Supporting Information

Electrochemical Synthesis of 2-Substituted Quinazolin-4(3*H*)-one from Primary Benzylic C(sp^3)–H and 2-Aminobenzamides

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1. General information

Experimental Details

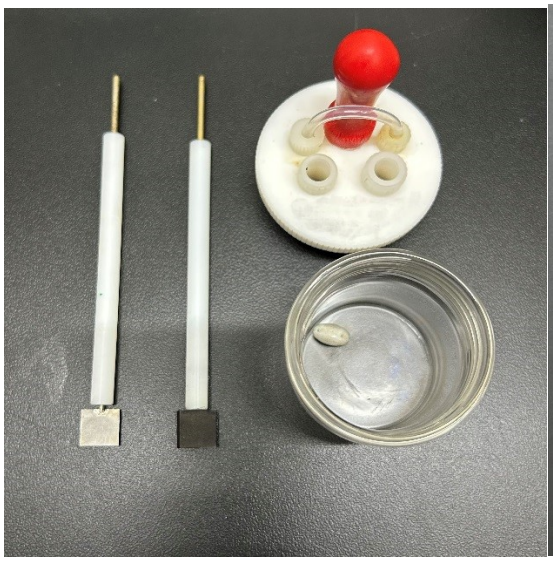
Unless otherwise noted, materials were obtained from commercial suppliers and used without further purification. The instrument for electrolysis is dual display potentiostat (DJS-292B) (made in China). The anodic electrode was graphite plate (10 mm×10mm×0.3 mm) and cathodic electrode was Pt plate (10 mm×10mm×0.3 mm). Thin layer chromatography (TLC) employed glass 0.25 mm silica gel plates. Flash chromatography columns were packed with 300-400 mesh silica gel in petroleum (boiling point is between 60-90 ℃). Gradient flash chromatography was conducted eluting with a continuous gradient from petroleum to the indicated solvent, and they are listed as volume/volume ratios.

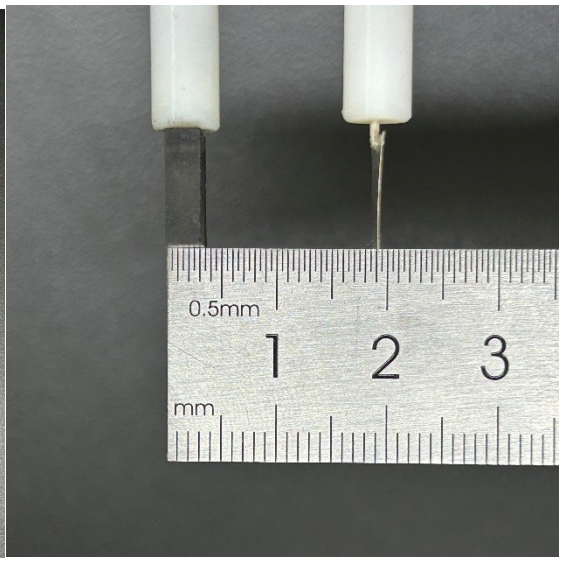
Analysis

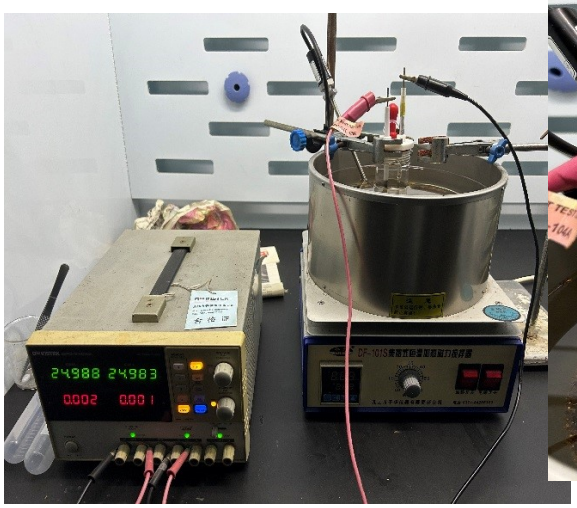
NMR samples were submitted in DMSO-d6 or $CDCl_3$ purchased from Sigma Aldrich and spectra were recorded on Brucker Advance 300 spectrometers. Chemical shifts are reported in parts per million (ppm). Coupling constants (J) are quoted in Hz. Multiplicities are reported as s (singlet), d (doublet), t (triplet), q (quartet), hept (heptet), m (multiplet). High Resolution Mass Spectrometry HRMS spectra were obtained by the ESI model from an ab sciex 500R QTOF or micr OTOF-Q II instrument at the University of Lishui mass spectrometry facility. Accurate masses are reported for the molecular ion + hydrogen ($[M+H]^+$).

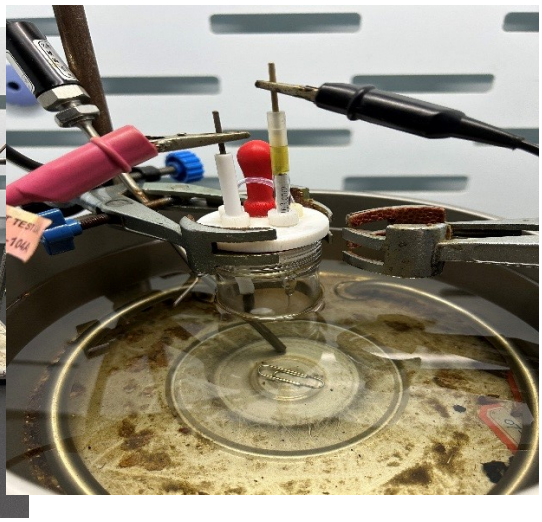
2. General procedures

In a 25 mL three-necked bottle equipped with a magnetic stir bar, graphite plate (10 mm×10mm×0.3 mm) was used as anode and Pt plate (10 mm×10mm×0.3 mm) was used as cathode. **1a** (0.6 mmol), **2a** (0.5 mmol), $LutH^+PF_6^-$ (0.25 mmol), TBAI (0.05 mmol), EtOH (10 mL), were added. The Electrolysis experiment was performed at 25 mA at 60 °C for 6 hours. When the reaction was finished, the reaction mixture was washed with water and extracted with ethyl acetate (10 mL x 3). The organic layers were combined, dried with Na_2SO_4, and concentrated. The pure product was obtained by flash column chromatography on silica gel.



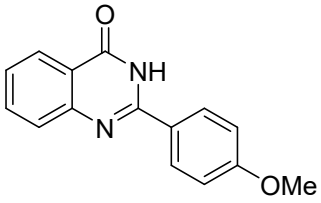






3.Detail descriptions for products

2-(4-methoxyphenyl)quinazolin-4(3*H*)-one (3a)[1]:

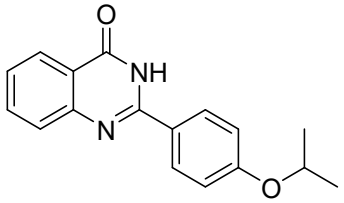


^{1}H NMR (300 MHz, DMSO) δ 12.45 (s, 1H), 8.21 (d, *J* = 8.4 Hz, 2H), 8.15 (d, *J* = 7.8 Hz, 1H), 7.82 (t, *J* = 7.3 Hz, 1H), 7.72 (d, *J* = 7.9 Hz, 1H), 7.50 (t, *J* = 7.2 Hz, 1H), 7.10 (d, *J* = 8.3 Hz, 2H), 3.86 (s, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 167.55, 167.08, 157.08, 154.17, 139.77, 134.69, 132.52, 131.35, 131.06, 130.01, 125.92, 119.21, 60.68.

HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{15}H_{12}N_2O_2$ 253.0977; Found 253.0971.

2-(4-isopropoxyphenyl)quinazolin-4(3*H*)-one (3b):

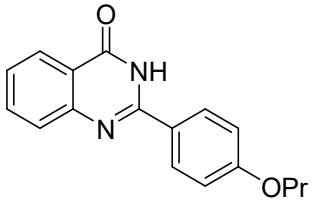


^{1}H NMR (300 MHz, DMSO) δ 12.41 (s, 1H), 8.17 (t, *J* = 9.2 Hz, 3H), 7.90 – 7.77 (m, 1H), 7.72 (d, *J* = 7.8 Hz, 1H), 7.50 (t, *J* = 7.4 Hz, 1H), 7.07 (d, *J* = 8.9 Hz, 2H), 4.77 (dt, *J* = 12.0, 6.0 Hz, 1H), 1.33 (s, 3H), 1.31 (s, 3H).

^{13}C NMR (75 MHz, DMSO) δ 162.78, 160.67, 152.38, 149.45, 135.03, 130.00, 127.76, 126.58, 126.31, 124.89, 121.16, 115.77, 70.00, 22.24.

HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{17}H_{16}N_2O_2$ 281.1290; Found 281.1284.

2-(4-propoxyphenyl)quinazolin-4(3*H*)-one (3c):

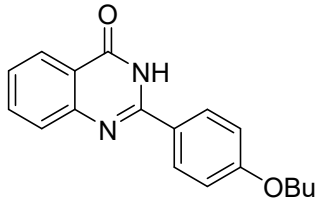


^{1}H NMR (300 MHz, DMSO) δ 8.31 – 8.05 (m, 3H), 7.83 (t, *J* = 7.5 Hz, 1H), 7.72 (d, *J* = 8.1 Hz, 1H), 7.50 (t, *J* = 7.4 Hz, 1H), 7.08 (d, *J* = 8.6 Hz, 2H), 4.03 (t, *J* = 6.5 Hz, 2H), 1.77 (dd, *J* = 14.0, 7.0 Hz, 2H), 1.00 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (75 MHz, DMSO) δ 162.86, 161.82, 152.44, 149.28, 135.05, 129.96, 127.62, 126.61, 126.32, 125.03, 121.11, 114.88, 69.70, 22.44, 10.83.

HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{17}H_{16}N_2O_2$ 281.1290; Found 281.1284.

2-(4-butoxyphenyl)quinazolin-4(3*H*)-one (3d):

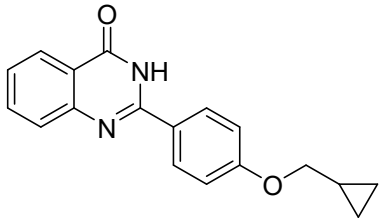


^{1}H NMR (300 MHz, DMSO) δ 12.44 (s, 1H), 8.17 (dd, *J* = 11.7, 8.5 Hz, 3H), 7.89 – 7.77 (m, 1H), 7.72 (d, *J* = 7.9 Hz, 1H), 7.50 (t, *J* = 7.4 Hz, 1H), 7.09 (d, *J* = 8.9 Hz, 2H), 4.07 (t, *J* = 6.5 Hz, 2H), 1.83 – 1.59 (m, 2H), 1.54 – 1.40 (m, 2H), 0.96 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (75 MHz, DMSO) δ 162.82, 161.82, 152.38, 149.40, 135.05, 129.94, 127.75, 126.62, 126.32, 125.07, 121.12, 114.90, 67.96, 31.12, 19.19, 14.18.

HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{18}H_{18}N_2O_2$ 295.1446; Found 295.1440.

2-(4-(cyclopropylmethoxy)phenyl)quinazolin-4(3*H*)-one (3e):



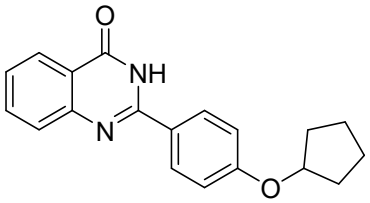
^{1}H NMR (300 MHz, DMSO) δ 12.41 (s, 1H), 8.19 (d, *J* = 8.8 Hz, 2H), 8.15 (d, *J* = 8.1 Hz, 1H), 7.83 (dd, *J* = 11.1, 4.1 Hz, 1H), 7.71 (d, *J* = 8.0 Hz, 1H), 7.49 (t, *J* = 7.4 Hz, 1H), 7.08 (d, *J* = 8.8

Hz, 2H), 3.98 (dd, *J* = 32.6, 6.8 Hz, 2H), 1.26 (ddd, *J* = 9.9, 7.8, 3.8 Hz, 1H), 0.75 – 0.48 (m, 2H), 0.36 (q, *J* = 4.6 Hz, 2H).

^{13}C NMR (75 MHz, DMSO) δ 162.78, 161.76, 152.35, 149.44, 135.01, 129.91, 127.76, 126.58, 126.30, 125.06, 121.17, 114.92, 79.66, 72.83, 10.53, 3.61.

HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{18}H_{16}N_2O_2$ 293.1290; Found 293.1282.

2-(4-(cyclopentyloxy)phenyl)quinazolin-4(3*H*)-one (3f):

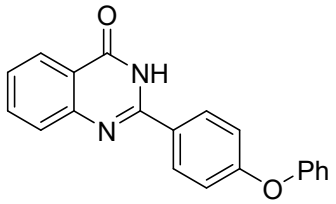


^{1}H NMR (300 MHz, DMSO) δ 12.41 (s, 1H), 8.16 (t, *J* = 8.6 Hz, 3H), 7.95 – 7.78 (m, 1H), 7.71 (d, *J* = 7.9 Hz, 1H), 7.50 (t, *J* = 7.4 Hz, 1H), 7.05 (d, *J* = 8.8 Hz, 2H), 4.94 (t, *J* = 5.7 Hz, 1H), 1.98 (dd, *J* = 12.2, 6.7 Hz, 2H), 1.86 – 1.46 (m, 6H).

^{13}C NMR (75 MHz, DMSO) δ 162.79, 160.83, 152.39, 149.46, 135.02, 129.93, 127.76, 126.57, 126.31, 124.87, 121.16, 115.73, 79.53, 32.76, 24.12.

HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{19}H_{18}N_2O_2$ 307.1446; Found 307.1438.

2-(4-phenoxyphenyl)quinazolin-4(3*H*)-one (3g):

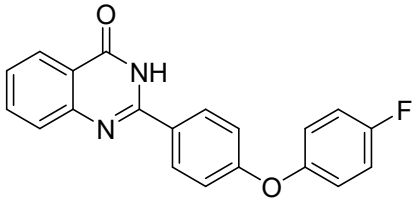


^{1}H NMR (300 MHz, DMSO) δ 12.54 (s, 1H), 8.24 (d, *J* = 8.8 Hz, 2H), 8.16 (d, *J* = 7.5 Hz, 1H), 7.85 (dd, *J* = 11.1, 4.1 Hz, 1H), 7.73 (d, *J* = 7.9 Hz, 1H), 7.58 – 7.42 (m, 3H), 7.26 (t, *J* = 7.4 Hz, 1H), 7.14 (t, *J* = 8.7 Hz, 4H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 167.50, 165.07, 160.63, 156.87, 154.04, 139.84, 135.55, 135.11, 132.62, 132.47, 131.63, 131.08, 129.74, 126.04, 124.98, 122.79.

HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{20}H_{14}N_2O_2$ 315.1133; Found 315.1127.

2-(4-(4-fluorophenoxy)phenyl)quinazolin-4(3*H*)-one (3h):



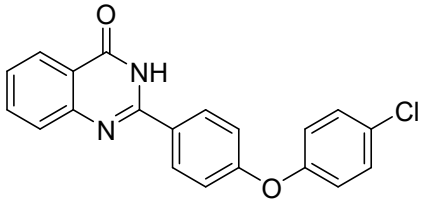
^{1}H NMR (300 MHz, DMSO) δ 12.54 (s, 1H), 8.23 (d, *J* = 8.8 Hz, 2H), 8.16 (d, *J* = 7.6 Hz, 1H), 7.84 (t, *J* = 7.1 Hz, 1H), 7.73 (d, *J* = 8.0 Hz, 1H), 7.52 (t, *J* = 7.3 Hz, 1H), 7.32 (t, *J* = 8.7 Hz, 2H), 7.21 (dd, *J* = 9.0, 4.6 Hz, 2H), 7.10 (d, *J* = 8.8 Hz, 2H).

^{13}C NMR (75 MHz, DMSO) δ 162.76, 160.89, 160.65, 157.70, 151.95 (d, *J* = 21.1 Hz), 149.28, 135.09, 130.37, 127.76 (d, *J* = 16.5 Hz), 126.88, 126.33, 122.35 (d, *J* = 8.3 Hz), 121.28, 117.61, 117.53, 117.22.

^{19}F NMR (565 MHz, DMSO) δ -118.48.

HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{20}H_{13}FN_2O_2$ 333.1039; Found 333.1032.

2-(4-(4-chlorophenoxy)phenyl)quinazolin-4(3*H*)-one (3i):

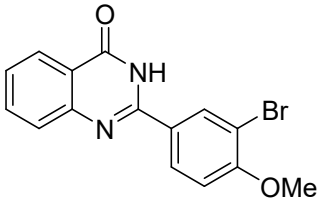


^{1}H NMR (300 MHz, DMSO) δ 12.55 (s, 1H), 8.25 (d, *J* = 8.7 Hz, 2H), 8.16 (d, *J* = 7.8 Hz, 1H), 7.84 (t, *J* = 7.6 Hz, 1H), 7.73 (d, *J* = 8.1 Hz, 1H), 7.60 – 7.43 (m, 3H), 7.16 (dd, *J* = 8.3, 5.4 Hz, 4H).

^{13}C NMR (75 MHz, DMSO) δ 162.74, 159.85, 154.91, 152.04, 149.26, 135.09, 130.64, 130.43, 128.75, 128.15, 127.89, 126.92, 126.33, 121.88, 121.31, 118.32.

HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{20}H_{13}ClN_2O_2$ 349.0744; Found 349.0736.

2-(3-bromo-4-methoxyphenyl)quinazolin-4(3*H*)-one (3j):

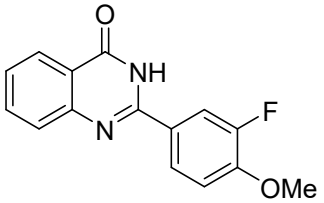


^{1}H NMR (300 MHz, DMSO) δ 12.53 (s, 1H), 8.49 (s, 1H), 8.26 (d, *J* = 8.6 Hz, 1H), 8.15 (d, *J* = 7.6 Hz, 1H), 7.83 (d, *J* = 6.9 Hz, 1H), 7.75 (d, *J* = 7.7 Hz, 1H), 7.52 (t, *J* = 7.0 Hz, 1H), 7.30 (d, *J* = 8.9 Hz, 1H), 3.97 (s, 3H).

^{13}C NMR (75 MHz, DMSO) δ 162.68, 158.32, 151.08, 149.16, 135.12, 132.71, 129.20, 127.89, 126.94, 126.56, 126.33, 121.30, 112.88, 111.30, 57.14.

HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{15}H_{11}BrN_2O_2$ 331.0082; Found 331.0076.

2-(3-fluoro-4-methoxyphenyl)quinazolin-4(3*H*)-one (3k):



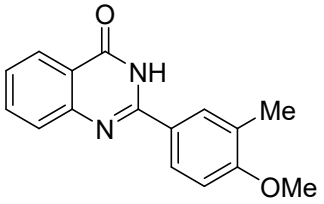
^{1}H NMR (300 MHz, DMSO) δ 12.51 (s, 1H), 8.13 (dd, *J* = 15.7, 9.4 Hz, 3H), 7.85 (t, *J* = 7.1 Hz, 1H), 7.74 (d, *J* = 8.0 Hz, 1H), 7.52 (t, *J* = 7.2 Hz, 1H), 7.36 (t, *J* = 8.6 Hz, 1H), 3.96 (s, 3H).

^{13}C NMR (75 MHz, DMSO) δ 162.70, 153.20, 151.27, 150.33 (d, *J* = 10.5 Hz), 149.14, 135.14, 127.88, 126.96, 126.34, 125.60 (d, *J* = 7.5 Hz), 125.21 (d, *J* = 3.0 Hz), 121.28, 115.56 (d, *J* = 18.7 Hz), 114.06, 56.75.

^{19}F NMR (565 MHz, DMSO) δ -114.13.

HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{15}H_{11}FN_2O_2$ 271.0883; Found 271.0877.

2-(3-methyl-4-methoxyphenyl)quinazolin-4(3*H*)-one (3l):



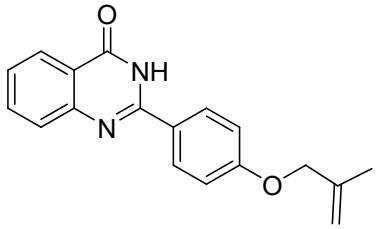
^{1}H NMR (300 MHz, DMSO) δ 12.36 (s, 1H), 8.15-8.08 (m, 3H), 7.82 (t, *J* = 7.2 Hz, 1H), 7.72 (d,

J = 7.8 Hz, 1H), 7.49 (t, *J* = 7.2 Hz, 1H), 7.09 (d, *J* = 8.4 Hz, 1H), 3.89 (s, 3H), 2.24 (s, 3H).

^{13}C NMR (75 MHz, DMSO) δ 162.79, 160.52, 152.46, 149.47, 135.03, 130.33, 127.73, 127.61, 126.55, 126.32, 124.70, 121.14, 110.60, 56.10, 16.59.

HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{16}H_{14}N_2O_2$ 267.1133; Found 267.1127.

2-(4-((2-methylallyl)oxy)phenyl)quinazolin-4(3*H*)-one (3m):

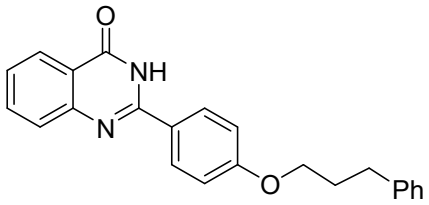


^{1}H NMR (300 MHz, DMSO) δ 12.44 (s, 1H), 8.27 – 8.09 (m, 3H), 7.89 – 7.77 (m, 1H), 7.72 (d, *J* = 7.8 Hz, 1H), 7.58 – 7.43 (m, 1H), 7.11 (d, *J* = 8.9 Hz, 2H), 5.04 (d, *J* = 29.4 Hz, 2H), 4.58 (s, 2H), 1.80 (s, 3H).

^{13}C NMR (75 MHz, DMSO) δ 162.81, 161.36, 152.33, 149.40, 140.98, 135.01, 129.91, 127.76, 126.61, 126.31, 125.39, 121.15, 115.16, 112.97, 71.46, 49.09, 19.65.

HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{18}H_{16}N_2O_2$ 293.1290; Found 293.1284.

2-(4-(3-phenylpropoxy)phenyl)quinazolin-4(3*H*)-one (3n):

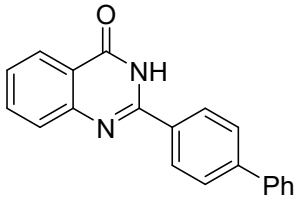


^{1}H NMR (300 MHz, DMSO) δ 12.45 (s, 1H), 8.21 – 8.14 (m, 3H), 7.83 (t, *J* = 7.2 Hz, 1H), 7.72 (d, *J* = 7.9 Hz, 1H), 7.50 (t, *J* = 7.2 Hz, 1H), 7.29 – 7.21 (m, 5H), 7.10 (d, *J* = 8.2 Hz, 2H), 4.08 (t, *J* = 5.4 Hz, 2H), 2.78 (t, *J* = 7.2 Hz, 2H), 2.07 (t, *J* = 6.1 Hz, 2H).

^{13}C NMR (75 MHz, DMSO) δ 162.80, 161.73, 152.36, 149.43, 141.78, 135.05, 129.98, 128.85, 127.77, 126.62, 126.37,126.32, 125.22, 121.17, 114.93, 79.66, 67.47, 31.89, 30.76.

HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{23}H_{20}N_2O_2$ 357.1603; Found 357.1597.

2-([1,1'-biphenyl]-4-yl)quinazolin-4(3*H*)-one (3o):

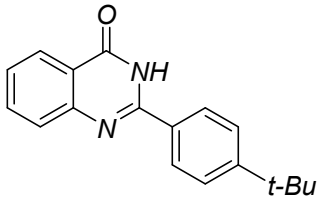


^{1}H NMR (300 MHz, DMSO) δ 12.62 (s, 1H), 8.32 (d, *J* = 7.2 Hz, 2H), 8.19 (d, *J* = 7.0 Hz, 1H), 7.88 (d, *J* = 7.0 Hz, 3H), 7.79 (s, 3H), 7.53 (s, 3H), 7.45 (d, *J* = 5.8 Hz, 1H).

^{13}C NMR (75 MHz, DMSO) δ 162.74, 152.41, 149.27, 143.33, 139.46, 135.11, 132.05, 129.56, 128.87, 128.67, 128.02, 127.34, 127.24, 127.07, 126.36, 121.50.

HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{20}H_{14}N_2O$ 299.1184; Found 299.1177.

2-(4-(tert-butyl)phenyl)quinazolin-4(3*H*)-one (3p):

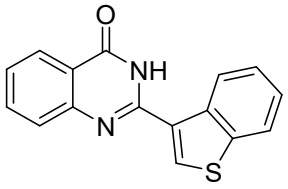


^{1}H NMR (300 MHz, $CDCl_3$) δ 11.22 (s, 1H), 8.34 (d, *J* = 7.9 Hz, 1H), 8.15 (d, *J* = 8.4 Hz, 2H), 7.83 (t, *J* = 7.3 Hz, 2H), 7.60 (d, *J* = 8.4 Hz, 2H), 7.51 (t, *J* = 7.2 Hz, 1H), 1.39 (s, 9H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 163.65, 155.36, 151.68, 149.59, 134.92, 129.90, 127.97, 127.06, 126.68, 126.43, 126.16, 120.83, 35.08, 31.21.

HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{18}H_{18}N_2O$ 279.1497; Found 279.1491.

2-(benzo[b]thiophen-3-yl)quinazolin-4(3*H*)-one (3q):

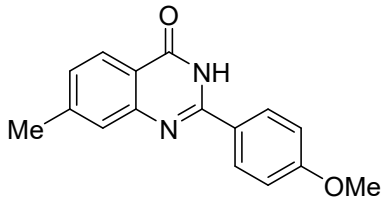


^{1}H NMR (300 MHz, DMSO) δ 12.58 (s, 1H), 9.04 (d, *J* = 7.7 Hz, 1H), 8.82 (s, 1H), 8.17 (dd, *J* = 19.3, 7.8 Hz, 2H), 7.89-7.85 (m, 2H), 7.58-7.49 (m, 3H).

^{13}C NMR (75 MHz, DMSO) δ 162.50, 149.22, 149.10, 140.19, 136.98, 135.16, 133.00, 128.57, 128.10, 127.24, 126.35, 125.95, 125.72, 125.66, 123.41, 121.67.

HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{16}H_{10}N_2OS$ 279.0592; Found 279.0586.

2-(4-methoxyphenyl)-7-methylquinazolin-4(3*H*)-one (4a):

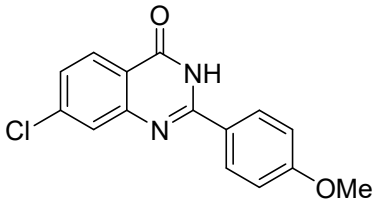


^{1}H NMR (300 MHz, $CDCl_3$) δ 11.64 (s, 1H), 8.21 (t, *J* = 8.8 Hz, 3H), 7.60 (s, 1H), 7.42 – 7.20 (m, 1H), 7.07 (d, *J* = 7.8 Hz, 2H), 3.91 (s, 3H), 2.53 (s, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 163.78, 162.42, 151.61, 149.73, 145.93, 129.10, 128.04, 127.45, 126.17, 125.12, 118.12, 114.38, 55.55, 22.06.

HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{16}H_{14}N_2O_2$ 267.1133; Found 267.1127.

7-chloro-2-(4-methoxyphenyl)quinazolin-4(3H)-one (4b)[2]:

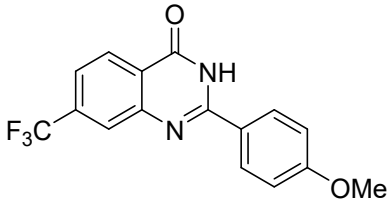


^{1}H NMR (300 MHz, DMSO) δ 12.56 (s, 1H), 8.20 (d, *J* = 8.5 Hz, 2H), 8.12 (d, *J* = 8.4 Hz, 1H), 7.75 (s, 1H), 7.51 (d, *J* = 8.2 Hz, 1H), 7.11 (d, *J* = 8.4 Hz, 2H), 3.87 (s, 3H).

^{13}C NMR (75 MHz, DMSO) δ 162.61, 162.23, 153.79, 150.57, 139.62, 130.16, 128.42, 126.82, 124.87, 119.98, 114.53, 55.98.

HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{15}H_{11}ClN_2O_2$ 287.0587; Found 287.0581.

2-(4-methoxyphenyl)-7-(trifluoromethyl)quinazolin-4(3*H*)-one (4c):



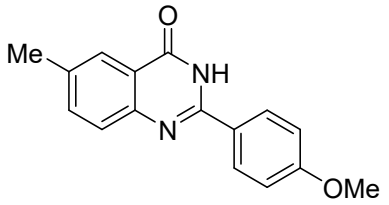
^{1}H NMR (300 MHz, DMSO) δ 12.44 (s, 1H), 8.18 (dd, *J* = 16.3, 7.9 Hz, 3H), 7.82 (t, *J* = 6.8 Hz, 1H), 7.71 (d, *J* = 7.6 Hz, 1H), 7.49 (t, *J* = 6.7 Hz, 1H), 7.10 (d, *J* = 8.0 Hz, 2H), 3.86 (s, 3H).

^{13}C NMR (75 MHz, DMSO) δ 162.82, 162.33, 152.34, 149.40, 134.99, 129.93, 127.75, 126.58, 126.31, 125.26, 121.15, 114.44, 55.91.

^{19}F NMR (565 MHz, DMSO) δ -61.74.

HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{16}H_{11}F_3N_2O_2$ 321.0851; Found 321.0845.

2-(4-methoxyphenyl)-6-methylquinazolin-4(3*H*)-one (4d):

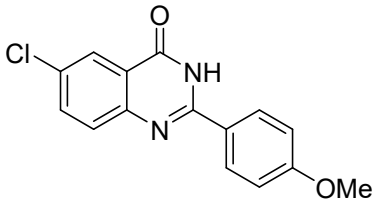


^{1}H NMR (300 MHz, DMSO) δ 12.37 (s, 1H), 8.19 (d, *J* = 7.8 Hz, 2H), 7.94 (s, 1H), 7.63 (s, 2H), 7.09 (d, *J* = 7.7 Hz, 2H), 3.86 (s, 3H), 2.46 (s, 3H).

^{13}C NMR (75 MHz, DMSO) δ 162.72, 162.20, 151.51, 147.42, 136.31, 136.26, 129.78, 127.65, 125.70, 125.36, 120.91, 114.45, 55.92, 21.31.

HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{16}H_{14}N_2O_2$ 267.1133; Found 267.1126.

6-chloro-2-(4-methoxyphenyl)quinazolin-4(3*H*)-one (4e):

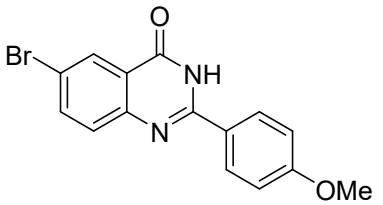


^{1}H NMR (300 MHz, DMSO) δ 12.57 (s, 1H), 8.19 (d, *J* = 8.7 Hz, 2H), 8.06 (d, *J* = 1.8 Hz, 1H), 7.83 (dd, *J* = 8.7, 2.1 Hz, 1H), 7.72 (d, *J* = 8.7 Hz, 1H), 7.09 (d, *J* = 8.7 Hz, 2H), 3.86 (s, 3H).

^{13}C NMR (75 MHz, DMSO) δ 162.51, 161.84, 152.83, 148.16, 135.10, 130.74, 130.05, 129.99, 125.31, 124.97, 122.38, 114.51, 55.96.

HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{15}H_{11}ClN_2O_2$ 287.0587; Found 287.0583.

6-bromo-2-(4-methoxyphenyl)quinazolin-4(3*H*)-one (4f):

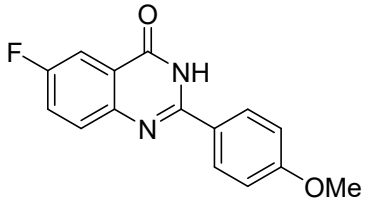


^{1}H NMR (300 MHz, DMSO) δ 12.61 (s, 1H), 8.21 (s, 1H), 8.19 (d, *J* = 7.4 Hz, 2H), 7.96 (dd, *J* = 8.7, 2.3 Hz, 1H), 7.66 (d, *J* = 8.7 Hz, 1H), 7.10 (d, *J* = 8.9 Hz, 2H), 3.86 (s, 3H).

^{13}C NMR (75 MHz, DMSO) δ 162.53, 161.77, 152.97, 137.83, 130.07, 128.44, 124.96, 122.75, 118.87, 114.52, 55.97.

HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{15}H_{11}BrN_2O_2$ 331.0082; Found 331.0076.

6-fluoro-2-(4-methoxyphenyl)quinazolin-4(3*H*)-one (4g):



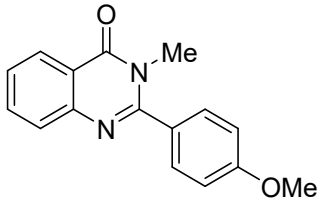
^{1}H NMR (300 MHz, DMSO) δ 12.56 (s, 1H), 8.18 (d, *J* = 8.8 Hz, 2H), 7.75 (dtd, *J* = 26.2, 8.7, 2.7 Hz, 3H), 7.09 (d, *J* = 8.8 Hz, 2H), 3.86 (s, 3H).

^{13}C NMR (75 MHz, DMSO) δ 162.30 (d, *J* = 8.8 Hz), 162.01 (d, *J* = 12.1 Hz), 158.59, 151.90, 146.31, 130.50 (d, *J* = 8.2 Hz), 129.91, 125.11, 123.45 (d, *J* = 18.2 Hz), 122.31 (d, *J* = 8.2 Hz), 114.49(d, *J* = 23.3 Hz), 110.90(d, *J* = 18.8 Hz), 55.95.

^{19}F NMR (565 MHz, DMSO) δ -113.94.

HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{15}H_{11}FN_2O_2$ 271.0883; Found 271.0876.

2-(4-methoxyphenyl)-3-methylquinazolin-4(3*H*)-one (4h):

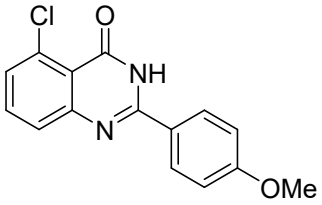


^{1}H NMR (300 MHz, DMSO) δ 8.18 (d, *J* = 7.9 Hz, 1H), 7.83 (t, *J* = 7.6 Hz, 1H), 7.67 (dd, *J* = 8.3, 3.7 Hz, 3H), 7.55 (t, *J* = 7.5 Hz, 1H), 7.10 (d, *J* = 8.6 Hz, 2H), 3.86 (s, 3H), 3.42 (s, 3H).

^{13}C NMR (75 MHz, DMSO) δ 162.33, 160.80, 156.50, 147.61, 134.76, 130.61, 128.14, 127.59, 127.12, 126.55, 120.43, 114.17, 55.82, 34.59.

HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{16}H_{14}N_2O_2$ 267.1133; Found 267.1128.

5-chloro-2-(4-methoxyphenyl)quinazolin-4(3*H*)-one (4i):

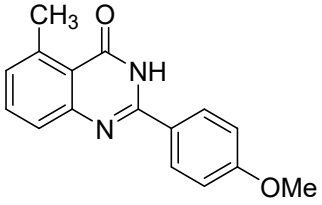


^{1}H NMR (300 MHz, DMSO) δ 12.44 (s, 1H), 8.20 (s, 2H), 7.73-7.66 (m, 2H), 7.50 (s, 1H), 7.11 (s, 2H), 3.87 (s, 3H).

^{13}C NMR (75 MHz, DMSO) δ 162.59, 160.95, 152.98, 151.96, 134.77, 132.94, 130.08, 128.92, 127.36, 124.62, 118.09, 114.51, 55.98.

HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{15}H_{11}ClN_2O_2$ 287.0587; Found 287.0582.

2-(4-methoxyphenyl)-5-methylquinazolin-4(3*H*)-one (4j):

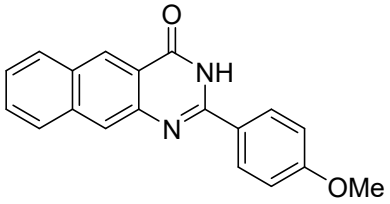


^{1}H NMR (300 MHz, DMSO) δ 12.43 (s, 1H), 8.25 (d, *J* = 8.9 Hz, 2H), 7.98 (d, *J* = 7.6 Hz, 1H), 7.68 (d, *J* = 7.1 Hz, 1H), 7.37 (t, *J* = 7.6 Hz, 1H), 7.11 (d, *J* = 8.9 Hz, 2H), 3.87 (s, 3H), 2.62 (s, 3H).

^{13}C NMR (75 MHz, DMSO) δ 163.11, 162.31, 151.09, 147.79, 135.80, 135.31, 129.89, 126.06, 125.56, 123.95, 121.04, 114.49, 55.94, 17.67.

HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{16}H_{14}N_2O_2$ 267.1133; Found 267.1129.

2-(4-methoxyphenyl)benzo[g]quinazolin-4(3*H*)-one (4k):



^{1}H NMR (300 MHz, DMSO) δ 12.27 (s, 1H), 8.85 (s, 1H), 8.49 – 7.94 (m, 5H), 7.61 (d, *J* = 26.4 Hz, 2H), 7.12 (s, 2H), 3.86 (s, 3H).

^{13}C NMR (75 MHz, DMSO) δ 163.28, 162.31, 151.31, 144.81, 136.91, 131.18, 129.88, 129.75, 128.91, 128.21, 127.71, 126.54, 125.47, 125.00, 120.46, 114.48, 55.93.

HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{19}H_{14}N_2O_2$ 303.1133; Found 303.1126.

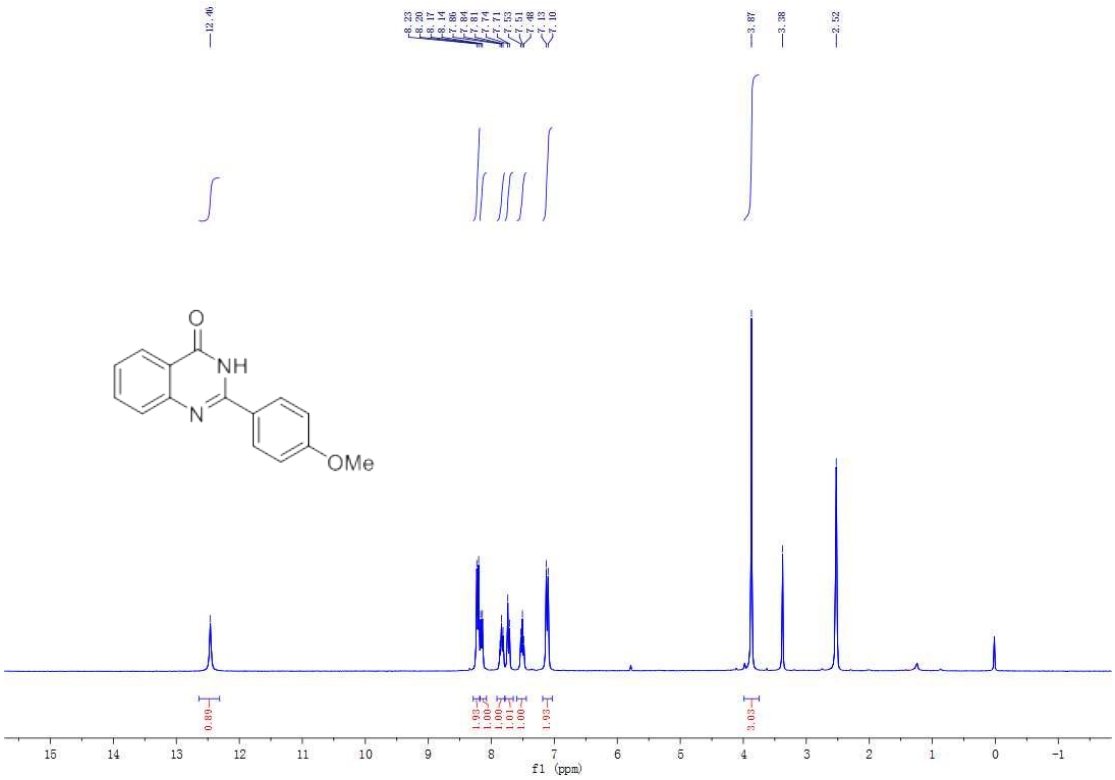
4. Reference

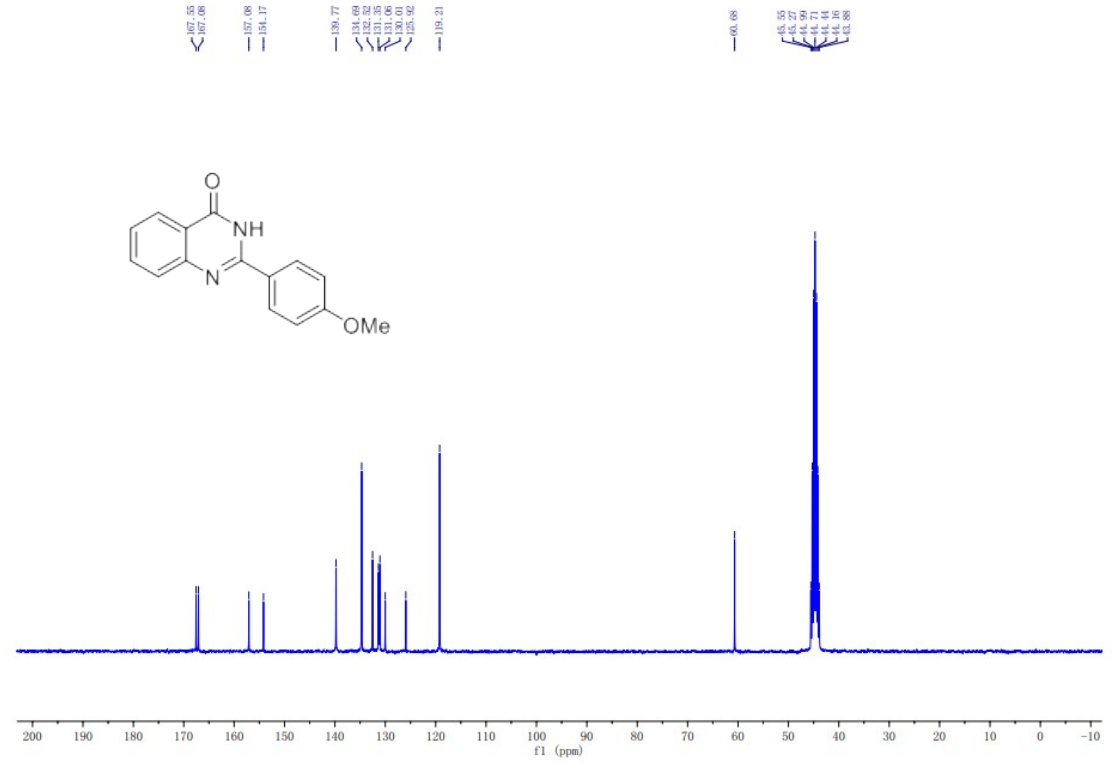
(1) Sharma, M.; Pandey, S.; Chauhan, K.; Sharma, D.; Kumar, B.; Chauhan, P. M. J. Org. Chem. 2012, 77, 929-937.

(2) Dutta, N.; Dutta, B.; Dutta, A.; Sarma, B. Sarma, D. *Org. Biomol. Chem.*, 2023, 21, 748-753.

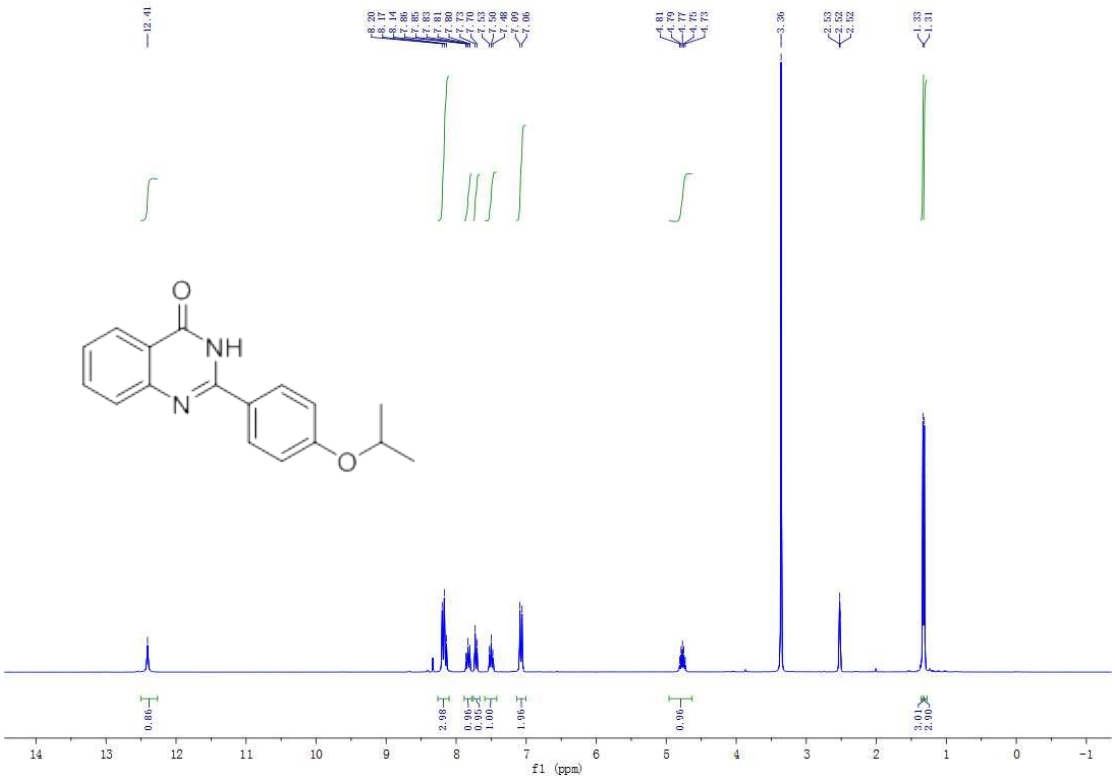
5. Copies of product NMR spectra

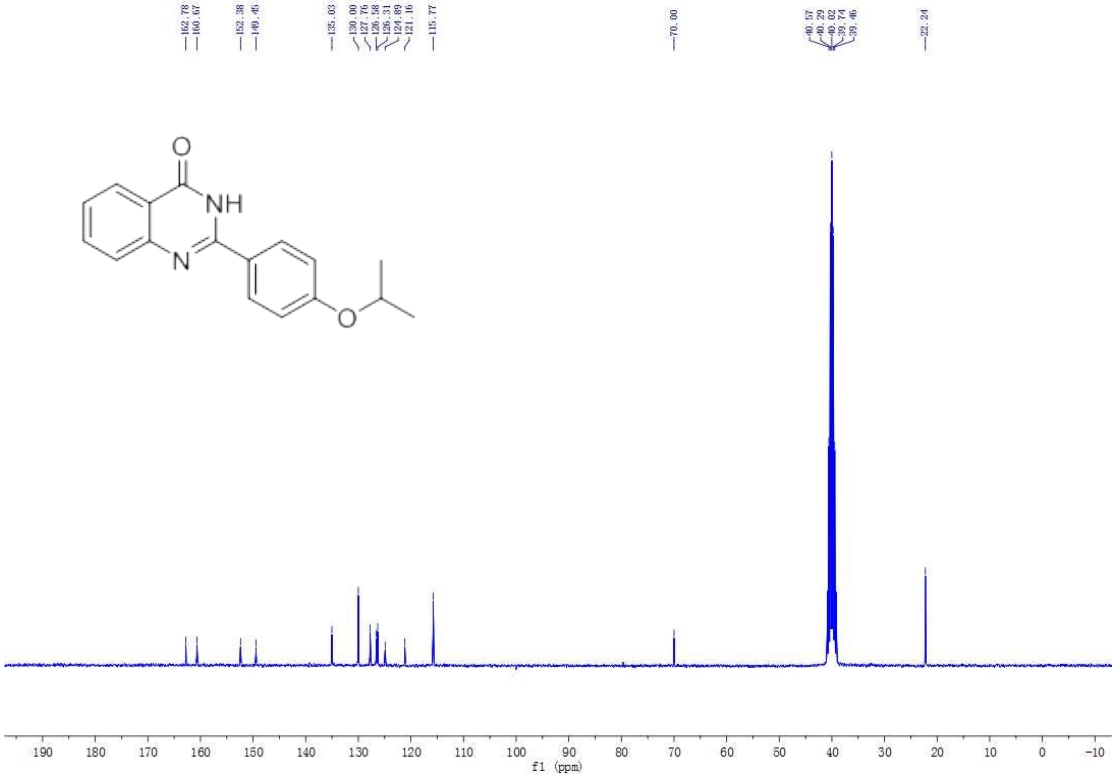
2-(4-methoxyphenyl)quinazolin-4(3*H*)-one (3a)



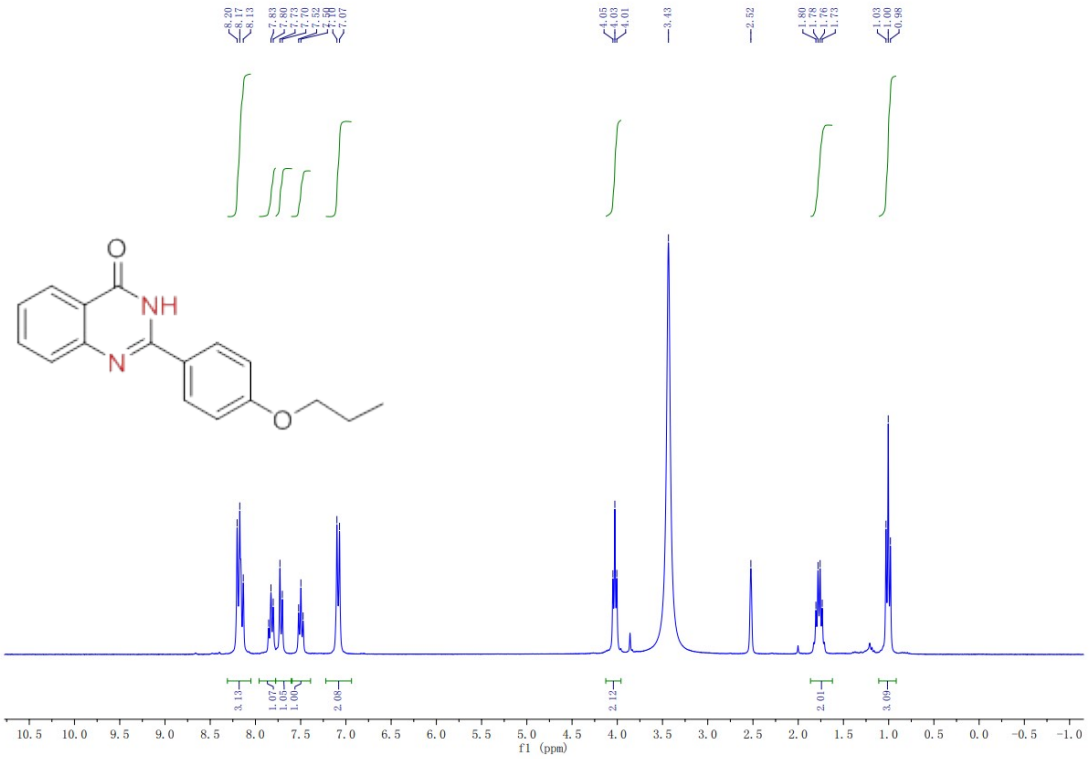


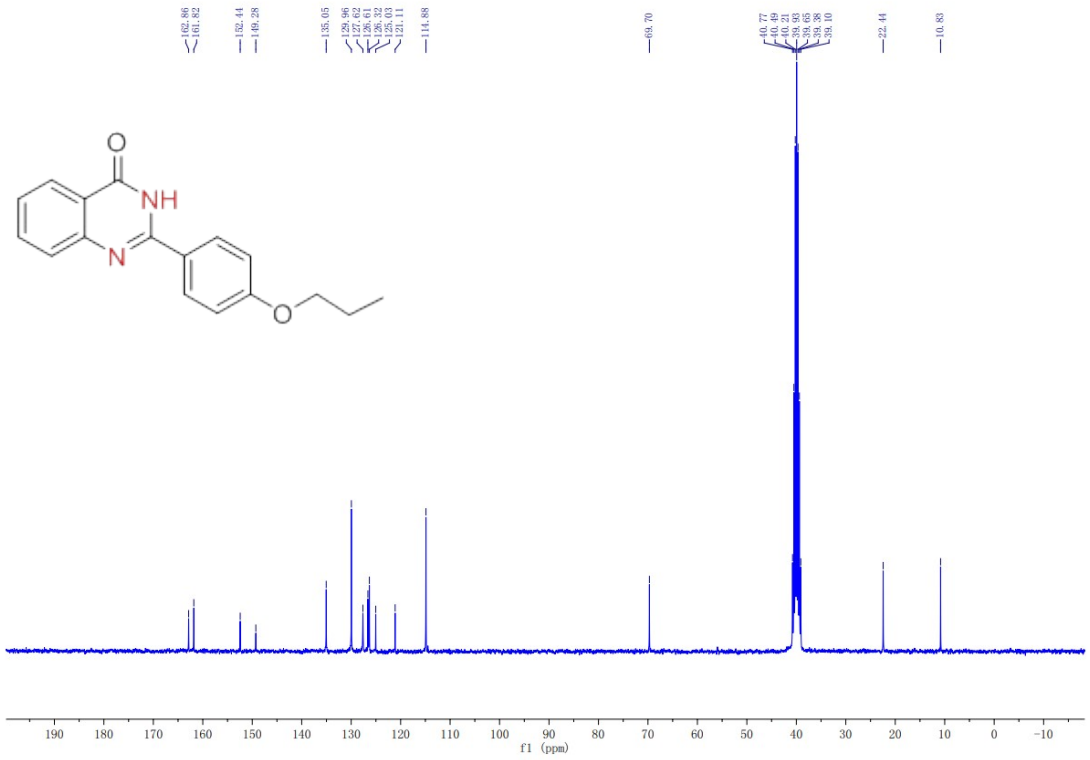
2-(4-isopropoxyphenyl)quinazolin-4(3*H*)-one (3b)



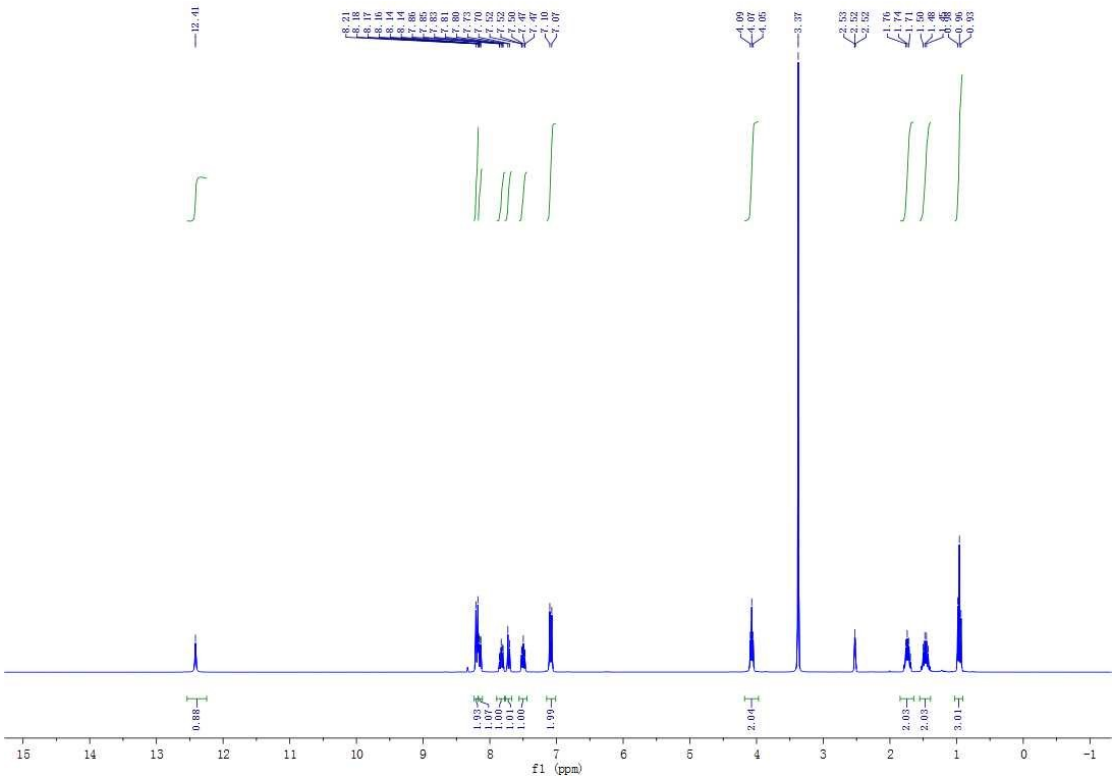


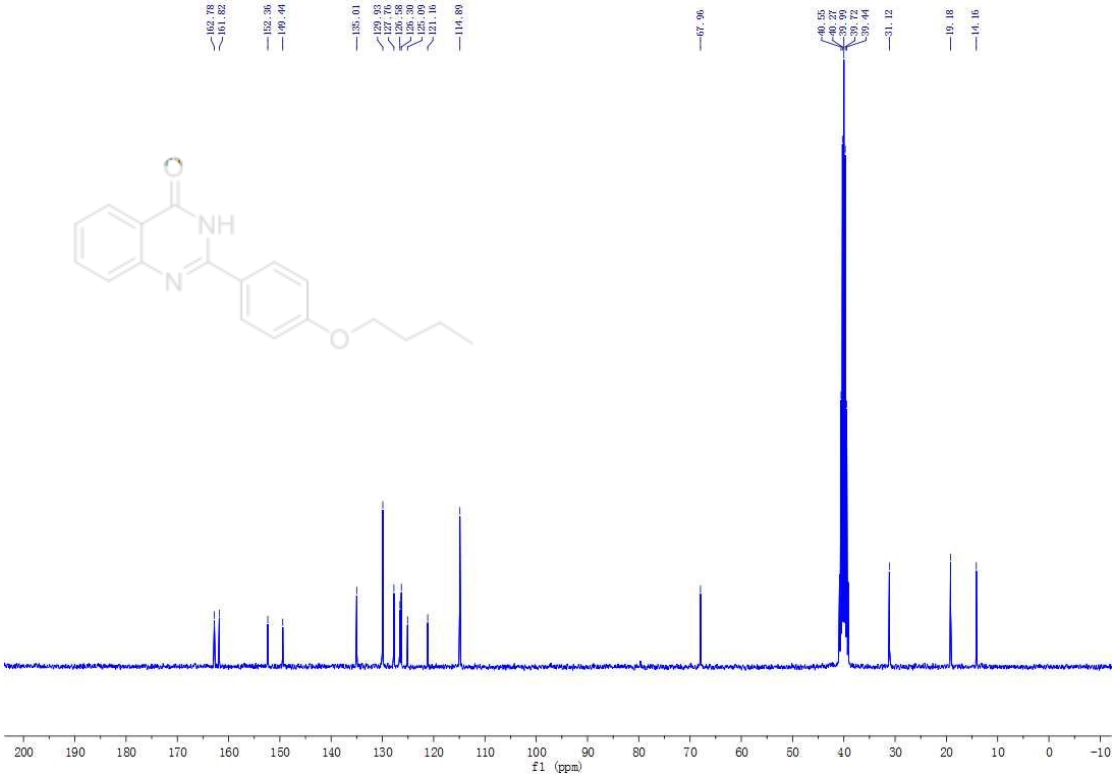
2-(4-propoxyphenyl)quinazolin-4(3*H*)-one (3c):



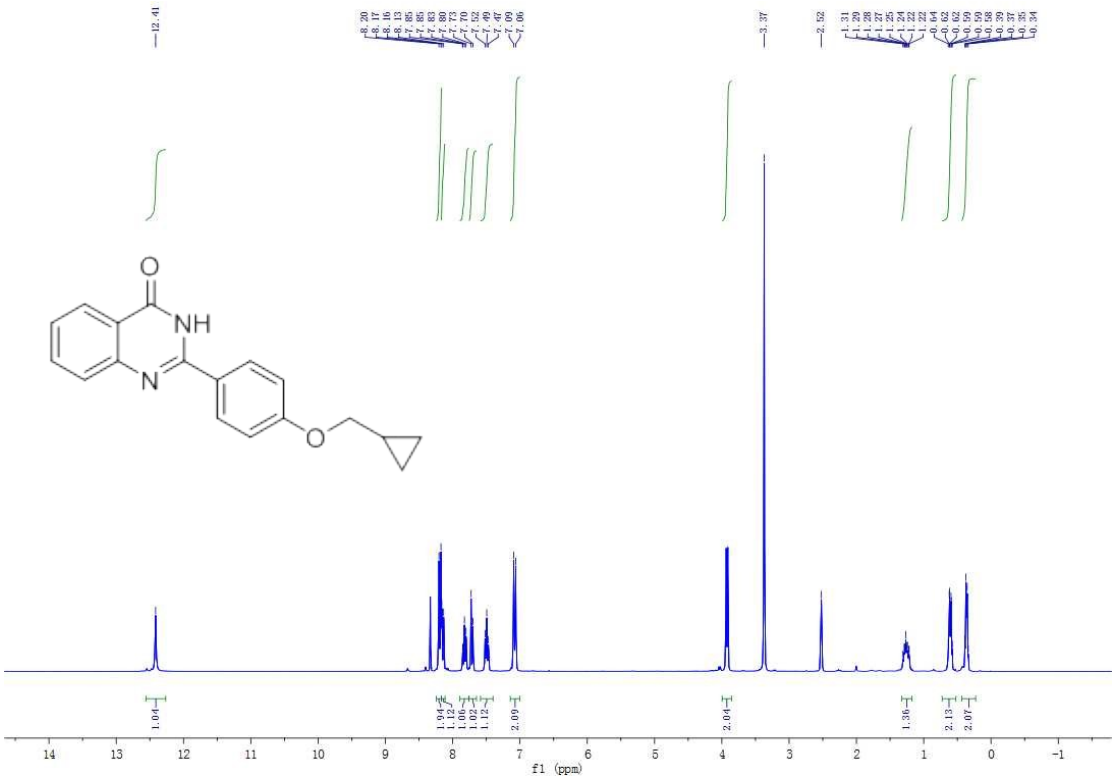


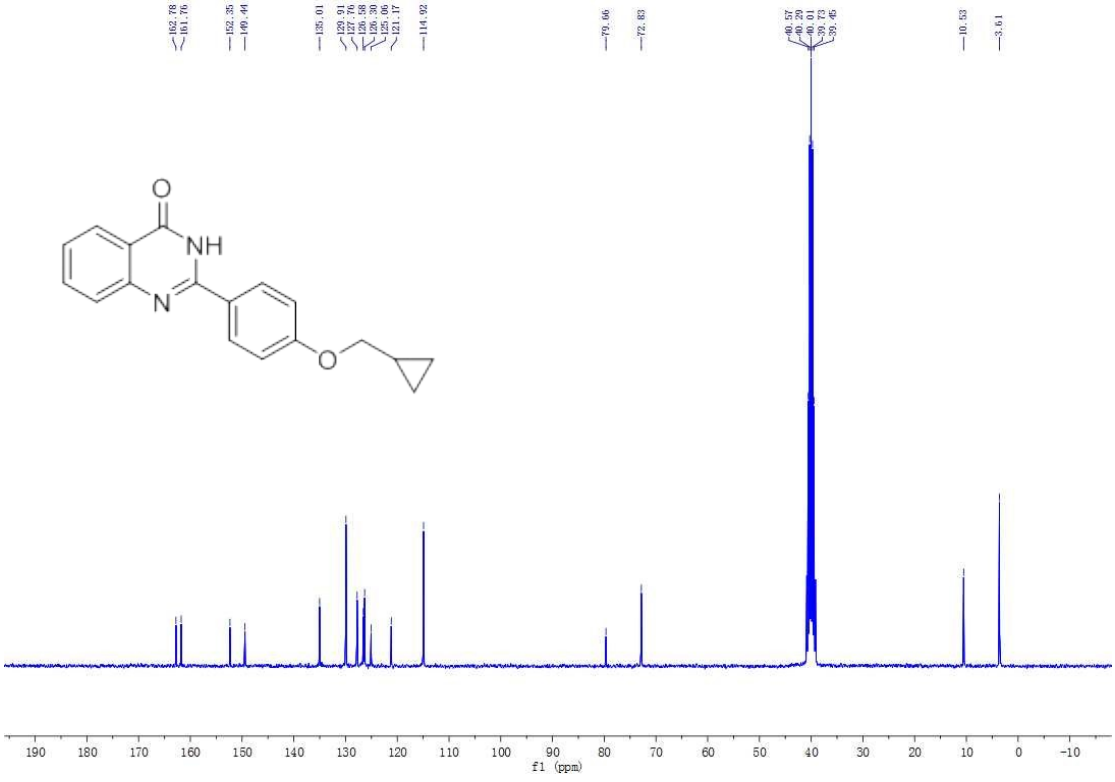
2-(4-butoxyphenyl)quinazolin-4(3*H*)-one (3d):



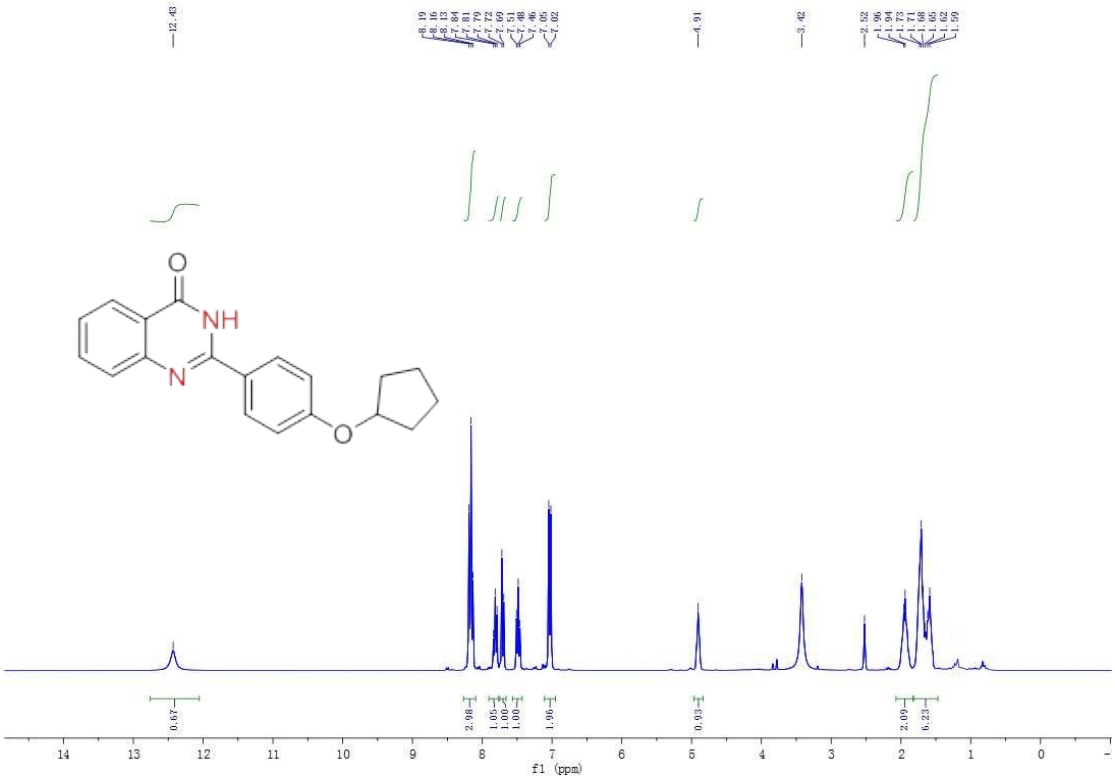


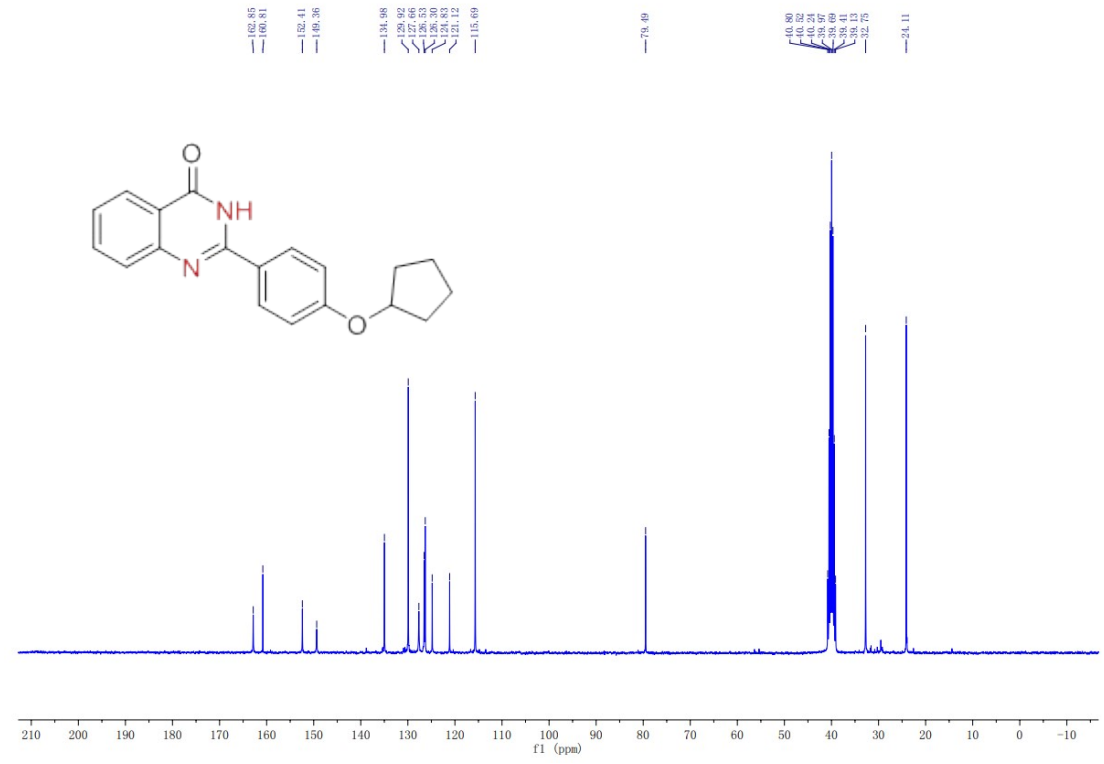
2-(4-(cyclopropylmethoxy)phenyl)quinazolin-4(3*H*)-one (3e):



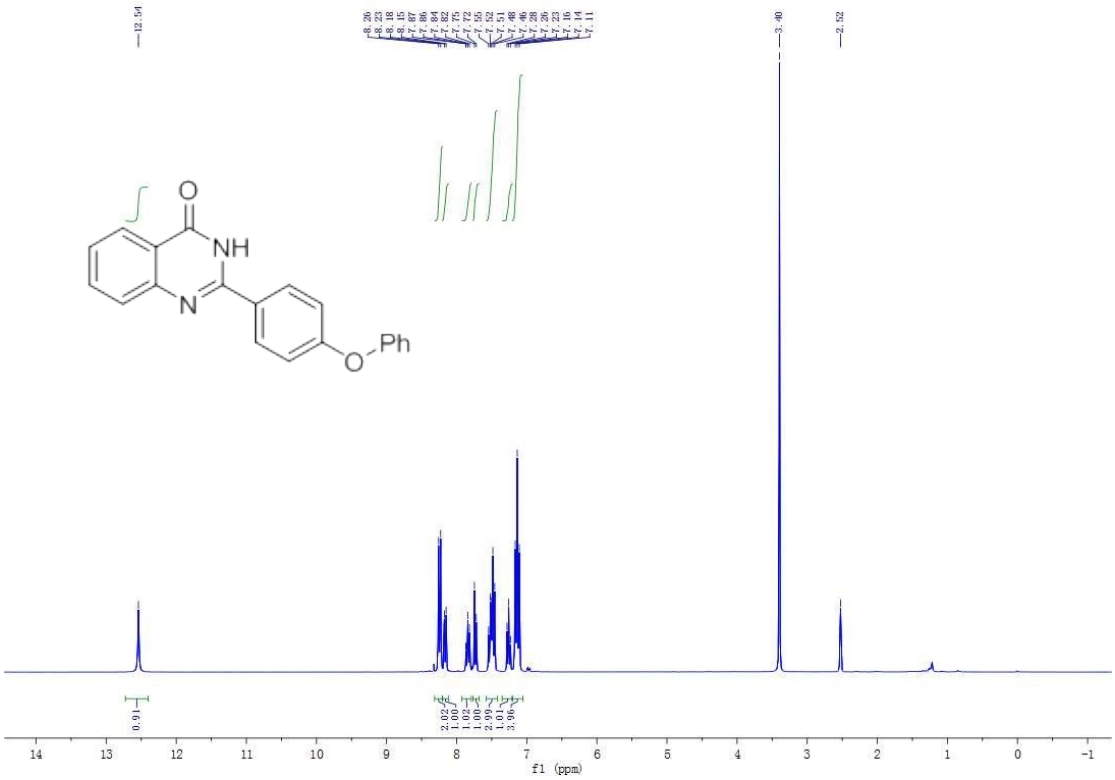


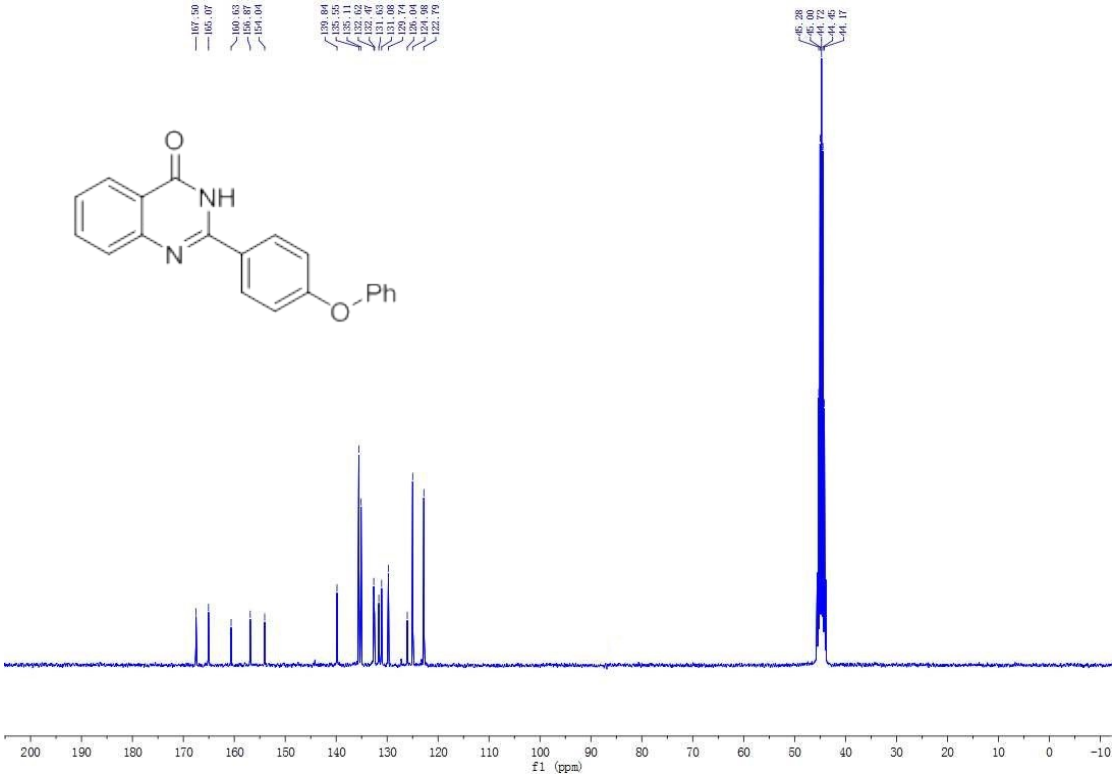
2-(4-(cyclopentyloxy)phenyl)quinazolin-4(3*H*)-one (3f):



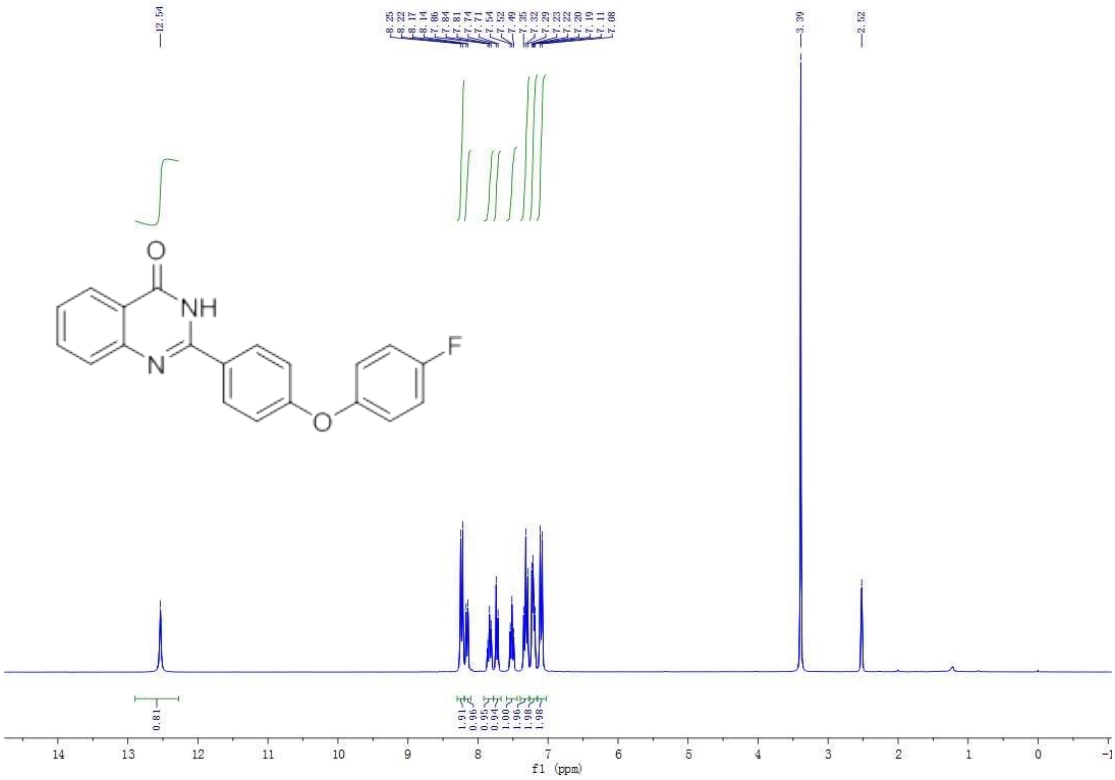


2-(4-phenoxyphenyl)quinazolin-4(3*H*)-one (3g)





2-(4-(4-fluorophenoxy)phenyl)quinazolin-4(3*H*)-one (3h)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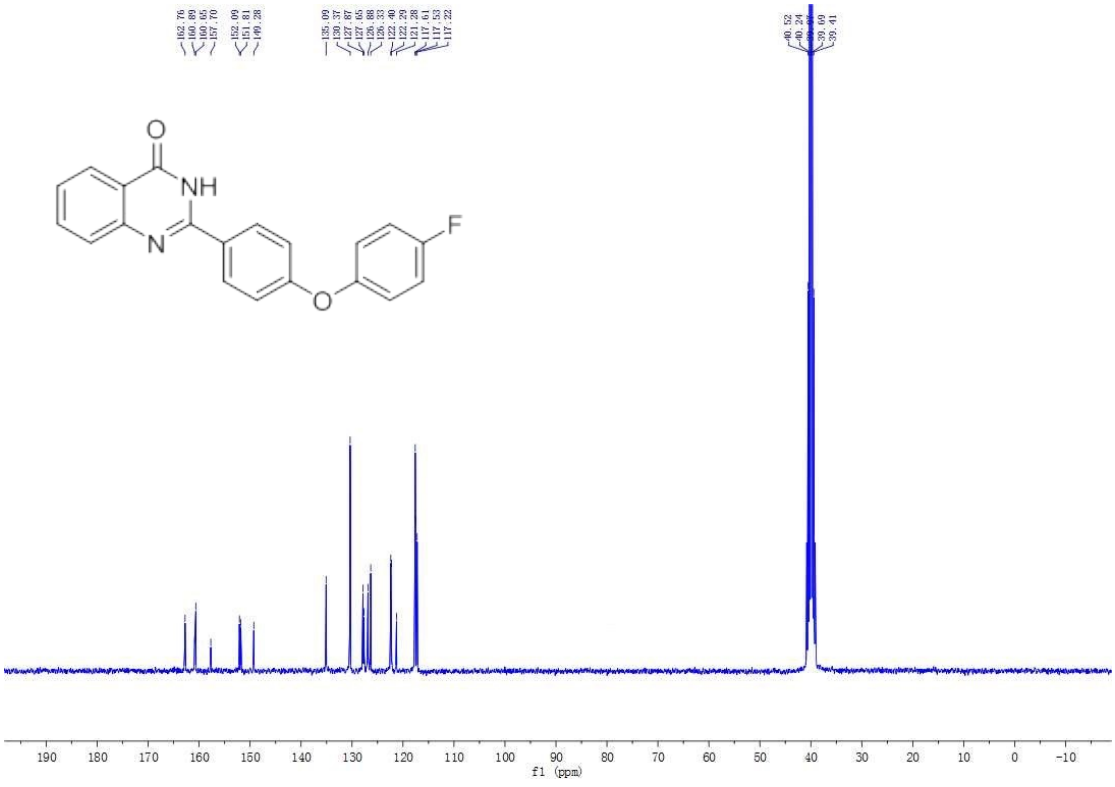
8.22
8.17
8.14
7.86
7.84
7.81
7.74
7.71
7.54
7.52
7.49
7.35
7.32
7.25
7.23
7.22
7.20
7.19
7.11
7.08
3.39
2.52
O
NH
N
F
O
0.81
1.91
0.99
0.95
0.94
1.00
1.96
1.98
1.98
f1 (ppm)


162.76
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127.87
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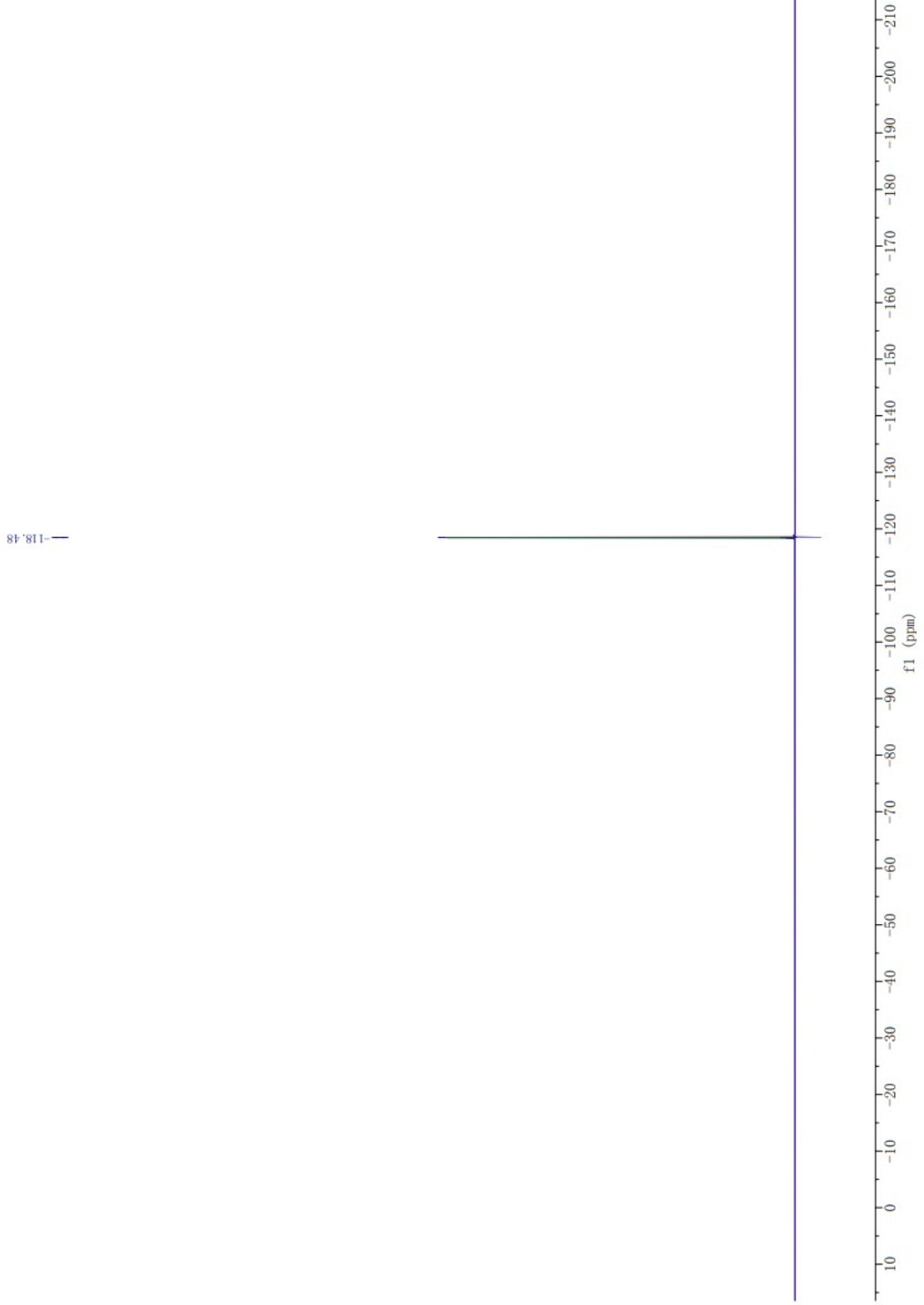
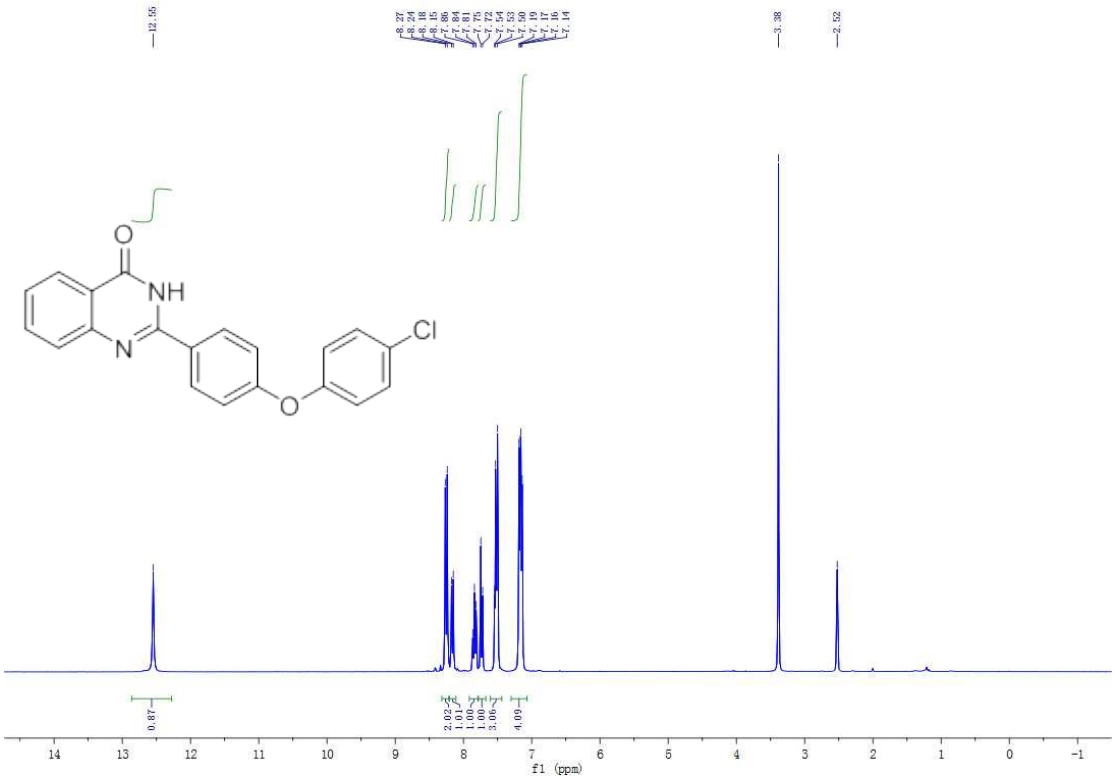
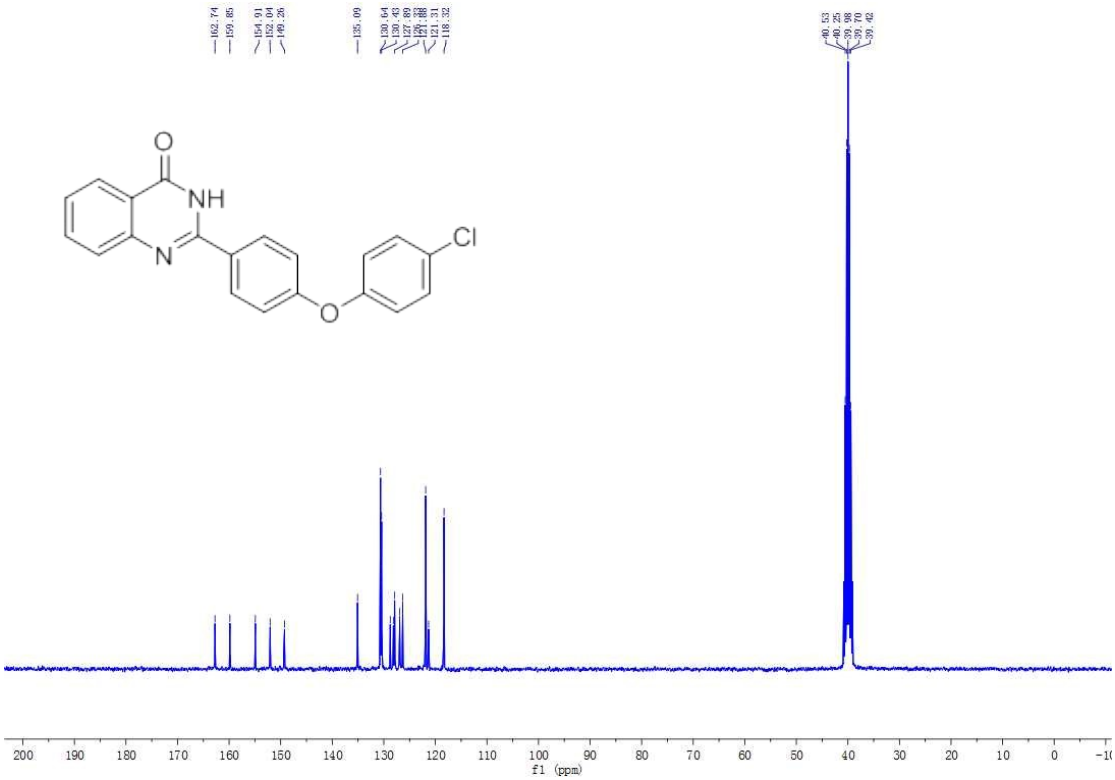
125.49
122.29
121.28
117.61
117.53
117.22
40.52
40.31
40.10
39.89
39.69
39.48
39.41
O
NH
N
F
O
f1 (ppm)

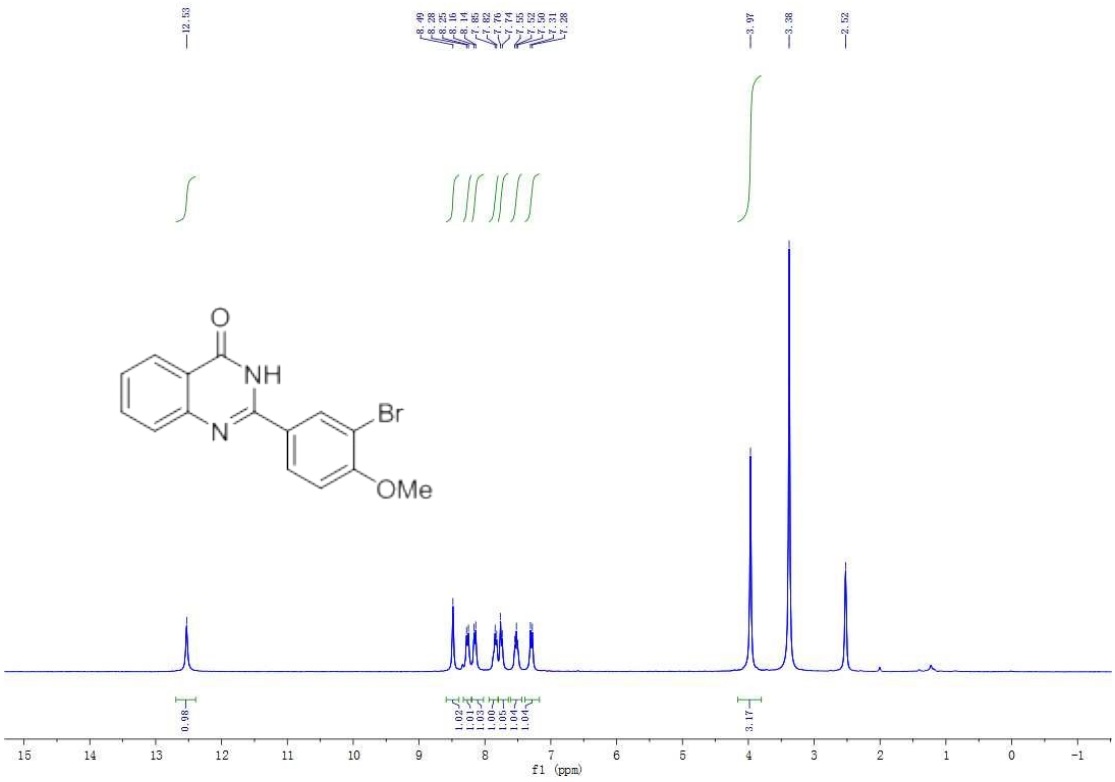


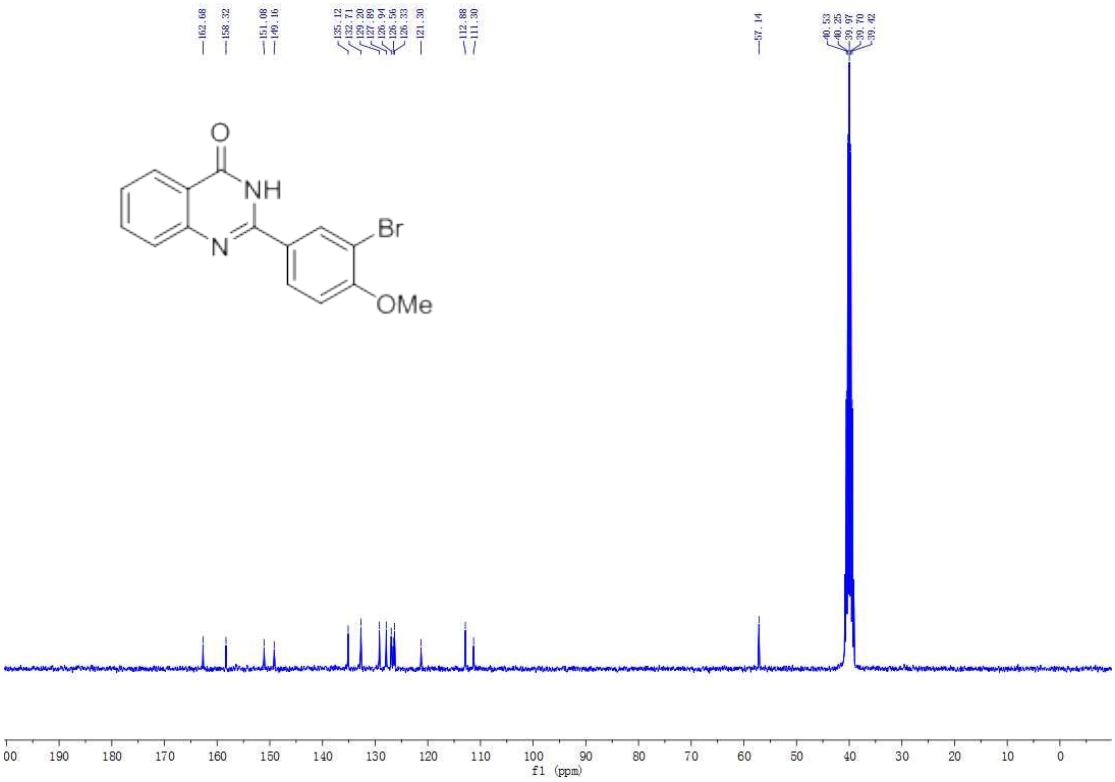
2-(4-(4-chlorophenoxy)phenyl)quinazolin-4(3*H*)-one (3i):



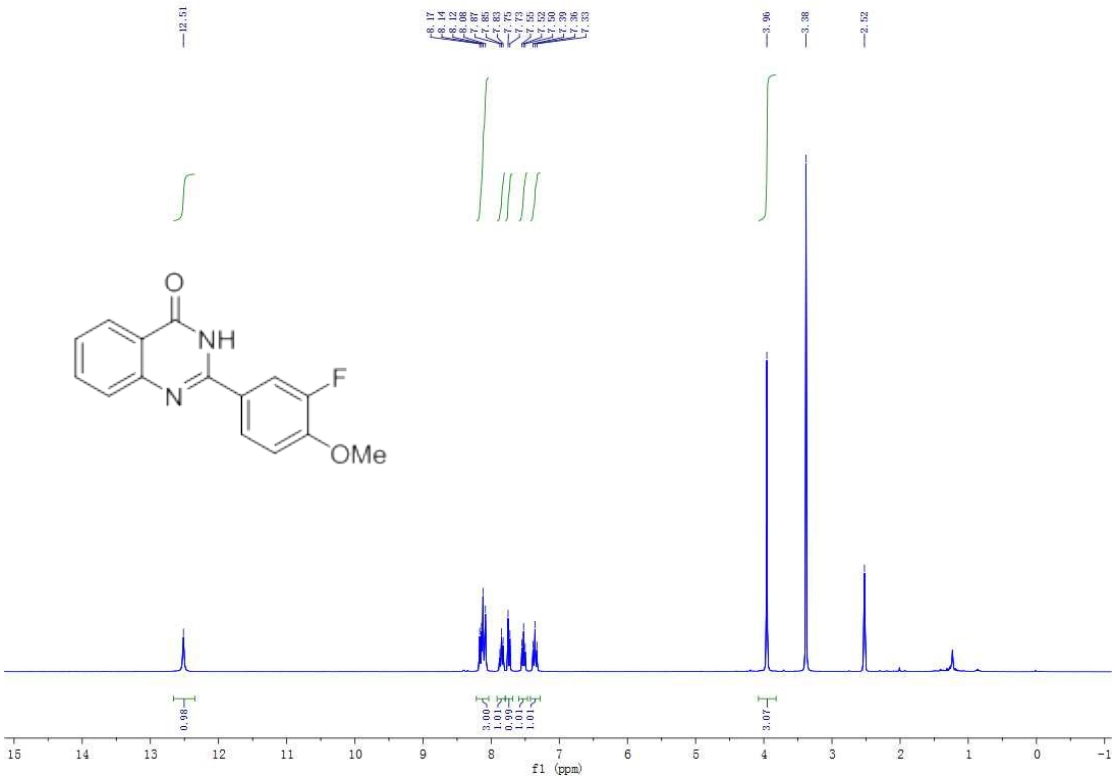


2-(3-bromo-4-methoxyphenyl)quinazolin-4(3*H*)-one (3j)





2-(3-fluoro-4-methoxyphenyl)quinazolin-4(3*H*)-one (3k)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7.33
3.96
3.38
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O
NH
N
F
OMe
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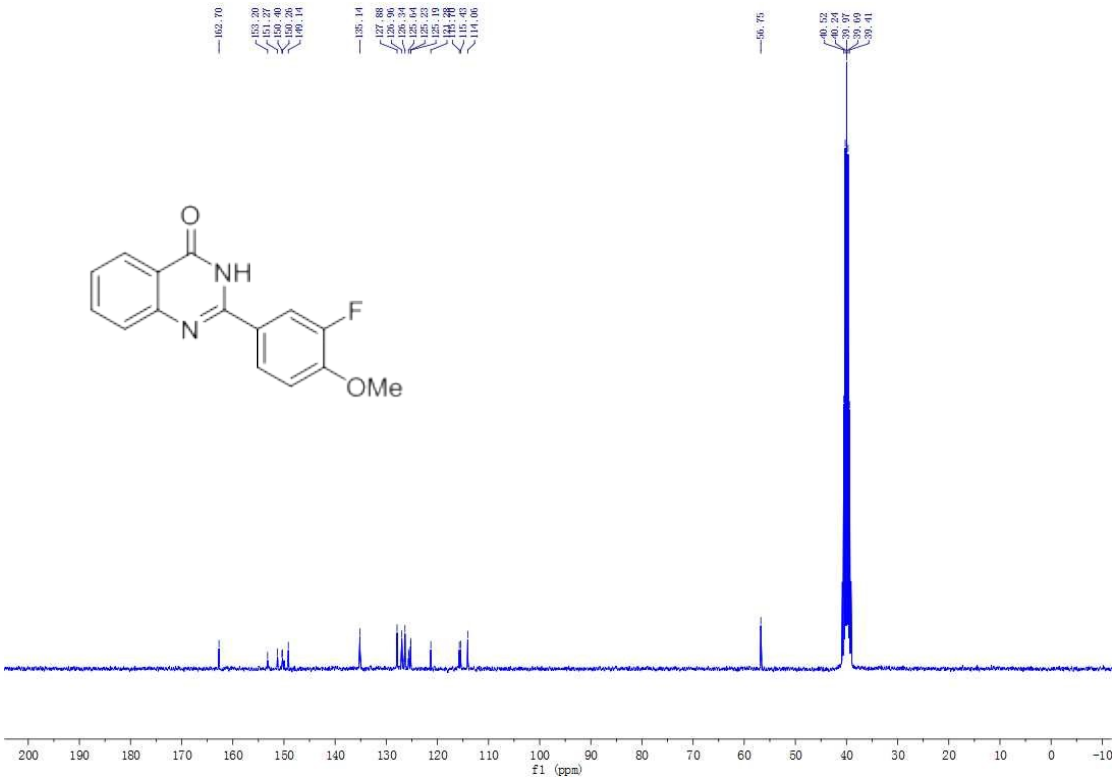
0.99
1.01
1.01
3.07
f1 (ppm)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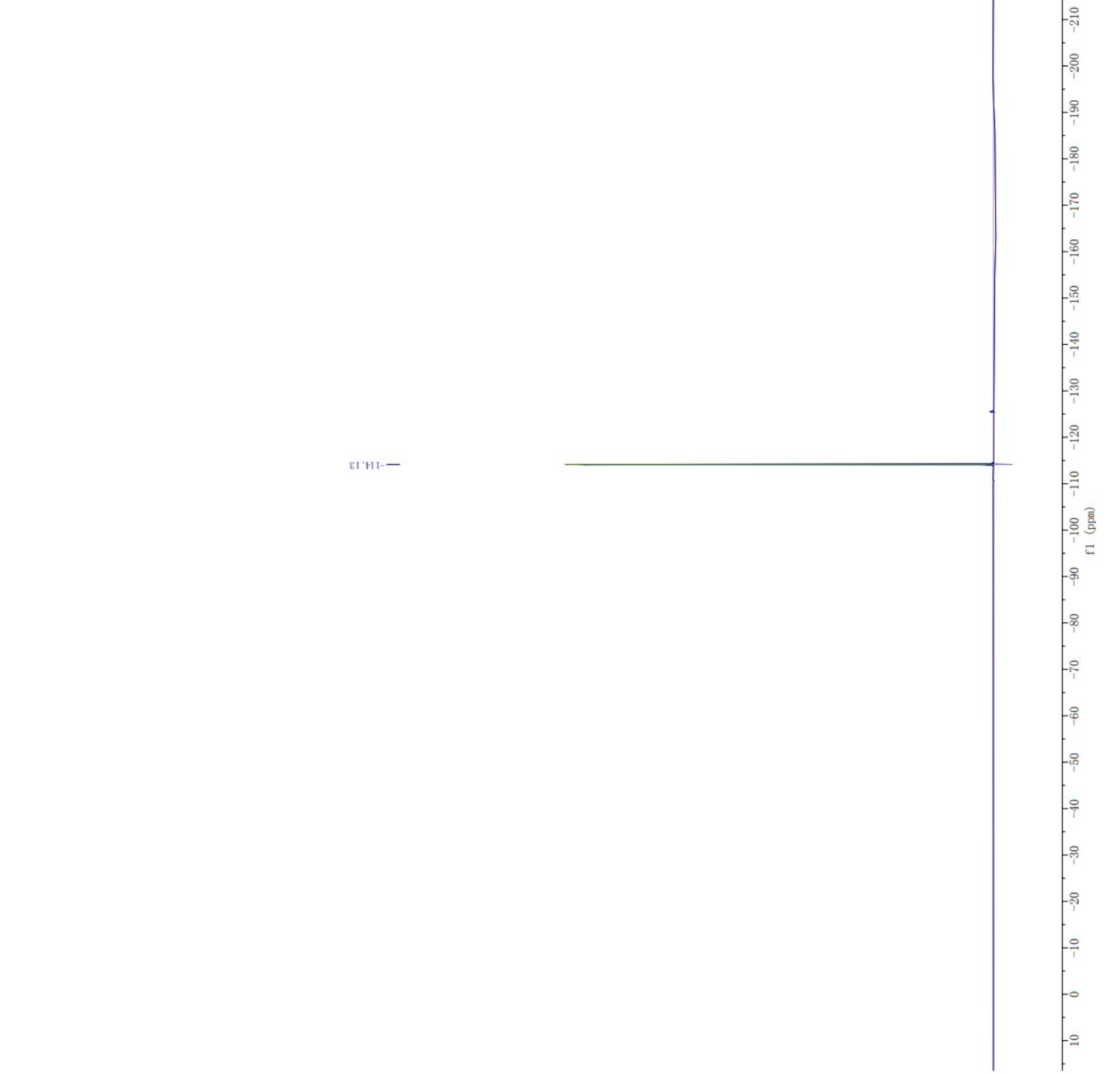
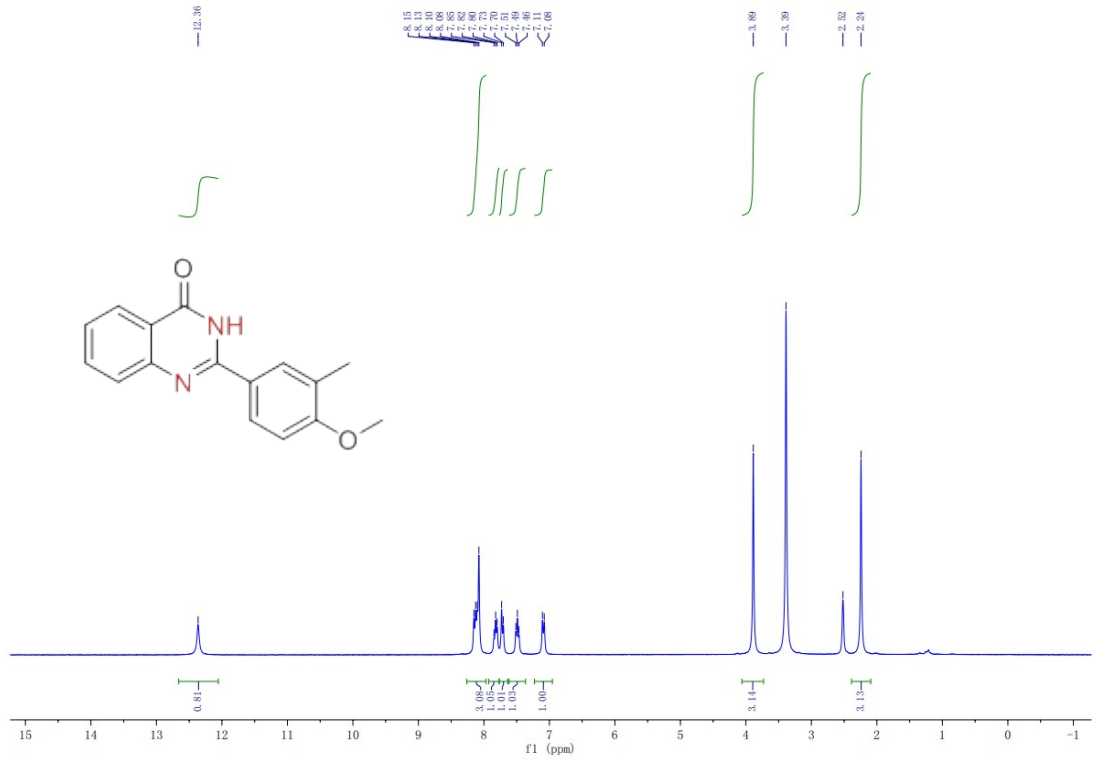
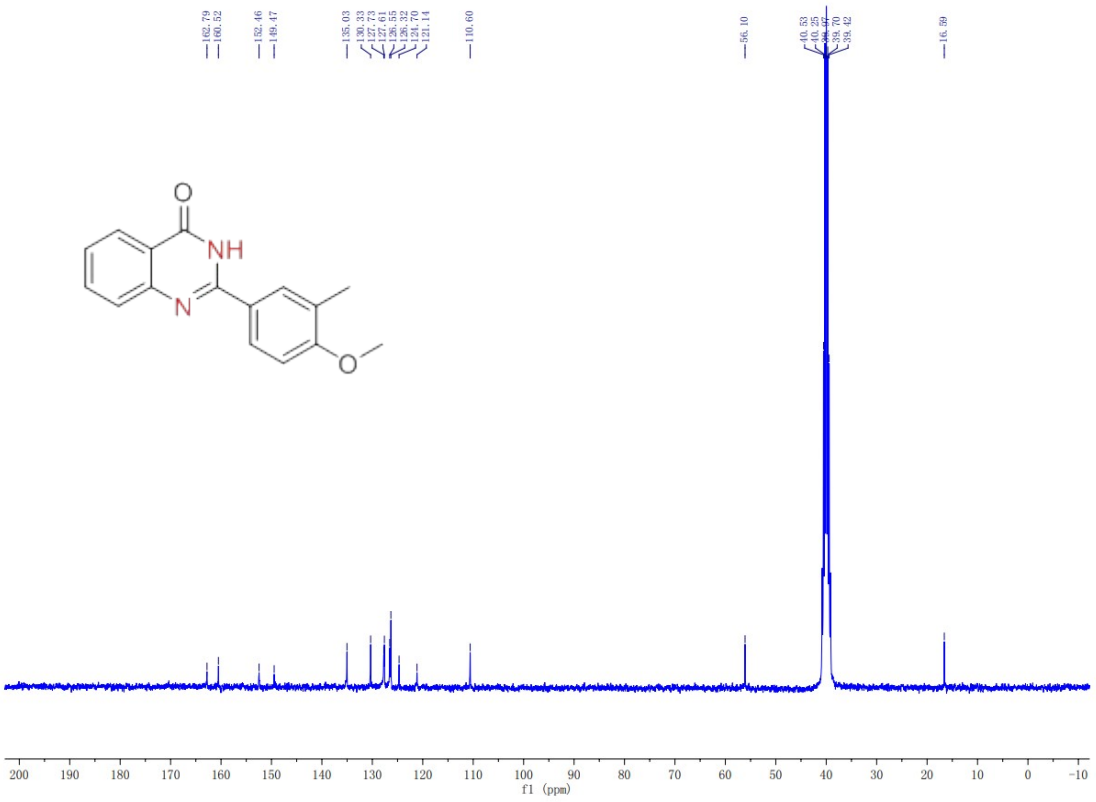
39.97
39.69
39.41
O
NH
N
F
OMe
f1 (ppm)

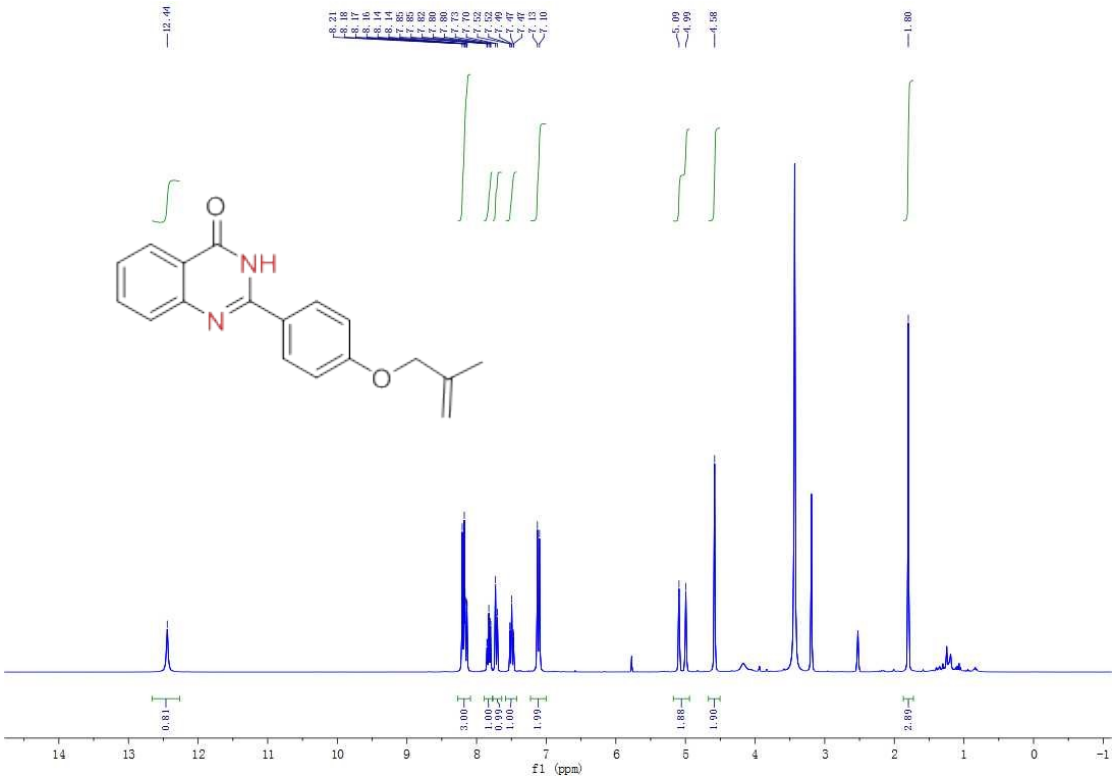


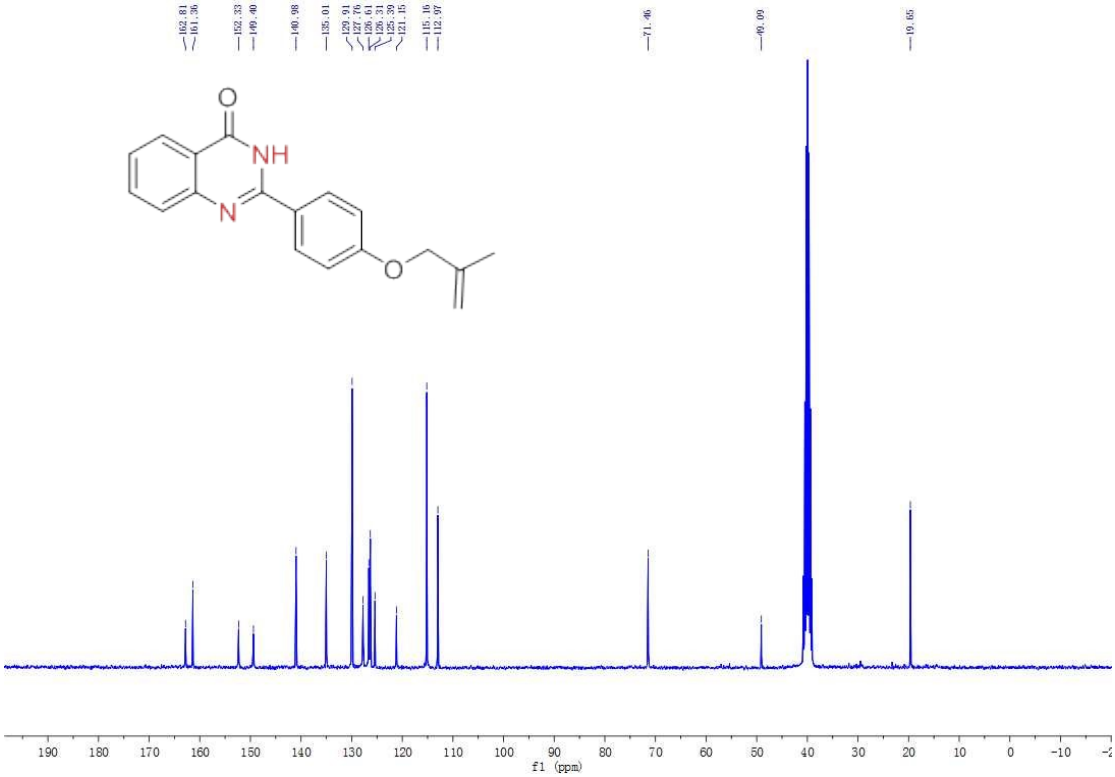
2-(3-methyl-4-methoxyphenyl)quinazolin-4(3*H*)-one (3l)



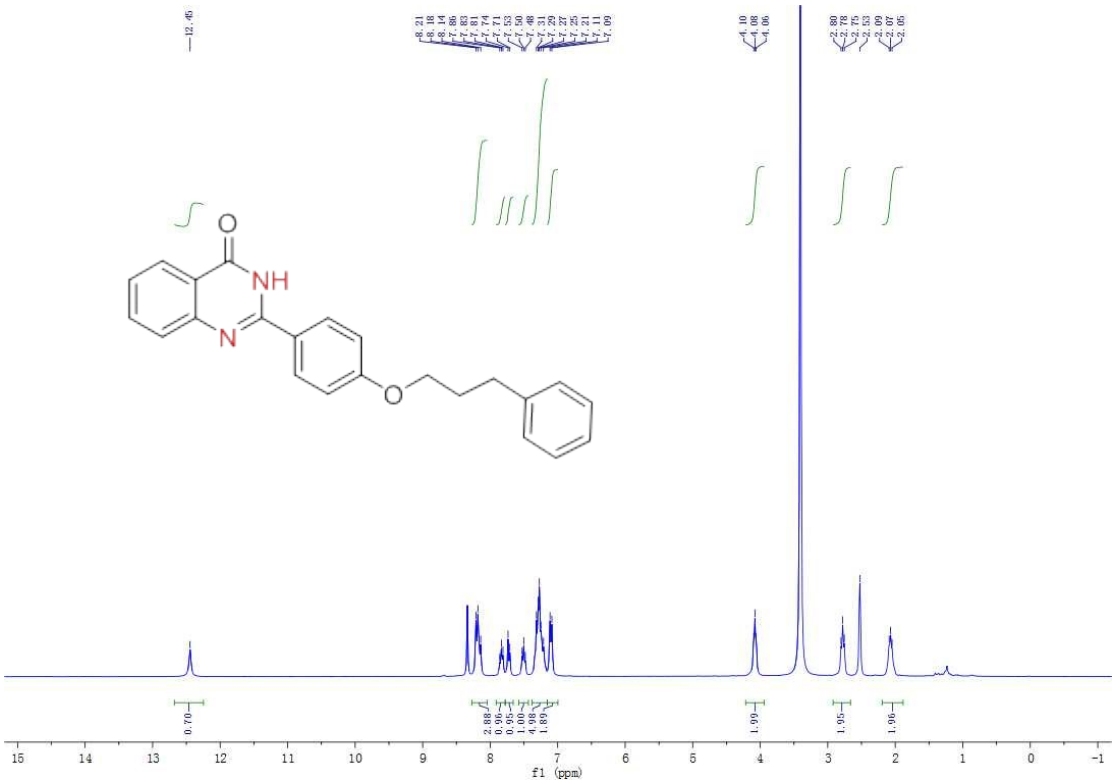


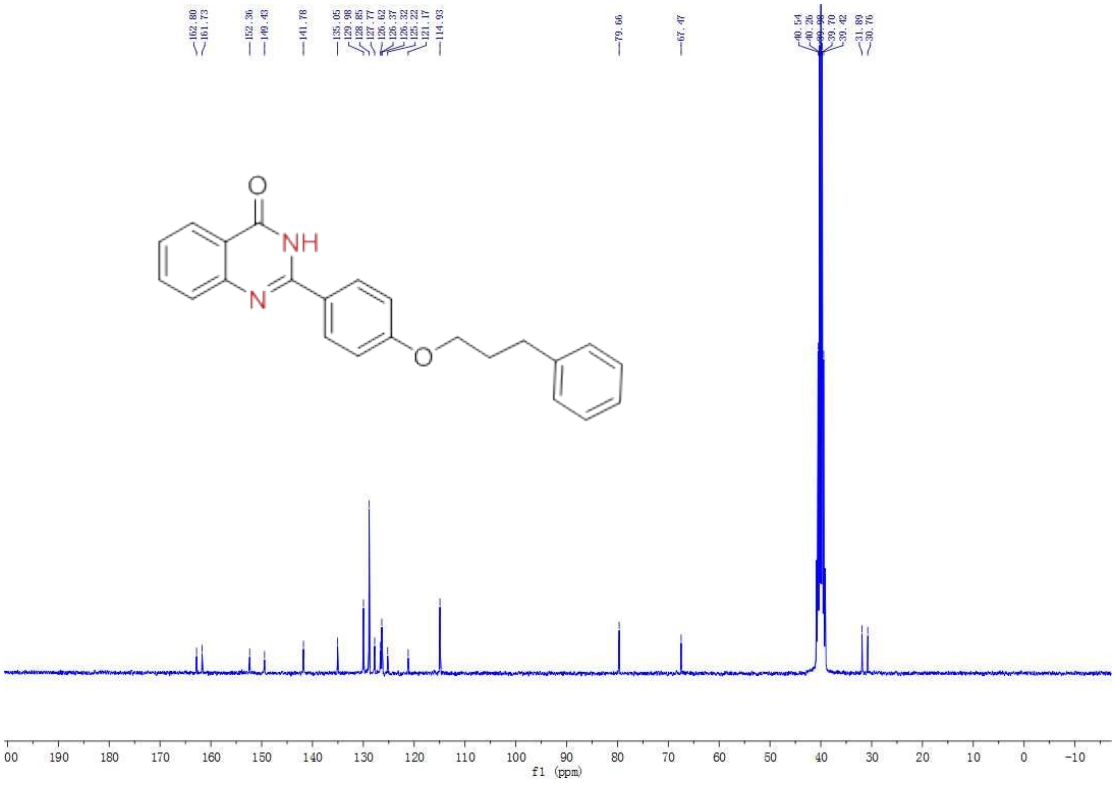
2-(4-((2-methylallyl)oxy)phenyl)quinazolin-4(3*H*)-one (3m)



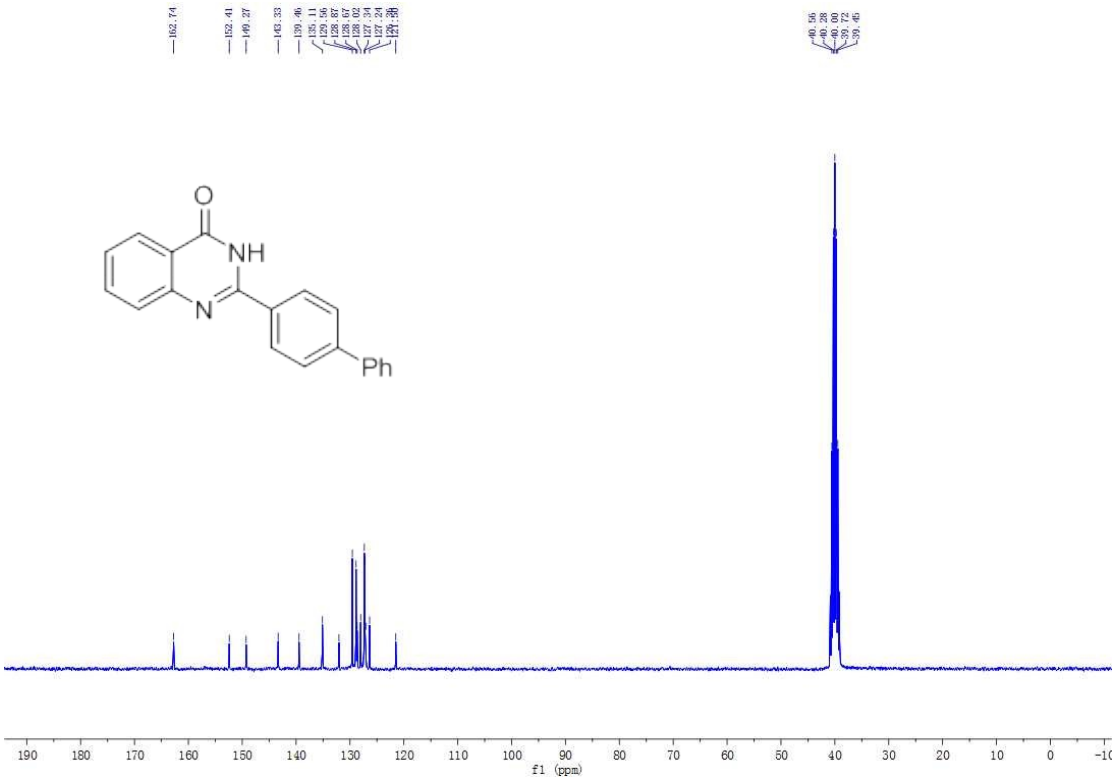


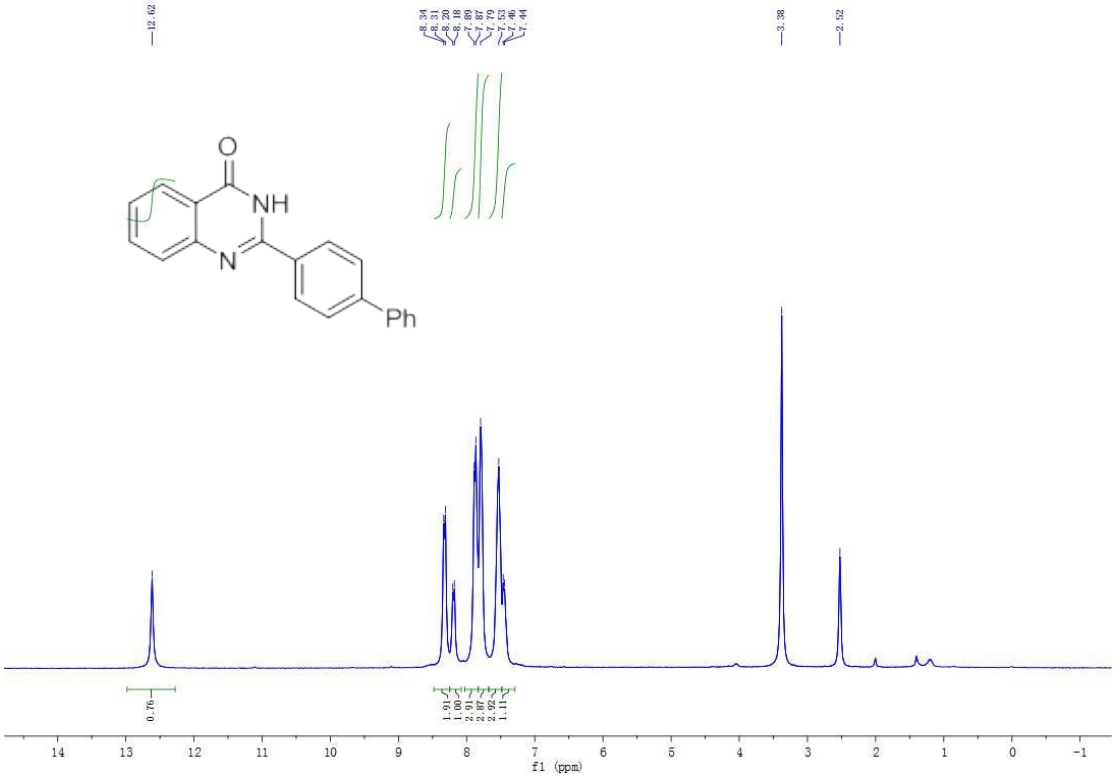
2-(4-(3-phenylpropoxy)phenyl)quinazolin-4(3*H*)-one (3n)



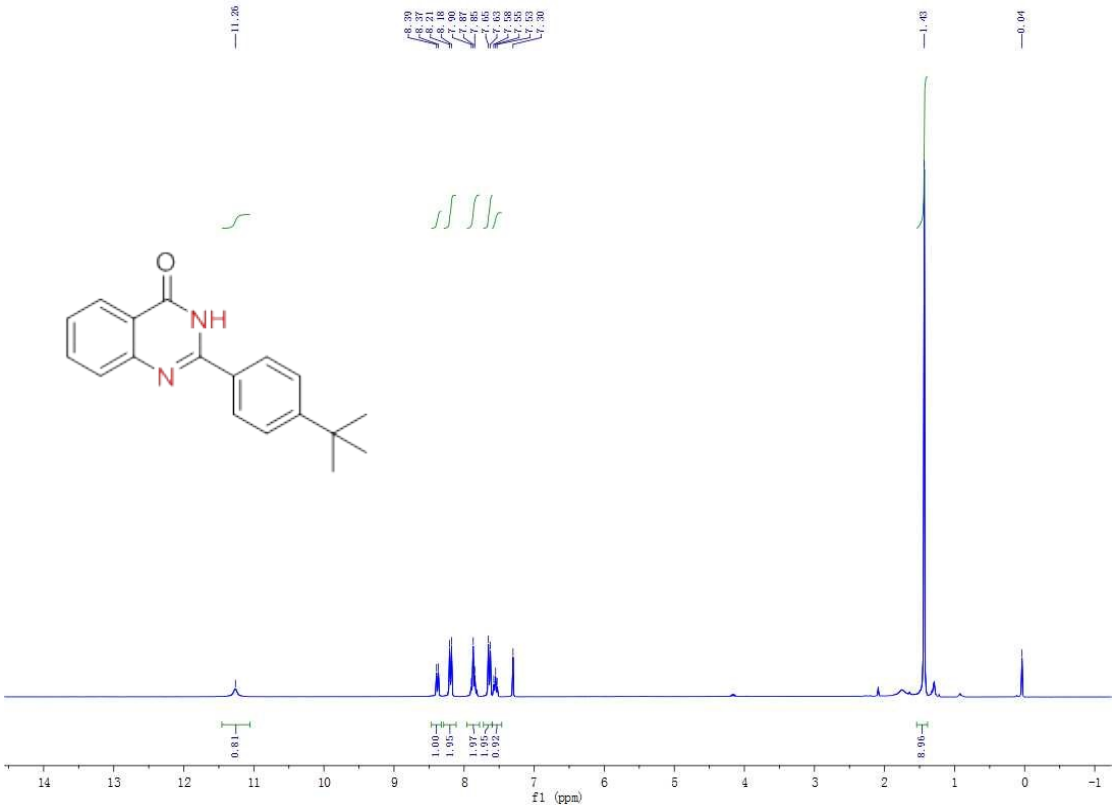


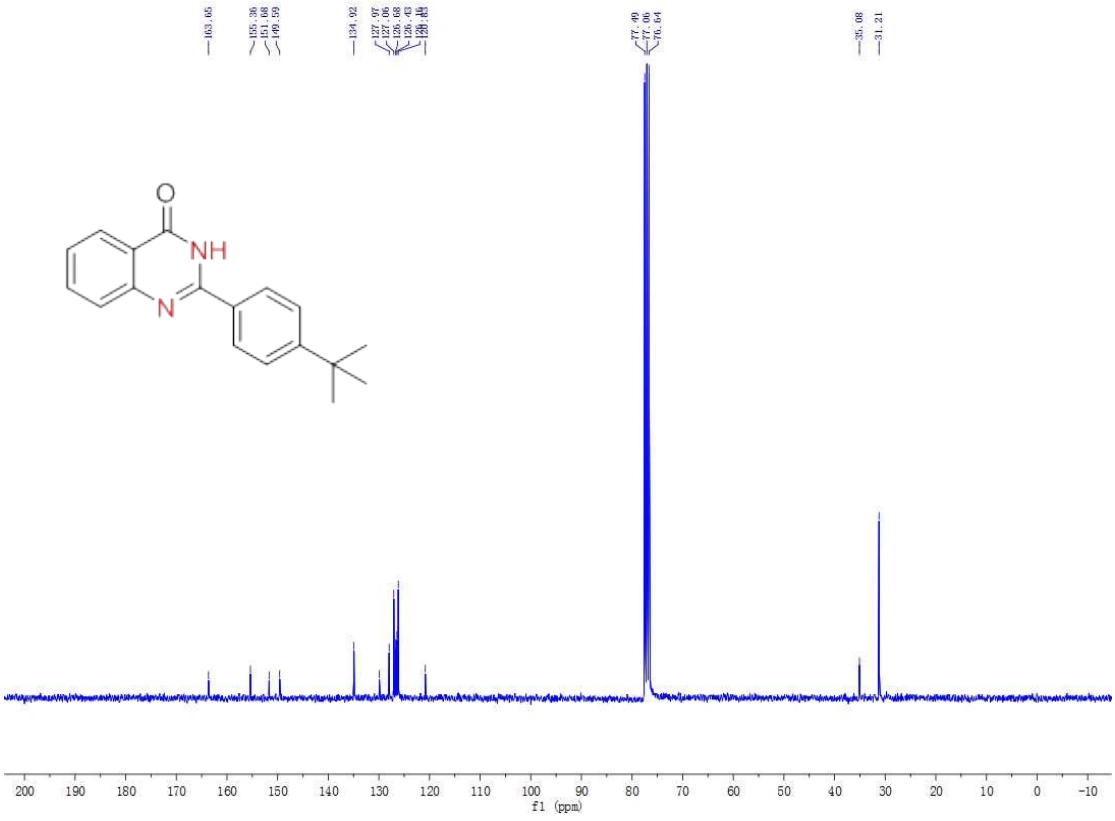
2-([1,1'-biphenyl]-4-yl)quinazolin-4(3*H*)-one (3o)



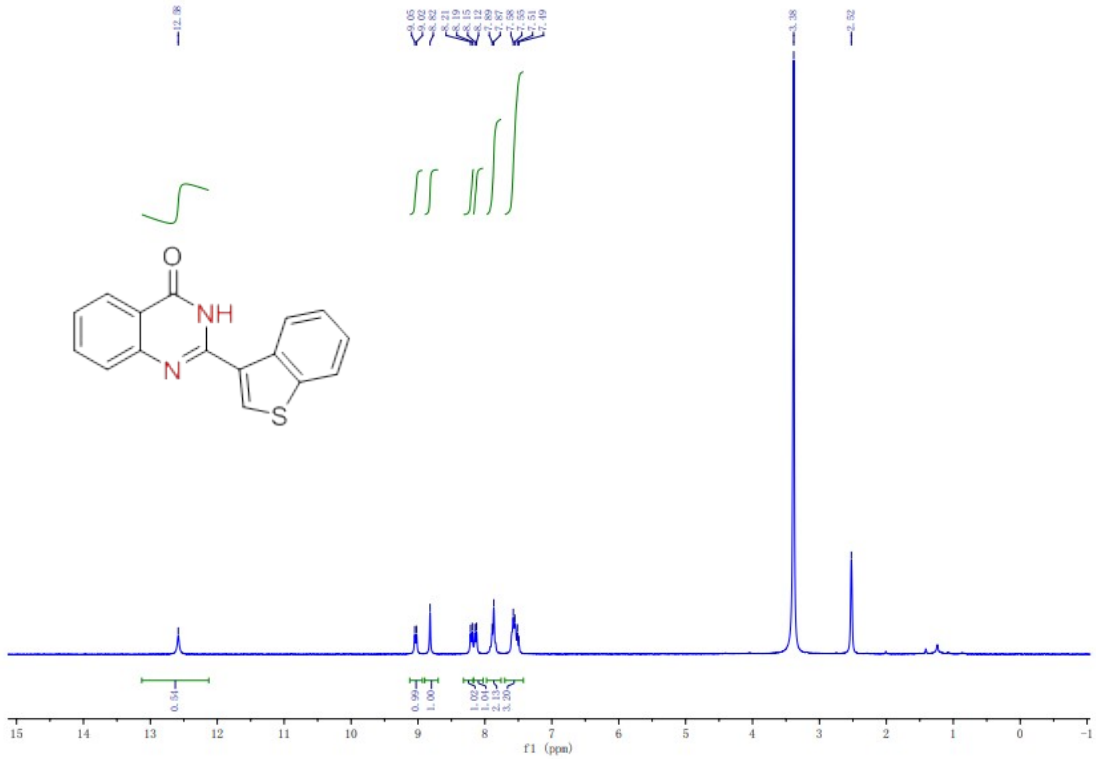


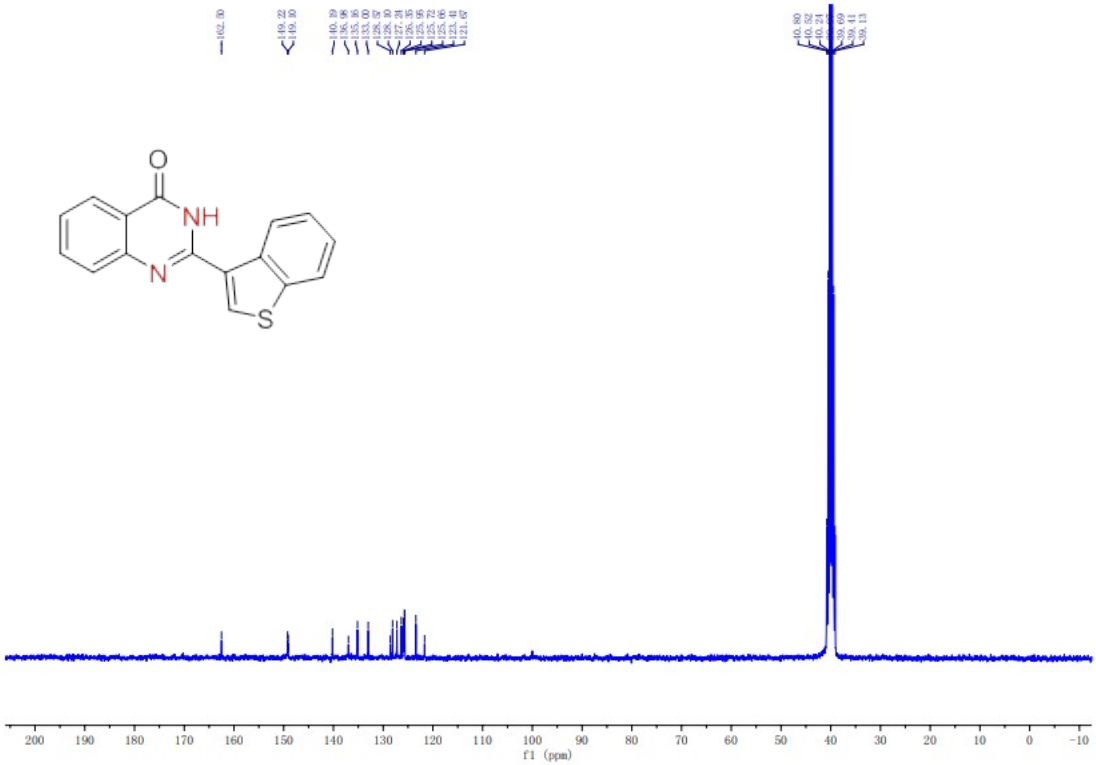
2-(4-(tert-butyl)phenyl)quinazolin-4(3*H*)-one (3p)



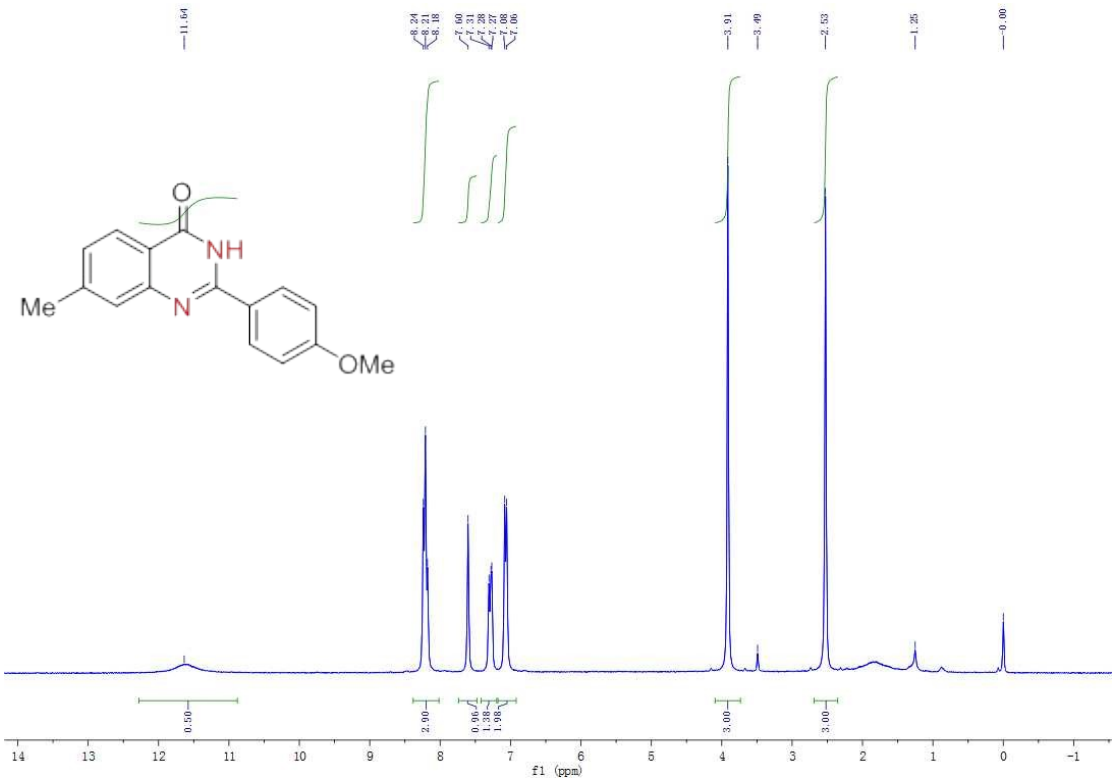


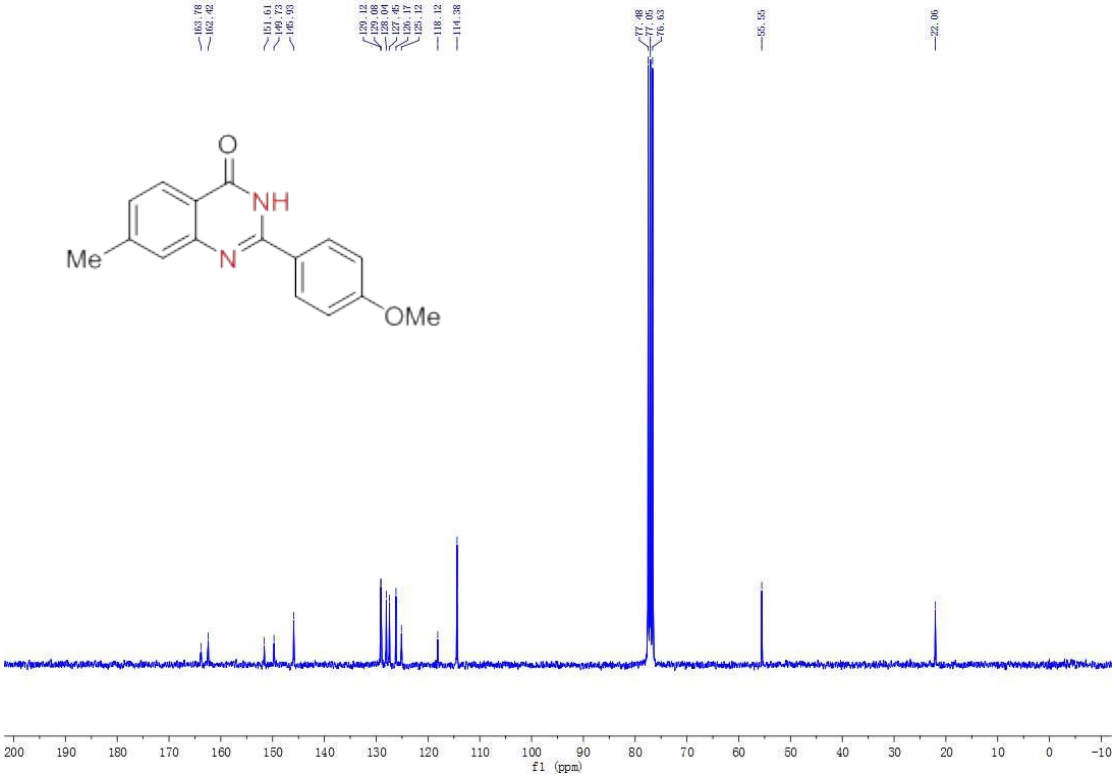
2-(benzo[b]thiophen-3-yl)quinazolin-4(3*H*)-one (3q)



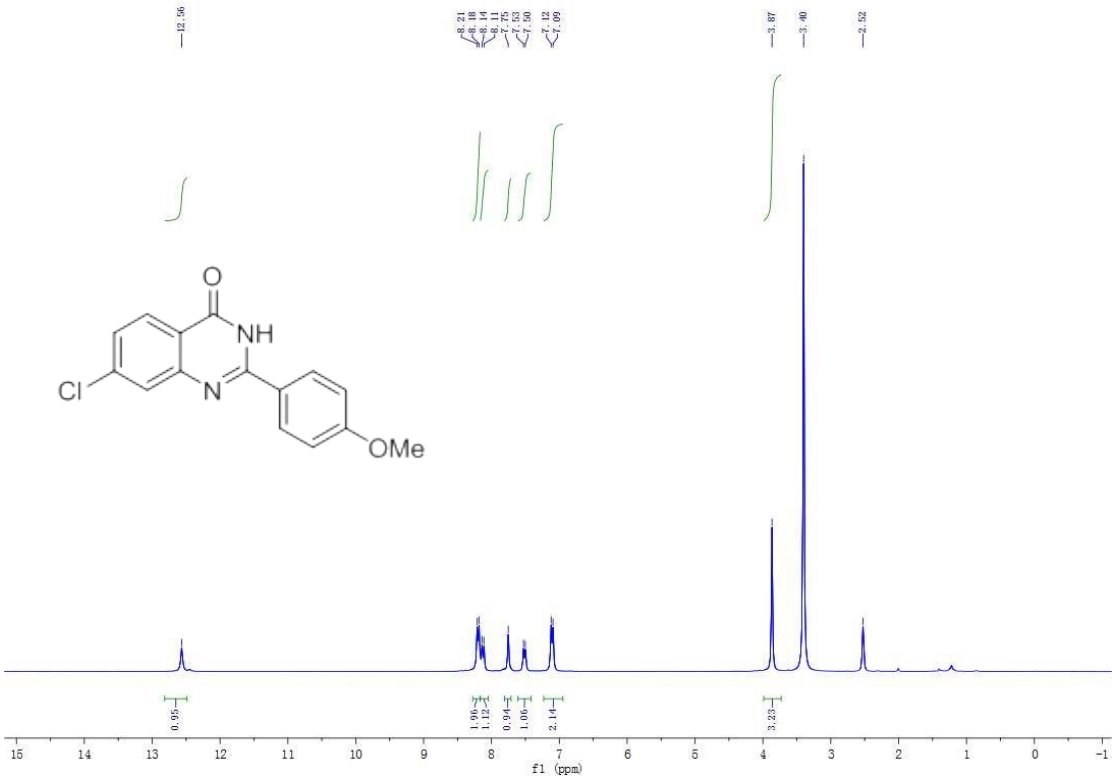


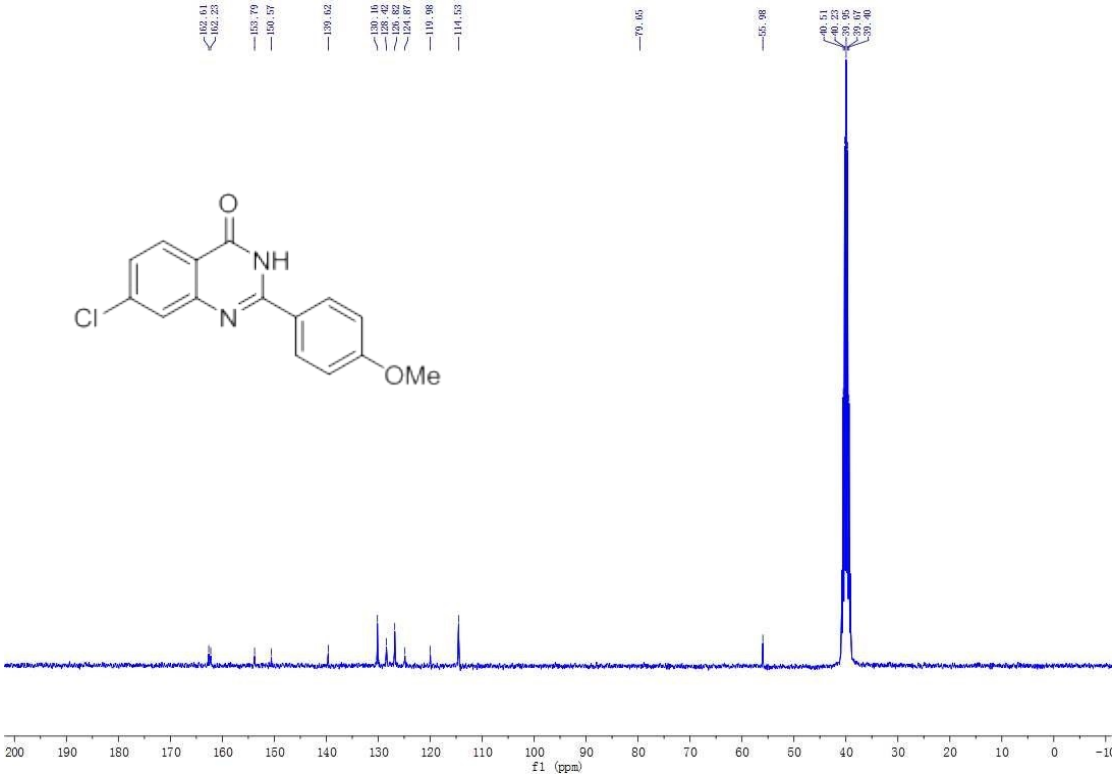
2-(4-methoxyphenyl)-7-methylquinazolin-4(3*H*)-one (4a)



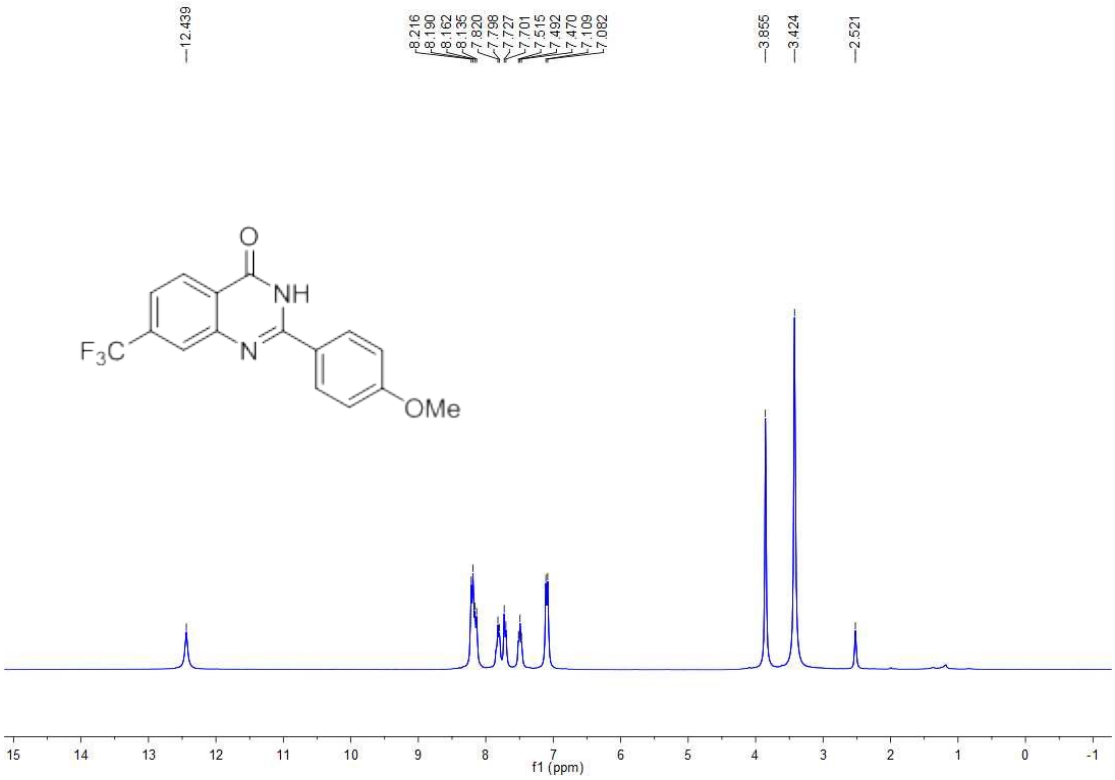


7-chloro-2-(4-methoxyphenyl)quinazolin-4(3H)-one (4b)





2-(4-methoxyphenyl)-7-(trifluoromethyl)quinazolin-4(3*H*)-one (4c)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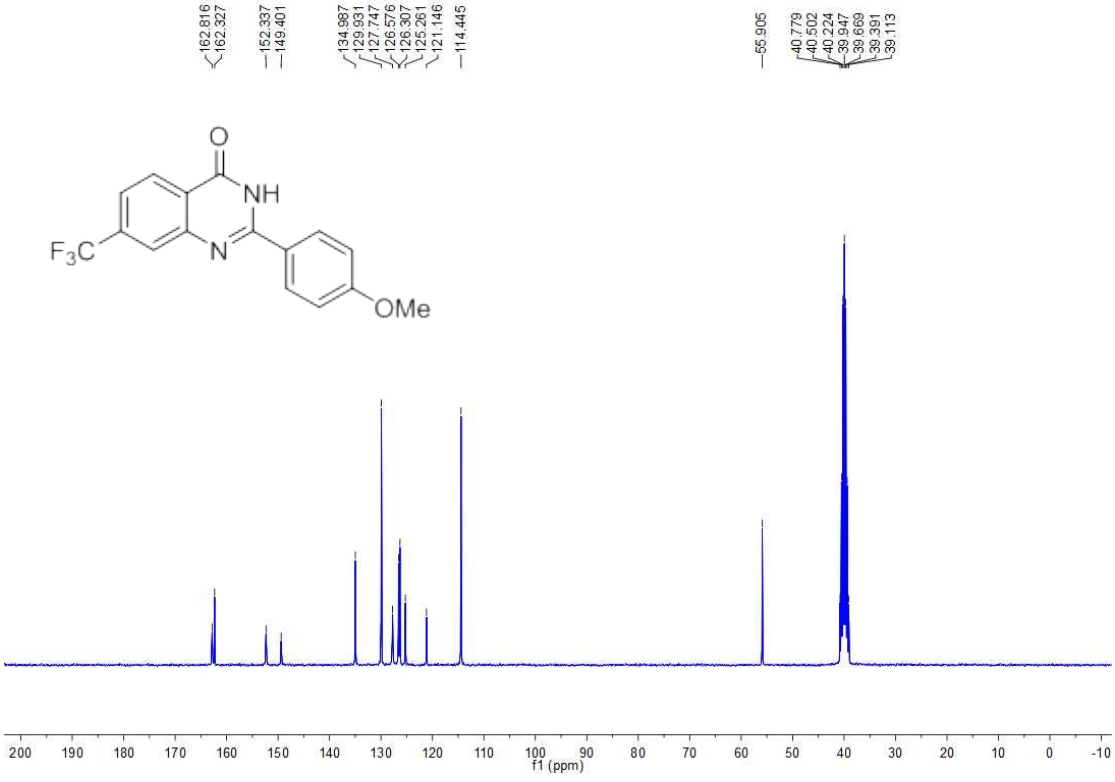
7.820
7.798
7.727
7.701
7.515
7.492
7.470
7.109
7.082
3.855
3.424
2.521
O
NH
N
F3C
OMe
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)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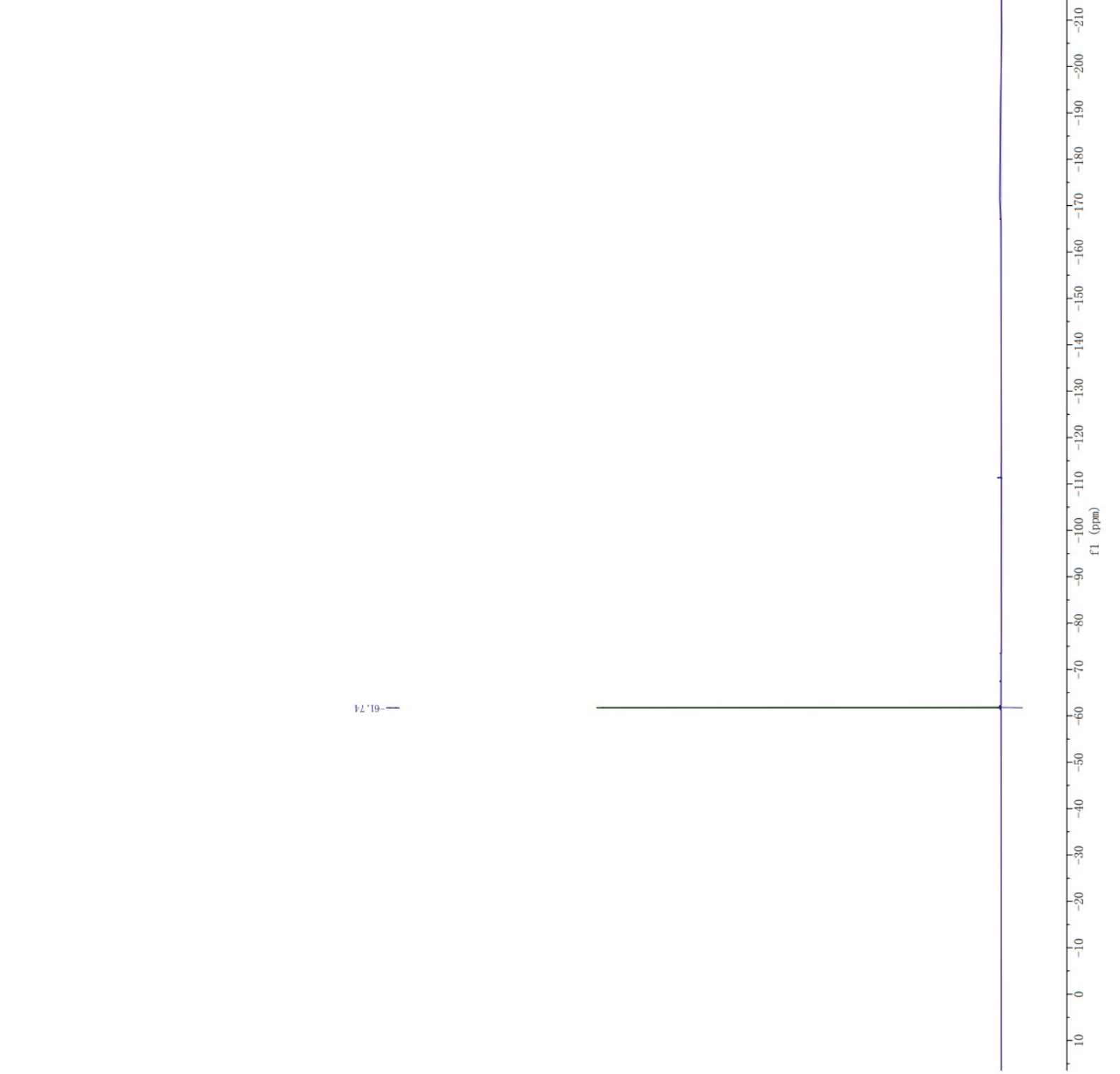
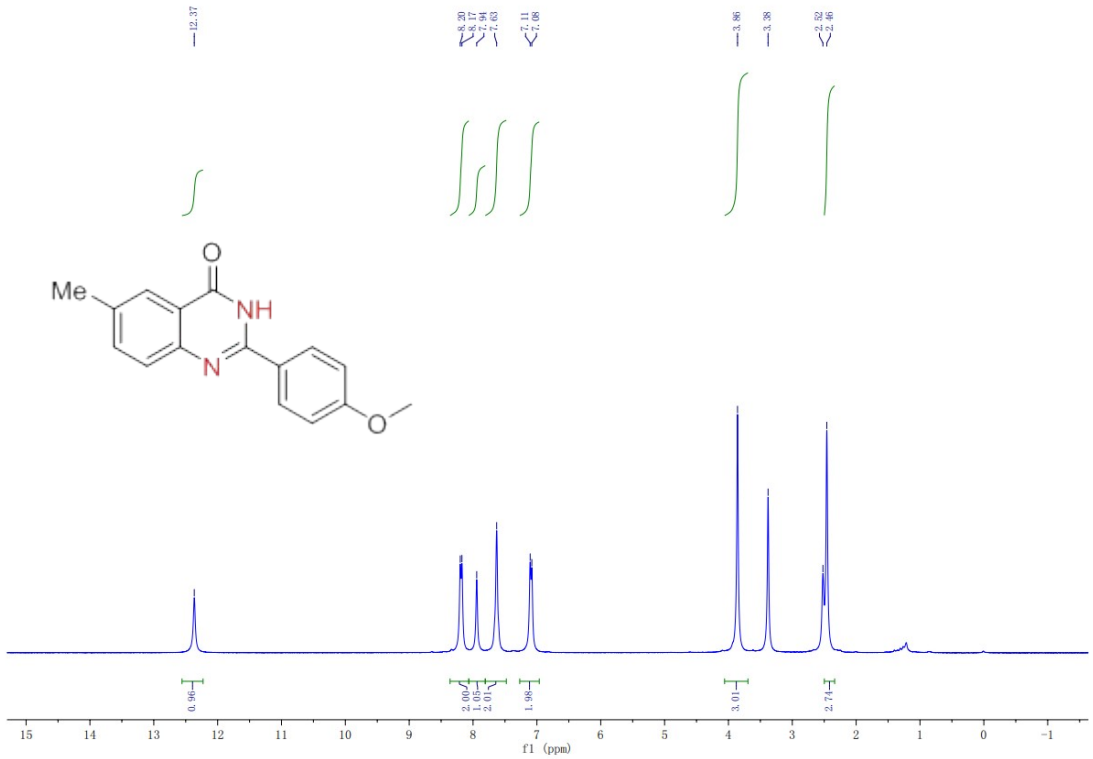
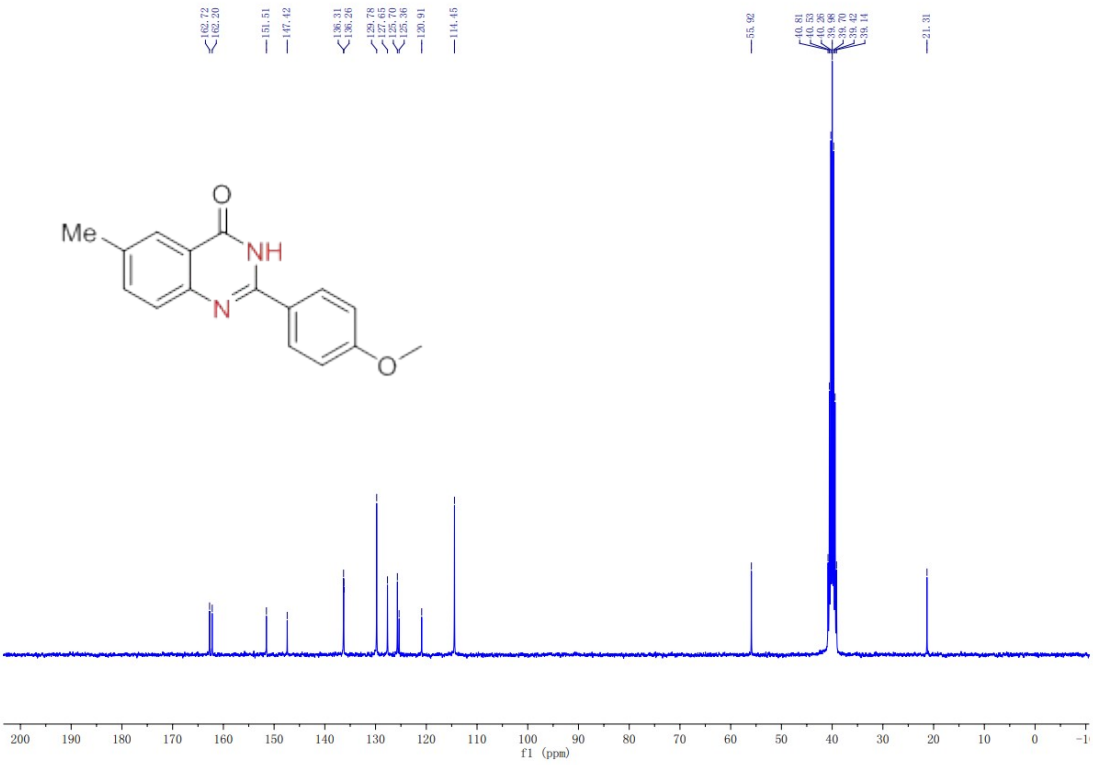
126.307
125.261
121.146
114.445
55.905
40.779
40.502
40.224
39.947
39.669
39.391
39.113
O
NH
N
F3C
OMe
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

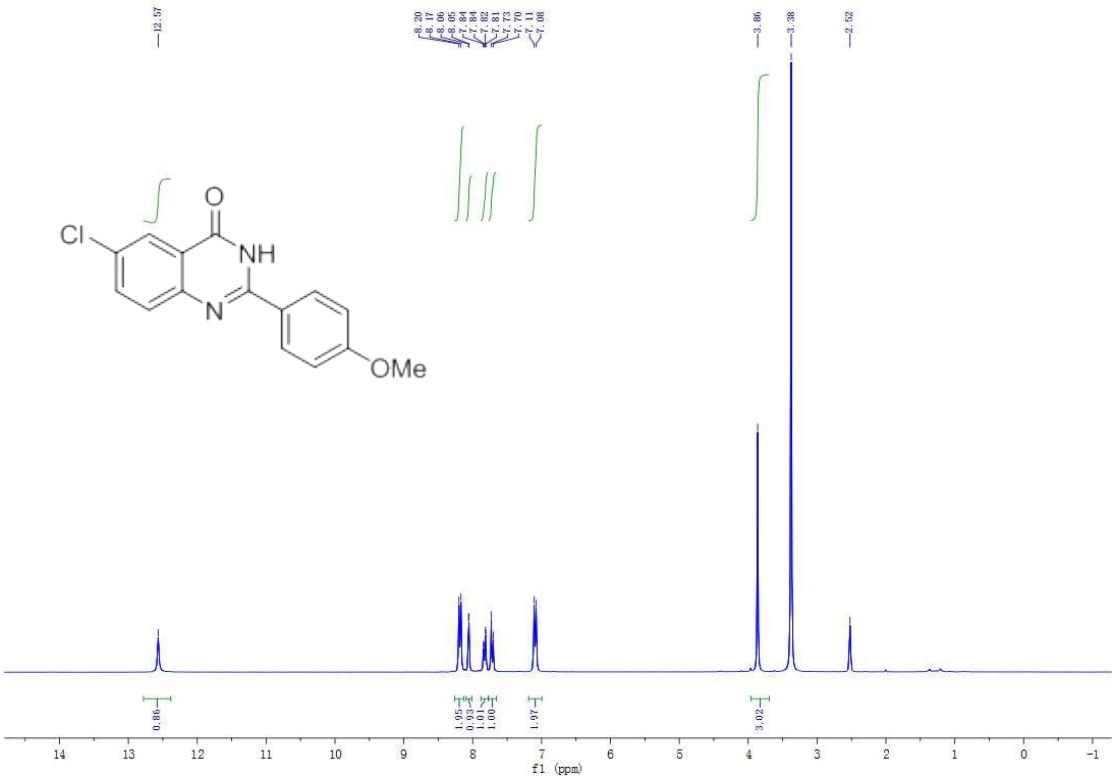


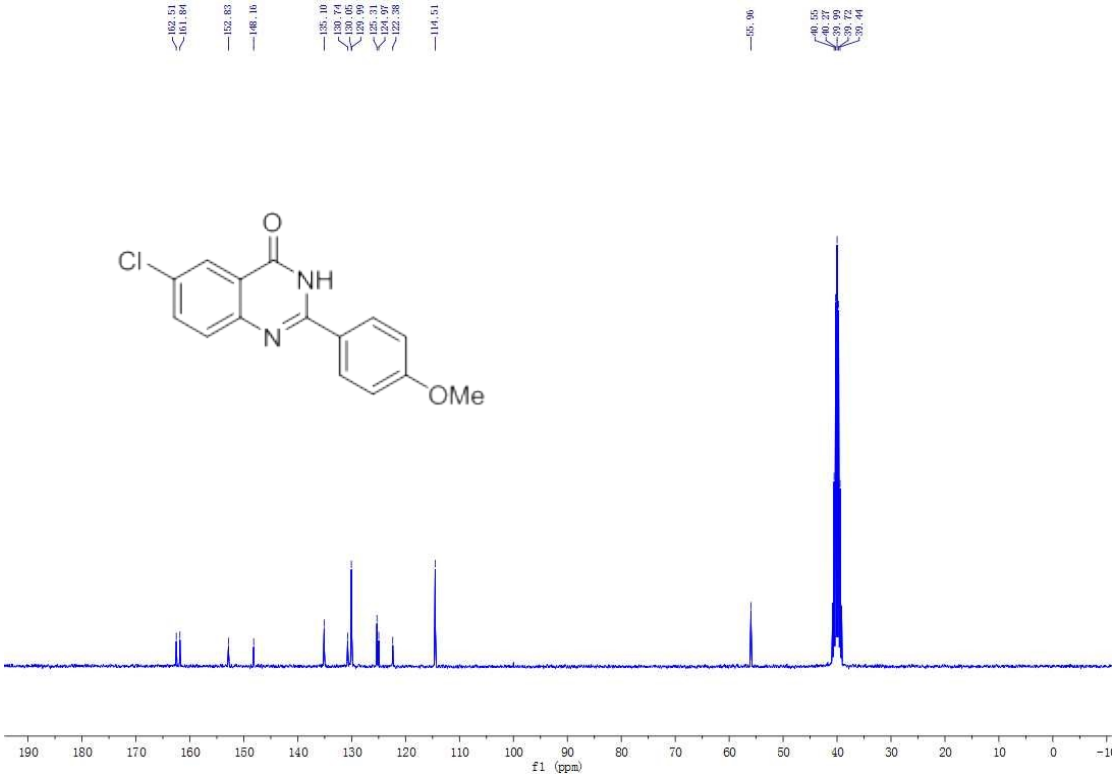
2-(4-methoxyphenyl)-6-methylquinazolin-4(3H)-one (4d):



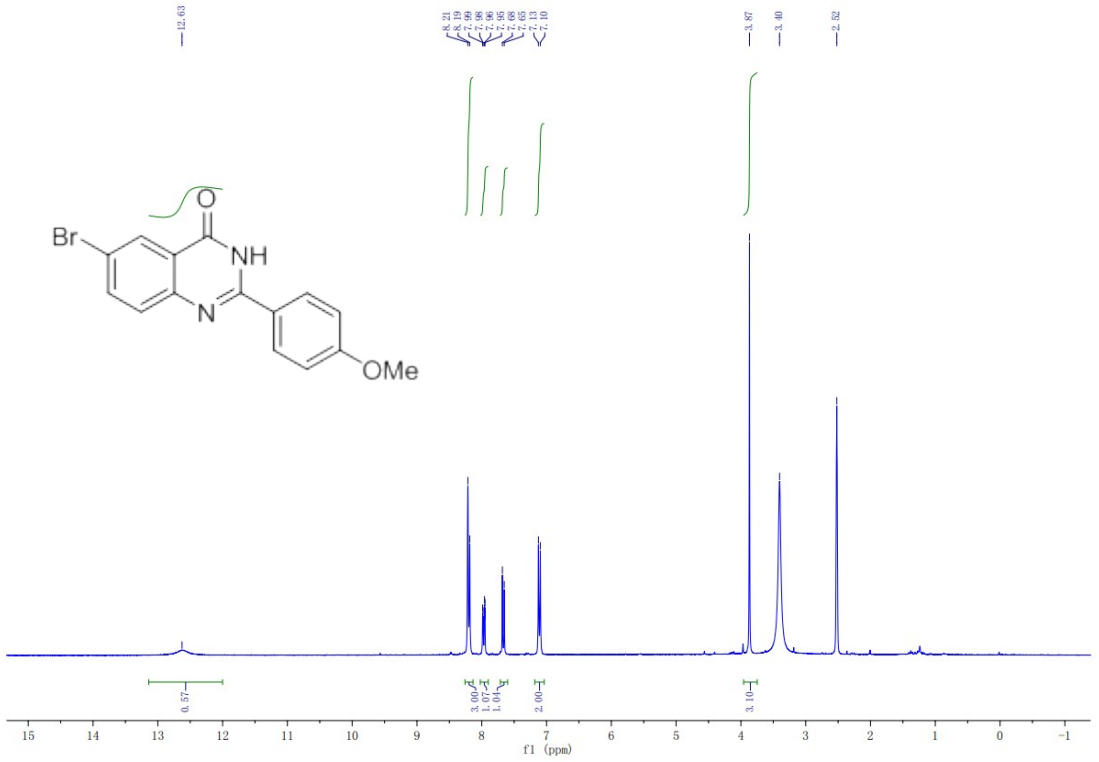


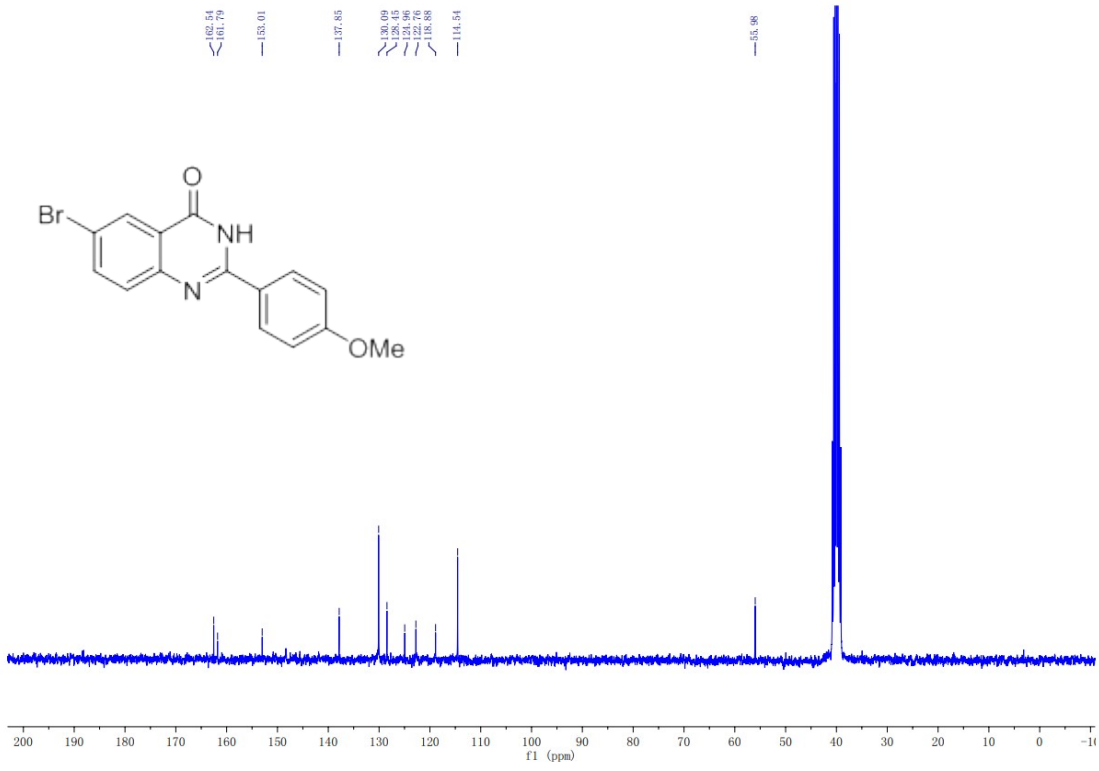
6-chloro-2-(4-methoxyphenyl)quinazolin-4(3H)-one (4e)



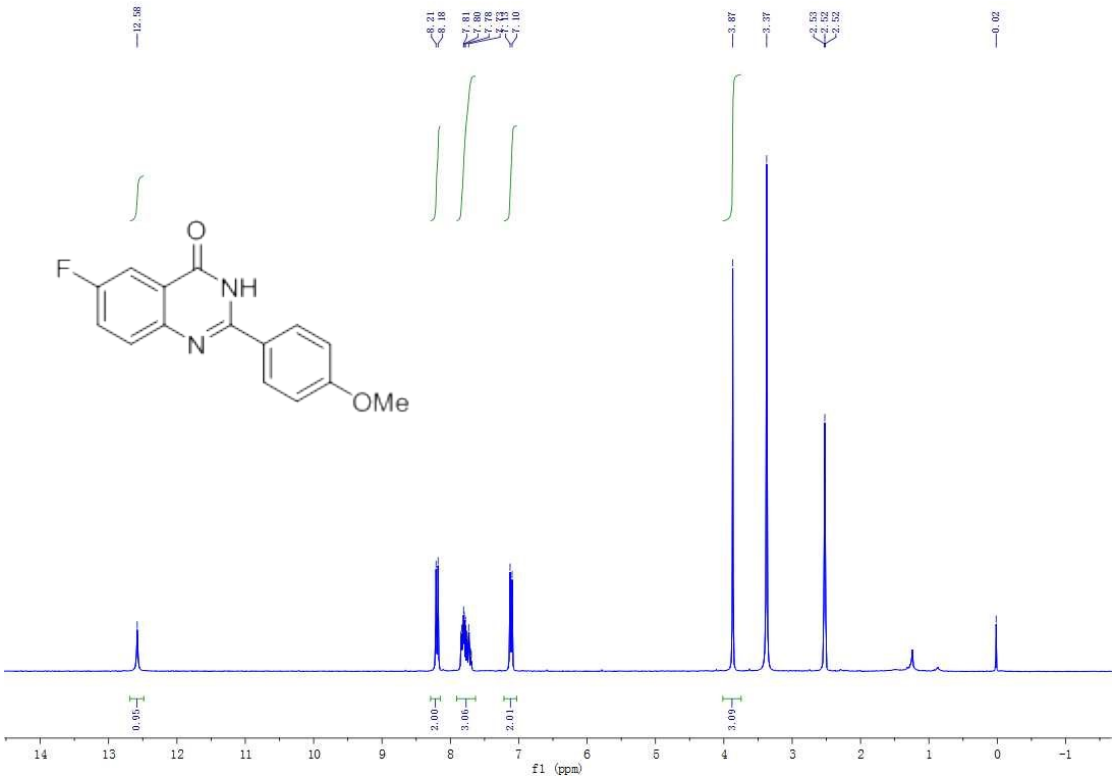


6-bromo-2-(4-methoxyphenyl)quinazolin-4(3H)-one (4f)





6-fluoro-2-(4-methoxyphenyl)quinazolin-4(3H)-one (4g)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3.37
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2.52
2.52
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O
F
NH
N
OMe
0.95
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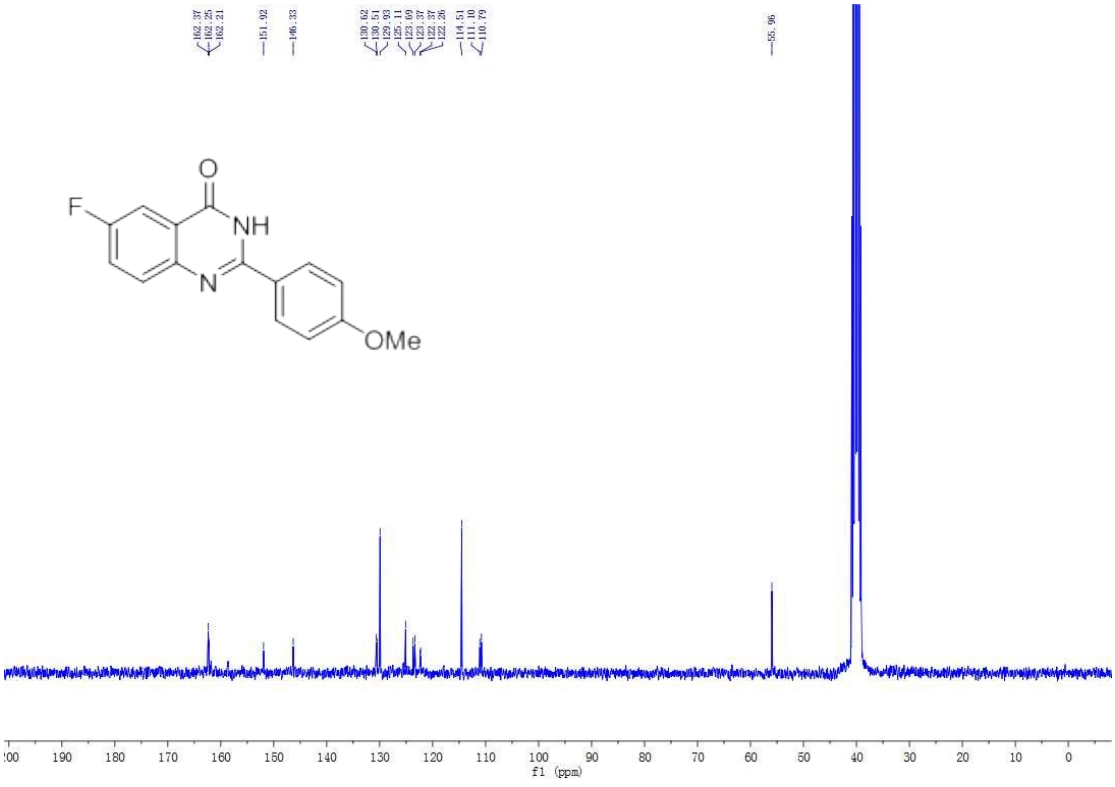
3.06
2.01
3.09
f1 (ppm)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146.33
130.62
130.51
129.93
125.11
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123.07
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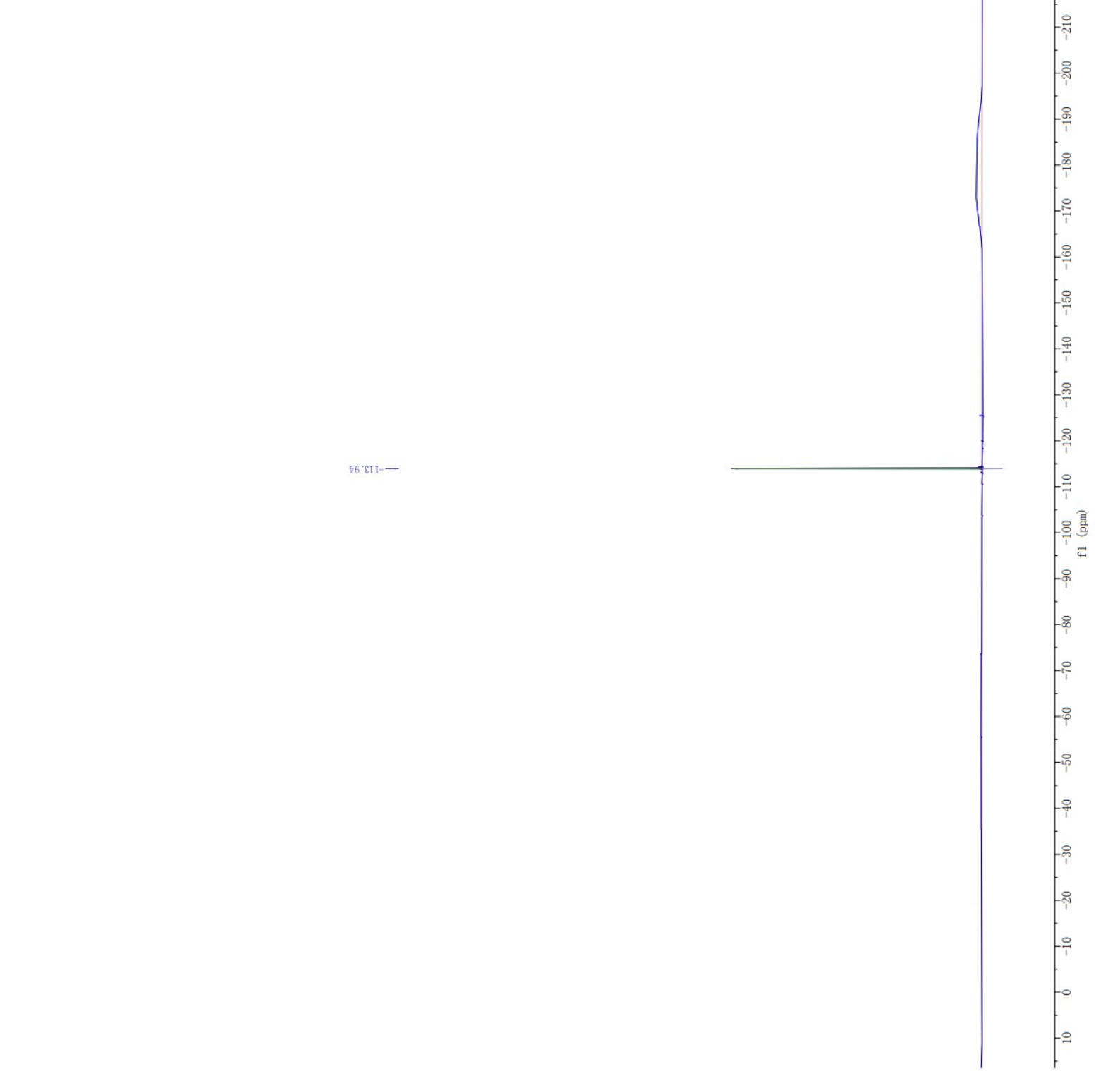
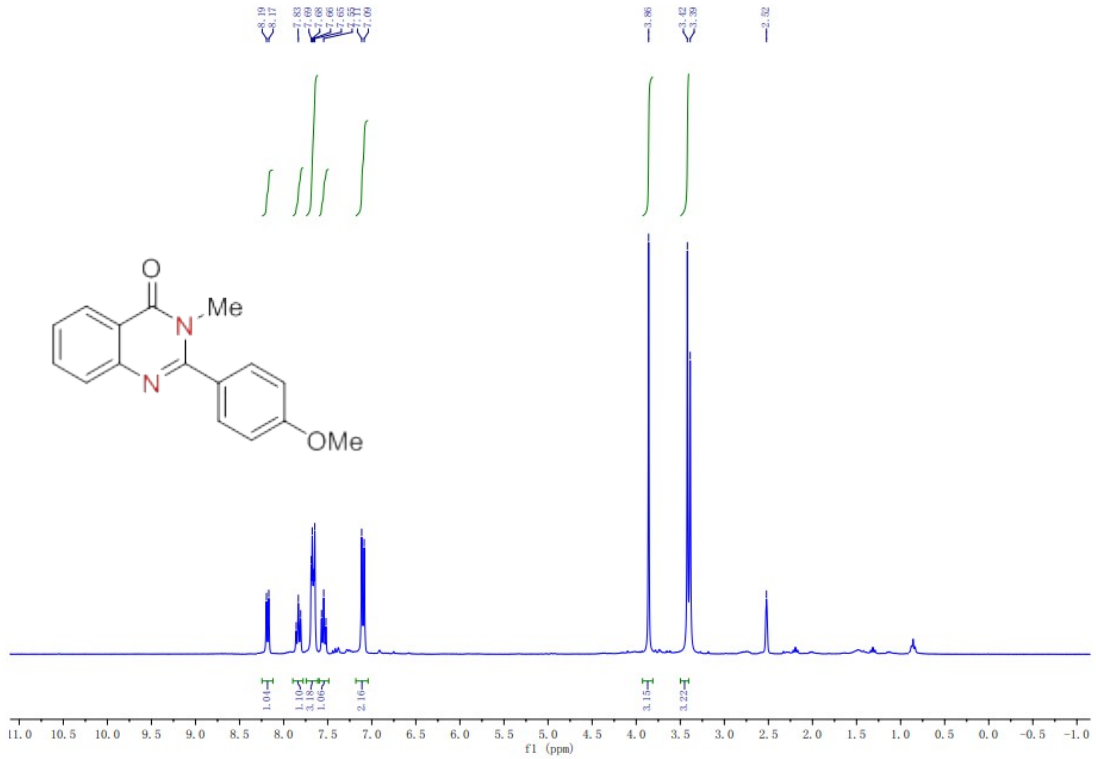
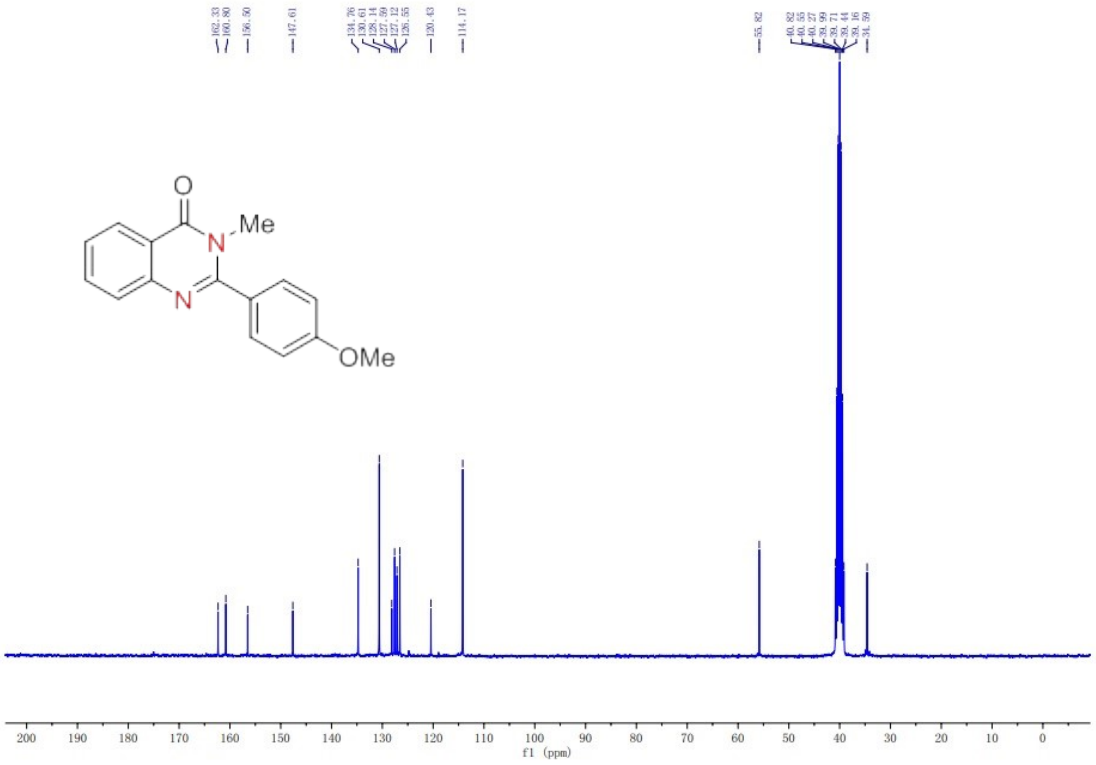
122.26
114.51
111.10
110.79
55.96
O
F
NH
N
OMe
f1 (ppm)

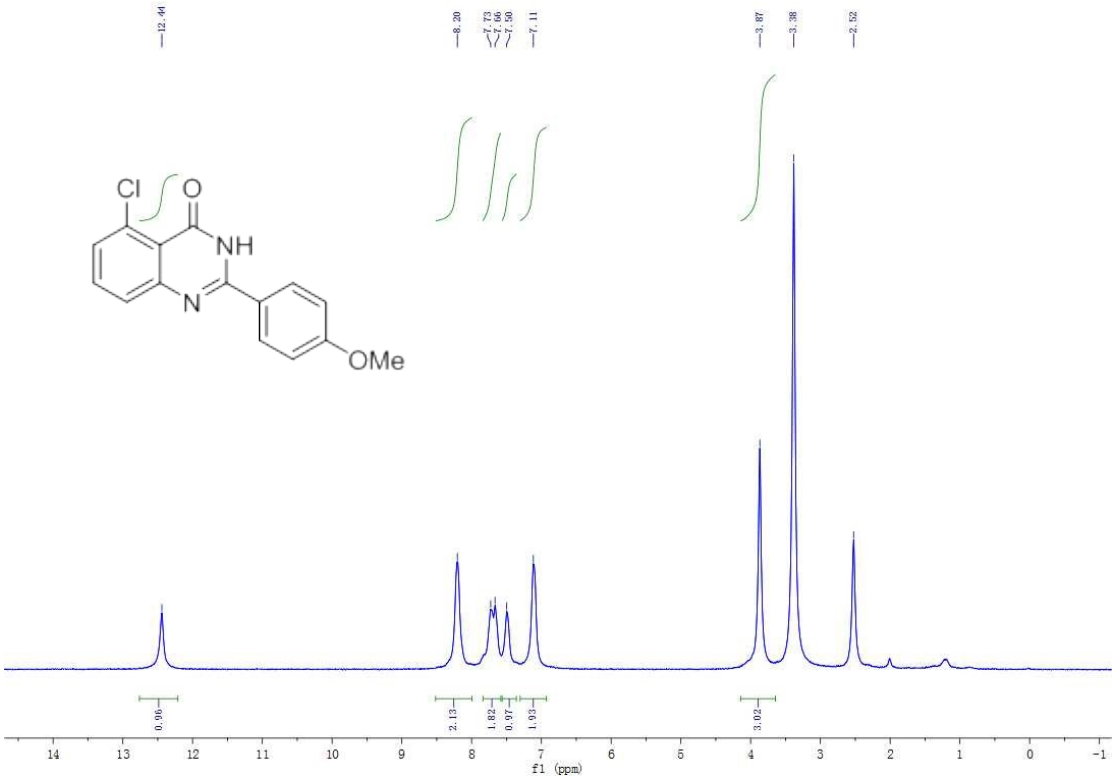


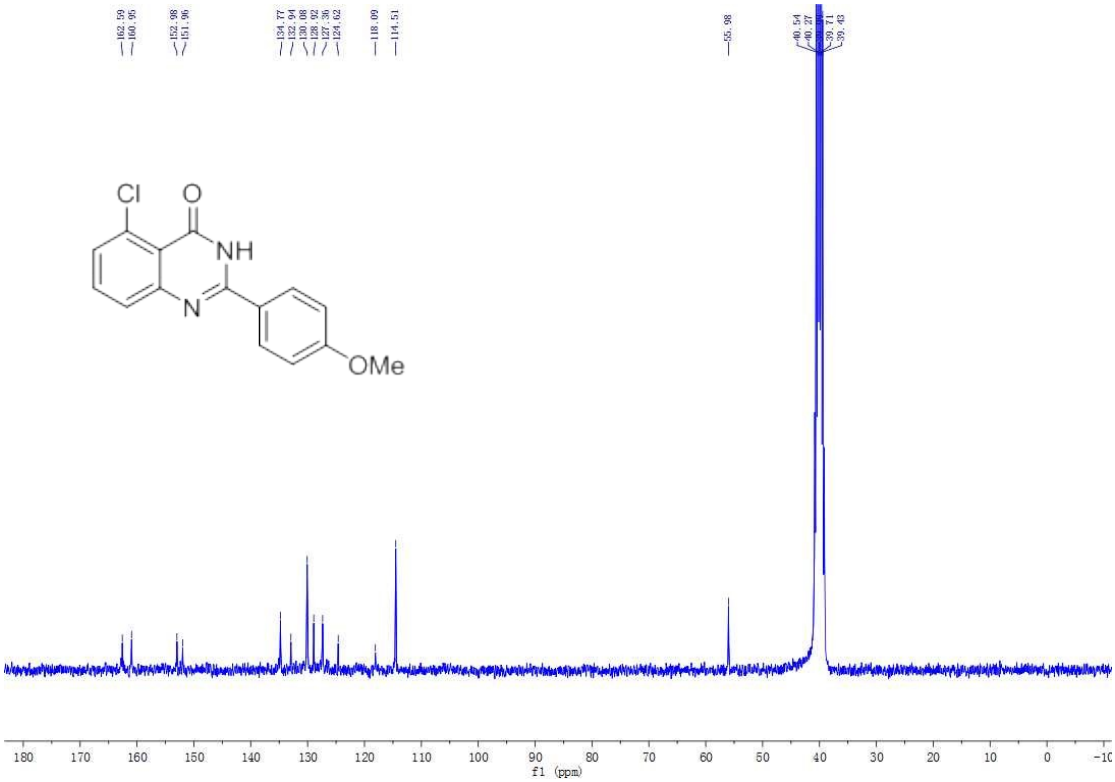
2-(4-methoxyphenyl)-3-methylquinazolin-4(3*H*)-one (4h)



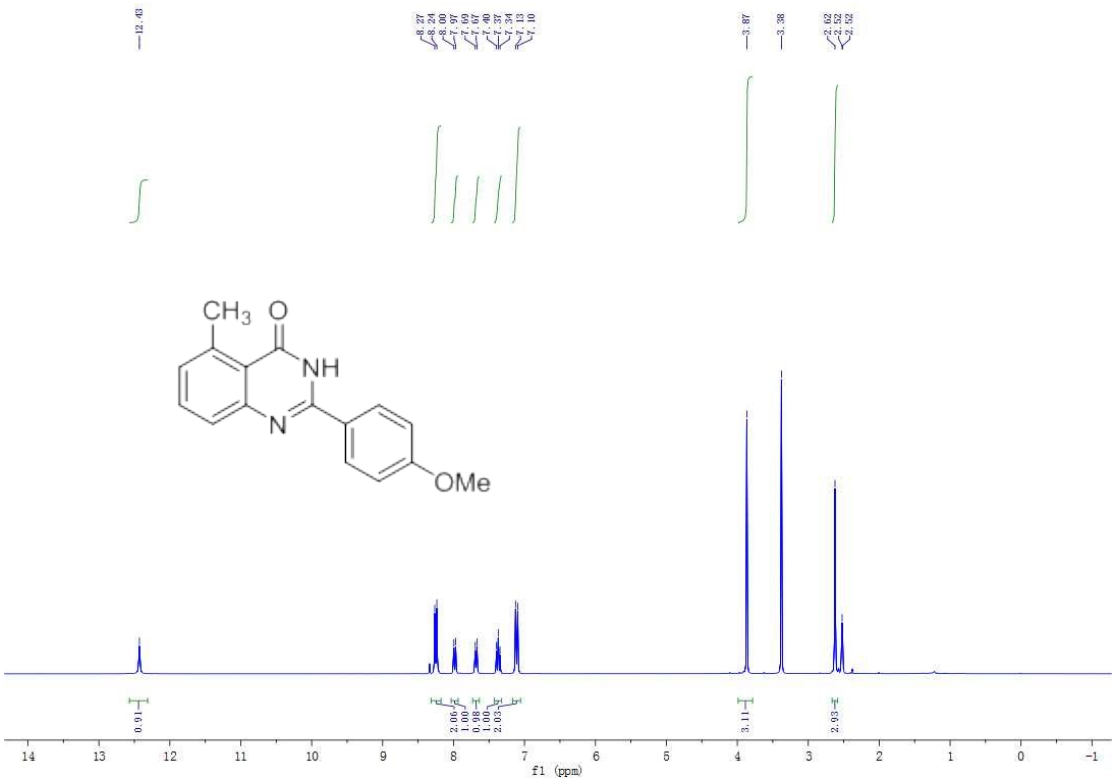


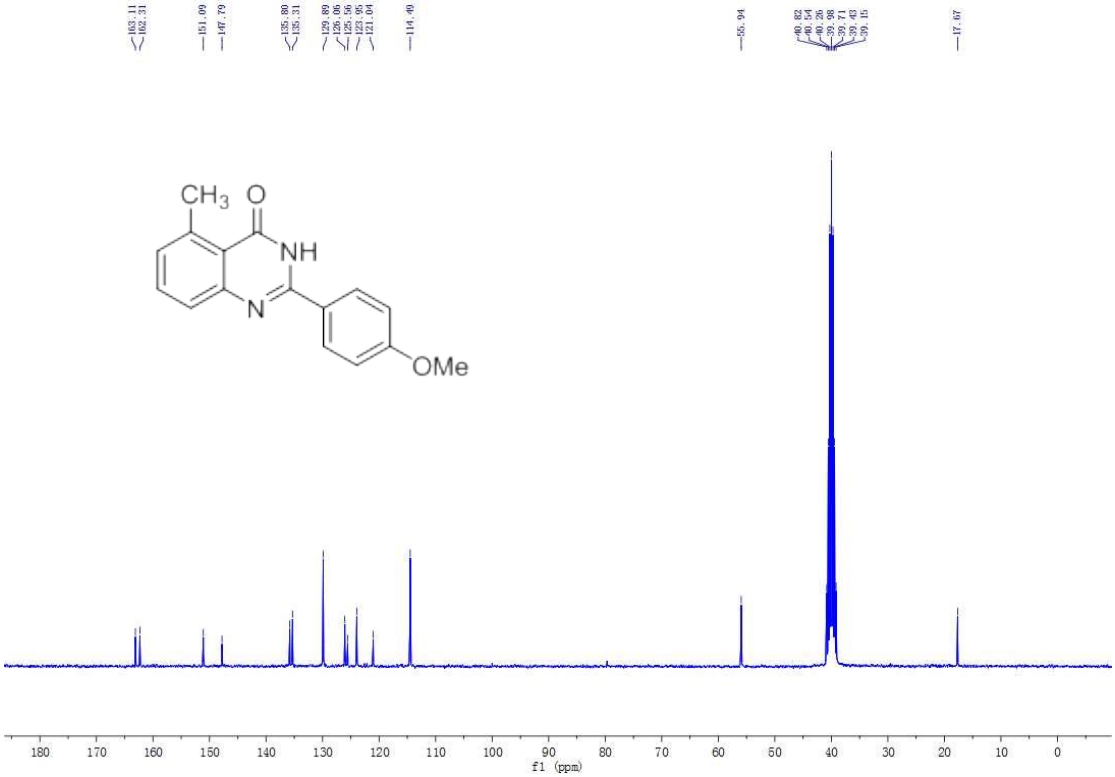
5-chloro-2-(4-methoxyphenyl)quinazolin-4(3*H*)-one (4i)



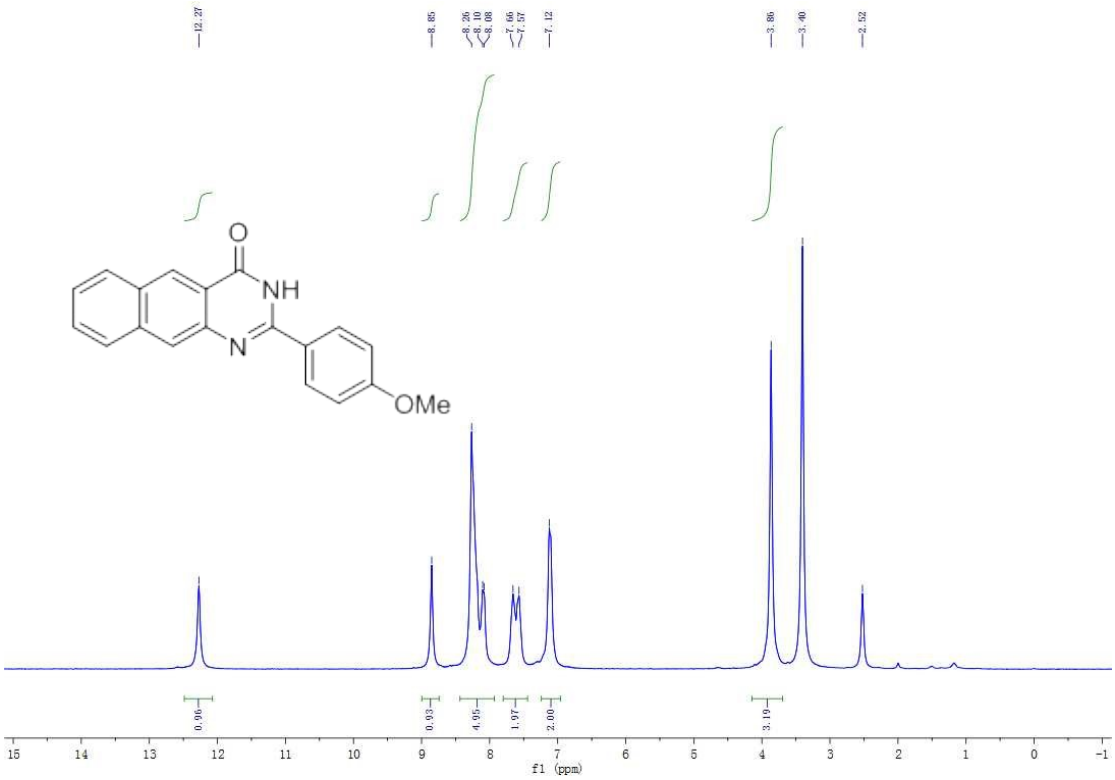


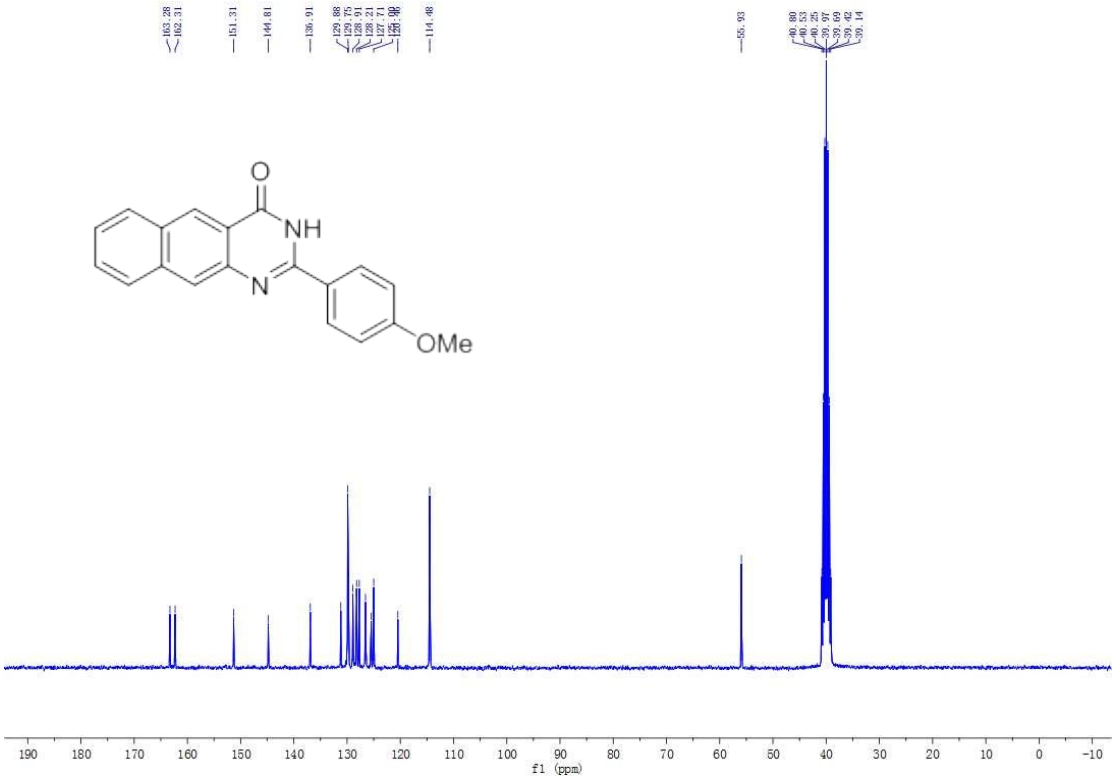
2-(4-methoxyphenyl)-5-methylquinazolin-4(3*H*)-one (4j)





2-(4-methoxyphenyl)benzo[g]quinazolin-4(3*H*)-one (4k)


12.27
8.85
8.26
8.10
8.08
7.66
7.57
7.12
3.86
3.40
2.52
O
NH
N
OMe
0.96
0.93
4.95
1.97
2.00
3.19
f1 (ppm)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162.31
151.31
144.61
136.91
129.88
129.75
128.91
128.21
127.71
125.98
120.48
114.48
55.93
40.80
40.53
40.25
39.97
39.69
39.42
39.14
O
NH
N
OMe
f1 (ppm)