

Supplementary Information

Ultrasound-assisted condensation cyclization reaction: fast synthesis of quinazolinones from *o*-aminobenzamides and aldehydes under ambient conditions

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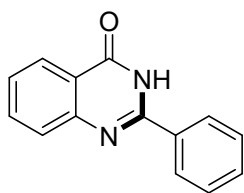
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General Information

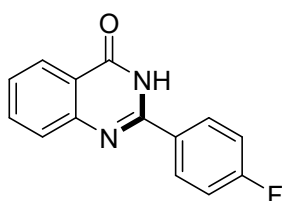
Commercially available reagents were purchased and used without further purification, unless otherwise stated. For the ultrasound irradiation, ultrasound apparatus from KQ3200DV ultrasonic cleaner with a frequency of 40 kHz and an output power of 150 W were used. The reactions were monitored by thin layer chromatography (TLC) on 0.25 mm silica gel plates (GF254) and visualized under UV light. Silica gel (200-300 mesh) was used for flash column chromatography. Nuclear magnetic resonance spectra (^1H NMR and ^{13}C NMR) were recorded on a Bruker Avance 400 spectrometer at 400 MHz and 100 MHz in $\text{DMSO}-d_6$, and chemical shifts were reported as parts per million (ppm). The resonance patterns were annotated as s (singlet), d (doublet), t (triplet) and m (multiplet). The coupling constants (J) were reported in Hertz (Hz). HRMS data were recorded using an Agilent Accurate-Mass Q-TOF LC/MS 6520 instrument with an ESI source.

General procedure for synthesis of products 3

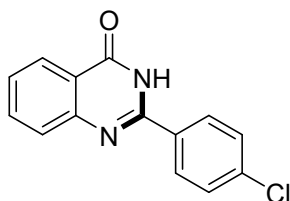
A mixture of *o*-aminobenzamides **1** (1.0 mmol) and aldehydes **2** (1.0 mmol) was prepared in a round bottom flask. The mixture was dissolved in CH_3OH (10 mL) and DDQ (1.2 mmol) was loaded into the round bottom flask. Afterwards, the reaction mixture was subjected to ultrasound irradiation at 60 W for 15 minutes at room temperature. After completion of the reaction, the organic solvent was evaporated. The obtained mixture was quenched by the aqueous sodium sulfite solution, extracted with ethyl acetate (25ml \times 3). The combined organic layer was dried with anhydrous MgSO_4 , and then remove the solvent. The crude product was purified by silica gel column chromatography to give the desired product **3**.



2-Phenylquinazolin-4(3H)-one (3aa). White solid; 90% yield; mp 229-231°C (lit. mp 230-232°C)¹; Rf = 0.48 (petroleum ether/ethyl acetate = 2:1); ¹H NMR (400 MHz, DMSO-*d*₆): δ (ppm) 12.56 (s, 1H), 8.21-8.16 (m, 3H), 7.86-7.83 (m, 1H), 7.76 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.62-7.52 (m, 4H); ¹³C NMR (100 MHz, DMSO-*d*₆): δ (ppm) 162.70, 152.78, 149.22, 135.08, 133.20, 131.86, 129.07, 128.24, 127.99, 127.06, 126.32, 121.47; HRMS (ESI) *m/z*: calcd for C₁₄H₁₁N₂O [M + H]⁺ 223.0866, found 223.0867.

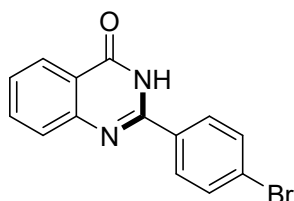


2-(4-Fluorophenyl)quinazolin-4(3H)-one (3ab). Yellow solid; 92% yield; mp 285-287°C (lit. mp 284-286°C)¹; Rf = 0.51 (petroleum ether/ethyl acetate = 2:1); ¹H NMR (400 MHz, DMSO-*d*₆): δ (ppm) 12.61 (s, 1H), 8.23-8.19 (m, 2H), 8.16 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.87-7.83 (m, 1H), 7.75 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.65-7.62 (m, 2H), 7.56-7.52 (m, 1H); ¹³C NMR (100 MHz, DMSO-*d*₆): δ (ppm) 162.67, 151.86, 149.13, 136.78, 135.15, 132.03, 130.10, 129.17, 127.94, 127.26, 126.35, 121.47; ¹⁹F NMR (376 MHz, DMSO-*d*₆): δ (ppm) -109.06; HRMS (ESI) *m/z*: calcd for C₁₄H₁₀FN₂O [M + H]⁺ 241.0772, found 241.0768.

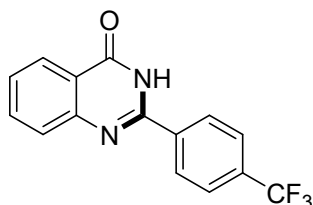


2-(4-Chlorophenyl)quinazolin-4(3H)-one (3ac). White solid; 87% yield; Rf = 0.51 (petroleum ether/ethyl acetate = 2:1); mp >300°C (lit. mp >300°C)¹; ¹H NMR (400 MHz, DMSO-*d*₆): δ

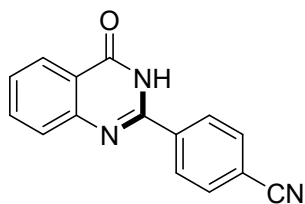
(ppm) 12.61 (s, 1H), 8.23-8.19 (m, 2H), 8.16 (dd, $J = 8.0, 1.5$ Hz, 1H), 7.87-7.83 (m, 1H), 7.75 (dd, $J = 8.3, 1.2$ Hz, 1H), 7.65-7.61 (m, 2H), 7.56-7.52 (m, 1H); ^{13}C NMR (100 MHz, DMSO- d_6): δ (ppm) 162.63, 151.81, 149.05, 136.77, 135.16, 132.03, 130.10, 129.16, 128.00, 127.26, 126.34, 121.49; HRMS (ESI) m/z : calcd for $\text{C}_{14}\text{H}_{10}\text{ClN}_2\text{O}$ [$\text{M} + \text{H}$] $^+$ 257.0476, found 257.0479.



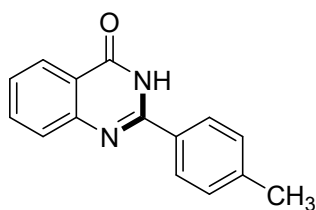
2-(4-Bromophenyl)quinazolin-4(3H)-one (3ad). Yellow solid; 91% yield; mp 292-293°C (lit. mp 292-294°C)¹; $R_f = 0.48$ (petroleum ether/ethyl acetate = 2:1); ^1H NMR (400 MHz, DMSO- d_6): δ (ppm) 12.61 (s, 1H), 8.17-8.12 (m, 3H), 7.87-7.83 (m, 1H), 7.79-7.74 (m, 3H), 7.56-7.52 (m, 1H); ^{13}C NMR (100 MHz, DMSO- d_6): δ (ppm) 162.62, 151.94, 149.05, 135.16, 132.40, 132.10, 130.28, 128.01, 127.28, 126.35, 125.70, 121.50; HRMS (ESI) m/z : calcd for $\text{C}_{14}\text{H}_{10}\text{BrN}_2\text{O}$ [$\text{M} + \text{H}$] $^+$ 300.9971, found 300.9969.



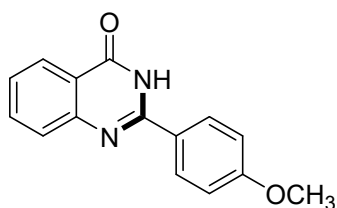
2-(4-(Trifluoromethyl)phenyl)quinazolin-4(3H)-one (3ae): White solid; 91% yield; mp 280-282°C (lit. mp 284-286°C)²; $R_f = 0.55$ (petroleum ether/ethyl acetate = 2:1); ^1H NMR (400 MHz, DMSO- d_6): δ (ppm) 12.76 (s, 1H), 8.38 (d, $J = 8.1$ Hz, 2H), 8.19 (dd, $J = 8.0, 1.6$ Hz, 1H), 7.93 (d, $J = 8.2$ Hz, 2H), 7.87 (td, $J = 7.6, 1.6$ Hz, 1H), 7.79 (d, $J = 8.1$ Hz, 1H), 7.57 (t, $J = 7.5$ Hz, 1H); ^{13}C NMR (100 MHz, DMSO- d_6): δ (ppm) 162.59, 151.66, 148.91, 137.09, 135.21, 131.74, 131.43, 129.21, 128.16, 127.59, 126.37, 125.91, 121.68; ^{19}F NMR (376 MHz, DMSO- d_6): δ (ppm) -61.34; HRMS (ESI) m/z : calcd for $\text{C}_{15}\text{H}_{10}\text{F}_3\text{N}_2\text{O}$ [$\text{M} + \text{H}$] $^+$ 291.0669, found 291.0667.



2-(4-Cyanophenyl)quinazolin-4(3H)-one (3af): White solid; 88% yield; mp > 300°C (lit. mp > 300°C)³; Rf = 0.47 (petroleum ether/ethyl acetate = 1:1); ¹H NMR (400 MHz, DMSO-*d*₆): δ (ppm) 12.75 (s, 1H), 8.36-8.33 (m, 2H), 8.18 (dd, *J* = 8.0, 1.6 Hz, 1H), 8.06-8.03 (m, 2H), 7.88 (ddd, *J* = 8.5, 7.1, 1.6 Hz, 1H), 7.80-7.77 (m, 1H), 7.58 (ddd, *J* = 8.2, 7.1, 1.3 Hz, 1H); ¹³C NMR (100 MHz, DMSO-*d*₆): δ (ppm) 162.54, 137.37, 135.26, 133.01, 129.11, 127.74, 126.39, 121.68, 118.82, 114.07; HRMS (ESI) *m/z*: calcd for C₁₅H₁₀N₃O [M + H]⁺ 248.0749, found 248.0746.

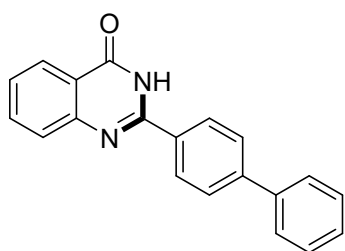


2-(4-Methylphenyl)quinazolin-4(3H)-one (3ag): White solid; 80% yield; mp 240-242°C (lit. mp 241-243°C)²; Rf = 0.48 (petroleum ether/ethyl acetate = 2:1); ¹H NMR (400 MHz, DMSO-*d*₆): δ (ppm) 12.47 (s, 1H), 8.15 (dd, *J* = 7.9, 1.5 Hz, 1H), 8.11 (d, *J* = 8.3 Hz, 2H), 7.86-7.81 (m, 1H), 7.73 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.53-7.49 (m, 1H), 7.36 (d, *J* = 8.3 Hz, 2H), 2.40 (s, 3H); ¹³C NMR (100 MHz, DMSO-*d*₆): δ (ppm) 162.37, 152.31, 148.83, 141.52, 134.63, 129.92, 129.25, 127.73, 127.42, 126.45, 125.89, 120.91, 21.04; HRMS (ESI) *m/z*: calcd for C₁₅H₁₃N₂O [M + H]⁺ 237.1022, found 237.1020.

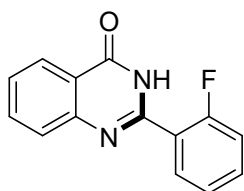


2-(4-Methoxyphenyl)quinazolin-4(3H)-one (3ah): White solid; 82% yield; mp 228-230°C (lit. mp

230-232°C)⁴; Rf = 0.57 (petroleum ether/ethyl acetate = 1:1); ¹H NMR (400 MHz, DMSO-*d*₆): δ (ppm) 12.42 (s, 1H), 8.22-8.18 (m, 2H), 8.14 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.84-7.80 (m, 1H), 7.71 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.51-7.47 (m, 1H), 7.11-7.08 (m, 2H), 3.86 (s, 3H); ¹³C NMR (100 MHz, DMSO-*d*₆): δ (ppm) 162.21, 161.77, 151.76, 148.85, 134.46, 129.36, 127.20, 126.04, 125.73, 124.70, 120.60, 113.90, 55.37; HRMS (ESI) *m/z*: calcd for C₁₅H₁₃N₂O₂ [M + H]⁺ 253.0972, found 253.0976.

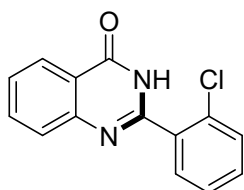


2-(Biphenyl-4-yl)quinazolin-4(3H)-one (3ai): White solid; 85% yield; mp 265-267°C (lit. mp 265-267°C)⁵; Rf = 0.46 (petroleum ether/ethyl acetate = 1:1); ¹H NMR (400 MHz, DMSO-*d*₆): δ (ppm) 12.59 (s, 1H), 8.32-8.30 (m, 2H), 8.17 (d, *J* = 7.9 Hz, 1H), 7.87 (dd, *J* = 8.5, 2.2 Hz, 3H), 7.80-7.76 (m, 3H), 7.52 (t, *J* = 7.4 Hz, 3H), 7.45-7.43 (m, 1H); ¹³C NMR (100 MHz, DMSO-*d*₆): δ (ppm) 162.75, 152.44, 149.23, 143.34, 139.44, 135.11, 132.04, 129.56, 128.87, 128.67, 127.33, 127.24, 127.07, 126.36, 121.46; HRMS (ESI) *m/z*: calcd for C₂₀H₁₅N₂O [M + H]⁺ 299.1110, found 299.1106.

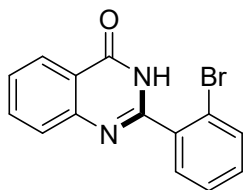


2-(2-Fluorophenyl)quinazolin-4(3H)-one (3aj): White solid; 90% yield; mp 163-164°C (lit. mp 162-163°C)⁶; Rf = 0.40 (petroleum ether/ethyl acetate = 2:1) ¹H NMR (400 MHz, DMSO-*d*₆): δ (ppm) 12.59 (s, 1H), 8.19 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.87 (td, *J* = 7.6, 1.6 Hz, 1H), 7.81 (td, *J* = 7.6,

1.7 Hz, 1H), 7.75 (d, $J = 8.1$ Hz, 1H), 7.67-7.61 (m, 1H), 7.60 – 7.56 (m, 1H), 7.42 (d, $J = 10.6$ Hz, 1H), 7.38 (d, $J = 7.3$ Hz, 1H); ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$): δ (ppm) 161.96, 150.42, 149.16, 135.07, 133.27, 131.50, 127.98, 127.50, 126.33, 125.10, 122.82, 121.59, 116.75; ^{19}F NMR (376 MHz, $\text{DMSO-}d_6$): δ (ppm) -114.65; HRMS (ESI) m/z : calcd for $\text{C}_{14}\text{H}_9\text{FN}_2\text{O}$ $[\text{M} + \text{H}]^+$ 241.0770, found 241.0769.

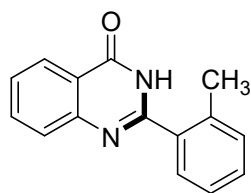


2-(2-Chlorophenyl)quinazolin-4(3H)-one (3ak): White solid; 86% yield; mp 194-196°C (lit. mp 196-197°C)⁷; $R_f = 0.58$ (petroleum ether/ethyl acetate = 1:1); ^1H NMR (400 MHz, $\text{DMSO-}d_6$): δ (ppm) 12.65 (s, 1H), 8.19 (d, $J = 7.9$ Hz, 1H), 7.87 (t, $J = 7.6$ Hz, 1H), 7.72 (d, $J = 8.1$ Hz, 1H), 7.69 (dd, $J = 7.5, 1.6$ Hz, 1H), 7.63 (d, $J = 7.9$ Hz, 1H), 7.58 (t, $J = 7.6$ Hz, 2H), 7.51 (t, $J = 7.4$ Hz, 1H); ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$): δ (ppm) 161.90, 152.74, 149.04, 135.06, 134.29, 132.09, 131.96, 131.35, 130.07, 127.94, 127.70, 127.54, 126.32, 121.71; HRMS (ESI) m/z : calcd for $\text{C}_{14}\text{H}_{10}\text{ClN}_2\text{O}$ $[\text{M} + \text{H}]^+$ 257.0478, found 257.0475.

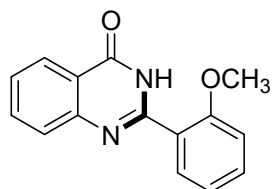


2-(2-Bromophenyl)quinazolin-4(3H)-one (3al): White solid; 91% yield; mp 174-176°C (lit. mp 174-176°C)⁴; $R_f = 0.32$ (petroleum ether/ethyl acetate = 2:1); ^1H NMR (400 MHz, $\text{DMSO-}d_6$): δ (ppm) 12.62 (s, 1H), 8.18 (dd, $J = 7.9, 1.6$ Hz, 1H), 7.88-7.84 (m, 1H), 7.78 (dd, $J = 7.9, 1.3$ Hz, 1H), 7.71 (dd, $J = 8.3, 1.1$ Hz, 1H), 7.65 (dd, $J = 7.5, 1.9$ Hz, 1H), 7.60-7.46 (m, 3H); ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$): δ (ppm) 161.89, 153.81, 149.03, 136.34, 135.06, 133.11, 132.14, 131.25, 128.15,

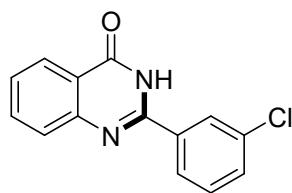
127.95, 127.52, 126.31, 121.74, 121.44; HRMS (ESI) m/z : calcd for $C_{14}H_{10}BrN_2O$ $[M + H]^+$
300.9971, found 300.9972.



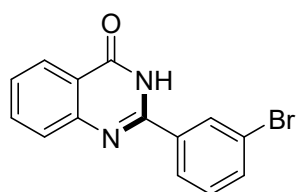
2-(2-Methylphenyl)quinazolin-4(3H)-one (3am): White solid; 84% yield; mp 214-215°C (lit. mp 216-218°C)²; R_f = 0.40 (petroleum ether/ethyl acetate = 2:1); 1H NMR (400 MHz, $DMSO-d_6$): δ (ppm) 12.44 (s, 1H), 8.17 (dd, J = 7.9, 1.6 Hz, 1H), 7.86-7.82 (m, 1H), 7.69 (dd, J = 8.3, 1.2 Hz, 1H), 7.57-7.50 (m, 2H), 7.44 (td, J = 7.4, 1.5 Hz, 1H), 7.36-7.31 (m, 2H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, $DMSO-d_6$): δ (ppm) 161.66, 154.26, 148.62, 135.99, 134.37, 134.12, 130.42, 129.78, 129.02, 127.26, 126.53, 125.67, 125.58, 120.87, 19.45; HRMS (ESI) m/z : calcd for $C_{15}H_{13}N_2O$ $[M + H]^+$ 237.1022, found 237.1022.



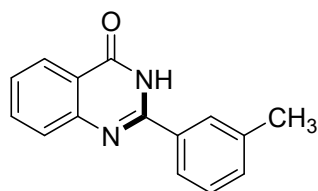
2-(2-Methoxyphenyl)quinazolin-4(3H)-one (3an): White solid; 80% yield; mp 200-202°C (lit. mp 200-202°C)¹; R_f = 0.48 (petroleum ether/ethyl acetate = 1:1); 1H NMR (500 MHz, $DMSO-d_6$): δ (ppm) 12.11 (s, 1H), 8.16 (dd, J = 8.0, 1.6 Hz, 1H), 7.86-7.80 (m, 1H), 7.72 (td, J = 5.9, 3.0 Hz, 2H), 7.58-7.51 (m, 2H), 7.20 (d, J = 8.4 Hz, 1H), 7.10 (t, J = 7.5 Hz, 1H), 3.87 (s, 3H); ^{13}C NMR (125 MHz, $DMSO-d_6$): δ (ppm) 161.71, 157.62, 152.84, 149.51, 134.89, 132.70, 130.93, 127.86, 127.03, 126.26, 123.14, 121.48, 120.91, 112.35, 56.26; HRMS (ESI) m/z : calcd for $C_{15}H_{13}N_2O_2$ $[M + H]^+$ 253.0975, found 253.0976.



2-(3-Chlorophenyl)quinazolin-4(3H)-one (3ao): White solid; 88% yield; mp 253-254°C (lit. mp 252-254°C)⁸; R_f = 0.51 (petroleum ether/ethyl acetate = 2:1); ¹H NMR (400 MHz, DMSO-*d*₆): δ (ppm) 12.63 (s, 1H), 8.25 (t, *J* = 1.9 Hz, 1H), 8.16 (tt, *J* = 5.9, 1.4 Hz, 2H), 7.86 (ddd, *J* = 8.5, 7.0, 1.6 Hz, 1H), 7.79-7.76 (m, 1H), 7.68-7.66 (m, 1H), 7.59 (d, *J* = 7.9 Hz, 1H), 7.57-7.54 (m, 1H); ¹³C NMR (100 MHz, DMSO-*d*₆): δ (ppm) 162.57, 151.46, 148.94, 135.18, 133.93, 131.64, 131.01, 128.10, 127.42, 126.90, 126.35, 121.59; HRMS (ESI) *m/z*: calcd for C₁₄H₁₀ClN₂O [M + H]⁺ 257.0475, found 257.0478

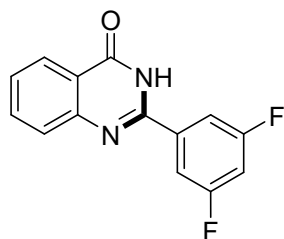


2-(3-Bromophenyl)quinazolin-4(3H)-one (3ap): Yellow solid; 89% yield; mp 295-296°C (lit. mp 295-296°C)⁷; R_f = 0.5 (petroleum ether/ethyl acetate = 2:1); ¹H NMR (400 MHz, DMSO-*d*₆): δ (ppm) 12.63 (s, 1H), 8.38 (t, *J* = 1.9 Hz, 1H), 8.21-8.15 (m, 2H), 7.88-7.76 (m, 3H), 7.57-7.51 (m, 2H); ¹³C NMR (100 MHz, DMSO-*d*₆): δ (ppm) 161.98, 150.79, 148.36, 134.82, 134.59, 133.94, 130.65, 130.30, 127.52, 126.83, 126.68, 125.77, 121.79, 121.03; HRMS (ESI) *m/z*: calcd for C₁₄H₁₀BrN₂O [M + H]⁺ 300.9971, found 300.9974.

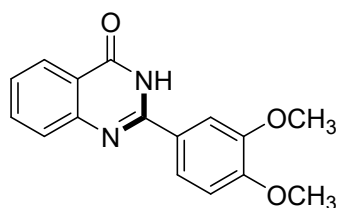


2-(3-Methylphenyl)quinazolin-4(3H)-one (3aq): White solid; 83% yield; mp 212-214°C (lit. mp 211-212°C)⁹; R_f = 0.53 (petroleum ether/ethyl acetate = 2:1); ¹H NMR (400 MHz, DMSO-*d*₆): δ

(ppm) 12.48 (s, 1H), 8.17 (dd, $J = 7.9, 1.6$ Hz, 1H), 8.04 (s, 1H), 8.00-7.97 (m, 1H), 7.87-7.82 (m, 1H), 7.75 (d, $J = 8.1$ Hz, 1H), 7.55-7.51 (m, 1H), 7.46-7.42 (m, 2H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, DMSO- d_6): δ (ppm) 162.72, 152.90, 149.17, 138.39, 135.05, 133.10, 132.48, 128.97, 128.76, 127.87, 127.00, 126.32, 125.36, 121.43, 21.44; HRMS (ESI) m/z : calcd for $\text{C}_{15}\text{H}_{13}\text{N}_2\text{O}$ [$\text{M} + \text{H}$] $^+$ 237.1026, found 237.1024.

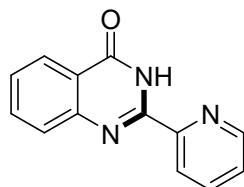


2-(3,5-Difluorophenyl)quinazolin-4(3H)-one (3ar): White solid; 89% yield; mp 260-262°C (lit. mp 259-260°C)⁵; $R_f = 0.51$ (petroleum ether/ethyl acetate = 3:1); ^1H NMR (400 MHz, DMSO- d_6): δ (ppm) 12.65 (s, 1H), 8.17 (dd, $J = 7.8, 1.5$ Hz, 1H), 7.94 (d, $J = 2.1$ Hz, 1H), 7.92-7.91 (m, 1H), 7.87 (ddd, $J = 8.5, 7.1, 1.5$ Hz, 1H), 7.78 (d, $J = 8.1$ Hz, 1H), 7.59-7.55 (m, 1H), 7.51 (dt, $J = 9.1, 2.3$ Hz, 1H); ^{13}C NMR (100 MHz, DMSO- d_6): δ (ppm) 163.99, 162.49, 161.67, 150.39, 148.63, 136.68, 135.26, 127.71, 126.37, 121.70, 107.28, 107.02; ^{19}F NMR (376 MHz, DMSO- d_6): δ (ppm) -108.72; HRMS (ESI) m/z : calcd for $\text{C}_{14}\text{H}_9\text{F}_2\text{N}_2\text{O}$ [$\text{M} + \text{H}$] $^+$ 259.0605, found 259.0608.

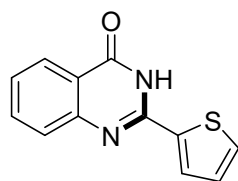


2-(3,4-Dimethoxyphenyl)quinazolin-4(3H)-one (3as): White solid; 80% yield; mp 241-242°C (lit. mp 242-243°C)⁶; $R_f = 0.38$ (petroleum ether/ethyl acetate = 1:1); ^1H NMR (400 MHz, DMSO- d_6): δ (ppm) 12.44 (s, 1H), 8.14 (dd, $J = 8.0, 1.5$ Hz, 1H), 7.88 (dd, $J = 8.5, 2.2$ Hz, 1H), 7.84-7.80 (m, 2H), 7.72 (dd, $J = 8.3, 1.2$ Hz, 1H), 7.51-7.47 (m, 1H), 7.12 (d, $J = 8.5$ Hz, 1H), 3.89 (s, 3H), 3.85

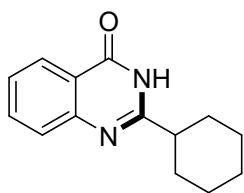
(s, 3H); ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$): δ (ppm) 162.26, 151.73, 151.47, 148.81, 148.44, 134.46, 127.23, 126.04, 125.74, 124.63, 121.04, 120.60, 111.25, 110.54, 55.57; HRMS (ESI) m/z : calcd for $\text{C}_{16}\text{H}_{15}\text{N}_2\text{O}_3$ $[\text{M} + \text{H}]^+$ 253.0972, found 253.0976.



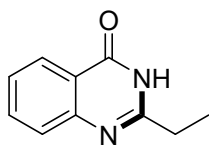
2-(Pyridin-2-yl)quinazolin-4(3H)-one (3at): White solid; 88% yield; mp 171-173°C (lit. mp 170-173°C)²; R_f = 0.5 (dichloromethane/methanol = 16:1); ^1H NMR (400 MHz, $\text{DMSO-}d_6$): δ (ppm) 11.78 (s, 1H), 8.75 (d, J = 4.8 Hz, 1H), 8.44 (d, J = 7.9 Hz, 1H), 8.19 (d, J = 7.9 Hz, 1H), 8.06 (t, J = 7.9 Hz, 1H), 7.88-7.78 (m, 2H), 7.66-7.55 (m, 2H); ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$): δ (ppm) 160.69, 149.87, 148.90, 148.60, 148.32, 137.91, 134.63, 127.62, 127.19, 126.49, 126.01, 122.08, 121.92; HRMS (ESI) m/z : calcd for $\text{C}_{13}\text{H}_{10}\text{N}_3\text{O}$ $[\text{M} + \text{H}]^+$ 224.0818, found 224.0821.



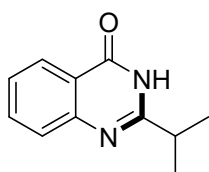
2-(Thiophene-2-yl)quinazolin-4(3H)-one (3au): White solid; 81% yield; mp 272-273°C (lit. mp 275-276°C)¹; R_f = 0.42 (petroleum ether/ethyl acetate = 2:1); ^1H NMR (400 MHz, $\text{DMSO-}d_6$): δ (ppm) 12.67 (s, 1H), 8.25 (d, J = 4.4 Hz, 1H), 8.14 (d, J = 7.8 Hz, 1H), 7.88 (d, J = 5.0 Hz, 1H), 7.83-7.80 (m, 1H), 7.66 (d, J = 8.1 Hz, 1H), 7.50 (t, J = 7.8 Hz, 1H), 7.25 (t, J = 4.4 Hz, 1H); ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$): δ (ppm) 161.70, 148.56, 147.74, 137.29, 134.61, 132.08, 129.32, 128.43, 126.87, 126.25, 125.90, 120.80; HRMS (ESI) m/z : calcd for $\text{C}_{12}\text{H}_9\text{N}_2\text{OS}$ $[\text{M} + \text{H}]^+$ 229.0430, found 229.0432.



2-Cyclohexylquinazolin-4(3H)-one (3av): White solid; 75% yield; mp 229-230°C (lit. mp 229-230°C)⁶; Rf = 0.46 (petroleum ether/ethyl acetate = 2:1); ¹H NMR (400 MHz, DMSO-*d*₆): δ (ppm) 12.09 (s, 1H), 8.09 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.77 (ddd, *J* = 8.5, 7.1, 1.6 Hz, 1H), 7.61 (d, *J* = 8.2 Hz, 1H), 7.48-7.44 (m, 1H), 2.59 (tt, *J* = 11.7, 3.4 Hz, 1H), 1.92 (dd, *J* = 12.8, 3.3 Hz, 2H), 1.80 (dt, *J* = 12.2, 3.1 Hz, 2H), 1.70 -1.66 (m, 1H), 1.59 (qd, *J* = 12.4, 3.1 Hz, 2H), 1.37-1.21 (m, 3H); ¹³C NMR (100 MHz, DMSO-*d*₆): δ (ppm) 162.39, 161.22, 149.40, 134.66, 127.42, 126.34, 126.12, 121.42, 43.30, 30.66, 25.97, 25.80; HRMS (ESI) *m/z*: calcd for C₁₄H₁₇N₂O [M + H]⁺ 229.1260, found 229.1263.

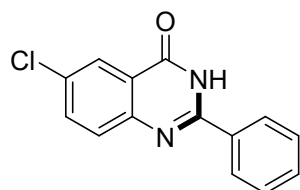


2-Ethylquinazolin-4(3H)-one (3aw): White solid; 76% yield; mp 226-227°C (lit. mp 228-230°C)⁷; Rf = 0.38 (petroleum ether/ethyl acetate = 1:1); ¹H NMR (400 MHz, DMSO-*d*₆): δ (ppm) 12.18 (s, 1H), 8.09 (d, *J* = 7.9 Hz, 1H), 7.78 (t, *J* = 7.7 Hz, 1H), 7.61 (d, *J* = 8.1 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 1H), 2.63 (q, *J* = 7.5 Hz, 2H), 1.26 (t, *J* = 7.5 Hz, 3H); ¹³C NMR (100 MHz, DMSO-*d*₆): δ (ppm) 161.70, 158.22, 148.86, 134.15, 126.71, 125.81, 125.59, 120.73, 27.74, 11.19; HRMS (ESI) *m/z*: calcd for C₁₀H₁₁N₂O [M + H]⁺ 175.0866, found 175.0868.

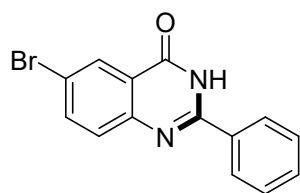


2-Isopropylquinazolin-4(3H)-one (3ax): White solid; 78% yield; mp 222-224°C (lit. mp 225-

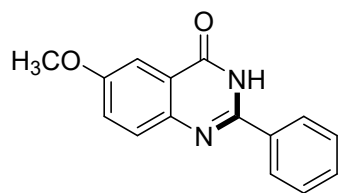
228°C)¹⁰; Rf = 0.39 (petroleum ether/ethyl acetate = 2:1); ¹H NMR (400 MHz, DMSO-*d*₆): δ (ppm) 12.14 (s, 1H), 8.09 (d, *J* = 7.8 Hz, 1H), 7.78 (t, *J* = 7.7 Hz, 1H), 7.62 (d, *J* = 8.2 Hz, 1H), 7.47 (t, *J* = 7.5 Hz, 1H), 2.89 (m, 1H), 1.27 (d, *J* = 6.9 Hz, 6H); ¹³C NMR (100 MHz, DMSO-*d*₆): δ (ppm) 161.83, 161.46, 148.77, 134.16, 126.87, 125.86, 125.56, 120.82, 33.19, 20.27; HRMS (ESI) *m/z*: calcd for C₁₁H₁₃N₂O [M + H]⁺ 189.1022, found 189.1026.



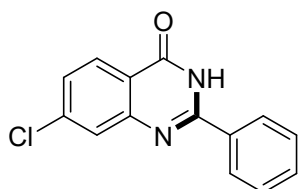
6-Chloro-2-phenylquinazolin-4(3H)-one (3ba): White solid; 90% yield; mp 295-296°C (lit. mp 296-297°C)⁷; Rf = 0.56 (petroleum ether/ethyl acetate = 2:1); ¹H NMR (400 MHz, DMSO-*d*₆): δ (ppm) 12.72 (s, 1H), 8.19-8.16 (m, 2H), 8.09 (d, *J* = 2.5 Hz, 1H), 7.87 (dd, *J* = 8.7, 2.5 Hz, 1H), 7.77 (d, *J* = 8.7 Hz, 1H), 7.61-7.53 (m, 3H); ¹³C NMR (100 MHz, DMSO-*d*₆): δ (ppm) 161.79, 153.33, 147.95, 135.19, 132.94, 132.09, 131.25, 130.22, 129.12, 128.33, 125.36, 122.72; HRMS (ESI) *m/z*: calcd for C₁₄H₁₀ClN₂O [M + H]⁺ 257.0476, found 257.0478.



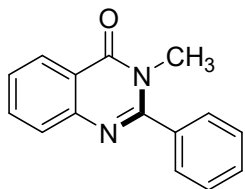
6-Bromo-2-phenylquinazolin-4(3H)-one (3ca): Yellow solid; 88% yield; mp 285-287°C (lit. mp 284-286°C)²; Rf = 0.54 (petroleum ether/ethyl acetate = 2:1); ¹H NMR (400 MHz, DMSO-*d*₆): δ (ppm) 12.73 (m, 1H), 8.23 (d, *J* = 2.3 Hz, 1H), 8.19-8.17 (m, 2H), 7.98 (dd, *J* = 8.7, 2.3 Hz, 1H), 7.70 (d, *J* = 8.7 Hz, 1H), 7.61-7.54 (m, 3H); ¹³C NMR (100 MHz, DMSO-*d*₆): δ (ppm) 161.08, 152.83, 147.65, 137.33, 132.35, 131.53, 129.79, 128.54, 127.89, 127.75, 122.51, 118.83; HRMS (ESI) *m/z*: calcd for C₁₄H₁₀BrN₂O [M + H]⁺ 300.9971, found 300.9973.



6-Methoxy-2-phenylquinazolin-4(3H)-one (3da): White solid; 82% yield; mp 249-251°C (lit. mp 244-246°C)²; R_f = 0.5 (petroleum ether/ethyl acetate = 1:1); ¹H NMR (400 MHz, DMSO-*d*₆): δ (ppm) 12.53 (s, 1H), 8.17 (d, *J* = 7.3 Hz, 2H), 7.72 (d, *J* = 8.9 Hz, 1H), 7.58-7.53 (m, 4H), 7.46 (dd, *J* = 8.9, 2.9 Hz, 1H), 3.91 (s, 3H); ¹³C NMR (100 MHz, DMSO-*d*₆): δ (ppm) 161.95, 157.65, 149.98, 143.12, 132.70, 130.95, 129.14, 128.49, 127.40, 124.02, 121.70, 105.75, 55.55; HRMS (ESI) *m/z*: calcd for C₁₅H₁₃N₂O₂ [M + H]⁺ 253.0972, found 253.0975.

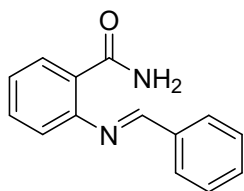


7-Chloro-2-phenylquinazolin-4(3H)-one (3ea): White solid; 89% yield; mp 283-285°C (lit. mp 284-286°C)²; R_f = 0.47 (petroleum ether/ethyl acetate = 2:1); ¹H NMR (400 MHz, DMSO-*d*₆): δ (ppm) 12.68 (s, 1H), 8.19-8.14 (m, 3H), 7.80 (d, *J* = 2.0 Hz, 1H), 7.64-7.54 (m, 4H); ¹³C NMR (100 MHz, DMSO-*d*₆): δ (ppm) 161.57, 153.66, 149.78, 139.07, 132.28, 131.61, 128.54, 127.83, 126.69, 126.49, 119.72; HRMS (ESI) *m/z*: calcd for C₁₄H₁₀ClN₂O [M + H]⁺ 257.0476, found 257.0475.



3-Methyl-2-phenylquinazolin-4(3H)-one (3fa): White solid; 79% yield; mp 123-125°C (lit. mp 125-127°C)²; R_f = 0.55 (petroleum ether/ethyl acetate = 2:1); ¹H NMR (400 MHz, DMSO-*d*₆): δ (ppm) 8.19 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.86-7.82 (m, 1H), 7.69-7.67 (m, 3H), 7.58-7.54 (m, 4H), 3.37 (s, 3H); ¹³C NMR (100 MHz, DMSO-*d*₆): δ (ppm) 161.55, 156.05, 146.96, 135.30, 134.26, 129.70,

128.31, 128.17, 127.08, 126.79, 125.99, 120.05, 33.80; HRMS (ESI) m/z : calcd for $C_{15}H_{13}N_2O$ [$M + H$]⁺ 237.1022, found 237.1025.

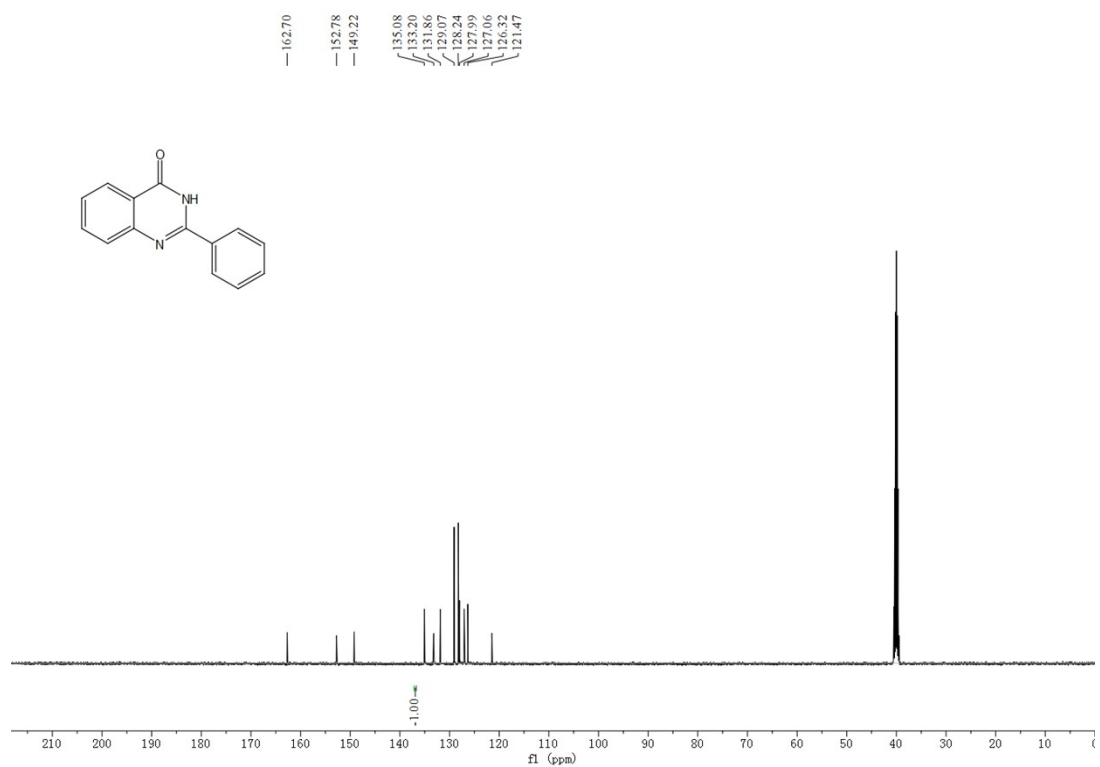
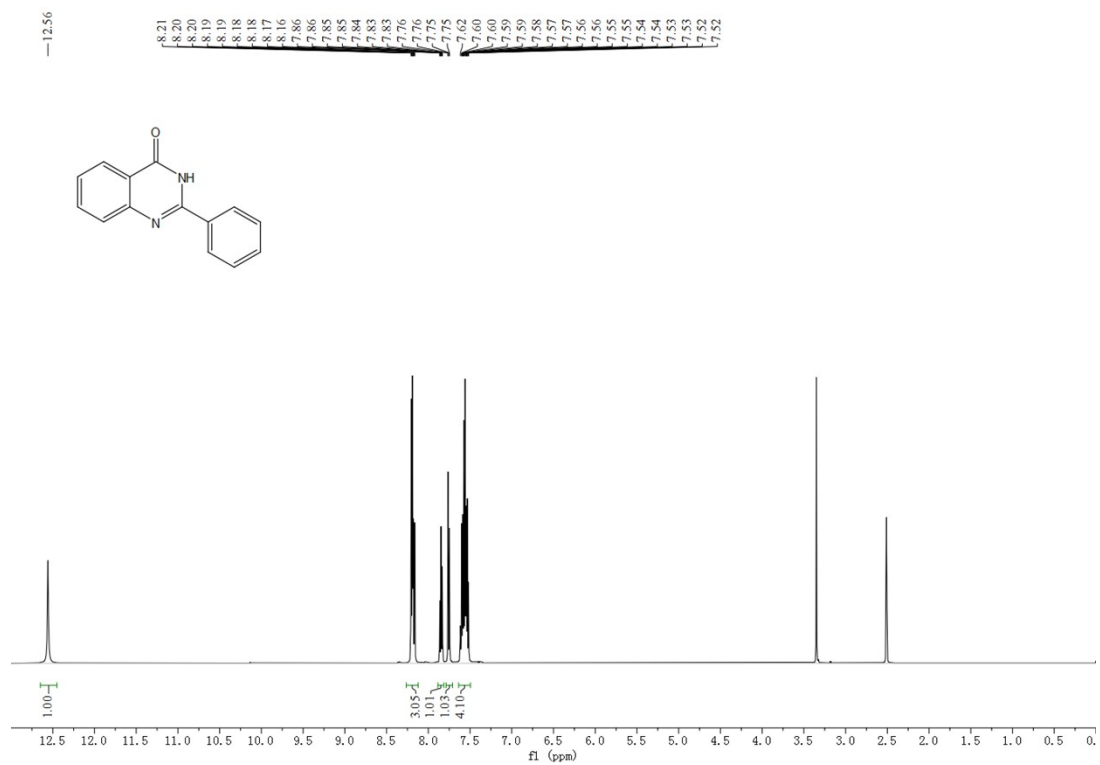


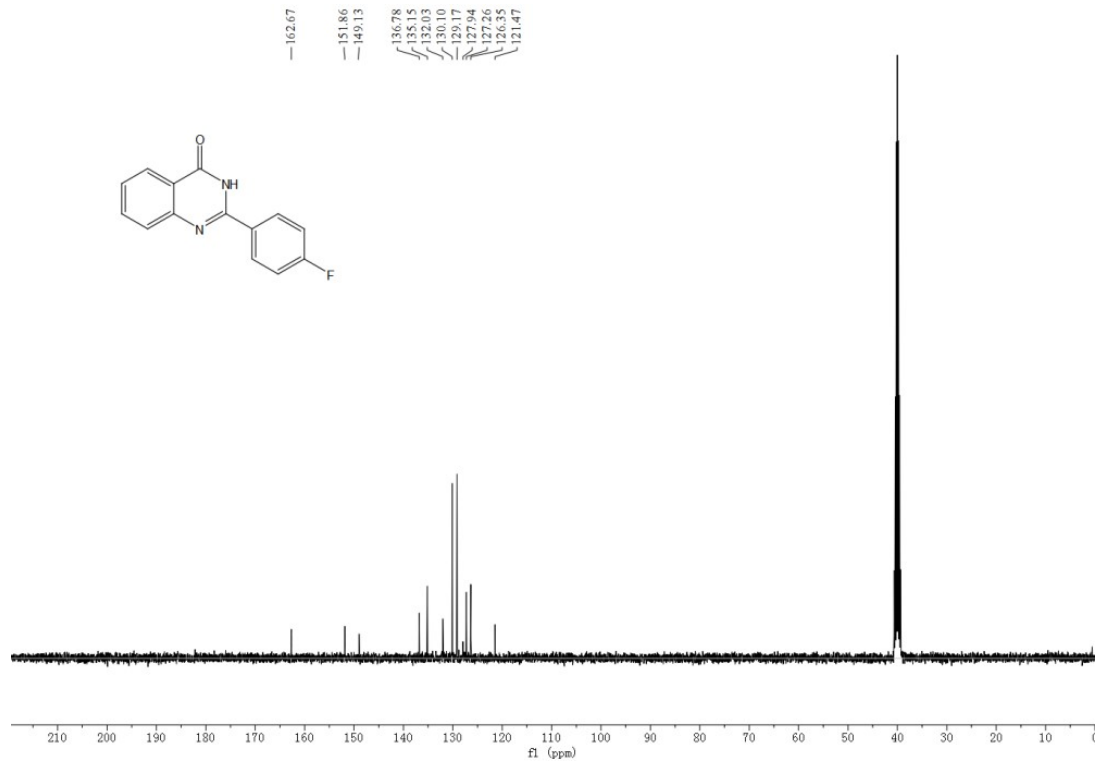
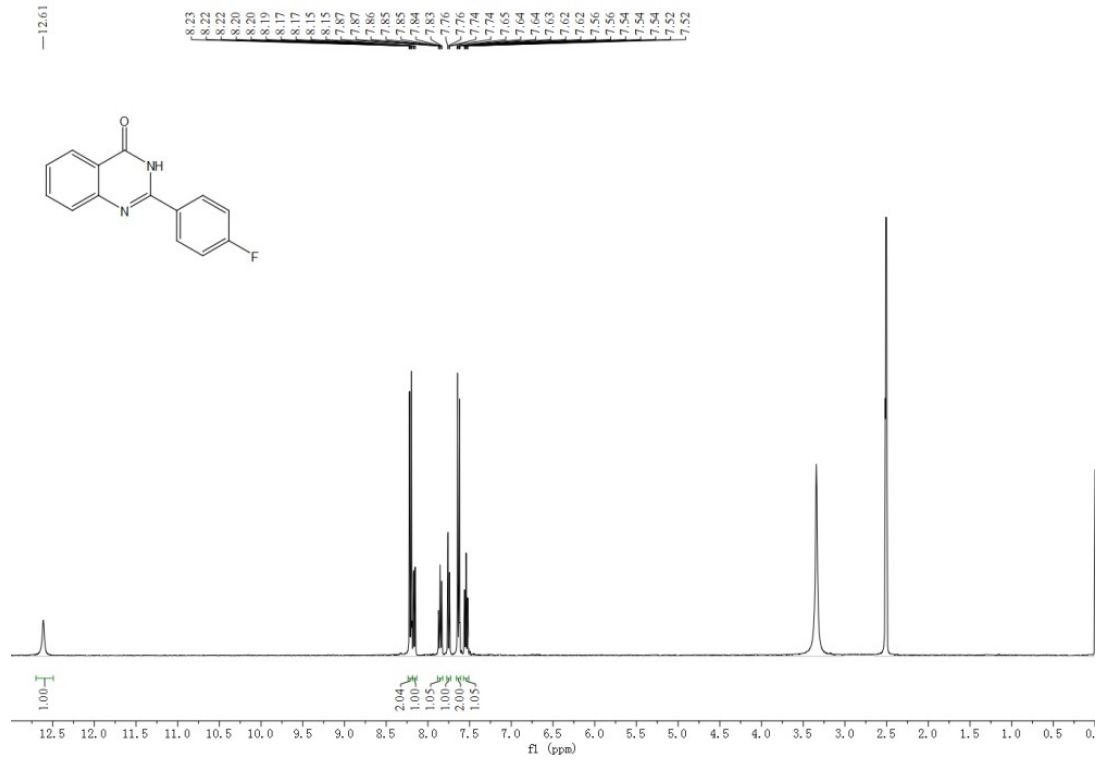
2-(Benzylideneamino)benzamide (A): White solid; 45% yield; mp 200-202°C; R_f = 0.59 (petroleum ether/ethyl acetate = 1:1); 1H NMR (400 MHz, $DMSO-d_6$): δ (ppm) 8.62 (s, 1H), 8.25 (s, 1H), 7.99-7.96 (m, 2H), 7.94 (dd, J = 7.8, 1.6 Hz, 1H), 7.67 (s, 1H), 7.61-7.54 (m, 4H), 7.38-7.34 (m, 1H), 7.24 (dd, J = 7.9, 1.2 Hz, 1H); ^{13}C NMR (100 MHz, $DMSO-d_6$): δ (ppm) 167.16, 162.23, 149.28, 135.41, 132.06, 131.89, 129.74, 128.92, 127.82, 125.90, 119.30; HRMS (ESI) m/z : calcd for $C_{14}H_{13}N_2O$ [$M + H$]⁺ 225.1029, found 225.1028.

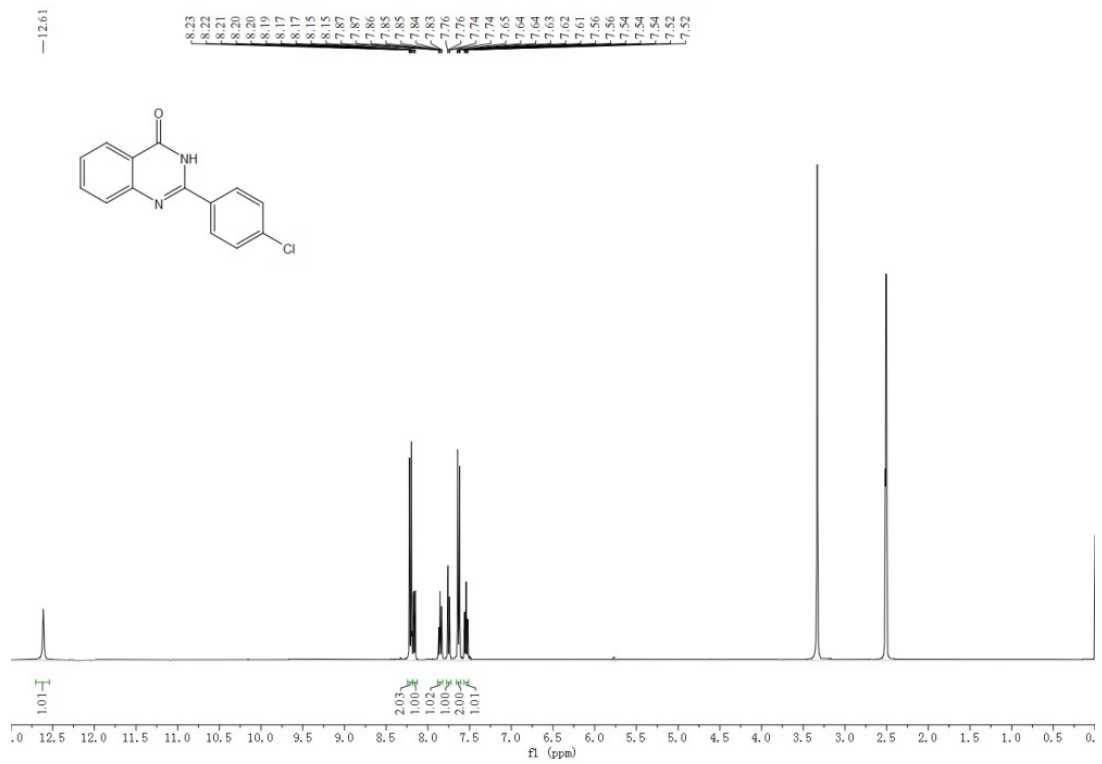
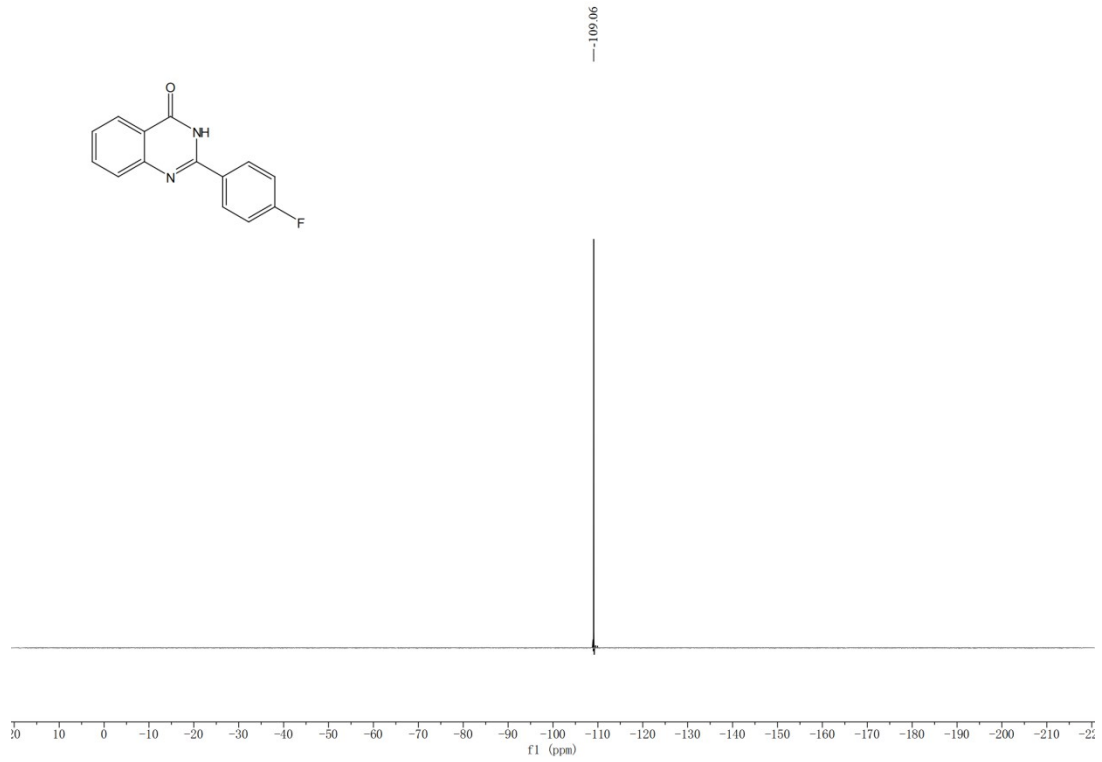
References

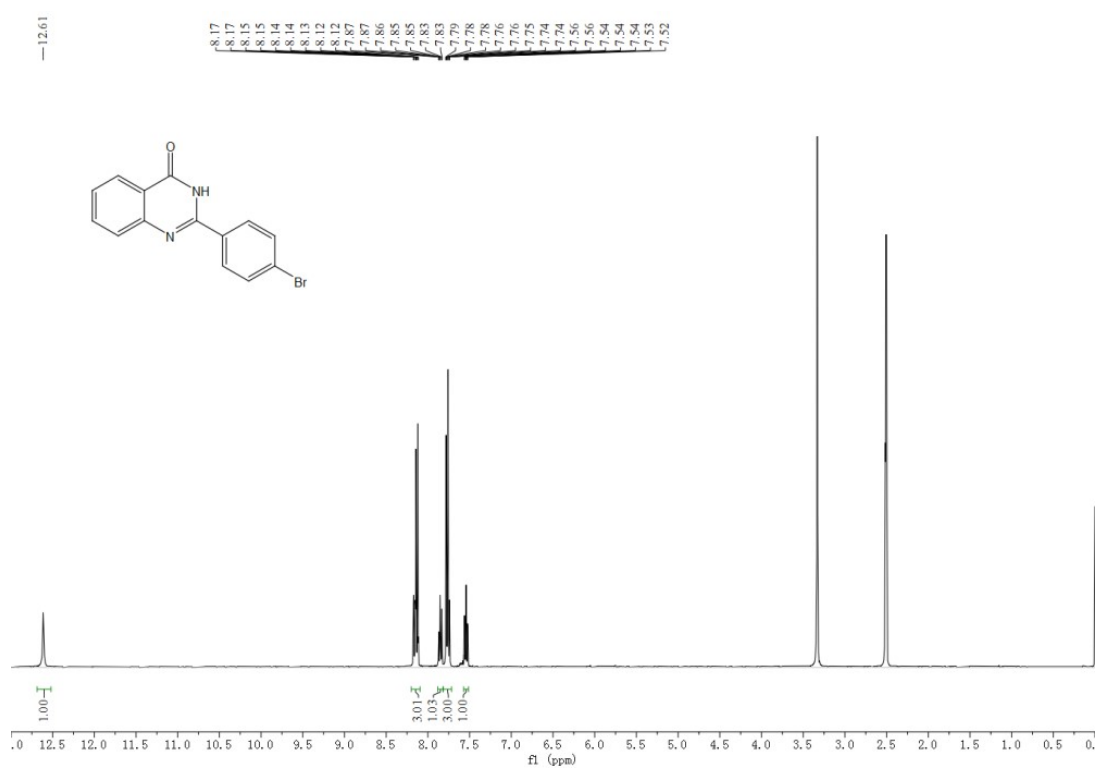
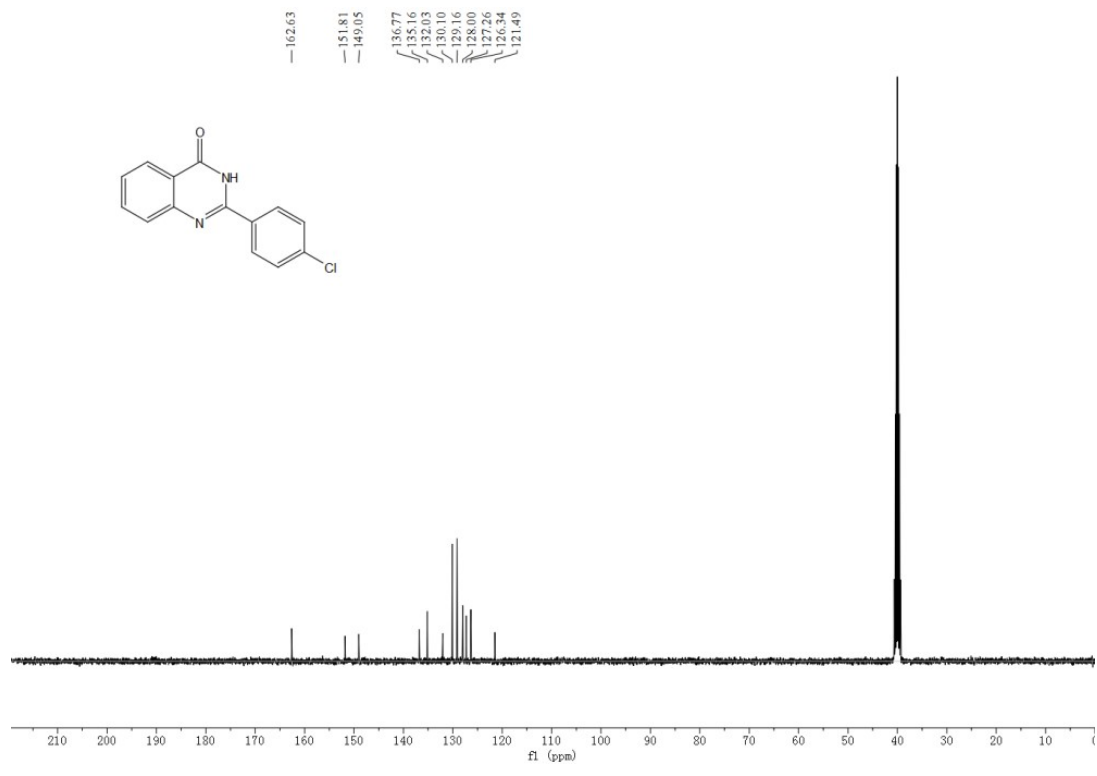
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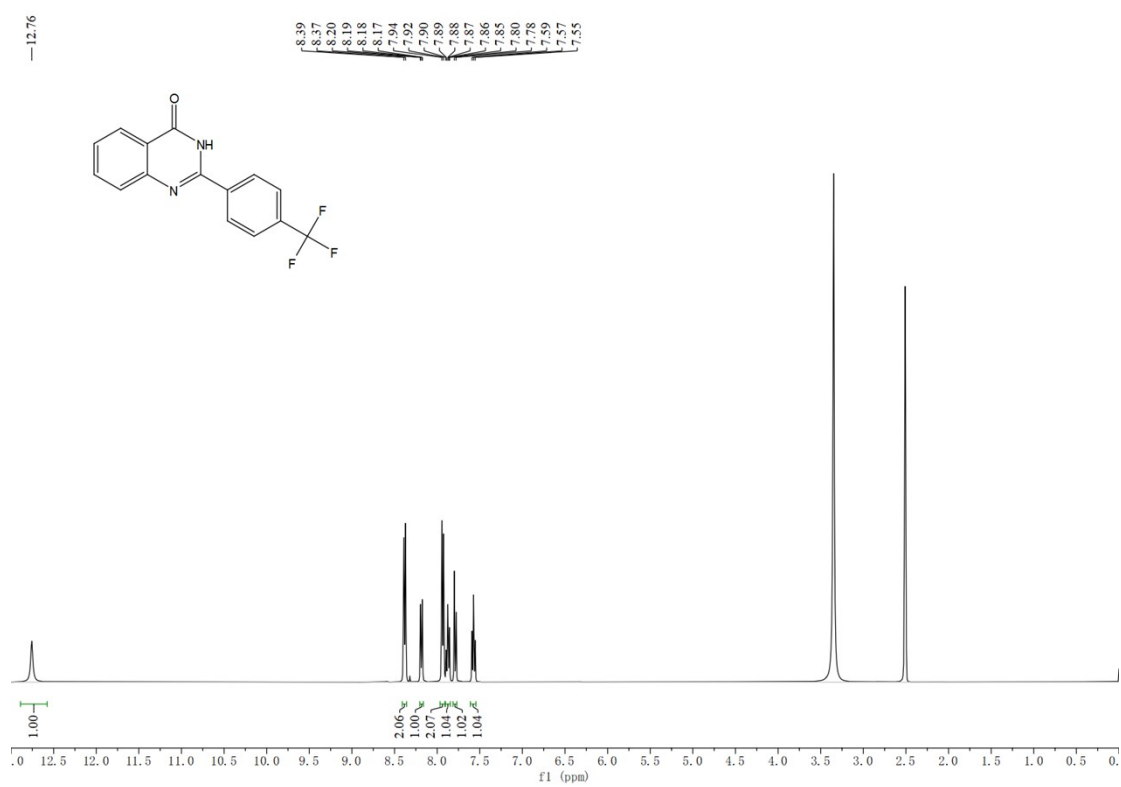
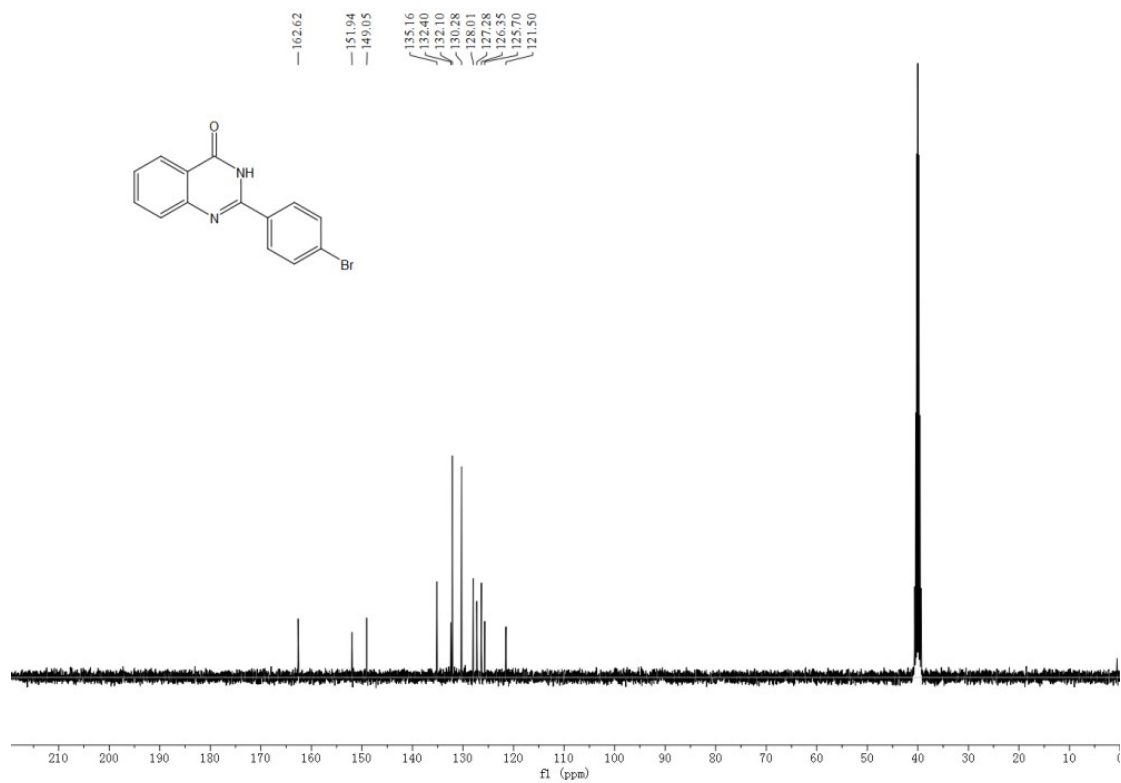
Structure characterization spectra of quinazolinones

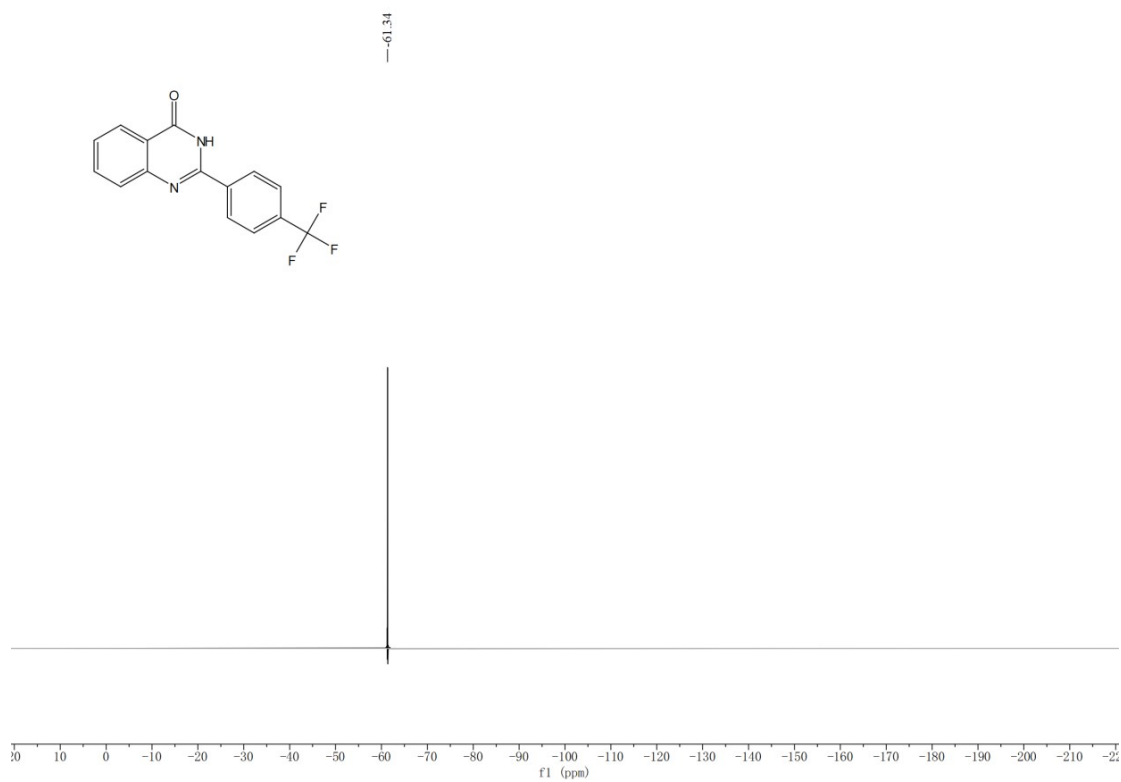
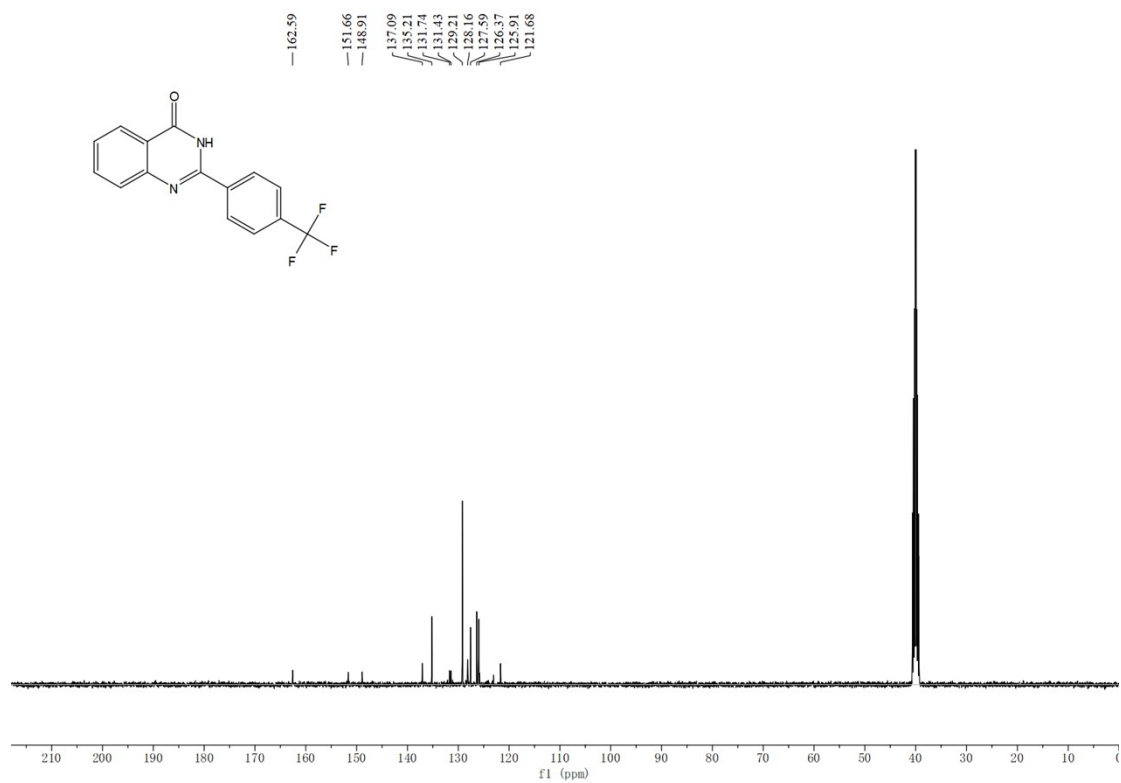


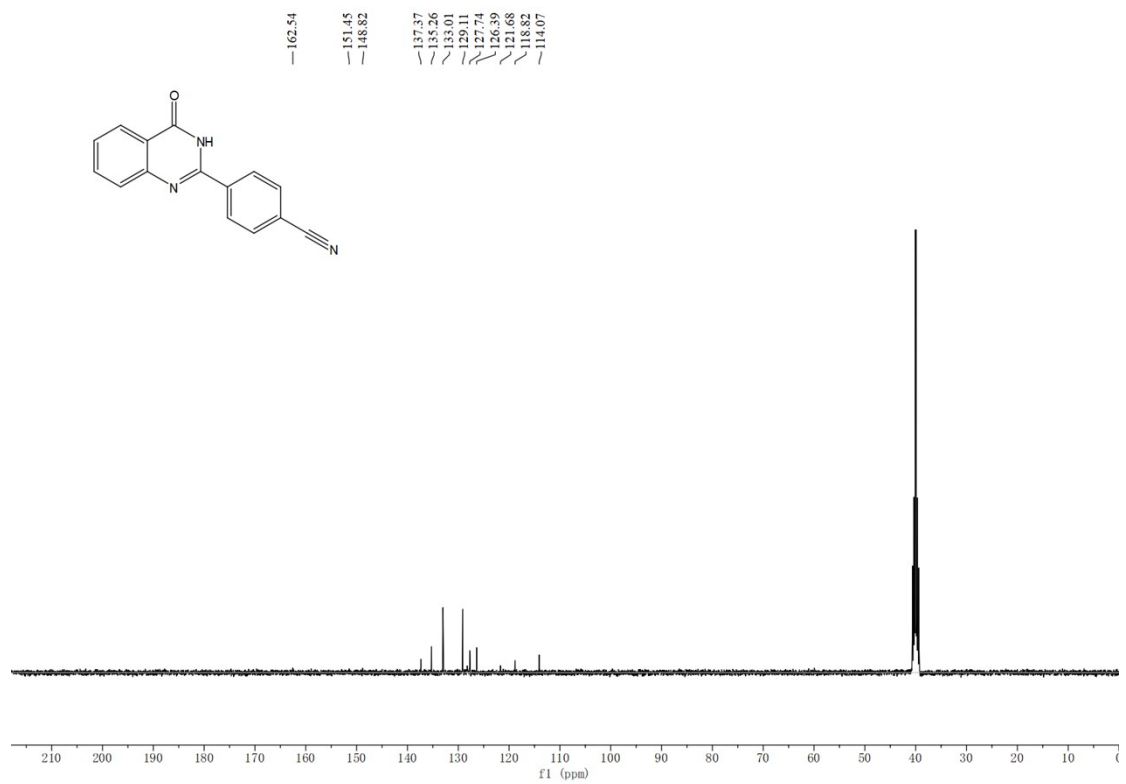
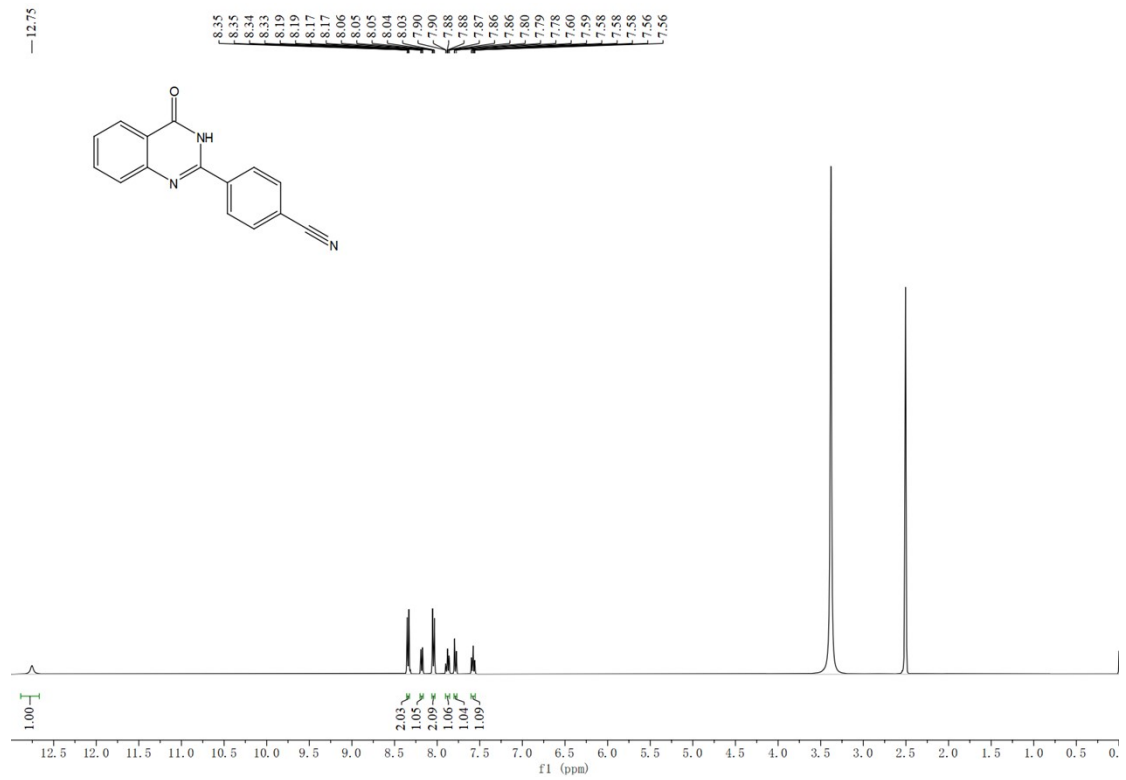


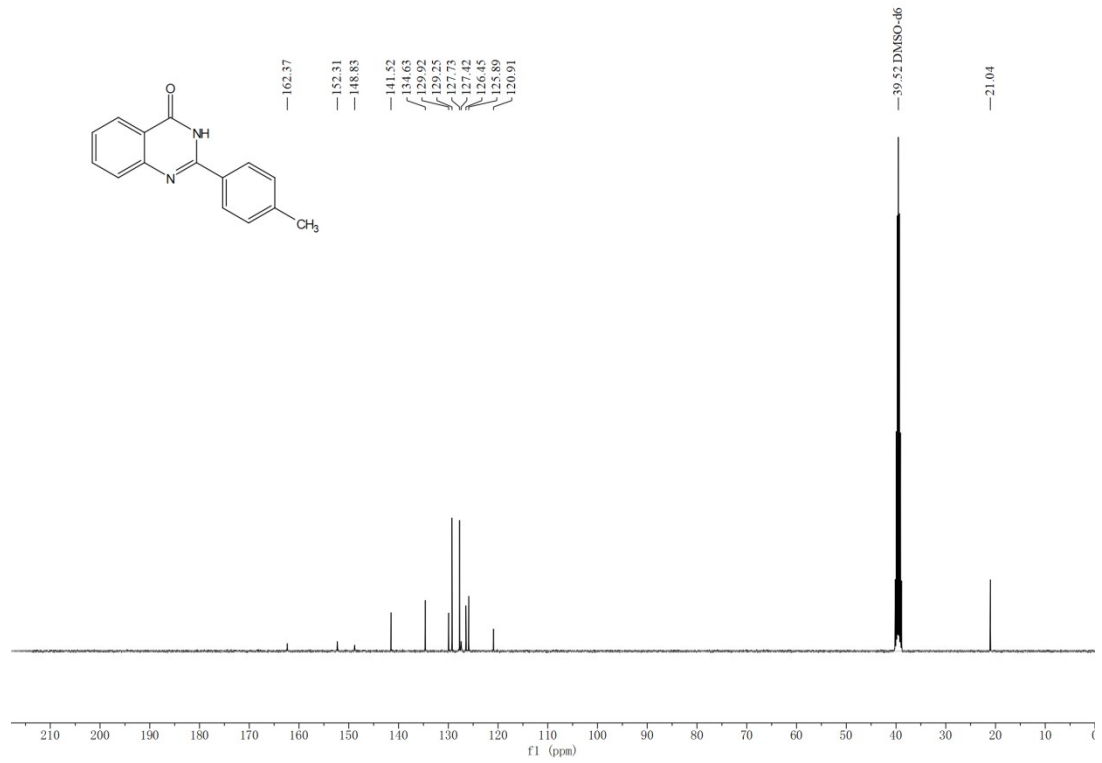
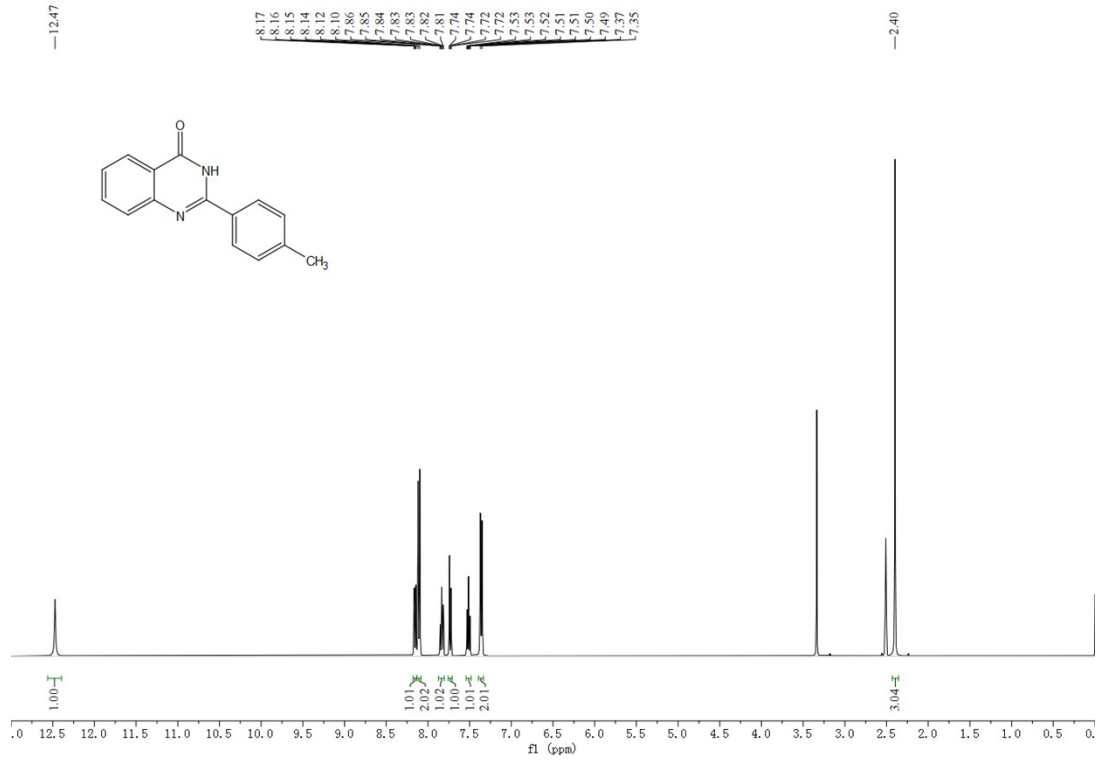


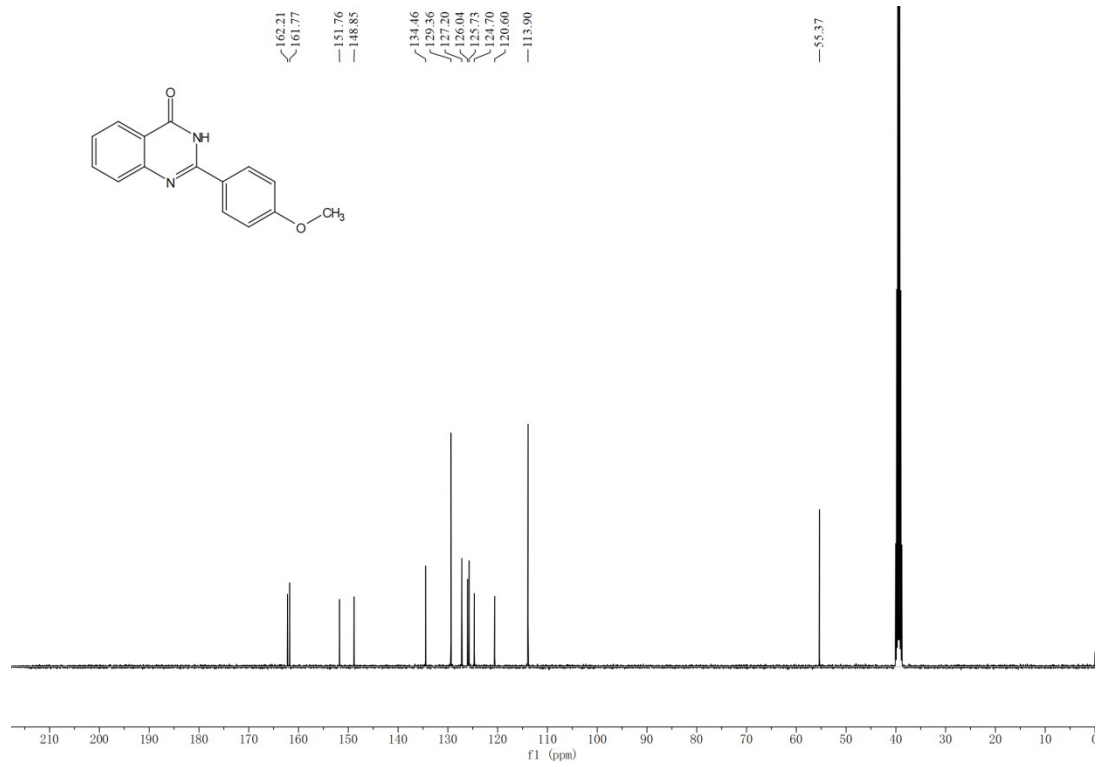
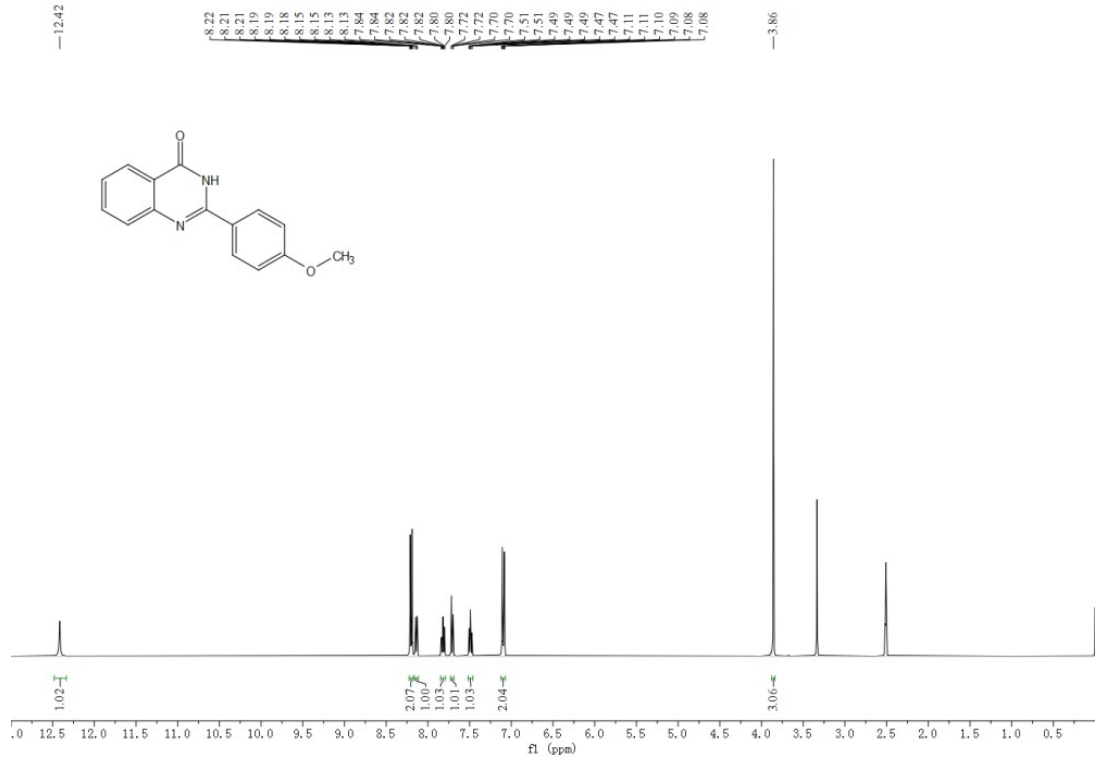


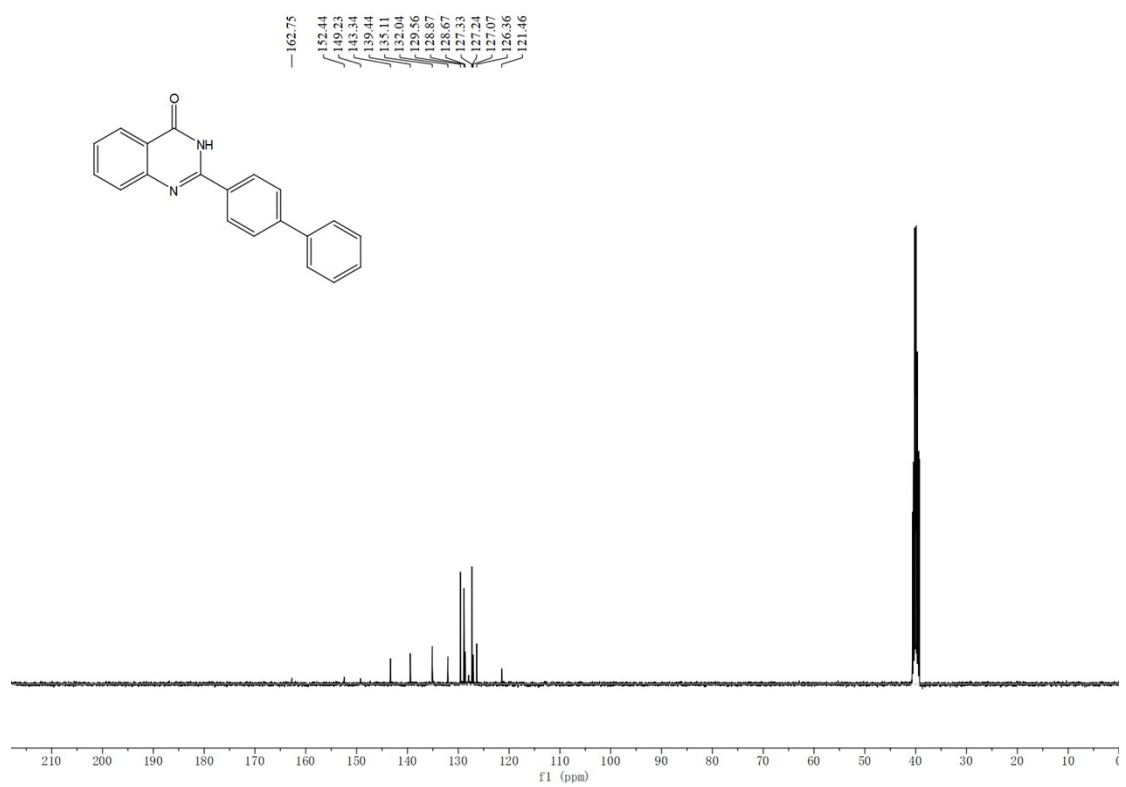
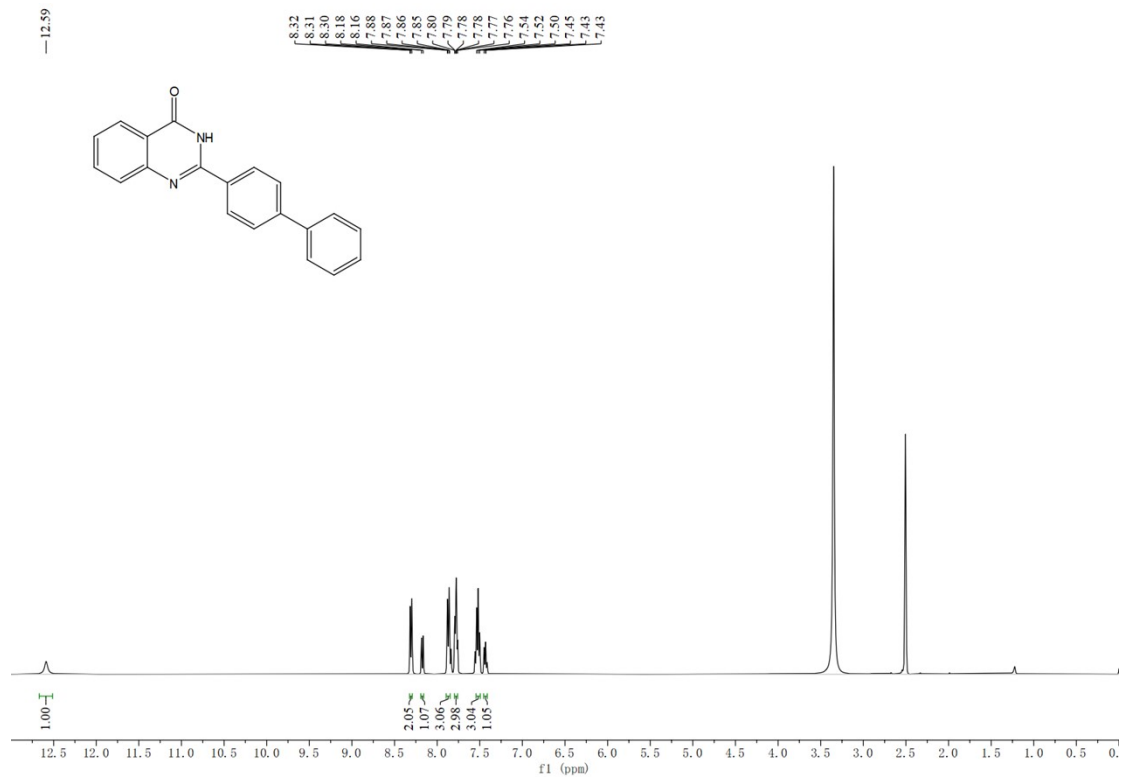


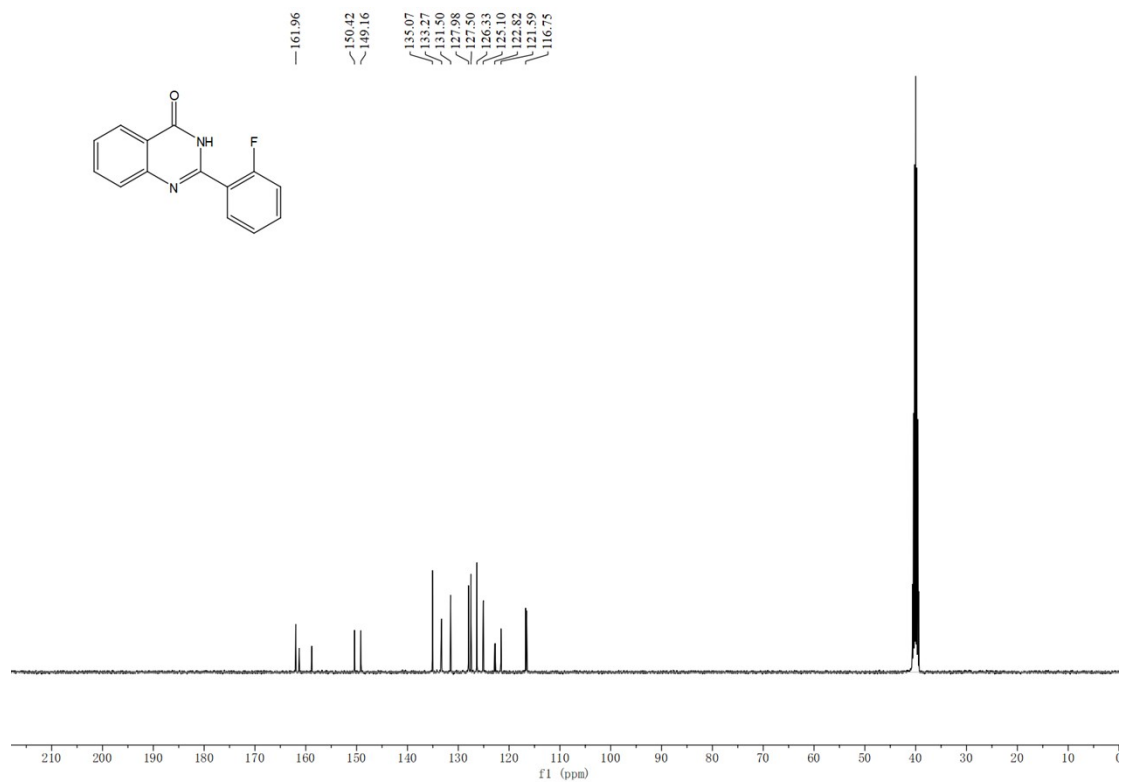
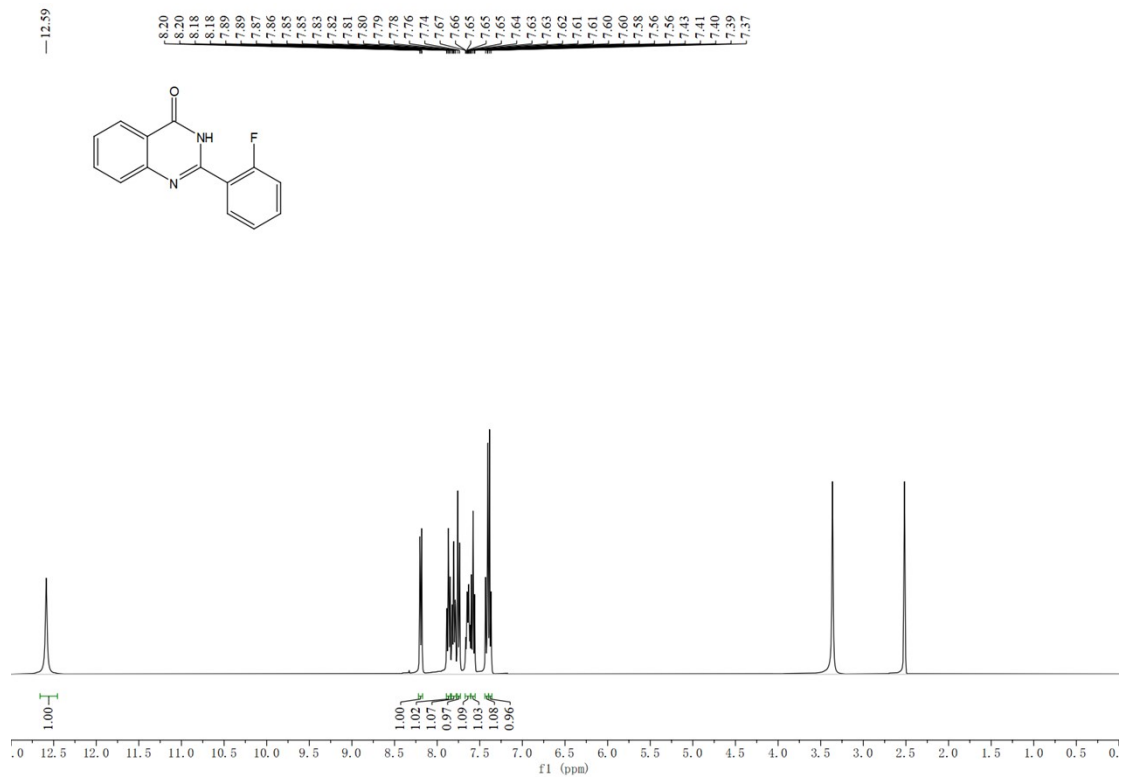


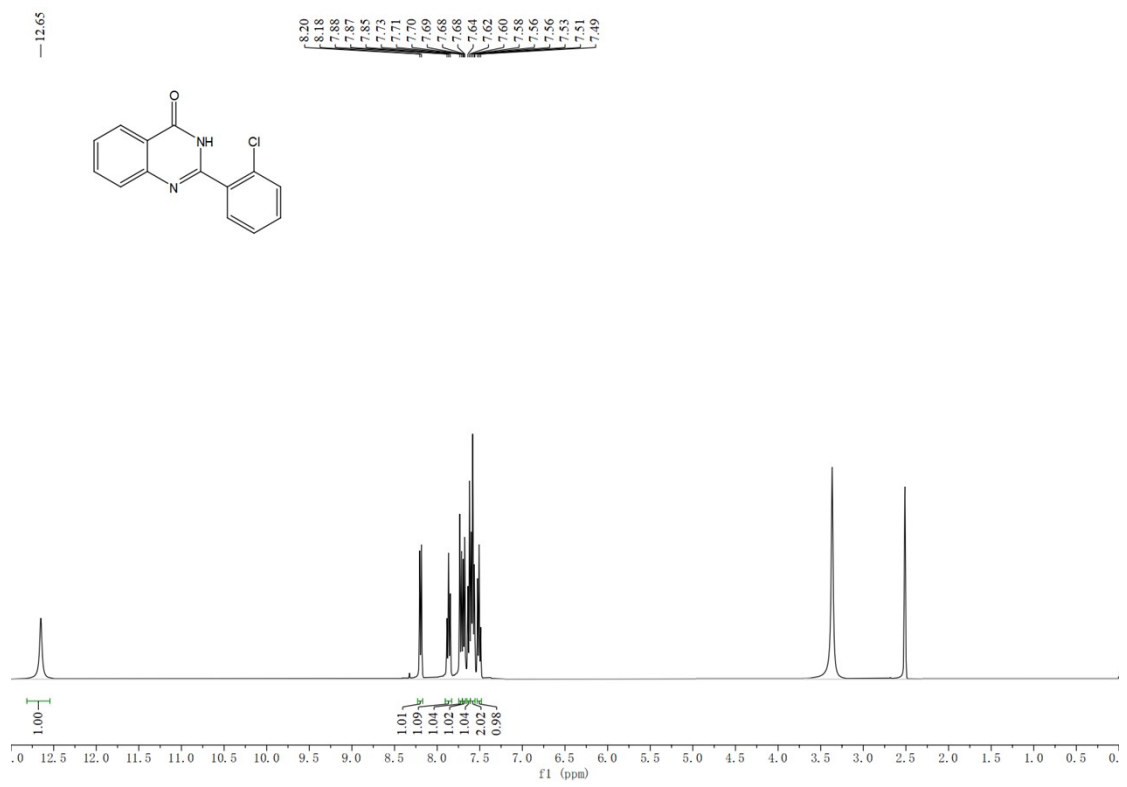
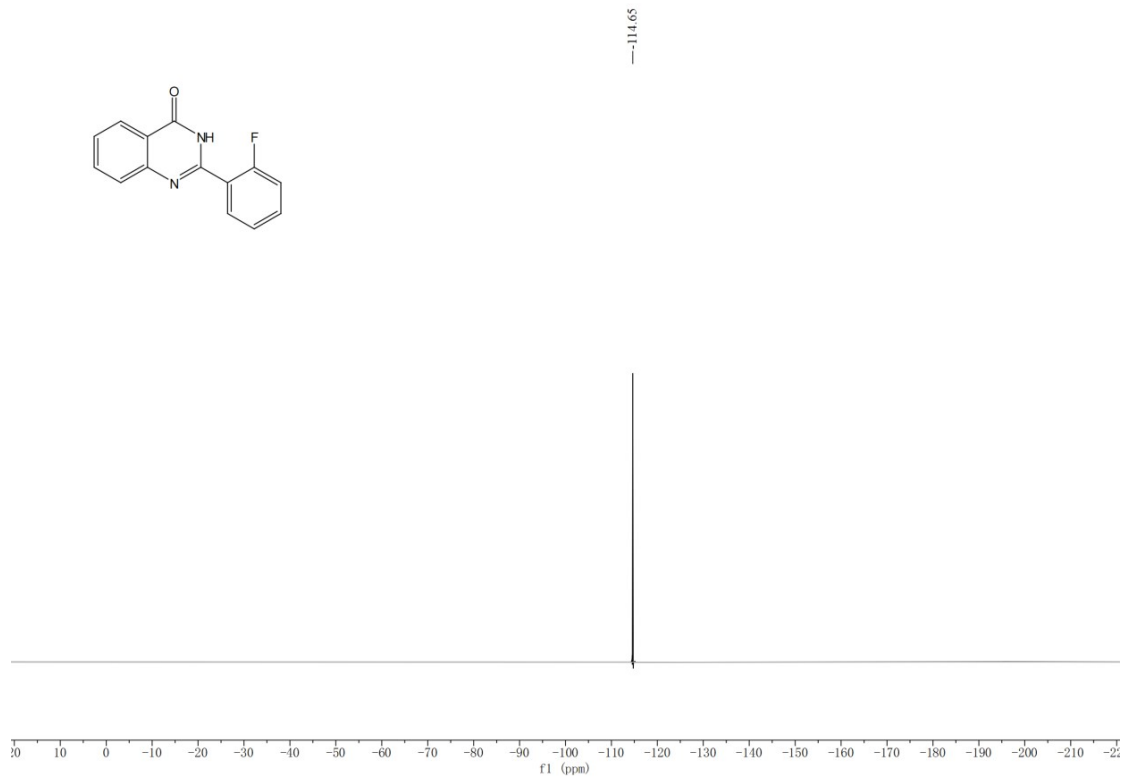


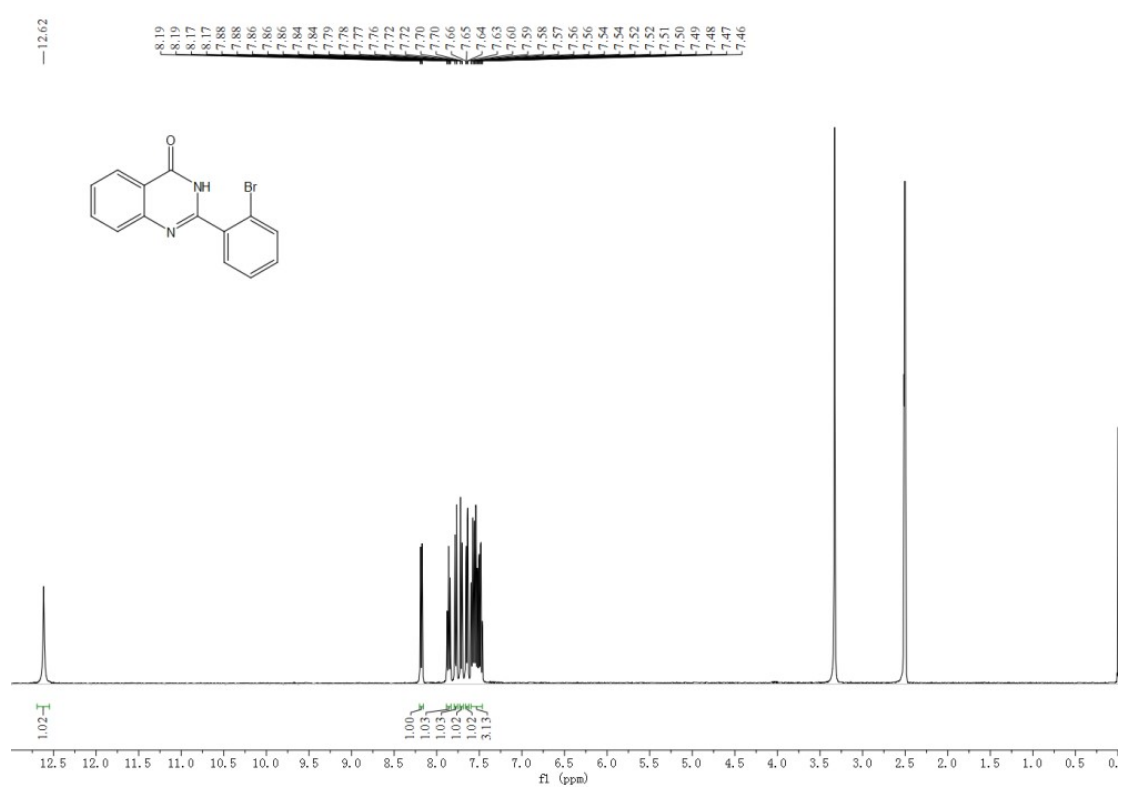
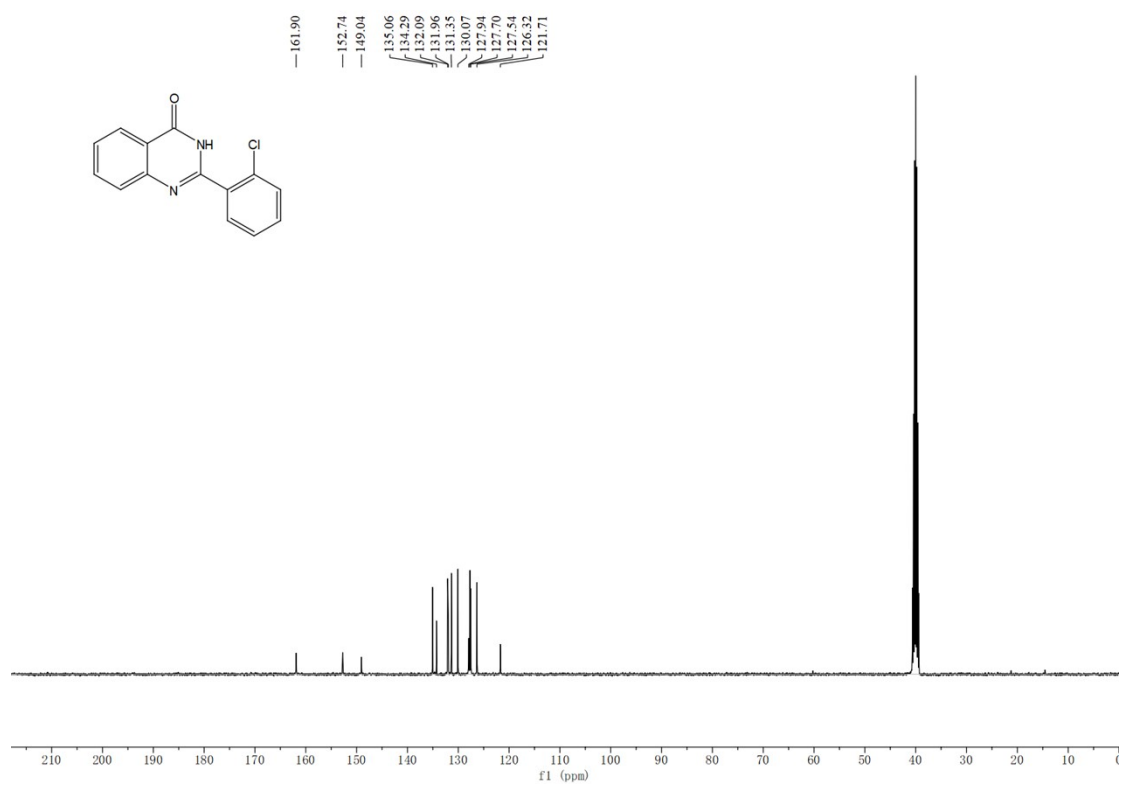


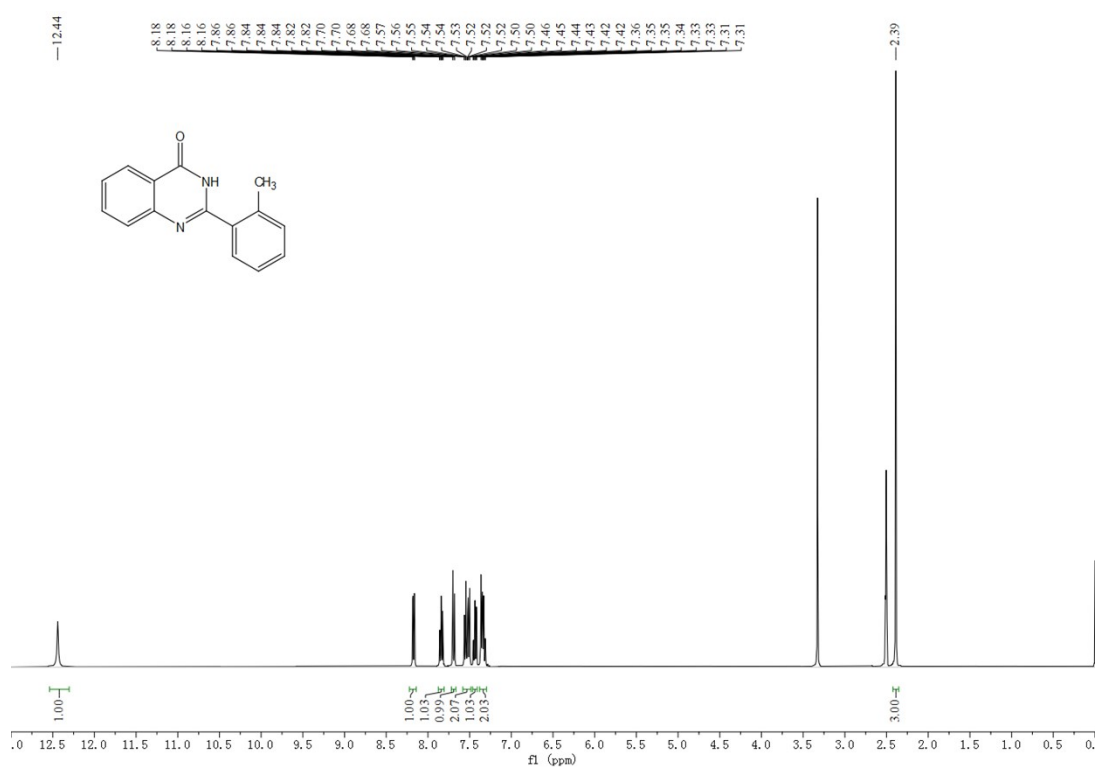
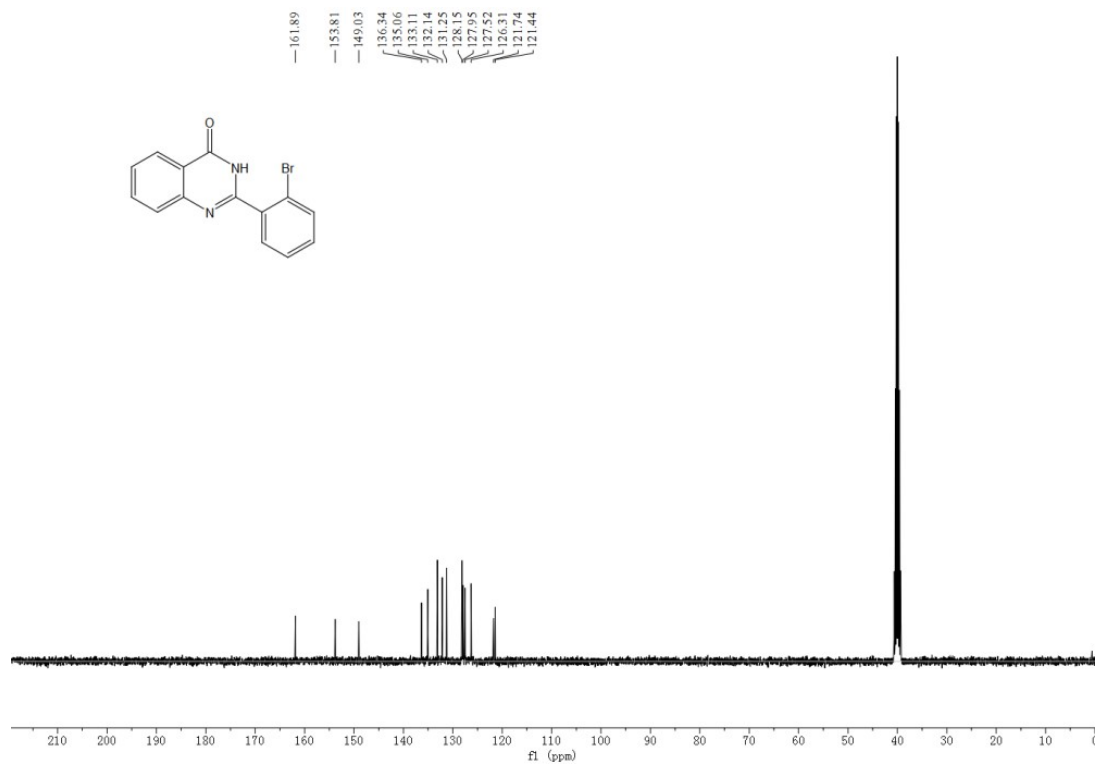


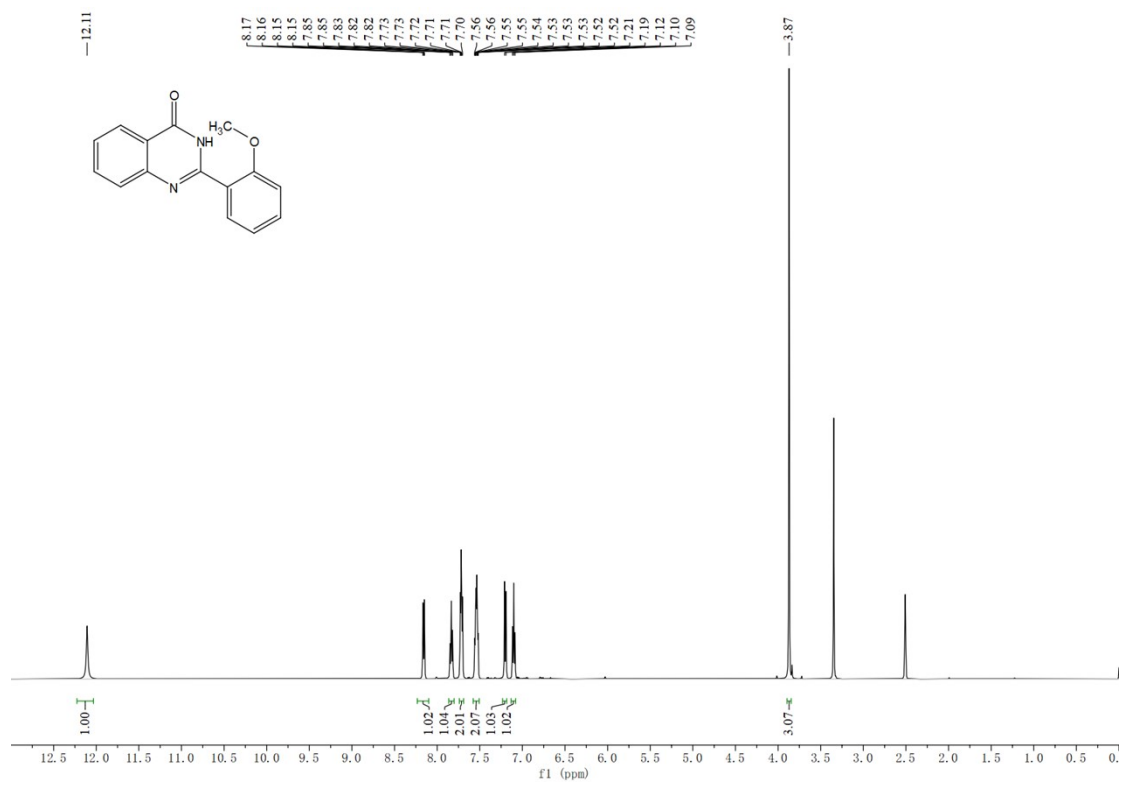
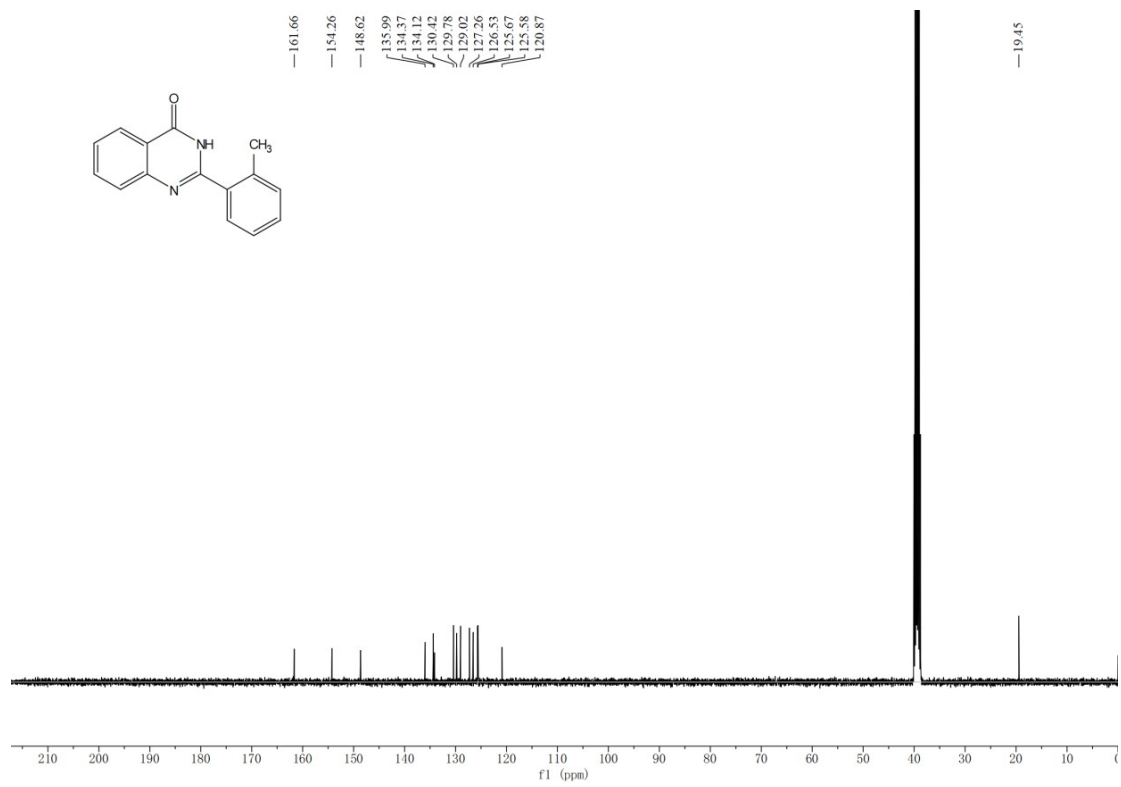


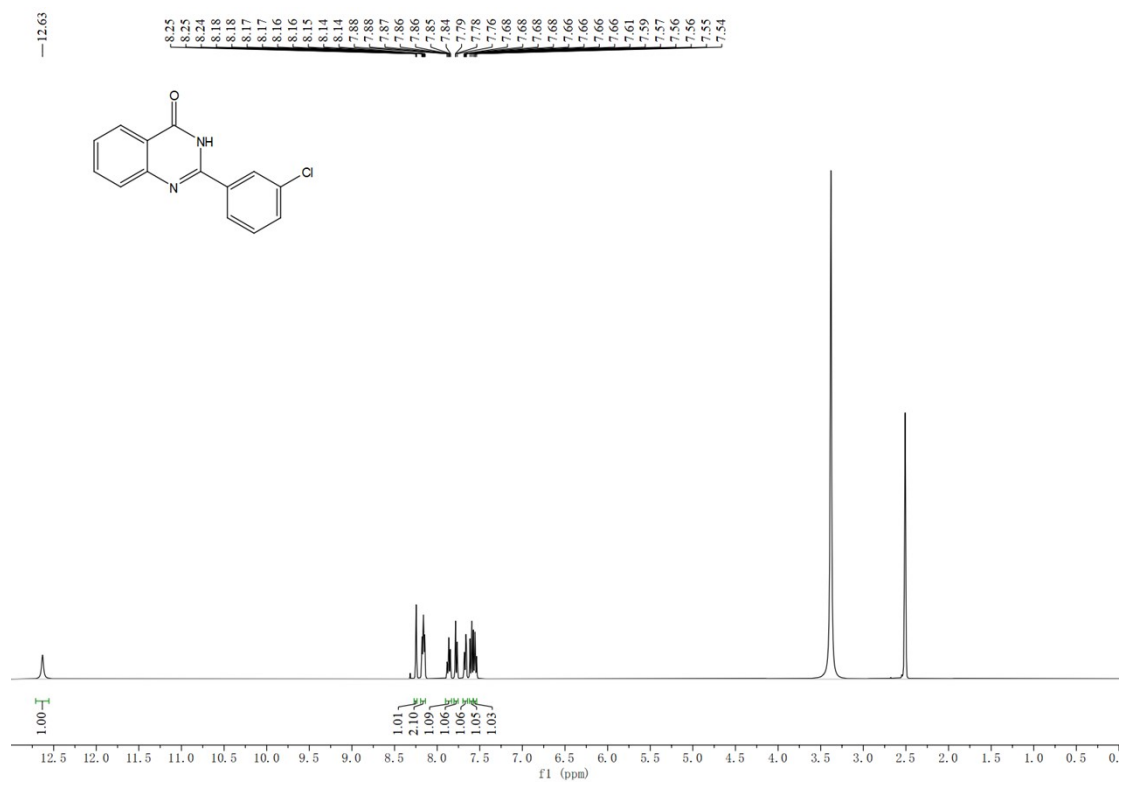
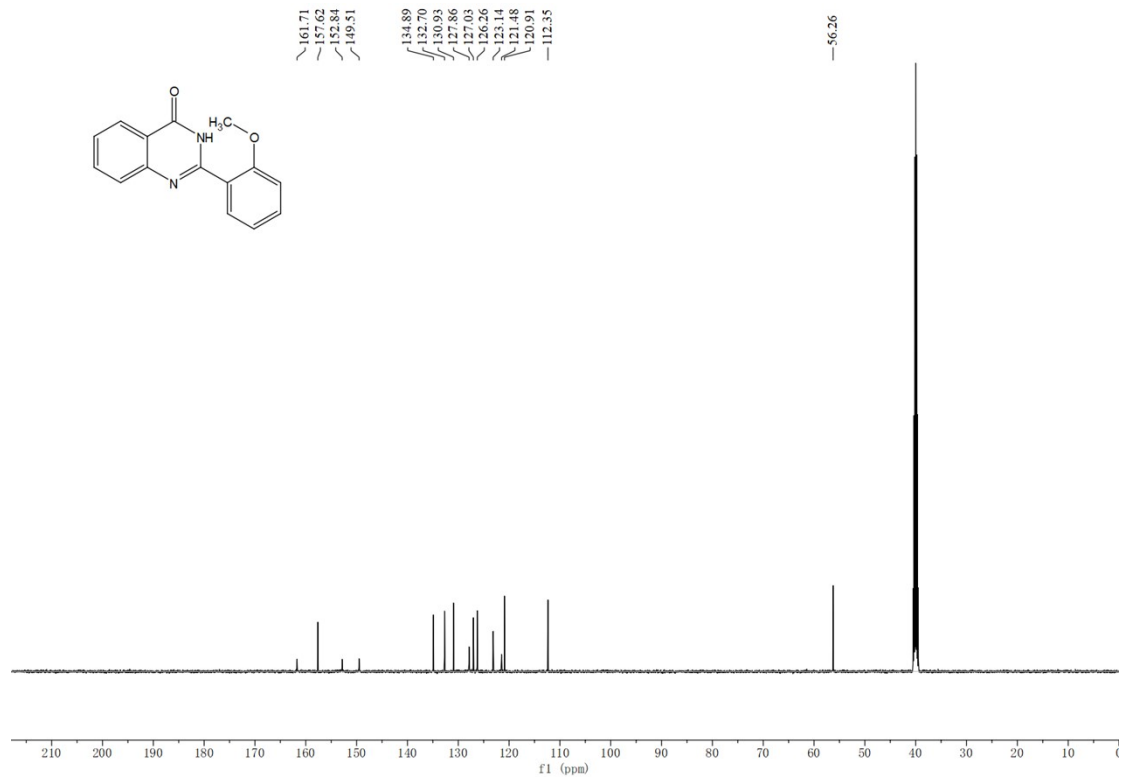


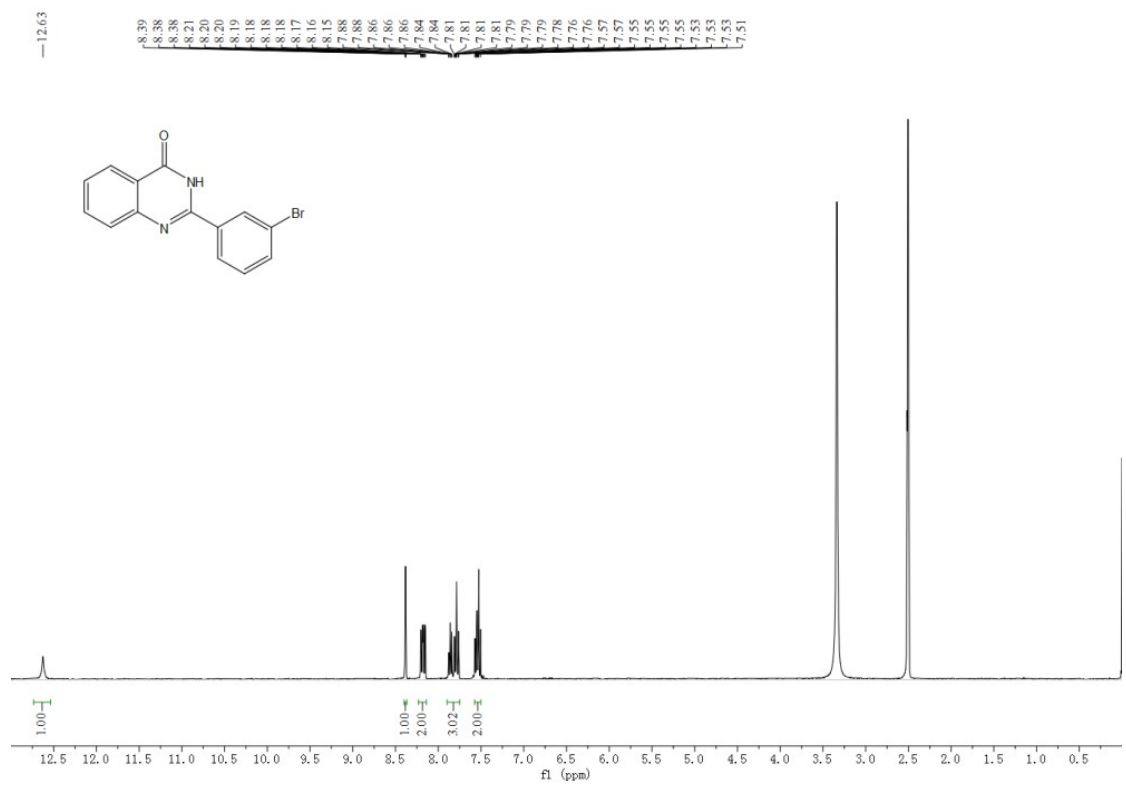
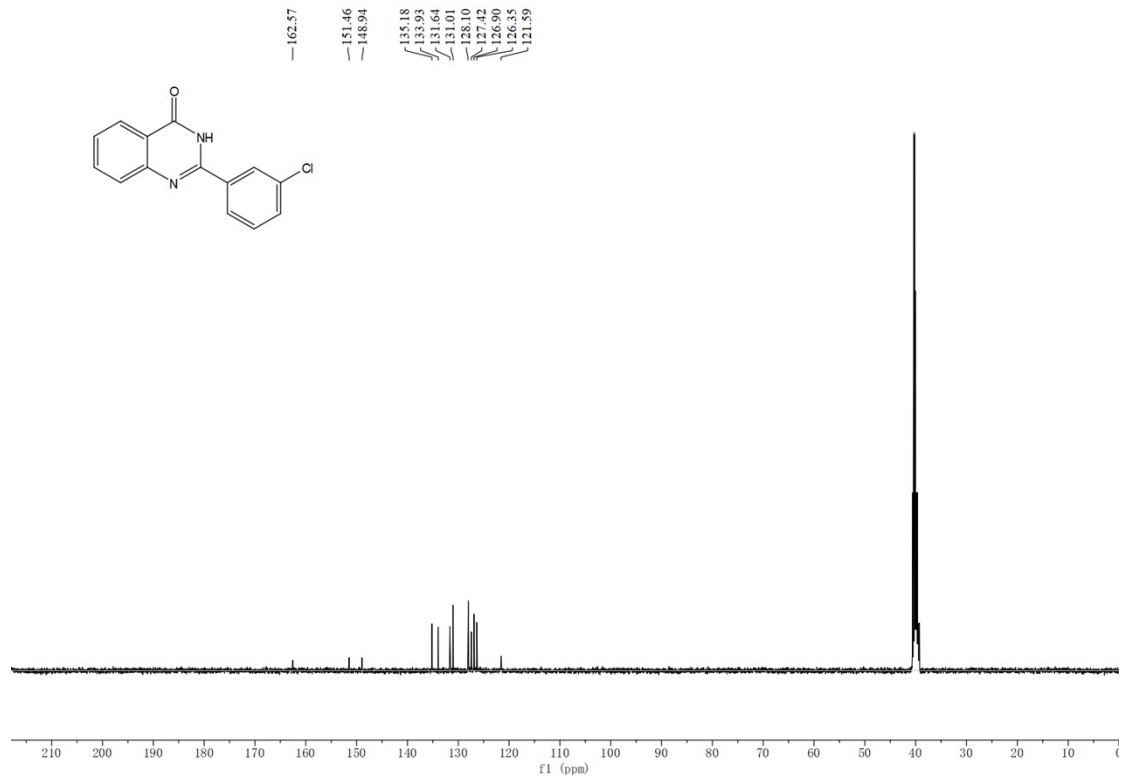


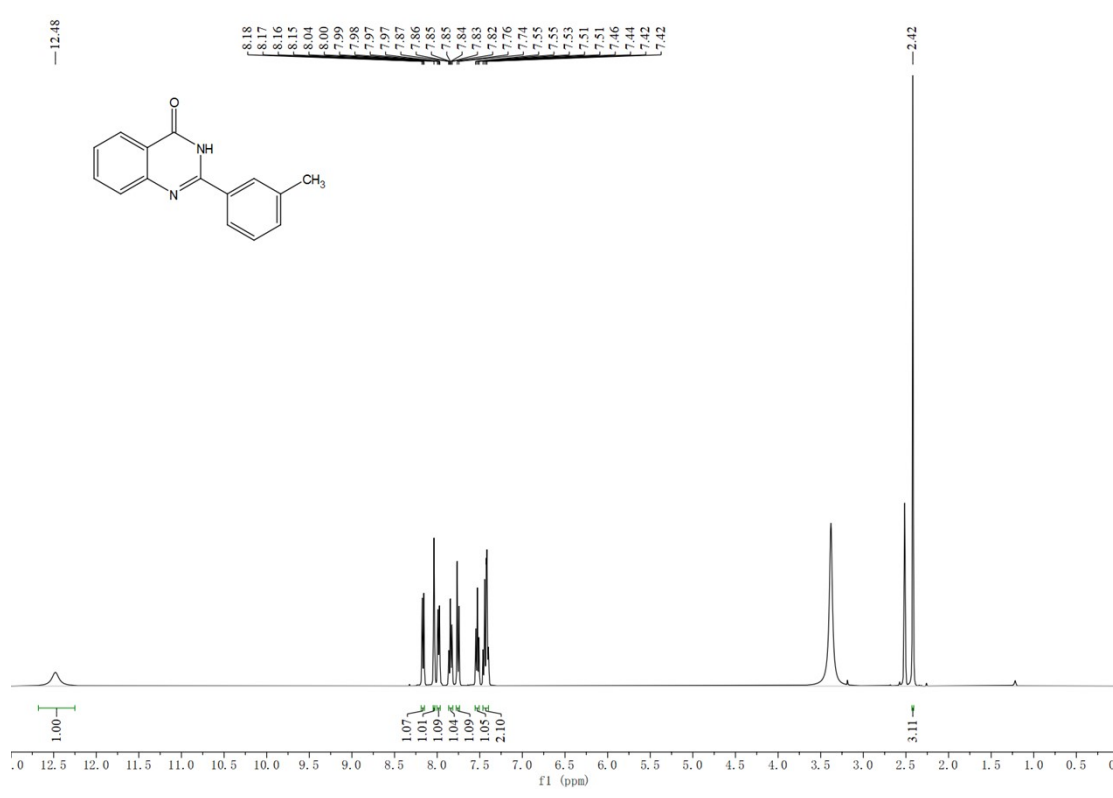


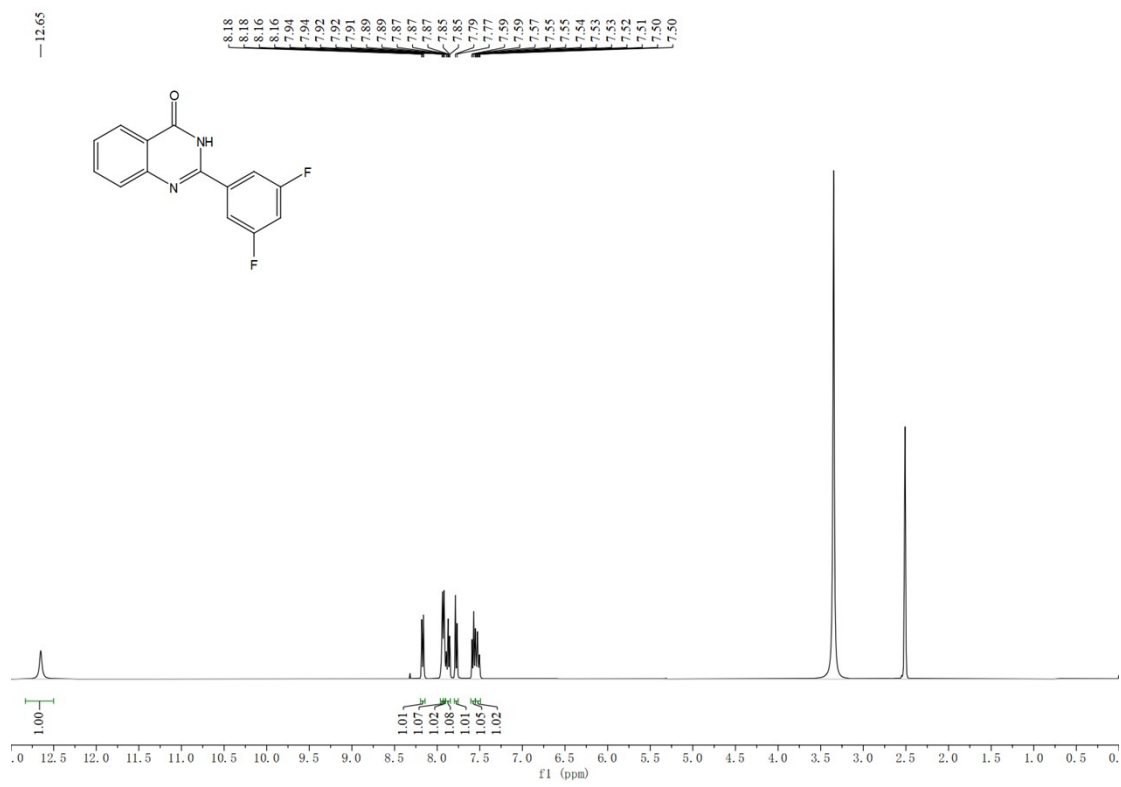
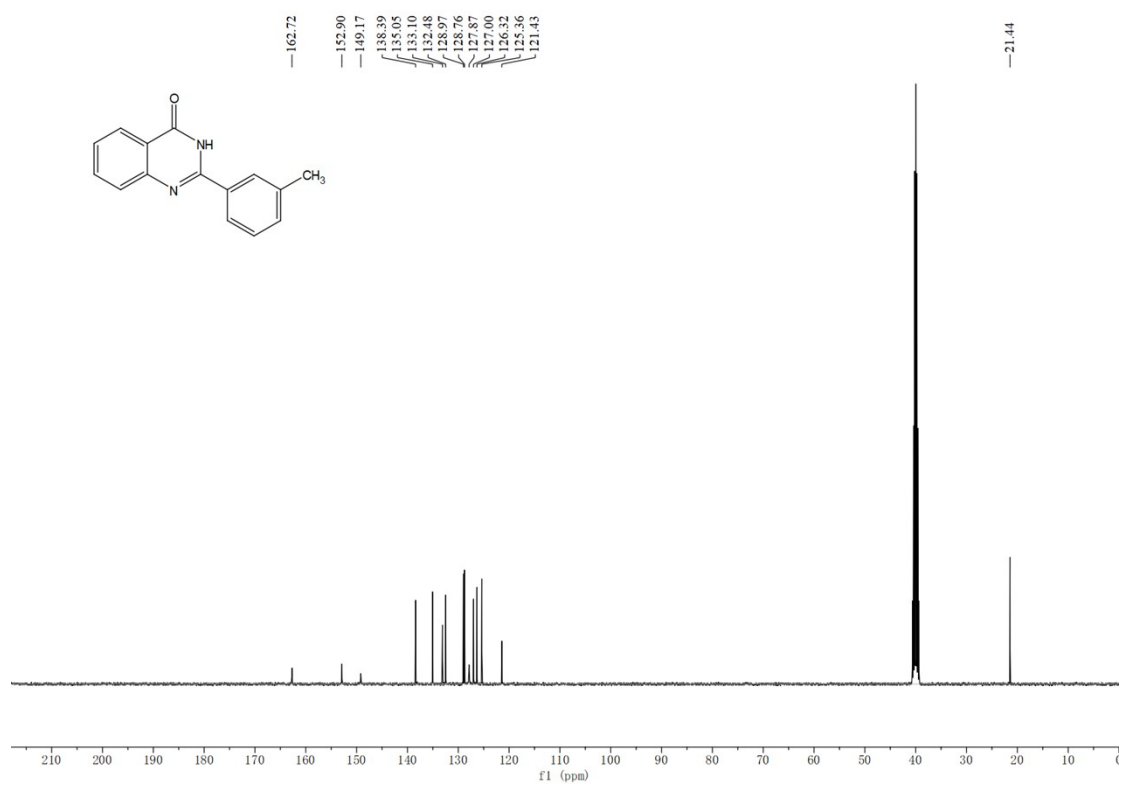


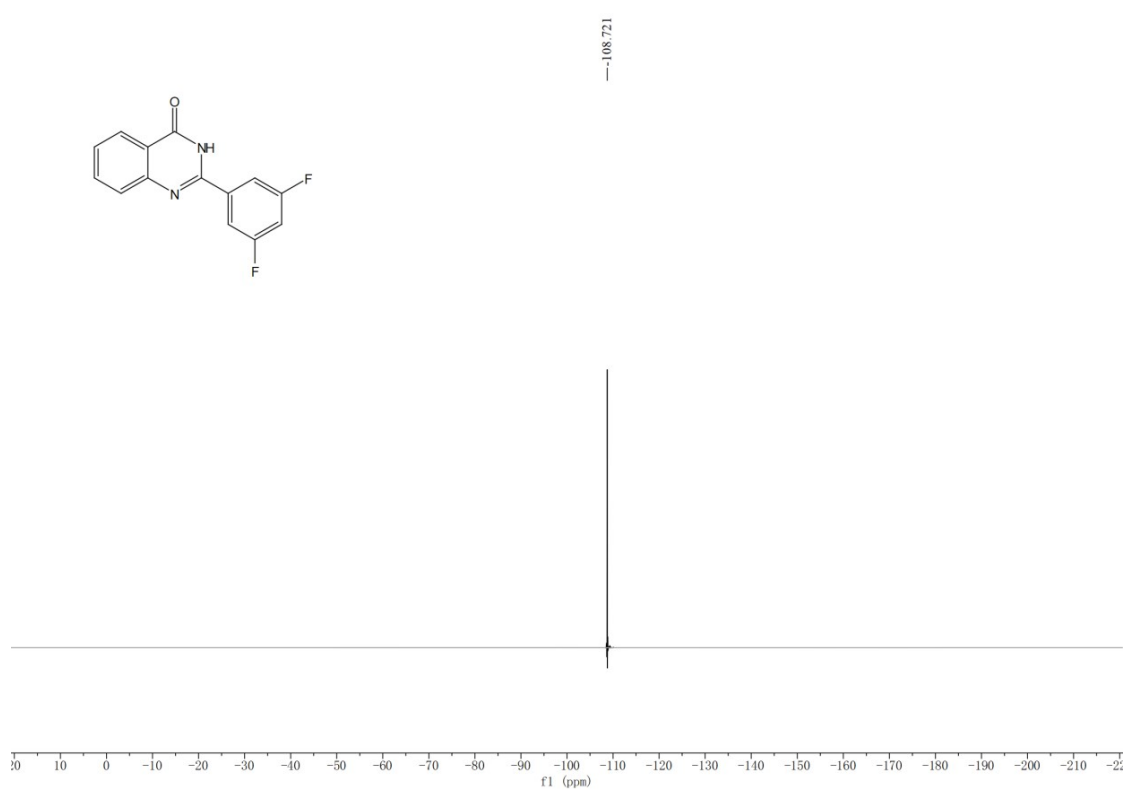
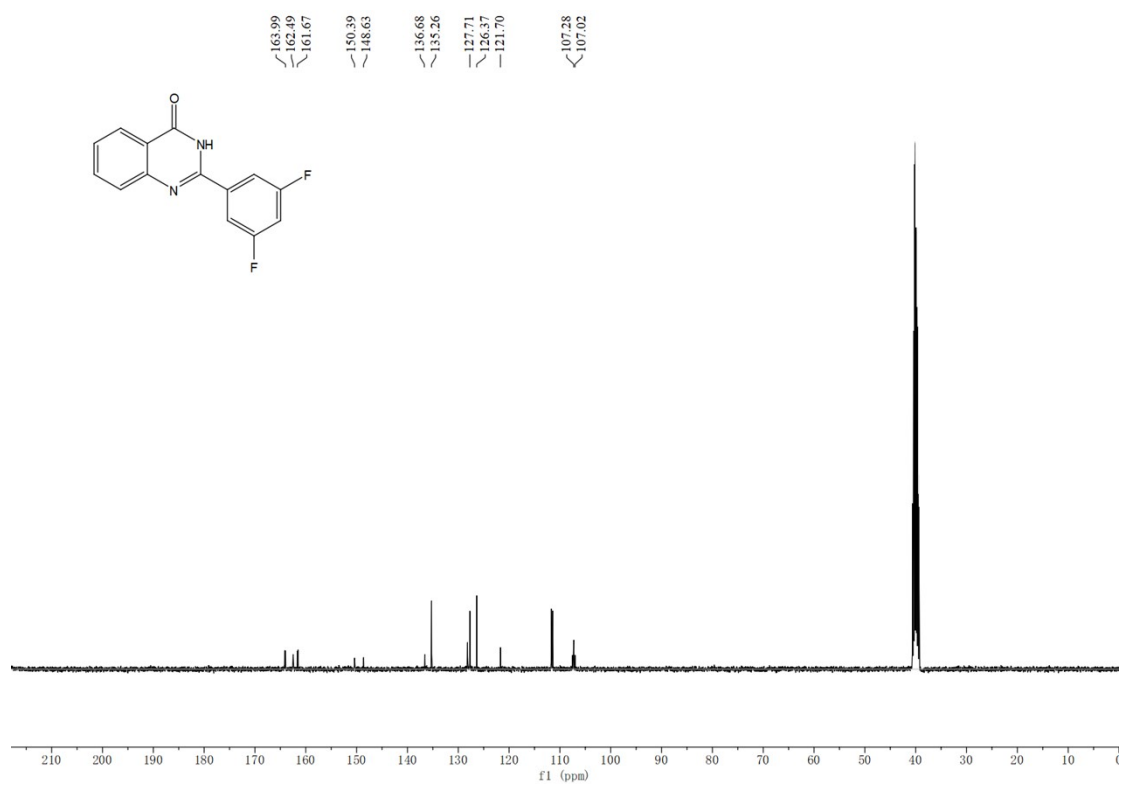


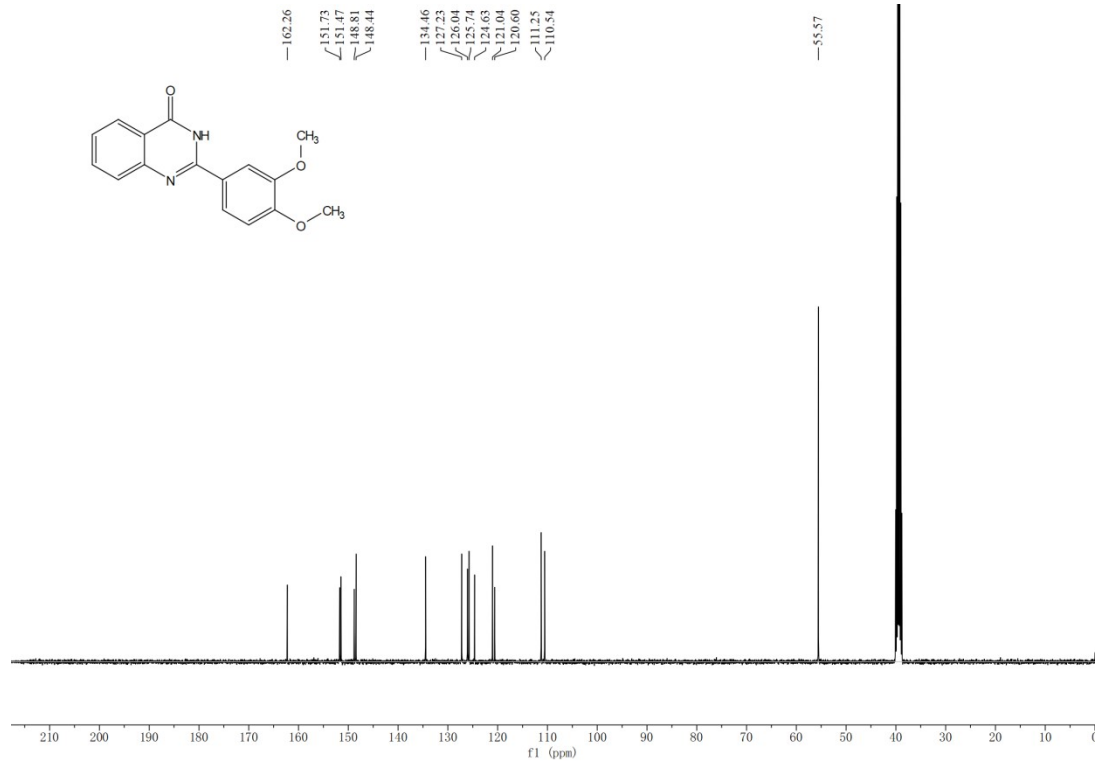
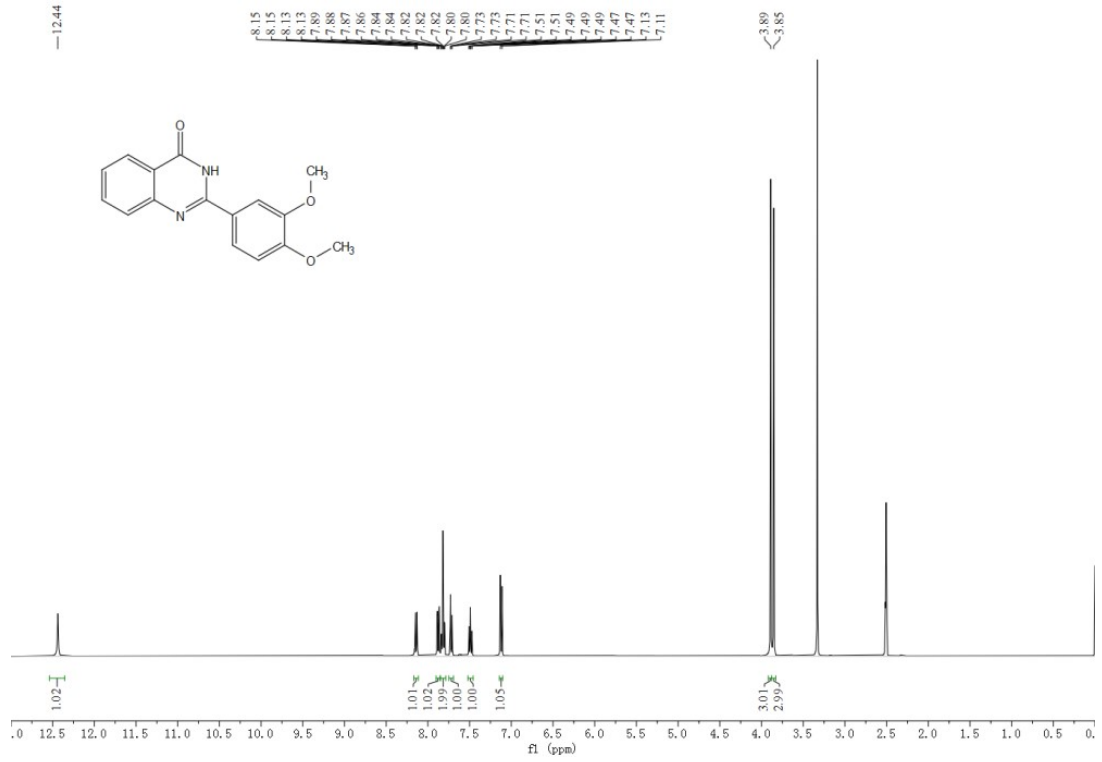


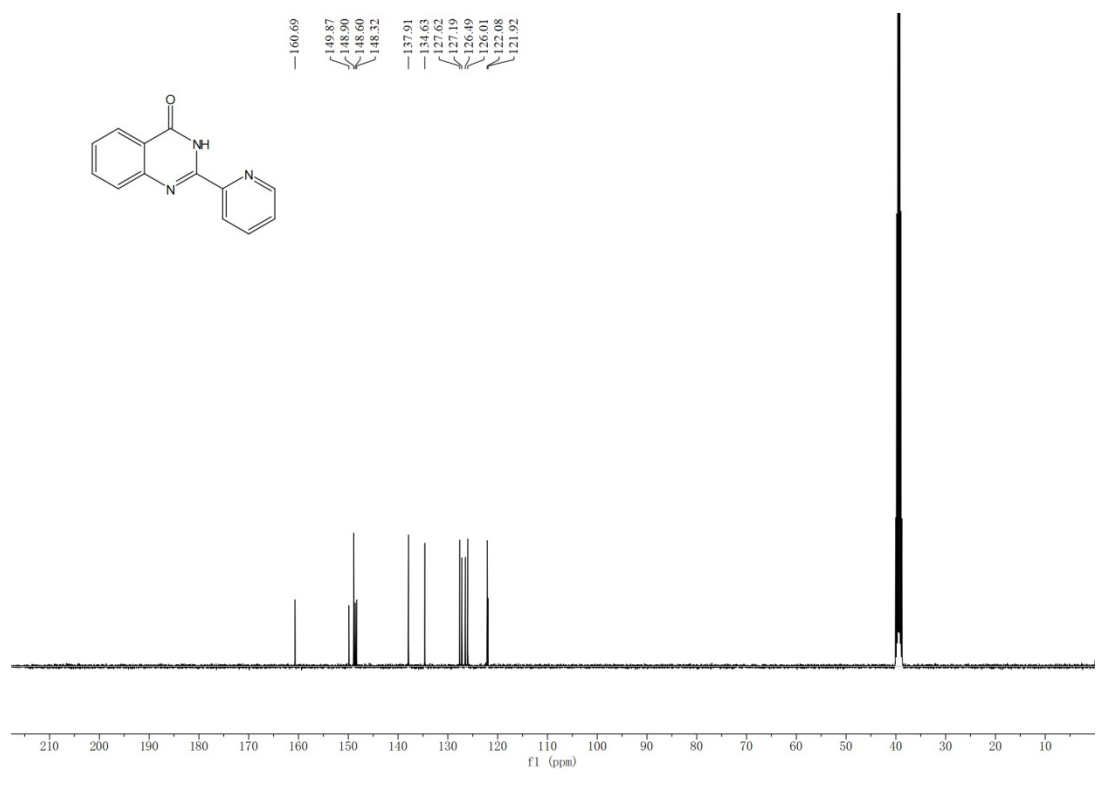
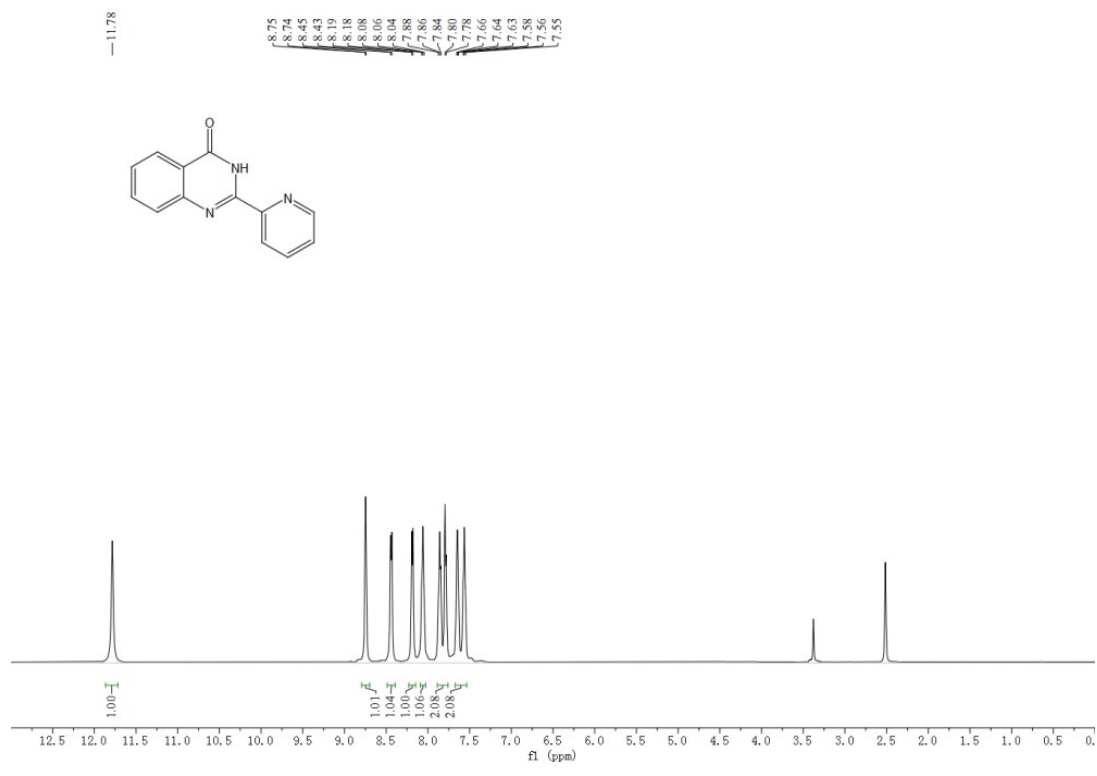






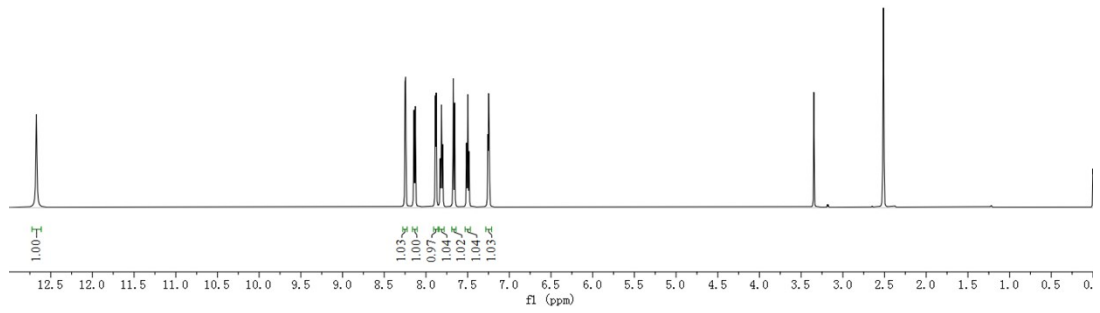
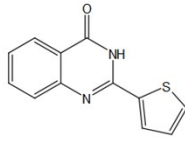






-12.67

8.25
8.24
8.14
8.10
7.80
7.88
7.83
7.83
7.81
7.80
7.67
7.66
7.51
7.50
7.48
7.26
7.25
7.24



-161.70

148.56
147.74
137.29
136.68
135.08
129.32
128.45
126.87
126.25
125.90
120.80

