Supplementary Materials: An amino-chain modified β-cyclodextrin: a supramolecular ligand for $Pd(OAc)_2$ acceleration in Suzuki–Miyaura coupling reactions in water.

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Succinyl-β-cyclodextrin-β-cyclodextrin (Suc-β-CD)

MALDI-TOF MS: m/z 1177 [M + H]+.^{1}H NMR (600 MHz, D_2O 99.9 atom% D, TMS): δ 5.05 (s, 7H, H1), 3.95-3.86 (m, 28H, H3, H5 and H6), 3.64-3.57 (m, 14H, H2 and H4), 3.45(m, 1H, H4'), 3.07-2.84 (br, 4H, H6'and H7), 2.73-2.67 (m, 2H, H8).

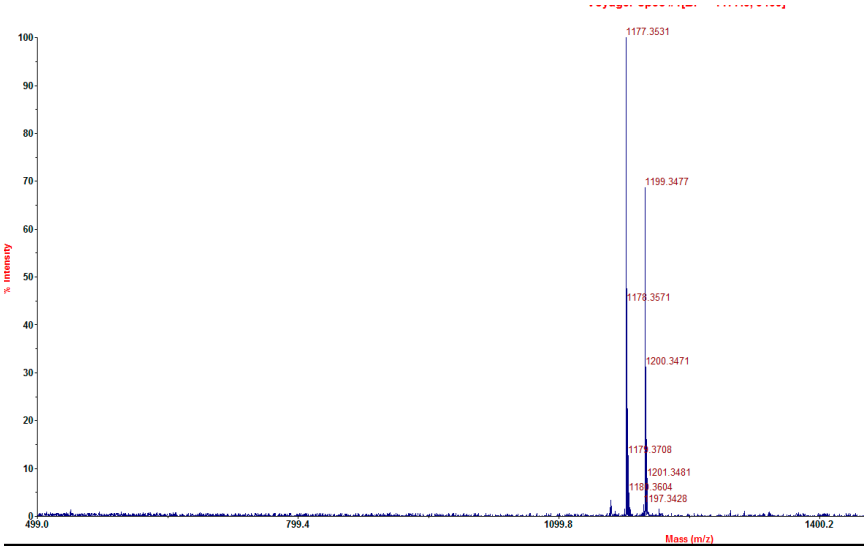


Figure S1. MALDI-TOF-MS of Et-β-CD.

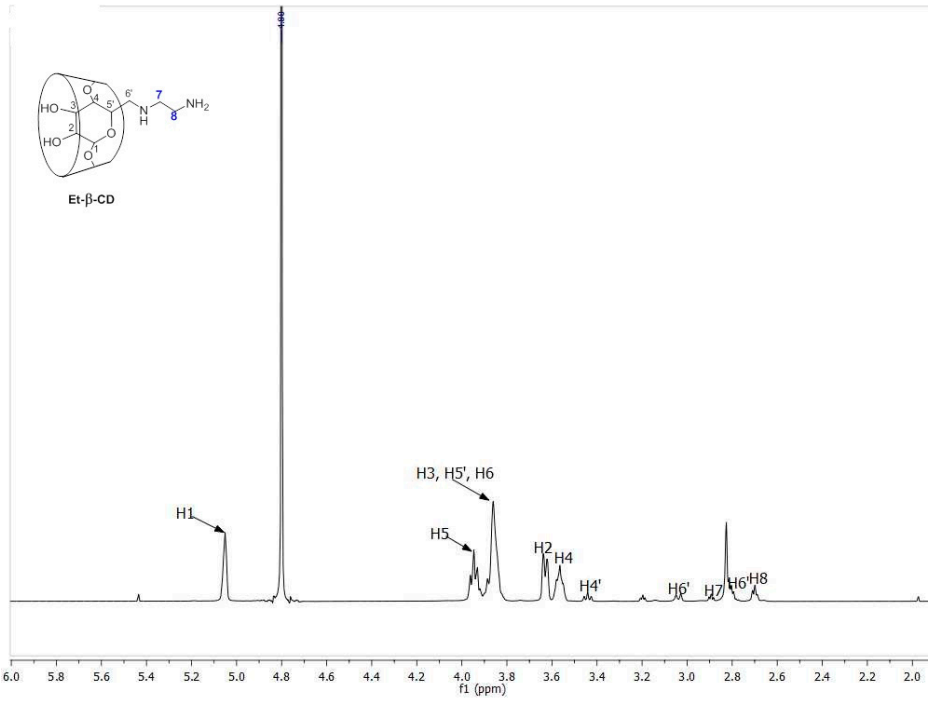


Figure S2. ^{1}H NMR of Et-β-CD measured in D_2O.

Spectral data of the Compounds

3-methoxy-4'-nitro-1,1'-biphenyle (**3a**)

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.31 – 8.27 (2 H, m), 7.74 – 7.70 (2 H, m), 7.43 – 7.39 (1 H, m), 7.20 (1 H, d, *J* = 7.7), 7.15 – 7.12 (1 H, m), 6.99 (1 H, dd, *J* = 8.3, 2.5), 3.88 (3 H, s). 13C NMR (125 MHz, $CDCl_3$) δ 163.80, 160.28, 147.62, 140.36, 130.35, 128.00, 124.23, 124.20, 119.95, 114.26, 113.39, 77.16, 55.54.

4-nitro-1,1'-biphenyl (**3b**)

NMR (500 MHz, CDCl3): δ 8.32 – 8.27 (2 H, m), 7.76 – 7.72 (2 H, m), 7.65 – 7.60 (2 H, m), 7.52 – 7.48 (2 H, m), 7.47 – 7.42 (1 H, m). 13C NMR (125 MHz, $CDCl_3$) δ 147.75, 138.89, 129.28, 129.05, 127.92, 127.89, 127.54, 127.51, 127.48, 124.26, 124.23.

1-(4-nitrophenyl) naphthalene (**3c**)

NMR (500 MHz, CDCl3): δ 8.37 – 8.32 (2 H, m), 7.93 (2 H, dd, *J* 8.0, 4.2), 7.79 – 7.76 (1 H, m), 7.68 – 7.64 (2 H, m), 7.57 – 7.51 (2 H, m), 7.47 (1 H, ddd, *J* 8.2, 6.8, 1.4), 7.42 (1 H, dd, *J* 7.0, 1.2). 13C NMR

(125 MHz, $CDCl_3$) δ 147.80, 137.90, 133.91, 131.05, 129.10, 128.71, 127.23, 126.87, 126.36, 125.45, 125.26, 123.72.

2,4-difluoro-4'-nitro-1,1'-biphenyl (**3d**)

NMR (500 MHz, CDCl3): δ 8.32 – 8.27 (2 H, m), 7.70 – 7.66 (2 H, m), 7.46 (1 H, td, *J* 8.7, 6.3), 7.05 – 7.00 (1 H, m), 6.99 – 6.94 (1 H, m). 13C NMR (125 MHz, $CDCl_3$) δ 164.38, 164.29, 162.38, 162.28, 147.34, 141.60, 131.62, 131.58, 131.54, 131.51, 129.84, 129.81, 123.88, 112.39, 112.36, 112.22, 112.19, 105.16, 104.96, 104.75.

2,4-difluoro-4'-nitro-1,1'-biphenyl (**3e**)

NMR (500 MHz, CDCl3): δ 7.40 – 7.37 (2 H, m), 7.36 – 7.32 (2 H, m), 6.91 – 6.90 (2 H, m), 6.74 – 6.71 (1 H, m), 4.94 (1 H, s).13C NMR (125 MHz, $CDCl_3$) δ 163.11, 163.02, 161.14, 161.04, 155.33, 132.62, 131.31, 131.27, 131.24, 131.20, 130.42, 130.40, 117.33, 115.59, 111.70, 111.67, 111.53, 111.50, 104.65, 104.44, 104.24.

4'-nitro-3,5-bis(trifluoromethyl)-1,1'-biphenyl (**3f**)

NMR (500 MHz, CDCl3): δ 8.40 – 8.36 (2 H, m), 8.06 (2 H, s), 7.97 (1 H, s), 7.82 – 7.78 (2 H, m). 13C NMR (125 MHz, $CDCl_3$) δ 148.27, 144.46, 141.10, 133.02, 132.70, 128.42, 127.68, 127.66, 124.68, 122.69, 122.66, 122.63, 122.60, 122.57.

3-methyl-1,1'-biphenyl (**3g**)

NMR (500 MHz, CDCl3): δ 7.61 – 7.56 (3 H, m), 7.44 – 7.40 (3 H, m), 7.33 (2 H, dt, *J* 5.2, 2.4), 7.16 (1 H, d, *J* 7.5), 2.41 (3 H, s). 13C NMR (125 MHz, $CDCl_3$) δ 141.49, 141.37, 138.46, 128.89, 128.86, 128.83, 128.80, 128.13, 128.12, 127.39, 127.31, 124.41, 21.69.

1,1'-biphenyl (**3h**)

NMR (500 MHz, CDCl3): δ 7.59 (4 H, dt, *J* 8.1, 1.7), 7.46 – 7.41 (4H, m), 7.36 – 7.32 (2 H, m). 13C NMR (125 MHz, $CDCl_3$) δ 141.38, 128.90, 127.39, 127.31.

3-methyl-1,1'-biphenyl (**3i**)

NMR (500 MHz, CDCl3): δ 8.25 (1 H, s), 7.99 (1 H, d, *J* 8.5), 7.91 (1 H, d, *J* 8.1), 7.85 (1 H, d, *J* 8.0), 7.76 (1 H, dd, *J* 3.0, 2.3), 7.55 – 7.51 (1 H, m), 7.51 – 7.46 (3 H, m), 7.40 (1 H, ddd, *J* 8.2, 6.8, 1.3), 7.35 – 7.33 (1 H, m), 7.30 – 7.28 (1 H, m), 6.63 (1 H, ddd, *J* 3.0, 2.1, 0.8). 13C NMR (125 MHz, $CDCl_3$) δ 141.57, 135.26, 133.97, 132.66, 128.29, 127.41, 127.16, 126.70, 125.87, 125.72, 125.54, 124.91, 124.79, 122.21, 110.76, 103.04.

2-([1,1'-biphenyl]-4-yl)propan-2-ol (**3j**)

NMR (500 MHz, CDCl3): δ 7.61 – 7.55 (6 H, m), 7.46 – 7.41 (2 H, m), 7.36 – 7.32 (1 H, m), 1.63 (6 H, s). 13C NMR (125 MHz, $CDCl_3$) δ 148.29, 140.98, 139.79, 128.90, 127.35, 127.22, 127.12, 125.02, 31.92.

4-methoxy-1,1'-biphenyl (**3k**)

NMR (500 MHz, CDCl3): δ 7.57 – 7.51 (4 H, m), 7.44 – 7.39 (2 H, m), 7.32 – 7.28 (1 H, m), 7.00 – 6.96 (2 H, m), 3.84 (3 H, s). 13C NMR (125 MHz, $CDCl_3$) δ 159.28, 140.96, 133.91, 128.86, 128.29, 126.88, 126.79, 114.33, 55.48.

2-methyl-1,1'-biphenyl (**3l**)

NMR (500 MHz, CDCl3): δ 7.43 – 7.38 (2 H, m), 7.35 – 7.30 (3 H, m), 7.28 – 7.25 (2 H, m), 7.25 – 7.22 (2 H, m), 2.27 (3 H, s). 13C NMR (125 MHz, $CDCl_3$) δ 142.10, 142.07, 135.48, 130.44, 129.93, 129.33, 128.20, 127.38, 126.89, 125.89, 20.61.

4-methyl-1,1'-biphenyl (**3m**)

NMR (500 MHz, CDCl3): 7.57 (2 H, dt, *J* 8.1, 1.6), 7.51 – 7.47 (2 H, m), 7.44 – 7.40 (2 H, m), 7.34 – 7.29 (1 H, m), 7.24 (2 H, d, *J* 7.9), 2.39 (3 H, s). 13C NMR (125 MHz, $CDCl_3$) δ 141.30, 138.50, 137.16, 129.62, 128.85, 127.13, 127.11, 21.24.

[1,1'-biphenyl]-2-carbaldehyde (**3n**)

NMR (500 MHz, CDCl3): δ 9.99 (1 H, s), 8.03 (1 H, dd, *J* 7.8, 1.3), 7.66 – 7.61 (1 H, m), 7.51 – 7.44 (4 H, m), 7.40 – 7.37 (2 H, m).13C NMR (125 MHz, $CDCl_3$) δ 92.64, 159.39, 146.12, 137.88, 133.71, 130.91, 130.24, 128.56, 128.26, 127.91, 127.70.

3'-methoxy-[1,1'-biphenyl]-4-ol (**3o**)

NMR (500 MHz, CDCl3): δ 7.49 – 7.45 (2 H, m), 7.35 – 7.31 (1 H, m), 7.14 – 7.11 (1 H, m), 7.08 – 7.06 (1 H, m), 6.91 – 6.88 (2 H, m), 6.86 (1 H, dd, *J* 8.2, 2.5), 4.92 (1 H, s), 3.86 (3 H, s). 13C NMR (125 MHz, $CDCl_3$) δ 160.03, 155.32, 142.43, 133.99, 129.86, 128.58, 119.44, 115.75, 112.65, 112.23, 55.45.

3',5'-bis(trifluoromethyl)-[1,1'-biphenyl]-4-ol (**3p**)

NMR (500 MHz, CDCl3): δ 7.95 (2 H, s), 7.80 (1 H, s), 7.53 – 7.48 (2 H, m), 6.99 – 6.94 (2 H, m), 5.23 (1 H, s).13C NMR (125 MHz, $CDCl_3$) δ 156.44, 154.68, 132.59, 128.80, 126.80, 120.47, 120.44, 120.41, 120.38, 120.35, 117.34, 116.32.

2-phenylpyridine (**3q**)
1H NMR (500 MHz, CDCl3) δ 8.68 (d, *J* = 4.6 Hz, 1H), 7.98 (d, *J* = 7.7 Hz, 2H), 7.71 (m, *J* = 6.9 Hz, 2H), 7.45 (t, *J* = 7.5 Hz, 2H), 7.41 (t, *J* = 7.3 Hz, 1H), 7.22 (t, *J* = 5.6 Hz, 1H).

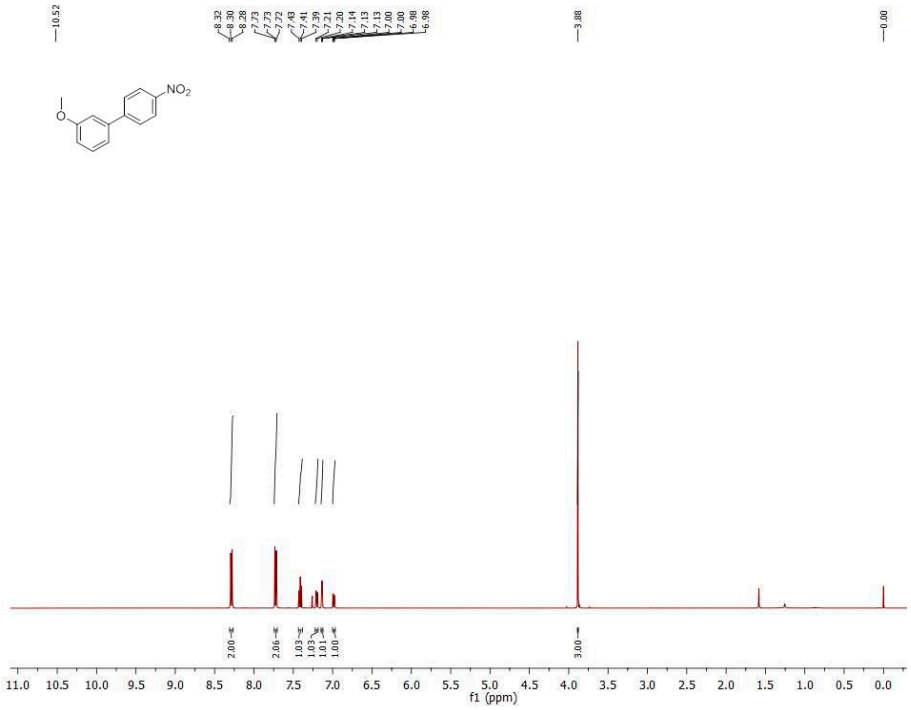
4-chloro-4'-methoxy-1,1'-biphenyl (**3r**)
1H NMR (500 MHz, CDCl3) δ 7.46 (m, *J* = 9.0 Hz, 4H), 7.36 (d, *J* = 8.3 Hz, 2H), 6.97 (d, *J* = 8.5 Hz, 2H), 3.84 (s, 3H).

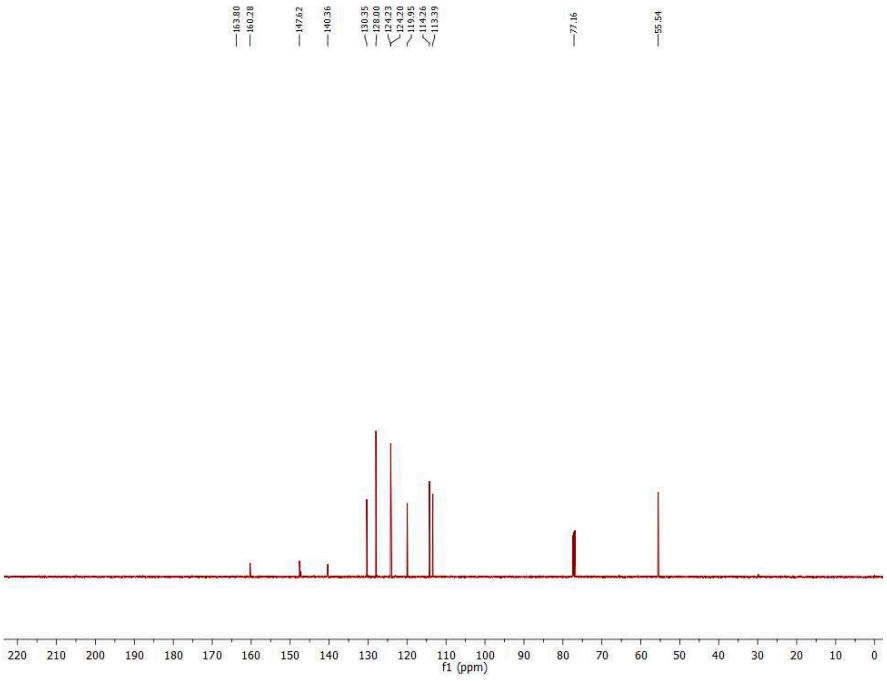
4-nitro-1,1'-biphenyl (**3s**)

NMR (500 MHz, CDCl3): δ 8.31 – 8.26 (2 H, m), 7.75 – 7.72 (2 H, m), 7.65 – 7.61 (2 H, m), 7.51 – 7.47 (2 H, m), 7.47 – 7.42 (1 H, m). 13C NMR (125 MHz, $CDCl_3$) δ 147.75, 138.89, 129.28, 129.05, 127.92, 127.89, 127.54, 127.51, 127.48, 124.26, 124.23.

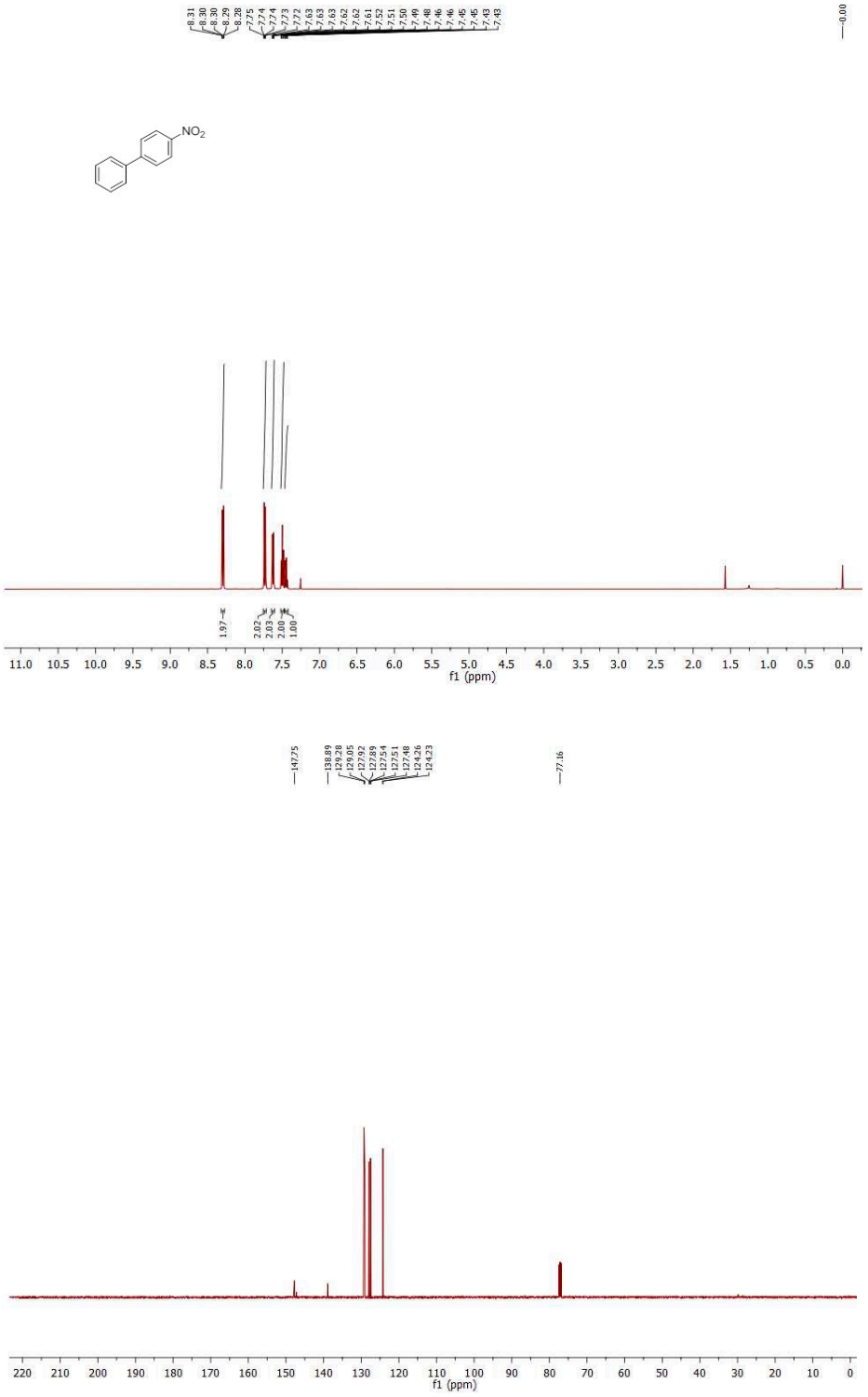
^{1}H NMR and ^{13}C NMR Spectra of all compounds

^{1}H and ^{13}C NMR of compound 3a

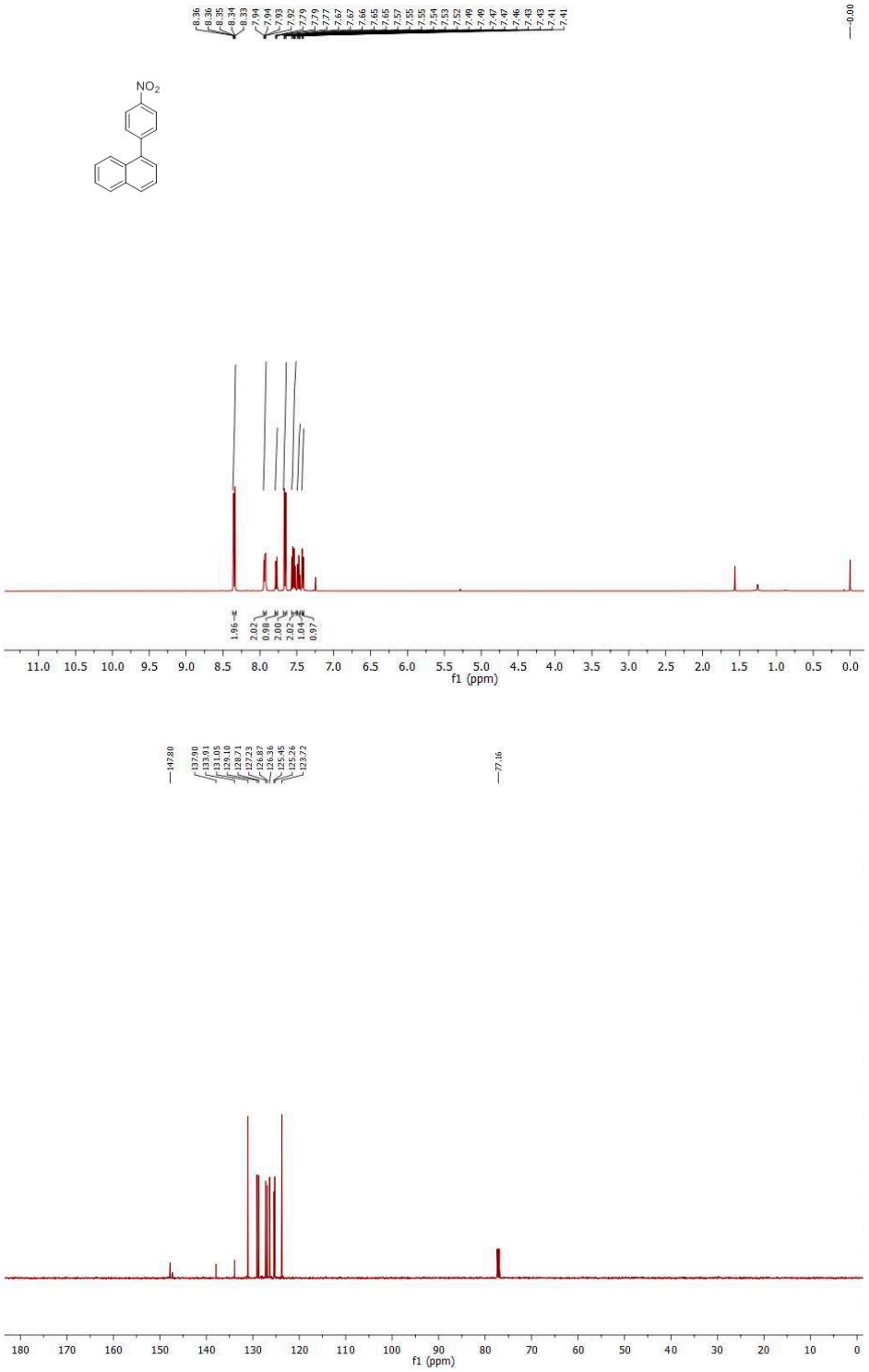




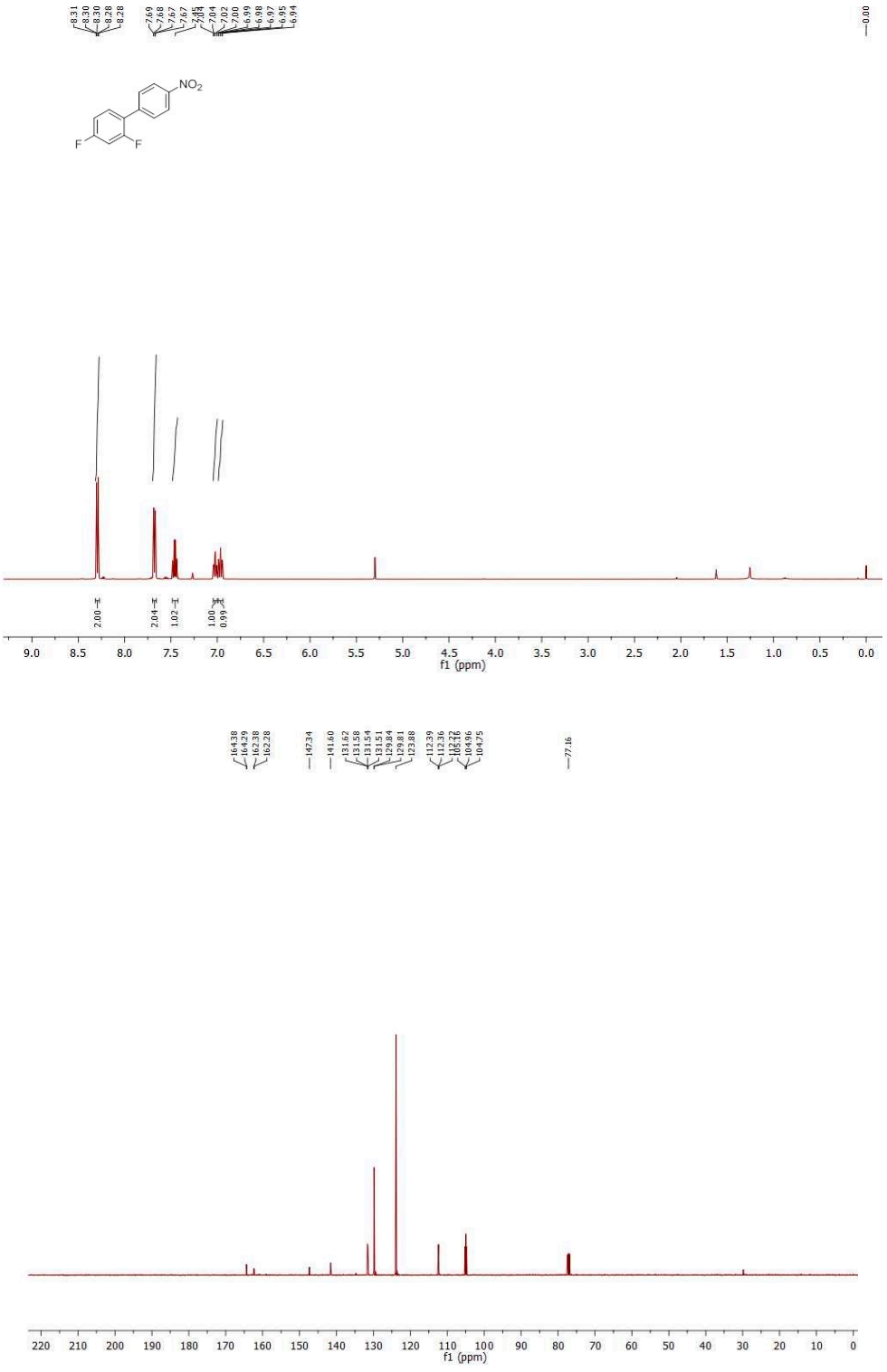
^{1}H and ^{13}C NMR of compound 3b



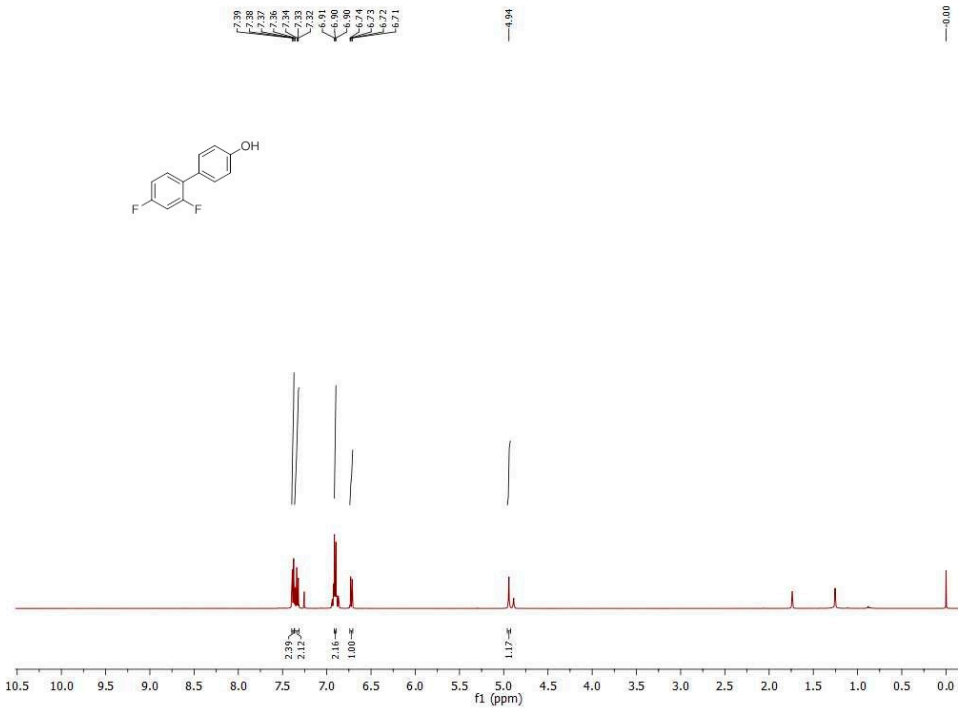
^{1}H and ^{13}C NMR of compound 3c

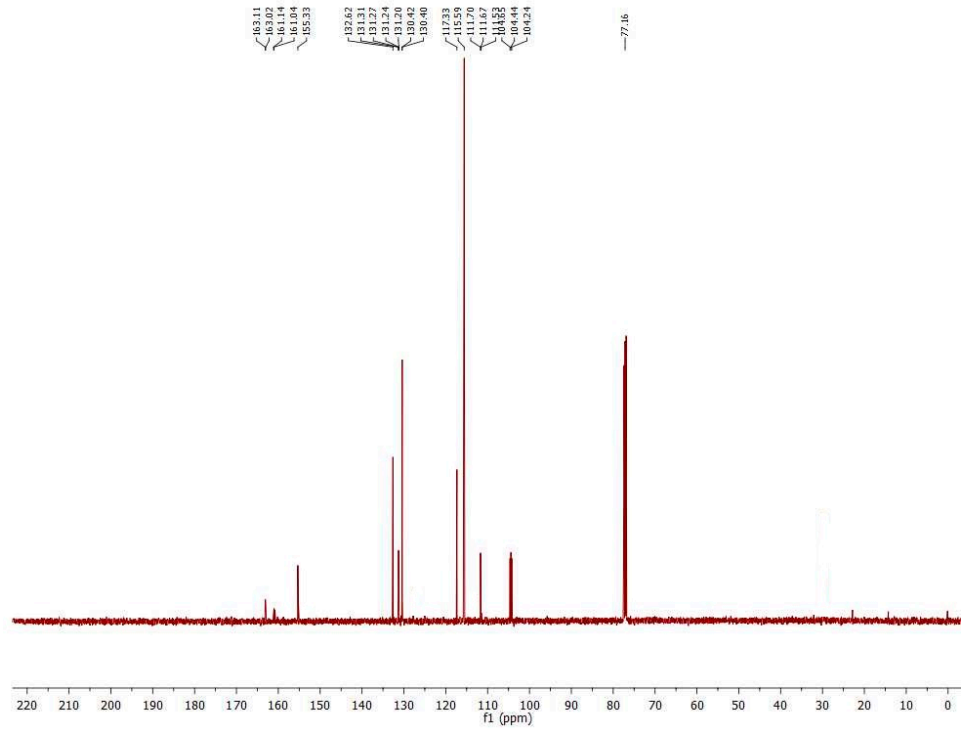


^{1}H and ^{13}C NMR of compound 3d

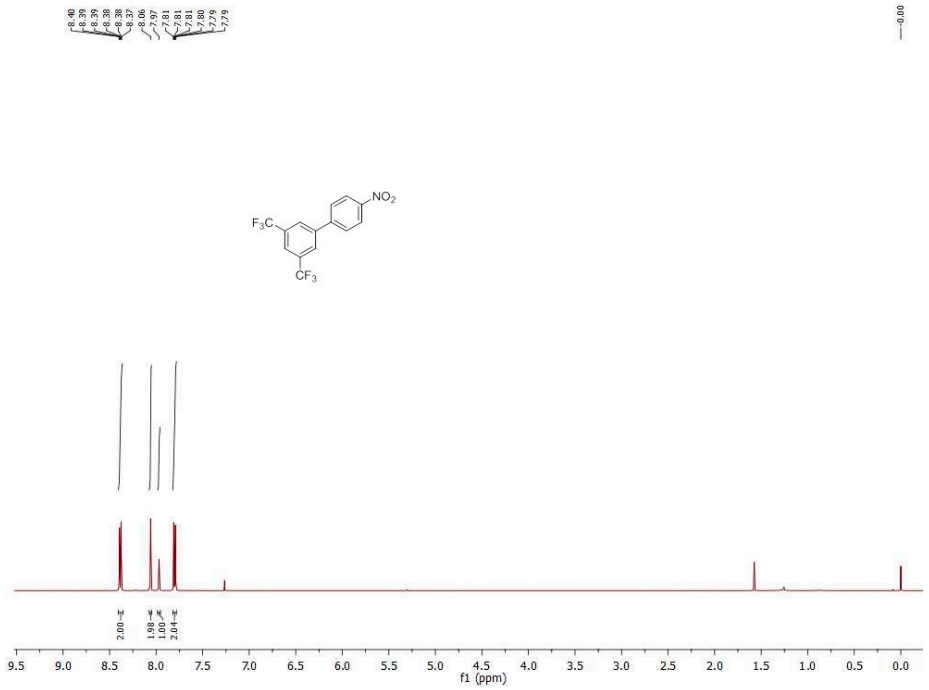


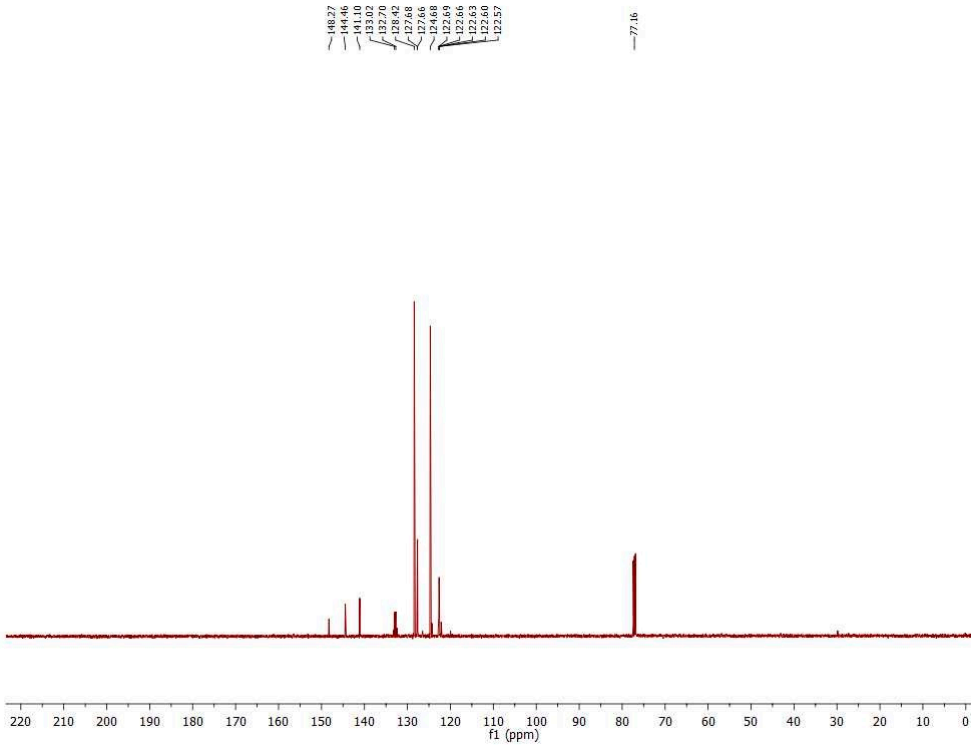
^{1}H and ^{13}C NMR of compound 3e



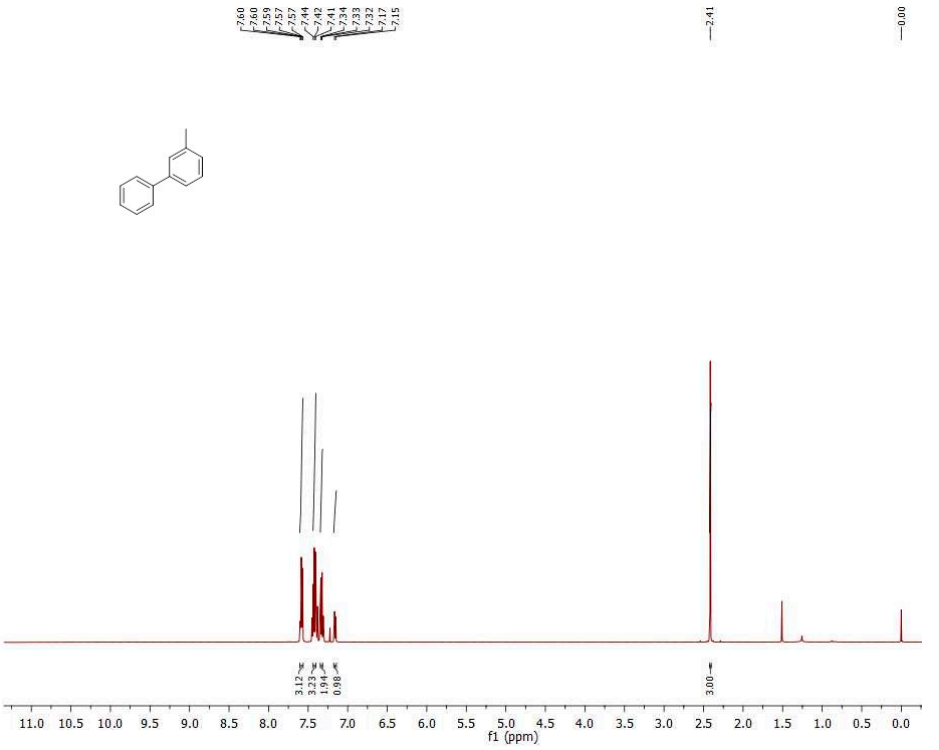


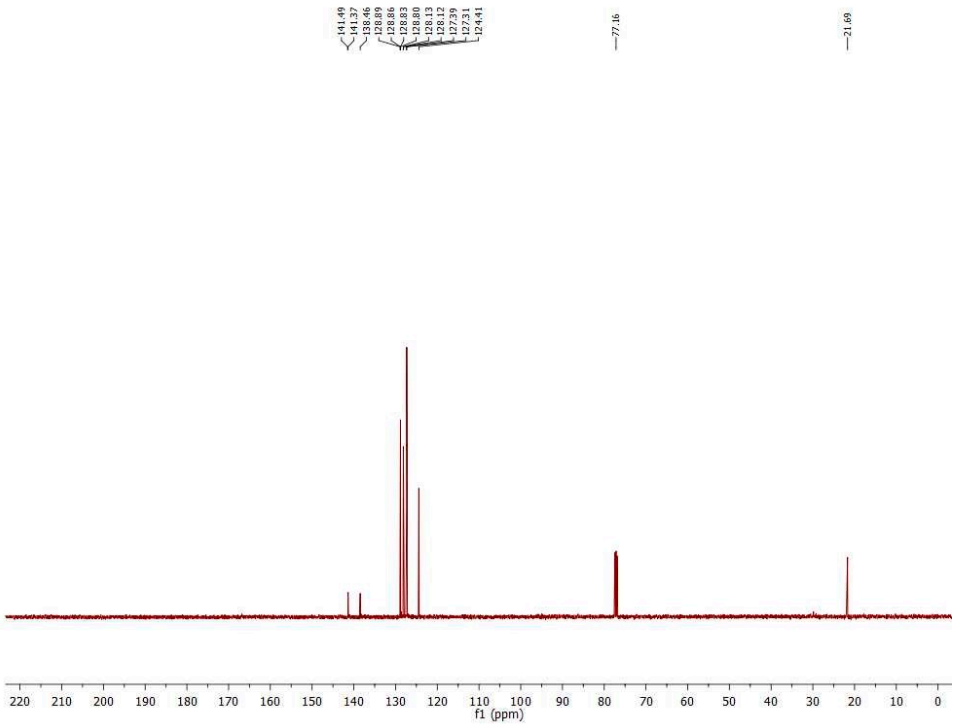
^{1}H and ^{13}C NMR of compound 3f



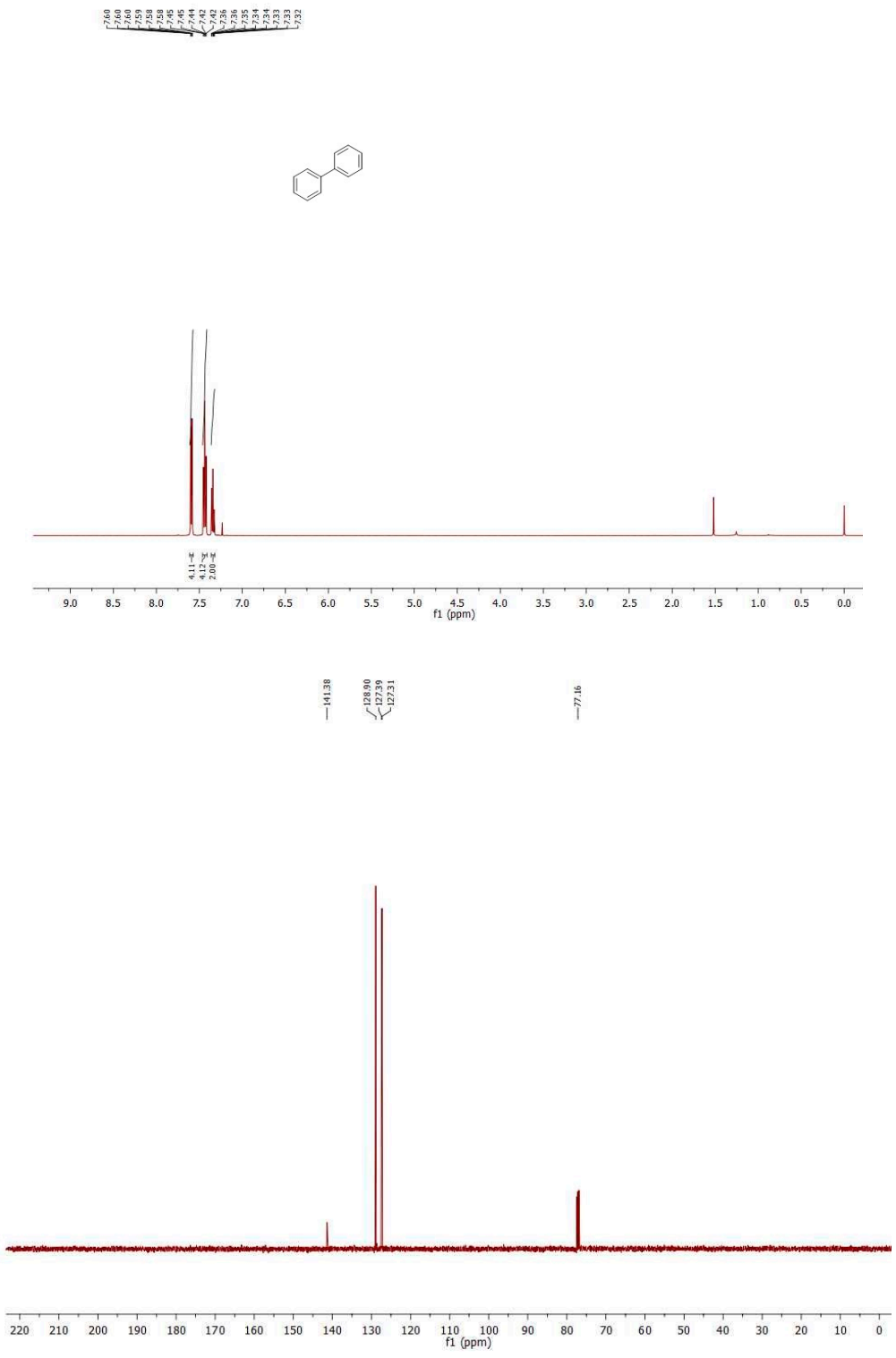


^{1}H and ^{13}C NMR of compound 3g

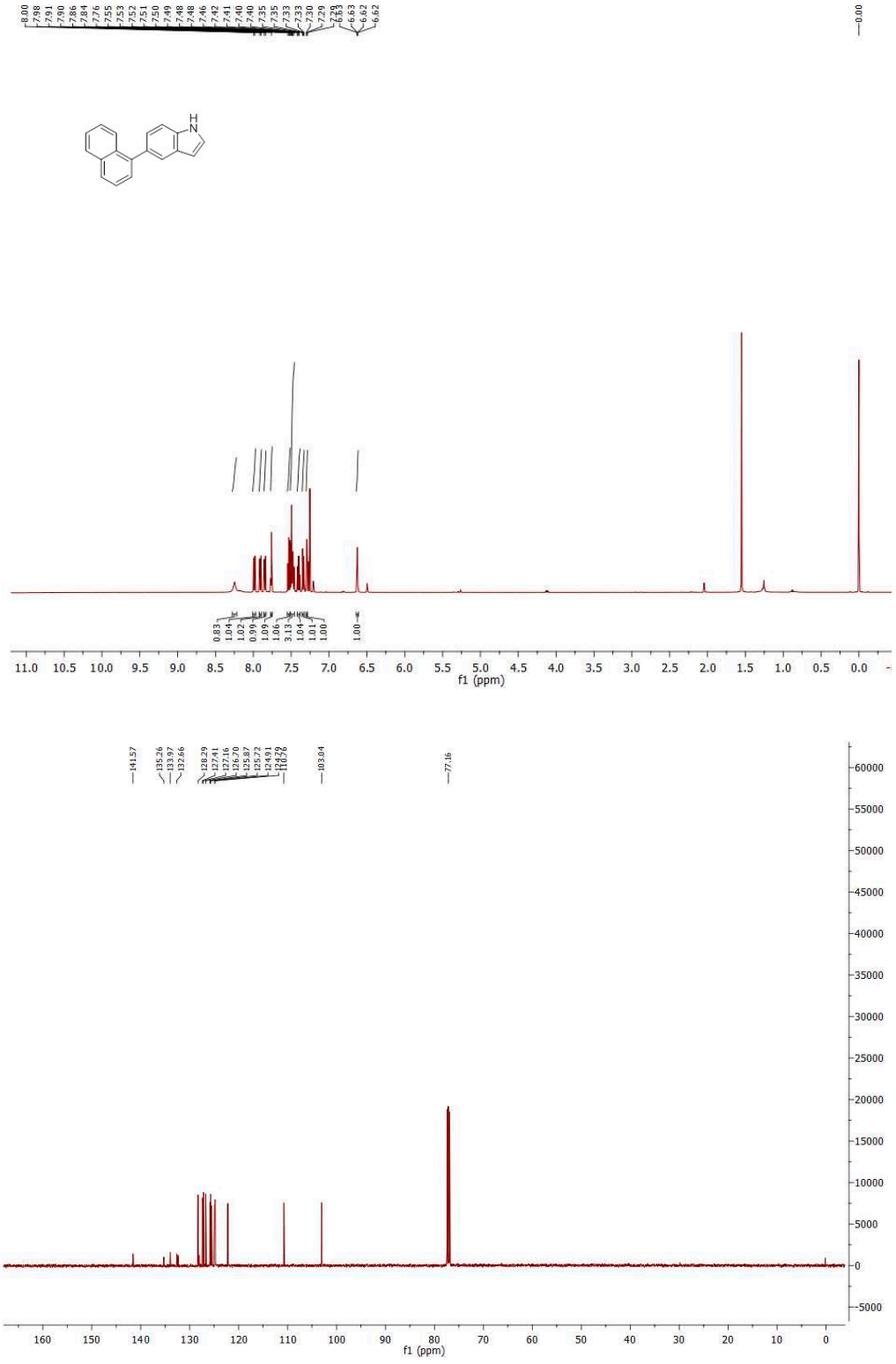




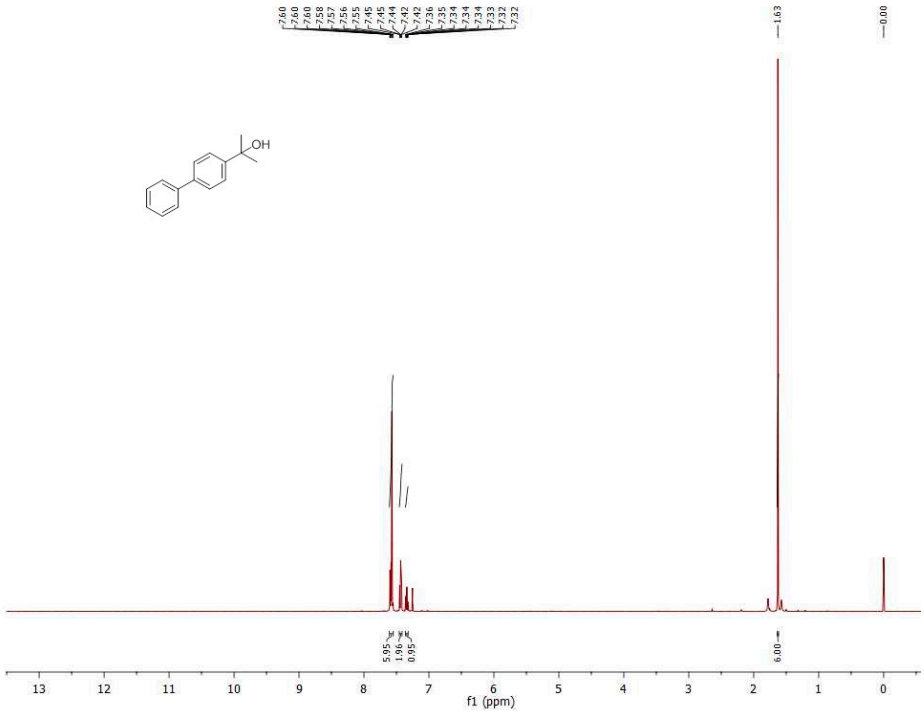
^{1}H and ^{13}C NMR of compound 3h

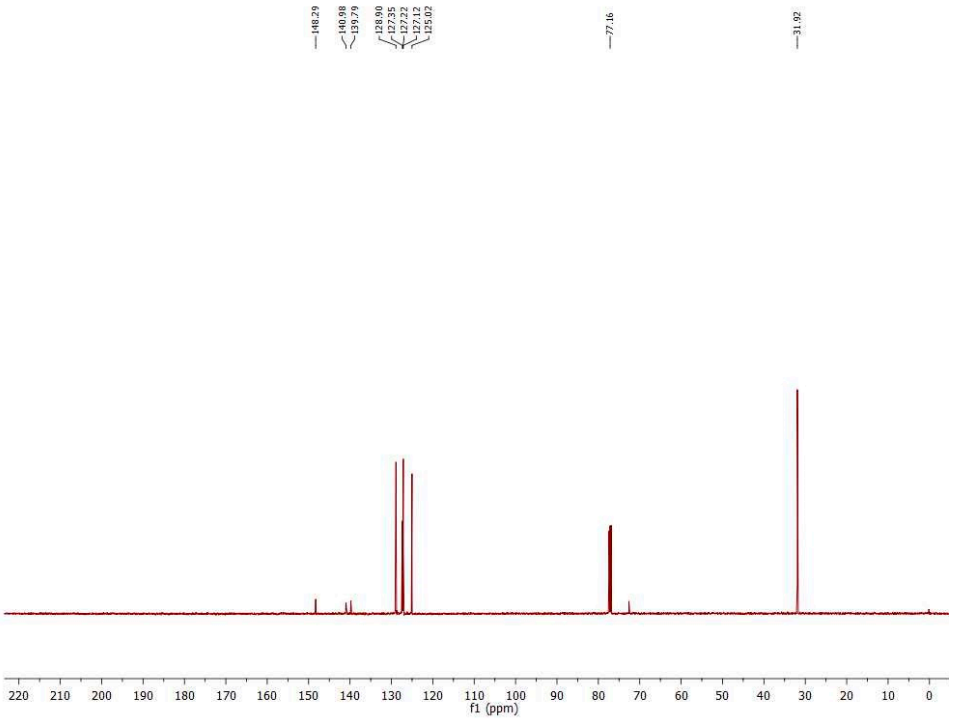


^{1}H and ^{13}C NMR of compound 3i

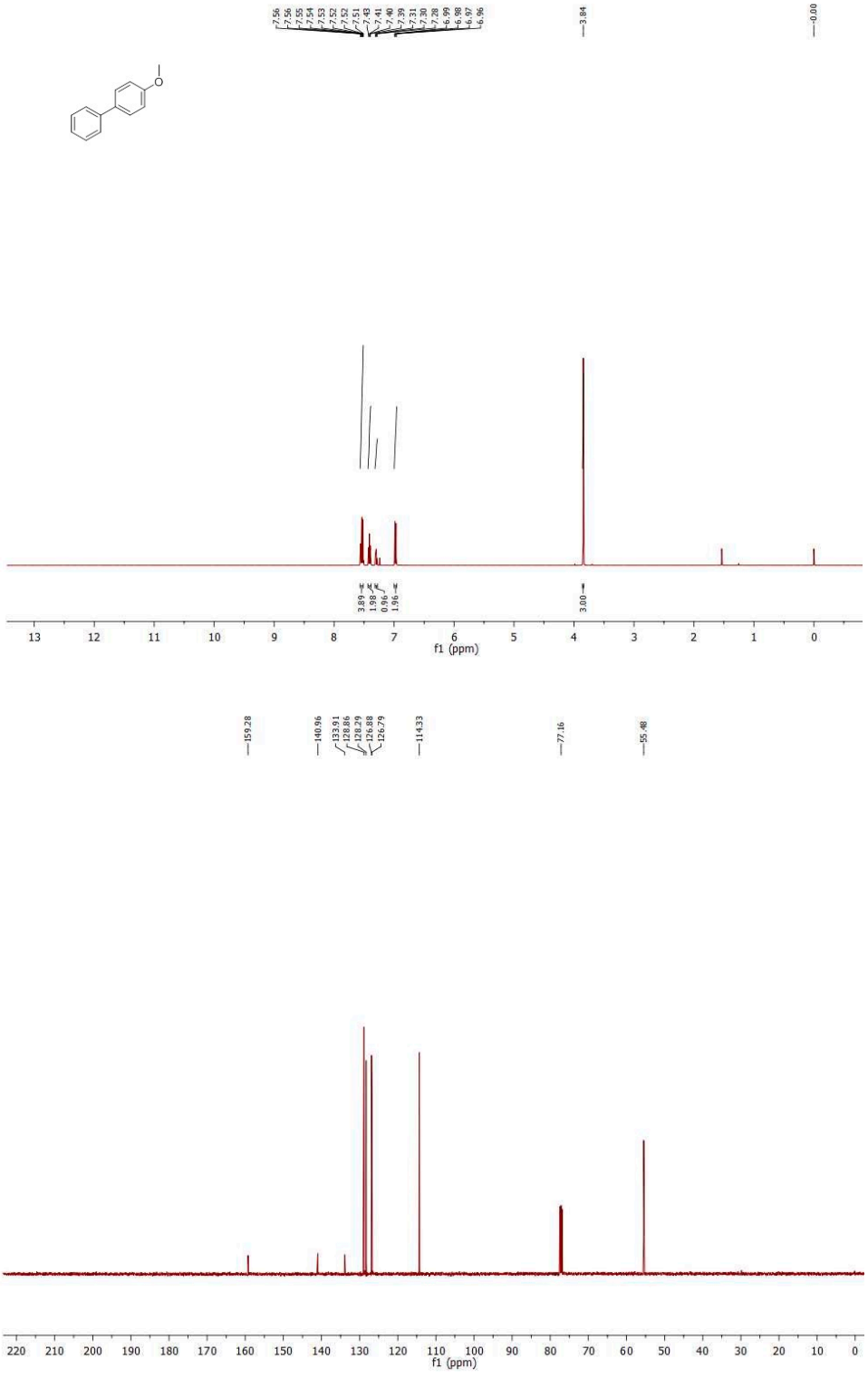


^{1}H and ^{13}C NMR of compound 3j

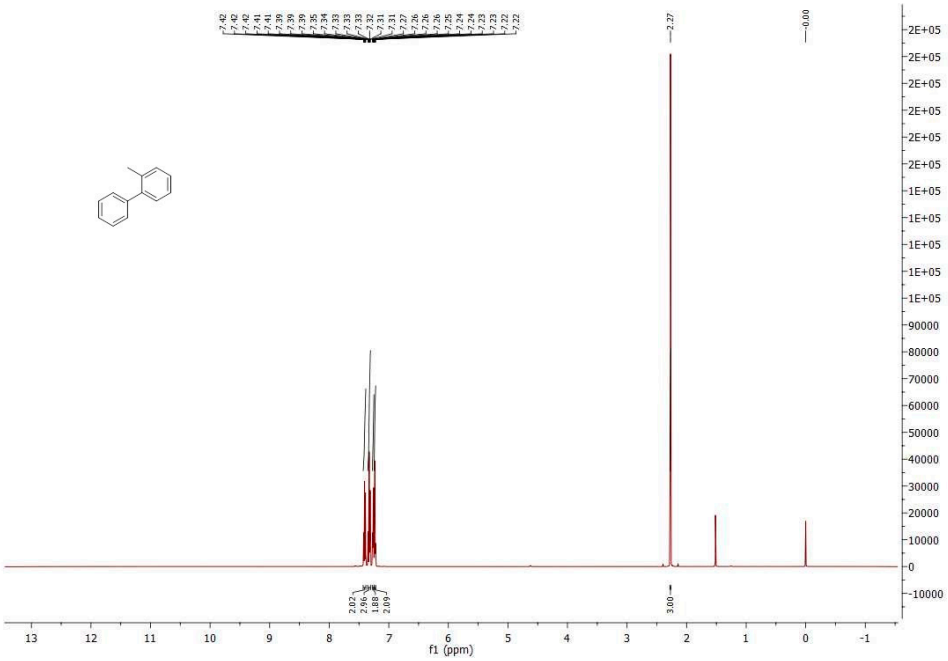


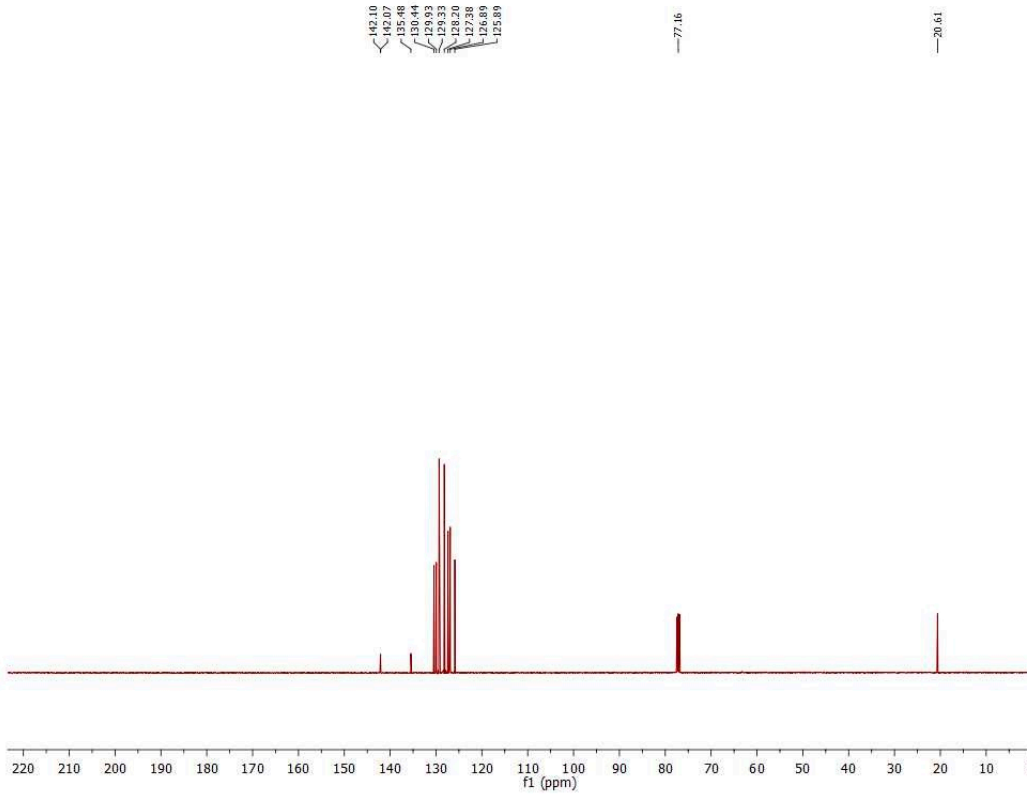


^{1}H and ^{13}C NMR of compound 3k

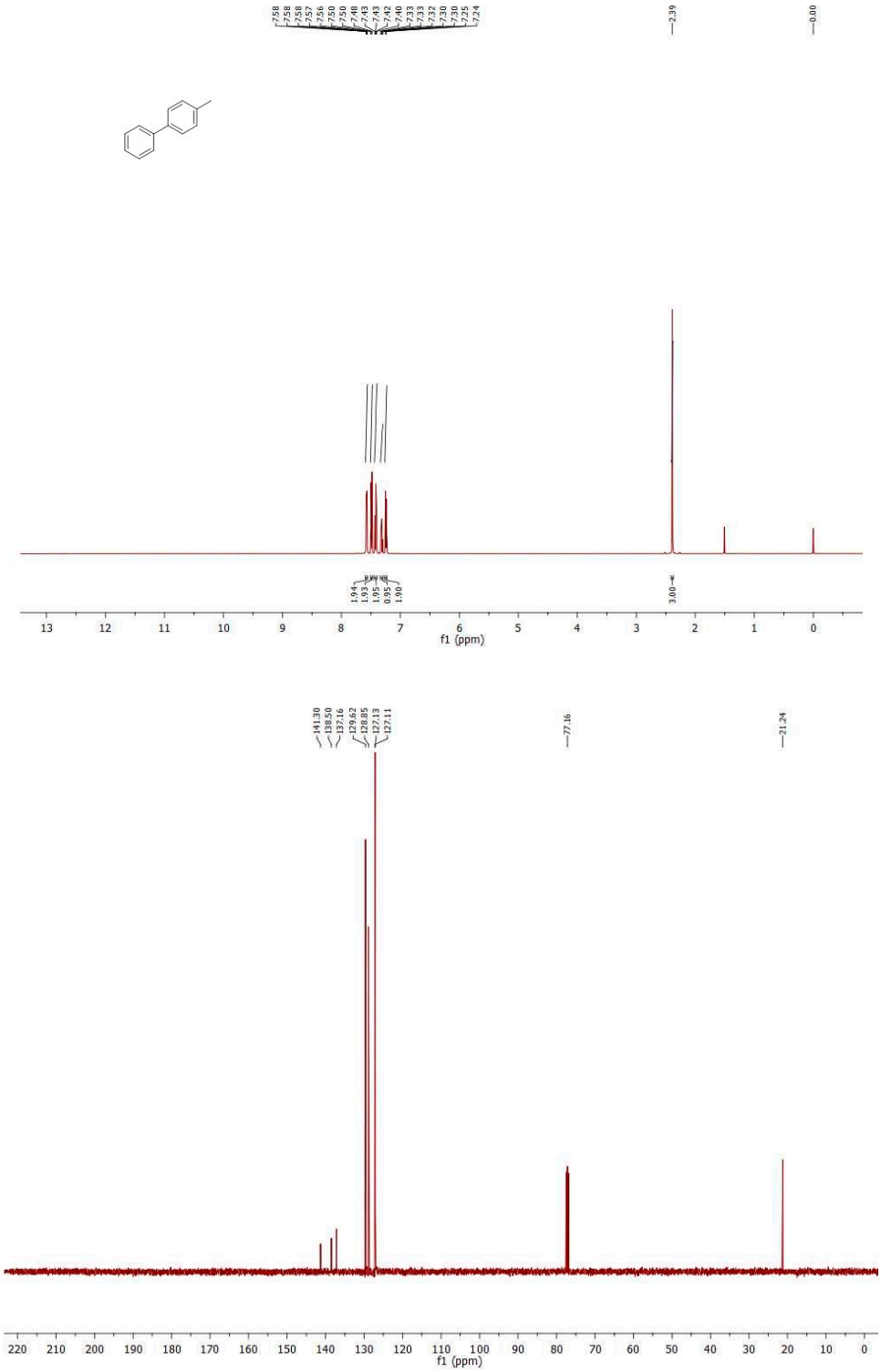


^{1}H and ^{13}C NMR of compound 3l





^{1}H and ^{13}C NMR of compound 3m



^{1}H and ^{13}C NMR of compound 3n