Copper(I)-Catalyzed Intermolecular Cyanoarylation of Alkenes: Convenient Access to α-Alkylated Arylacetonitriles

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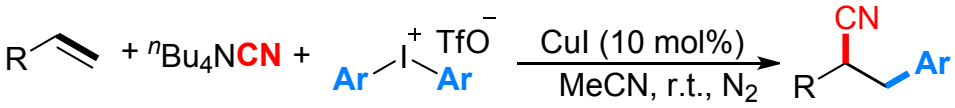
Contents

1. General Information

Reactions requiring inert conditions were carried out in glove box. All glassware was oven or flame dried prior to use. All solvents were purified and dried according to standard methods prior to use, unless stated otherwise. All reagents were obtained from commercial sources and used without further purification. The diaryliodonium salts were prepared according to literature.[1] NMR spectra were recorded at room temperature on the following spectrometers: Agilent (400 MHz) and VARIAN (400 MHz). Chemical shifts are given in ppm and coupling constants in Hz. ^{1}H spectra were calibrated in relation to the reference measurement of TMS (0.00 ppm). ^{13}C spectra were calibrated in relation to deuterated solvents, namely $CDCl_3$ (77.16 ppm). Chemical shifts are given in ppm and coupling constants in Hz. Data for ^{1}H NMR are recorded as follows: chemical shift (δ, ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet or unresolved, br = broad singlet, coupling constant(s) in Hz, integration). IR spectra were recorded on a Nicolet FT-IR spectrometer and only major peaks are reported in cm^{-1}. Mass spectra were performed on a spectrometer operating on ESI-TOF. Column chromatography was performed on silica gel (200-300 mesh).

2. Experimental Details

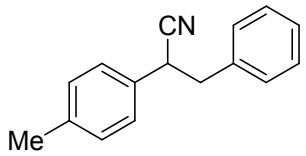
General procedure for the synthesis of α-alkylated arylacetonitriles



In a nitrogen-filled glovebox, an oven-dried 2 mL vial, CuI (1.9 mg, 0.01 mmol, 10 mol %) were dissolved in CH_3CN (1 mL). The mixture was stirred for 1-3 min. Then, alkene substrate (0.40 mmol) was added, followed by the diaryliodonium salts (0.1 mmol). The mixture was stirred for 5-10 min, then the $(n\text{-}C_4H_9)_4N^+CN^-$ (0.1 mmol) were added into the vial. Next, the reaction mixture was stirring at r.t .for 24 h. The resulting mixture was passed through a pad of silica gel and eluted with ethyl acetate. The combined organic layer was washed with water (20 mL), and brine (10 mL) sequentially, dried over $MgSO_4$. The filtrate was concentrated under reduced pressure. The residue was purified by silica gel flash chromatography (hexane/ EtOAc= 20/1) to give pure product.

3. Characterization Dates

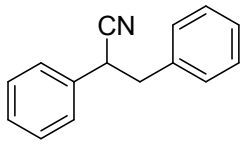
3-phenyl-2-(p-tolyl)propanenitrile (4ba)[2]



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.24 (m, 3 H), 7.15 (m, *J* = 5.9 Hz, 6 H), 3.97 (dd, *J* = 8.1, 6.7 Hz, 1 H), 3.14 (qd, *J* = 13.6, 7.4 Hz, 2 H), 2.36 (s, 3 H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 138.00, 136.41, 132.21, 129.65, 129.20, 128.60, 127.32, 127.32, 120.54, 42.24, 39.46, 21.09.

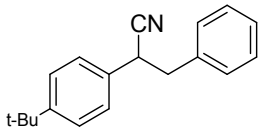
2,3-diphenylpropanenitrile (4aa)[2]



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.32 (m, 3 H), 7.32 – 7.23 (m, 5 H), 7.18 – 7.11 (m, 2 H), 4.05 – 3.96 (m, 1 H), 3.16 (qd, *J* = 13.6, 7.4 Hz, 2 H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 136.25, 135.18, 129.21, 129.01, 128.62, 128.20, 127.48, 127.38, 120.37, 42.20, 39.82.

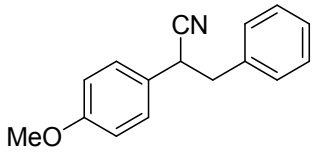
2-(4-(tert-butyl)phenyl)-3-phenylpropanenitrile (4ca)[2]



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, *J* = 8.4 Hz, 2 H), 7.41 – 7.33 (m, 3 H), 7.31 (d, *J* =8.4 Hz, 2 H), 7.29 – 7.20 (m, 2 H), 4.04 (dd, *J* = 8.6, 6.4 Hz, 1 H), 3.28 – 3.17 (m, 2 H), 1.40 (s, 9 H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.28, 136.55, 132.27, 129.13, 128.60, 127.31, 127.06, 125.93, 120.47, 42.21, 39.46, 34.56, 31.25.

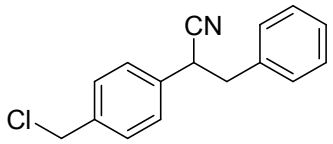
2-(4-methoxyphenyl)-3-phenylpropanenitrile (4da)[2]



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.27 (m, 3 H), 7.18 (d, *J* =8.7 Hz, 2 H), 7.15 (d, *J* =7.6 Hz, 2 H), 6.89 (d, *J* = 8.7 Hz, 2 H), 3.99 – 3.95 (m, 1 H), 3.82 (s, 3 H), 3.14 (qd, *J* =13.5, 7.3 Hz, 2 H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 159.36, 136.34, 129.22, 128.60, 128.57, 127.29, 127.15, 120.62, 114.31, 55.31, 42.26, 38.96.

2-(4-(chloromethyl)phenyl)-3-phenylpropanenitrile (4ea)



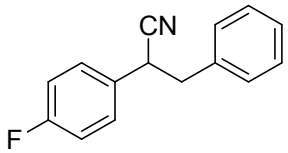
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (d, *J* = 8.0 Hz, 2 H), 7.29 – 7.23 (m, 5 H), 7.12 (d, *J* = 8.0 Hz, 2 H), 4.56 (s, 2 H), 4.01 – 3.97 (m, 1 H), 3.14 (qd, *J* = 13.7, 7.4 Hz, 2 H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 136.58, 135.01, 134.35, 128.18, 128.16, 127.65, 126.86, 126.44, 119.06, 44.49, 41.07, 38.50.

IR (neat) cm^{-1}: 3032, 2946, 2857, 2240, 1603, 1512, 1496, 1453, 1265, 976, 828, 742.

HRMS (ESI) m/z calcd. for $C_{16}H_{14}ClN$ $[M+Na]^+$: 278.0712; found 278.0710.

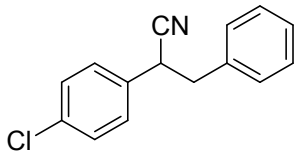
2-(4-fluorophenyl)-3-phenylpropanenitrile (4fa)[2]



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 – 7.26 (m, 3 H), 7.20 (dd, *J* = 8.5, 5.2 Hz, 2 H), 7.11 (d, *J* = 7.6 Hz, 2 H), 7.04 (t, *J* = 8.6 Hz, 2 H), 3.99 (t, *J* = 7.3 Hz, 1 H), 3.15 (qd, *J* = 13.6, 7.3 Hz, 2 H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.42 (d, $J_{C\text{-}F}$ = 247.6 Hz,) 135.88, 130.87, 129.20 (d, $J_{C\text{-}F}$ = 4.2 Hz), 128.65, 127.46, 120.18, 125.9, 115.96 (d, $J_{C\text{-}F}$ = 21.8 Hz), 42.16, 38.99.

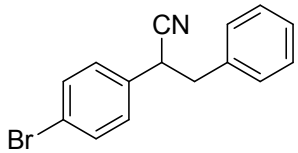
2-(4-chlorophenyl)-3-phenylpropanenitrile (4ga)[2]



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (d, *J* =8.4 Hz, 2 H), 7.31–7.25 (m, 3 H), 7.17 (d, *J* = 8.4 Hz, 2 H), 7.13 – 7.07 (m, 2 H), 3.99 (t, *J* = 7.3 Hz, 1 H), 3.15 (qd, *J* = 13.6, 7.2 Hz, 2 H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 135.73, 134.20, 133.54, 129.20, 129.16, 128.86, 128.67, 127.51, 119.94, 41.99, 39.13.

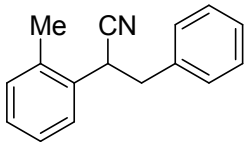
2-(4-bromophenyl)-3-phenylpropanenitrile (4ha)[2]



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (d, *J* = 8.2 Hz, 2 H), 7.34 – 7.25 (m, 3 H), 7.11 (d, *J* = 8.2 Hz, 4 H), 3.97 (t, *J* = 7.3 Hz, 1 H), 3.15 (qd, *J* = 13.6, 7.3 Hz, 2 H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 135.72, 134.09, 132.12, 129.20, 129.18, 128.68, 127.52, 122.29, 119.85, 41.93, 39.20.

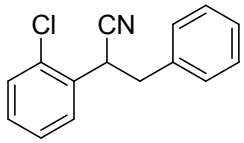
2-phenyl-2-(o-tolyl)propanenitrile (4ia)[2]



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.38 (m, 1 H), 7.33 – 7.26 (m, 3 H), 7.25 – 7.21 (m, 2 H), 7.19 – 7.14 (m, 3 H), 4.14 (dd, *J* = 8.7, 6.0 Hz, 1 H), 3.11 (q, *J* = 13.6, 6.0 Hz, 2 H), 2.25 (s, 3 H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 136.51, 135.00, 133.66, 130.90, 129.11, 128.66, 128.24, 127.64, 127.40, 126.87, 120.71, 40.98, 36.60, 19.03.

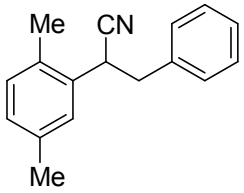
2-(2-chlorophenyl)-3-phenylpropanenitrile (4ja)[3]



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.43 (m, 1 H), 7.42 – 7.39 (m, 1 H), 7.33 – 7.26 (m, 5 H), 7.24 – 7.21 (m, 2 H), 4.51 (dd, *J* = 9.4, 4.8 Hz, 1 H), 3.20 (dd, *J* = 13.6, 4.8 Hz, 1 H), 3.04 (dd, *J* = 13.6, 9.4 Hz, 1 H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 136.05, 132.98, 132.58, 129.98, 129.64, 129.20, 129.16, 128.65, 127.53, 127.49, 119.74, 40.11, 37.32.

2-(2,5-dimethylphenyl)-3-phenylpropanenitrile (4ka)



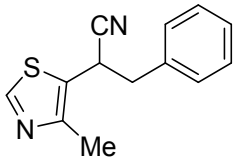
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 – 7.27 (m, 4 H), 7.23 – 7.15 (m, 2 H), 7.09 – 7.02 (m, 2 H), 4.11 (dd, *J* = 9.0, 5.8 Hz, 1 H), 3.10 (qd, *J* = 13.6, 7.4 Hz, 2 H), 2.34 (s, 3 H), 2.22 (s, 3 H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 136.65, 136.51, 133.47, 131.71, 130.77, 129.08, 128.92, 128.65, 128.19, 127.38, 120.85, 41.14, 36.66, 20.95, 18.55.

IR (neat) cm^{-1}: 3027, 2923, 2864, 2239, 1603, 1501, 1452, 1381, 1181, 911, 811, 727.

HRMS (ESI) m/z calcd. for $C_{17}H_{17}N$ $[M+Na]^+$: 258.1259, found 258.1258.

2-(4-methylthiazol-5-yl)-3-phenylpropanenitrile (4la)



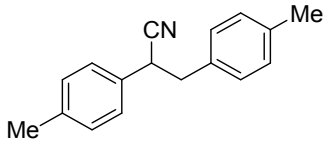
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68 (s, 1 H), 7.30 (m, 3 H), 7.12 (dd, *J* = 7.0, 2.2 Hz, 2 H), 4.25 (t, *J* = 7.5 Hz, 1 H), 3.31 (dd, *J* = 13.5, 7.5 Hz, 1 H), 3.13 (dd, *J* = 13.5, 7.5 Hz, 1 H), 2.22 (s, 3 H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 150.23, 150.08, 134.31, 128.03, 127.84, 126.79, 124.02, 118.05, 40.59, 30.57, 13.89.

IR (neat) cm^{-1}: 3063, 3029, 2925, 2860, 2241, 1729, 1603, 1539, 1452, 1259, 1237, 938, 843, 754.

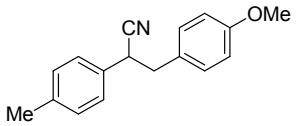
HRMS (ESI) m/z calcd. for $C_{13}H_{12}N_2S$ $[M+Na]^+$: 251.0619, found 251.0620.

2,3-di-p-tolylpropanenitrile (4ab)[4]



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.16 (s, 4 H), 7.11 (d, *J* = 7.8 Hz, 2 H), 7.04 (d, *J* = 7.8 Hz, 2 H), 3.95 – 3.92 (m, 1 H), 3.10 (qd, *J* = 13.7, 7.6 Hz, 2 H), 2.35 (s, 3 H), 2.33 (s, 3 H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 136.93, 135.92, 132.37, 131.34, 128.63, 128.27, 128.04, 126.31, 119.60, 40.85, 38.59, 20.07. 20.07.

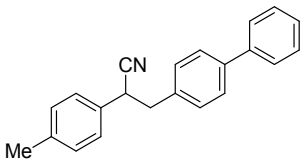
3-(4-methoxyphenyl)-2-(p-tolyl)propanenitrile (4ac)[5]



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18 – 7.11 (m, 4 H), 7.05 (d, *J* = 8.6 Hz, 2 H), 6.83 (d, *J* = 8.6 Hz, 2 H), 3.94 – 3.90 (m, 1 H), 3.79 (s, 3 H), 3.14 – 3.03 (m, 2 H), 2.35 (s, 3 H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.77, 137.90, 132.22, 130.25, 129.60, 128.43, 127.32, 120.62, 113.92, 55.21, 41.41, 39.70, 21.07.

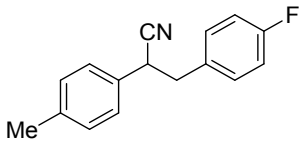
3-([1,1'-biphenyl]-4-yl)-2-(p-tolyl)propanenitrile (4ad)[5]



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 7.8 Hz, 2 H), 7.53 (d, *J* = 8.1 Hz, 2 H), 7.43 (t, *J* = 7.6 Hz, 2 H), 7.34 (m, 1 H), 7.21 (d, *J* = 7.8 Hz, 2 H), 7.17 (s, 4 H), 3.99 (dd, *J* = 8.2, 6.5 Hz, 1 H), 3.17 (qd, *J* = 13.6, 7.4 Hz, 2 H), 2.35 (s, 3 H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 140.63, 140.20, 138.06, 135.43, 132.18, 129.70, 129.65, 128.78, 127.36, 127.33, 127.30, 127.03, 120.57, 41.90, 39.45, 21.13.

3-(4-fluorophenyl)-2-(p-tolyl)propanenitrile (4ae)



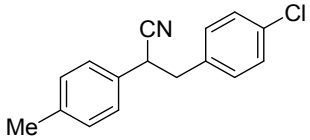
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.16 (d, *J* = 8.1 Hz, 2 H), 7.12 (d, *J* = 8.1 Hz, 2 H), 7.08 (dd, *J* =8.4 Hz, 5.5 Hz, 2 H), 6.98 (t, J =8.6 Hz, 2 H), 3.94 (t, *J* = 7.3 Hz, 1 H), 3.17 – 3.07 (m, 2 H), 2.35 (s, 3 H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.09 (d, J_{C-F} =245.9 Hz), 138.10, 131.98 (d, J_{C-F} =3.3 Hz), 131.81, 130.80 (d, J_{C-F} = 8.1 Hz), 129.67, 127.30, 120.32, 115.44 (d, J_{C-F} =21.4 Hz), 41.30, 39.41, 21.07.

IR (neat) cm^{-1}: 2923, 2852, 2242, 1599, 1508, 1445, 1416, 1260, 1219, 975, 843, 779.

HRMS (ESI) m/z calcd. for $C_{16}H_{14}FN$ $[M+Na]^+$: 262.1008, found 262.1010.

3-(4-chlorophenyl)-2-(p-tolyl)propanenitrile(4af)

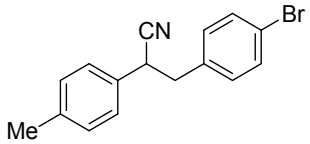


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27 – 7.25 (m, 2 H), 7.16 (d, *J* = 8.0 Hz, 2 H), 7.12 (d, *J* = 8.1 Hz, 2 H), 7.05 (d, *J* = 8.2 Hz, 2 H), 3.95 (t, *J* = 7.2 Hz, 1 H), 3.17 – 3.06 (m, 2 H), 2.35 (s, 3 H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 137.17, 133.70, 132.30, 130.71, 129.60, 128.71, 127.73, 126.31, 119.23, 40.42, 38.18, 20.07.

IR (neat) cm^{-1}: 2958, 2920, 2850, 2242, 1645, 1511, 1445, 1260, 1184, 939, 845, 765.

HRMS (ESI) m/z calcd. for $C_{16}H_{14}ClN$ $[M+Na]^+$: 278.0712, found 278.0717.

3-(4-bromophenyl)-2-(p-tolyl)propanenitrile(4ag)

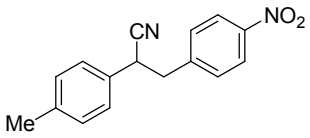


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (d, *J* =8.4 Hz, 2 H), 7.15 (d, *J* =8.1 Hz, 2 H), 7.10 (d, *J* =8.1 Hz, 2 H), 6.97 (d, *J* =8.4 Hz, 2 H), 3.95 – 3.91 (m, 1 H), 3.13 – 3.03 (m, 2 H), 2.34 (s, 3 H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 138.17, 135.19, 131.67, 131.76, 130.95, 129.71, 127.30, 121.40, 120.20, 41.48, 39.09, 21.08.

IR (neat) cm^{-1}: 2961, 2923, 2860, 2241, 1591, 1511, 1484, 1443, 1260, 1184, 942, 838, 762.

HRMS (ESI) m/z calcd. for $C_{16}H_{14}BrN$ $[M+Na]^+$: 322.0207, found 322.0203.

3-(4-nitrophenyl)-2-(p-tolyl)propanenitrile(4ah)



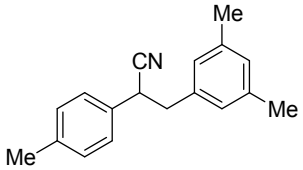
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, *J* = 8.6 Hz, 2 H), 7.26 (d, *J* = 8.6 Hz, 2 H), 7.17 (d, *J* = 8.0 Hz, 2 H), 7.11 (d, *J* = 8.0 Hz, 2 H), 4.04 (t, *J* = 7.1 Hz, 1 H), 3.29 – 3.23 (m, 2 H), 2.36 (s, 3 H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 147.30, 143.46, 138.52, 131.00, 130.27, 129.86, 127.24, 123.75, 119.74, 41.59, 38.61, 21.09.

IR (neat) cm^{-1}: 2921, 2850, 2244, 1662, 1599, 1513, 1448, 1260, 1183, 883, 737, 695.

HRMS (ESI) m/z calcd. for $C_{16}H_{14}N_2O_2$ $[M+Na]^+$: 289.0953, found 289.0956.

3-(3,5-dimethylphenyl)-2-(p-tolyl)propanenitrile(4ai)



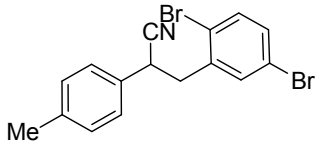
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.20 – 7.17 (s, 4 H), 6.91 (s, 1 H), 6.80 (s, 2 H), 3.94 (dd, *J* =9.0, 6.2 Hz, 1 H), 3.06 (qd, *J* =13.5, 7.6 Hz, 2 H), 2.36 (s, 3 H), 2.29 – 2.25 (m, 6 H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 137.10, 136.92, 135.42, 128.66, 128.61, 127.92, 126.26, 125.89, 119.62, 41.26, 38.58, 20.23, 20.07.

IR (neat) cm^{-1}: 3010, 2919, 2860, 2239, 1606, 1512, 1446, 1308, 1186, 849.36, 770, 733.

HRMS (ESI) m/z calcd. for $C_{18}H_{19}N$ $[M+Na]^+$: 272.1415, found 272.1412.

3-(2,5-dibromophenyl)-2-(p-tolyl)propanenitrile (4aj)

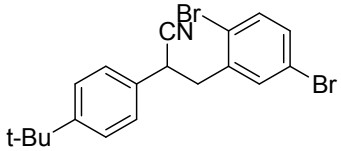


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, *J* = 8.5 Hz, 1 H), 7.35 (d, *J* = 2.2 Hz, 1 H), 7.30 (dd, *J* =8.5, 2.2 Hz, 1 H), 7.25 (d, *J* = 8.1 Hz, 2 H), 7.20 (d, *J* = 8.1 Hz, 2 H), 4.14 (dd, *J* = 9.5, 6.3 Hz, 1 H), 3.25 – 3.14 (m, 2 H), 2.37 (s, 3 H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 138.52, 138.05, 134.65, 134.45, 132.44, 131.92, 129.98, 127.24, 123.17, 121.64, 119.97, 42.65, 37.21, 21.25.

IR (neat) cm^{-1}: 2959, 2901, 2866, 2244, 1511, 1459, 1412, 1263, 1106, 897, 825, 801, 733.

HRMS (ESI) m/z calcd. for $C_{16}H_{13}Br_2N$ $[M+Na]^+$: 401.9292, found 401.9292.

2-(4-(tert-butyl)phenyl)-3-(2,5-dibromophenyl)propanenitrile(4ak)

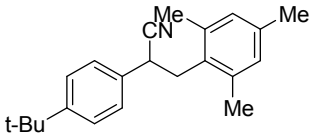


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (dd, *J* = 14.0, 8.3 Hz, 3H), 7.20 – 7.16 (m, 4H), 4.05 – 4.01 (m, 1H), 3.11 (dd, *J* = 7.9, 3.9 Hz, 2H), 1.23 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 151.65, 137.89, 134.56, 134.27, 132.26, 131.71, 126.93, 126.10, 122.99, 121.45, 119.81, 42.45, 36.94, 34.61, 31.24.

IR (neat) cm^{-1}: 2959, 2901, 2866, 2244, 1511, 1459, 1412, 1263, 1198, 825, 801, 682.

HRMS (ESI) m/z calcd. for $C_{19}H_{19}Br_2N$ $[M+Na]^+$: 443.9761, found 443.9766.

2-(4-(tert-butyl)phenyl)-3-mesitylpropanenitrile(4al)



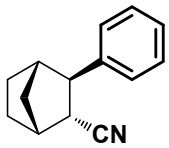
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (d, *J* = 8.3 Hz, 2 H), 7.26 – 7.23 (m, 2 H), 6.86 (s, 2 H), 3.90 (dd, *J* = 9.1, 6.7 Hz, 1 H), 3.34 (dd, *J* = 14.0, 9.3 Hz, 1 H), 3.02 (dd, *J* = 14.0, 6.7 Hz, 1 H), 2.26 (d, *J* = 3.2 Hz, 9 H), 1.32 (s, 9 H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.46, 136.89, 136.78, 133.01, 130.70, 129.54, 127.03, 126.12, 121.00, 37.21, 35.99, 34.74, 31.43, 21.04, 20.09.

IR (neat) cm^{-1}: 3395, 2962, 2920, 2849, 2240, 1645, 1511, 1465, 1415, 1260, 853, 798, 694.

HRMS (ESI) m/z calcd. for $C_{22}H_{27}N$ $[M+Na]^+$: 328.2041, found 328.2044.

(1R, 2R, 4S)-3-phenylbicyclo[2.2.1]heptane-2-carbonitrile(4am)



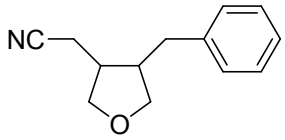
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (dd, *J* = 9.1, 5.9 Hz, 2 H), 7.25 (t, *J* = 5.2 Hz, 3 H), 2.98 (d, *J* = 5.9 Hz, 1 H), 2.73 (ddd, *J* = 6.0, 3.9, 2.0 Hz, 1 H), 2.64 (s, 1 H), 2.59 (d, *J* = 2.9 Hz, 1 H), 1.93 - 1.82 (m, 1 H), 1.78 - 1.65 (m, 3 H), 1.55 - 1.45 (m, 2 H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 143.27, 128.79, 126.76, 126.40, 122.22, 52.93, 42.07, 40.52, 40.29, 37.12, 30.08, 24.32.

IR (neat) cm^{-1}: 3060, 3027, 2877, 2234, 1600, 1452, 1302.41, 1258, 1208, 1155, 923, 730.

HRMS (ESI) m/z calcd. for $C_{14}H_{15}N$ $[M+Na]^+$: 220.1097, found 220.1021.

2-(4-benzyltetrahydrofuran-3-yl)acetonitrile (5aa)



^{1}H NMR (400 MHz, CDCl3) δ 7.33-7.27 (m, 2H), 7.25-7.15 (m, 3H), 4.04- 3.80 (m, 3H), 3.60-3.55 (m, 1H), 2.82-2.71 (m, 2H), 2.65- 2.54 (m, 2H), 2.48-2.40 (m, 1H), 2.25-2.22 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 139.25, 128.90,128.89, 128.76,128.54,126.73, 118.94, 72.39,71.69, 46.38, 38.94,33.57,16.66.

IR (neat) cm^{-1}: 3648.67, 3061.78, 2929.68, 2246.96, 1959.60, 1731.83, 1602.45, 1453.06, 1354.67, 1053.17, 989.86, 907.33.

HRMS (ESI) m/z calcd. for $C_{13}H_{15}NO$ $[M+Na]^+$: 224.1048, found 224.1053.

4. Reference

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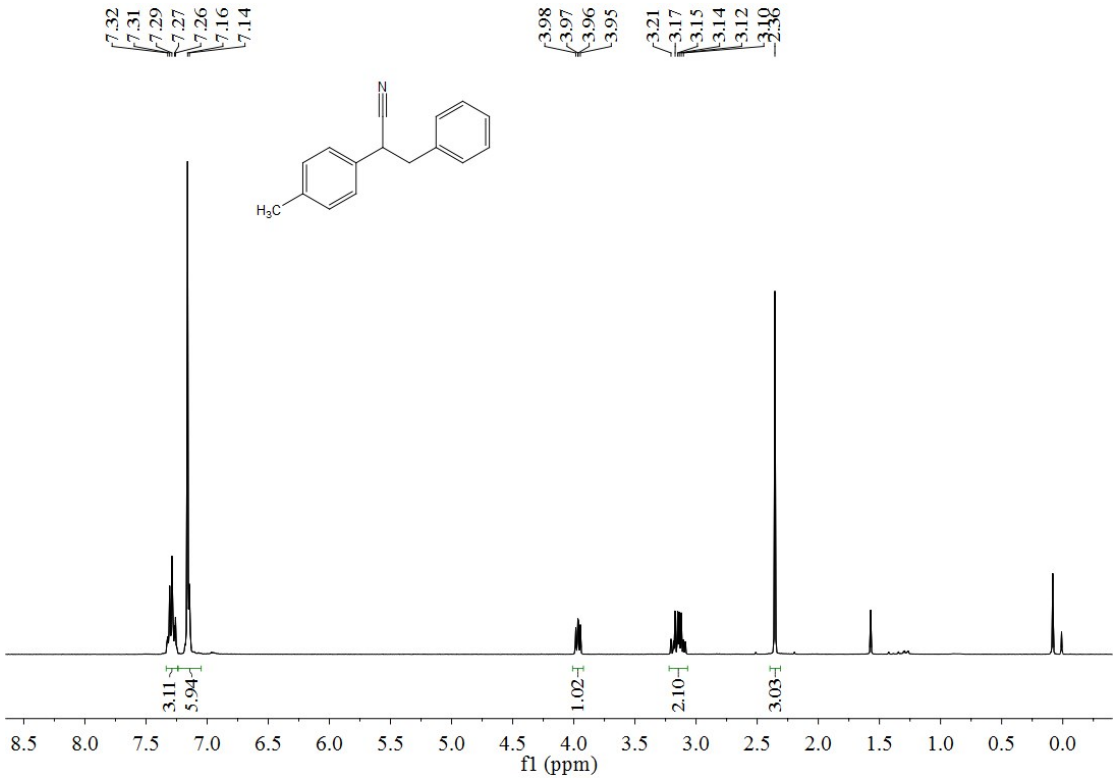
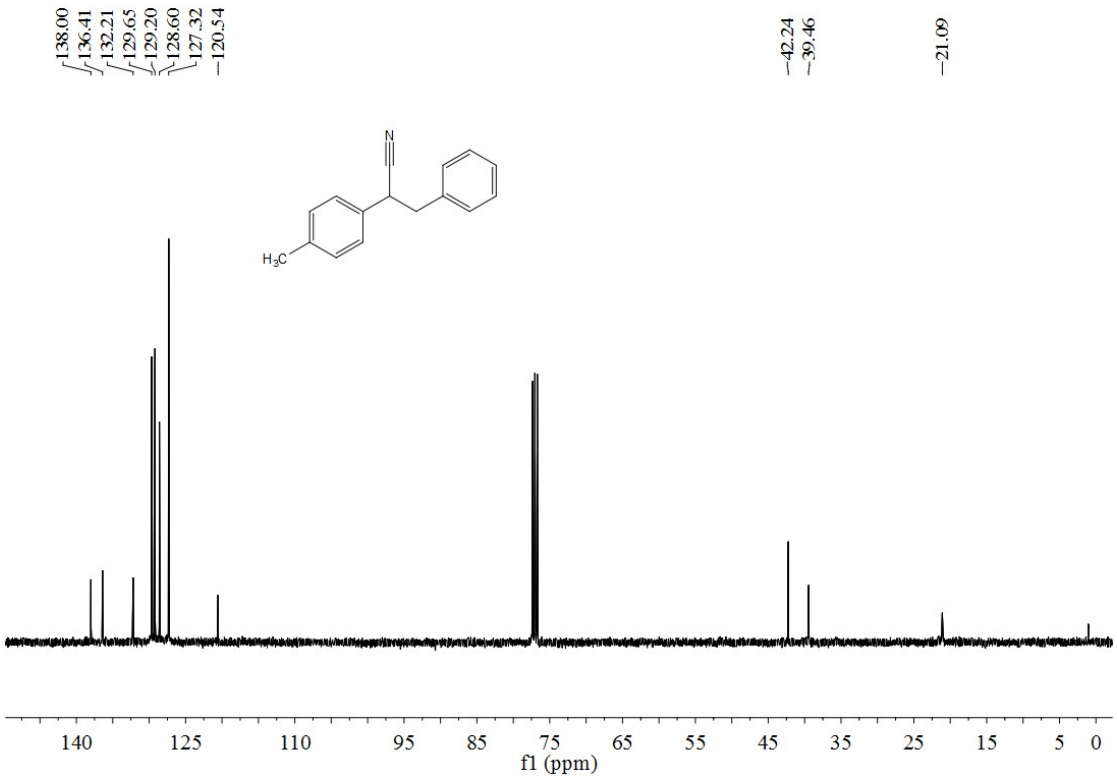
2. Z.-H. Zhu, Y. Li, Y.-B. Wang, Z.-G. Lan, X. Zhu, X.-Q. Hao and M.-P. Song, *Organometallics*, 2019, **38**, 2156.
3. B. C. Roy, I. A. Ansari, S. A. Samim and S. Kundu, *Chem. Asian J.*, 2019, **14**, 2215.
4. W. Ma, S. Cui, H. Sun, W. Tang, D. Xue, C. Li, J. Fan, J. Xiao and C. Wang, *Chem - Eur. J.*, 2018, **24**, 13118.
5. A. Jana, C. B. Reddy and B. Maji, *ACS Catal.*, 2018, **8**, 9226.

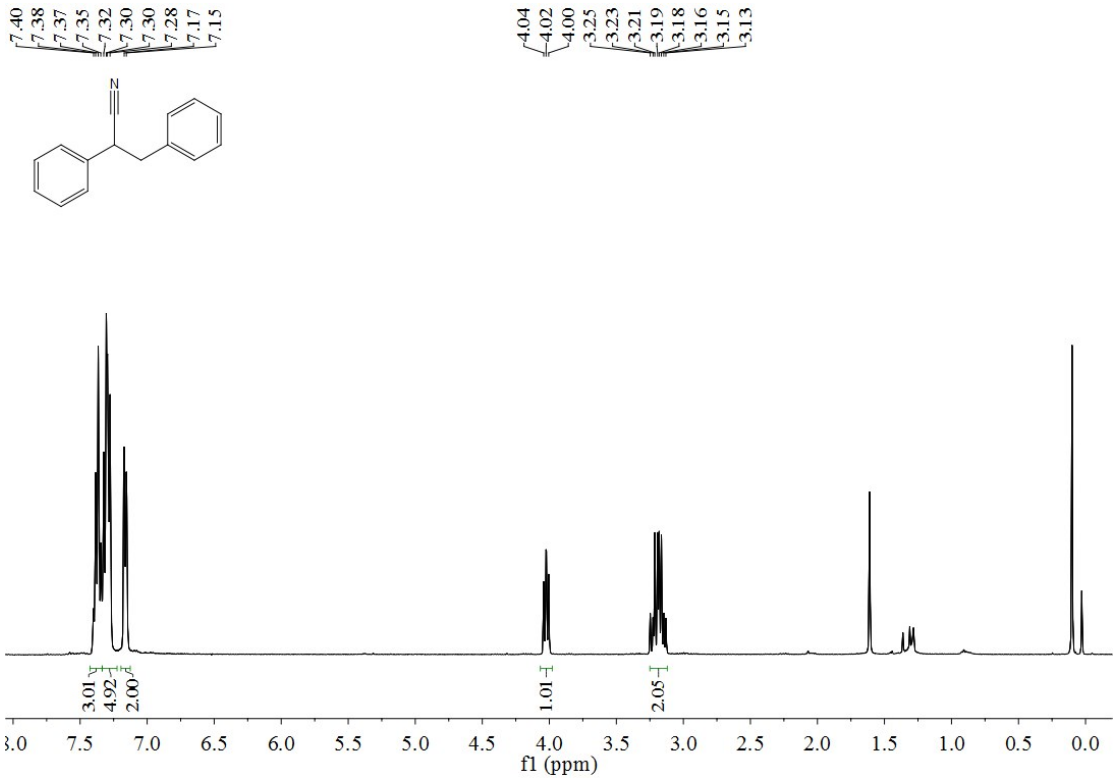
5. Copies of NMR spectra

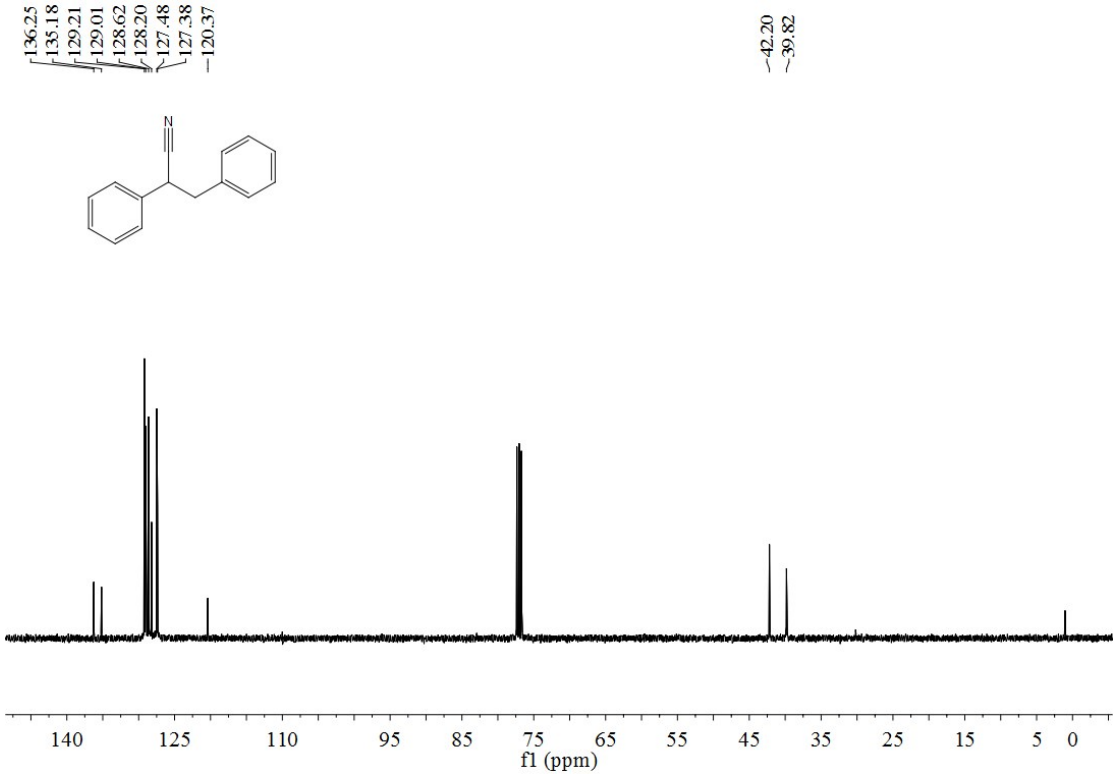
3-phenyl-2-(p-tolyl)propanenitrile(4aa)



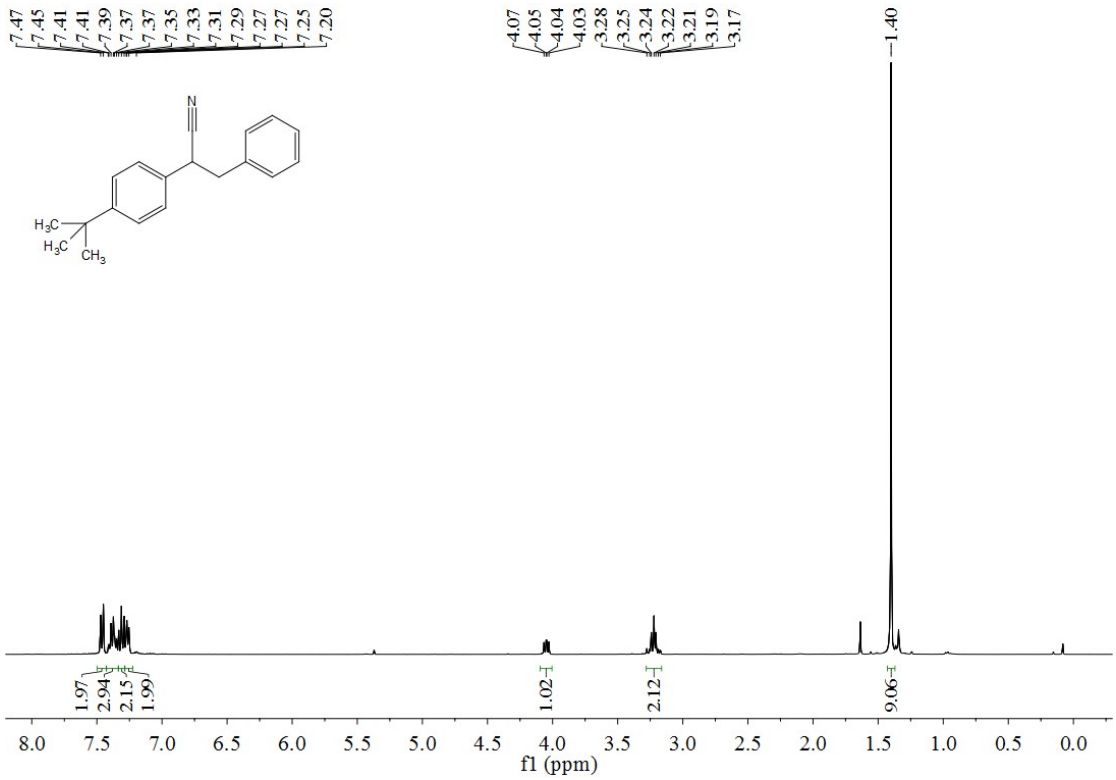


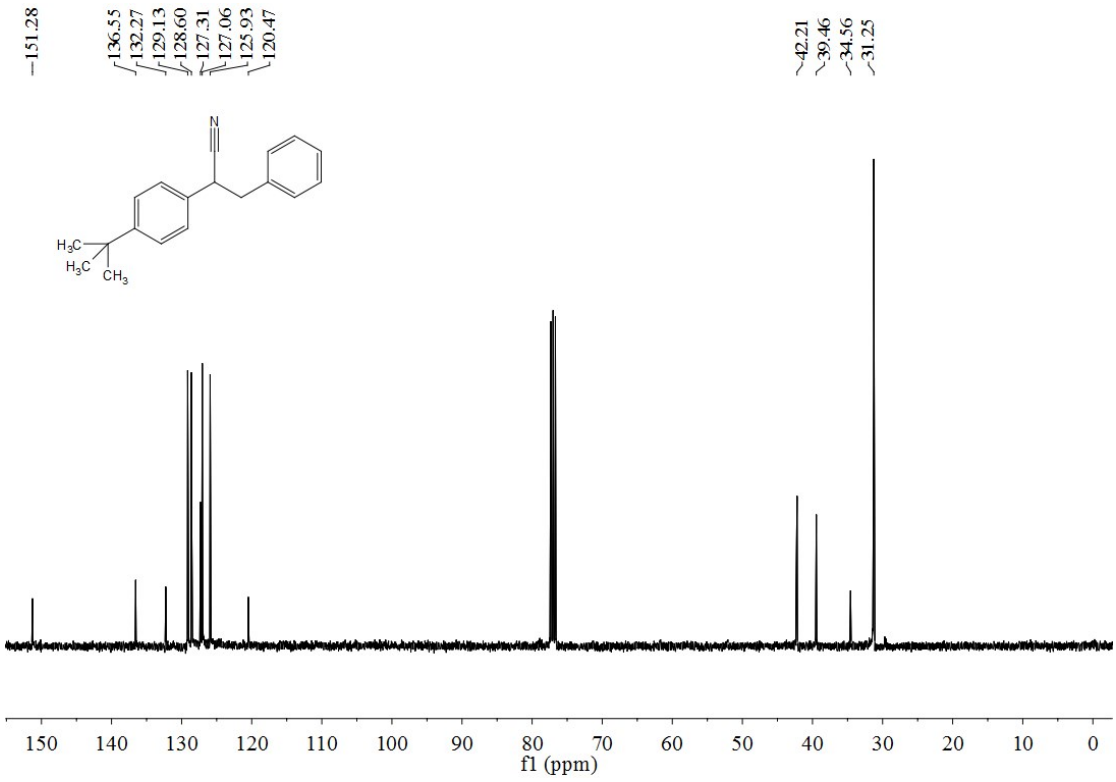
2,3-diphenylpropanenitrile (4ba)



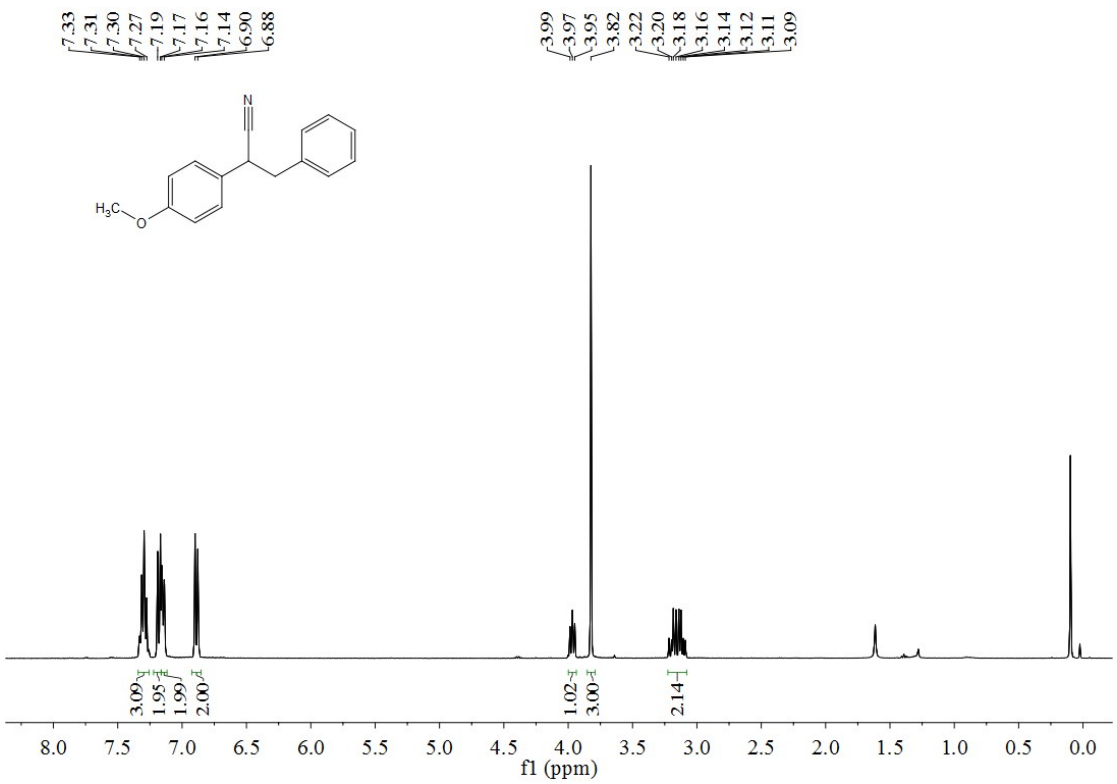


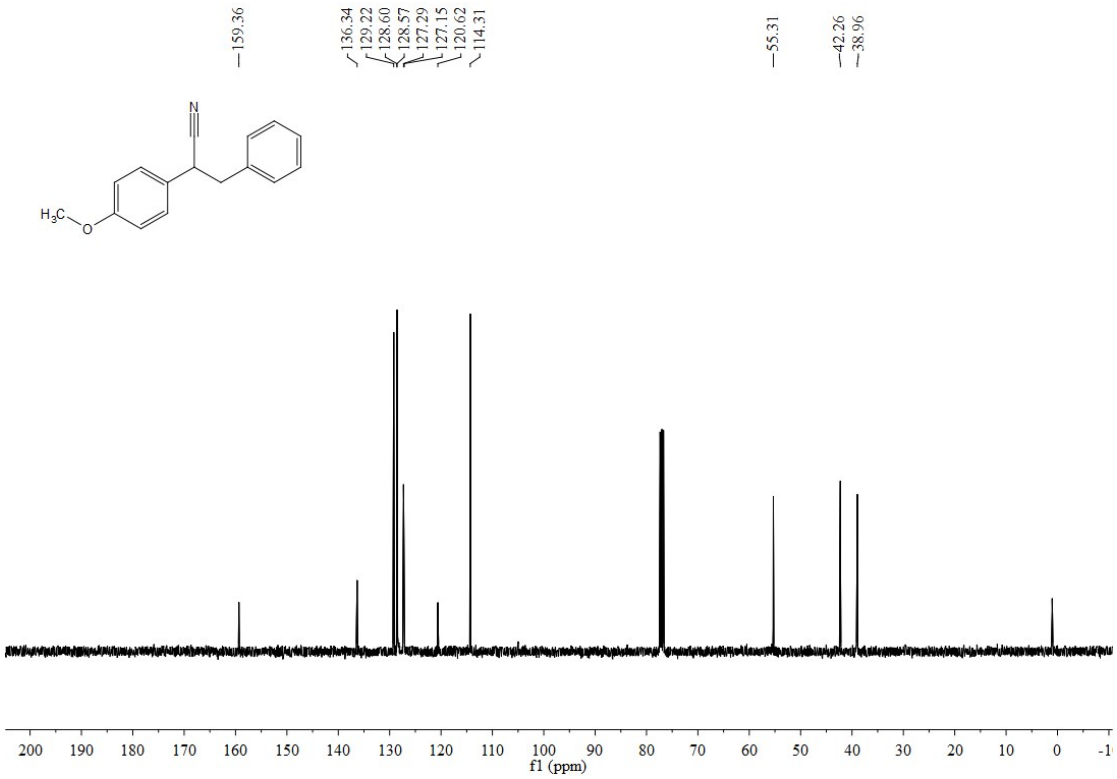
2-(4-(tert-butyl)phenyl)-3-phenylpropanenitrile(4ca)



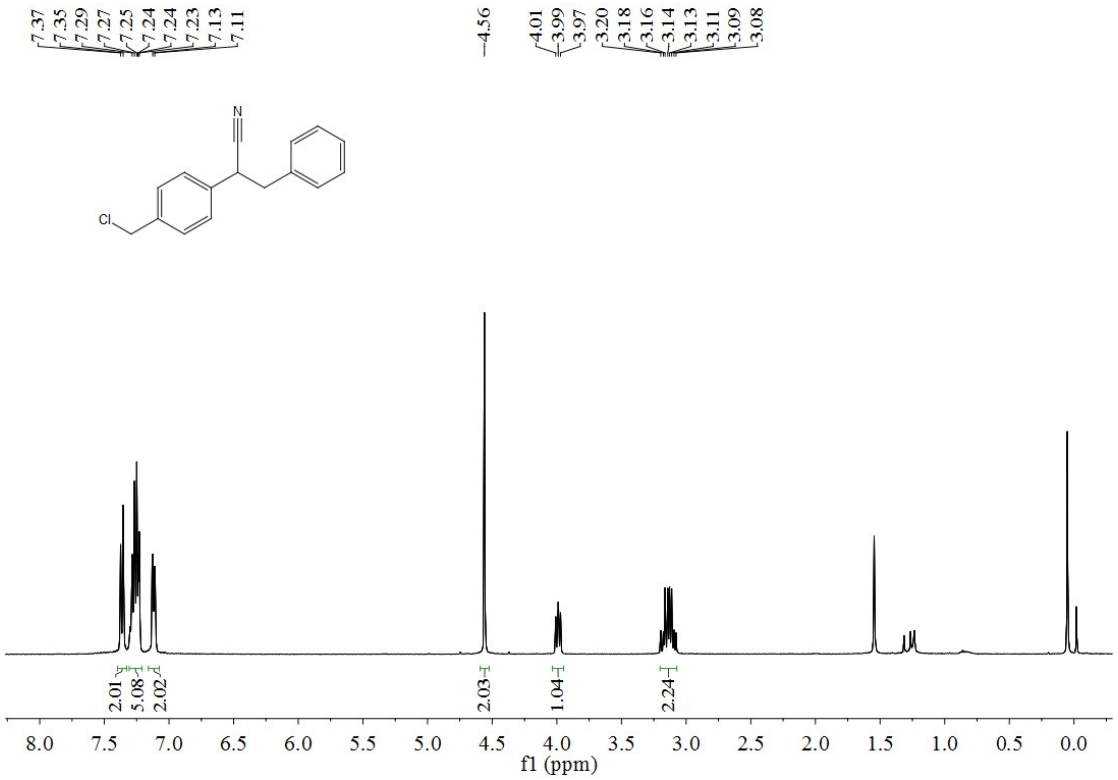


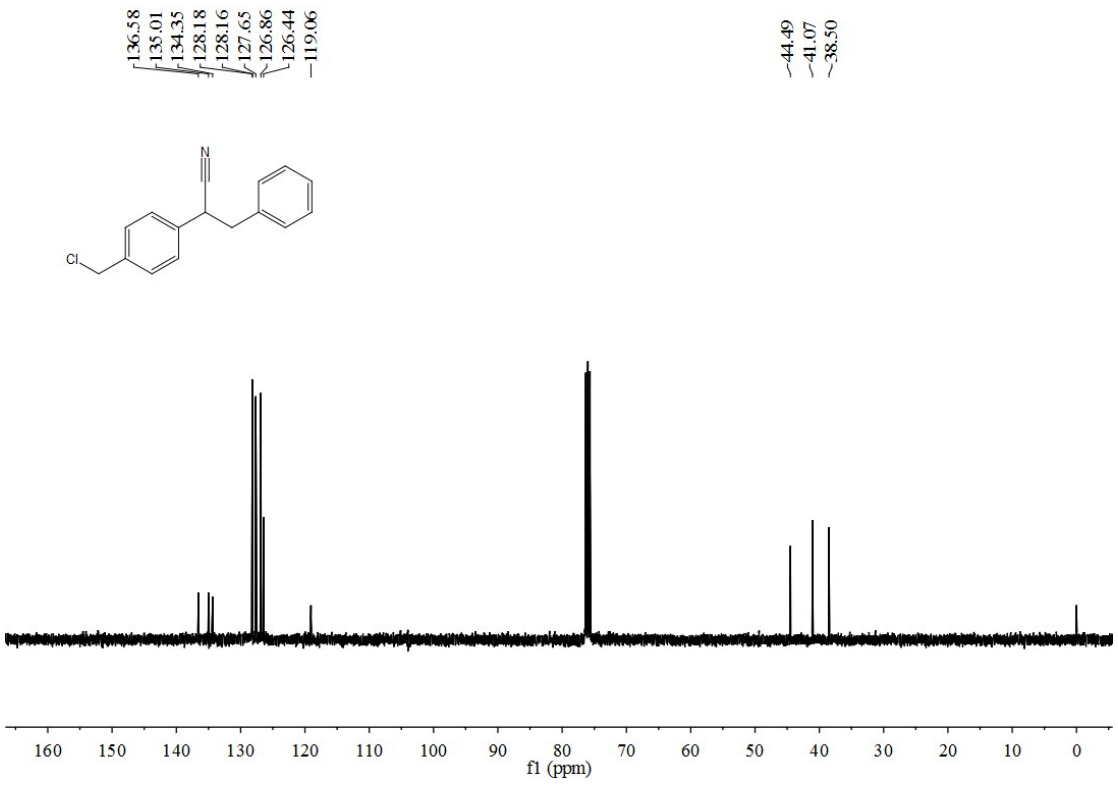
2-(4-methoxyphenyl)-3-phenylpropanenitrile(4da)



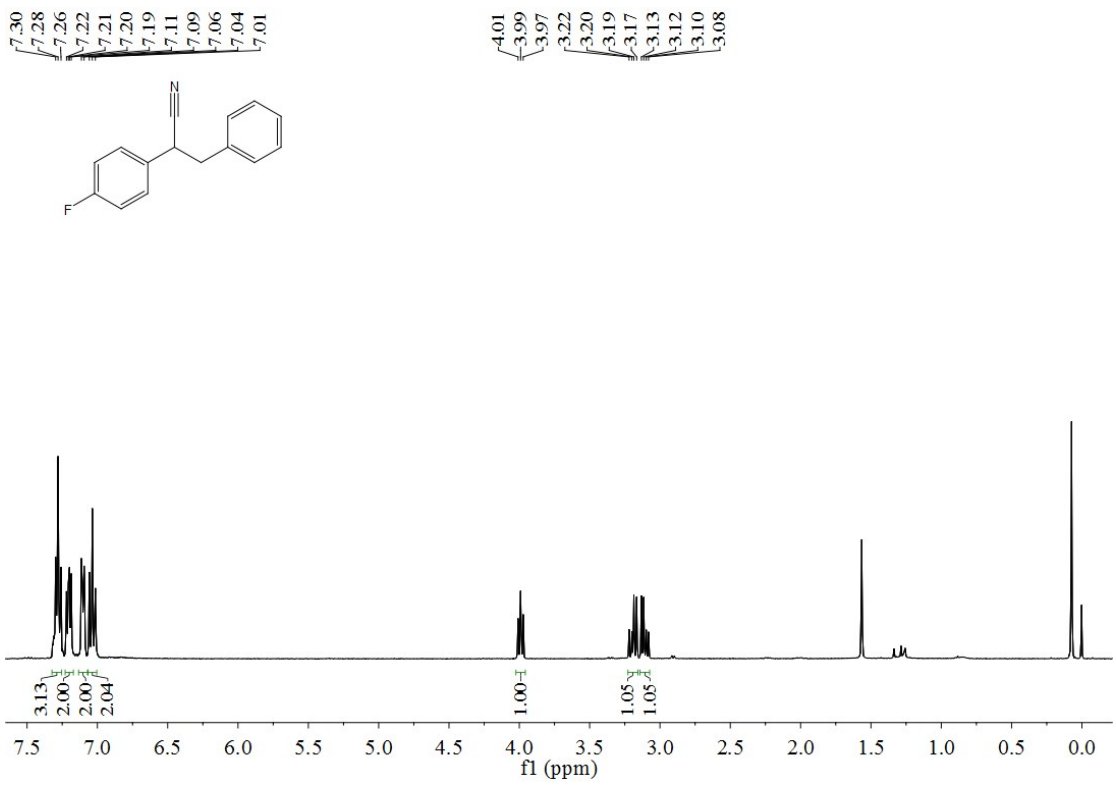


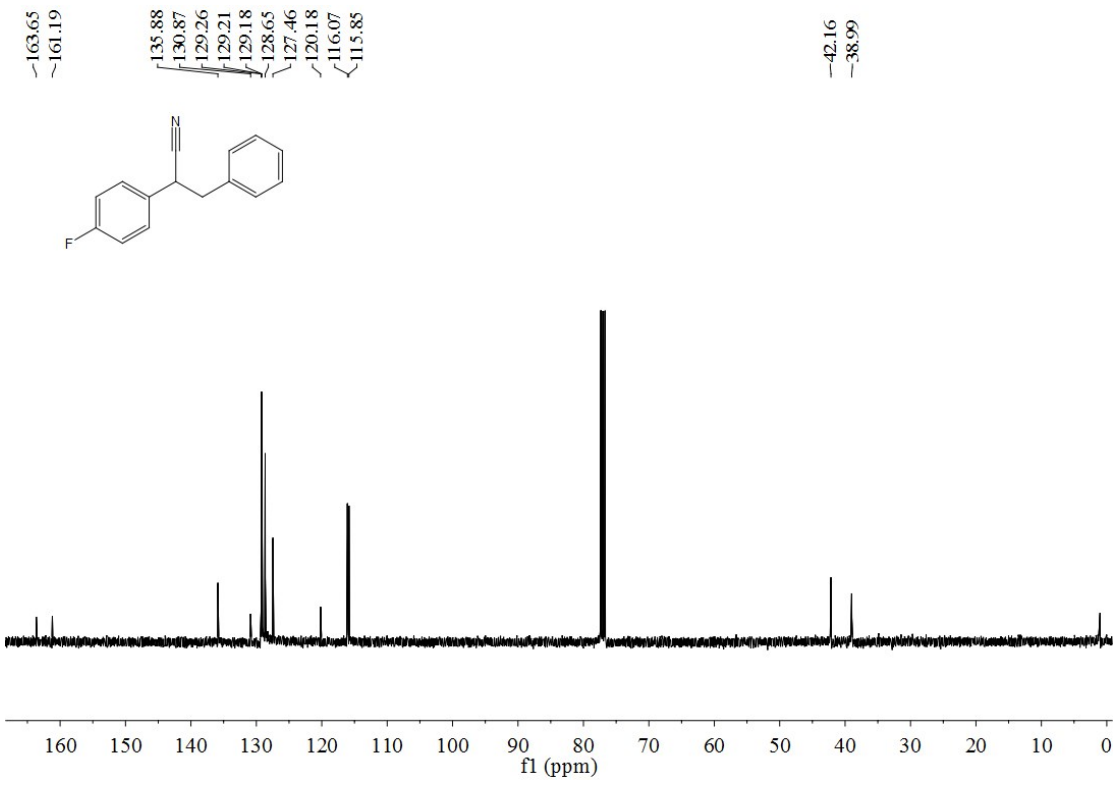
2-(4-(chloromethyl)phenyl)-3-phenylpropanenitrile(4ea)



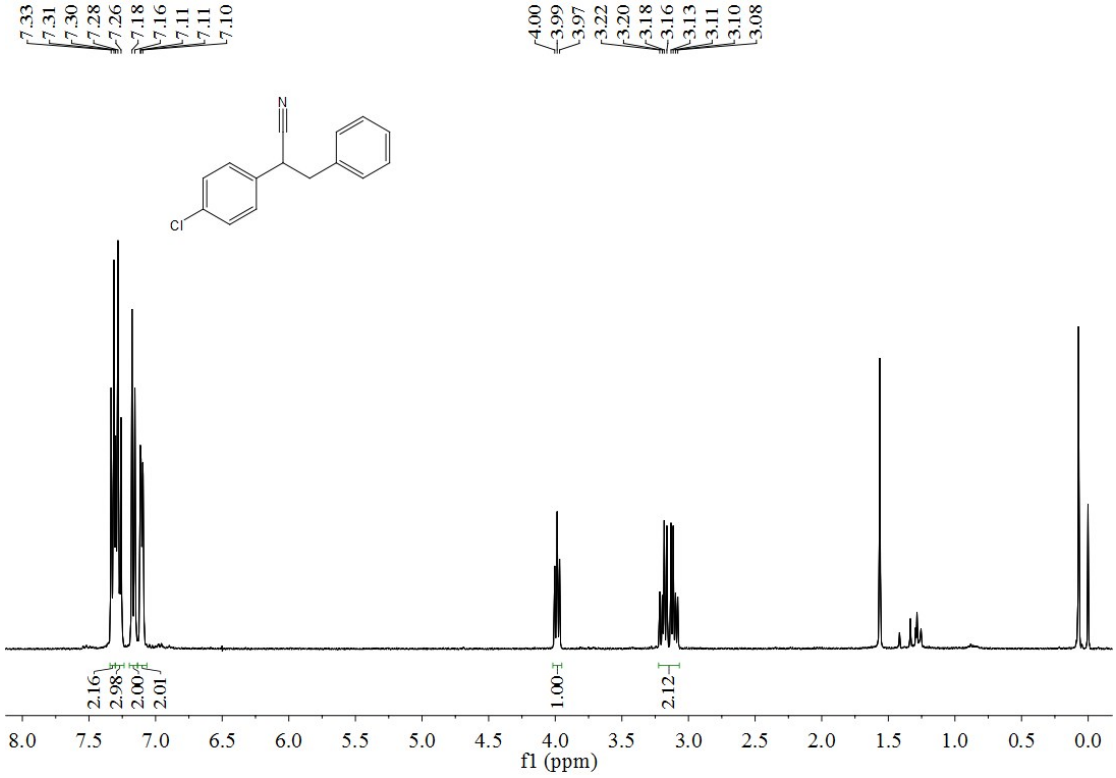


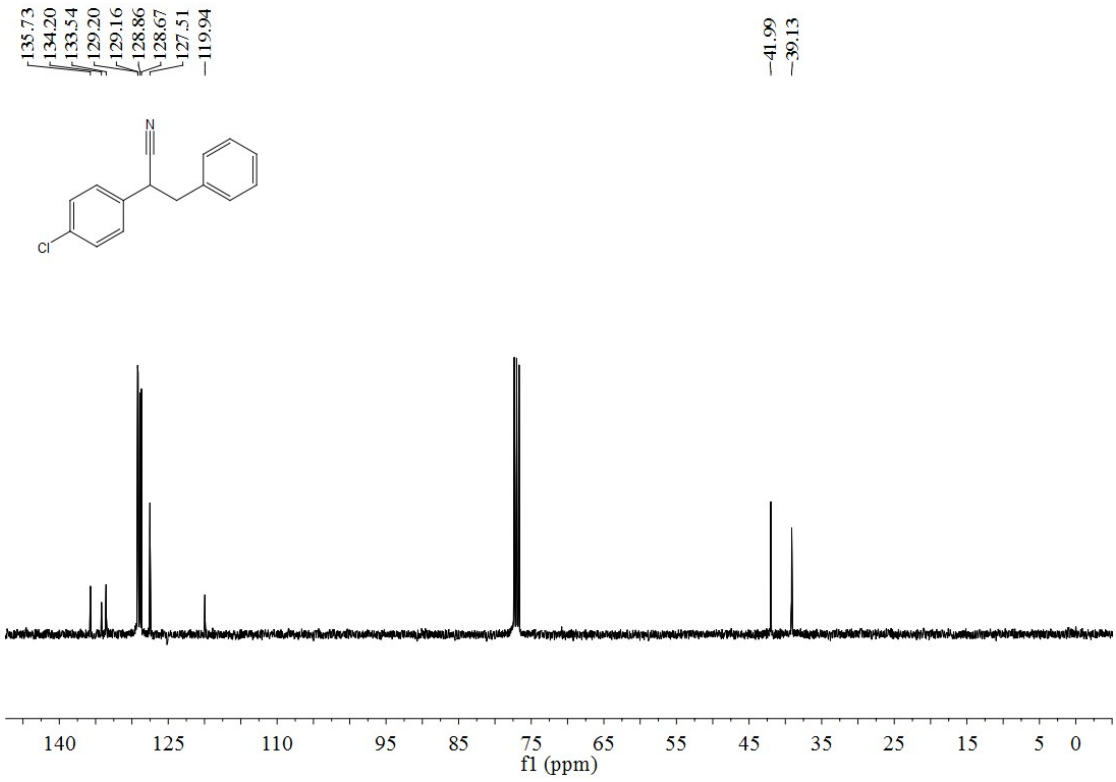
2-(4-fluorophenyl)-3-phenylpropanenitrile(4fa)



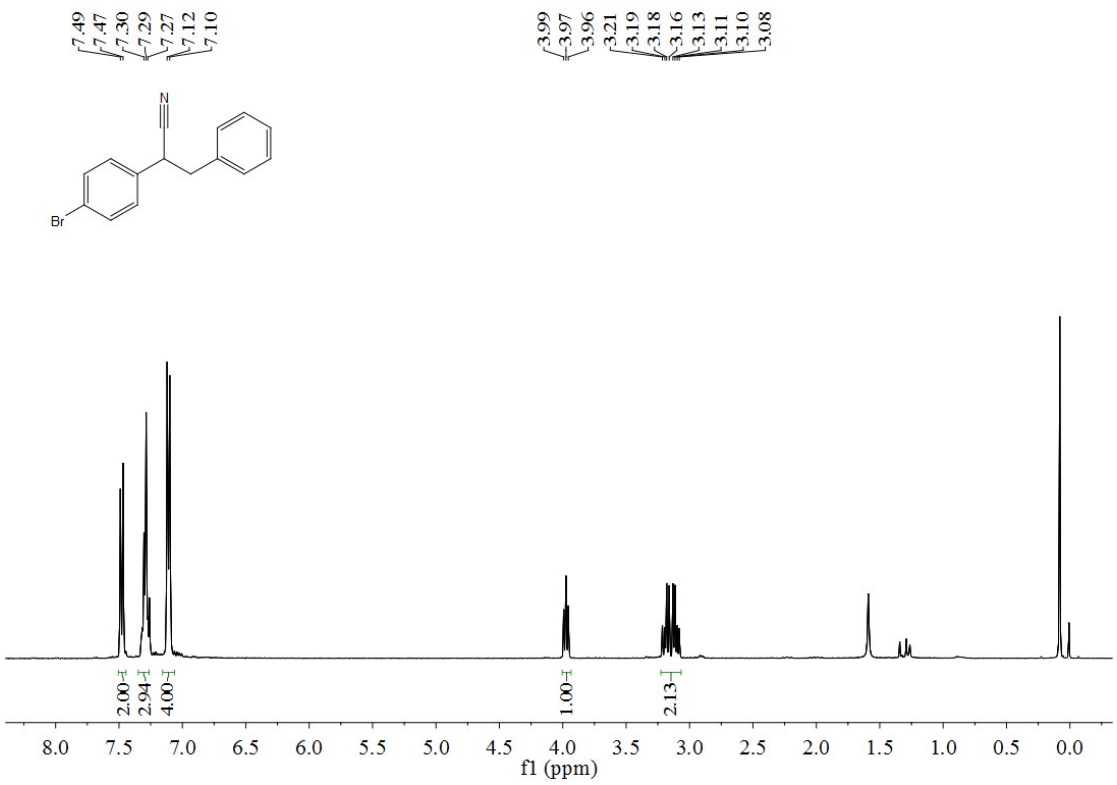


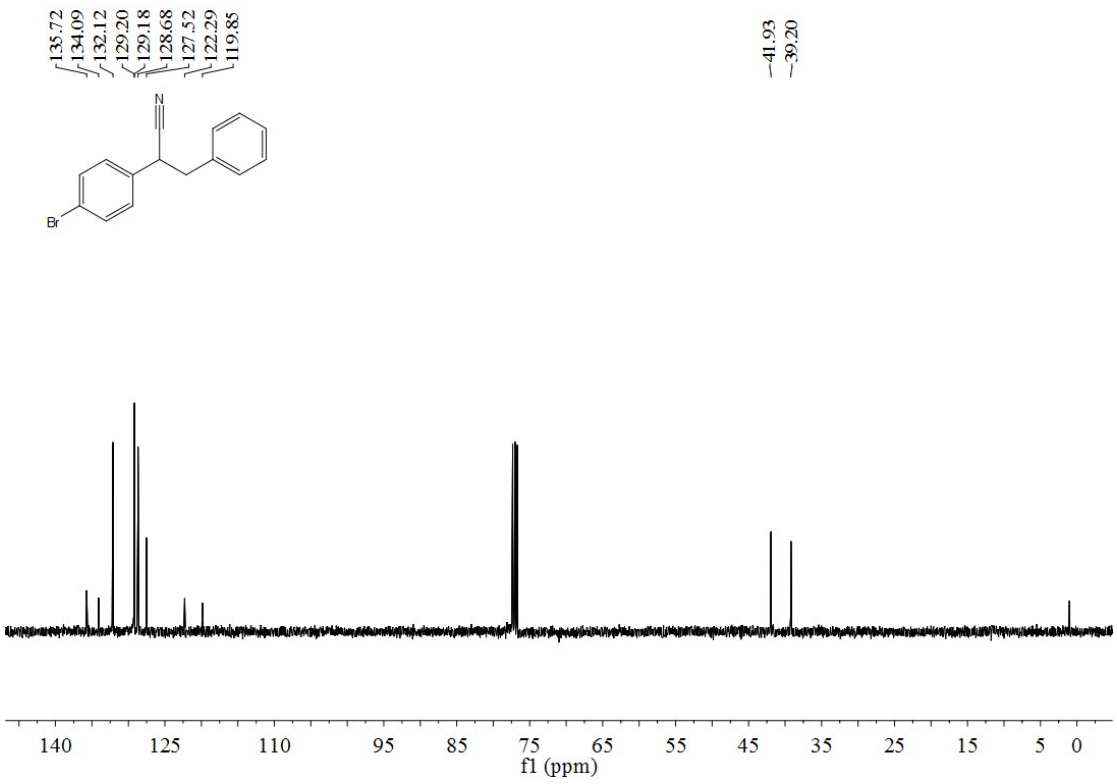
2-(4-chlorophenyl)-3-phenylpropanenitrile(4ga)



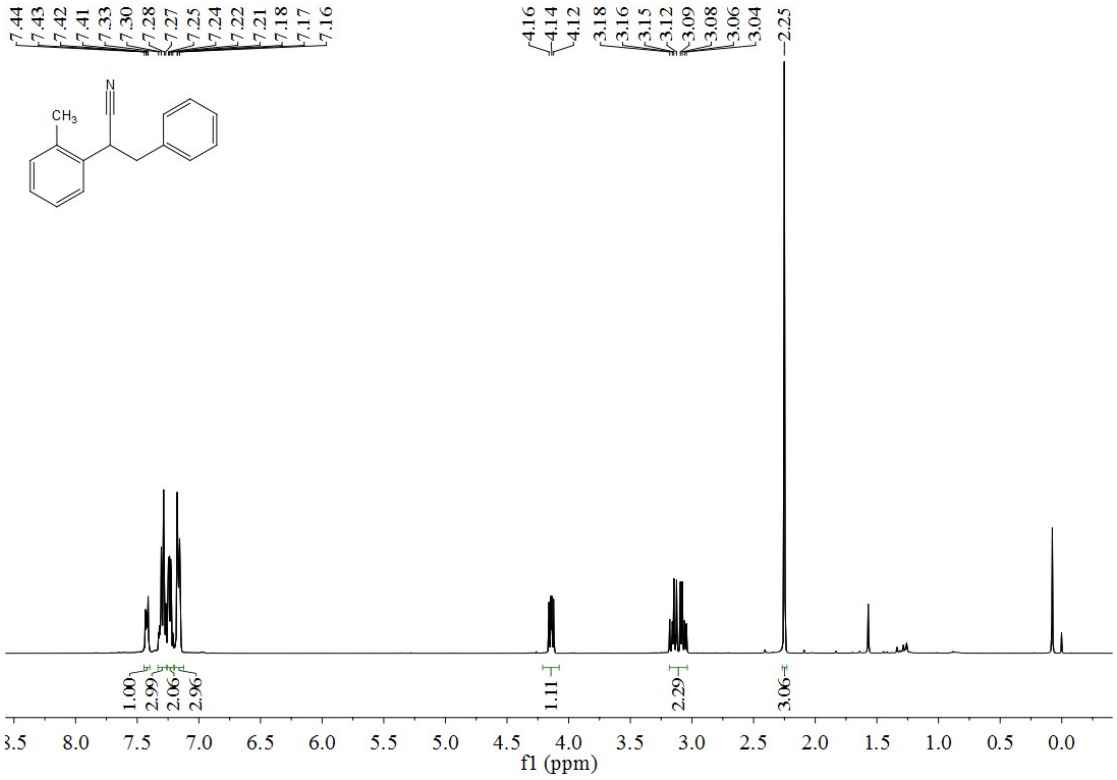


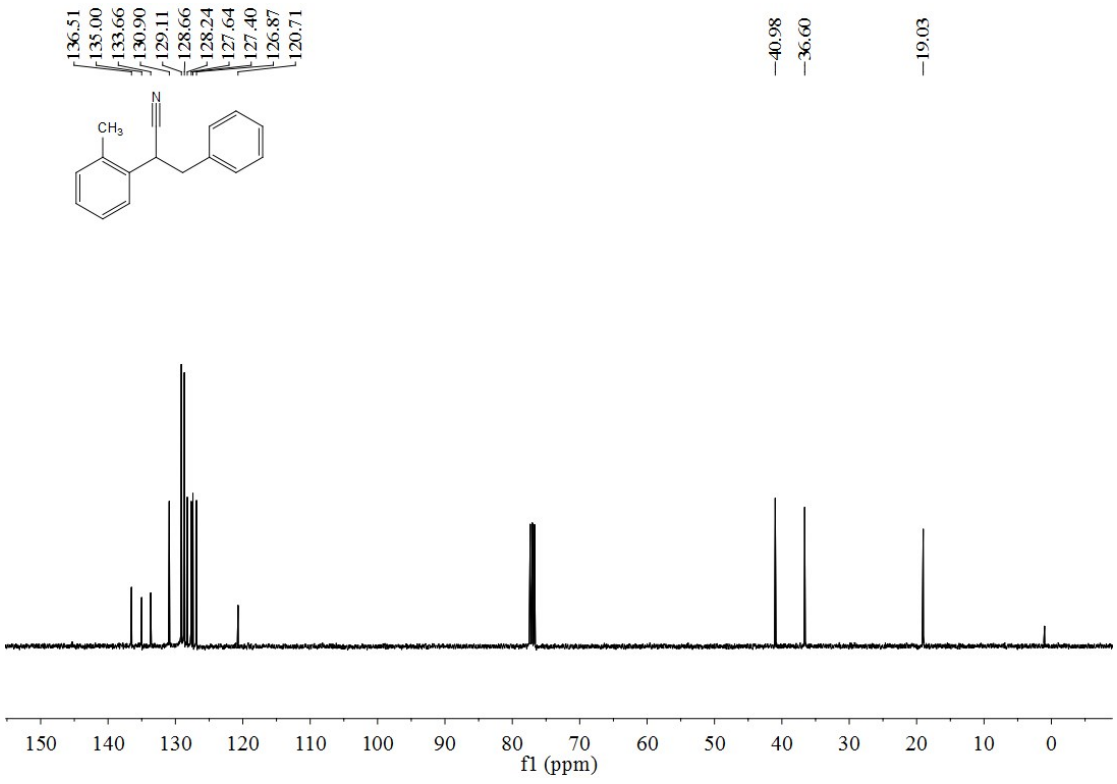
2-(4-bromophenyl)-3-phenylpropanenitrile (4ha)



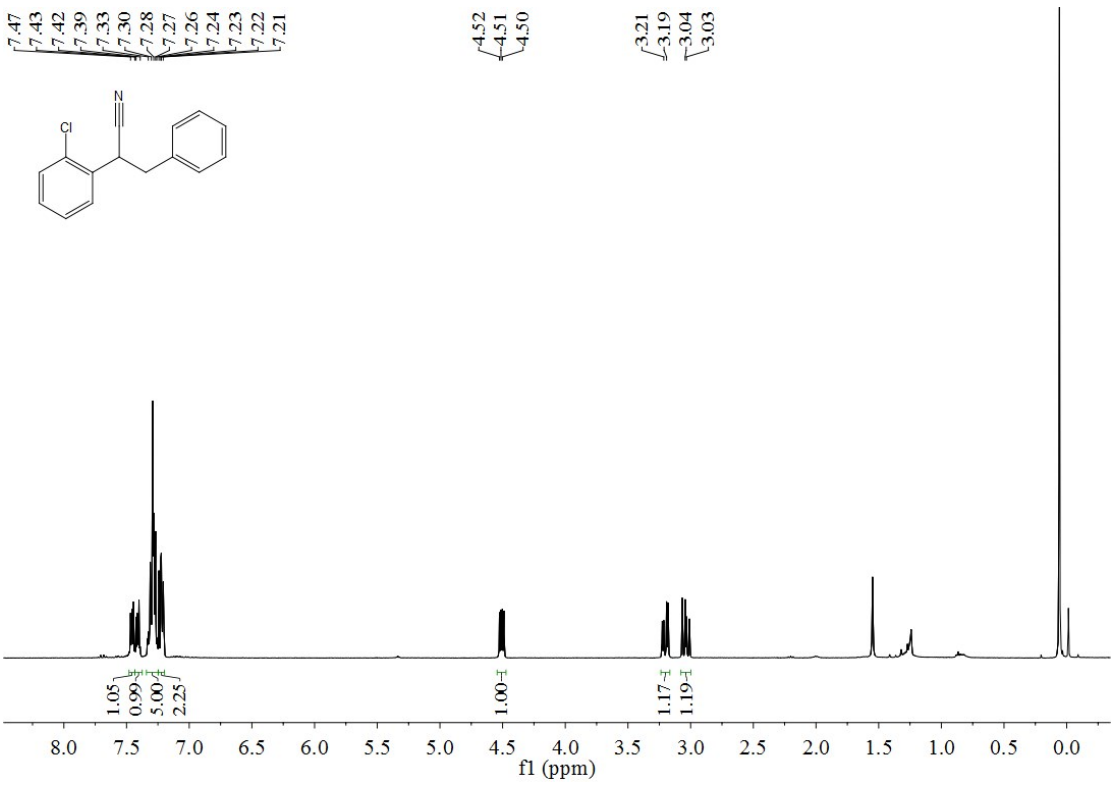


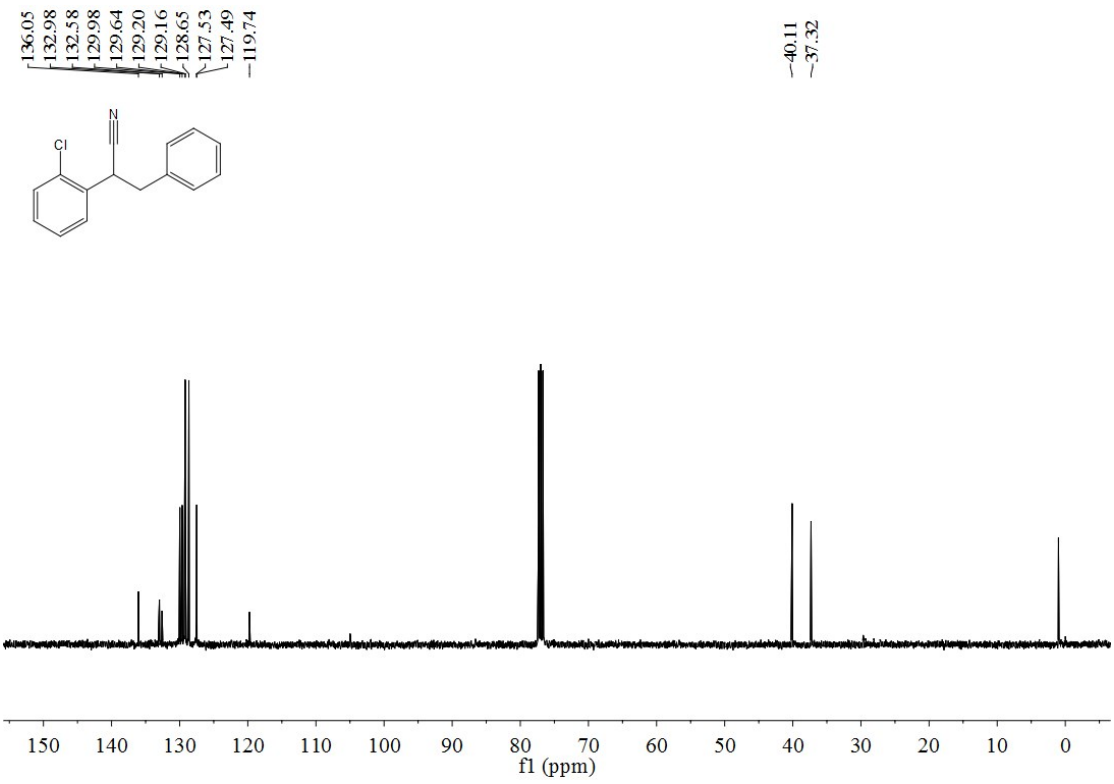
2-phenyl-2-(o-tolyl)propanenitrile (4ia)



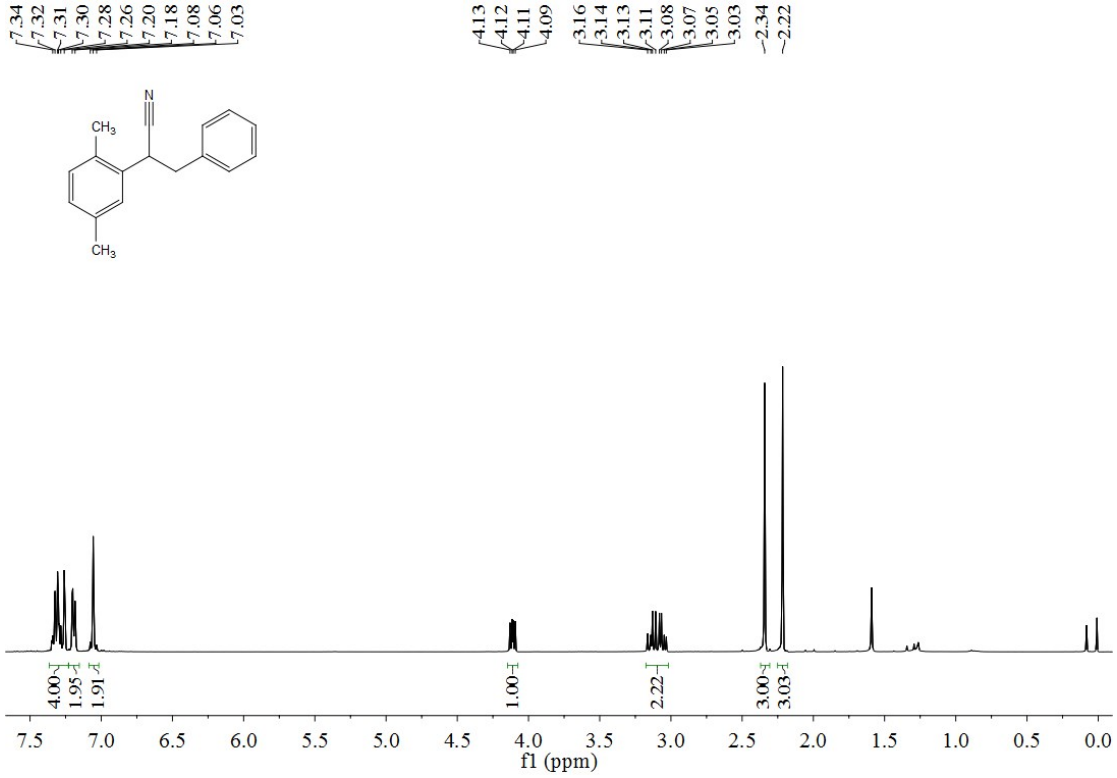


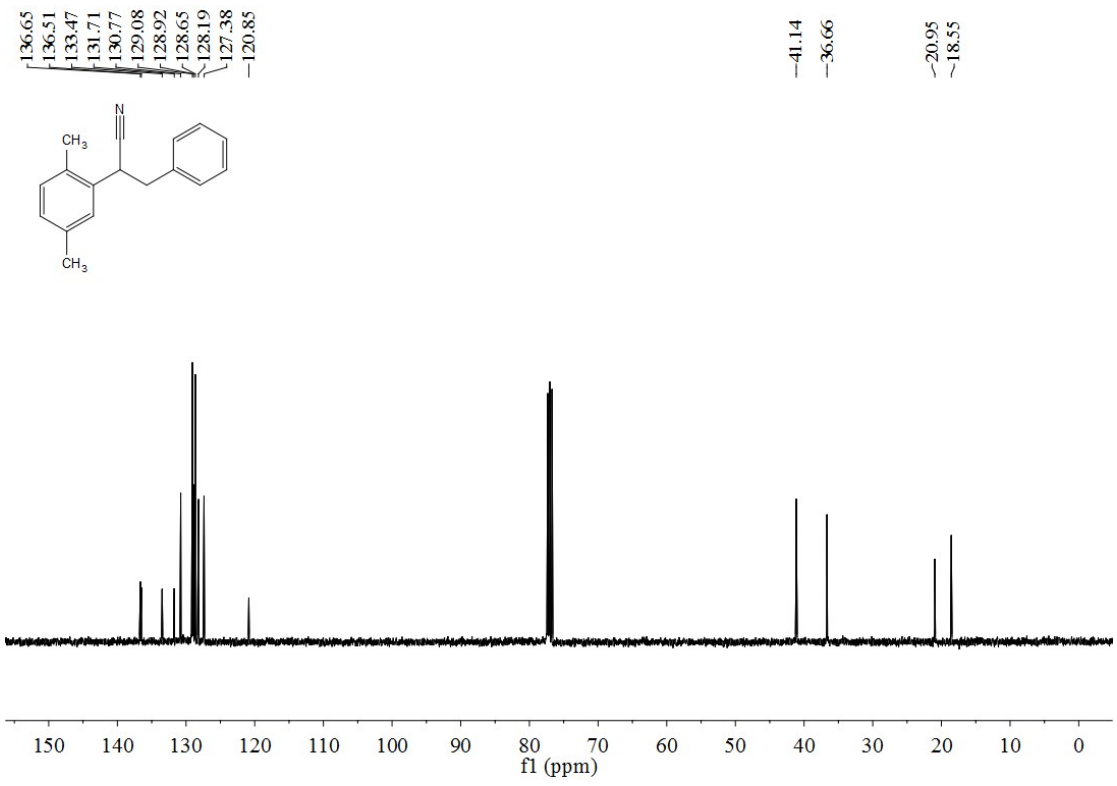
2-(2-chlorophenyl)-3-phenylpropanenitrile (4ja)



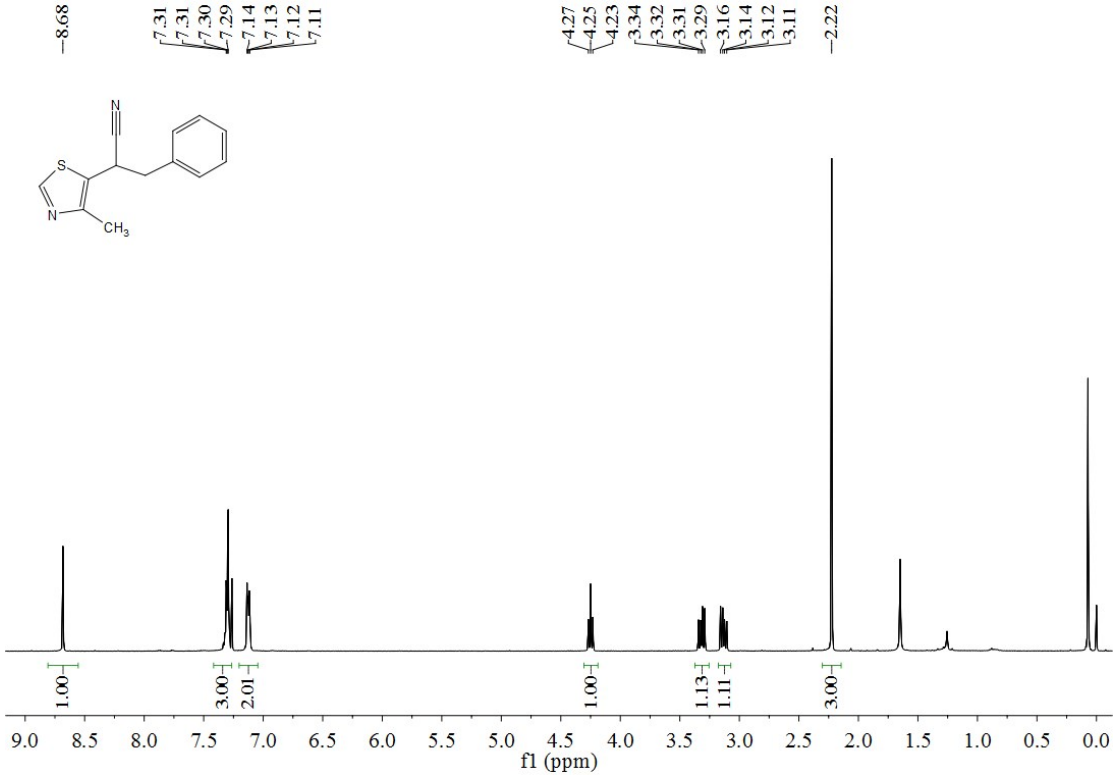


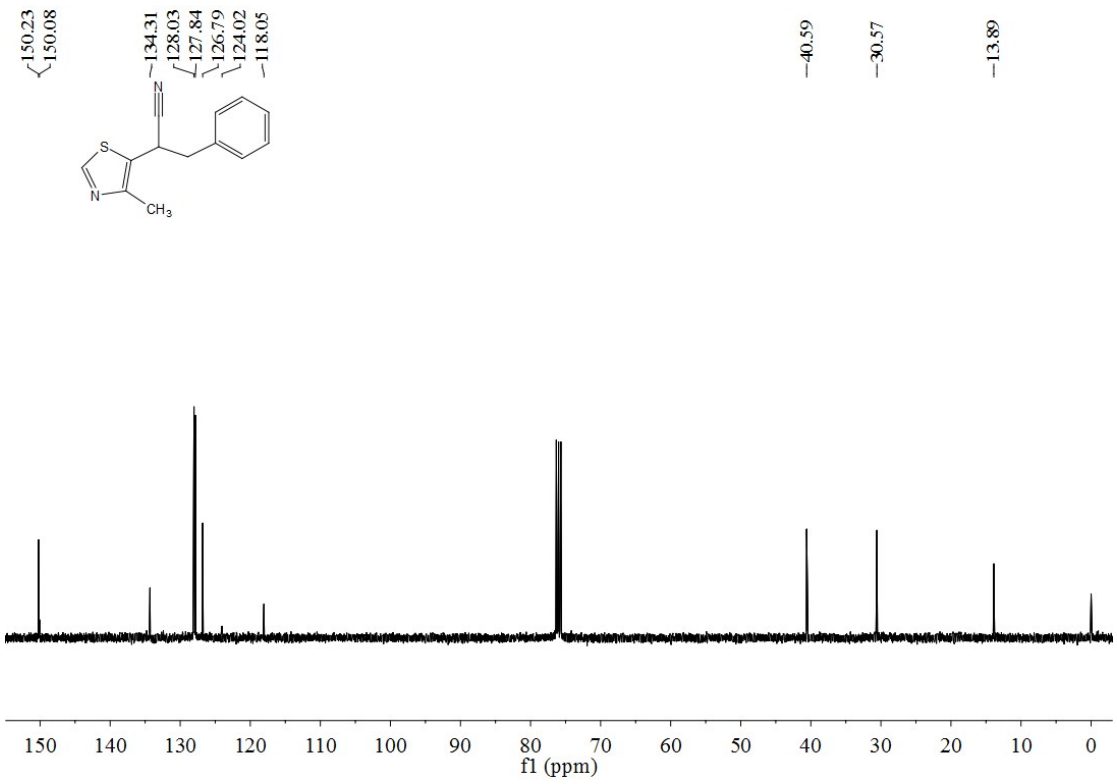
2-(2,5-dimethylphenyl)-3-phenylpropanenitrile (4ka)



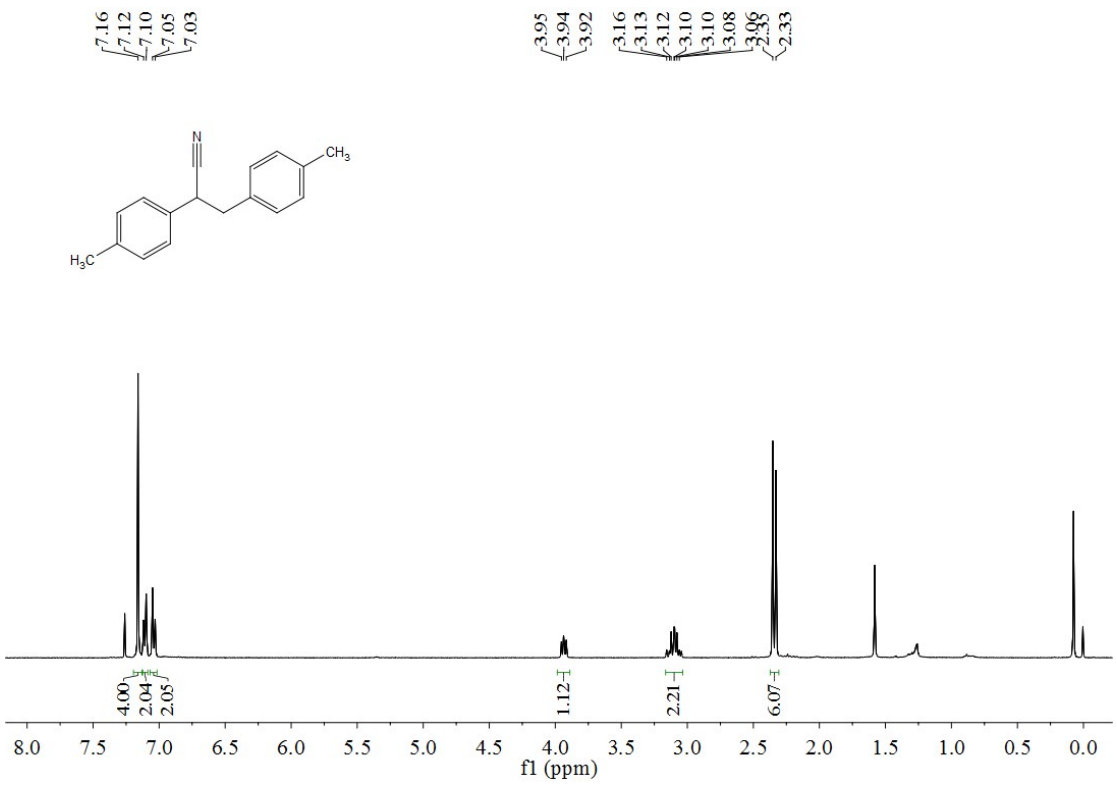


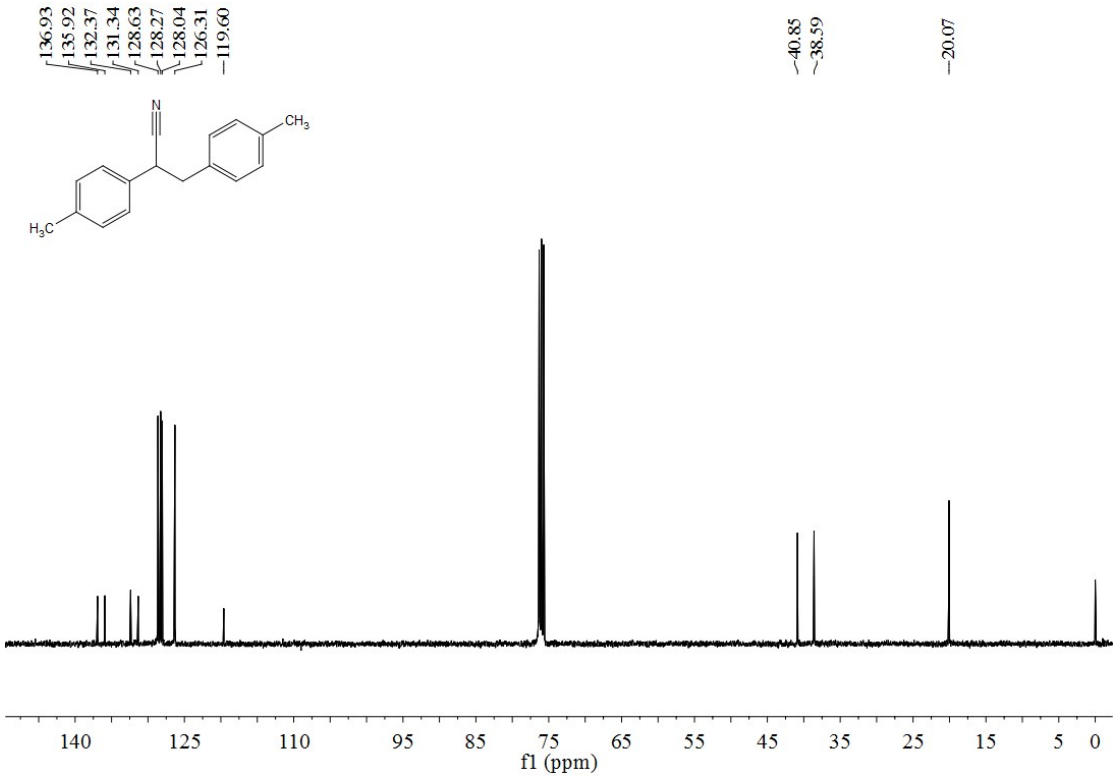
2-(4-methylthiazol-5-yl)-3-phenylpropanenitrile(4la)



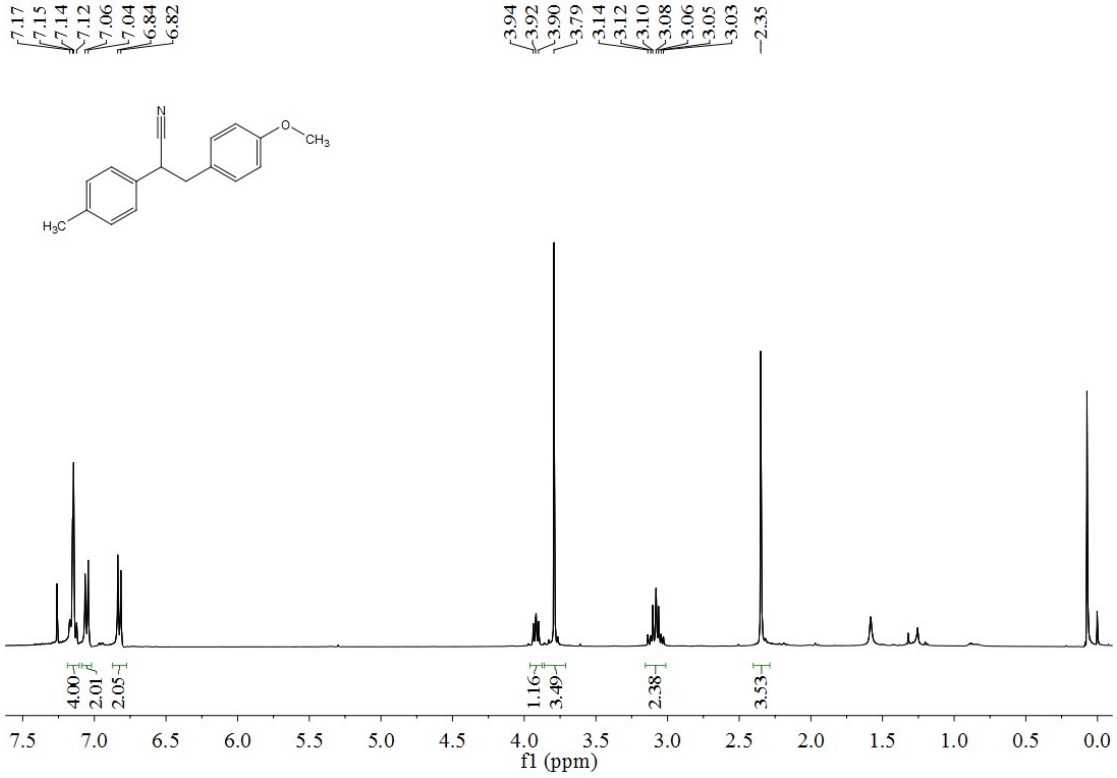


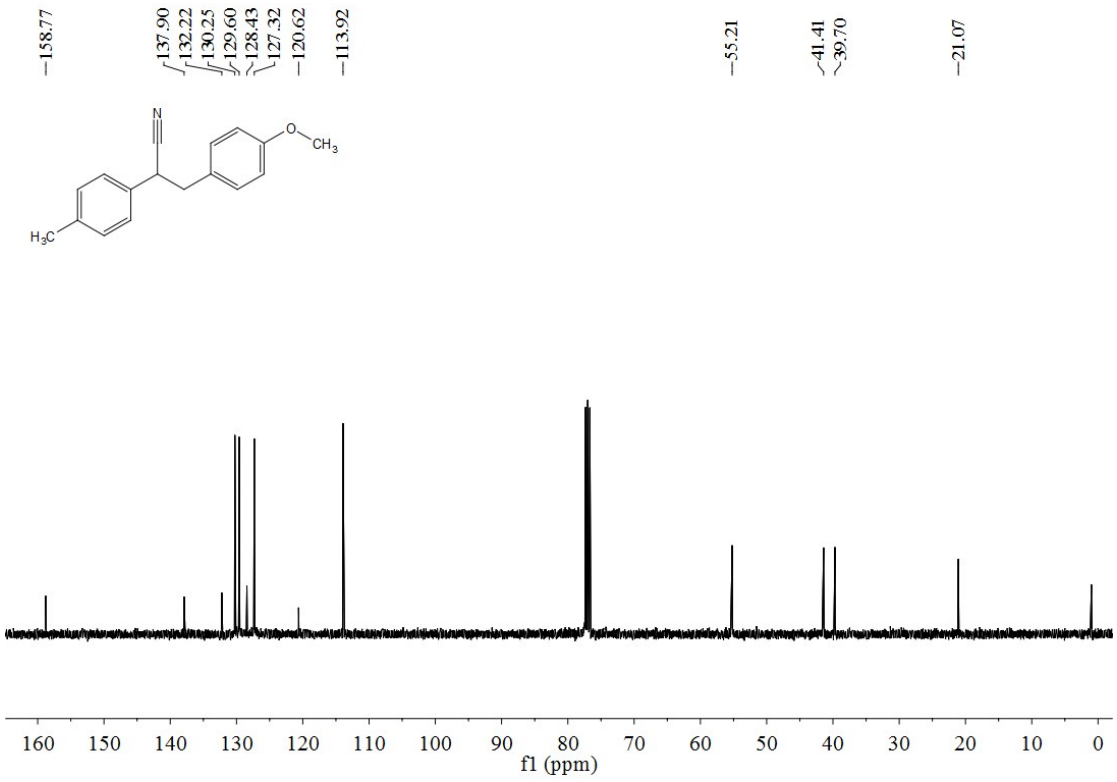
2,3-di-p-tolylpropanenitrile(4ab)



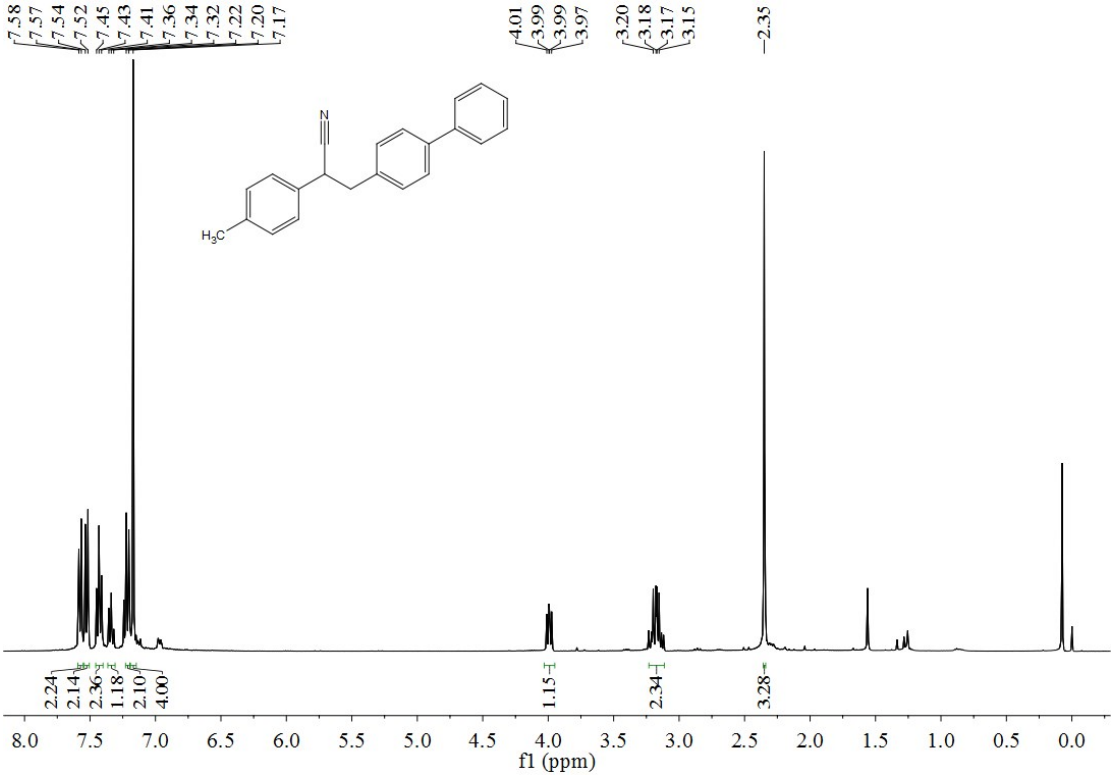


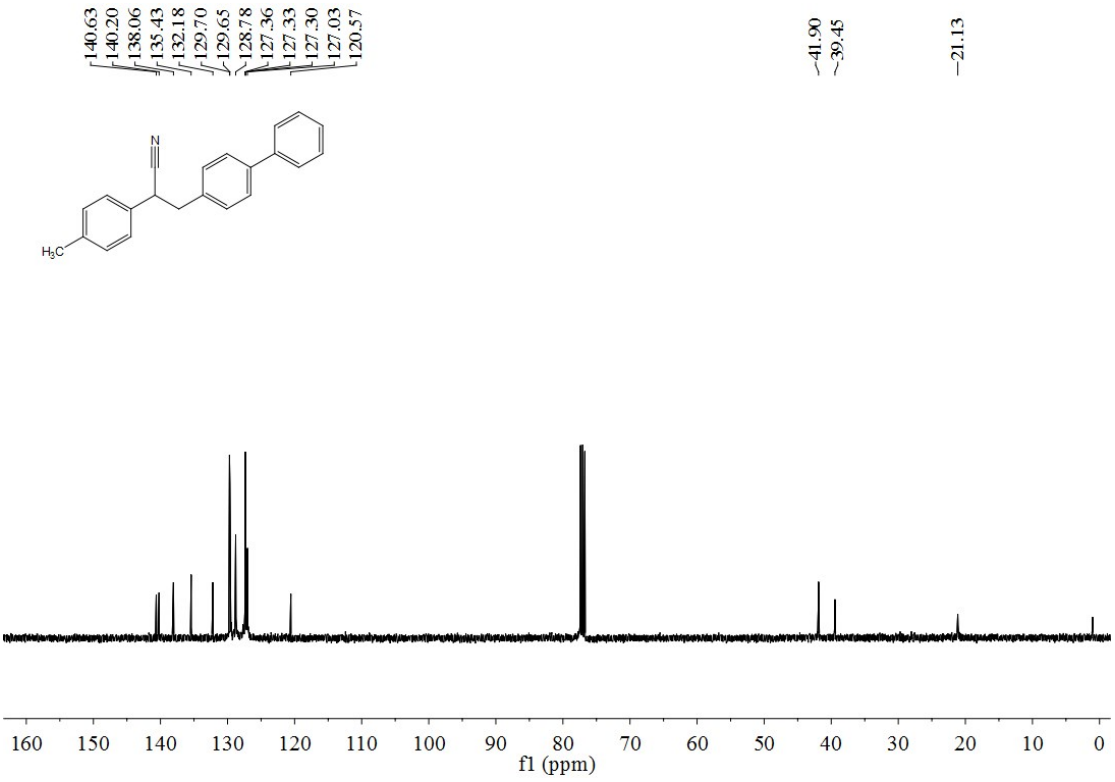
3-(4-methoxyphenyl)-2-(p-tolyl)propanenitrile(4ac)



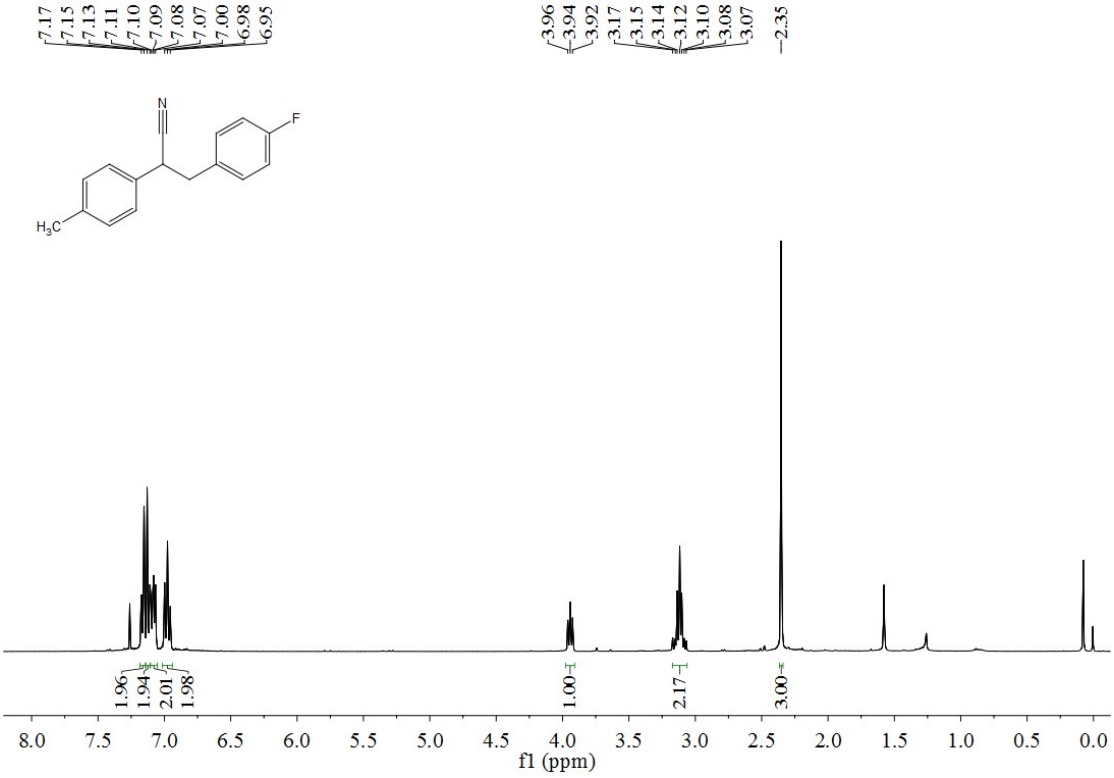


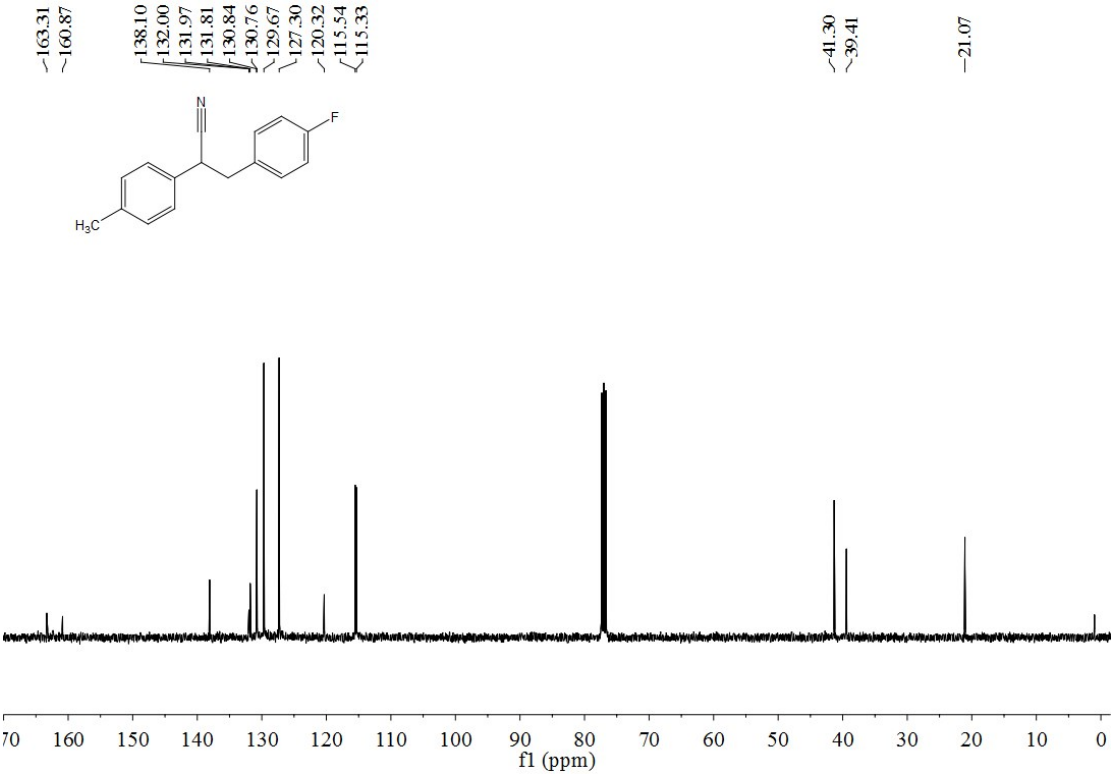
3-([1,1'-biphenyl]-4-yl)-2-(p-tolyl)propanenitrile(4ad)



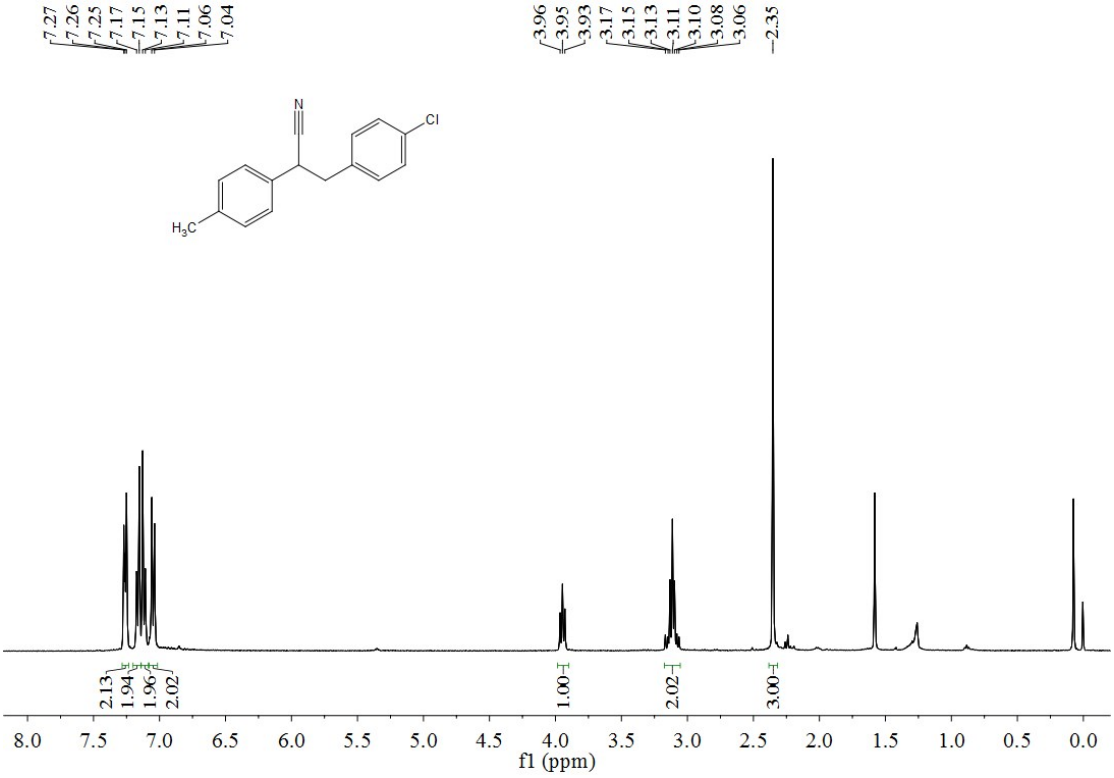


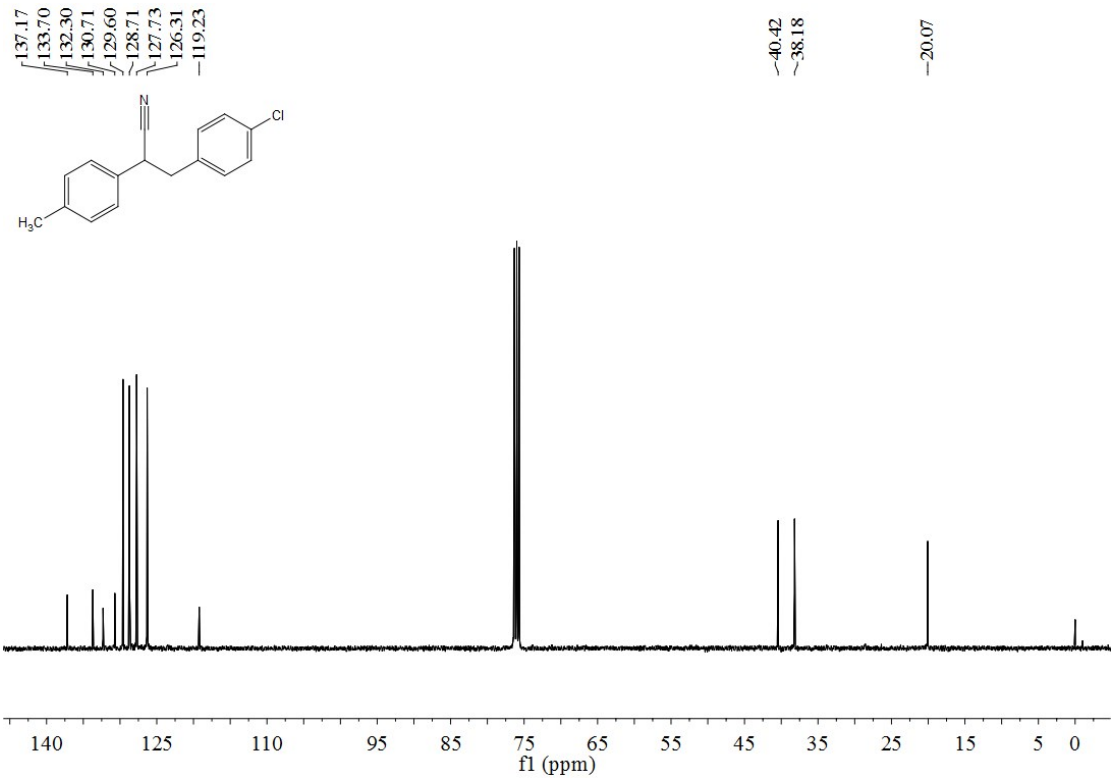
3-(4-fluorophenyl)-2-(p-tolyl)propanenitrile(4ae)



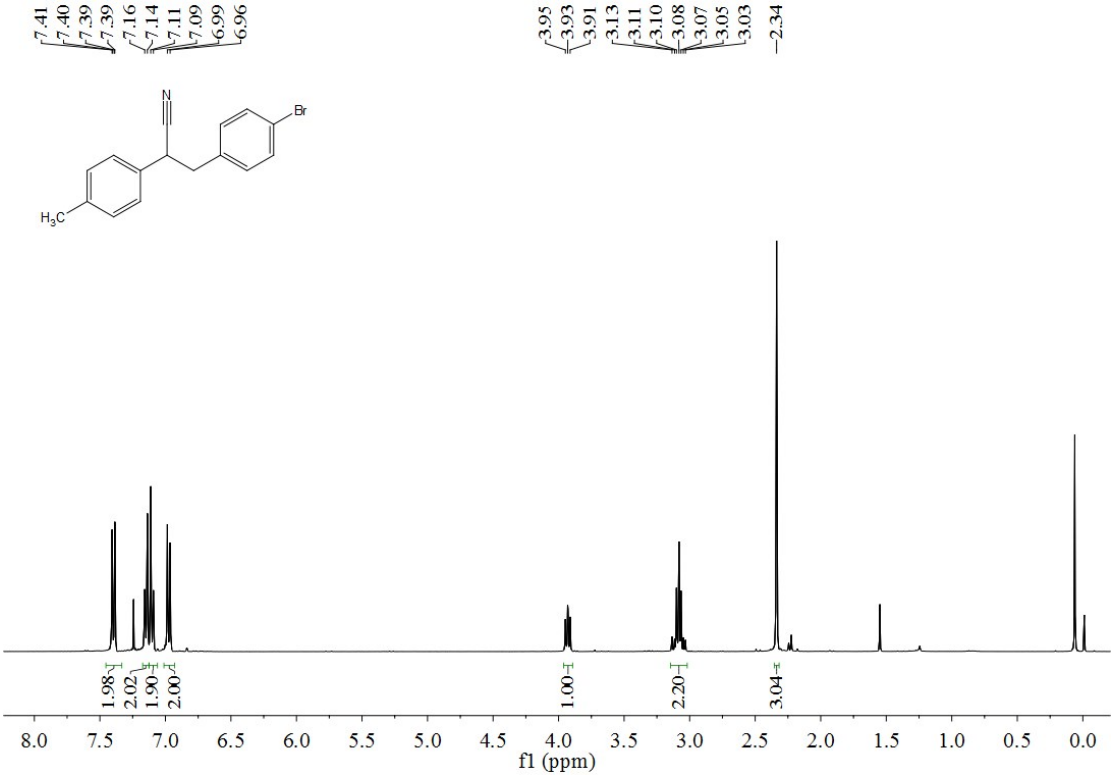


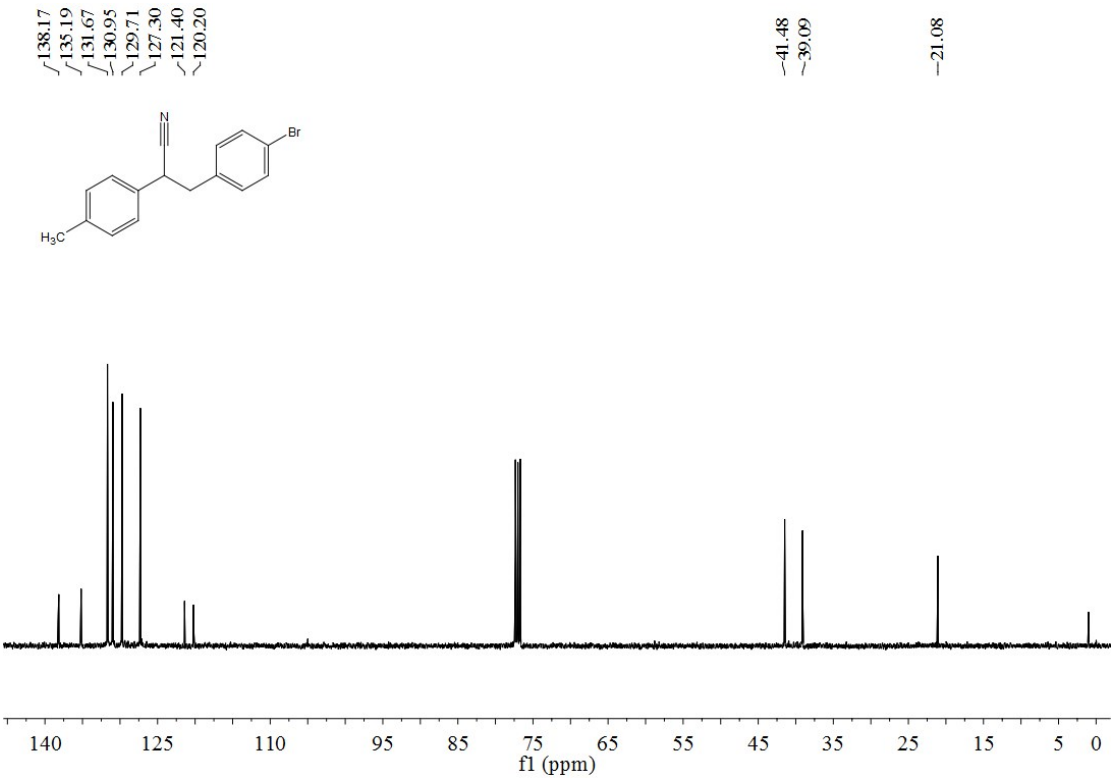
3-(4-chlorophenyl)-2-(p-tolyl)propanenitrile(4af)



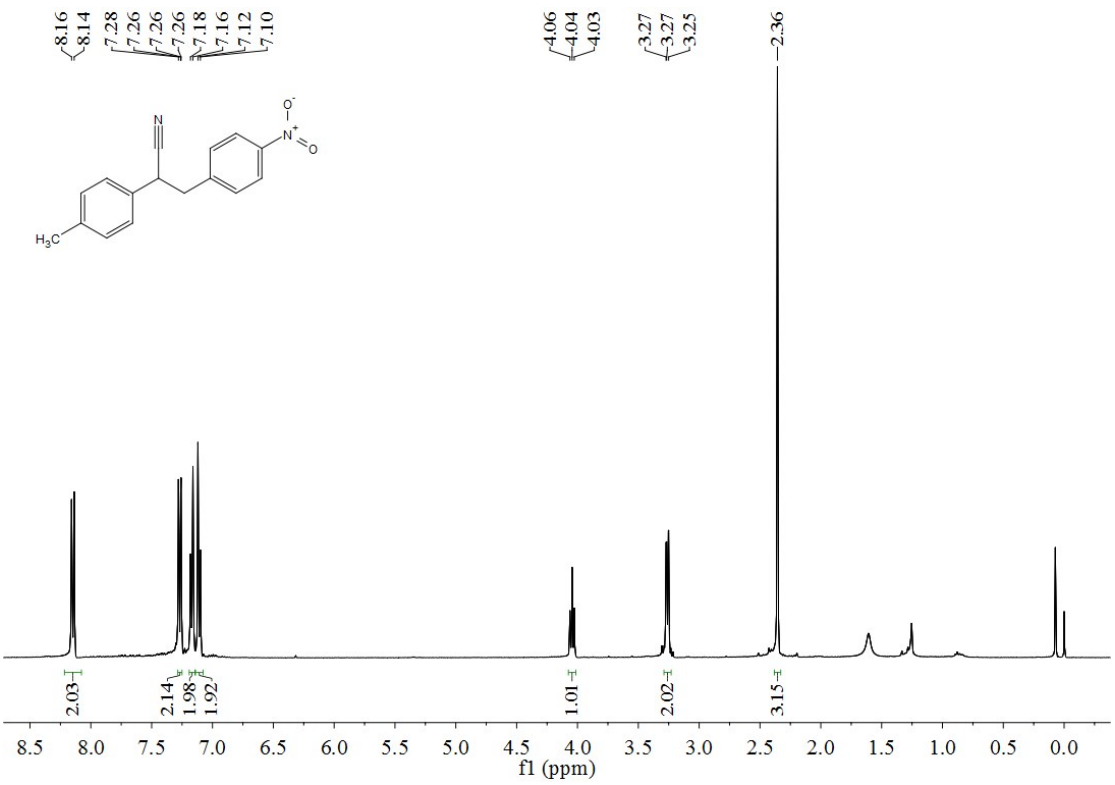


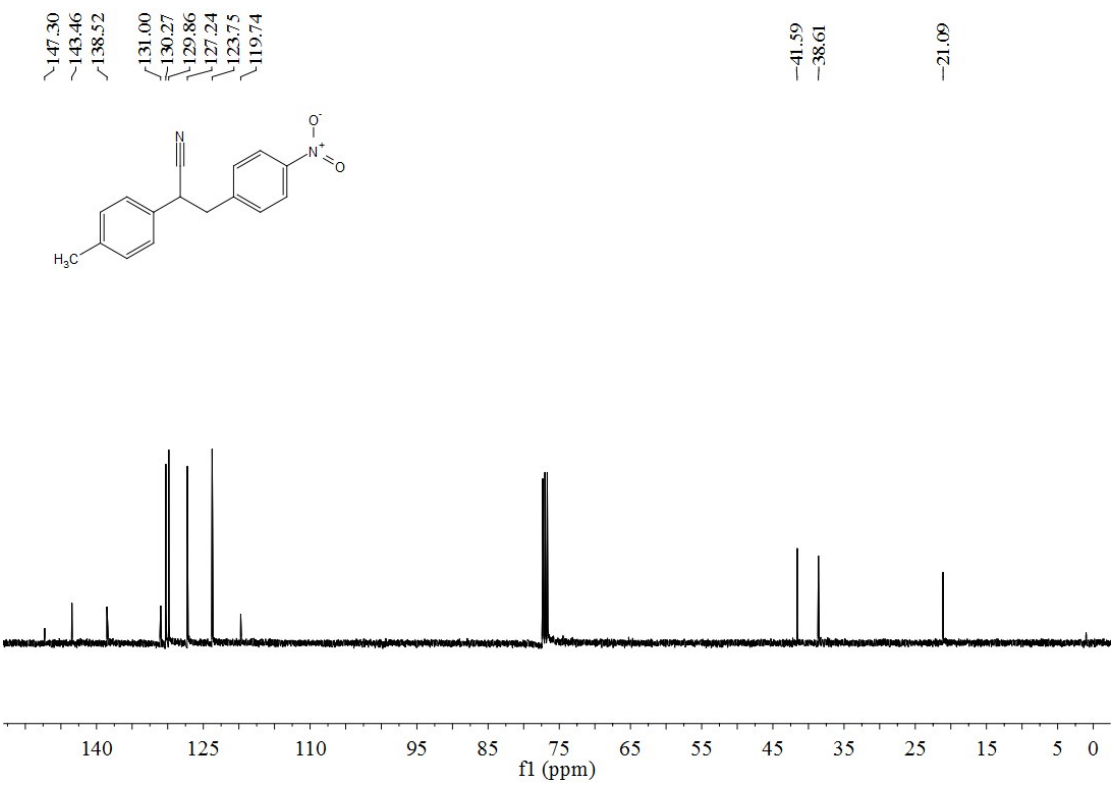
3-(4-bromophenyl)-2-(p-tolyl)propanenitrile(4ag)



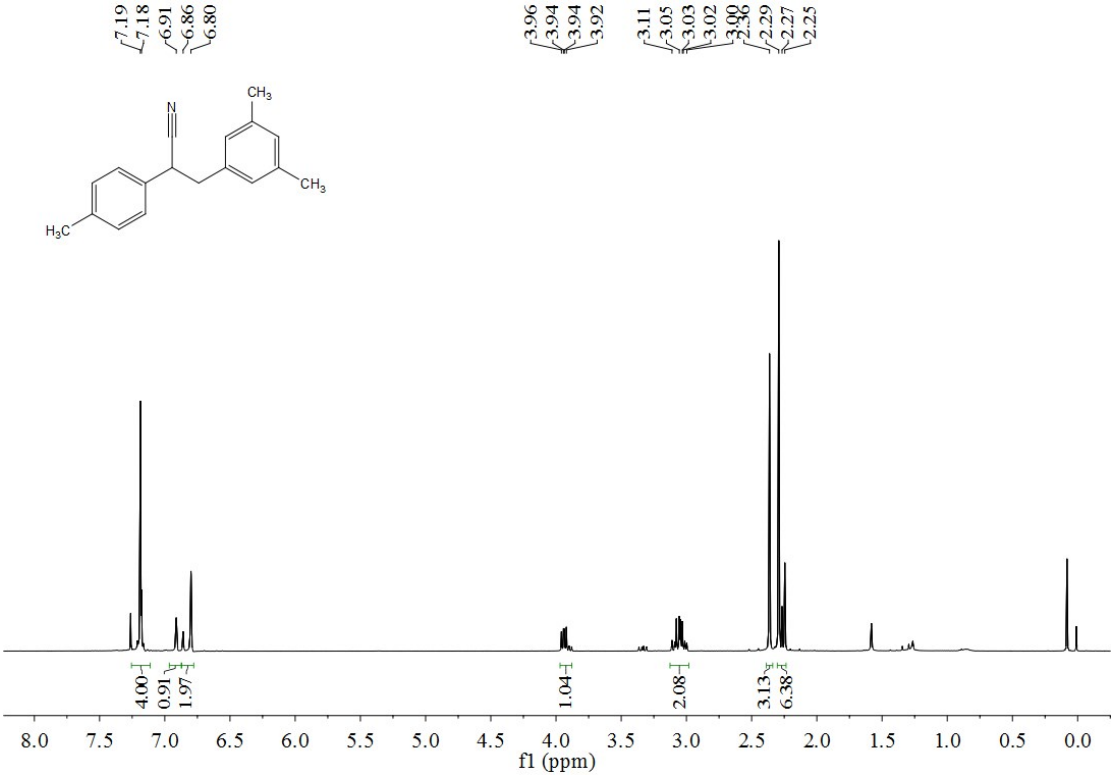


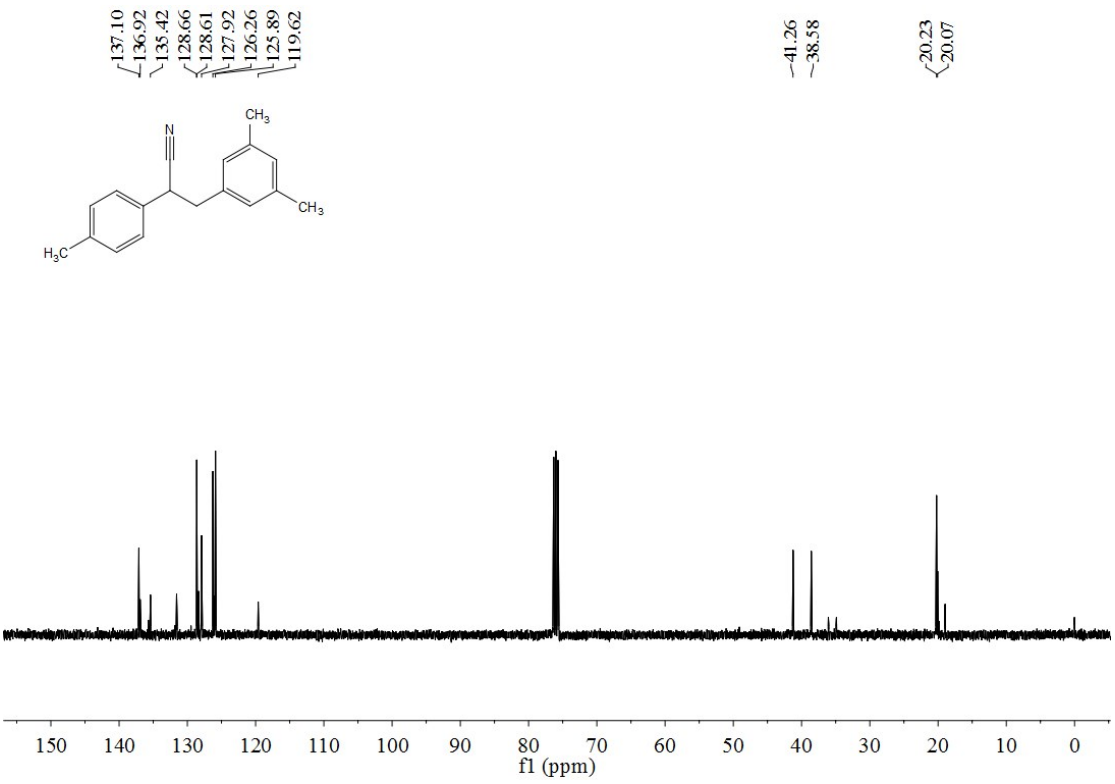
3-(4-nitrophenyl)-2-(p-tolyl)propanenitrile(4ah)



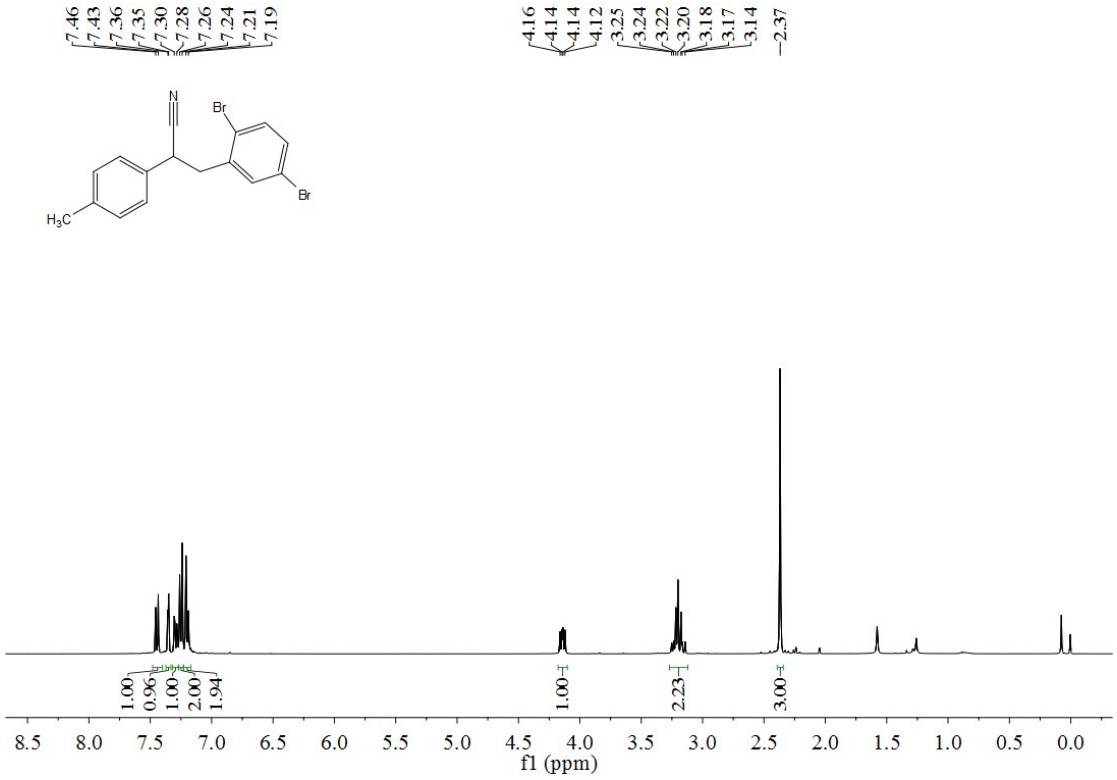


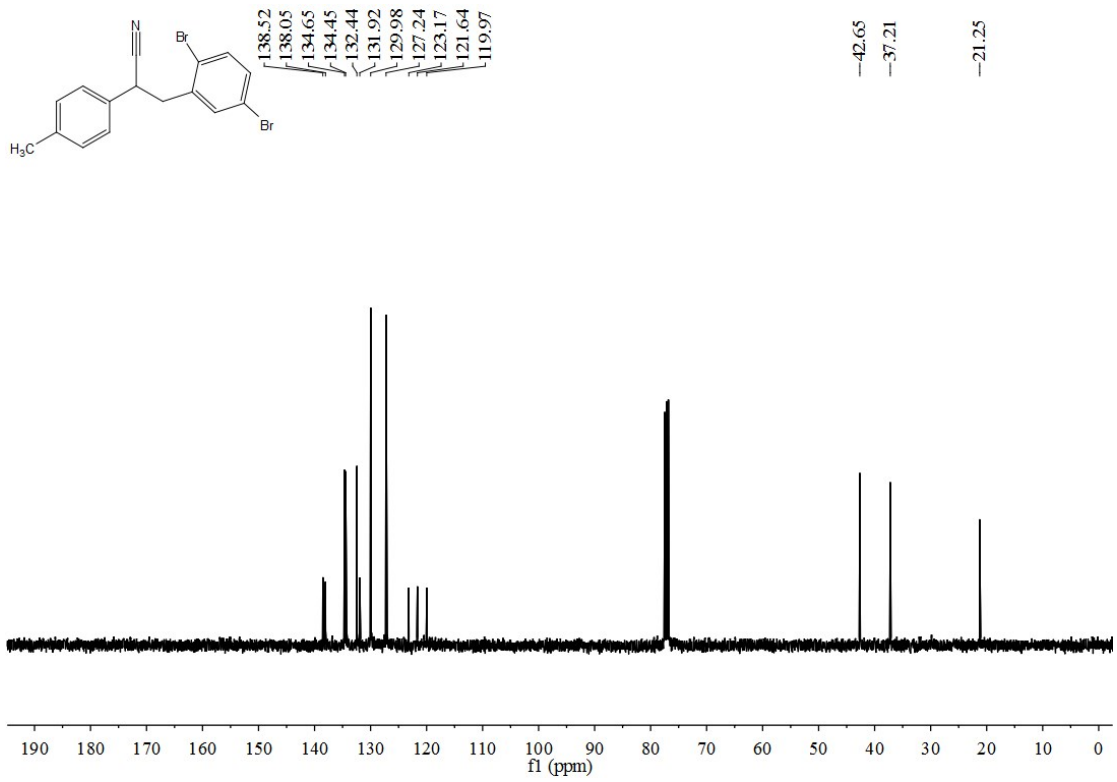
3-(3,5-dimethylphenyl)-2-(p-tolyl)propanenitrile(4ai)



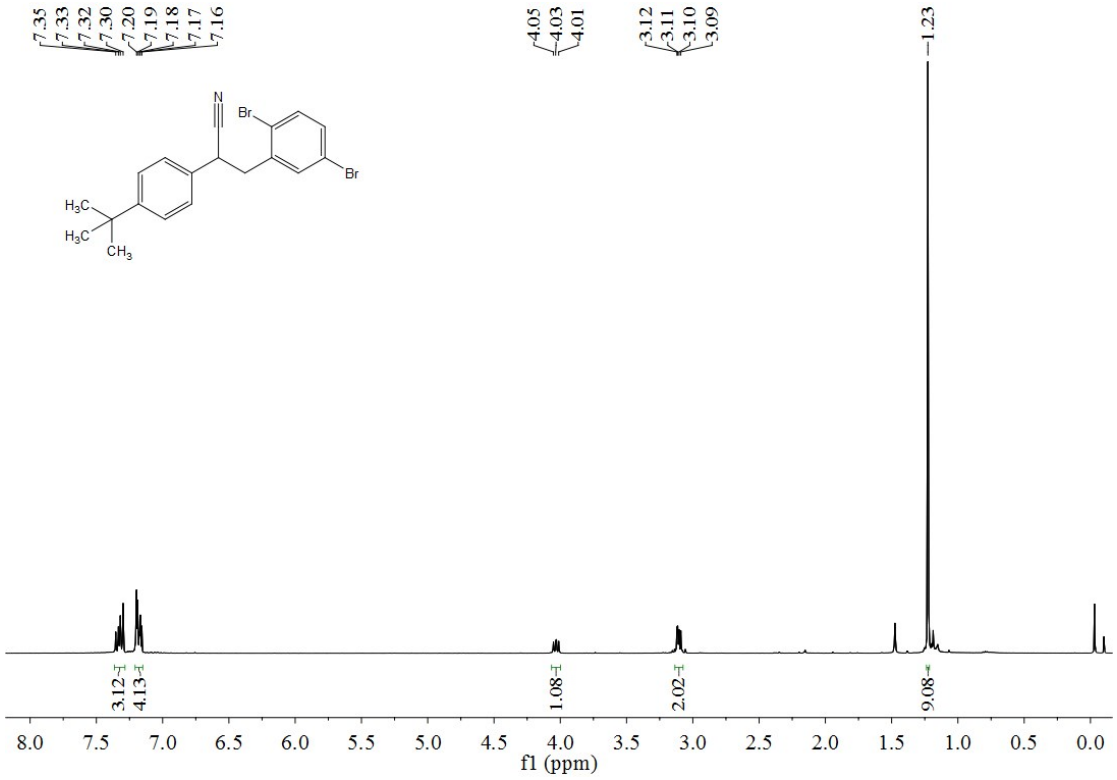


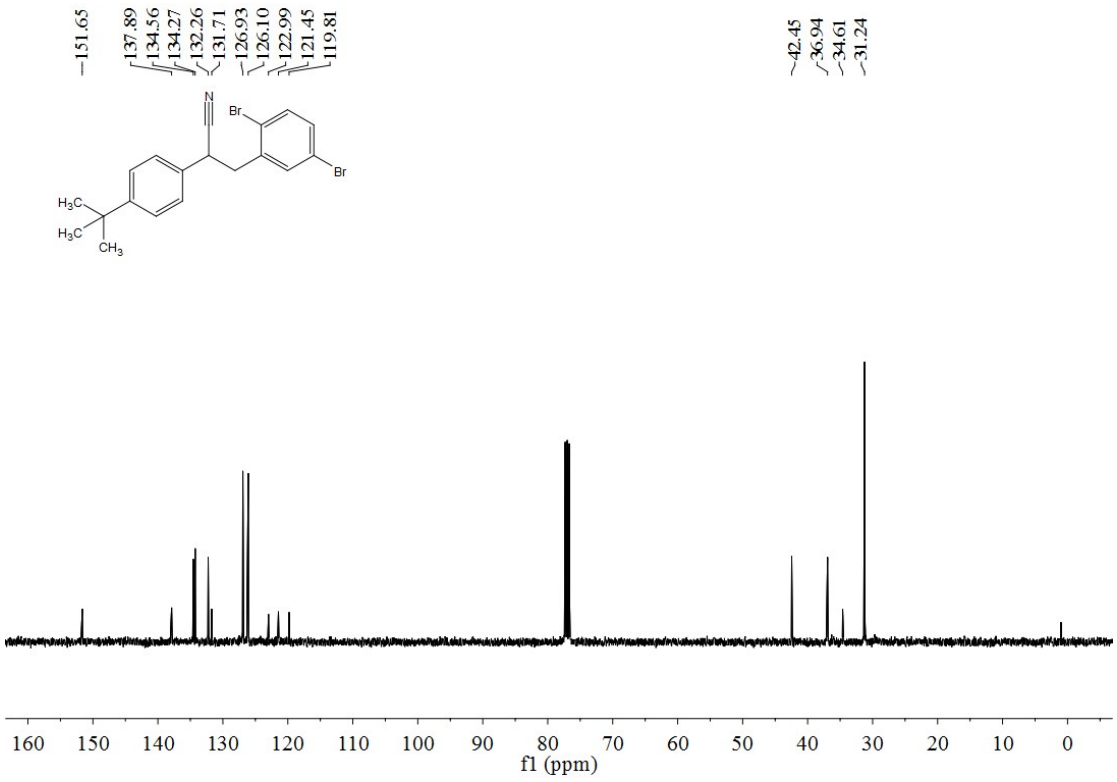
3-(2,5-dibromophenyl)-2-(p-tolyl)propanenitrile(4aj)



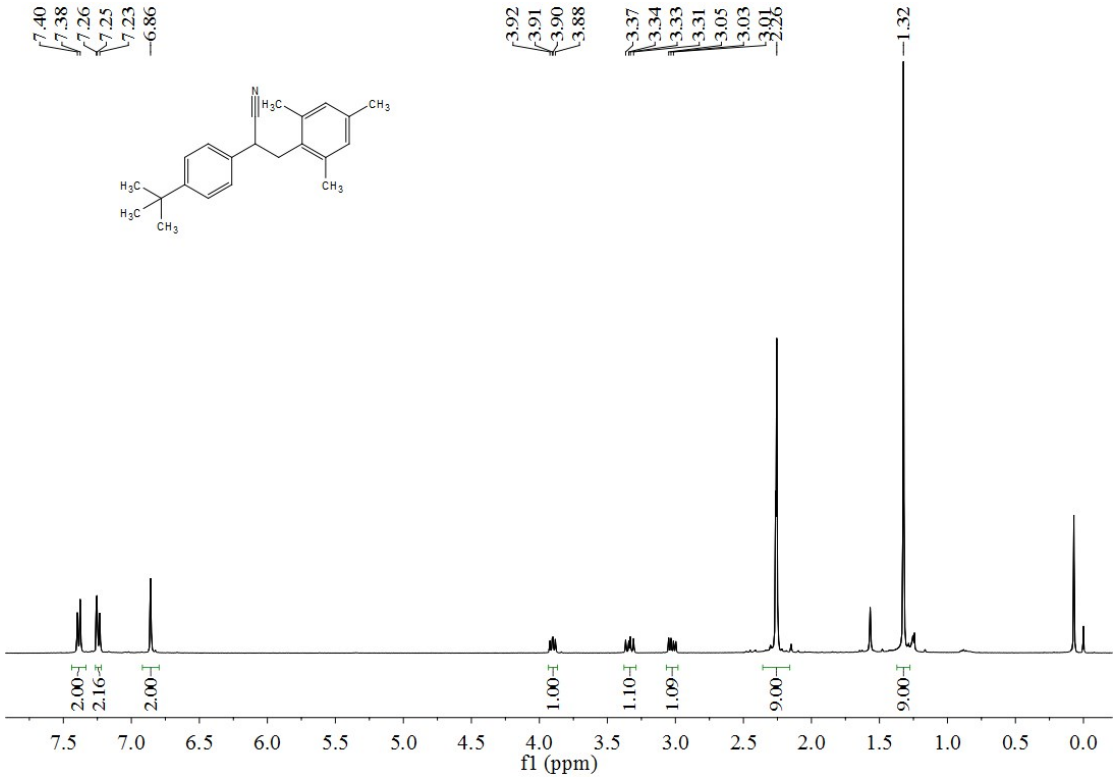


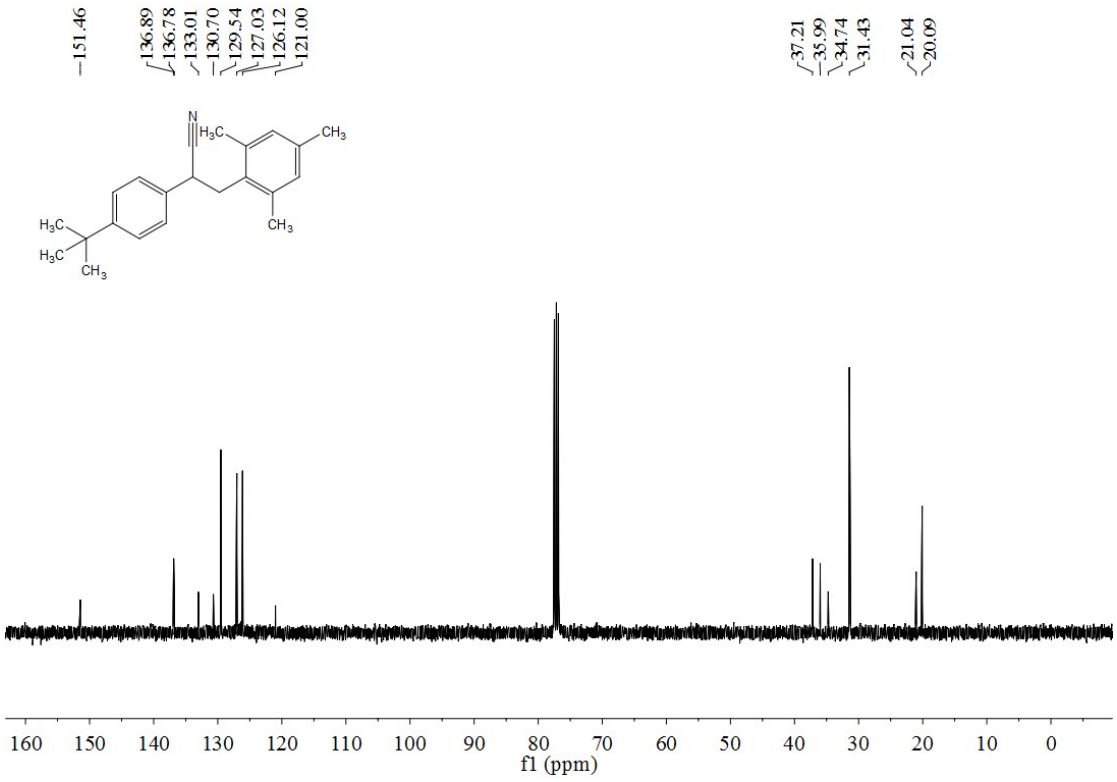
2-(4-(tert-butyl)phenyl)-3-(2,5-dibromophenyl)propanenitrile(4ak)



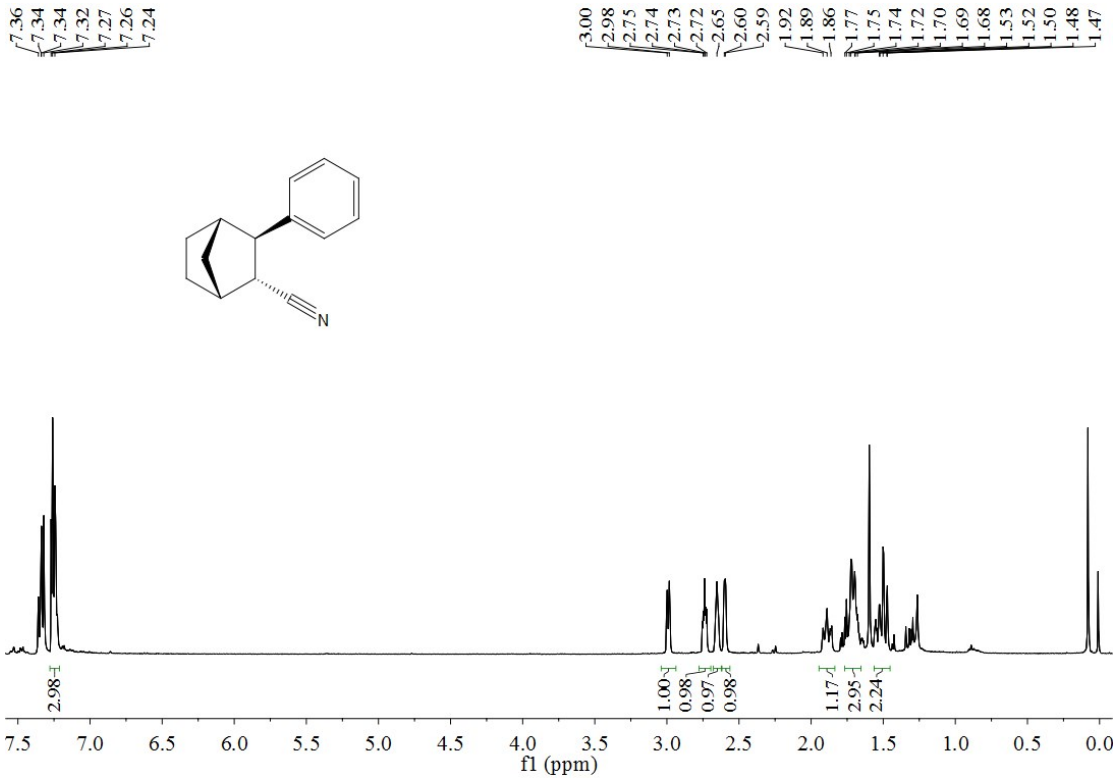


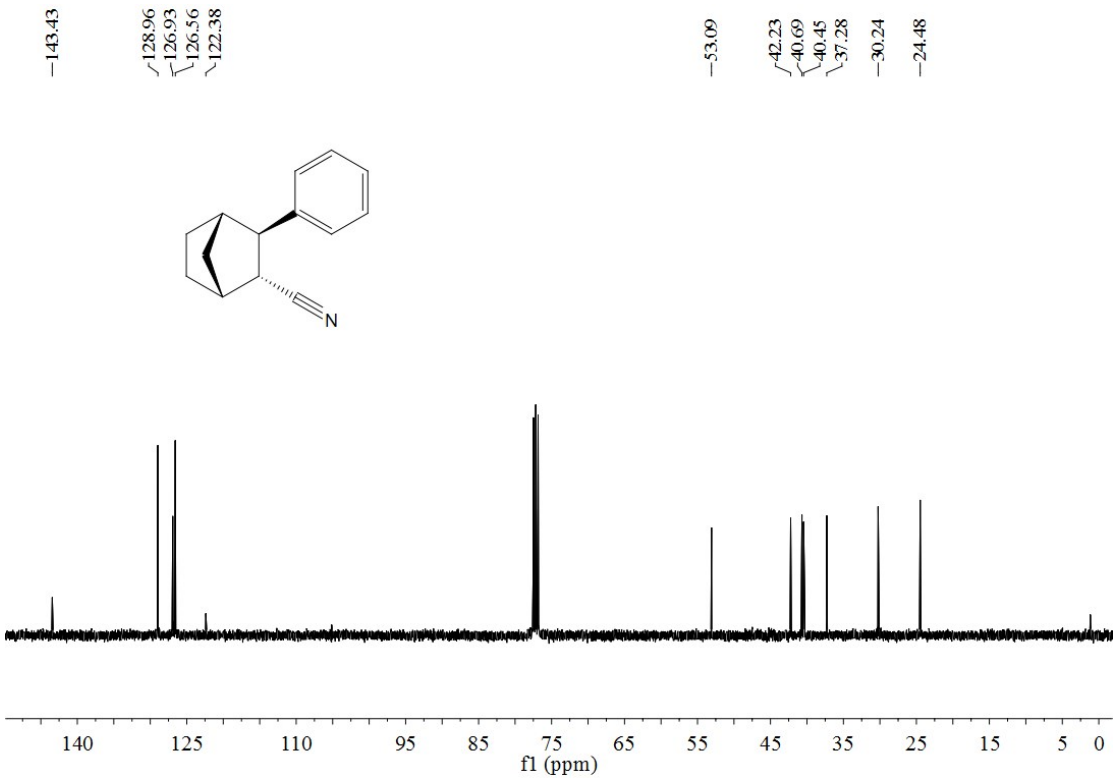
2-(4-(tert-butyl)phenyl)-3-mesitylpropanenitrile (4al)





(1R, 2R, 4S)-3-phenylbicyclo[2.2.1]heptane-2-carbonitrile (4am)





2-(4-benzyltetrahydrofuran-3-yl)acetonitrile (5aa)