Direct C−H aminocarbonylation of *N*-heteroarenes with isocyanides under transition metal-free conditions

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Supplementary Information

Content

Experimental Section

Instrumentation and chemicals

^{1}H NMR, ^{13}C NMR spectra were recorded on a Bruker DPX-400 spectrometer with $CDCl_3$ as the solvent and TMS as an internal standard, operating at 400 MHz for ^{1}H NMR and 100 MHz for ^{13}C NMR. Melting points were measured by SGW X-4A microscopic apparatus. The X-ray crystallography was measured on Bruker D8 VENTURE PHOTON instrument. HRMS-ESI were measured by Q Exactive LC/HRMS spectrometer. An Agilent 7890A-5975C GC/MS spectrometer was used for isotopic labeling analysis.

Eethyl acetate and hexane were used for column chromatography without further purification. All solvents and chemicals were obtained from commercial sources and used as received unless otherwise noted. Benzyl and phenyl isocyanides was synthesized according to known methods[1] and the others were obtained from commercial sources.

Experimental procedures

General procedure for the direct C−H aminocarbonylation of *N*-heteroarenes.

Heteroarenes (**1**, 0.2 mmol), isocyanide (**2**, 0.6mmol), and $Na_2S_2O_8$ (2 equiv) were added into a vial containing a stirring bar and sealed with a Teflo*N*-lined cap. Then CH_3CN (2 mL) was introduced. The resulting mixture was stirred at 120 ℃ for 24 h. After reaction, the mixture was added into H_2O (25 mL) and extracted with dichloromethane (10 mL) for three times. The combined organic layer was dried over anhydrous $MgSO_4$ and filtered. After removal of the solvent *in vacuo*, column chromatography (ethyl acetate/hexane) of the residue afforded the pure product.

Characterization Data

N-(*tert*-butyl)isoquinoline-1-carboxamide (3a)

White solid, mp 99–101 ℃; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.58–9.55 (m, 1H), 8.40 (d, J = 5.56 Hz, 1H), 8.09 (s, 1H), 7.81–7.78 (m, 1H), 7.73 (d, J = 5.52 Hz, 1H), 7.69–7.61 (m, 2H), 1.54 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.4, 154.8, 149.8, 148.2, 138.3, 128.7, 127.9, 127.5, 122.9, 119.4, 79.1, 69.1, 43.5, 34.4, 25.9. HRMS–ESI(m/z): calcd for $C_{14}H_{17}N_2O$ ($M+H^+$): 229.1335, found:: 229.1339.

N-(*tert*-butyl)-3-methylisoquinoline-1-carboxamide (3b)

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.56 (d, J = 8.77 Hz, 1H), 8.22 (s, 1H), 7.72 (d, J = 8.15 Hz, 1H), 7.63 (t, J = 6.86 Hz, 1H), 7.58 (s, 1H), 7.55 (d, J = 5.43 Hz, 1H), 2.68 (s, 3H), 1.54 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.5, 159.9, 148.6, 143.2, 135.8, 127.9, 127.6, 126.4, 121.2, 119.1, 52.7, 28.9, 25.3. HRMS–ESI(m/z): calcd for $C_{15}H_{19}N_2O$ ($M+H^+$): 243.1492, found:: 243.1495.

N-(*tert*-butyl)-6-methylisoquinoline-1-carboxamide (3c)

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.47 (d, J = 8.89 Hz, 1H), 8.36 (d, J = 5.53 Hz, 1H), 8.12 (s, 1H), 7.65 (d, J = 5.52 Hz, 1H), 7.56 (s, 1H), 7.47 (dd, J = 8.91 Hz, J = 1.65 Hz, 1H), 2.52 (s, 3H), 1.54 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.7, 148.9, 140.7, 140.0, 137.8, 130.8, 127.7, 125.6, 125.3, 123.5, 51.1, 28.8, 21.9. HRMS–ESI(m/z): calcd for $C_{15}H_{19}N_2O$ ($M+H^+$): 243.1492, found:: 242.1494.

***N*-(*tert*-butyl)-4-chloroisoquinoline-1-carboxamide (3d)**

White solid, mp 57–59 ℃; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.65 (d, J = 8.71 Hz, 1H), 8.48 (S, 1H), 8.25 (d, J = 8.46 Hz, 1H), 7.98 (S, 1H), 7.85–7.80 (m, 1H), 7.75–7.70 (m, 1H), 1.54 (S, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.9, 147.9, 138.9, 134.6, 131.4, 131.3, 129.2, 128.5, 127.7, 123.3, 51.3, 28.7. HRMS–ESI(m/z): calcd for $C_{14}H_{16}ClN_2O$ ($M+H^+$): 263.0946, found:: 263.0943.

***N*-(*tert*-butyl)-5-chloroisoquinoline-1-carboxamide (3e)**

Yellow solid, mp 69–71 ℃; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.58 (d, J = 8.77 Hz, 1H), 8.54 (d, J = 5.78 Hz, 1H), 8.21 (dd, J = 5.78 Hz, J = 0.73 Hz, 1H), 8.09 (S, 1H), 7.79 (dd, J = 7.46 Hz, J = 0.92 Hz, 1H), 7.57 (dd, J = 8.73 Hz, J = 7.52 Hz, 1H), 1.54 (S, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.1, 149.6, 141.1, 135.2, 130.9, 130.5, 128.2, 127.8, 127.2, 120.3, 51.3, 28.7. HRMS–ESI(m/z): calcd for $C_{14}H_{16}ClN_2O$ ($M+H^+$): 263.0946, found:: 263.0947.

4-bromo-*N*-(*tert*-butyl)isoquinoline-1-carboxamide (3f)

Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.60 (d, J = 8.66 Hz, 1H), 8.60 (s, 1H), 8.18 (d, J = 8.43 Hz, 1H), 7.97 (s, 1H), 7.85–7.75 (m, 1H), 7.75–7.67 (m, 1H),1.53 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.9, 148.6, 141.8, 135.9, 131.7, 129.2, 128.5, 128.0, 126.0, 122.9, 51.3, 28.7. HRMS–ESI(m/z): calcd for $C_{14}H_{16}BrN_2O$ ($M+H^+$): 307.0441, found: 307.0438.

5-bromo-*N*-(*tert*-butyl)isoquinoline-1-carboxamide (3g)

Yellow solid, mp 87–89 ℃; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.61 (d, J = 8.74 Hz, 1H), 8.52 (d, J = 5.80 Hz, 1H), 8.16 (d, J = 6.58 Hz, 1H), 8.08 (s, 1H), 7.98 (d, J = 8.38 Hz, 1H), 7.56–7.42 (m, 1H), 1.54 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.0, 149.7, 141.3, 136.4, 134.3, 128.6, 128.0, 127.8, 122.9, 121.5, 51.3, 28.7. HRMS–ESI(m/z): calcd for $C_{14}H_{16}BrN_2O$ ($M+H^+$):307.0441, found: 307.0437.

7-bromo-*N*-(*tert*-butyl)isoquinoline-1-carboxamide (3h)

Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.92 (m, 1H), 8.45 (d, J = 5.50 Hz, 1H), 8.18 (S, 1H), 7.78 (dd, J = 8.77 Hz, J = 1.95 Hz, 1H), 7.74 (d, J = 5.42 Hz, 1H), 7.70 (d, J = 8.77 Hz, 1H), 1.54 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.0, 147.8, 140.3, 135.9, 134.0, 130.3, 128.3, 127.7, 123.9, 122.8, 51.2, 28.8. HRMS–ESI(m/z): calcd for $C_{14}H_{16}BrN_2O$ ($M+H^+$): 307.0441, found: 307.0443.

***N*-(*tert*-butyl)phenanthridine-6-carboxamide (3i)**

Yellow solid, mp 106–108 ℃; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.59 (d, J = 8.39 Hz, 1H), 8.60 (d, J = 8.28 Hz, 1H), 8.54 (d, J = 7.91 Hz, 1H), 8.15 (d, J = 7.78 Hz, 1H), 8.07 (s, 1H), 7.84 (t, J = 7.62 Hz, 1H), 7.72 (t, J = 8.20 Hz, 3H), 1.60 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.6, 150.4, 141.8, 133.8, 130.8, 130.4, 129.2, 128.7, 128.2, 127.8, 125.4, 124.3, 122.1, 121.7, 51.3, 28.8. HRMS–ESI(m/z): calcd for $C_{18}H_{19}N_2O$ ($M+H^+$): 279.1492, found: 279.1496.

***N*-(*tert*-butyl)-4-methylpicolinamide (3j)**

Pale green oil; ^{1}H NMR (400 MHz, CDCl3) δ ppm 8.36 (d, J =4.92 Hz, 1H), 8.00–7.99 (m, 2H), 7.22–7.18 (m, 1H), 2.40 (s, 3H), 1.48 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.7, 149.6, 147.8, 146.6, 125.6, 121.6, 49.8, 27.7, 20.1.

HRMS–ESI (m/z): calcd for $C_{11}H_{17}N_2O$ ($M+H^+$): 193.1335, found: 193.1338.

_N_-(*tert*-butyl)-2-methoxyisonicotinamide (3k)

White solid, mp 129–131 ℃; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.79 (s, 1H), 7.75 (dd, J = 7.29 Hz, J = 0.90 Hz, 1H), 7.68 (dd, J = 8.12 Hz, J = 7.34 Hz, 1H), 6.84 (dd, J = 8.16 Hz, J = 0.92 Hz, 1H), 3.93 (s, 3H), 1.46 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.3, 161.5, 147.1, 138.7, 113.9, 112.7, 52.2, 49.7, 27.7. HRMS–ESI(m/z): calcd for $C_{11}H_{17}N_2O_2$ ($M+H^+$): 209.1285, found: 209.1289.

_N_-(*tert*-butyl)-4-cyanopicolinamide (3l)

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.69 (dd, J = 4.94 Hz, J = 0.85 Hz, 1H), 8.38 (dd, J = 1.49 Hz, J = 0.93 Hz, 1H), 7.86 (s, 1H), 7.63 (dd, J = 4.94 Hz, J = 1.58 Hz, 1H), 1.47 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.3, 152.2, 148.7, 127.2, 123.7, 122.0, 116.1, 51.3, 28.6. HRMS–ESI(m/z): calcd for $C_{11}H_{14}N_3O$ ($M+H^+$): 204.1131, found: 204.1136.

_N_-(*tert*-butyl)-2,6-dimethylisonicotinamide (3m)

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.17 (s, 2H), 6.01 (s, 1H), 2.52 (s, 3H), 1.43 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.6, 158.7, 143.7, 117.4, 52.0, 28.7, 24.5. HRMS–ESI(m/z): calcd for $C_{12}H_{19}N_2O$ ($M+H^+$): 207.1492, found: 207.1493.

N,2,6-tri-*tert*-butylisonicotinamide (3n)

White solid, mp 139–141 ℃; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.31 (s, 2H), 5.96 (s, 1H), 1.47 (s, 9H), 1.35 (s, 18H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.7, 166.8, 143.5, 112.6, 51.9, 37.8, 30.1, 28.8. HRMS–ESI(m/z): calcd for $C_{18}H_{31}N_2O$ ($M+H^+$): 291.2431, found: 291.2432.

4-bromo-_N_-(*tert*-butyl)-6-methylpicolinamide (3o)

White solid, mp 81–83 ℃; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.13 (s, 1H), 7.93 (s, 1H), 7.41 (s, 1H), 2.53 (s, 3H), 1.47 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.3, 158.2, 151.2, 134.4, 128.5, 122.5, 51.0, 28.7, 24.0. HRMS–ESI(m/z): calcd for $C_{11}H_{16}BrN_2O$ ($M+H^+$): 271.0441, found: 271.0445.

_N_-(*tert*-butyl)-2-methylquinoline-4-carboxamide (3p)

White solid, mp 123–125 ℃; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.07 (dd, J = 8.35 Hz, J = 0.78 Hz, 1H), 8.00 (d, J = 8.46 Hz, 1H), 7.72–7.66 (m, 1H), 7.56–7.48 (m, 1H), 7.21 (s, 1H), 5.98 (s, 1H), 2.69 (s, 3H), 1.54 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.0, 158.6, 148.2, 143.4, 129.9, 128.9, 126.6, 124.9, 122.7, 119.0, 52.6, 28.9, 25.2. HRMS–ESI(m/z): calcd for $C_{15}H_{19}N_2O$ ($M+H^+$): 243.1492, found: 243.1496.

_N_-(*tert*-butyl)-2,6-dimethylquinoline-4-carboxamide (3q)

White solid, mp 158–160 ℃; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.86 (d, J = 8.59 Hz, 1H), 7.76 (s, 1H), 7.48 (d, J = 8.59 Hz, 1H), 7.05 (s, 1H), 6.22 (s, 1H), 2.59 (s, 3H), 2.48 (s, 3H), 1.55 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.2, 157.4, 146.7, 142.7, 136.4, 132.0, 128.4, 123.8, 122.6, 118.8, 52.5, 28.9, 25.0, 21.8. HRMS–ESI(m/z): calcd for

$C_{16}H_{21}N_2O$ ($M+H^+$): 257.1648, found: 257.1652.

***N*-(*tert*-butyl)-2-phenylquinoline-4-carboxamide (3r)**

White solid, mp 169–171 ℃; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.16–7.97 (m, 4H), 7.78–7.63 (m, 2H), 7.49 (d, J = 7.19 Hz, 4H), 6.21 (s, 1H), 1.55 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.1, 156.7, 148.5, 143.9, 138.8, 130.0, 129.9, 129.7, 128.9, 127.5, 127.1, 124.9, 123.3, 116.1, 52.6, 28.9. HRMS–ESI(m/z): calcd for $C_{20}H_{21}N_2O$ ($M+H^+$): 305.1648, found: 305.1644.

4-bromo-*N*-(*tert*-butyl)quinoline-2-carboxamid (3s)

White solid, mp 48–50 ℃; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.57 (s, 1H), 8.21 (d, J = 7.58 Hz, 1H), 8.09 (d, J = 6.84 Hz, 2H), 7.78 (d, J = 6.38 Hz, 1H), 7.69 (d, J = 6.74 Hz, 1H), 1.54 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.4, 150.4, 146.9, 135.6, 130.8, 130.0, 129.0, 128.6, 126.9, 122.7, 51.2, 28.8. HRMS–ESI(m/z): calcd for $C_{14}H_{16}BrN_2O$ ($M+H^+$): 307.0441, found: 307.0438.

***N*-(*tert*-butyl)benzo[d]thiazole-2-carboxamide (3ta)**

Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.07–8.00 (m, 1H), 7.98–7.91 (m, 1H), 7.55–7.50 (m, 1H), 7.48–7.43 (m, 1H), 7.33 (s, 1H), 1.52 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.5, 158.0, 151.8, 136.1, 125.7, 125.5, 123.0, 121.4, 51.0, 27.7. HRMS–ESI(m/z): calcd for $C_{12}H_{15}N_2OS$ ($M+H^+$): 235.0900, found: 235.0903.

***N*-(2,4,4-trimethylpenta*N*-2-yl)isoquinoline-1-carboxamide (4a)**

Colourless oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.62 (dd, J = 8.45 Hz, J = 0.86 Hz, 1H), 8.43 (d, J = 5.52 Hz, 1H), 8.24 (s, 1H), 7.82 (d, J = 7.58 Hz, 1H), 7.76 (d, J = 5.43 Hz, 1H), 7.72–7.62 (m, 2H), 1.93 (s, 2H), 1.60 (s, 6H), 1.06 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.1, 148.2, 139.0, 136.4, 129.3, 127.3, 127.0, 125.9, 125.7, 122.9, 53.8, 50.7, 30.7, 30.5, 28.2. HRMS–ESI(m/z): calcd for $C_{18}H_{25}N_2O$ ($M+H^+$): 285.1961, found: 285.1963.

***N*-cyclohexylisoquinoline-1-carboxamide (4b)**

White solid, mp 118–120 ℃; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.60 (d, J = 8.29 Hz, 1H), 8.44 (d, J = 5.52 Hz, 1H), 8.10 (d, J = 7.12 Hz, 1H), 7.85–7.80 (m, 1H), 7.77 (d, J = 5.49 Hz, 1H), 7.73–7.63 (m, 2H), 4.08–3.95 (m, 1H), 2.07 (dd, J = 12.01 Hz, J = 2.77 Hz, 2H), 1.87–1.73 (m, 2H), 1.65 (dd, J = 10.15 Hz, J = 6.34 Hz, 1H), 1.54–1.43 (m, 2H), 1.42–1.30 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.2, 148.7, 140.2, 137.4, 130.4, 128.5, 128.0, 127.1, 126.8, 124.2, 48.3, 33.1, 25.7, 25.0. HRMS–ESI(m/z): calcd for $C_{16}H_{19}N_2O$ ($M+H^+$): 255.1492, found: 255.1496.

***N*-benzylisoquinoline-1-carboxamide (4c)**

White solid, mp 85–87 ℃; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.61 (d, J = 8.27 Hz, 1H), 8.62 (s, 1H), 8.42 (d, J = 5.53 Hz, 1H), 7.83 (d, J = 7.66 Hz, 1H), 7.79 (d, J = 5.57 Hz, 1H), 7.75–7.65 (m, 2H), 7.41 (d, J = 7.43 Hz, 2H), 7.34 (t, J = 7.45 Hz, 2H), 7.27 (m, 1H), 4.71 (d, J = 6.02 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.7, 146.9, 138.8, 137.3, 136.4, 129.7, 127.7, 127.6, 126.8, 126.4, 126.0, 125.8, 123.5, 42.5. HRMS–ESI(m/z): calcd for $C_{17}H_{15}N_2O$ ($M+H^+$): 263.1179, found: 263.1182.

_N_-phenylisoquinoline-1-carboxamide (4d)

White solid, mp 119–120 ℃; ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.36 (s, 1H), 9.81–9.67 (m, 1H), 8.53 (d, J = 5.49 Hz, 1H), 7.95–7.80 (m, 4H), 7.77–7.71 (m, 2H), 7.47–7.37 (m, 2H), 7.21–7.13 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.6, 146.5, 138.9, 137.0, 136.6, 129.6, 128.3, 128.0, 127.9, 126.8, 126.3, 125.9,123.9, 123.2, 118.8, 118.7. HRMS–ESI(m/z): calcd for $C_{16}H_{13}N_2O$ ($M+H^+$): 249.1022, found: 249.1019.

4-cyano-_N_-(2,4,4-trimethylpenta_N_-2-yl)picolinamide (5a)

Yellow solid, mp 48–50 ℃; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.70 (d, J = 3.90 Hz, 1H), 8.39 (s, 1H), 7.97 (s, 1H), 7.63 (d, J = 3.17 Hz, 1H), 1.84 (s, 2H), 1.53 (s, 6H), 1.01 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.0, 152.3, 148.8, 127.2, 123.7, 122.0, 116.1, 55.1, 51.9, 31.7, 31.5, 29.0. HRMS–ESI(m/z): calcd for $C_{15}H_{22}N_3O$ ($M+H^+$): 260.1757, found: 260.1762.

4-cyano-_N_-cyclohexylpicolinamide (5b)

Yellow solid, mp 56–58 ℃; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.73 (dd, J = 4.94 Hz, J = 0.84 Hz, 1H), 8.42 (dd, J = 1.49 Hz, J = 0.92 Hz, 1H), 7.84 (d, J = 6.74 Hz, 1H), 7.65 (dd, J = 4.93 Hz, J = 1.58 Hz, 1H), 4.10–3.86 (m, 1H), 2.00 (dd, J = 12.34 Hz, J = 3.31 Hz, 2H), 1.89–1.71 (m, 2H), 1.69–1.61 (m, 1H), 1.48–1.37 (m, 2H), 1.36–1.27 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.3, 150.6, 147..9, 126.3, 123.1, 120.9, 115.0, 47.4, 31.9, 24.5, 23.7. HRMS–ESI(m/z): calcd for $C_{13}H_{16}N_3O$ ($M+H^+$): 230.1288, found: 230.1291.

ethyl (4-cyanopicolinoyl)glycinate (5c)

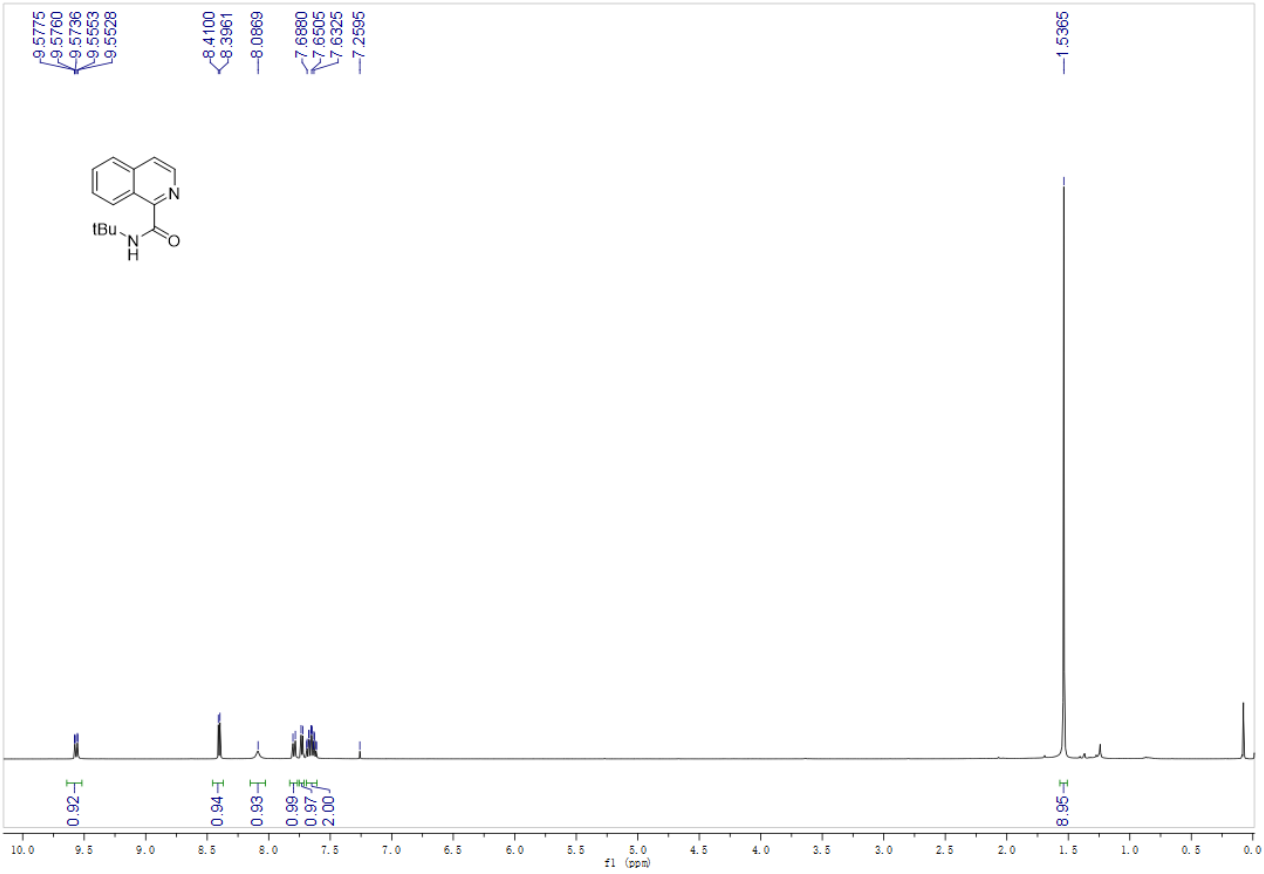
White solid, mp 123–125 ℃; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.79 (d, J = 4.92 Hz, 1H), 8.42 (s, 1H), 8.38 (s, 1H), 7.69 (dd, J = 1.54 Hz, J = 4.93 Hz, 1H), 4.42–4.18 (m, 4H), 1.32 (t, J = 7.10 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.4, 162.6, 150.7, 149.3, 127.8, 124.2, 122.1, 115.9, 61.8, 41.5, 14.2. HRMS–ESI(m/z): calcd for $C_{11}H_{12}N_3O_3$ ($M+H^+$): 234.0873, found: 234.0871.

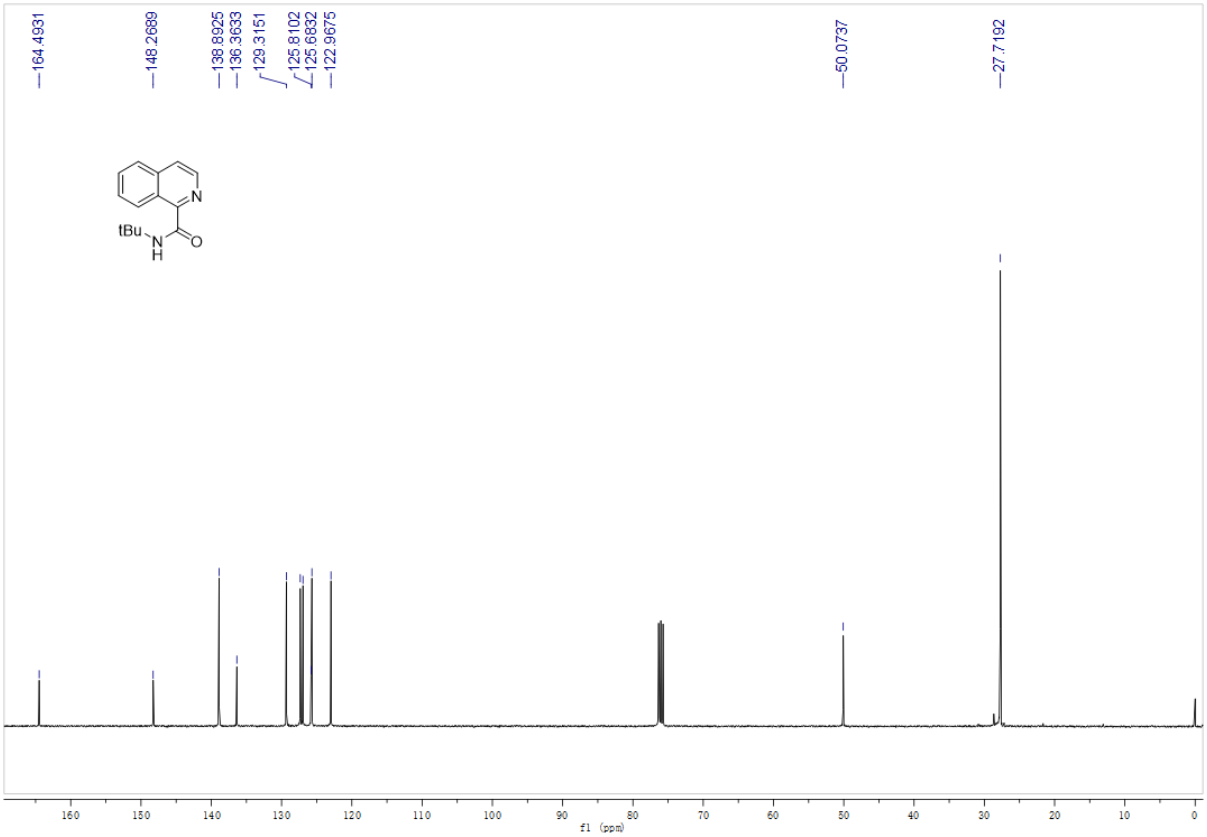
References:

[1] S. Ghorai and D. Lee, *Org. Lett.* **2019**, *21*, 7390–7393.

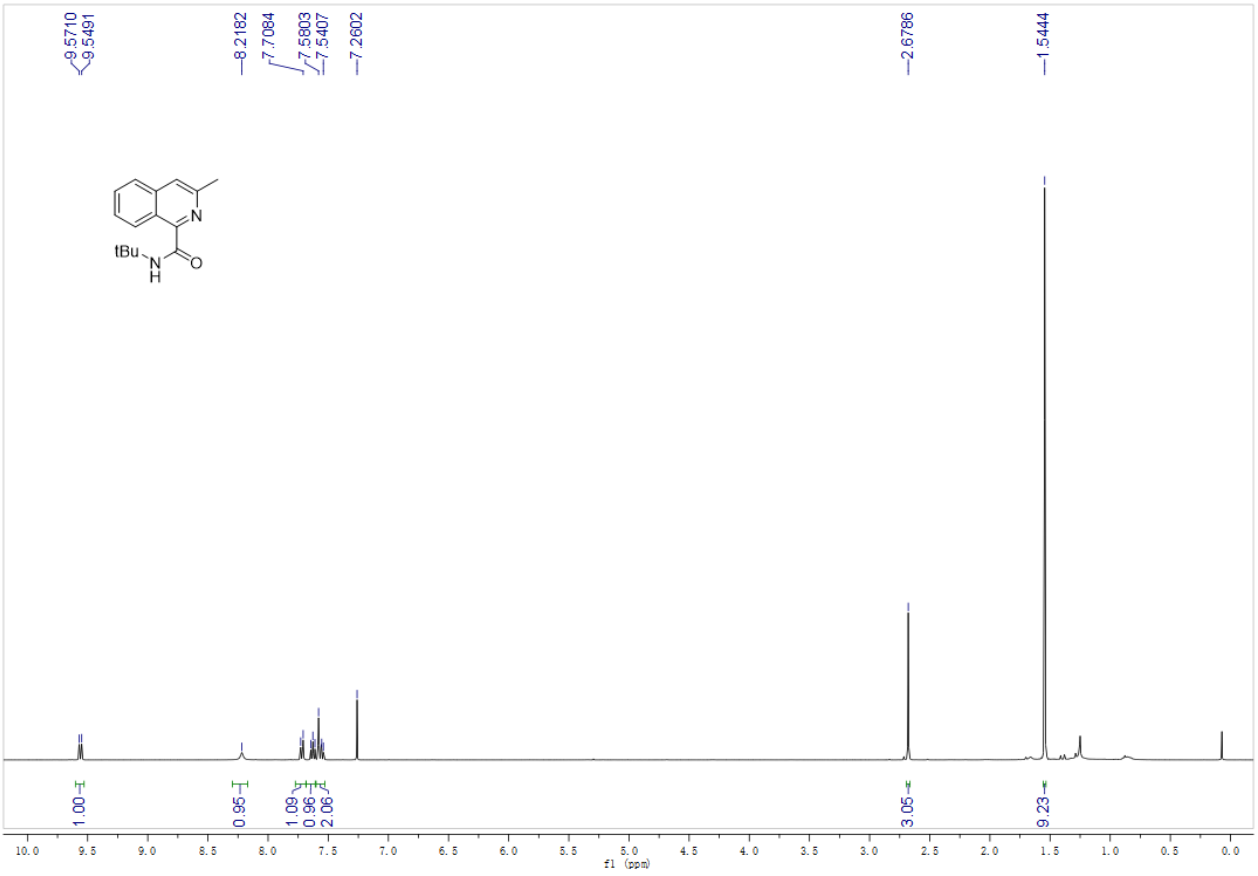
Copies of ^{1}H and ^{13}C NMR spectra

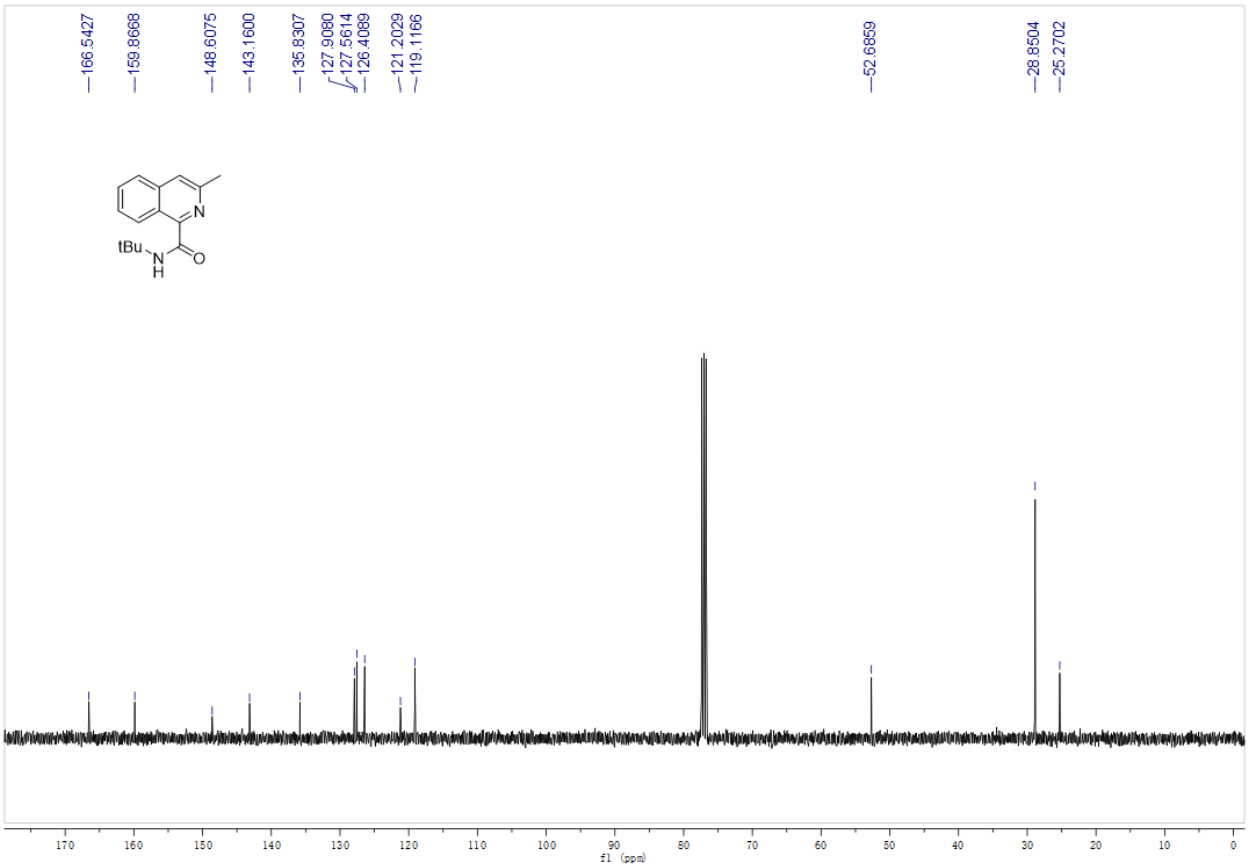
N-(*tert*-butyl)isoquinoline-1-carboxamide (3a)



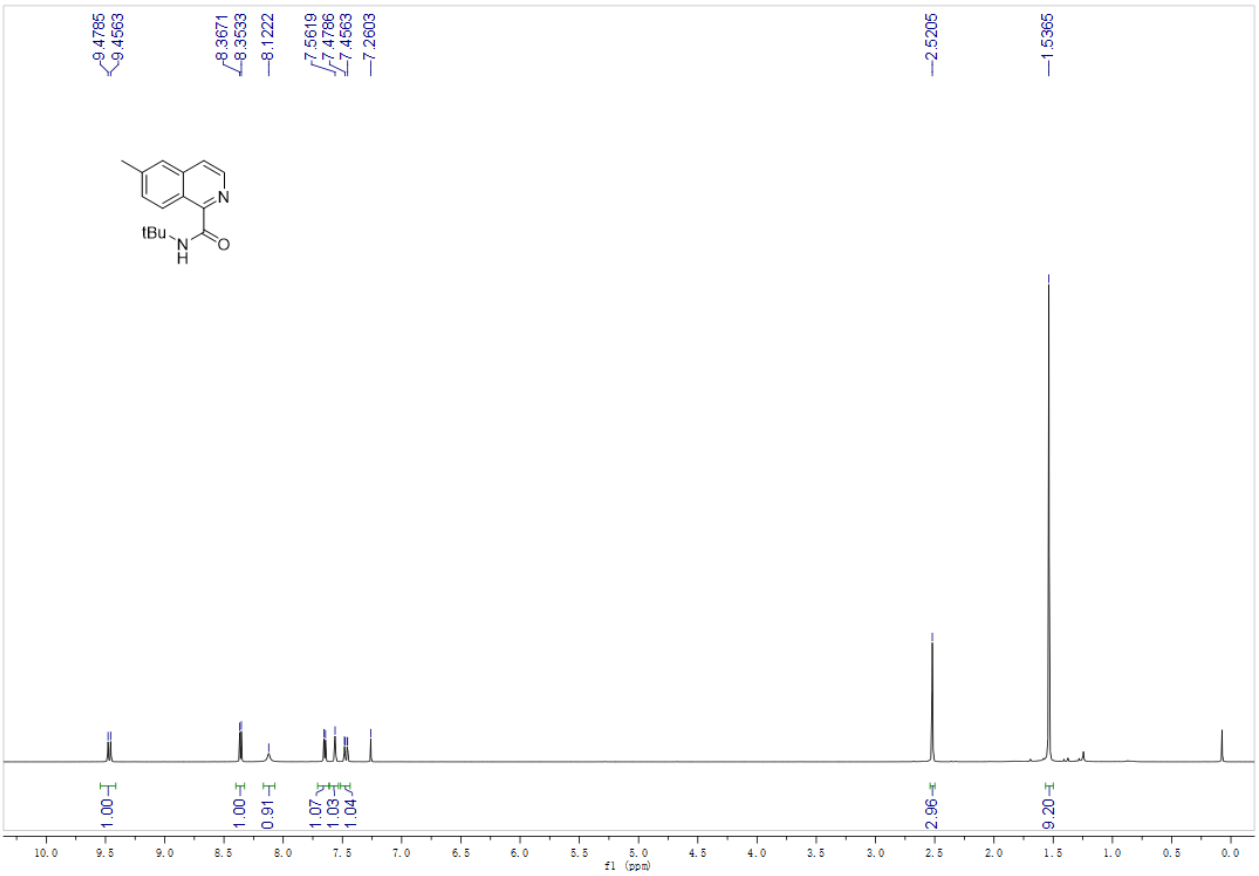


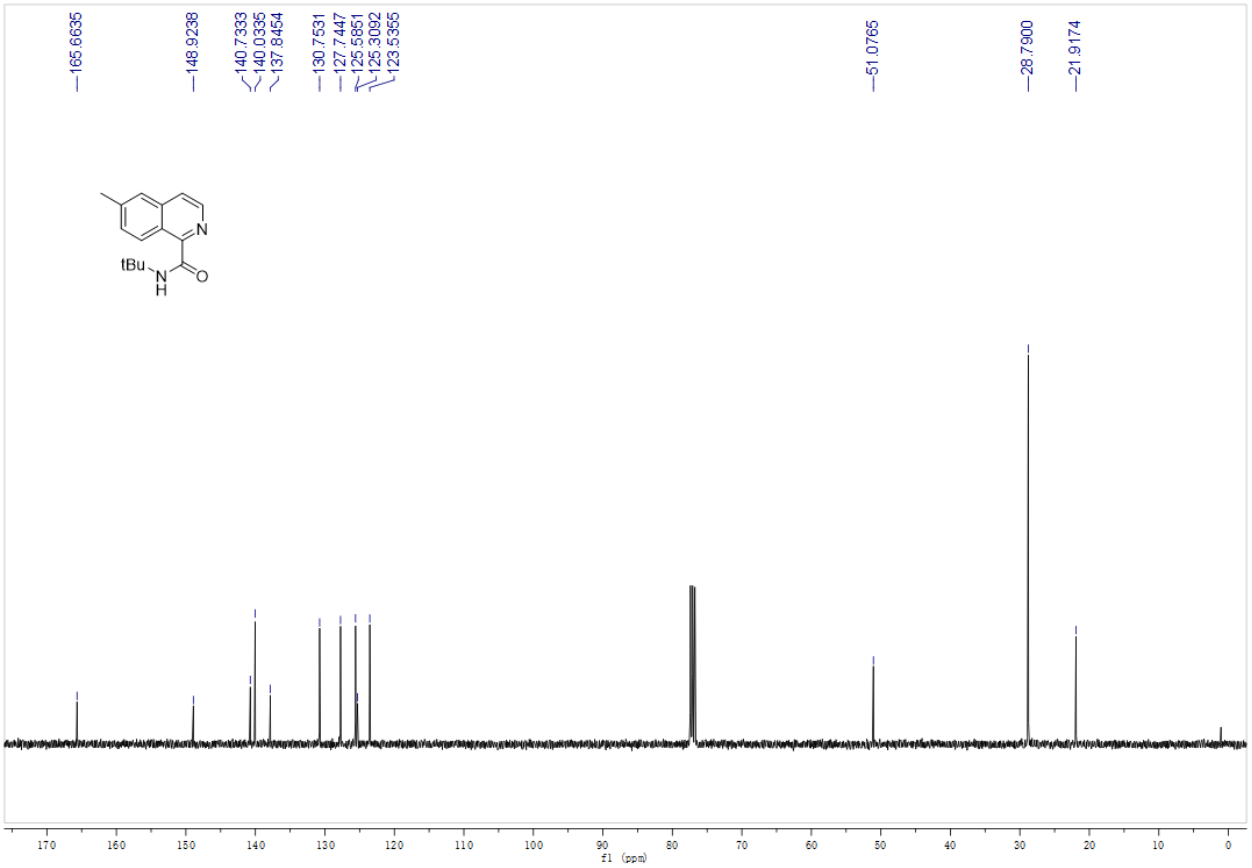
N-(*tert*-butyl)-3-methylisoquinoline-1-carboxamide (3b)



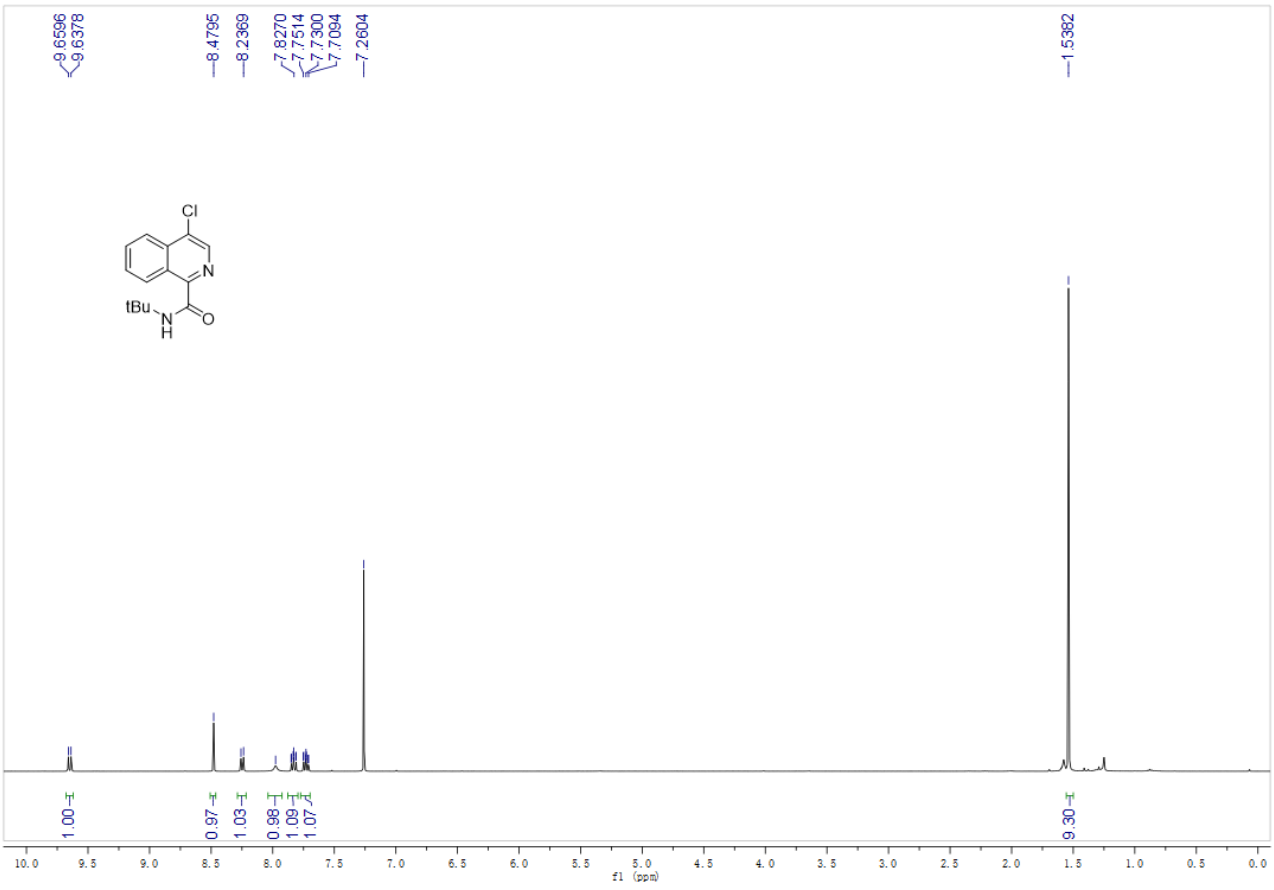


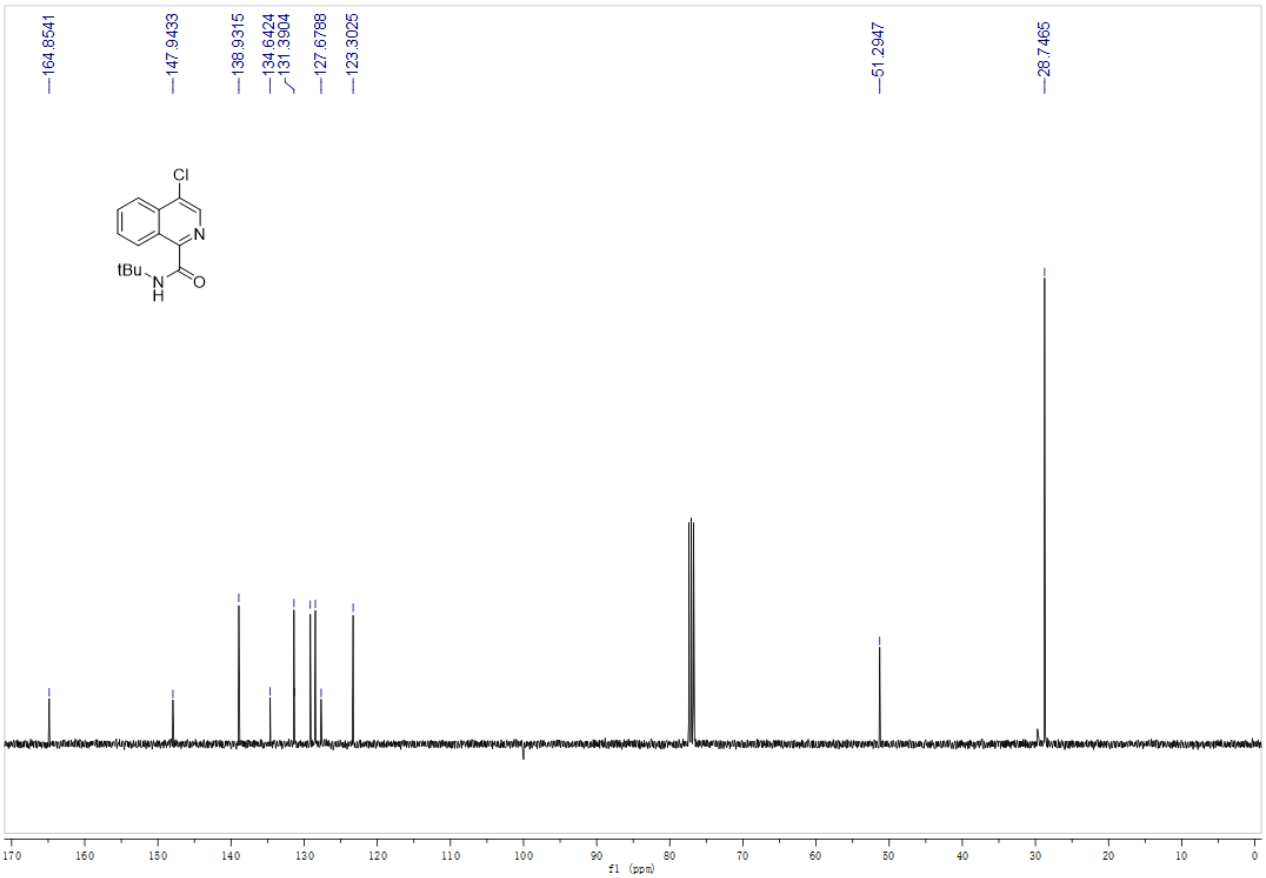
N-(*tert*-butyl)-6-methylisoquinoline-1-carboxamide (3c)



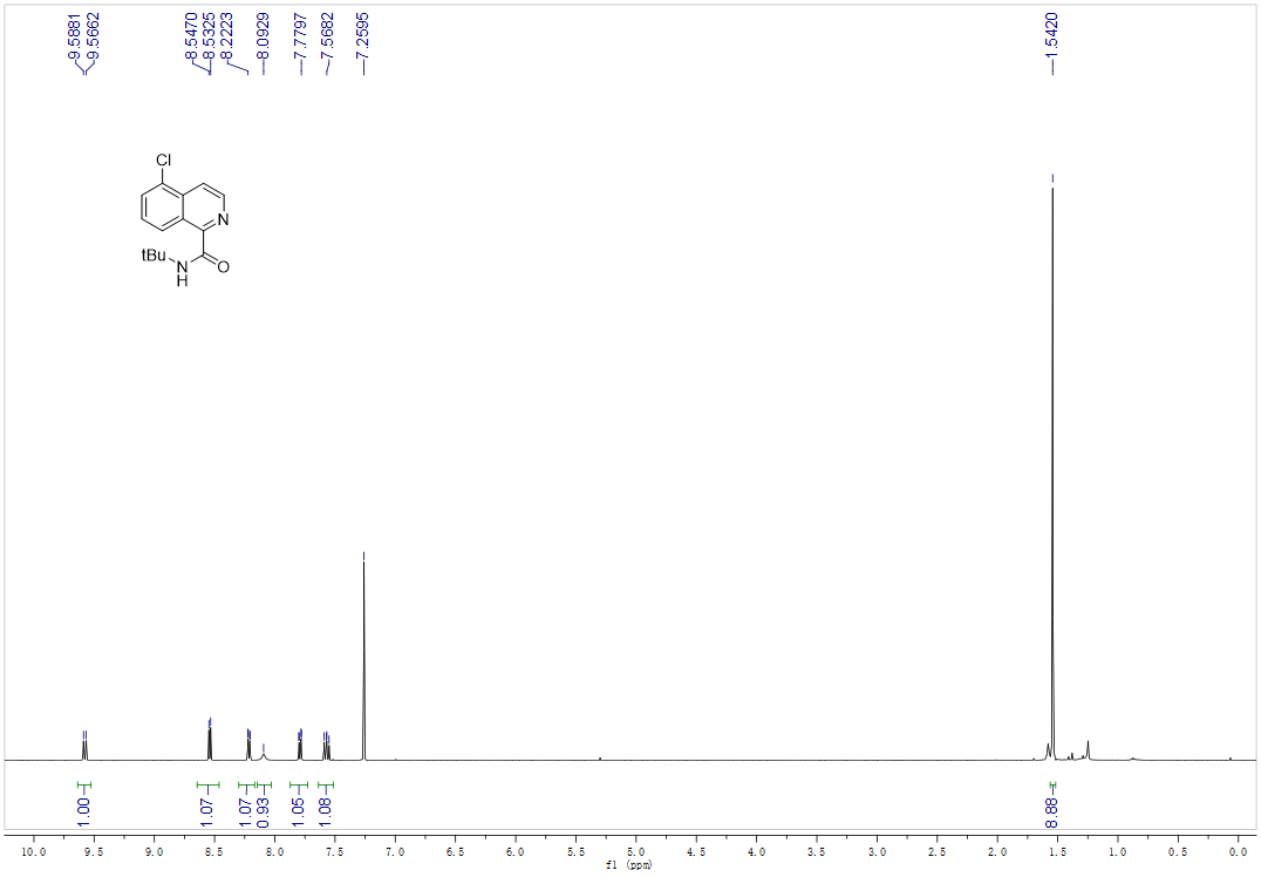


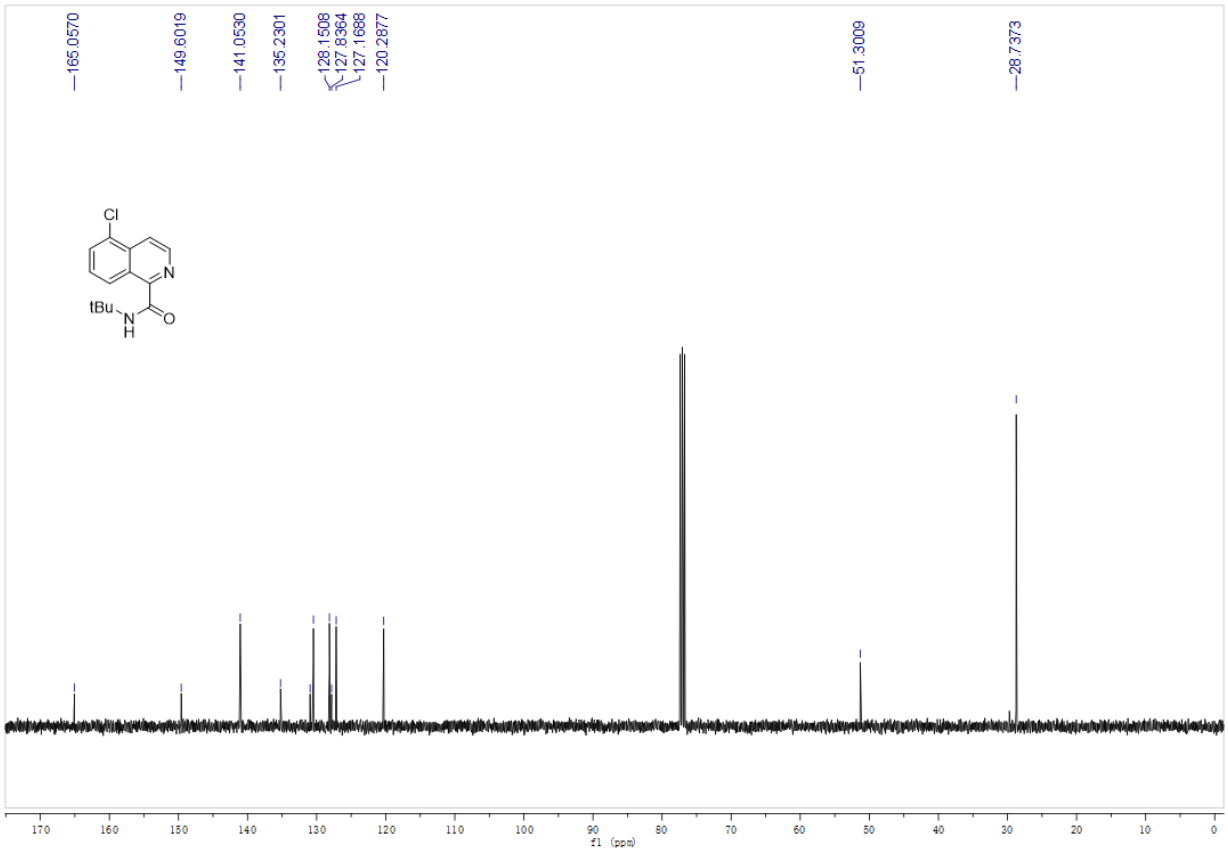
N-(*tert*-butyl)-4-chloroisoquinoline-1-carboxamide (3d)



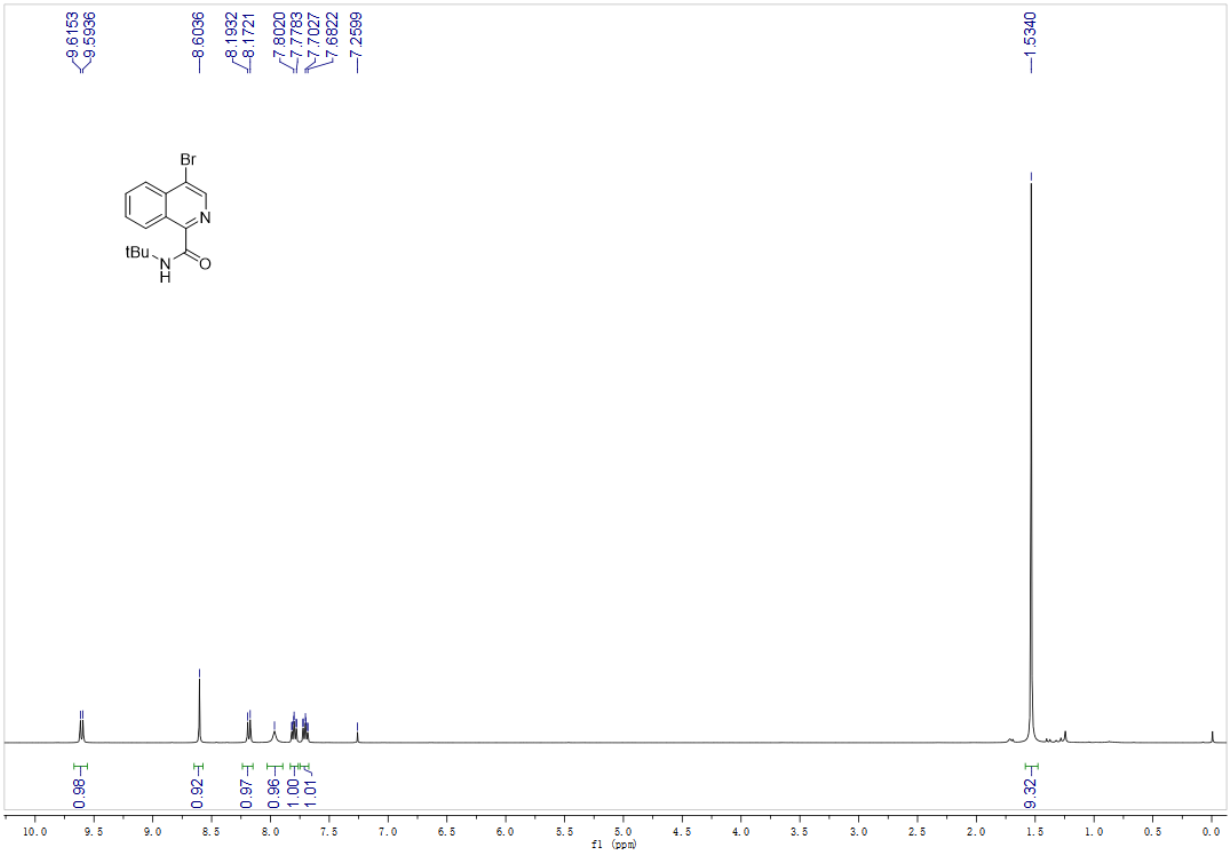


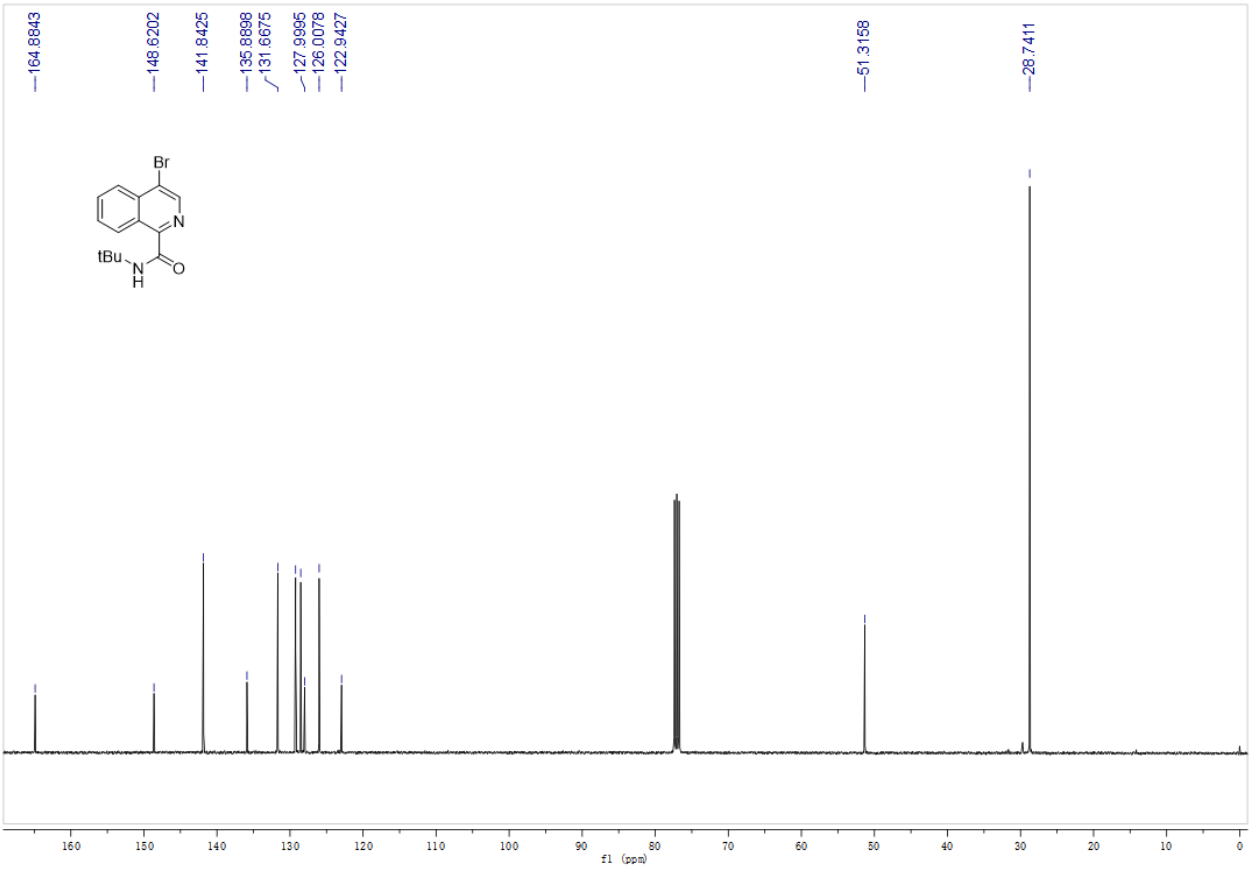
N-(*tert*-butyl)-5-chloroisoquinoline-1-carboxamide (3e)



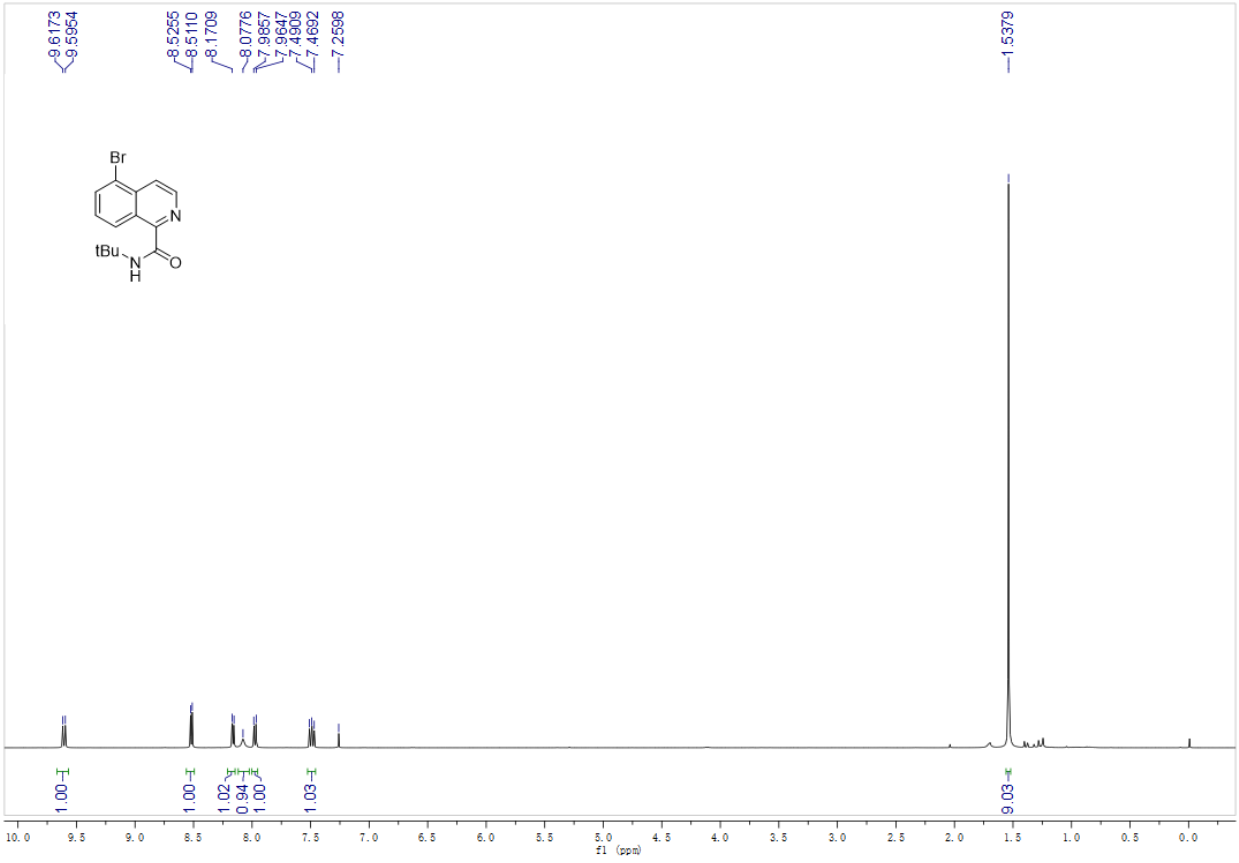


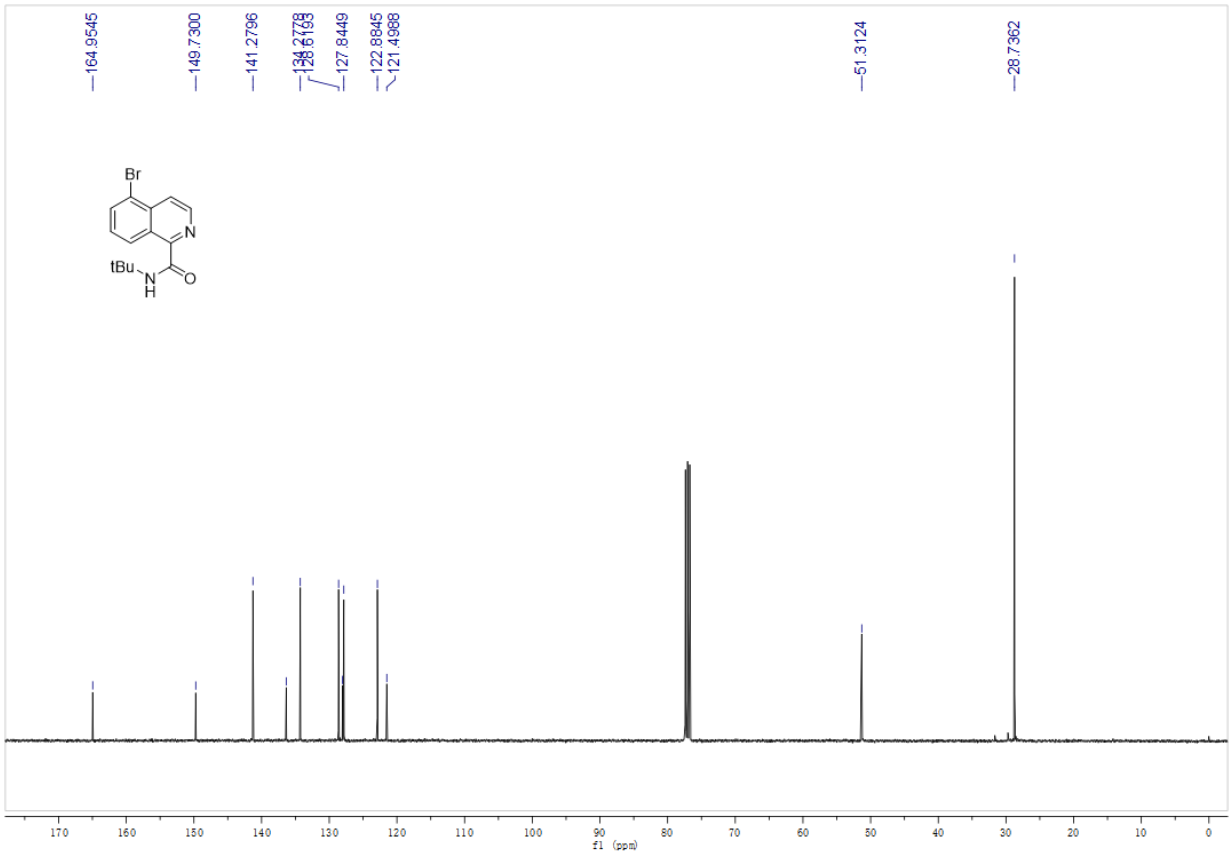
4-bromo-*N*-(*tert*-butyl)isoquinoline-1-carboxamide (3f)



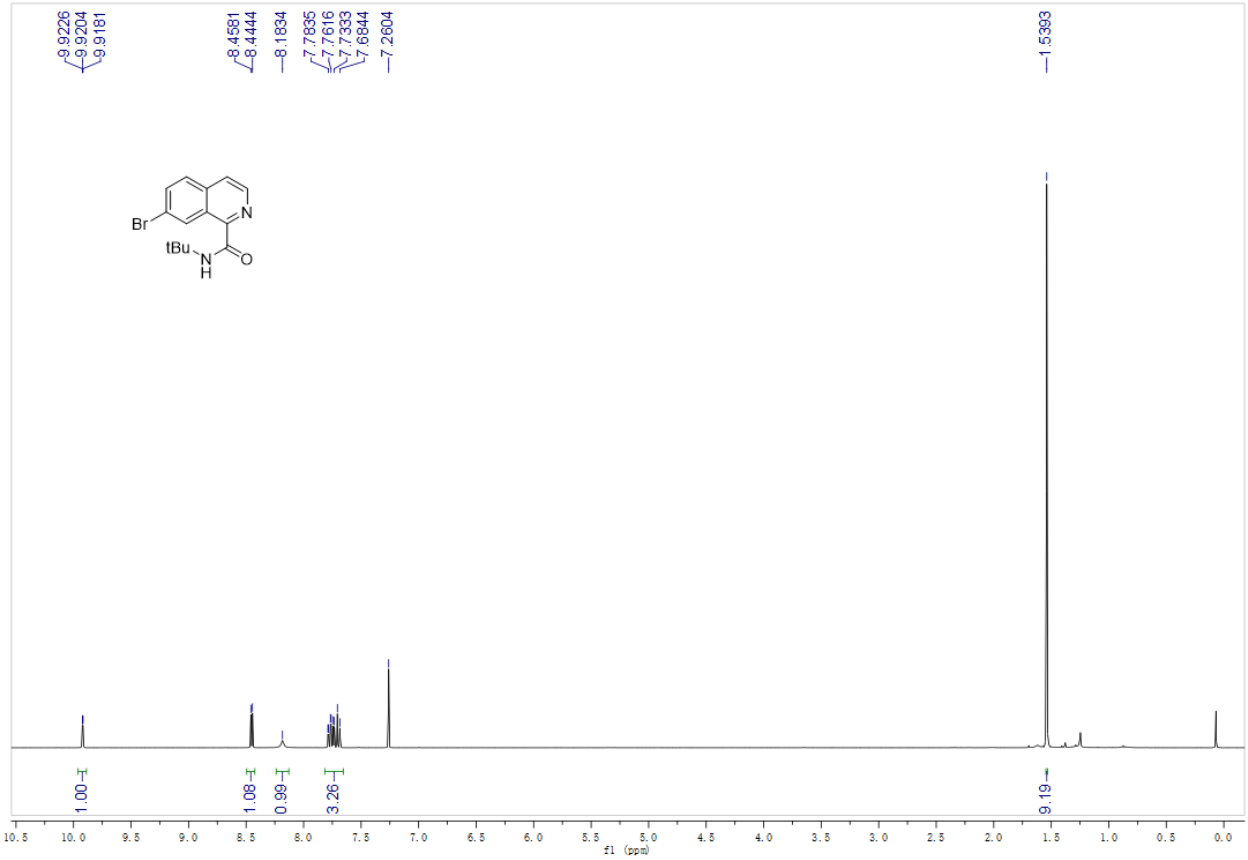


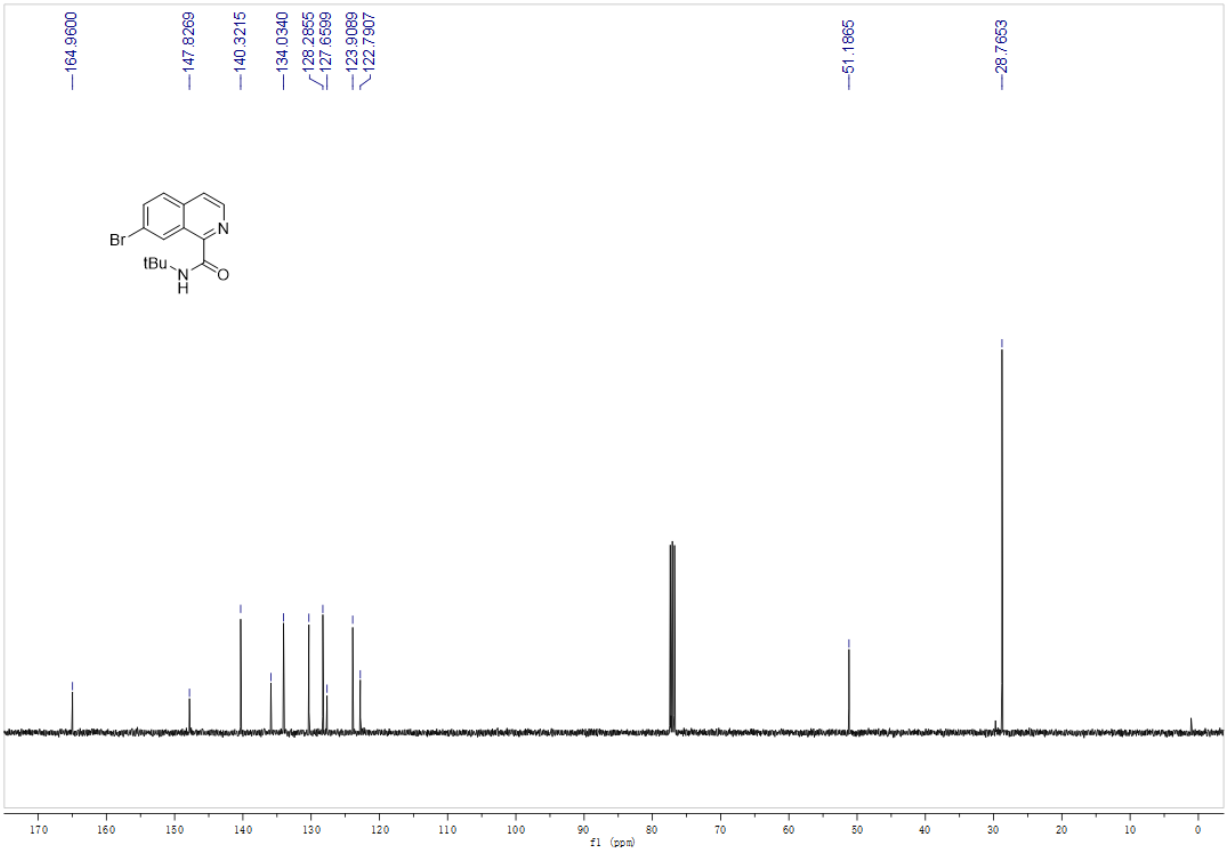
5-bromo-*N*-(*tert*-butyl)isoquinoline-1-carboxamide (3g)



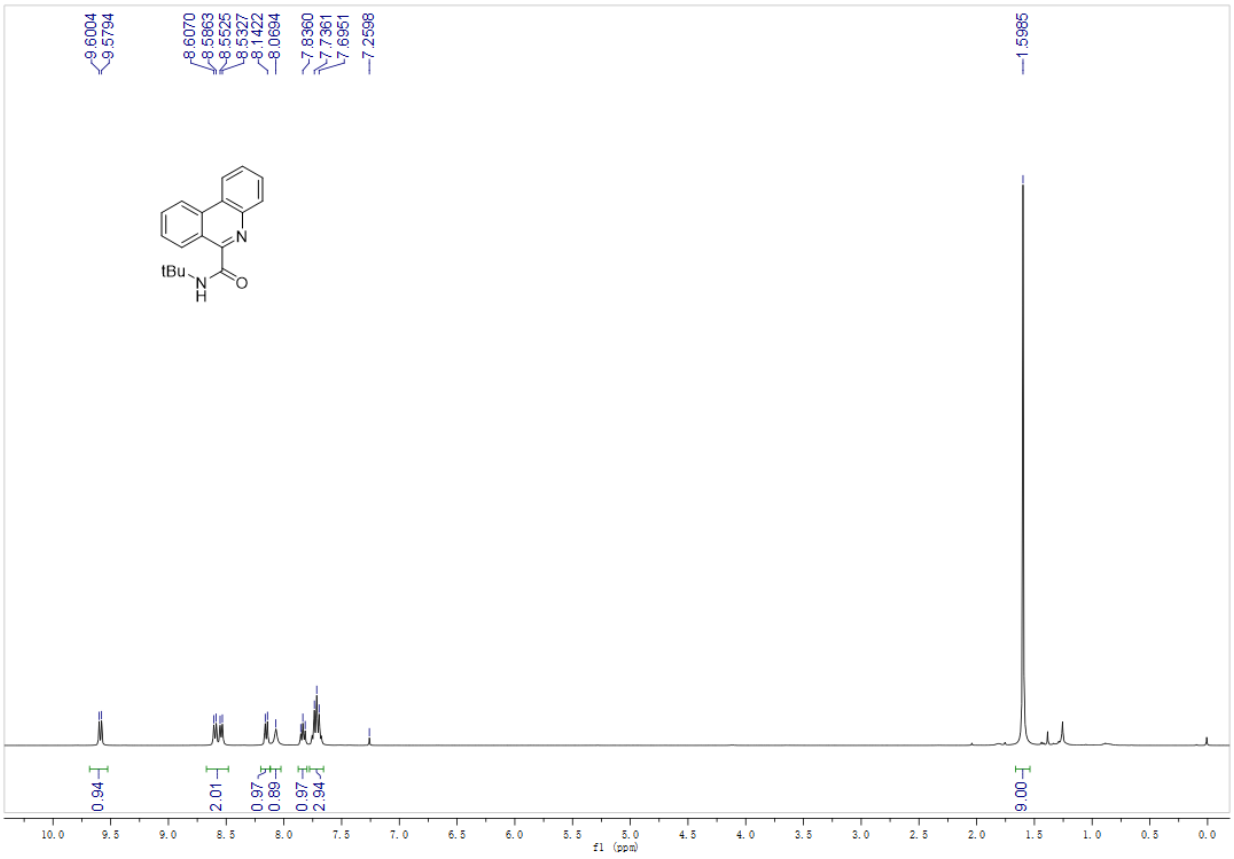


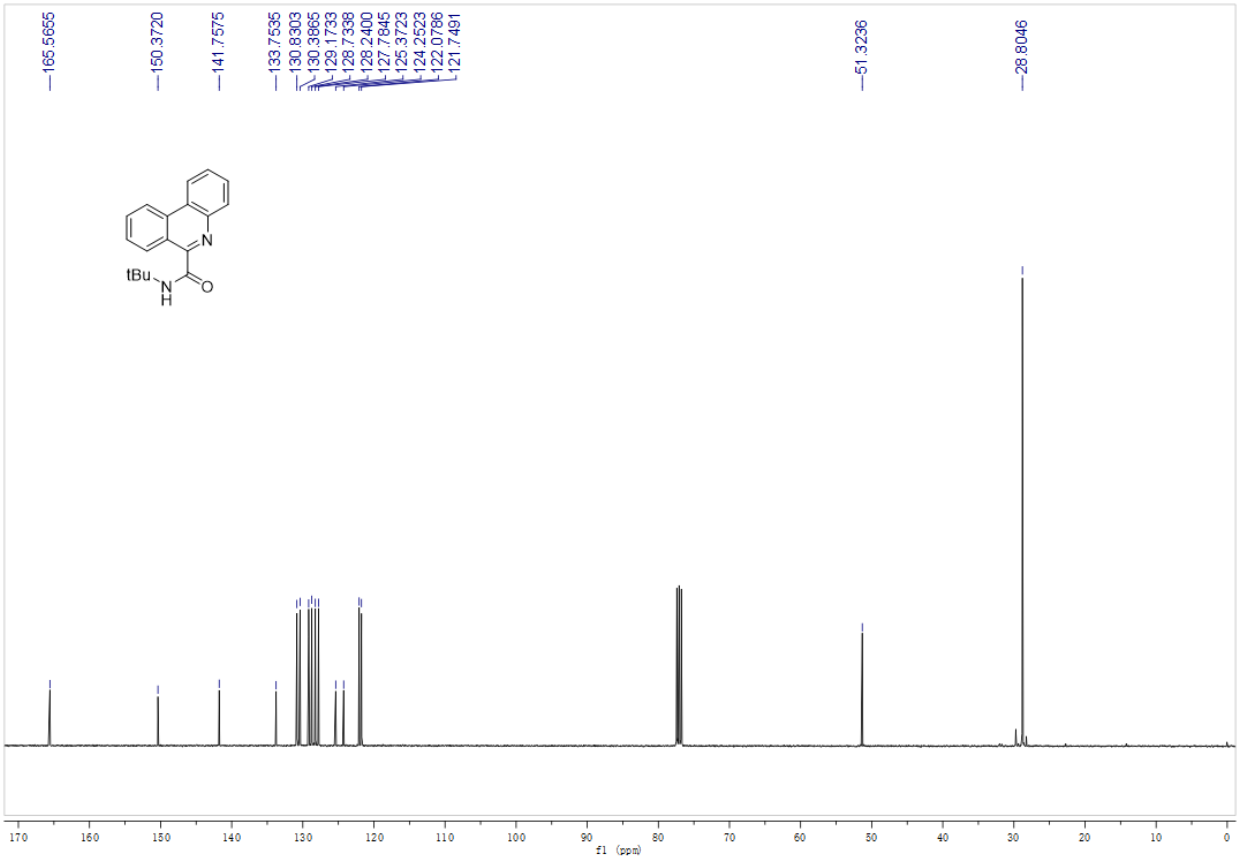
7-bromo-*N*-(*tert*-butyl)isoquinoline-1-carboxamide (3h)



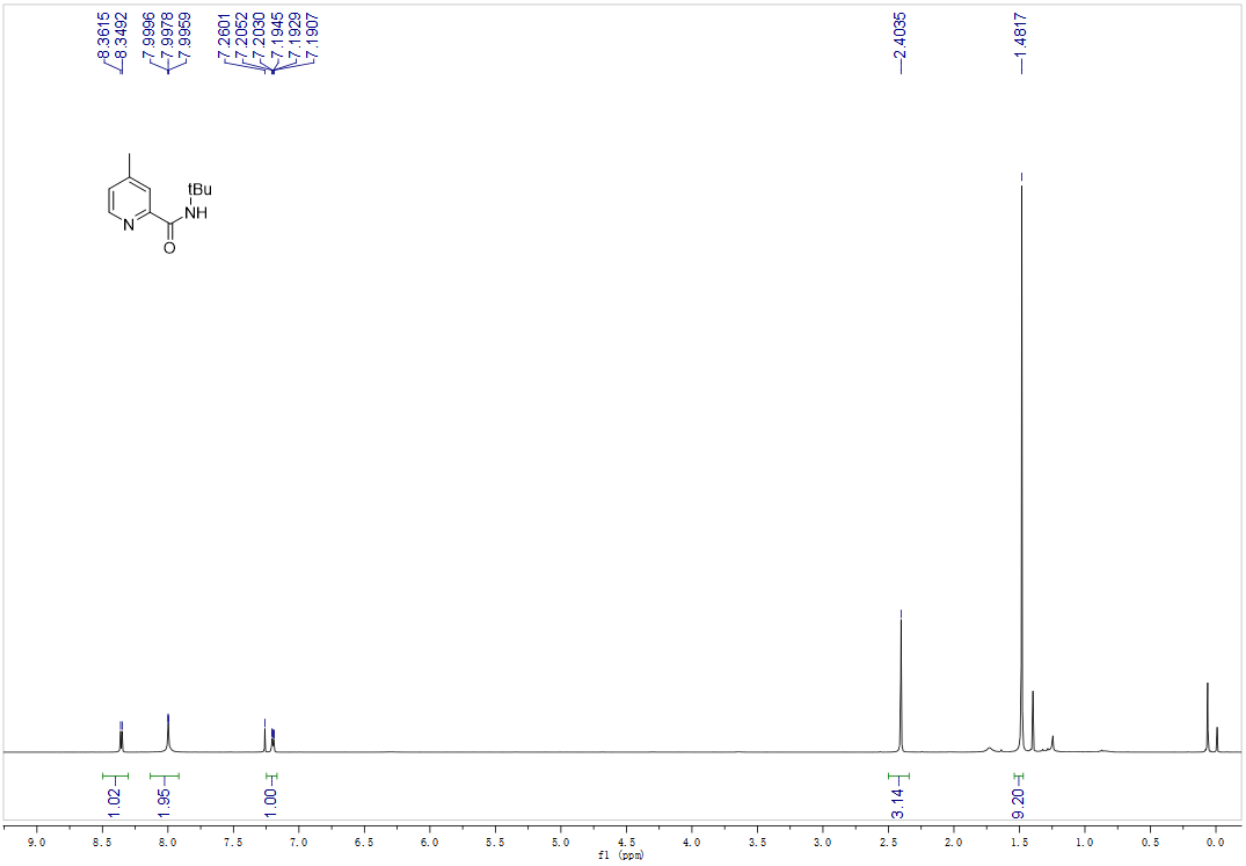


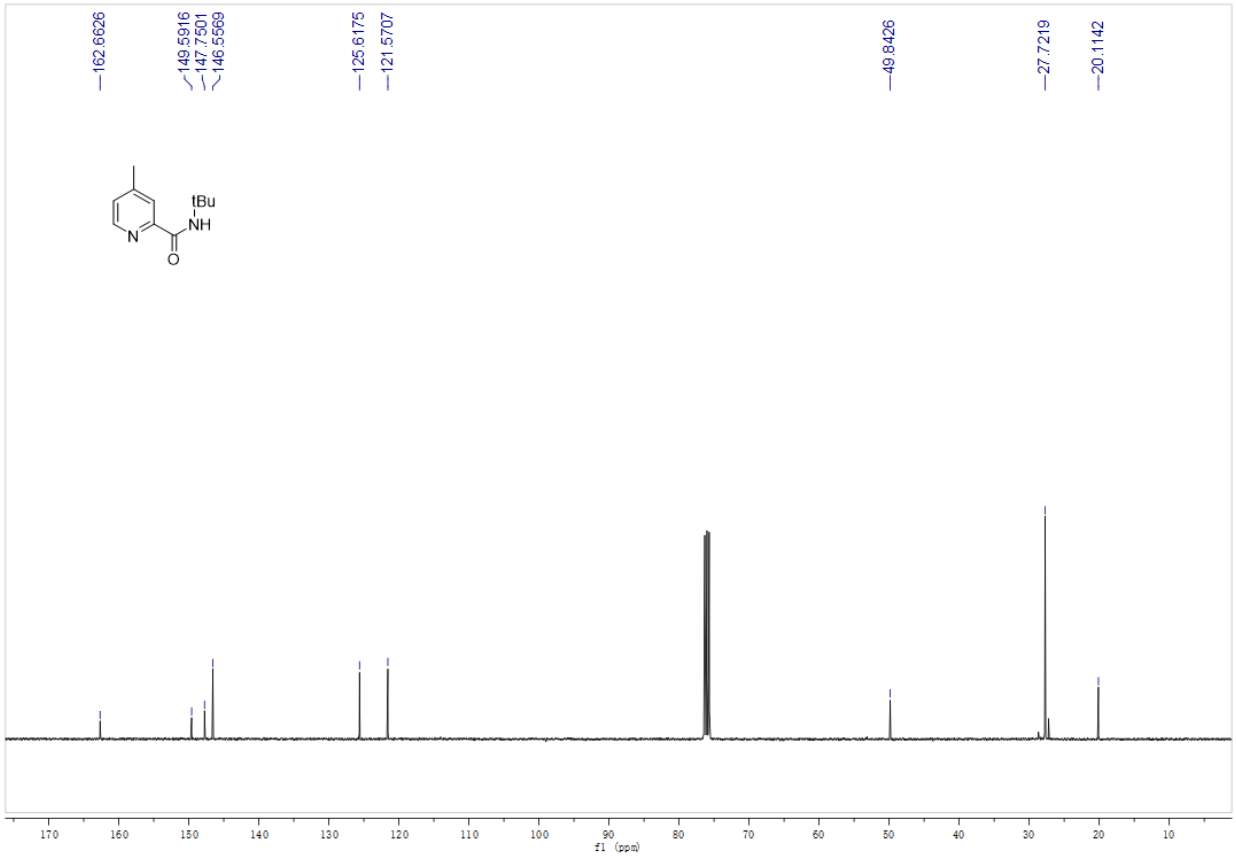
N-(*tert*-butyl)phenanthridine-6-carboxamide (3i)



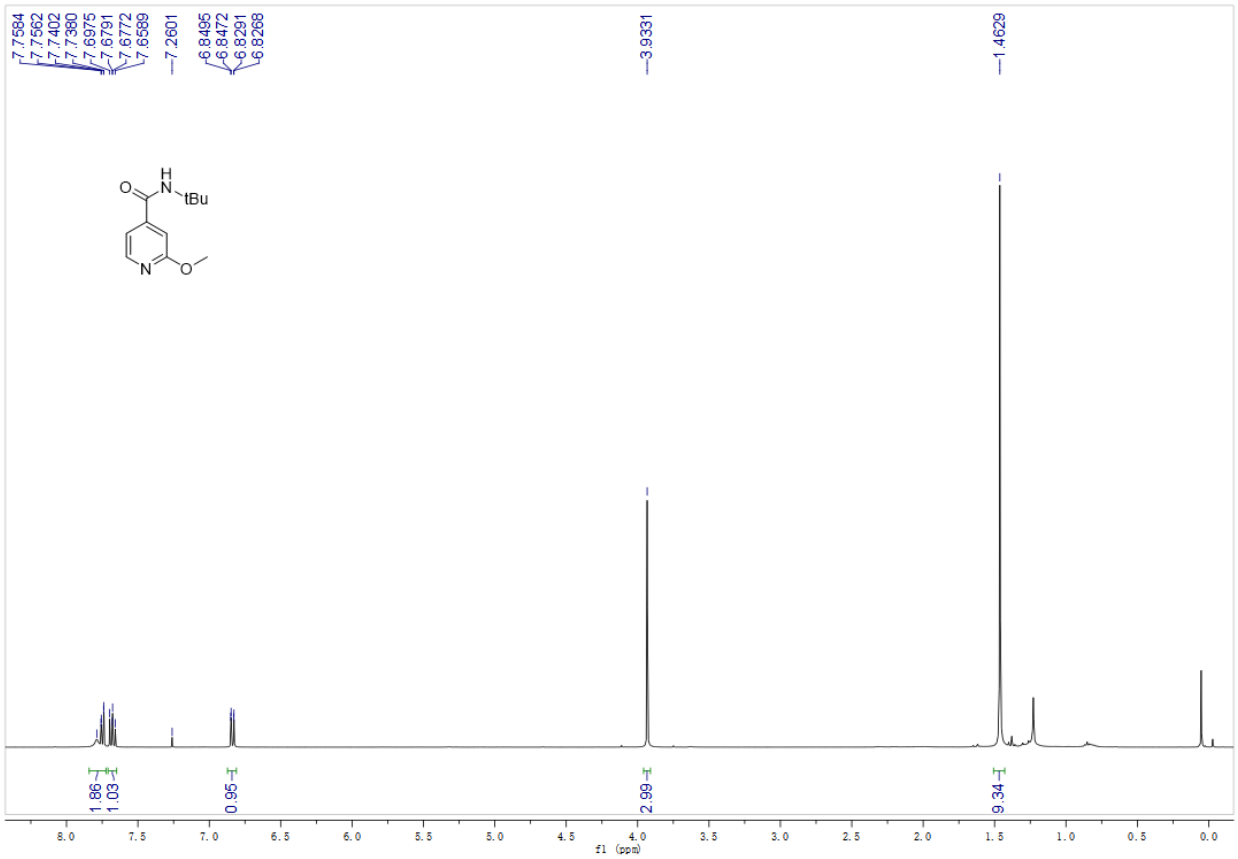


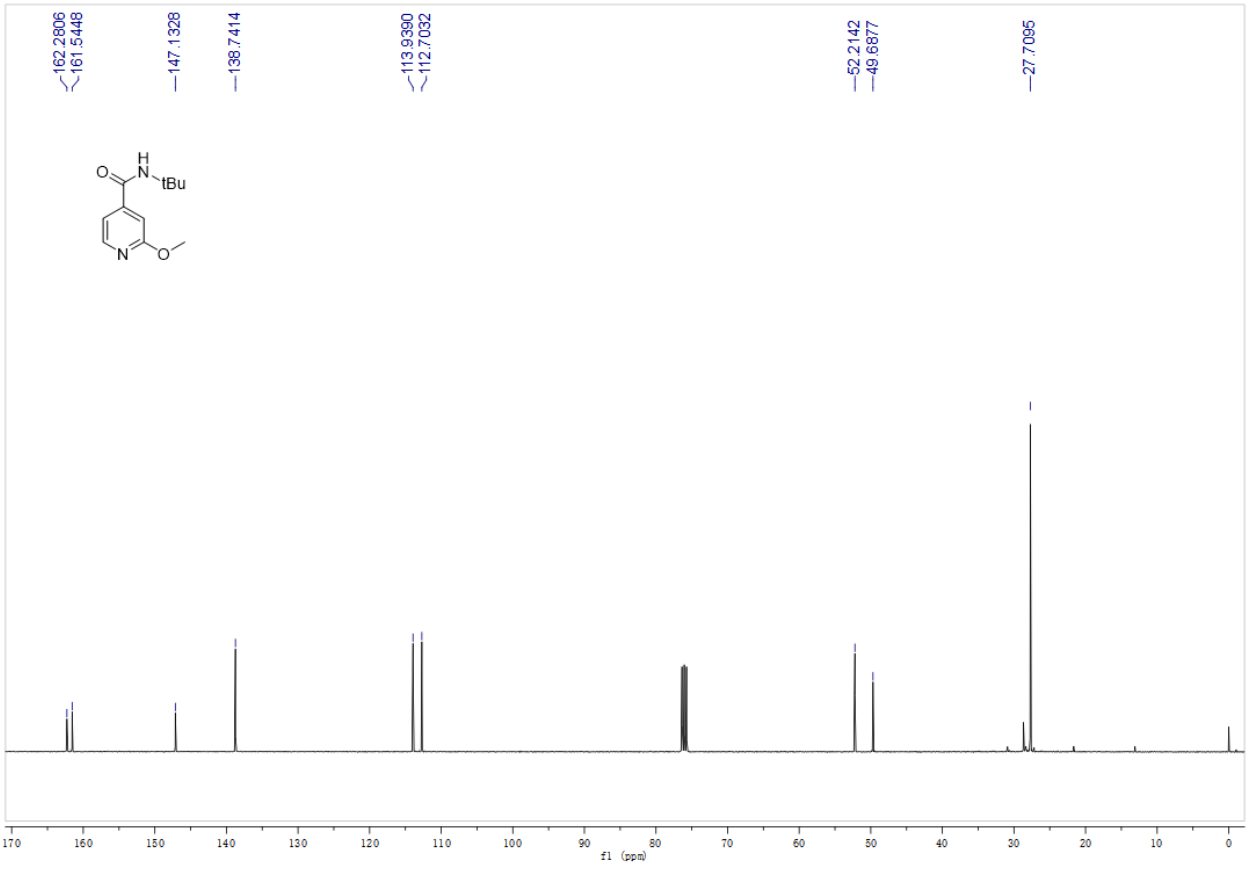
N-(*tert*-butyl)-4-methylpicolinamide (3j)



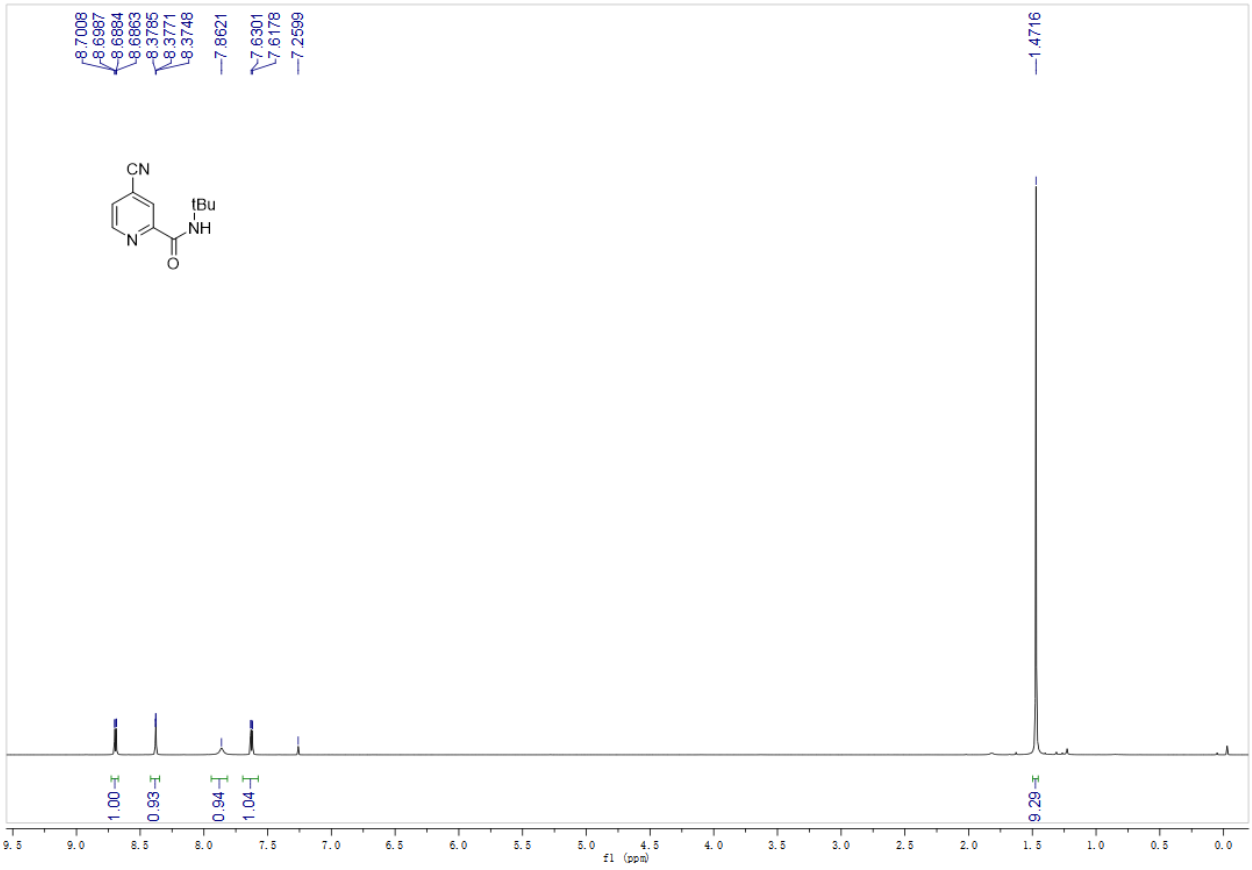


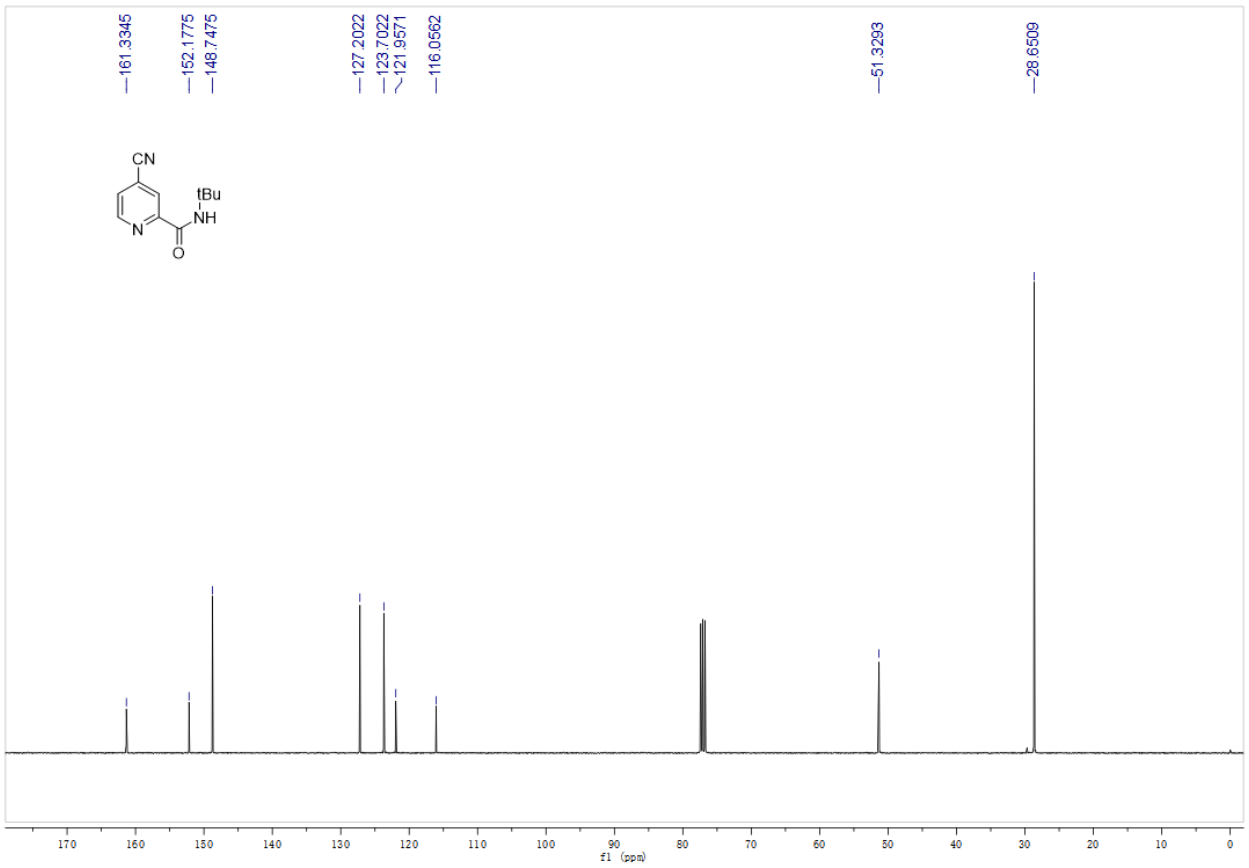
N-(*tert*-butyl)-2-methoxyisonicotinamide (3k)



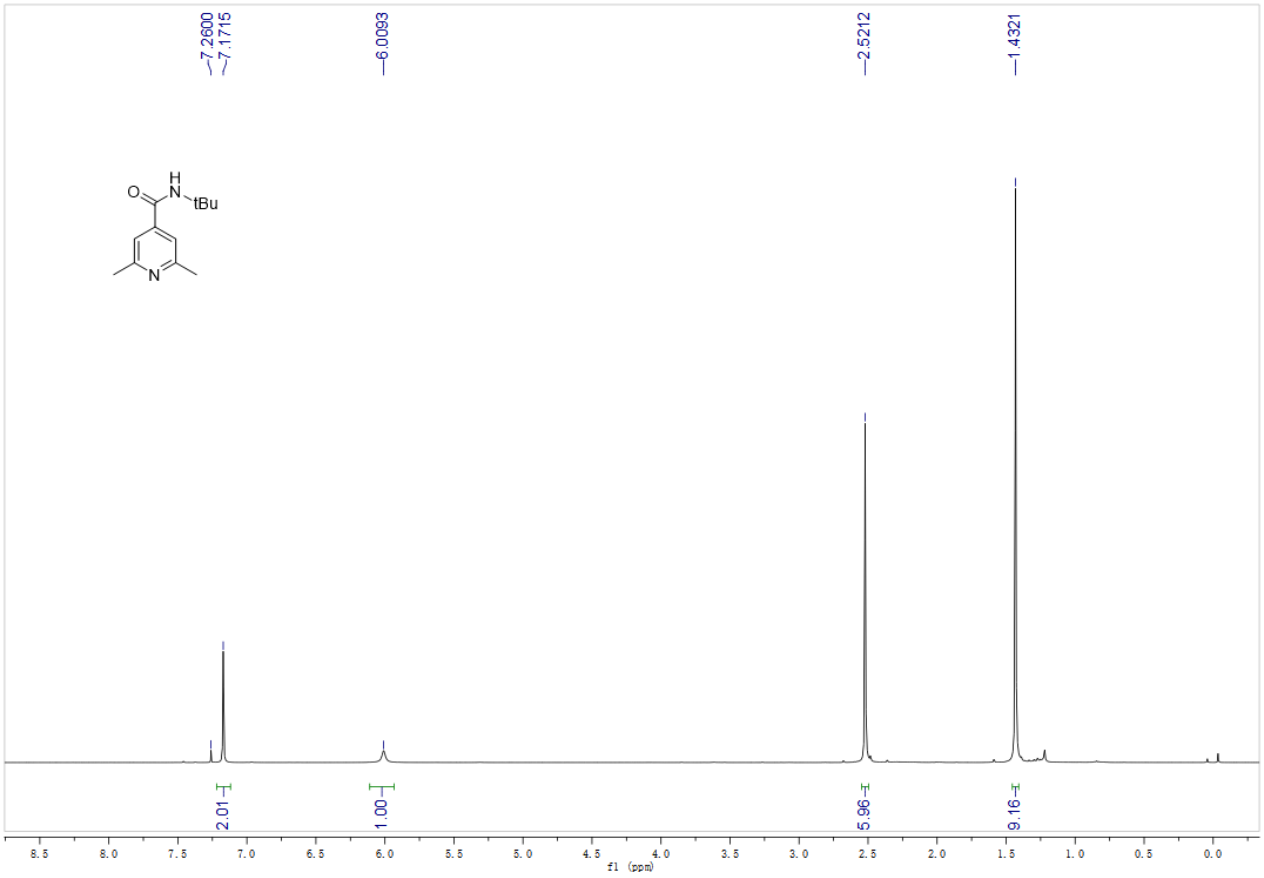


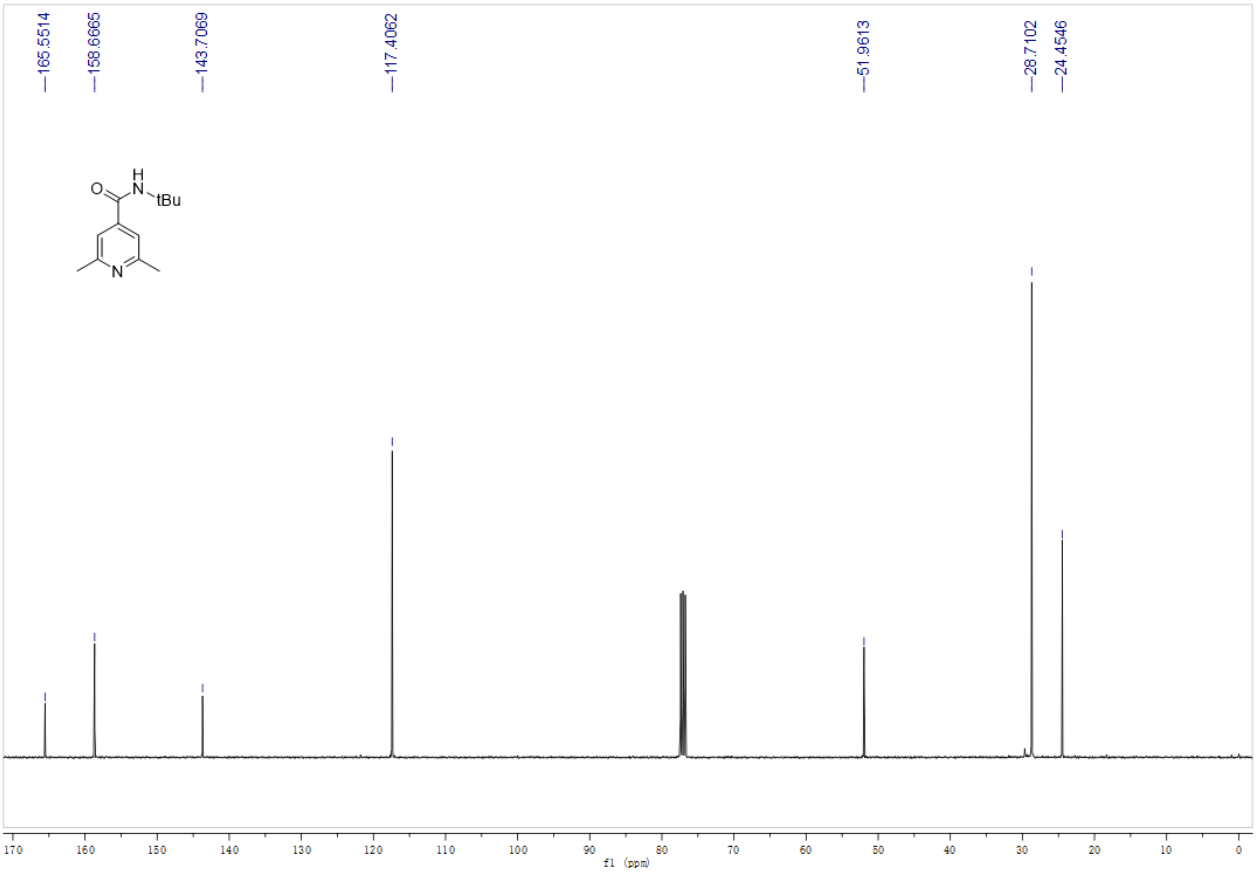
N-(*tert*-butyl)-4-cyanopicolinamide (3l)



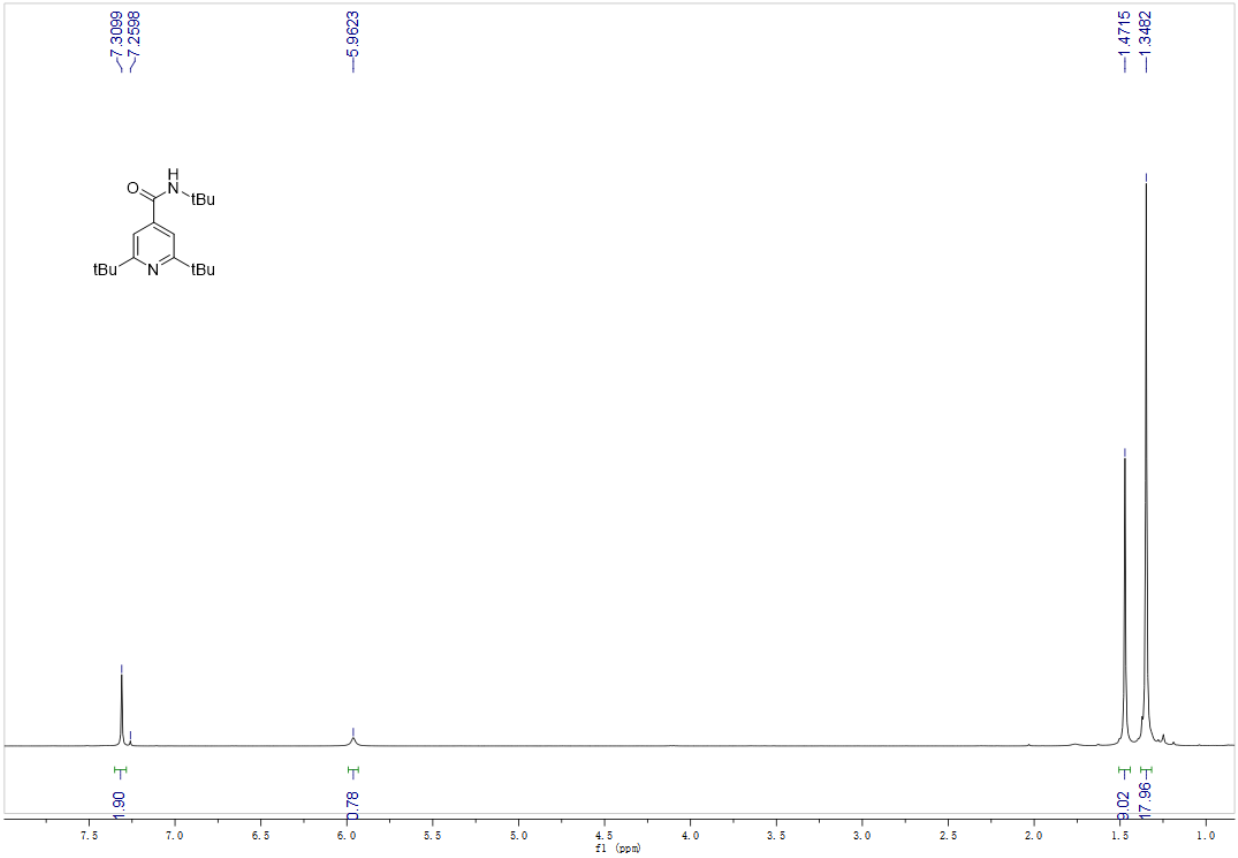


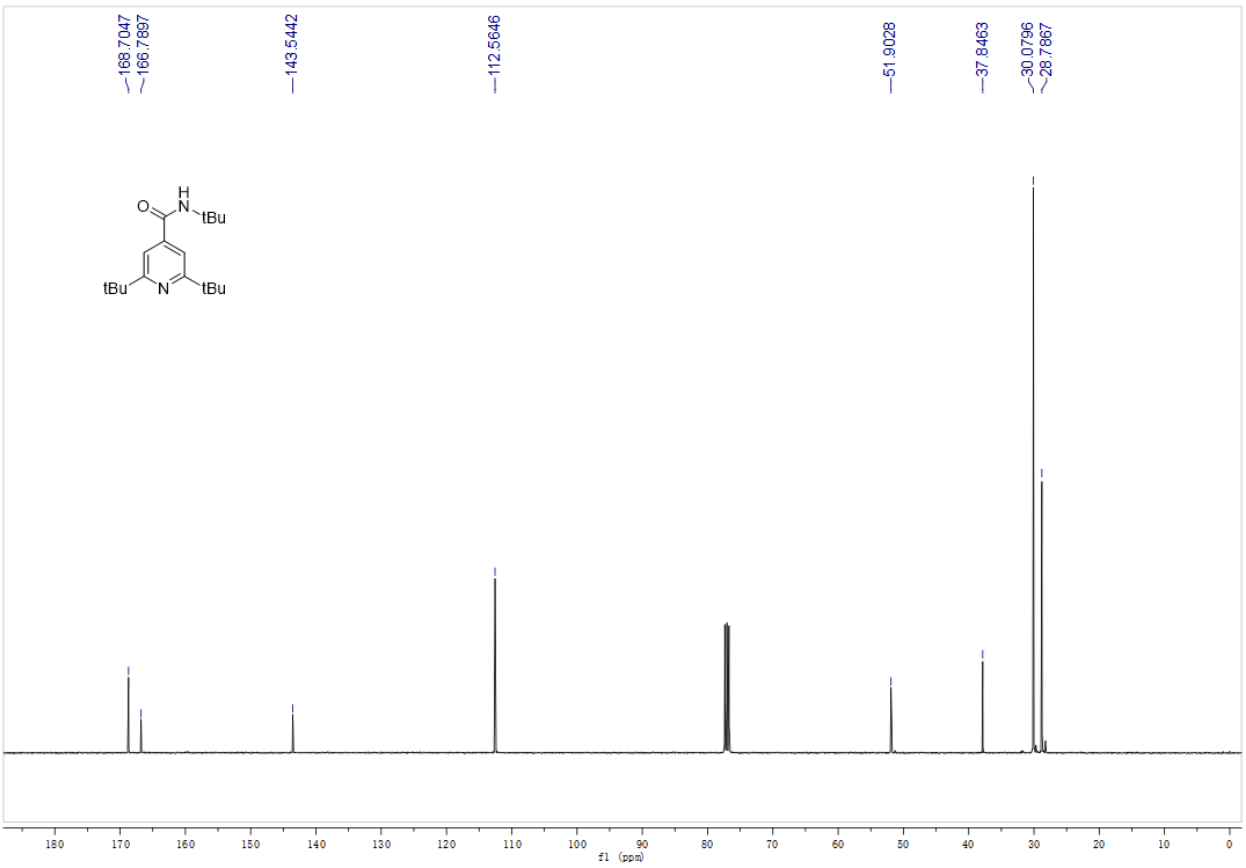
N-(*tert*-butyl)-2,6-dimethylisonicotinamide (3m)



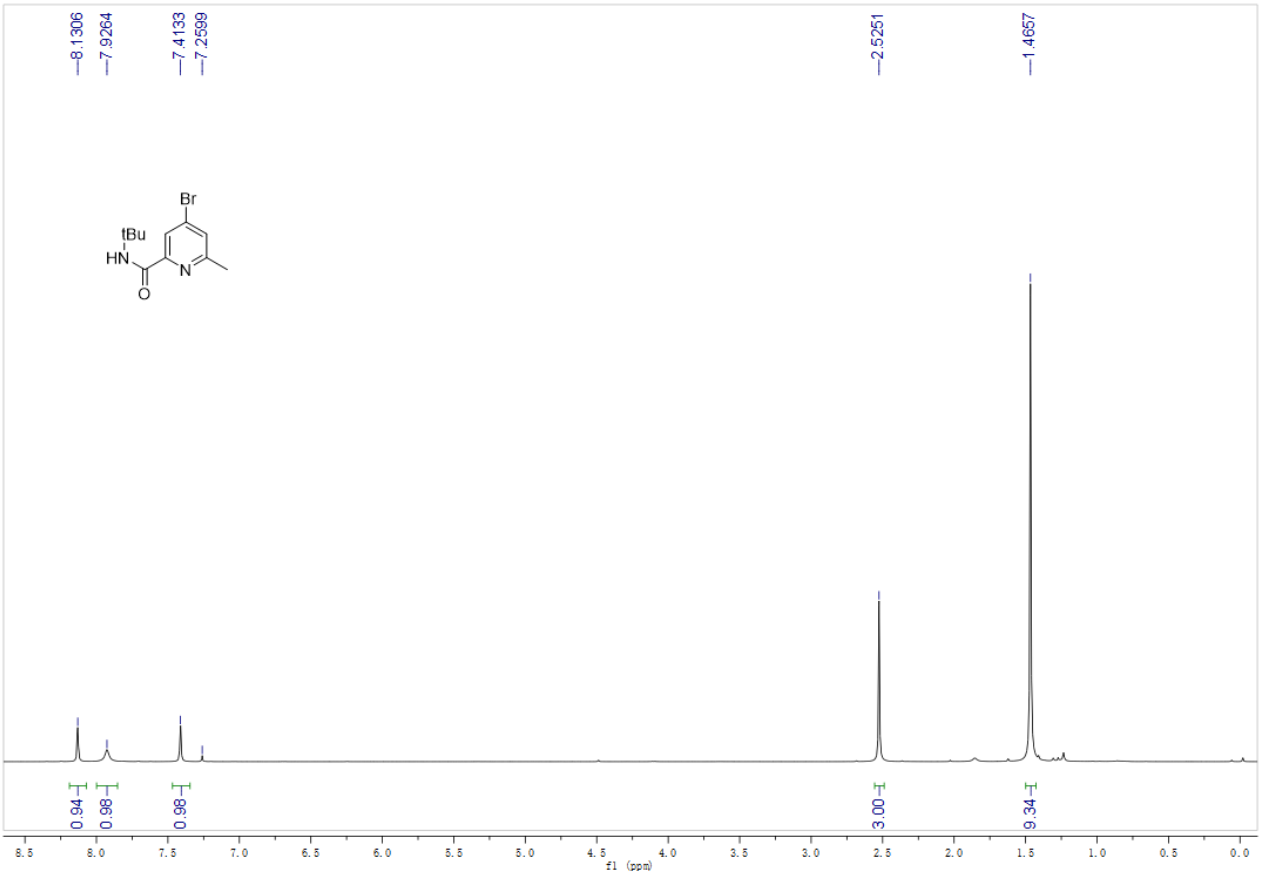


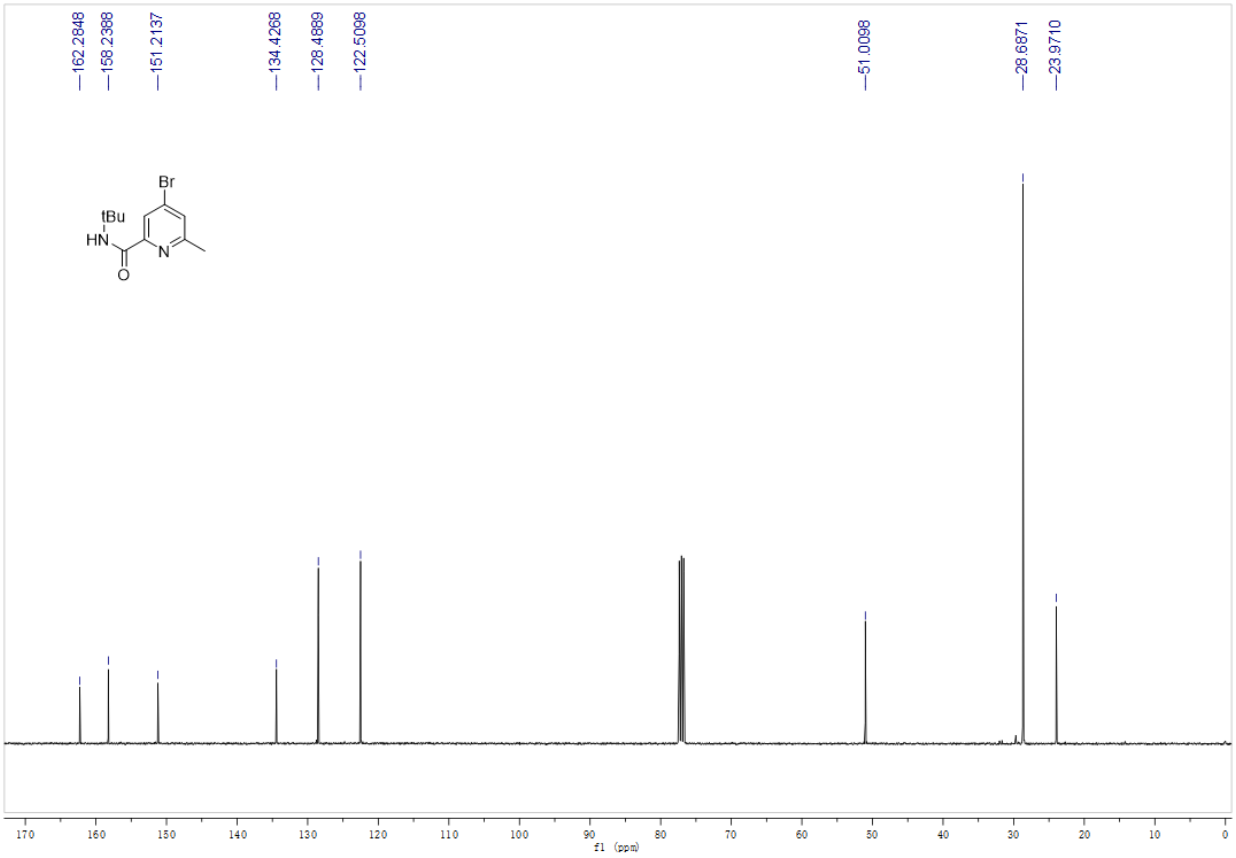
N,2,6-tri-*tert*-butylisonicotinamide (3n)



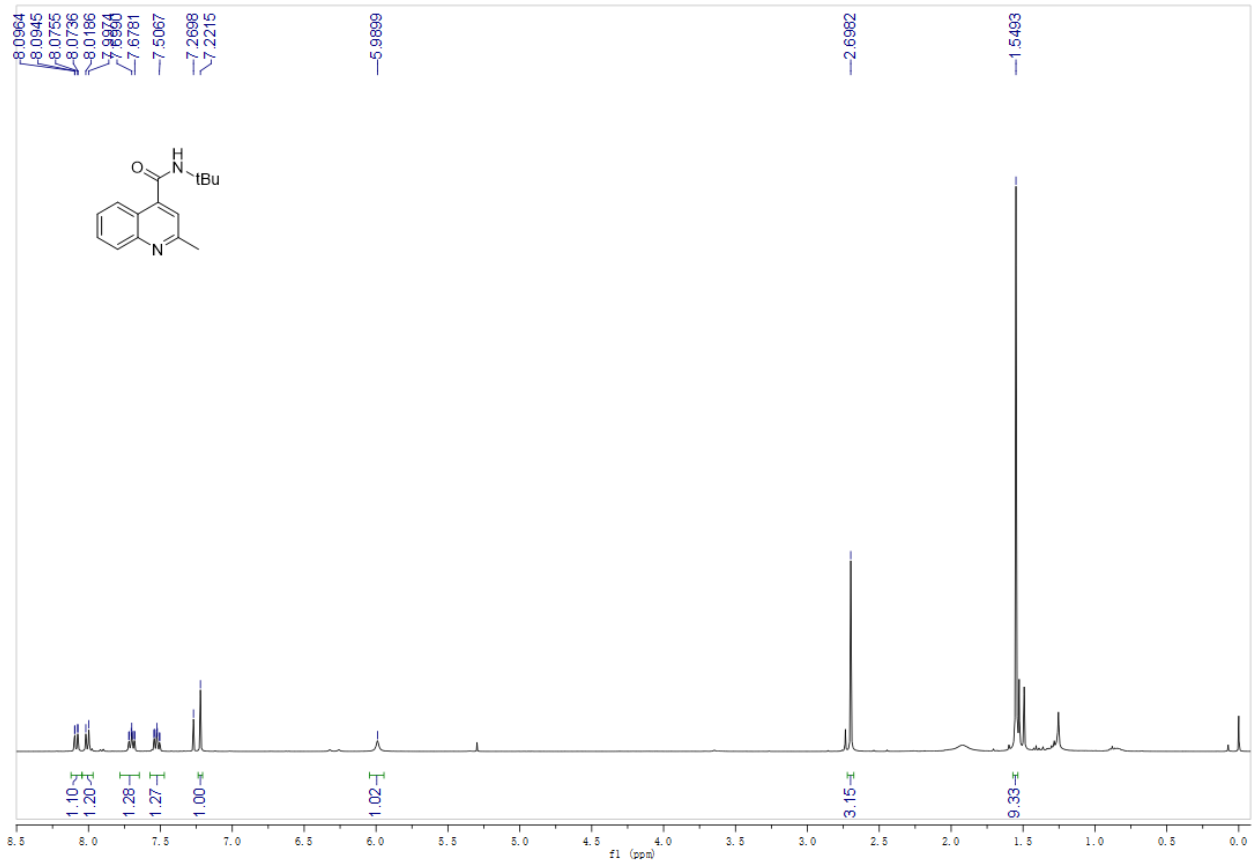


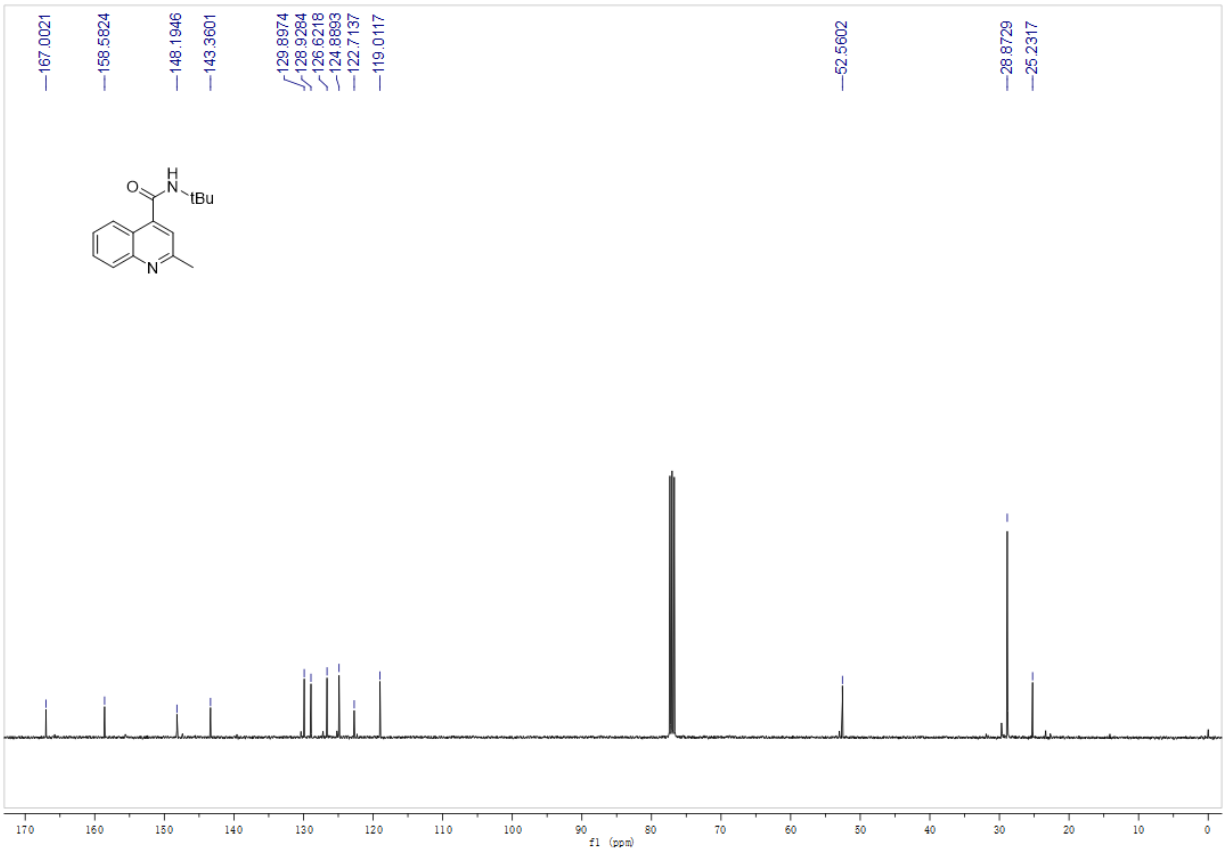
4-bromo-*N*-(*tert*-butyl)-6-methylpicolinamide (3o)



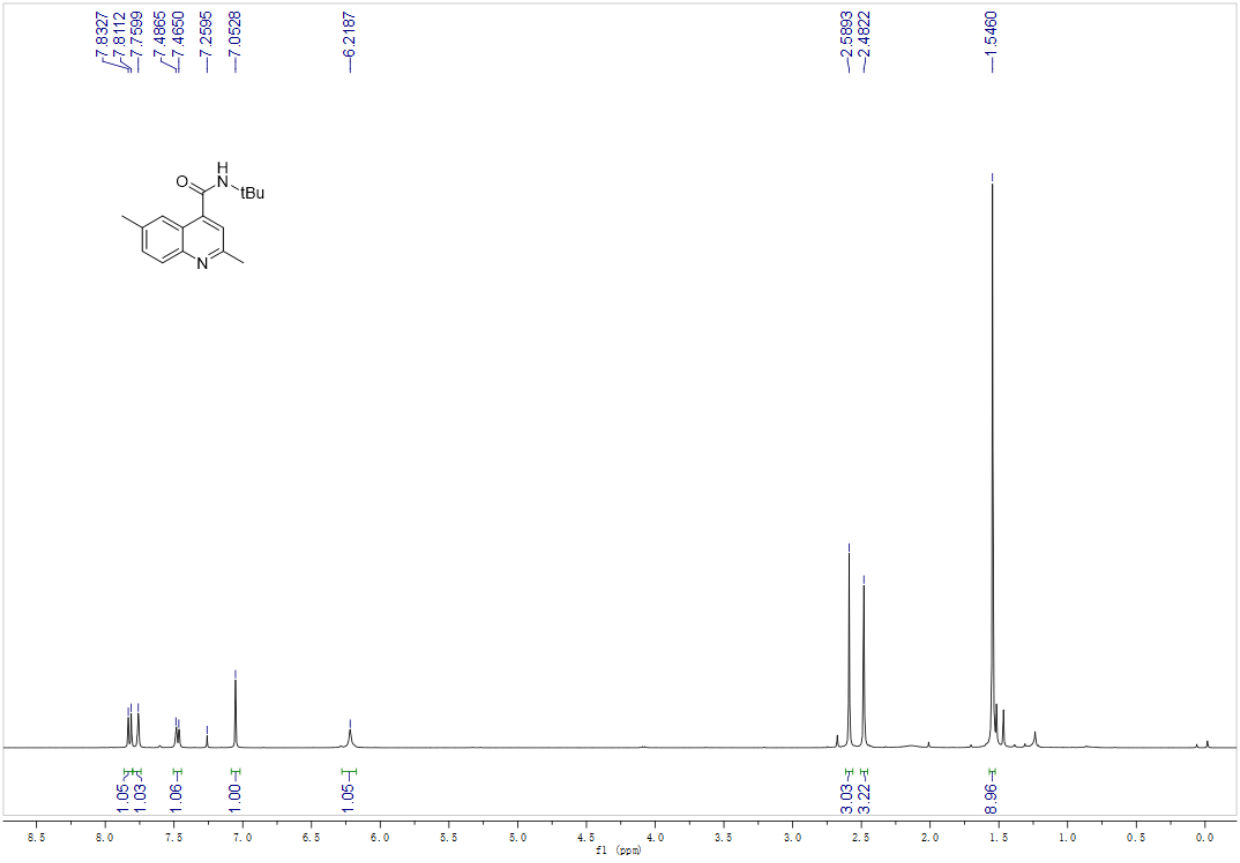


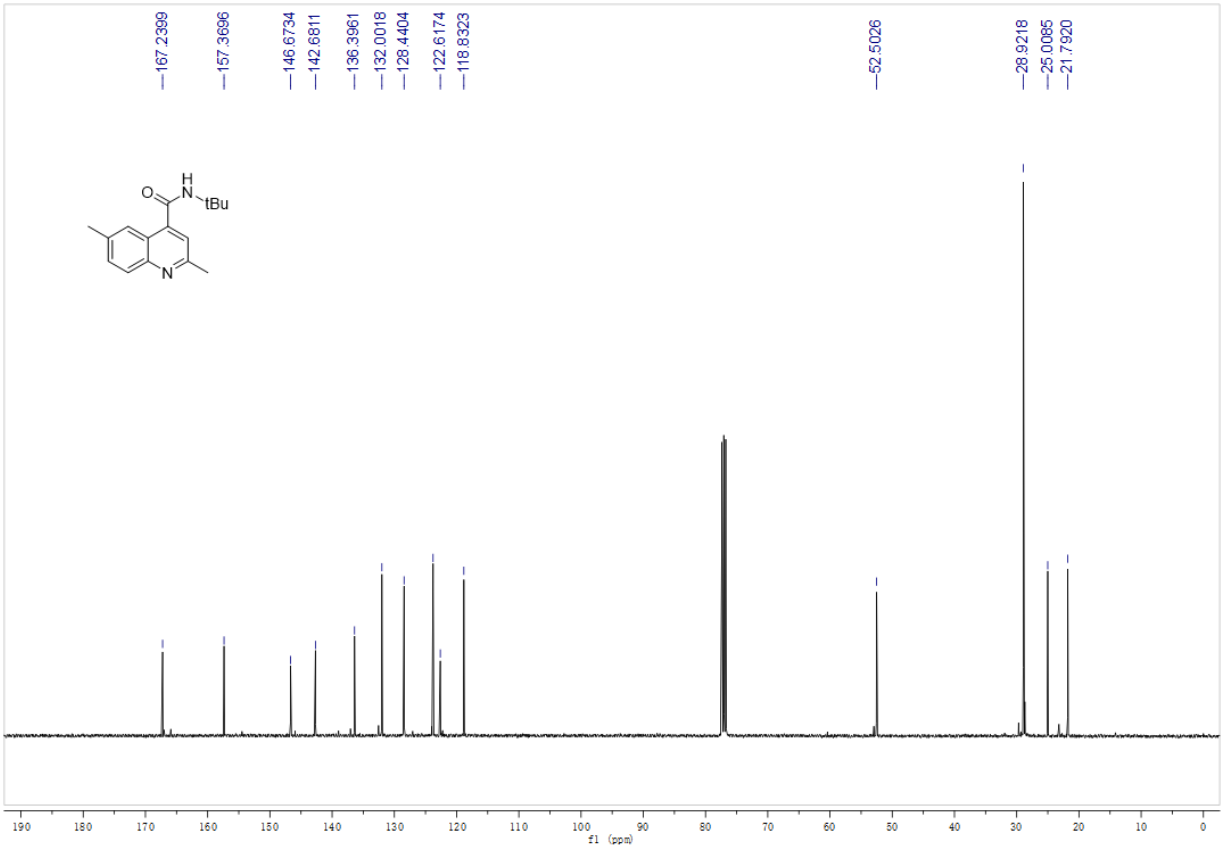
N-(*tert*-butyl)-2-methylquinoline-4-carboxamide (3p)



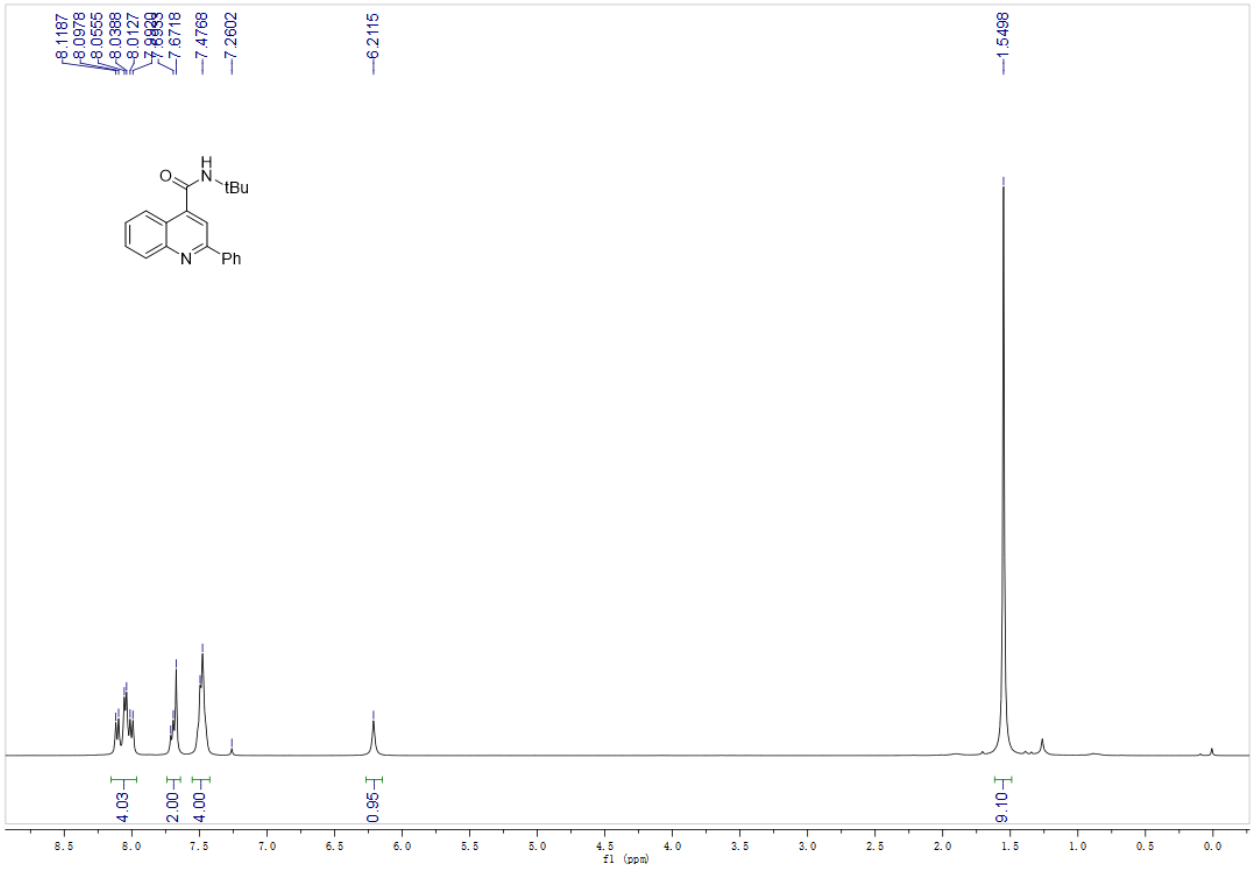


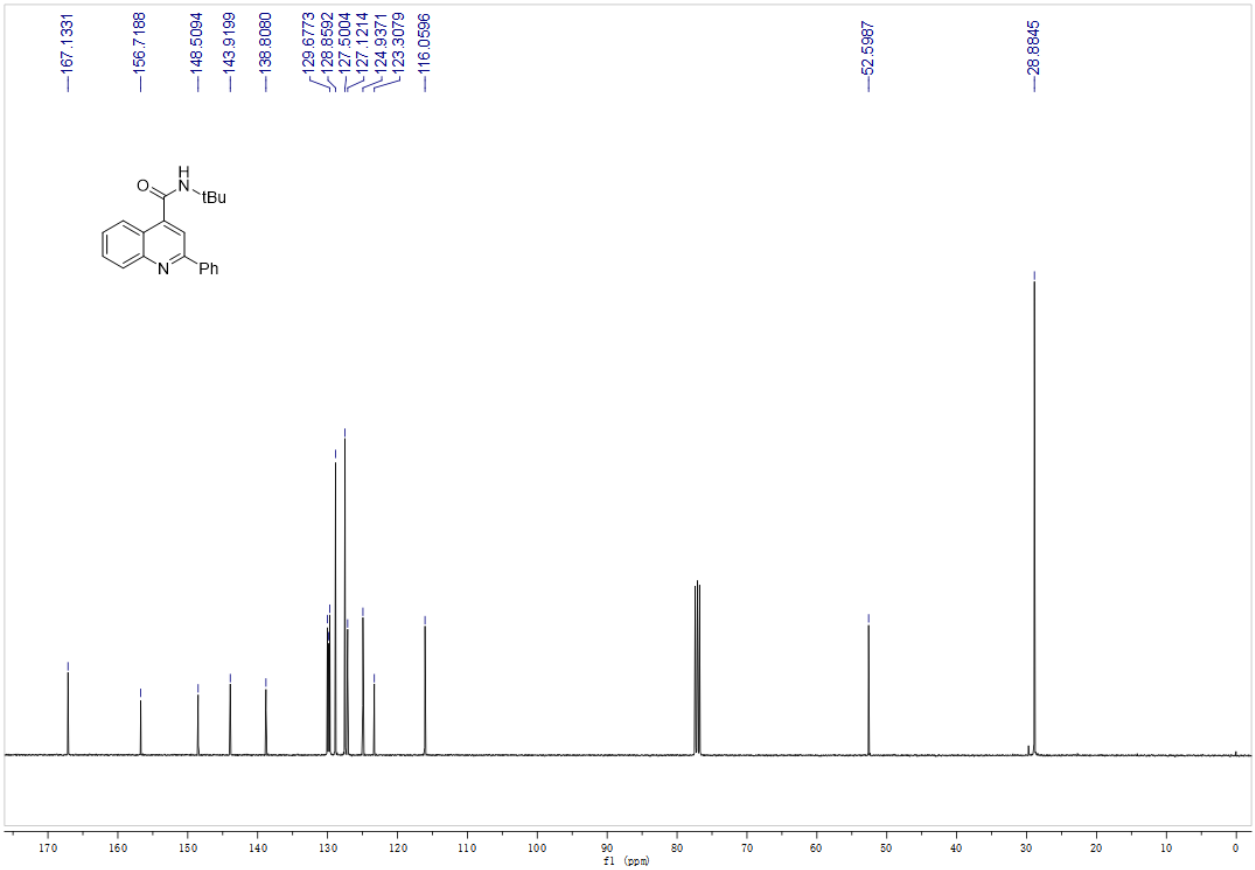
N-(*tert*-butyl)-2,6-dimethylquinoline-4-carboxamide (3q)



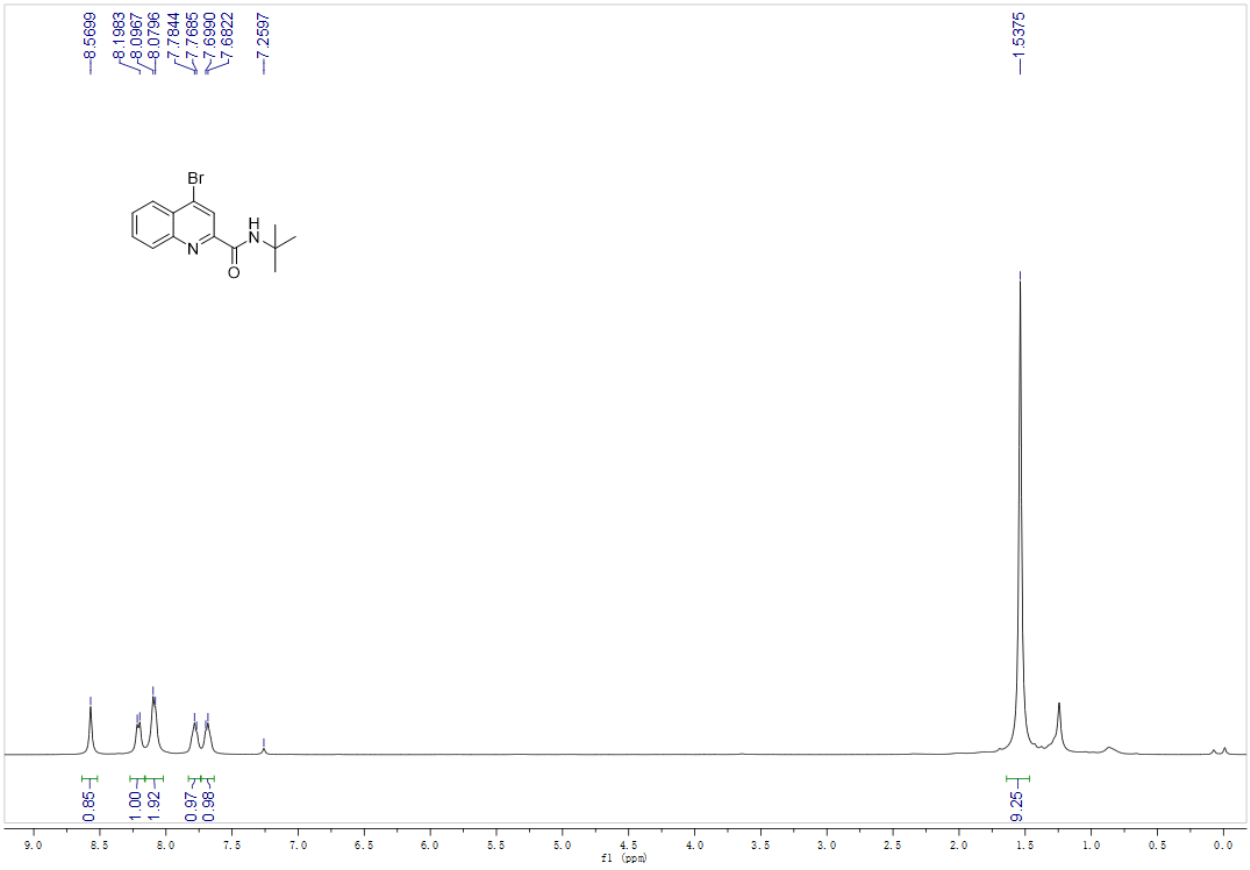


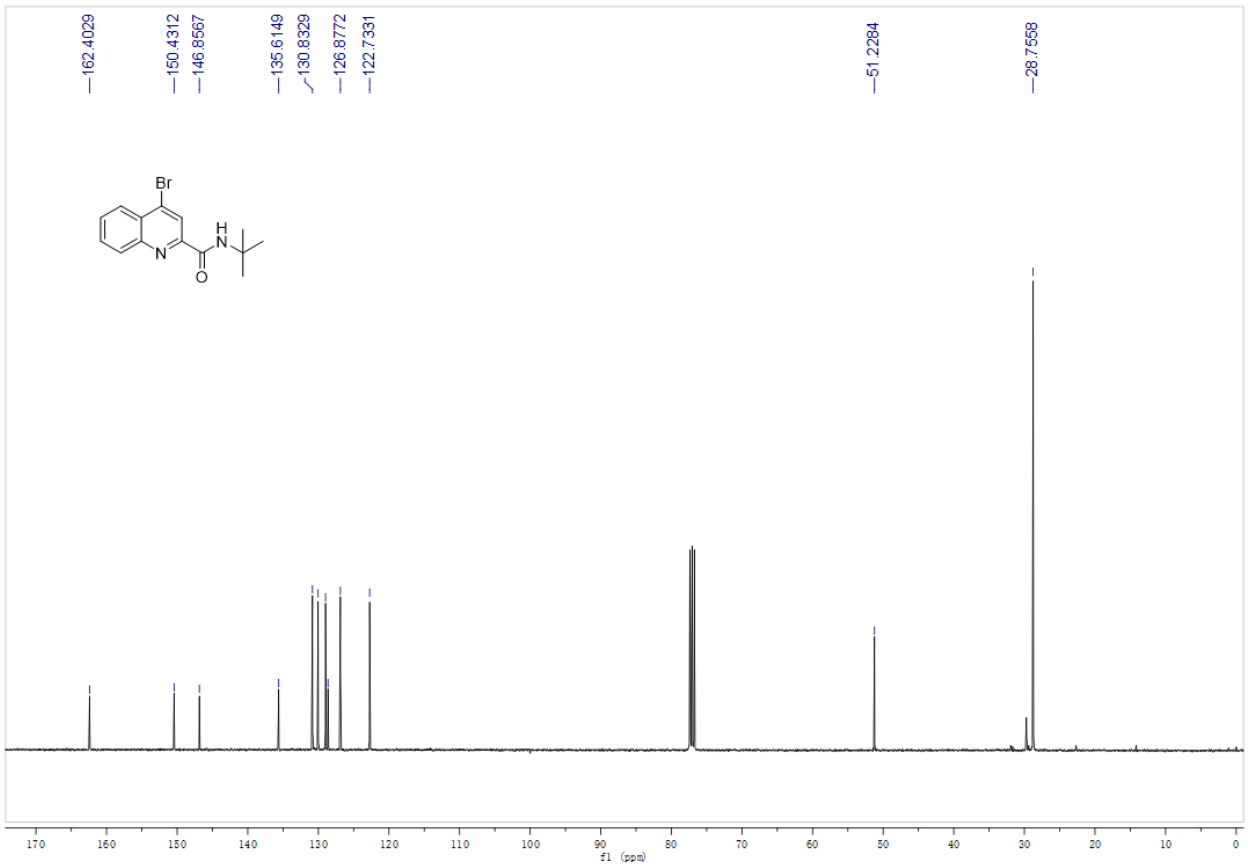
N-(*tert*-butyl)-2-phenylquinoline-4-carboxamide (3r)



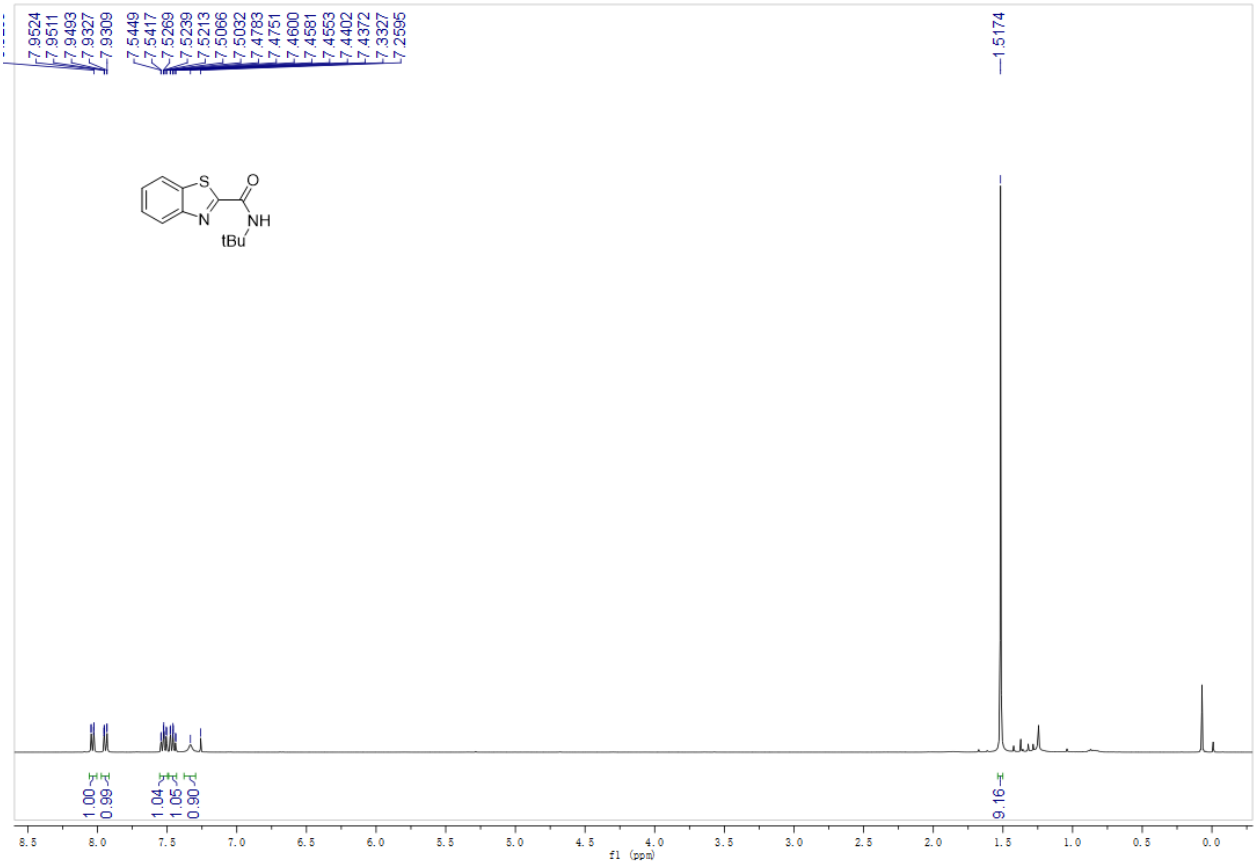


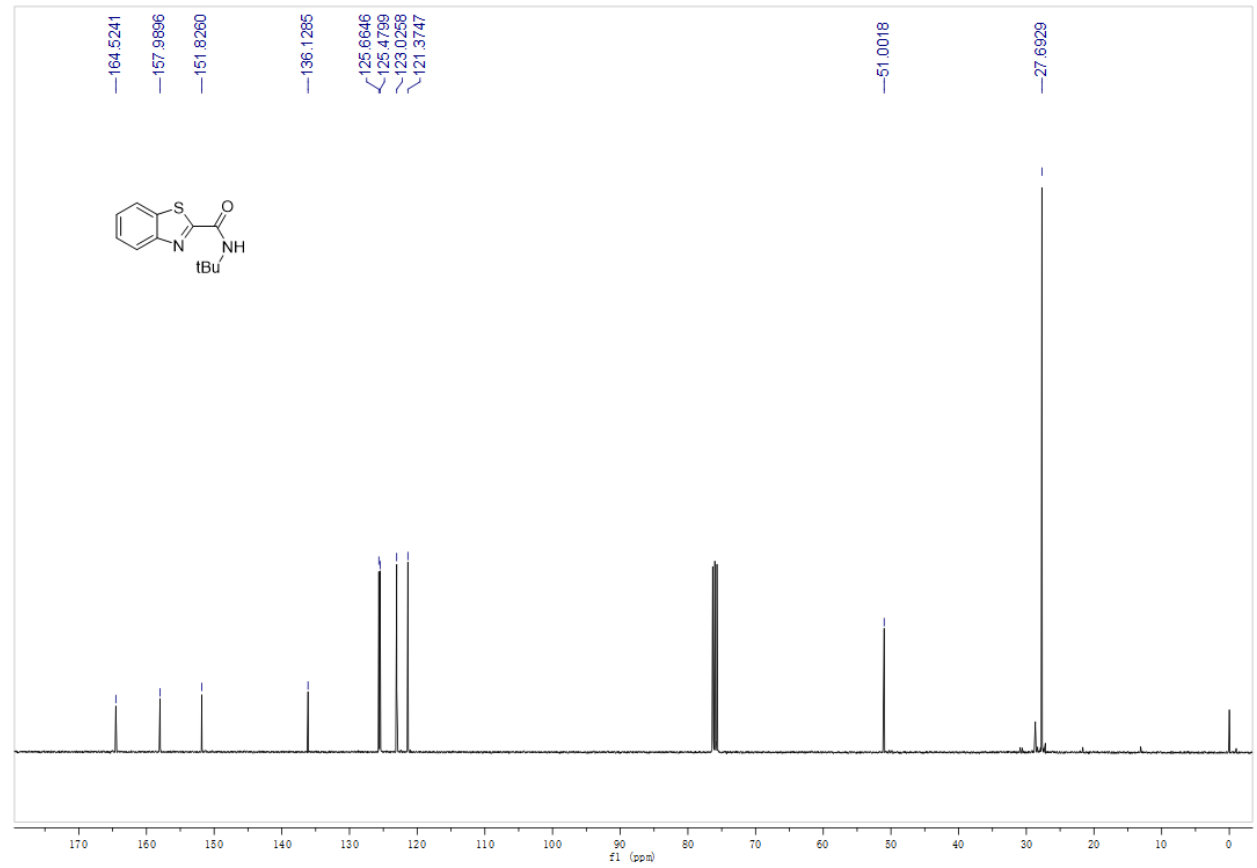
4-bromo-*N*-(*tert*-butyl)quinoline-2-carboxamid (3s)



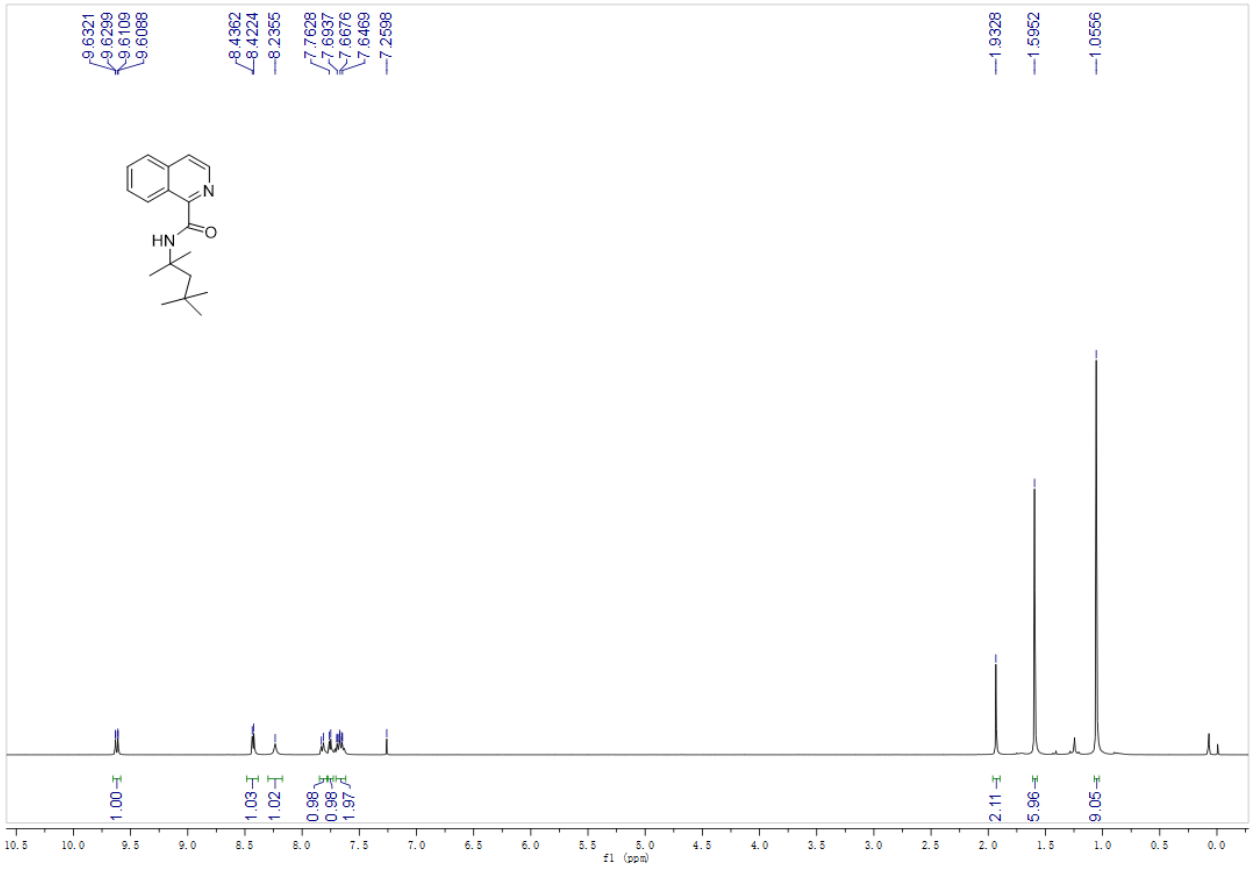


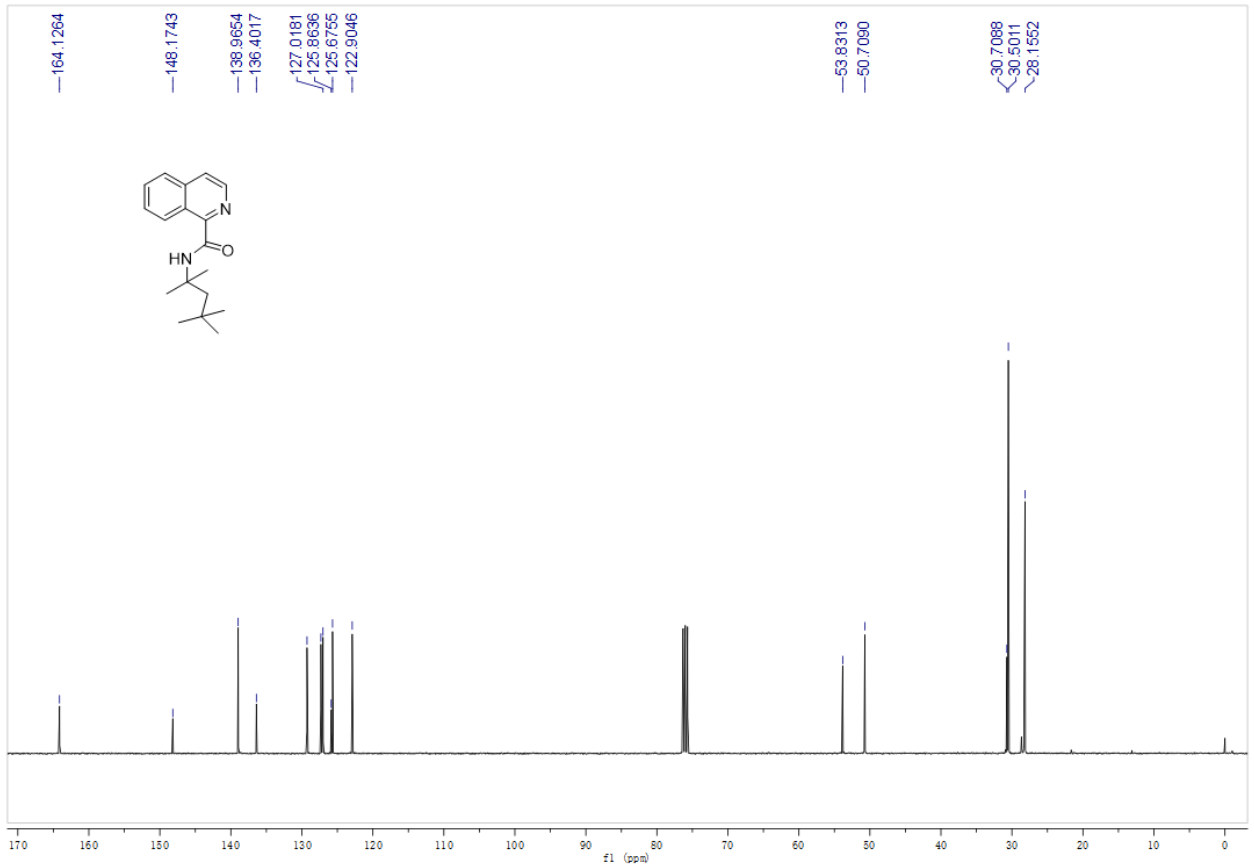
N-(*tert*-butyl)benzo[d]thiazole-2-carboxamide (3t)



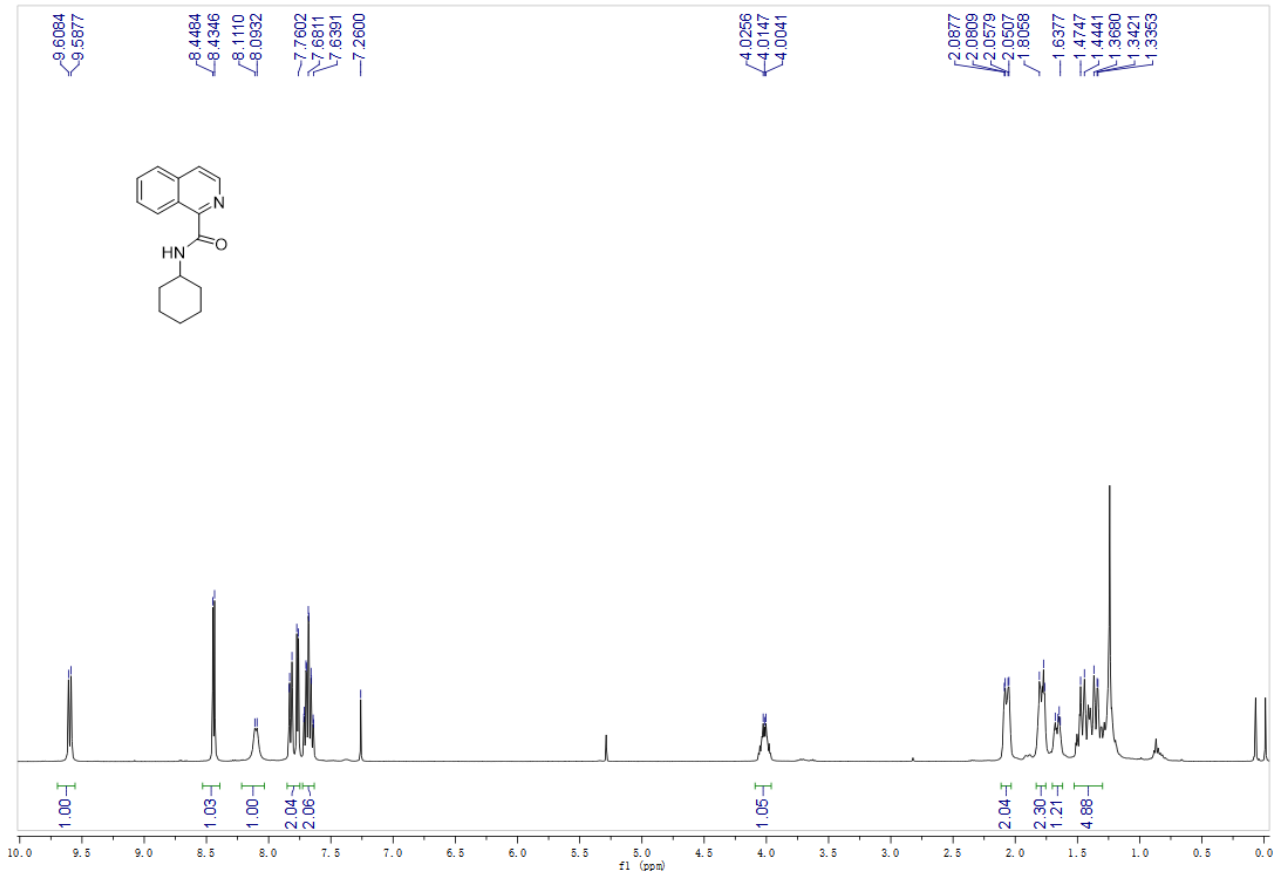


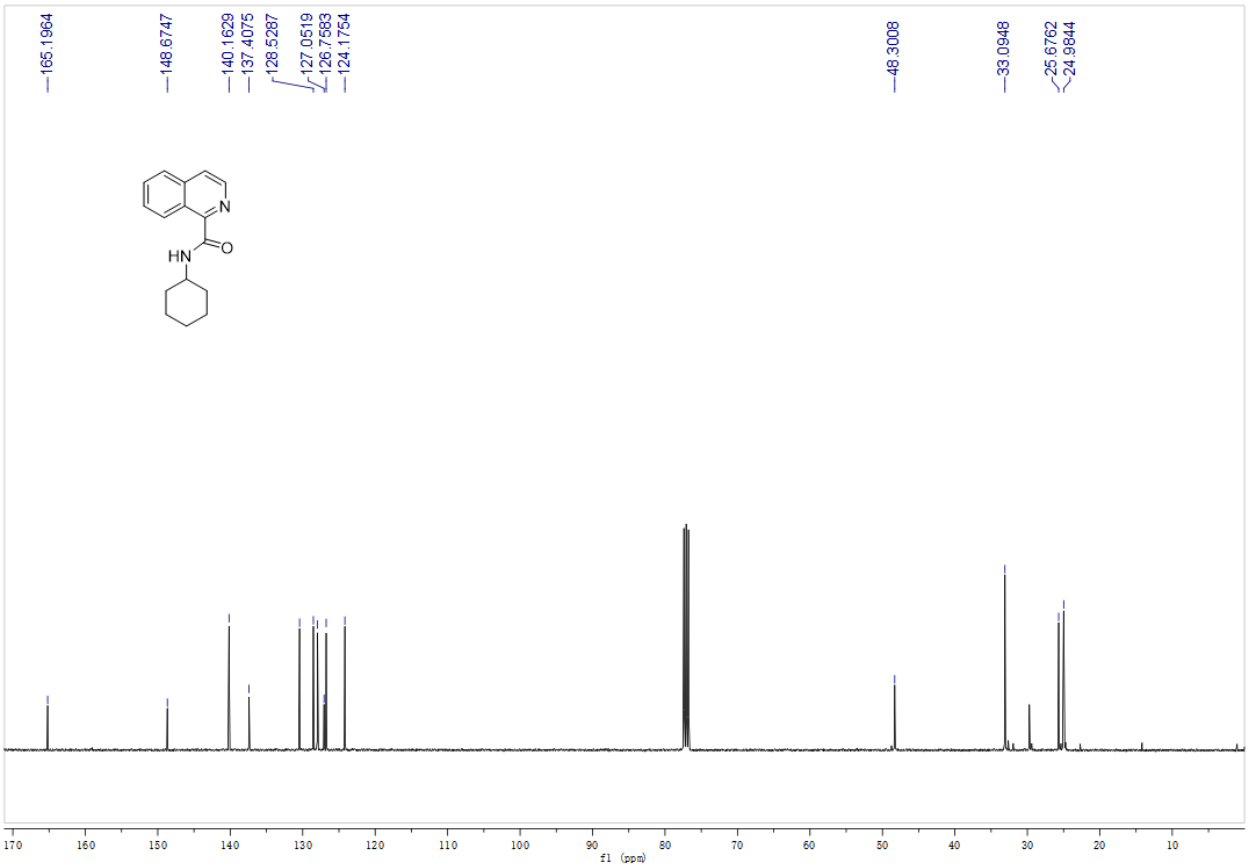
N-(2,4,4-trimethylpenta*N*-2-yl)isoquinoline-1-carboxamide (4a)



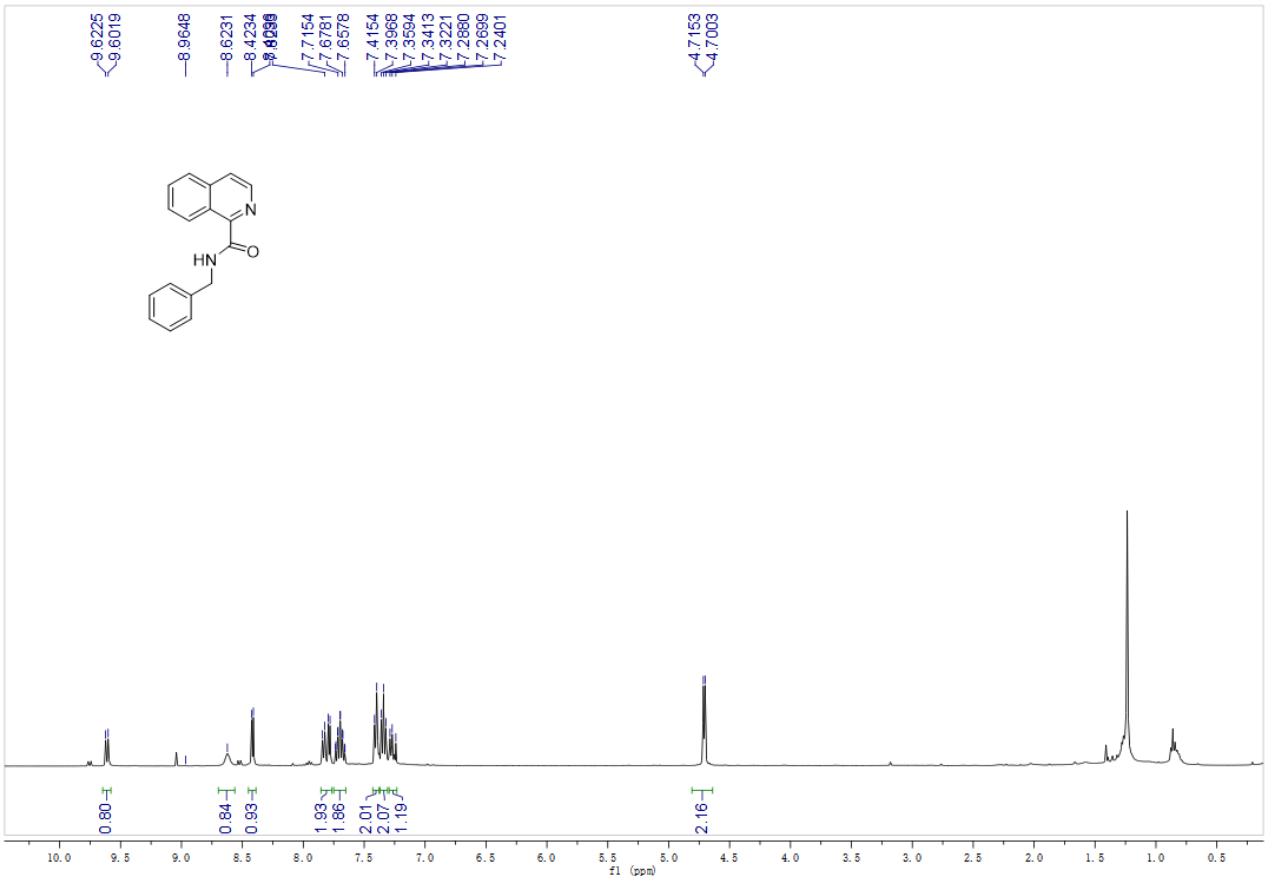


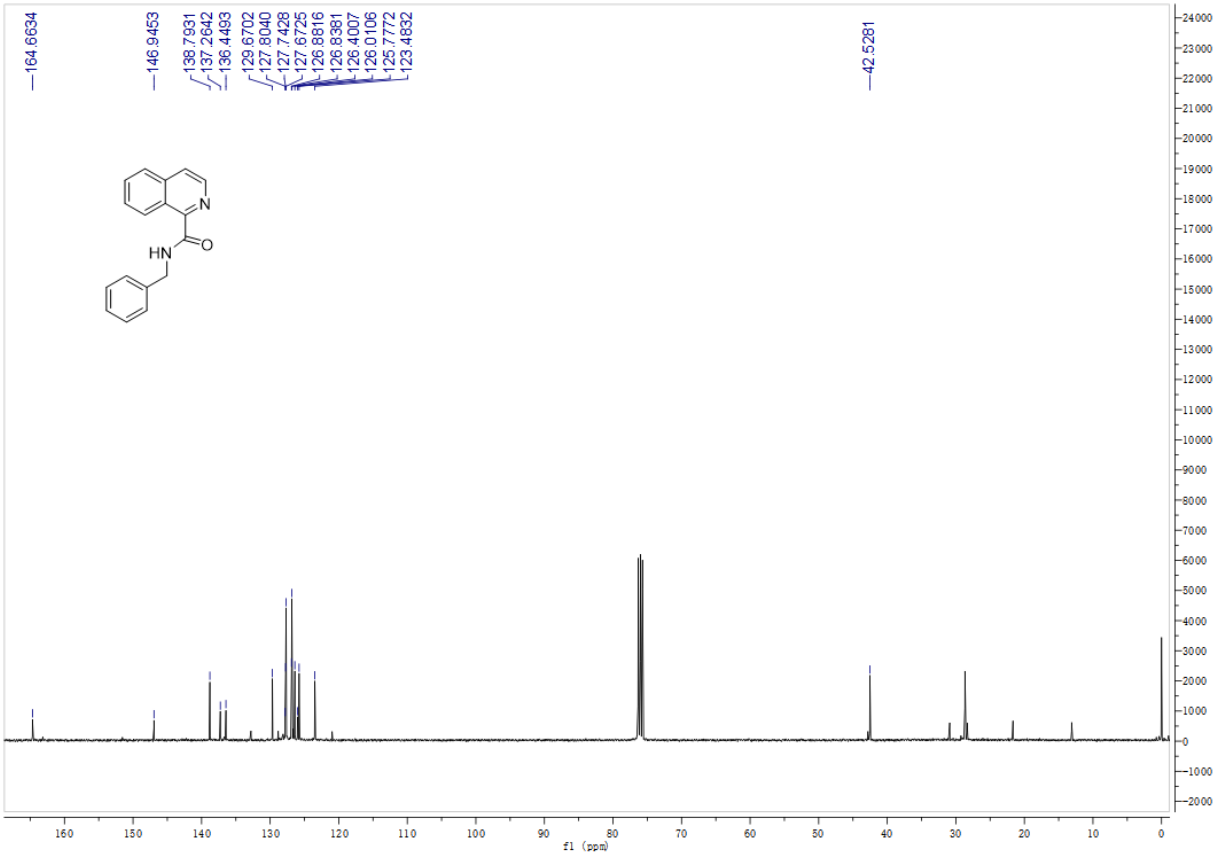
N-cyclohexylisoquinoline-1-carboxamide (4b)



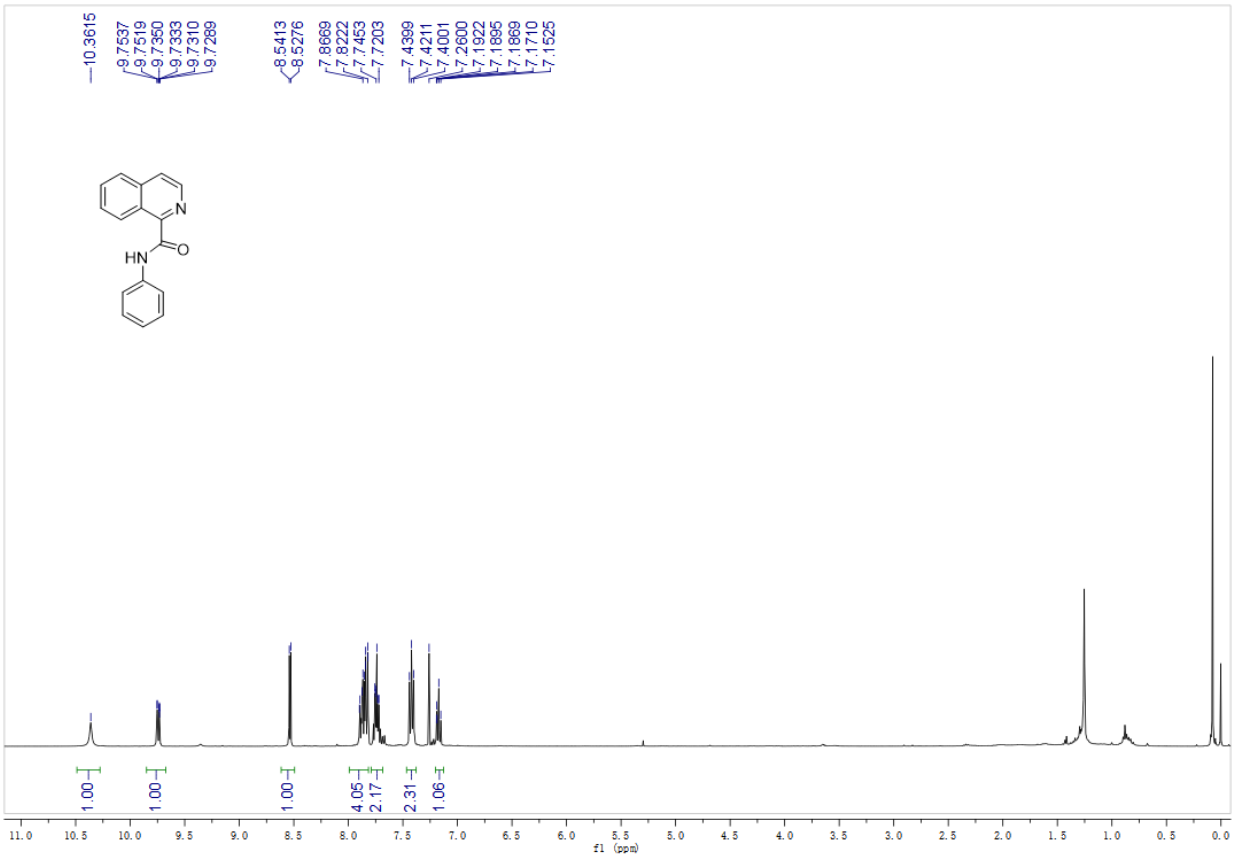


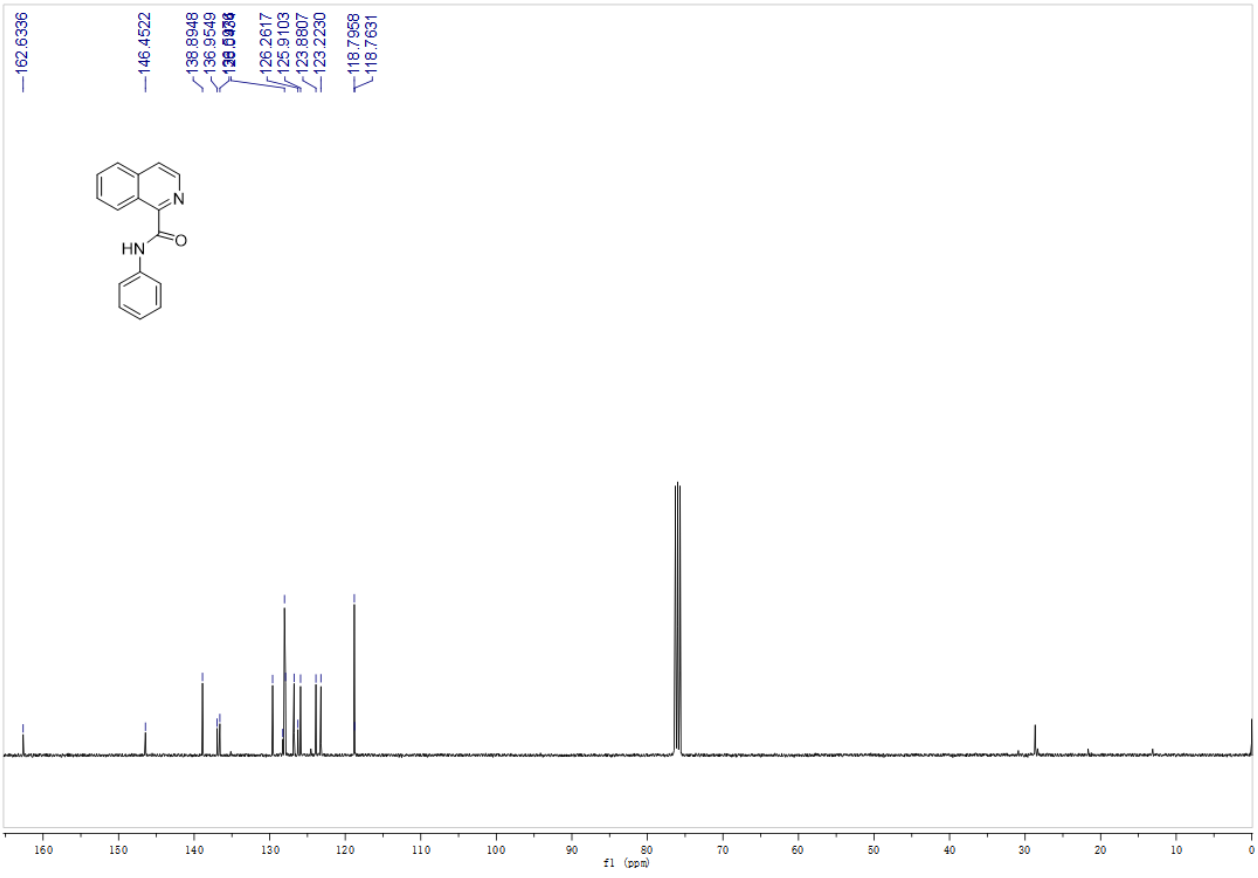
N-benzylisoquinoline-1-carboxamide (4c)



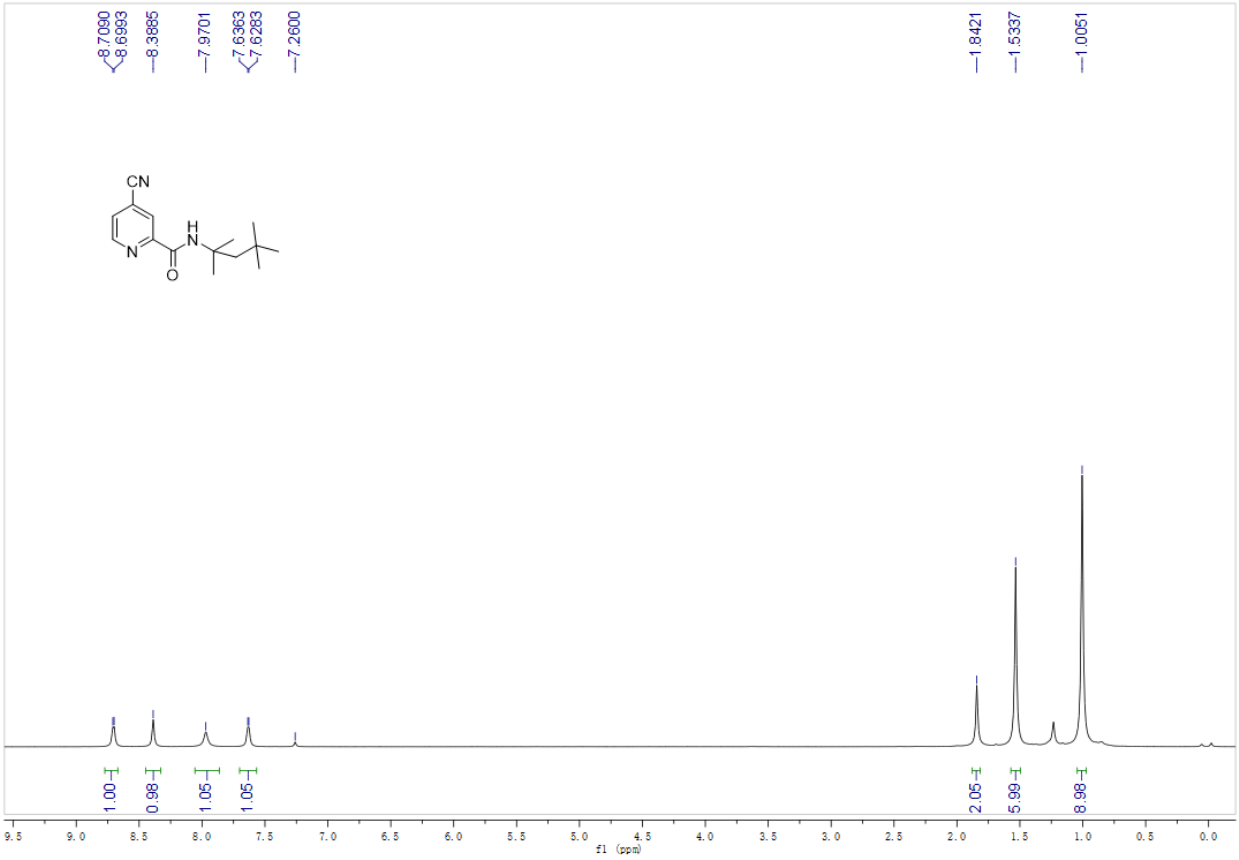


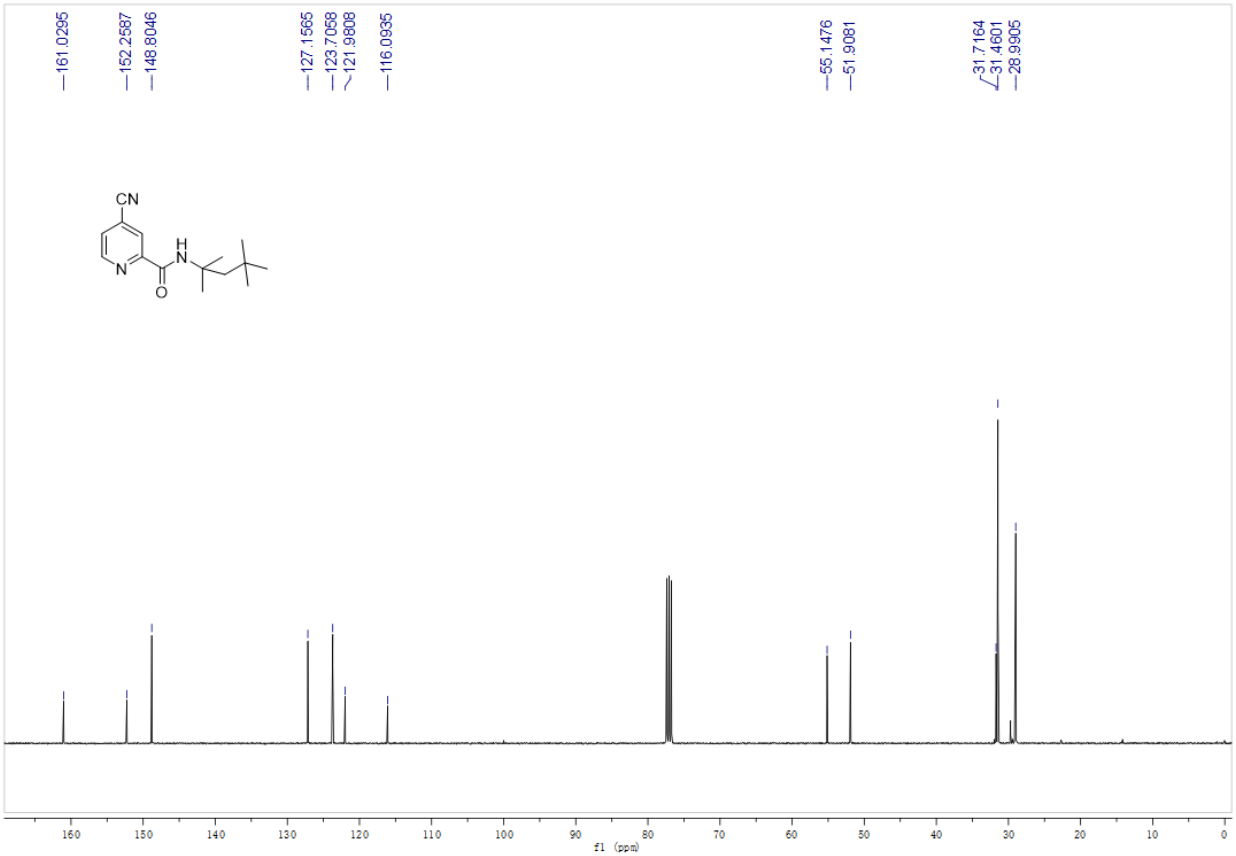
N-phenylisoquinoline-1-carboxamide (4d)



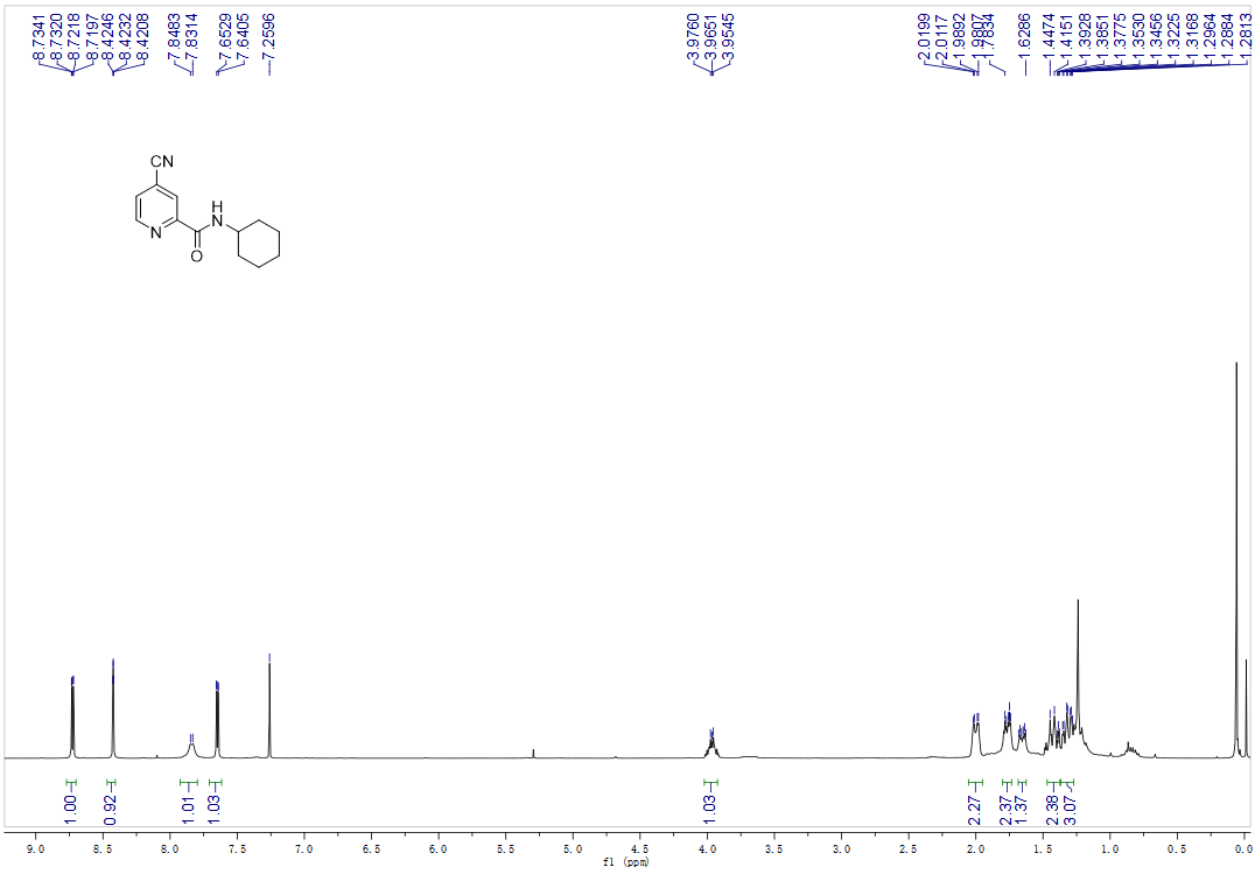


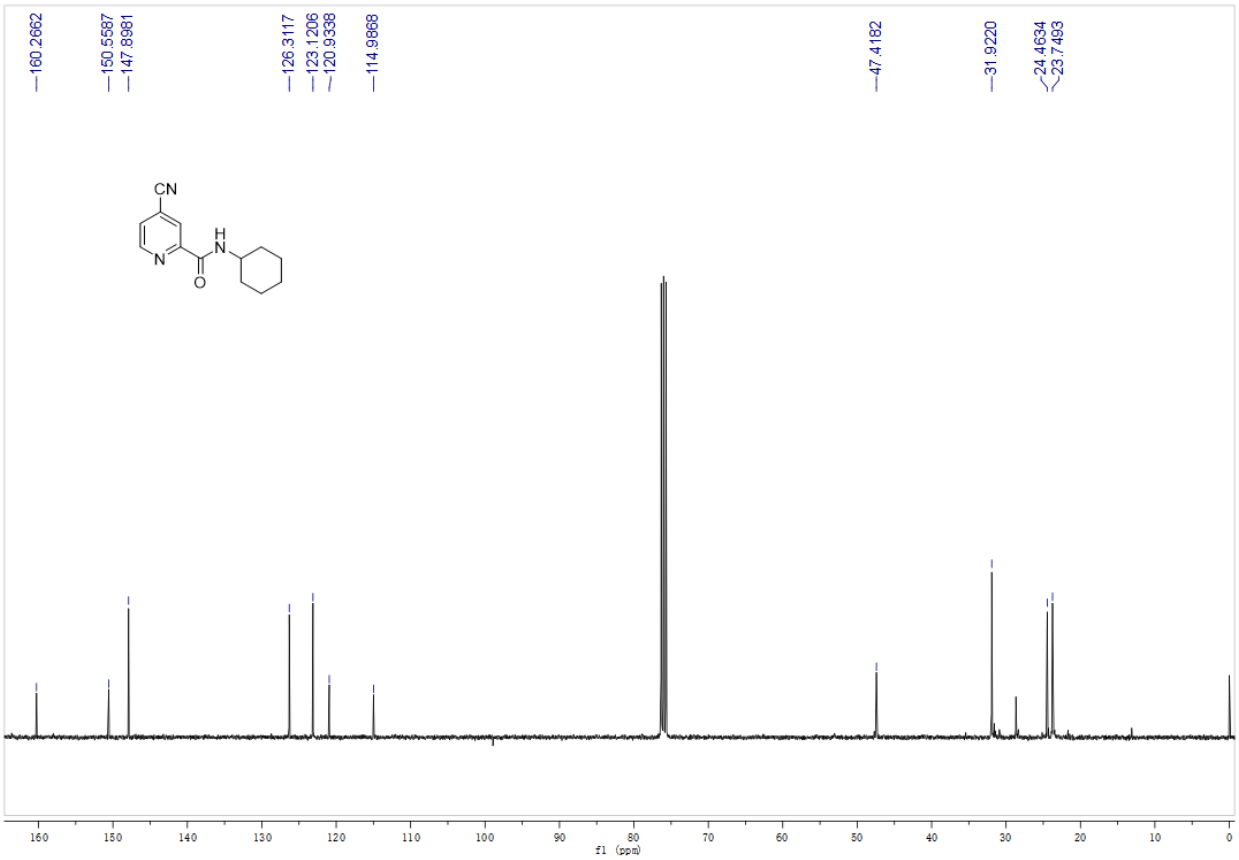
4-cyano-*N*-(2,4,4-trimethylpenta*N*-2-yl)picolinamide (5a)





4-cyano-*N*-cyclohexylpicolinamide (5b)





ethyl (4-cyanopicolinoyl)glycinate (5c)