

Supporting Information

Pd(OAc)₂ without added ligand as an active catalyst
for Mizoroki–Heck reaction in aqueous media

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Contents:

1. Experimental characterization data for compounds
2. Copies of product ¹H NMR and ¹³C NMR

(E)- Stilbene

^1H NMR (500 MHz; CDCl_3) δ : 7.60 (d, $J=1.0$ Hz, 4H), 7.43 (t, $J=7.5$ Hz, 4H), 7.32 (t, $J=7.2$ Hz, 2H), 7.19 (s, 2H); ^{13}C NMR δ : 127.0, 128.1, 129.1, 129.2, 137.8; Anal. calcd. for $\text{C}_{14}\text{H}_{12}$: C 93.29, H 6.71; found C 83.18, H 6.78.

(E)-Cinnamionitrile:

^1H NMR (500 MHz, CDCl_3) δ : 7.71-7.66 (3H, m), 7.55-7.50 (2H, m), 7.41 (1H, $J=16.8$ Hz, d), 6.18 (1H, $J=16.8$ Hz, d); ^{13}C NMR δ : 151.5, 134.4, 132.1, 130.0, 128.3, 119.1, 97.2; Anal. Calc. for $\text{C}_9\text{H}_7\text{N}$: C, 83.72; H, 5.43; N, 10.85. Found: C, 83.63; H, 5.37; N, 10.91.

(E)-n-butyl cinnamate:

^1H NMR (500 MHz, CDCl_3) δ : 7.72 (1 H, $J=16.0$ Hz, d), 7.56 (2 H, $J=3.7$ Hz, q), 7.41 (3 H, $J=1.0$ Hz, t), 6.48 (1 H, $J=16.0$ Hz, d), 4.26 (2 H, $J=6.7$ Hz, t), 1.76-1.72 (2 H, m), 1.51-1.47 (2 H, m), 1.01 (3 H, $J=7.4$ Hz, t); ^{13}C NMR δ : 14.2, 19.6, 31.2, 64.8, 118.8, 128.5, 129.3, 130.6, 134.9, 145.0, 167.5; Anal. Calc. for $\text{C}_{13}\text{H}_{16}\text{O}_2$: C, 76.44; H, 7.90. Found: C, 76.37; H, 7.81.

4-Acetylstilbene:

^1H NMR (500 MHz, CDCl_3) δ : 7.90 (2 H, $J=8.4$ Hz, d), 7.53 (2 H, $J=8.4$ Hz, d), 7.50-7.47 (2 H, m), 7.37-7.34 (2 H, m), 7.30-7.27 (1 H, m), 7.17 (1 H, $J=16.3$ Hz, d), 7.07 (1 H, $J=16.3$ Hz, d), 2.55 (3

H, s); ^{13}C NMR δ : 197.3, 141.9, 136.6, 135.9, 131.4, 128.8, 128.7, 128.2, 127.4, 126.7, 126.4, 29.6; Anal. Calc. for $\text{C}_{16}\text{H}_{14}\text{O}$: C, 86.45; H, 6.35. Found: C, 86.37; H, 6.31.

4-Methoxystilbene:

^1H NMR (500 MHz, CDCl_3) δ : 7.36 (2 H, $J=7.4$ Hz, d), 7.33 (2 H, $J=8.7$ Hz, d), 7.26-7.22 (2 H, m), 7.13-7.09 (1 H, m), 6.94 (1 H, $J=16.3$ Hz, d), 6.84 (1 H, $J=16.3$ Hz, d), 6.76 (2 H, $J=8.7$ Hz, d), 3.71 (3 H, s); ^{13}C NMR δ : 159.2, 137.7, 130.1, 128.7, 128.1, 127.6, 127.1, 126.6, 126.2, 114.1, 55.2; Anal. Calc. for $\text{C}_{15}\text{H}_{14}\text{O}$: C, 85.68; H, 6.71. Found: C, 85.59; H, 6.63.

4-Methylstilbene:

^1H NMR (500 MHz, CDCl_3) δ : 7.55 (2 H, $J=7.54$ Hz, d), 7.46 (2 H, $J=8.03$ Hz, d), 7.39 (2 H, $J=7.54$ Hz, t), 7.33-7.28 (1 H, m), 7.21 (2 H, $J=8.03$ Hz, d), 7.14 (1 H, $J=16.0$ Hz, d), 7.09 (1 H, $J=16.0$ Hz, d), 2.40 (3 H, s); ^{13}C NMR δ : 137.0, 134.1, 128.9, 128.2, 128.1, 127.2, 126.9, 125.9, 125.9, 20.8; Anal. Calc. for $\text{C}_{15}\text{H}_{14}$: C, 92.74; H, 7.26. Found: C, 92.71; H, 7.18.

(E)- Methyl-cinnamate

^1H NMR (500 MHz, CDCl_3) δ : 7.63 (d, $J=16.2$ Hz, 1H), 7.43-7.40 (m, 2H), 7.33-7.30 (m, 3H), 6.37 (d, $J=16.2$ Hz, 1H), 3.73 (s, 3H); ^{13}C NMR δ : 167.2, 144.6, 134.2, 130.0, 128.7, 127.7, 117.5, 51.4; Anal. Calc. for $\text{C}_{10}\text{H}_{10}\text{O}_2$: C, 74.06; H, 6.21. Found: C, 73.98; H, 6.18.

(E)-Ethyl cinnamate

^1H NMR (500 MHz, CDCl_3) δ : 7.68 (d, $J=16.2$ Hz, 1H), 7.54-7.51(m, 2H), 7.38-7.35 (m, 3H), 6.46-6.42 (m, 1H), 4.28-4.25 (m, 2H) 1.35- 1.32(m, 3H); ^{13}C NMR δ : 166.9, 144.5, 134.4, 130.1, 128.8, 128.0, 118.2, 60.4, 14.3; Anal. Calc. for $\text{C}_{11}\text{H}_{12}\text{O}_2$: C, 74.98; H, 6.86. Found: C, 74.86; H, 6.91.

(E)-butyl 3-(4-acetylphenyl)acrylate

^1H NMR (500 MHz, CDCl_3) δ : 7.98-7.94 (m, 2H); 7.69 (d, $J=16.0$ Hz, 1H), 7.60-7.57 (m, 2H), 6.53 (d, $J=16.0$ Hz, 1H), 4.22 (t, $J=6.6$ Hz, 2H), 2.57 (s, 3H), 1.71-1.68 (m, 2H), 1.47-1.44 (m, 2H), 0.96 (t, $J=7.4$ Hz, 3H); ^{13}C NMR δ : 197.3; 166.6, 143.0, 138.8, 137.9, 128.8, 128.1, 120.8, 64.7, 30.7, 26.7, 19.2, 13.7; Anal. Calc. for $\text{C}_{15}\text{H}_{18}\text{O}_3$: C, 73.15; H, 7.37. Found: C, 73.06; H, 7.41.

(E)-Butyl 3-(2-methoxyphenyl)acrylate

^1H NMR (500 MHz, CDCl_3) δ : 8.07 (d, $J=16.2$ Hz, 1H), 7.55-7.58 (m, 1H), 7.38-7.44 (m, 1H), 6.95-7.04 (m, 2H), 6.59 (d, $J=16.2$ Hz, 1H), 4.28 (t, $J=6.7\text{Hz}$, 2H), 3.94 (s, 3H), 1.70-1.80 (m, 2H), 1.44-1.56 (m, 2H), 1.03 (t, $J=7.3\text{Hz}$, 3H); ^{13}C NMR δ : 167.5, 158.2, 139.9, 131.3, 128.8, 123.4, 120.6, 118.7, 111.0, 64.2, 55.4, 30.8, 19.1, 13.7; Anal. Calc. for $\text{C}_{14}\text{H}_{18}\text{O}_3$: C, 71.77; H, 7.74. Found: C, 71.53; H, 7.62.

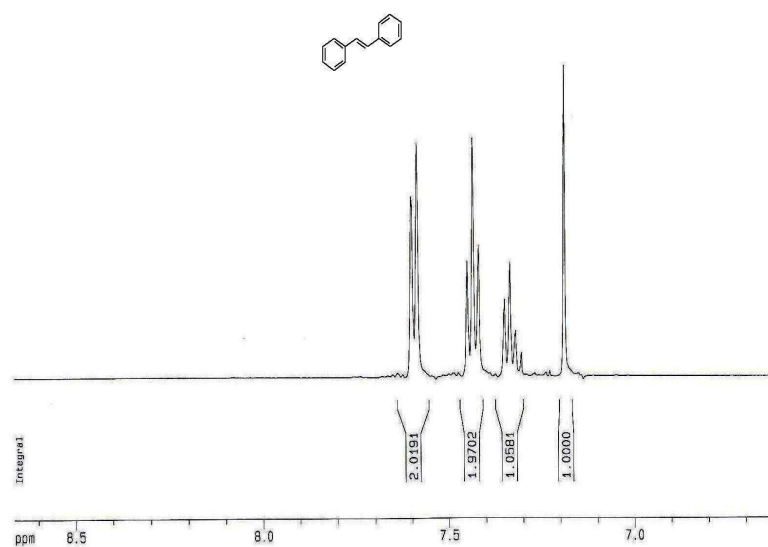
(E)-Butyl 3-(4-methoxyphenyl)acrylate

^1H NMR (500 MHz, CDCl_3) δ : 7.68 (d, $J = 16.0$ Hz, 1H), 7.50-7.52 (m, 2H), 6.92-6.95 (m, 2H), 6.35 (d, $J=16.0\text{Hz}$, 1H), 4.24 (t, J

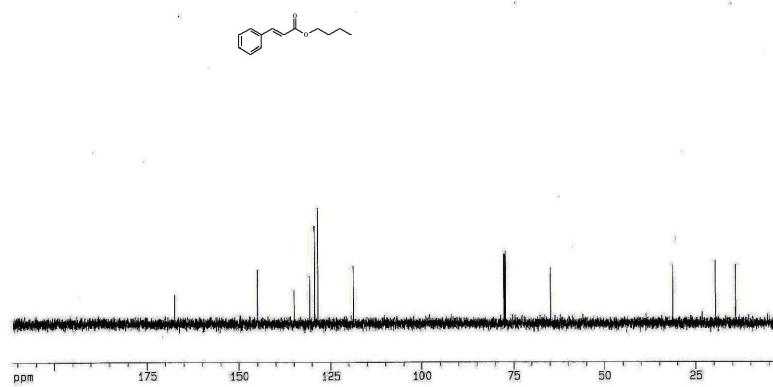
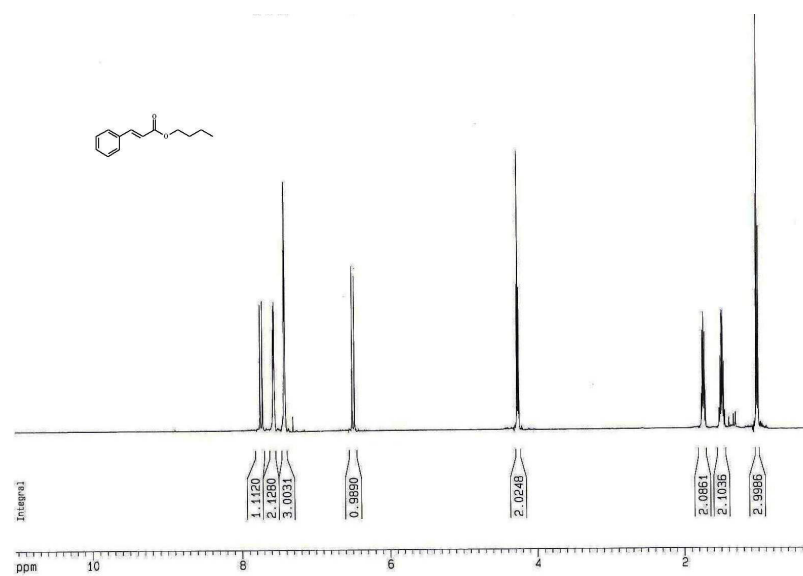
= 6.6 Hz, 2H), 3.86 (s, 3H), 1.68-1.75 (m, 2H), 1.42-1.51 (m, 2H), 0.99 (t, J = 7.3Hz, 3H); ^{13}C NMR δ : 167.3, 161.3, 144.1, 129.6, 127.2, 115.7, 114.2, 64.2, 55.3, 30.8, 19.1, 13.7; Anal. Calc. for $\text{C}_{14}\text{H}_{18}\text{O}_3$: C, 71.77; H, 7.74. Found: C, 71.59; H, 7.64.

(E)- Stilbene

^1H NMR Spectra

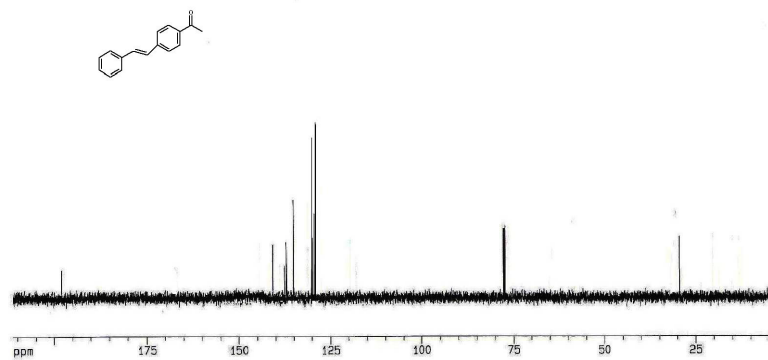
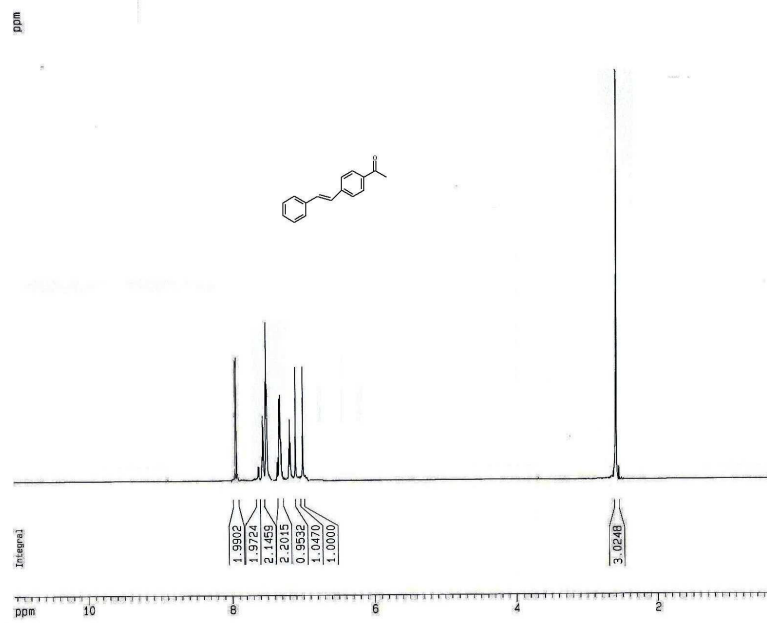


(E)-n-butyl cinnamate:
 ^1H , ^{13}C NMR Spectra

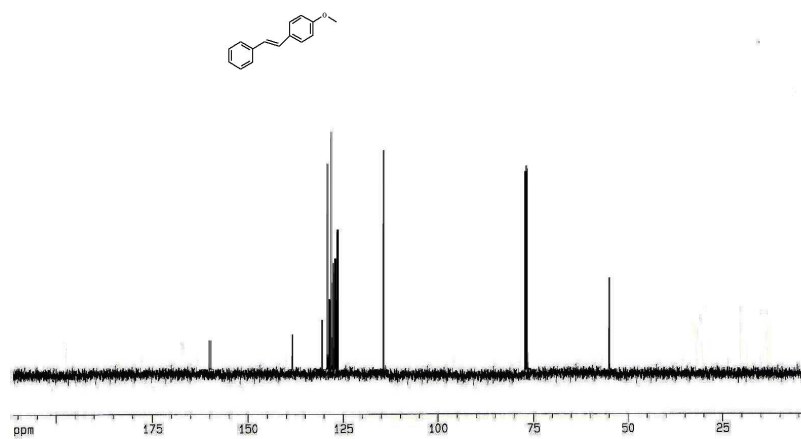
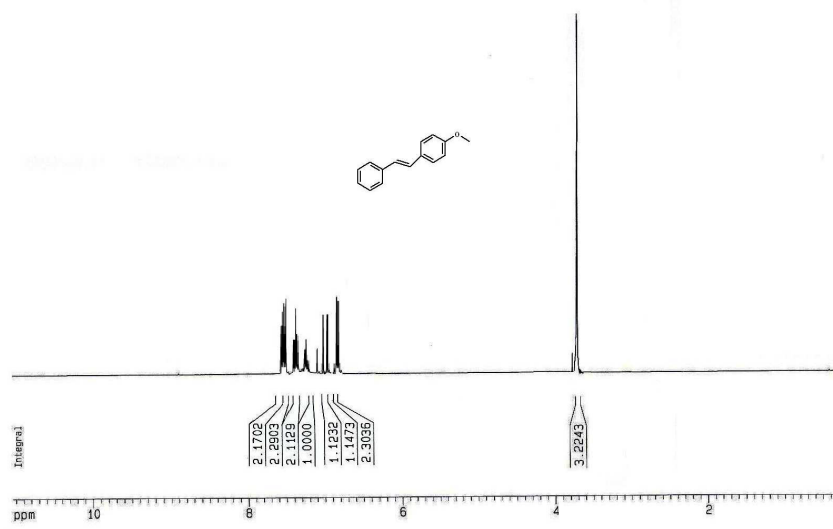


4-Acetylstilbene:

^1H , ^{13}C NMR Spectra

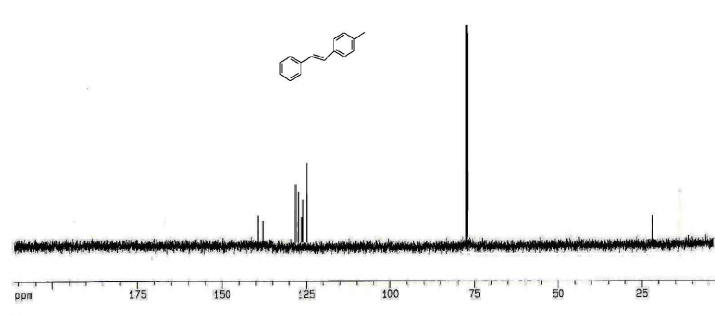
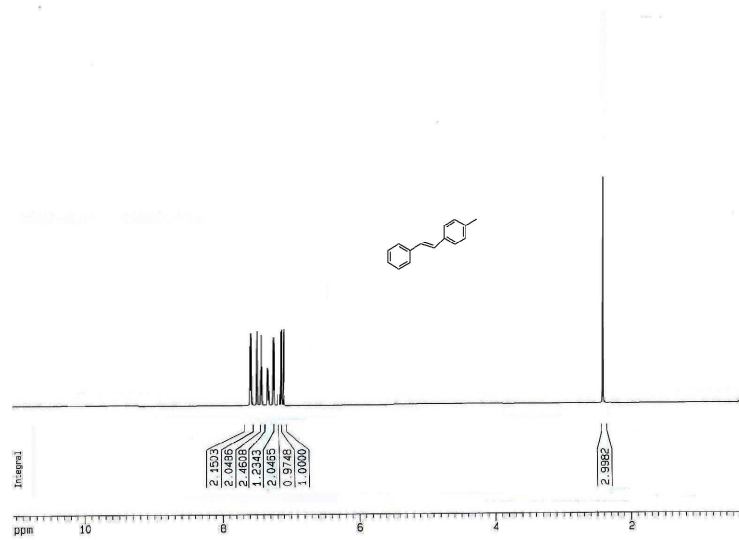


4-Methoxystilbene:
 ^1H , ^{13}C NMR Spectra

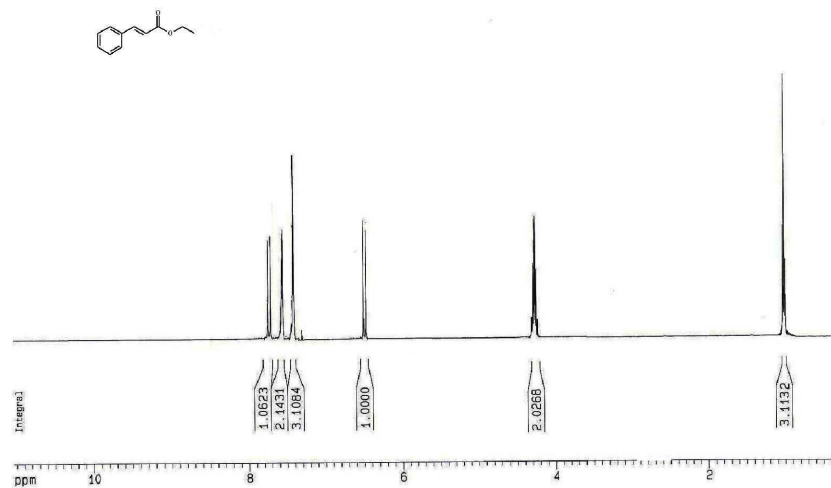


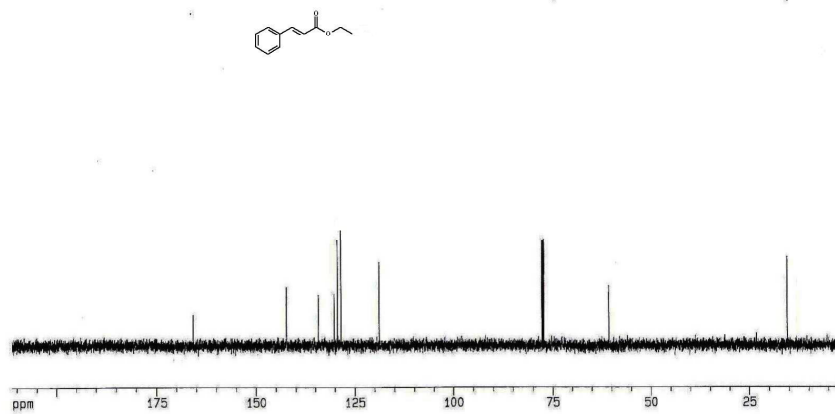
4-Methylstilbene:

^1H , ^{13}C NMR Spectra



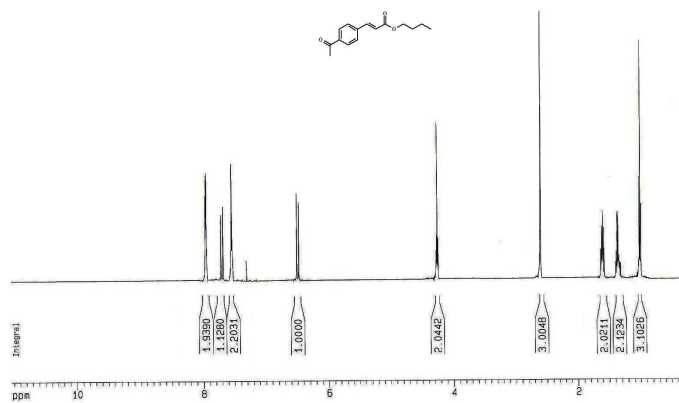
(E)-Ethyl cinnamate
 ^1H , ^{13}C NMR Spectra

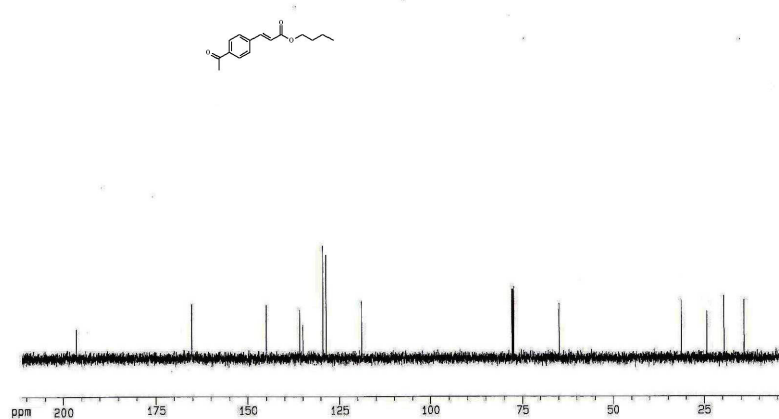




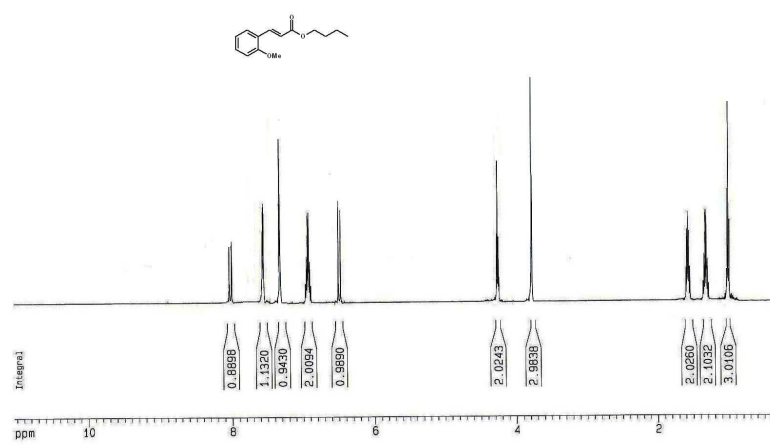
(E)-butyl 3-(4-acetylphenyl)acrylate

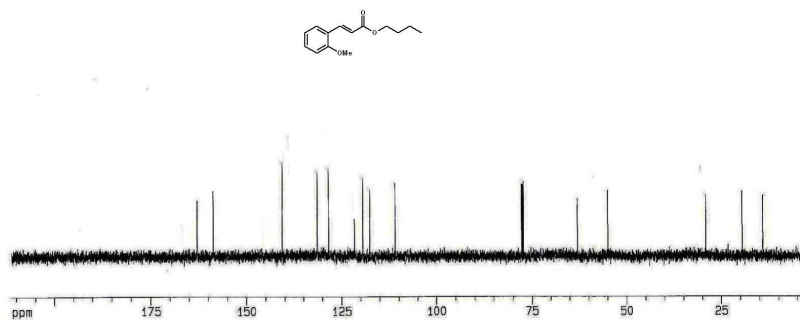
¹H, ¹³C NMR Spectra





(E)-Butyl 3-(2-methoxyphenyl)acrylate





(E)-Butyl 3-(4-methoxyphenyl)acrylate

