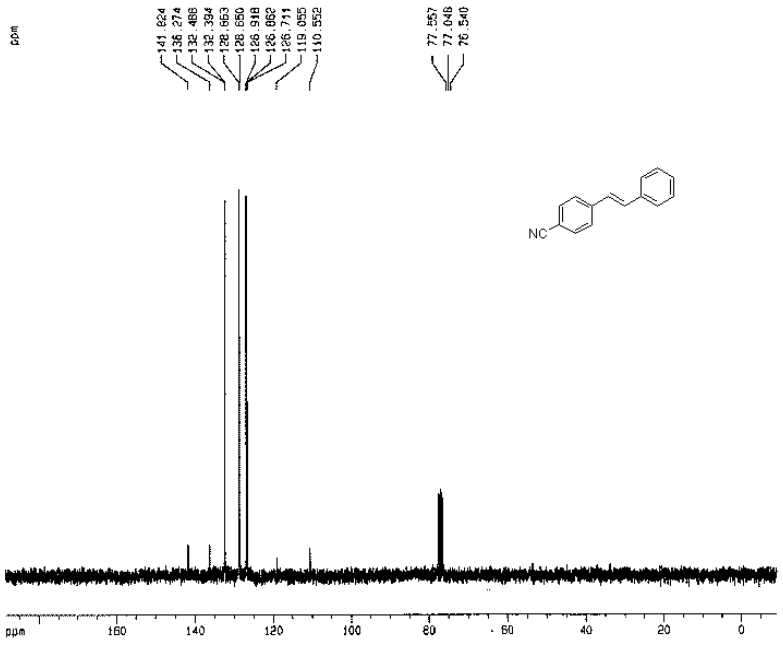
128.553
127.020
126.852
126.273
124.135
123.552
77.535
77.027
76.519
O2N
ppm
160
140
120
100
80
60
40
20
0

11)(E)-1-cyano-4-styryl-benzene: ^{1}H-NMR (250 MHz, $CDCl_3$): δ 7.51-7.67 (m, 4H), 7.12-7.39 (m, 4H), 6.99 (d, 1H,), 7.13 (d, 1H) ppm; ^{13}C NMR (60 MHz, $CDCl_3$): δ 141.8, 136.2, 132.4, 132.3, 128.8, 128.6, 126.9, 126.8, 126.7, 119.0,110.5 ppm, white solid, m.p. 117^{o} C[1-3].







References

1. B. Tamami, F. Farjadian, S. Ghasemi and H. Allahyari, *New Journal of Chemistry*, 2013, **37**, 2011-2018.
2. H. Firouzabadi, N. Iranpoor and A. Ghaderi, *Journal of Molecular Catalysis A: Chemical*, 2011, **347**, 38-45.
3. H. Firouzabadi, N. Iranpoor and M. Gholinejad, *Tetrahedron*, 2009, **65**, 7079-7084.