Supporting Information

# Manganese Catalyzed Cross-Coupling of Allylic Alcohols and Nitriles: An Elegant Route for Access of *δ*-Hydroxynitriles

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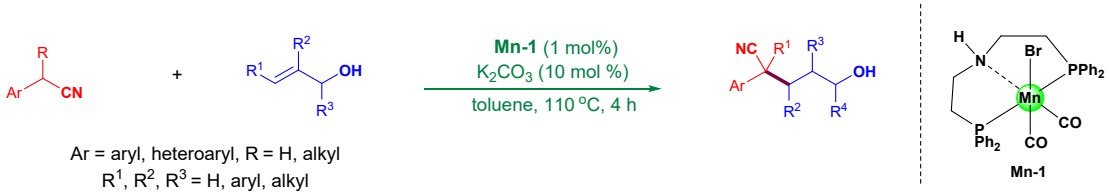
## 1. General information

NMR spectra were recorded with tetramethylsilane (TMS) as the internal standard. $^{1}H$ NMR spectra were recorded at 400 MHz, $^{13}C$ NMR spectra were recorded at 100 MHz and $^{19}F$ NMR (376 MHz) spectra were recorded at 376 MHz on Bruker AV ANCE II instruments. $^{1}H$ NMR chemical shifts (δ) are reported in ppm relative to tetramethylsilane (TMS) with the solvent signal as the internal standard ($CDCl_3$ at 7.26 ppm). $^{13}C$ NMR chemical shifts are reported in ppm from tetramethylsilane (TMS) with the solvent resonance as the internal standard ($CDCl_3$ at 77.16 ppm). Data are given as: s (singlet), d (doublet), t (triplet), q (quartet), dd (double of doublet) or m (multiplets), coupling constants (Hz) and integration. High resolution mass spectra were obtained with the Q-TOF-Premier mass spectrometer (Agilent 1200HPLC-6210TOFMS). Reactions were monitored by TLC and visualized with ultraviolet light. All the solvents were used directly without any purification. The allylic alcohols were synthesized according to the references 1 and 2.

## 2. General Procedure for the Synthesis of *δ*-Hydroxynitriles



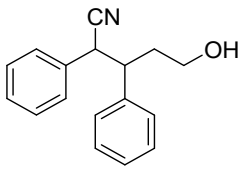

Ar = aryl, heteroaryl, R = H, alkyl
$R^1$, $R^2$, $R^3$ = H, aryl, alkyl

To a mixture of **Mn-1** catalyst (1 mol %), $K_2CO_3$ (10 mol %), nitriles (0.5 mmol) and cinnamyl alcohol (1.0 mmol), 1.0 mL of toluene was added. Then, the reaction was stirred at 110 °C for 4 h under Ar in a pressure tube (ACE pressure tube, 15 mL). After cooling to room temperature, the reaction was diluted with ethyl acetate (10 mL) and water (10 mL). The organic layer was separated, and the aqueous layer was extracted with ethyl acetate (10 mL) for three times. The combined organic layers were washed by brine and dried over magnesium sulfate and the volatiles were removed under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1-2:1) to give the desired product *δ*-hydroxynitrile.

## 3.Spectra data of products

**5-Hydroxy-2,3-diphenyl pentanenitrile (3):**

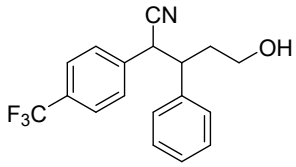
Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent.




Colorless liquid. Yield: 106 mg, 85%. $^1$H NMR analysis of the crude reaction mixture showed a *d.r.* of 60:40. $^1$H NMR (400 MHz, $CDCl_3$, ppm): δ 7.24 – 7.30 (m, 6H), 7.09 – 7.18 (m, 4H), 4.08 (m, 1H), 3.49 – 3.59 (m, 1H), 3.25 – 3.43 (m, 2H), 2.03 – 2.28 (m, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm): δ 139.3, 138.6, 134.3, 134.3, 128.7, 128.5, 128.5, 128.3, 128.2, 128.1, 128.1, 127.7, 127.6, 120.0, 119.8, 60.1, 60.1, 47.3, 47.1, 44.8, 44.3, 35.7, 34.4. HRMS (ESI) m/z calcd for $C_{17}H_{18}NO$ $[M+H]^+$: 252.1388, found: 252.1384.

**5-Hydroxy-3-phenyl-2-(4-(trifluoromethyl) phenyl) pentanenitrile (4)**:

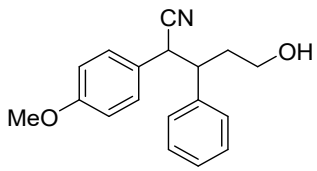
Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent.




Colorless liquid. Yield: 79 mg, 50%. $^1$H NMR analysis of the crude reaction mixture showed a *d.r.* of 75:25. $^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 7.55 (d, $J$ = 8.0 Hz, 1H), 7.20 – 7.31 (m, 5H), 7.07 – 7.14 (m, 2H), 4.18 (m, 1H), 3.59 – 3.72 (m, 1H), 3.30 – 3.53 (m, 2H), 2.06 – 2.36 (m, 2H), 1.64 (s, 1H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 138.3, 137.8, 128.9, 128.7, 128.6, 128.5, 128.1, 128.0, 127.9, 125.7, 125.7, 125.6, 125.6, 60.0, 59.9, 47.3, 47.0, 44.5, 44.0, 35.6, 34.6. HRMS (ESI) m/z calcd for $C_{18}H_{17}F_3NO$ $[M+H]^+$: 320.1262, found: 320.1266.

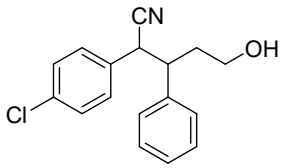
**5-Hydroxy-2-(4-methoxyphenyl)-3-phenylpentanenitrile (5)**:

Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent.



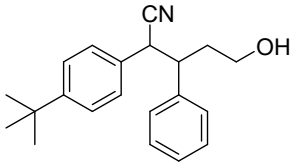

Colorless liquid. Yield: 126 mg, 90%. $^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 7.23 – 7.33 (m, 3H), 7.15 (d, $J$ = 6.4 Hz, 2H), 7.09 (d, $J$ = 8.4 Hz, 2H), 6.81 (d, $J$ = 8.8 Hz, 2H), 3.98 (d, $J$ = 7.2 Hz, 1H), 3.79 (s, 3H), 3.56 – 3.61 (m, 1H), 3.35 – 3.41 (m, 1H), 3.23 – 3.28 (m, 1H), 2.21 – 2.31 (m, 1H), 2.06 – 2.18 (m, 1H), 1.51 (s, 1H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 159.3, 139.3, 129.2, 128.7, 128.2, 127.6, 126.3, 120.2, 114.1, 60.2, 60.2, 55.3, 47.4, 44.0, 34.5. HRMS (ESI) m/z calcd for $C_{18}H_{20}NO_2$ $[M+H]^+$: 282.1494, found: 282.1497.

**2-(4-Chlorophenyl)-5-hydroxy-3-phenylpentanenitrile (6):**




Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless liquid. Yield: 111 mg, 78%. $^1$H NMR analysis of the crude reaction mixture showed a *d.r.* of 80:20. $^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 7.25 – 7.31 (m, 5H), 7.01 – 7.13 (m, 4H), 4.08 (m, 1H), 3.58 – 3.70 (m, 1H), 3.35 – 3.51 (m, 1H), 3.25 – 3.30 (m, 1H), 2.08 – 2.17 (m, 2H), 1.66 (s, 1H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 138.8, 138.1, 134.1, 132.8, 132.8, 129.5, 129.5, 128.9, 128.9, 128.8, 128.6, 128.5, 128.2, 127.8, 127.8, 119.6, 119.3, 60.0, 60.0, 47.3, 47.0, 44.1, 43.6, 35.6, 34.6. HRMS (ESI) m/z calcd for $C_{17}H_{17}ClNO$ $[M+H]^+$: 286.0998, found: 286.0994.

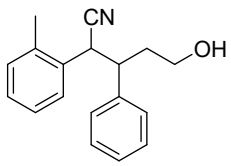
**2-(4-(*Tert*-butyl)phenyl)-5-hydroxy-3-phenylpentanenitrile（7）:**



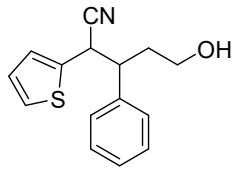

Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless liquid. Yield: 130 mg, 85%. $^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 7.28 – 7.34 (m, 5H), 7.14 – 7.17 (m, 2H), 7.06 – 7.09 (m, 2H), 4.05 (d, $J$ = 7.6 Hz, 1H), 3.58 – 3.63 (m, 1H), 3.40 – 3.47 (m, 1H), 3.24 – 3.30 (m, 1H), 2.01 – 2.07 (m, 2H), 1.51 (s, 1H), 1.32 (s, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 151.3, 139.0, 131.2, 128.6, 128.4, 127.9, 127.7, 125.7, 119.9, 60.3, 47.2, 44.0, 35.6, 34.6, 31.3. HRMS (ESI) m/z calcd for $C_{21}H_{26}NO$ $[M+H]^+$: 308.2014, found: 308.2018.

**5-Hydroxy-3-phenyl-2-(*m*-tolyl) pentanenitrile (8)**:

Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless liquid. Yield: 111 mg, 84%. $^1$H NMR analysis of the crude reaction mixture showed a d.r. of 84:16. $^1$H NMR (400 MHz, $CDCl_3$, ppm): δ 7.28 – 7.33 (m, 3H), 7.10 – 7.21 (m, 4H), 6.91 – 6.93 (m, 2H), 4.03 (m, 1H), 3.58 – 3.66 (m, 1H), 3.43 – 3.49 (m, 1H), 3.25 – 3.30 (m, 1H), 2.31 – 2.33 (d, $J$ = 4.8 Hz, 3H), 2.04 – 2.09 (m, 2H), 1.55 (s, 1H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm): δ 139.4, 138.7, 138.5, 134.2, 134.1, 128.9, 128.9, 128.8, 128.7, 128.6, 128.5, 128.5, 128.2, 127.7, 127.6, 125.3, 125.1, 119.9, 60.2, 60.2,

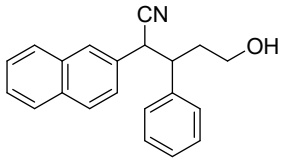


47.3, 47.2, 44.8, 44.4, 35.7, 34.1, 21.3. HRMS (ESI) m/z calcd for $C_{18}H_{20}NO$ $[M+H]^+$: 266.1545, found: 266.1547.



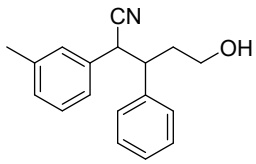

**5-Hydroxy-3-phenyl-2-(*o*-tolyl)pentanenitrile (9):**

Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless liquid. Yield: 112 mg, 85%. $^1$H NMR analysis of the crude reaction mixture showed a d.r. of 60:40. $^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 7.28 – 7.49 (m, 3H), 6.94 – 7.27 (m, 6H), 4.28 (m, 1H), 3.54 – 3.67 (m, 1H), 3.20 – 3.51 (m, 2H), 2.08 – 2.38 (m, 5H), 1.57 (s, 1H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 139.9, 138.8, 135.2, 133.1, 132.6, 131.0, 130.8, 128.9, 128.8, 128.6,128.6, 128.5, 128.2, 128.1, 127.8, 127.7, 127.7, 126.5, 126.4, 120.2, 120.1, 60.2, 60.1, 45.6, 45.4, 41.7, 40.7, 35.5, 33.8, 19.3, 19.3. HRMS (ESI) m/z calcd for $C_{18}H_{20}NO$ $[M+H]^+$: 266.1545 found: 266.1542.




**5-Hydroxy-2-(naphthalen-2-yl)-3-phenylpentanenitrile (10)**:

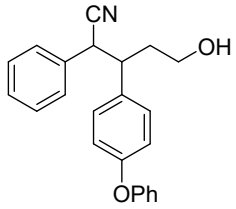
Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless liquid. Yield: 117 mg, 78%. $^1$H NMR analysis of the crude reaction mixture showed a *d.r.* of 66:34. $^1$H NMR (400 MHz, $CDCl_3$, ppm): δ 7.75 – 7.85 (m, 3H), 7.65 (dd, $J_1$ = 2.0 Hz, $J_2$ = 2.0 Hz, 1H), 7.50 – 7.54 (m, 2H), 7.12 – 7.30 (m, 6H), 4.26 (m, 1H), 3.54 – 3.65 (m, 1H), 3.33 – 3.48 (m, 2H), 2.07 – 2.20 (m, 2H), 1.66 (s, 1H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm): δ 139.3, 138.6, 133.1, 133.1, 132.8, 132.8, 131.6, 128.8, 128.7, 128.6, 128.6, 128.5, 128.2, 127.9, 127.9,127.7, 127.7, 127.7, 127.6, 127.4, 126.6, 126.6, 126.5, 126.5, 125.5, 125.5, 120.0, 119.8, 60.1, 60.0, 47.1, 47.1, 45.0, 44.5, 35.8, 34.3, 30.9. HRMS (ESI) m/z calcd for $C_{21}H_{20}NO$ $[M+H]^+$: 302.1539, found: 302.1537.




**5-Hydroxy-3-phenyl-2-(thiophen-2-yl)pentanenitrile (11):**

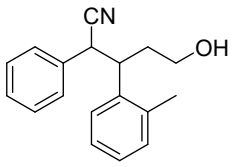
Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless liquid. Yield: 105 mg, 82%. $^1$H NMR analysis of the crude reaction mixture showed a *d.r.* of 73:27. $^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 7.28 – 7.32 (m, 4H), 7.13 – 7.21 (m, 2H), 7.00 – 7.11

(m, 1H), 6.86 – 6.90 (m, 1H), 4.20 (m, 1H), 3.58 – 3.69 (m, 1H), 3.29 – 3.51 (m, 2H), 2.09 – 2.27 (m, 2H), 1.60 (s, 1H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 139.4, 138.7, 134.3, 134.2, 128.8, 128.6, 128.4, 128.1, 127.7, 126.8, 126.8, 126.6, 126.6, 123.6, 123.6, 119.8, 119.5, 60.1, 60.1, 46.5, 46.4, 40.1, 39.5, 35.6, 34.5. HRMS (ESI) m/z calcd for $C_{15}H_{16}NOS$ $[M+H]^+$: 258.0952, found: 258.0948



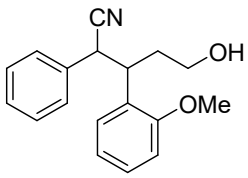

**5-Hydroxy-2-phenyl-3-(*o*-tolyl)pentanenitrile (12):**

Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless liquid. Yield: 100 mg, 76%. $^1$H NMR analysis of the crude reaction mixture showed a *d.r.* of 96:4. $^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 7.41 – 7.44 (d, $J$ =7.6 Hz, 1H), 7.29 – 7.31 (m, 3H), 7.25 – 7.28 (m, 1H), 7.08 – 7.20 (m, 4H), 4.03 (m, 1H), 3.67 – 3.72 (m, 1H), 3.58 – 3.63 (m, 1H), 3.35 – 3.41 (m, 1H), 2.01 – 2.19 (m, 5H), 1.62 (s, 1H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 137.6, 137.2, 134.4, 130.5, 128.7, 128.3, 128.2, 127.3, 126.4, 120.0, 60.1, 44.3, 40.9, 36.1, 19.5. HRMS (ESI) m/z calcd for $C_{18}H_{20}NO$ $[M+H]^+$: 266.1545, found: 266.1542




**5-Hydroxy-3-(2-methoxyphenyl)-2-phenylpentanenitrile (13):**

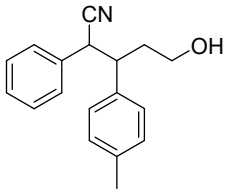
Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless liquid. Yield: 112 mg, 80%. $^1$H NMR analysis of the crude reaction mixture showed a *d.r.* of 67:33. $^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 7.19 – 7.32 (m, 7H), 6.84 – 7.01 (m, 2H), 4.19 (m, 1H), 3.67 – 3.84 (m, 4H), 3.49 – 3.58 (m, 1H), 3.32 – 3.39 (m, 1H), 1.93 – 2.30 (m, 2H), 1.69 (s, 1H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 157.5, 157.2, 135.1, 134.5, 128.7, 128.7, 128.6, 128.6, 138.5, 128.4, 128.2, 128.0, 127.9, 127.8, 127.3, 127.2, 121.1, 120.9, 120.4, 120.0, 111.0, 110.8, 60.4, 55.5, 55.5, 43.0, 42.9, 34.5, 32.6. HRMS (ESI) m/z calcd for $C_{18}H_{20}NO_2$ $[M+H]^+$: 282.1494, found: 282.1490




**5-Hydroxy-3-(4-phenoxyphenyl)-2-phenylpentanenitrile（14）：**

Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless liquid. Yield: 145 mg, 85%. $^1$H NMR analysis of the crude reaction mixture showed a *d.r.* of 77:23. $^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 7.24 – 7.36 (m, 6H), 7.09 – 7.18 (m, 3H), 6.87 – 7.00

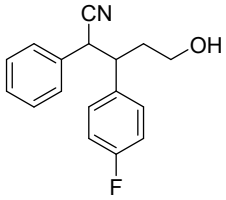
(m, 4H), 6.70 – 6.75 (m, 1H), 4.06 (m, 1H), 3.59 – 3.68 (m, 1H), 3.37 – 3.50 (m, 1H), 3.24 – 3.31 (m, 1H), 2.04 – 2.34 (m, 2H), 1.53 (s, 1H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 157.1, 157.0, 141.3, 140.7, 134.2, 134.2, 130.1, 130.0, 129.8, 129.7, 128.8, 128.8, 128.2, 128.1, 128.1, 123.3, 123.2, 123.1, 122.9, 119.6, 119.3, 119.0, 118.7, 118.6, 118.3, 118.2, 60.0, 47.3, 47.0, 44.6, 44.1, 35.7, 34.8.




HRMS(ESI) m/z calcd for $C_{23}H_{22}NO_2$ $[M+H]^+$: 344.1651, found: 344.1657.

**3-(4-Fluorophenyl)-5-hydroxy-2-phenylpentanenitrile（15）:**

Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless liquid. Yield: 105 mg, 78%. $^1$H NMR analysis of the crude reaction mixture showed a *d.r.* of 77:23. $^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 7.29 – 7.31 (m, 3H), 7.04 – 7.17 (m, 4H), 6.94 – 7.00 (m, 2H), 4.07 (m, 1H), 3.64 – 3.76 (m, 1H), 3.43 – 3.62 (m, 1H), 3.28 – 3.39 (m, 1H), 2.05 – 2.31 (m, 2H), 1.65 (s, 1H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 163.5, 161.0, 134.1, 134.0, 130.1,130.0, 129.8, 129.7, 128.8, 128.8, 128.2, 128.2, 128.1, 128.1, 119.5, 115.5, 115.3, 59.9, 59.9, 46.5, 46.4, 44.8, 44.3, 35.8, 34.5. HRMS (ESI) m/z calcd for $C_{17}H_{17}FNO$ $[M+H]^+$: 270.1294, found: 270.1297.



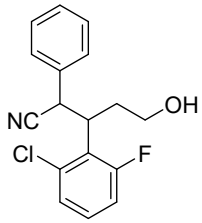

**5-Hydroxy-2-phenyl-3-(*p*-tolyl)pentanenitrile (16):**

Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless liquid. Yield: 112 mg, 85%. $^1$H NMR analysis of the crude reaction mixture showed a *d.r.* of 70:30. $^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 7.28 – 7.32 (m, 3H), 7.06 – 7.22 (m, 4H), 6.92 – 6.99 (m, 2H), 4.06 (m, 1H), 3.59 – 3.64 (m, 1H), 3.35 – 3.48 (m, 1H), 3.20 – 3.27 (m, 1H), 2.31 – 2.32 (m, 3H), 1.98 – 2.07 (m, 2H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 139.3, 138.6, 138.4, 138.1, 134.5, 134.4, 129.2, 128.9, 128.7, 128.6, 128.5, 128.4, 128.4, 128.2, 128.1, 128.1, 128.0, 125.4, 125.1,

119.9, 119.8, 60.3, 60.2, 47.3, 47.1, 44.9, 44.4, 35.6, 34.2, 21.4. HRMS (ESI) m/z calcd for $C_{18}H_{20}NO$ $[M+H]^+$: 266.1545, found: 266.1548.

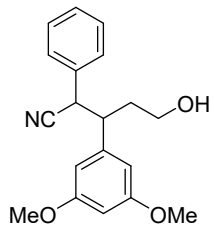
**3-(2-Chloro-6-fluorophenyl)-5-hydroxy-2-phenylpentanenitrile (17):**

Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless liquid. Yield: 94 mg, 62%. $^1$H NMR analysis of the crude reaction mixture showed a *d.r.* of 60:40. $^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 7.38 – 7.47 (m, 2H), 7.28 – 7.32 (m, 1H), 7.19 – 7.23 (m, 3H), 6.96 – 7.07 (m, 2H), 4.26 (m, 1H), 4.05 – 4.17 (m, 1H), 3.28 – 3.69 (m, 2H), 2.34 – 2.55 (m, 1H), 1.73 – 2.08 (m, 1H), 1.67 (s, 1H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ134.5, 134.1, 129.7, 129.6, 129.3, 129.3, 129.2, 128.7, 128.7, 128.5, 128.3, 127.7, 126.1, 126.1, 125.7, 120.5, 119.6, 115.4, 115.1, 60.5, 60.3, 42.1, 42.1, 41.3, 41.3, 33.4, 33.4. HRMS (ESI) m/z calcd for $C_{17}H_{16}ClFNO$ $[M+H]^+$: 304.0904, found: 304.0907.

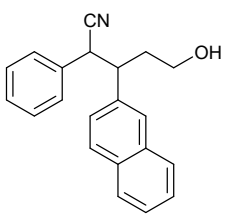



**3-(3,5-Dimethoxyphenyl)-5-hydroxy-2-phenylpentanenitrile（18）:**

Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless liquid. Yield: 133 mg, 86%. $^1$H NMR analysis of the crude reaction mixture showed a *d.r.* of 80:20. $^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 7.28 – 7.32 (m, 3H), 7.14 – 7.22 (m, 2H), 6.34 – 6.37 (m, 1H), 6.26 – 6.31 (m, 2H) 4.05 (m, 1H), 3.72 – 3.74 (d, $J$ = 6.8 Hz, 6H), 3.59 – 3.65 (m, 1H), 3.43 – 3.50 (m, 1H), 3.18 – 3.24 (m, 1H), 1.99 – 2.06 (m, 2H), 1.65 (s, 1H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 161.0, 160.8, 141.8, 141.0, 134.4, 134.3, 128.7, 128.2, 128.1, 128.1, 128.1, 120.0, 119.8, 106.6, 106.3, 99.7, 99.4, 60.1, 55.3, 55.3, 55.3, 47.6, 47.4, 44.6, 44.2, 35.6, 34.3. HRMS (ESI) m/z calcd for $C_{19}H_{22}NO_3$ $[M+H]^+$: 312.1599, found: 312.1595.

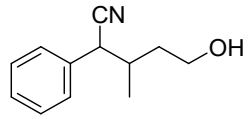



**5-hydroxy-3-(naphthalen-2-yl)-2-phenyl pentanenitrile (19):**

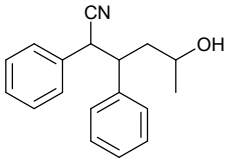



Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless liquid. Yield: 80 mg, 85%. $^1$H NMR analysis of the crude reaction mixture showed a *d.r.* of 71:29. $^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 7.77 – 7.84 (m, 3H), 7.48 – 7.59(m, 3H), 7.16 – 7.33 (m, 6H), 4.16 (m, 1H),3.44 –

3.64 (m, 3H), 2.13 – 2.34 (m, 2H), 1.67 (s, 1H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 136.6, 136.1, 134.3, 134.2, 133.3, 133.3, 132.9, 132.8, 128.8, 128.6, 128.3, 128.2, 128.1, 128.1, 127.9, 127.8, 127.7, 127.5, 126.3, 126.2, 126.1, 126.0, 126.0, 125.6, 120.0, 119.8, 60.1, 60.1, 47.4, 47.2, 44.7, 44.3, 35.6, 34.4. HRMS (ESI) m/z calcd for $C_{21}H_{20}NO$ $[M+H]^+$: 302.1537, found: 302.1533.




**5-hydroxy-2,3-diphenyl hexanenitrile (20):**

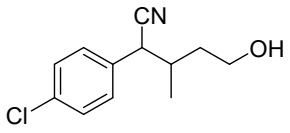



Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless liquid. Yield: 80 mg, 85%. $^1$H NMR analysis of the crude reaction mixture showed a *d.r.* of 56:44. $^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 7.28 (s, 5H), 7.10 – 7.15 (d, $J$ = 20.0 Hz, 4H), 4.11 (m, 1H), 3.63 – 3.85 (m, 1H), 3.13 – 3.23 (m, 1H), 1.98 – 2.30 (m, 2H), 1.61 (s, 1H), 1.11 – 1.20 (dd, $J_1$ = 6.8 Hz, $J_2$ = 6.4 Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 139.4, 138.9, 134.2, 134.1, 128.8, 128.7, 128.7, 128.6, 128.5, 128.4, 128.2, 128.1, 128.1, 128.1, 127.7, 120.0, 119.6, 66.3, 65.7, 48.4, 47.4, 44.9, 43.7, 42.1, 41.2, 23.5, 22.9. HRMS (ESI) m/z calcd for $C_{18}H_{20}NO$ $[M+H]^+$: 266.1537, found: 266.1532.

**5-Hydroxy-3-methyl-2-phenylpentanenitrile (21):**

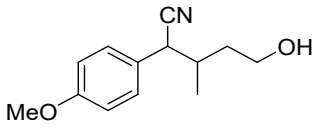
Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless liquid. Yield: 80 mg, 85%. $^1$H NMR analysis of the crude reaction mixture showed a *d.r.* of 78:22. $^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 7.32 – 7.41 (m, 5H), 3.82 – 4.01 (m, 1H), 3.60 – 3.79 (m, 2H), 2.18 – 2.28 (m, 1H), 1.98 (s, 1H), 1.77 – 1.86 (m, 1H), 1.45 – 1.67 (m, 2H), 1.04 (dd, $J_1$ = 6.8 Hz, $J_2$ = 6.4 Hz, 1H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 134.8, 134.3, 128.9, 128.9, 128.1, 128.1, 128.0, 127.8, 127.8, 120.1, 119.5, 60.1, 60.1, 44.2, 43.4, 37.5, 35.4, 35.3, 35.1, 17.5, 15.6. HRMS (ESI) m/z calcd for $C_{12}H_{16}NO$ $[M+H]^+$: 190.1232, found: 190.1230.

**2-(4-Chlorophenyl)-5-hydroxy-3-methylpentanenitrile (22)**:



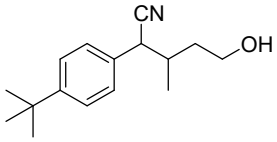

Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless liquid. Yield: 89 mg, 80%.$^{1}$H NMR analysis of the crude reaction mixture showed a d.r. of 60:40. $^{1}$H NMR (400 MHz, $CDCl_3$, ppm) δ 7.37 – 7.39 (d, *J* = 8.0 Hz, 2H), 7.27 – 7.30 (m, 2H), 4.08 (m, 1H), 3.62 – 4.01 (m, 3H), 2.19 – 2.26 (m, 1H), 1.61 – 1.83 (m, 3H), 1.04 (m, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 134.2, 134.0, 133.3, 132.8, 129.4, 129.2, 129.1, 129.1, 119.6, 119.0, 60.1, 60.1, 43.6, 42.8, 37.3, 35.4, 35.3, 35.1, 17.5, 15.5. HRMS (ESI) m/z calcd for $C_{12}H_{15}ClNO$ $[M+H]^+$: 224.0842, found: 224.0837.

**5-Hydroxy-2-(4-methoxyphenyl)-3-methylpentanenitrile (23):**




Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless liquid. Yield: 97 mg, 89%. $^{1}$H NMR analysis of the crude reaction mixture showed a d.r. of 48:52. $^{1}$H NMR (400 MHz, $CDCl_3$, ppm) δ 7.23 – 7.26 (m, 2H), 6.89 – 6.92 (m, 2H), 3.81 – 3.93 (m, 4H), 3.62 – 3.78 (m, 2H), 2.15 – 2.22 (m, 1H), 1.78 – 1.84 (m, 1H), 1.44 – 1.64 (m, 2H), 1.04 (m, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 159.4, 159.3, 129.2, 128.9, 126.7, 126.2, 120.3, 119.7, 114.3, 114.3, 60.2, 55.3, 43.4, 42.7, 37.4, 35.5, 35.4, 35.1, 17.5, 15.7. HRMS (ESI) m/z calcd for $C_{13}H_{18}NO_2$ $[M+H]^+$: 220.1337, found: 220.1335.

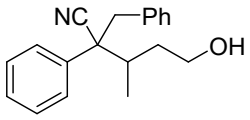
**2-(4-(Tert-butyl)phenyl)-5-hydroxy-3-methylpentanenitrile (24):**




Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless liquid. Yield: 110 mg, 90%. $^{1}$H NMR analysis of the crude reaction mixture showed a d.r. of 56:44. $^{1}$H NMR (400 MHz, $CDCl_3$, ppm) δ 7.39 – 7.41 (m, 2H), 7.25 – 7.28 (m, 2H), 3.60 – 3.96 (m, 3H), 2.18 – 2.27 (m, 1H), 1.78 – 1.86 (m, 2H), 1.49 – 1.66 (m, 1H), 1.05 (m, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 151.1, 151.0, 131.6, 131.2, 127.7, 127.5, 125.8, 125.8, 120.2,119.7, 60.2, 43.8, 43.0, 37.5, 35.4, 35.2, 35.0, 34.6, 34.5, 31.3, 17.6, 15.7. HRMS (ESI) m/z calcd for $C_{16}H_{24}NO$ $[M+H]^+$: 246.1858, found: 246.1857.

**3-(2-Hydroxyethyl)-2-phenylhexanenitrile (25):**

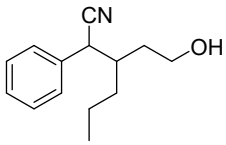
Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless liquid. Yield: 86 mg, 80%. $^1$H NMR analysis of the crude reaction mixture showed a *d.r.* of 50:50. $^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 7.37 – 7.42 (m, 5H), 4.11 (m, 1H), 3.52 – 3.83 (m, 2H), 2.05 – 2.11 (m, 1H), 1.62 – 1.83 (m, 3H), 1.41 – 1.51 (m, 4H), 0.82 – 0.99 (m, 3H). $^{13}$C NMR




(100 MHz, $CDCl_3$, ppm) δ 134.8, 134.7, 129.0, 128.9, 128.0, 127.9, 127.9, 127.8, 119.9, 119.6, 60.5, 60.3, 41.4, 41.3, 40.0, 39.9, 34.2, 34.1, 33.2, 32.4, 20.0, 19.8, 14.1, 14.0. HRMS (ESI) m/z calcd for $C_{14}H_{20}NO$ $[M+H]^+$: 218.1545, found: 218.1542.

**5-Hydroxy-2,3-dimethyl-2-phenylpentanenitrile (26):**

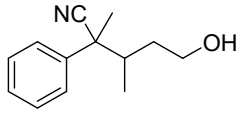
Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent.




Colorless liquid. Yield: 95mg, 94%. $^1$H NMR analysis of the crude reaction mixture showed a *d.r.* of 57:43. $^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 7.29 – 7.46 (m, 5H), 7.47 (t, $J$ = 5.8 Hz, 2H), 7.04 (t, $J$ = 7.6 Hz, 2H), 7.32 (d, $J$ = 7.2 Hz, 1H), 3.47 – 3.80 (m, 2H), 2.13 – 2.20 (m, 1H), 1.95 – 2.02 (m, 1H), 1.72 (d, $J$ = 9.6 Hz, 3H), 1.20 – 1.61(m, 2H), 1.02 (m ,3H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 140.3, 140.2, 128.9, 128.8, 128.8, 127.7, 127.7, 126.0, 125.9, 122.6, 122.4, 60.3, 60.3, 47.6, 47.4, 39.4, 39.2, 35.5, 34.6, 25.2, 24.6, 15.4, 14.7. HRMS (ESI) m/z calcd for $C_{13}H_{18}NO$ $[M+H]^+$: 204.1388, found: 204.1385.

**2-Benzyl-5-hydroxy-3-methyl-2-phenylpentanenitrile (27):**

Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent.

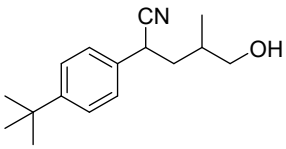



Colorless liquid. Yield: 125 mg, 90%. $^1$H NMR analysis of the crude reaction mixture showed a *d.r.* of 70:30. $^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 7.25 – 7.29 (m, 5H), 7.07 – 7.13 (m, 3H), 6.82 – 6.87 (m, 2H), 3.75 – 3.95 (m, 2H), 3.03 – 3.54 (m, 2H), 2.34 – 2.51 (m, 2H), 1.68 – 1.74 (m, 1H), 1.15 (m, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 137.4, 137.3, 135.4, 135.3, 135.3, 130.2, 128.6, 128.5, 128.5, 127.8, 127.8, 127.7, 127.6, 127.1, 127.0, 127.0, 126.9, 120.8, 120.7, 60.4, 60.4, 55.4, 55.2, 44.6, 44.1, 38.2, 37.8, 35.6, 35.5, 15.7, 15.4. HRMS (ESI) m/z calcd for $C_{19}H_{22}NO$ $[M+H]^+$: 280.1701, found: 280.1708.

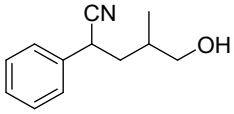
**5-Hydroxy-4-methyl-2-phenylpentanenitrile (28)**:

Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless liquid. Yield: 80 mg, 85%. $^{1}$H NMR analysis of the crude reaction mixture showed a d.r. of 53:47. $^{1}$H NMR (400 MHz, $CDCl_3$, ppm) δ 7.31 – 7.42 (m, 5H), 3.92 – 4.04 (m, 1H), 3.48 – 3.66 (m, 2H), 1.88 – 2.22 (m, 2H), 1.61 – 1.84 (m, 2H), 1.02 (m ,3H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 136.2, 129.2, 128.1, 127.3, 127.3, 121.4, 120.8, 67.6, 67.2, 40.1, 39.8, 35.5, 35.3, 33.8, 33.5, 16.9, 16.0. HRMS (ESI) m/z calcd for $C_{12}H_{16}NO$ $[M+H]^+$: 190.1232, found: 190.1230.

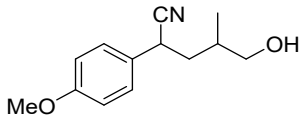
**2-(4-(*Tert*-butyl)phenyl)-5-hydroxy-4-methylpentanenitrile (29):**




Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless liquid. Yield: 104 mg, 85%. $^{1}$H NMR analysis of the crude reaction mixture showed a d.r. of 50:50. $^{1}$H NMR (400 MHz, $CDCl_3$, ppm) δ 7.40 – 7.43 (m, 2H), 7.27 – 7.31 (m, 2H), 3.89 – 4.00 (m, 1H), 3.50 – 3.66 (m, 2H), 2.02 – 2.19 (m, 1H), 1.82 – 1.99 (m, 2H), 1.61 – 1.68 (m, 2H), 1.34 (s, 9H), 1.33 (m, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 151.2, 151.1, 133.2, 133.1, 127.0, 126.9, 126.1, 121.5, 121.0, 67.7, 67.3, 40.0, 39.8, 34.9, 34.8, 34.6, 33.8, 33.4, 31.3, 16.9, 16.0. HRMS (ESI) m/z calcd for $C_{16}H_{24}NO$ $[M+H]^+$: 246.1858, found: 246.1855.

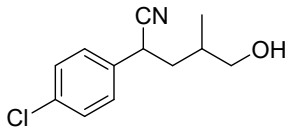



**5-Hydroxy-2-(4-methoxyphenyl)-4-methylpentanenitrile (30):**




Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless liquid. Yield: 96 mg, 88%. $^{1}$H NMR analysis of the crude reaction mixture showed a d.r. of 48:52. $^{1}$H NMR (400 MHz, $CDCl_3$, ppm) δ 7.26 – 7.29 (m, 2H), 6.90 – 6.93 (m, 2H), 3.88 – 3.97 (m, 1H), 3.83 (s, 3H), 3.49 – 3.65 (m, 2H), 1.97 – 2.18 (m, 1H), 1.80 – 1.88 (m, 1H), 1.59 – 1.66 (m, 2H), 1.02 (m, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 159.4, 128.4, 128.4, 128.2, 128.1, 121.6, 121.1, 114.5, 67.7, 67.3, 55.4, 40.1, 39.8, 34.6, 34.5, 33.8, 33.4, 16.8, 16.1. HRMS (ESI) m/z calcd for $C_{13}H_{18}NO_2$ $[M+H]^+$: 220.1337, found: 220.1335.

**2-(4-Chlorophenyl)-5-hydroxy-4-methylpentanenitrile (31):**

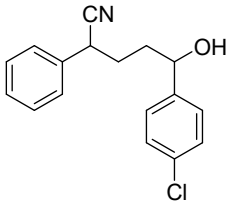



Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless liquid. Yield: 88 mg, 79%. $^{1}$H NMR analysis of the crude reaction mixture showed a d.r. of 48:52. $^{1}$H NMR (400 MHz, $CDCl_3$, ppm) δ 7.36 – 7.39 (m, 2H), 7.28 – 7.32 (m, 2H), 3.92 – 4.05 (m, 1H), 3.49 – 3.68 (m, 2H), 1.95 – 2.20 (m, 2H), 1.59 – 1.89 (m, 3H), 1.02 (m, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 134.8, 134.7, 134.1, 134.1, 129.3, 128.7, 128.7, 120.9, 120.4, 67.6, 67.2, 40.2, 39.8, 35.0, 34.8, 33.7, 33.4, 16.9, 16.0. HRMS (ESI) m/z calcd for $C_{12}H_{15}ClNO$ $[M+H]^+$: 224.0842, found: 224.0838.

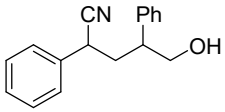
**5-Hydroxy-2,4-diphenylpentanenitrile (32)**:

Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless liquid. Yield: 106 mg, 85%. $^{1}$H NMR (400 MHz, $CDCl_3$, ppm) δ 7.32 – 7.45 (m, 7H), 7.18 – 7.27 (m, 3H), 3.70 – 3.87 (m, 2H), 3.49 – 3.68 (m, 1H), 2.77 – 3.25 (m, 1H), 2.09 – 2.46 (m, 2H), 1.85 (s, 1H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 140.2, 140.2, 140.0, 140.0, 136.1, 135.4, 129.2, 129.2, 129.1, 129.0, 128.3, 128.1, 128.0, 127.8, 127.6, 127.5, 127.1, 121.3, 120.4, 67.0, 66.9, 46.9, 45.3, 38.8, 37.8, 35.5, 34.8. HRMS (ESI) m/z calcd for $C_{17}H_{18}NO$ $[M+H]^+$: 252.1388, found: 252.1386.

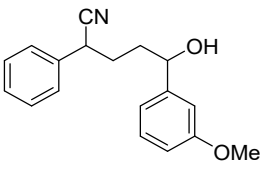
**5-(4-Chlorophenyl)-5-hydroxy-2-phenylpentanenitrile (33):**




Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless liquid. Yield: 114 mg, 80%. $^{1}$H NMR (400 MHz, $CDCl_3$, ppm) δ 7.31 – 7.42 (m, 9H), 4.72 – 4.77 (m, 1H), 3.83 – 3.89 (m, 1H), 1.86 – 2.03 (m, 4H), 1.64 (s, 1H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 143.9, 135.7, 129.1, 128.7, 128.7, 128.1, 127.9, 127.9, 127.3, 127.3, 125.7, 120.7, 74.0, 73.7, 37.3, 37.0, 36.1, 35.8, 32.3, 31.9. HRMS (ESI) m/z calcd for $C_{17}H_{17}ClNO$ $[M+H]^+$: 286.0998, found: 286.0994.



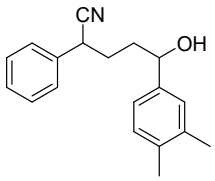

**5-Hydroxy-2-(4-methoxyphenyl)-4-methylpentanenitrile (34):**




Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless liquid. Yield: 122 mg, 87%. $^{1}$H NMR

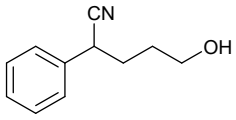
analysis of the crude reaction mixture showed a *d.r.* of 50:50. $^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 7.27 – 7.41 (m, 6H), 6.83 – 6.92 (m, 3H), 4.69 – 4.74 (m, 1H), 3.83 (d, *J* = 2.0 Hz, 3H), 2.04 – 2.15 (m, 2H), 1.87 – 1.96 (m, 2H), 1.72 (s, 1H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 159.9, 145.6, 145.6, 135.7, 135.7, 129.7, 129.7, 129.1, 128.1, 127.3, 127.3, 120.7, 120.7, 118.0, 113.3, 113.3, 111.3, 111.3, 73.9, 73.6, 55.3, 37.3, 37.0, 36.0, 35.7, 32.2, 31.8. HRMS (ESI) m/z calcd for $C_{17}H_{18}NO_2$ $[M+H]^+$: 282.1494, found: 282.1489.

**5-(3,4-Dimethylphenyl)-5-hydroxy-2-phenylpentanenitrile (35):**



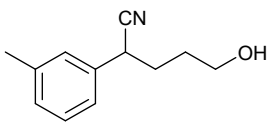

Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless liquid. Yield: 118 mg, 85%. $^1$H NMR analysis of the crude reaction mixture showed a d.r. of 50:50. $^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 7.32 – 7.44 (m, 5H), 7.05 – 7.17 (m, 3H), 4.65 – 4.69 (m, 1H), 3.83 – 3.97 (m, 1H), 2.28 (s, 6H), 2.16 – 1.84 (m, 4H), 1.64 (s, 1H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 141.4, 136.9, 136.3, 135.8, 135.8, 135.7, 129.9, 129.1, 129.1, 128.7, 128.1, 127.3, 127.3, 127.0, 123.2, 120.7, 73.9, 73.6, 37.3, 37.0, 36.0, 35.7, 32.4, 32.0, 19.8, 19.4. HRMS (ESI) m/z calcd for $C_{19}H_{22}NO$ $[M+H]^+$: 280.1701, found: 280.1703.

**5-Hydroxy-2-phenylpentanenitrile (36)**:




Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless oil. Yield: 74 mg, 85%. $^1$H NMR (400 MHz, $CDCl_3$, ppm): δ 7.34 – 7.42 (m, 5H), 3.88 (t, *J* = 7.4 Hz, 1H), 3.68 – 3.71 (m, 2H), 2.00 – 2.06 (m, 2H), 1.86 (s, 1H), 1.70 – 1.77 (m, 2H). $^{13}$C NMR (100. MHz, $CDCl_3$, ppm): δ 135.8, 129.1, 128.1, 127.3, 120.8, 61.8, 37.2, 32.4, 29.8. HRMS (ESI) m/z calcd for $C_{11}H_{14}NO$ $[M+H]^+$: 176.1075, found: 176.1073.

**5-Hydroxy-2-(*m*-tolyl) pentanenitrile (37)**:

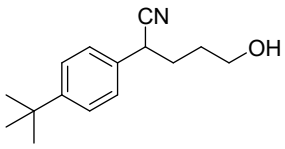



Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless liquid. Yield: 77 mg, 82%. $^1$H NMR (400 MHz, $CDCl_3$, ppm): δ 7.26 – 7.29 (m, 1H), 7.13 – 7.17 (m, 3H), 3.84 (t, *J* = 7.4 Hz, 1H), 3.67 – 3.70 (m, 2H), 2.38 (s, 3H), 1.98 – 2.04 (m, 2H), 1.69

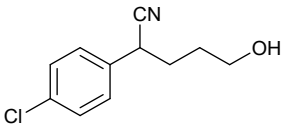
– 1.78 (m, 2H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm): δ 138.9, 135.7, 129.0, 128.9, 127.9, 124.3, 121.0, 61.8, 37.1, 32.4, 29.9, 21.4. HRMS (ESI) m/z calcd for $C_{12}H_{16}NO$ $[M+H]^+$: 190.1232, found: 190.1225.

**5-Hydroxy-2-(*o*-tolyl)pentanenitrile (38):**

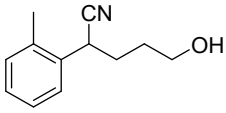
Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless oil. Yield: 80 mg, 85%. $^1$H NMR (400 MHz, $CDCl_3$, ppm): δ 7.43 – 7.45 (m, 1H), 7.19 – 7.28 (m, 3H), 4.03 – 4.07 (m, 1H), 3.66 – 3.76 (m, 2H), 2.37 (s, 3H), 2.06 (s, 1H), 1.95 – 2.02 (m, 2H), 1.75 – 1.87 (m, 2H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm): δ 135.0, 134.1, 131.0, 128.1, 127.4, 126.9, 121.1, 61.7, 34.0, 31.1, 30.1, 19.1. HRMS (ESI) m/z calcd for $C_{12}H_{16}NO$ $[M+H]^+$: 190.1232, found: 190.1227.




**2-(4-Chlorophenyl)-5-hydroxypentanenitrile (39):**




Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless liquid. Yield: 85 mg, 82%. $^1$H NMR (400 MHz, $CDCl_3$, ppm): δ 7.34 (dd, $J_1$ = 31.6 Hz, $J_2$ = 8.4 Hz, 2H), 3.88 (t, $J$ = 7.4 Hz, 1H), 3.70 – 3.74 (m, 2H), 2.00 – 2.06 (m, 2H), 1.71 – 1.79 (m, 2H), 1.60 (s, 1H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm): δ 134.3, 134.2, 129.3, 128.6, 120.3, 61.8, 36.6, 32.4, 29.7. HRMS (ESI) m/z calcd for $C_{11}H_{13}ClNO$ $[M+H]^+$: 210.0685, found: 210.0688.

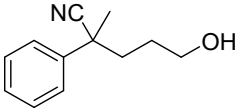



**2-(4-(*Tert*-butyl)phenyl)-5-hydroxypentanenitrile (40):**

Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless liquid. Yield: 98 mg, 85%. $^1$H NMR (400 MHz, $CDCl_3$, ppm): δ 7.40 – 7.42 (dd, $J_1$ = 52 Hz, $J_2$ = 8.4 Hz, 4H), 3.84 – 3.88 (t, $J$ = 7.4 Hz, 1H), 3.67 – 3.71 (m, 2H), 1.99 – 2.05 (m, 2H), 1.89 (s, 1H), 1.73 – 1.80 (m, 2H), 1.34 (s, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm): δ 151.2, 132.7, 127.0, 126.0, 121.0, 61.8, 61.7, 36.7, 34.6, 32.3, 31.3, 29.9. HRMS (ESI) m/z calcd for $C_{15}H_{22}NO$ $[M+H]^+$: 232.1701, found: 232.1707.

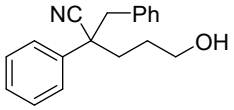
**5-Hydroxy-2-(naphthalen-2-yl) pentanenitrile (41):**

Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless liquid. Yield: 85 mg, 76%. $^1$H NMR (400 MHz, $CDCl_3$, ppm): δ 7.89 – 7.84 (m, 4H), 7.52 – 7.54 (m, 2H), 7.41 – 7.44 (m, 1H), 4.03 – 4.06 (m, 1H), 3.68 – 3.71 (m, 2H), 2.14 – 2.09 (q, *J* = 7.6 Hz, 2H), 1.88 (s, 1H), 1.75 – 1.79 (m, 2H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm): δ133.0, 129.1, 127.9, 127.7, 126.8, 126.5, 126.4, 124.8, 120.8, 61.8, 37.3, 32.3, 29.9. HRMS (ESI) m/z calcd for $C_{15}H_{16}NO$ $[M+H]^+$: 226.1232, found: 226.1228.

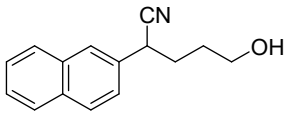



**2-(3,4-Dimethoxyphenyl)-5-hydroxypentanenitrile (42):**

Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless liquid. Yield: 82 mg, 70%. $^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 6.84 – 6.90 (m, 3H), 7.14 – 7.22 (m, 2H), 6.34 – 6.40 (m, 1H), 6.23 – 6.32 (m, 2H), 3.99 (d, *J* = 8.0 Hz, 6H), 3.82 (t, *J* = 7.4 Hz, 1H), 3.66 – 3.73 (m, 2H), 1.99 – 2.03 (m, 2H), 1.74 – 1.81 (m, 2H), 1.70 (s, 1H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 149.5, 148.9, 128.2, 121.0, 119.6, 111.6, 110.4, 61.8, 56.0, 56.0, 36.8, 32.4, 29.9. HRMS (ESI) m/z calcd for $C_{13}H_{18}NO_3$ $[M+H]^+$: 236.1286, found: 236.1282.

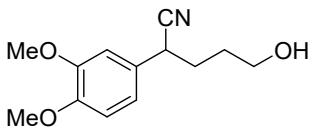



**5-Hydroxy-2-methyl-2-phenylpentanenitrile (43):**




Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless liquid. Yield: 87 mg, 92%. $^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 7.44 – 7.46 (m, 2H), 7.39 (t, *J* = 7.6 Hz, 2H), 7.32 (d, *J* = 7.2 Hz, 1H), 3.59 (t, *J* = 6.2 Hz, 2H), 2.01 – 2.07 (m, 3H), 1.73 (s, 3H), 1.67 – 1.73 (m, 1H), 1.42 – 1.51 (m 1H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 140.0, 129.0, 127.8, 125.4, 123.4, 61.9, 61.9, 42.3, 38.5, 28.7, 27.8. HRMS (ESI) m/z calcd for $C_{12}H_{16}NO$ $[M+H]^+$: 190.1232, found: 190.1230.

**2-Benzyl-5-hydroxy-2-phenylpentanenitrile (44):**



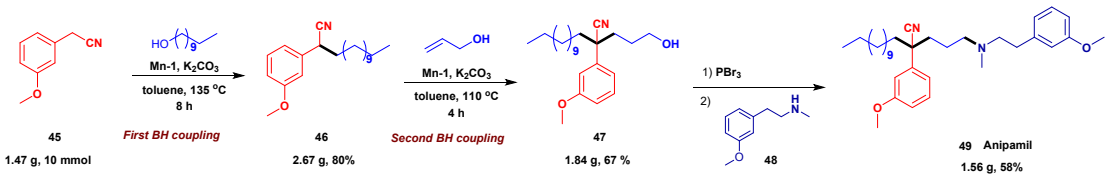

Purified by silica-gel column chromatography using ethyl acetate/hexane (1:2) mixture as eluent. Colorless liquid. Yield: 119 mg, 90%. $^1$H NMR (400 MHz, $CDCl_3$, ppm) δ 7.32 – 7.36 (m, 6H),

7.21 – 7.23 (m, 2H), 6.99 – 7.01 (m, 1H), 3.62 (t, $J$ = 6.4 Hz, 2H), 3.15 – 3.25 (m, 2H), 2.12 – 2.27 (m, 2H), 1.66 – 1.78 (m 1H), 1.66 (s, 1H), 1.41 – 1.50 (m, 1H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) δ 137.6, 134.9, 130.4, 128.8, 128.1, 127.9, 127.3, 126.4, 121.9, 62.1, 49.4, 48.0, 35.8, 28.6. HRMS (ESI) m/z calcd for $C_{18}H_{20}NO$ $[M+H]^+$: 266.1545, found: 266.1542.

## 4. Experimental for Synthesis of Biologically Active Molecules

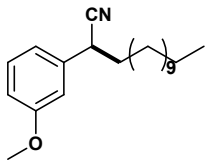
### General Procedure for the Synthesis of Anipamil (49) and verapamil intermediate (52)

Synthesis of Anipamil (**49**):




**Experimental Procedure for Synthesis of 2-(3-Methoxyphenyl) tetradecanenitrile (46):** A Schlenk flask (150 mL) was equipped with a stir bar, **Mn-1** (0.1 mmol), $K_2CO_3$ (1 mmol), 3-methoxy phenyl acetonitrile (10 mmol), 1-dodecanol (20 mmol), and toluene (30 mL) were added in sequence under nitrogen atmosphere. The flask was taken out of the glove box and fitted with a condenser, and the reaction mixture refluxed (oil bath temperature 135 °C) with stirring under $N_2$ for 4 h. Upon completion, the solvent was evaporated, and the crude reaction mixture was purified by silica-gel (100-200 mesh) column chromatography using ethyl acetate/hexane (2:98) mixture as eluent. **46** was isolated in 2.67 g, 80% yield.

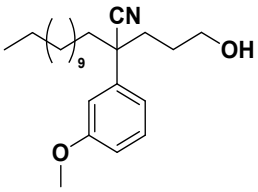
**2-(3-Methoxyphenyl) tetradecanenitrile (46)**:




Purified by silica-gel column chromatography using ethyl acetate/hexane (1:99) mixture as eluent. Colorless liquid. Yield: 312 mg, 99%. $^1$H NMR (400 MHz, $CDCl_3$, ppm): δ 7.30 – 7.33 (m, 1H), 6.86 – 6.94 (m, 3H), 3.84 (s, 3H), 3.75 (dd, $J_1$ = 4.0 Hz, $J_2$ = 4.0 Hz, 1H), 1.82 – 1.99 (m, 2H), 1.34 – 1.45 (m, 2H), 1.28 – 1.34 (m, 18H), 0.80 (t, $J$ = 8.0 Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm): δ 160.1, 137.6, 130.1, 120.8, 119.5, 113.3, 113.1, 55.3, 37.4, 35.8, 31.9, 29.6, 29.6, 29.5, 29.3, 29.3, 29.0, 27.1, 22.7, 14.1. HRMS (ESI) m/z calcd for $C_{21}H_{34}NO$ $[M+H]^+$: 316.2641, found: 316.2647.

**Experimental Procedure for Synthesis of 2-(3-Hydroxypropyl)-2-(3-methoxyphenyl) tetradecanenitrile (47)**: A Schlenk flask (38 mL) was equipped with a stir bar, **Mn-1** (0.05 mmol), $K_2CO_3$ (0.5 mmol), 2-(3-methoxyphenyl)tetradecanenitrile (**46**, 5 mmol), allyl alcohol (7.5 mmol) and toluene (10 mL) were added under nitrogen atmosphere. The solution was heated at 110 °C (oil bath temperature) with stirring under $N_2$ for 4 h. Then, the solvent was evaporated, and the resulted residue was purified by silica-gel (100-200 mesh) column chromatography using ethyl acetate/hexane (20:80) mixture as eluent. **47** was isolated in 1.84 g, 67 %.

**2-(3-Hydroxypropyl)-2-(3-methoxyphenyl) tetradecanenitrile** (**47**):



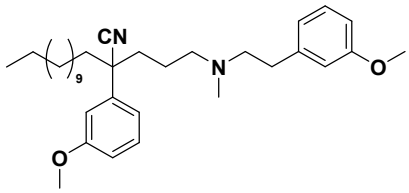

Purified by silica-gel column hromatography using ethyl acetate/hexane (30:70) mixture as eluent. Colorless liquid. Yield: 1.84 g, 67%. $^1$H-NMR (400 MHz, $CDCl_3$, ppm): δ 7.27 – 7.31 (m, 1H), 6.94 – 6.99 (m, 2H), 6.82 – 6.84 (m, 1H), 3.82 (s, 3H), 3.56 (t, $J$ = 6.2 Hz, 2H), 1.83 – 2.13 (m, 6H), 1.62 – 1.74 (m, 1H), 1.34 – 1.49 (m, 2H), 1.12 – 1.32 (m, 20H), 0.88 (t, $J$ = 6.8 Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm): δ 160.0, 140.1, 130.0, 122.6, 118.2, 112.5, 112.4, 62.1, 55.3, 48.2, 41.3, 37.5, 32.0, 29.8, 29.7, 29.7, 29.6, 29.6, 29.5, 29.4, 29.3, 28.6, 25.3, 22.8, 14.2. HRMS (ESI) m/z calcd for $C_{24}H_{40}NO_2$ $[M+H]^+$: 374.3054, found:374.3037.

**Experimental Procedure for Synthesis of Anipamil (49):** Step 1: To a round bottom flask, a magnetic stir bar, 2-(3-hydroxypropyl)-2-(3-methoxyphenyl) tetradecanenitrile (47, 0.5 mmol, 1 equiv) and toluene (1 mL) were added under nitrogen atmosphere and cooled to -5 °C. To this solution, $PBr_3$ (0.6 mmol, 1.1 equiv) was added dropwise and stirred for 30 minutes. The reaction mixture was allowed to warm to room temperature and then heated at 100 °C for 2 h. Upon completion, reaction mixture was cooled to room temperature, poured into ice, and the resulted aqueous solution was extracted using diethyl ether (2 × 10 mL). The combined organic layer was washed with brine and dried over anhydrous $Na_2SO_4$. The solvent was removed under reduced pressure using a rotavapor, and the residue was used directly in next step.

Step two: Residue (above), 2-(3-methoxyphenyl)-*N*-methylethan-1-amine (**48**, 0.3 mmol, 1 equiv.) and acetonitrile (1 mL) were charged S10 in a round bottom flask. Freshly ground anhydrous $Na_2CO_3$ (0.9 mmol, 3 equiv.) was added as one portion, and the solution was heated at 80 °C for 6

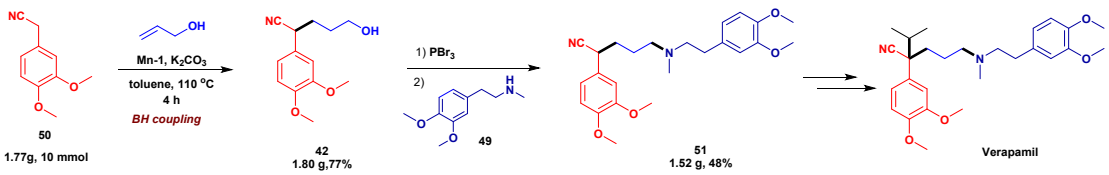
h. Upon completion of the reaction, the solvent was removed under reduced pressure using a rotavapor, and the residue obtained was dissolved in water (2 mL). The aqueous solution was extracted using ethyl acetate (3 × 10 mL), the combined organic layer washed with brine, and dried over anhydrous $Na_2SO_4$. The solvent was removed, and resulted residue purified by silica gel column chromatography using DCM/MeOH (95:5) mixture as eluent. Yields were calculated for pure isolated products. The aqueous solution was extracted using ethyl acetate (3 × 10 mL), the combined organic layer washed with brine, and dried over anhydrous $Na_2SO_4$. The solvent was removed, and the resulted residue was purified by silica gel column chromatography using DCM/MeOH (90:10) mixture as eluent. Anipamil (**49**) was isolated in 1.56 g, 58% yield.

**2-(3-((3-Methoxyphenethyl) (methyl)amino) propyl)-2-(3-methoxyphenyl) tetradecanenitrile (49):**




Purified by silica-gel column chromatography using ethyl acetate/hexane (70:30) mixture as eluent. Viscous yellow oil. Yield: 1.56 g, 58%. $^1$H NMR (400 MHz, $CDCl_3$, ppm): δ 7.30 (t, *J* = 8.0 Hz, 1H), 7.19 – 7.23 (m, 1H), 6.95-6.98 (m, 2H), 6.83 – 6.86 (m, 2H), 6.74 – 6.78 (m, 4H), 3.84 (d, *J* = 12.0 Hz, 6H), 2.72 (m, 2H), 2.55 (t, *J* = 6.0 Hz, 2H), 2.36 (m, 2H), 2.23 (s, 3H), 1.81 – 1.99 (m, 4H), 1.43 – 1.69 (m, 2H), 1.23 – 1.35 (m, 21H), 0.90 (t, *J* = 6.0 Hz, 3H). $^{13}$CNMR (100 MHz, $CDCl_3$, ppm): δ 160.0, 159.7, 142.1, 140.3, 129.9, 129.3, 122.6, 121.1, 118.2, 114.6, 112.5, 112.4, 111.3, 59.2, 56.8, 55.3, 55.1, 48.2, 41.9, 41.2, 38.7, 33.7, 31.9, 29.6, 29.5, 29.5, 29.5, 29.3, 29.3, 25.2, 23.0, 22.7, 14.1. HRMS (ESI) m/z calcd for $C_{34}H_{53}N_2O_2$ $[M+H]^+$: 521.4102, found: 521.4105.

**Synthesis of verapamil intermediate (51):**

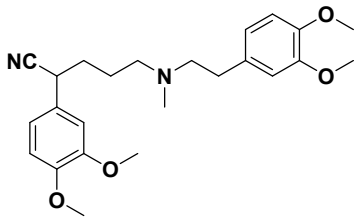


**Experimental Procedure for Synthesis of 2-(3,4-Dimethoxyphenyl)-5-hydroxypentanenitrile (42):** A Schlenk flask (38 mL) was equipped with a stir bar, **Mn-1** (0.1 mmol), $K_2CO_3$ (0.5 mmol), 2-(3,4-dimethoxyphenyl) acetonitrile (**50**, 1.77g, 10 mmol), allyl alcohol (15 mmol) and toluene (10 mL) under nitrogen atmosphere. the solution was heated at 110 °C (oil bath temperature) with stirring under $N_2$ for 4 h. Then, the solvent was evaporated, and the resulted residue was purified by silica-gel (100-200 mesh) column chromatography using ethyl acetate/hexane (20:80) mixture as eluent. **42** was isolated in 1.80 g, 77% yield.

**Experimental Procedure for Synthesis of product (51)[3]:** Step 1: To a round bottom flask, a magnetic stir bar, 2-(3,4-Dimethoxyphenyl)-5-hydroxypentanenitrile (**42**, 0.5 mmol, 1 equiv) and toluene (1 mL) were added under nitrogen atmosphere and cooled to -5 °C. To this solution, $PBr_3$ (0.6 mmol, 1.1 equiv) was added dropwise and stirred for 30 minutes. The reaction mixture was allowed to warm to room temperature and then heated at 100 °C for 2 h. Upon completion, reaction mixture was cooled to room temperature, poured into ice, and the resulted aqueous solution was extracted using diethyl ether (2 × 10 mL). The combined organic layer was washed with brine and dried over anhydrous $Na_2SO_4$. The solvent was removed under reduced pressure using a rotavapor, and the residue was used directly in next step.

Step two: Residue (above), 2-(3,4-dimethoxyphenyl)-N-methylethan-1-amine (**49**, 0.3 mmol, 1 equiv.) and acetonitrile (1 mL) were charged S10 in a round bottom flask. Freshly ground anhydrous $Na_2CO_3$ (0.9 mmol, 3 equiv.) was added as one portion, and the solution was heated at 80 °C for 6 h. Upon completion of the reaction, the solvent was removed under reduced pressure using a rotavapor, and the residue obtained was dissolved in water (2 mL). The aqueous solution was extracted using ethyl acetate (3 × 10 mL), the combined organic layer washed with brine, and dried over anhydrous $Na_2SO_4$. The solvent was removed, and resulted residue purified by silica gel column chromatography using DCM/MeOH (95:5) mixture as eluent. Yields were calculated for pure isolated products. The aqueous solution was extracted using ethyl acetate (3 × 10 mL), the combined organic layer washed with brine, and dried over anhydrous $Na_2SO_4$. The solvent was removed, and the resulted residue was purified by silica gel column chromatography using DCM/MeOH (90:10) mixture as eluent. product (**52**) was isolated in 1.52 g, 48% yield.

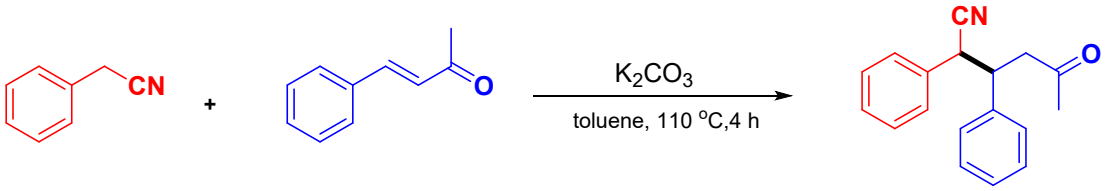
**5-((3,4-Dimethoxyphenethyl) (methyl)amino)-2-(3,4-dimethoxyphenyl) pentanenitrile (51):**



Purified by silica-gel column chromatography using DCM/MeOH (95:5) mixture as eluent. Viscous yellow oil. Yield: 1.52 g, 48%. $^{1}$H NMR (400 MHz, $CDCl_3$, ppm): δ 6.78 – 6.85 (m, 4H), 6.72 – 6.75 (m, 2H), 3.85 – 3.91 (m, 12H), 3.76 – 3.79(m, 1H), 2.69 – 2.73 (m, 2H), 2.56 – 2.60 (m, 2H), 2.42 – 2.46 (m, 2H), 2.28 (s, 3H), 1.84 – 2.00 (m, 2H), 1.59 – 1.74 (m, 2H). $^{13}$C NMR (100 MHz, $CDCl_3$, ppm): δ 149.4, 148.9, 148.9, 147.4, 133.1, 128.4, 121.0, 120.5, 119.6, 112.2, 111.5, 111.4, 110.4, 59.7, 56.7, 56.0, 56.0, 55.9, 55.9, 42.1, 36.8, 33.8, 33.5, 24.0. HRMS (ESI) m/z calcd for $C_{24}H_{33}N_2O_4$ $[M+H]^+$: 413.2440, found: 413.2445.

## 5. Mechanism Studies

**Synthesis of Products 54**

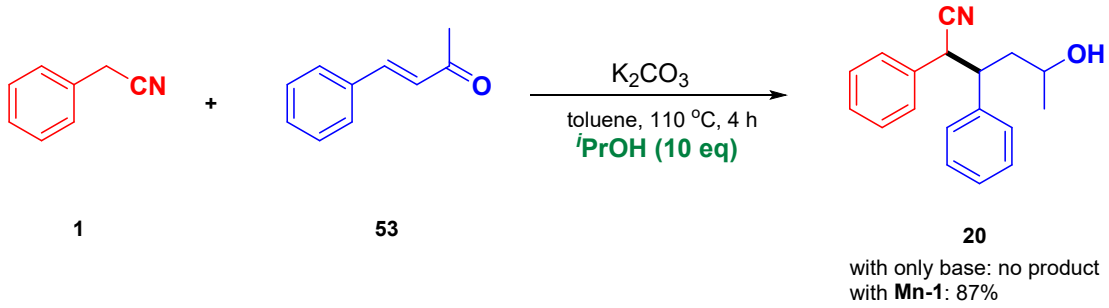



**1** **53** **54**

with only base: 25%
with **Mn-1** and base: 87%

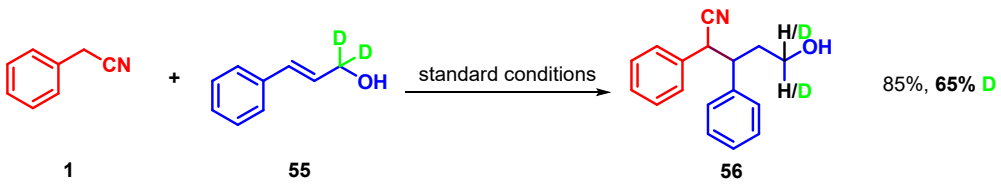
A mixture of $K_2CO_3$ (10 mol % mmol), nitriles **1** (0.5mmol), Cinnamone **53** (0.75 mmol) and toluene (1 mL) was stirred at 110 °C for 4 h under Ar in a pressure tube (ACE pressure tube, 15 mL). After cooling to room temperature, the reaction was diluted with ethyl acetate (10 mL) and water (10 mL). The organic layer was separated, and the aqueous layer was extracted with ethyl acetate (10 mL) for three times. The combined organic layer was washed by brine and dried over magnesium sulfate and the volatiles were removed under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 20:1) to give the products **54** in 33 mg, 25% yield. (give the products **54** in 114 mg, 87% yield with Mn-1)

**Synthesis of Products 20**




A mixture of $K_2CO_3$ (10 mol % mmol), nitriles **1** (0.5mmol), Cinnamone **53** (0.75 mmol), $^i$PrOH (0.4 mL) and toluene (1 mL) was stirred at 110 °C for 4 h under Ar in a pressure tube (ACE pressure tube, 15 mL). After cooling to room temperature, the reaction was diluted with ethyl acetate (10 mL) and water (10 mL). The organic layer was separated, and the aqueous layer was extracted with ethyl acetate (10 mL) for three times. The combined organic layer was washed by brine and dried over magnesium sulfate and the volatiles were removed under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1-2:1) to give the products **20** in 0 mg, 0% yield. (give the products **20** in 115 mg, 87% yield with Mn-1)

**Synthesis of Products 56**



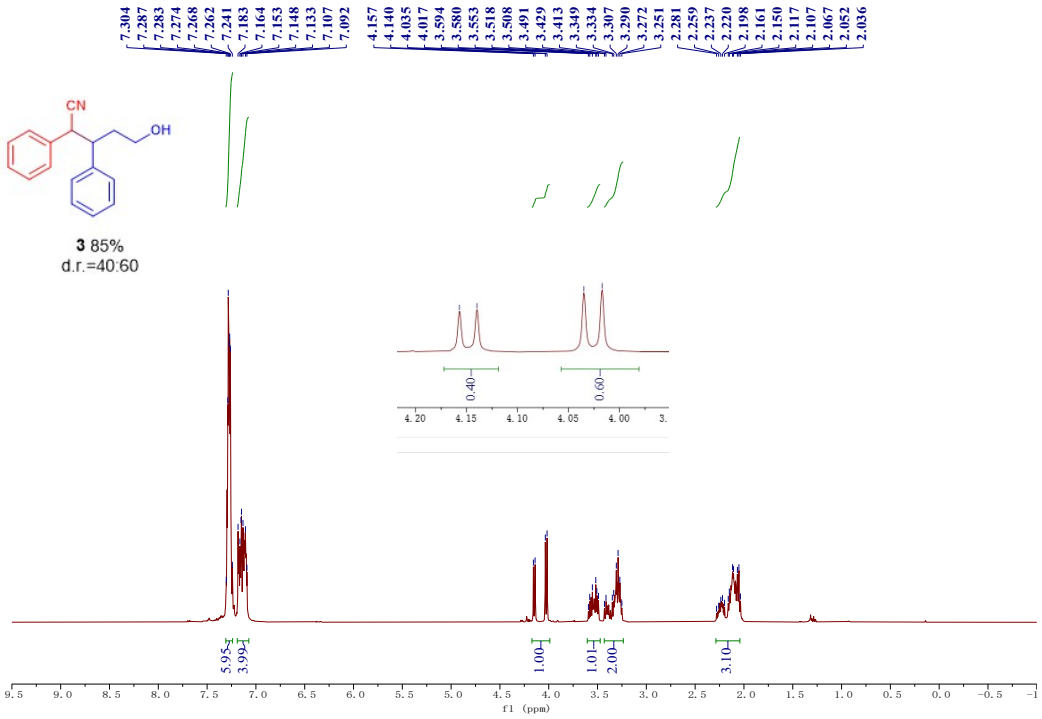

**Mn-1** (1 mol % mmol), $K_2CO_3$ (10 mol % mmol), nitrile **1** (0.5mmol), cinnamyl alcohol **55** (1 mmol) and toluene (1 mL) was stirred at 110 °C for 4 h under Ar in a pressure tube (ACE pressure tube, 15 mL). After cooling to room temperature, the reaction was diluted with ethyl acetate (10 mL) and water (10 mL). The organic layer was separated, and the aqueous layer was extracted with ethyl acetate (10 mL) for three times. The combined organic layer was washed by brine and dried over magnesium sulfate and the volatiles were removed under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1-2:1) to give the deuterated products **56**.

## 6. Reference

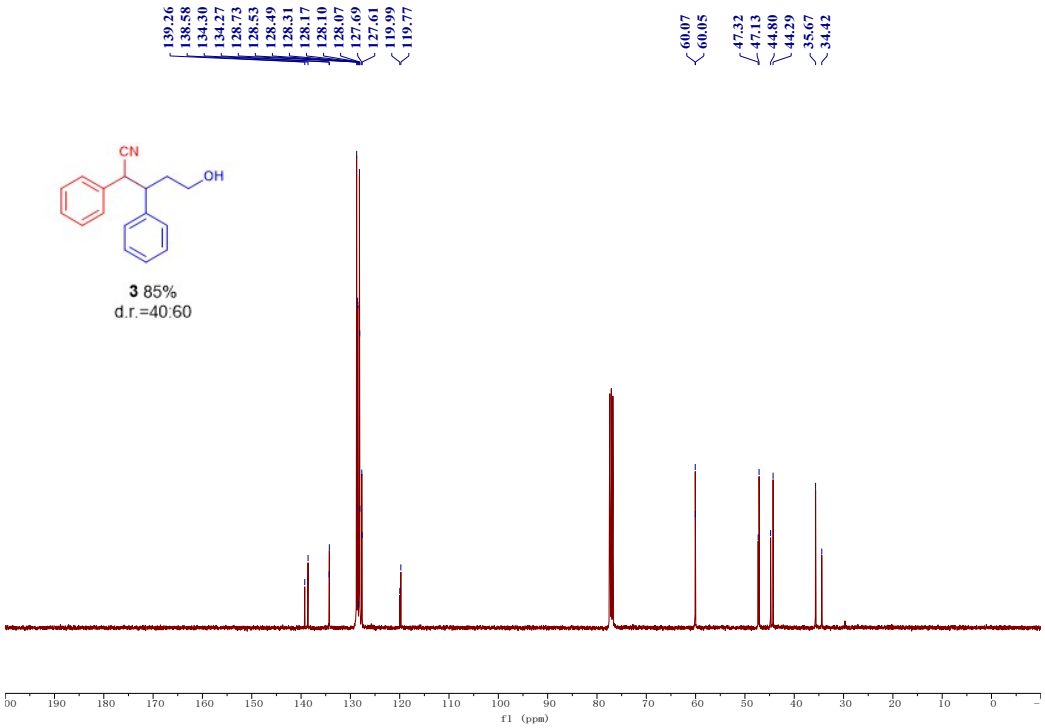
1. J. Dorfler, T. Preuss, A. Schischko, M. Schmidtmann and S. Doye, A 2,6-Bis(phenylamino)pyridinato Titanium Catalyst for theHighly Regioselective Hydroaminoalkylation of Styrenes and1,3-Butadienes. *Angew. Chem., Int. Ed.*, 2014, **53**, 7918-7922.
2. S. Estopina-Duran, E. B. McLean, L. J. Donnelly, B. M. Hockin and J. E. Taylor, Arylboronic Acid Catalyzed C-Alkylation and Allylation Reactions Using Benzylic Alcohols. *Org. Lett.*, 2020, **22**, 7547-7551.
3. S. Thiyagarajan, R. V. Sankar, P. K. Anjalikrishna, C. H. Suresh and C. Gunanathan, Catalytic Formal Conjugate Addition: Direct Synthesis of $\delta$-Hydroxynitriles from Nitriles and Allylic Alcohols. *ACS Catalysis*, 2022, **12**, 2191-2204.

## 7. NMR spectra

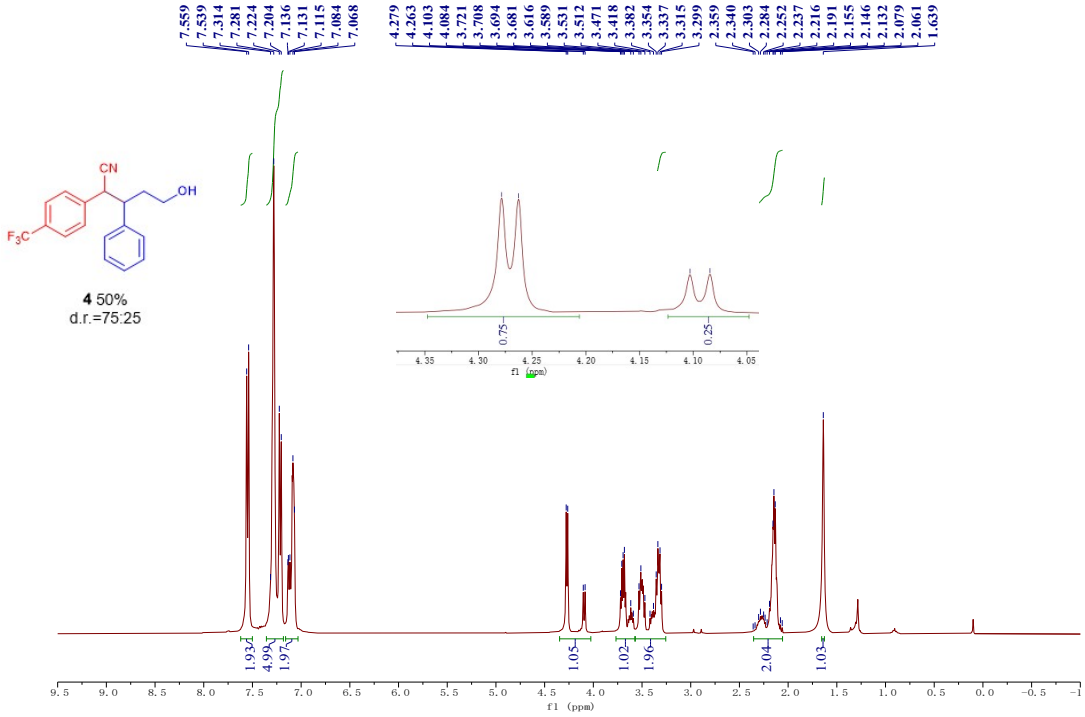
$^{1}$H NMR spectrum of 5-hydroxy-2,3-diphenylpentanenitrile (**3**, 400 MHz, $CDCl_3$):



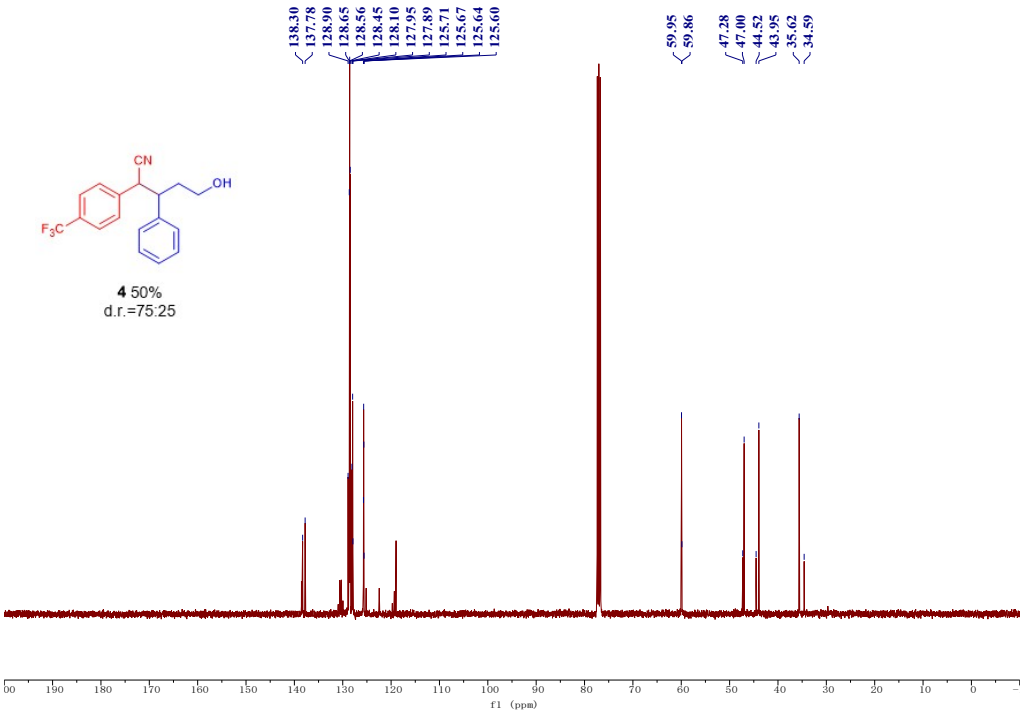

$^{13}$C NMR spectrum of 5-hydroxy-2,3-diphenylpentanenitrile (**3**, 100 MHz, $CDCl_3$):



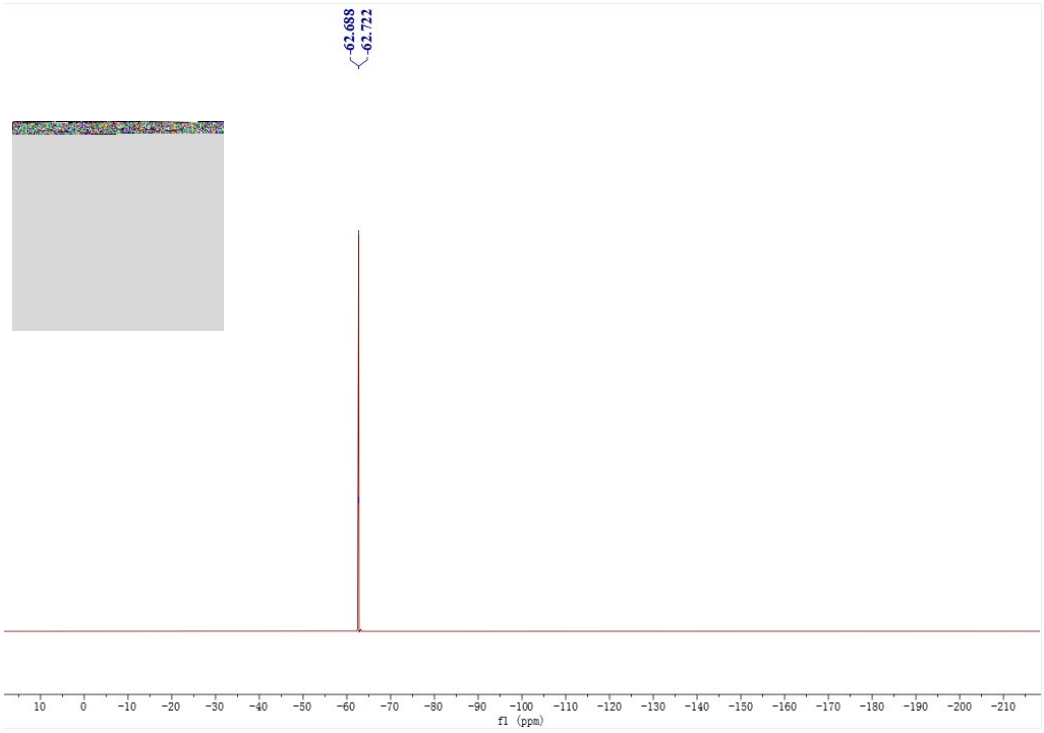
$^{1}$H NMR spectrum of 5-hydroxy-3-phenyl-2-(4-(tri-fluoromethyl)phenyl) pentan-enitrile (**4**, 400 MHz, $CDCl_3$):



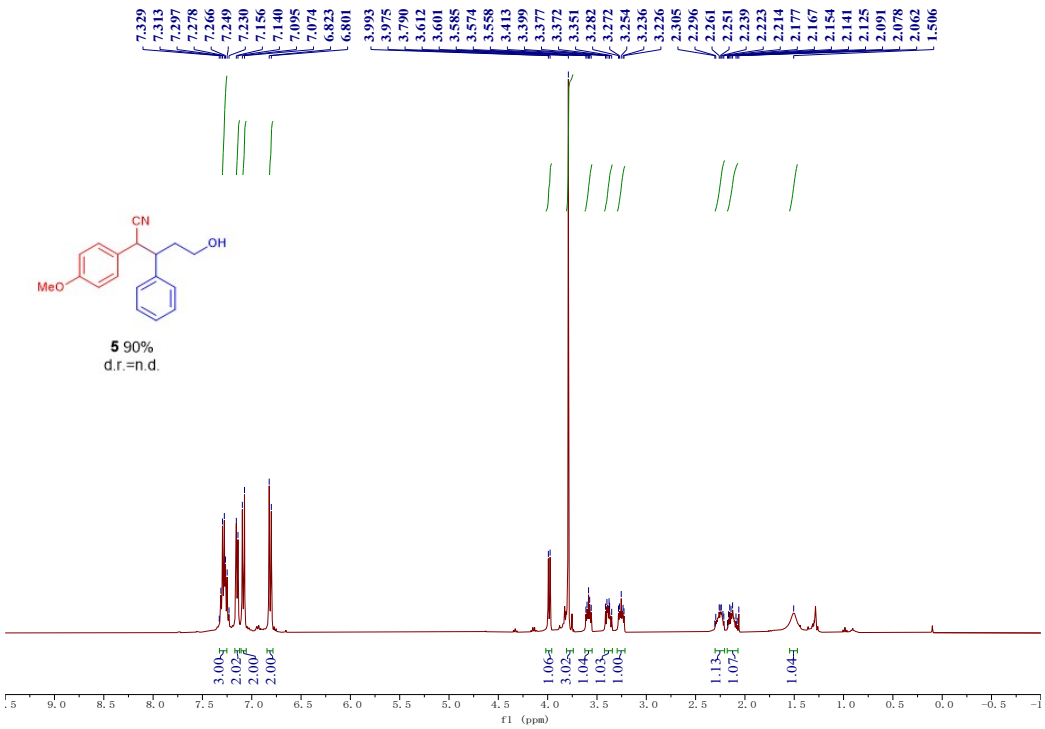

$^{13}$C NMR spectrum of 5-hydroxy-3-phenyl-2-(4-(tri-fluoromethyl)phenyl) pentan-enitrile (**4**, 100 MHz, $CDCl_3$):



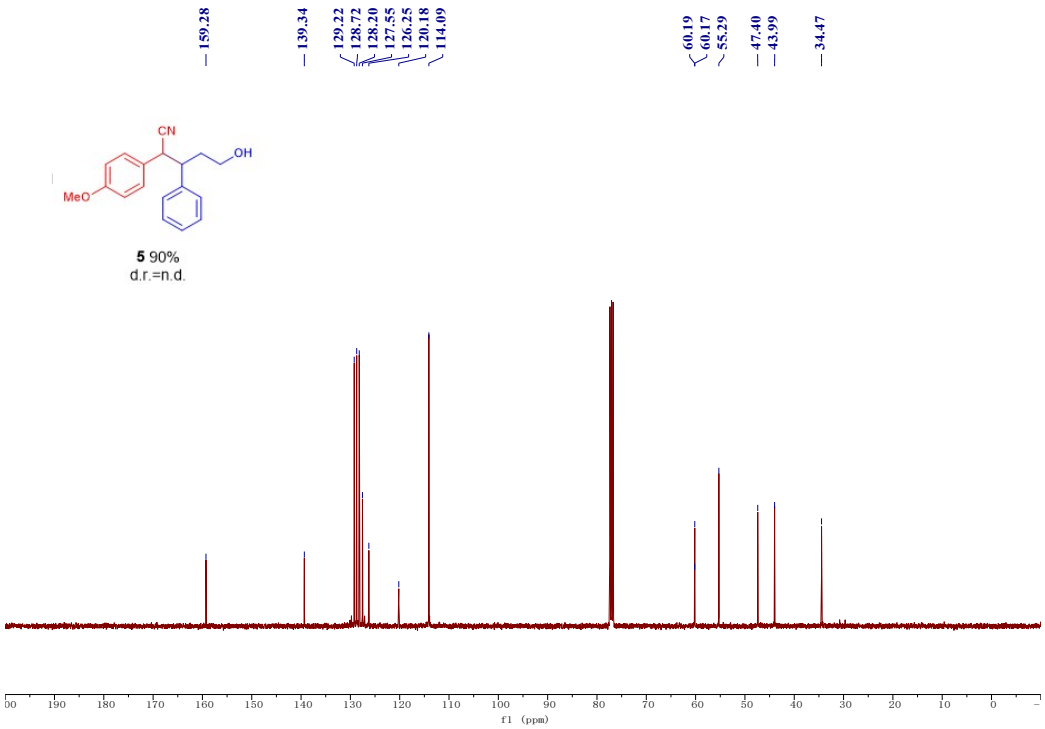
$^{19}F$ NMR spectrum of 5-hydroxy-3-phenyl-2-(4-(tri-fluoromethyl) phenyl) pentan-enitrile (**4**, 376 MHz, $CDCl_3$):



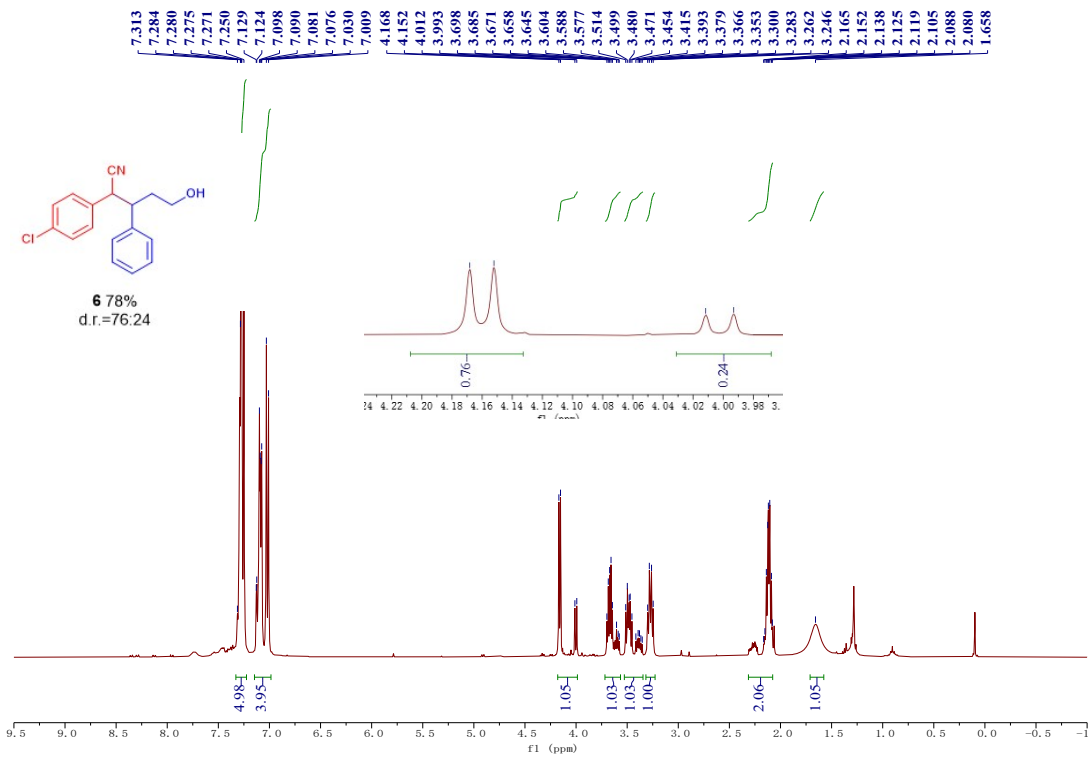

$^{1}H$ NMR spectrum of 5-Hydroxy-2-(4-methoxyphenyl)-3-phenylpentanenitrile (**5**, 400 MHz, $CDCl_3$):



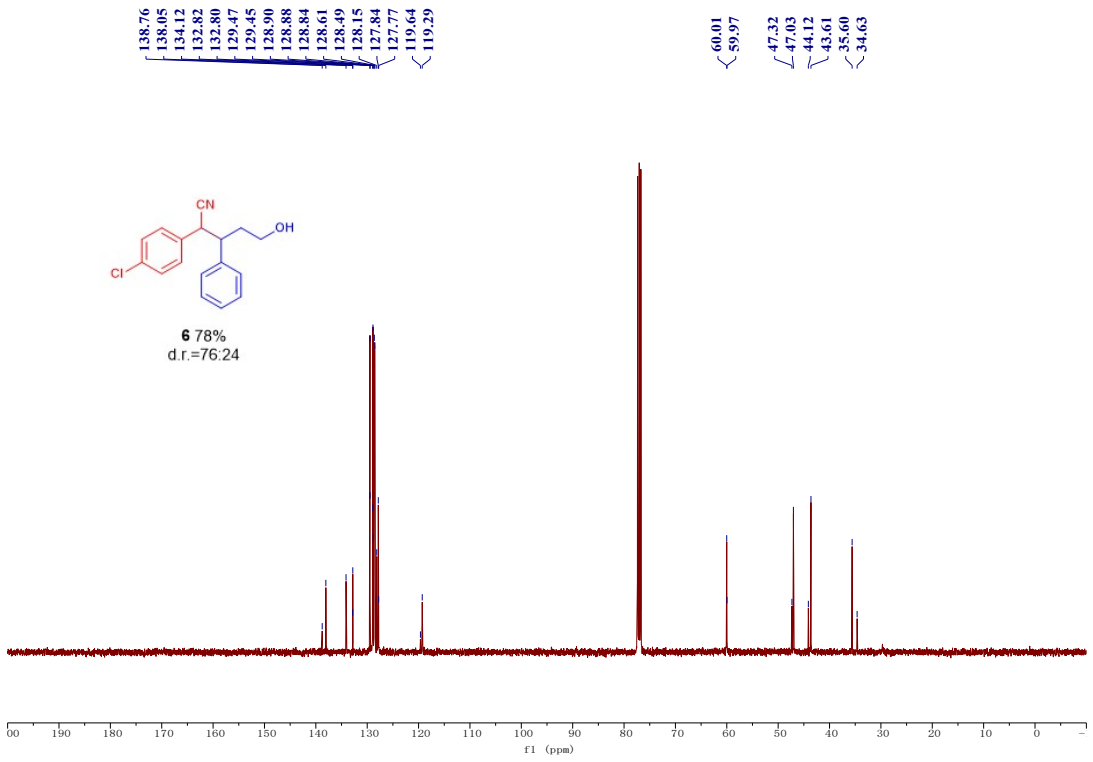

$^{13}$C NMR spectrum of 5-Hydroxy-2-(4-methoxyphenyl)-3-phenylpentanenitrile (**5**, 100 MHz, $CDCl_3$):



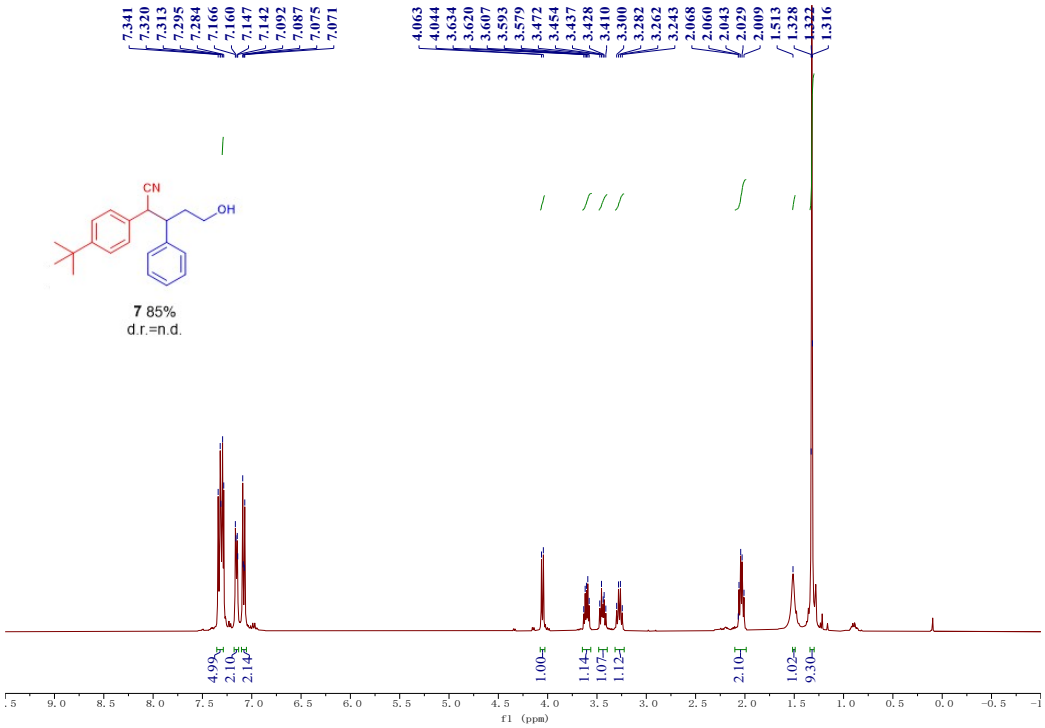

$^{1}$H NMR spectrum of 2-(4-Chlorophenyl)-5-hydroxy-3-phenylpentanenitrile (**6**, 400 MHz, $CDCl_3$):



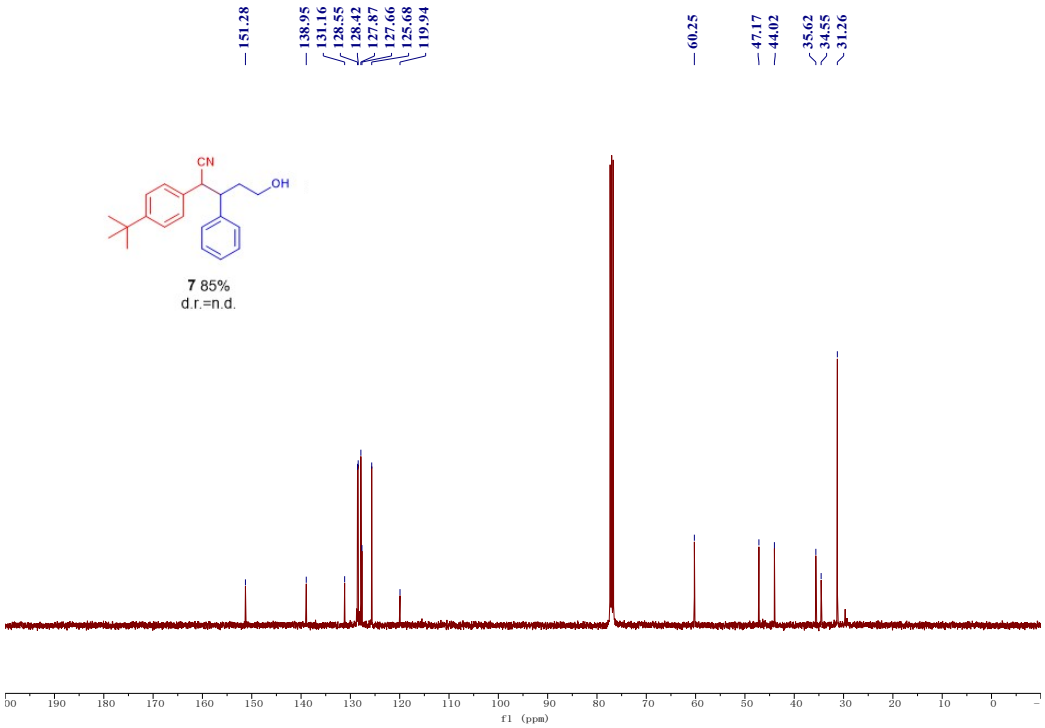

$^{13}$C NMR spectrum of 2-(4-Chlorophenyl)-5-hydroxy-3-phenylpentanenitrile (**6**, 100 MHz, $CDCl_3$):



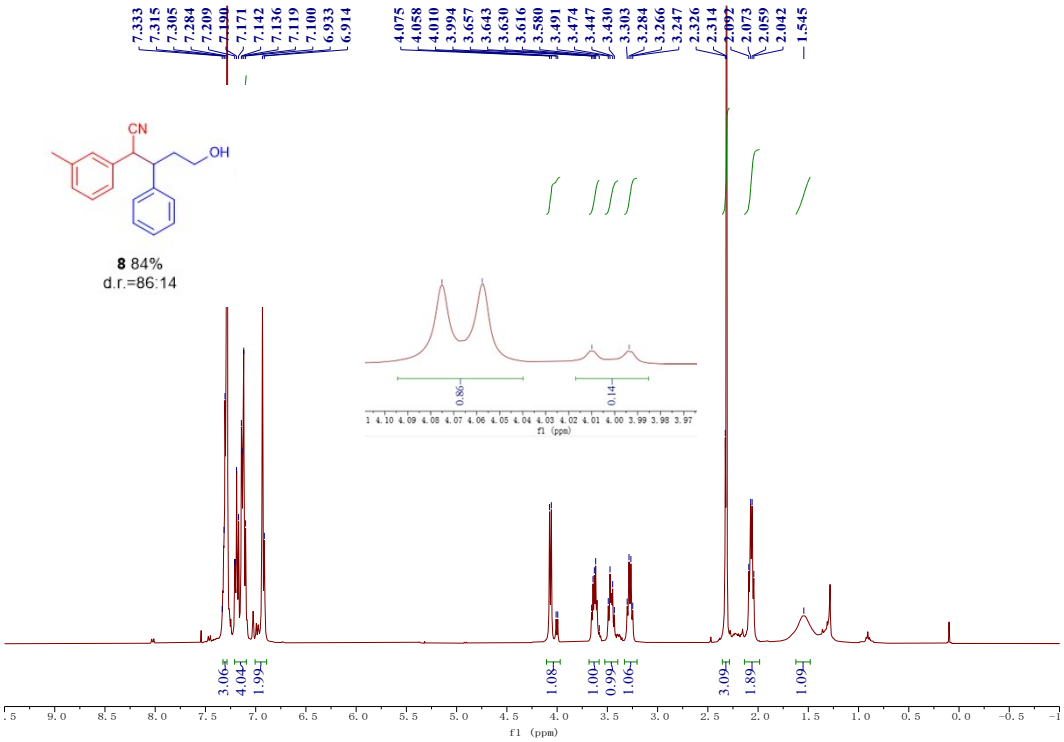
$^{1}$H NMR spectrum of 2-(4-(tert-butyl) phenyl)-5-hydroxy-3-phenylpentanenitrile (**7**, 400 MHz, $CDCl_3$):



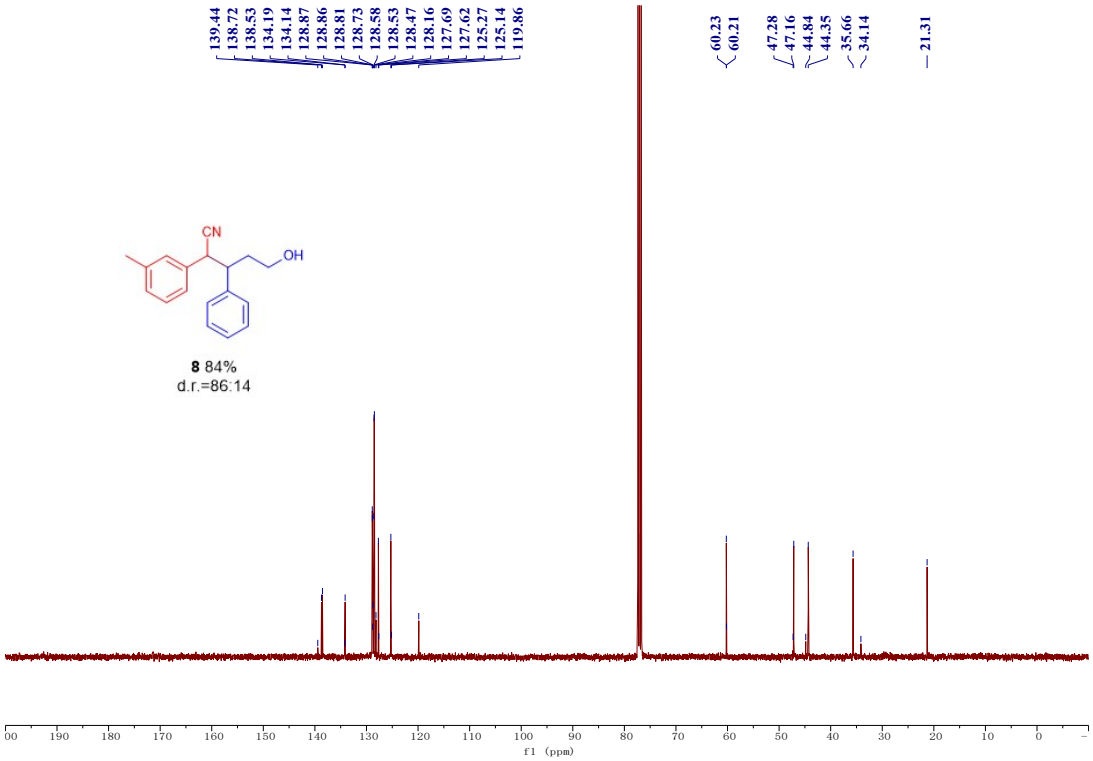

$^{13}$C NMR spectrum of 2-(4-(tert-butyl) phenyl)-5-hydroxy-3-phenylpentanenitrile (**7**, 100 MHz, $CDCl_3$):



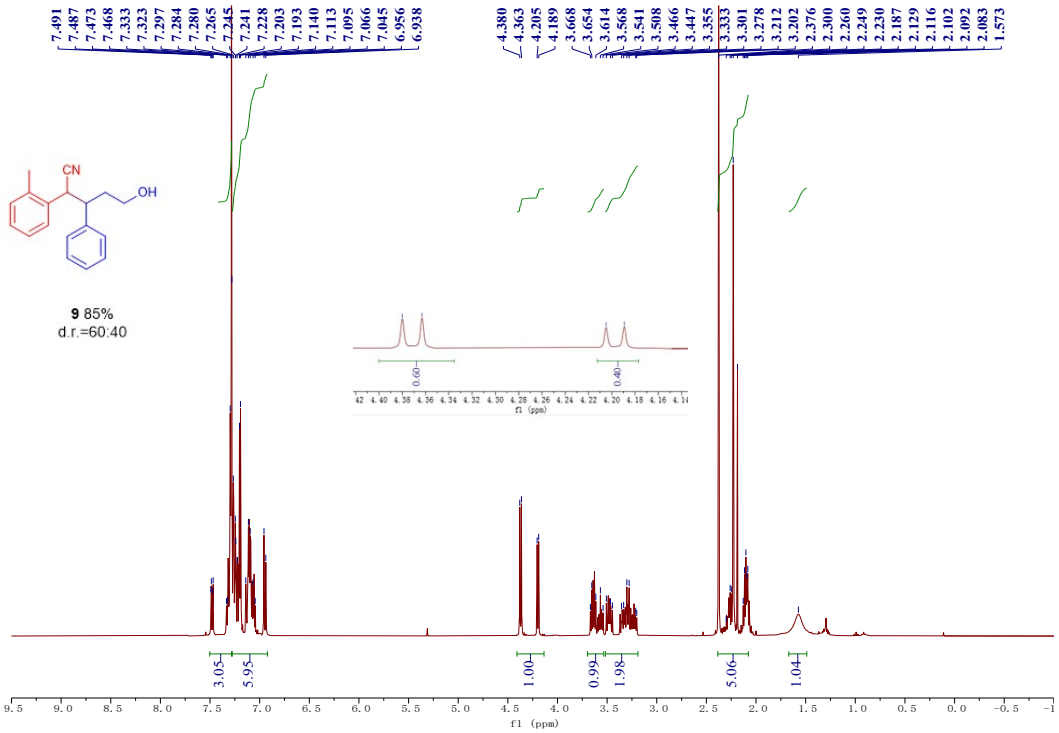

$^{1}$H NMR spectrum of 5-Hydroxy-3-phenyl-2-(m-tolyl) pentanenitrile (**8**, 400 MHz, $CDCl_3$):



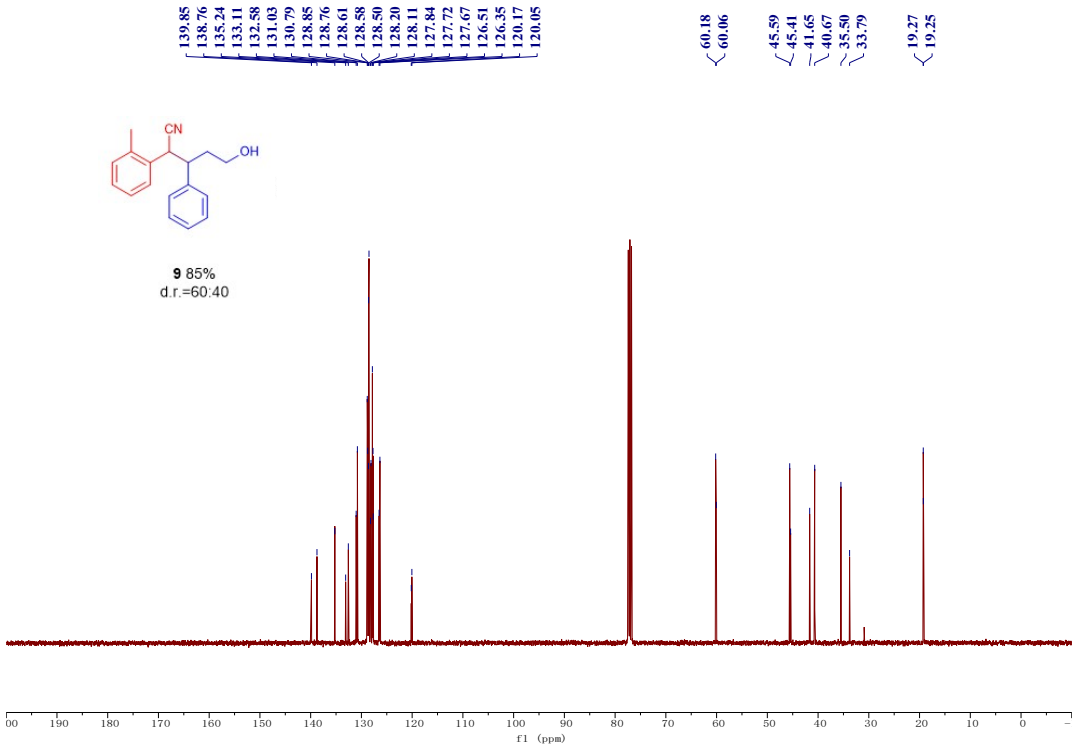

$^{13}$C NMR spectrum of 5-Hydroxy-3-phenyl-2-(m-tolyl) pentanenitrile (**8**, 100 MHz, $CDCl_3$):



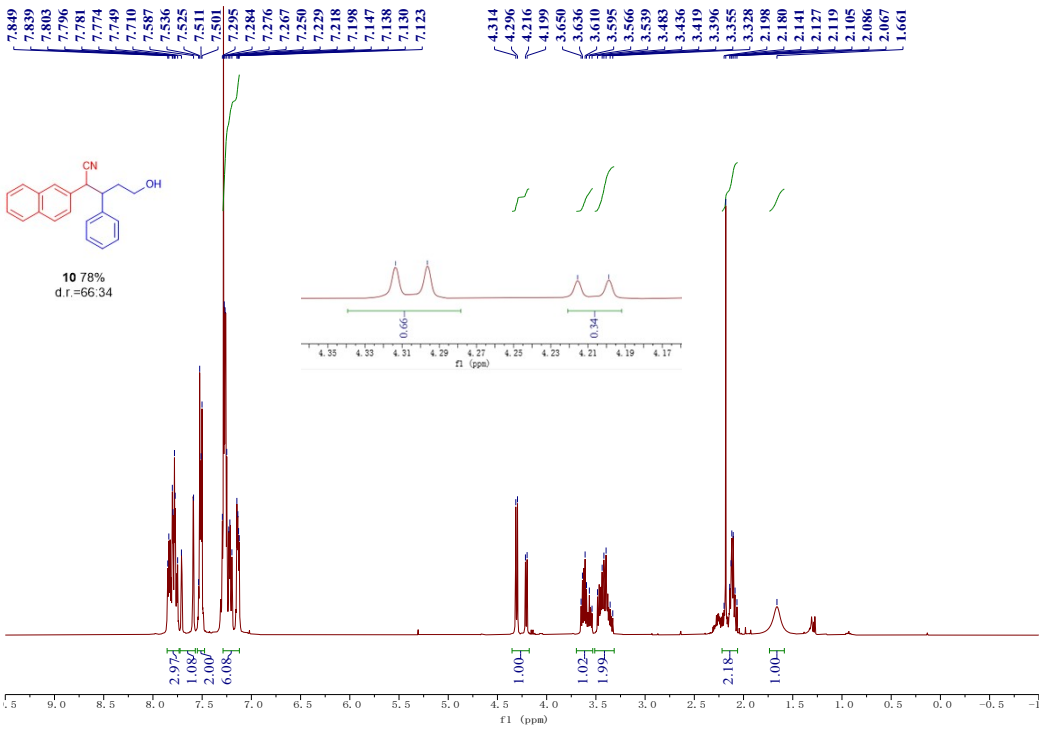
$^{1}$H NMR spectrum of 5-Hydroxy-3-phenyl-2-(o-tolyl) pentanenitrile (**9**, 400 MHz, $CDCl_3$):



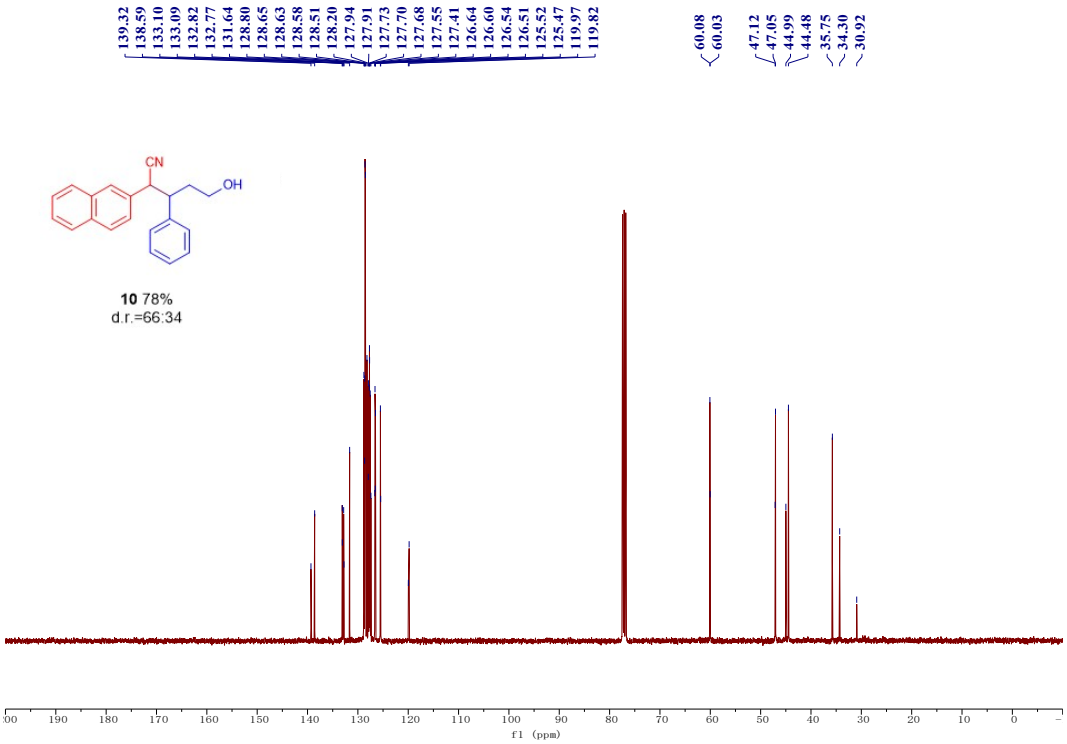

$^{13}$C NMR spectrum of 5-Hydroxy-3-phenyl-2-(o-tolyl) pentanenitrile (**9**, 100 MHz, $CDCl_3$):



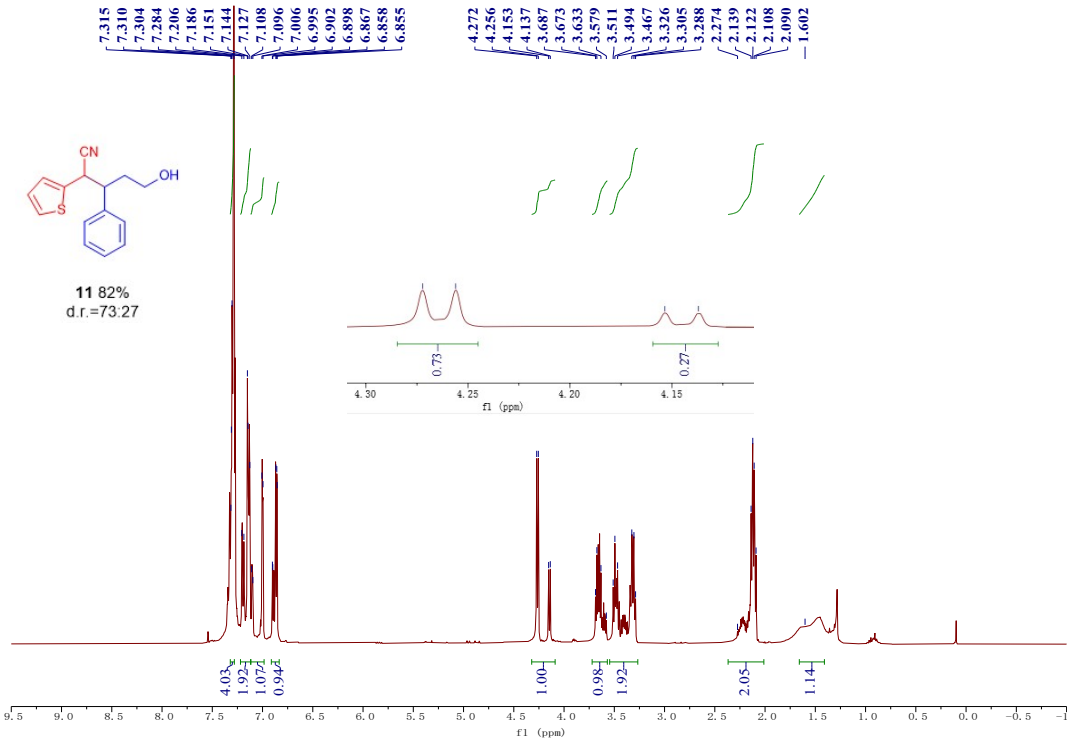

$^{1}$H NMR spectrum of 5-Hydroxy-2-(naphthalen-2-yl)-3-phenylpentanenitrile (**10**, 400 MHz, $CDCl_3$):



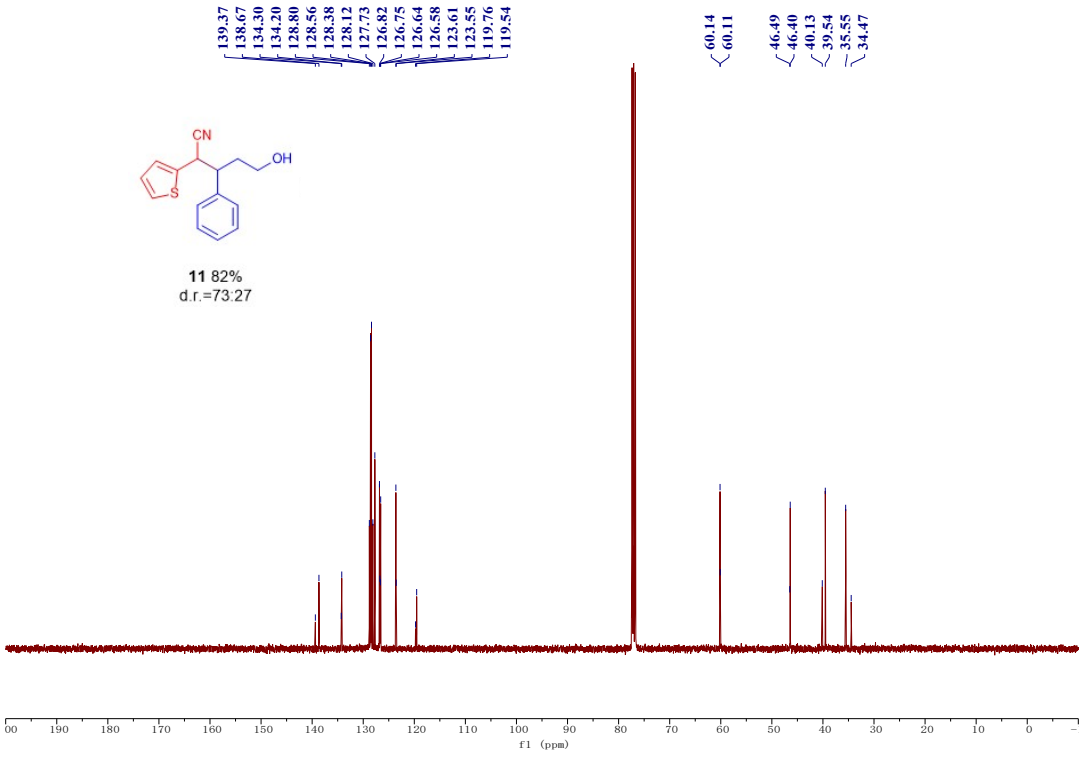

$^{13}C$ NMR spectrum of 5-Hydroxy-2-(naphthalen-2-yl)-3-phenylpentanenitrile (**10**, 100 MHz, $CDCl_3$):



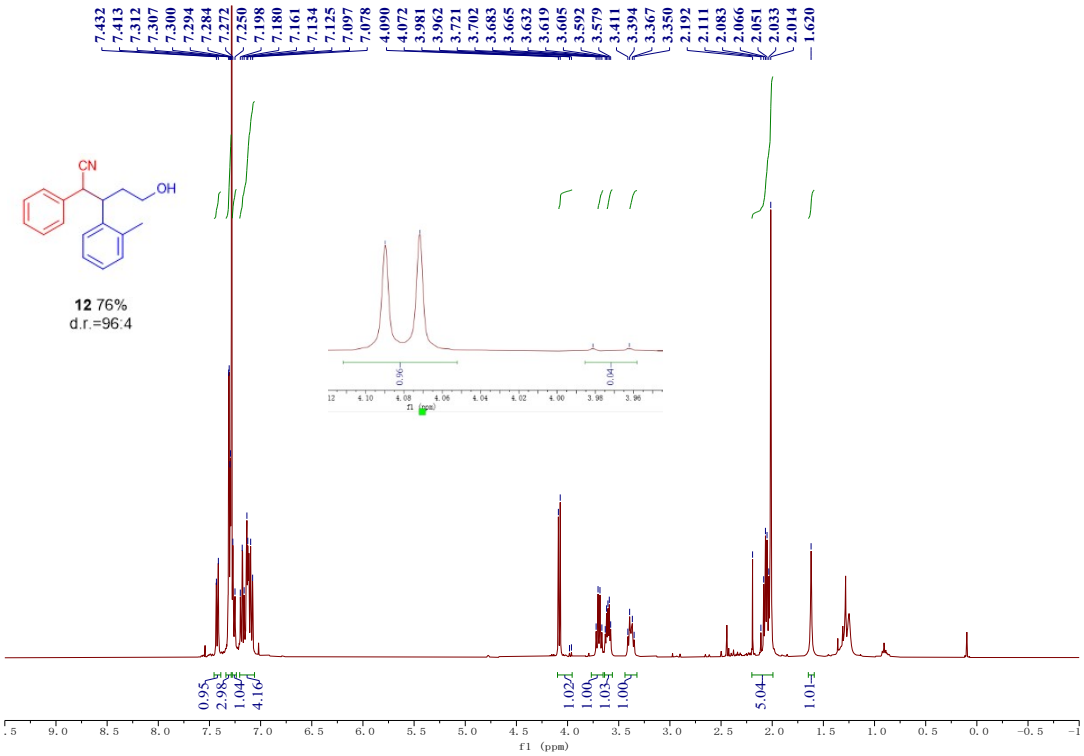

$^{1}H$ NMR spectrum of 5-Hydroxy-3-phenyl-2-(thiophen-2-yl) pentanenitrile (**11**, 400 MHz, $CDCl_3$):



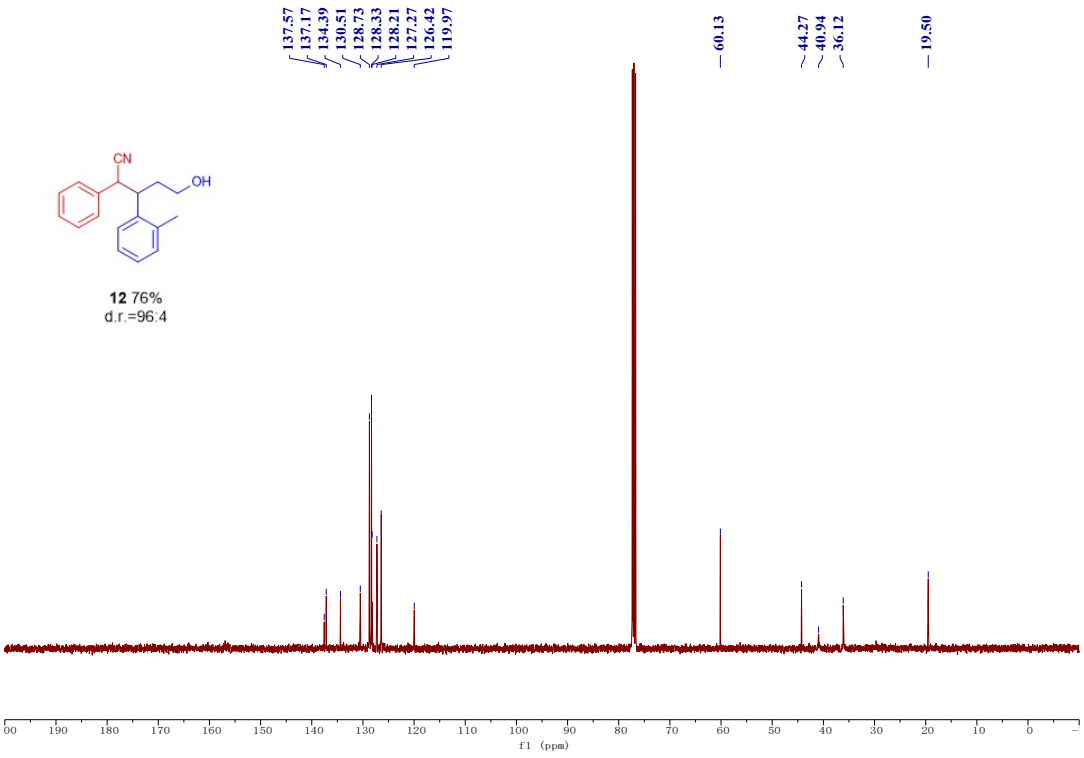

$^{13}$C NMR spectrum of 5-Hydroxy-3-phenyl-2-(thiophen-2-yl) pentanenitrile (**11**, 100 MHz, $CDCl_3$):



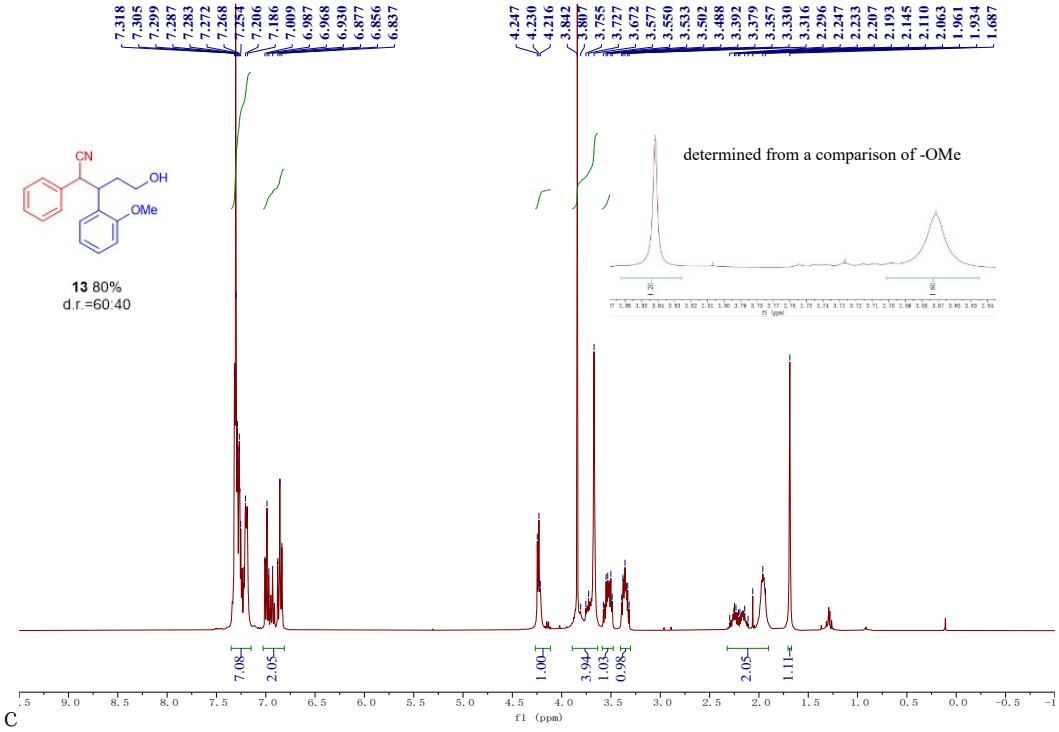
$^{1}$H NMR spectrum of 5-Hydroxy-2-phenyl-3-(*o*-tolyl) pentanenitrile (**12**, 400 MHz, $CDCl_3$):



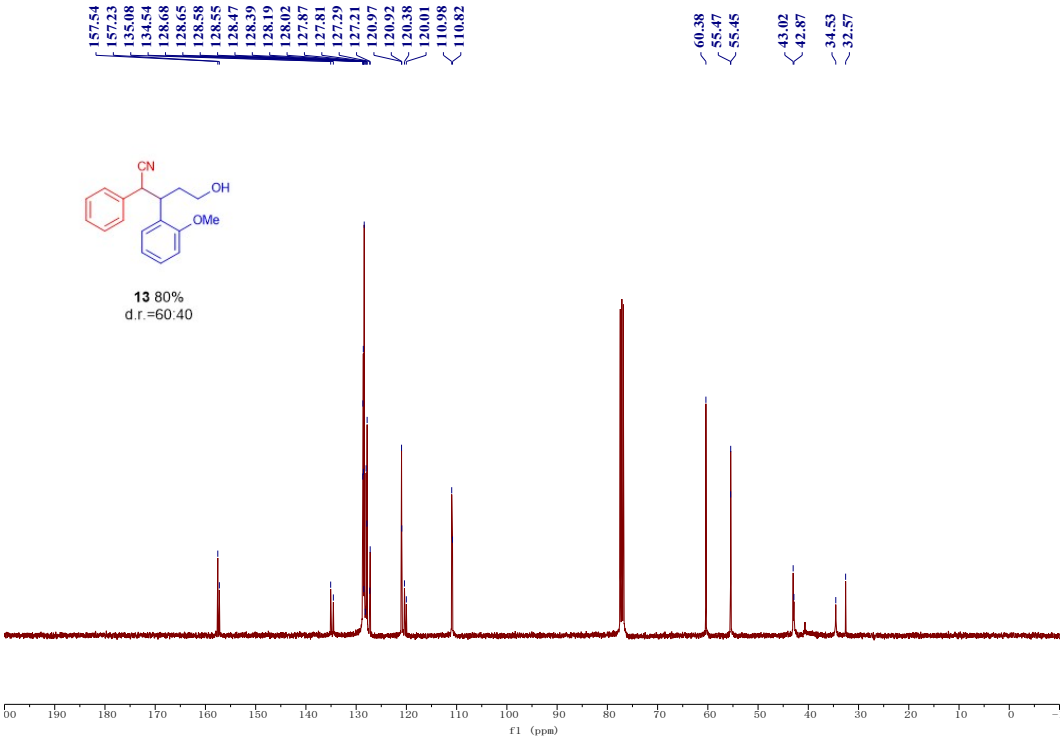

$^{13}$C NMR spectrum of 5-Hydroxy-2-phenyl-3-(o-tolyl) pentanenitrile (**12**, 100 MHz, $CDCl_3$):



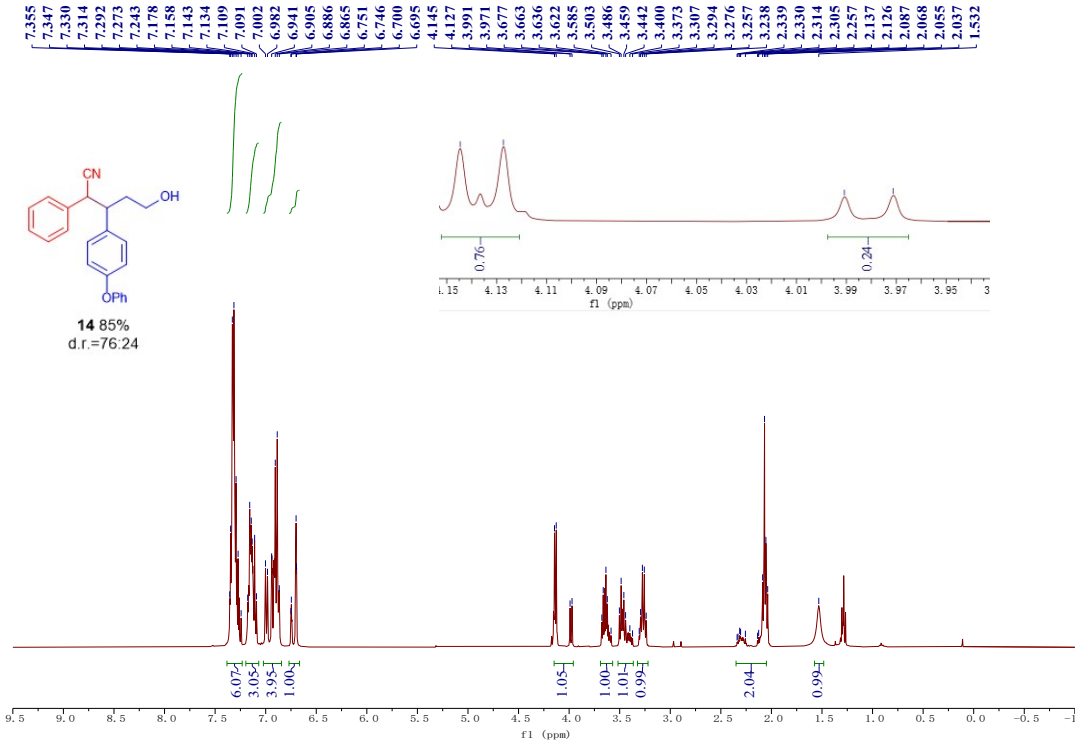
$^{1}$H NMR spectrum of 5-Hydroxy-3-(2-methoxyphenyl)-2-phenylpentanenitrile (**13**, 400 MHz, $CDCl_3$):



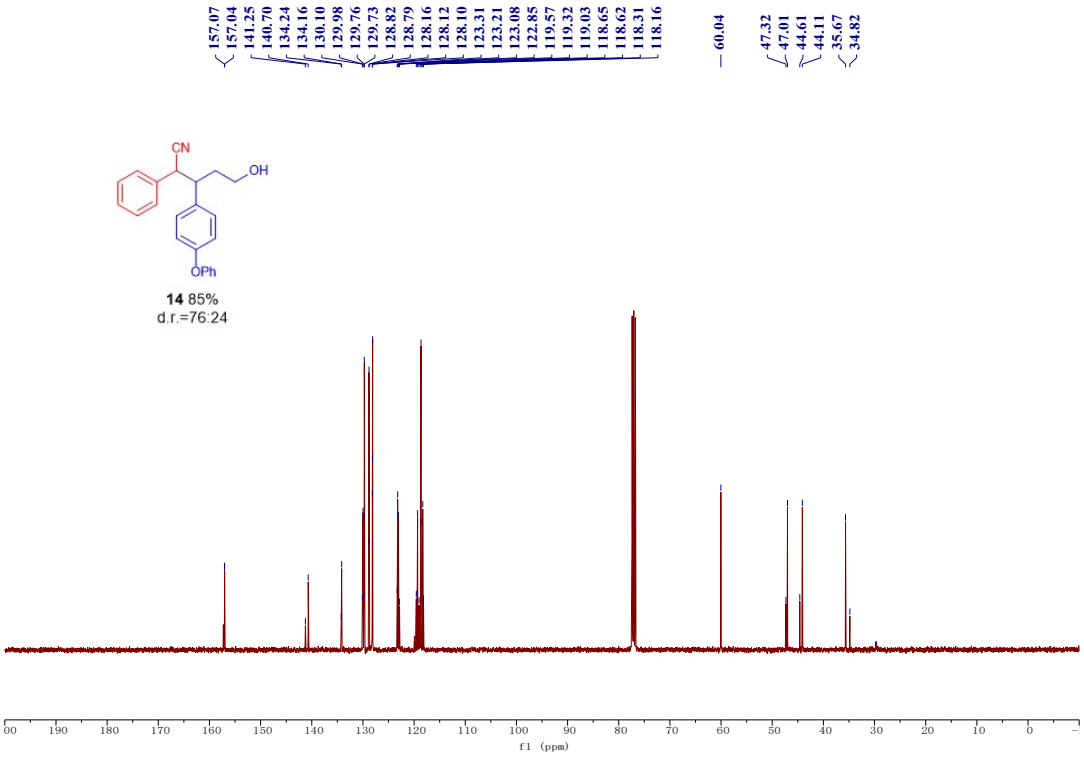

$^{13}$C NMR spectrum of 5-Hydroxy-3-(2-methoxyphenyl)-2-phenylpentanenitrile (**13**, 100 MHz, $CDCl_3$):



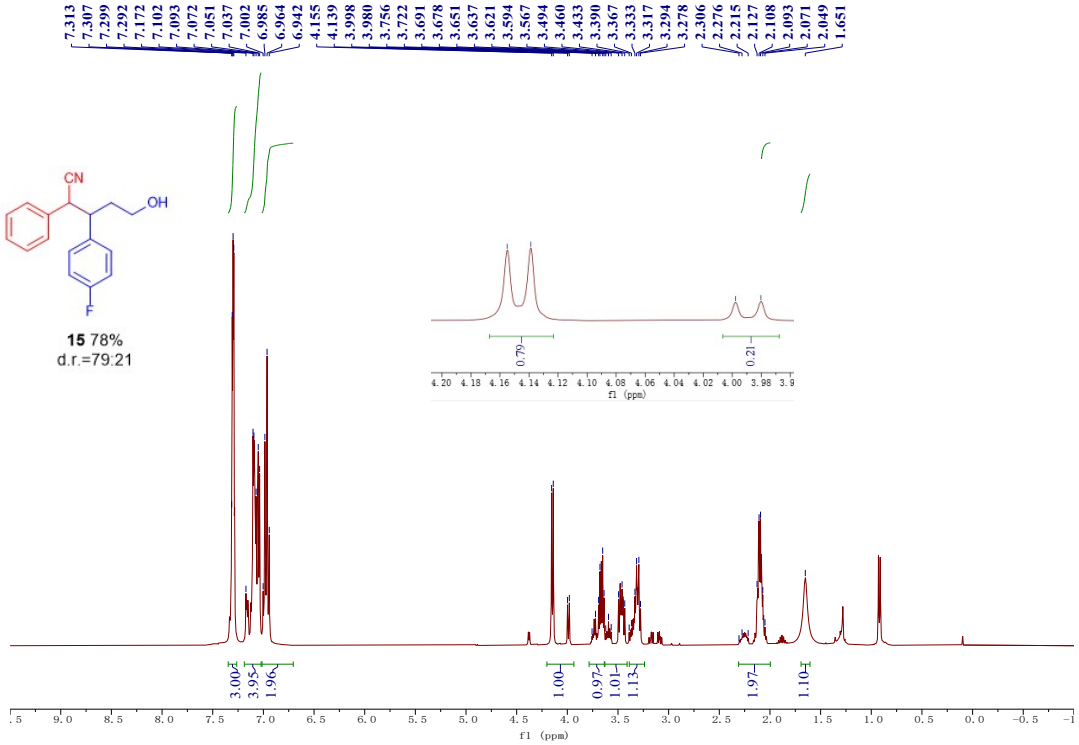
$^{1}$H NMR spectrum of 5-Hydroxy-3-(4-phenoxyphenyl)-2-phenylpentanenitrile (**14**, 400 MHz, $CDCl_3$):



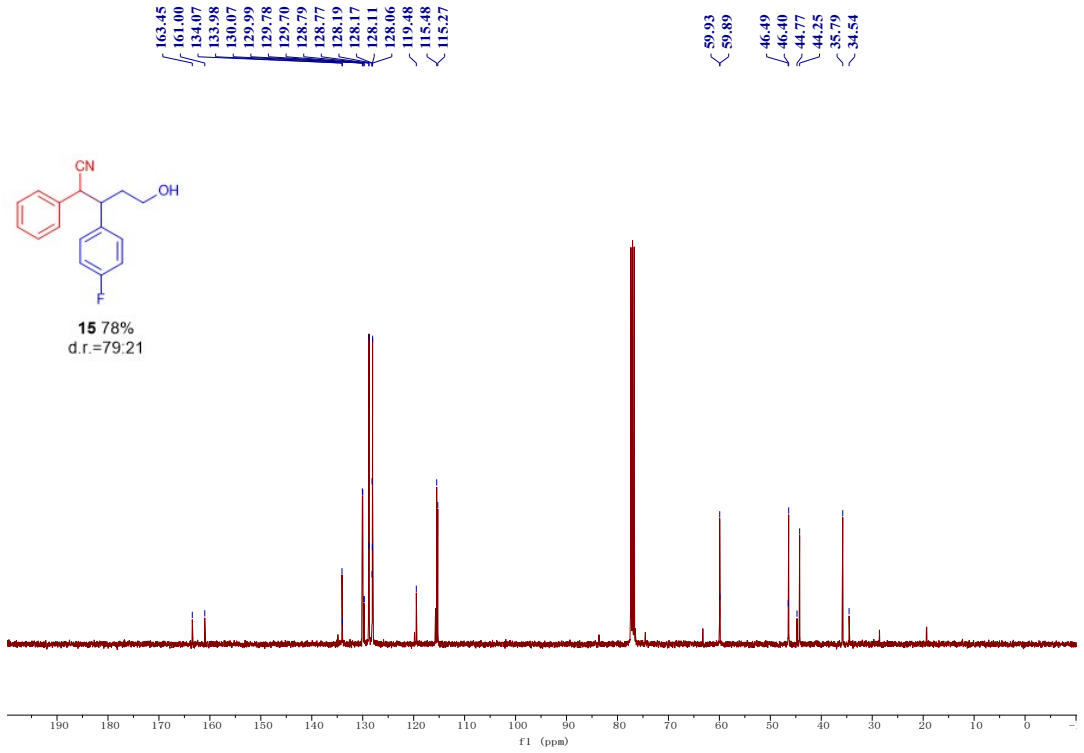

$^{13}$C NMR spectrum of 5-Hydroxy-3-(4-phenoxyphenyl)-2-phenylpentanenitrile (**14**, 100 MHz, $CDCl_3$):



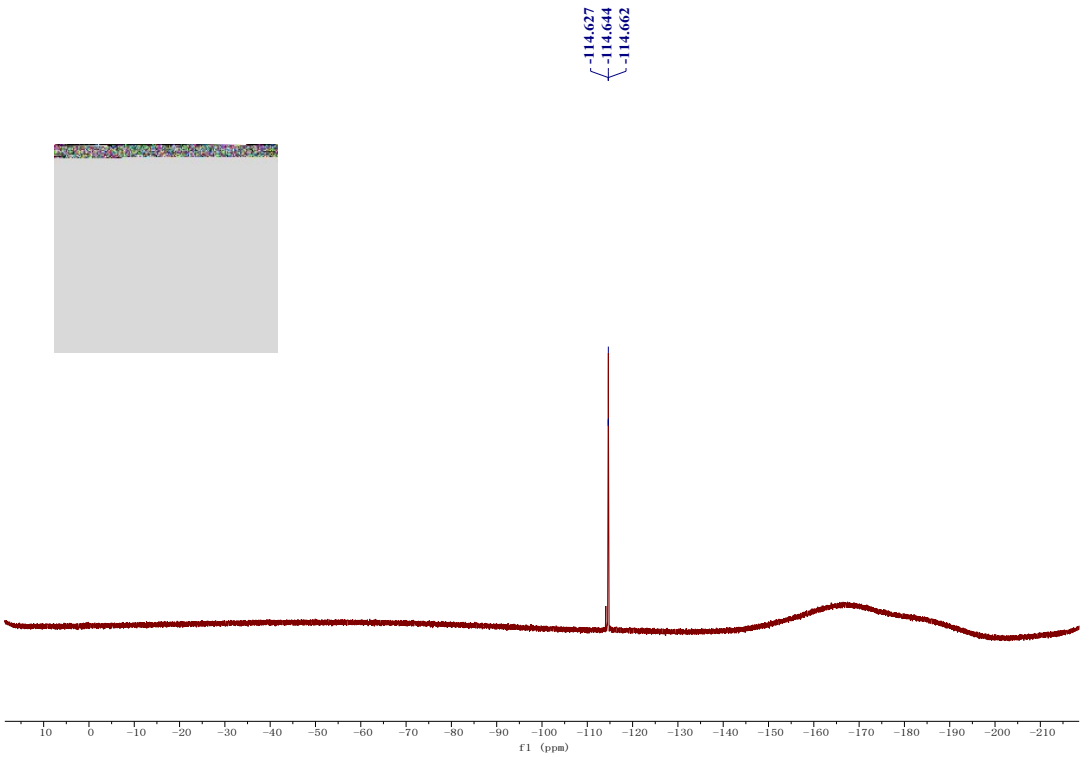
$^{1}$H NMR spectrum of 3-(4-Fluorophenyl)-5-hydroxy-2-phenylpentanenitrile (**15**, 400 MHz, $CDCl_3$):



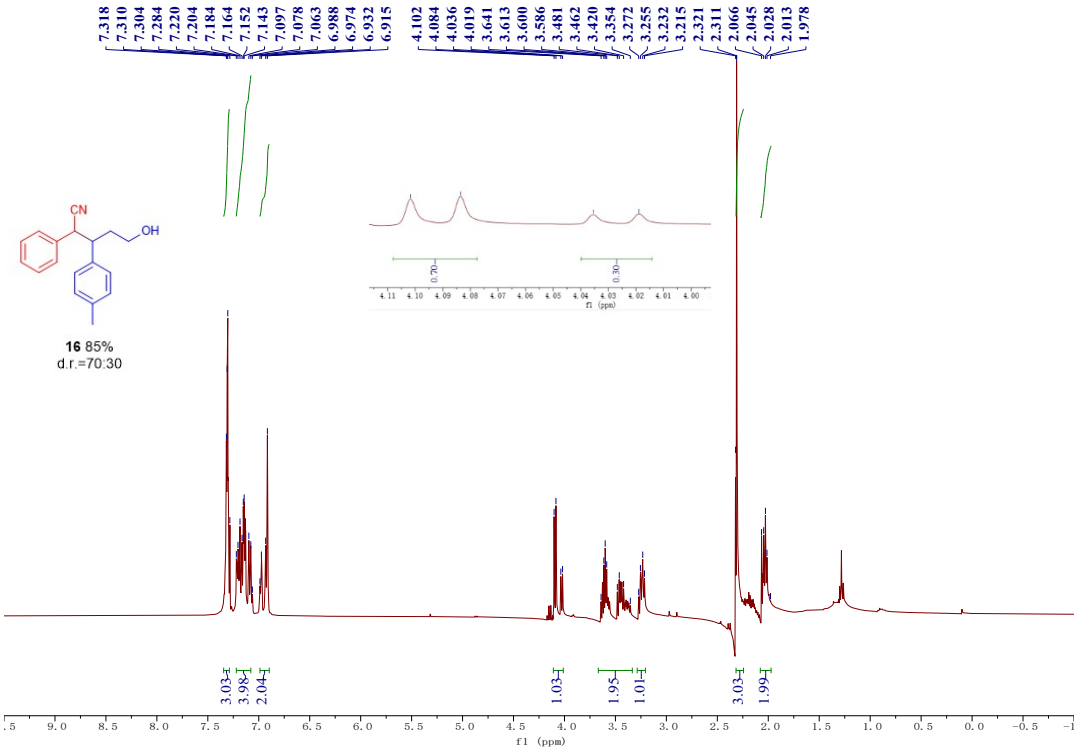

$^{13}$C NMR spectrum of 3-(4-Fluorophenyl)-5-hydroxy-2-phenylpentanenitrile (**15**, 100 MHz, $CDCl_3$):



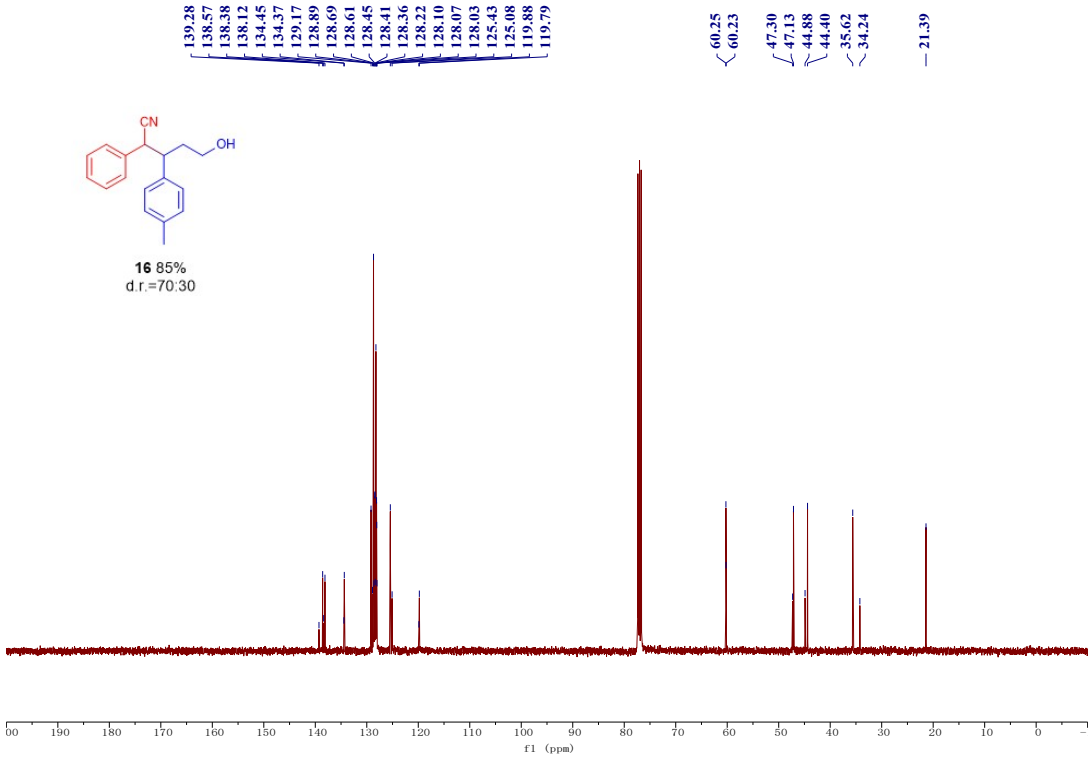
$^{19}F$ NMR spectrum of 3-(4-Fluorophenyl)-5-hydroxy-2-phenylpentanenitrile (**15**, 376 MHz, $CDCl_3$):



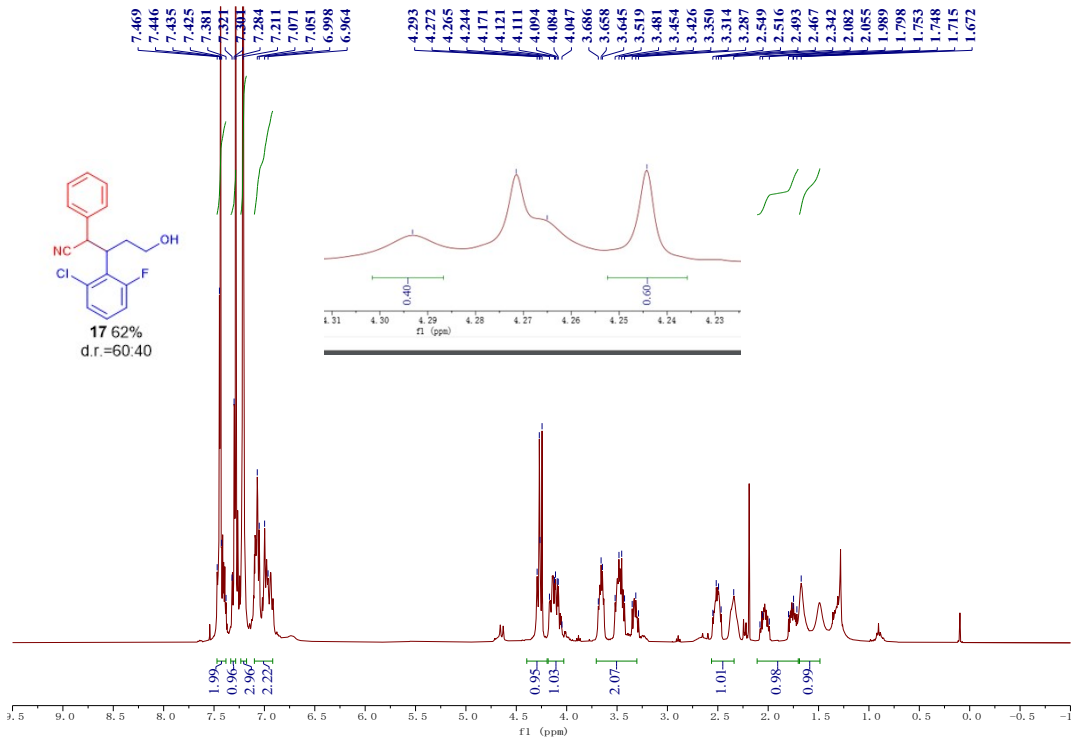
$^{1}$H NMR spectrum of 5-Hydroxy-2-phenyl-3-(*p*-tolyl) pentanenitrile (**16**, 400 MHz, $CDCl_3$):



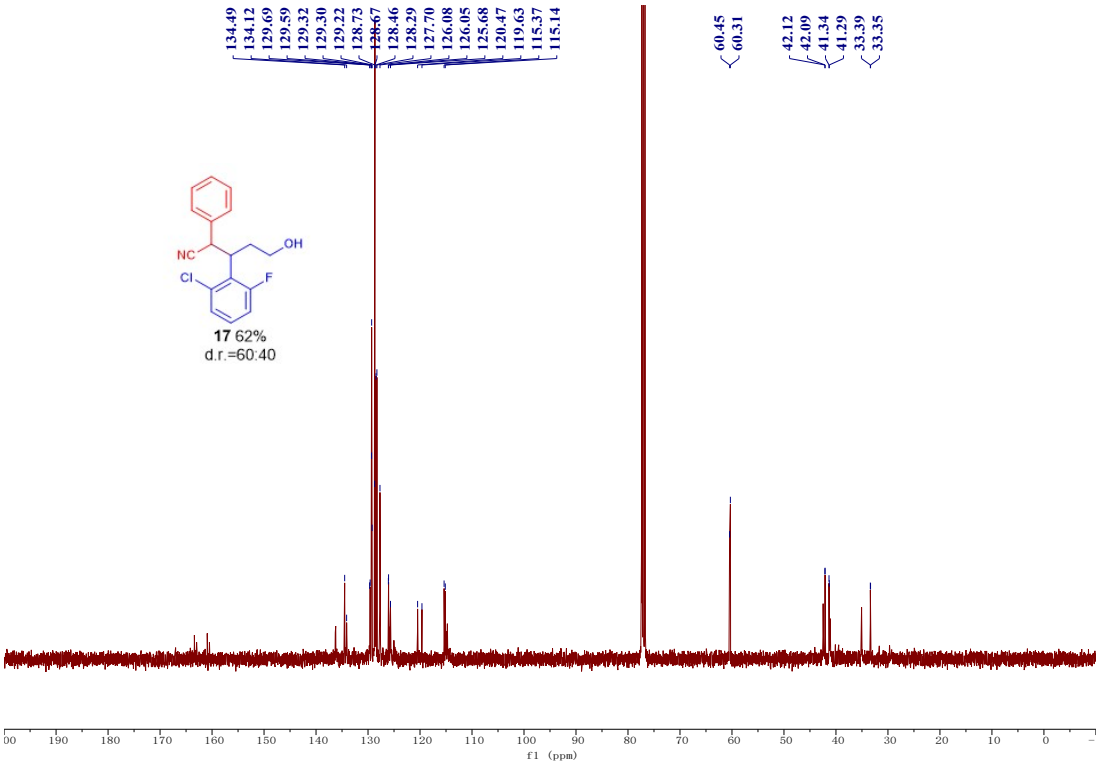

$^{13}$C NMR spectrum of 5-Hydroxy-2-phenyl-3-(p-tolyl) pentanenitrile (**16**, 100 MHz, $CDCl_3$):



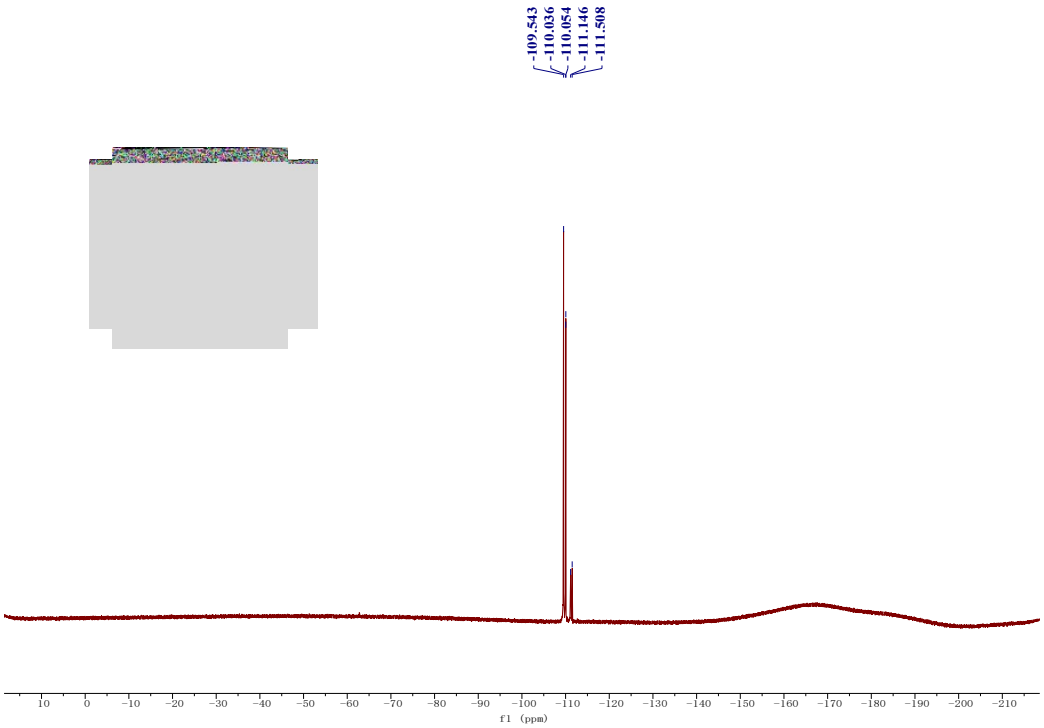
$^{1}$H NMR spectrum of 3-(2-Chloro-6-fluorophenyl)-5-hydroxy-2-phenylpentanenitrile (**17**, 400 MHz, $CDCl_3$):



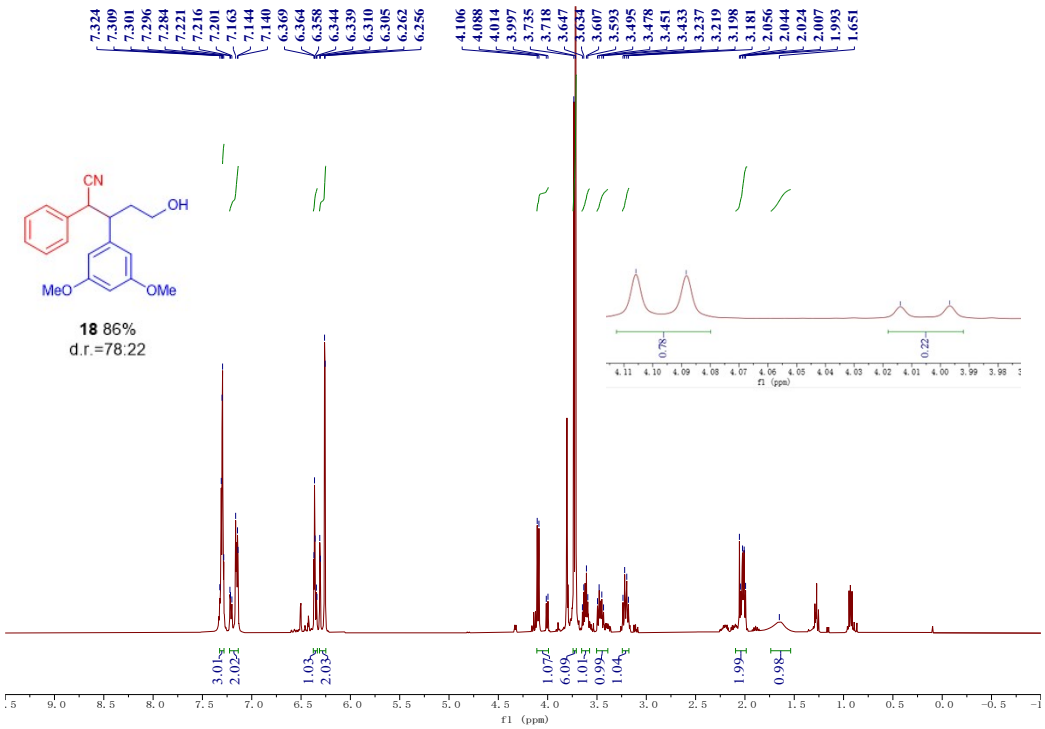

$^{13}$C NMR spectrum of 3-(2-Chloro-6-fluorophenyl)-5-hydroxy-2-phenylpentanenitrile (**17**, 100 MHz, $CDCl_3$):



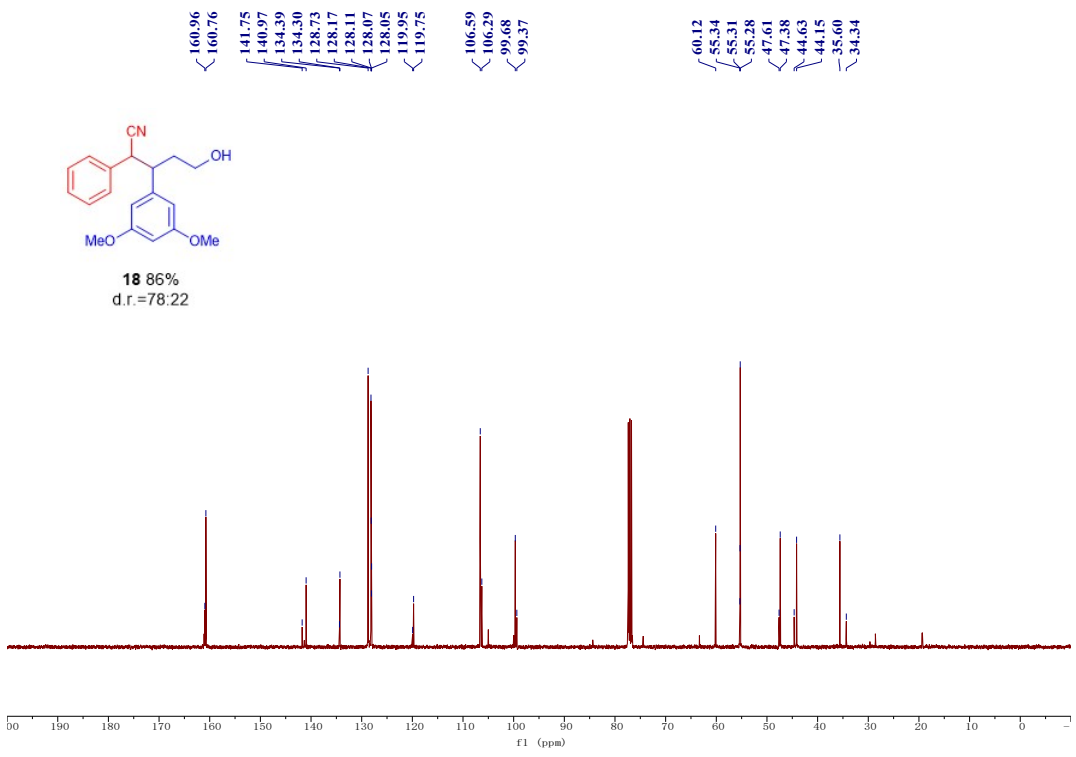
$^{19}$F NMR spectrum of 3-(2-Chloro-6-fluorophenyl)-5-hydroxy-2-phenylpentanenitrile (**17**, 376 MHz, $CDCl_3$):



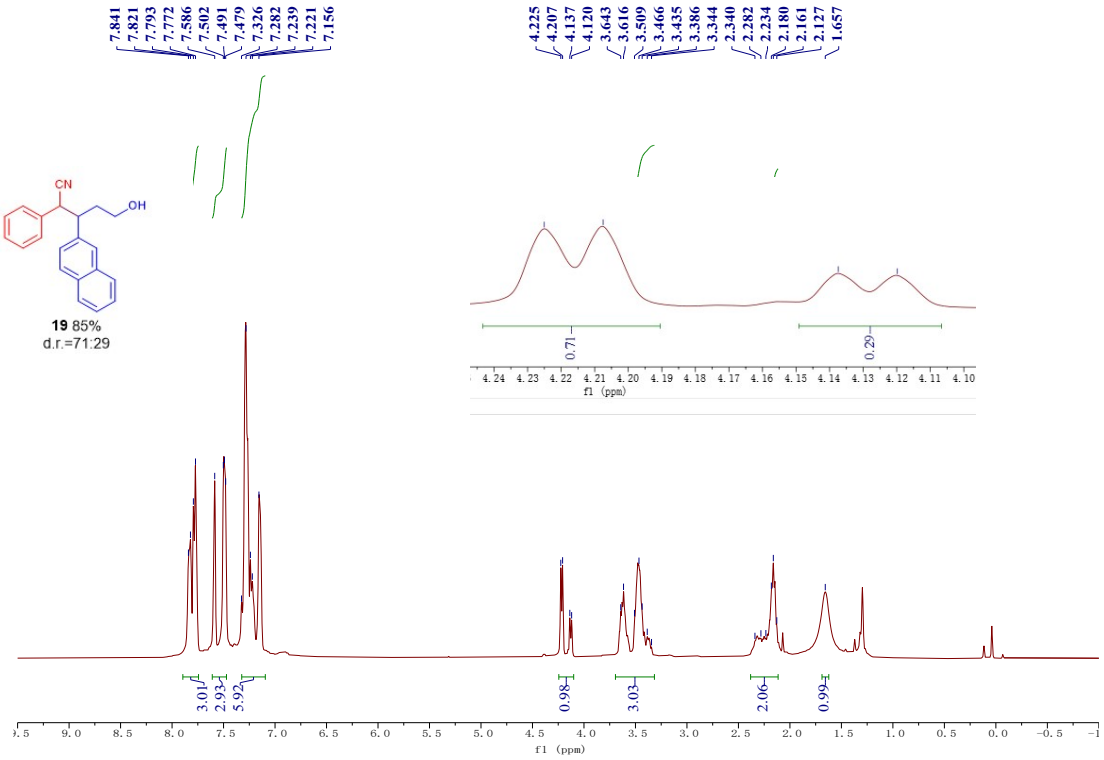

$^{1}$H NMR spectrum of 3-(3,5-Dimethoxyphenyl)-5-hydroxy-2-phenylpentanenitrile (**18**, 400 MHz, $CDCl_3$):



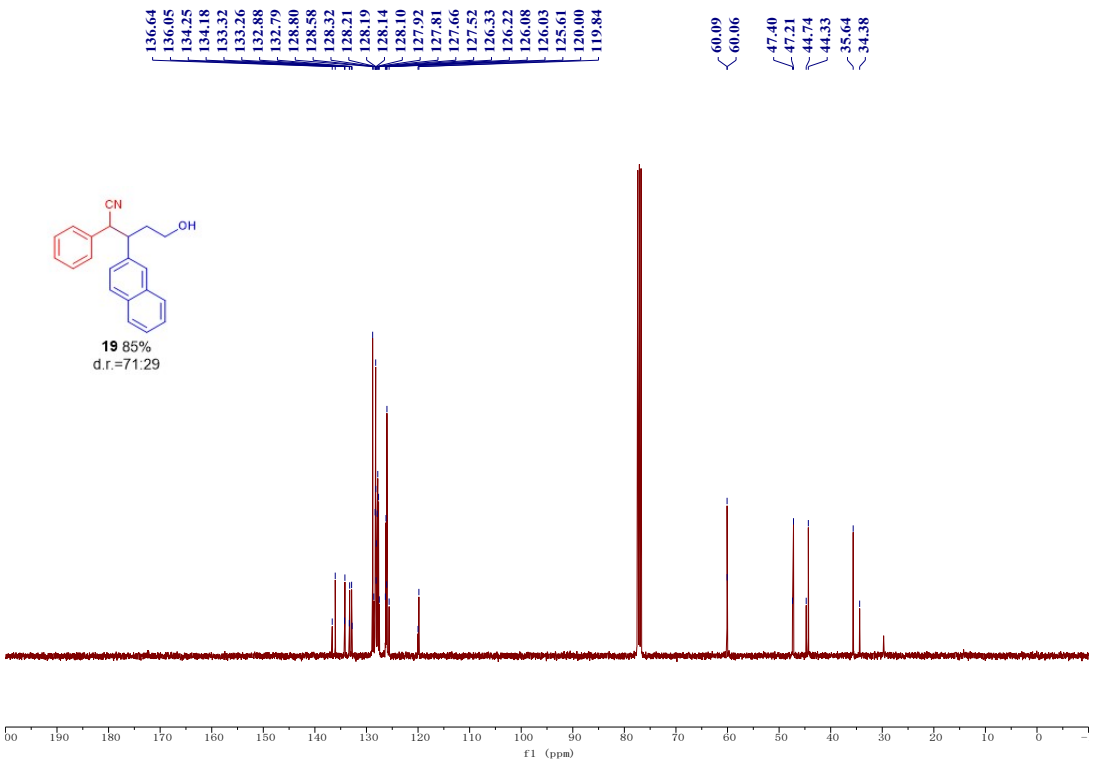

$^{13}$C NMR spectrum of 3-(3,5-Dimethoxyphenyl)-5-hydroxy-2-phenylpentanenitrile (**18**, 100 MHz, $CDCl_3$):



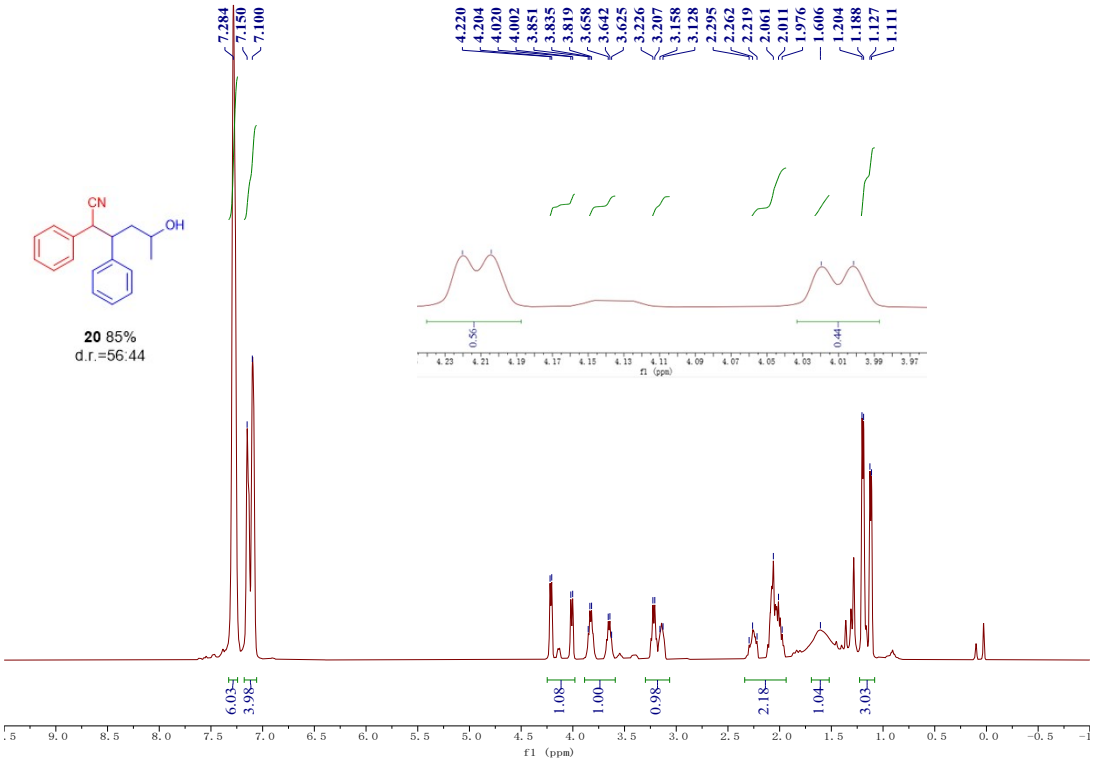

$^{1}$H NMR spectrum of 5-hydroxy-3-(naphthalen-2-yl)-2-phenylpentanenitrile (**19**, 400 MHz, $CDCl_3$):



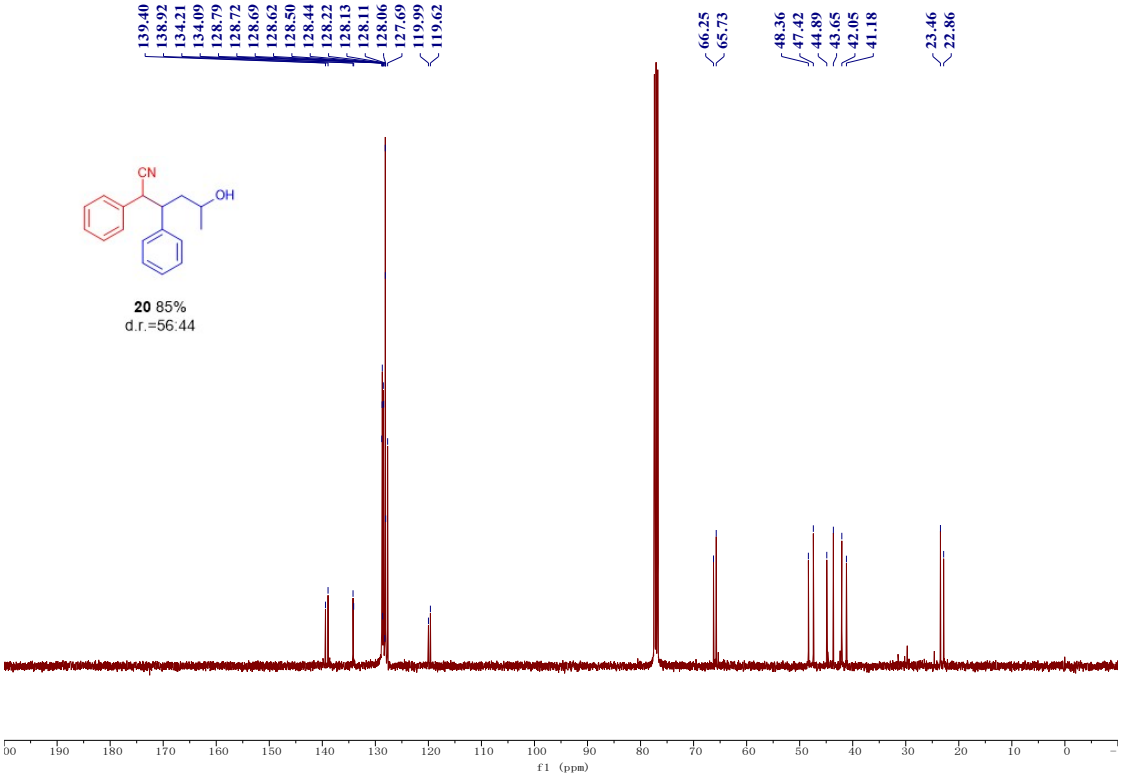

$^{13}C$ NMR spectrum of 5-hydroxy-3-(naphthalen-2-yl)-2-phenylpentanenitrile (**19**, 100 MHz, $CDCl_3$):



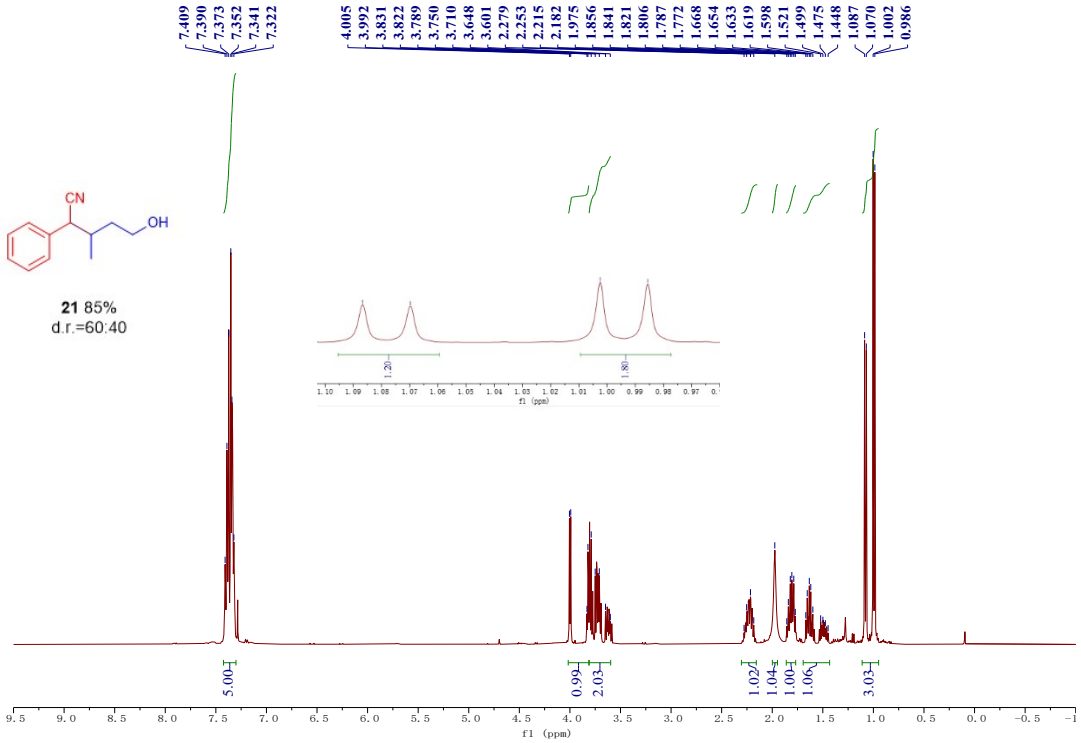

$^{1}H$ NMR spectrum of 5-hydroxy-2,3-diphenylhexanenitrile (**20**, 400 MHz, $CDCl_3$):



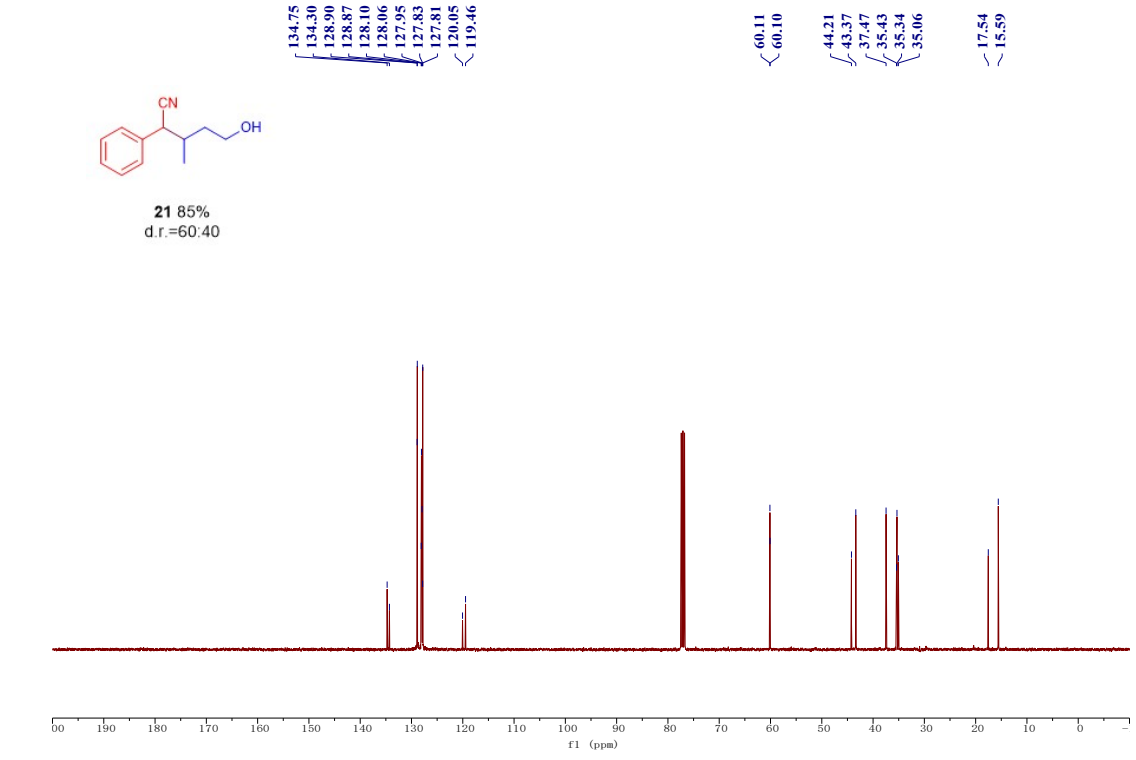

$^{13}$C NMR spectrum of 5-hydroxy-2,3-diphenylhexanenitrile (**20**, 100 MHz, $CDCl_3$):



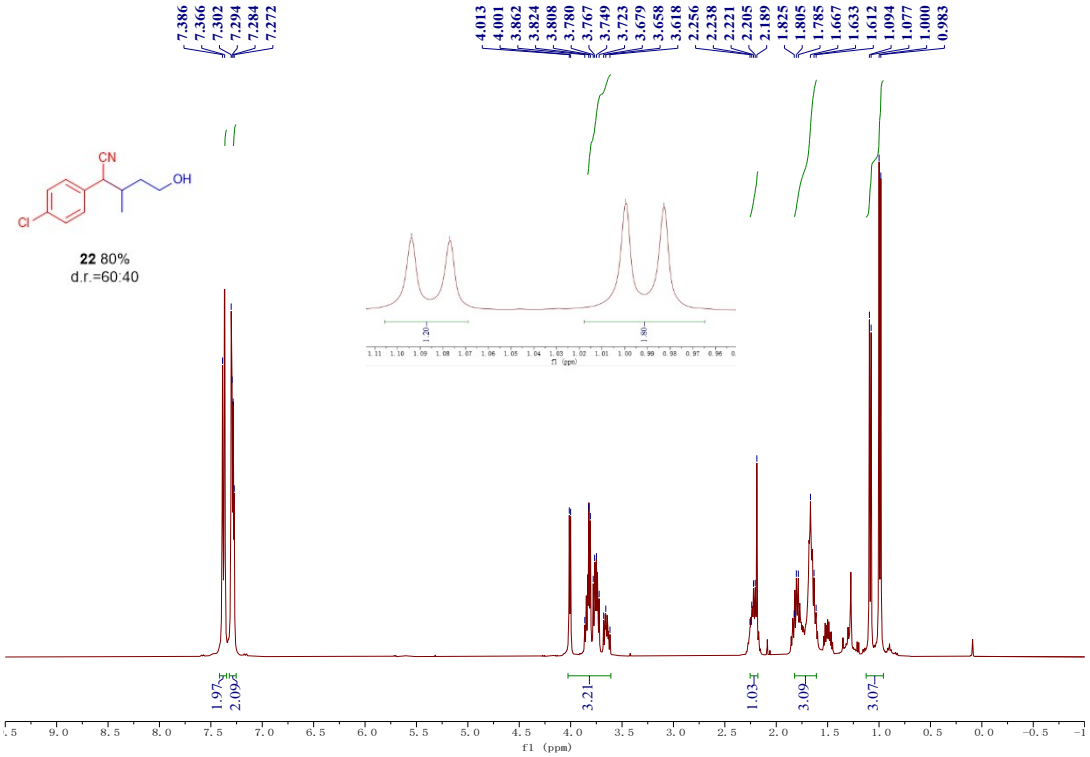
$^{1}$H NMR spectrum of 5-Hydroxy-3-methyl-2-phenylpentanenitrile (**21**, 400 MHz, $CDCl_3$):



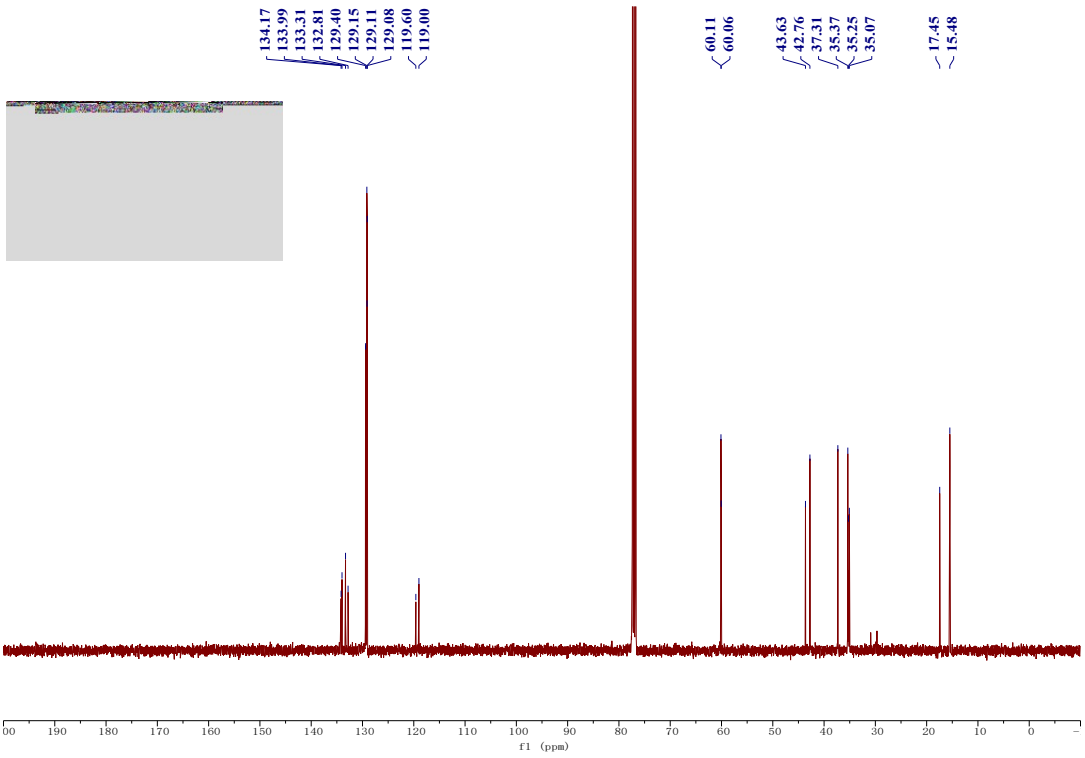

$^{13}$C NMR spectrum of 5-Hydroxy-3-methyl-2-phenylpentanenitrile (**21**, 100 MHz, $CDCl_3$):



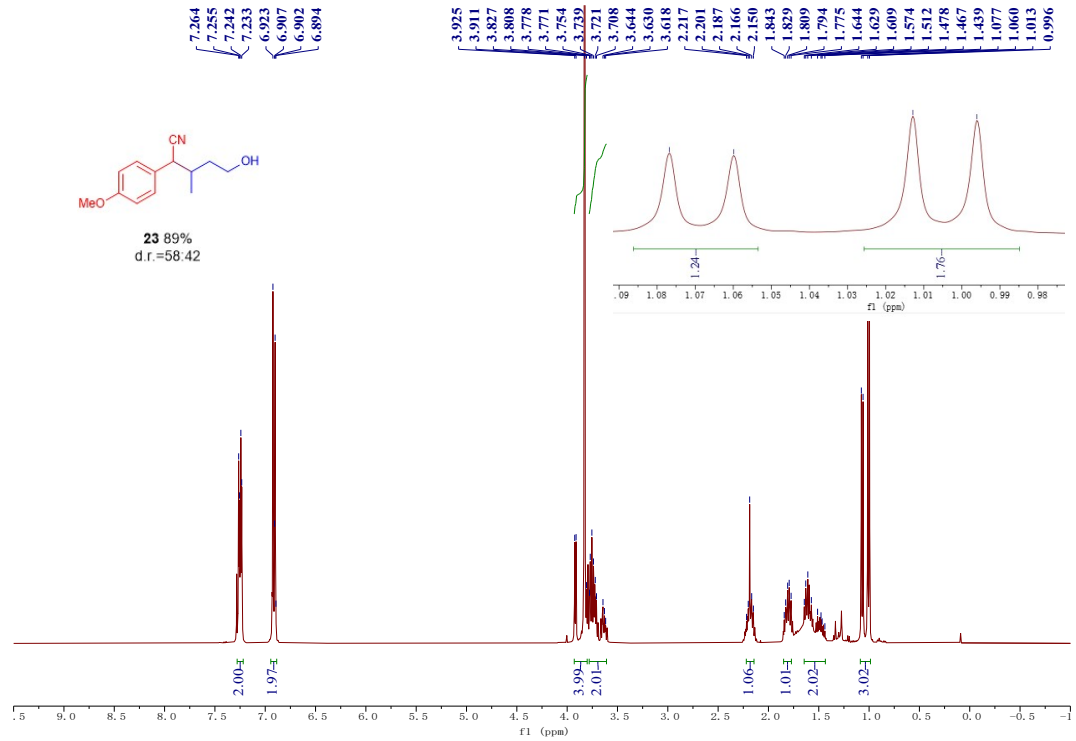
$^{1}$H NMR spectrum of 2-(4-Chlorophenyl)-5-hydroxy-3-methylpentanenitrile (**22**, 400 MHz, $CDCl_3$):



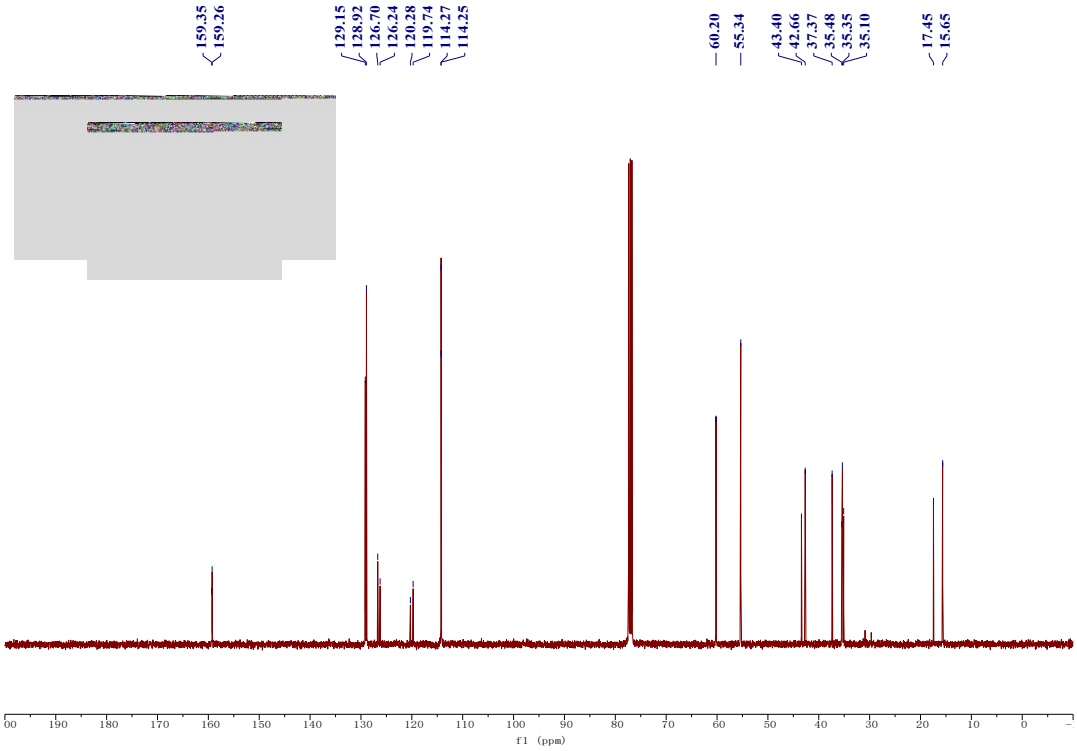

$^{13}$C NMR spectrum of 2-(4-Chlorophenyl)-5-hydroxy-3-methylpentanenitrile (**22**, 100 MHz, $CDCl_3$):



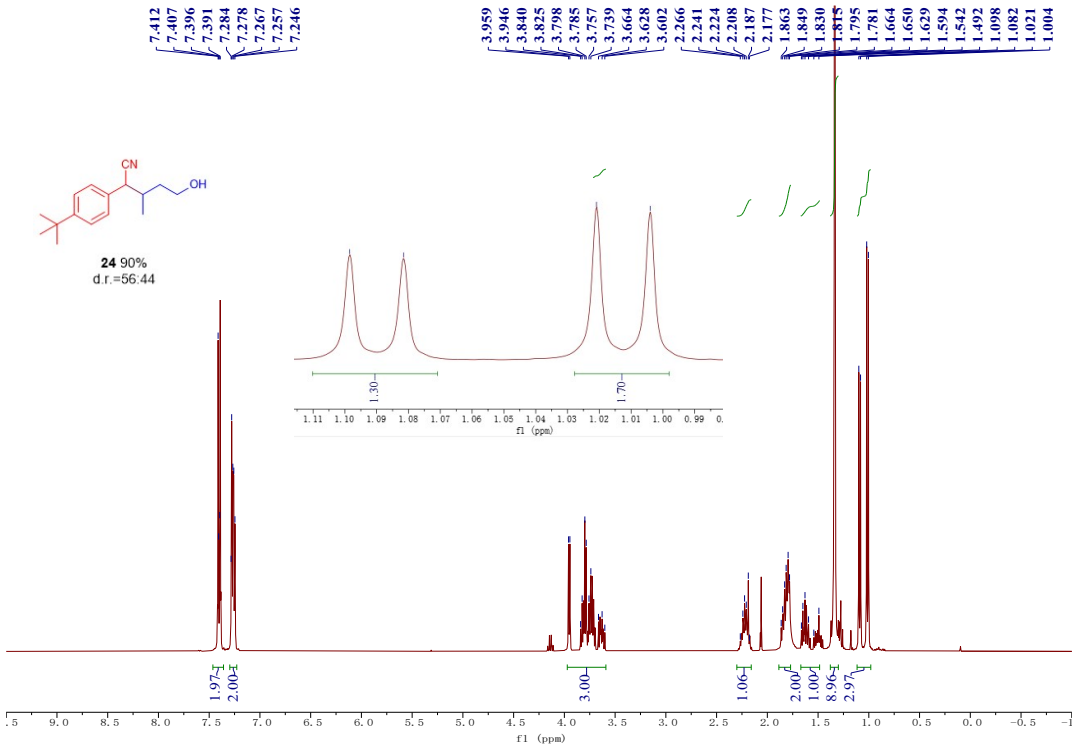

$^{1}$H NMR spectrum of 5-Hydroxy-2-(4-methoxyphenyl)-3-methylpentanenitrile (**23**, 400 MHz, $CDCl_3$):



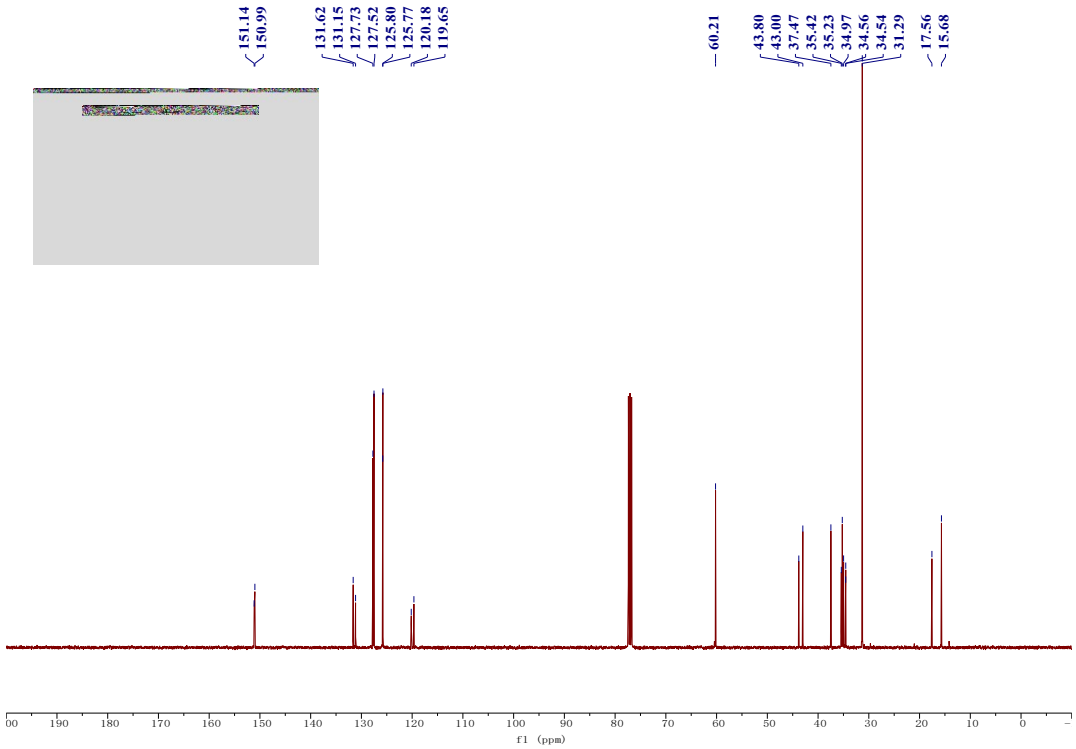

$^{13}$C NMR spectrum of 5-Hydroxy-2-(4-methoxyphenyl)-3-methylpentanenitrile (**23**, 100 MHz, $CDCl_3$):



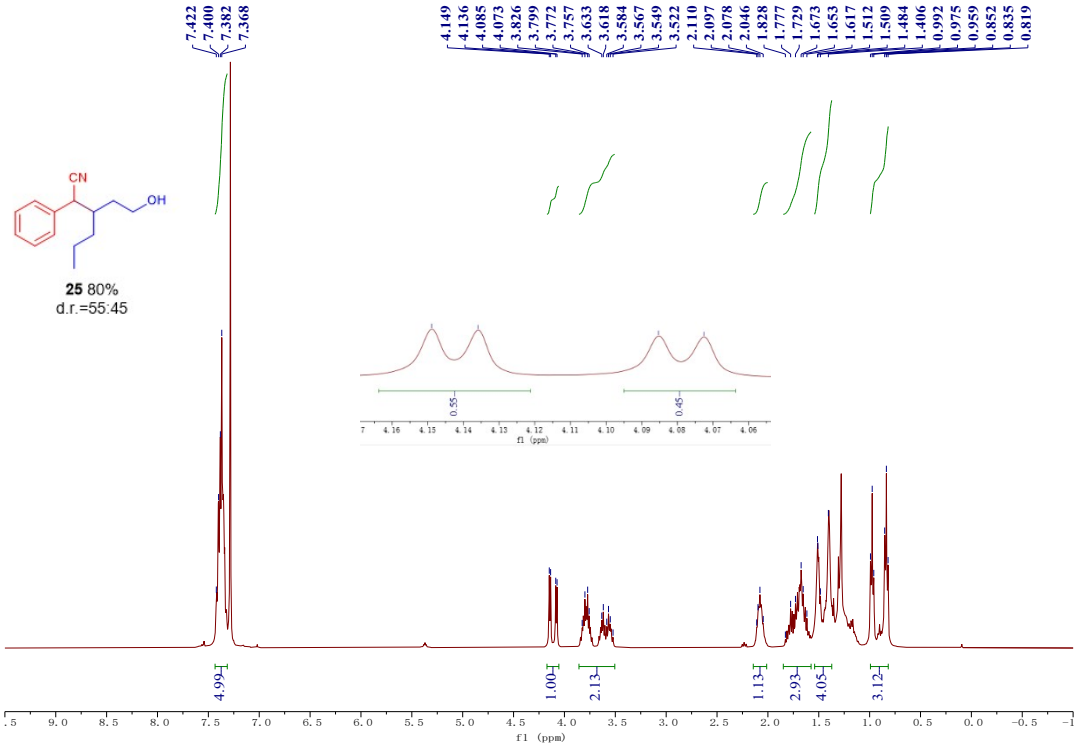

$^{1}$H NMR spectrum of 2-(4-(Tert-butyl) phenyl)-5-hydroxy-3-methylpentanenitrile (**24**, 400 MHz, $CDCl_3$):



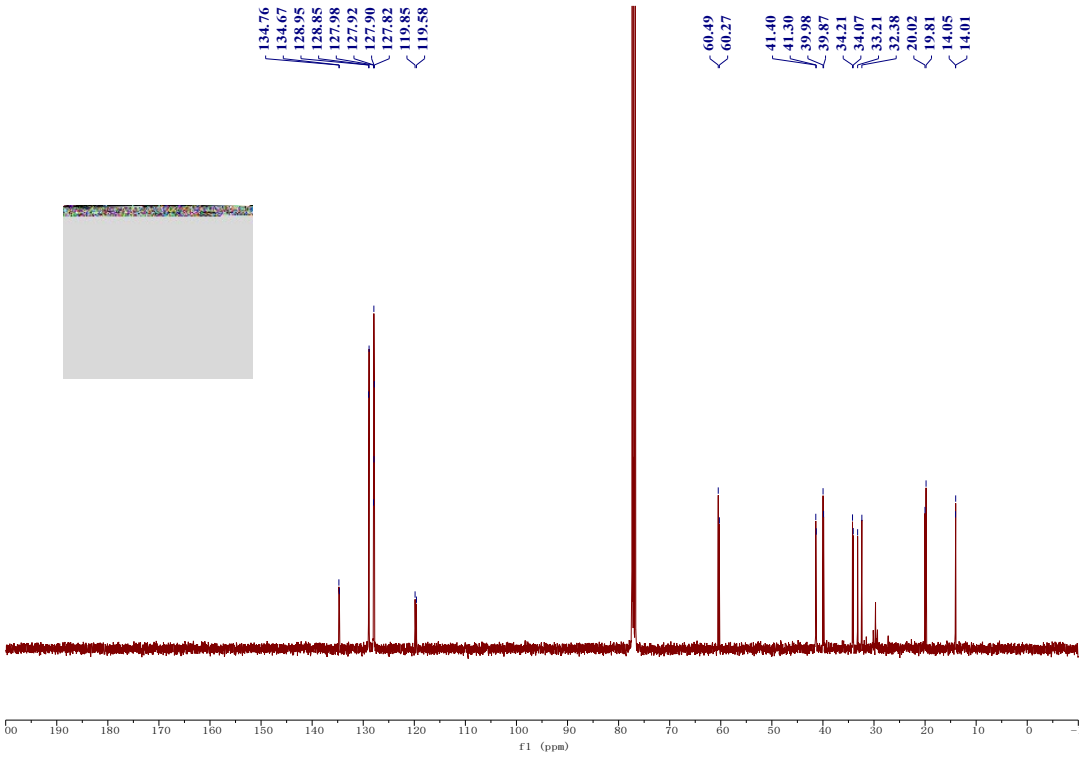

$^{13}$C NMR spectrum of 2-(4-(Tert-butyl) phenyl)-5-hydroxy-3-methylpentanenitrile (**24**, 100 MHz, $CDCl_3$):



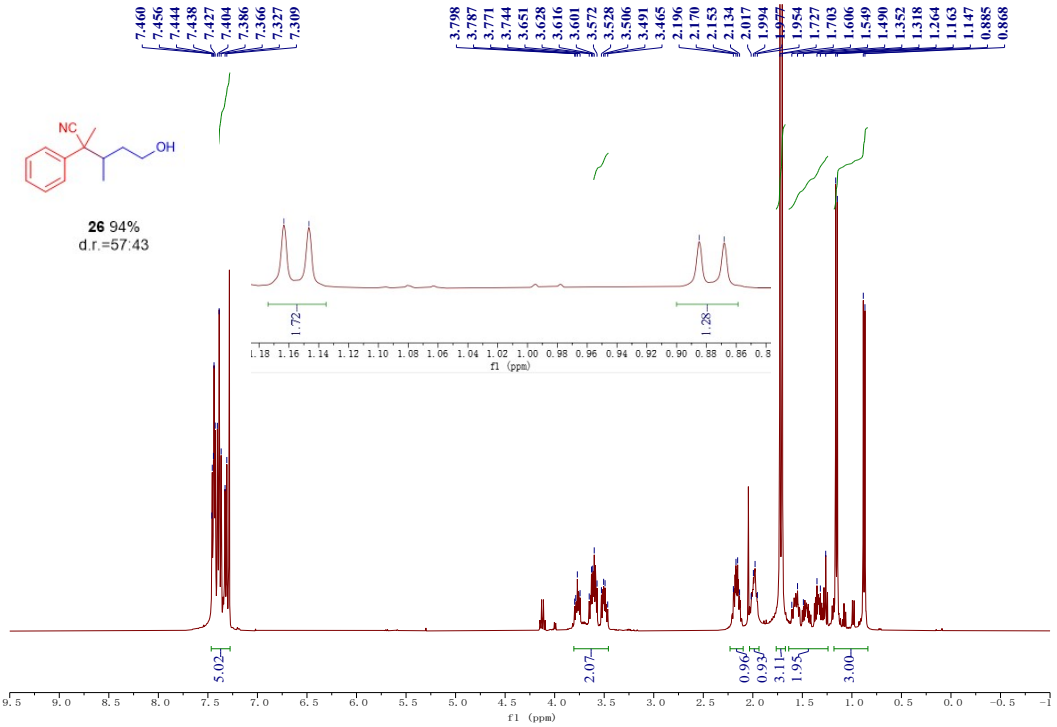

$^1$H NMR spectrum of 3-(2-Hydroxyethyl)-2-phenylhexanenitrile (**25**, 400 MHz, $CDCl_3$):



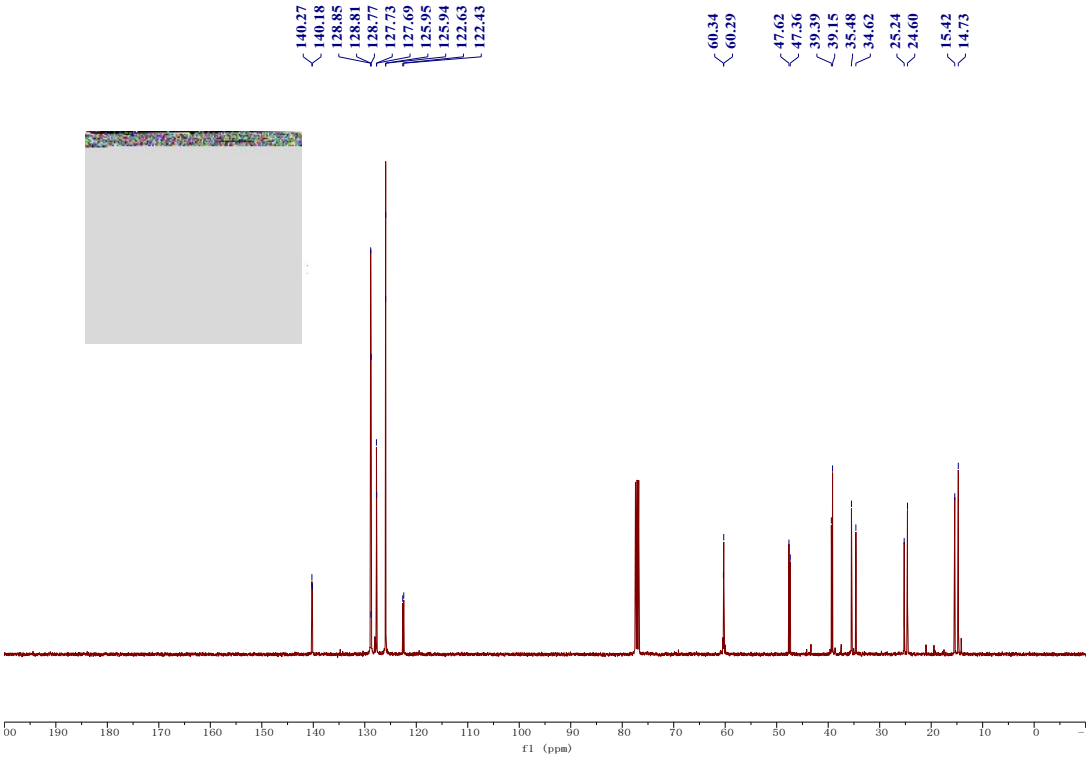
$^{13}$C NMR spectrum of 3-(2-Hydroxyethyl)-2-phenylhexanenitrile (**25**, 100 MHz, $CDCl_3$):



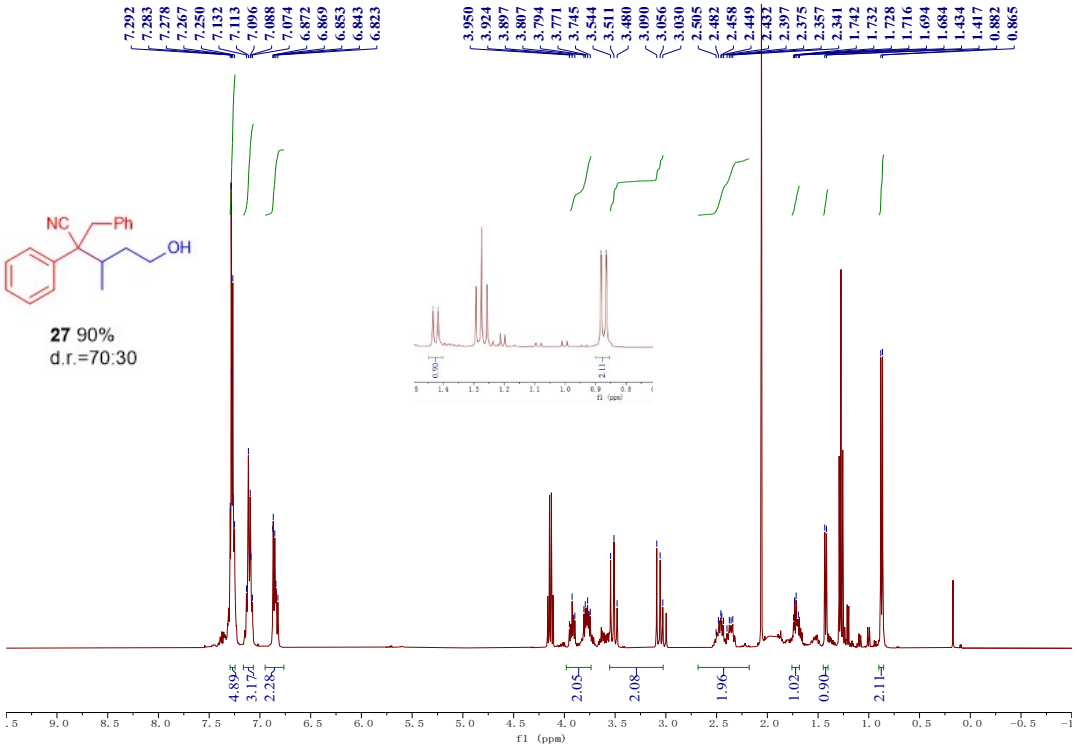

$^{1}$H NMR spectrum of 5-Hydroxy-2,3-dimethyl-2-phenylpentanenitrile (**26**, 400 MHz, $CDCl_3$):



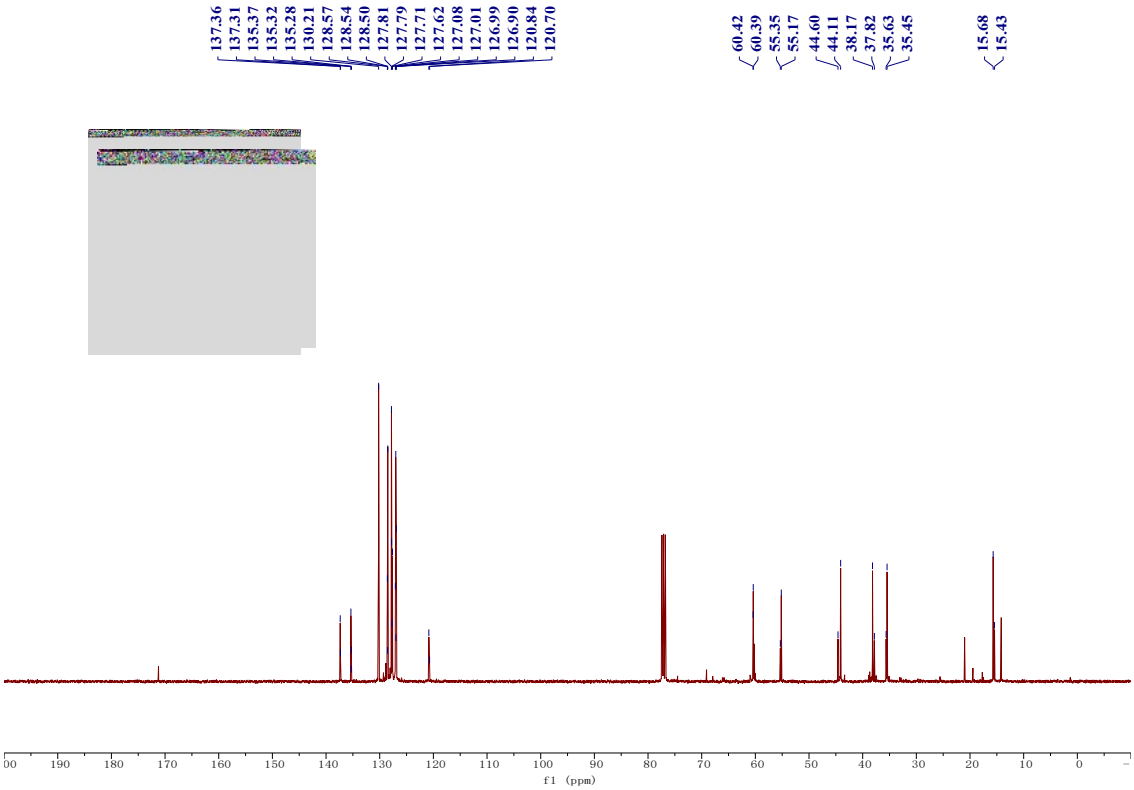
$^{13}$C NMR spectrum of 5-Hydroxy-2,3-dimethyl-2-phenylpentanenitrile (**26**, 100 MHz, $CDCl_3$):



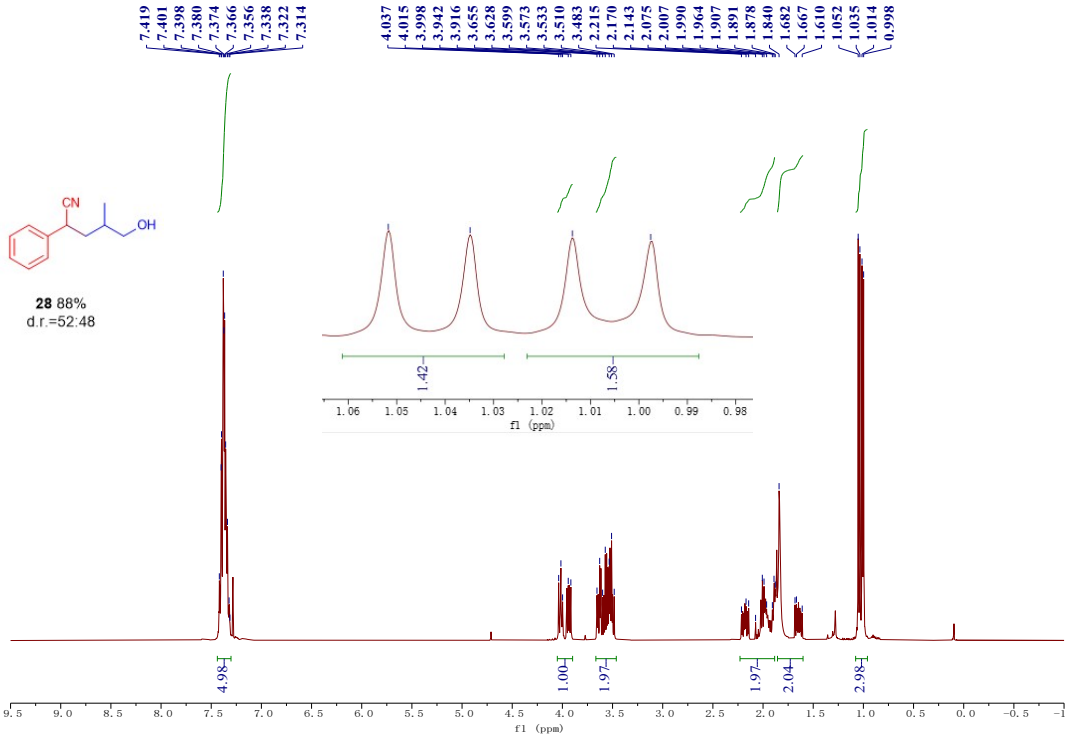
$^{1}$H NMR spectrum of 2-Benzyl-5-hydroxy-3-methyl-2-phenylpentanenitrile (**27**, 400 MHz, $CDCl_3$):



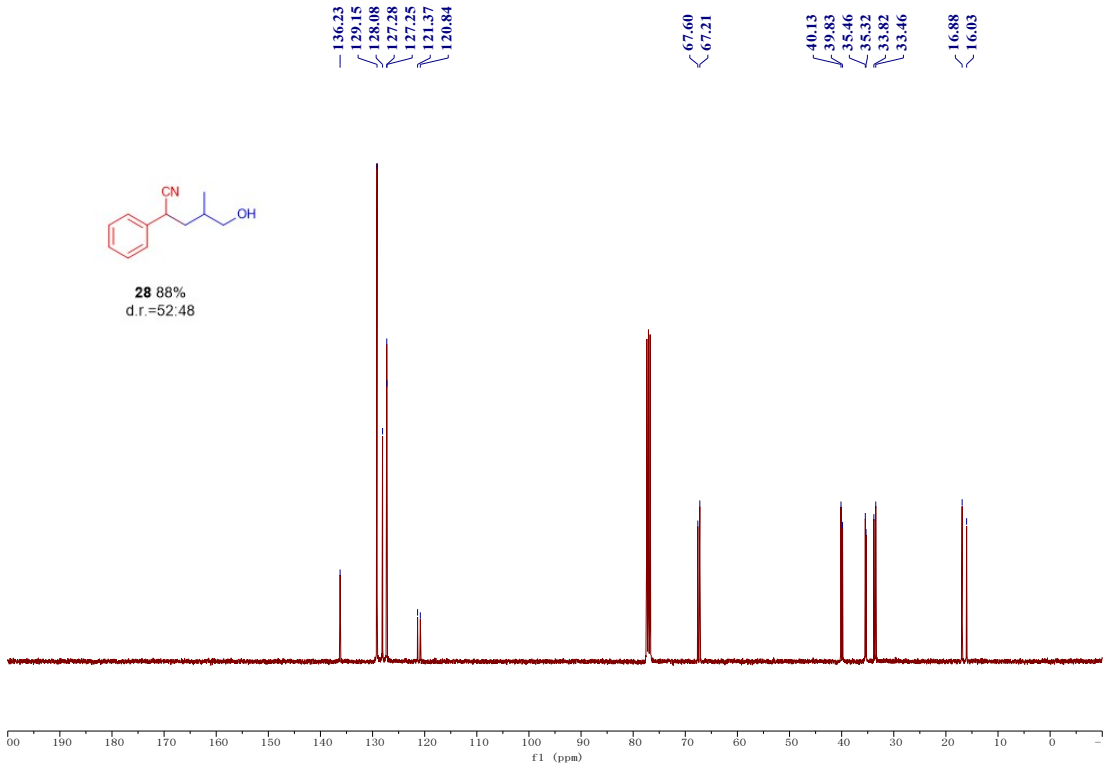

$^{13}$C NMR spectrum of 2-Benzyl-5-hydroxy-3-methyl-2-phenylpentanenitrile (**27**, 100 MHz, $CDCl_3$):


137.36
137.31
135.37
135.32
135.28
130.21
128.57
128.54
128.50
127.81
127.79
127.71
127.62
127.08
127.01
126.99
126.90
120.84
120.70
60.42
60.39
55.35
55.17
44.60
44.11
38.17
37.82
35.63
35.45
15.68
15.43
f1 (ppm)

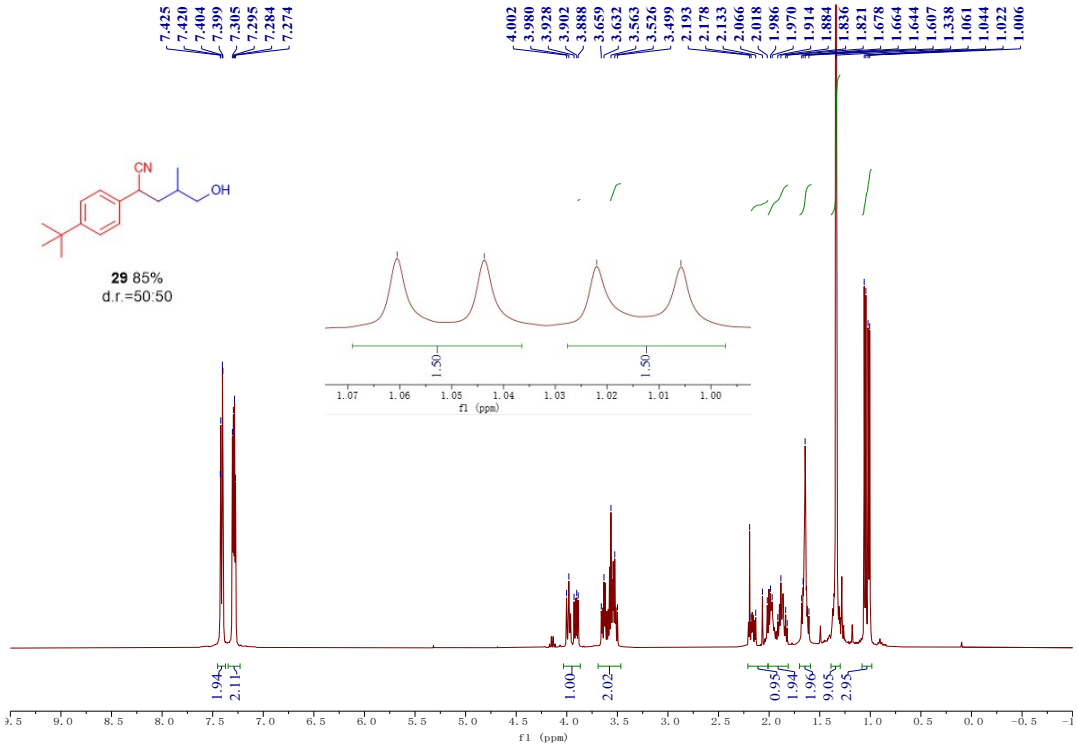
$^{1}$H NMR spectrum of 5-Hydroxy-4-methyl-2-phenylpentanenitrile (**28**, 400 MHz, $CDCl_3$):



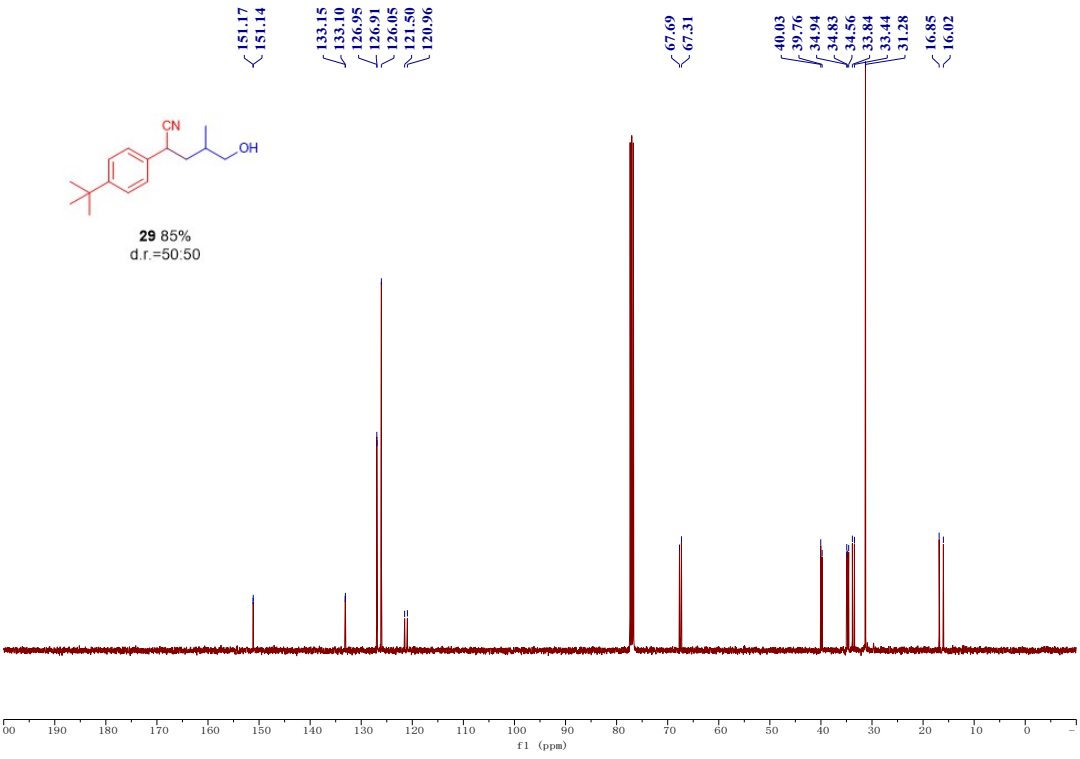

$^{13}$C NMR spectrum of 5-Hydroxy-4-methyl-2-phenylpentanenitrile (**28**, 100 MHz, $CDCl_3$):



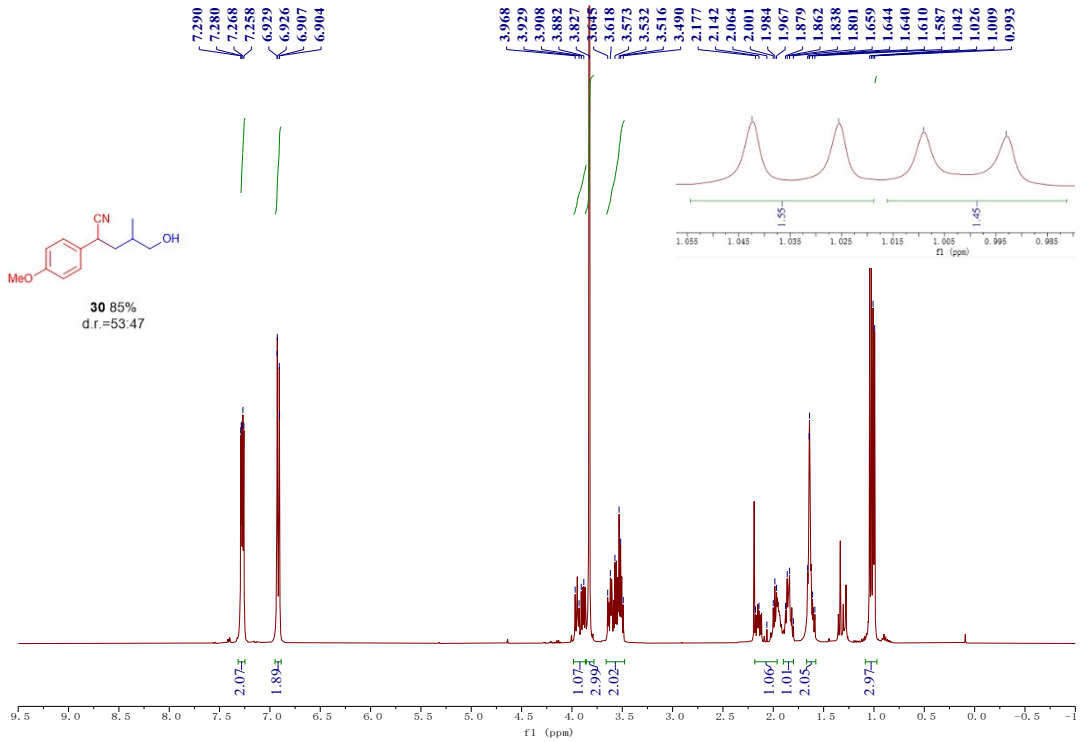
$^{1}$H NMR spectrum of 2-(4-(Tert-butyl) phenyl)-5-hydroxy-4-methylpentanenitrile (**29**, 400 MHz, $CDCl_3$):



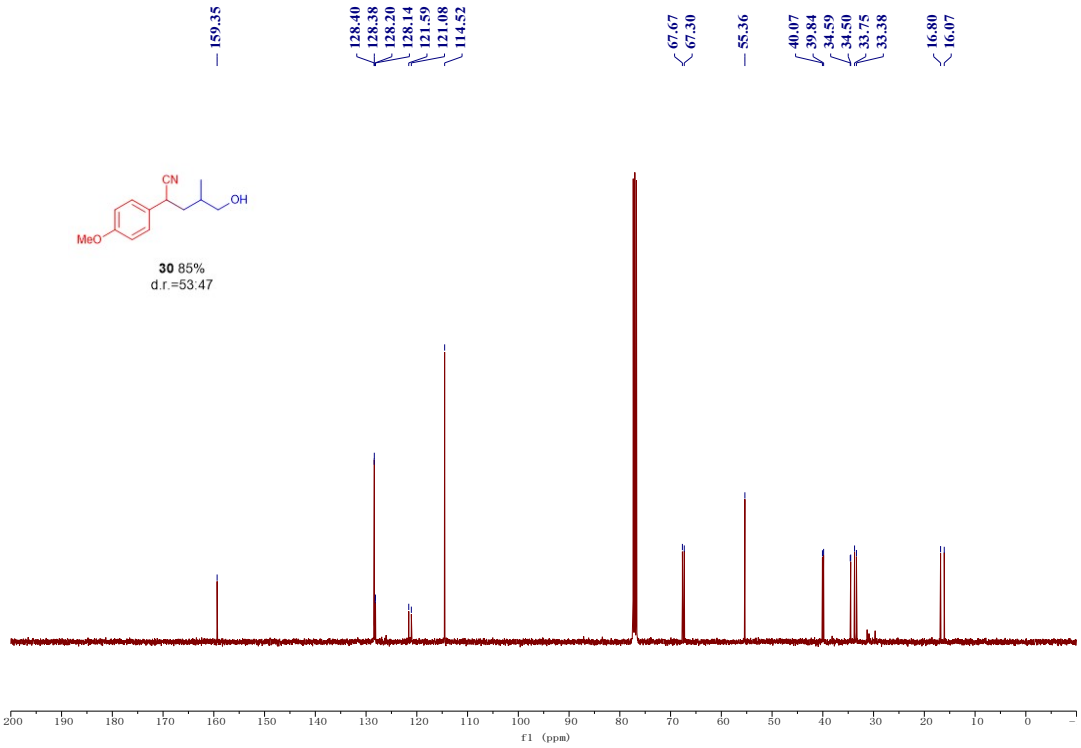

$^{13}$C NMR spectrum of 2-(4-(Tert-butyl) phenyl)-5-hydroxy-4-methylpentanenitrile (**29**, 100 MHz, $CDCl_3$):



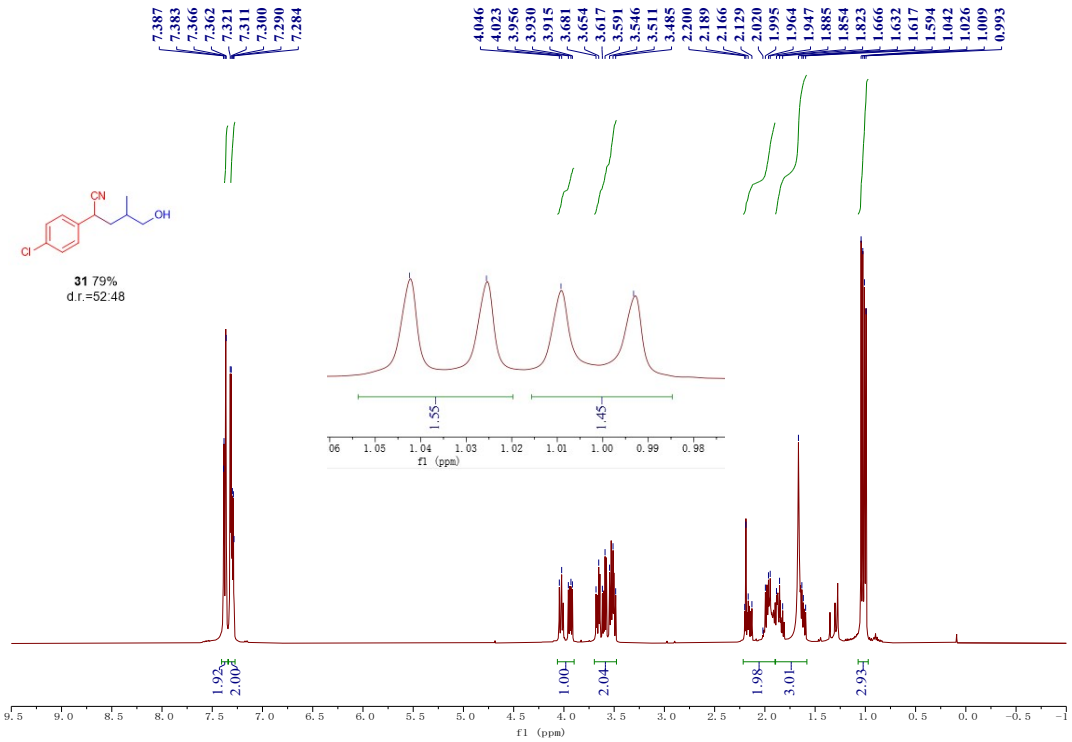
$^{1}$H NMR spectrum of 5-Hydroxy-2-(4-methoxyphenyl)-4-methylpentanenitrile (**30**, 400 MHz, $CDCl_3$):



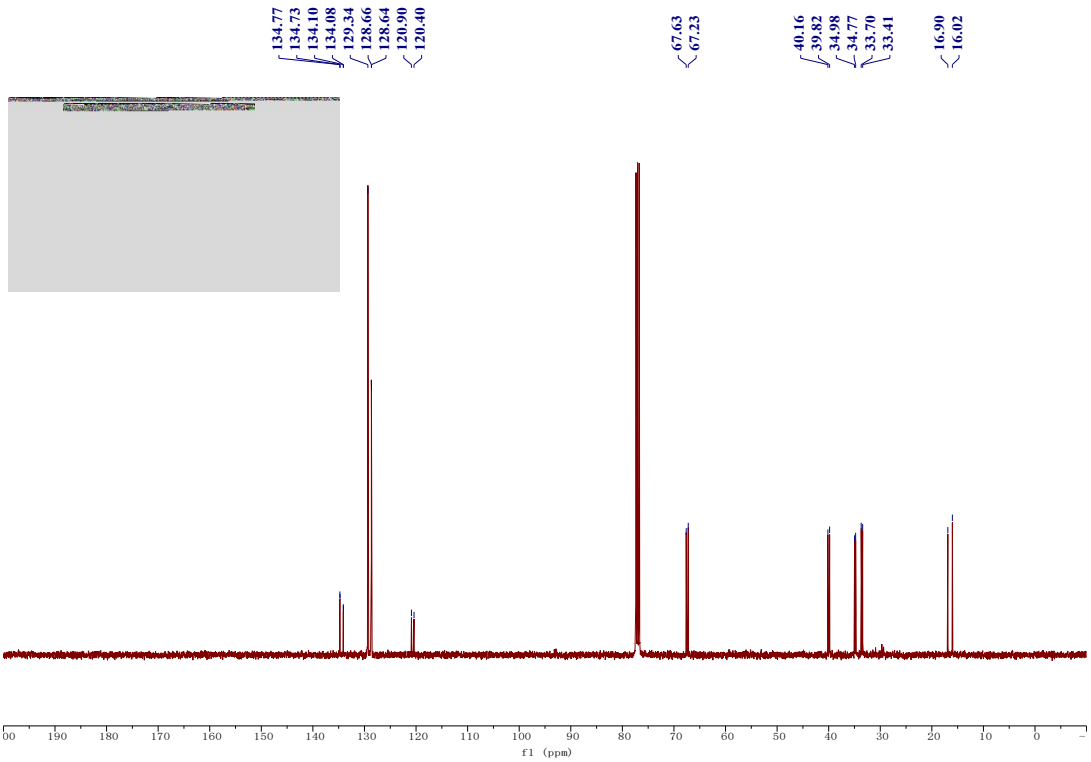

$^{13}$C NMR spectrum of 5-Hydroxy-2-(4-methoxyphenyl)-4-methylpentanenitrile (**30**, 100 MHz, $CDCl_3$):



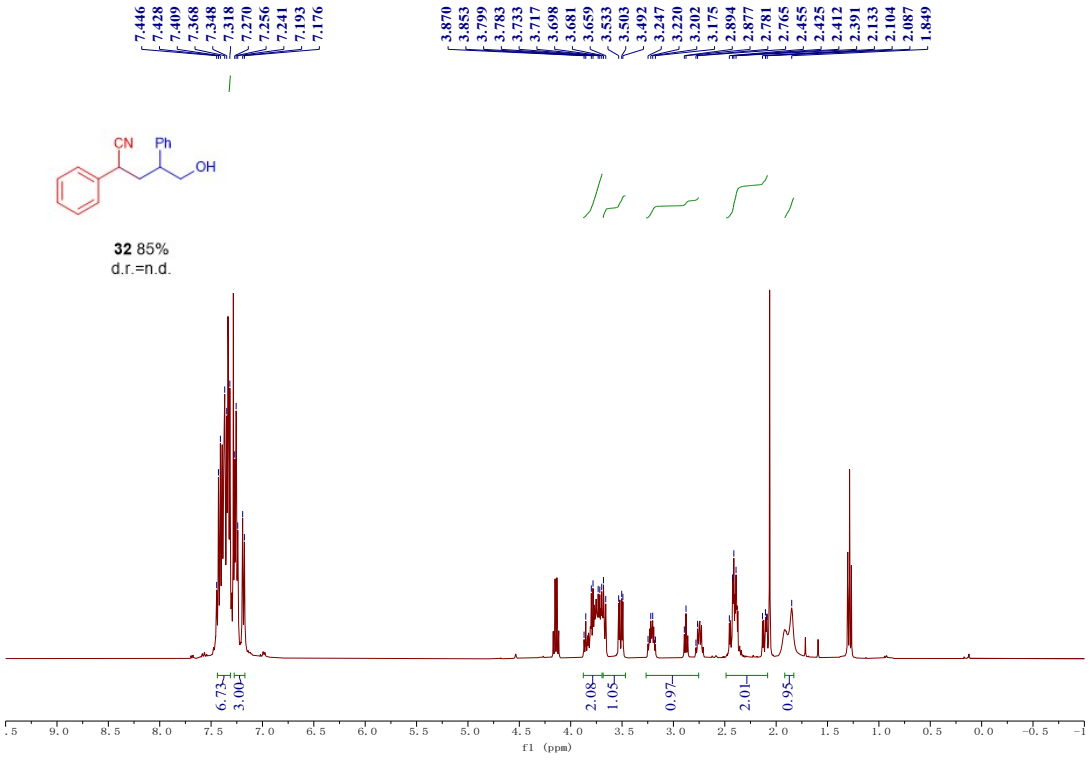
$^{1}$H NMR spectrum of 2-(4-Chlorophenyl)-5-hydroxy-4-methylpentanenitrile (**31**, 400 MHz, $CDCl_3$):



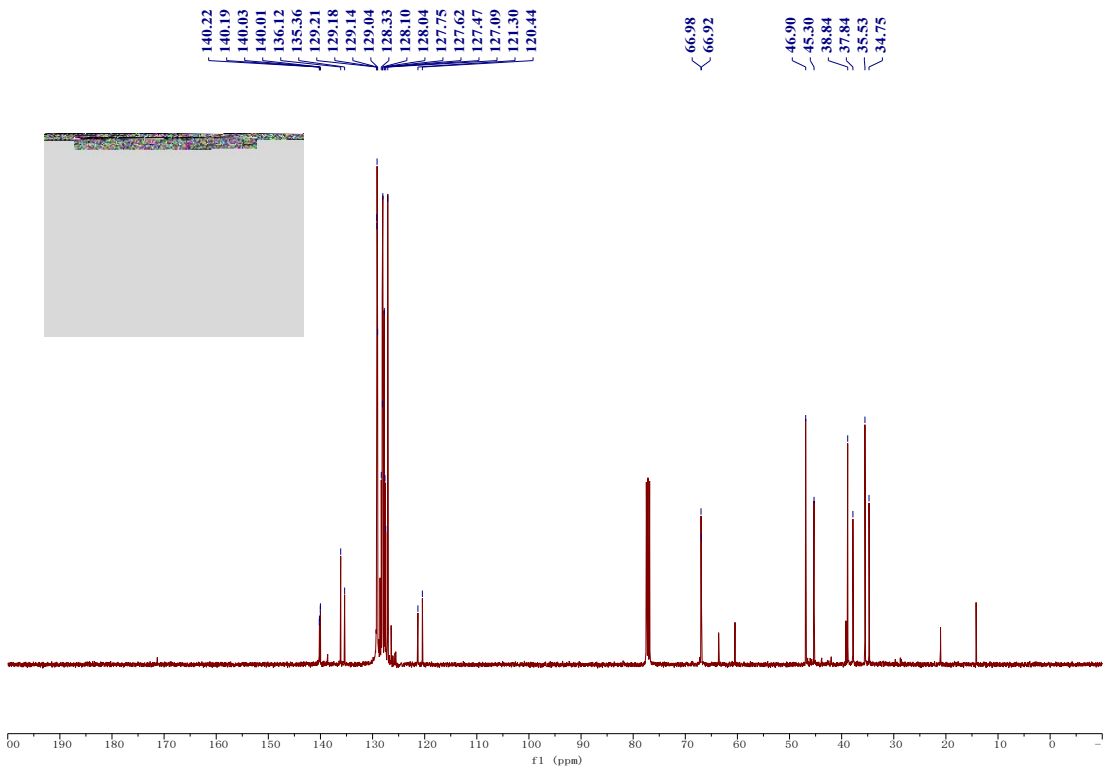

$^{13}$C NMR spectrum of 2-(4-Chlorophenyl)-5-hydroxy-4-methylpentanenitrile (**31**, 100 MHz, $CDCl_3$):



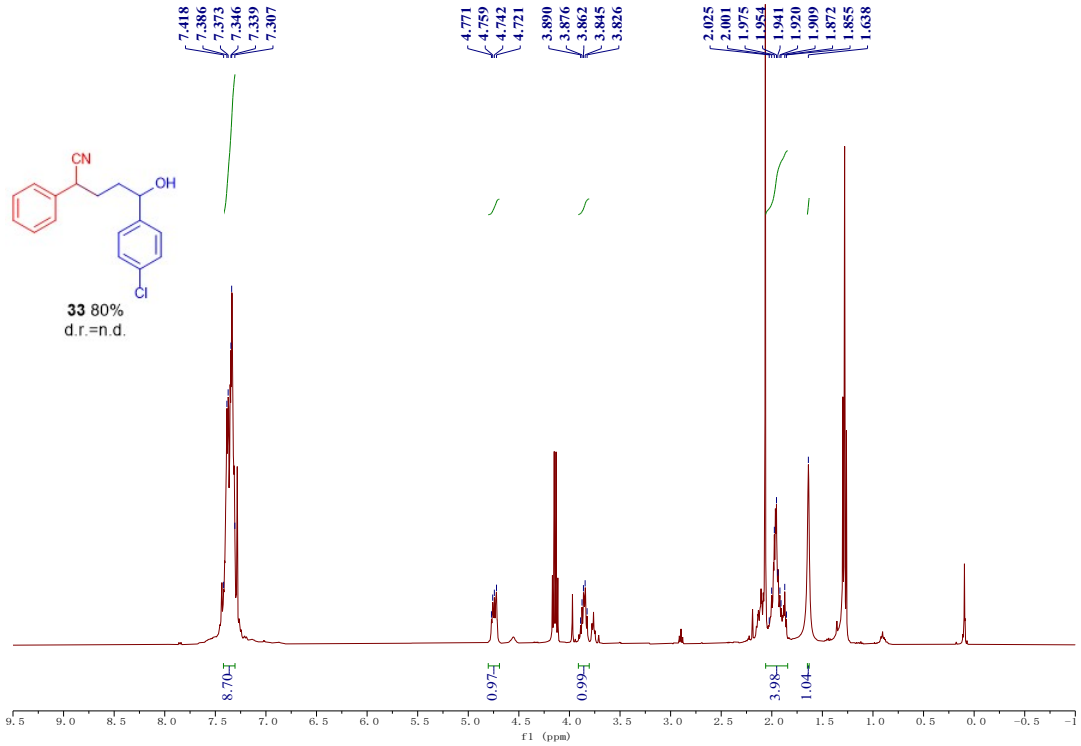

$^{1}$H NMR spectrum of 5-Hydroxy-2,4-diphenylpentanenitrile (**32**, 400 MHz, $CDCl_3$):



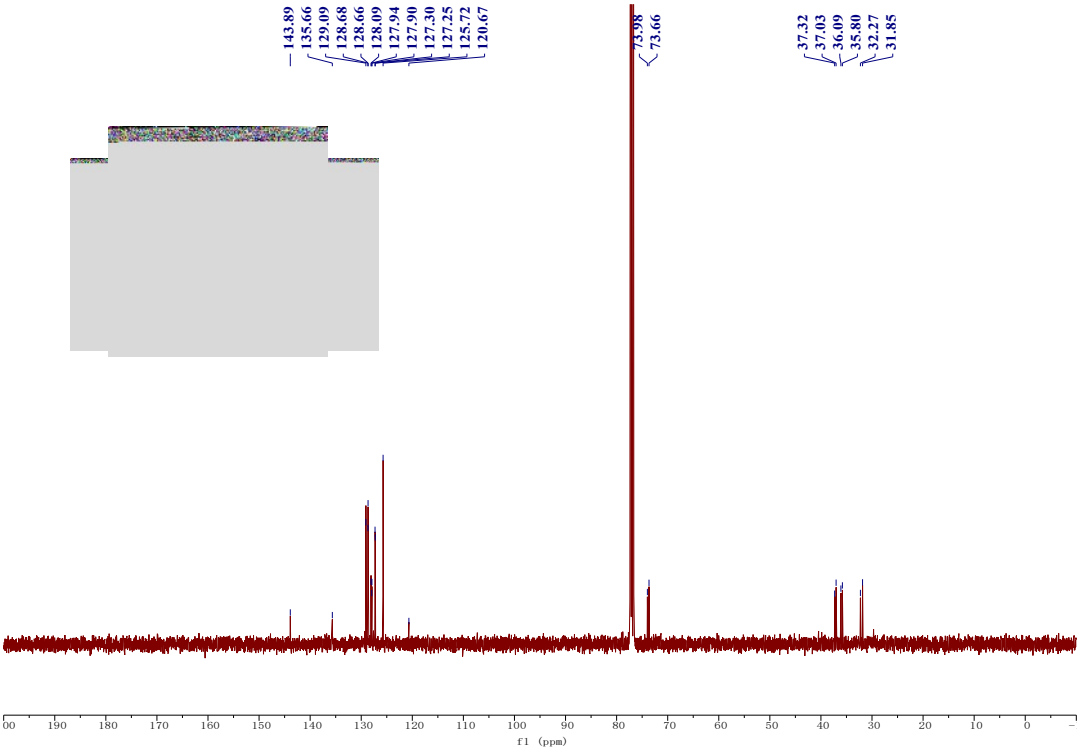

$^{13}$C NMR spectrum of 5-Hydroxy-2,4-diphenylpentanenitrile (**32**, 100 MHz, $CDCl_3$):



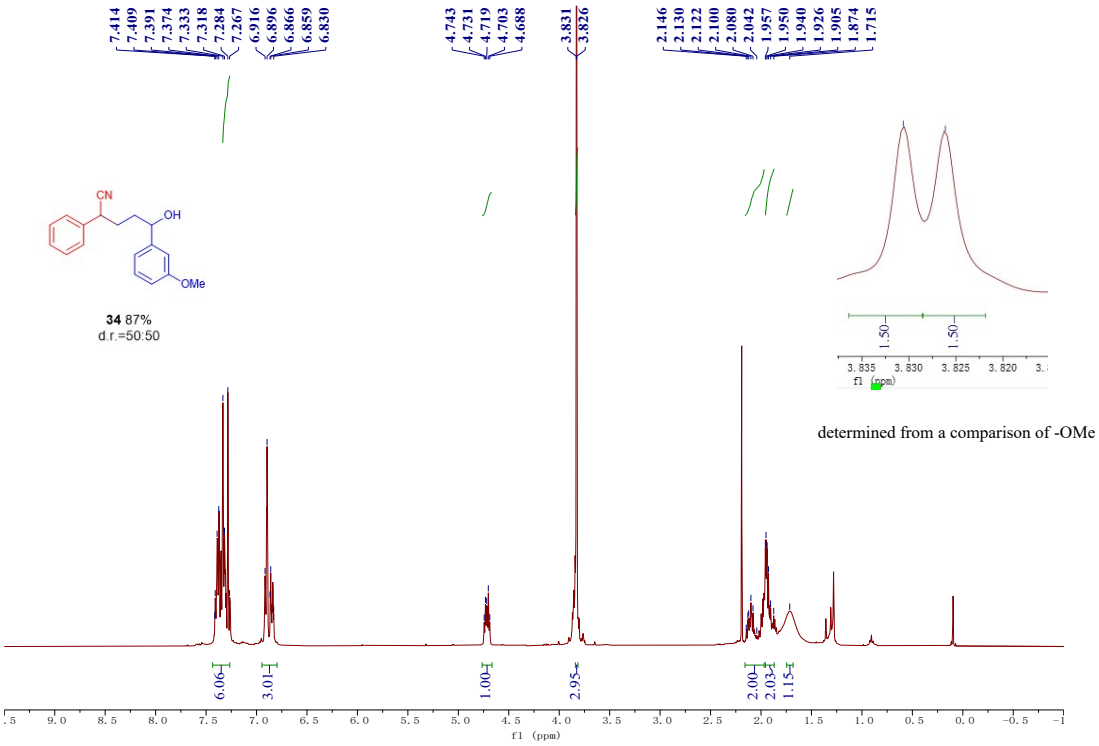

$^1$H NMR spectrum of 5-(4-Chlorophenyl)-5-hydroxy-2-phenylpentanenitrile (**33**, 400 MHz, $CDCl_3$):



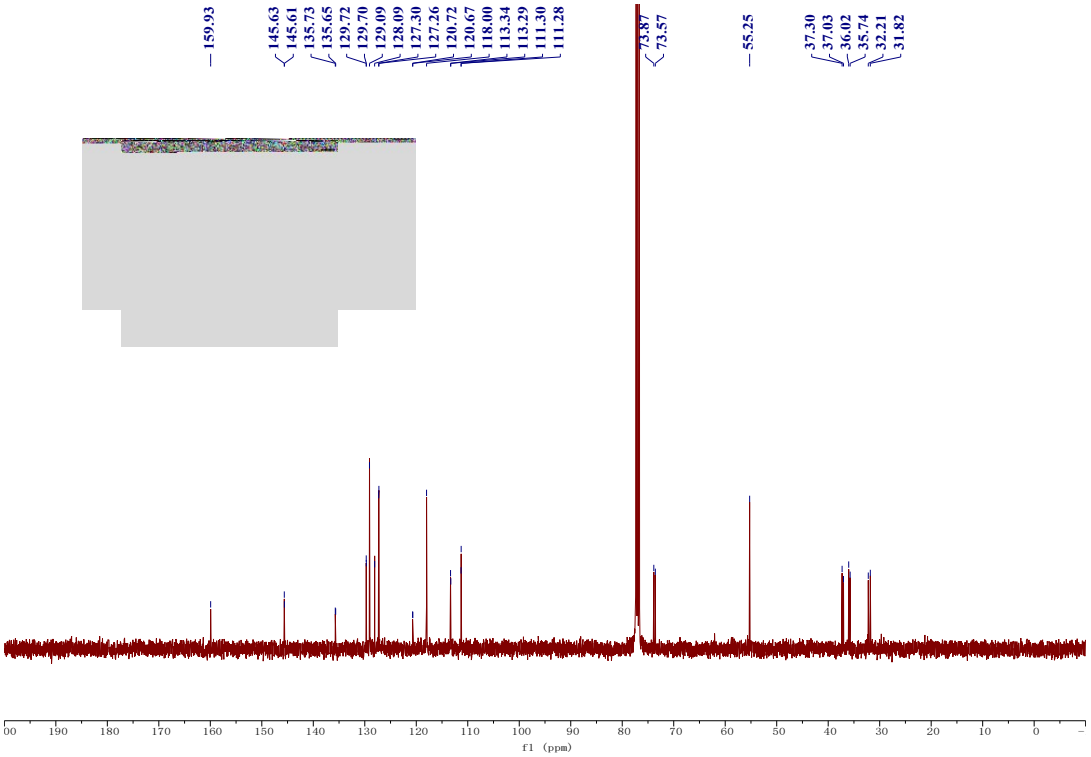
$^{13}C$ NMR spectrum of 5-(4-Chlorophenyl)-5-hydroxy-2-phenylpentanenitrile (**33**, 100 MHz, $CDCl_3$):



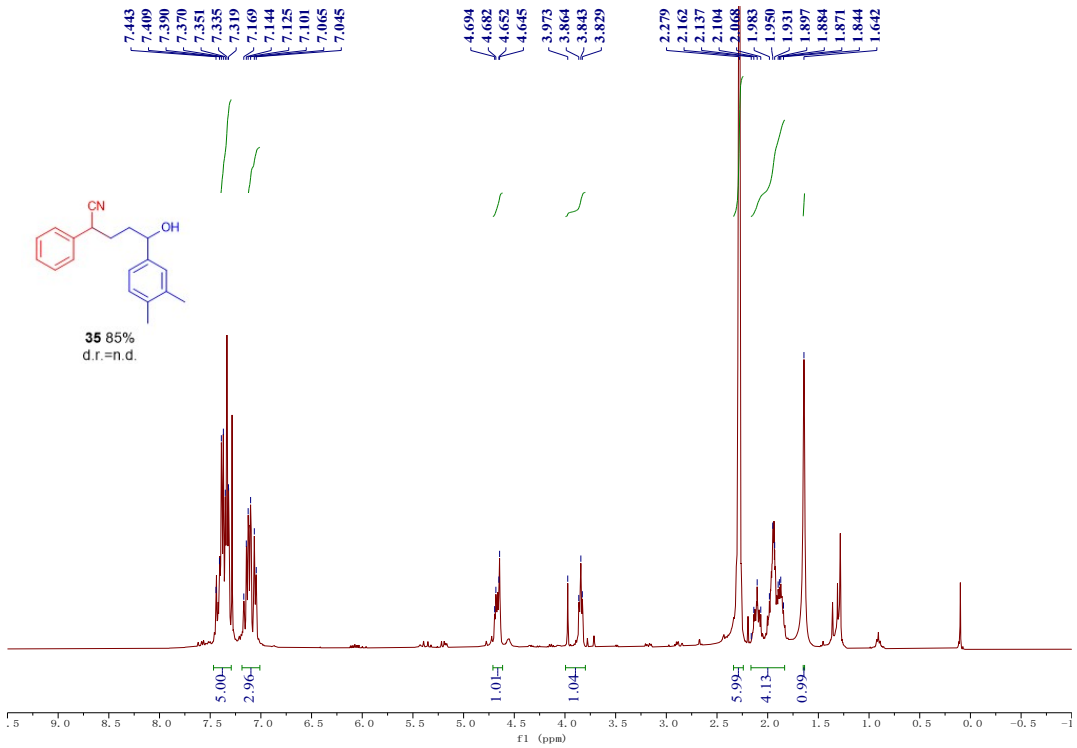

$^{1}H$ NMR spectrum of 5-hydroxy-2-(4-methoxyphenyl)-4-methylpentanenitrile (**34**, 400 MHz, $CDCl_3$):



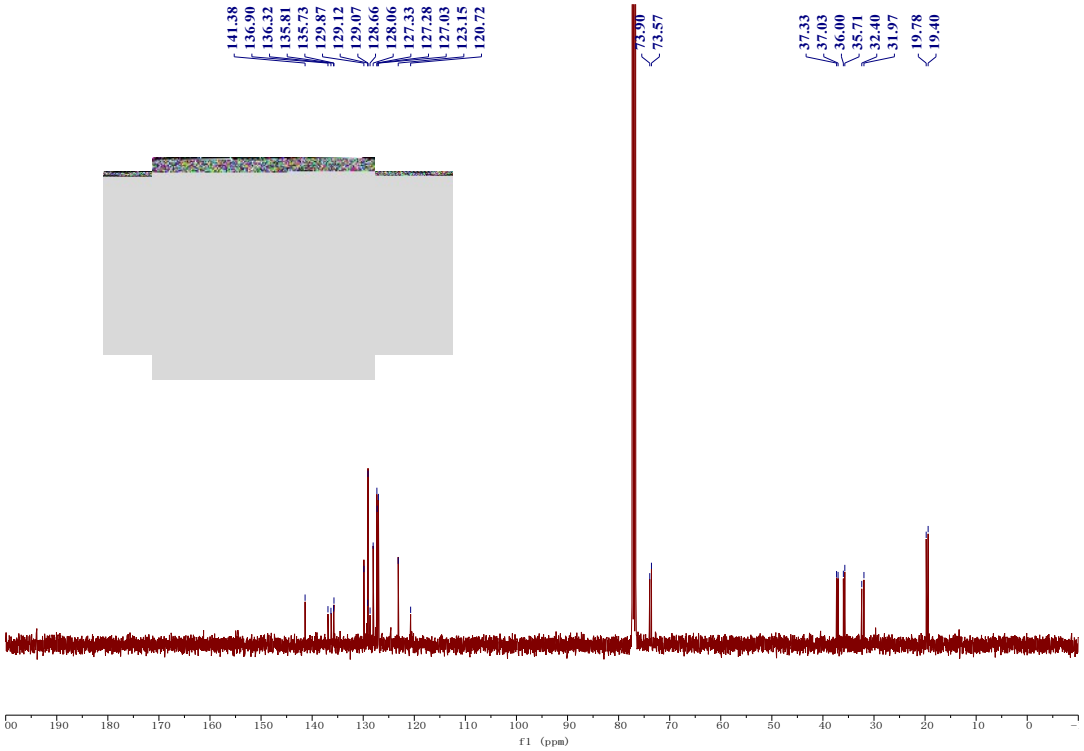
$^{13}C$ NMR spectrum of 5-hydroxy-2-(4-methoxyphenyl)-4-methylpentanenitrile (**34**, 100 MHz, $CDCl_3$):



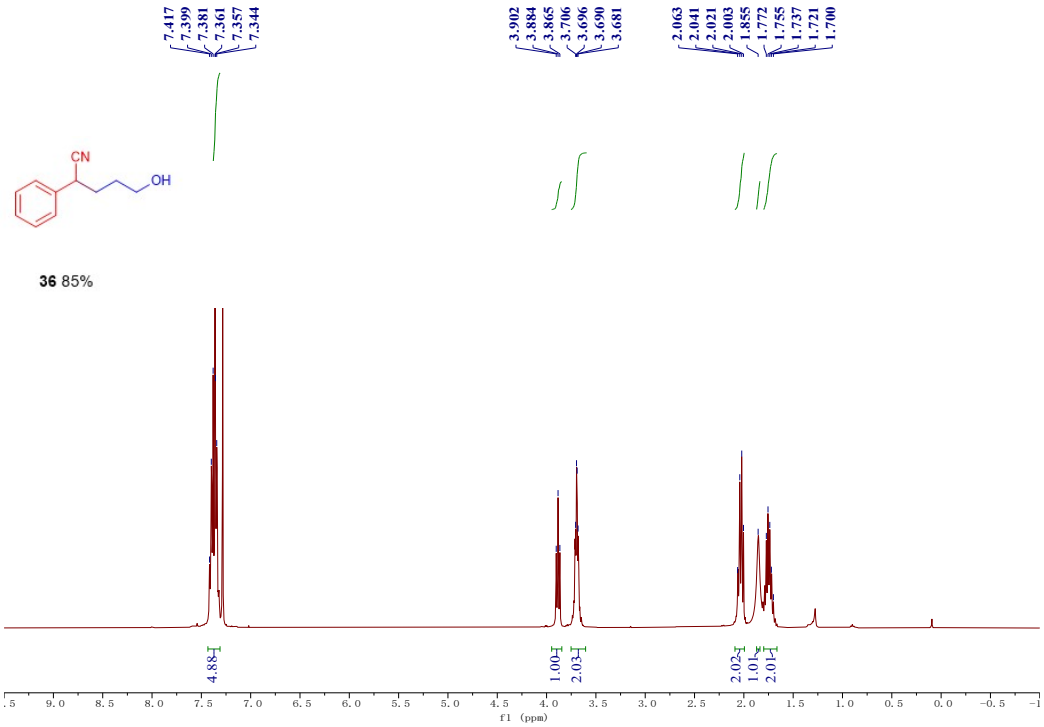

$^{1}H$ NMR spectrum of 5-(3,4-dimethylphenyl)-5-hydroxy-2-phenylpentanenitrile (**35**, 400 MHz, $CDCl_3$):



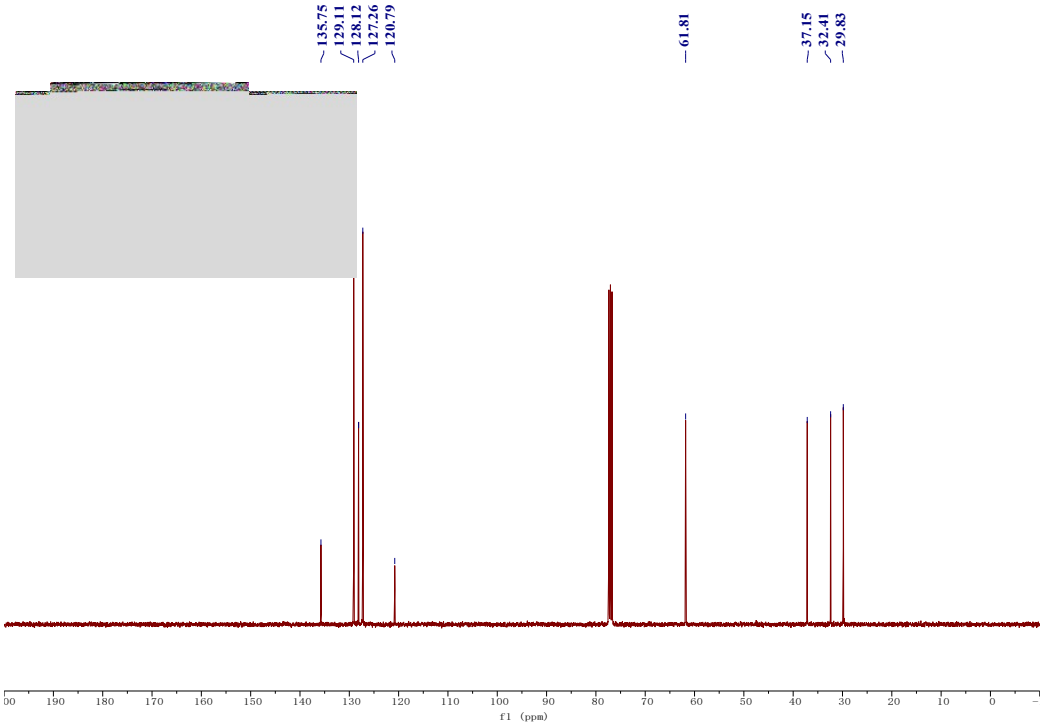
$^{13}C$ NMR spectrum of 5-(3,4-dimethylphenyl)-5-hydroxy-2-phenylpentanenitrile (**35**, 100 MHz, $CDCl_3$):



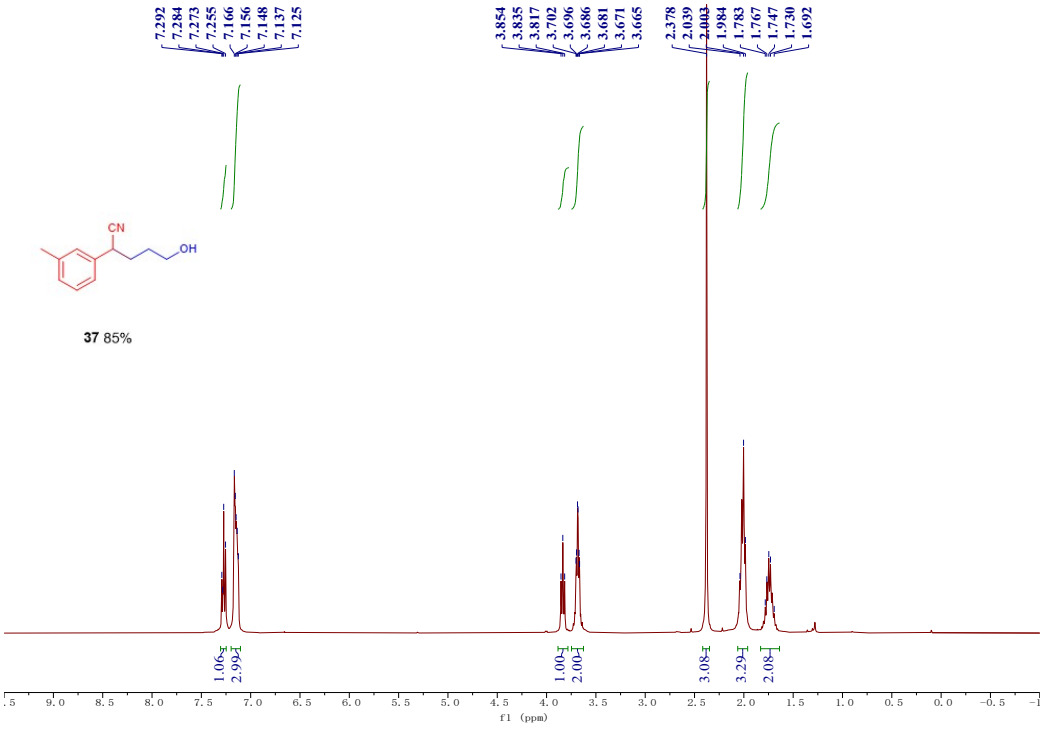

$^{1}H$ NMR spectrum of 5-hydroxy-2-phenylpentanenitrile (**36**, 400 MHz, $CDCl_3$):



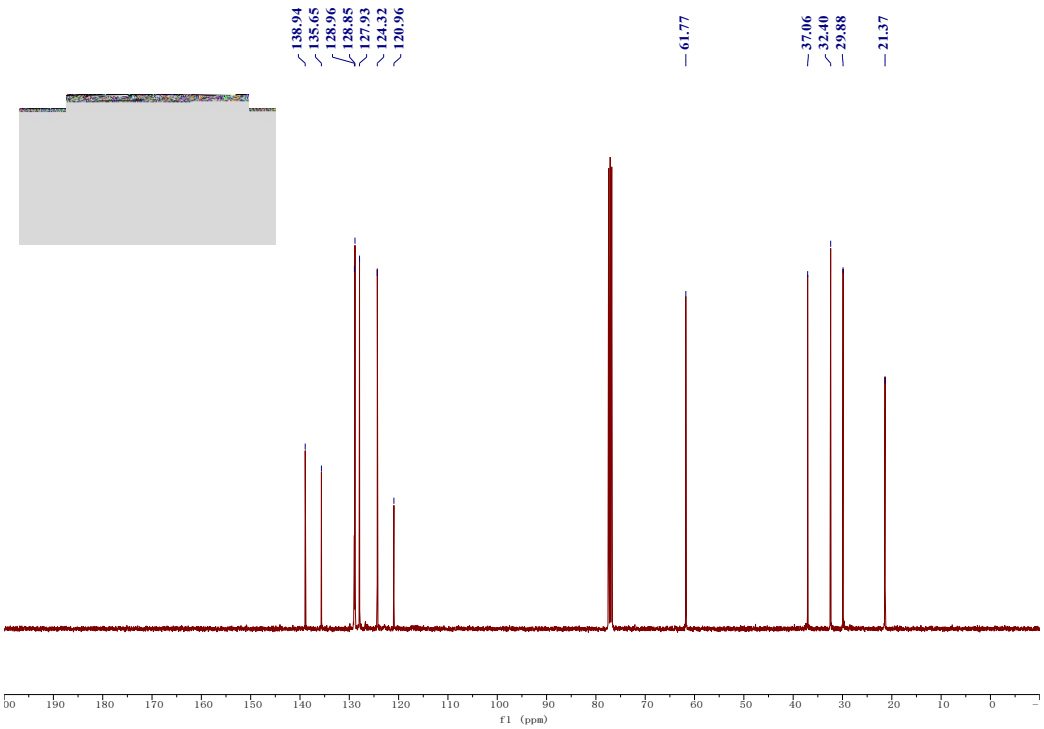
$^{13}$C NMR spectrum of 5-hydroxy-2-phenylpentanenitrile (**36**, 100 MHz, $CDCl_3$):



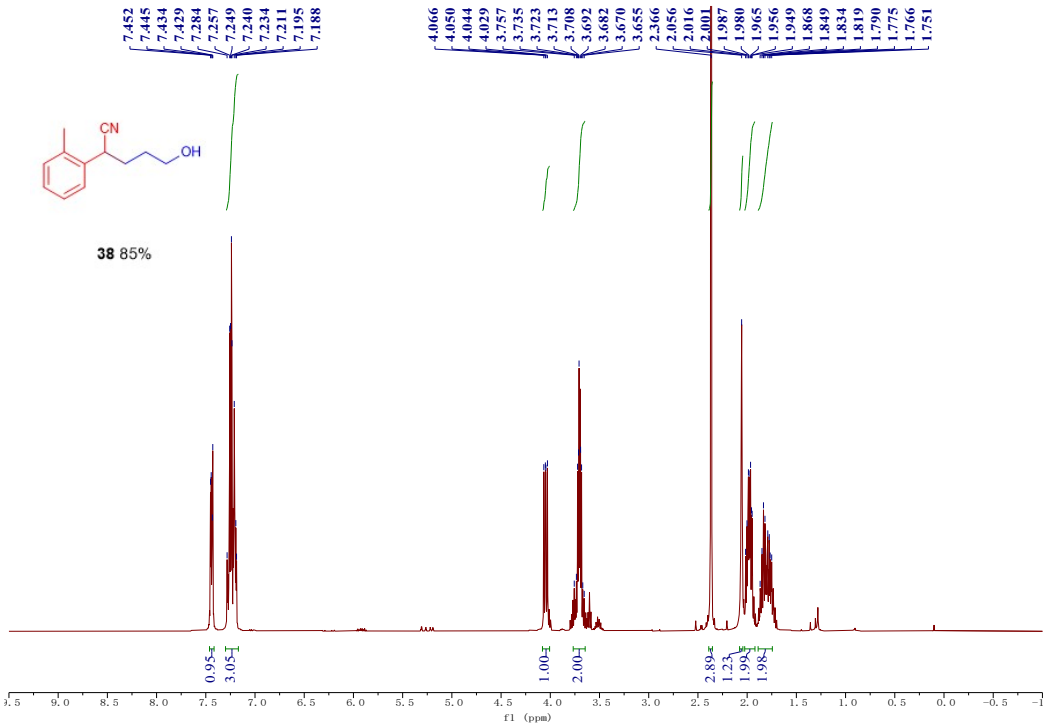

$^{1}$H NMR spectrum of 5-Hydroxy-2-(*m*-tolyl) pentanenitrile (**37**, 400 MHz, $CDCl_3$):



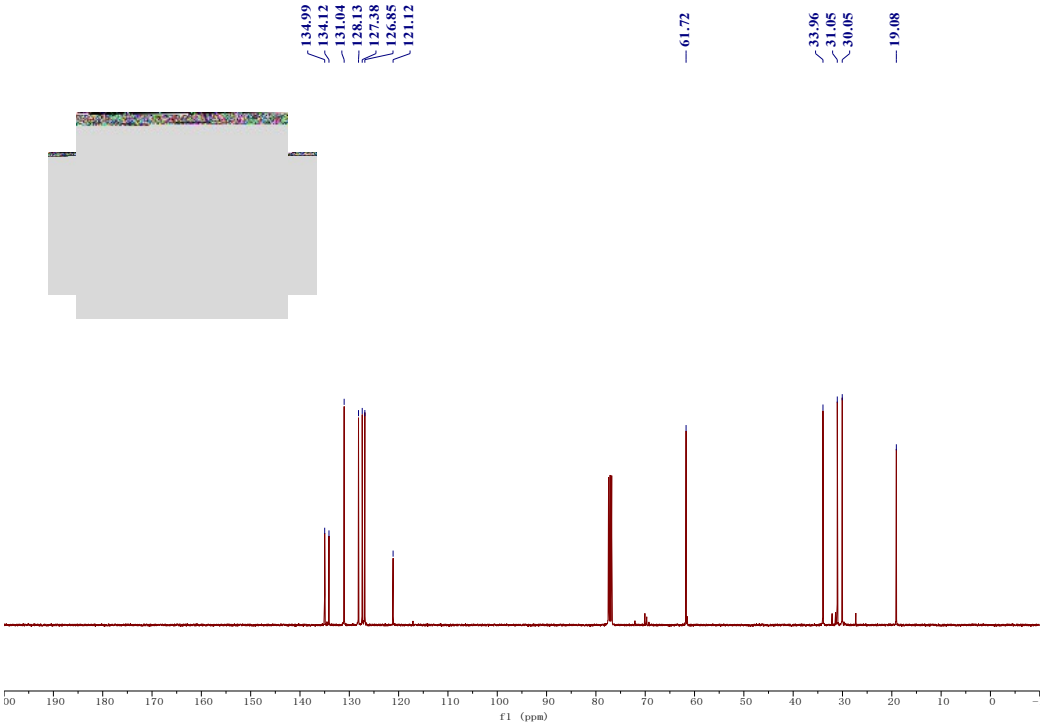

$^{13}$C NMR spectrum of 5-Hydroxy-2-(*m*-tolyl) pentanenitrile (**37**, 100 MHz, $CDCl_3$):



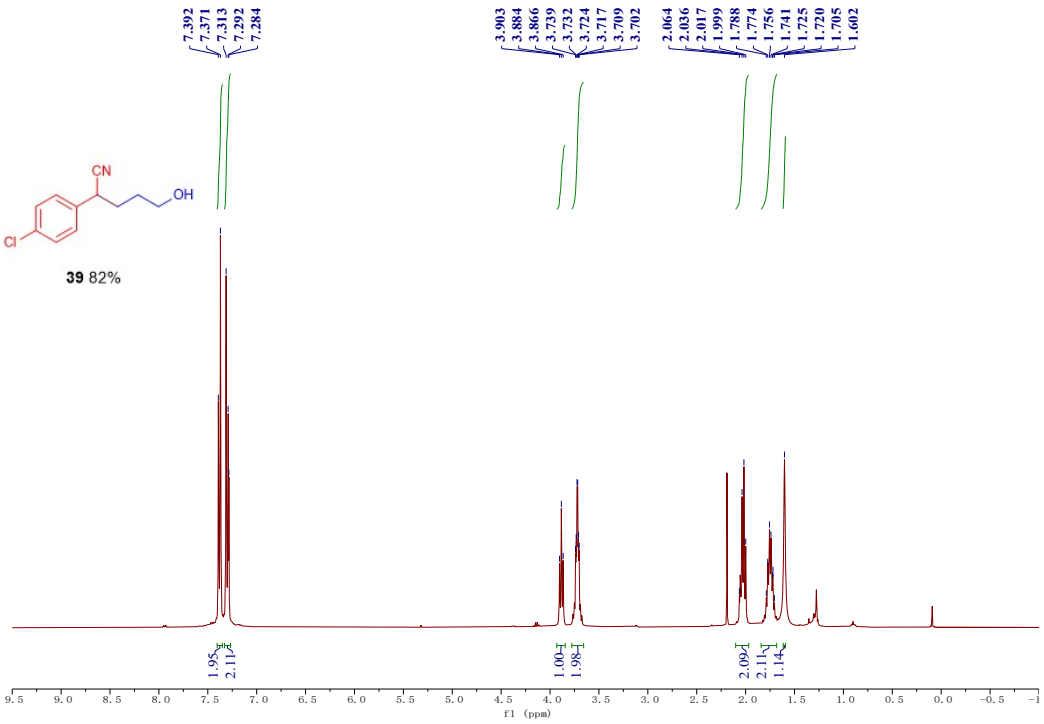

$^1$H NMR spectrum of 5-Hydroxy-2-(*o*-tolyl) pentanenitrile (**38**, 400 MHz, $CDCl_3$):



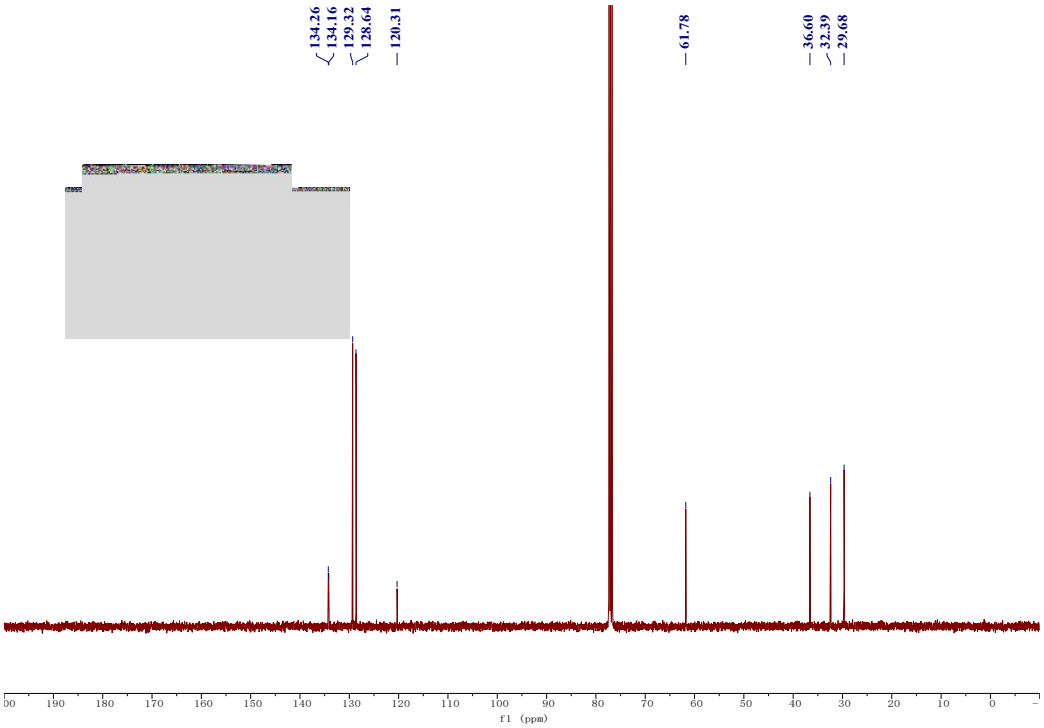
$^{13}$C NMR spectrum of 5-Hydroxy-2-(*o*-tolyl) pentanenitrile (**38**, 100 MHz, $CDCl_3$):



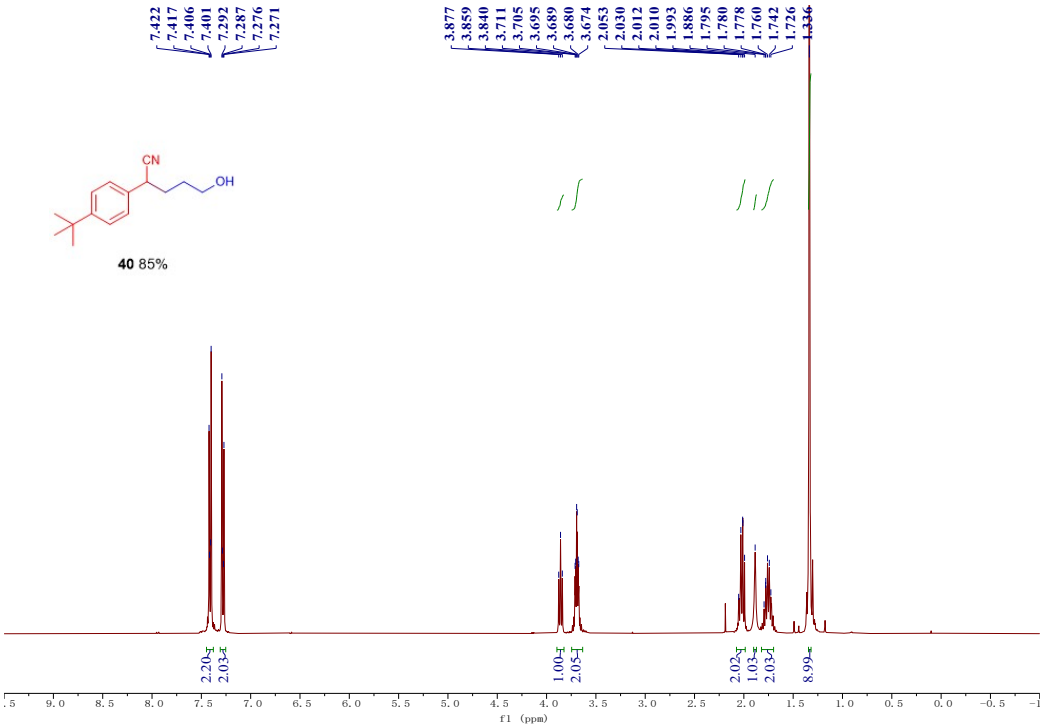

$^{1}$H NMR spectrum of 2-(4-Chlorophenyl)-5-hydroxypentanenitrile (**39**, 400 MHz, $CDCl_3$):



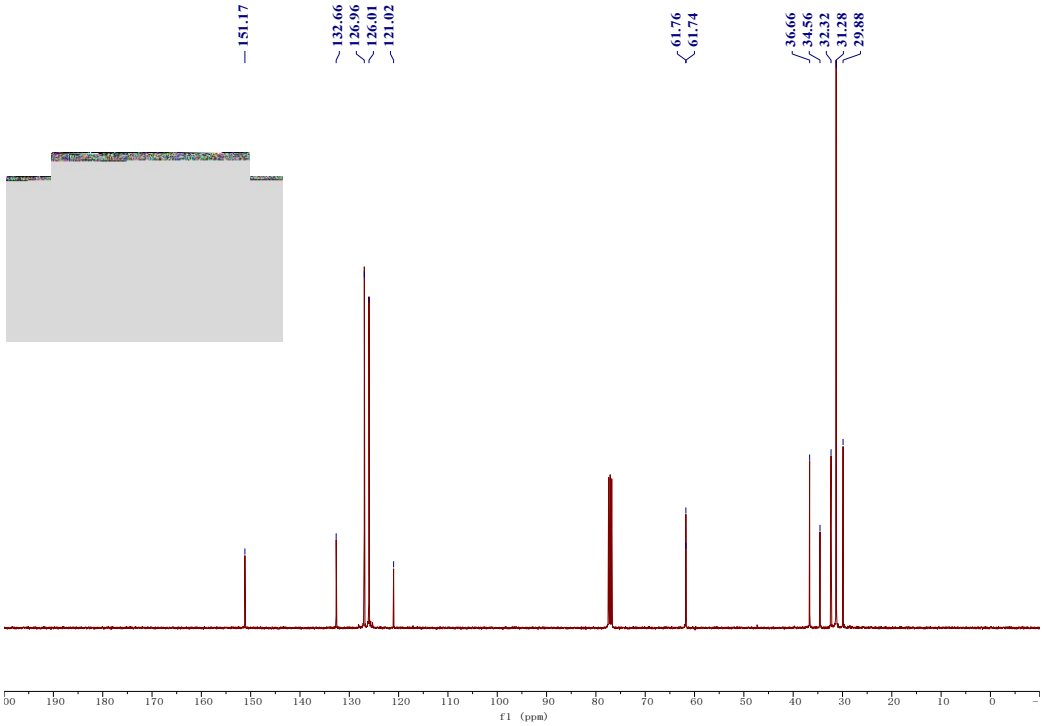
$^{13}C$ NMR spectrum of 2-(4-Chlorophenyl)-5-hydroxypentanenitrile (**39**, 100 MHz, $CDCl_3$):



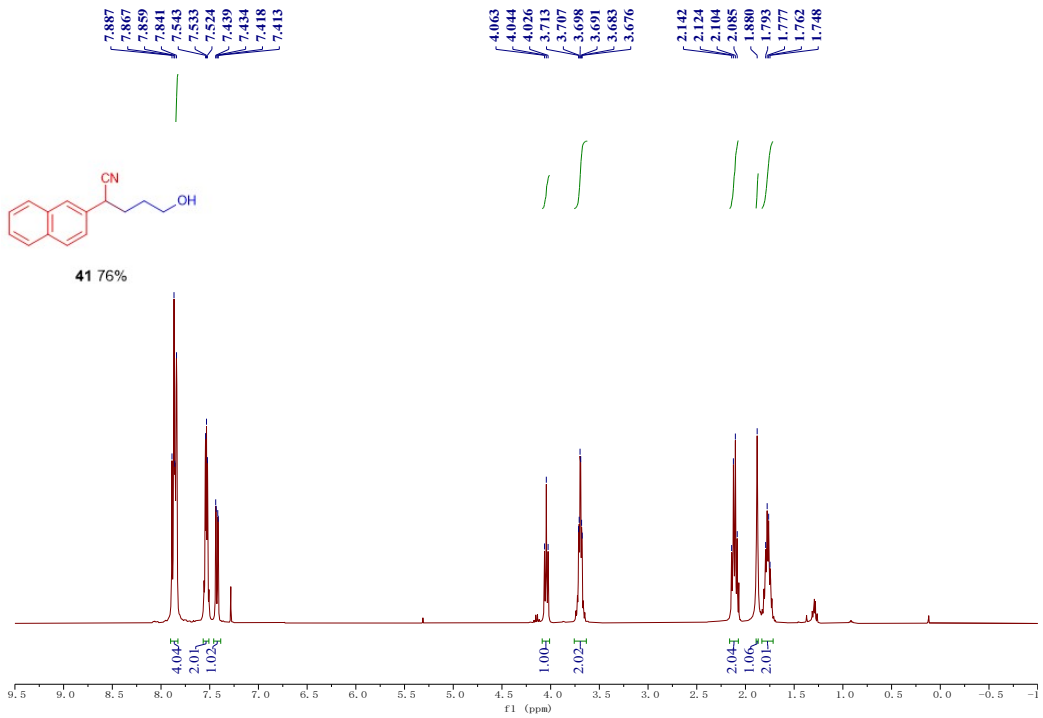

$^{1}H$ NMR spectrum of 2-(4-(Tert-butyl) phenyl)-5-hydroxypentanenitrile (**40**, 400 MHz, $CDCl_3$):



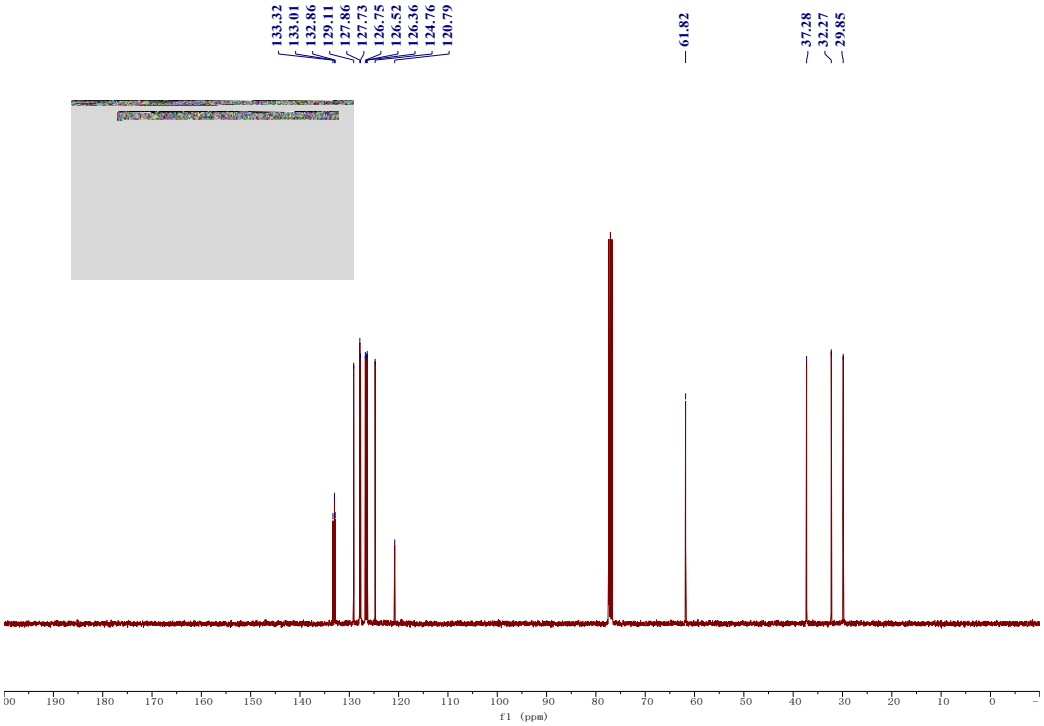
$^{13}C$ NMR spectrum of 2-(4-(Tert-butyl) phenyl)-5-hydroxypentanenitrile (**40**, 100 MHz, $CDCl_3$):



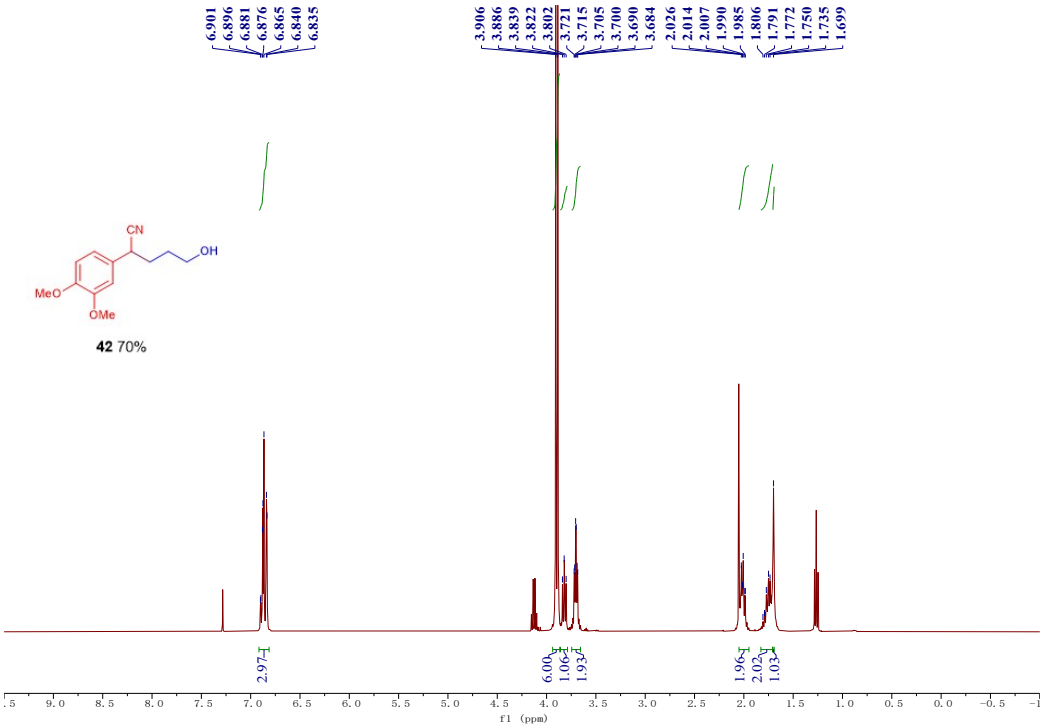

$^{1}H$ NMR spectrum of 5-Hydroxy-2-(naphthalen-2-yl) pentanenitrile (**41**, 400 MHz, $CDCl_3$):



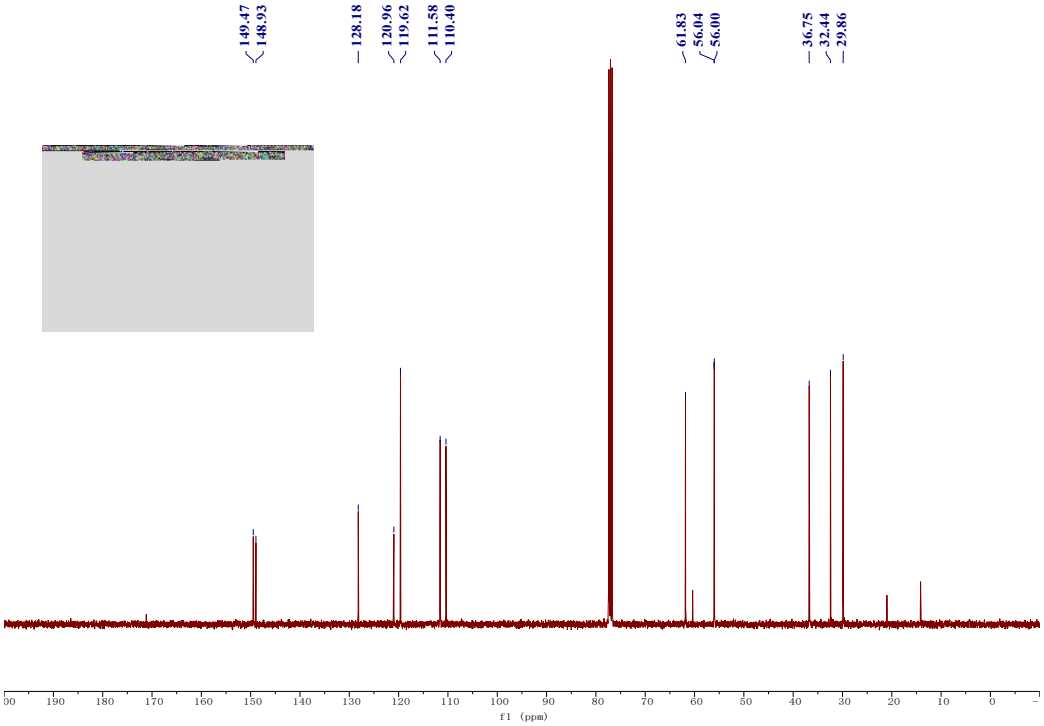
$^{13}$C NMR spectrum of 5-Hydroxy-2-(naphthalen-2-yl) pentanenitrile (**41**, 100 MHz, $CDCl_3$):



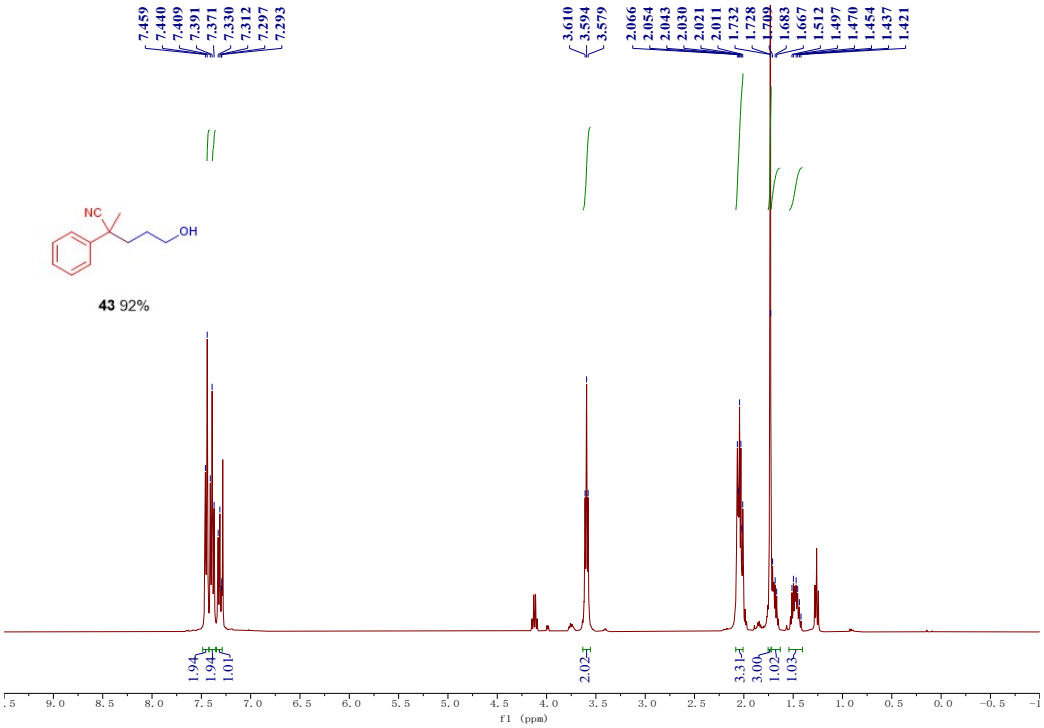

$^{1}$H NMR spectrum of 2-(3,4-Dimethoxyphenyl)-5-hydroxypentanenitrile (**42**, 400 MHz, $CDCl_3$):



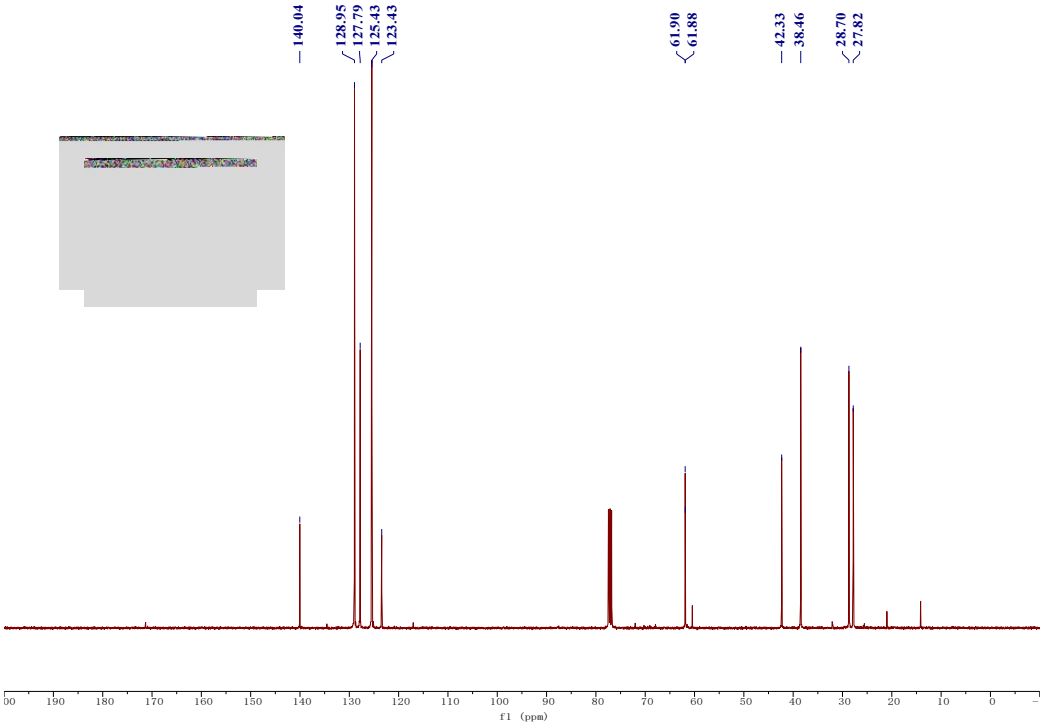
$^{13}C$ NMR spectrum of 2-(3,4-Dimethoxyphenyl)-5-hydroxypentanenitrile (**42**, 100 MHz, $CDCl_3$):



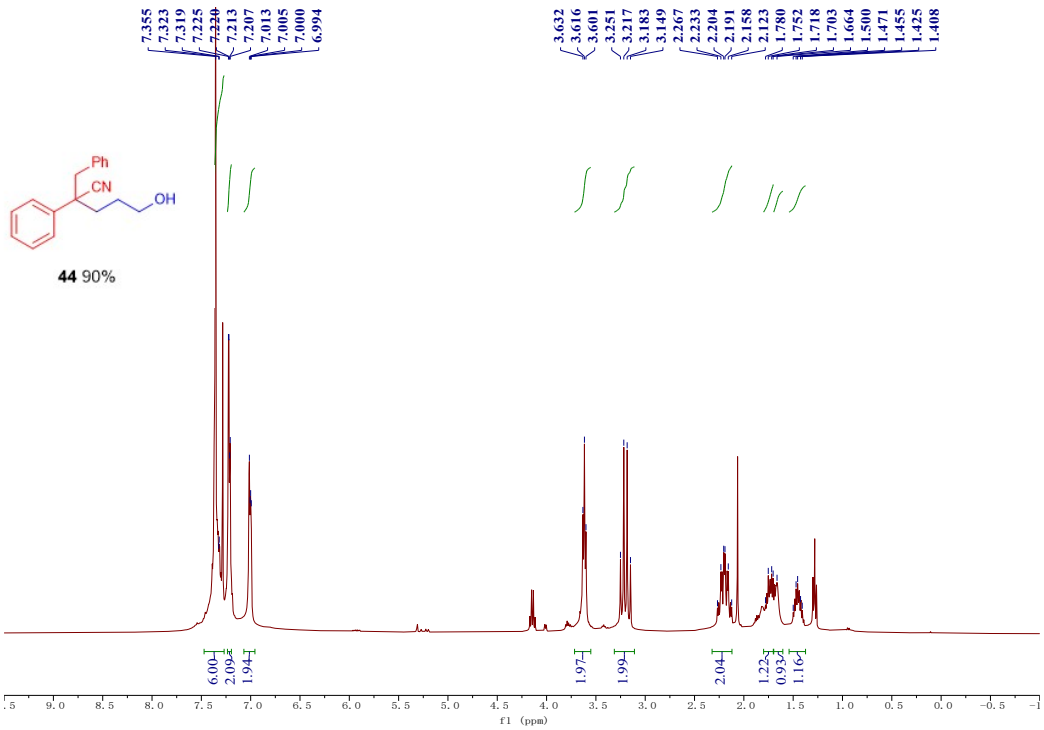

$^{1}H$ NMR spectrum of 5-Hydroxy-2-methyl-2-phenylpentanenitrile (**43**, 400 MHz, $CDCl_3$):



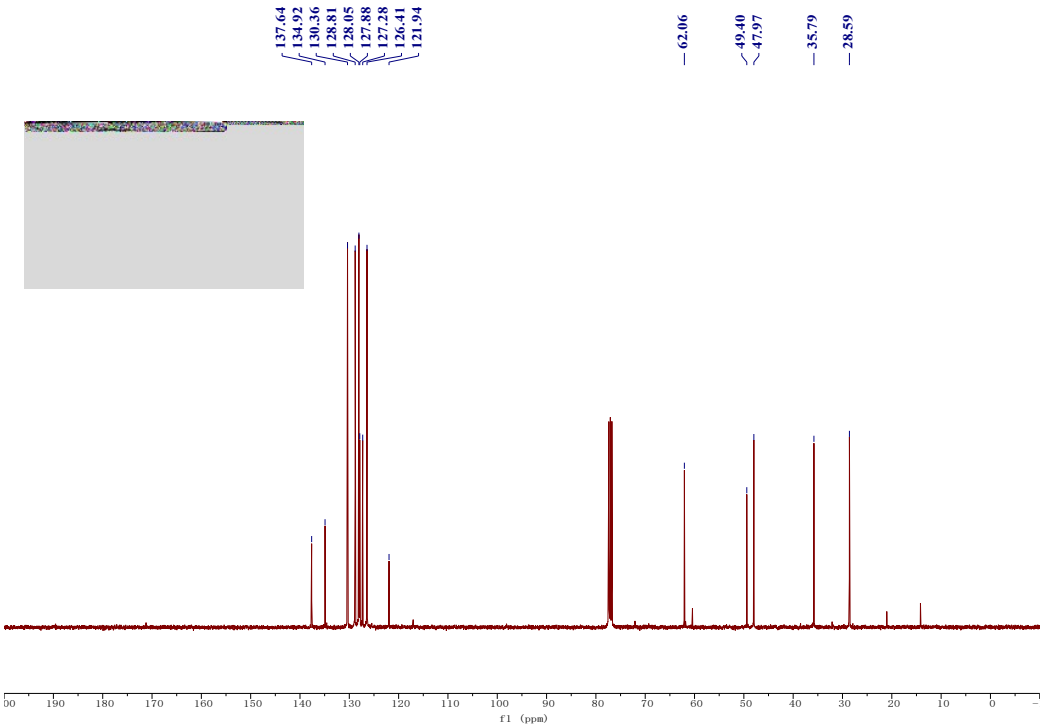
$^{13}C$ NMR spectrum of 5-Hydroxy-2-methyl-2-phenylpentanenitrile (**43**, 100 MHz, $CDCl_3$):



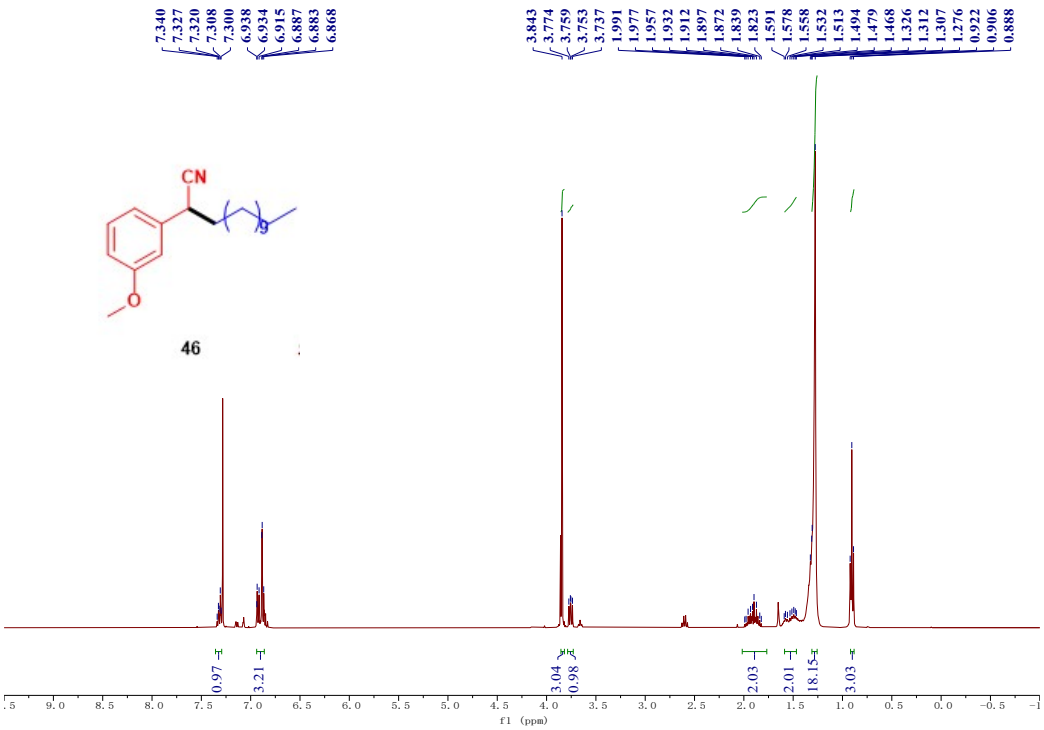

$^{1}H$ NMR spectrum of 2-Benzyl-5-hydroxy-2-phenylpentanenitrile (**44**, 400 MHz, $CDCl_3$):



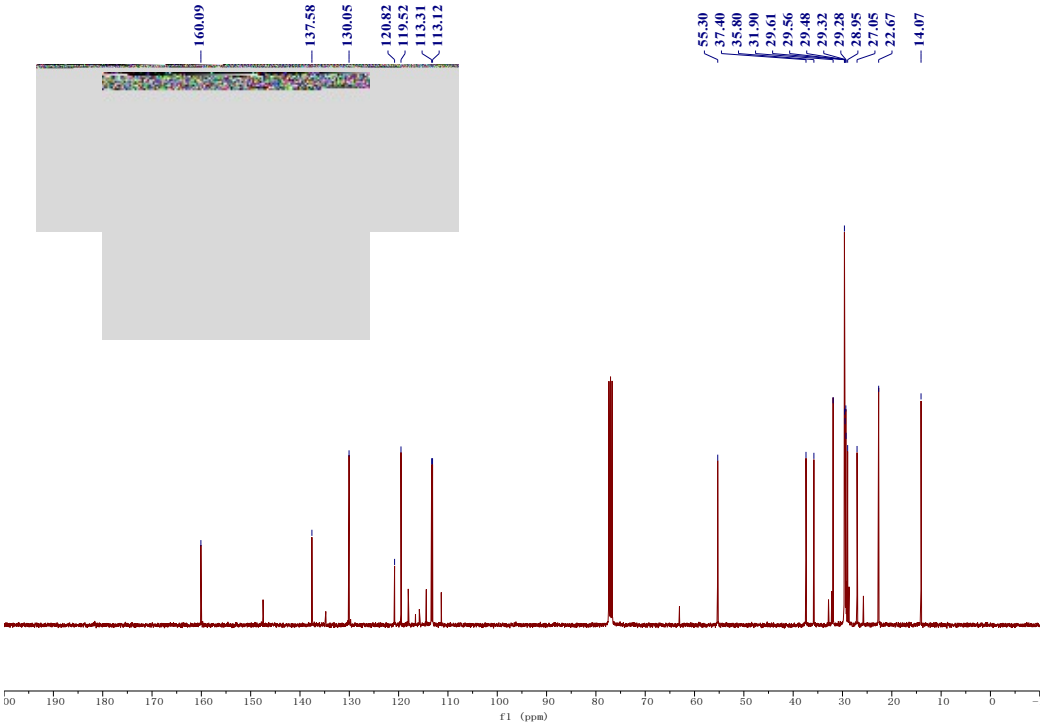
$^{13}C$ NMR spectrum of 2-Benzyl-5-hydroxy-2-phenylpentanenitrile (**44**, 100 MHz, $CDCl_3$):



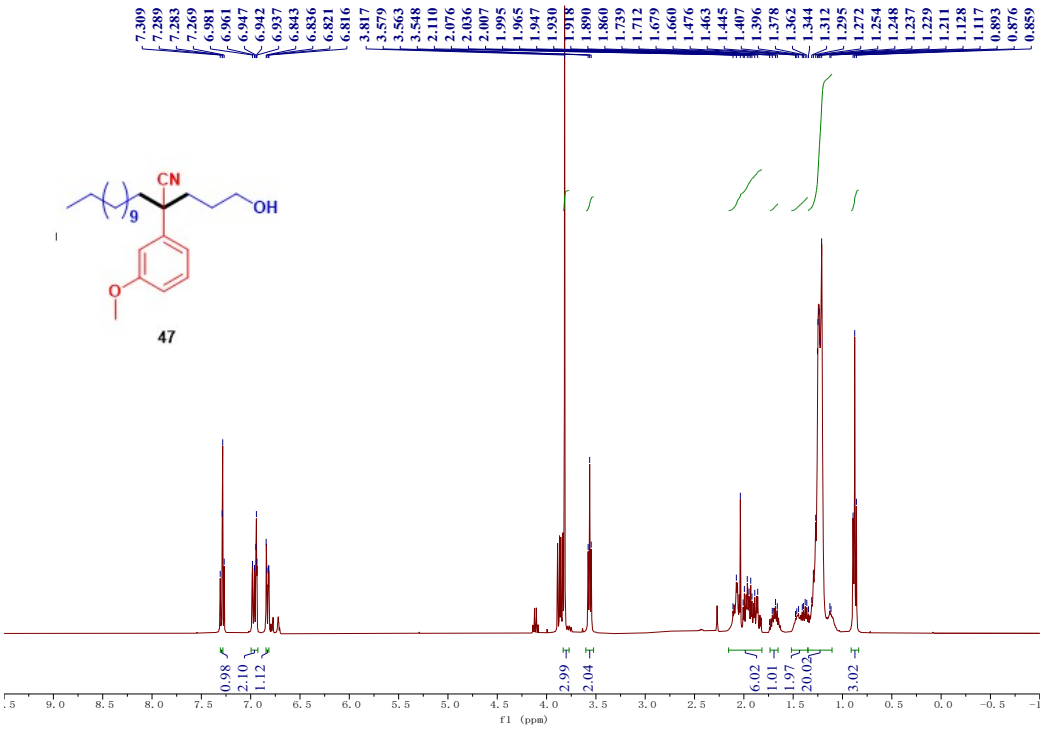

$^{1}H$ NMR spectrum of 2-(3-Methoxyphenyl) tetradecanenitrile (**46**, 400 MHz, $CDCl_3$):



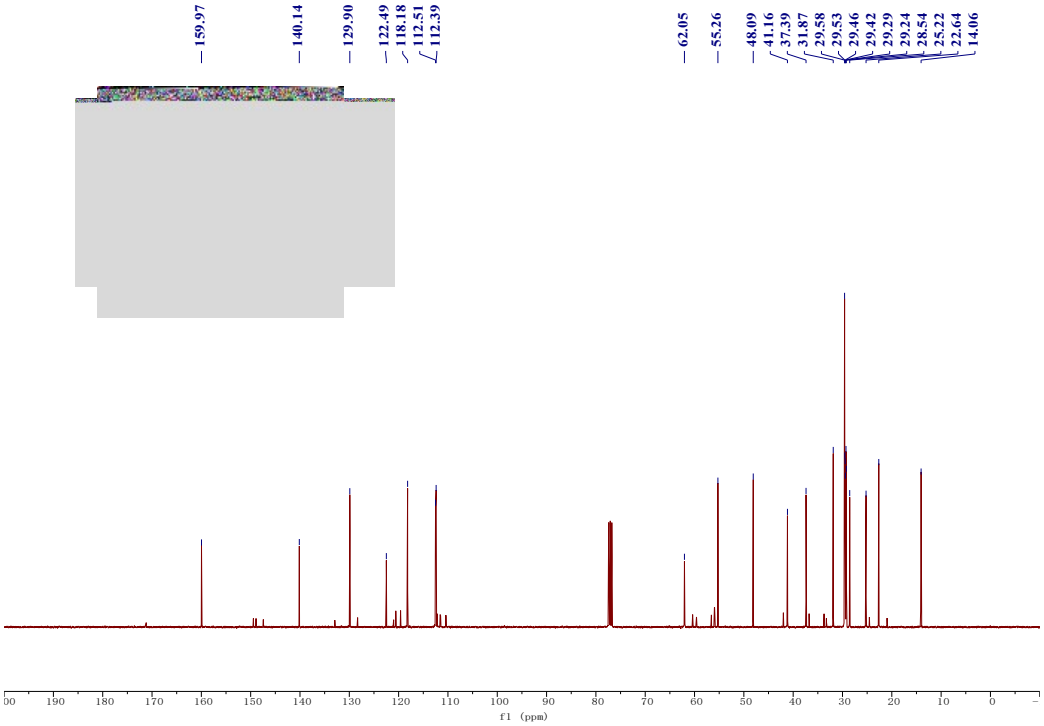
$^{13}$C NMR spectrum of 2-(3-Methoxyphenyl) tetradecanenitrile (**46**, 100 MHz, $CDCl_3$):



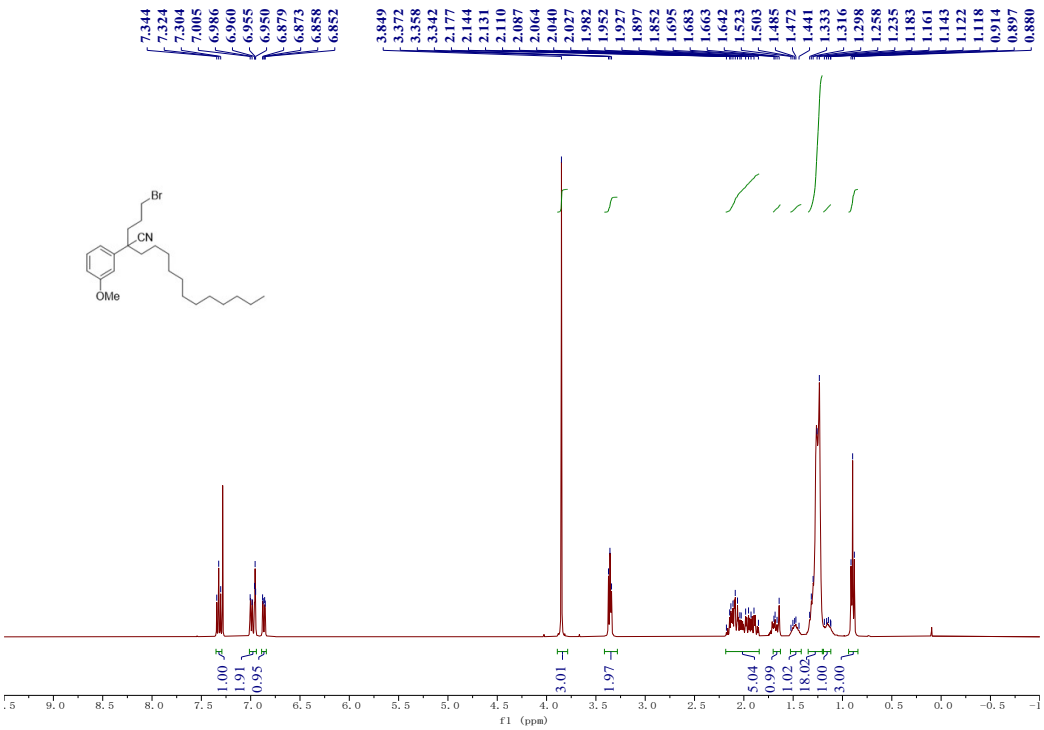

$^{1}$H NMR spectrum of 2-(3-Hydroxypropyl)-2-(3-methoxyphenyl) tetradecanenitrile (**47**, 400 MHz, $CDCl_3$):



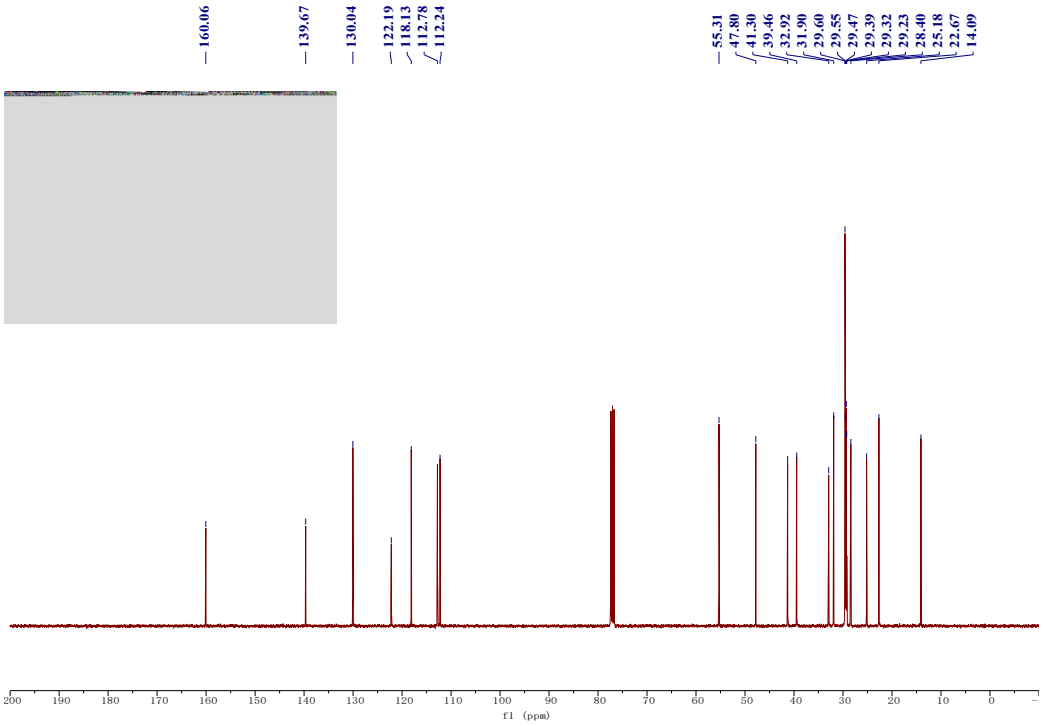
$^{13}$C NMR spectrum of 2-(3-Hydroxypropyl)-2-(3-methoxyphenyl) tetradecanenitrile (**47**, 100 MHz, $CDCl_3$):



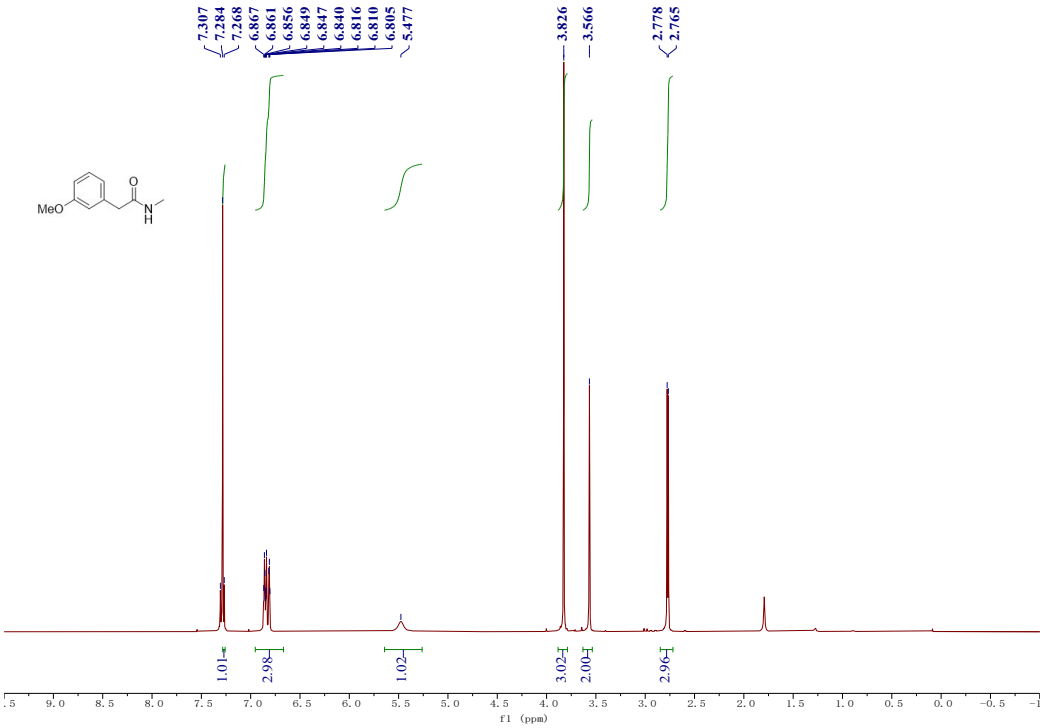

$^{1}$H NMR spectrum of 2-(3-Bromopropyl)-2-(3-methoxyphenyl) tetradecanenitrile (**48A**, 400 MHz, $CDCl_3$):



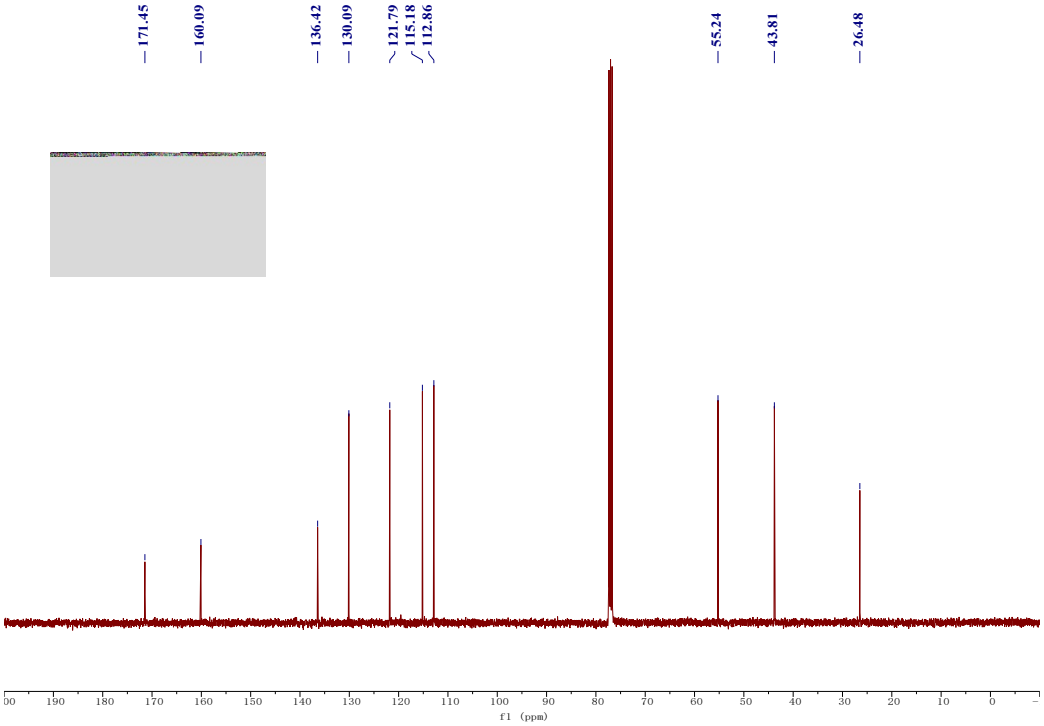
$^{13}C$ NMR spectrum of 2-(3-Bromopropyl)-2-(3-methoxyphenyl) tetradecanenitrile (**48A**, 100 MHz, $CDCl_3$):



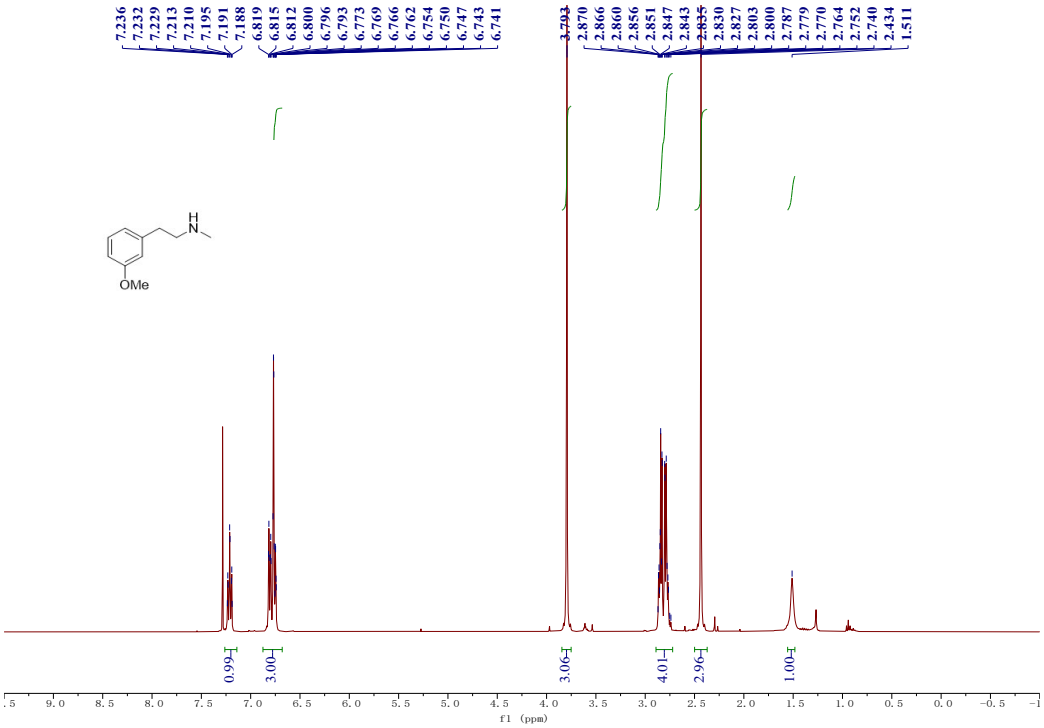

$^{1}H$ NMR spectrum of 2-(3-Methoxyphenyl)-*N*-methylacetamide (**48a**, 400 MHz, $CDCl_3$):



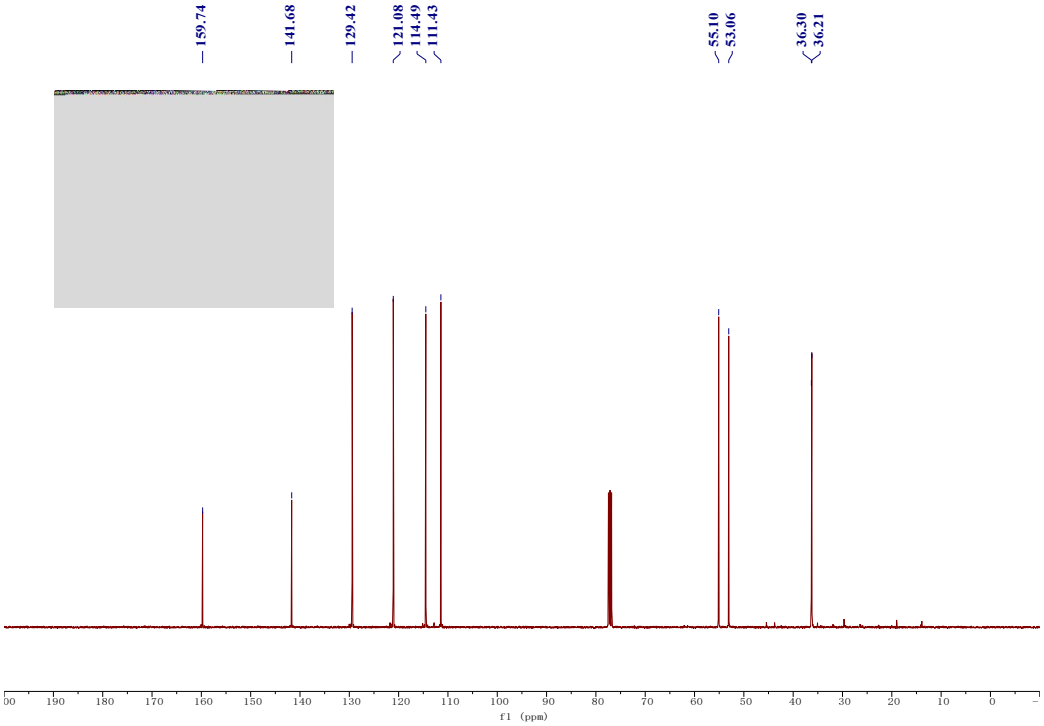
$^{13}$C NMR spectrum of 2-(3-Methoxyphenyl)-*N*-methylacetamide (**48a**, 100 MHz, $CDCl_3$):



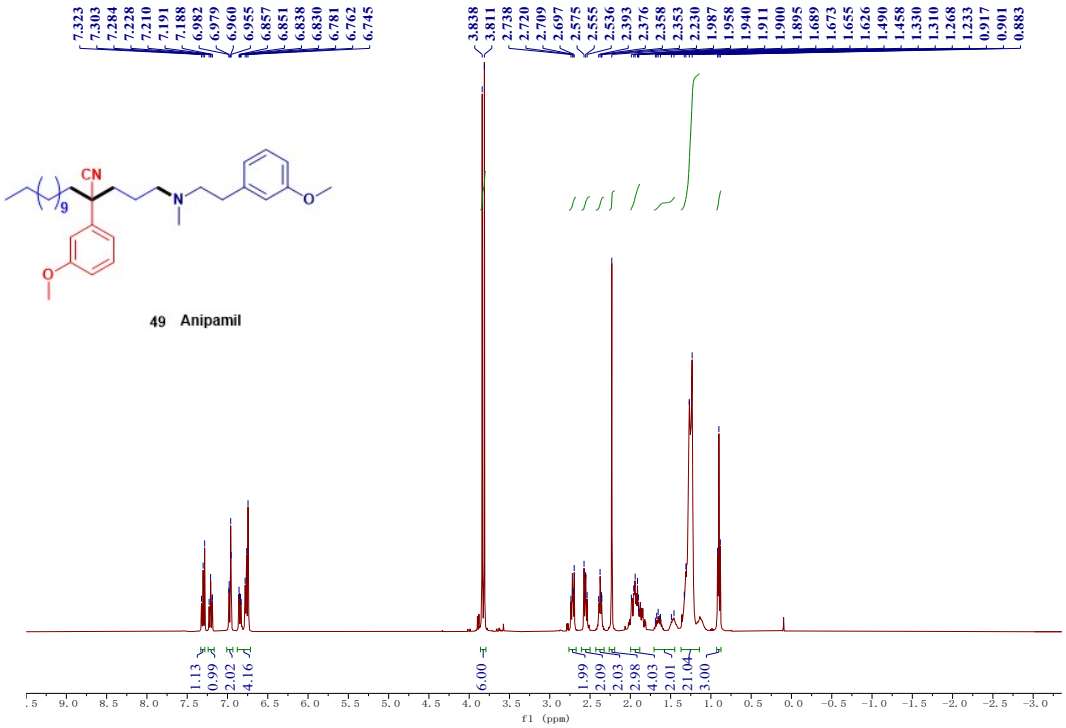

$^{1}$H NMR spectrum of 2-(3-Methoxyphenyl)-*N*-methylethan-1-amine (**48**, 400 MHz, $CDCl_3$):



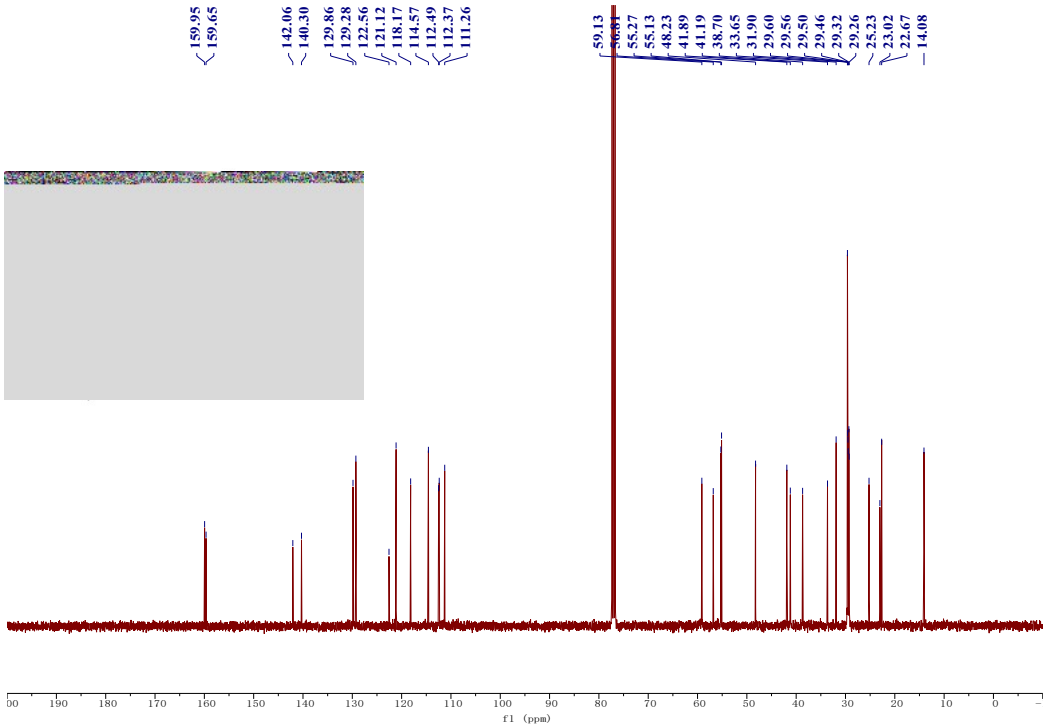
$^{13}C$ NMR spectrum of 2-(3-Methoxyphenyl)-*N*-methylethan-1-amine (**48**, 100 MHz, $CDCl_3$):



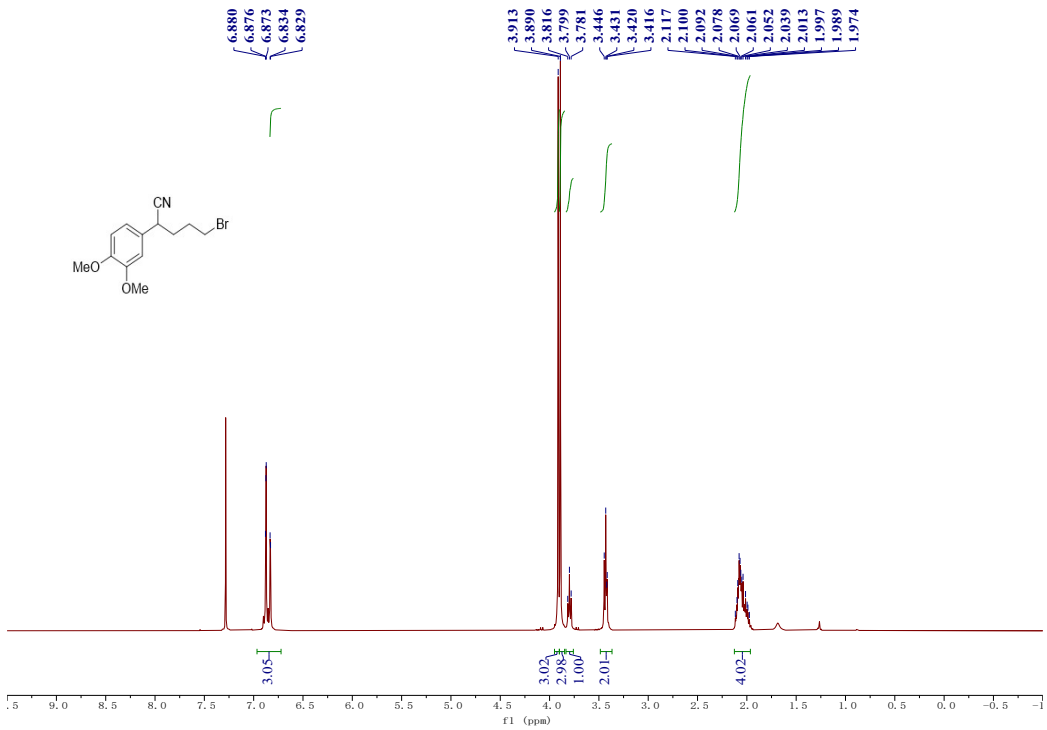

$^{1}H$ NMR spectrum of 2-(3-((3-Methoxyphenethyl) (methyl)amino) propyl)-2-(3-methoxyphenyl) tetradecanenitrile (**49**, 400 MHz, $CDCl_3$):



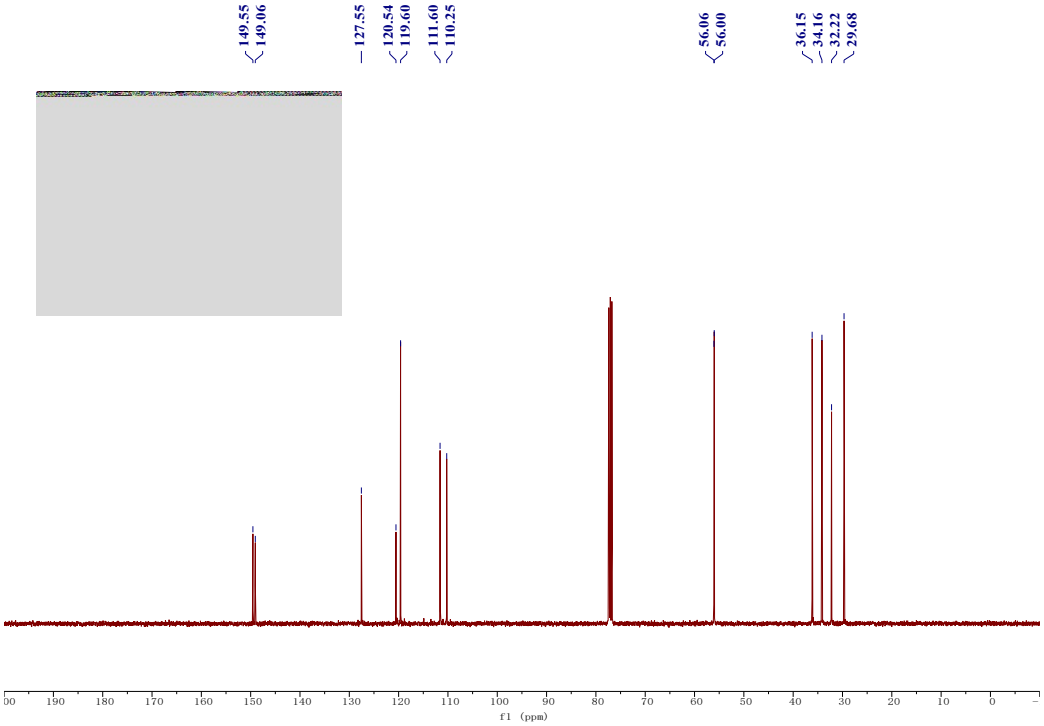
$^{13}$C NMR spectrum of 2-(3-((3-Methoxyphenethyl) (methyl)amino) propyl)-2-(3-methoxyphenyl) tetradecanenitrile (**49**, 100 MHz, $CDCl_3$):



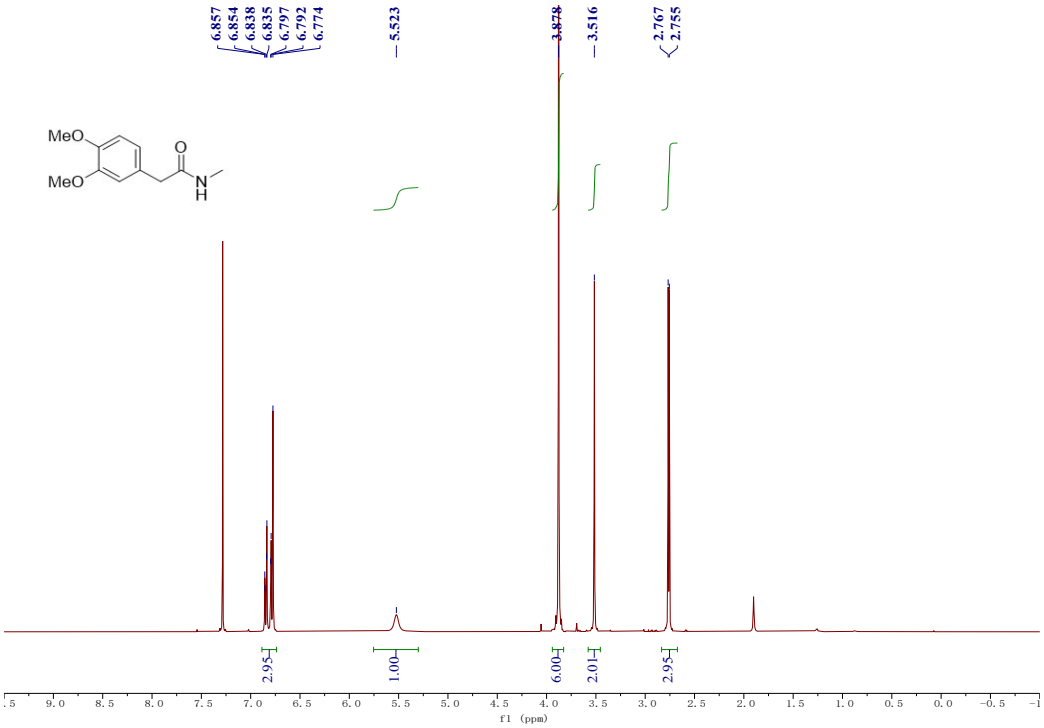

$^{1}$H NMR spectrum of 5-Bromo-2-(3,4-dimethoxyphenyl) pentanenitrile (**49A**, 400 MHz, $CDCl_3$):



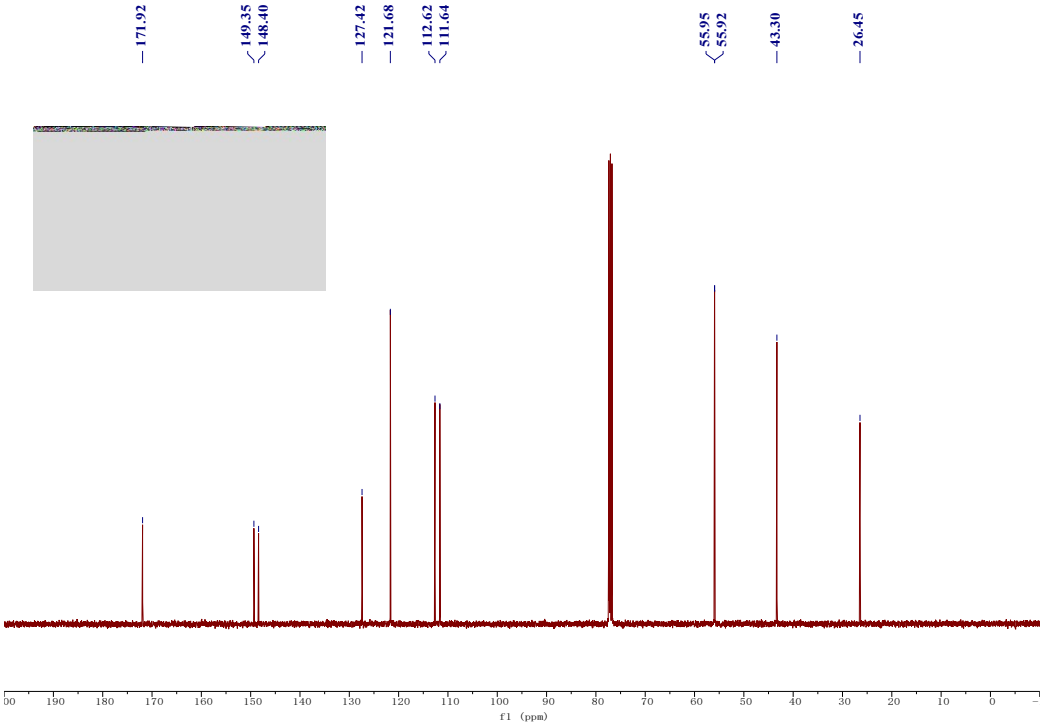
$^{13}$C NMR spectrum of 5-Bromo-2-(3,4-dimethoxyphenyl) pentanenitrile (**49A**, 100 MHz, $CDCl_3$):



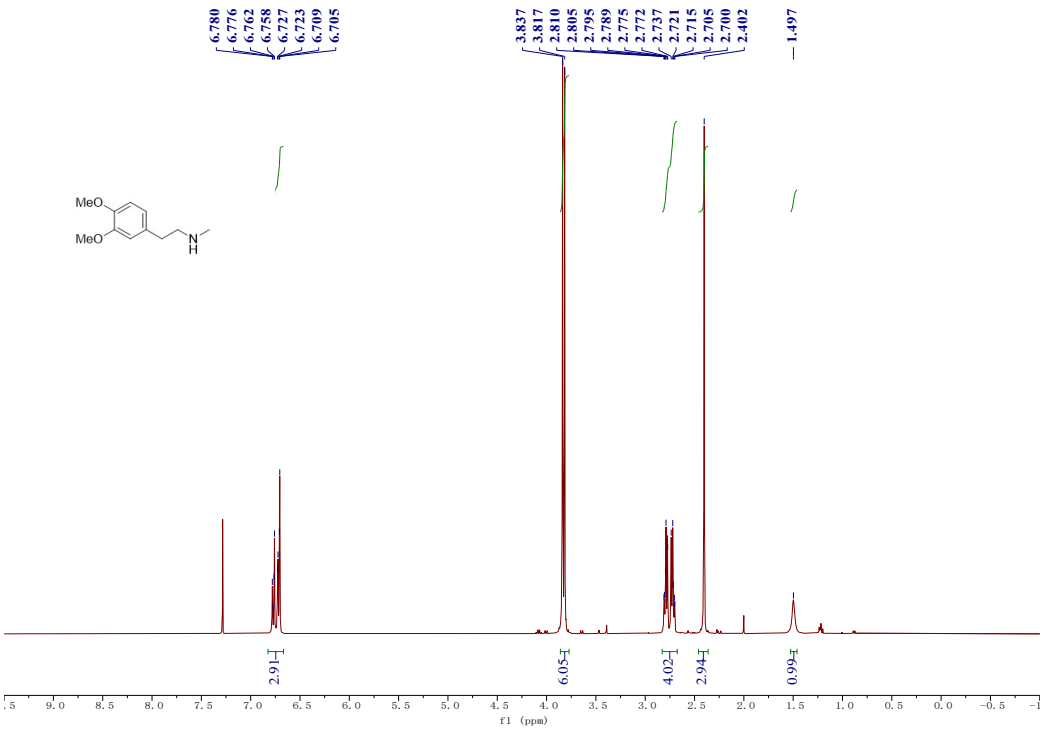

$^{1}$H NMR spectrum of 2-(3,4-Dimethoxyphenyl)-*N*-methylacetamide (**49a**, 400 MHz, $CDCl_3$):



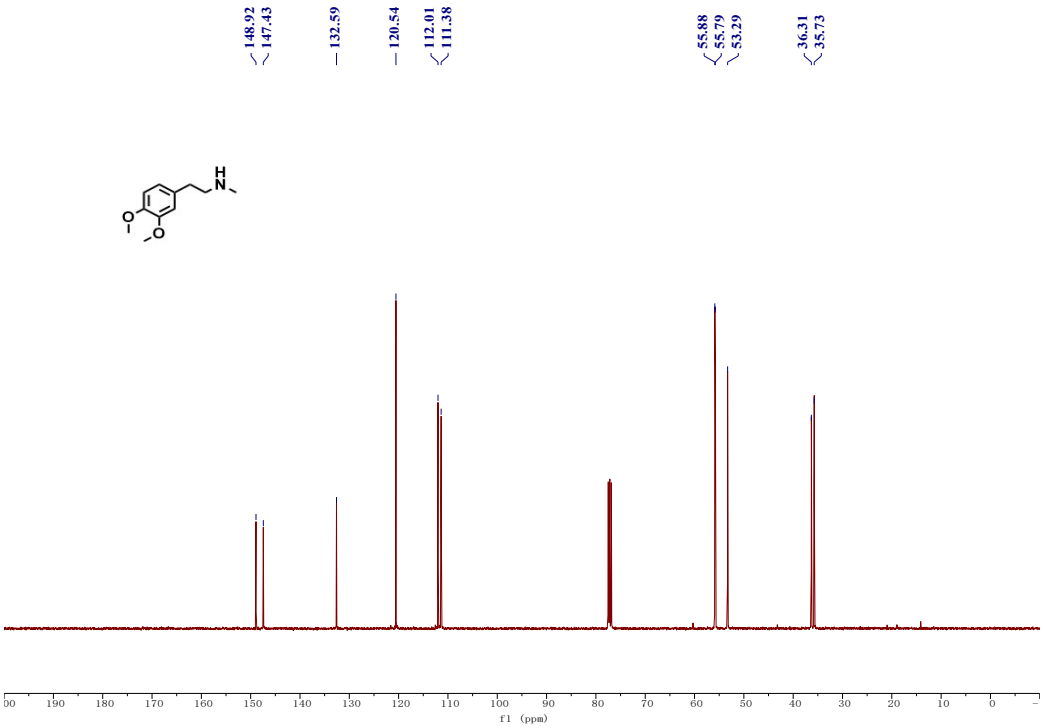
$^{13}$C NMR spectrum of 2-(3,4-Dimethoxyphenyl)-*N*-methylacetamide (**49a**, 100 MHz, $CDCl_3$):



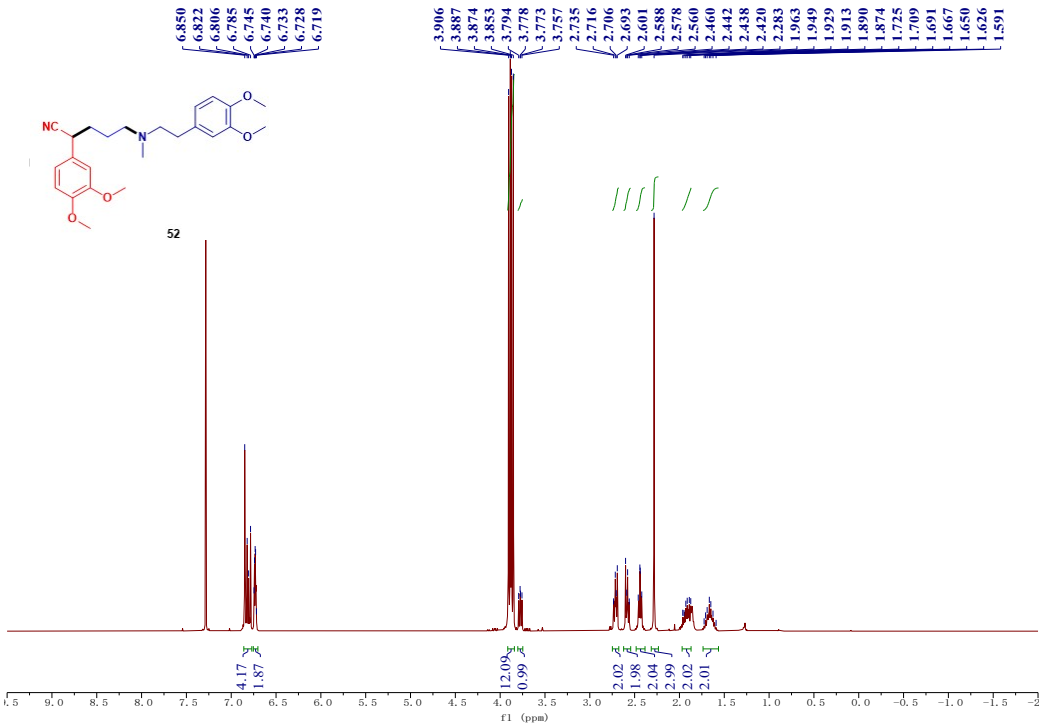

$^{1}$H NMR spectrum of 2-(3,4-Dimethoxyphenyl)-*N*-methylethan-1-amine (**49**, 400 MHz, $CDCl_3$):



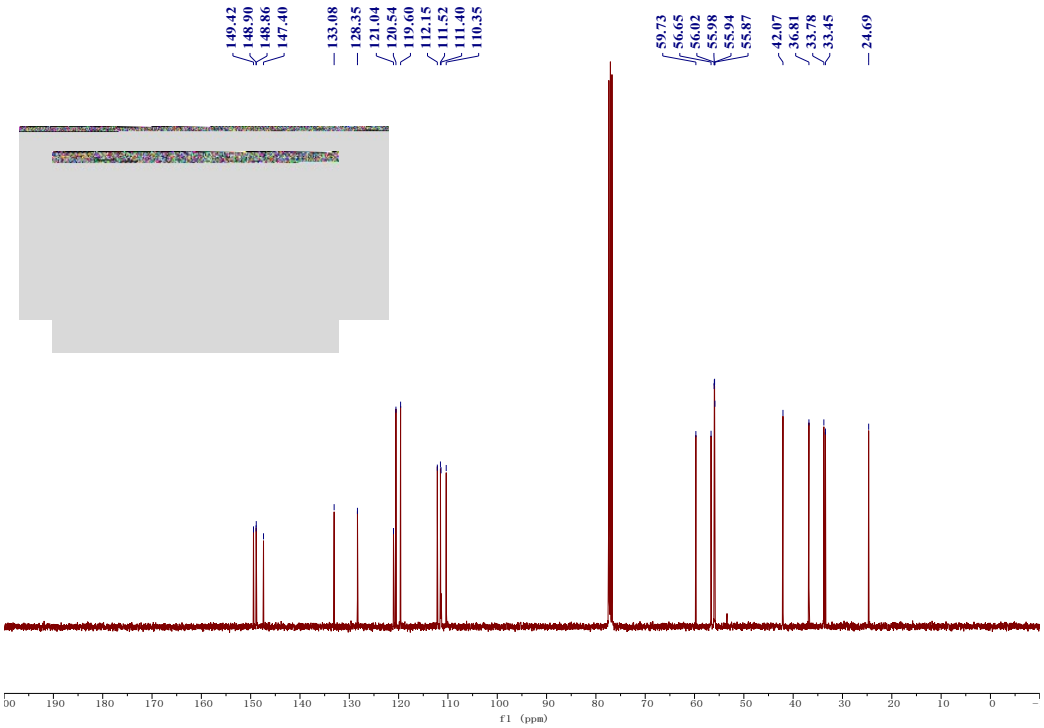
$^{13}$C NMR spectrum of 2-(3,4-Dimethoxyphenyl)-*N*-methylethan-1-amine (**49**, 100 MHz, $CDCl_3$):



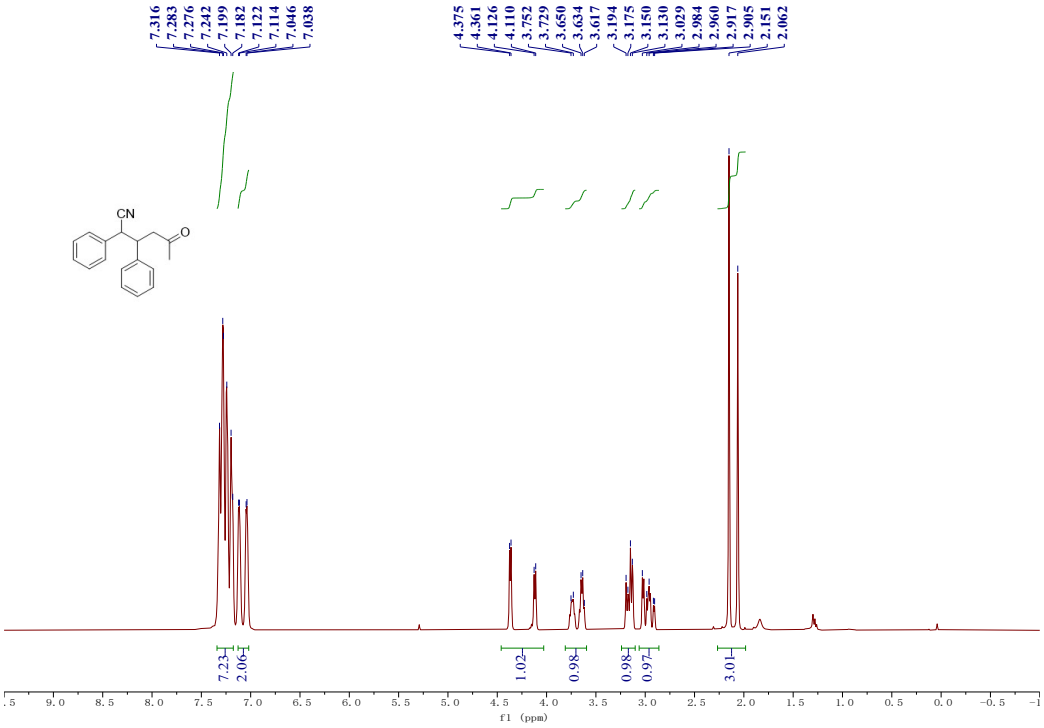

$^{1}$H NMR spectrum of 5-((3,4-Dimethoxyphenethyl) (methyl)amino)-2-(3,4-dimethoxyphenyl) pentanenitrile (**51**, 400 MHz, $CDCl_3$):



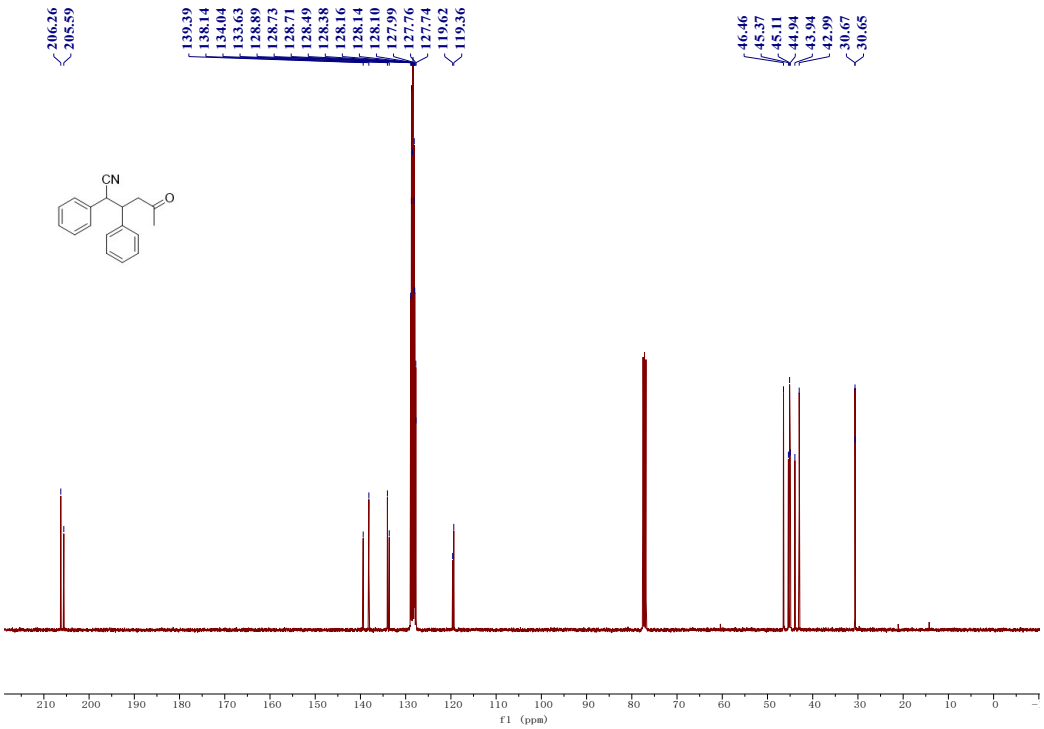
$^{13}$C NMR spectrum of 5-((3,4-Dimethoxyphenethyl) (methyl)amino)-2-(3,4-dimethoxyphenyl) pentanenitrile (**51**, 100 MHz, $CDCl_3$):



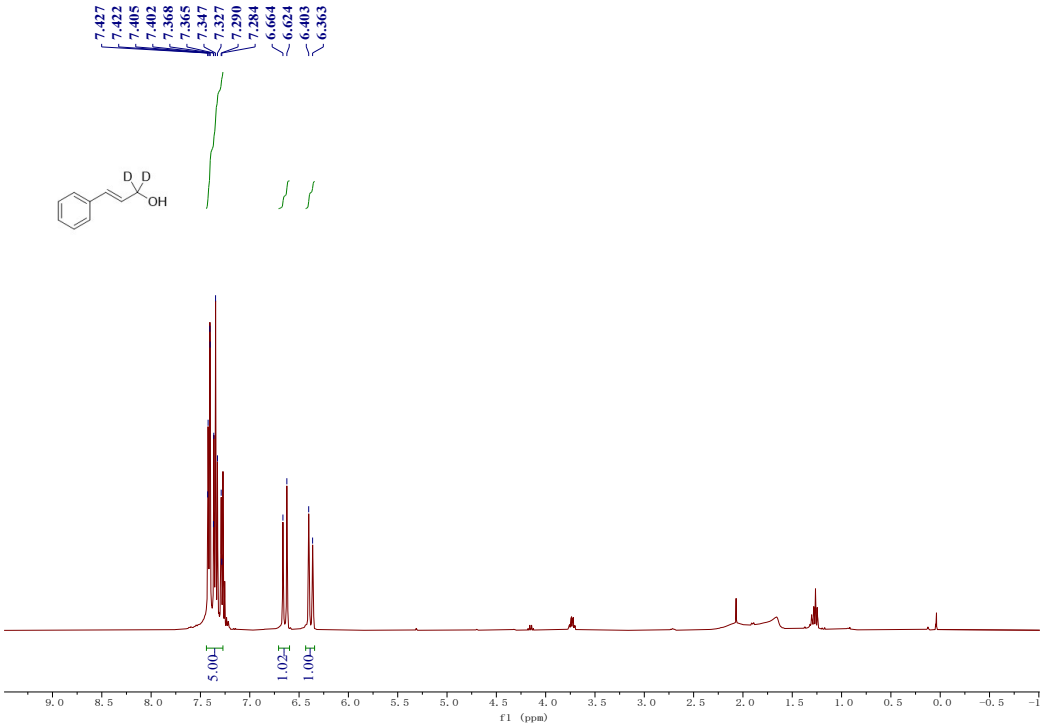

$^{1}$H NMR spectrum of 5-oxo-2,3-diphenylhexanenitrile (**54**, 400 MHz, $CDCl_3$):




$^{13}$C NMR spectrum of 5-oxo-2,3-diphenylhexanenitrile (**54**, 100 MHz, $CDCl_3$):




$^1$H NMR spectrum of product (**55**, 400 MHz, $CDCl_3$):



$^1$H NMR spectrum of product (**56**, 400 MHz, $CDCl_3$):