Electronic Supplementary Material (ESI) for ChemComm.

Supplementary Information

Oxidative Three-Component 1,2-Alkylarylation of Alkenes with Alkyl Nitriles and *N*-Heteroarenes

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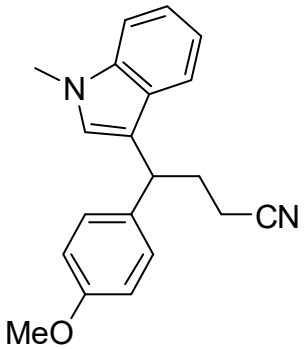
(A) Typical experimental procedure

(a) Typical Experimental Procedure for the Indium-Promoted Intermolecular Oxidative 1,2-Alkylarylation of Alkenes with Alkyl Nitriles and N-Heteroarenes：

To a Schlenk tube were added alkenes **1** (0.2 mmol), α-carbonyl alkyl bromides **2** (0.4 mol), indoles **3** (0.24 mmol), $In(OTf)_3$ (5 mol%; 0.01 mmol), Ag_2CO_3 (2 equiv; 0.4 mmol) and MeCN (2 mL). The tube was charged with argon and sealed, and then was stirred at 120 ºC for 24 h until complete consumption of starting material as monitored by TLC and/or GC-MS analysis. After the reaction was finished, the concentrated in vacuum, and the resulting residue was purified by silica gel column chromatography (hexane/ethyl acetate) to afford the desired products **4**.

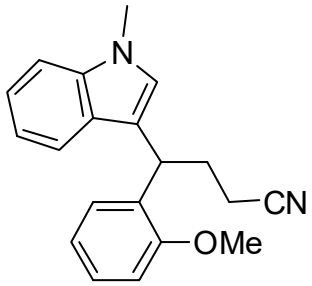
(B) Analytical data



4-(4-Methoxyphenyl)-4-(1-methyl-1*H*-indol-3-yl)butanenitrile (4aaa):

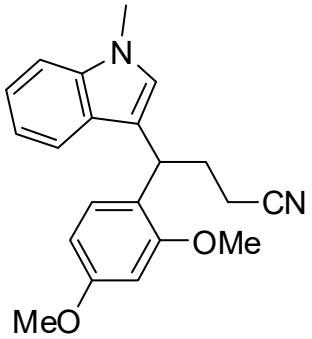
Brown oil; ^1H NMR (400 MHz, $CDCl_3$) δ: 7.43 (d, J = 8.0 Hz, 1H), 7.28-7.17 (m, 4H), 7.03 (t, J = 7.6 Hz, 1H), 6.87-6.80 (m, 3H), 4.25 (t, J = 7.2 Hz, 1H), 3.76 (s, 3H), 3.74 (s, 3H), 2.54-2.48 (m, 1H), 2.32-2.27 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 158.2, 137.3, 135.0, 128.6, 126.8, 125.9, 121.8, 119.7, 119.4, 119.0, 116.8, 114.0, 109.3, 55.2, 40.89, 32.7, 31.5, 15.8; LRMS (EI, 70 eV) *m/z* (%): 304 (M^+, 22), 250 (100),

235 (11), 206 (23); HRMS *m/z* (ESI) calcd for $C_{20}H_{21}N_2O$ ($[M+H]^+$) 305.1648, found 305.1661.



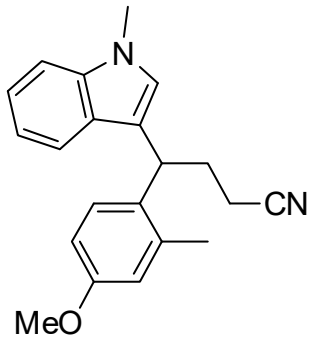
4-(2-Methoxyphenyl)-4-(1-methyl-1*H*-indol-3-yl)butanenitrile (4baa):

Yellow solid, mp 134.2-135.6 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.47 (d, *J* = 8.0 Hz, 1H), 7.26 (d, *J* = 8.4 Hz, 1H), 7.23-7.14 (m, 3H), 7.02 (t, *J* = 7.6 Hz, 1H), 6.91-6.81 (m, 3H), 4.79-4.77 (m, 1H), 3.88 (s, 3H), 3.74 (s, 3H), 2.46-2.41 (m, 1H), 2.39-2.28 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 156.8, 137.1, 131.5, 128.0, 127.5, 127.3, 126.2, 121.7, 120.7, 120.0, 119.4, 118.9, 116.2, 110.5, 109.2, 55.4, 34.1, 32.7, 31.1, 15.8; LRMS (EI, 70 eV) *m/z* (%):304 (M^+, 12), 250 (100), 235 (13), 206 (27); HRMS *m/z* (ESI) calcd for $C_{20}H_{21}N_2O$ ($[M+H]^+$) 305.1648, found 305.1655.



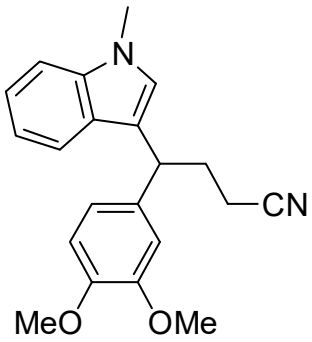
4-(2,4-Dimethoxyphenyl)-4-(1-methyl-1*H*-indol-3-yl)butanenitrile (4caa):

Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.88 (s, 1H), 7.38 (d, *J* = 8.4 Hz, 1H), 7.27-7.20 (m, 3H), 6.93 (s, 1H), 6.81 (d, *J* = 7.6 Hz, 2H), 4.29 (t, *J* = 6.4 Hz, 1H), 4.01-3.81 (m, 4H), 3.77 (s, 3H), 3.74 (s, 3H), 2.80-2.67 (m, 2H), 1.40 (s, 3H), 1.16-1.08 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 159.3, 157.8, 137.1, 128.5, 127.3, 126.1, 124.0, 121.6, 120.1, 119.5, 118.8, 116.5, 109.1, 104.3, 98.4, 55.4, 55.2, 33.7, 32.7, 31.2, 15.7; (EI, 70 eV) *m/z* (%): 334 (M^+, 22), 280 (100), 264 (13), 144 (51); HRMS *m/z* (ESI) calcd for $C_{21}H_{23}N_2O_2$ ($[M+H]^+$) 335.1754, found 335.1763.



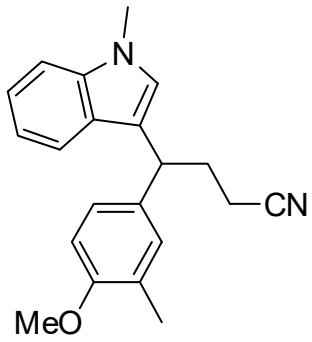
4-(4-Methoxy-2-methylphenyl)-4-(1-methyl-1*H*-indol-3-yl)butanenitrile (4daa):

Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.51 (d, *J* = 8.0 Hz, 1H), 7.26 (d, *J* = 8.0 Hz, 1H), 7.20 (t, *J* = 8.0 Hz, 2H), 7.06 (t, *J* = 7.6 Hz, 1H), 6.73-6.68 (m, 3H), 4.47 (t, *J* = 7.2 Hz, 1H), 3.76 (s, 3H), 3.69 (s, 3H), 2.52-2.45 (m, 1H), 2.35-2.25 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 157.8, 137.6, 137.1, 133.0, 127.1, 127.0, 126.5, 121.7, 119.8, 119.0, 116.8, 116.2, 111.4, 109.3, 55.01, 36.3, 32.6, 31.6, 19.9, 15.7; (EI, 70 eV) *m/z* (%): 318 (M^+, 22), 264 (100), 248 (5), 220 (8); HRMS *m/z* (ESI) calcd for $C_{21}H_{23}N_2O$ ($[M+H]^+$) 319.1805, found 319.1811.



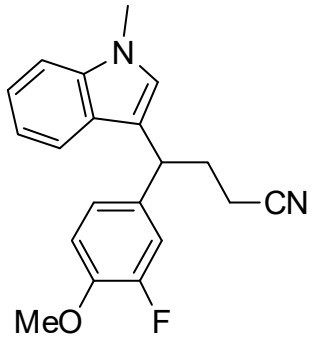
4-(3,4-Dimethoxyphenyl)-4-(1-methyl-1*H*-indol-3-yl)butanenitrile (4eaa):

Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.46 (d, *J* = 8.0 Hz, 1H), 7.27 (t, *J* = 8.4 Hz, 1H), 7.20 (t, *J* = 7.6 Hz, 1H), 7.04 (t, *J* = 7.6 Hz, 1H), 6.89-6.86 (m, 2H), 6.82-6.78 (m, 2H), 4.26 (t, *J* = 7.2 Hz, 1H), 3.84 (s, 3H), 3.82 (s, 3H), 3.75 (s, 3H), 2.56-2.49 (m, 1H), 2.35-2.28 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 149.0, 147.7, 137.3, 135.5, 126.8, 125.9, 121.8, 119.7, 119.5, 119.4, 119.0, 116.7, 111.2, 111.1, 109.3, 55.8, 55.8, 41.4, 32.7, 31.5, 15.8; (EI, 70 eV) *m/z* (%): 334 (M^+, 20), 280 (100), 264 (12), 144 (8); HRMS *m/z* (ESI) calcd for $C_{21}H_{23}N_2O_2$ ($[M+H]^+$) 335.1754, found 335.1768.



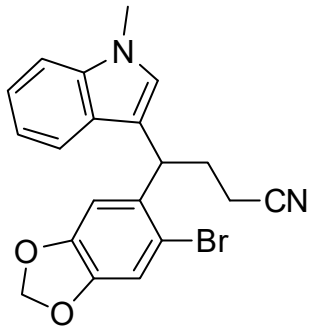
4-(4-Methoxy-3-methylphenyl)-4-(1-methyl-1*H*-indol-3-yl)butanenitrile (4faa)：

Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.45 (d, *J* = 8.0 Hz, 1H), 7.26-7.16 (m, 2H), 7.09-7.00 (m, 3H), 6.83 (s, 1H), 6.72 (d, *J* = 8.0 Hz, 1H), 4.19 (t, *J* = 8.8 Hz, 1H), 3.76 (s, 3H), 3.70 (s, 3H), 2.51-2.44 (m, 1H), 2.26-2.10 (m, 3H), 2.16 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 156.4, 137.2, 134.5, 129.8, 126.9, 126.67, 125.7, 121.7, 119.8, 119.3, 118.9, 117.0, 109.8, 109.2, 55.2, 40.9, 32.6, 31.6, 16.3, 15.7; (EI, 70 eV) *m/z* (%): 318 (M^+, 17), 264 (100), 249 (13), 220 (13);HRMS *m/z* (ESI) calcd for $C_{21}H_{23}N_2O$ ($[M+H]^+$) 319.1805, found 319.1819.



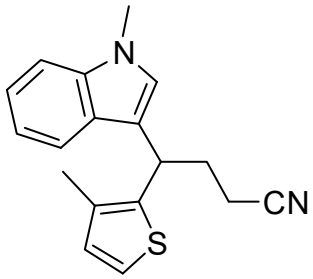
4-(3-Fluoro-4-methoxyphenyl)-4-(1-methyl-1H-indol-3-yl)butanenitrile (4gaa):

Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.40 (d, *J* = 8.0 Hz, 1H), 7.28 (d, *J* = 8. Hz, 1H), 7.20 (t, *J* = 7.6 Hz, 1H), 7.50-6.97 (m, 3H), 6.89-6.85 (m, 2H), 4.26-4,22 (m, 1H), 3.83 (s, 3H), 3.74 (s, 3H), 2.51-2.44 (m, 1H), 2.33-2.22 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 153.6, 151.2 (d, J_{CF} = 244.5 Hz), 146.2, 146.1 (d, J_{CF} = 10.8 Hz), 137.3, 136.3, 136.2 (d, J_{CF} = 5.1 Hz), 126.7, 125.8, 123.3, 123.3, 121.9, 119.5, 119.2, 119.1, 116.0, 115.2, 115.0 (d, J_{CF} = 18 Hz), 113.4 (2C), (d, J_{CF} = 1.8 Hz), 109.3, 56.2, 40.7, 32.7, 31.3, 15.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ : -134.5; (EI, 70 eV) *m/z* (%): 332 (M^+, 22), 268 (100), 253 (17), 224 (15);HRMS *m/z* (ESI) calcd for $C_{20}H_{20}FN_2O$ ($[M+H]^+$) 323.1554, found 323.1563.



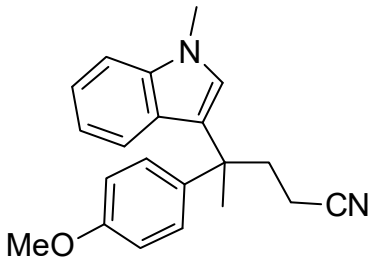
4-(6-Bromobenzo[*d*][1,3]dioxol-5-yl)-4-(1-methyl-1*H*-indol-3-yl)butanenitrile (4haa):

Light yellow oil; 1H NMR (400 MHz, CDCl3) δ: 7.44 (d, *J* = 8.0 Hz, 1H), 7.29-7.19 (m, 2H), 7.07-7.02 (m, 2H), 6.96 (s, 1H), 6.64 (s, 1H), 5.90 (s, 1H), 5.84 (s, 1H), 4.76 (t, *J* = 7.6 Hz, 1H), 3.78 (s, 3H), 2.51-2.41 (m, 2H), 2.36-2.25 (m, 2H); ^{13}C NMR (100 MHz, CDCl3) δ: 147.8, 147.0, 137.2, 135.7, 127.0, 125.7, 122.1, 119.6, 119.4, 119.3, 115.6, 114.4, 112.5, 109.3, 108.4, 101.7, 40.5, 32.8, 31.6, 15.5; LRMS (EI, 70 eV) m/z (%): 398 (M^++2, 28), 396 (M^+, 28), 344 (83), 342 (84), 263 (100); HRMS m/z (ESI) calcd for $C_{20}H_{18}BrN_2O_2$ ([M+H]$^+$) 397.0546, found 397.0561.



4-(1-Methyl-1*H*-indol-3-yl)-4-(3-methylthiophen-2-yl)butanenitrile (4iaa):

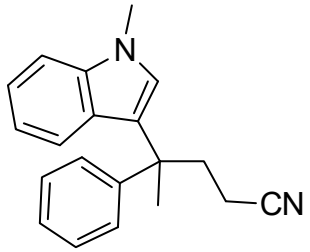
Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.58 (d, J = 7.6 Hz, 1H), 7.29-7.20 (m, 2H), 7.11-7.07 (m, 2H), 6.89 (s, 1H), 6.79 (d, J = 4.8 Hz, 1H), 4.65 (t, J = 8.0 Hz, 1H), 3.74 (s, 3H), 2.57-2.51 (m, 1H), 2.38-2.30 (m, 3H), 2.25 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 140.3, 137.1, 133.6, 130.2, 126.6, 126.2, 121.9, 119.6, 119.2, 119.0, 116.3, 109.4, 34.8, 33.0, 32.8, 15.7, 14.0; (EI, 70 eV) *m/z* (%): 294 (M^+, 21), 240 (100), 224 (10); HRMS *m/z* (ESI) calcd for $C_{18}H_{19}N_2S$ ([M+H]$^+$) 295.1263, found 295.1272.



4-(4-Methoxyphenyl)-4-(1-methyl-1*H*-indol-3-yl)pentanenitrile (4kaa):

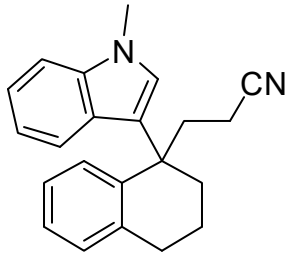
Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.27 (d,

J = 8.5 Hz, 1H), 7.18-7.13 (m, 3H), 6.94 (d, *J* = 8.0 Hz, 2H), 6.87 (t, *J* = 7.5 Hz, 1H), 6.79 (d, *J* = 8.5 Hz, 2H), 3.77 (s, 3H), 3.76 (s, 3H), 2.66-2.60 (m, 1H), 2.52-2.46 (m, 1H), 2.14-2.01 (m, 2H), 1.67 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 157.7, 139.0, 137.7, 127.6, 126.3, 125.8, 121.5, 121.0, 120.7, 120.4, 118.6, 113.5, 109.2, 55.0, 41.4, 36.9, 32.6, 27.6, 13.1; LRMS (EI, 70 eV) *m/z* (%): 318 (M^+, 18), 303 (7), 264 (100), 133 (20); HRMS *m/z* (ESI) calcd for $C_{21}H_{23}N_2O$ ($[M+H]^+$) 319.1805, found 319.1813.



4-(1-methyl-1*H*-indol-3-yl)-4-phenylpentanenitrile (4laa):

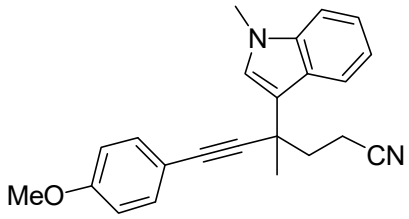
Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.30-7.25 (m, 5H), 7.21 (m, 2H), 6.96 (s, 1H), 6.92-6.87 (m, 2H), 3.80 (s, 3H), 2.70-2.64 (m, 1H), 2.57-2.51 (m, 1H), 2.14-2.04 (m, 2H), 1.71 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 147.0, 137.8, 128.3, 126.6, 126.5, 126.3, 125.9, 121.7, 121.0, 120.5, 120.4, 118.8, 109.3, 42.1, 36.7, 32.8, 27.6, 13.2; LRMS (EI, 70 eV) *m/z* (%): 288 (M^+, 18), 234 (100); HRMS *m/z* (ESI) calcd for $C_{20}H_{21}N_2$ ($[M+H]^+$) 289.1699, found 289.1712.



3-(1-(1-Methyl-1*H*-indol-3-yl)-1,2,3,4-tetrahydronaphthalen-1-yl)propanenitrile (4maa)：

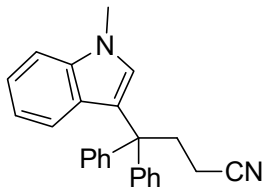
Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.38 (d, *J* = 8.0 Hz, 1H), 7.28 (d, *J* = 8.0 Hz, 1H), 7.21-7.14 (m, 5H), 7.02 (t, *J* = 7.5 Hz, 1H), 6.29 (s, 1H), 3.66 (s, 3H), 2.86-2.81 (m, 3H), 2.64-2.58 (m, 1H), 2.45-2.43 (m, 1H), 2.32-2.26 (m, 2H), 1.95-1.89 (m, 1H), 1.77-1.65 (m, 2H); ^{13}C NMR (100 MHz, CDCl3) δ: 139.4, 138.0, 137.8, 129.7, 128.3, 128.2, 126.5, 125.9, 125.3, 123.0, 121.4, 120.9, 120.5, 118.7, 109.5, 42.4, 36.4, 34.5, 32.6, 30.0, 19.4, 13.4;

(EI, 70 eV) *m/z* (%): 314 (M^+, 27), 260 (100), 183 (26), 129 (43); HRMS *m/z* (ESI) calcd for $C_{22}H_{23}N_2$ ($[M+H]^+$) 315.1856, found 315.1870.



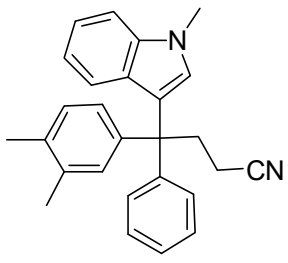
6-(4-Methoxyphenyl)-4-methyl-4-(1-methyl-1*H*-indol-3-yl)hex-5-ynenitrile (4naa):

Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.80 (d, *J* = 8.0 Hz, 1H), 7.42 (d, *J* = 8.4 Hz, 2H), 7.33 (d, *J* = 8.2 Hz, 1H), 7.27 – 7.23 (m, 2H), 7.15-7.10 (m, 2H), 6.86 (d, *J* = 8.4 Hz, 2H), 3.82 (s, 3H), 3.76 (s, 3H), 2.58-2.54 (m, 2H), 2.34-2.24 (m, 2H), 1.83 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 159.5, 138.0, 133.0, 127.1, 124.9, 121.8, 120.3, 120.2, 119.1, 116.8, 115.2, 113.9, 109.8, 91.7, 83.1, 55.3, 37.8, 35.9, 32.7, 29.1, 14.1; LRMS (EI, 70 eV) m/z (%): 342 (M^+, 12), 288 (100), 273 (7); HRMS *m/z* (ESI) calcd for $C_{23}H_{23}N_2O$ ($[M+H]^+$) 343.1805, found 343.1813.



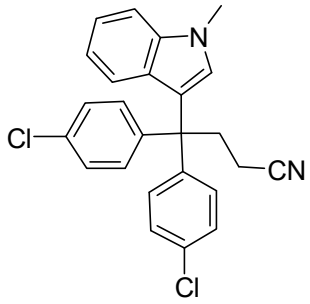
Phenyl 4-(4-methoxyphenyl)-2,3-dimethyl-4-(1-methyl-1*H*-indol-3-yl)butanoate (4oaa):

Yellow solid, mp 183.2-184.6 ºC (uncorrected); ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.35-7.18 (m, 13H), 7.03 (d, *J* = 8.0 Hz, 1H), 6.93 (t, *J* = 7.5 Hz, 1H), 6.66 (s, 1H), 3.74 (s, 3H), 3.09-3.06 (m, 2H), 2.13-2.09 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 145.4, 137.8, 129.0, 128.3, 128.1, 126.4, 121.8, 121.8, 120.2, 119.0, 118.5, 109.8, 51.6, 35.5, 32.8, 14.4; LRMS (EI, 70 eV) *m/z* (%): 350 (M^+, 10), 296 (100), 218 (8); HRMS *m/z* (ESI) calcd for $C_{25}H_{23}N_2$ ($[M+H]^+$) 351.1856, found 351.1867.



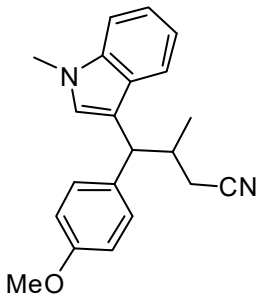
4-(3,4-Dimethylphenyl)-4-(1-methyl-1*H*-indol-3-yl)-4-phenylbutanenitrile (4paa):

Yellow solid, mp 157.8-158.9 °C (uncorrected); ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.33 (d, *J* = 7.5 Hz, 2H), 7.29-7.23 (m, 3H), 7.18 (t, *J* = 7.5 Hz, 2H), 7.09-7.00 (m, 4H), 6.92 (t, *J* = 7.5 Hz, 1H), 6.66 (s, 1H), 3.72 (s, 3H), 3.06-3.04 (m, 2H), 2.20 (s, 3H), 2.18 (s, 3H), 2.12-2.07 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 157.8, 137.0, 135.8, 134.3, 128.3, 126.1, 120.6, 119.9, 119.0, 118.9, 113.8, 110.5, 108.9, 55.1, 40.0, 30.0, 29.6, 15.9, 10.5; LRMS (EI, 70 eV) *m/z* (%): 378 (M^+, 9), 324 (100), 294 (4); HRMS *m/z* (ESI) calcd for $C_{27}H_{27}N_2$ ($[M+H]^+$) 379.2169, found 379.2177.



4,4-Bis(4-chlorophenyl)-4-(1-methyl-1*H*-indol-3-yl)butanenitrile (4qaa):

Yellow solid, mp 209.1-209.6 °C (uncorrected); ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.32-7.21 (m, 11H), 7.00-6.95 (m, 2H), 6.63 (s, 1H), 3.75 (s, 3H), 3.02 (t, *J* = 8.0 Hz, 2H), 2.08 (t, *J* = 8.4 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 143.6, 137.8, 132.5, 129.4, 128.9, 128.6, 125.9, 122.1, 121.5, 119.7, 119.4, 117.5, 109.7, 50.9, 35.3, 32.9, 14.3; HRMS *m/z* (ESI) calcd for $C_{25}H_{21}Cl_2N_2$ ($[M+H]^+$) 419.1076, found 419.1085.

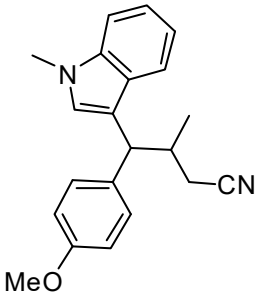


4-(4-Methoxyphenyl)-3-methyl-4-(1-methyl-1*H*-indol-3-yl)butanenitrile (4raa- from trans **1r):**

d.r. = 1.2

Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.57 (t, *J* = 8.8 Hz, 1.01H), 7.26-7.22 (m, 3.06H), 7.18 (t, *J* = 7.4 Hz, 1.07H), 7.06 (t, *J* = 7.6, 1.00H), 6.94 (d, *J* = 4.8 Hz, 0.97H), 6.80 (d, *J* = 8.8 Hz, 2.02H), 3.99 (d, *J* = 10.0 Hz, 0.46H), 3.93 (d, *J* = 10.4 Hz, 0.56H), 3.73 (s, 4.6H),3.73 (s, 1.39H), 2.74-2.63 (m, 1.02H),

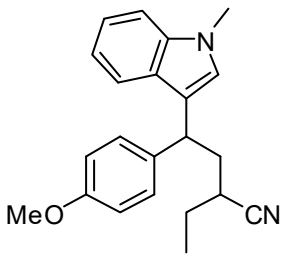
2.49 (d, *J* = 16.8, 0.55H), 2.35 (d, *J* = 16.4, 0.48H), 2.24 (d, *J* = 16.8, 0.56H), 2.10 (dd, *J* = 16.4, 0.49H), 1.20 (d, *J* = 6.6 Hz, 1.41H), 1.08 (d, *J* = 6.6 Hz, 1.63H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 158.1(2C), 137.0, 136.9, 135.2, 135.1, 128.9, 128.7, 127.5, 127.0, 125.7, 125.5, 121.8, 121.7, 119.2(2C), 119.1(3C), 118.9, 116.5, 116.4, 114.0, 113.8, 109.3, 109.2, 55.1(2C), 47.7, 47.5, 35.4, 35.1, 32.7(2C), 23.8, 23.5, 18.7, 18.5; LRMS (EI, 70 eV) *m/z* (%):318 (M^+, 10), 250 (100), 235 (9), 206 (19); HRMS *m/z* (ESI) calcd for $C_{21}H_{23}N_2O$ ($[M+H]^+$) 319.1805, found 319.1821.



4-(4-Methoxyphenyl)-3-methyl-4-(1-methyl-1*H*-indol-3-yl)butanenitrile (4raa- from cis **1r):**

d.r = 1.2

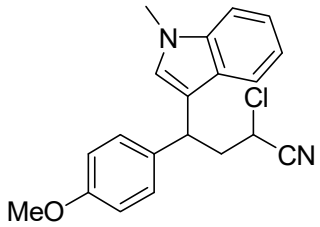
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.57 (t, *J* = 8.8 Hz, 1.06H), 7.26-7.22 (m, 3.08H), 7.19 (t, *J* = 7.2 Hz, 1.06H), 7.07 (t, *J* = 7.4 Hz, 1.08H), 6.95 (d, *J* = 4.4 Hz, 1.00H), 6.80 (d, *J* = 8.4 Hz, 2.00H), 3.99 (d, *J* = 10.4 Hz, 0.48H), 3.94 (d, *J* = 10.4 Hz, 0.58H), 3.73 (s, 4.54H), 3.72 (s, 1.62H), 2.73-2.65 (m, 1.05H), 2.49 (d, *J* = 16.8, 0.58H), 2.35 (d, *J* = 16.4, 0.51H), 2.24 (d, *J* = 16.4, 0.57H), 2.10 (dd, *J* = 16.4, 0.54H), 1.21 (d, *J* = 6.6 Hz, 1.34H), 1.09 (d, *J* = 6.6 Hz, 1.64H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 158.1, 158., 137.0, 136.9, 135.2, 135.1, 128.9, 128.7, 127.5, 127.00, 125.7, 125.5, 121.9, 121.7, 119.3, 119.2, 119.1(3C), 118.9, 116.5, 116.4, 114.1, 113.8, 109.3, 109.2, 55.1(2C), 47.7, 47.5, 35.4, 35.1, 32.7(2C), 23.8, 23.5, 18.7, 18.5; LRMS (EI, 70 eV) *m/z* (%): 318 (M^+, 9), 250 (100), 235 (8), 206 (16).



2-Ethyl-4-(4-methoxyphenyl)-4-(1-methyl-1*H*-indol-3-yl)butanenitrile (4aba):

d.r. = 1.1:1

Lihgt yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.48 (d, *J* = 8.0 Hz, 1H), 7.30-7.18 (m, 4H), 7.04 (t, *J* = 7.2 Hz, 1H), 6.84-6.79 (m, 3H), 4.44-4.34 (m, 1H), 3.79 (s, 1.47H), 3.76 (s, 3H), 3.74 (s, 1.56H), 2.47-2.31 (m, 2H), 1.65-1.58 (m, 4H), 1.04 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 158.3, 158.1, 137.5, 137.3, 136.1, 135.0, 128.8, 128.4, 126.9, 126.9, 126.5, 125.5, 122.2, 122.1, 121.8, 121.8, 119.6, 119.4, 119.0(2C), 118.1, 116.2, 114.1, 113.9, 109.4, 109.2, 55.2, 340.0, 39.8, 38.5, 38.2, 32.7, 32.7, 31.8, 31.6, 25.8, 25.4, 11.4(2C); LRMS (EI, 70 eV) *m/z* (%): 332 (M^+, 15), 250 (100), 206 (16); HRMS *m/z* (ESI) calcd for $C_{22}H_{25}N_2O$ ($[M+H]^+$) 333.1961, found 333.1975.

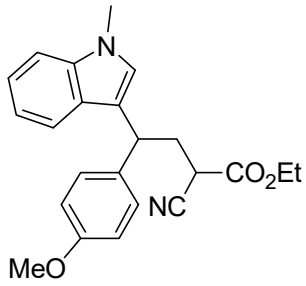


2-Chloro-4-(4-methoxyphenyl)-4-(1-methyl-1*H*-indol-3-yl)butanenitrile (4aca):

d.r. = 1:1

Lihgt yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.44 (t, *J* = 7.2 Hz, 1H), 7.30-7.19 (m, 4H), 7.05 (t, *J* = 7.6 Hz, 1H), 6.88-6.84 (m, 3H), 4.48 (t, *J* = 8.0 Hz, 1H), 4.23-4.16 (m, 1H), 3.77 (s, 3H), 3.75 (s, 3H), 2.95-2.83 (m, 1H), 2.74-2.64 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 158.6, 158.5, 137.3(2C), 134.0, 133.5, 128.7, 128.5, 126.6(2C), 126.1, 126.0, 122.05(2C), 119.3(2C), 119.2(2C), 117.3, 117.2, 115.7, 115.4, 114.3, 114.2, 109.4(2C), 55.2(2C), 42.6, 42.4, 41.2(2C), 38.8, 38.5, 32.8(2C);

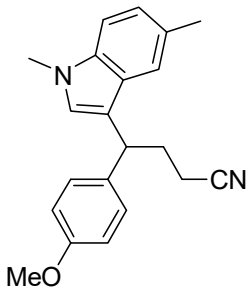
LRMS (EI, 70 eV) *m/z* (%): 340 (M^++2, 3), 338 (M^+, 10), 304 (5), 250 (100); HRMS *m/z* (ESI) calcd for $C_{20}H_{20}ClN_2O$ ($[M+H]^+$) 339.1259, found 339.1266.



Ethyl 2-cyano-4-(4-methoxyphenyl)-4-(1-methyl-1*H*-indol-3-yl)butanoate (4ada):

d.r. = 1.2:1

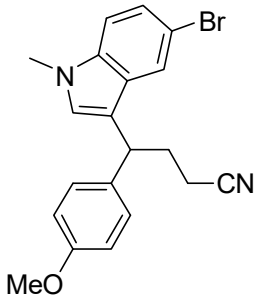
Light yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.50 (d, *J* = 8.0 Hz, 0.48H), 7.44 (d, *J* = 8.0 Hz, 0.56H), 7.29-7.18 (m, 4.21H), 7.06 (d, *J* = 6.8Hz, 0.59H), 7.06 (d, *J* = 7.2Hz, 0.49H) 6.94 (s, 0.48H), 6.87-6.81(m, 2.68H), 4.46-4.39 (m, 1.00H), 4.22-4.16 (m, 2.03H), 3.78, 3.76 (s, 3.05H), 3.75,3.74 (s, 2.97H), 3.47-3.43 (m, 0.47H), 3.35-3.31 (m, 0.60H), 2.90-2.83 (m, 0.48H), 2.75-2.68 (m, 0.55H), 2.66-2.50 (m, 1.02H), 1.29 (d, *J* = 6.4 Hz, 1.48H), 1.26 (d, *J* = 6.8 Hz, 1.63H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 166.2(2C), 158.5, 158.3, 137.4, 137.2, 134.9, 133.8, 128.8, 128.6, 126.8, 126.7, 126.4, 125.8, 121.9(2C), 121.9, 119.5, 119.3, 119.2, 119.1, 116.9, 116.7, 116.5, 115.4, 114.3, 114.0, 109.4, 109.2, 62.8(2C), 55.2(2C), 39.5, 39.5, 36.3, 36.1, 36.0, 35.8, 32.8, 32.7, 13.9(2C); LRMS (EI, 70 eV) m/z (%): 376 (M^+, 17), 250 (100), 206 (16); HRMS *m/z* (ESI) calcd for $C_{23}H_{25}N_2O_3$ ($[M+H]^+$) 377.1860, found 377.1875.



4-(1,5-Dimethyl-1*H*-indol-3-yl)-4-(4-methoxyphenyl)butanenitrile (4aab):

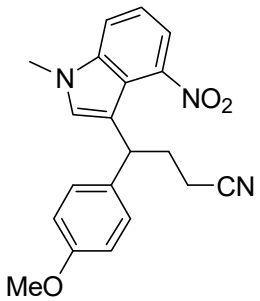
Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.23-7.21 (m, 3H), 7.15 (d, *J* = 8.4 Hz, 1H), 7.01 (d, *J* = 8.4 Hz, 1H), 6.83 (d, *J* = 8.0 Hz, 2H), 6.79 (s, 1H), 4.21 (t, *J* = 7.6 Hz, 1H), 3.76 (s, 3H), 3.69 (s, 3H), 2.54-

2.43 (m, 1H), 2.39 (s, 3H), 2.29-2.22 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 158.2, 135.7, 135.1, 128.6, 128.2, 127.0, 126.0, 123.4, 119.8, 118.9, 116.2, 114.0, 109.0, 55.2, 40.9, 32.7, 31.6, 21.5, 15.8; LRMS (EI, 70 eV) *m/z* (%): 318 (M^+, 17), 264 (100), 249 (8), 206 (14); HRMS *m/z* (ESI) calcd for $C_{21}H_{23}N_2O$ ($[M+H]^+$) 319.1805, found 319.1817.



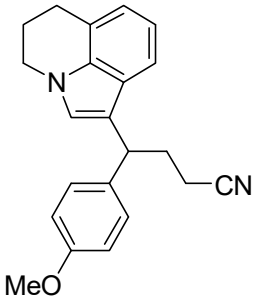
4-(5-Bromo-1-methyl-1*H*-indol-3-yl)-4-(4-methoxyphenyl)butanenitrile (4aac):

Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.52 (s, 1H), 7.25 (d, *J* = 7.2 Hz, 1H), 7.18 (d, *J* = 8.8 Hz, 2H), 7.11 (d, *J* = 8.4 Hz, 1H), 6.68-6.82 (m, 3H), 4.16 (t, *J* = 7.6 Hz, 1H), 3.76 (s, 3H), 3.71 (s, 3H), 2.48-2.42 (m, 1H), 2.28-2.23 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 158.3, 135.9, 134.4, 128.5, 128.4, 127.0, 124.6, 121.7, 119.5, 116.5, 114.1, 112.4, 110.8, 55.2, 40.7, 32.9, 31.4, 15.7; LRMS (EI, 70 eV) *m/z* (%): 384 (M^++2, 17), 382 (M^+, 16), 328 (100), 206 (16); HRMS *m/z* (ESI) calcd for $C_{20}H_{20}BrN_2O$ ($[M+H]^+$) 383.0754, found 383.0762.



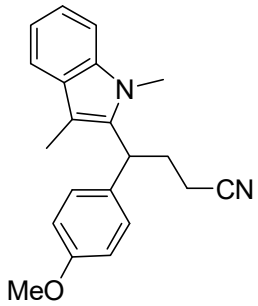
4-(4-Methoxyphenyl)-4-(1-methyl-4-nitro-1*H*-indol-3-yl)butanenitrile (4aad)：

Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.35 (d, *J* = 2.0 Hz, 1H), 8.09 (d, *J* = 9.0, 2.0 Hz, 1H), 7.29-7.21 (m, 3H), 7.06 (s, 1H), 6.86 (d, *J* = 8.5 Hz, 2H), 4.27 (t, *J* = 7.0 Hz, 1H), 3.83 (s, 3H), 3.78 (s, 3H), 2.55-2.50 (m, 1H), 2.36-2.30 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 158.6, 141.2, 140.0, 133.8, 128.7, 128.5, 126.1, 120.2, 119.3, 117.6, 116.7, 114.3, 109.3, 55.21, 40.7, 33.2, 31.3, 15.7; (EI, 70 eV) *m/z* (%): 349 (M^+, 15), 295 (100), 249 (30); HRMS *m/z* (ESI) calcd for $C_{20}H_{20}N_3O_3$ ($[M+H]^+$) 350.1499, found 350.1511.



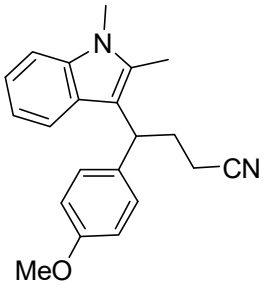
4-(5,6-Dihydro-4*H*-pyrrolo[3,2,1-*ij*]quinolin-1-yl)-4-(4-methoxyphenyl)butanenitrile (4aae):

Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.24-7.22 (m, 3H), 6.93 (t, *J* = 7.6 Hz, 1H), 6.87 (d, *J* = 5.6 Hz, 2H), 6.82 (d, *J* = 8.4 Hz, 2H), 4.23 (t, *J* = 7.6 Hz, 1H), 4.20-4.06 (m, 2H), 3.75 (s, 3H), 2.94 (t, *J* = 6.0 Hz, 2H), 2.56-2.46 (m, 1H), 2.34-2.26 (m, 3H), 2.22-2.16 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 158.1, 135.3, 134.7, 128.6, 124.3, 123.3, 121.8, 119.8, 119.3, 118.6, 116.9, 116.8, 113.9, 55.2, 43.9, 41.3, 31.5, 24.6, 22.7, 15.8; LRMS (EI, 70 eV) *m/z* (%): 330 (M^+, 17), 276 (100), 232 (11), 204 (10); HRMS *m/z* (ESI) calcd for $C_{22}H_{23}N_2O$ ($[M+H]^+$) 331.1805, found 331.1813.



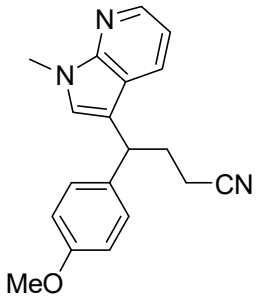
4-(1,3-Dimethyl-1*H*-indol-2-yl)-4-(4-methoxyphenyl)butanenitrile (4aaf):

Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.56 (d, *J* = 7.6 Hz, 1H), 7.24-7.18 (m, 2H), 7.14-7.09 (m, 3H), 6.82 (d, *J* = 8.0 Hz, 2H), 4.53-4.49 (m, 1H), 3.76 (s, 3H), 3.45 (s, 3H), 2.64-2.57 (m, 1H), 2.50-2.20 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 158.3, 137.0, 134.6, 132.7, 128.3, 128.2, 122.4, 121.5, 119.4, 118.9, 118.3, 114.0, 108.8, 55.2, 39.5, 30.4, 29.1, 15.7, 9.5; LRMS (EI, 70 eV) *m/z* (%): 318 (M^+, 45), 264 (100), 249 (7), 218 (9); HRMS *m/z* (ESI) calcd for $C_{21}H_{23}N_2O$ ($[M+H]^+$) 319.1805, found 319.1809.



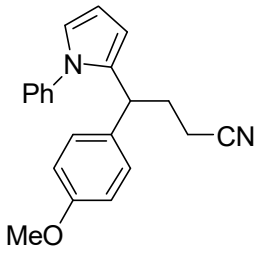
4-(1,2-Dimethyl-1*H*-indol-3-yl)-4-(4-methoxyphenyl)butanenitrile (4aag):

Yellow solid, mp 163.2-164.7 (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.43 (d, *J* = 8.0 Hz, 1H), 7.26-7.22 (m, 3H), 7.13 (t, *J* = 7.6 Hz, 1H), 6.99 (t, *J* = 7.6 Hz, 1H), 6.78 (d, *J* = 8.0 Hz, 2H), 4.33 (t, *J* = 8.0 Hz, , 1H), 3.73 (s, 3H), 3.64 (s, 3H), 2.58-2.54 (m, 2H), 2.40 (s, 3H), 2.33-2.26 (m, 1H), 2.18-2.10 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 145.8, 142.8, 137.7, 136.2, 134.5, 129.4, 129.1, 128.9, 128.1, 128.0, 126.4, 126.2, 125.6, 121.9, 121.7, 120.3, 118.9, 118.7, 109.4, 51.2, 35.5, 32.8, 20.1, 19.2, 14.3; LRMS (EI, 70 eV) *m/z* (%):318 (M^+, 39), 264 (100), 218 (10); HRMS *m/z* (ESI) calcd for $C_{21}H_{23}N_2O$ ($[M+H]^+$) 319.1805, found 319.1814.



4-(4-Methoxyphenyl)-4-(1-methyl-1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)butanenitrile (4aah):

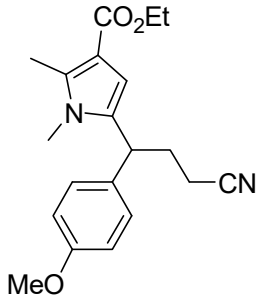
Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.29 (d, *J* = 4.8 Hz, 1H), 7.65 (d, *J* = 7.6 Hz, 1H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.01 (s, 1H), 6.97-6.94 (m, 1H), 6.85 (d, *J* = 8.4 Hz, 2H), 4.24 (t, *J* = 7.6 Hz, 1H), 3.86 (s, 3H), 3.78 (s, 3H), 2.56-2.45 (m, 1H), 2.35-2.27 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 158.4, 148.1, 143.1, 134.4, 128.6, 127.6, 125.7, 119.5, 119.2, 115.5, 115.1, 114.1, 55.2, 40.9, 31.2, 31.1, 15.7; LRMS (EI, 70 eV) *m/z* (%): 305 (M^+, 15), 251 (100), 236 (9), 207 (14); HRMS *m/z* (ESI) calcd for $C_{19}H_{20}N_3O$ ($[M+H]^+$) 306.1601, found 306.1615.



4-(4-Methoxyphenyl)-4-(1-phenyl-1*H*-pyrrol-2-yl)butanenitrile (4aai):

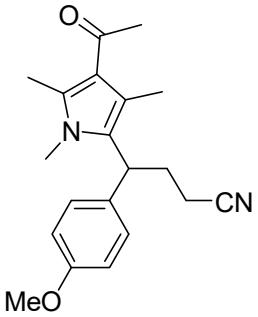
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.31-7.30 (m, 3H), 7.00-6.99 (m, 2H), 6.81 (d, *J* = 8.4 Hz, 2H), 6.70 (d, *J* = 8.8 Hz,

3H), 6.27-6.24 (m, 2H), 3.88 (t, *J* = 7.6 Hz, 1H), 3.75 (s, 3H), 2.36-2.07 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 158.2, 139.7, 134.4, 134.1, 128.9, 128.6, 127.6, 127.0, 122.7, 119.4, 113.8, 107.8, 106.1, 55.2, 41.1, 32.1, 15.6; LRMS (EI, 70 eV) *m/z* (%): 316 (M^+, 20), 262 (100), 154 (21); HRMS *m/z* (ESI) calcd for $C_{21}H_{21}N_2O$ ($[M+H]^+$) 317.1648, found 317.1655.



Ethyl 5-(3-cyano-1-(4-methoxyphenyl)propyl)-1,2-dimethyl-1*H*-pyrrole-3-carboxylate (4aaj):

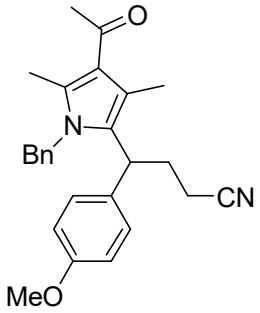
Light yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.06 (d, *J* = 8.4 Hz, 2H), 6.83 (d, *J* = 8.4 Hz, 2H), 6.48 (s, 1H), 4.28 (q, *J* = 7.2 Hz, 2H), 3.94 (t, *J* = 7.2 Hz, 1H), 3.78 (s, 3H), 3.19 (s, 3H), 2.46 (s, 3H), 2.44-2.25 (m, 3H), 2.17-2.08 (m, 1H), 1.36 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 165.6, 158.7, 136.5, 133.0, 132.7, 128.8, 119.4, 114.4, 110.8, 106.4, 59.3, 55.3, 41.2, 31.5, 30.4, 15.6, 14.6, 11.3; LRMS (EI, 70 eV) m/z (%): 376 (M^+, 17), 250 (100), 206 (16); HRMS *m/z* (ESI) calcd for $C_{20}H_{25}N_2O_3$ ($[M+H]^+$) 341.1860, found 341.1871.



4-(4-Acetyl-1,3,5-trimethyl-1*H*-pyrrol-2-yl)-4-(4-methoxyphenyl)butanenitri le (4aak):

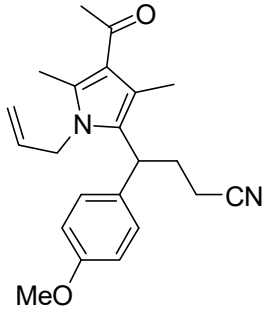
Brown oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.07 (d, J = 8.5 Hz, 2H), 6.85 (d, J = 8.5 Hz, 2H), 4.37-4.34 (m, 1H), 3.79 (s, 3H), 3.17 (s, 3H), 2.62-2.58 (m, 1H), 2.46-2.26 (m, 12H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 196.0, 158.3, 135.7, 132.9, 128.0, 127.5, 121.8, 119.4, 117.3, 114.1, 55.3, 38.4, 31.5, 31.2, 28.7, 15.7, 12.6, 12.4; LRMS (EI, 70 eV) *m/z*

(%): 324 (M^+, 27), 270 (100), 240 (5), 212 (11); HRMS *m/z* (ESI) calcd for $C_{20}H_{25}N_2O_2$ ($[M+H]^+$) 325.1911, found 325.1923.



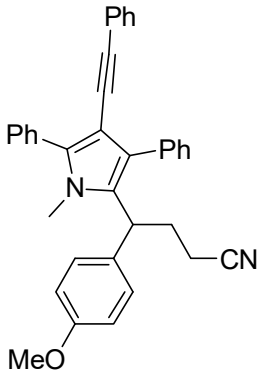
4-(4-Acetyl-1-benzyl-3,5-dimethyl-1*H*-pyrrol-2-yl)-4-(4-methoxyphenyl)butanenitrile (4aal):

Light yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.29-7.21 (m, 3H), 6.97 (d, *J* = 8.4 Hz, 2H), 6.79-6.74 (m, 4H), 4.85 (s, 2H), 4.24-4.22 (m, 1H), 3.76 (s, 3H), 2.50 (s, 3H), 2.38 (s, 3H), 2.34-2.27 (m, 4H), 2.18-2.02 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 196.1, 158.2, 136.8, 135.7, 132.7, 128.9, 128.0, 127.8, 127.5, 125.0, 122.3, 119.3, 117.9, 114.0, 55.2, 46.8, 38.7, 31.6, 28.9, 15.4, 12.6, 12.3; HRMS *m/z* (ESI) calcd for $C_{26}H_{29}N_2O_2$ ($[M+H]^+$) 401.2224, found 401.2236.



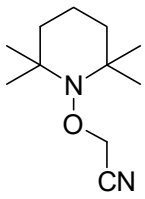
4-(4-Acetyl-1-allyl-3,5-dimethyl-1*H*-pyrrol-2-yl)-4-(4-methoxyphenyl)butanenitrile (4aam):

Light yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.05 (d, *J* = 8.4 Hz, 2H), 6.84 (d, *J* = 8.4 Hz, 2H), 5.72-5.64 (m, 1H), 5.11 (d, *J* = 10.4 Hz, 1H), 4.67 (d, *J* = 17.2 Hz, 1H), 4.28-4.15 (m, 3H), 3.79 (s, 3H), 2.53-2.44 (m, 4H), 2.37 (s, 3H), 2.35-2.22 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 196.1, 158.2, 135.7, 132.9, 132.9, 128.1, 127.3, 122.1, 119.5, 117.5, 116.1, 114.0, 55.2, 45.8, 38.6, 31.5, 29.0, 15.6, 12.6, 12.1; LRMS (EI, 70 eV) *m/z* (%): 350 (M^+, 43), 296 (100), 254 (21), 212 (14); HRMS *m/z* (ESI) calcd for $C_{22}H_{27}N_2O_2$ ($[M+H]^+$) 351.2067, found 351.2074.



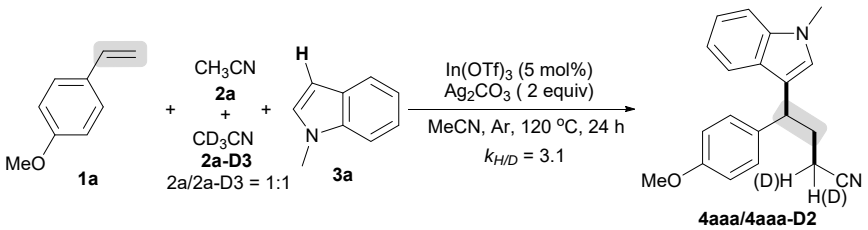
4-(4-Methoxyphenyl)-4-(1-methyl-3,5-diphenyl-4-(phenylethynyl)-1*H*-pyrrol-2-yl)butanenitrile (4aan):

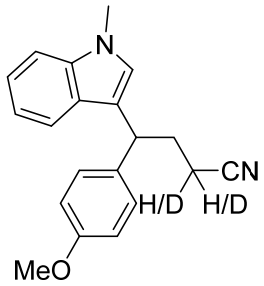
Light yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.57 (d, *J* = 7.6 Hz, 2H), 7.49-7.45 (m, 4H), 7.39-7.29 (m, 4H), 7.25-7.13 (m, 7H), 6.91 (d, *J* = 8.4 Hz, 2H), 4.47-4.43 (m, 1H), 3.81 (s, 3H), 3.32 (s, 3H), 2.37-2.30 (m, 1H), 2.26-2.10 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 158.4, 138.0, 135.1, 133.3, 131.2, 130.8, 130.3, 130.2, 128.3, 128.2, 128.2, 128.0(2C), 127.7, 126.9, 126.9, 126.6, 124.5, 119.3, 114.2, 103.9, 90.5, 85.4, 55.3, 40.0, 33.1, 28.5, 15.6; HRMS *m/z* (ESI) calcd for $C_{36}H_{31}N_2O$ ($[M+H]^+$) 507.2431, found 507.2446.



2-(2,2,6,6-Tetramethylpiperidin-1-yloxy)acetonitrile (5):

Light yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 4.52 (s, 2H), 1.58-1.31 (m, 6H), 1.20 (s, 6H), 1.10 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 116.0, 62.6, 60.3, 39.5, 32.9, 19.8, 16.8; LRMS (EI, 70 eV) *m/z* (%):196 (M^+, 2), 181 (70), 156 (100), 69 (92).



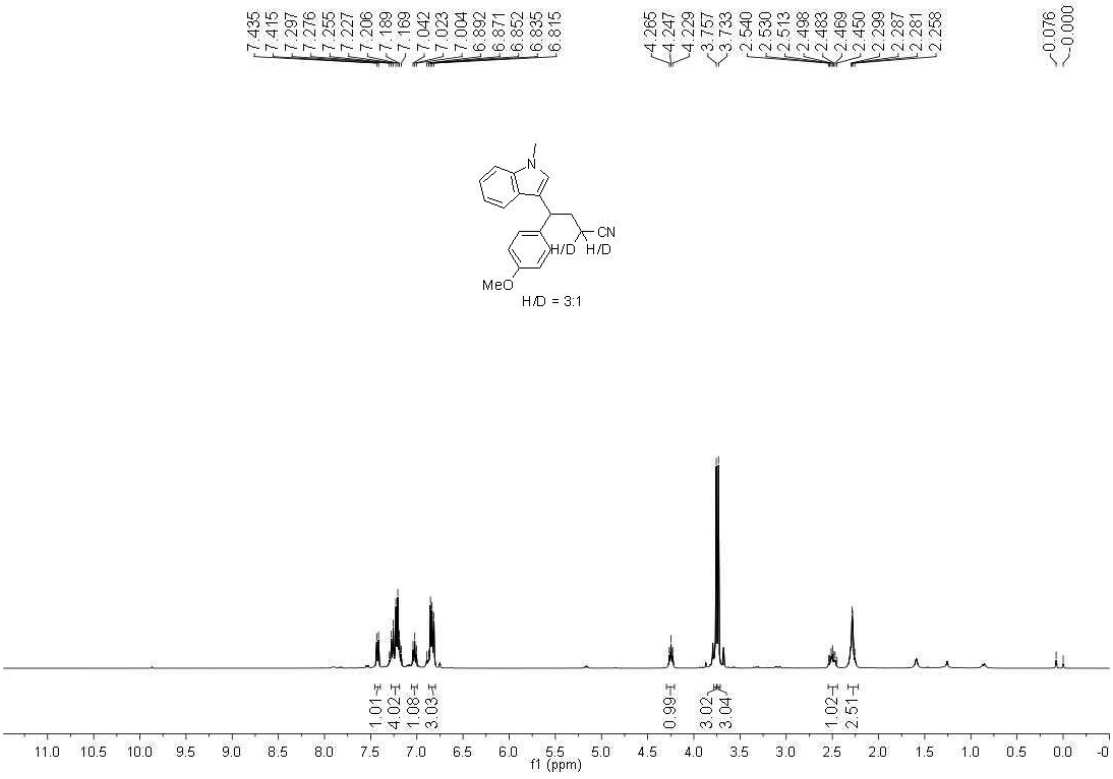


4-(4-Methoxyphenyl)-4-(1-methyl-1*H*-indol-3-yl)butanenitrile (4aaa+4aaa-2D):

H/D = 3:1

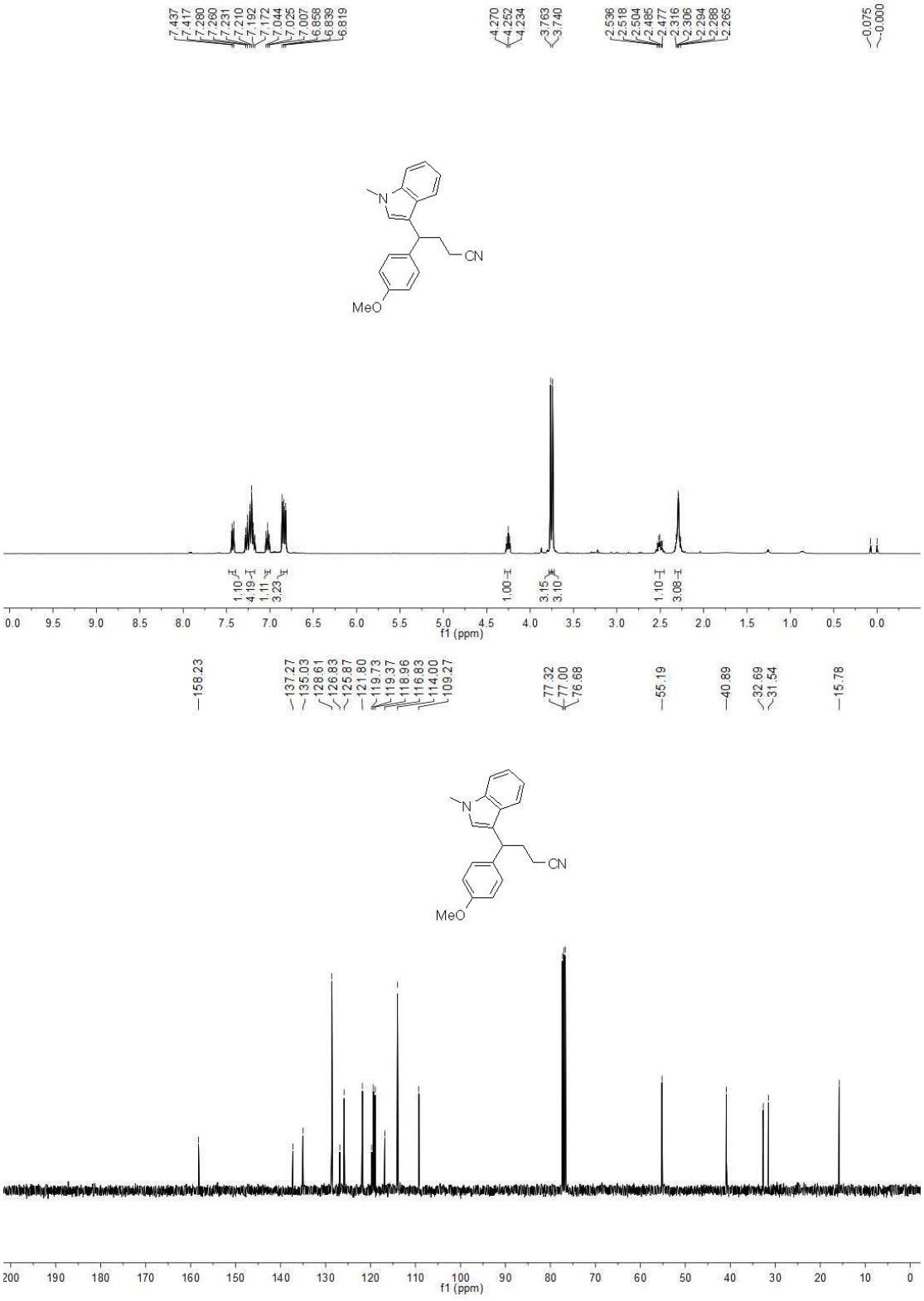
Light yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.42 (d, *J* = 8.0 Hz, 1H), 7.30-7.17 (m, 4H), 7.02 (t, *J* = 7.6 Hz, 1H), 6.89-6.82 (m, 3H), 4.25 (t, *J* = 7.2 Hz, 1H), 3.76 (s, 3H), 3.73 (s, 3H), 2.54-2.45 (m, 1H), 2.30-2.26 (m, 2.51H); LRMS (EI, 70 eV) *m/z* (%): 306 (M^++2, 5), 305 (M^++1, 4), 304 (M^+, 14), 250 (100), 206 (21).

4-(4-Methoxyphenyl)-4-(1-methyl-1*H*-indol-3-yl)butanenitrile-(4aaa+4aaa-2D)

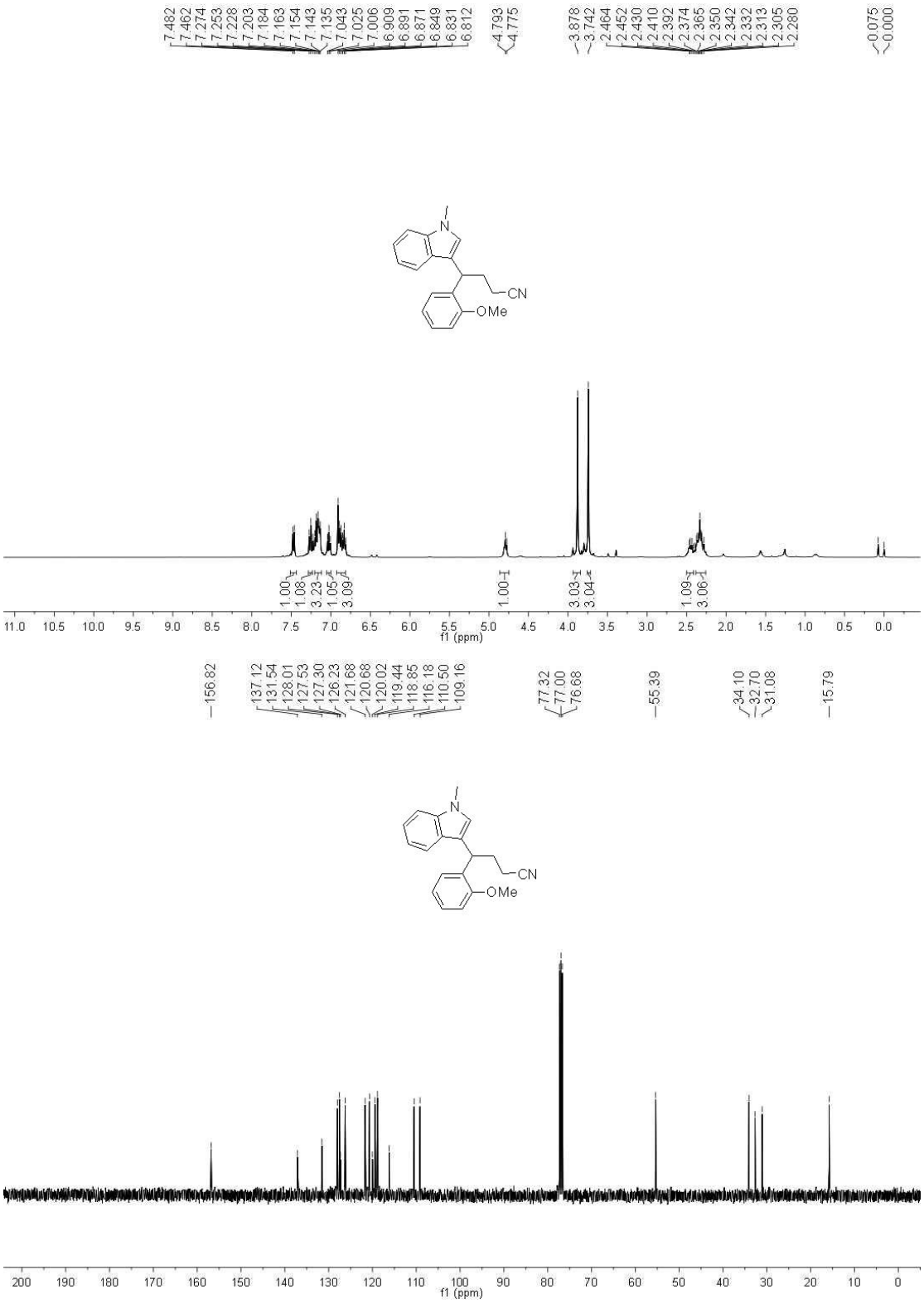


(D) Spectra

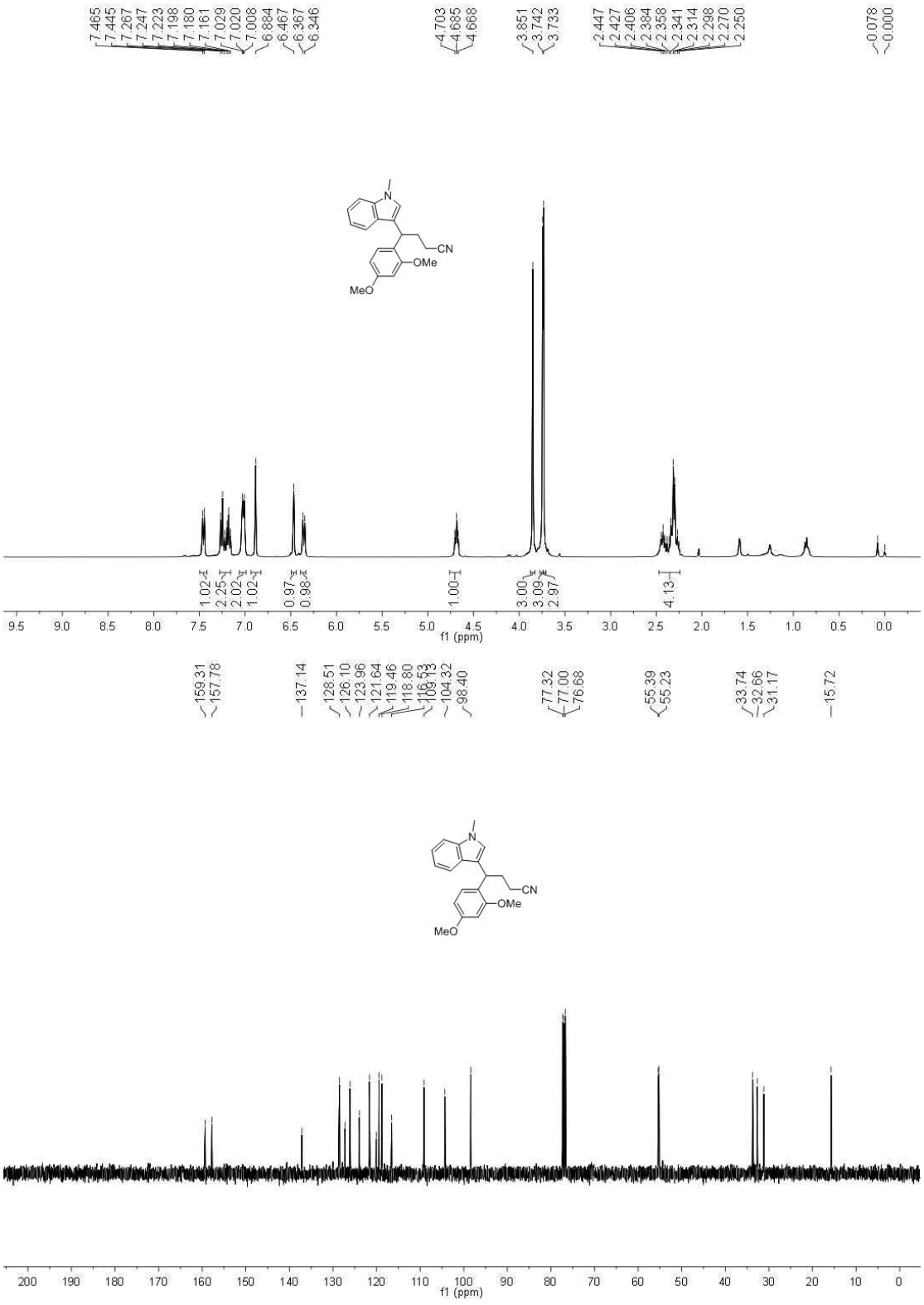
4-(4-Methoxyphenyl)-4-(1-methyl-1*H*-indol-3-yl)butanenitrile (4aaa)



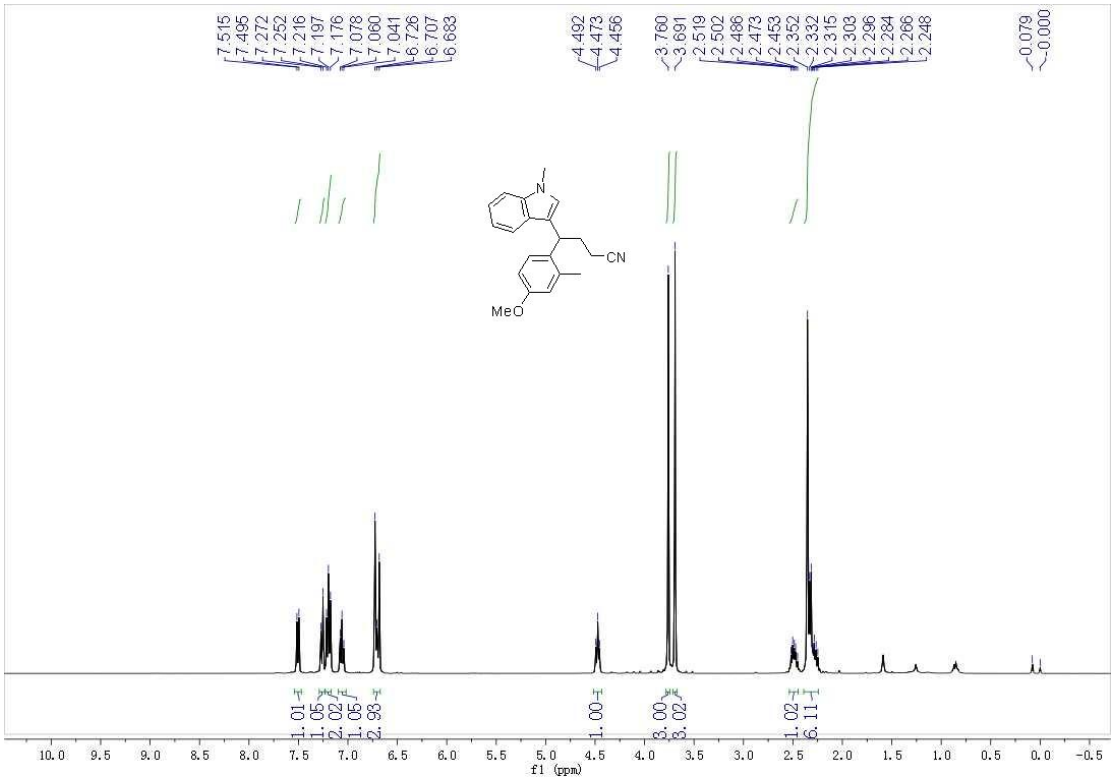
4-(2-Methoxyphenyl)-4-(1-methyl-1*H*-indol-3-yl)butanenitrile (4baa)

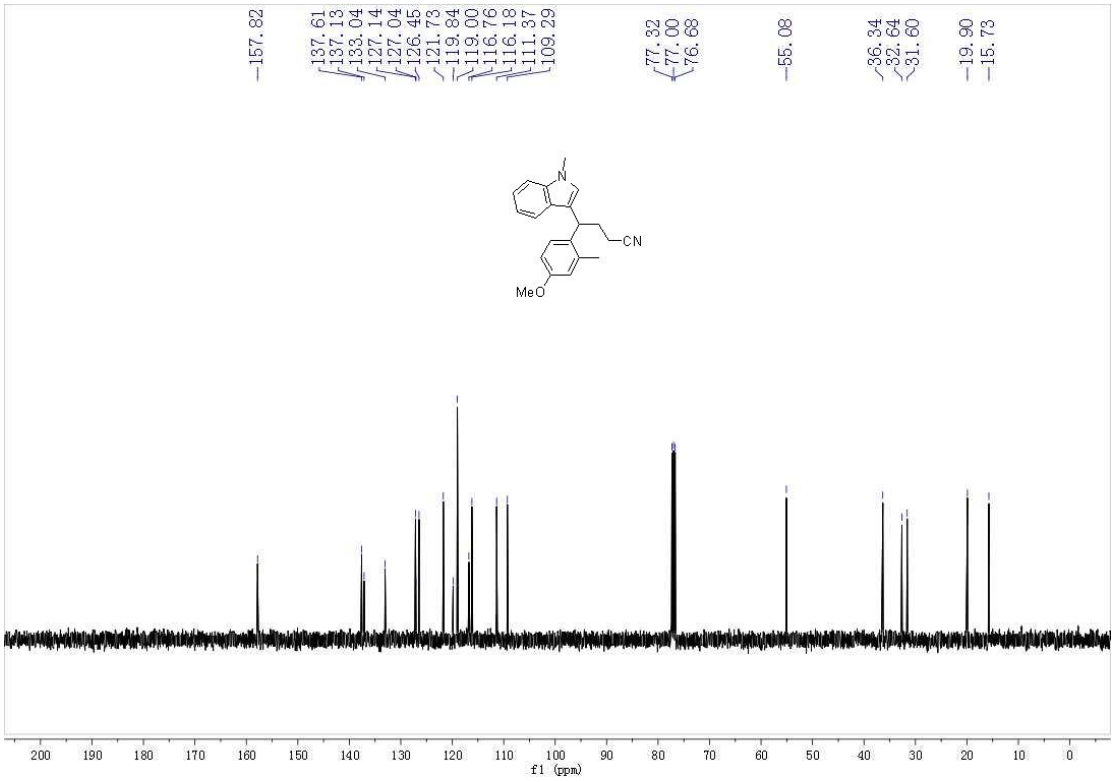


4-(2,4-Dimethoxyphenyl)-4-(1-methyl-1*H*-indol-3-yl)butanenitrile (4caa)

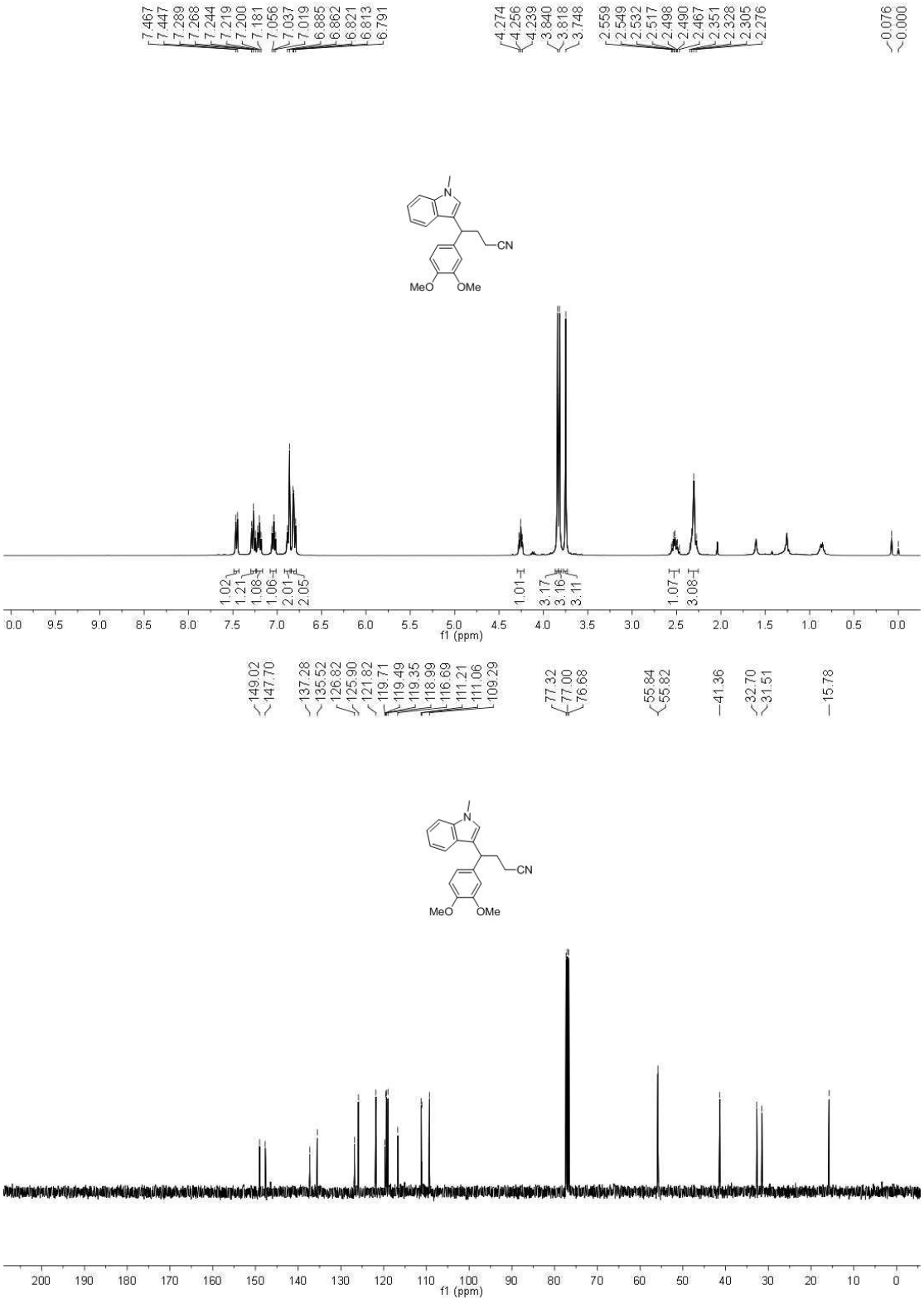


4-(4-Methoxy-2-methylphenyl)-4-(1-methyl-1*H*-indol-3-yl)butanenitrile (4daa)

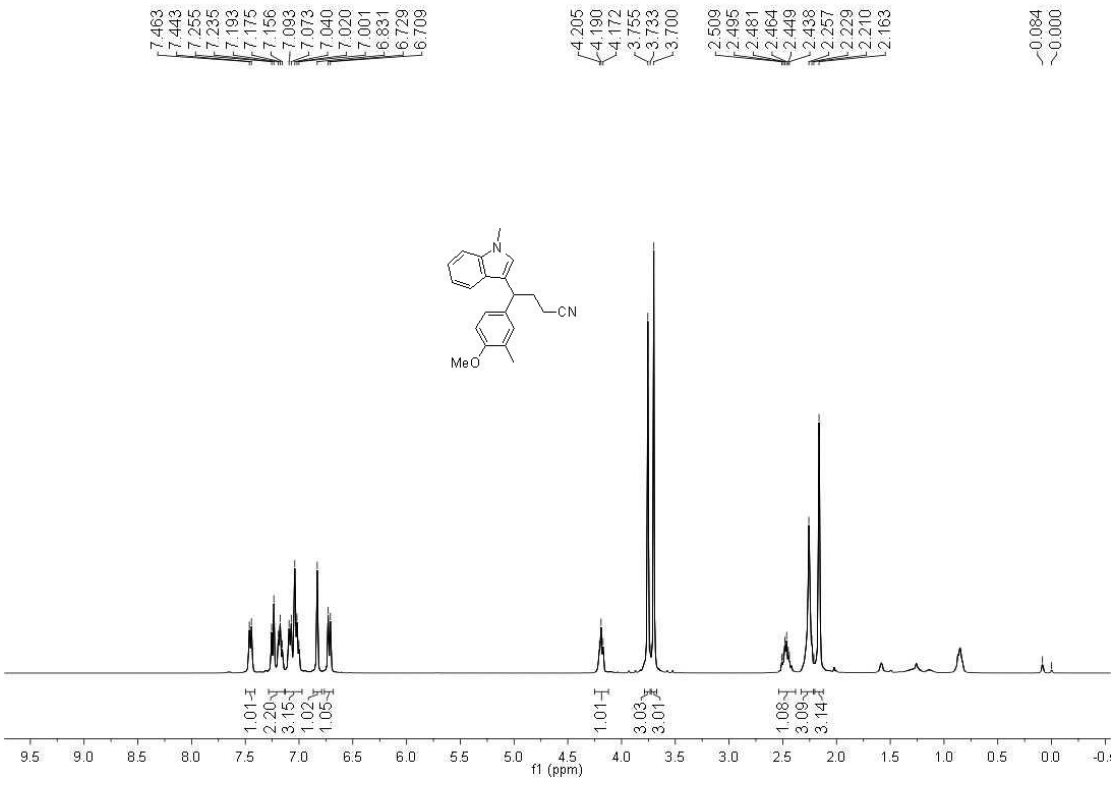


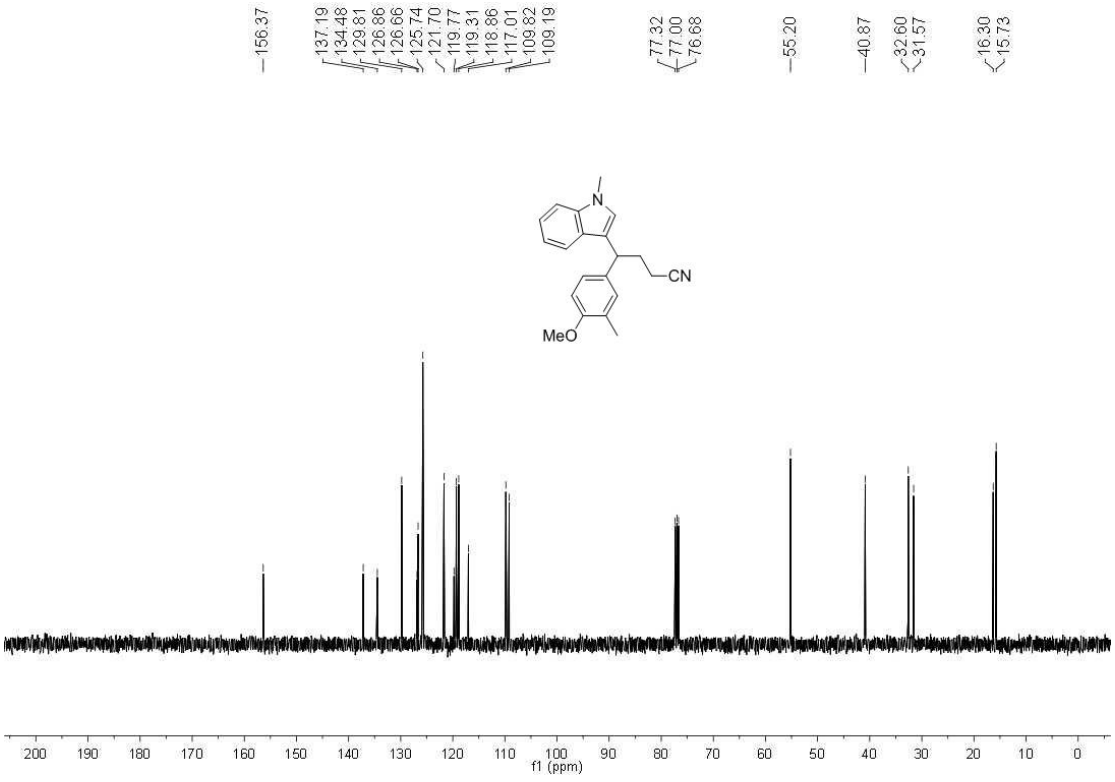


4-(3,4-Dimethoxyphenyl)-4-(1-methyl-1*H*-indol-3-yl)butanenitrile (4eaa)

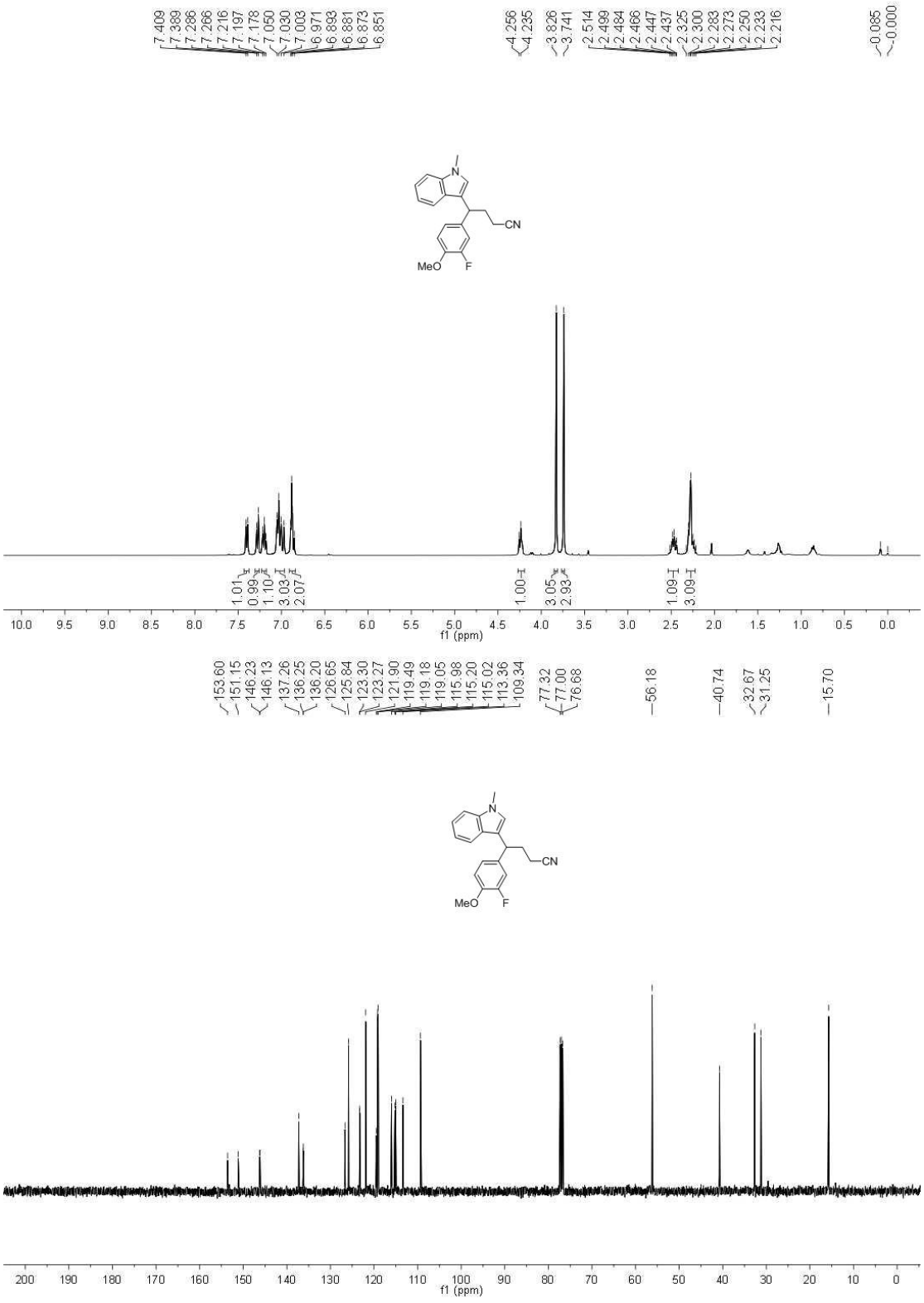


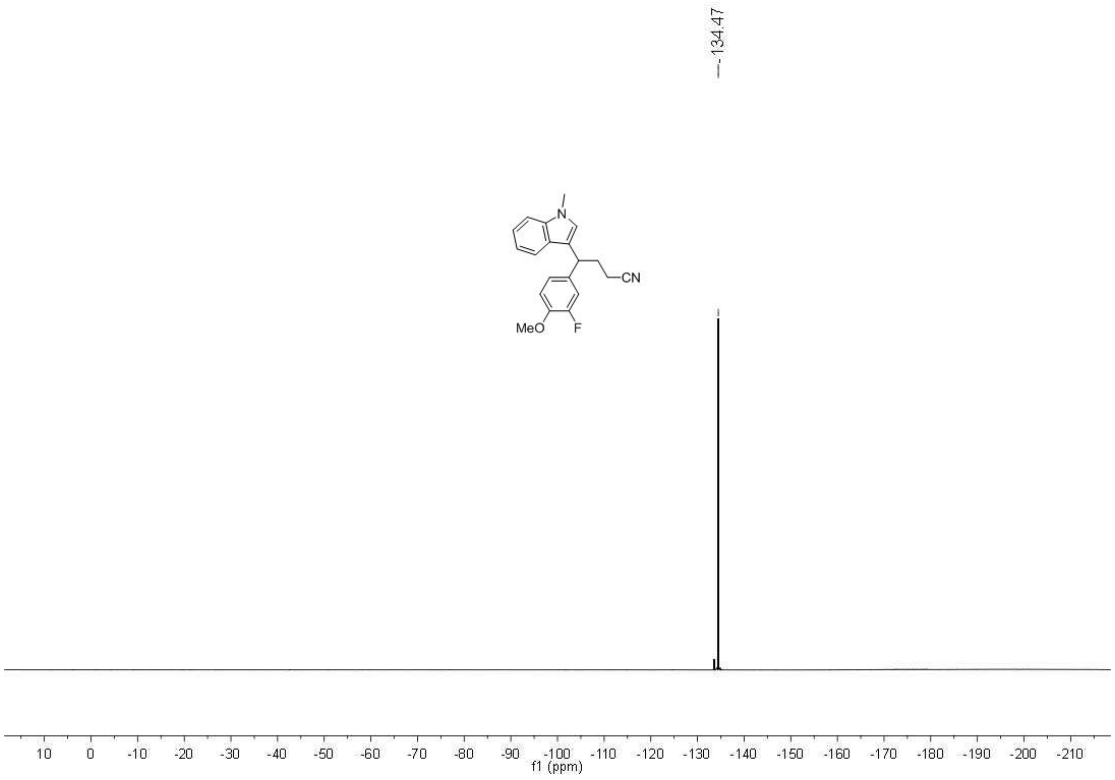
4-(4-Methoxy-3-methylphenyl)-4-(1-methyl-1*H*-indol-3-yl)butanenitrile (4faa)



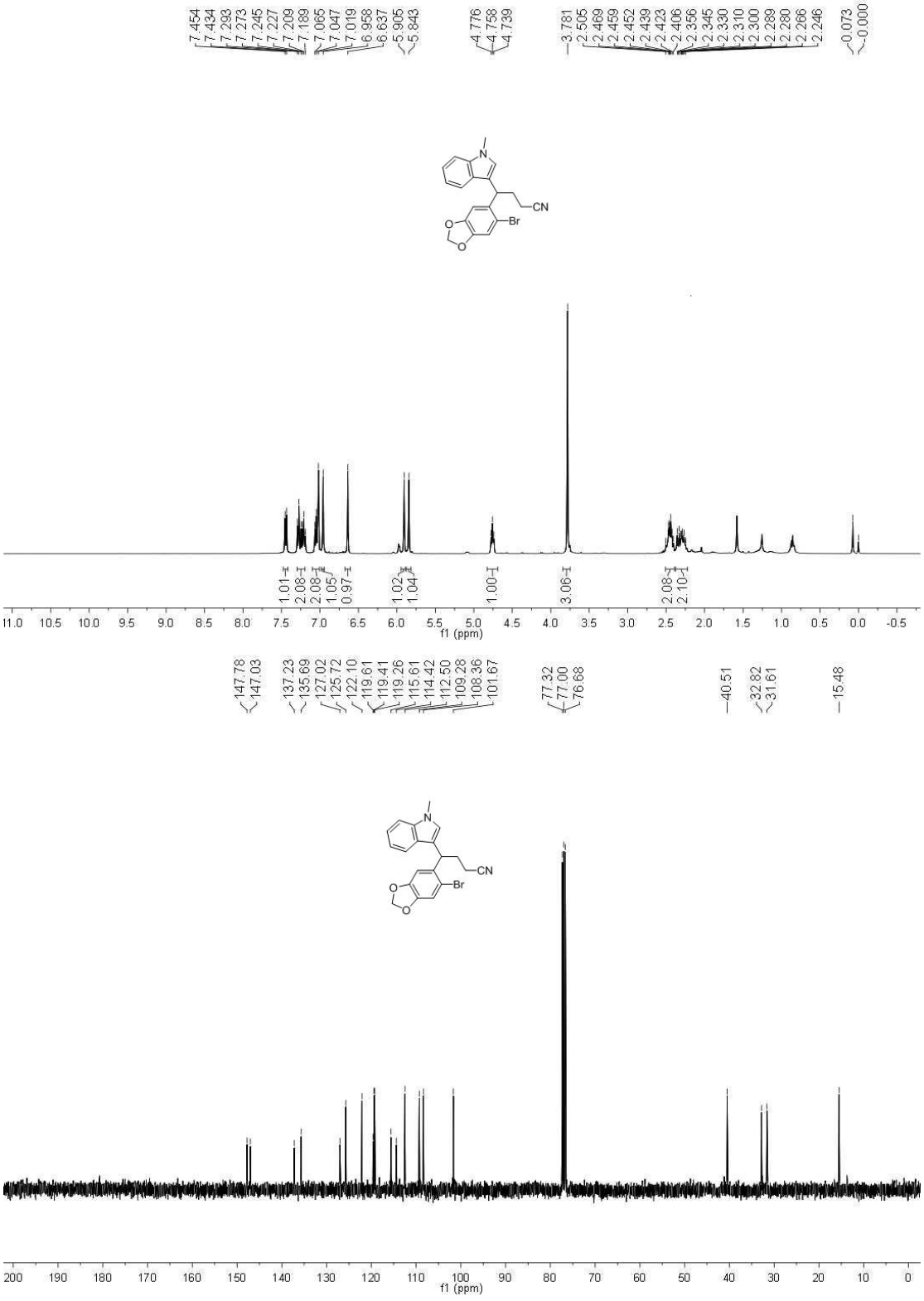


4-(3-Fluoro-4-methoxyphenyl)-4-(1-methyl-1*H*-indol-3-yl)butanenitrile (4gaa)

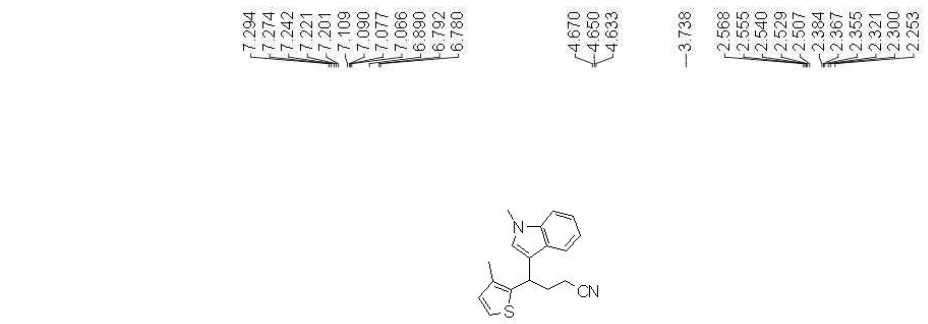


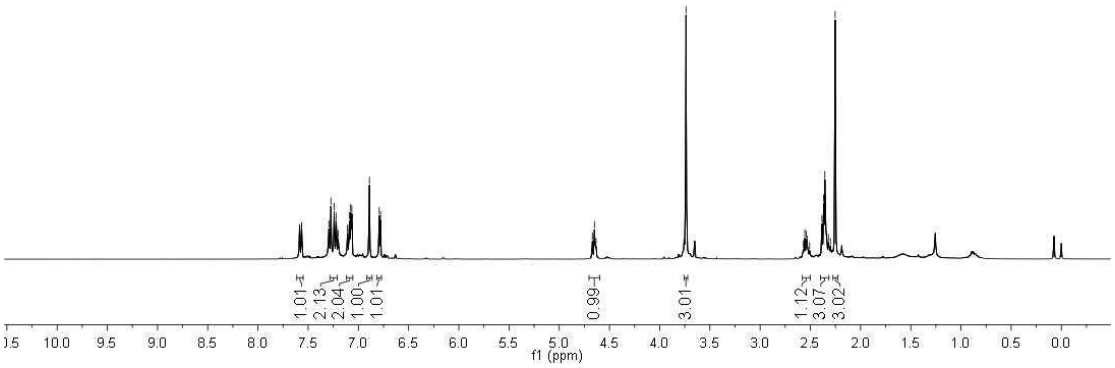

-134.47
N
CN
MeO
F
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

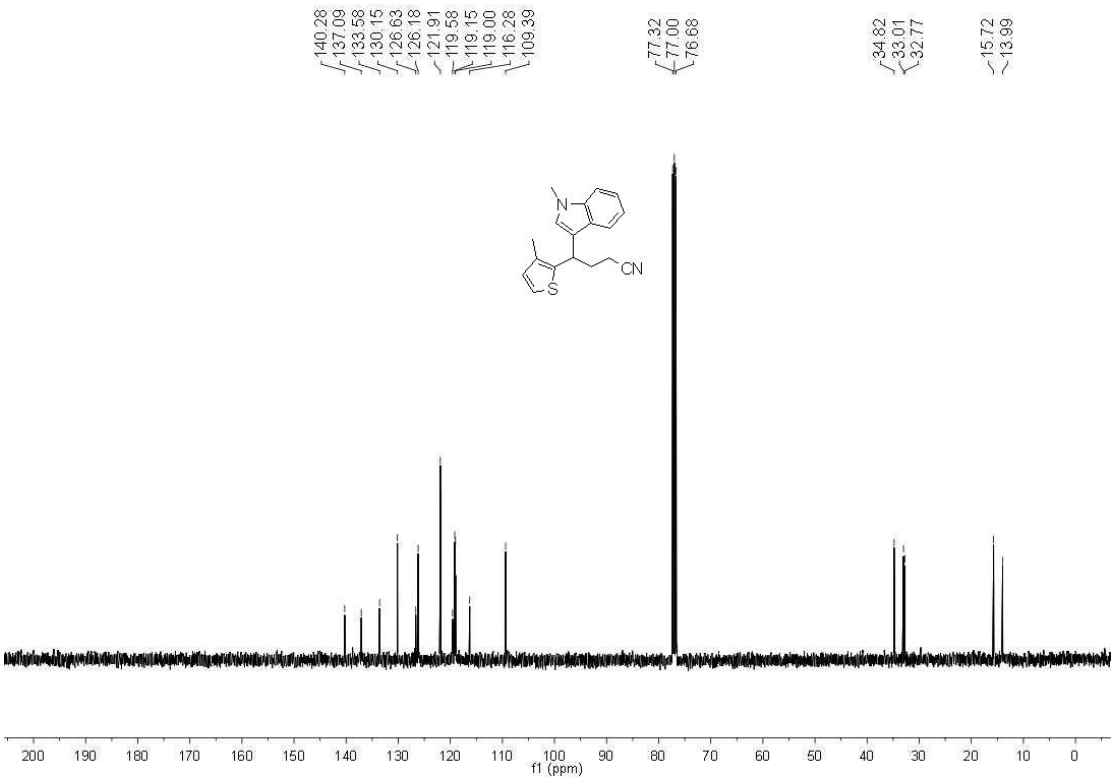
4-(6-Bromobenzo[*d*][1,3]dioxol-5-yl)-4-(1-methyl-1*H*-indol-3-yl)butanenitrile (4haa)



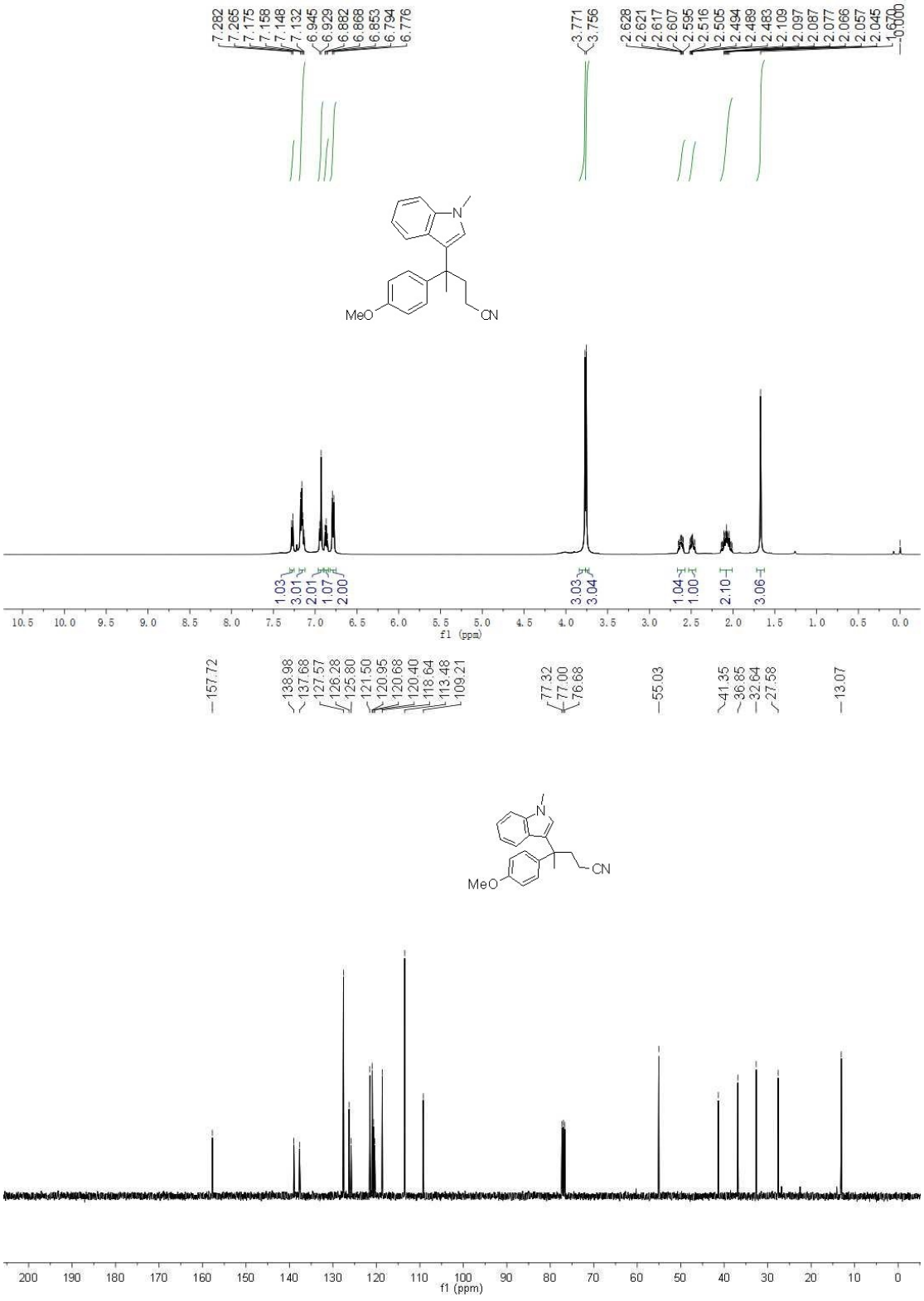
4-(1-Methyl-1*H*-indol-3-yl)-4-(3-methylthiophen-2-yl)butanenitrile (4iaa)



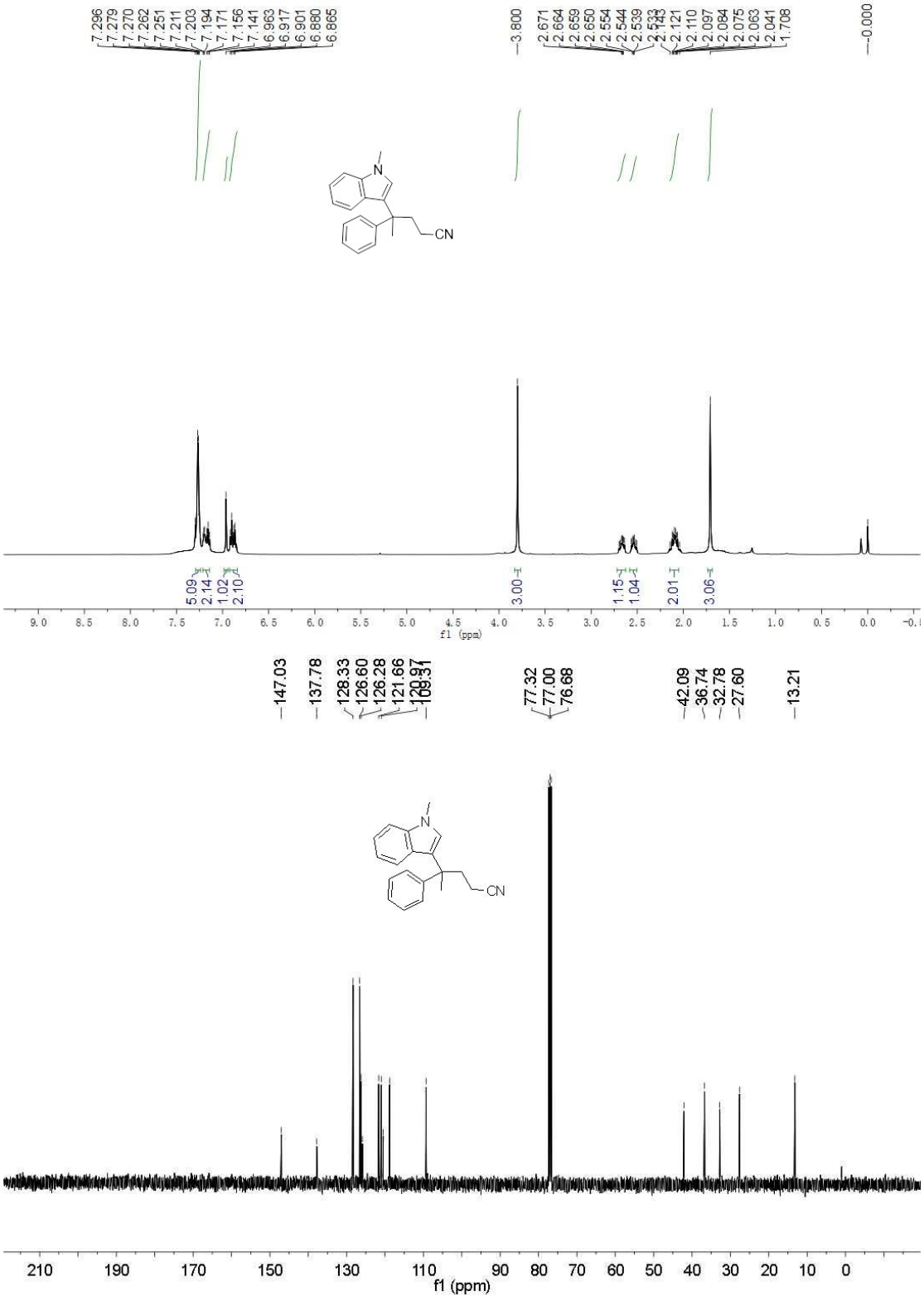




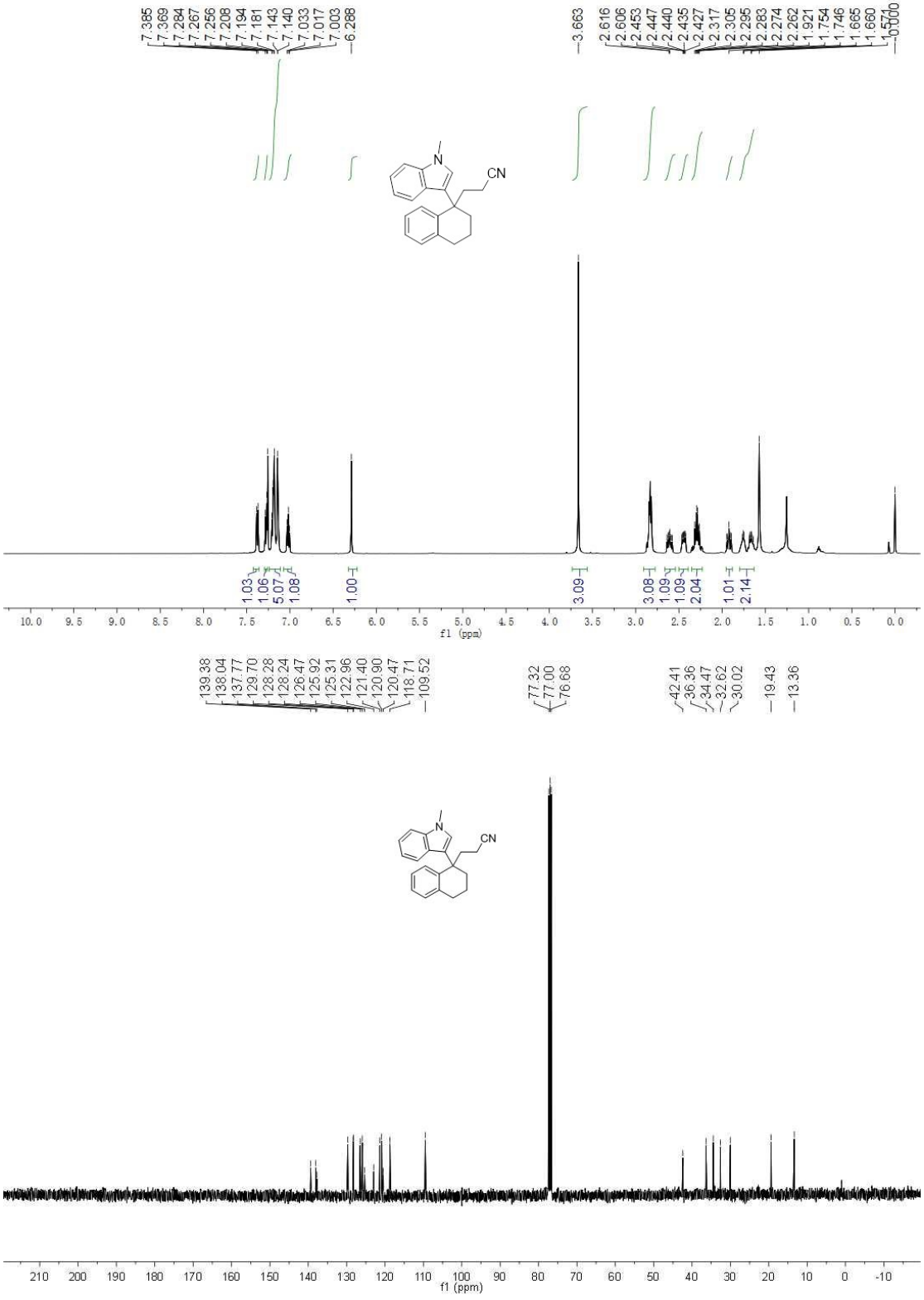
4-(4-Methoxyphenyl)-4-(1-methyl-1*H*-indol-3-yl)pentanenitrile (4kaa)



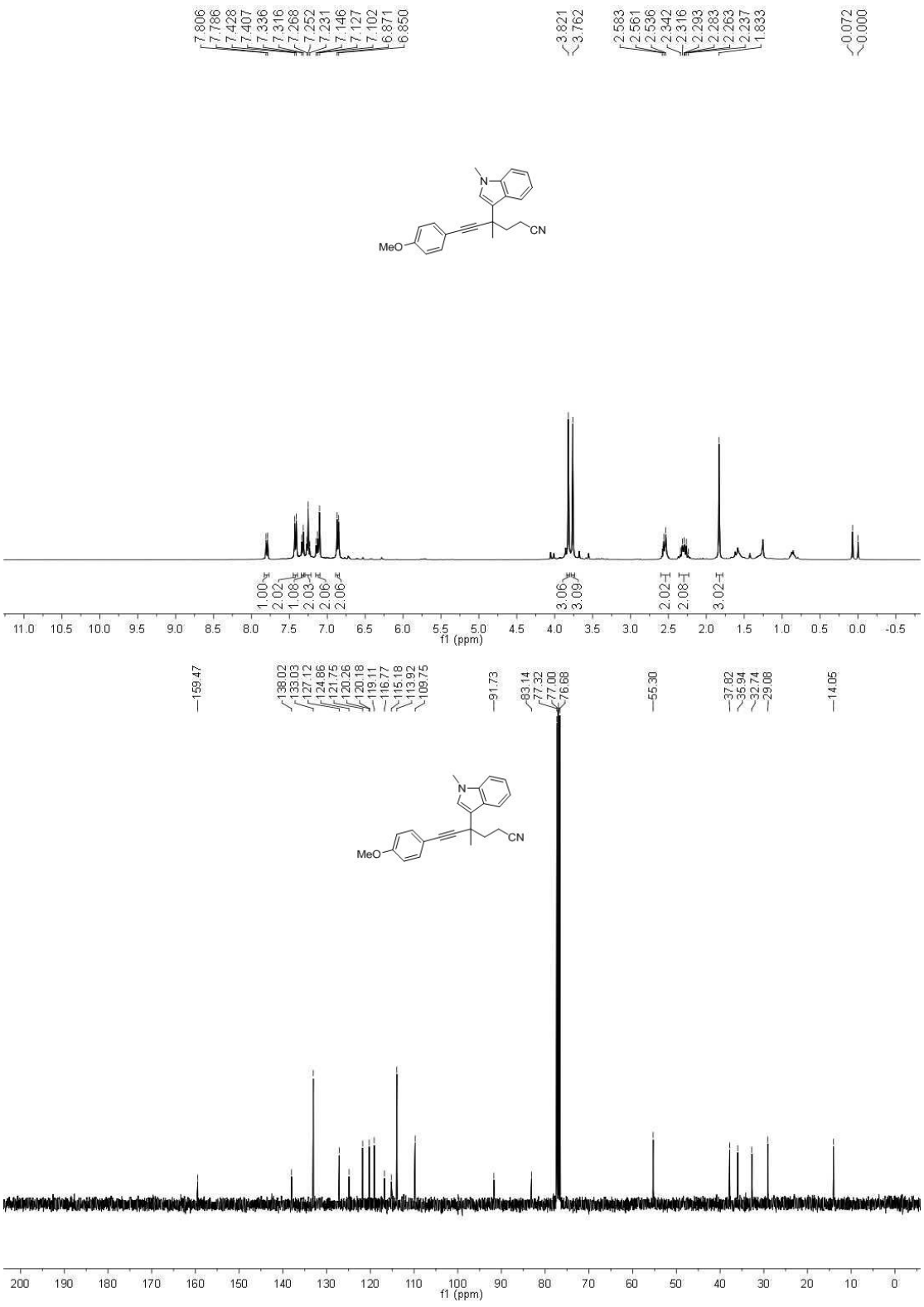
4-(1-methyl-1*H*-indol-3-yl)-4-phenylpentanenitrile (4laa)



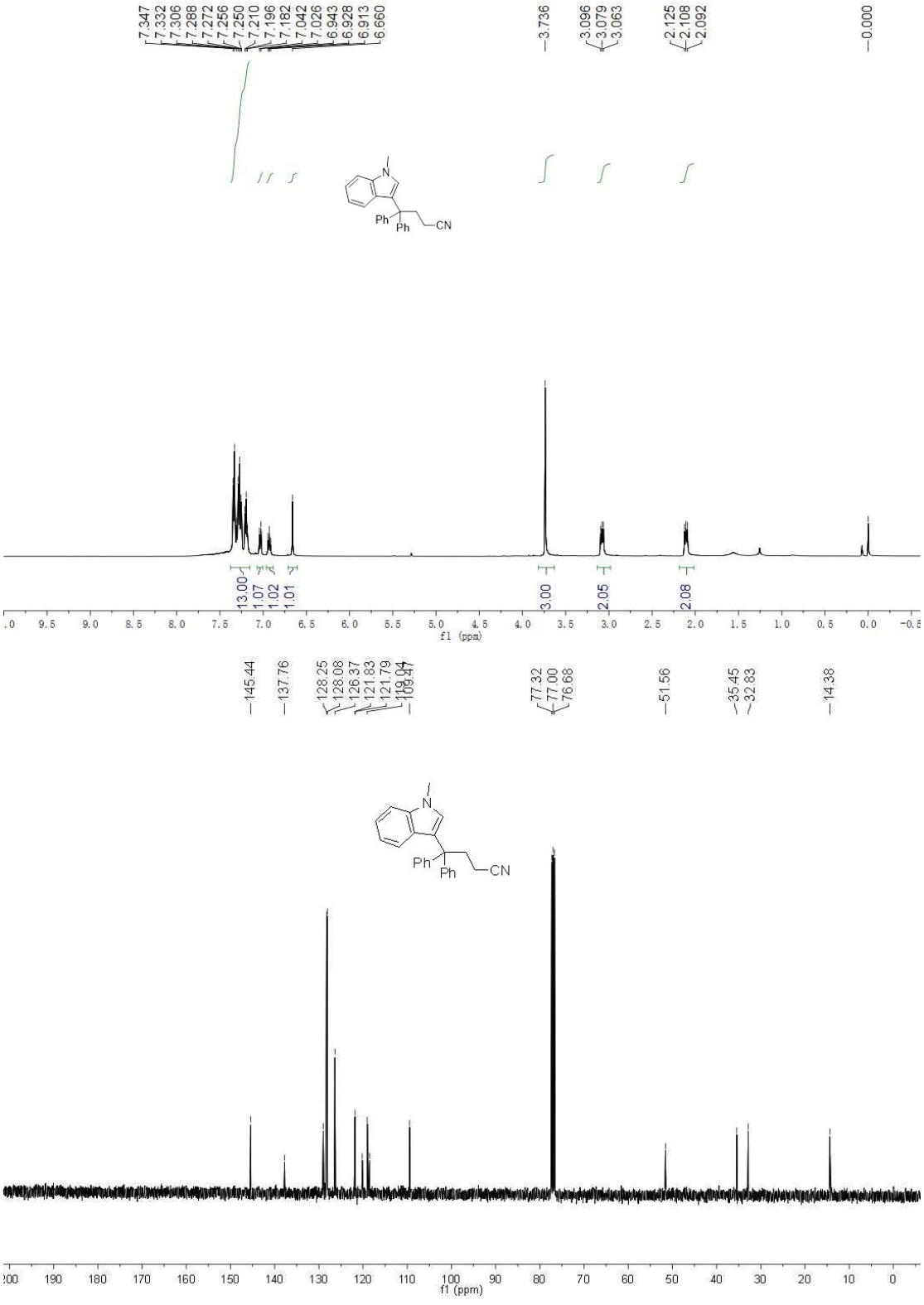
3-(1-(1-Methyl-1*H*-indol-3-yl)-1,2,3,4-tetrahydronaphthalen-1-yl)propanenitrile (4maa)



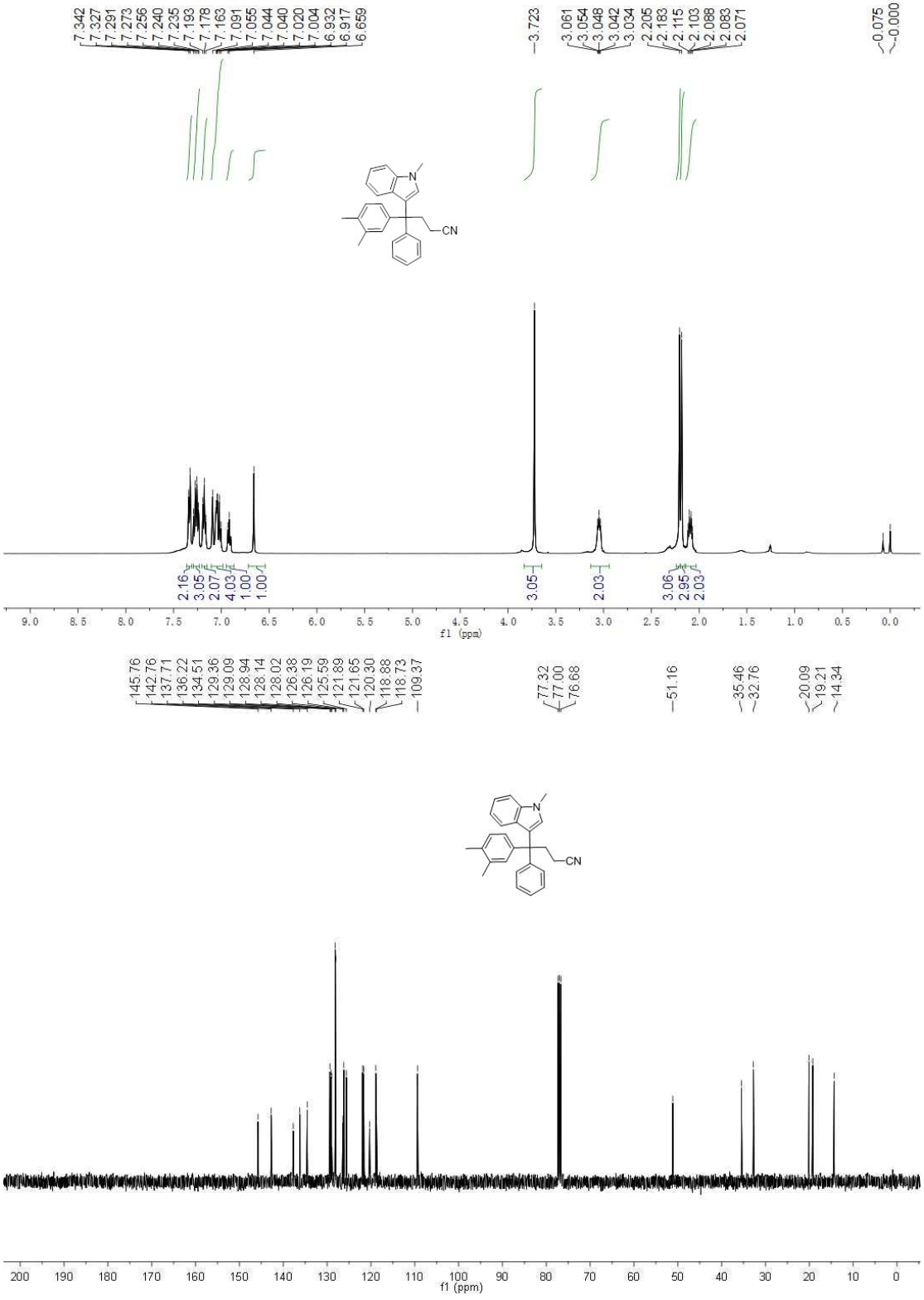
6-(4-Methoxyphenyl)-4-methyl-4-(1-methyl-1*H*-indol-3-yl)hex-5-ynenitrile (4naa):



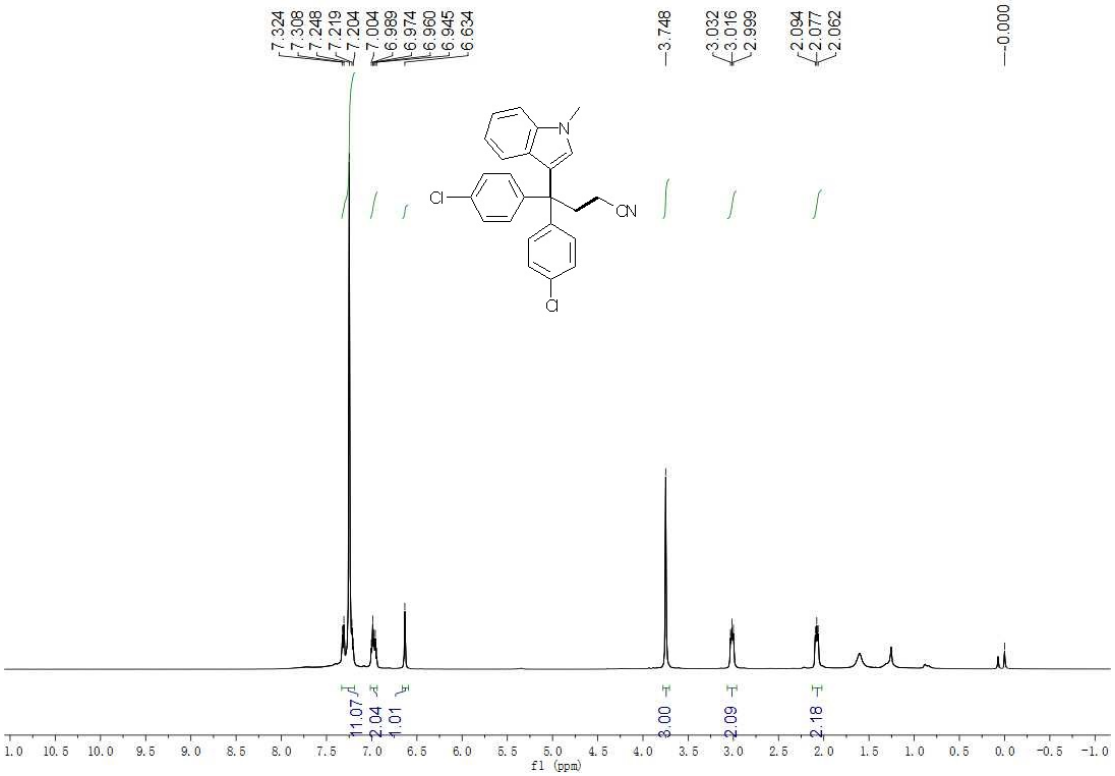
Phenyl 4-(4-methoxyphenyl)-2,3-dimethyl-4-(1-methyl-1*H*-indol-3-yl)butanoate (4oaa)

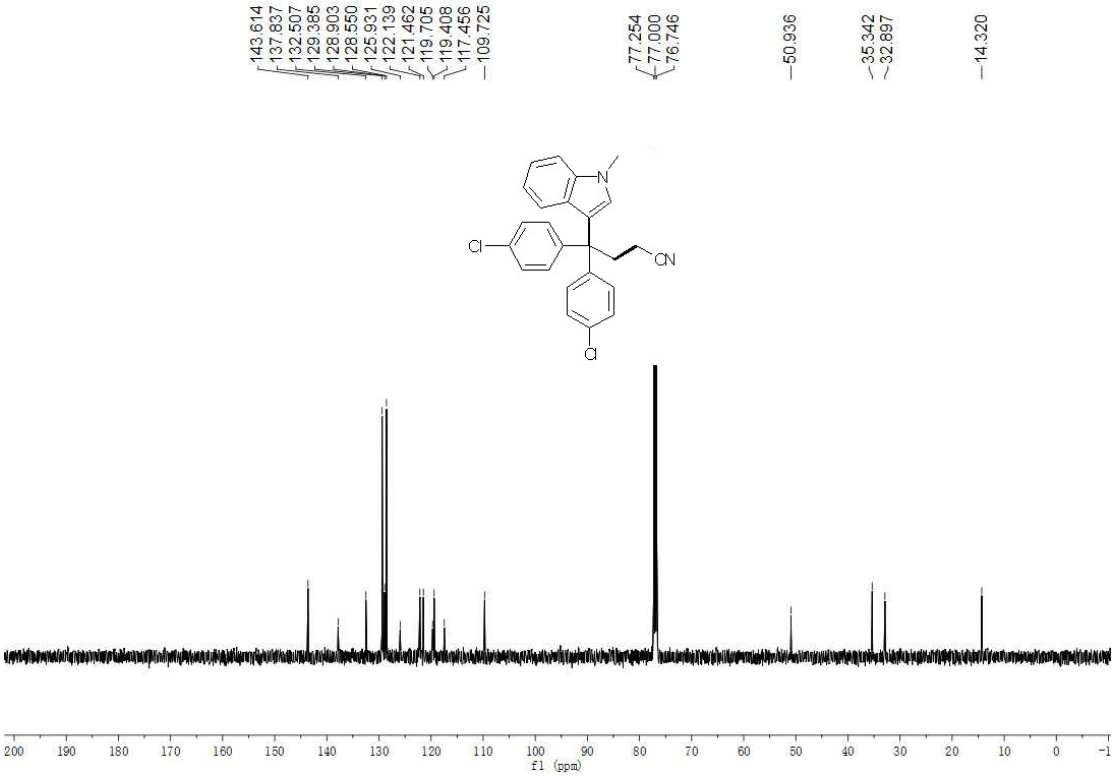


4-(3,4-Dimethylphenyl)-4-(1-methyl-1*H*-indol-3-yl)-4-phenylbutanenitrile (4paa)



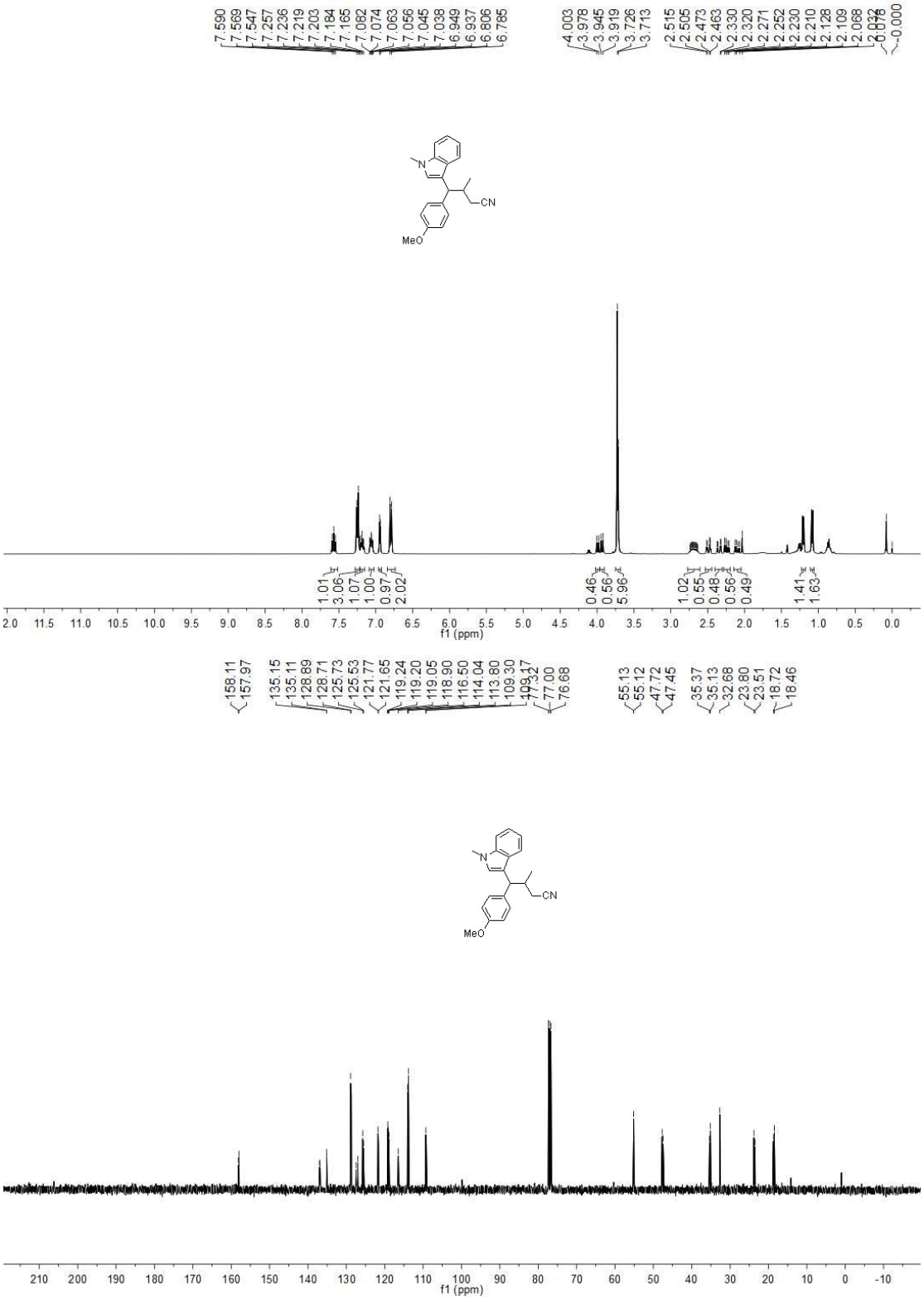
4,4-Bis(4-chlorophenyl)-4-(1-methyl-1*H*-indol-3-yl)butanenitrile (4qaa)





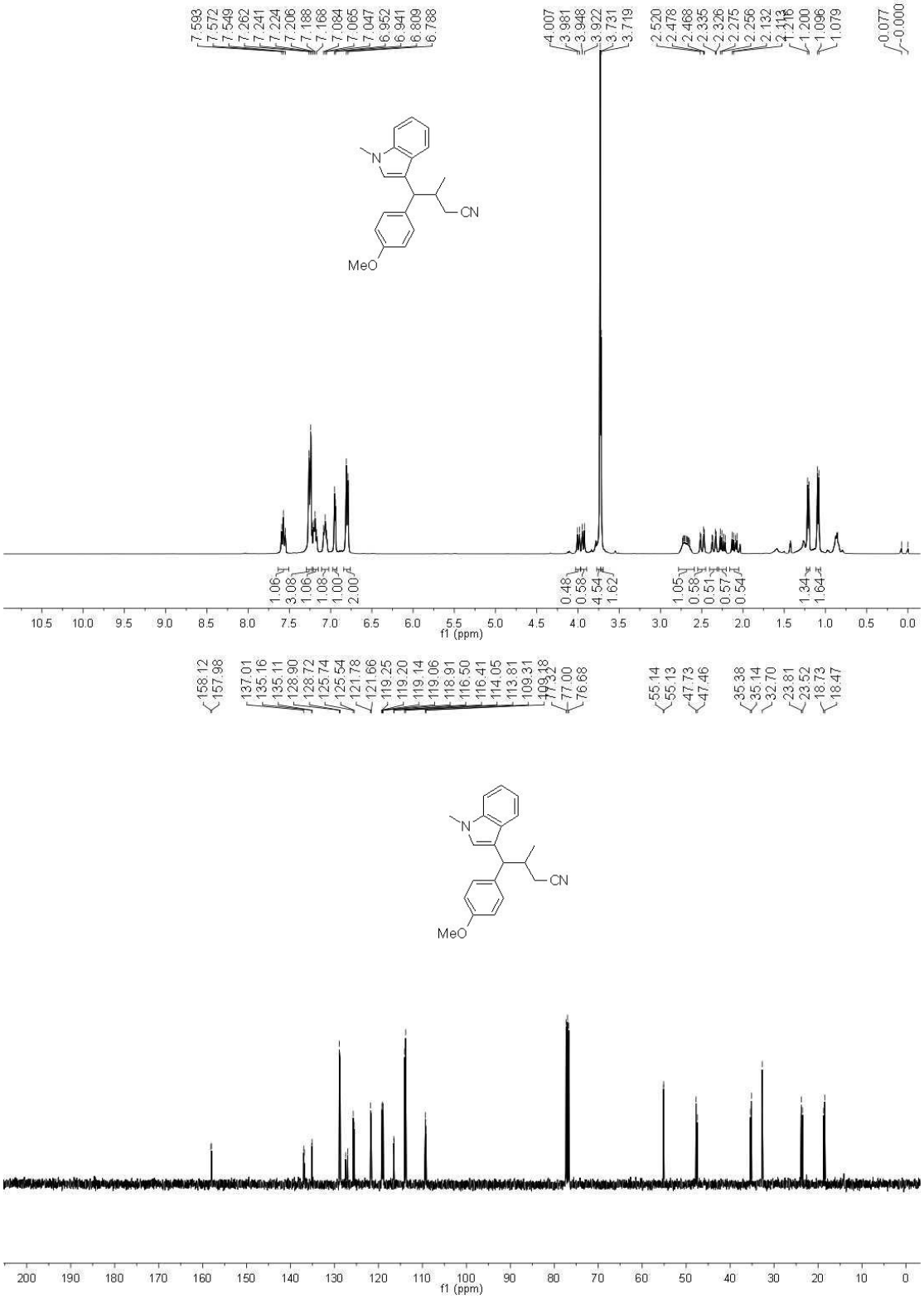
4-(4-Methoxyphenyl)-3-methyl-4-(1-methyl-1*H*-indol-3-yl)butanenitrile

(4raa-from trans **1r)**

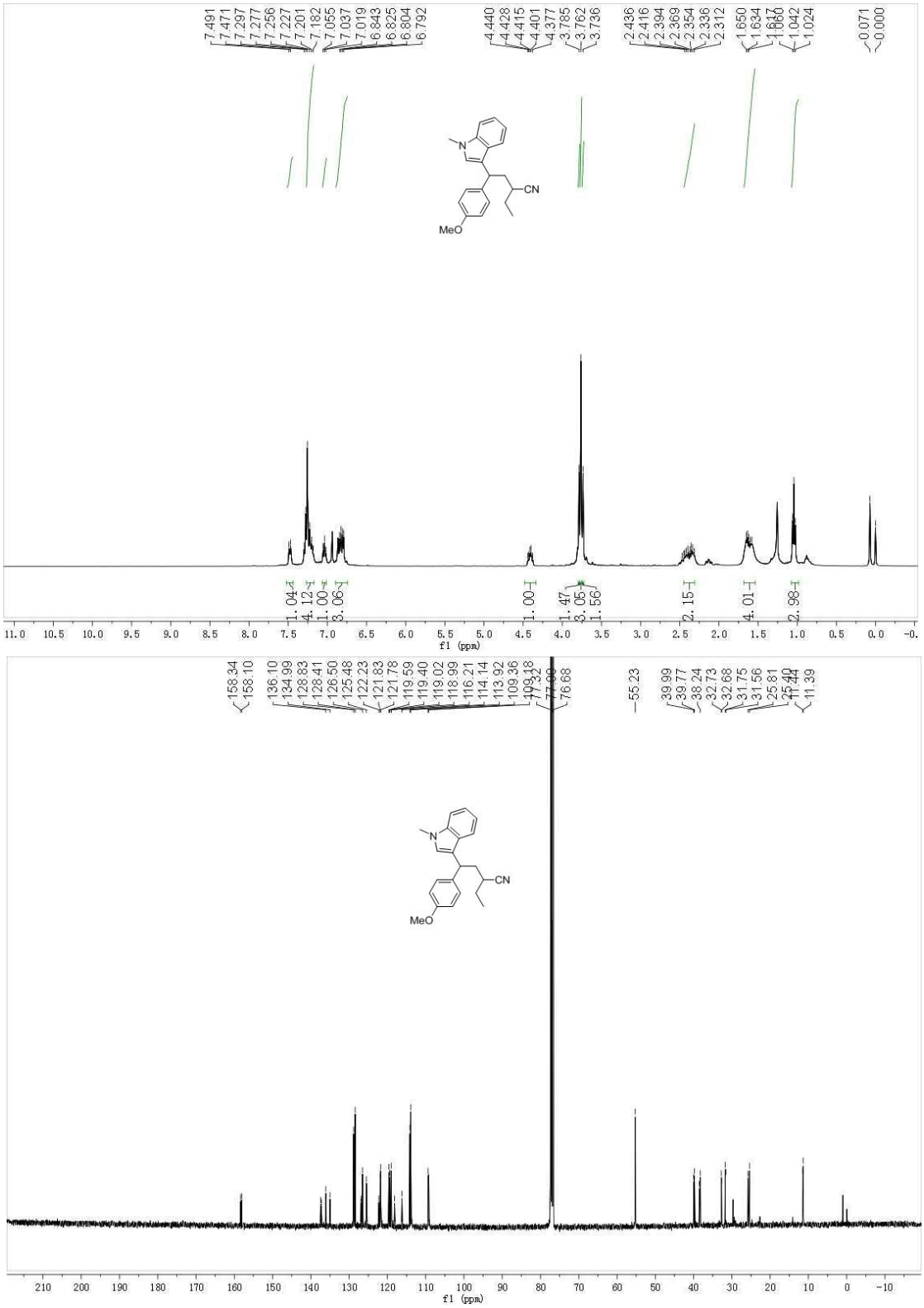


4-(4-Methoxyphenyl)-3-methyl-4-(1-methyl-1*H*-indol-3-yl)butanenitrile

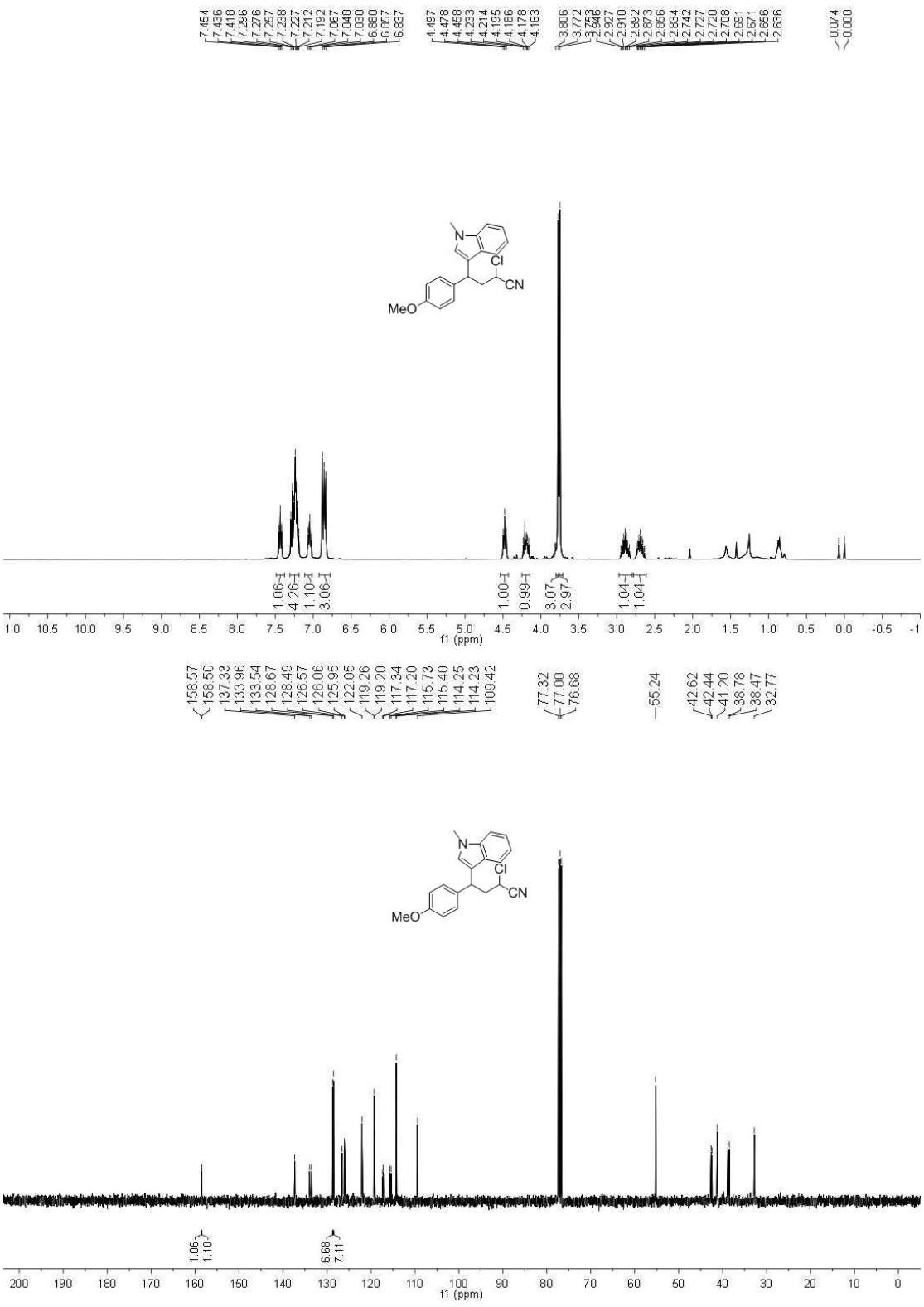
(4raa-from cis **1r)**



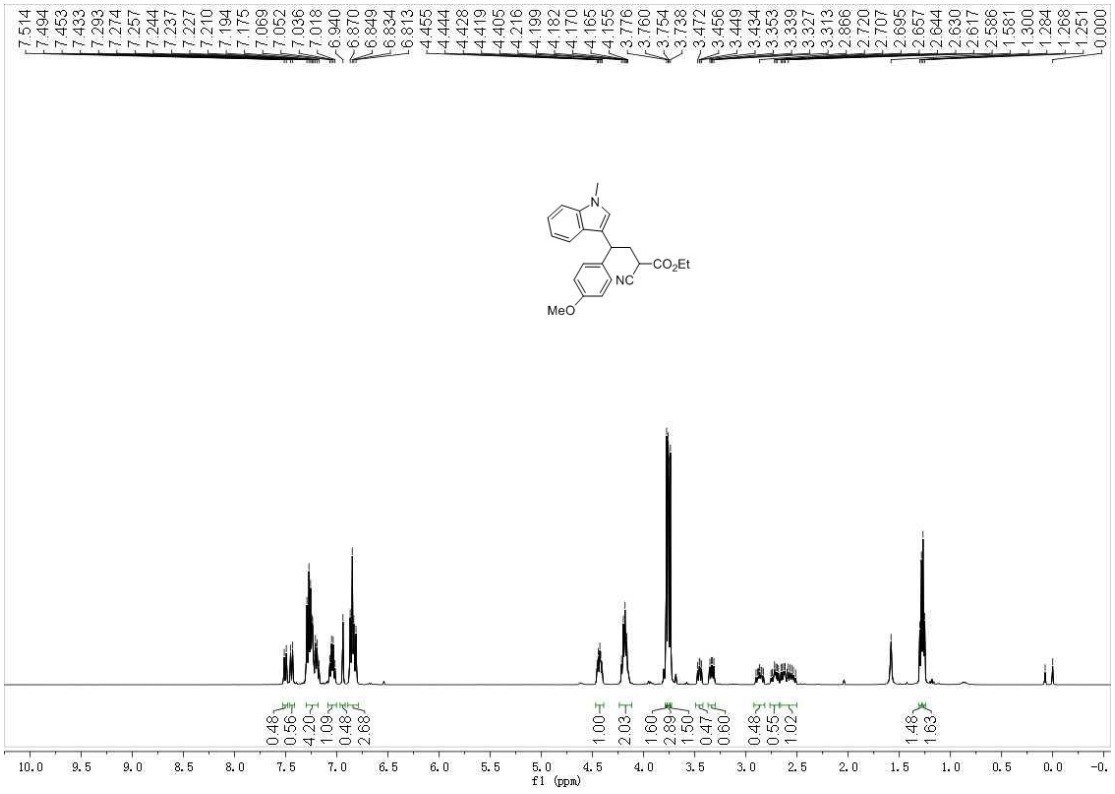
2-Ethyl-4-(4-methoxyphenyl)-4-(1-methyl-1*H*-indol-3-yl)butanenitrile (4aba)

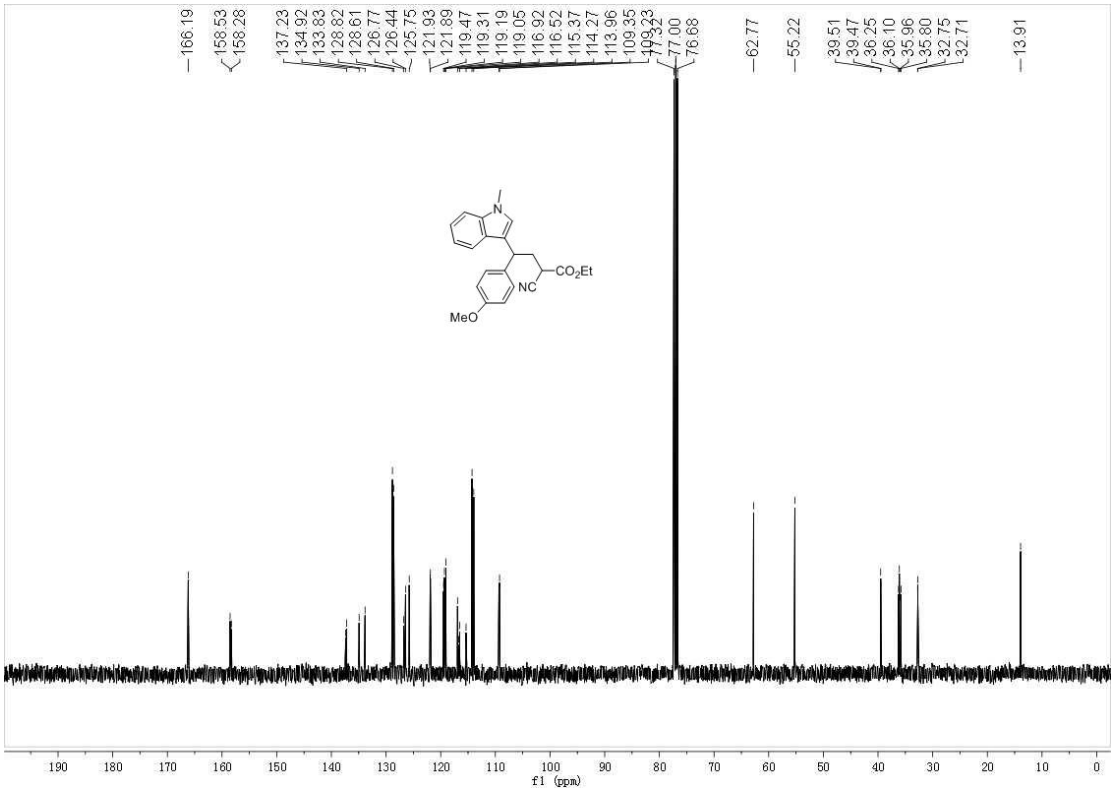


2-Chloro-4-(4-methoxyphenyl)-4-(1-methyl-1*H*-indol-3-yl)butanenitrile (4aca)

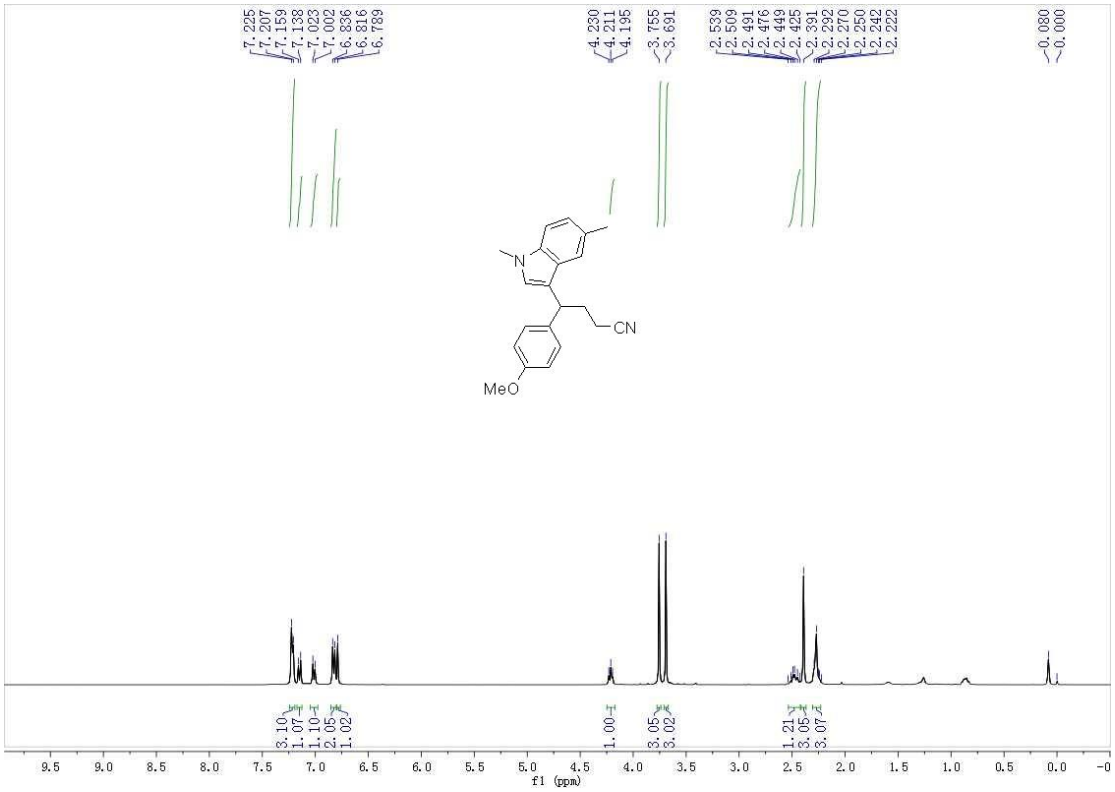


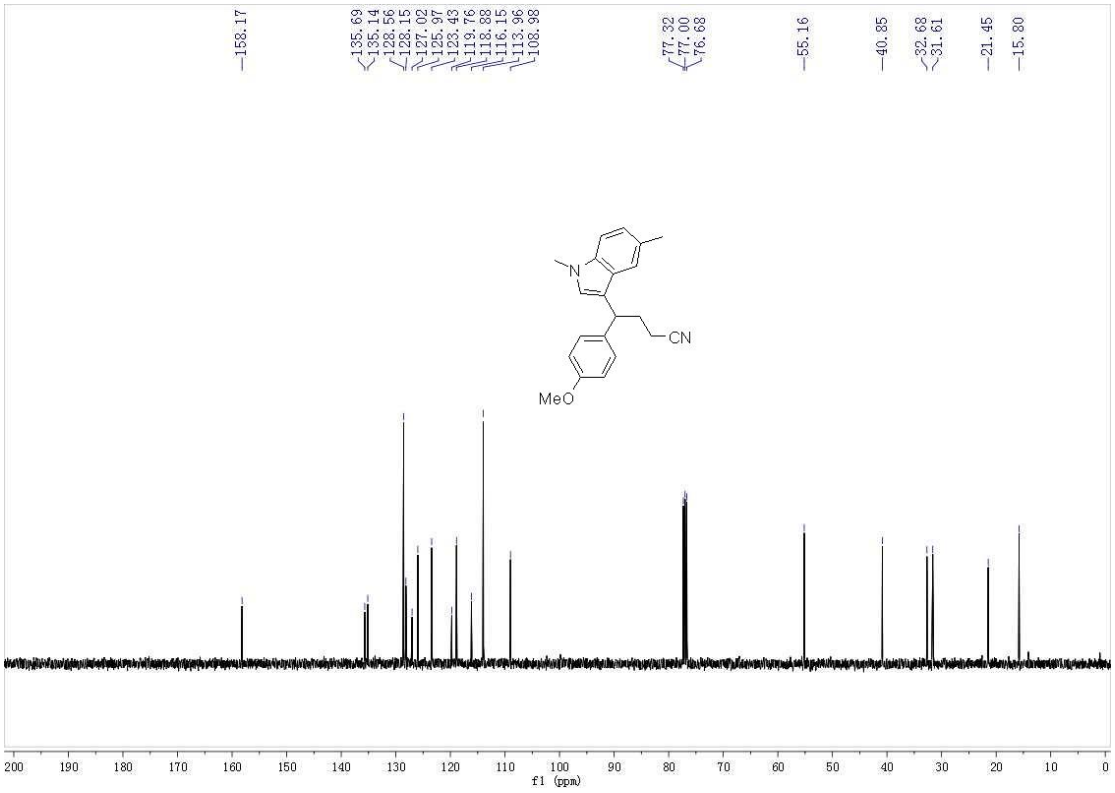
Ethyl 2-cyano-4-(4-methoxyphenyl)-4-(1-methyl-1*H*-indol-3-yl)butanoate (4ada)



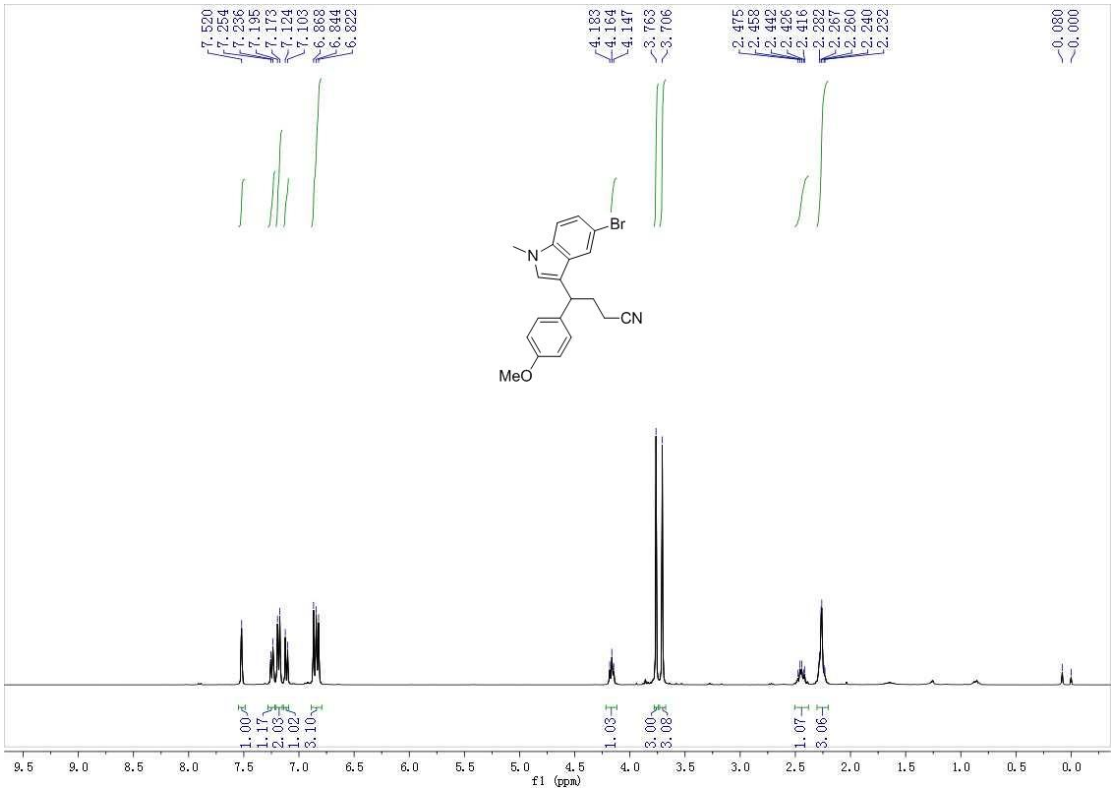


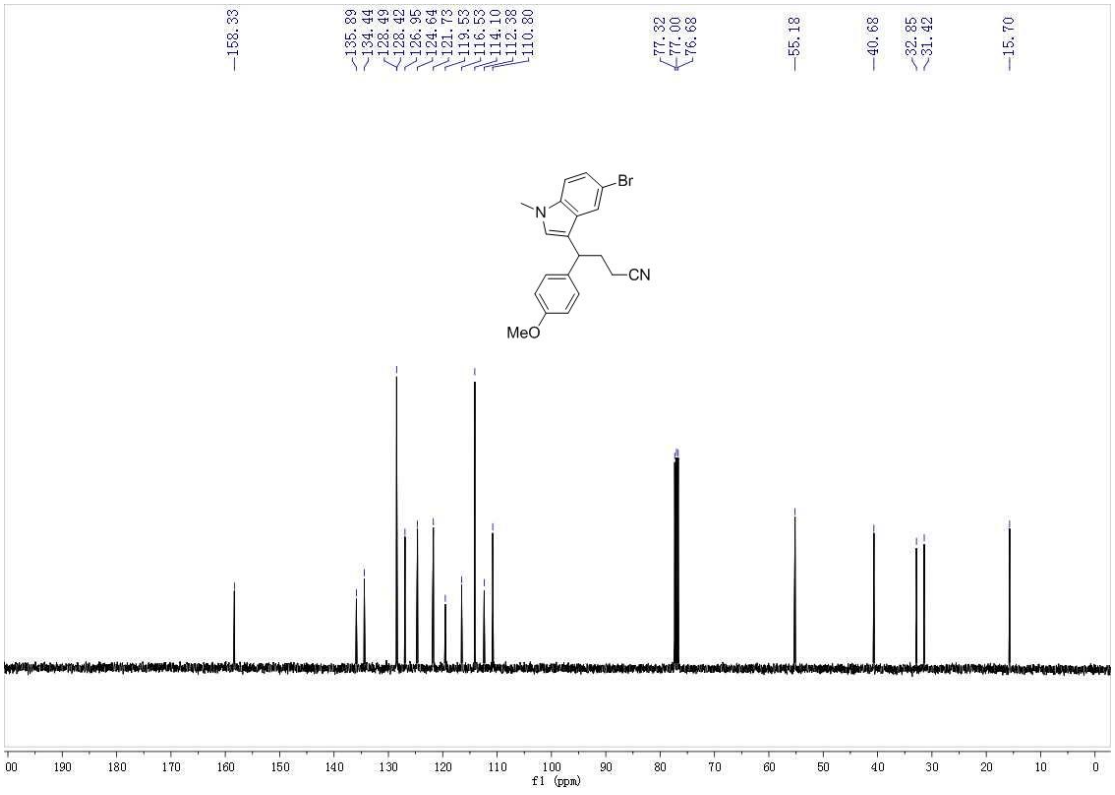
4-(1,5-Dimethyl-1*H*-indol-3-yl)-4-(4-methoxyphenyl)butanenitrile (4aab)



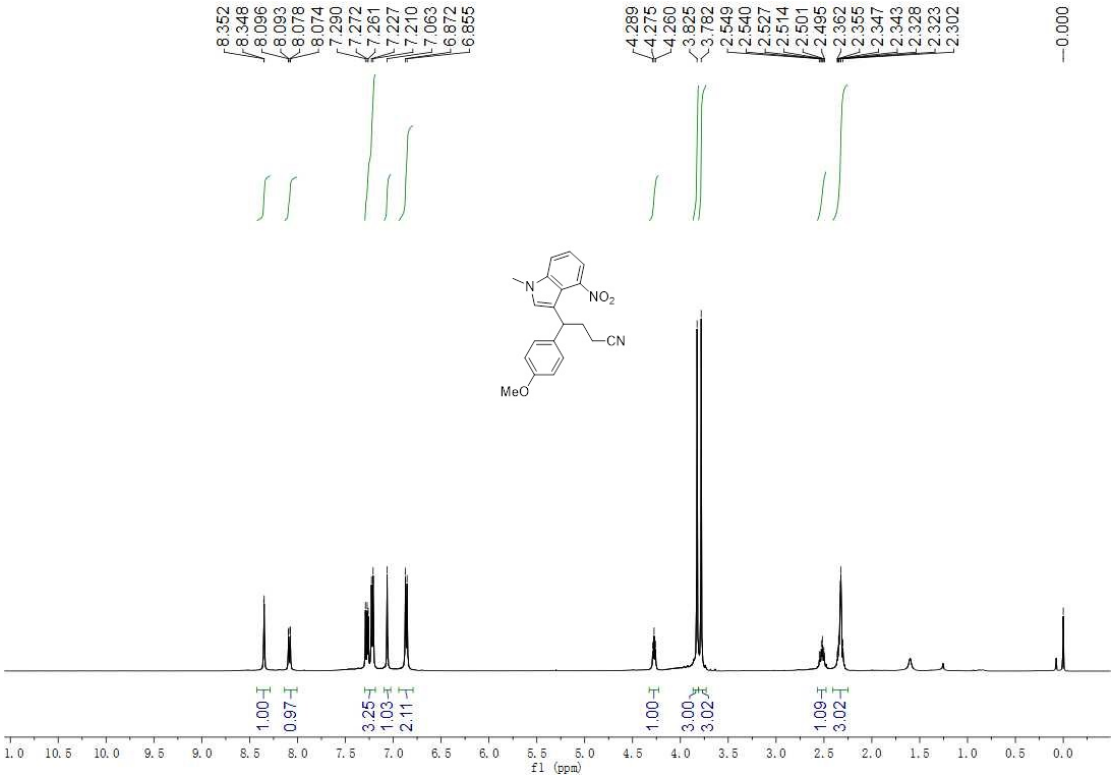


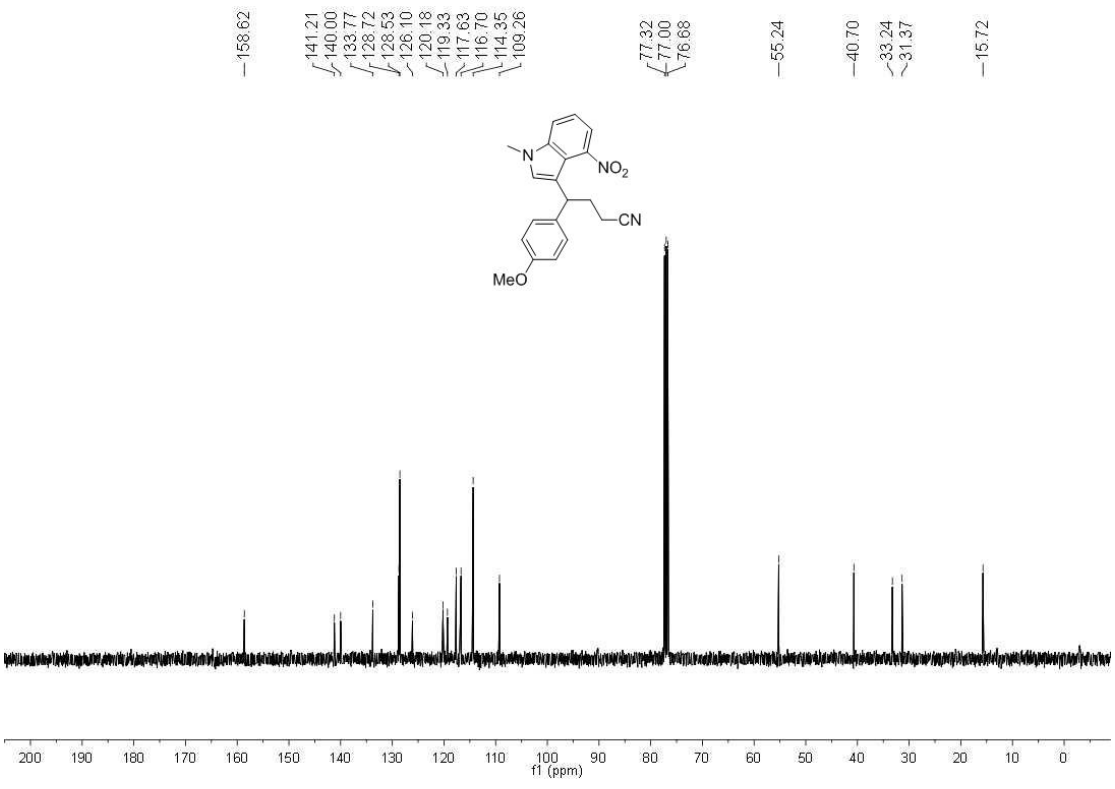
4-(5-Bromo-1-methyl-1*H*-indol-3-yl)-4-(4-methoxyphenyl)butanenitrile (4aac)



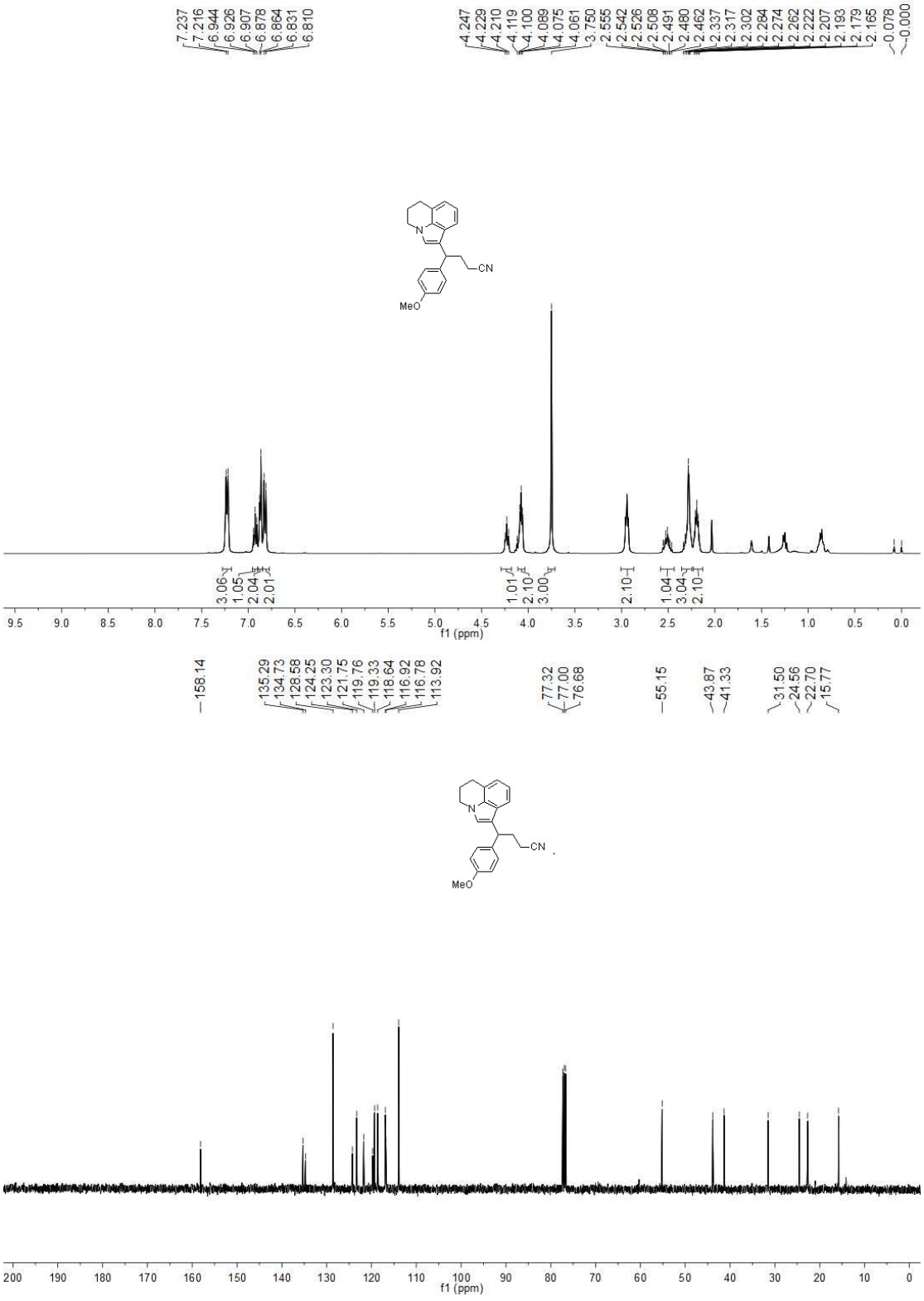


4-(4-Methoxyphenyl)-4-(1-methyl-4-nitro-1*H*-indol-3-yl)butanenitrile (4aad)

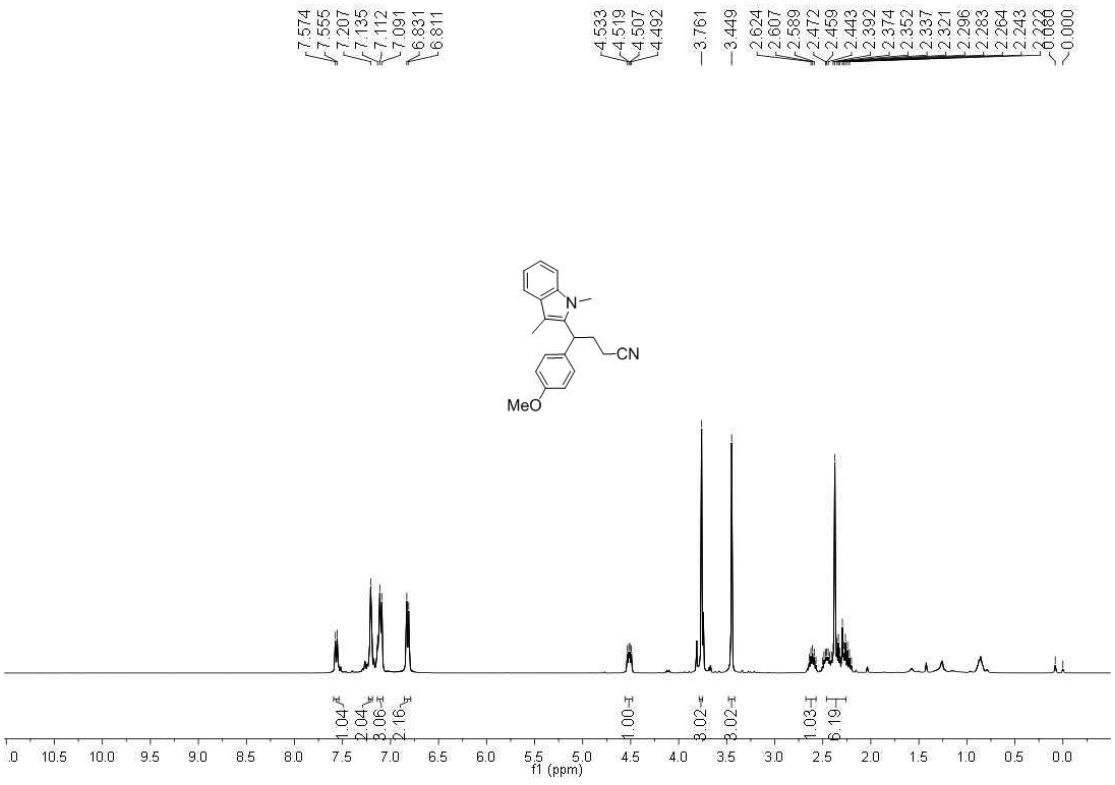


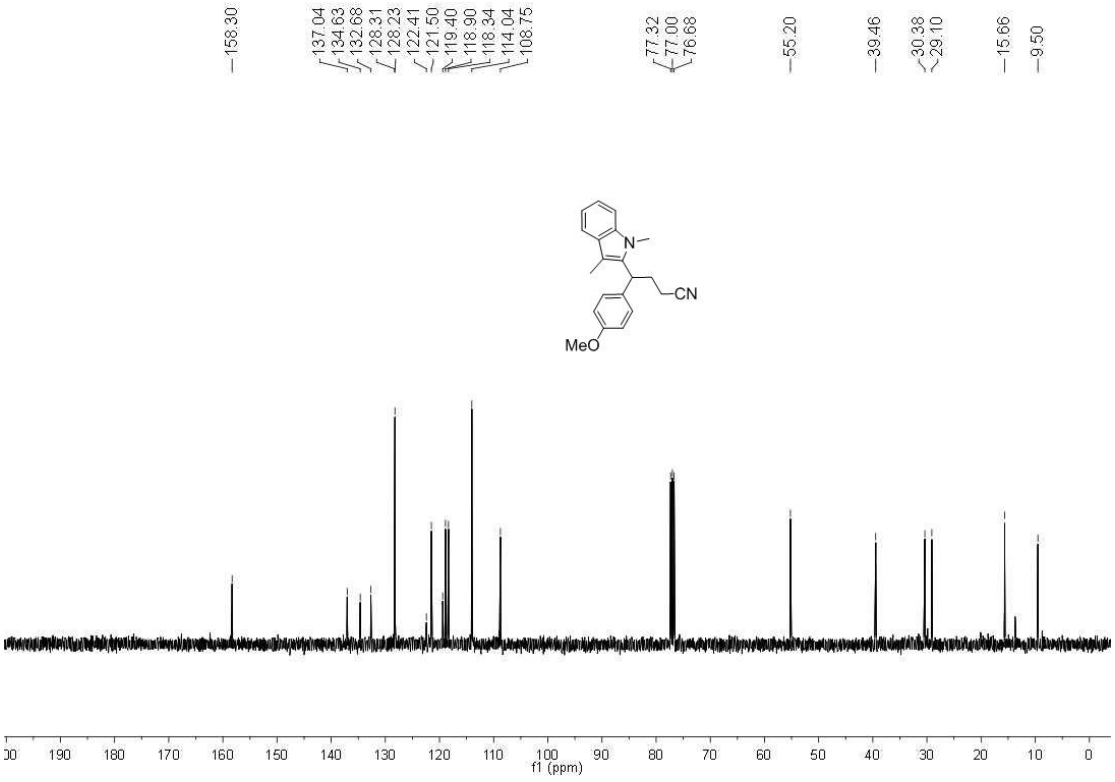


4-(5,6-Dihydro-4*H*-pyrrolo[3,2,1-*ij*]quinolin-1-yl)-4-(4-methoxyphenyl)butanenitrile (4aae)

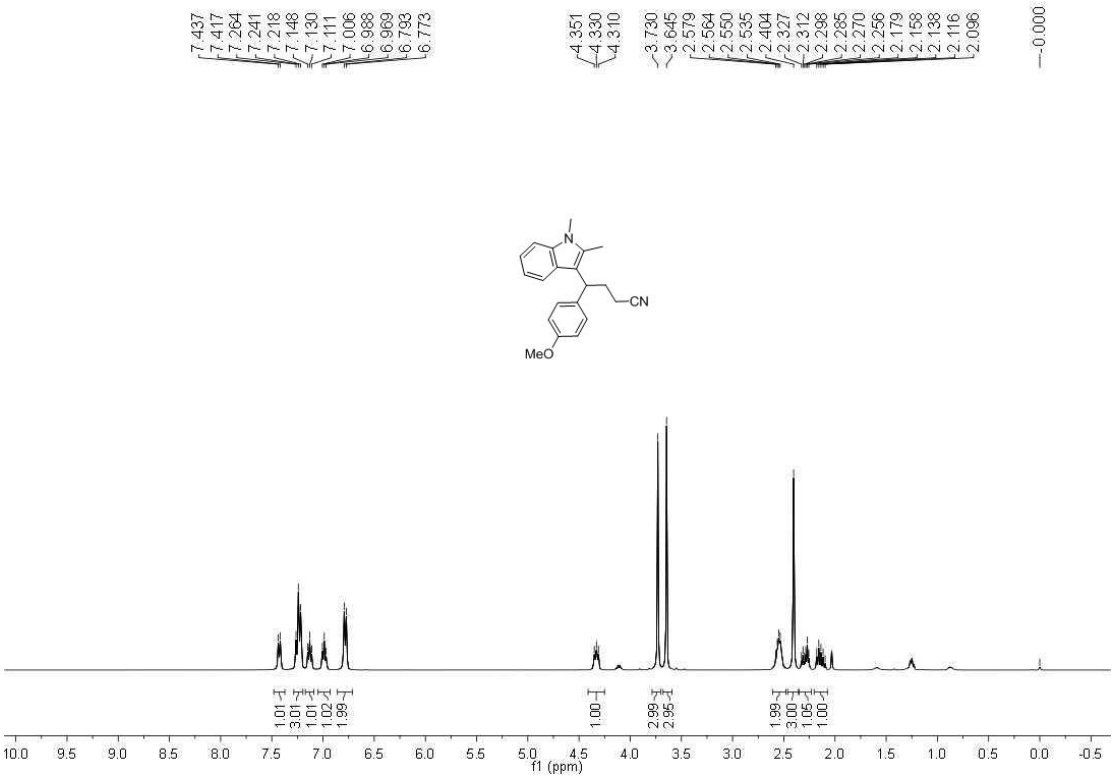


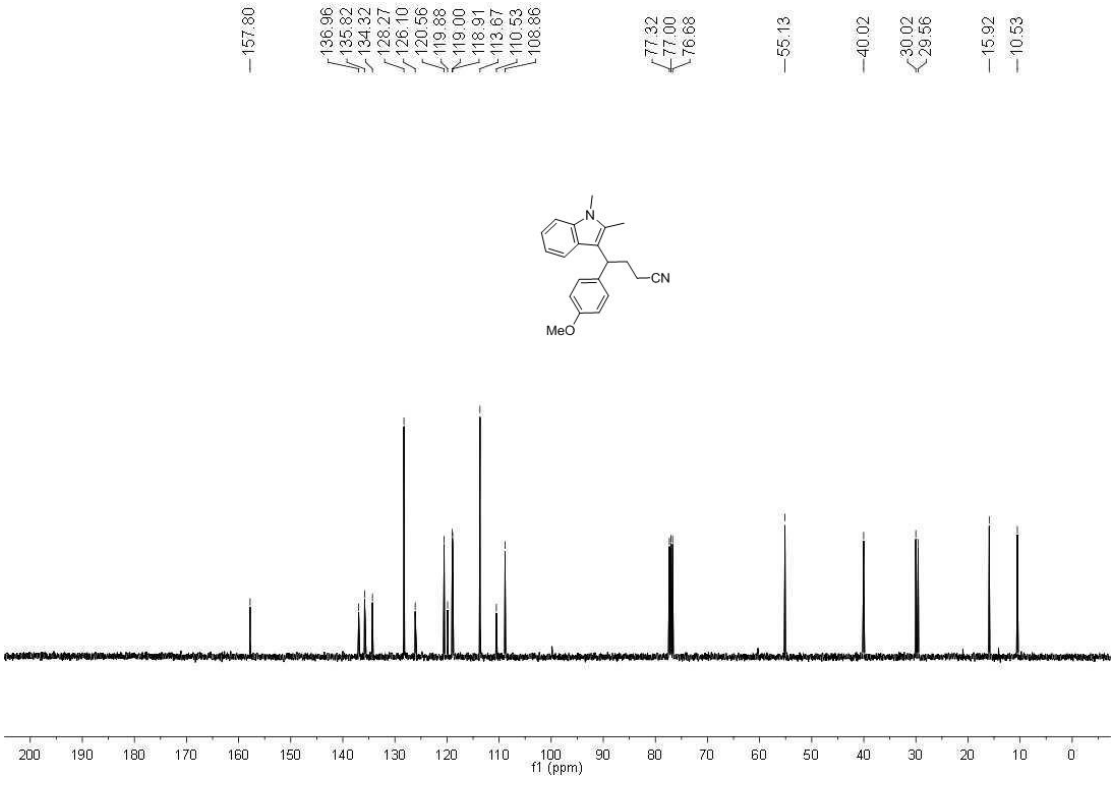
4-(1,3-Dimethyl-1*H*-indol-2-yl)-4-(4-methoxyphenyl)butanenitrile (4aaf)



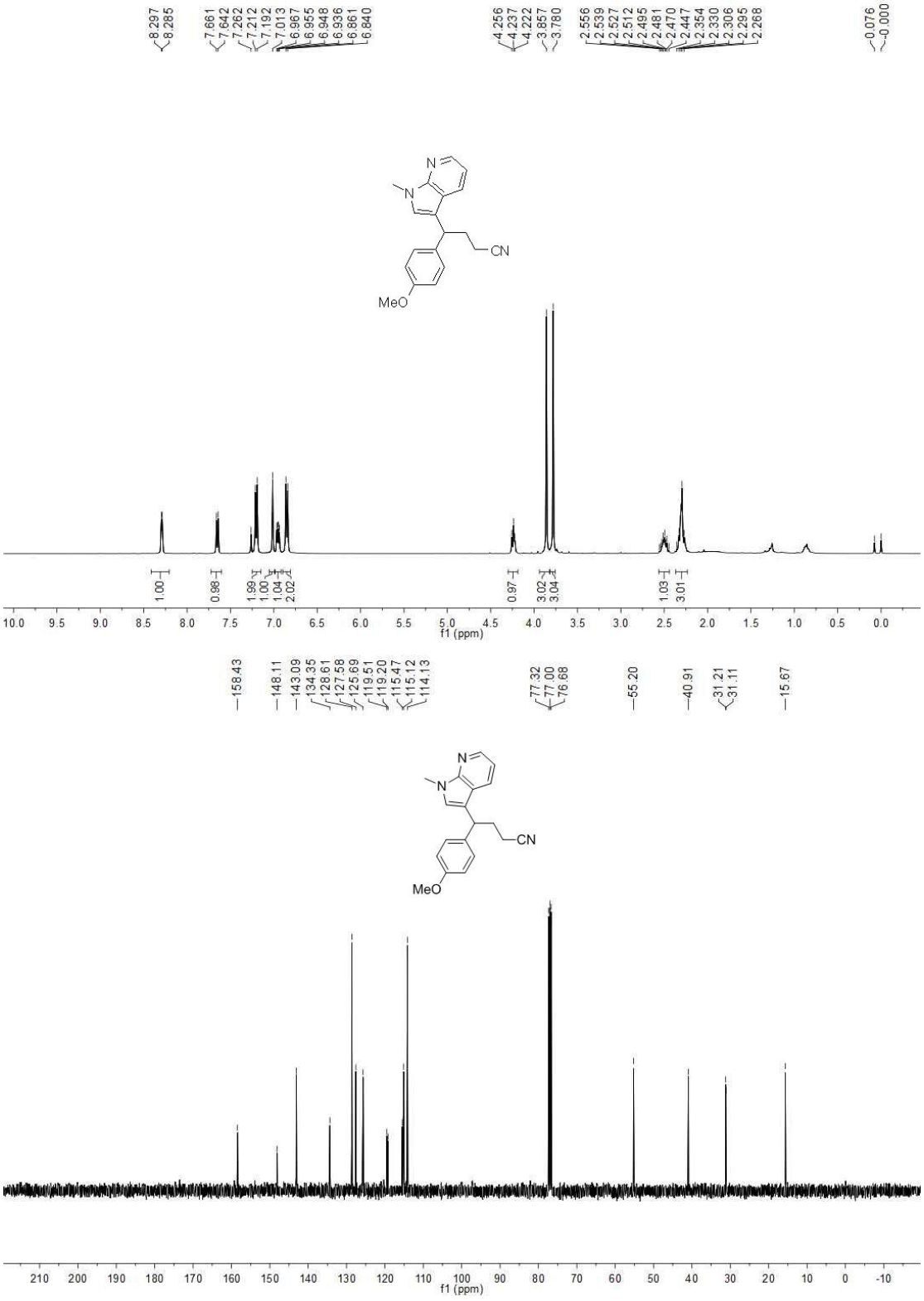


4-(1,2-Dimethyl-1*H*-indol-3-yl)-4-(4-methoxyphenyl)butanenitrile (4aag)

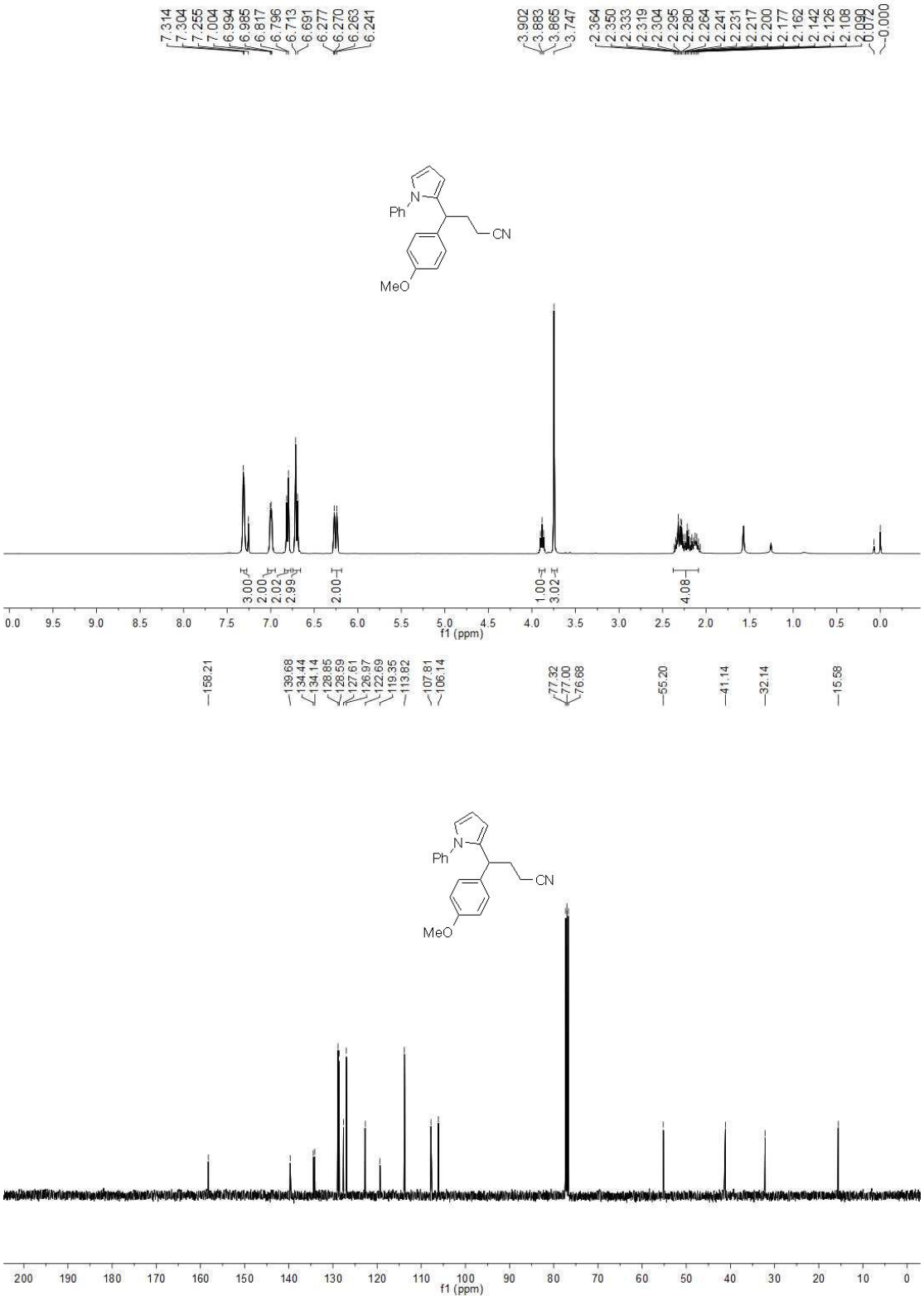




4-(4-Methoxyphenyl)-4-(1-methyl-1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)butanenitrile (4aah)

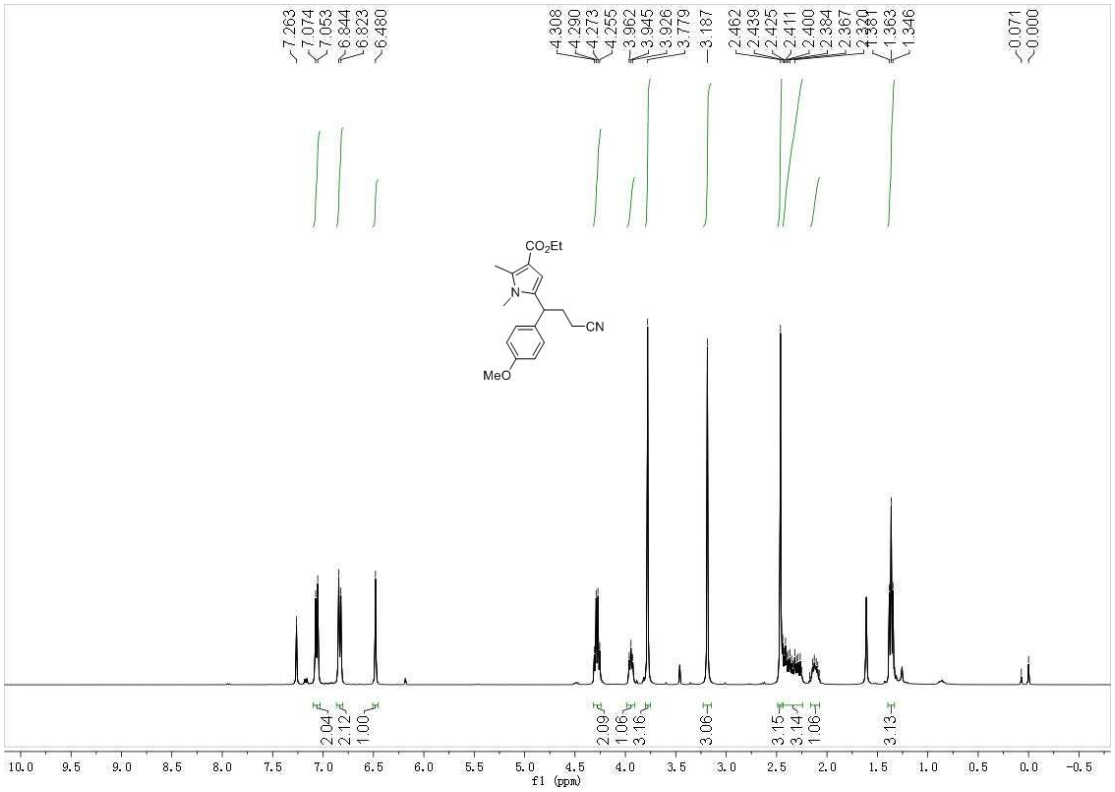


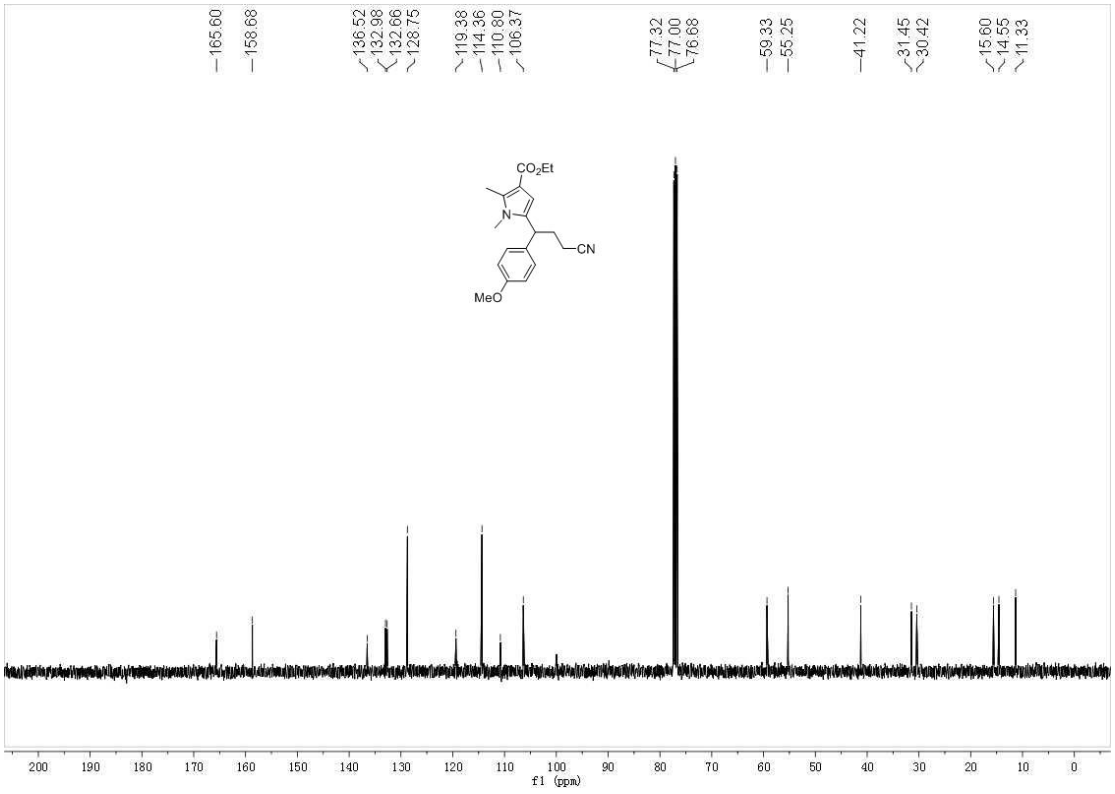
4-(4-Methoxyphenyl)-4-(1-phenyl-1*H*-pyrrol-2-yl)butanenitrile (4aai)



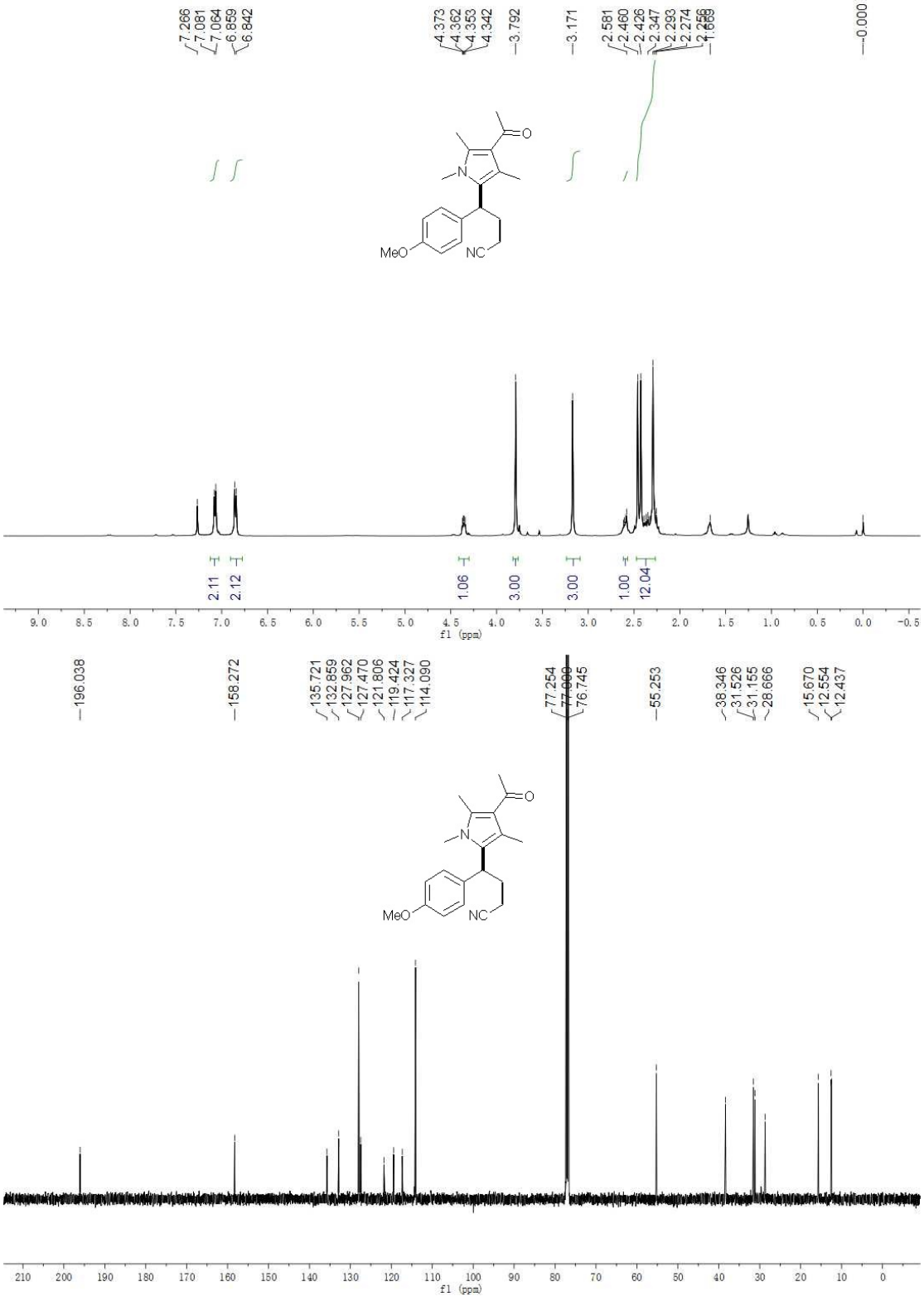
Ethyl 5-(3-cyano-1-(4-methoxyphenyl)propyl)-1,2-dimethyl-1*H*-pyrrole-3-carboxylate

(4aaj)



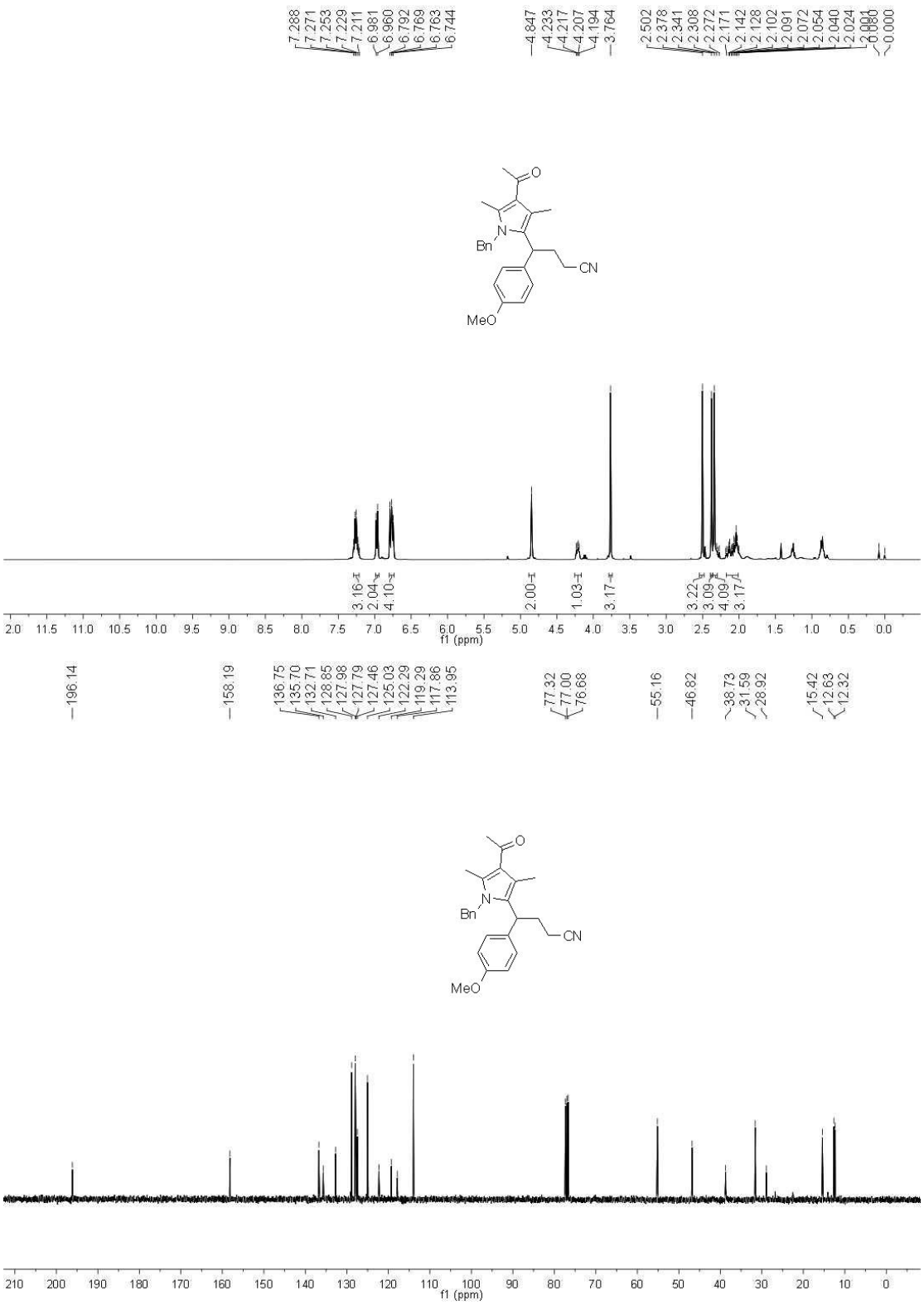


4-(4-Acetyl-1,3,5-trimethyl-1*H*-pyrrol-2-yl)-4-(4-methoxyphenyl)butanenitrile (4aak)

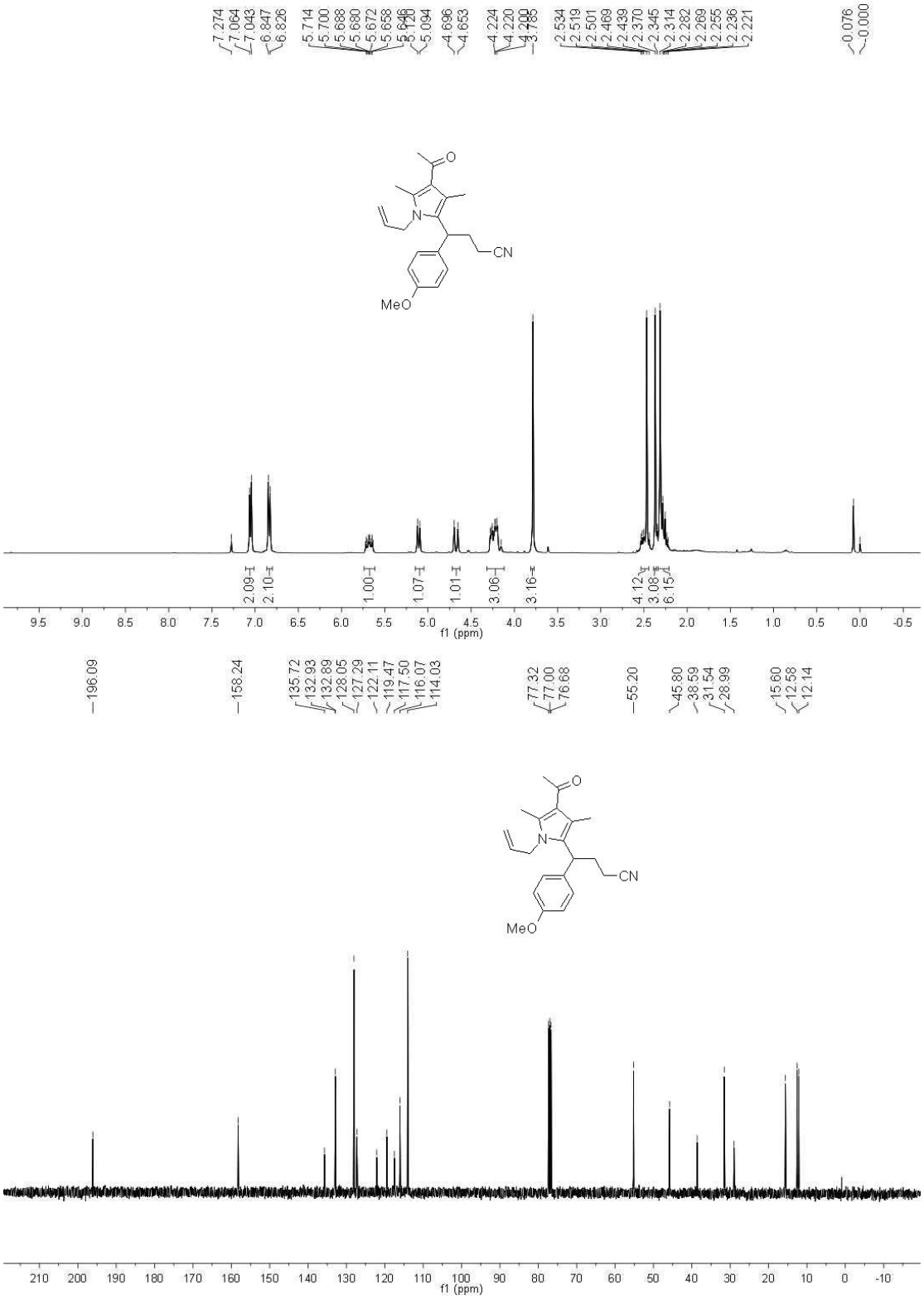


4-(4-Acetyl-1-benzyl-3,5-dimethyl-1*H*-pyrrol-2-yl)-4-(4-methoxyphenyl)butanenitrile

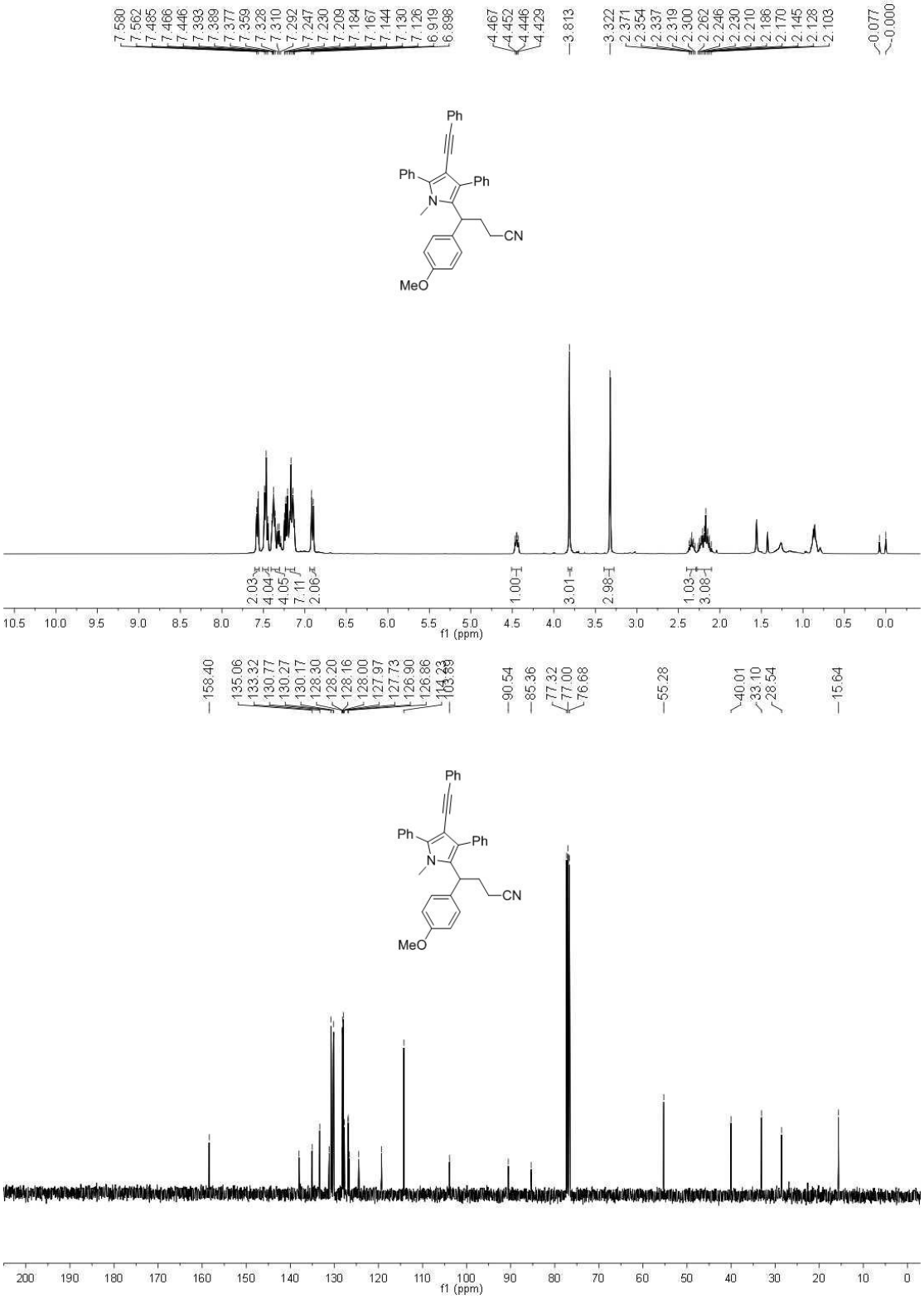
(4aal)



4-(4-Acetyl-1-allyl-3,5-dimethyl-1*H*-pyrrol-2-yl)-4-(4-methoxyphenyl)butanenitrile (4aam)



4-(4-Methoxyphenyl)-4-(1-methyl-3,5-diphenyl-4-(phenylethynyl)-1*H*-pyrrol-2-yl)butanenitrile (4aan)



2-(2,2,6,6-Tetramethylpiperidin-1-yloxy)acetonitrile (5):