Supporting Information for

Silver catalyzed decarboxylative direct C2-alkylation of benzothiazole with carboxylic acids

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General:

NMR spectra were recorded with a 400 NMR spectrometer for ^{1}H-NMR, 100 MHz for ^{13}C-NMR. Proton chemical shifts δ were given in ppm relative to tetramethylsilane (0.00 ppm) in $CDCl_3$. High resolution mass spectra were taken with a 3000 mass spectrometer, using Waters Q-Tof MS/MS system. For column chromatography 200-300 mesh silica gel (GF254) was used as the stationary phase. All reactions were monitored by thin layer chromatography (TLC). All reactions were set up in air (with no use of a glove box). Methy, bromo- and chloro- substituted benzothiazoles were prepared from the corresponding substituted 2-amino benzothiazoles.[1] All other chemicals were purchased commercially and used without further purification.

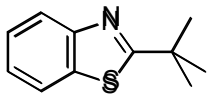
1. A. R. Katritzky, B. V. Rogovoy, C. Chassaing, V. Vvedensky, B. Forood, B. Flatt, H. Nakai, *J. Heterocyclic Chem.* **2000** , *37*, 1655.

General procedure for the silver catalyzed decarboxylative direct C2-alkylation of benzothiazole with carboxylic acids

A 25-mL round-bottom flask containing a stirbar was charged with Benzothiazole (0.5 mmol), carboxylic acids (1.0 mmol), $AgNO_3$ (0.1 mmol), $K_2S_2O_8$ (2.0 mmol) and CH_2Cl_2/ H_2O(2.5/ 2.5 mL). The reaction was stirred at room temperature for 8 h (monitored by TLC). Upon completion of the reaction, the mixture was diluted with brine (3 mL) and extracted with dichloromethane (10 mL × 3). The organic layers were combined, washed with brine, dried over anhydrous Na_2SO_4, and filtered. The solvents were removed via rotary evaporator under reduced pressure and the residue was purified with flash chromatography (silica gel, gradient eluent of petroleum ether/ ethyl acetate mixtures) to yield the desired product.

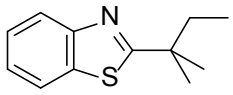
Characterization of compounds

2-(*tert*-butyl)benzo[*d*]thiazole (3a)



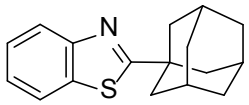
Yellow liquid. ^{1}H NMR($CDCl_3$, 400 MHz) :δ(ppm) 7.96 (d, *J*=10.8 Hz, 1H), 7.80 (d, *J*=11.0 Hz, 1H), 7.41 (s, 1H), 7.29 (t, *J*=5.0 Hz, 1H), 1.50 (d, *J*=11.6 Hz, 9H); ^{13}C NMR($CDCl_3$, 100 MHz): δ(ppm) 181.8, 153.3, 135.0, 125.7, 124.5, 122.7, 121.5, 38.3, 30.8; HRMS: calcd for $C_{11}H_{13}NS$ $[M+H]^+$ 192.0841, found 192.0841.

2-(*tert*-pentyl)benzo[*d*]thiazole (3b)



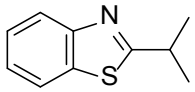
Yellow liquid. ^{1}H NMR($CDCl_3$, 400 MHz) :δ(ppm) 8.00 (d, *J*=8.2 Hz, 1H), 7.83 (d, *J*=7.9 Hz, 1H), 7.44-7.40 (m, 1H), 7.31 (q, *J*=7.6 Hz, 1H), 1.85 (q, *J*=7.5 Hz, 2H), 1.47 (s, 6H), 0.85 (t, *J*=7.4 Hz, 3H); ^{13}C NMR($CDCl_3$, 100 MHz): δ(ppm) 181.2, 153.3, 135.0, 125.7, 124.5, 122.7, 121.4, 41.8, 36.7, 28.1, 9.1; HRMS: calcd for $C_{12}H_{15}NS$ $[M+H]^+$ 206.0998, found 206.0999.

2-((3*r*,5*r*,7*r*)-adamantan-1-yl)benzo[*d*]thiazole (3c)



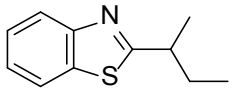
Yellow solid m.p. 70-72° C. ^{1}H NMR($CDCl_3$, 400 MHz) :δ(ppm) 8.00 (d, *J*=8.1 Hz, 1H), 7.84 (d, *J*=7.9 Hz, 1H), 7.43 (t, *J*=7.7 Hz, 1H), 7.31 (t, *J*=7.6 Hz, 1H), 2.15 (s, 9H), 1.81 (s, 6H); ^{13}C NMR($CDCl_3$, 100 MHz): δ(ppm) 182.2, 153.1, 134.3, 125.7, 124.4, 122.6, 121.6, 43.0, 40.2, 36.5, 28.6; HRMS: calcd for $C_{17}H_{19}NS$ $[M+H]^+$ 270.1311, found 270.1314.

2-isopropylbenzo[*d*]thiazole (3d)



Yellow liquid. ^{1}H NMR($CDCl_3$, 400 MHz) :δ(ppm) 8.00 (d, *J*=8.2 Hz, 1H), 7.85 (d, *J*=7.8 Hz, 1H), 7.48-7.43 (m, 1H), 7.36-7.32 (m, 1H), 3.49-3.39 (m, 1H), 1.50 (d, *J*=6.9 Hz, 6H); ^{13}C NMR($CDCl_3$, 100 MHz): δ(ppm) 178.6, 153.2, 134.7, 125.8, 124.6, 122.6, 121.5, 34.1, 22.9; HRMS: calcd for $C_{10}H_{11}NS$ $[M+H]^+$ 178.0685, found 178.0685.

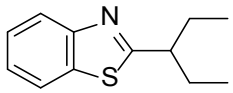
2-(*sec*-butyl)benzo[*d*]thiazole (3e)



Yellow liquid. ^{1}H NMR($CDCl_3$, 400 MHz) :δ(ppm) 7.98 (d, *J*=8.0 Hz, 1H), 7.85 (d, *J*=8.0 Hz, 1H), 7.47-7.43 (m, 1H), 7.36-7.32 (m, 1H), 3.26-3.17 (m, 1H), 1.97-1.73 (m, 2H), 1.45 (d, *J*=6.9 Hz, 3H),

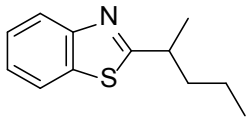
0.98 (t, *J*=7.4 Hz, 3H); ^{13}C NMR($CDCl_3$, 100 MHz): δ(ppm) 177.9, 153.1, 134.7, 125.8, 124.6, 122.6, 121.6, 41.1, 30.6, 20.7, 11.8; HRMS: calcd for $C_{11}H_{13}NS$ $[M+H]^+$ 192.0841, found 192.0842.

2-(pentan-3-yl)benzo[*d*]thiazole (3f)



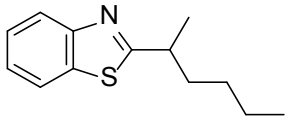
Yellow liquid. ^{1}H NMR($CDCl_3$, 400 MHz) :δ(ppm) 8.01 (d, *J*=8.2 Hz, 1H), 7.86 (d, *J*=8.0 Hz, 1H), 7.46 (t, *J*=7.7 Hz, 1H), 7.35 (t, *J*=7.6 Hz, 1H), 3.04-2.98 (m, 1H), 1.90-1.81 (m, 4H), 0.94 (t, *J*=7.4 Hz, 6H); ^{13}C NMR($CDCl_3$, 100 MHz): δ(ppm) 176.9, 153.1, 134.7, 125.7, 124.5, 122.6, 121.6, 48.7, 29.0, 11.9; HRMS: calcd for $C_{12}H_{15}NS$ $[M+H]^+$ 206.0998, found 206.1001.

2-(pentan-2-yl)benzo[*d*]thiazole (3g)



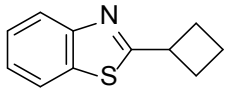
Yellow liquid. ^{1}H NMR($CDCl_3$, 400 MHz) :δ(ppm) 7.98 (d, *J*=8.1 Hz, 1H), 7.84 (d, *J*=7.5 Hz, 1H), 7.46-7.41 (m, 1H), 7.35-7.31 (m, 1H), 3,34-3.26 (m, 1H), 1.88-1.69 (m, 2H), 1.44 (d, *J*=6.9 Hz, 3H), 1.40-1.34 (m, 2H), 0.93 (t, *J*=7.3 Hz, 3H); ^{13}C NMR($CDCl_3$, 100 MHz): δ(ppm) 178.1, 153.1, 134.7, 125.8, 124.5, 122.6, 121.5, 39.8, 39.3, 21.2, 20.5, 14.0; HRMS: calcd for $C_{12}H_{15}NS$ $[M+H]^+$ 206.0998, found 206.0999.

2-(hexan-2-yl)benzo[*d*]thiazole (3h)



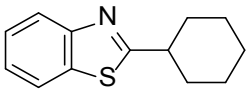
Orange liquid. ^{1}H NMR($CDCl_3$, 400 MHz) :δ(ppm) 7.98 (d, *J*=8.1 Hz, 1H), 7.83 (d, *J*=7.9 Hz, 1H), 7.45-7.41 (m, 1H), 7.34-7.30 (m, 1H), 3.32-3.23 (m, 1H), 1.91-1.68 (m, 2H), 1.44 (d, *J*=6.9 Hz, 3H), 1.36-1.31 (m, 4H), 0.88 (t, *J*=7.0 Hz, 3H); ^{13}C NMR($CDCl_3$, 75 MHz): δ(ppm) 178.1, 153.1, 134.7, 125.8, 124.5, 122.6, 121.5, 39.5, 37.4, 29.5, 22.6, 21.2, 13.9; HRMS: calcd for $C_{13}H_{17}NS$ $[M+H]^+$ 220.1154, found 220.1157.

2-cyclobutylbenzo[*d*]thiazole (3i)



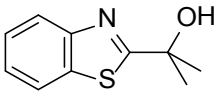
Yellow liquid. ^{1}H NMR($CDCl_3$, 400 MHz) :δ(ppm) 7.98 (d, *J*=8.0 Hz, 1H), 7.85-7.83 (m, 1H), 7.46-7.42 (m, 1H), 7.36-7.31 (m, 1H), 4.01-3.92 (m, 1H), 2.57-2.43 (m, 4H), 2.19-1.97 (m, 2H); ^{13}C NMR($CDCl_3$, 100 MHz): δ(ppm) 176.1, 153.4, 135.0, 125.9, 124.6, 122.6, 121.6, 39.0, 29.7, 18.5; HRMS: calcd for $C_{11}H_{11}NS$ $[M+H]^+$ 190.0685, found 190.0687.

2-cyclohexylbenzo[*d*]thiazole (3j)



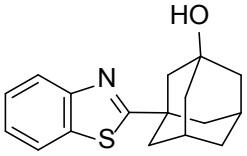
Yellow liquid. ^{1}H NMR($CDCl_3$, 400 MHz) :δ(ppm) 7.97 (d, *J*=8.1 Hz, 1H), 7.82 (d, *J*=8.0 Hz, 1H), 7.41 (t, *J*=7.2 Hz, 1H), 7.30 (t, *J*=7.2 Hz, 1H), 3.12-3.05 (m, 1H), 2.20 (d, *J*=11.6 Hz, 2H), 1.89-1.85 (m, 2H), 1.76-1.73 (m, 1H), 1.68-1.58 (m, 2H), 1.48-1.37 (m, 2H), 1.35-1.26 (m, 1H); ^{13}C NMR($CDCl_3$, 75 MHz): δ(ppm) 177.5, 153.1, 134.5, 125.8, 124.5, 122.5, 121.5, 43.4, 33.4, 26.1, 25.8; HRMS: calcd for $C_{13}H_{15}NS$ $[M+H]^+$ 218.0998, found 218.1000.

2-(benzo[*d*]thiazol-2-yl)propan-2-ol (3k)



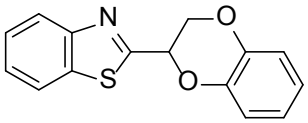
White solid. ^{1}H NMR($CDCl_3$, 400 MHz) :δ(ppm) 7.99 (d, *J*=8.1 Hz, 1H), 7.89 (d, *J*=7.9 Hz, 1H), 7.50-7.45 (m, 1H), 7.39-7.35 (m, 1H), 3.08 (s, 1H), 1.75 (s, 6H); ^{13}C NMR($CDCl_3$, 75 MHz): δ(ppm) 179.9, 153.1, 135.4, 126.0, 124.9, 122.9, 121.8, 73.6, 30.8; HRMS: calcd for $C_{10}H_{11}NOS$ $[M+H]^+$ 194.0634, found 194.0635.

(1*s*,3*r*,5*R*,7*S*)-3-(benzo[*d*]thiazol-2-yl)adamantan-1-ol (3l)



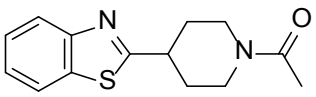
White solid. ^{1}H NMR($CDCl_3$, 400 MHz) :δ(ppm) 8.00 (d, *J*=8.2 Hz, 1H), 7.85 (d, *J*=7.9 Hz, 1H), 7.46-7.42 (m, 1H), 7.35-7.31 (m, 1H), 2.37 (s, 2H), 2.12 (s, 2H), 2.04 (t, *J*=13.1 Hz, 5H), 1.81 (d, *J*=2.6 Hz, 4H), 1.72-1.64 (m, 2H); ^{13}C NMR($CDCl_3$, 75 MHz): δ(ppm) 180.1, 153.1, 134.3, 125.9, 124.6, 122.8, 121.6, 68.7, 50.2, 44.3, 43.4, 41.8, 35.0, 30.7; HRMS: calcd for $C_{17}H_{19}NOS$ $[M+H]^+$ 286.1260, found 286.1265.

2-(2,3-dihydrobenzo[*b*][1,4]dioxin-2-yl)benzo[*d*]thiazole (3m)



White solid. ^{1}H NMR($CDCl_3$, 400 MHz) :δ(ppm) 8.05 (d, *J*=8.2 Hz, 1H), 7.91 (d, *J*=8.0 Hz, 1H), 7.53-7.49 (m, 1H), 7.43-7.39 (m, 1H), 7.08-7.06 (m, 1H), 6.96-6.91 (m, 3H), 5.64 (dd, *J*=4.3, 2.6 Hz, 1H), 4.72 (dd, *J*=8.8, 2.7 Hz, 1H), 4.42 (dd, *J*=7.0, 4.5 Hz, 1H); ^{13}C NMR($CDCl_3$, 75 MHz): δ(ppm) 167.7, 153.1, 143.1, 142.4, 135.0, 126.3, 125.4, 123.3, 122.3, 122.1, 121.9, 117.6, 117.5, 73.5, 67.1; HRMS: calcd for $C_{15}H_{11}NO_2S$ $[M+H]^+$ 270.0583, found 270.0586.

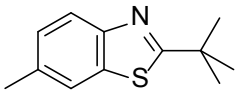
1-(4-(benzo[*d*]thiazol-2-yl)piperidin-1-yl)ethanone (3n)



Yellow liquid. ^{1}H NMR($CDCl_3$, 400 MHz) :δ(ppm) 7.98 (d, *J*=8.2 Hz, 1H), 7.87 (d, *J*=8.0 Hz, 1H), 7.47

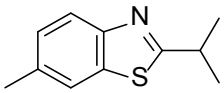
(t, *J*=7.6 Hz, 1H), 7.37 (t, *J*=7.6 Hz, 1H), 4.70 (d, *J*=13.4 Hz, 1H), 3.95 (d, *J*=13.7 Hz, 1H), 3.38-3.31 (m, 1H), 3.30-3.22 (m, 1H), 2.85-2.78 (m, 1H), 2.27-2.19 (m, 2H), 2.14 (s, 3H), 1.96-1.83 (m, 2H); ^{13}C NMR($CDCl_3$, 75 MHz): δ(ppm) 174.4, 168.9, 153.0, 134.5, 126.1, 125.0, 122.8, 121.7, 46.2, 41.3, 32.4, 31.9, 21.5**;** HRMS: calcd for $C_{14}H_{16}N_2OS$ $[M+H]^+$ 261.1056, found 261.1059.

2-(*tert*-butyl)-6-methylbenzo[*d*]thiazole (3o)



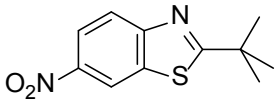
Yellow liquid. ^{1}H NMR($CDCl_3$, 400 MHz) :δ(ppm) 7.86 (d, *J*=8.3 Hz, 1H), 7.61 (s, 1H), 7.23 (d, *J*=8.3 Hz, 1H), 2.45 (s, 3H), 1.50 (s, 9H); ^{13}C NMR($CDCl_3$, 75 MHz): δ(ppm) 180.7, 151.3, 135.1, 134.5, 127.3, 122.1, 121.2, 38.2, 30.7, 21.4; HRMS: calcd for $C_{12}H_{15}NS$ $[M+H]^+$ 206.0998, found 206.0999.

2-isopropyl-6-methylbenzo[*d*]thiazole (3p)



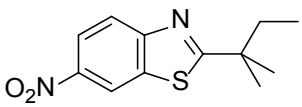
Yellow liquid. ^{1}H NMR($CDCl_3$, 400 MHz) :δ(ppm) 7.84 (d, *J*=8.3 Hz, 1H), 7.62 (s, 1H), 7.24 (d, *J*=8.7 Hz, 1H), 3.45-3.35 (m, 1H), 2.46 (s, 3H), 1.46 (d, *J*=6.9 Hz, 6H); ^{13}C NMR($CDCl_3$, 75 MHz): δ(ppm) 177.7, 151.2, 134.8, 134.6 127.4, 122.0, 121.3, 34.0, 22.9, 21.4; HRMS: calcd for $C_{11}H_{13}NS$ $[M+H]^+$ 192.0841, found 192.0843.

2-(*tert*-butyl)-6-nitrobenzo[*d*]thiazole (3q)



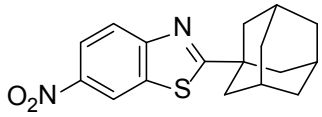
Yellow solid m.p. 89-91° C. ^{1}H NMR($CDCl_3$, 400 MHz) :δ(ppm) 8.79 (d, *J*=2.2 Hz, 1H), 8.33 (q, *J*=6.7 Hz, 1H), 8.06 (d, *J*=9.0 Hz, 1H), 1.55 (s, 9H); ^{13}C NMR($CDCl_3$, 100 MHz): δ(ppm) 188.3, 157.1, 144.6, 135.4, 122.9, 121.4, 118.1, 39.1, 30.6; HRMS: calcd for $C_{11}H_{12}N_2O_2S$ $[M+H]^+$ 237.0692, found 237.0693.

6-nitro-2-(*tert*-pentyl)benzo[*d*]thiazole (3r)



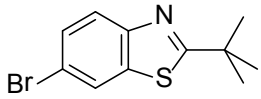
Yellow oil. ^{1}H NMR($CDCl_3$, 400 MHz) :δ(ppm) 8.79 (s, 1H), 8.33 (q, *J*=6.9 Hz, 1H), 8.06 (d, *J*=9.0 Hz, 1H), 1.89 (q, *J*=7.4 Hz, 2H), 1.51 (s, 6H), 0.87 (t, *J*=7.4 Hz, 3H); ^{13}C NMR($CDCl_3$, 100 MHz): δ(ppm) 187.8, 157.1, 144.6, 135.4, 122.9, 121.3, 118.1, 42.5, 36.6, 27.9, 9.0; HRMS: calcd for $C_{12}H_{14}N_2O_2S$ $[M+H]^+$ 251.0849, found 251.0850.

2-((3*r*,5*r*,7*r*)-adamantan-1-yl)-6-nitrobenzo[*d*]thiazole (3s)



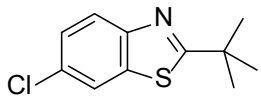
Yellow solid m.p. 179-181° C. ^{1}H NMR($CDCl_3$, 400 MHz) :δ(ppm) 8.80 (s, 1H), 8.32 (d, *J*=9.0 Hz, 1H), 8.05 (d, *J*=8.9 Hz, 1H), 2.16 (s, 9H), 1.84 (s, 6H); ^{13}C NMR($CDCl_3$, 100 MHz): δ(ppm) 188.6, 157.1, 144.5, 134.8, 122.9, 121.3, 118.2, 42.9, 41.0, 36.4, 28.4; HRMS: calcd for $C_{17}H_{18}N_2O_2S$ $[M+H]^+$ 315.1162, found 315.1163.

6-bromo-2-(*tert*-butyl)benzo[*d*]thiazole (3t)



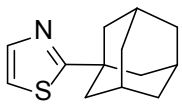
Colorless oil. ^{1}H NMR($CDCl_3$, 400 MHz) :δ(ppm) 7.98 (d, *J*=1.8 Hz, 1H), 7.83 (d, *J*=8.6 Hz, 1H), 7.54 (q, *J*=6.8 Hz, 1H), 1.51 (s, 9H); ^{13}C NMR($CDCl_3$, 75 MHz): δ(ppm) 182.5, 152.1, 136.7, 129.2, 124.0, 123.8, 118.0, 38.4, 30.6; HRMS: calcd for $C_{11}H_{12}BrNS$ $[M+H]^+$ 269.9947, found 269.9947.

2-(*tert*-butyl)-6-chlorobenzo[d]thiazole (3u)



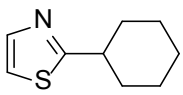
Brown liquid. ^{1}H NMR($CDCl_3$, 400 MHz) :δ(ppm) 7.88 (d, *J*=8.7 Hz, 1H), 7.81 (s, 1H), 7.39 (d, *J*=8.7 Hz, 1H), 1.51 (s, 9H); ^{13}C NMR($CDCl_3$, 100 MHz): δ(ppm) 182.3, 151.9, 136.3, 130.4, 126.4, 123.4, 121, 38.4, 30.6; HRMS: calcd for $C_{11}H_{12}ClNS$ $[M+H]^+$ 226.0452, found 226.0453.

2-((3*r*,5*r*,7*r*)-adamantan-1-yl)thiazole (3v)



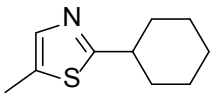
Yellow liquid. ^{1}H NMR($CDCl_3$, 400 MHz) :δ(ppm) 7.70 (d, *J*=3.3 Hz, 1H), 7.19 (d, *J*=3.3 Hz, 1H), 2.11 (s, 3H), 2.07 (d, *J*=2.6 Hz, 6H), 1.79 (s, 6H); ^{13}C NMR($CDCl_3$, 100 MHz): δ(ppm) 181.8, 141.9, 117.1, 43.3, 39.3, 36.5, 28.6; HRMS: calcd for $C_{13}H_{17}NS$ $[M+H]^+$ 220.1154, found 220.1156.

2-cyclohexylthiazole (3w)



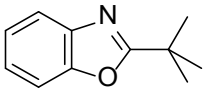
colorless liquid. ^{1}H NMR($CDCl_3$, 400 MHz) :δ(ppm) 7.68 (d, *J*=3.3 Hz, 1H), 7.18 (d, *J*=3.3 Hz, 1H), 3.05-2.98 (m, 1H), 2.17-2.13 (m, 2H), 1.88-1.83 (m, 2H), 1.78-1.73 (m, 1H), 1.60-1.50 (m, 2H), 1.47-1.37 (m, 2H), 1.34-1.22 (m, 1H); ^{13}C NMR($CDCl_3$, 100 MHz): δ(ppm) 177.1, 141.9, 117.3, 42.4, 33.8, 26.1, 25.8;HRMS: calcd for $C_9H_{13}NS$ $[M+H]^+$ 168.0841, found 168.0840.

2-cyclohexyl-5-methylthiazole (3x)



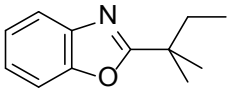
Pale yellow liquid. ^{1}H NMR($CDCl_3$, 400 MHz) :δ(ppm) 6.71 (d, *J*=0.8 Hz, 1H), 3.01-2.92 (m, 1H), 2.42 (d, *J*=0.8 Hz, 3H), 2.16-2.08 (m, 2H), 1.88-1.80 (m, 2H), 1.77-1.69 (m, 1H), 1.54-1.46 (m, 2H), 1.43-1.36 (m, 2H), 1.30-1.24 (m, 1H); ^{13}C NMR($CDCl_3$, 100 MHz): δ(ppm) 176.6, 151.8, 111.6, 42.6, 33.8, 26.1, 25.8, 17.1; HRMS: calcd for $C_{10}H_{15}NS$ $[M+H]^+$ 182.0998, found 182.0997.

2-(*tert*-butyl)benzo[*d*]oxazole (3y)



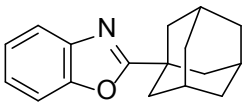
Yellow liquid. ^{1}H NMR($CDCl_3$, 400 MHz) :δ(ppm) 7.71-7.68 (m, 1H), 7.50-7.48 (m, 1H), 7.32-7.27 (m, 2H), 1.50 (s, 9H); ^{13}C NMR($CDCl_3$, 100 MHz): δ(ppm) 172.5, 149.8, 140.2, 123.4, 122.9, 118.7, 109.3, 27.5; HRMS: calcd for $C_{11}H_{13}NO$ $[M+H]^+$ 176.1070, found 176.1070.

2-(*tert*-pentyl)benzo[*d*]oxazole (3z)



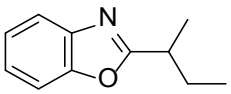
Brown liquid. ^{1}H NMR($CDCl_3$, 400 MHz) :δ(ppm) 7.71-7.69 (m, 1H), 7.50-7.47 (m, 1H), 7.31-7.28 (m, 2H), 1.85 (q, *J*=7.5 Hz, 2H), 1.46 (s, 6H), 0.84 (t, *J*=7.5 Hz, 3H); ^{13}C NMR($CDCl_3$, 100 MHz): δ(ppm) 172.9, 150.8, 141.2, 124.3, 123.9, 119.7, 110.3, 37.9, 34.5, 25.9, 9.2; HRMS: calcd for $C_{12}H_{15}NO$ $[M+H]^+$ 190.1226, found 190.1227.

2-((3*r*,5*r*,7*r*)-adamantan-1-yl)benzo[*d*]oxazole (3aa)



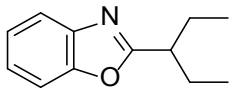
Yellow solid m.p. 94-96° C. ^{1}H NMR($CDCl_3$, 400 MHz) :δ(ppm) 7.70-7.68 (m, 1H), 7.49-7.47 (m, 1H), 7.31-7.27 (m, 2H), 2.16 (d, *J*=2.3 Hz, 6H), 2.13 (s, 3H), 1.82 (d, *J*=2.8 Hz, 6H); ^{13}C NMR($CDCl_3$, 100 MHz): δ(ppm) 173.0, 150.5, 141.2, 124.3, 123.9, 119.7, 110.3, 40.2, 36.5, 36.1, 28.0; HRMS: calcd for $C_{17}H_{19}NO$ $[M+H]^+$ 254.1539, found 254.1542.

2-(*sec*-butyl)benzo[*d*]oxazole (3ab)



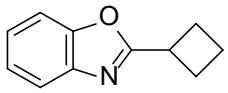
Yellow liquid. ^{1}H NMR($CDCl_3$, 400 MHz) :δ(ppm) 7.70-7.67 (m, 1H), 7.50-7.47 (m, 1H), 7.31-7.28 (m, 2H), 3.11-3.02 (m, 1H), 1.99-1.73 (m, 2H), 1.44 (d, *J*=7.0 Hz, 3H), 0.97 (t, *J*=7.4 Hz, 3H); ^{13}C NMR($CDCl_3$, 100 MHz): δ(ppm) 170.7, 150.7, 141.3, 124.4, 124.0, 119.6, 110.3, 35.8, 28.0, 17.9, 11.6; HRMS: calcd for $C_{11}H_{13}NO$ $[M+H]^+$ 176.1070, found 176.1070.

2-(pentan-3-yl)benzo[*d*]oxazole (3ac)



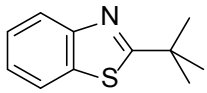
Purple oil. ^{1}H NMR($CDCl_3$, 400 MHz) :δ(ppm) 7.70-7.68 (m, 1H), 7.51-7.48 (m, 1H), 7.31-7.29 (m, 2H), 2.92-2.84 (m, 1H), 1.93-1.78 (m, 4H), 0.92 (t, *J*=7.4 Hz, 6H); ^{13}C NMR($CDCl_3$, 100 MHz): δ(ppm) 169.9, 150.7, 141.3, 124.3, 124.0, 119.6, 110.3, 43.4, 26.3, 11.8; HRMS: calcd for $C_{12}H_{15}NO$ $[M+H]^+$ 190.1226, found 190.1226.

2-cyclobutylbenzo[*d*]oxazole (3ad)

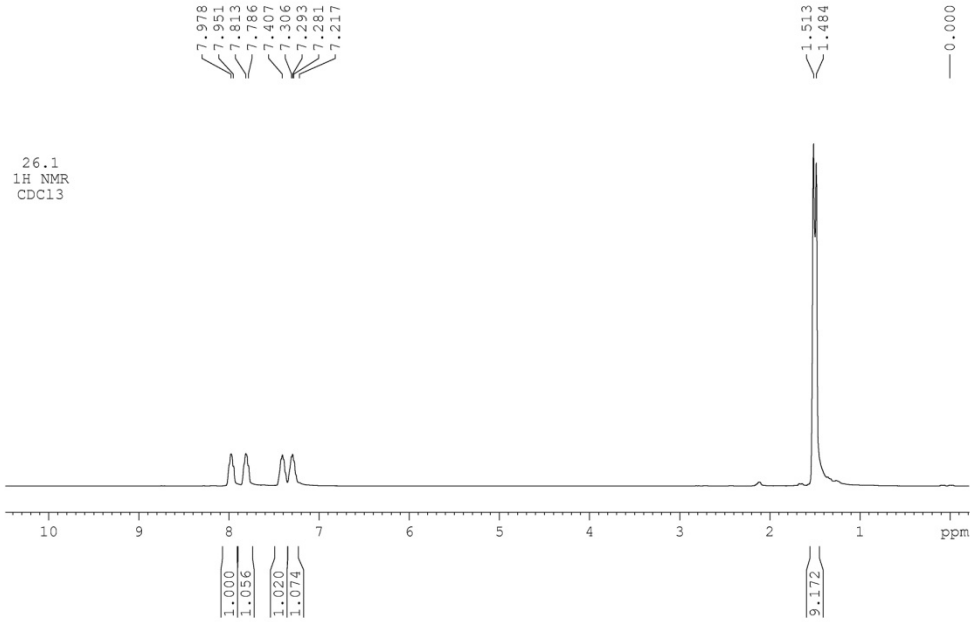


Brown liquid. ^{1}H NMR($CDCl_3$, 400 MHz) :δ(ppm) 7.69-7.67 (m, 1H), 7.49-7.47 (m, 1H), 7.32-7.28 (m, 2H), 3.84-3.75 (m, 1H), 2.59-2.51 (m, 2H), 2.49-2.44 (m, 2H), 2.18-2.11 (m, 1H), 2.11-2.04 (m, 1H); ^{13}C NMR($CDCl_3$, 100 MHz): δ(ppm) 169.4, 150.8, 141.4, 124.4, 124.1, 119.6, 110.3, 33.5, 27.1, 18.8; HRMS: calcd for $C_{11}H_{11}NO$ $[M+H]^+$ 174.0913, found 174.0912.

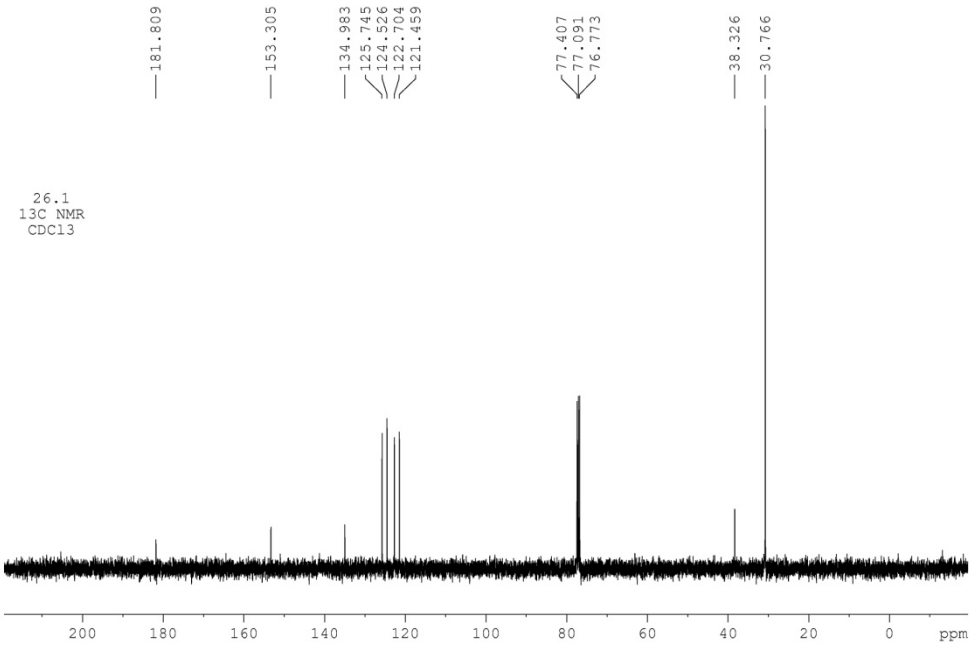
Copies of ^{1}H-NMR and ^{13}C-NMR spectra

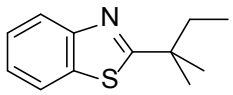


^{1}H-NMR spectrum of **3a**

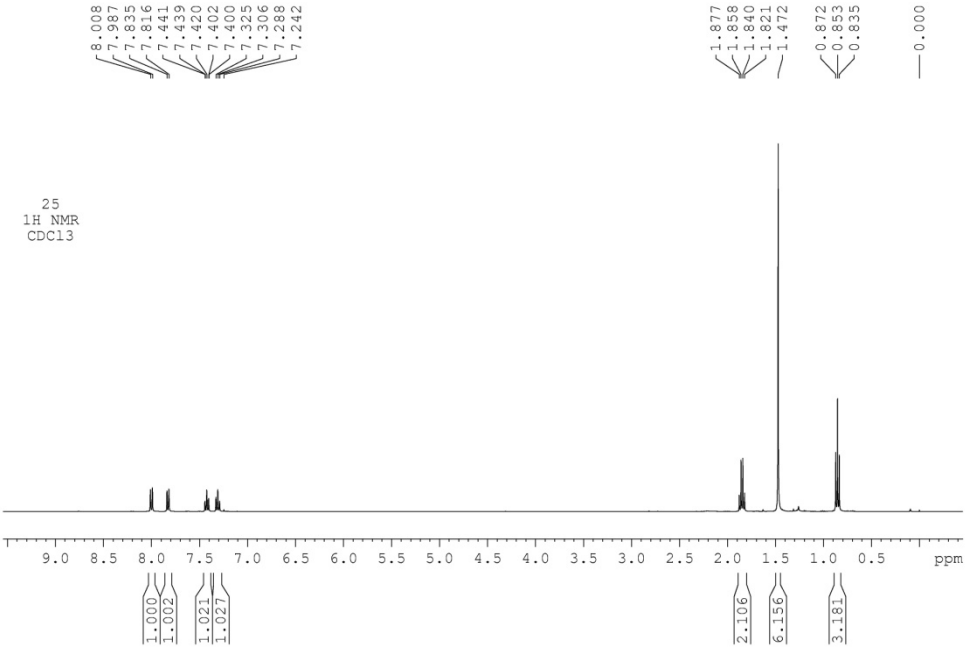


^{13}C-NMR spectrum of **3a**

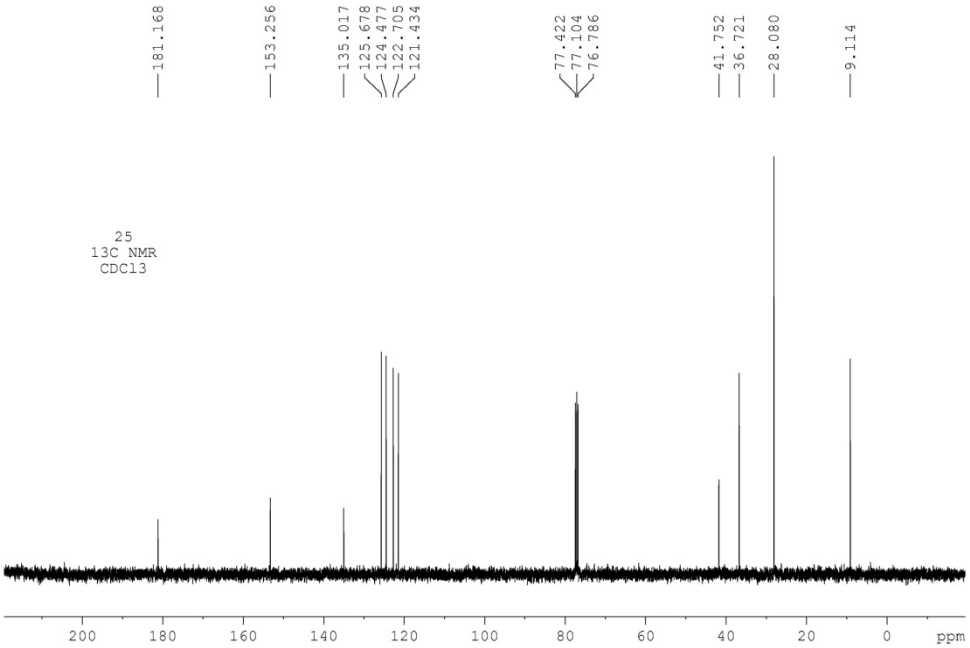


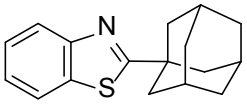


^{1}H-NMR spectrum of **3b**

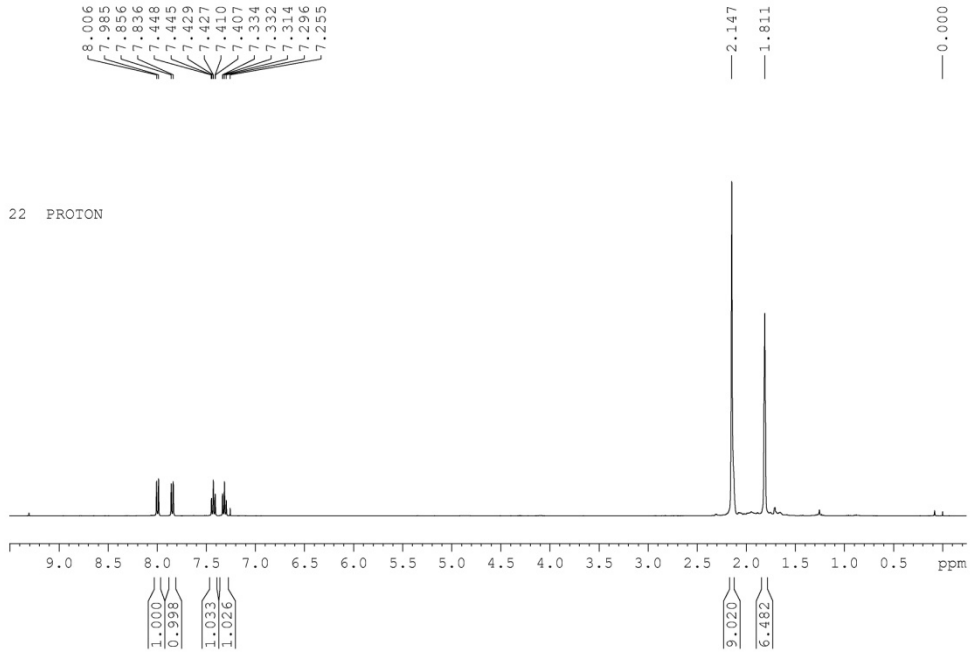


^{13}C-NMR spectrum of **3b**

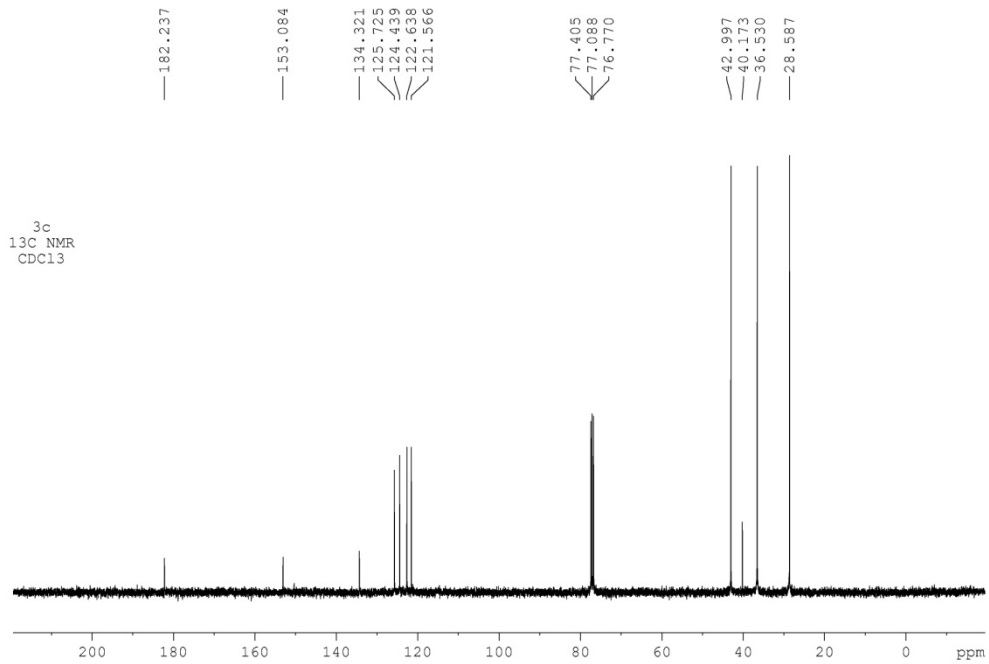


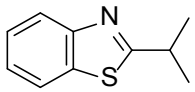


^{1}H-NMR spectrum of **3c**

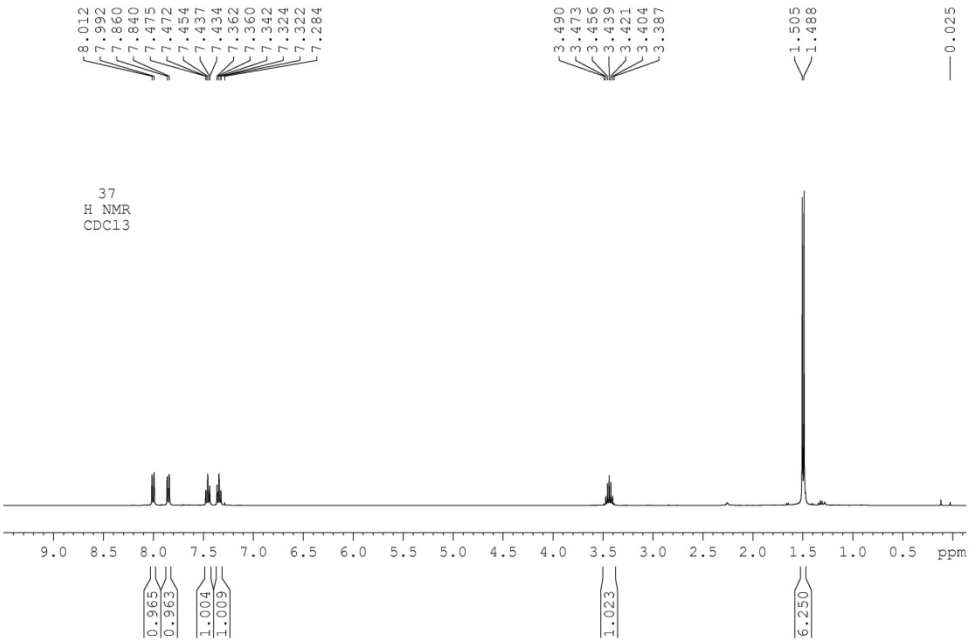


^{13}C-NMR spectrum of **3c**

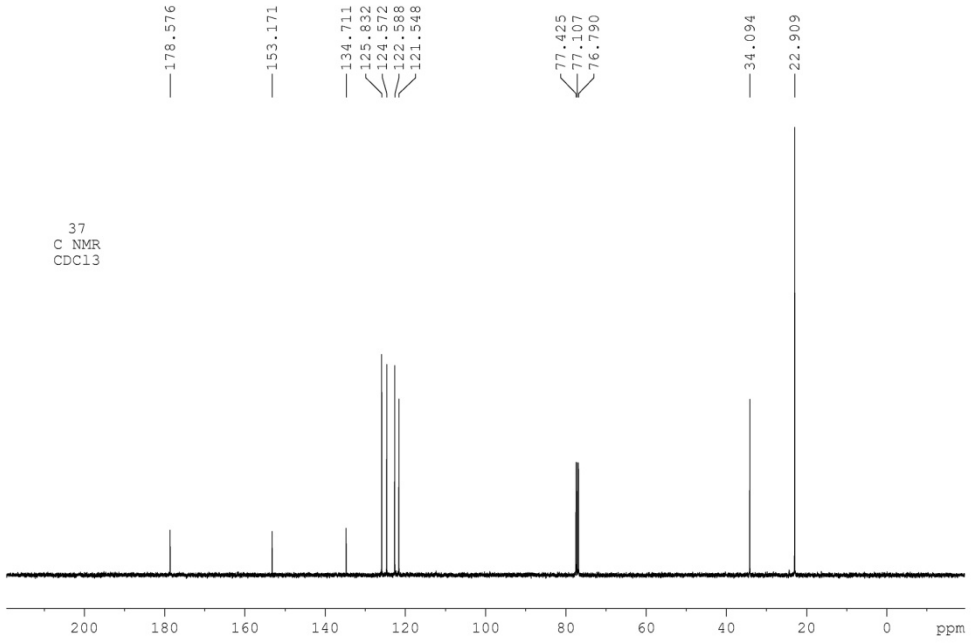


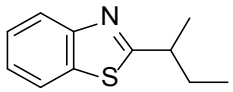


^{1}H-NMR spectrum of **3d**

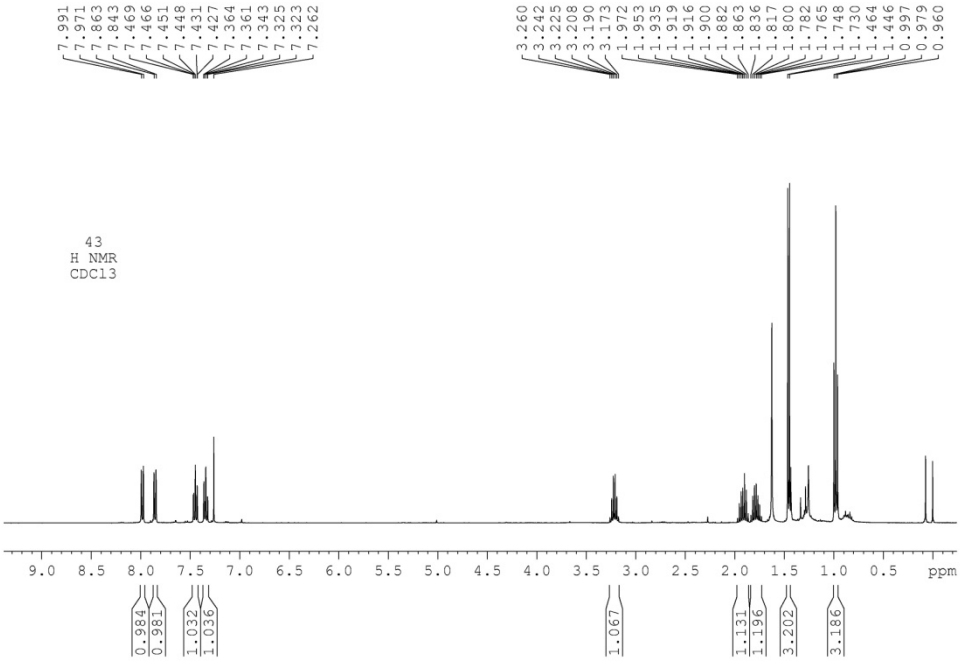


^{13}C-NMR spectrum of **3d**

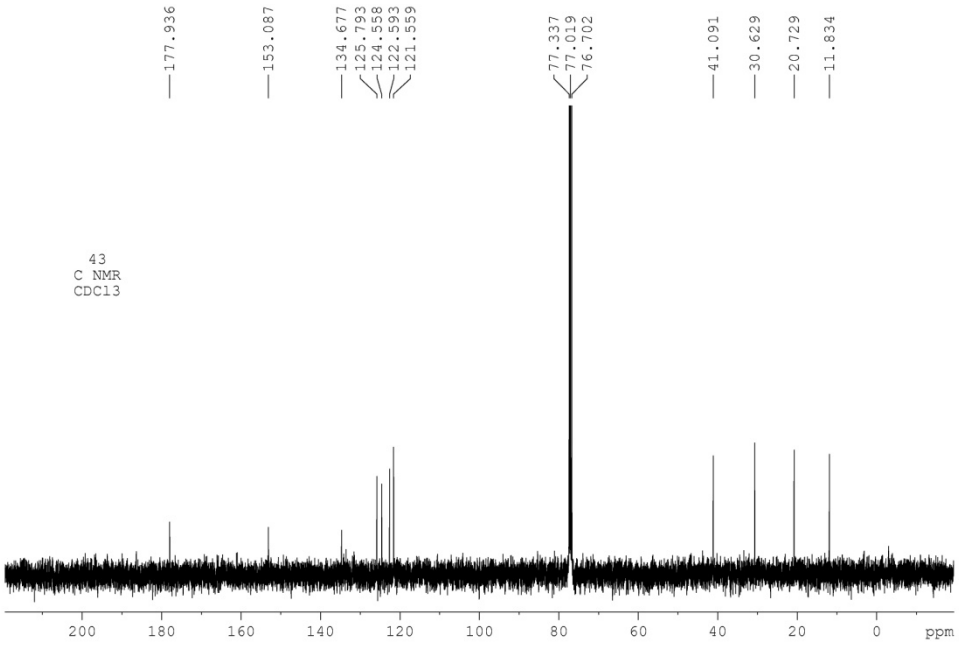


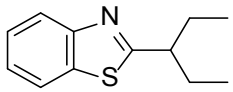


^{1}H-NMR spectrum of **3e**

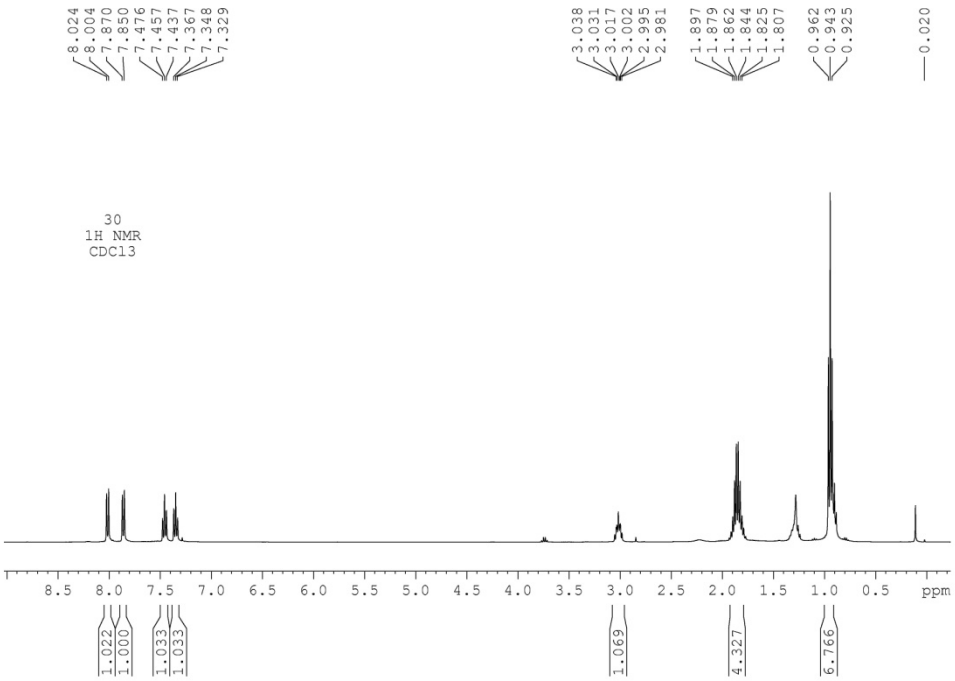


^{13}C-NMR spectrum of **3e**

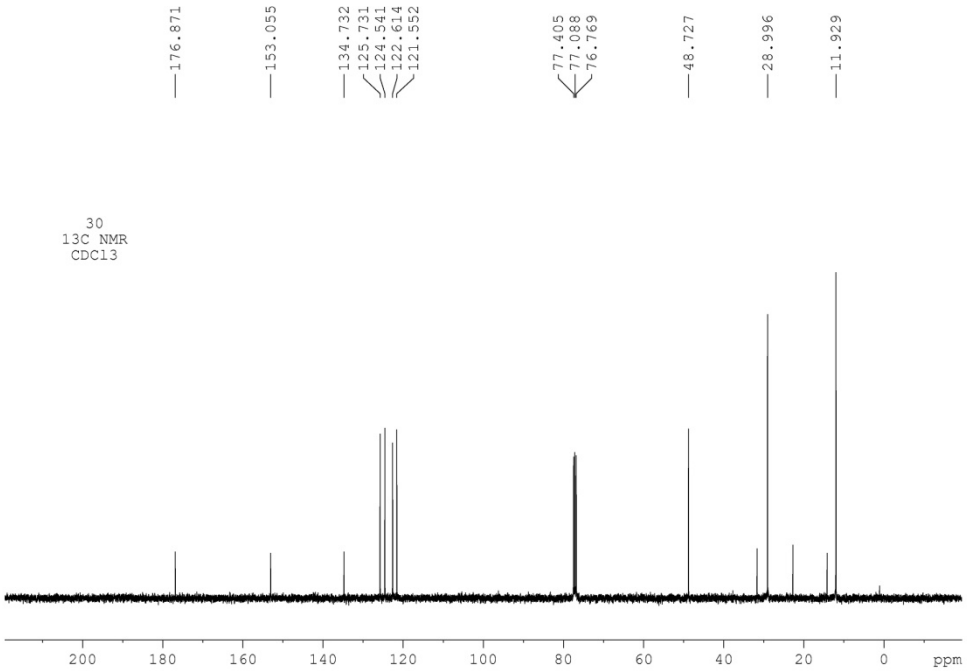


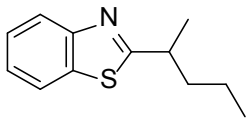


^{1}H-NMR spectrum of **3f**

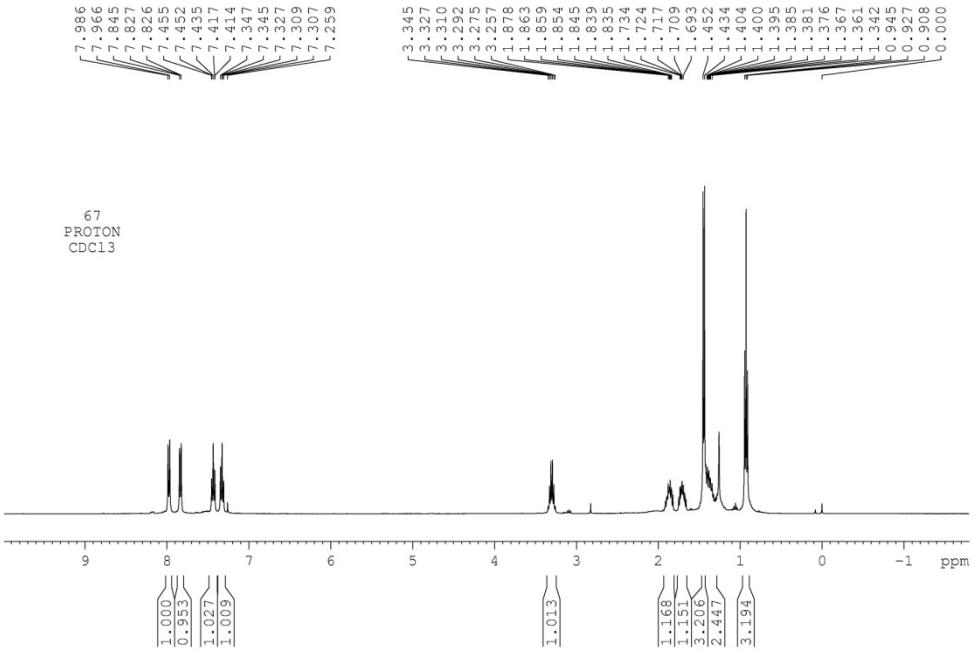


^{13}C-NMR spectrum of **3f**

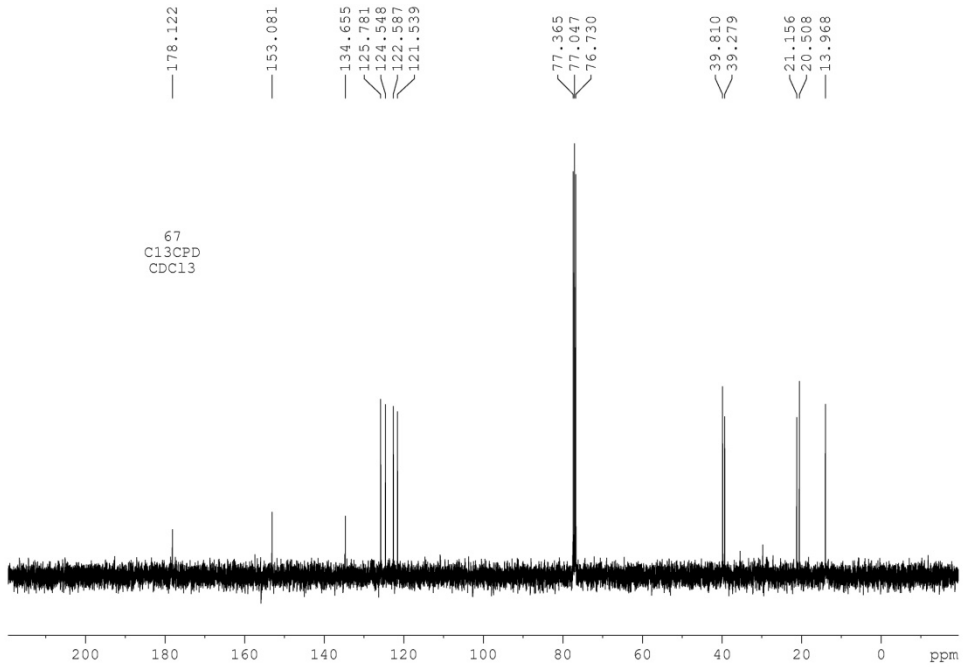


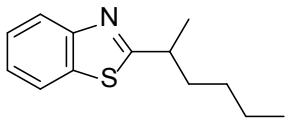


^{1}H-NMR spectrum of **3g**

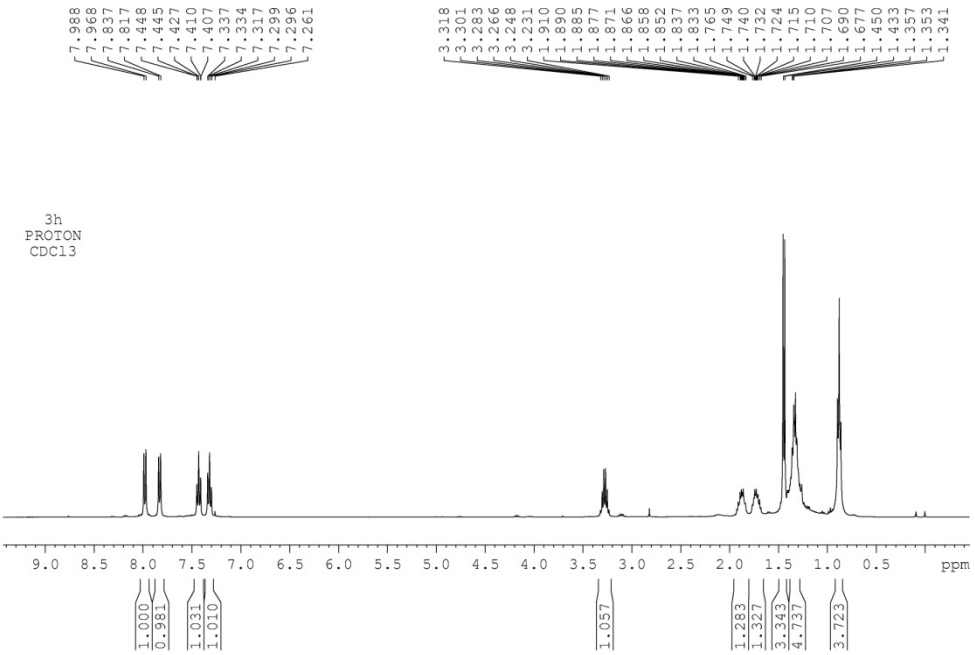


^{13}C-NMR spectrum of **3g**

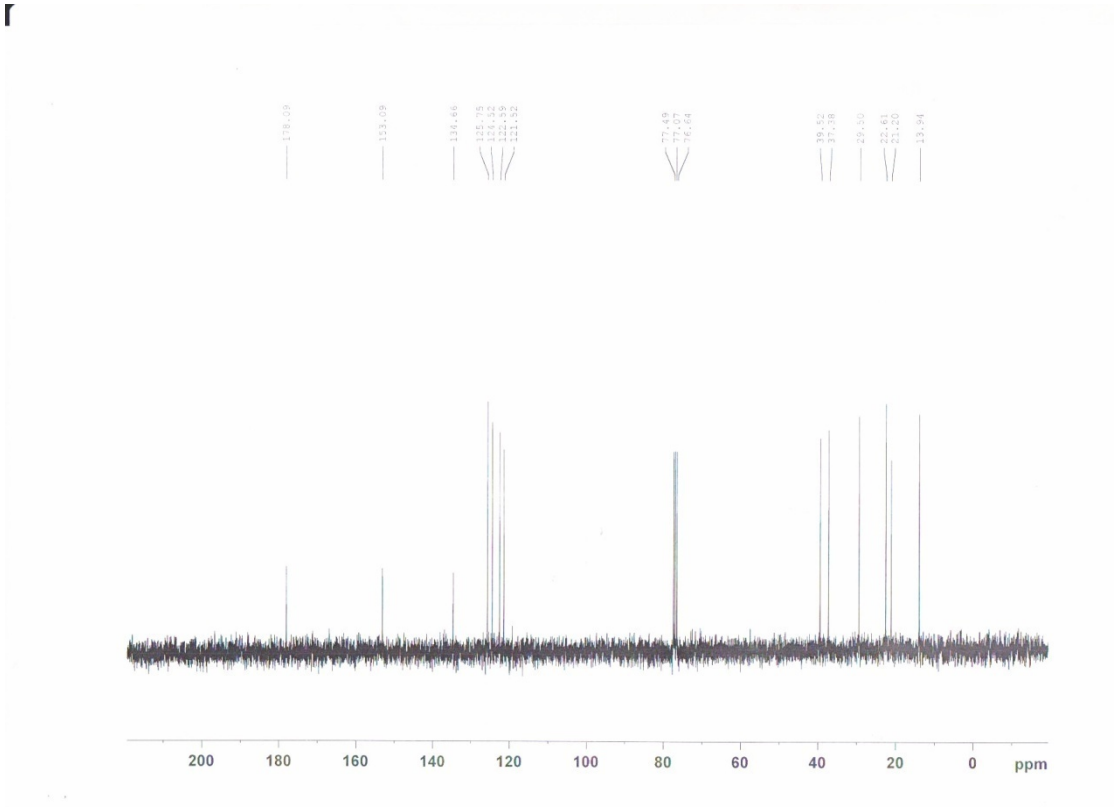


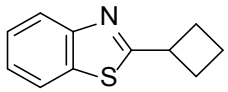


^{1}H-NMR spectrum of **3h**

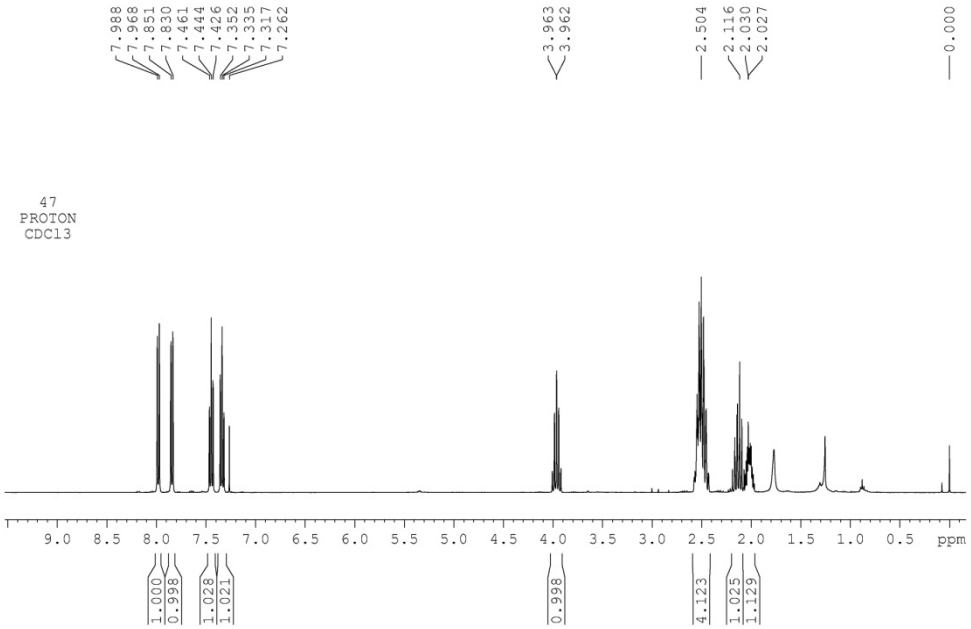


^{13}C-NMR spectrum of **3h**

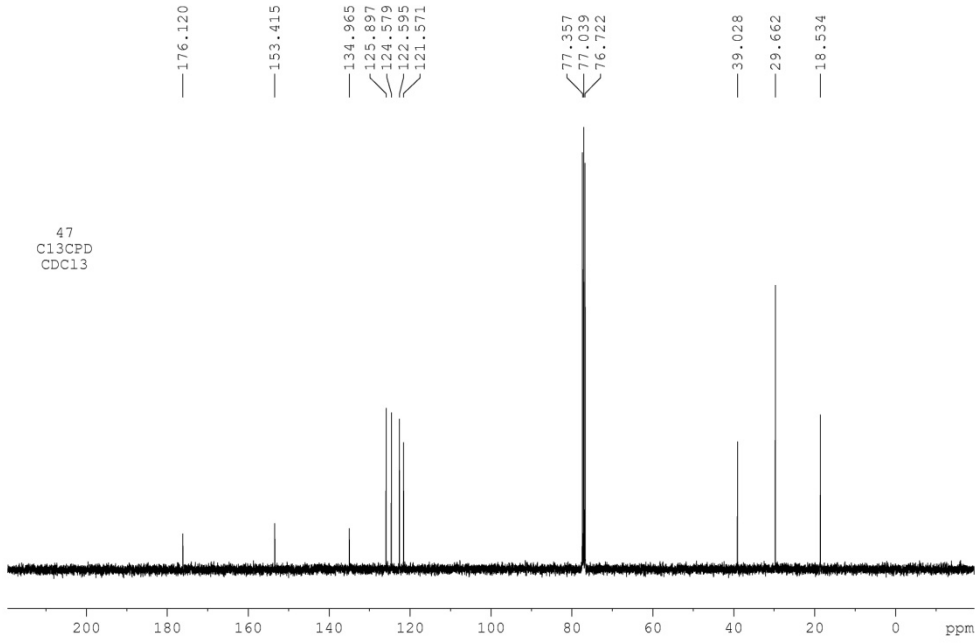


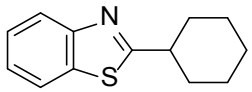


^{1}H-NMR spectrum of **3i**

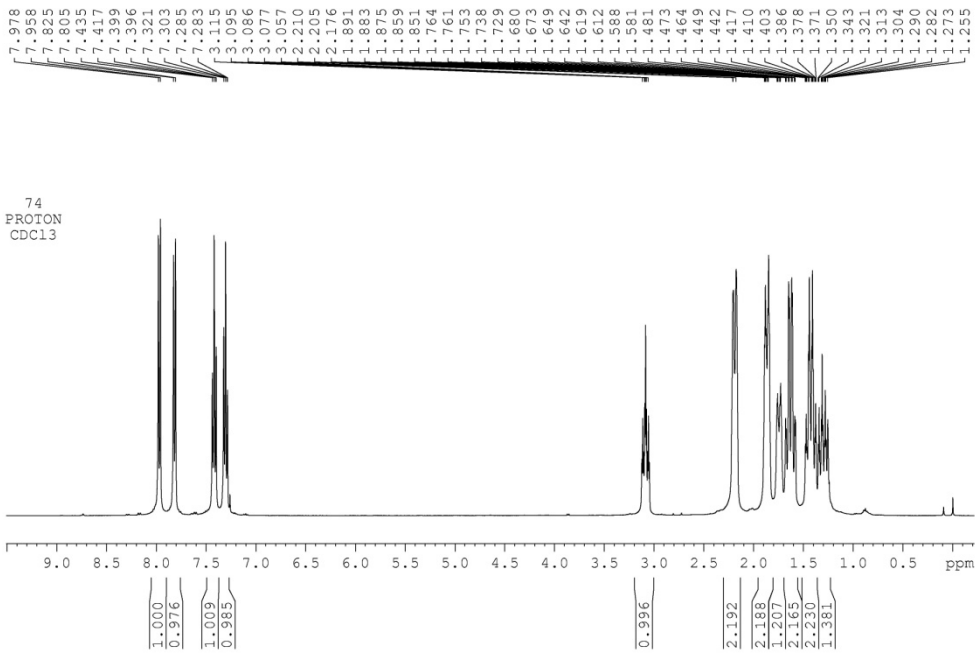


^{13}C-NMR spectrum of **3i**

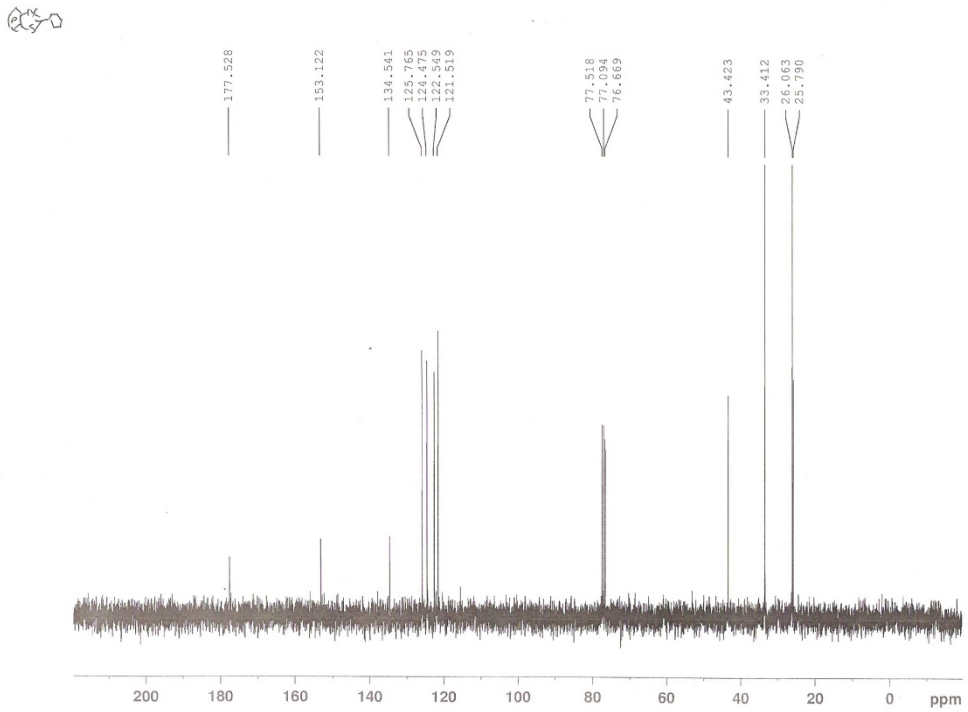


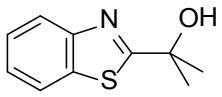


^{1}H-NMR spectrum of **3j**

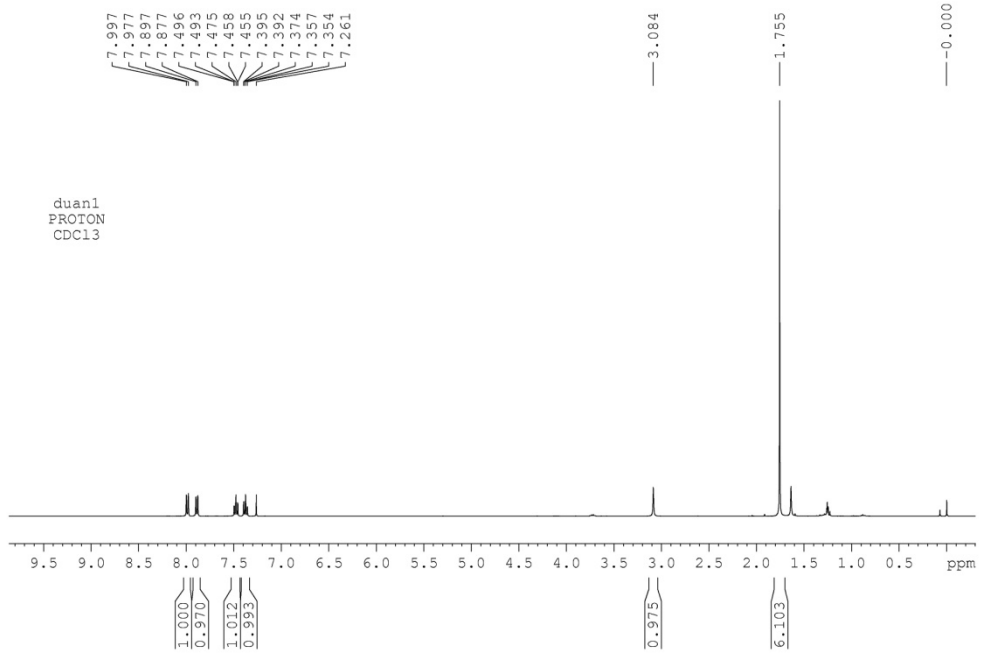


^{13}C-NMR spectrum of **3j**

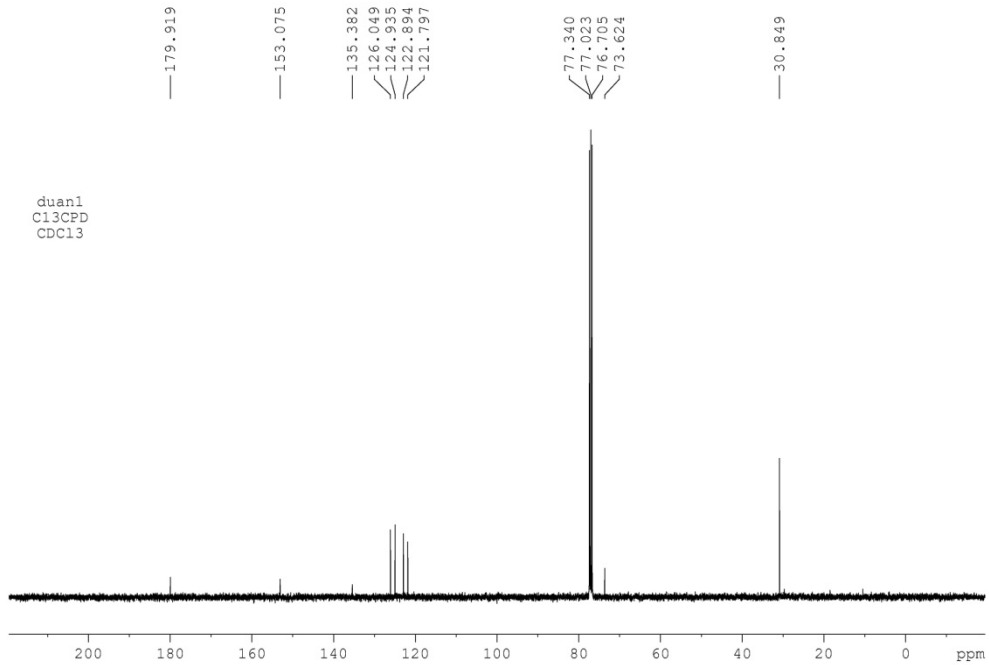


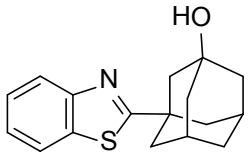


^{1}H-NMR spectrum of **3k**

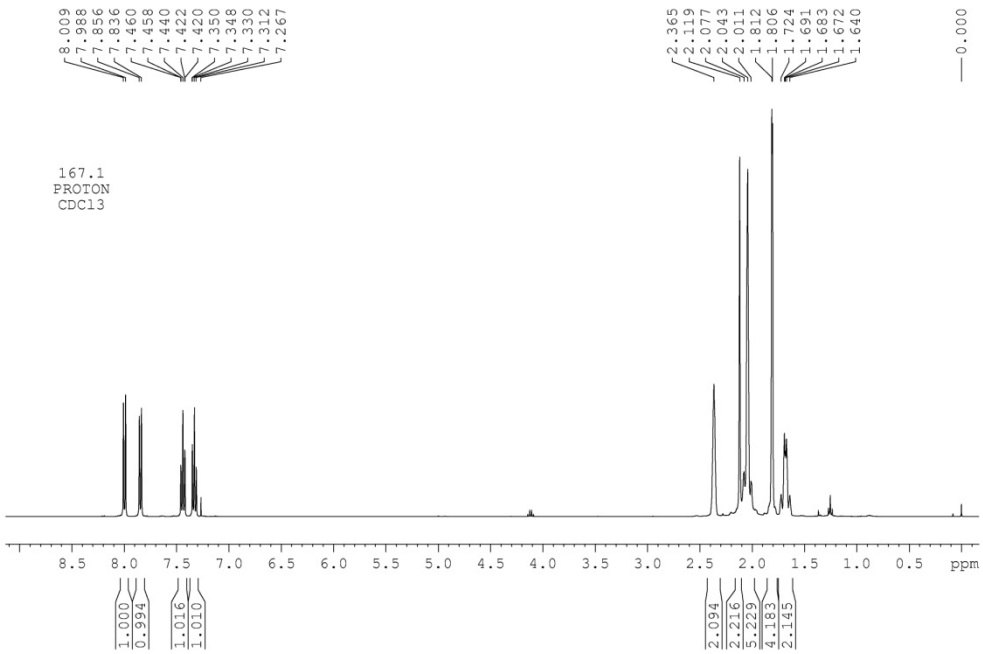


^{13}C-NMR spectrum of **3k**

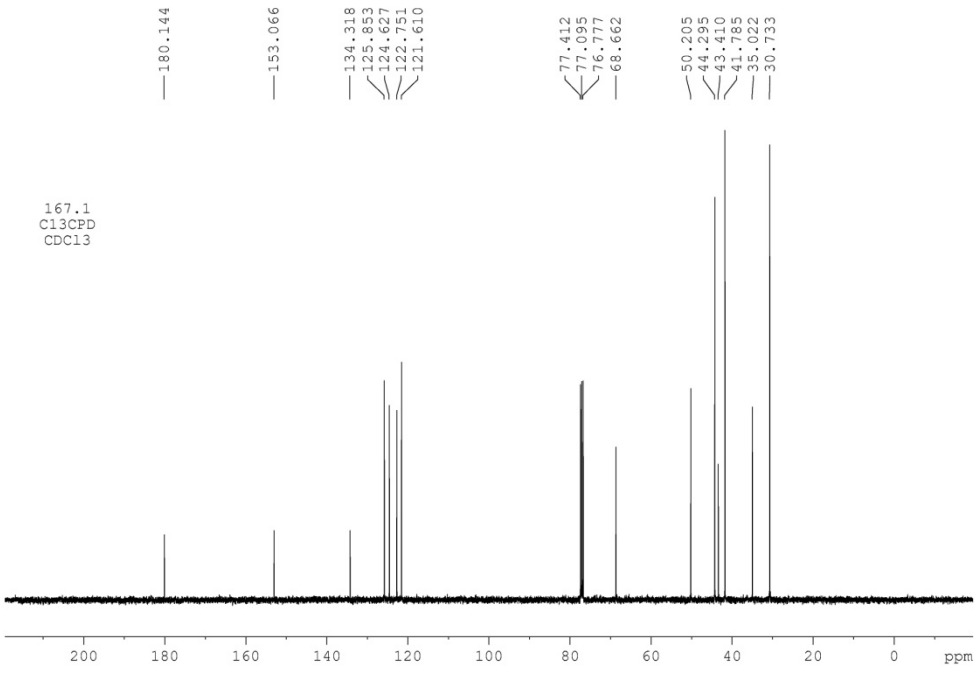


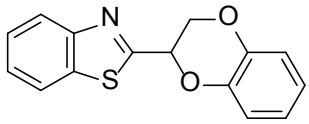


^{1}H-NMR spectrum of **3l**

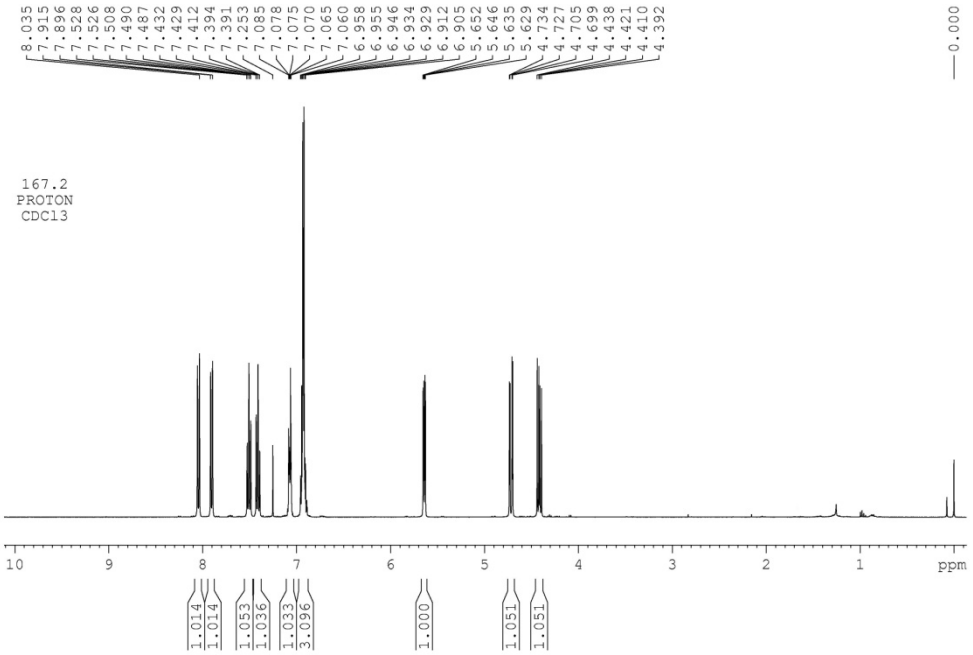


^{13}C-NMR spectrum of **3l**

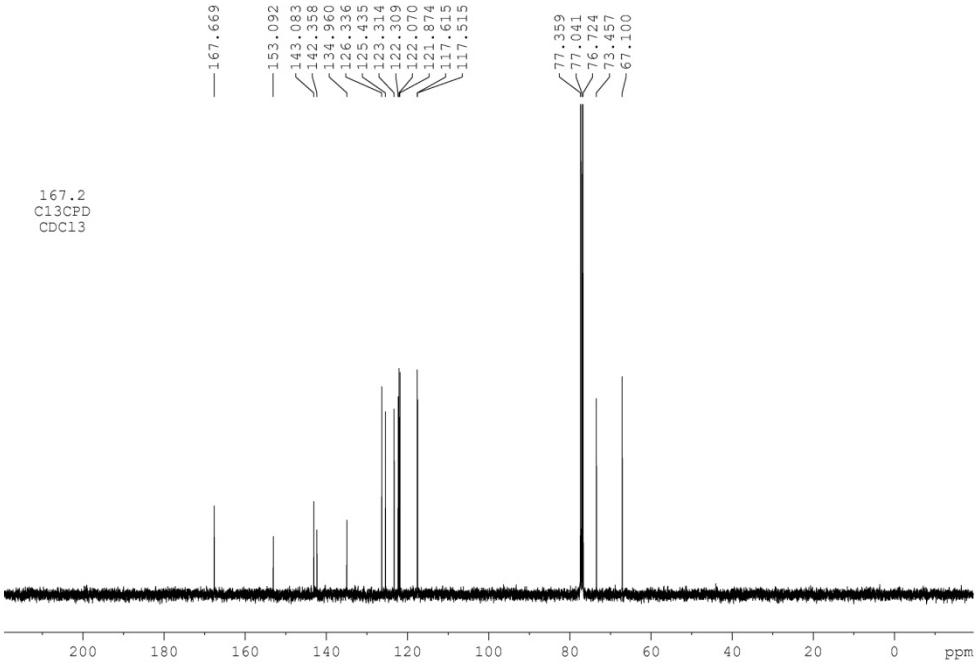


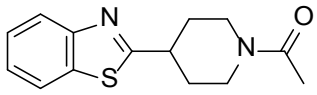


^{1}H-NMR spectrum of **3m**

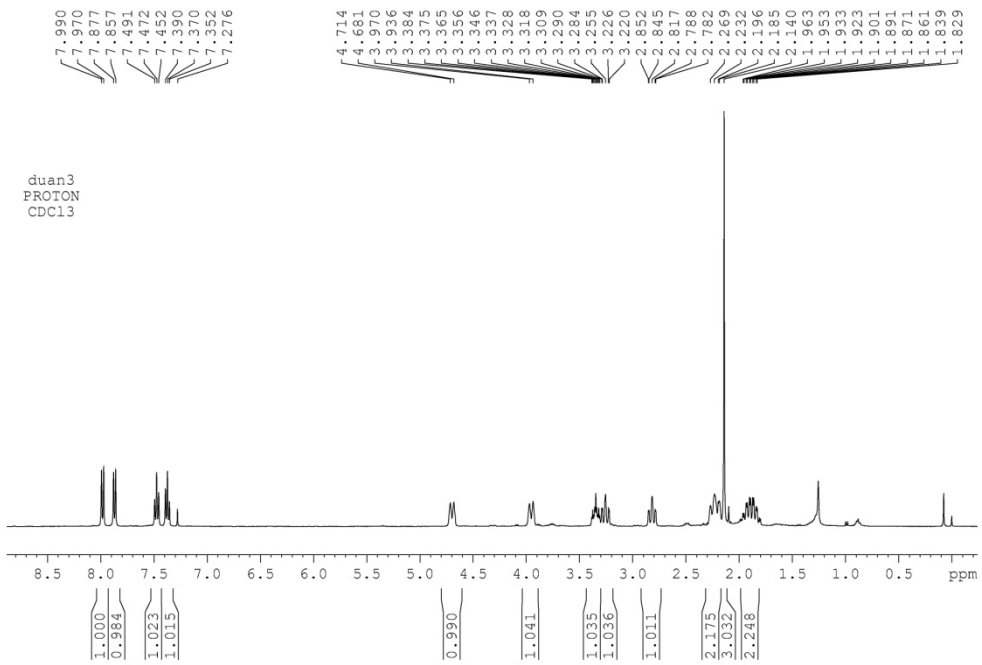


^{13}C-NMR spectrum of **3m**

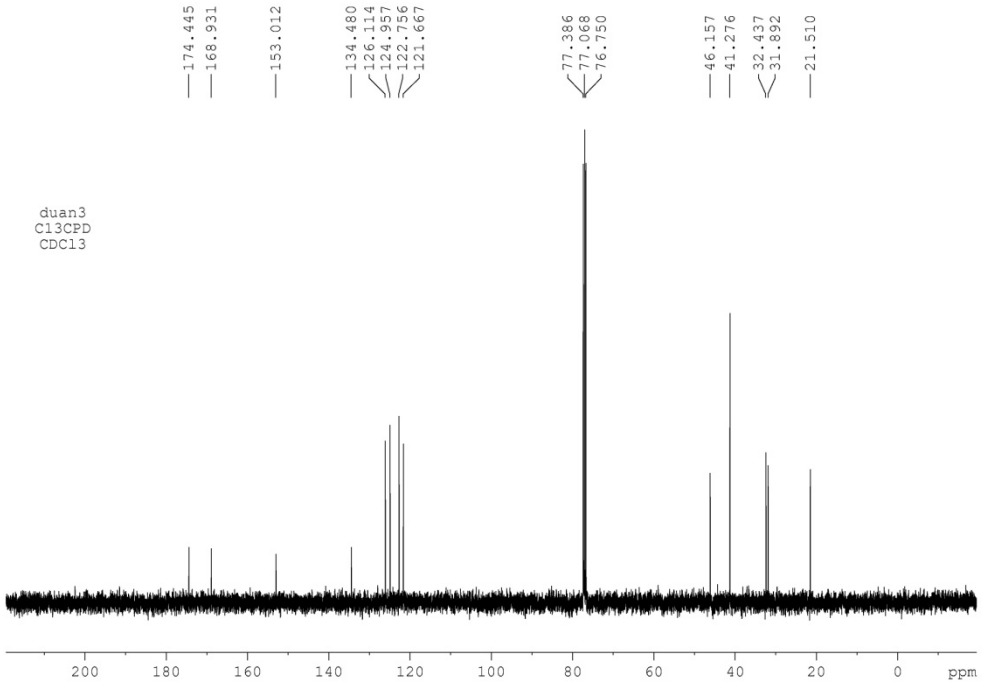


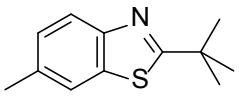


^{1}H-NMR spectrum of **3n**

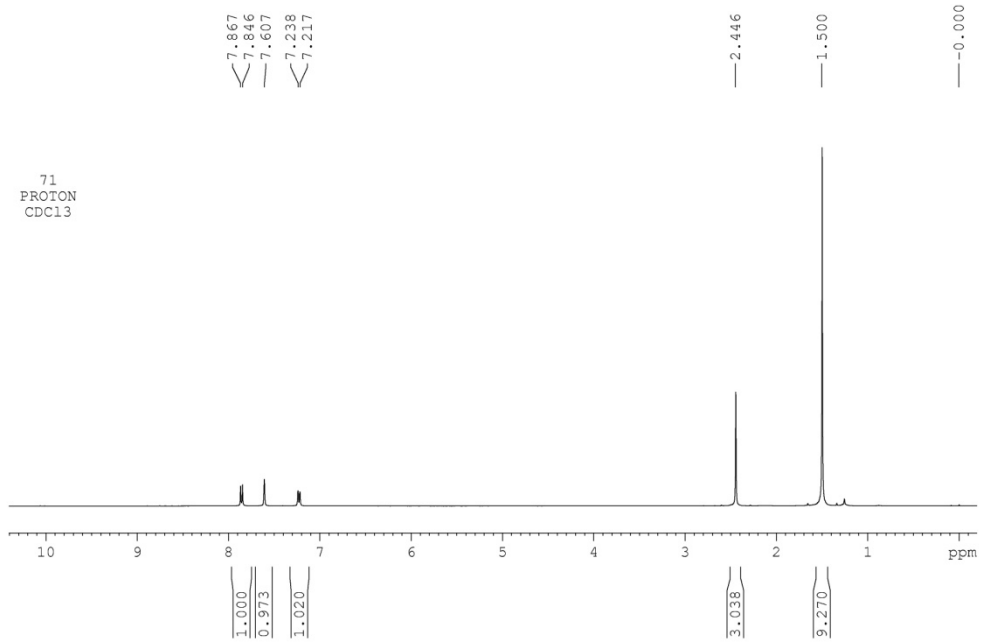


^{13}C-NMR spectrum of **3n**

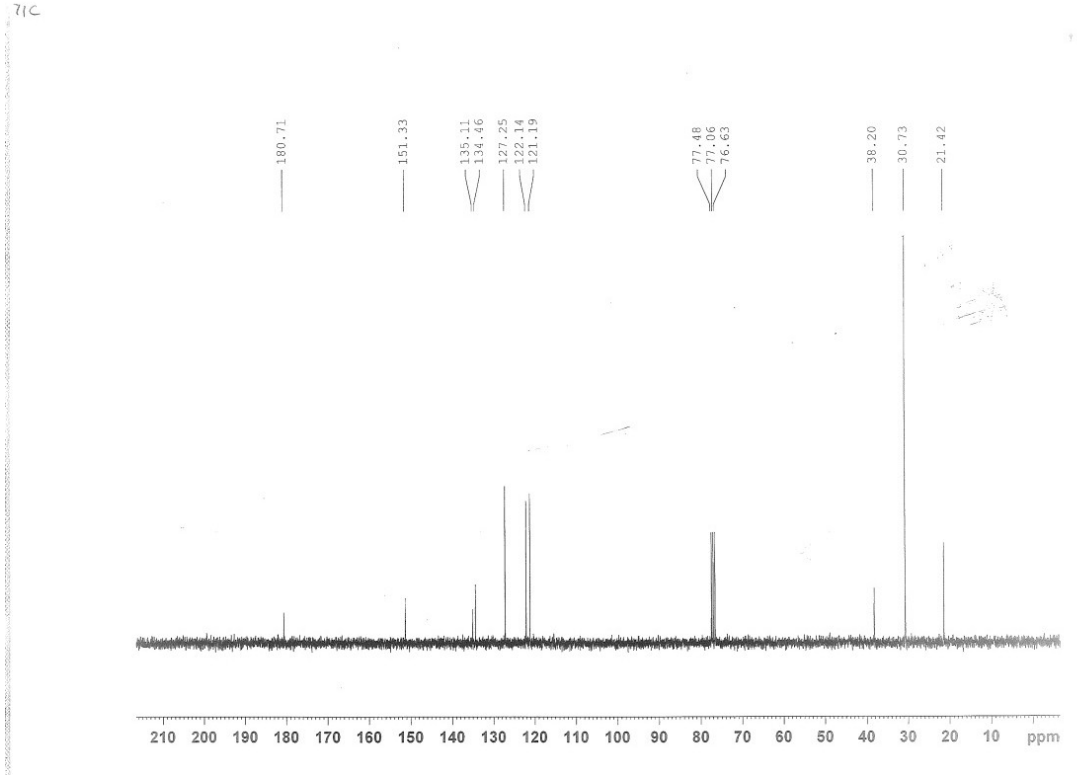


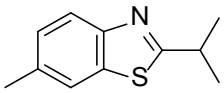


^{1}H-NMR spectrum of **3o**

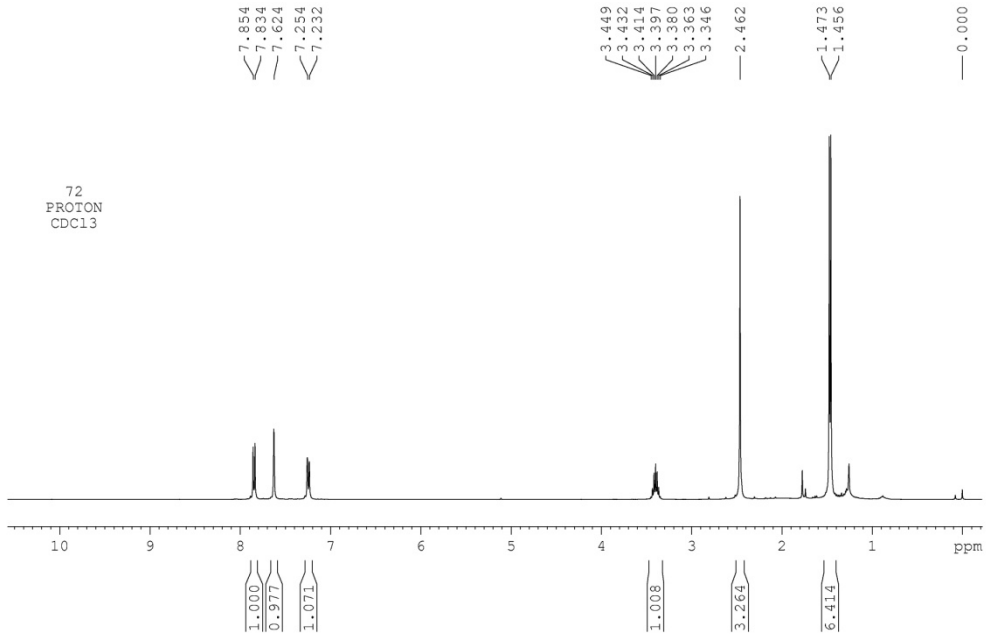


^{13}C-NMR spectrum of **3o**

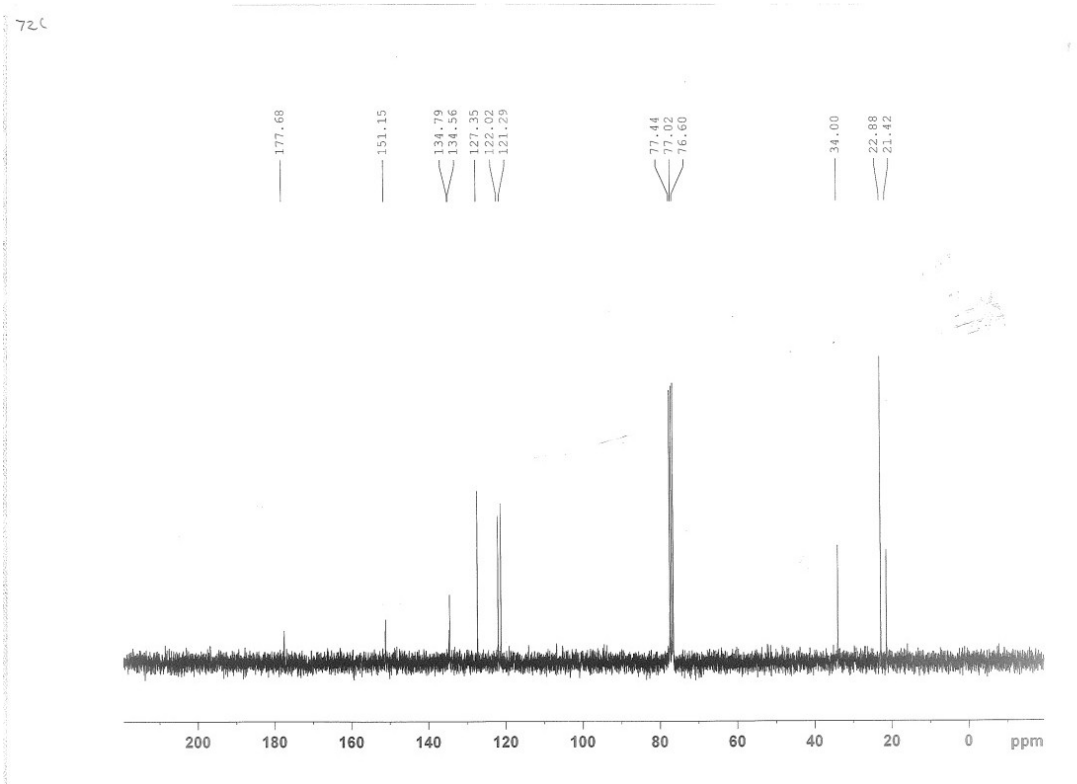


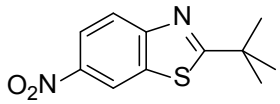


^{1}H-NMR spectrum of **3p**

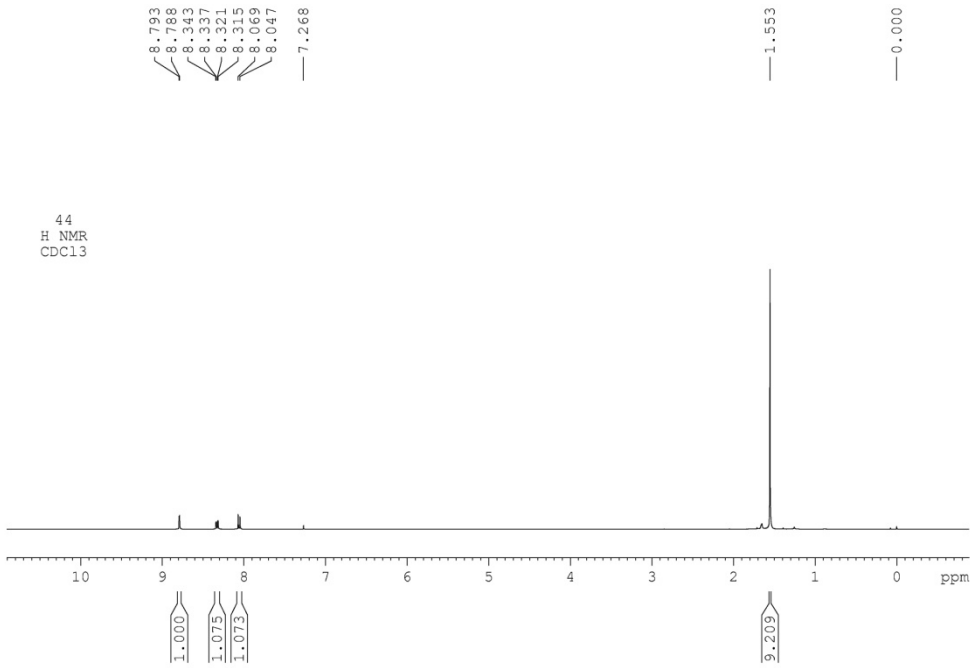


^{13}C-NMR spectrum of **3p**

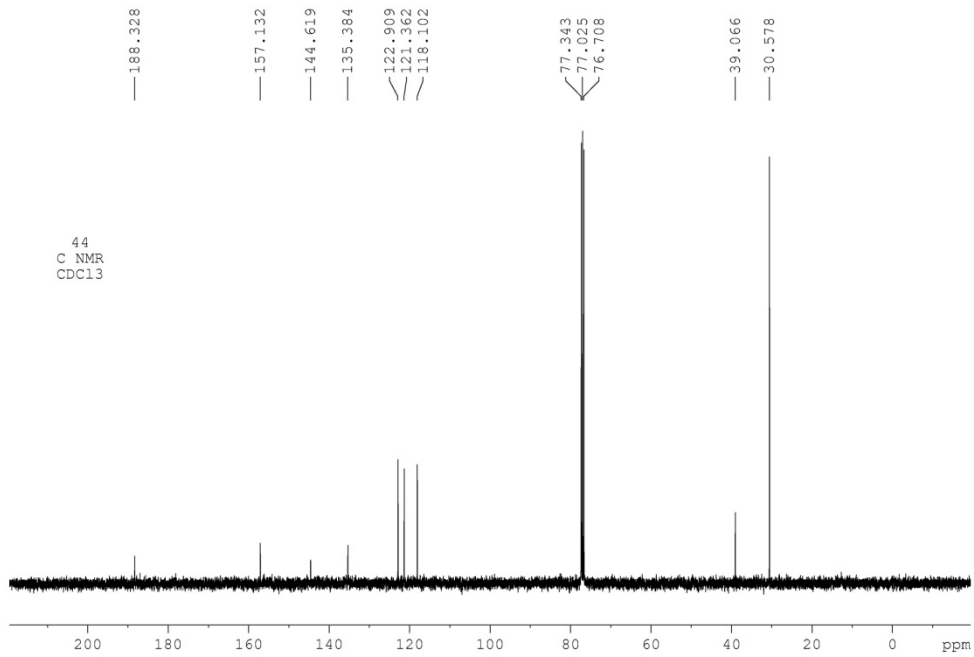


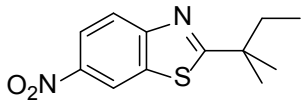


^{1}H-NMR spectrum of **3q**

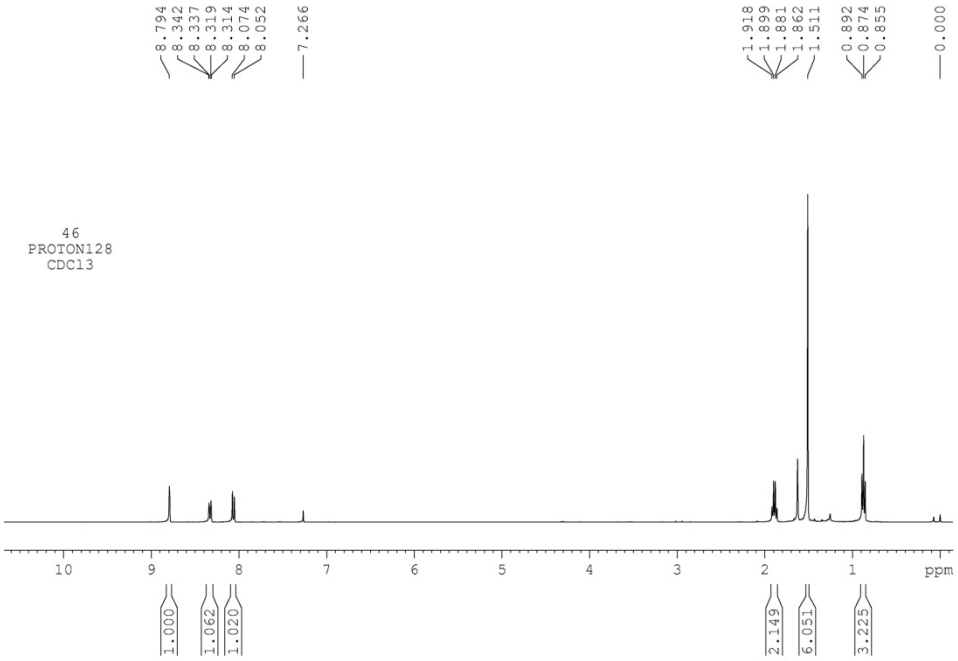


^{13}C-NMR spectrum of **3q**

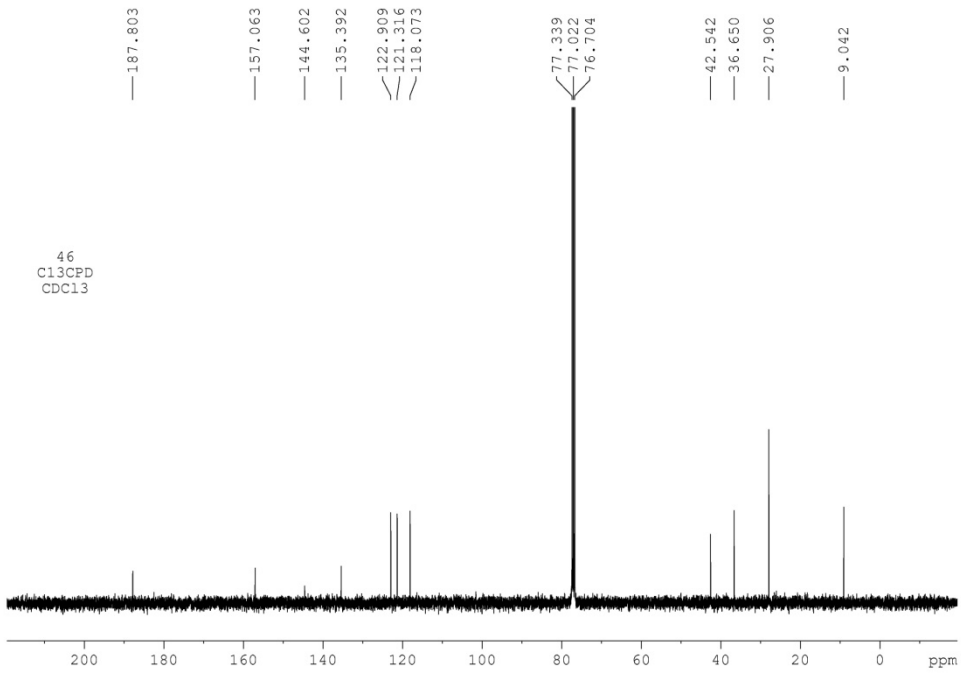


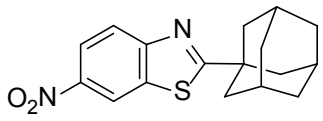


^{1}H-NMR spectrum of **3r**

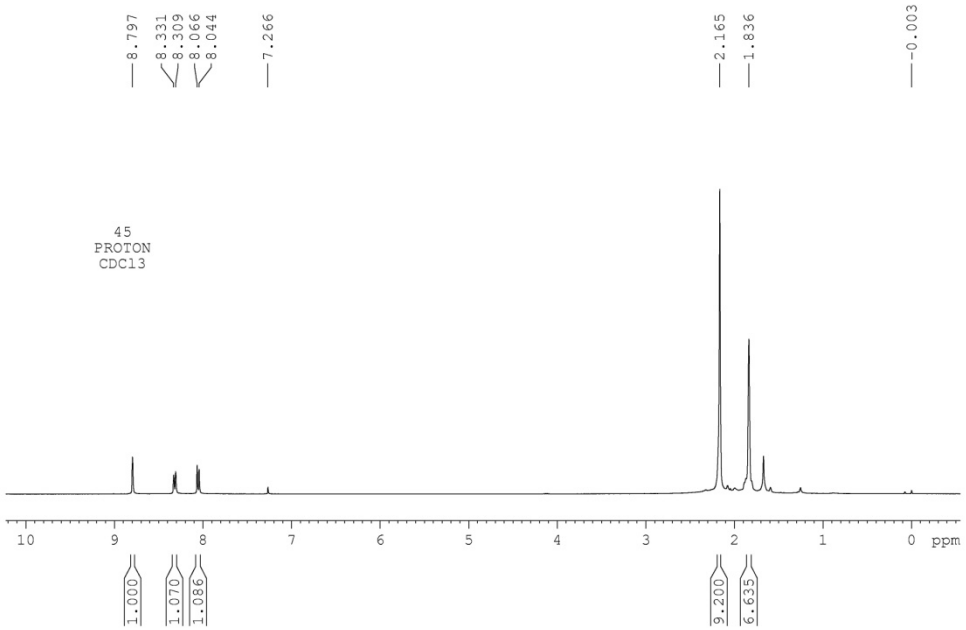


^{13}C-NMR spectrum of **3r**

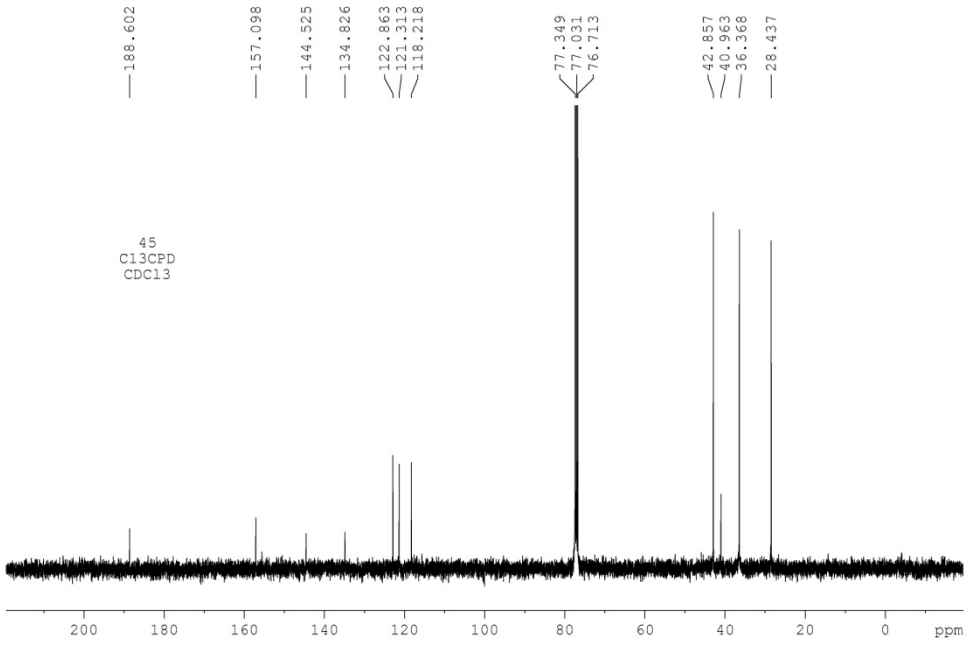


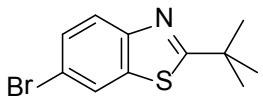


^{1}H-NMR spectrum of **3s**

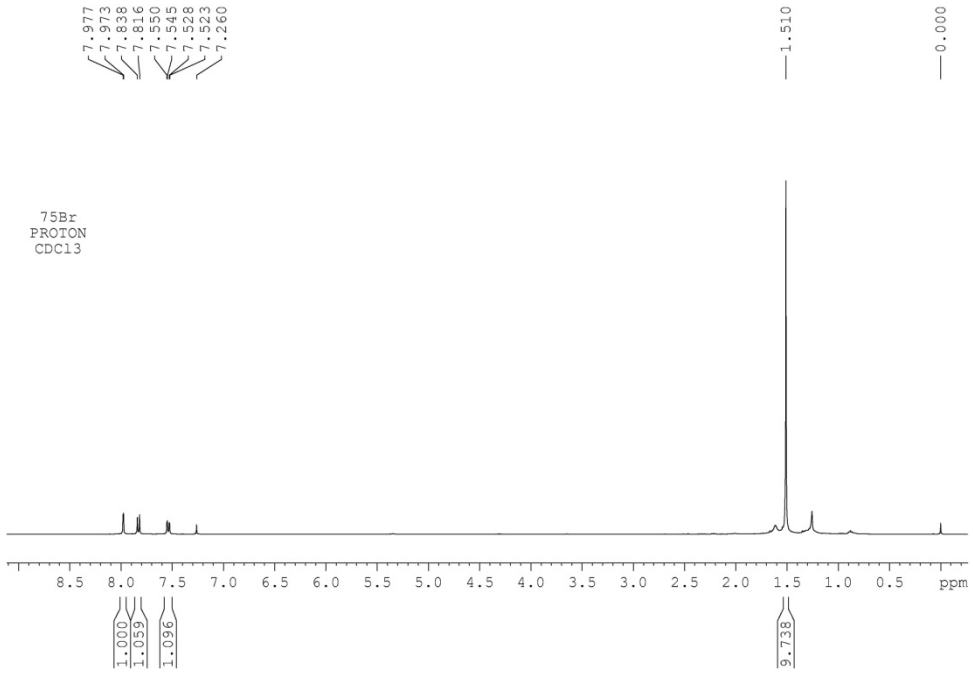


^{13}C-NMR spectrum of **3s**

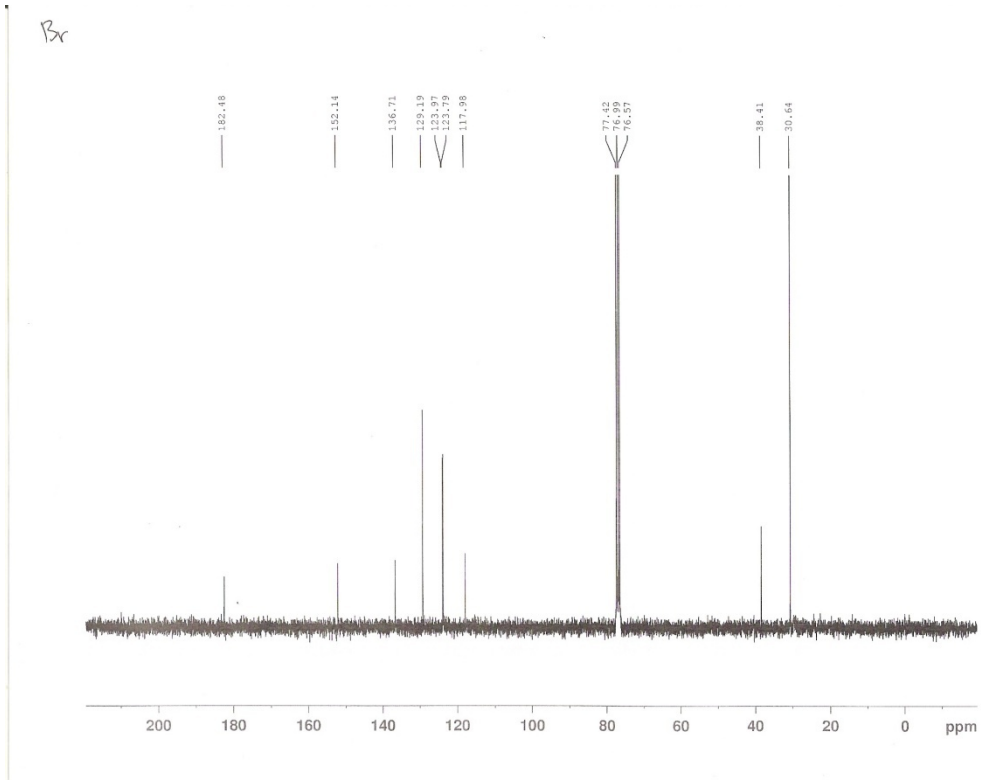


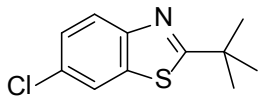


^{1}H-NMR spectrum of **3t**

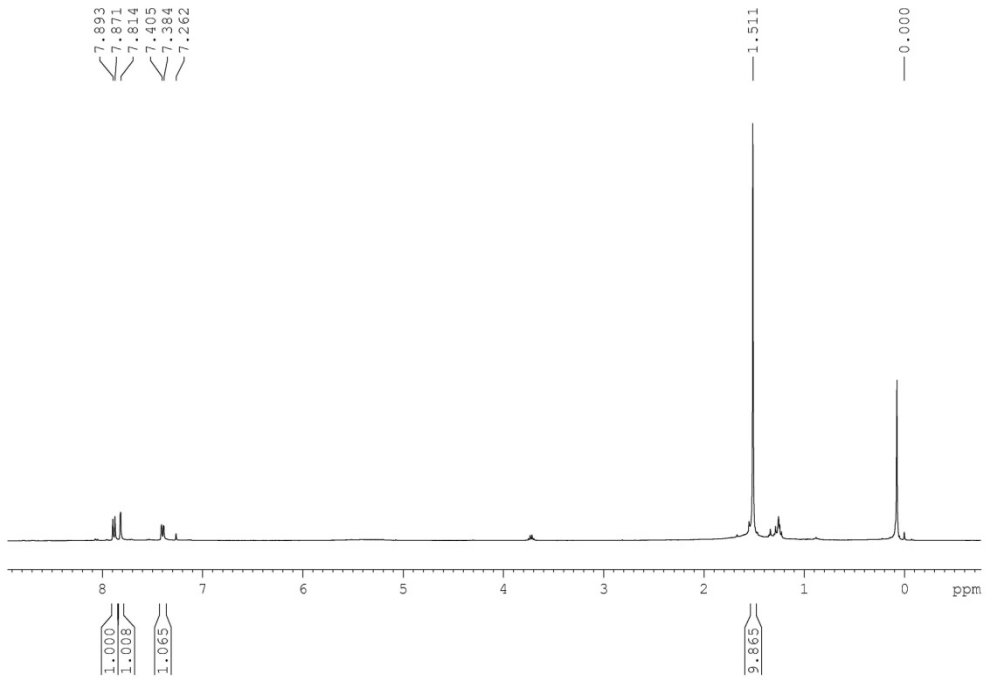


^{13}C-NMR spectrum of **3t**

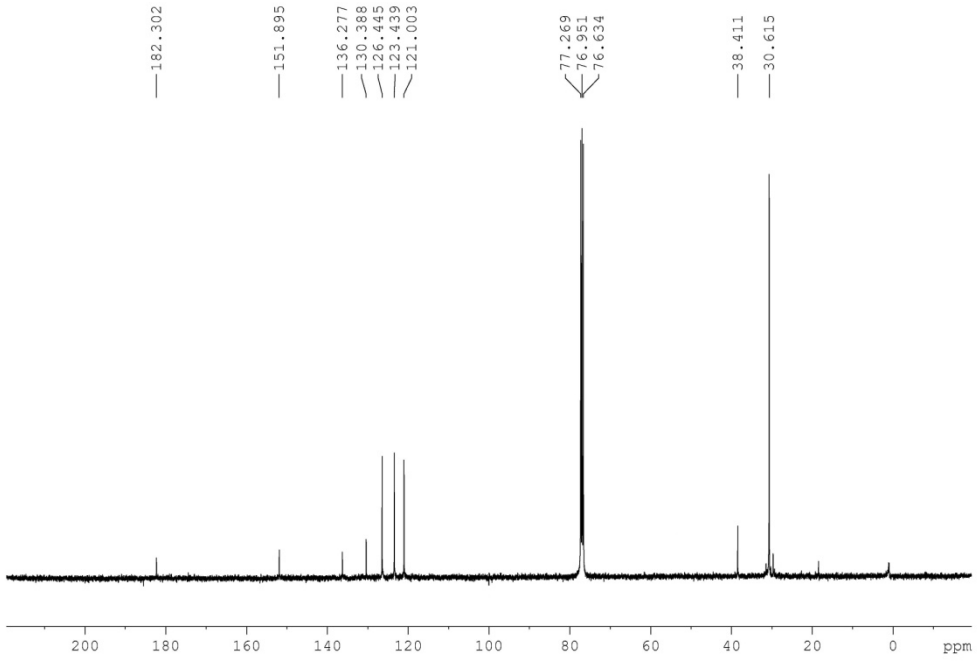


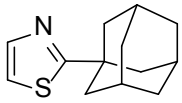


^{1}H-NMR spectrum of **3u**

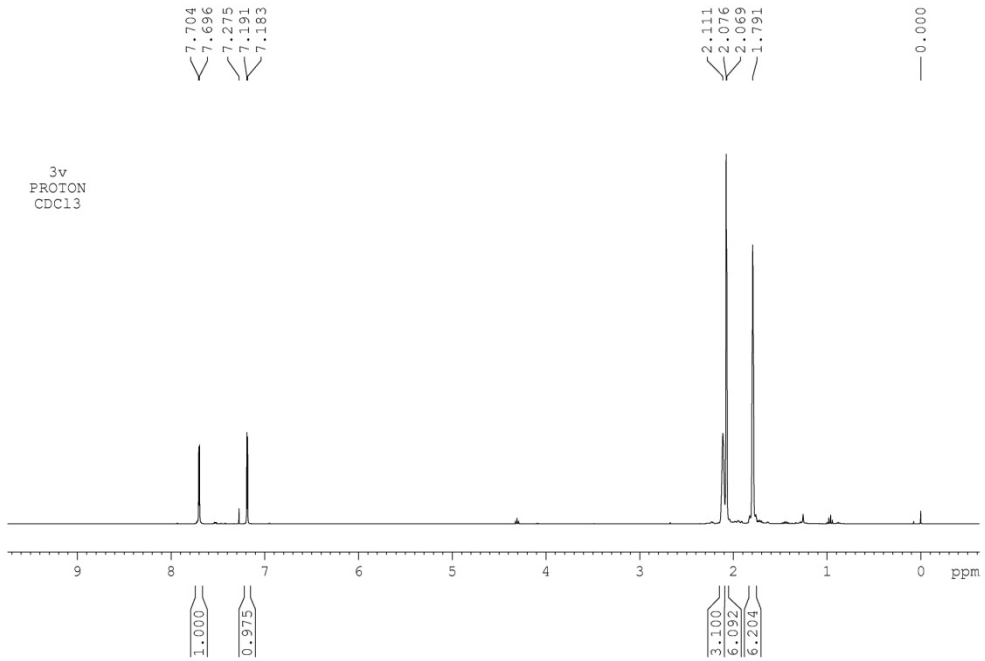


^{13}C-NMR spectrum of **3u**

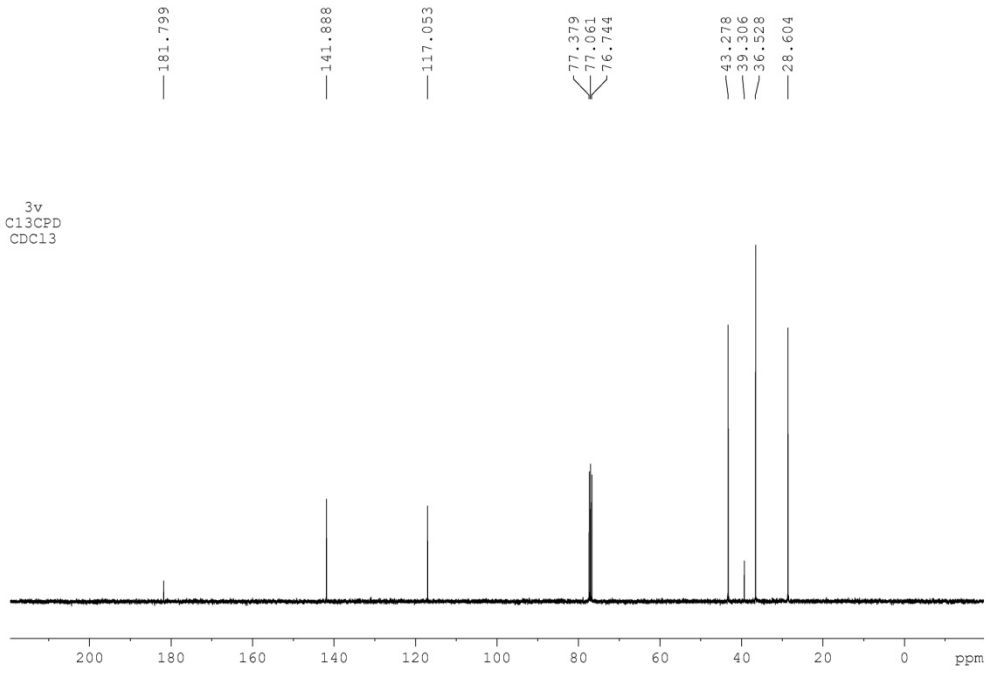


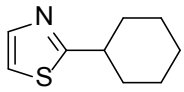


^{1}H-NMR spectrum of **3v**

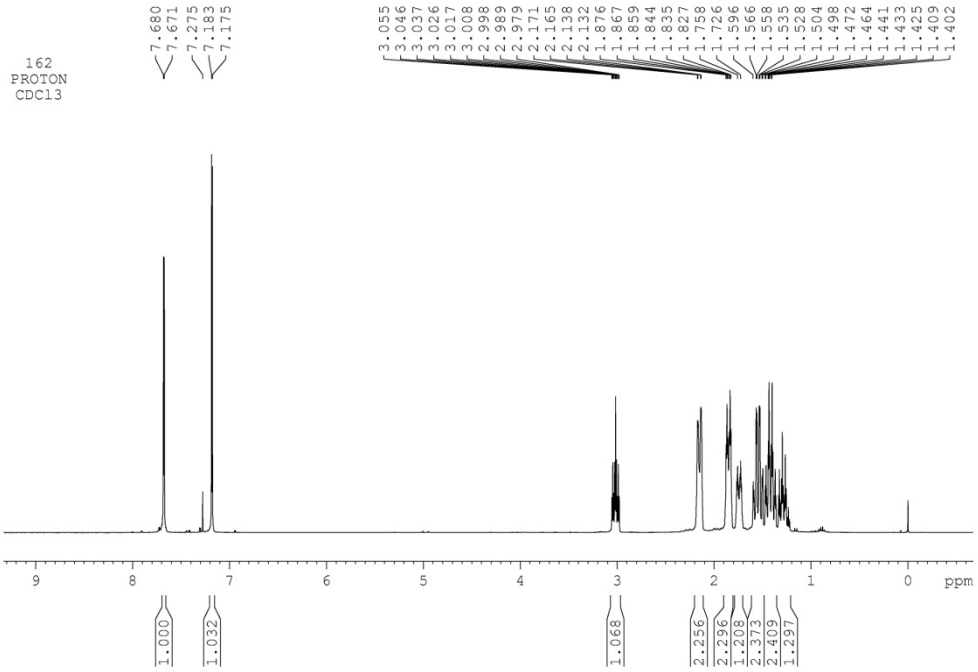


^{13}C-NMR spectrum of **3v**

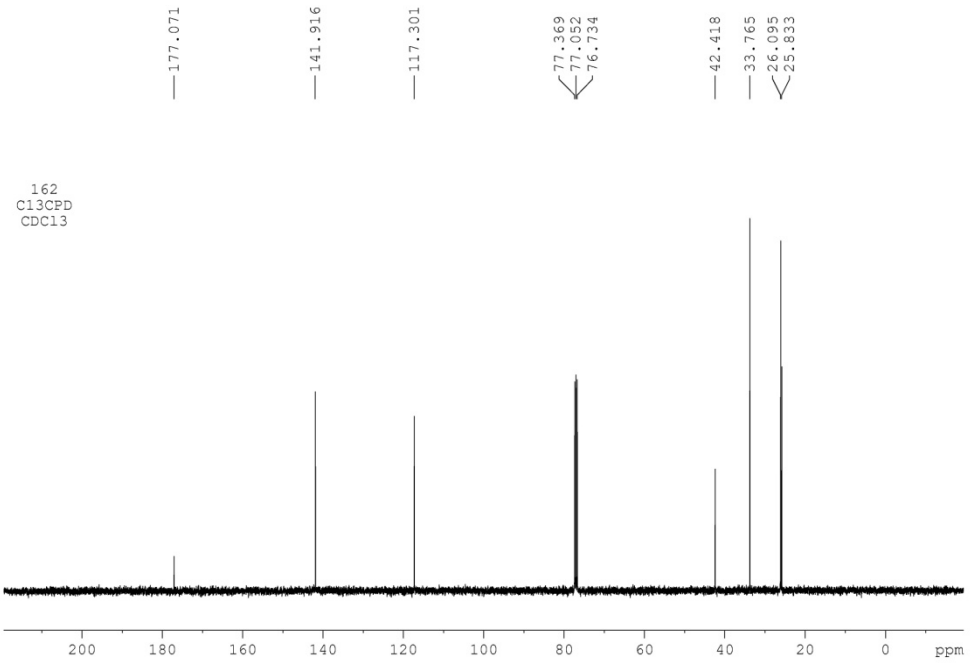


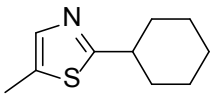


^{1}H-NMR spectrum of **3w**

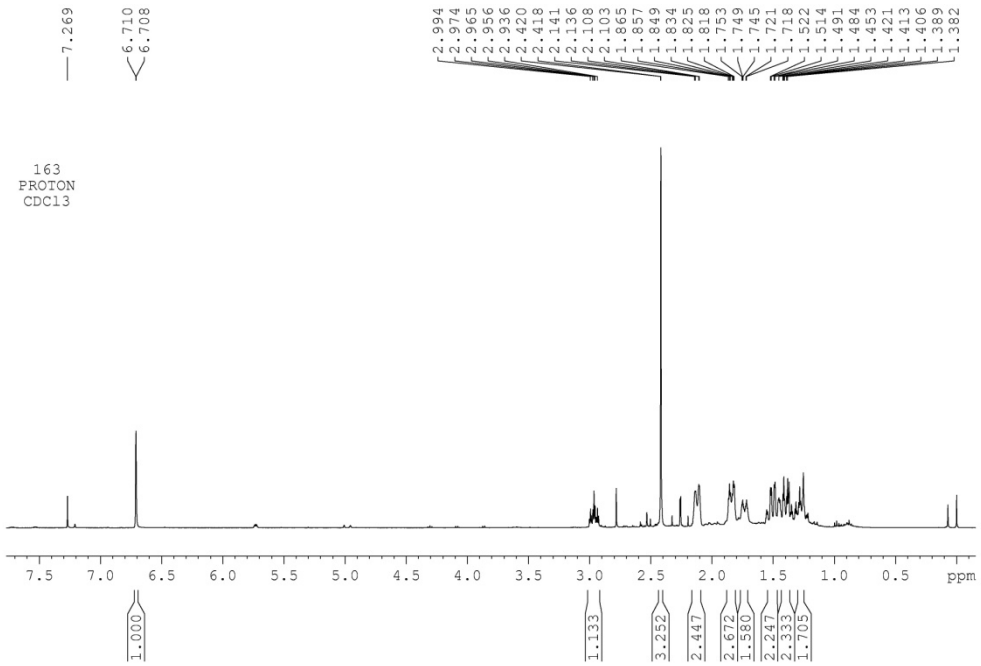


^{13}C-NMR spectrum of **3w**

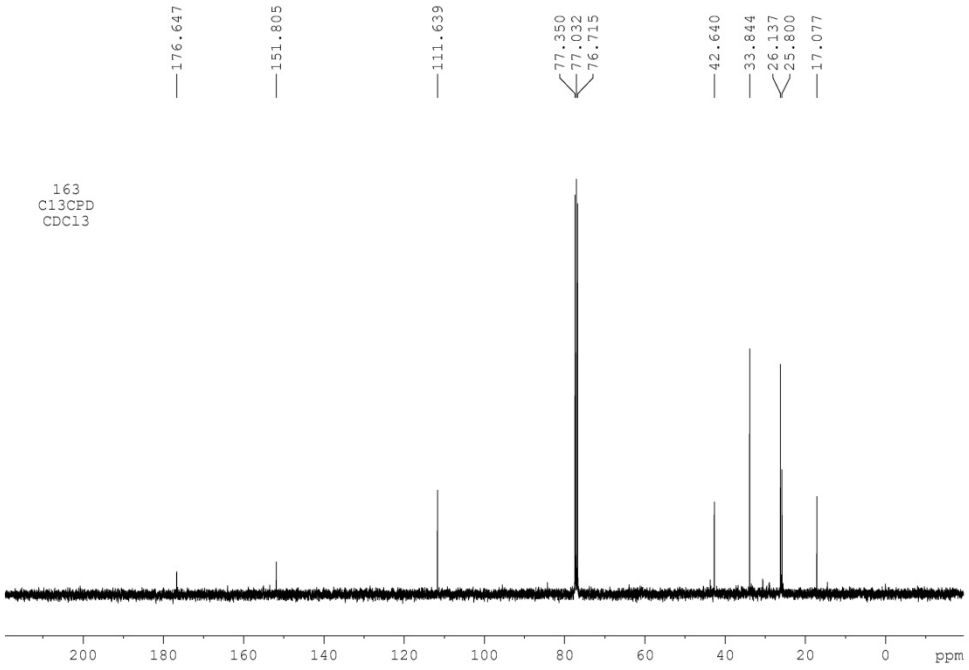


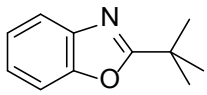


^{1}H-NMR spectrum of **3x**

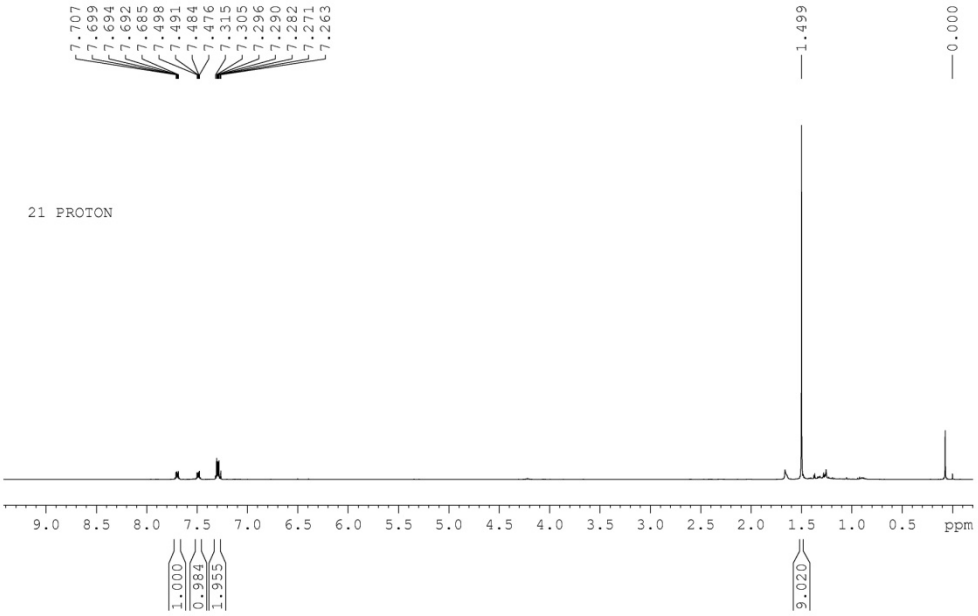


^{13}C-NMR spectrum of **3x**

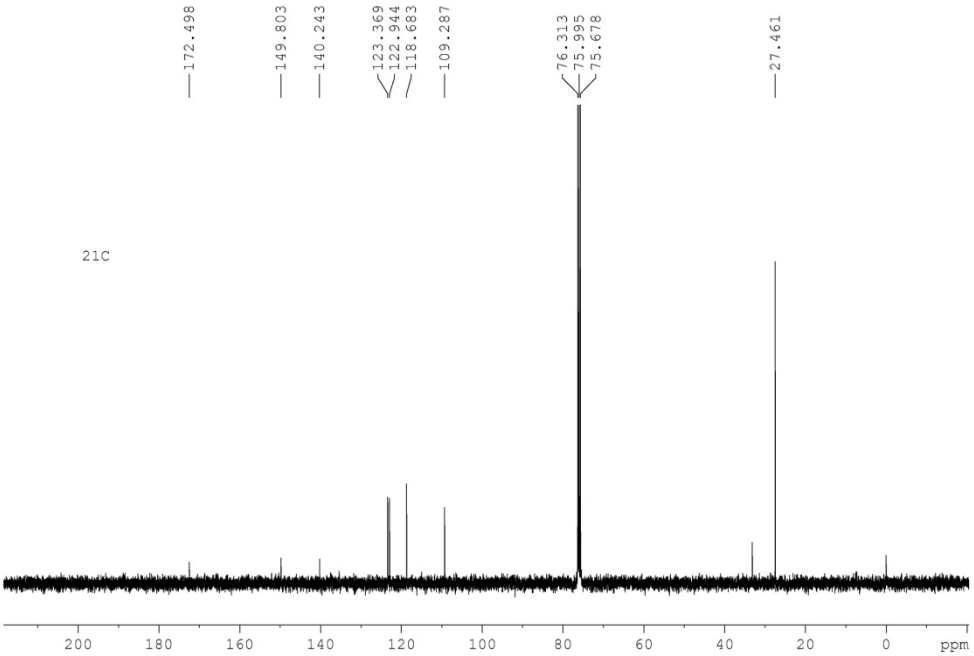


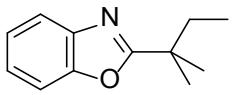


^{1}H-NMR spectrum of **3y**

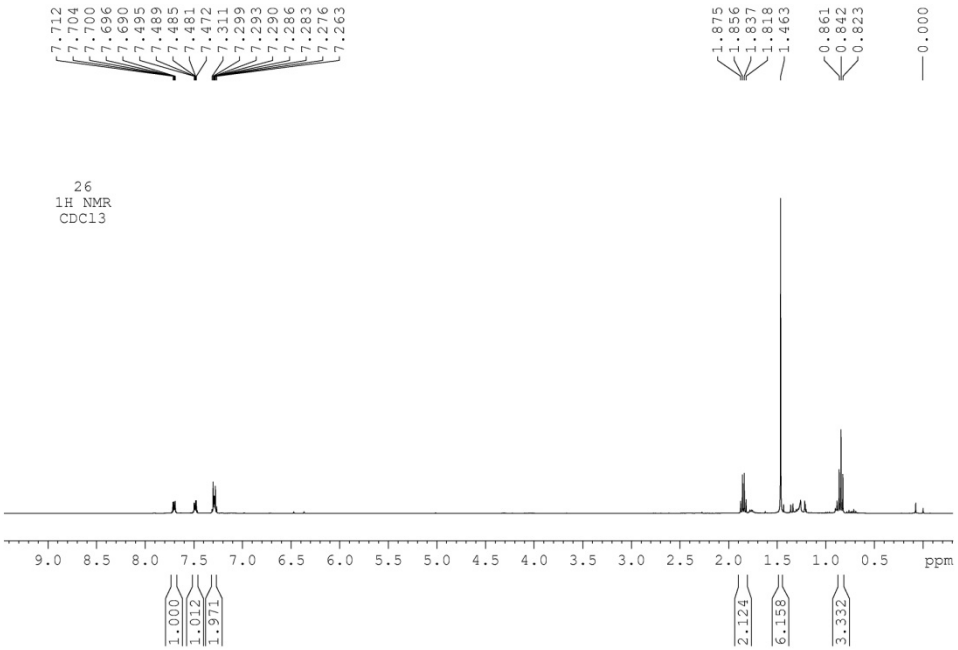


^{13}C-NMR spectrum of **3y**

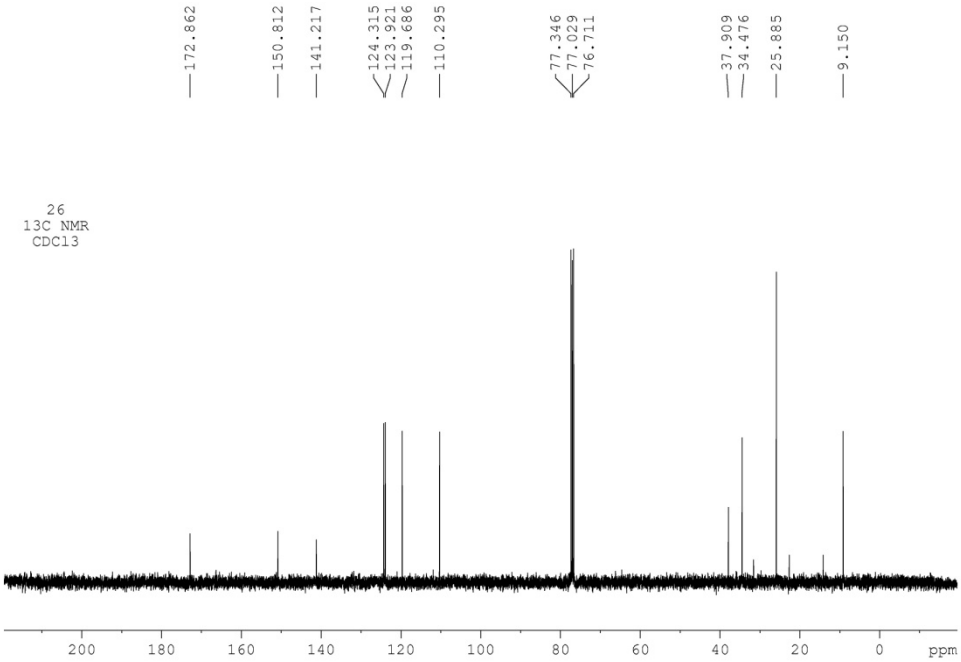


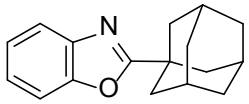


^{1}H-NMR spectrum of **3z**

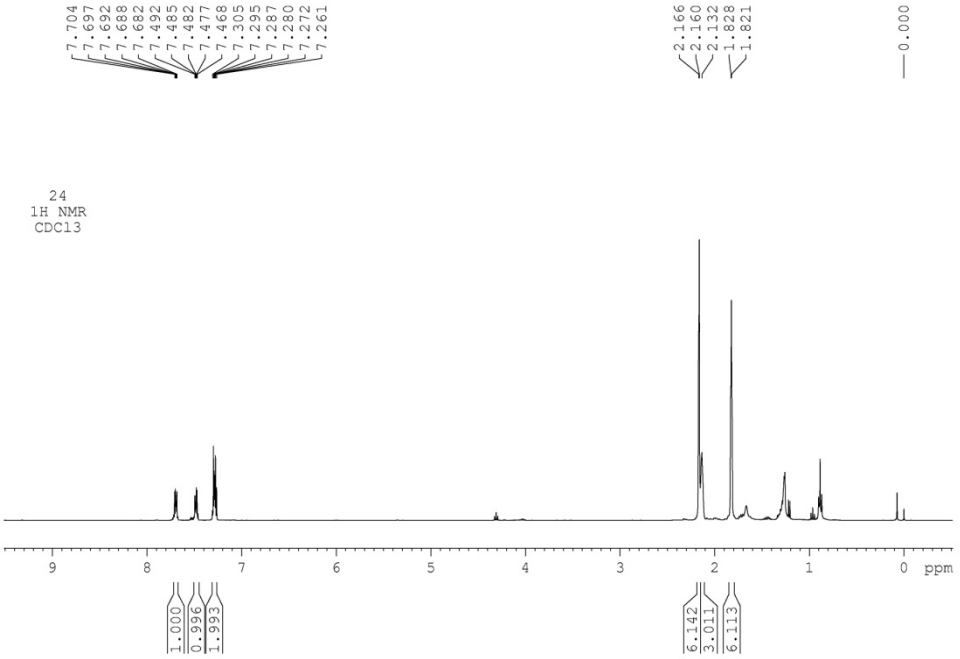


^{13}C-NMR spectrum of **3z**

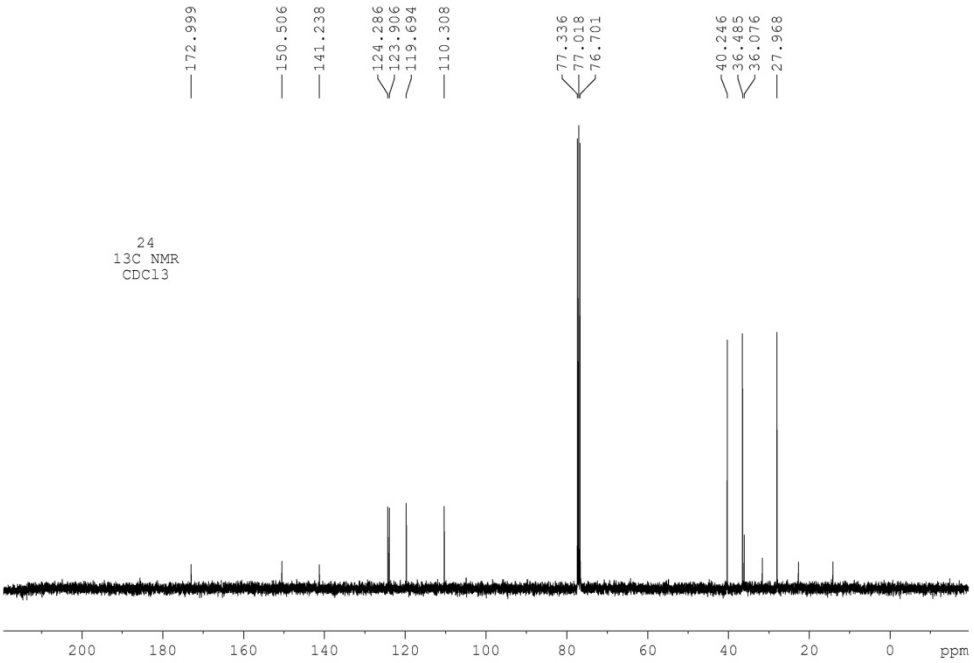


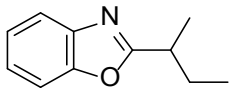


^{1}H-NMR spectrum of **3aa**

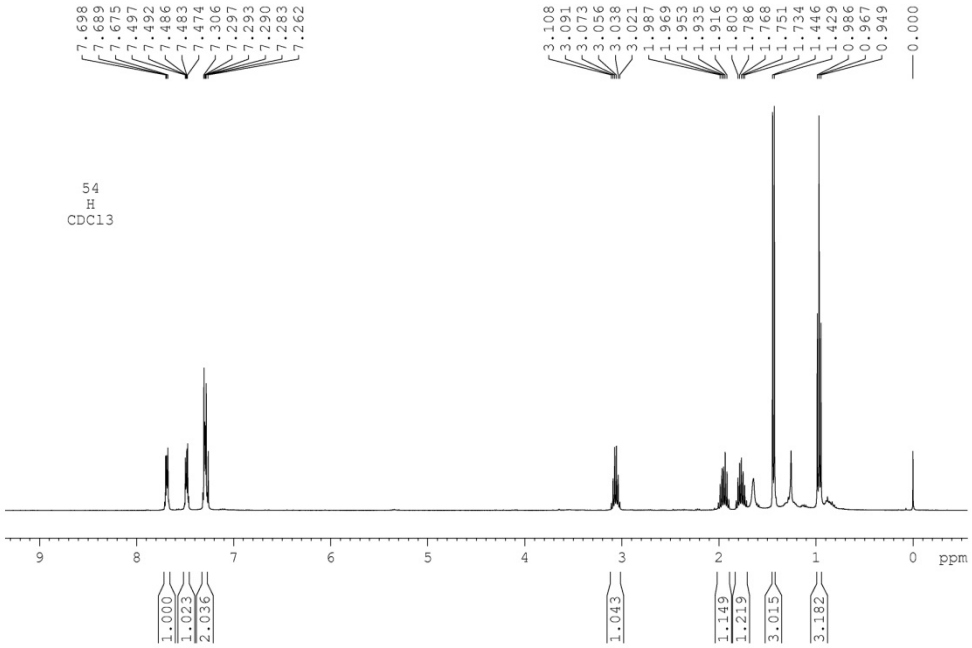


^{13}C-NMR spectrum of **3aa**

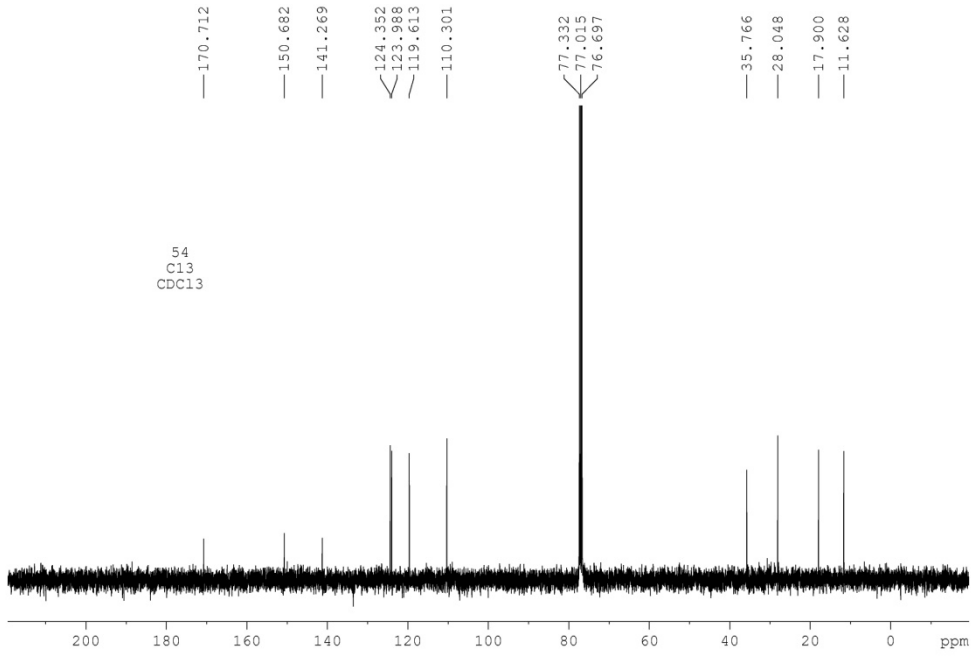


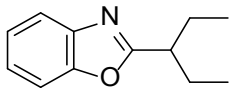


^{1}H-NMR spectrum of **3ab**

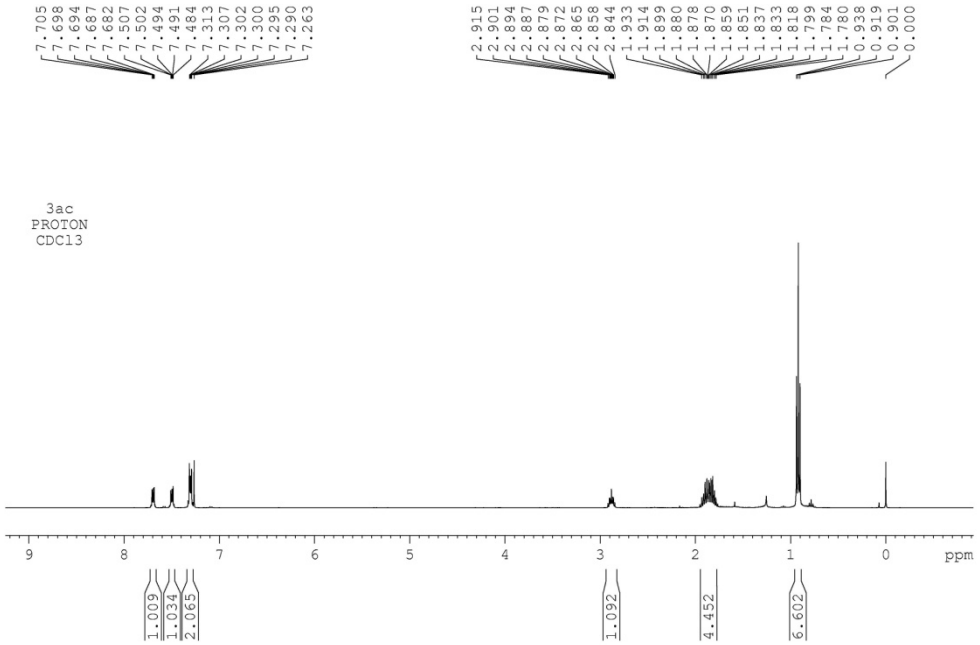


^{13}C-NMR spectrum of **3ab**

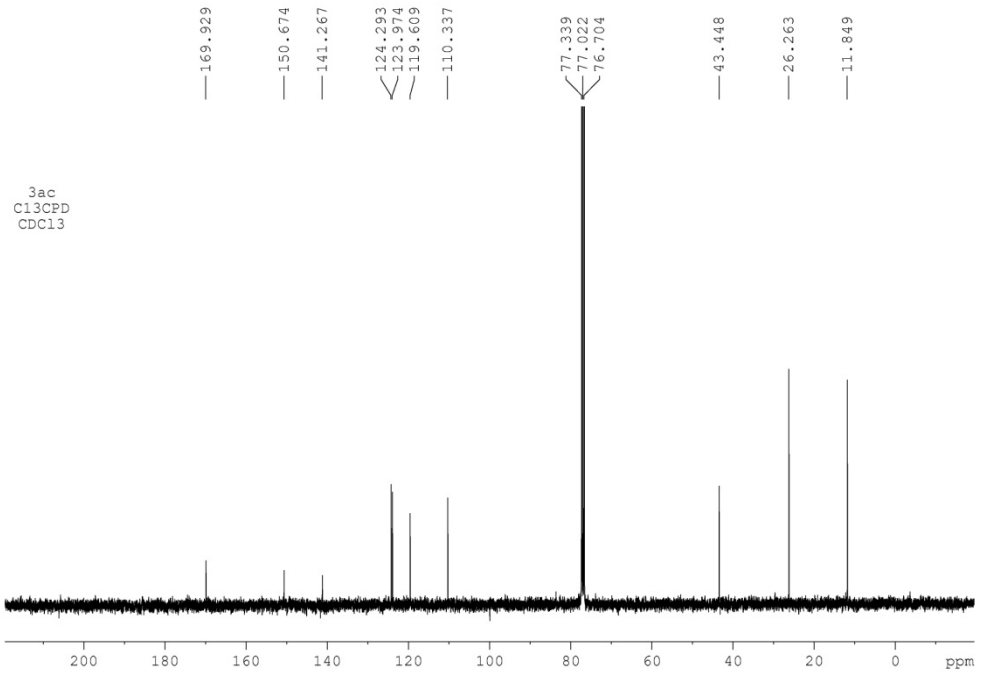


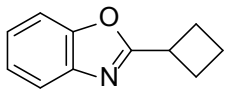


^{1}H-NMR spectrum of **3ac**

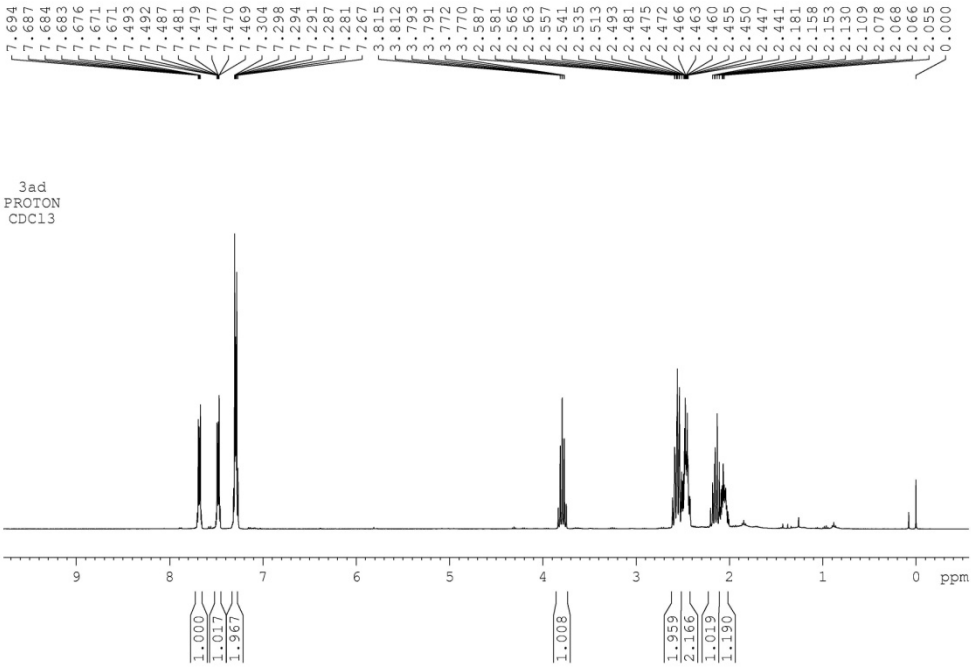


^{13}C-NMR spectrum of **3ac**





^{1}H-NMR spectrum of **3ad**



^{13}C-NMR spectrum of **3ad**