Supporting information

Palladium Nanoparticles on Noncovalently Functionalized Graphene-based Heterogeneous Catalyst for the Suzuki–Miyaura and Heck-Mizoroki Reactions in Water

Vittal Sharavath and Sutapa Ghosh*,

^{1}H and ^{13}C NMR Spectroscopic data for the Suzuki-Miyaura reaction products:

Compound-1 (Biphenyl)[2]

Colorless solid; ^{1}H NMR (300 MHz, $CDCl_3$): δ=7.29 (2 H, t, Ar-H), 7.39 (4 H, m, Ar-H), 7.53 (4 H, m, Ar-H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$): δ=127.10, 127.18, 128.67 and 141.15, ppm.

Compound-2 (1,1'-Biphenyl)-4-carboxaldehyde)[2]

Colorless solid; ^{1}H NMR (300 MHz, $CDCl_3$): δ=7.35-7.47 (3 H, m, Ar-H), 7.60 (2 H; d, Ar-H), 7.73 (2 H, d, Ar-H), 7.94 (2 H, d, Ar-H), 10.03 (1 H, s, -CHO) ppm.

^{13}C NMR (75 MHz, $CDCl_3$): δ=127.32, 127.64, 128.43, 128.97, 130.24, 135.13, 139.66, 147.16 and 192.1.ppm.

Compound-3 (2-(4-Methoxyphenyl) naphthalene) [3]

^{1}H NMR (300 MHz, $CDCl_3$): δ=3.85 (3 H; s, OCH_3), 6.93-6.98 (2 H, m; Ar-H), 7.37-7.47 (2 H, m, Ar-H), 7.57-7.62 (2 H, m, Ar-H), 7.64-7.68 (1 H, m, Ar-H), 7.78-7.85 (3 H, m, Ar-H), 7.92 (1 H, s, Ar-H)ppm.

^{13}C NMR (75 MHz, $CDCl_3$): δ=55.29, 114.16, 126.69, 128.11, 128.68, 133.72, 140.91 and 159.1 ppm.

Compound-4 (4-hydroxy-1, 1'-biphenyl) [2]

Colorless solid; ^{1}H NMR (300 MHz, $CDCl_3$): δ=6.83-6.85 (2 H, m, Ar-H), 7.25 (1 H, t; Ar-H), 7.36 (2 H, t, Ar-H), 7.41 (2 H, d, Ar-H), 7.47 (2 H, d, Ar-H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$+DMSO): δ=115.30, 125.76, 125.82, 127.40, 128.09, 131.51, 140.38 and 156.39.ppm.

Compound-5 (4-methyl-1, 1'-biphenyl)[1, 3,7]

Colorless solid; ^{1}H NMR (300 MHz, $CDCl_3$): δ=2.38 (3 H, s, CH_3), 7.17 (2 H, d, Ar-H), 7.26 (1 H; t Ar-H), 7.36 (2 H, t, Ar-H), 7.41 (2 H, d, Ar-H), 7.50 (2 H, d, Ar-H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$): δ=21.0, 126.7, 126.9, 128.6, 129.4, 136.6, 136.9, 138.3 and 141.1.ppm.

Compound-6 (2, 4-Dimethoxy-biphenyl) [1, 4]

Colorless oil; ^{1}H NMR (300 MHz, $CDCl_3$): δ=3.74 (3 H, s, -OCH_3), 3.83 (3 H, s, -OCH_3), 6.95-6.82 (3 H, m, Ar-H), 7.34 (1 H, t, Ar-H), 7.40 (2 H, t, Ar-H), 7.53 (2 H, d, Ar-H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$): δ=55.8, 56.2, 112.5, 112.8, 113.0, 116.0, 116.6, 127.0, 128.0, 129.4, 138.3 and 153.6.ppm.

Compound-7 (4-[1] Naphthylbenzonitrile)

White solid; ^{1}H NMR (500 MHz, $CDCl_3$): δ=7.37 (1 H, dd, Ar-H), 7.44 (1 H, t, Ar-H), 7.53-7.50 (2 H m, Ar-H), 7.58 (2 H, d, Ar-H), 7.76-7.74 (3 H, m, Ar-H), 7.90 (2H, t, Ar-H) ppm.

^{13}C NMR (125 MHz, $CDCl_3$): δ=111.2, 118.8, 125.1, 125.3, 126.1, 126.6, 127.0, 128.5, 128.7, 130.7, 130.9, 132.1, 133.8, 138.2 and 145.6 ppm.

Compound-8 (2-Phenylpyridine) [2]

Colorless liquid; ^{1}H NMR (300 MHz, $CDCl_3$): δ=7.17 (1 H, dd Ar-H), 7.3-7.46 (3 H, m, Ar-H), 7.69 (2 H, d, Ar-H), 7.95-7.98 (2 H, m, Ar-H), 8.67 (1 H, d, Ar-H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$): δ=120.30, 121.9, 126.7, 128.5, 128.7, 136.5, 139.2, 149.4 and 157 ppm.

Compound-9 (3-Phenylpyridine) [2, 4]

White solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ=7.43─7.35 (2 H, m, Ar-H), 7.49 (2 H, t; Ar-H), 7.60 (2H; d, Ar-H), 7.88 (1 H, d, Ar-H), 8.59 (1H, d, Ar-H), 8.85 (1 H, s Ar-H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ=123.5, 127.1, 128.1, 129.0, 134.3, 136.6, 137.8, 148.3 and 148.4 ppm.

Compound-10 (5-Phenylpyrimidine) [4]

White solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ=7.47 (1H, t, Ar-H), 7.53 (2 H, t, Ar-H), 7.58 (2 H, d, Ar-H), 8.96 (2 H, s; Ar-H), 9.21 (1 H, s, Ar-H) ppm.

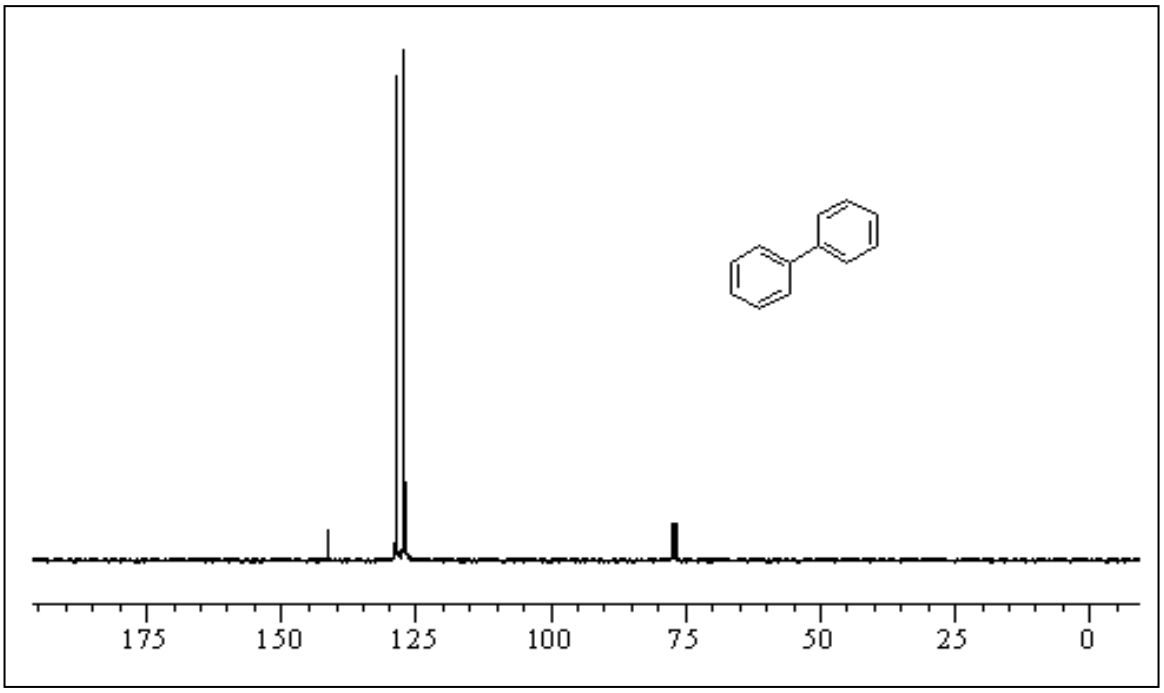
^{13}C NMR (100 MHz, $CDCl_3$): δ=126.7, 128.9, 129.3, 134.1, 134.2, 154.8 and 157.3 ppm.

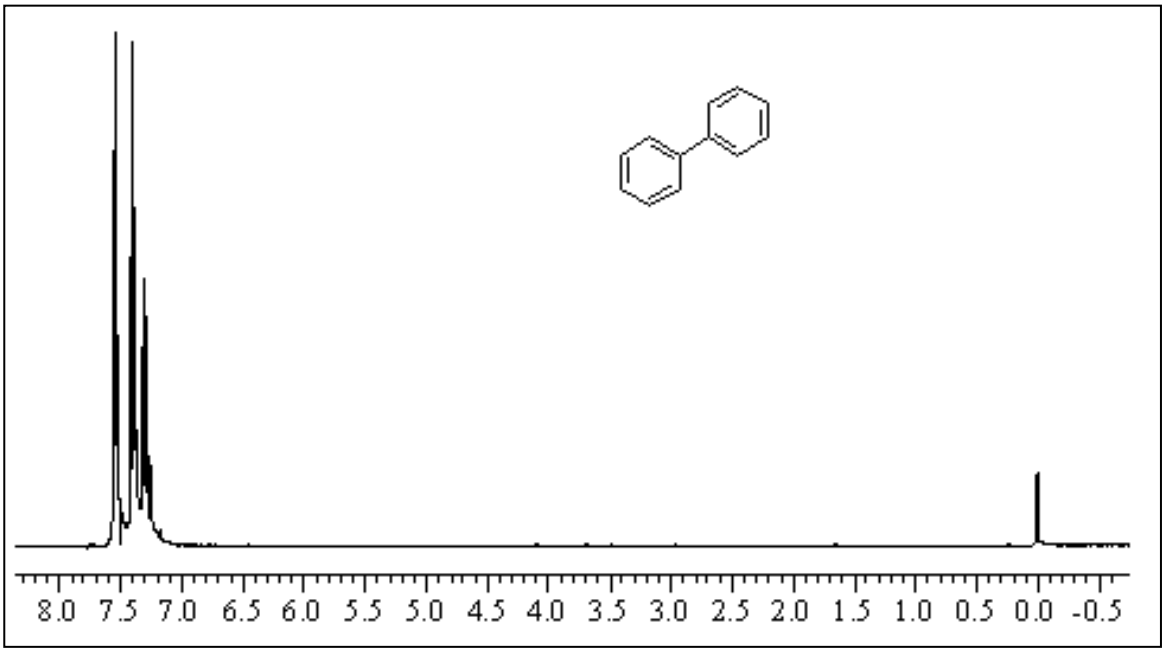
Compound-11 (3-Nitrobiphenyl-4-carbonitrile)

White solid; ^{1}H NMR (500 MHz, $CDCl_3$): δ=7.69 (1 H, t, Ar-H), 7.75 (2 H, dd, Ar-H), 7.81(2 H, dd, Ar-H), 7.93 (1 H, dd, Ar-H), 8.29 (1 H, dd, Ar-H), 8.46 (1 H, t, Ar-H) ppm.

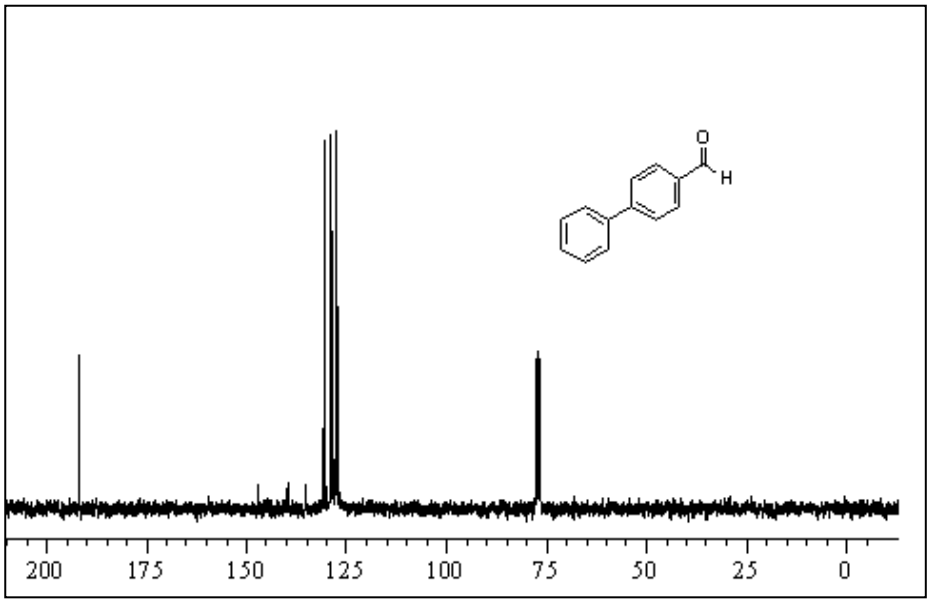
^{13}C NMR (125 MHz, $CDCl_3$): δ=112.4, 118.3, 122.1, 123.3, 127.9, 130.2, 132.9, 133.0, 140.8 and 143.0 ppm.

Compound-1 (Biphenyl)

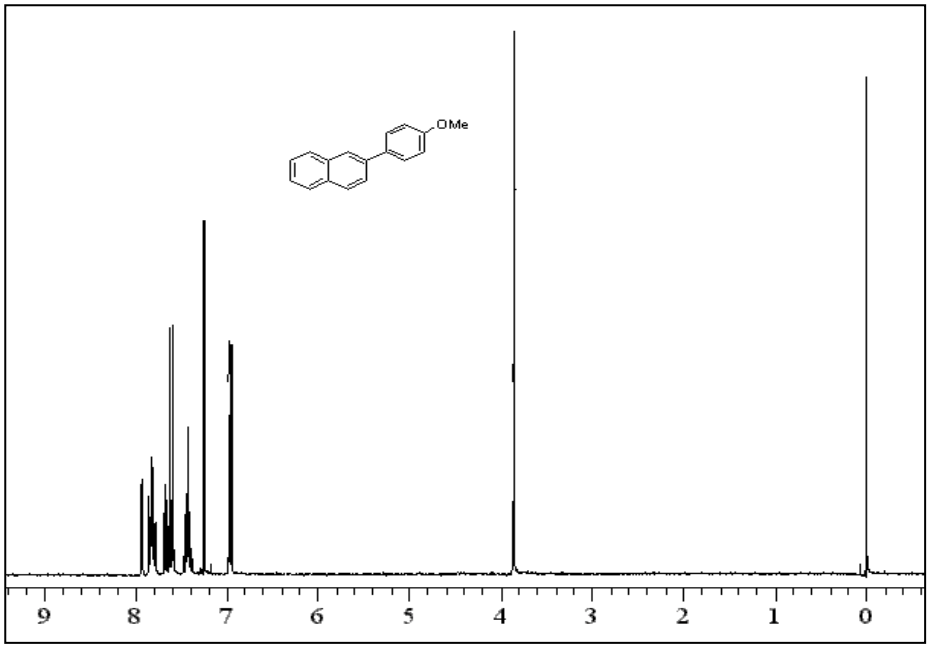


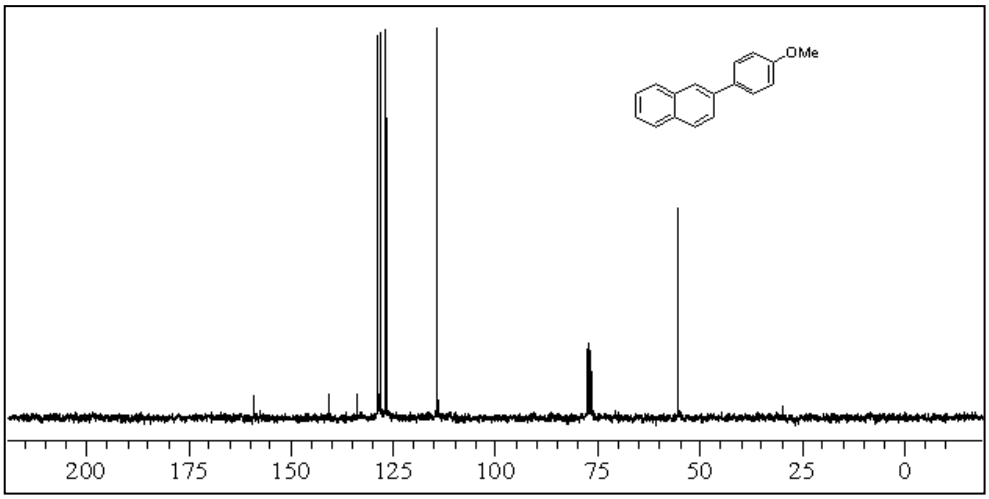


Compound-2 (1,1'-Biphenyl)-4-carboxaldehyde)

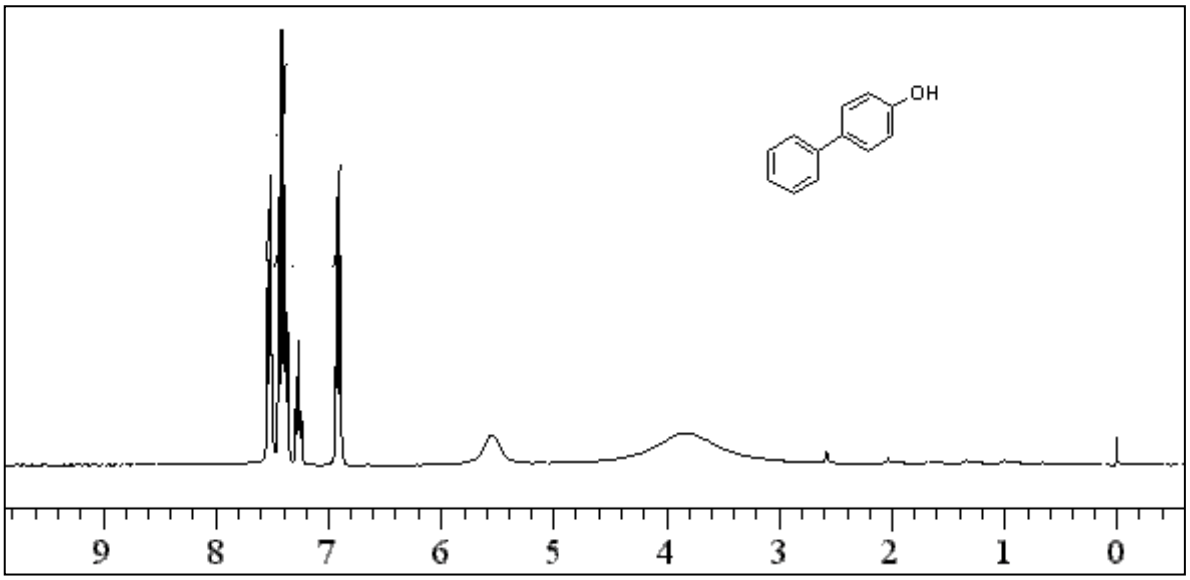


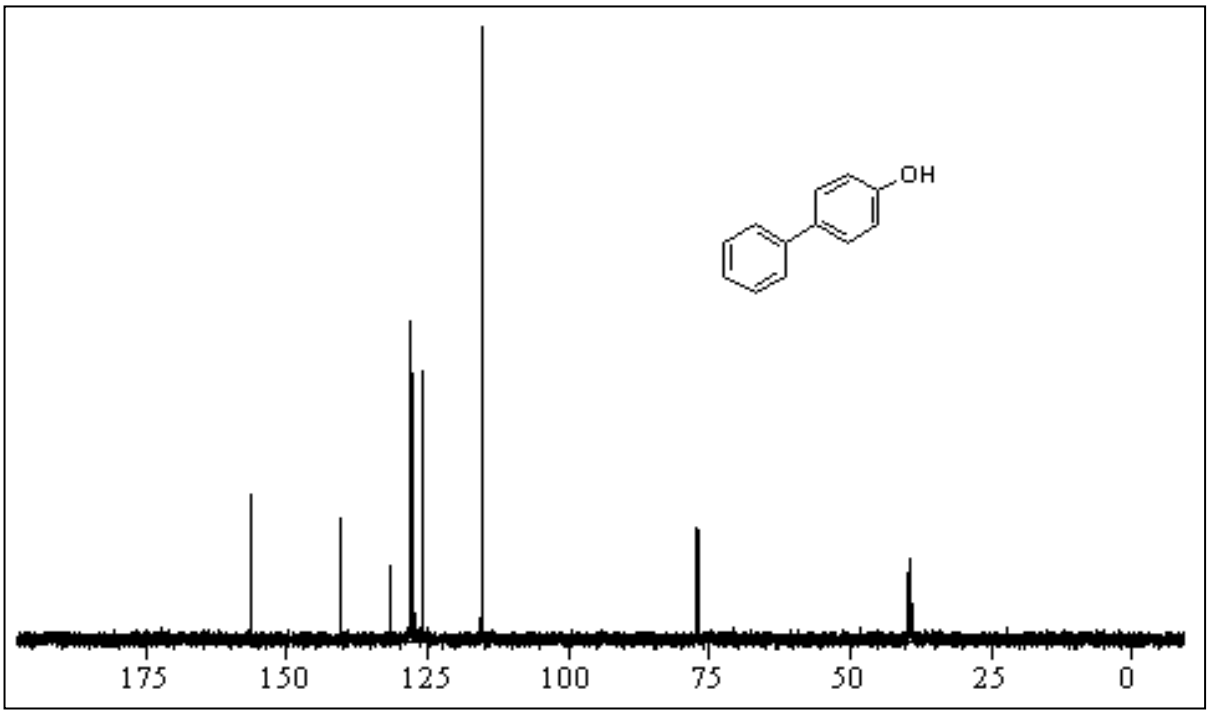
Compound-3 (2-(4-Methoxyphenyl) naphthalene)



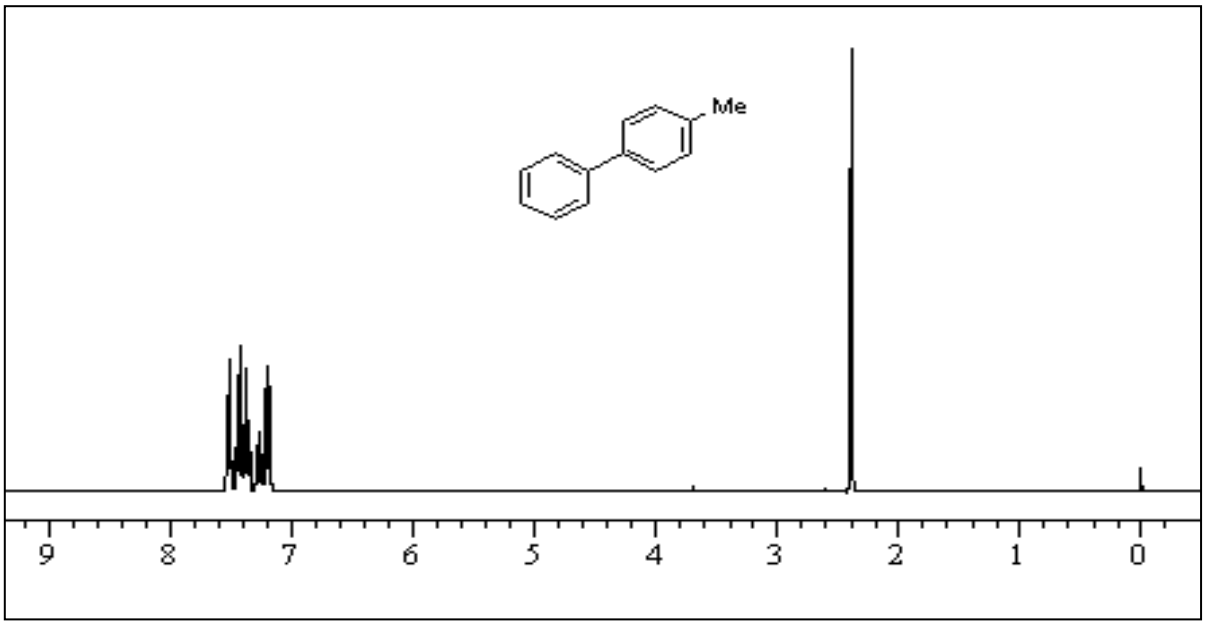


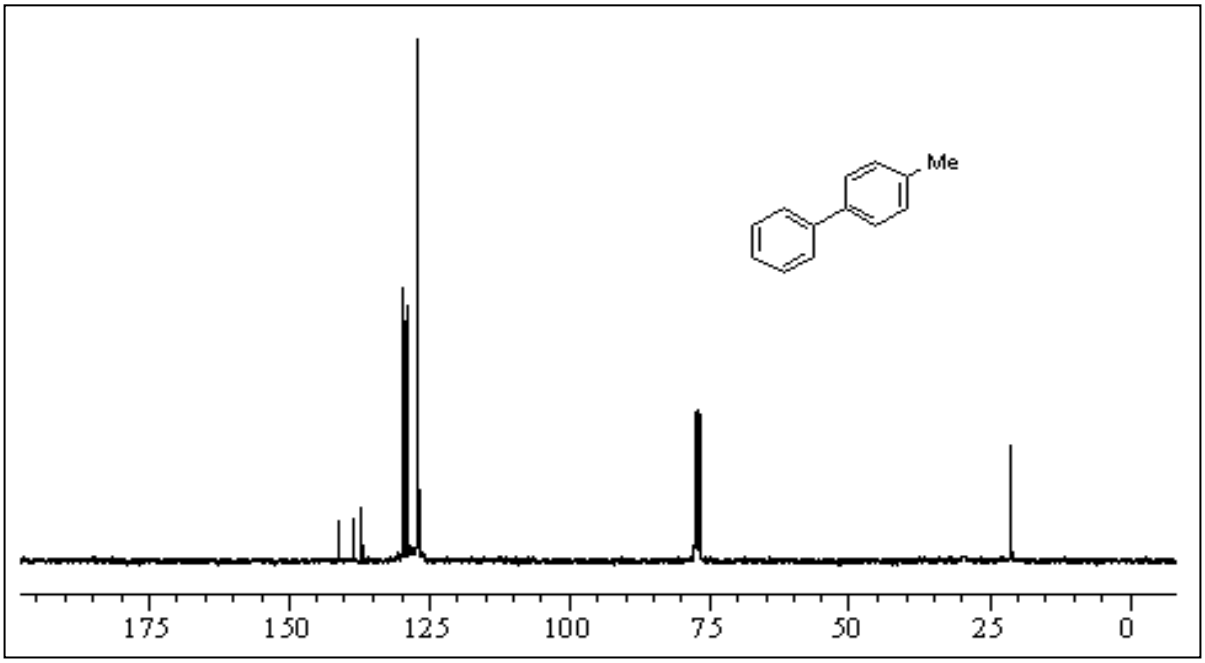
Compound-4 (4-hydroxy-1, 1'-biphenyl)



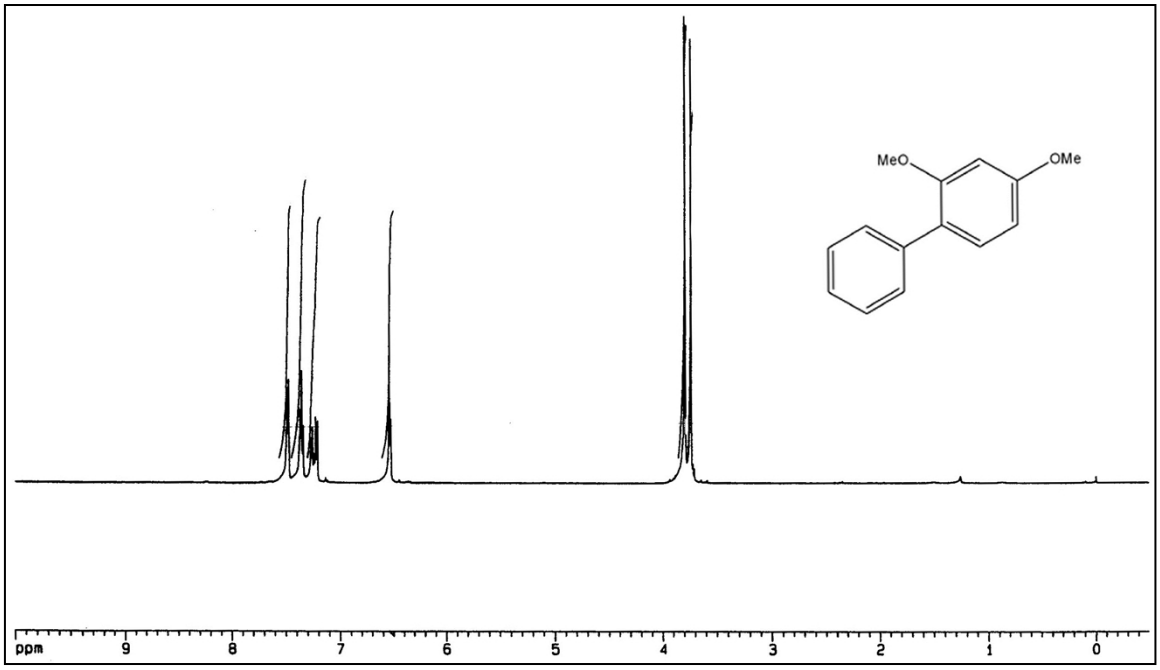


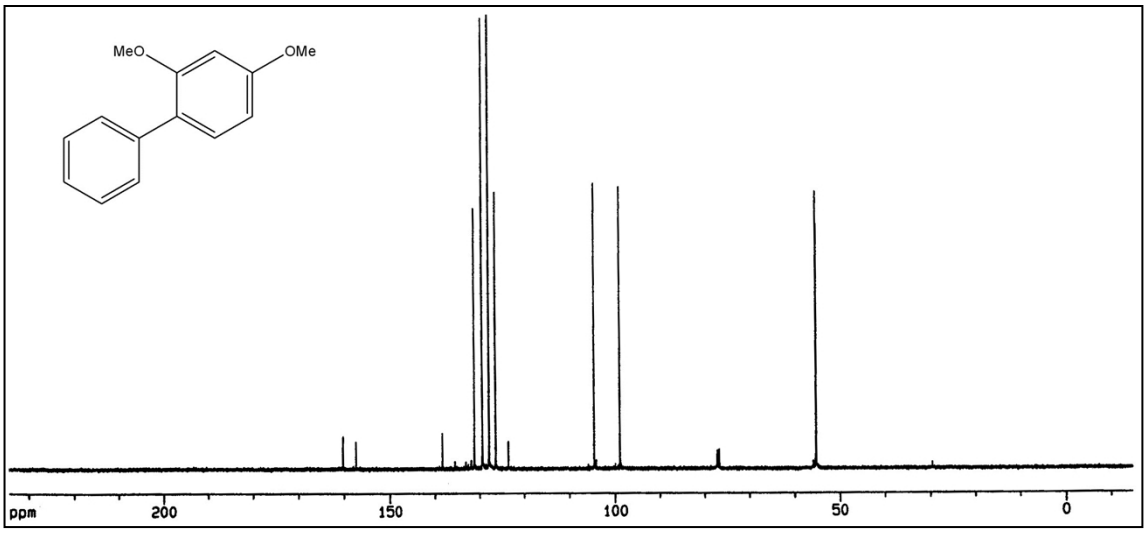
Compound-5 (4-methyl-1, 1'-biphenyl)



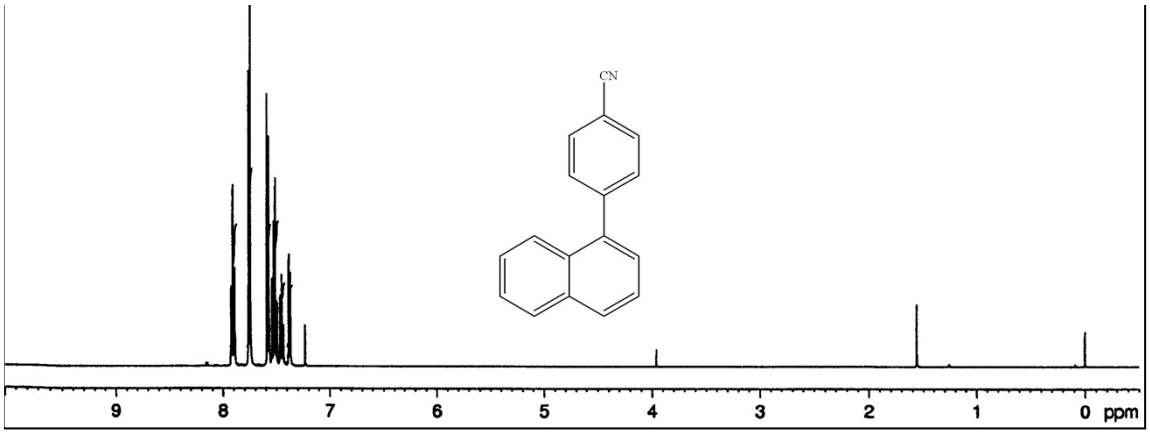


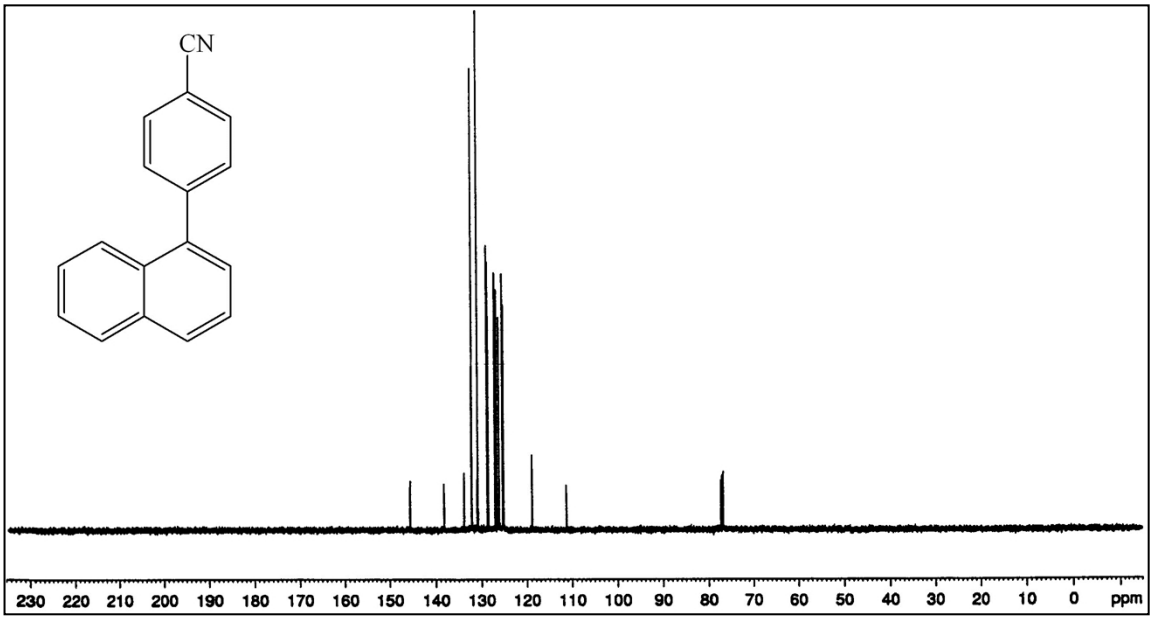
Compound-6 (2, 4-Dimethoxy-biphenyl)



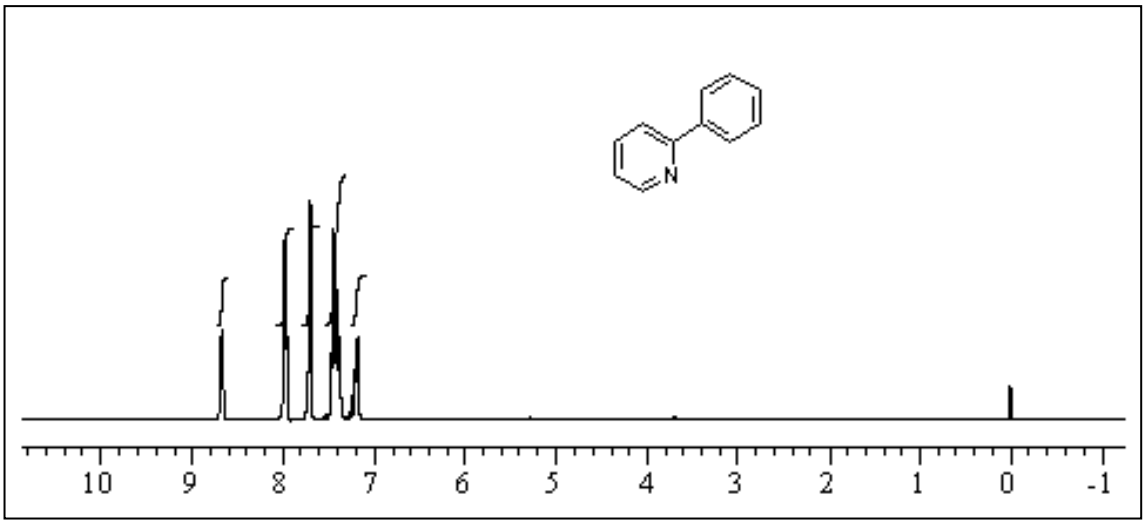


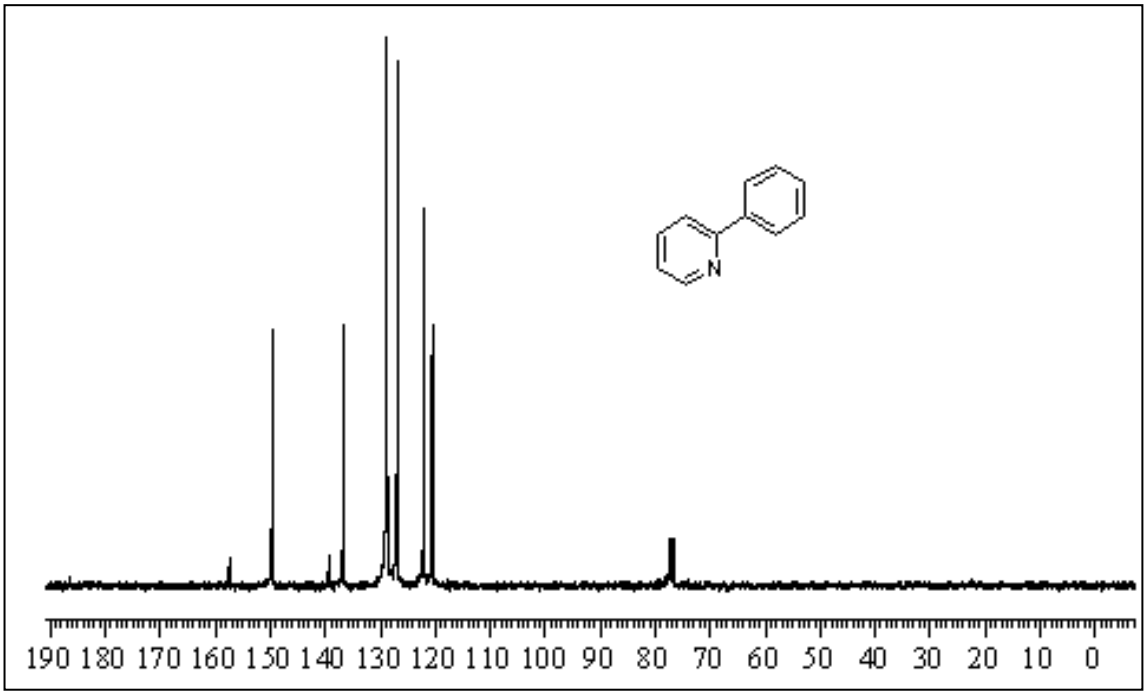
Compound-7 (4-[1] Naphthylbenzonitrile)



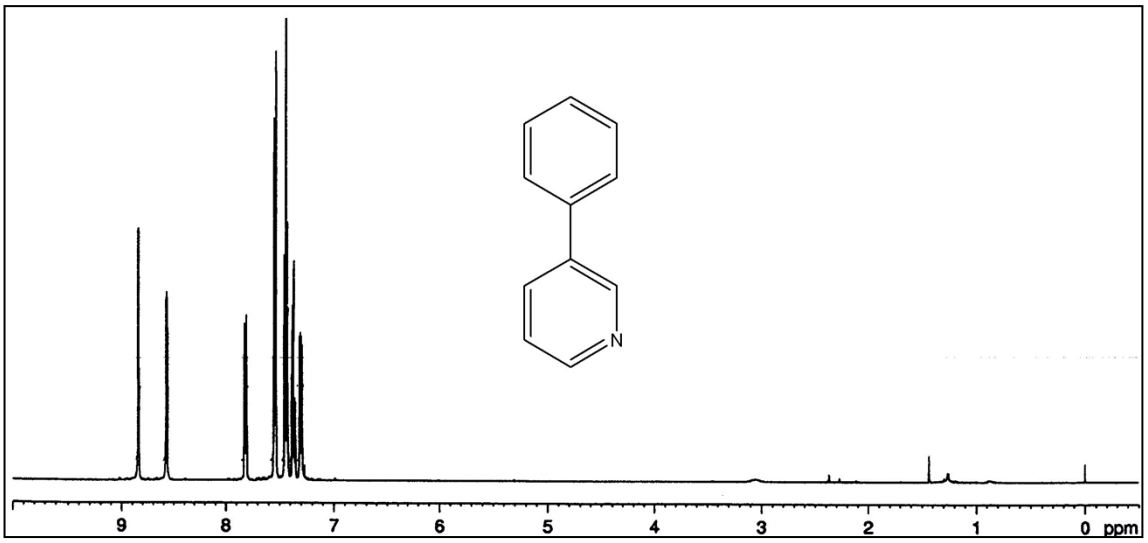


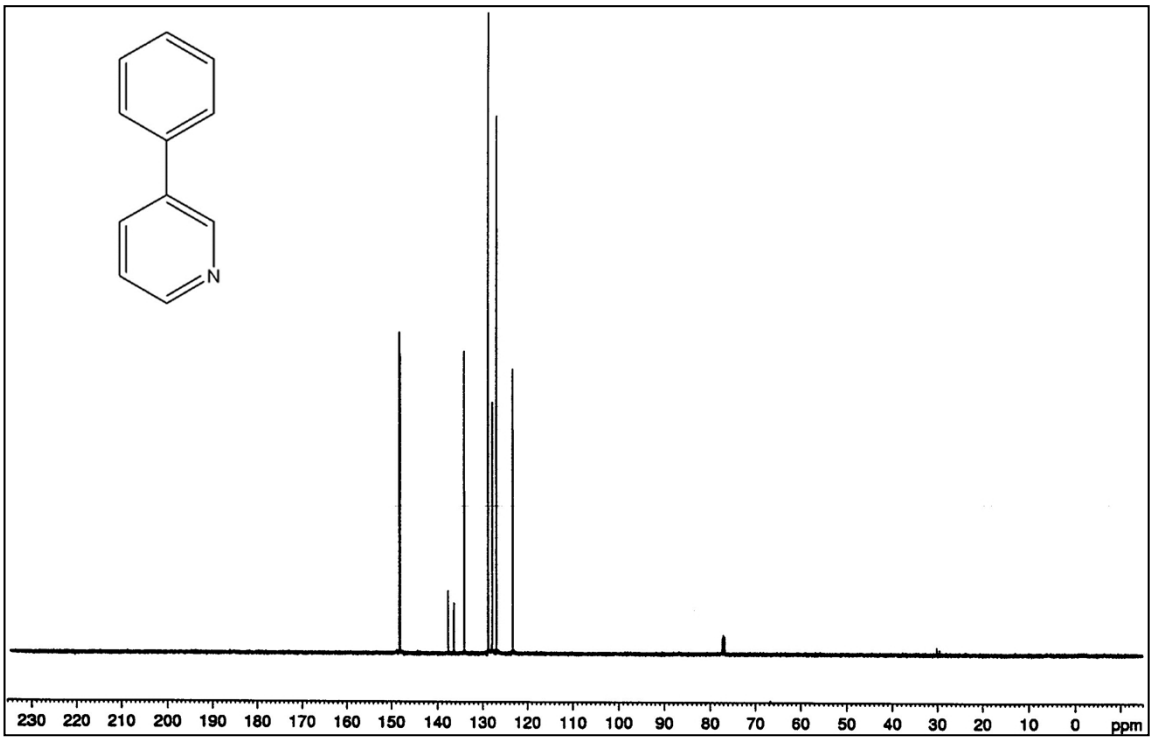
Compound-8 (2-Phenylpyridine)



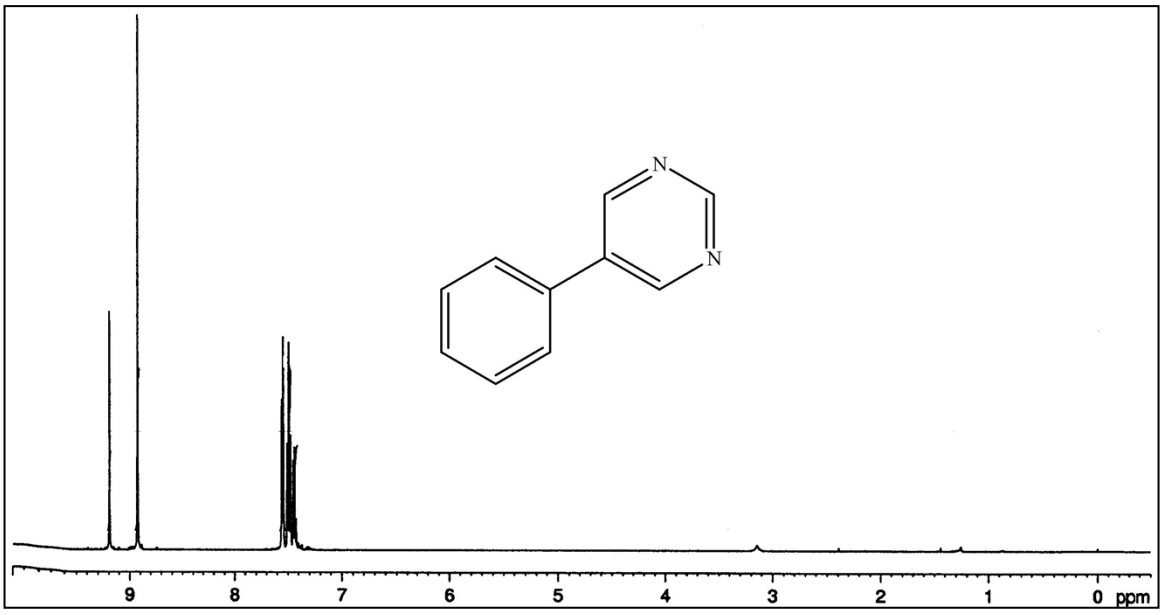


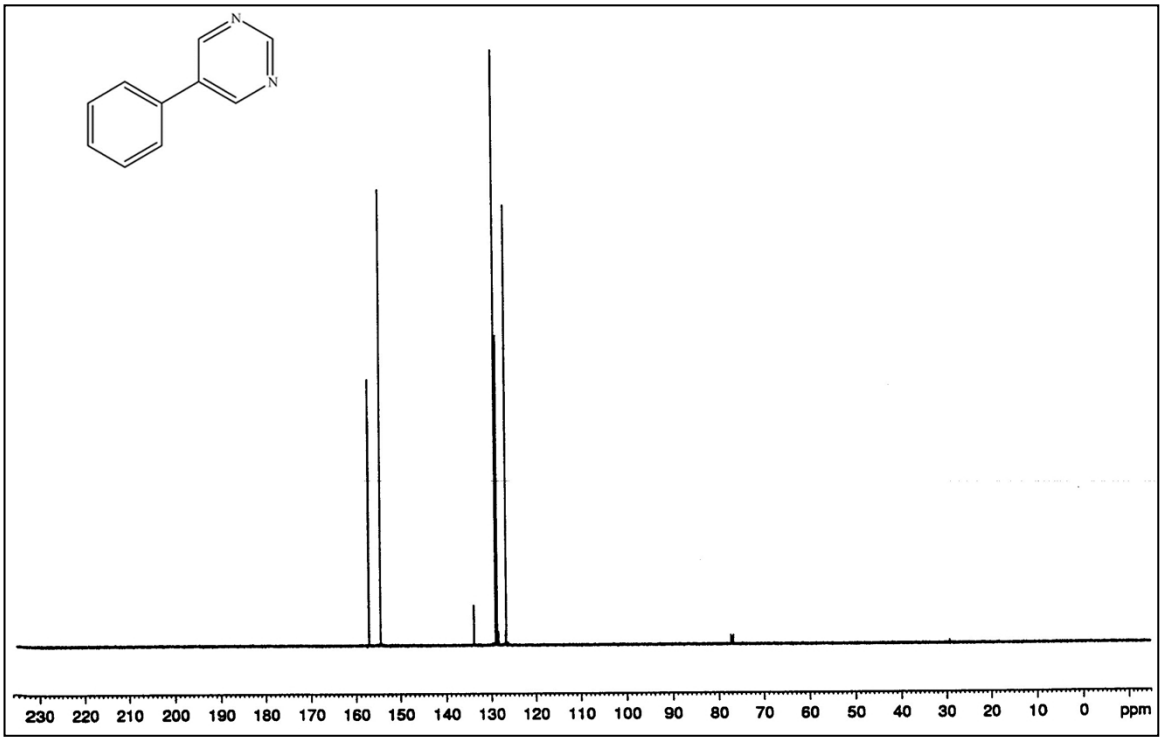
Compound-9 (3-Phenylpyridine)



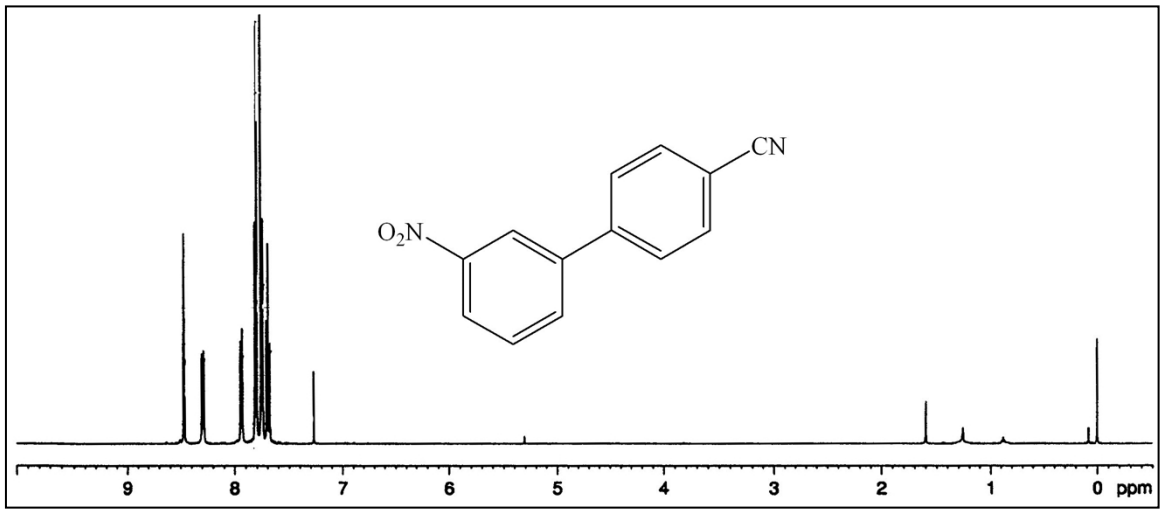


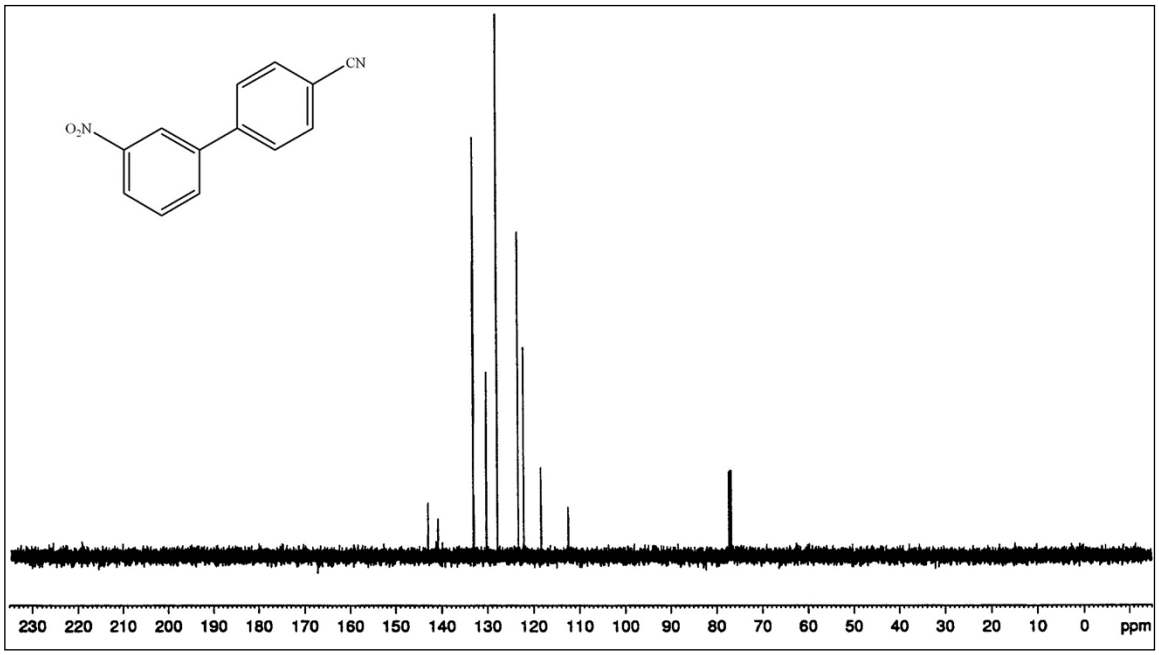
Compound-10 (5-Phenylpyrimidine)





Compound-11 (3-Nitrobiphenyl-4-carbonitrile)





^{1}H and ^{13}C NMR Spectroscopic data for the Heck-Mizoroki reaction products:

Compound-1 (*E*)-1,2-Diphenylethene.[5, 6]

White crystalline solid, ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.04 (2 H, s, Ar-H), 7.16–7.21 (2 H, m, Ar-H), 7.29 (4 H, t, Ar-H), 7.46 (4 H, d, Ar-H) ppm.

^{13}C NMR (75 MHz, CDCl3): δ 126.4, 127.5, 128.5, 128.6, 137.2 ppm

Compound-2 (*E*)-1-Methyl-4-styrylbenzene. [5-7]

White crystalline solid, ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.36 (3 H, s, CH_3), 7.02 (2 H, s, Ar-H), 7.11 (2 H, d, Ar-H), 7.16–7.24 (1 H, m, Ar-H), 7.29 (2 H, t, Ar-H), 7.34 (2 H, d, Ar-H), 7.45 (2 H, d, Ar-H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$): δ 21.2, 126.3, 127.3, 127.6, 128.6, 129.3, 134.5, 137.4 ppm.

Compound-3 (*E*)-1-Chloro-4-styrylbenzene. [6]

White crystalline solid, ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.01 (2 H, s, Ar-H), 7.19–7.39 (5H, m, Ar-H), 7.39–7.46 (4 H, m, Ar-H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$): δ 126.5, 127.3, 127.6, 127.8, 128.6, 128.9, 129.2, 133.1, 135.8, 136.9 ppm.

Compound-4 (*E*)-1-Methoxy-4-styrylbenzene. [5]

White crystalline solid, ^{1}H NMR (300 MHz, $CDCl_3$): δ 3.81(3 H, s, - OCH_3), 6.82 (2H, d, Ar-H), 6.88–7.04 (2 H, dd, Ar-H), 7.18 (1 H, t, Ar-H), 7.29 (2 H, t, Ar-H), 7.38–7.45 (4 H, m, Ar-H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$): δ 55.2, 114.0, 126.2, 126.5, 127.1, 127.6, 128.1, 128.5, 130.0, 137.6, 159.2 ppm.

Compound-5 (*E*)-1-Styryl-4-(trifluoromethyl)benzene.

White crystalline solid, ^{1}H NMR (300 MHz, $CDCl_3$): δ 6.98 (1 H, d, Ar-H) , 7.08 (1 H, d, Ar-H), 7.17–7.21 (1 H, m, Ar-H), 7.22–7.27 (2 H, m, Ar-H), 7.30–7.35 (3 H, m, Ar-H), 7.47 (3 H, t, Ar-H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$): δ 126.5, 127.3, 127.6, 127.8, 128.6, 128.7, 129.2, 133.1, 135.8, 136.9 ppm.

Compound-6 *Trans*-Cinnamic acid.[5]

White crystalline solid, ^{1}H NMR (300 MHz, $CDCl_3$): δ 6.43 (1 H, d, Ar-H), 7.34–7.41 (3 H, m, Ar-H), 7.52–7.55 (2 H, m, Ar-H), 7.79 (1H, d, Ar-H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$): δ 117.3, 128.3, 128.8, 130.6, 133.9, 147.0, 172.7 ppm.

Compound-7 *(E)*-n-Butyl cinnamate.

Yellow liquid, ^{1}H NMR (300 MHz, $CDCl_3$): δ 0.98 (3 H;t, - CH_3), 1.38–1.93 (2 H, m, -CH_2), 1.63–1.73 (2 H, m, -CH_2), 4.18 (2 H, t, -OCH_2), 6.39 (1 H, d, Ar-H), 7.32–7.38 (3 H, m, Ar-H), 7.49 (2 H; dd, Ar-H), 7.60 (1 H; d, Ar-H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$): δ 13.5, 18.9, 30.5, 64.1, 118.0, 127.8, 128.6, 129.9, 134.2, 144.3, 166.8 ppm.

Compound-8 (*E*)-Methyl cinnamate.[7]

Colorless liquid, ^{1}H NMR (300 MHz, $CDCl_3$): δ 3.79 (3 H, s, -OCH_3), 6.38 (1 H, d, Ar-H), 7.34–7.37 (3 H, m, Ar-H), 7.49–7.50 (2 H; m, Ar-H), 7.65 (1H, d, Ar-H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$): δ 51.5, 117.6, 127.9, 128.7, 130.1, 134.1, 144.6, 167.2 ppm.

Compound-9 *(E)*-3-(4-nitrophenyl) acrylic acid. [5]

Pale yellow solid, ^{1}H NMR (300 MHz, DMSO-d_6): δ 6.48 (1H; d, Ar-H), 7.62 (2 H, d Ar-H), 7.79 (1 H, d, Ar-H), 8.20 (2 H, d, Ar-H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$): δ=120.2, 128.6, 130.4, 143.0, 148.2, 160.0, 172.3 ppm.

Compound-10 *(E)*-3-(4-formylphenyl) acrylic acid.

White solid, ^{1}H NMR (300 MHz, $CDCl_3$): δ 6.42 (1 H; d, Ar-H), 7.72 (1 H; d, Ar-H), 7.80–7.85 (4H, m, Ar-H), 9.97 (1 H, s, - CHO) ppm.

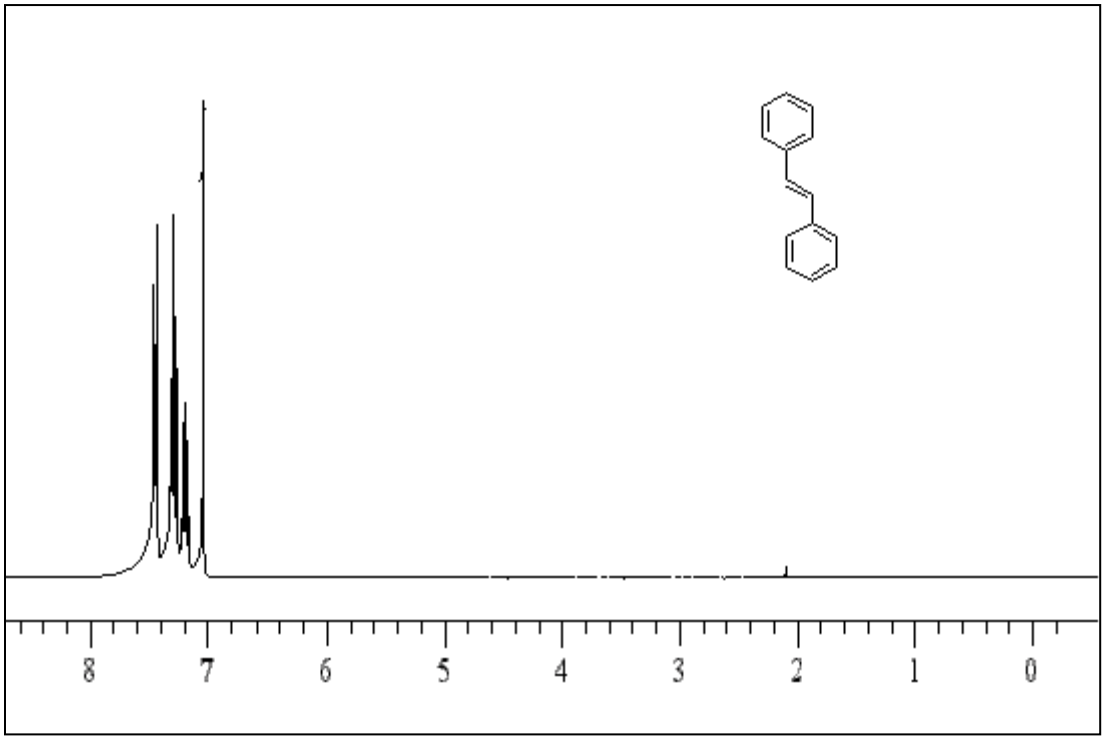
^{13}C NMR (75 MHz, $CDCl_3$): δ 116.9, 129.6, 130.1, 136.2, 141.2, 144.5, 171.5, 191.5 ppm.

Compound-11 *(E)*-3-(4-methoxyphenyl) acrylic acid. [5]

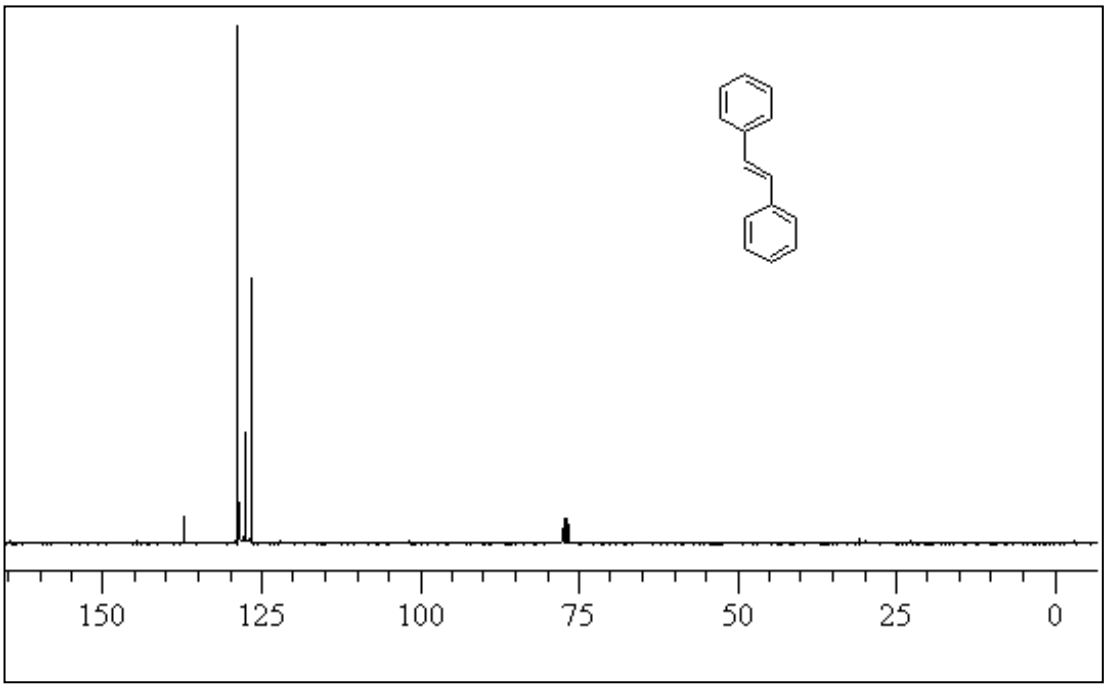
Pale brown crystalline solid, ^{1}H NMR (300 MHz, $CDCl_3$): δ 3.85 (3 H, s, - OCH_3), 6.42 (1 H, d, Ar-H), 6.99 (2 H, d, Ar-H), 7.58 (2 H, d, Ar-H), 7.82 (1 H, d, Ar-H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$): δ 55.2, 114.0, 117.2, 128.4, 130.2, 134.2, 147.0, 172.3 ppm.

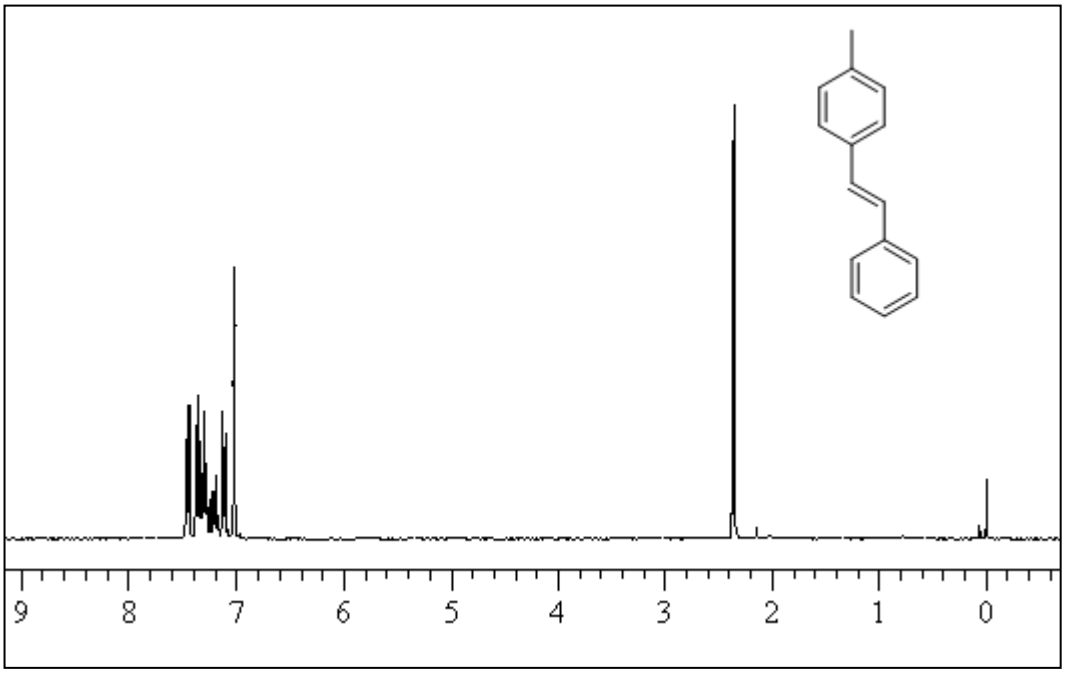
1. **^{1}H NMR (300 MHz, $CDCl_3$) spectrum of (*E*)-1,2-Diphenylethene.**



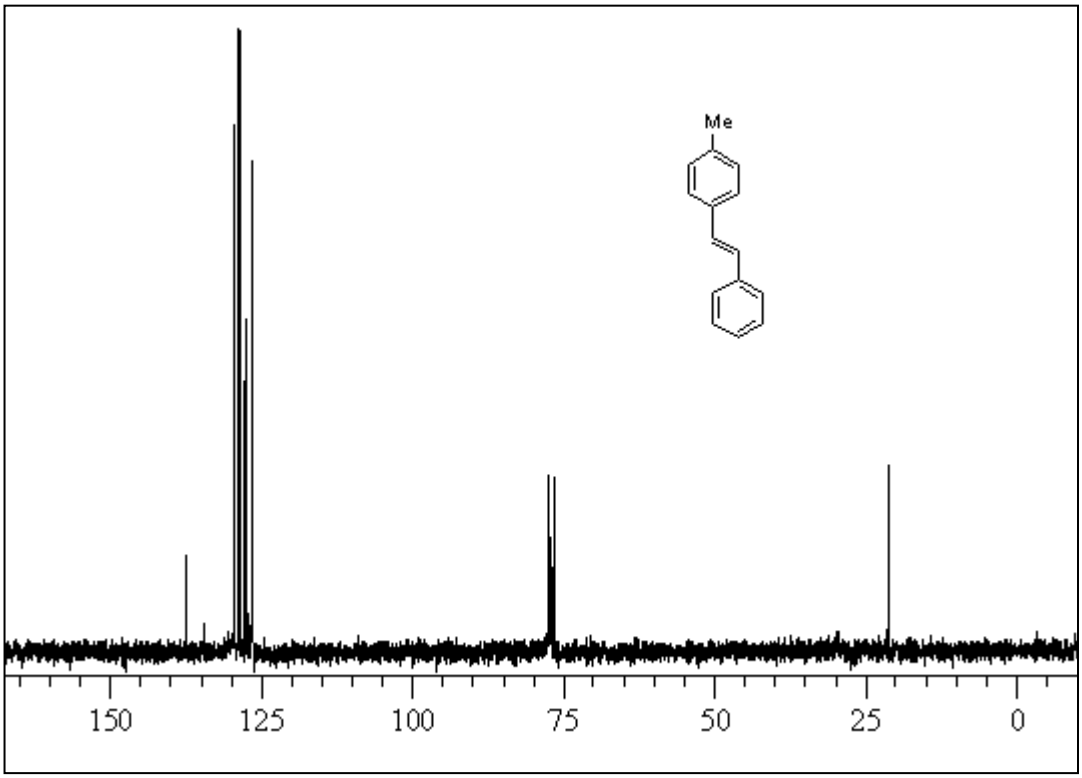
^{13}C NMR (50 MHz, $CDCl_3$) spectrum of (*E*)-1,2-Diphenylethene.



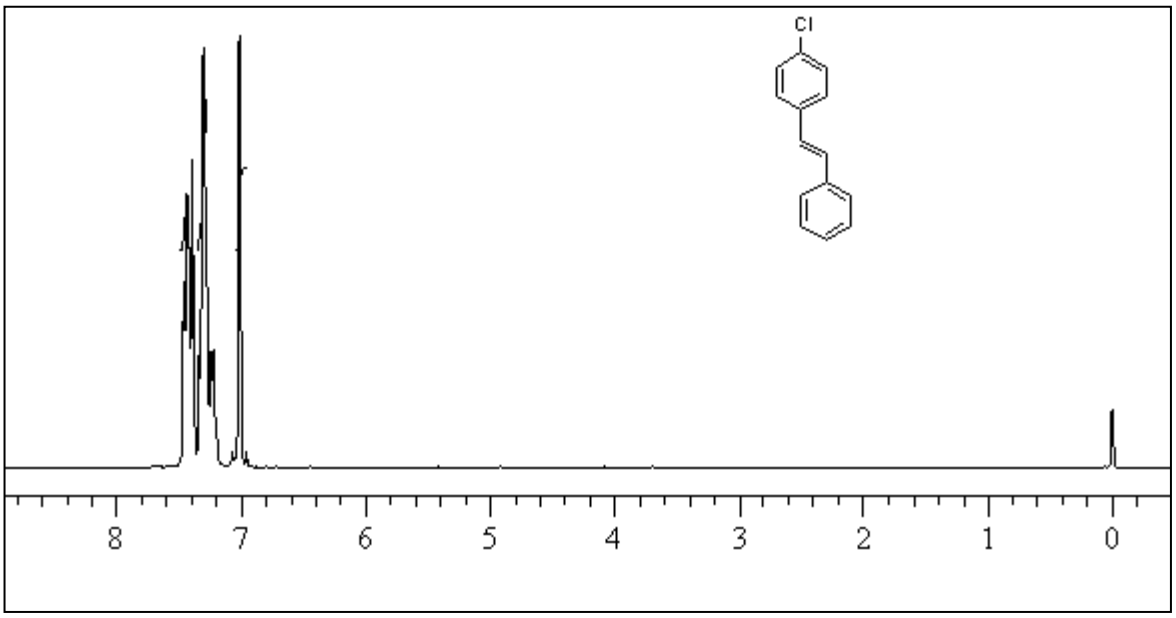
2. **^{1}H NMR (300 MHz, $CDCl_3$) spectrum of (*E*)-1-Methyl-4-styrylbenzene.**



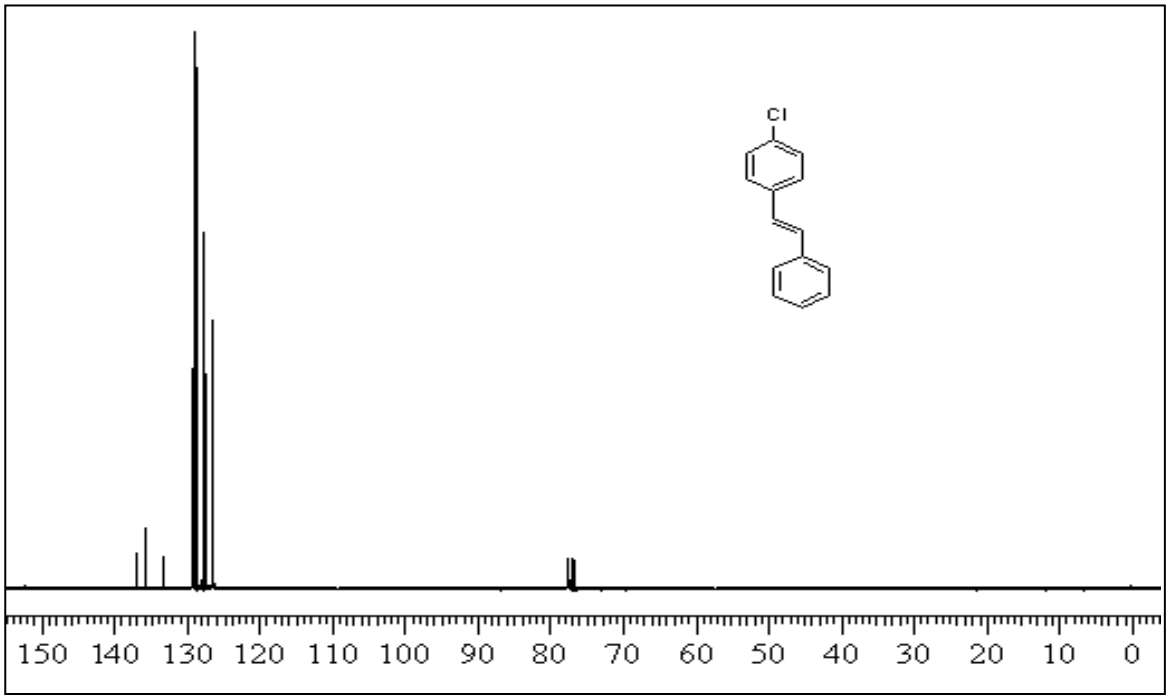
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of (*E*)-1-Methyl-4-styrylbenzene.



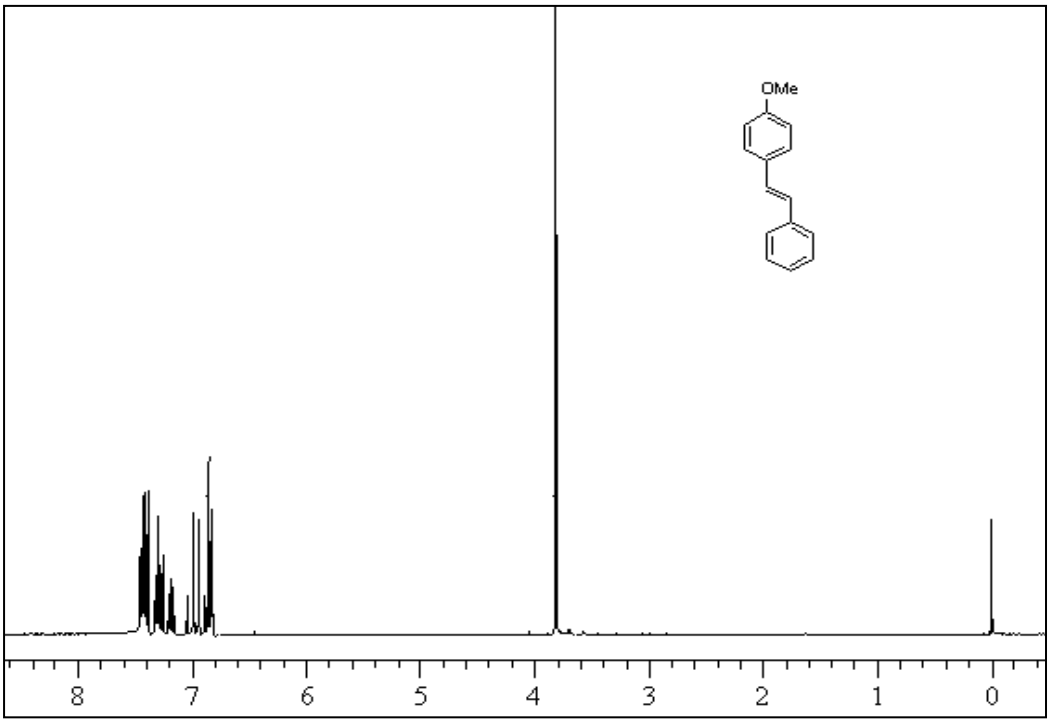
3. **^{1}H NMR (300 MHz $CDCl_3$) spectrum of (*E*)-1-Chloro-4-styrylbenzene**



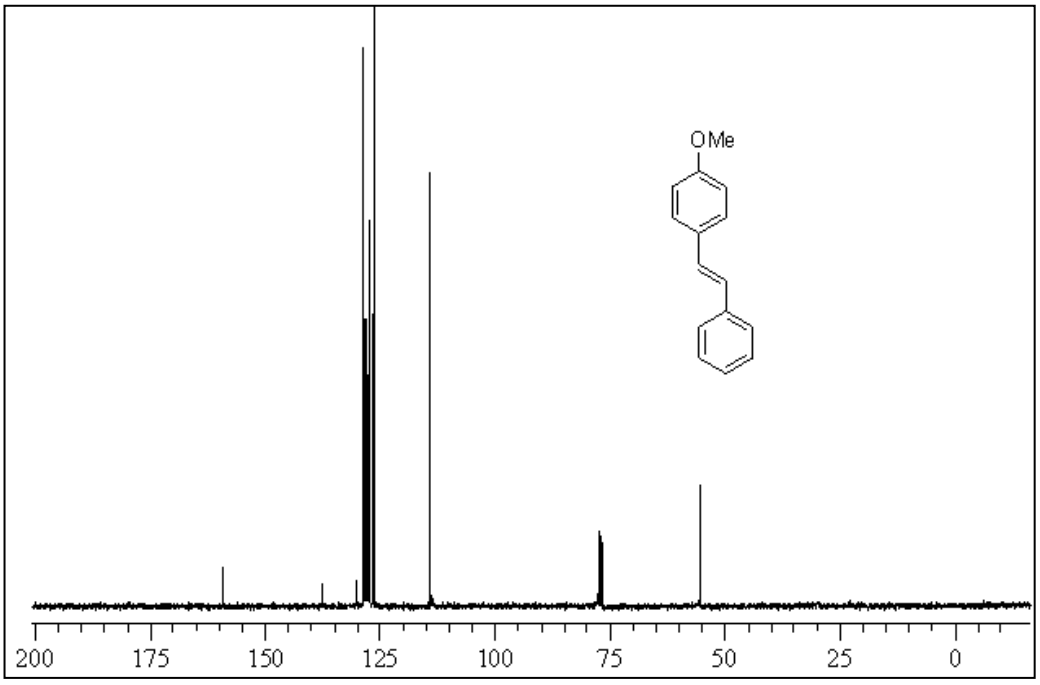
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of (*E*)-1-Chloro-4-styrylbenzene.



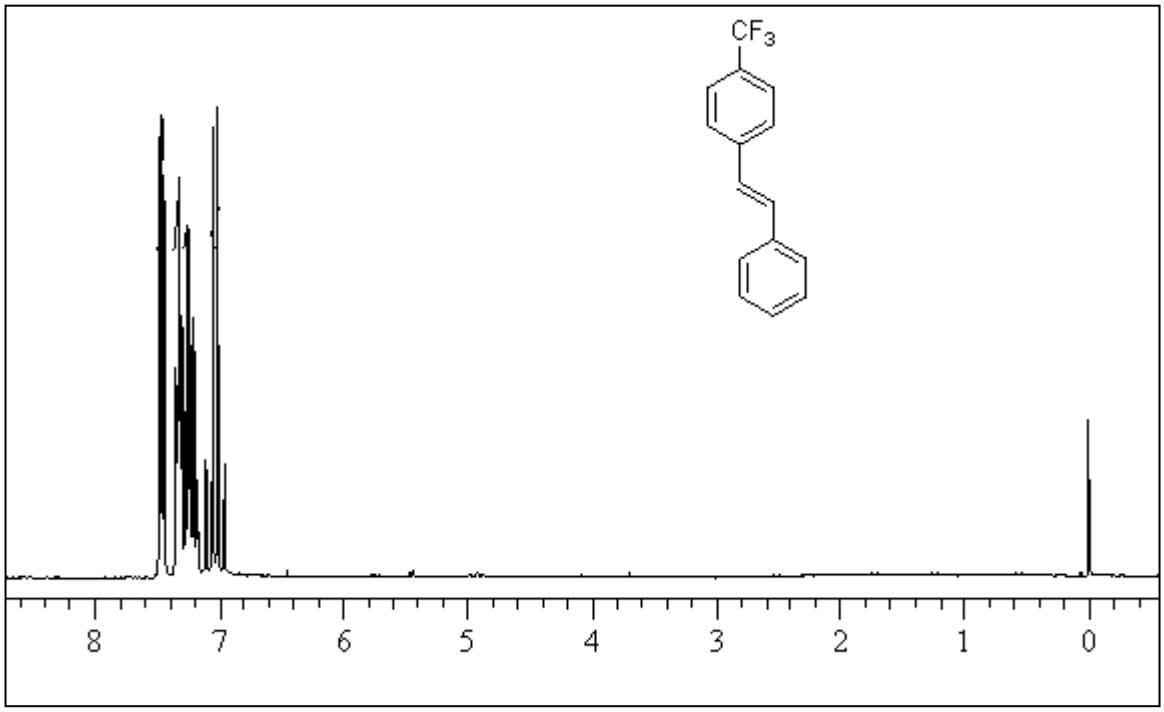
4. **^{1}H NMR (300 MHz $CDCl_3$) spectrum of (*E*)-1-Methoxy-4-styrylbenzene.**



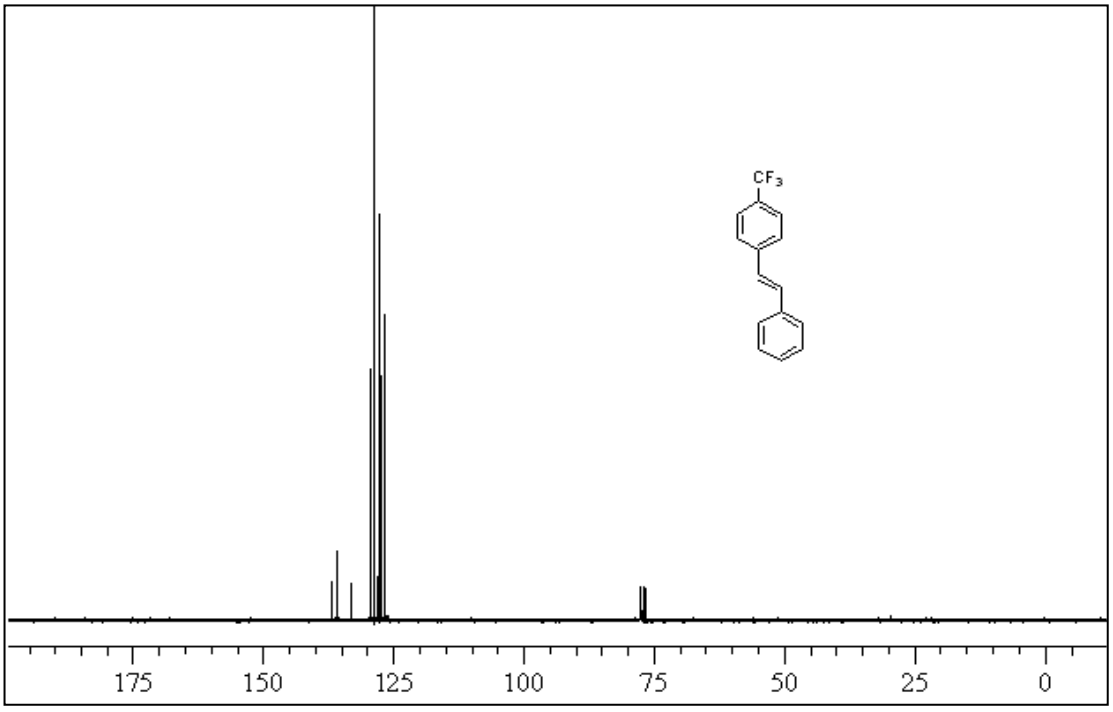
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of (*E*)-1-Methoxy-4-styrylbenzene.



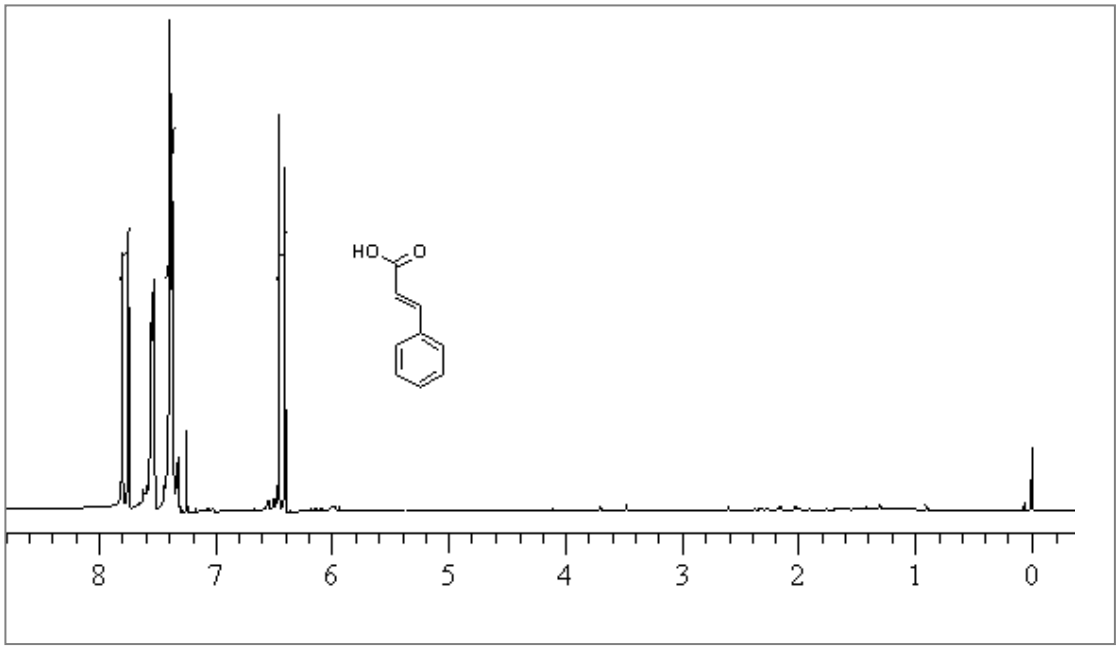
5. **^{1}H NMR (300 MHz $CDCl_3$) spectrum of (*E*)-1-Styryl-4-(trifluoromethyl)benzene.**



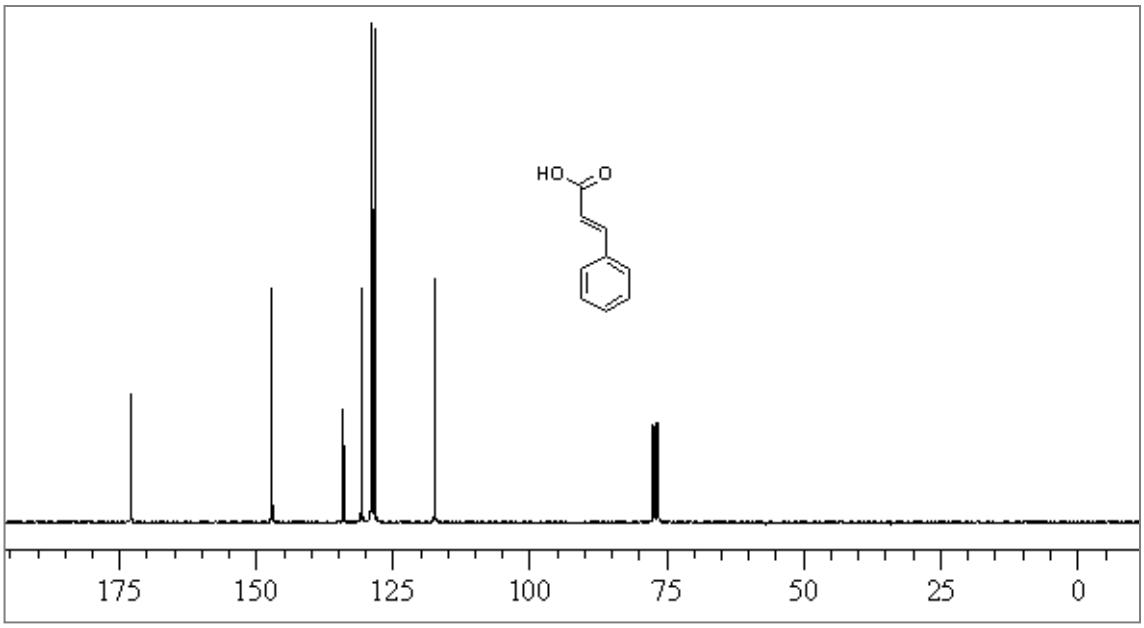
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of (*E*)-1-Styryl-4-(trifluoromethyl) benzene.



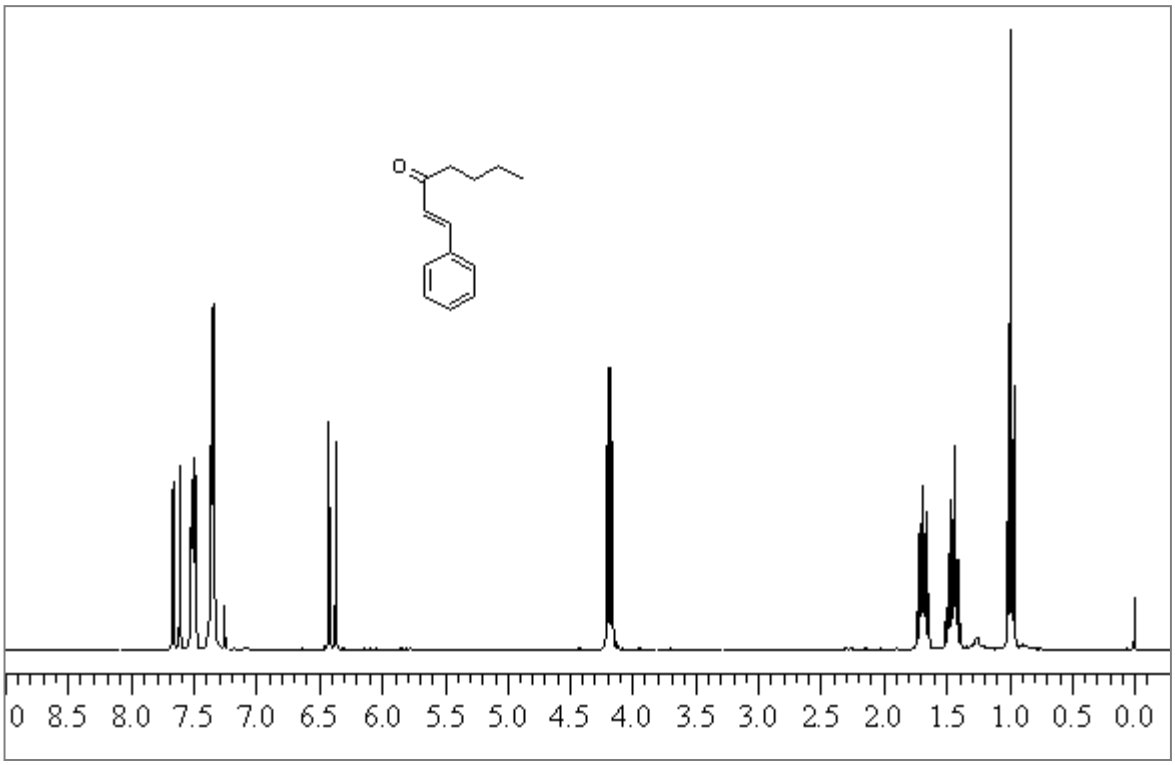
6. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of *trans* cinnamic acid.



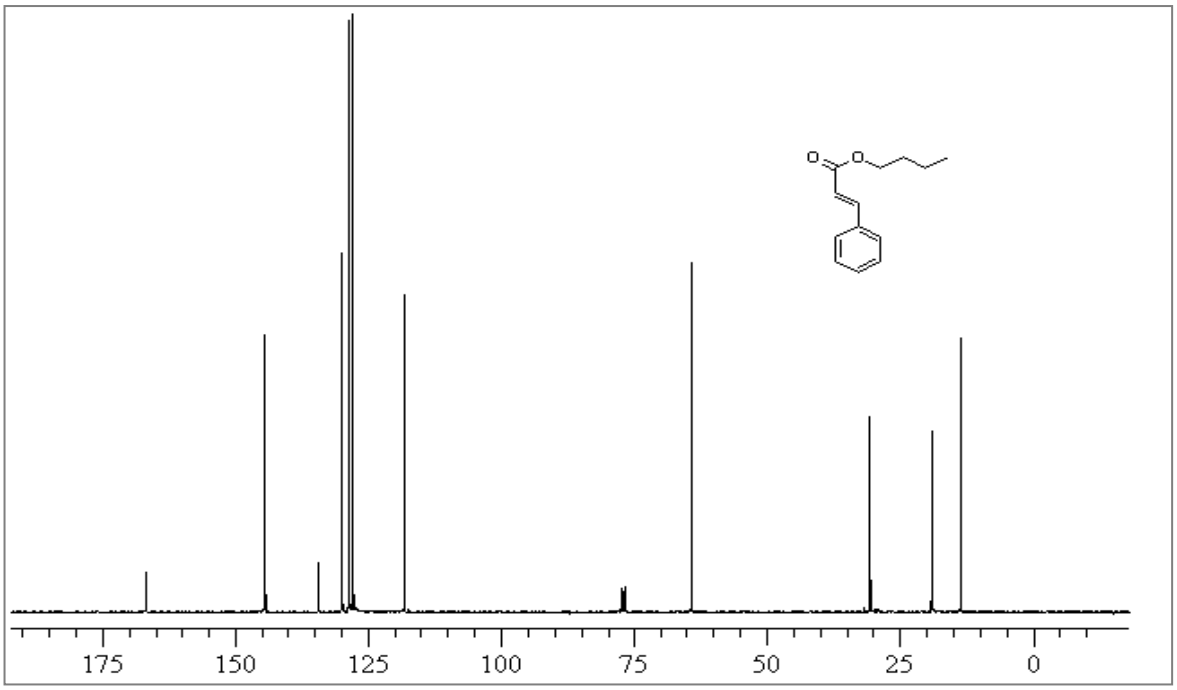
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of *trans* cinnamic acid.



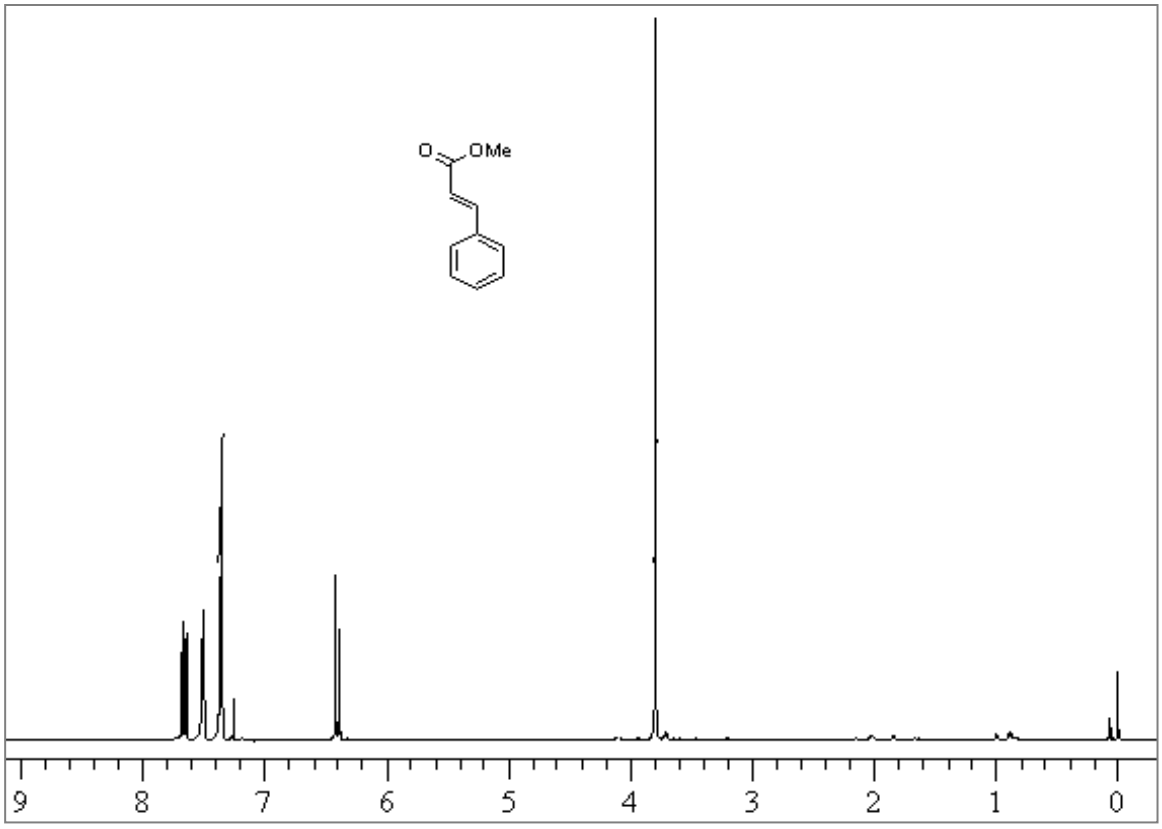
7. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of (*E*)-n-butyl cinnamate.



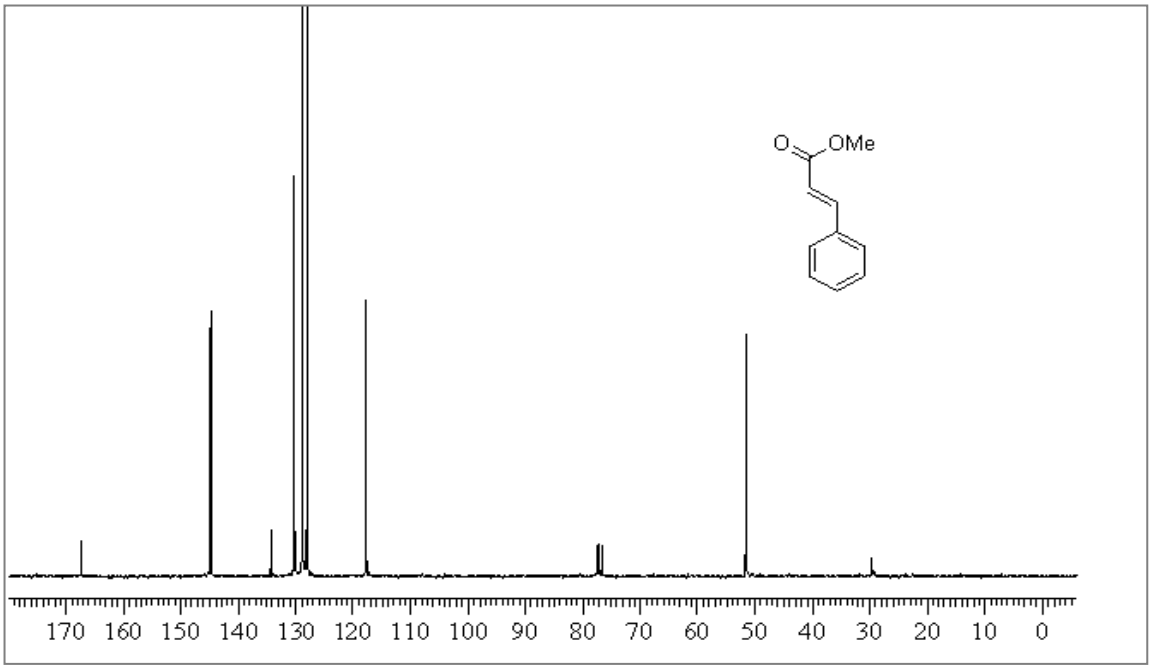
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of (*E*)-n-butyl cinnamate.



8. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of (*E*)-methyl cinnamate.



^{13}C NMR (75 MHz, $CDCl_3$) spectrum of (*E*)-methyl cinnamate.



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