

Supporting Information

Visible light-mediated synthesis of quinazolinones from benzyl bromides and 2-aminobenzamides without using any photocatalyst or additive

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1. Experimental section

1.1 Instruments and reagents

All major chemicals and solvents were obtained from commercial sources and used without further purification. ^1H NMR ^{13}C NMR and ^{19}F spectra were recorded on a Bruker Avance III-500 spectrometer (Bruker, Switzerland).

1.2 General Methods for the Synthesis of quinazolinone derivatives

A mixture of benzyl bromide (0.1 mmol), 2-aminobenzamide (0.2 mmol) and methanol (2 mL) as added to the test tube. The reaction mixture was irradiated with a Blue LED (18 W) for 28 h under air atmosphere and stirred at 300–400 rpm. The reaction was monitored using TLC (PE: EtOAc = 6:1, v/v). The organic phase was concentrated under reduced pressure to give the crude product, which was purified by column chromatography to obtain the pure product.

1.3 Cyclic Voltammetry Experiment

Cyclic voltammetry (CV) was taken using a CHI6043E potentiostation. CV measurement of A was carried out in 0.1 M of $^n\text{Bu}_4\text{NBF}_4/\text{MeOH}$ at a scan rate of 100 mV/s with the protection of N_2 . The working electrode is a glassy carbon, the counter electrode is a Pt wire, and the reference electrode is saturated calomel electrode (SCE).

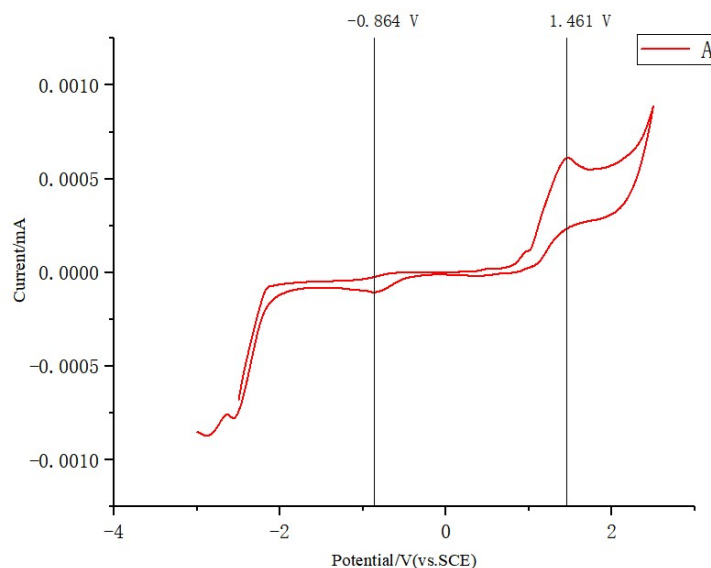


Figure S1. Cyclic voltammograms of A

1.4 UV-Visible Spectroscopy

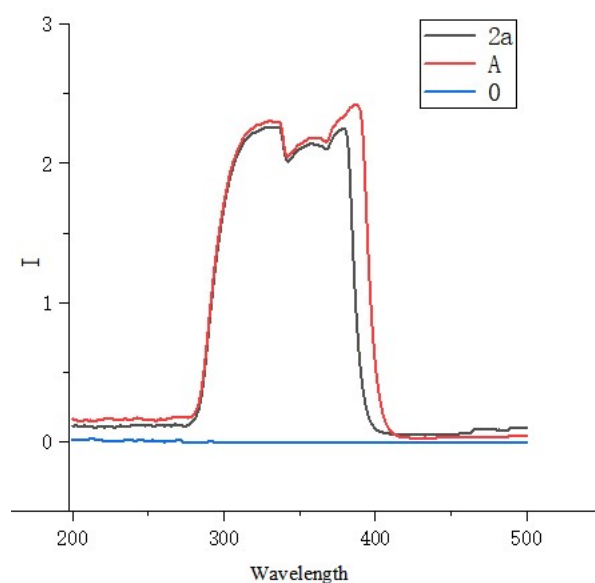


Figure S2. UV-Visible absorption spectra

1.5 Determination of electron spin resonance (EPR)

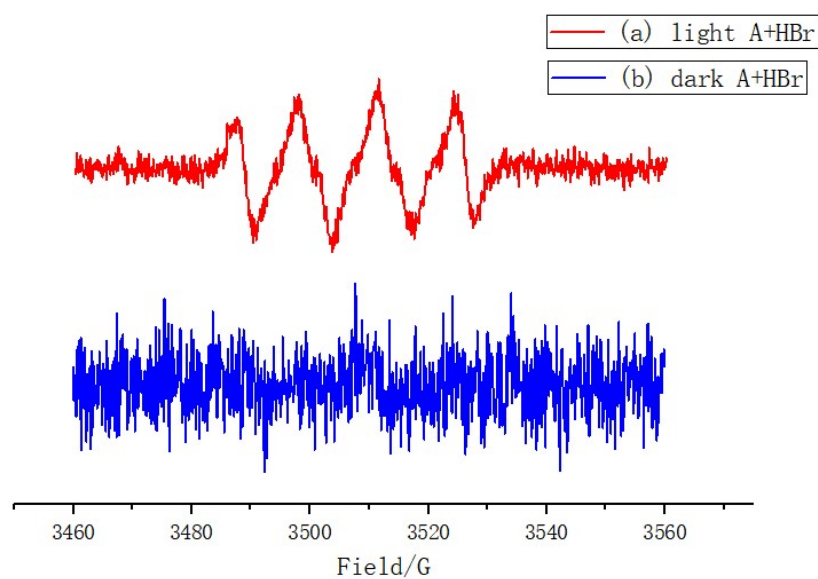


Figure S3. EPR spectra

(a) A and hydrobromic acid in MeOH, under blue LED irradiation 10 min;

(b) A and hydrobromic acid in MeOH, dark.

1.6 Confirmation of Formation of H_2O_2

We conducted the step of template reaction. After 28 hours of reaction, EtOAc (20 mL) was added in the reaction mixture. The organic phase was extracted with H_2O (3x10 mL). To this aqueous

layer, HCl and a solution of KI in H₂O were added successively and stirred well. Subsequently, a starch solution was added under vigorous stirring. Finally, the blue color appeared in several minutes. This experimental result indicated that the H₂O₂ was formed in the reaction could oxidize the iodide ions in acidic media to produce I₂, and then I₂ was trapped by the starch to form this deep blue complex (Figure S1).

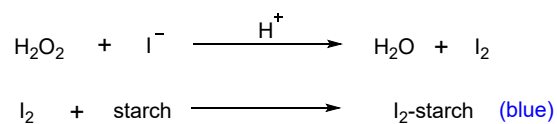
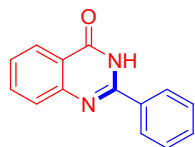


Figure S4. Confirmation of Formation of H₂O₂

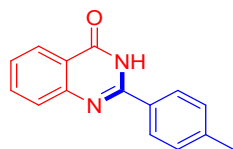
2. Characterization Data of Products

(3a) 2-phenylquinazolin-4(3H)-one ^[1]



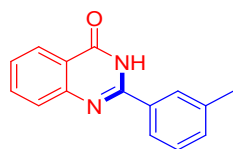
White solid, m.p. 235.2-236.4 °C. ¹H NMR (500 MHz, DMSO-*d*₆) δ 12.59 (s, 1H), 8.24 – 8.15 (m, 3H), 7.85 (td, *J* = 7.8, 7.2, 1.4 Hz, 1H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.64 – 7.50 (m, 4H). ¹³C NMR (126 MHz, DMSO-*d*₆) δ 162.74, 152.78, 149.19, 135.08, 133.18, 131.87, 129.08, 128.24, 127.98, 127.06, 126.33, 121.44.

(3b) 2-(p-tolyl)quinazolin-4(3H)-one ^[1]



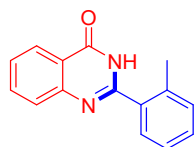
White solid, m.p. 240.3-242.4 °C. ¹H NMR (500 MHz, DMSO-*d*₆) δ 12.51 (s, 1H), 8.14 (dd, *J* = 24.1, 7.7 Hz, 3H), 7.88 – 7.81 (m, 1H), 7.74 (d, *J* = 8.1 Hz, 1H), 7.52 (t, *J* = 7.4 Hz, 1H), 7.36 (d, *J* = 8.1 Hz, 2H), 2.40 (s, 3H). ¹³C NMR (126 MHz, DMSO-*d*₆) δ 162.73, 152.65, 149.28, 141.89, 135.01, 130.33, 129.64, 128.13, 127.87, 126.83, 126.30, 121.35, 21.45.

(3c) 2-(m-tolyl)quinazolin-4(3H)-one ^[2]



White solid, m.p. 237.3-239.5 °C. ¹H NMR (500 MHz, DMSO-*d*₆) δ 12.51 (s, 1H), 8.16 (d, *J* = 7.7 Hz, 1H), 8.04 (s, 1H), 7.98 (d, *J* = 7.4 Hz, 1H), 7.85 (t, *J* = 7.5 Hz, 1H), 7.75 (d, *J* = 8.1 Hz, 1H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.47 – 7.34 (m, 2H), 2.42 (s, 3H). ¹³C NMR (126 MHz, DMSO-*d*₆) δ 162.74, 152.88, 149.16, 138.37, 135.04, 133.10, 132.46, 128.96, 128.75, 126.98, 126.31, 125.34, 121.42, 21.45.

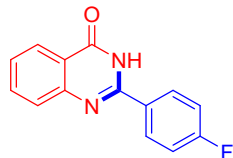
(3d) 2-(o-tolyl)quinazolin-4(3H)-one ^[2]



White solid, m.p. 212.5-213.8 °C. ¹H NMR (500 MHz, DMSO-*d*₆) δ 12.48 (s, 1H), 8.18 (d, *J* = 7.8 Hz, 1H), 7.89 – 7.80 (m, 1H), 7.70 (d, *J* = 8.1 Hz, 1H), 7.60 – 7.48 (m, 2H), 7.44 (t, *J* = 7.2 Hz, 1H), 7.39 –

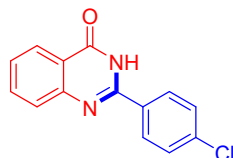
7.31 (m, 2H), 2.39 (s, 3H). ¹³C NMR (126 MHz, DMSO-*d*₆) δ 162.24, 154.83, 149.19, 136.57, 134.93, 134.68, 130.99, 130.36, 129.60, 127.83, 127.10, 126.25, 126.16, 121.44, 20.04.

(3e) 2-(4-Fluorophenyl)quinazolin-4(3H)-one ^[3]



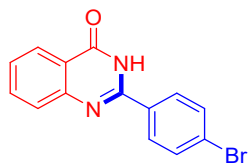
White solid, m.p. 283.1-284.9 °C. ¹H NMR (500 MHz, DMSO-*d*₆) δ 12.61 (s, 1H), 8.26 (dd, *J* = 8.6, 5.5 Hz, 2H), 8.16 (d, *J* = 7.7 Hz, 1H), 7.85 (t, *J* = 7.5 Hz, 1H), 7.75 (d, *J* = 8.1 Hz, 1H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.41 (t, *J* = 8.8 Hz, 2H). ¹³C NMR (126 MHz, DMSO-*d*₆) δ 165.49, 163.50, 162.71, 151.84, 149.08, 135.10, 130.87, 130.80, 129.67, 127.89, 127.07, 126.32, 121.32, 116.19, 116.01. ¹⁹F NMR (471 MHz, DMSO-*d*₆) δ -109.05.

(3f) 2-(4-chlorophenyl)quinazolin-4(3H)-one ^[3]



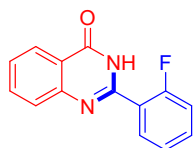
White solid, m.p. 297.8-299.6 °C. ¹H NMR (500 MHz, DMSO-*d*₆) δ 12.64 (s, 1H), 8.19 (dd, *J* = 24.0, 8.1 Hz, 3H), 7.85 (t, *J* = 7.1 Hz, 1H), 7.75 (d, *J* = 8.1 Hz, 1H), 7.64 (d, *J* = 8.5 Hz, 2H), 7.54 (t, *J* = 7.4 Hz, 1H). ¹³C NMR (126 MHz, DMSO-*d*₆) δ 162.64, 151.79, 149.02, 136.75, 135.13, 131.99, 130.08, 129.15, 127.98, 127.24, 126.34, 121.44.

(3g) 2-(4-bromophenyl)quinazolin-4(3H)-one ^[3]



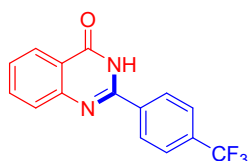
White solid, m.p. 293.1-295.2 °C. ¹H NMR (500 MHz, DMSO-*d*₆) δ 12.64 (s, 1H), 8.22 – 8.06 (m, 3H), 7.89 – 7.82 (m, 1H), 7.76 (t, *J* = 9.0 Hz, 3H), 7.55 (t, *J* = 7.4 Hz, 1H). ¹³C NMR (126 MHz, DMSO-*d*₆) δ 162.62, 151.90, 149.02, 135.15, 132.35, 132.08, 130.26, 127.99, 127.26, 126.34, 125.71, 121.47.

(3h) 2-(2-fluorophenyl)quinazolin-4(3H)-one ^[1]



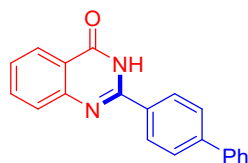
White solid, m.p. 240.5-242.6 °C. ¹H NMR (500 MHz, DMSO-*d*₆) δ 12.61 (s, 1H), 8.19 (d, *J* = 7.8 Hz, 1H), 7.87 (t, *J* = 7.6 Hz, 1H), 7.80 (t, *J* = 7.0 Hz, 1H), 7.75 (d, *J* = 8.1 Hz, 1H), 7.64 (q, *J* = 6.3 Hz, 1H), 7.58 (t, *J* = 7.5 Hz, 1H), 7.45 – 7.35 (m, 2H). ¹³C NMR (126 MHz, DMSO-*d*₆) δ 161.96, 161.02, 159.03, 150.41, 149.13, 135.07, 133.35, 133.28, 131.52, 131.51, 127.96, 127.50, 126.32, 125.09, 125.06, 122.79, 122.68, 121.56, 116.73, 116.56. ¹⁹F NMR (471 MHz, DMSO-*d*₆) δ -114.68.

(3i) 2-(4-(trifluoromethyl)phenyl)quinazolin-4(3H)-one ^[3]



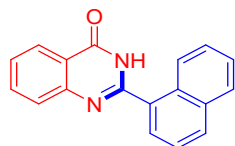
White solid, m.p. 283.8-295.7 °C. ¹H NMR (500 MHz, DMSO-*d*₆) δ 12.78 (s, 1H), 8.38 (d, *J* = 7.2 Hz, 2H), 8.19 (d, *J* = 7.2 Hz, 1H), 8.02 – 7.70 (m, 4H), 7.57 (t, *J* = 6.6 Hz, 1H). ¹³C NMR (126 MHz, DMSO-*d*₆) δ 151.60, 148.89, 137.04, 135.18, 131.68, 131.42, 129.17, 128.14, 127.56, 126.35, 125.96, 125.93, 125.49, 123.33, 121.65. ¹⁹F NMR (471 MHz, DMSO-*d*₆) δ -61.35.

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



White solid, m.p. 288.1-290.5 °C. ¹H NMR (500 MHz, DMSO-*d*₆) δ 12.63 (s, 1H), 8.32 (d, *J* = 8.4 Hz, 2H), 8.18 (d, *J* = 7.8 Hz, 1H), 7.86 (dd, *J* = 10.5, 7.9 Hz, 3H), 7.78 (t, *J* = 7.2 Hz, 3H), 7.53 (q, *J* = 8.0 Hz, 3H), 7.44 (t, *J* = 7.3 Hz, 1H). ¹³C NMR (126 MHz, DMSO-*d*₆) δ 162.72, 152.37, 149.24, 143.29, 139.41, 135.10, 132.00, 129.54, 128.84, 128.65, 127.99, 127.32, 127.22, 127.06, 126.34, 121.47.

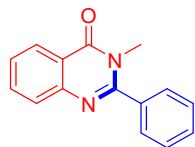
(3k) 2-(naphthalen-1-yl)quinazolin-4(3H)-one ^[3]



White solid, m.p. 289.8-291.9 °C. ¹H NMR (500 MHz, DMSO-*d*₆) δ 12.71 (s, 1H), 8.24 (d, *J* = 7.6 Hz, 1H), 8.19 (d, *J* = 7.6 Hz, 1H), 8.13 (d, *J* = 8.2 Hz, 1H), 8.09 – 8.04 (m, 1H), 7.88 (t, *J* = 7.5 Hz, 1H), 7.81 (d, *J* = 6.9 Hz, 1H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.69 – 7.56 (m, 4H). ¹³C NMR (126 MHz, DMSO-*d*₆) δ

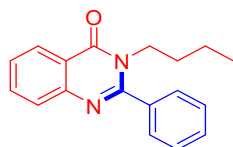
162.37, 154.13, 149.19, 135.01, 133.58, 132.18, 130.85, 130.71, 128.81, 128.16, 127.94, 127.55, 127.27, 126.84, 126.32, 125.69, 125.55, 121.70.

(3l) 3-methyl-2-phenylquinazolin-4(3H)-one ^[1]



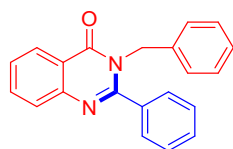
White solid, m.p. 127.9-129.8 °C. ¹H NMR (500 MHz, DMSO-*d*₆) δ 8.19 (d, *J* = 7.9 Hz, 1H), 7.84 (t, *J* = 7.5 Hz, 1H), 7.74 – 7.65 (m, 3H), 7.56 (s, 4H), 3.37 (s, 3H). ¹³C NMR (126 MHz, DMSO-*d*₆) δ 162.11, 156.60, 147.52, 135.86, 134.81, 130.26, 128.87, 128.73, 127.64, 127.34, 126.55, 120.61, 34.36.

(3m) 3-butyl-2-phenylquinazolin-4(3H)-one ^[5]



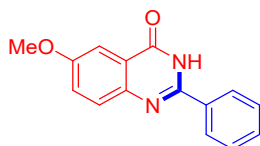
White solid, m.p. 112.4-114.1 °C. ¹H NMR (500 MHz, DMSO-*d*₆) δ 8.20 (d, *J* = 7.9 Hz, 1H), 7.85 (t, *J* = 7.5 Hz, 1H), 7.71 – 7.61 (m, 3H), 7.56 (d, *J* = 6.0 Hz, 4H), 3.97 – 3.81 (m, 2H), 1.48 (p, *J* = 7.4 Hz, 2H), 1.07 (h, *J* = 7.3 Hz, 2H), 0.66 (t, *J* = 7.3 Hz, 3H). ¹³C NMR (126 MHz, DMSO-*d*₆) δ 161.59, 156.51, 147.34, 135.87, 134.91, 130.04, 128.83, 128.44, 127.63, 127.43, 126.64, 120.89, 45.28, 30.31, 19.76, 13.64.

(3n) 3-benzyl-2-phenylquinazolin-4(3H)-one ^[1]



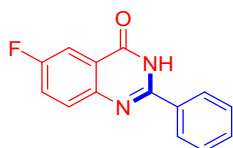
White solid, m.p. 138.4-140.6 °C. ¹H NMR (500 MHz, DMSO-*d*₆) δ 8.25 – 8.19 (m, 1H), 7.93 – 7.86 (m, 1H), 7.72 (d, *J* = 8.1 Hz, 1H), 7.61 (t, *J* = 7.4 Hz, 1H), 7.54 – 7.40 (m, 5H), 7.21 (t, *J* = 7.7 Hz, 3H), 6.92 (d, *J* = 6.6 Hz, 2H), 5.19 (s, 2H). ¹³C NMR (126 MHz, DMSO-*d*₆) δ 161.85, 156.61, 147.42, 137.18, 135.59, 135.22, 130.17, 128.88, 128.69, 128.44, 127.82, 127.70, 127.55, 126.88, 126.72, 120.84, 48.68.

(3o) 6-methoxy-2-phenylquinazolin-4(3H)-one ^[1]



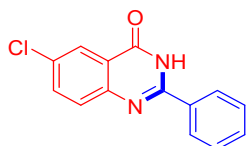
White solid, m.p. >300°C. ¹H NMR (500 MHz, DMSO-*d*₆) δ 12.53 (s, 1H), 8.17 (d, *J* = 7.0 Hz, 2H), 7.71 (d, *J* = 8.8 Hz, 1H), 7.55 (d, *J* = 7.4 Hz, 4H), 7.49 – 7.40 (m, 1H), 3.90 (s, 3H). ¹³C NMR (126 MHz, DMSO-*d*₆) δ 162.49, 158.20, 150.54, 143.67, 133.25, 129.69, 129.04, 127.95, 124.58, 122.25, 56.11.

(3p) 6-fluoro-2-phenylquinazolin-4(3H)-one ^[4]



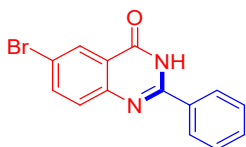
White solid; m.p: 274.2-276.6 °C. ¹H NMR (500 MHz, DMSO-*d*₆) δ 12.70 (s, 1H), 8.18 (d, *J* = 7.2 Hz, 2H), 7.84 (dd, *J* = 8.6, 3.2 Hz, 2H), 7.74 (td, *J* = 8.7, 2.9 Hz, 1H), 7.58 (dt, *J* = 14.5, 7.0 Hz, 3H). ¹³C NMR (126 MHz, DMSO-*d*₆) δ 162.16, 161.41, 159.46, 152.31, 146.08, 133.00, 131.89, 130.81, 130.75, 129.08, 128.21, 123.63, 123.43, 122.67, 122.61, 111.07, 110.89. ¹⁹F NMR (471 MHz, DMSO-*d*₆) δ - 113.50.

(3q) 6-chloro-2-phenylquinazolin-4(3H)-one ^[1]



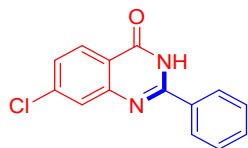
White solid, m.p. 276.9-279.0 °C. ¹H NMR (500 MHz, DMSO-*d*₆) δ 12.74 (s, 1H), 8.18 (d, *J* = 7.4 Hz, 2H), 8.08 (d, *J* = 2.2 Hz, 1H), 7.86 (dd, *J* = 8.7, 2.3 Hz, 1H), 7.76 (d, *J* = 8.7 Hz, 1H), 7.59 (dt, *J* = 25.5, 7.1 Hz, 3H). ¹³C NMR (126 MHz, DMSO-*d*₆) δ 161.76, 153.25, 147.93, 135.15, 132.89, 132.06, 131.21, 130.20, 129.10, 128.30, 125.33.

(3r) 6-bromo-2-phenylquinazolin-4(3H)-one ^[1]



White solid; m.p: 283.8-286.3 °C. ¹H NMR (500 MHz, DMSO-*d*₆) δ 12.74 (s, 1H), 8.31 – 8.11 (m, 3H), 7.98 (d, *J* = 7.8 Hz, 1H), 7.70 (d, *J* = 8.4 Hz, 1H), 7.66 – 7.50 (m, 3H). ¹³C NMR (126 MHz, DMSO-*d*₆) δ 161.62, 153.36, 148.18, 137.86, 132.90, 132.08, 130.34, 129.10, 128.45, 128.31, 123.05, 119.39.

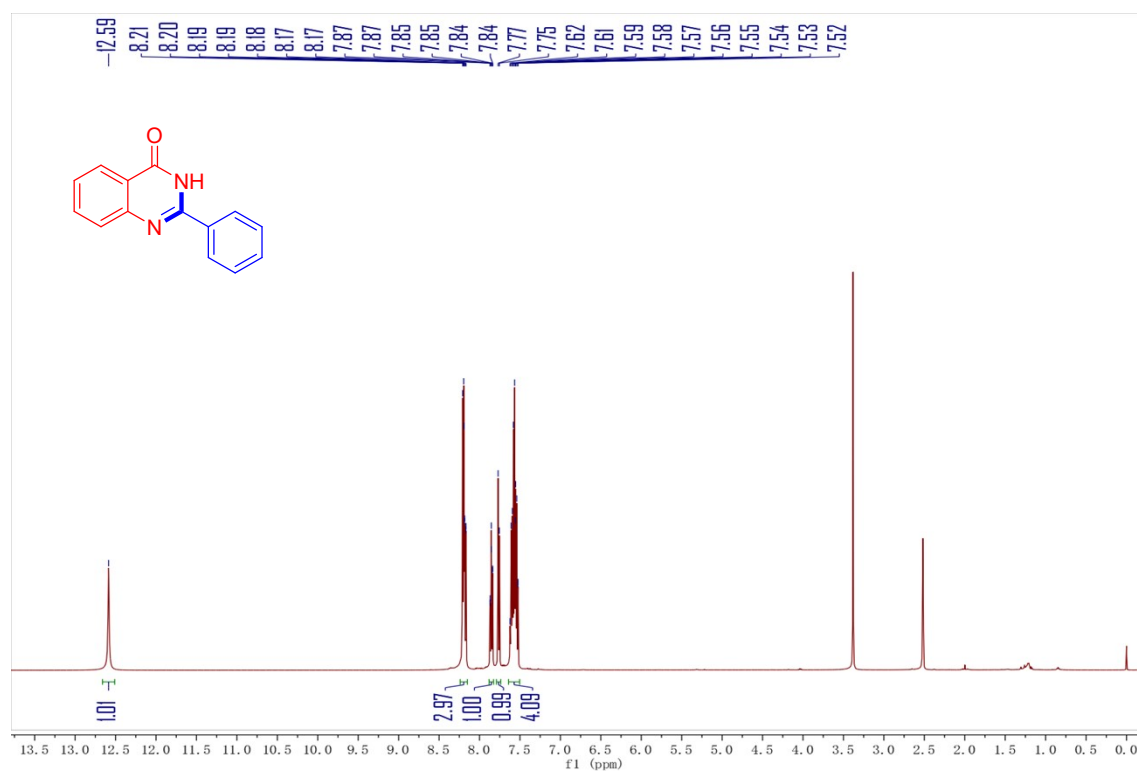
(3s) 7-chloro-2-phenylquinazolin-4(3H)-one ^[3]



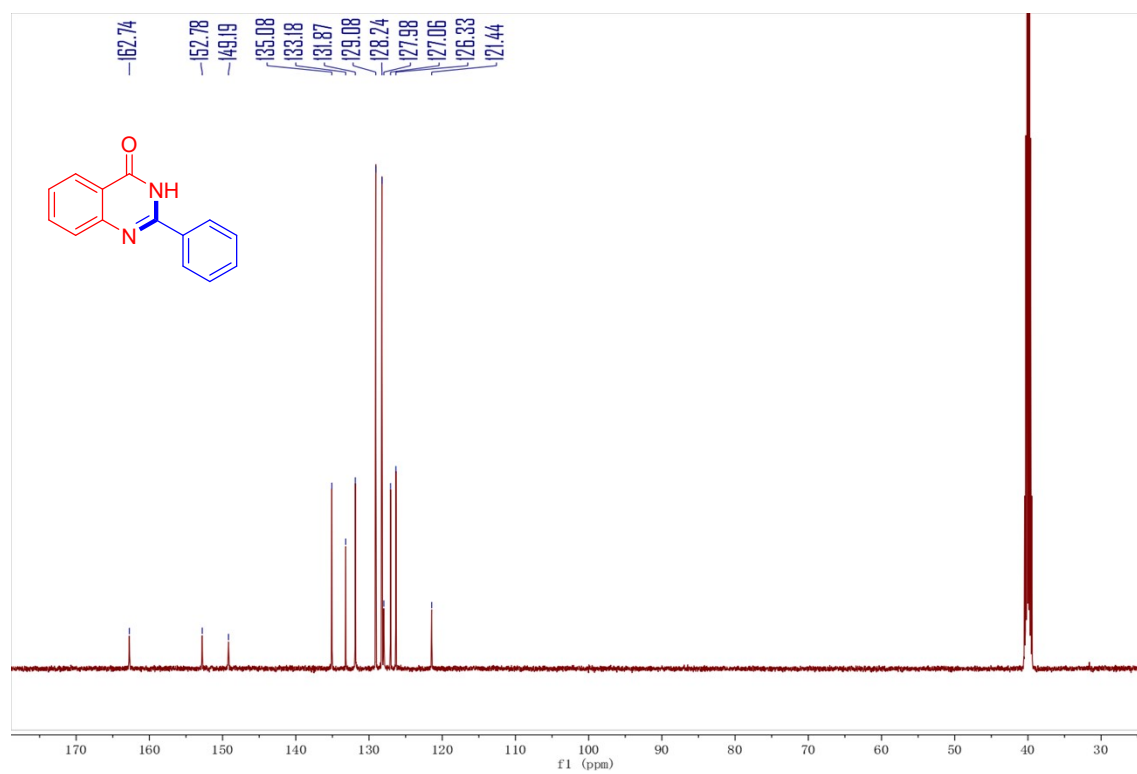
White solid; m.p: 284.1-286.3 °C. ^1H NMR (500 MHz, $\text{DMSO-}d_6$) δ 12.74 (s, 1H), 8.20 (dd, $J = 24.5$, 4.4 Hz, 3H), 8.03 – 7.93 (m, 1H), 7.69 (d, $J = 8.7$ Hz, 1H), 7.59 (dt, $J = 26.2$, 7.1 Hz, 3H). ^{13}C NMR (126 MHz, $\text{DMSO-}d_6$) δ 161.67, 153.40, 148.17, 137.87, 132.91, 132.08, 130.31, 129.10, 128.45, 128.31, 123.05, 119.39.

3. ^1H -NMR, ^{13}C -NMR and ^{19}F -NMR spectra of products

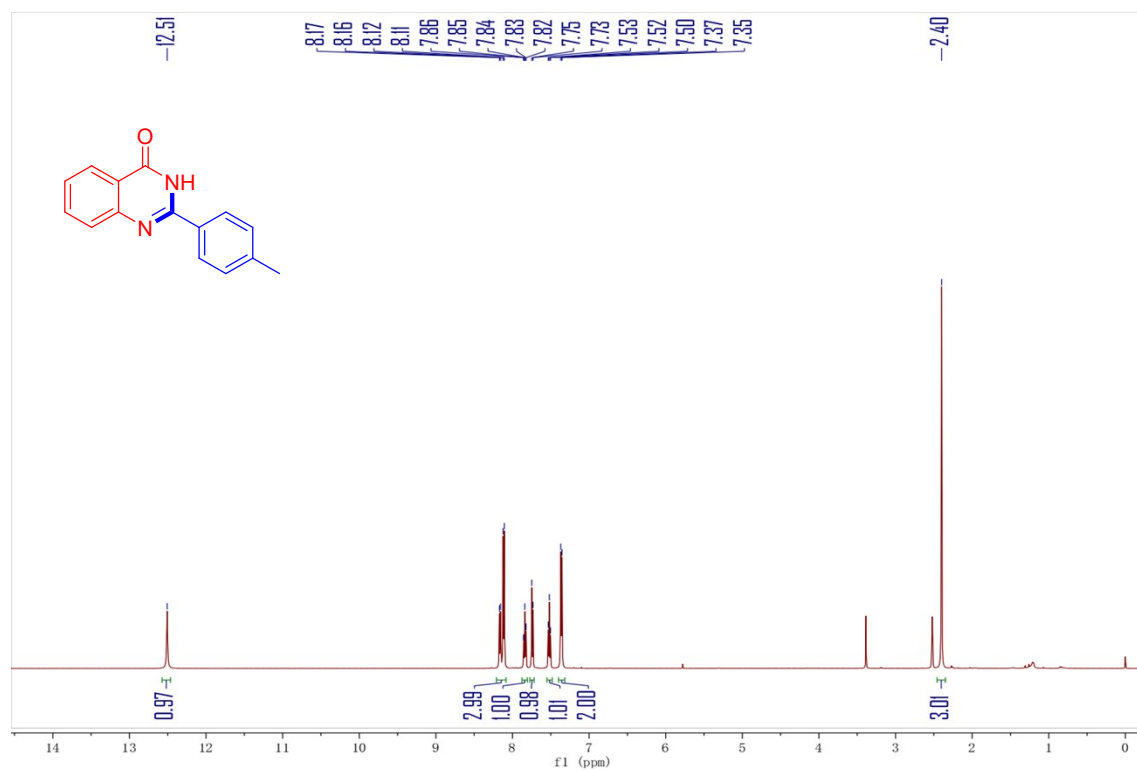
^1H NMR spectra of compound **3a**



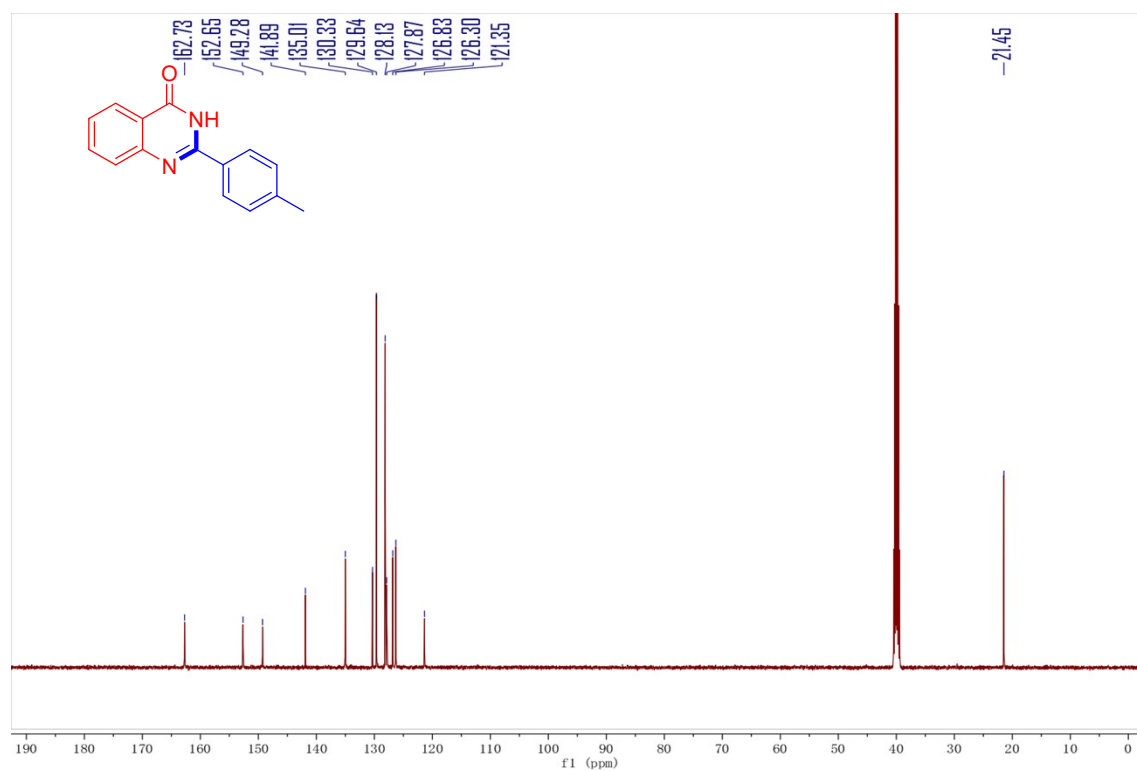
¹³C NMR spectra of compound 3a



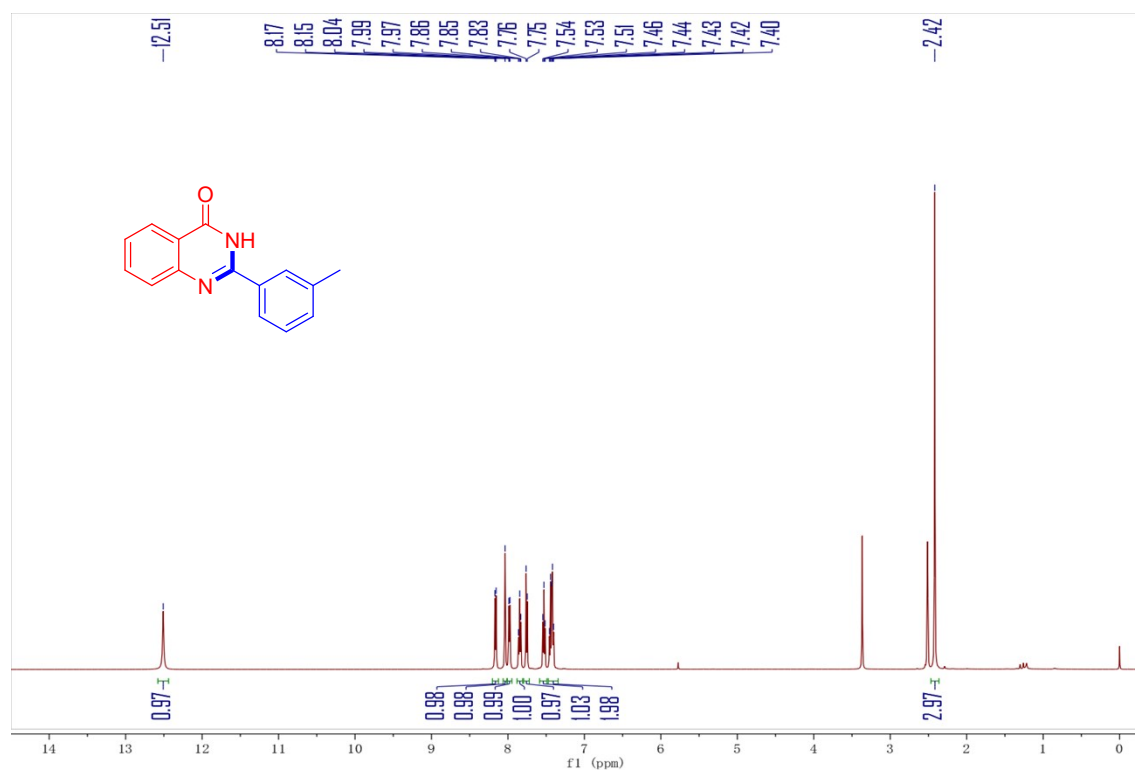
¹H NMR spectra of compound 3b



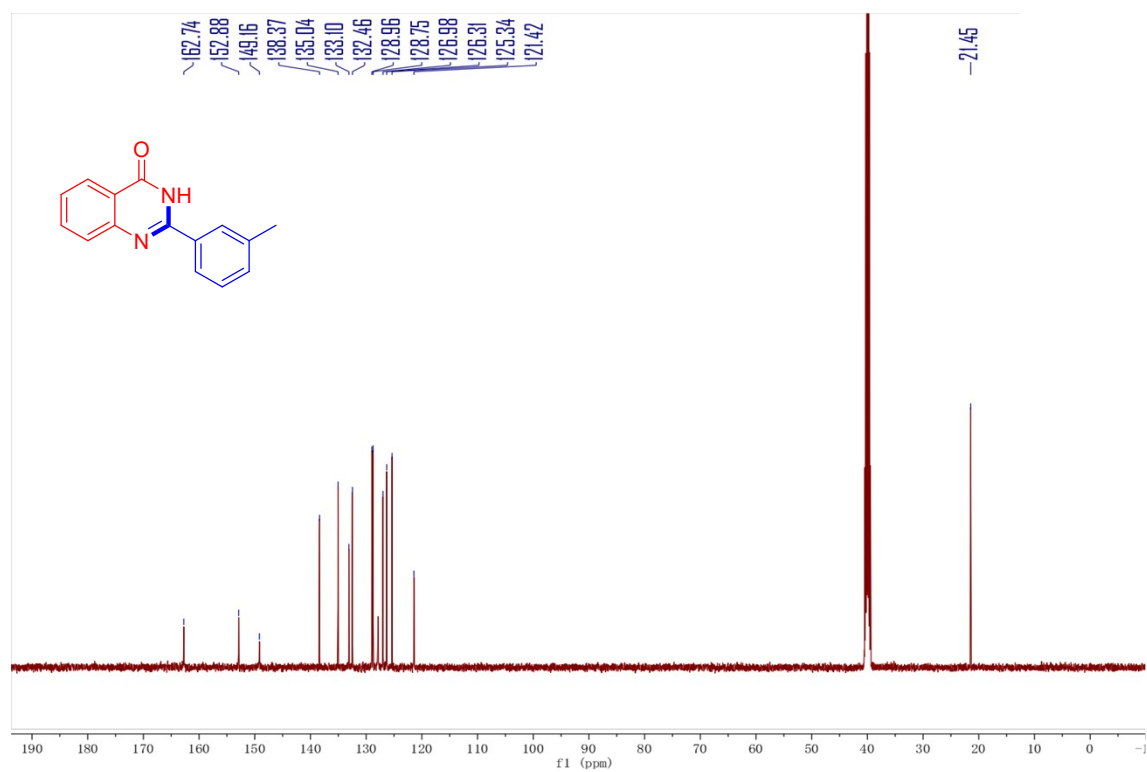
¹³C NMR spectra of compound 3b



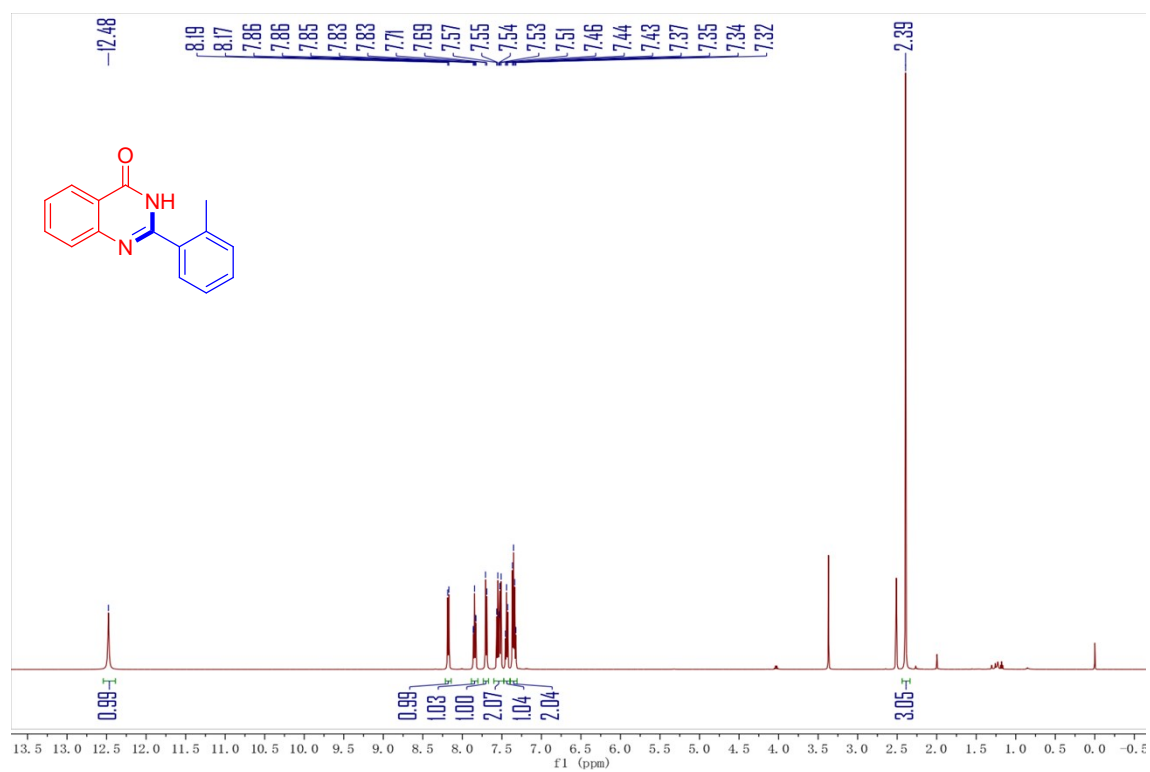
^1H NMR spectra of compound **3c**



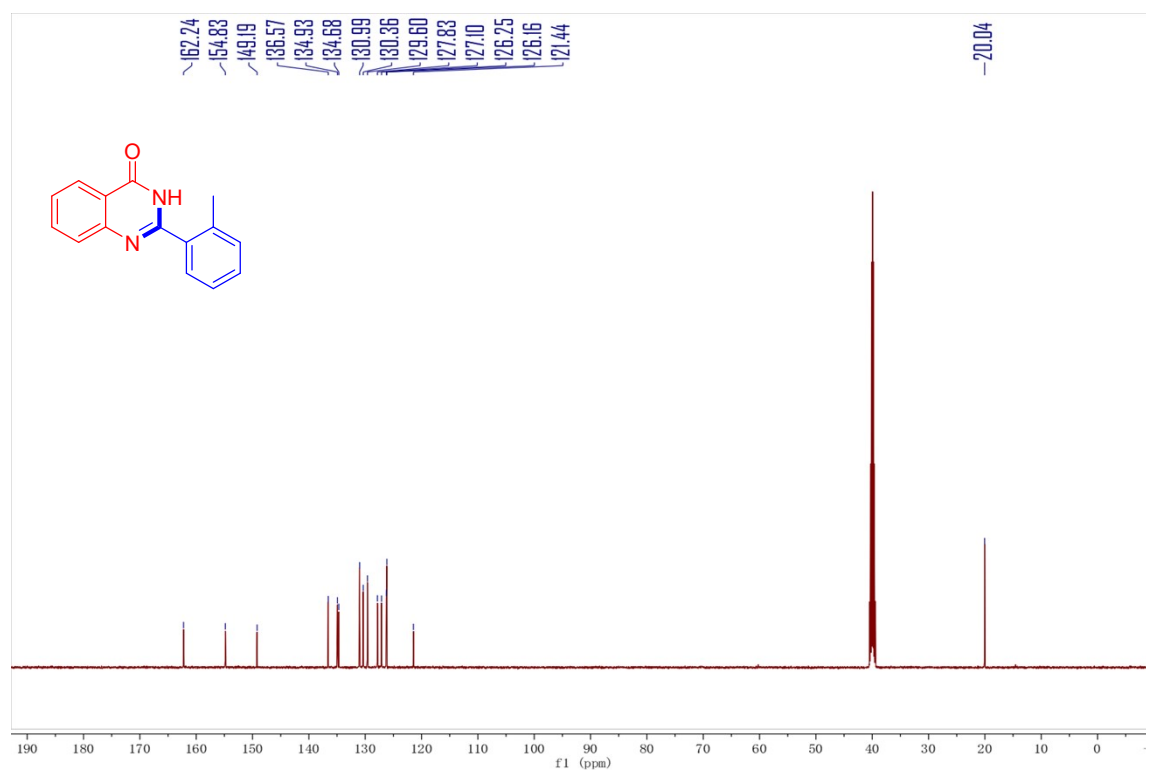
^{13}C NMR spectra of compound **3c**



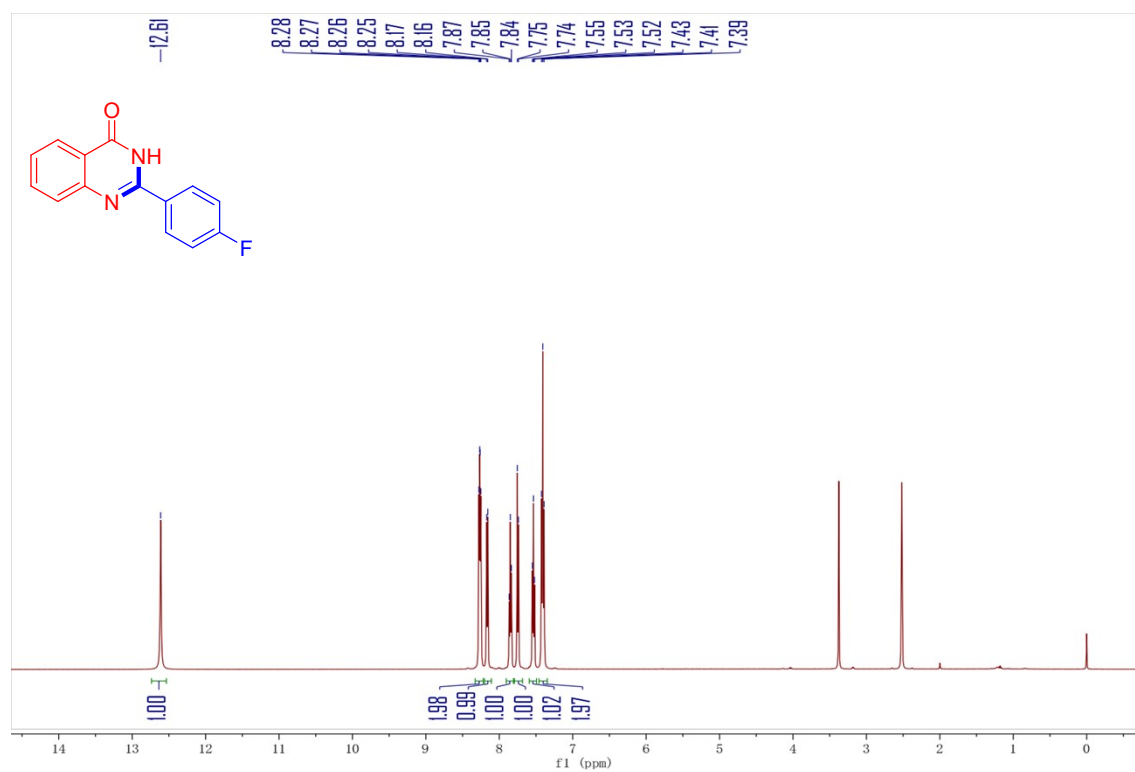
¹H NMR spectra of compound **3d**



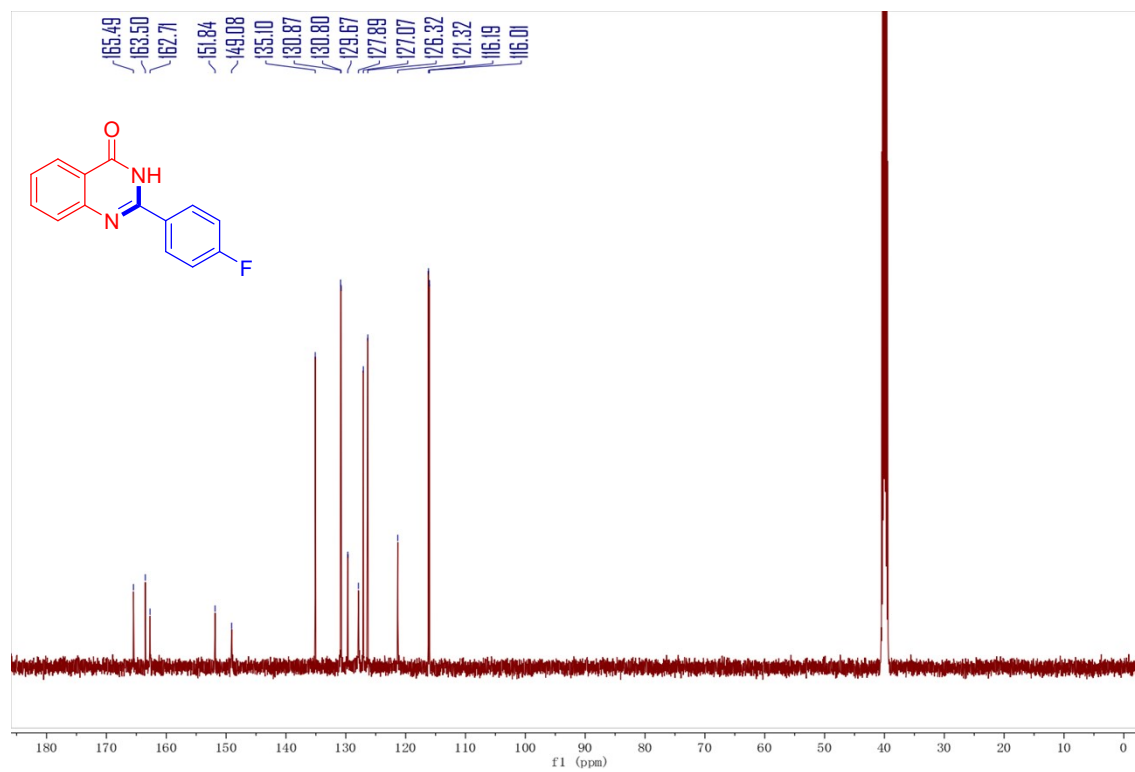
¹³C NMR spectra of compound **3d**



^1H NMR spectra of compound **3e**



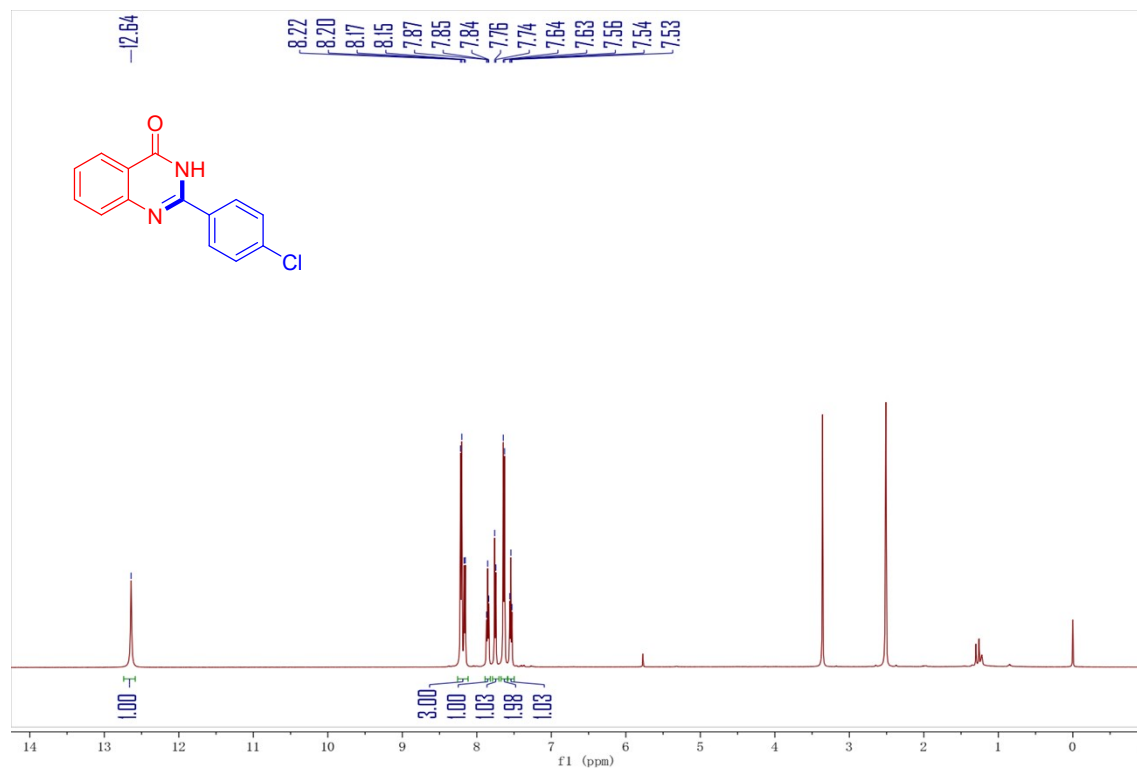
^{13}C NMR spectra of compound **3e**



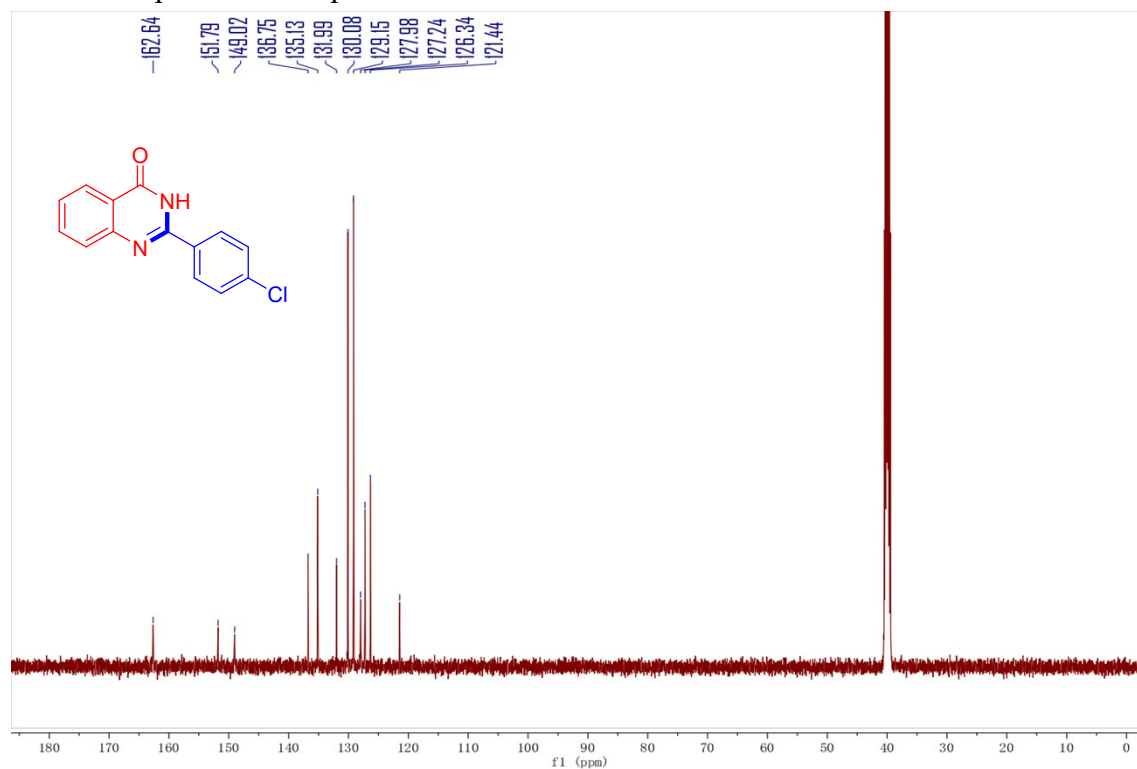
^{19}F NMR spectra of compound **3e**



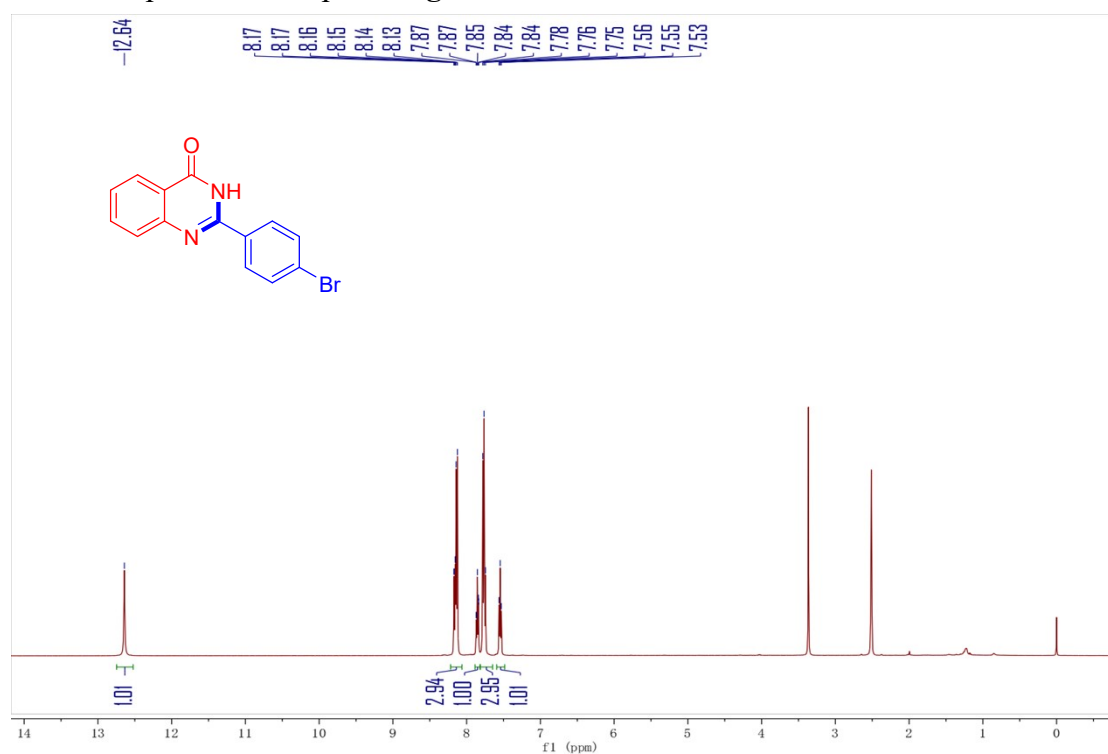
^1H NMR spectra of compound **3f**



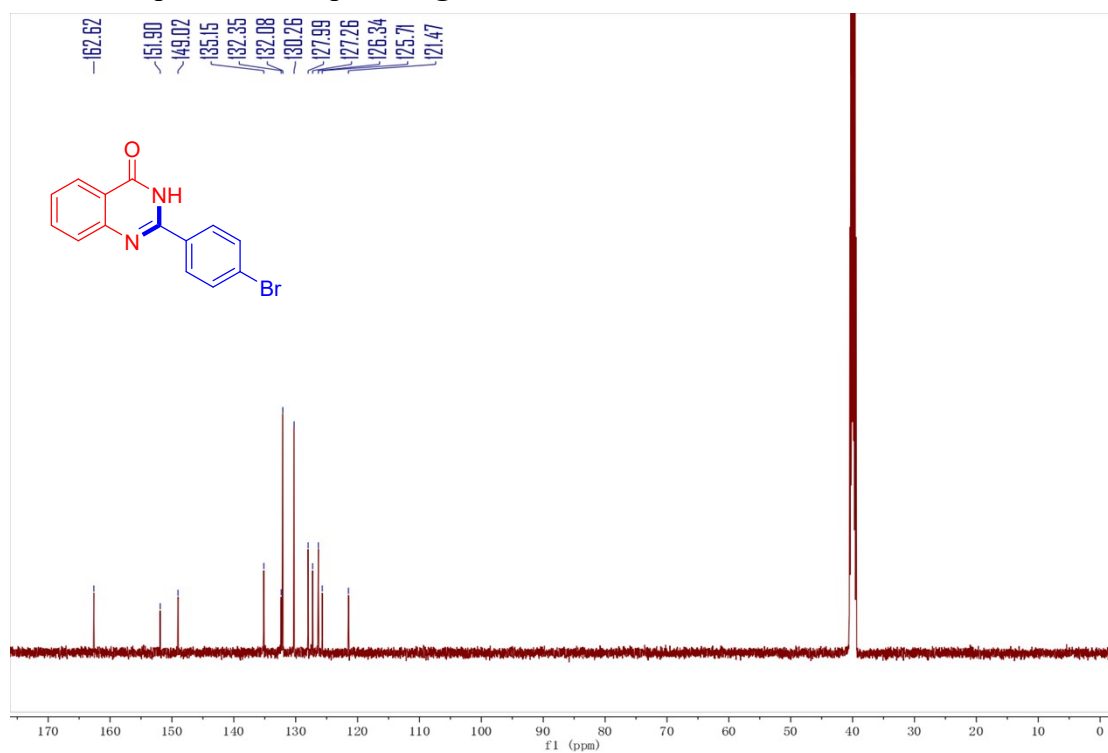
^{13}C NMR spectra of compound **3f**



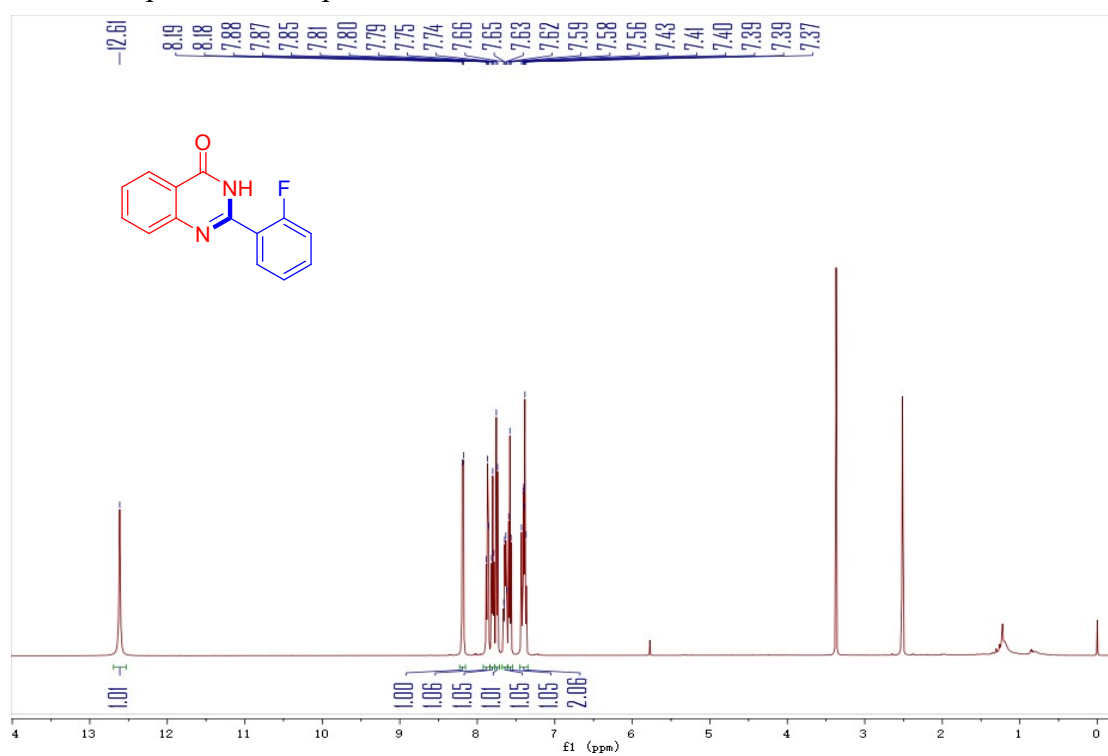
^1H NMR spectra of compound **3g**



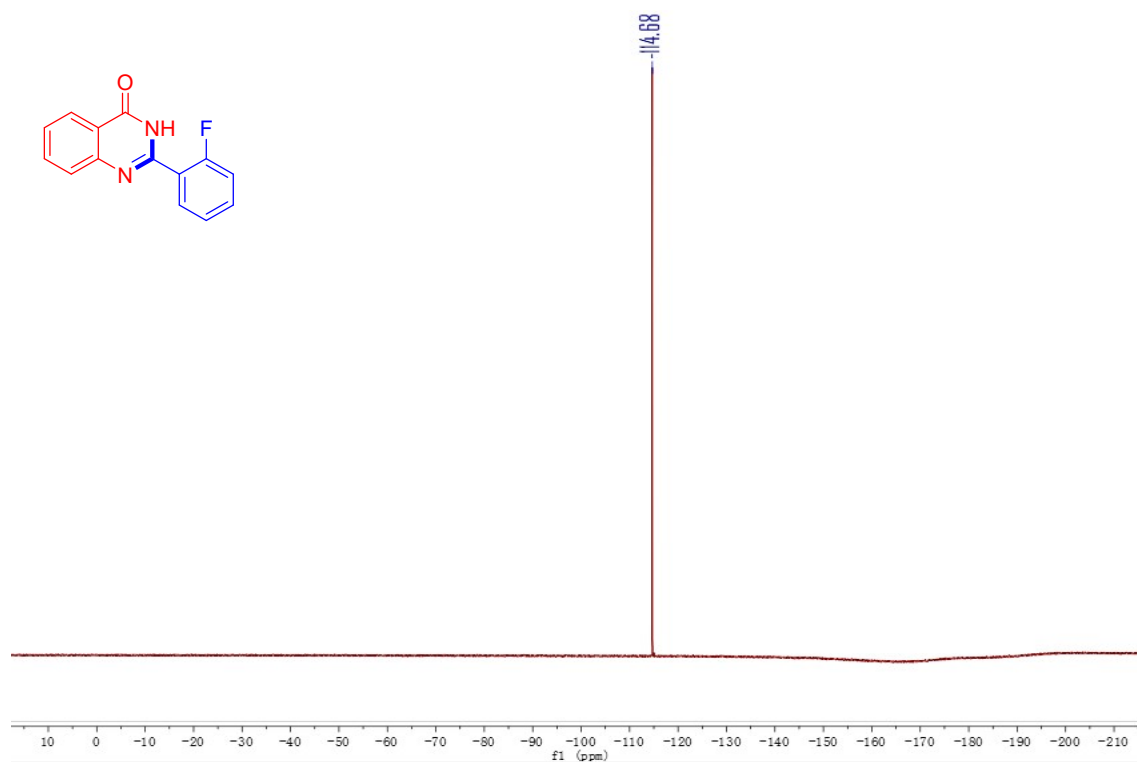
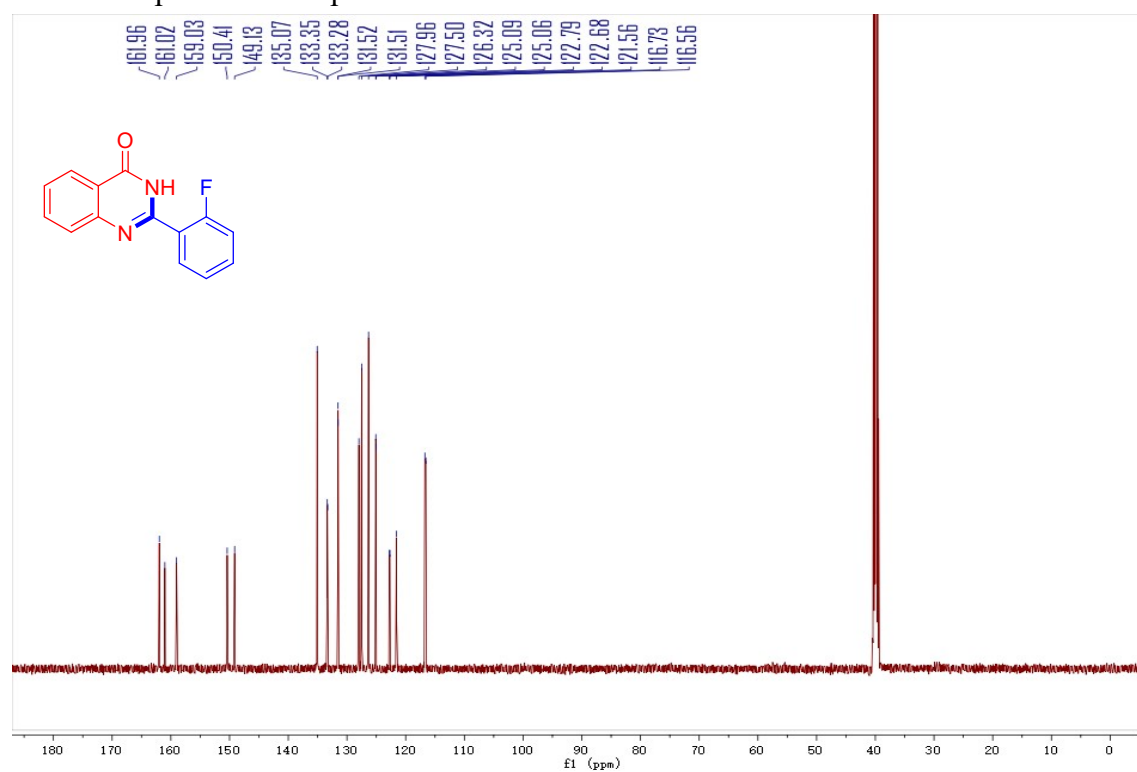
¹³C NMR spectra of compound **3g**



¹H NMR spectra of compound **3h**

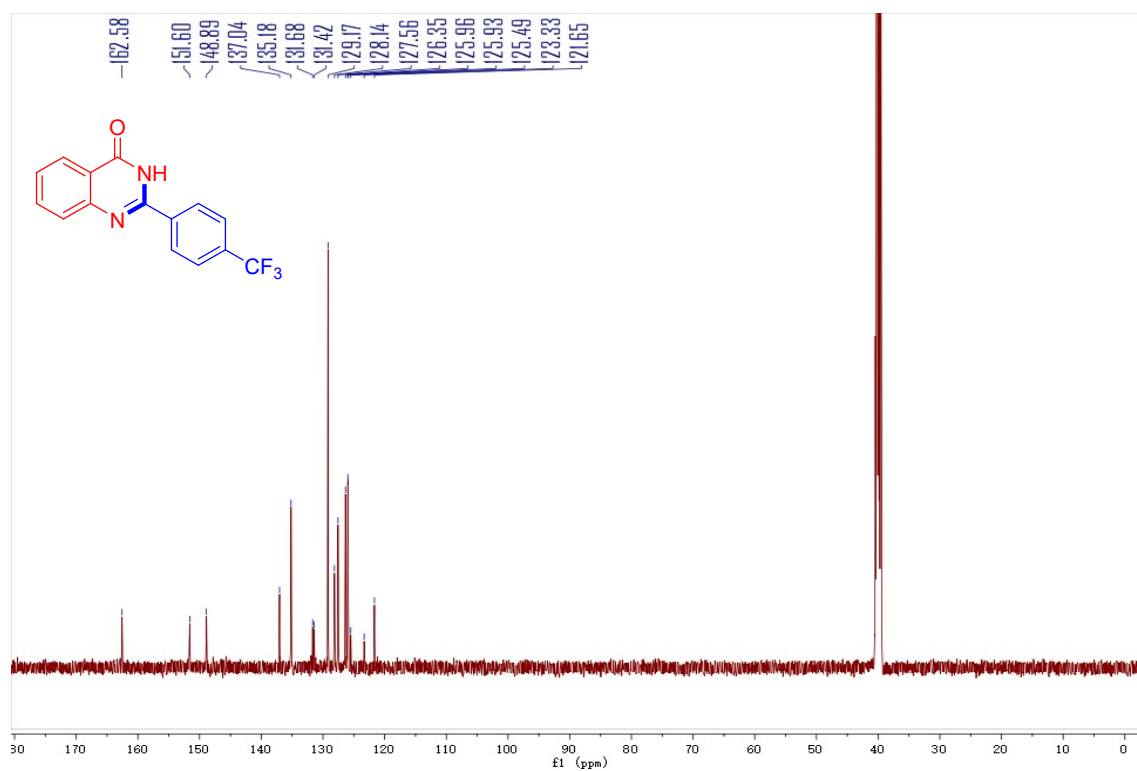
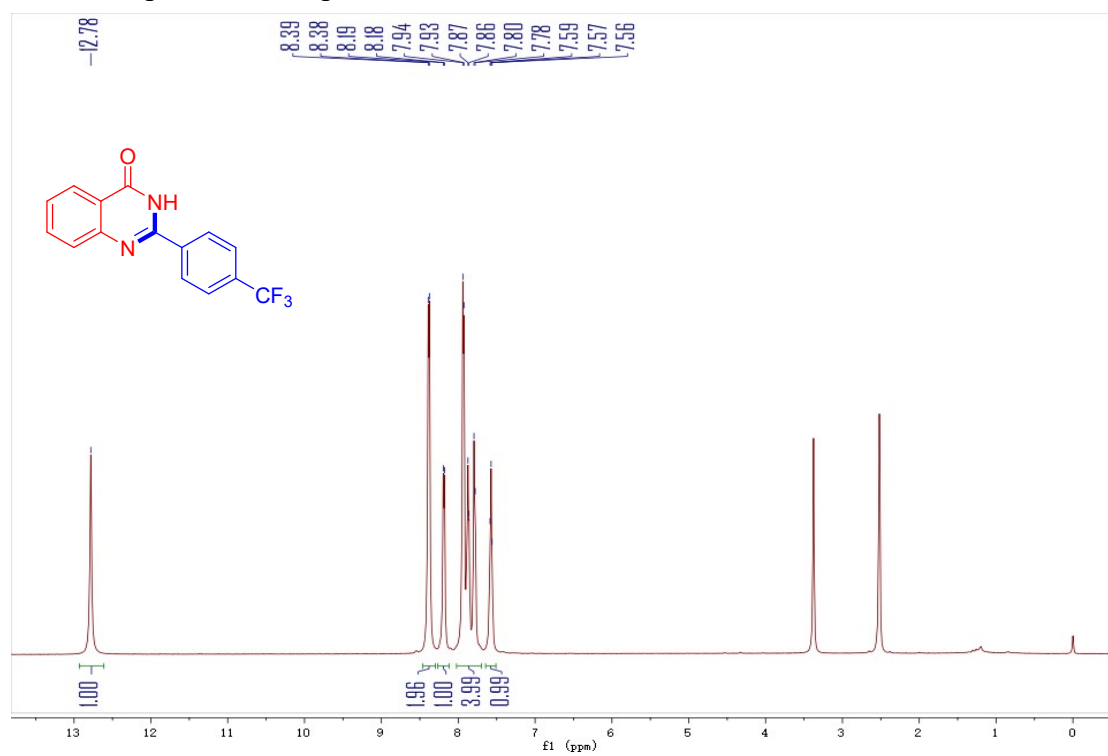


¹³C NMR spectra of compound **3h**

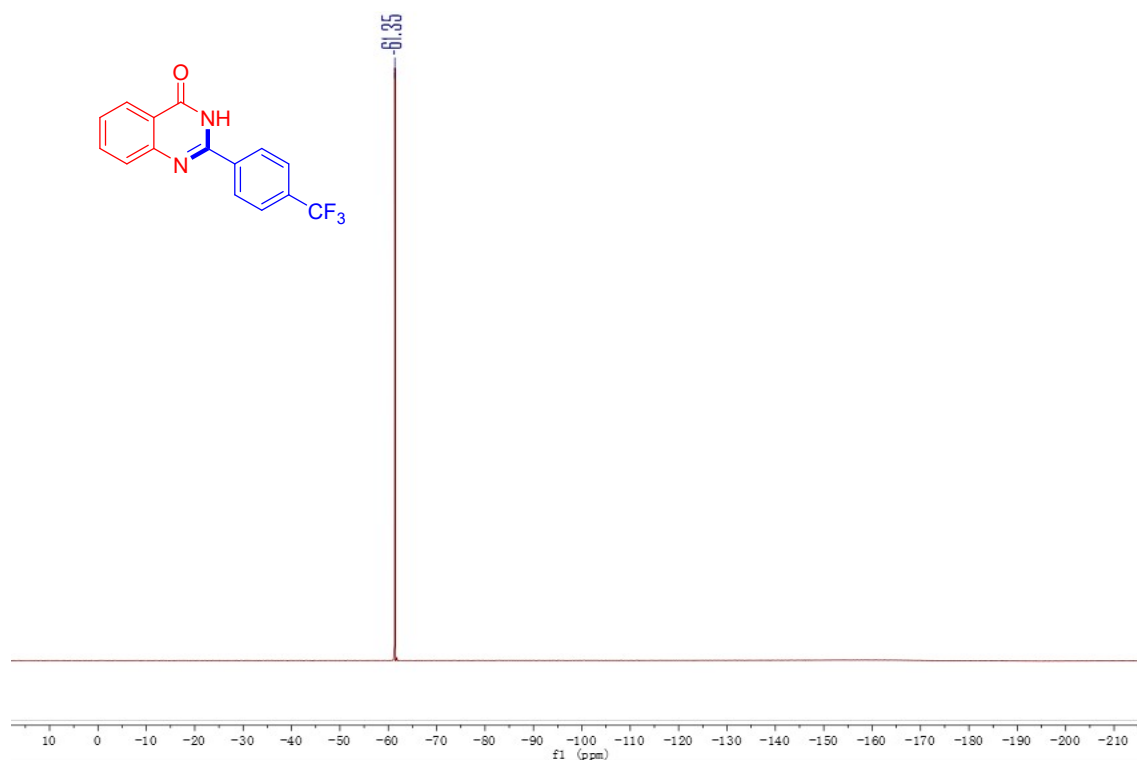


¹⁹F NMR spectra of compound **3h**

¹H NMR spectra of compound **3i**

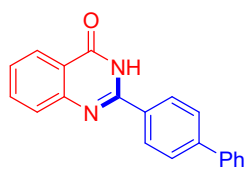


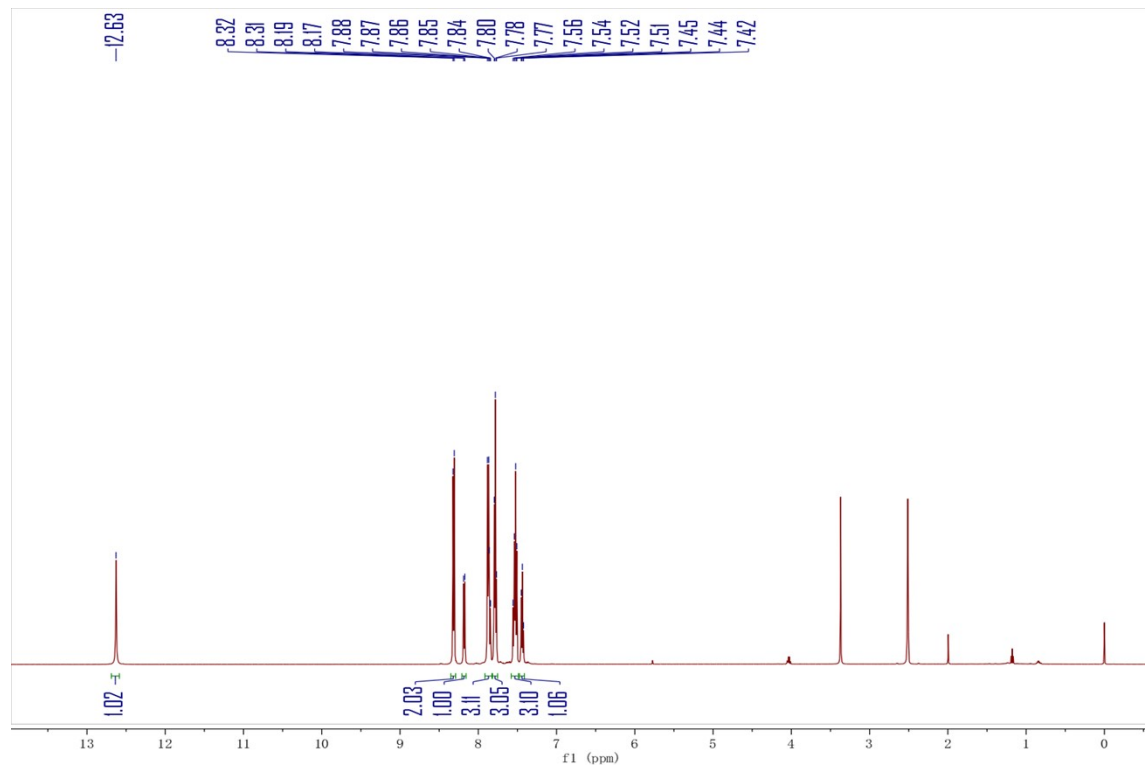
¹³C NMR spectra of compound **3i**

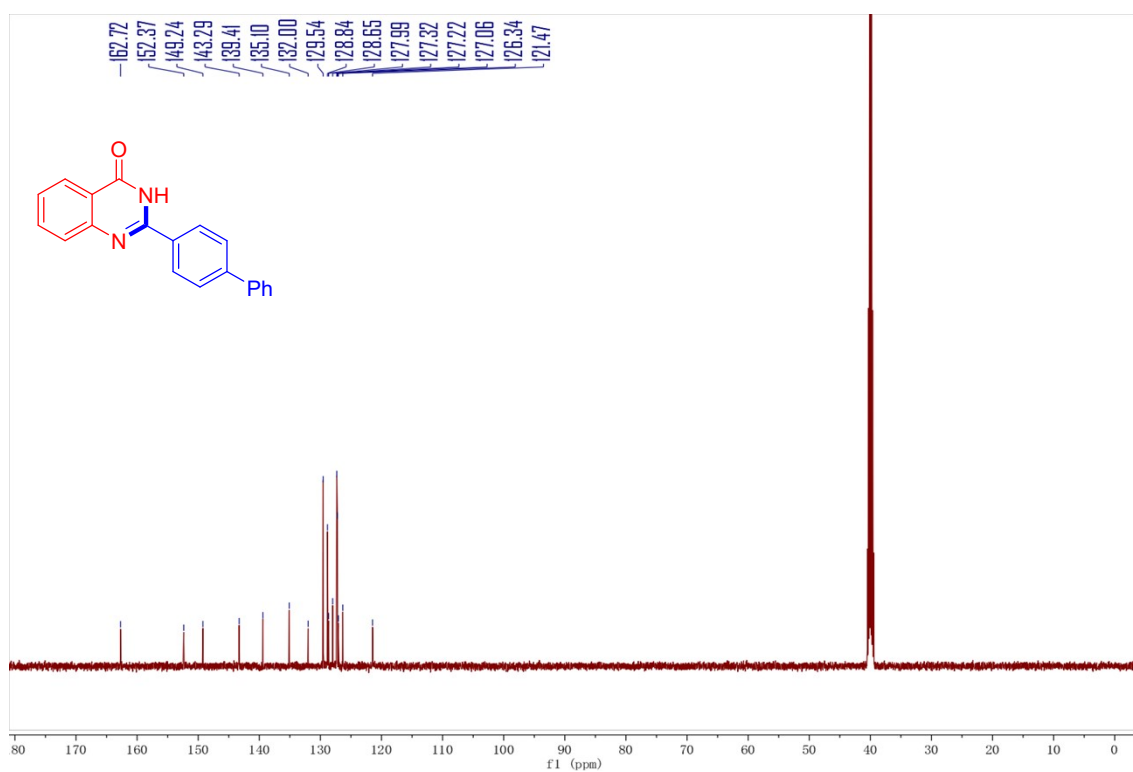


^{19}F NMR spectra of compound **3i**

^1H NMR spectra of compound **3j**

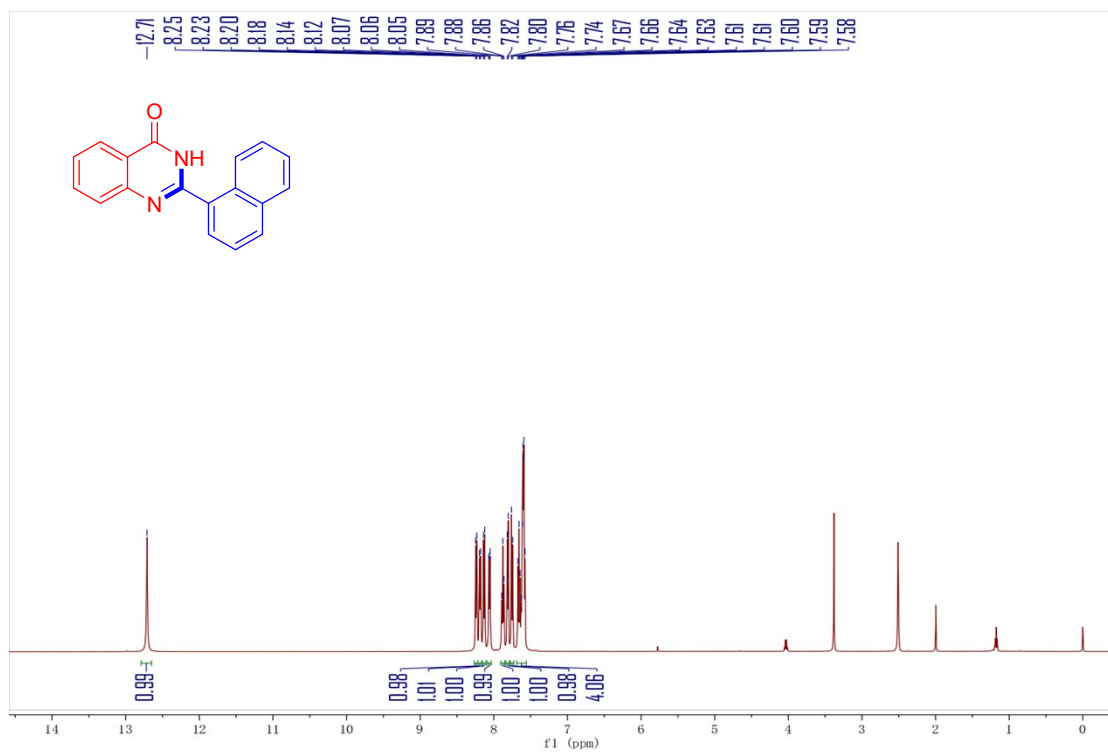




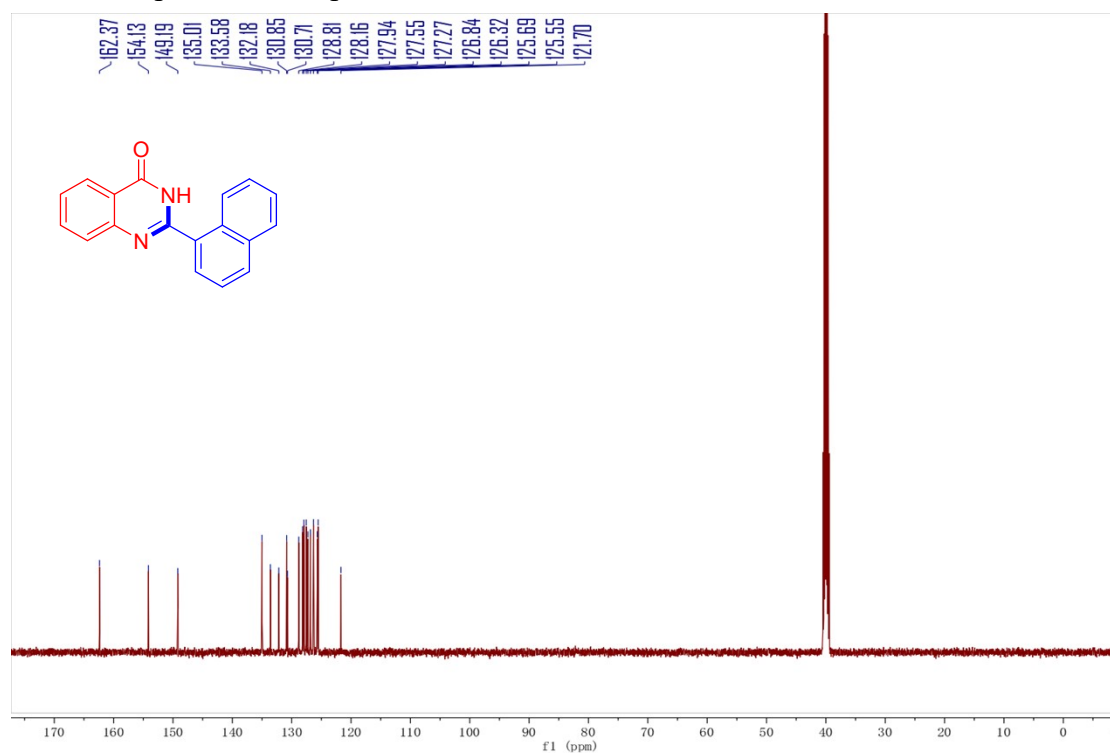


¹³C NMR spectra of compound **3j**

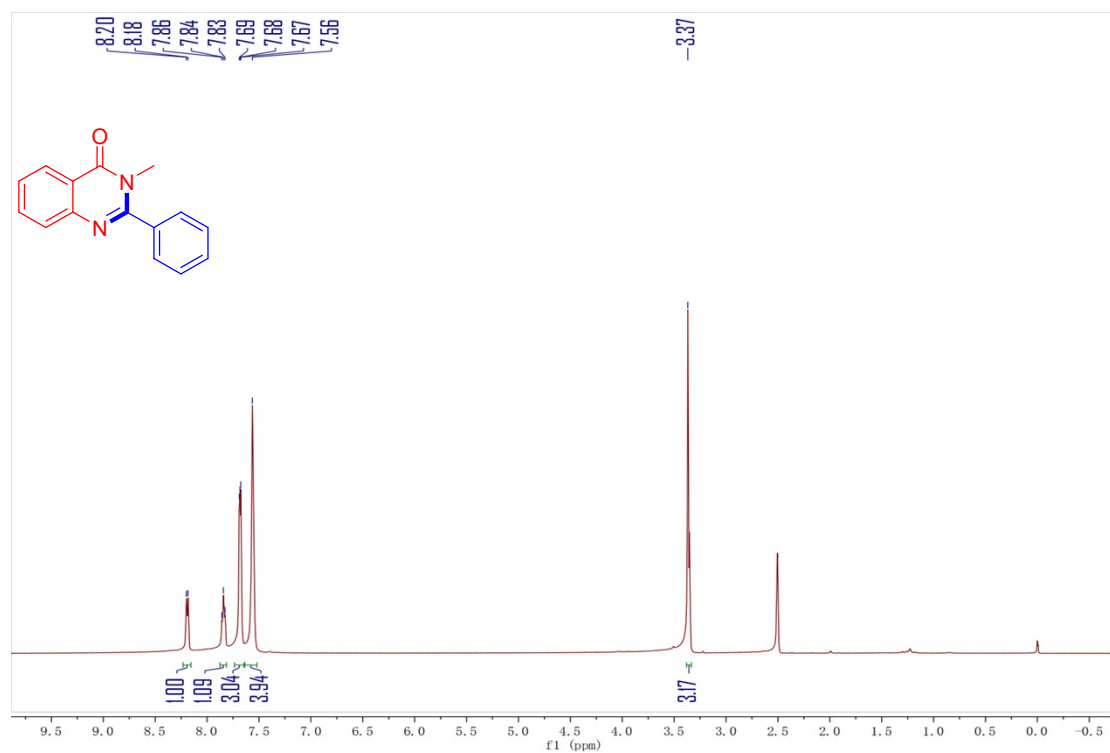
¹H NMR spectra of compound **3k**



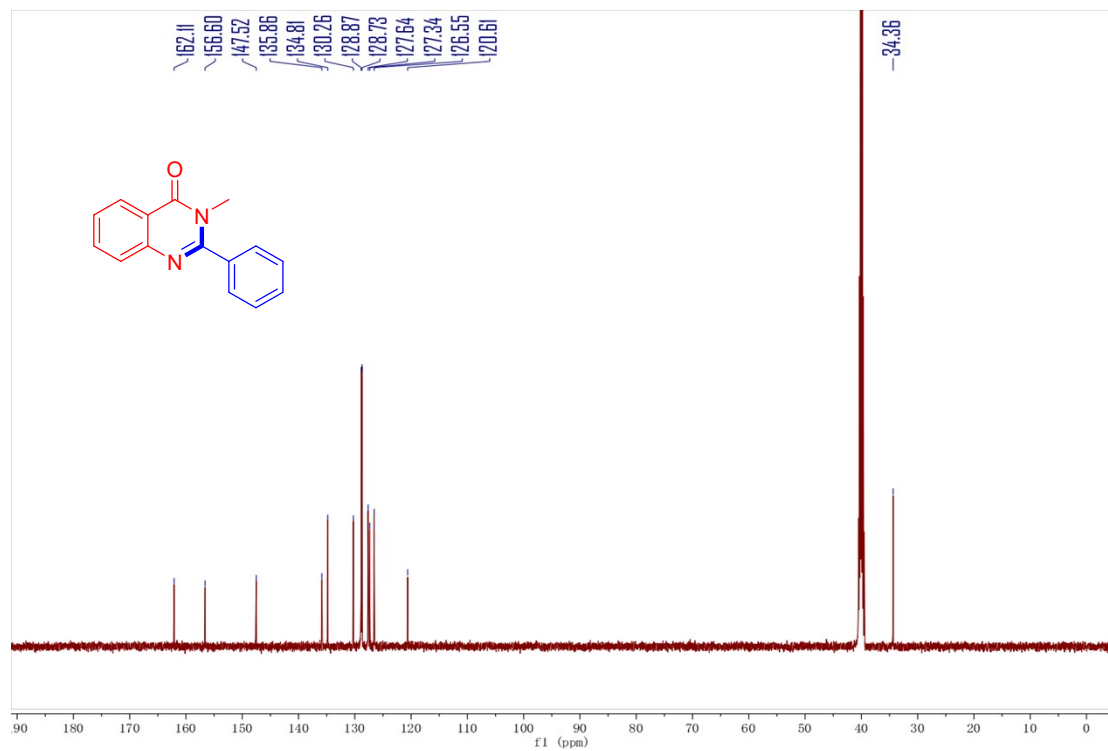
¹³C NMR spectra of compound **3k**



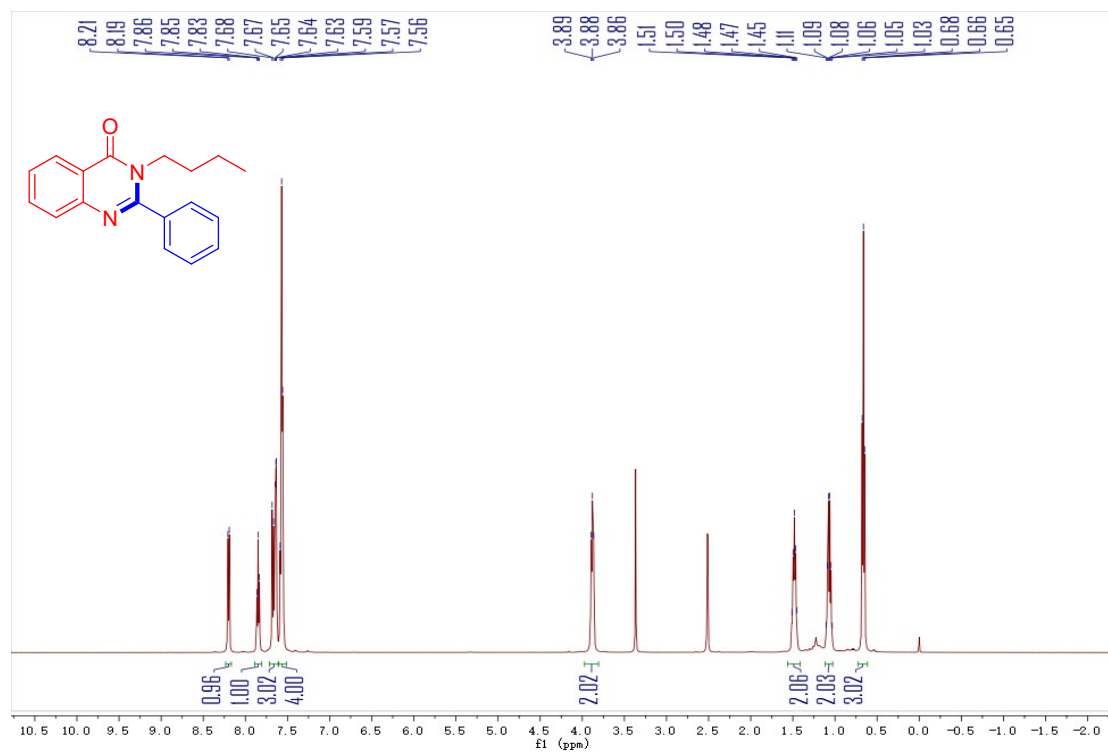
¹H NMR spectra of compound **3l**

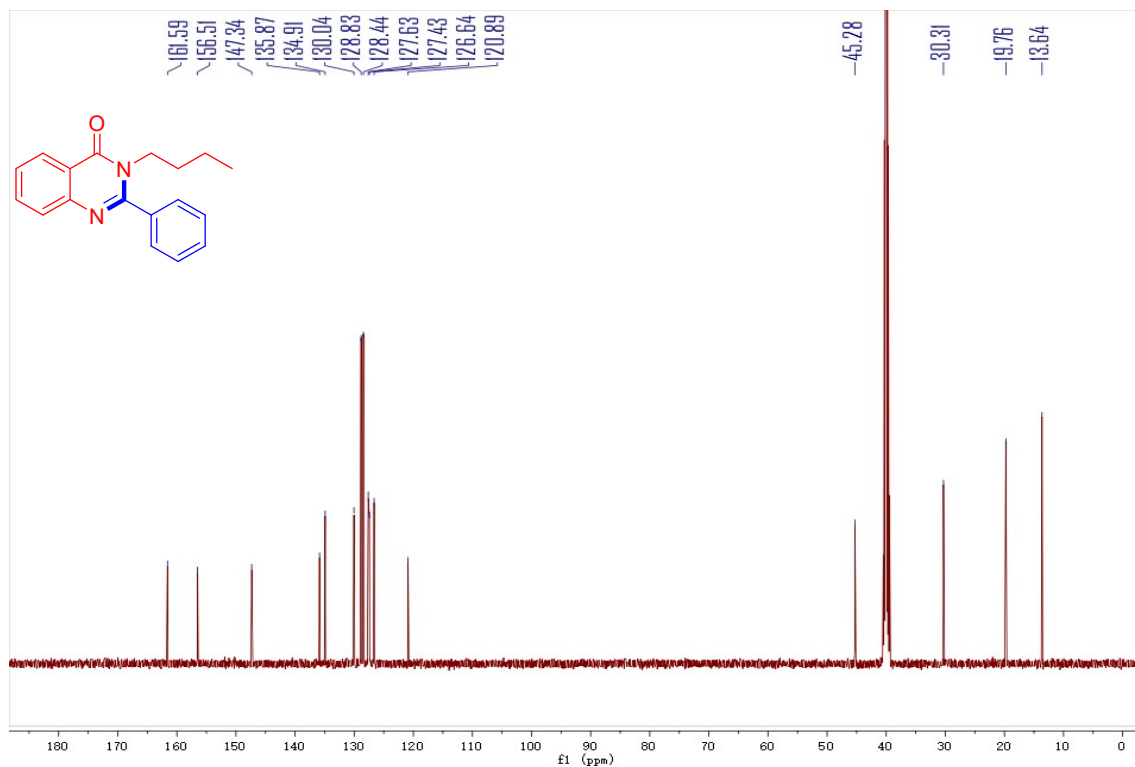


^{13}C NMR spectra of compound **3l**



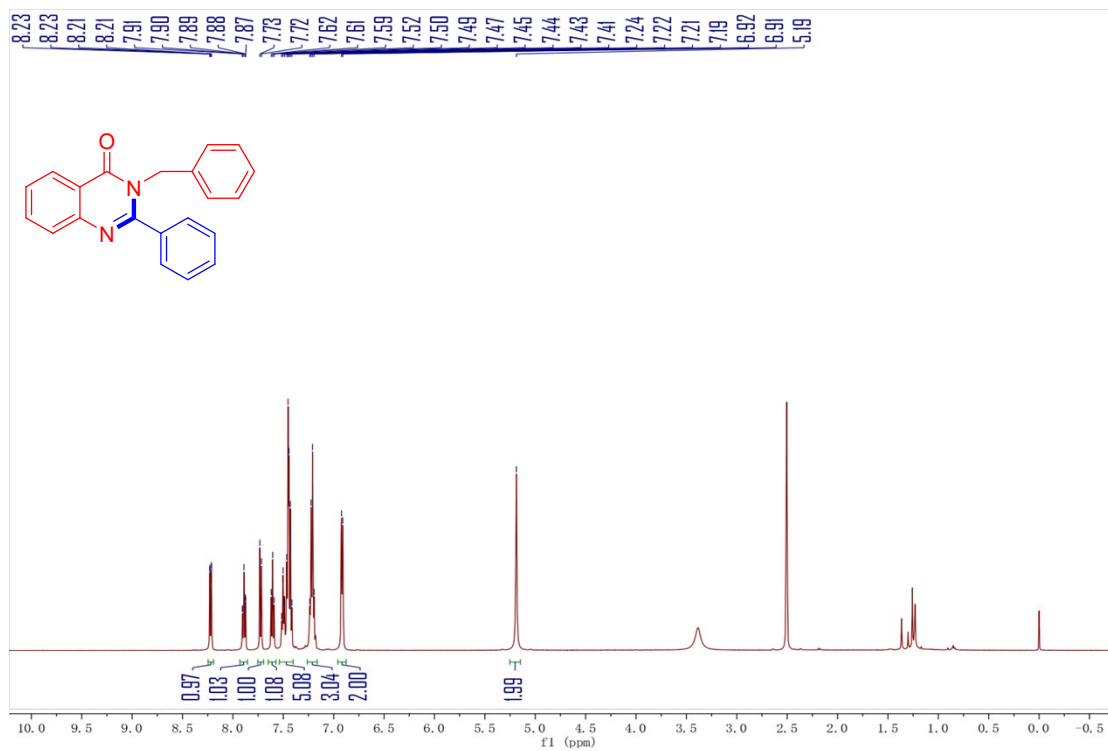
^1H NMR spectra of compound **3m**



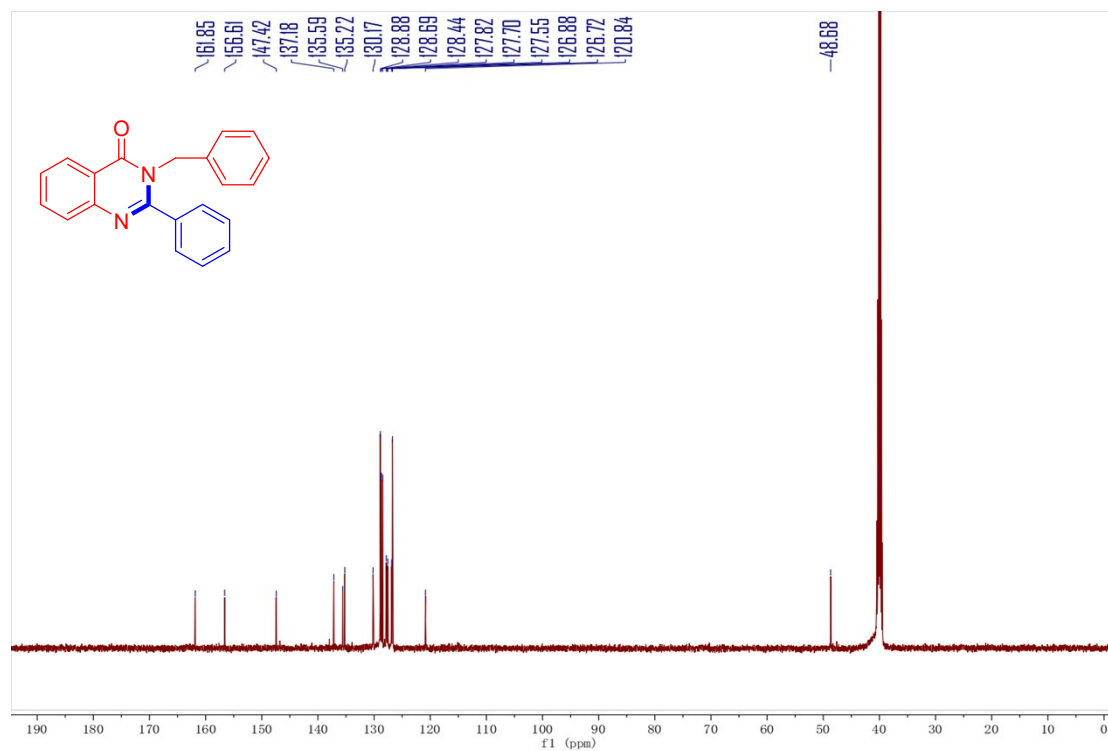


¹³C NMR spectra of compound 3m

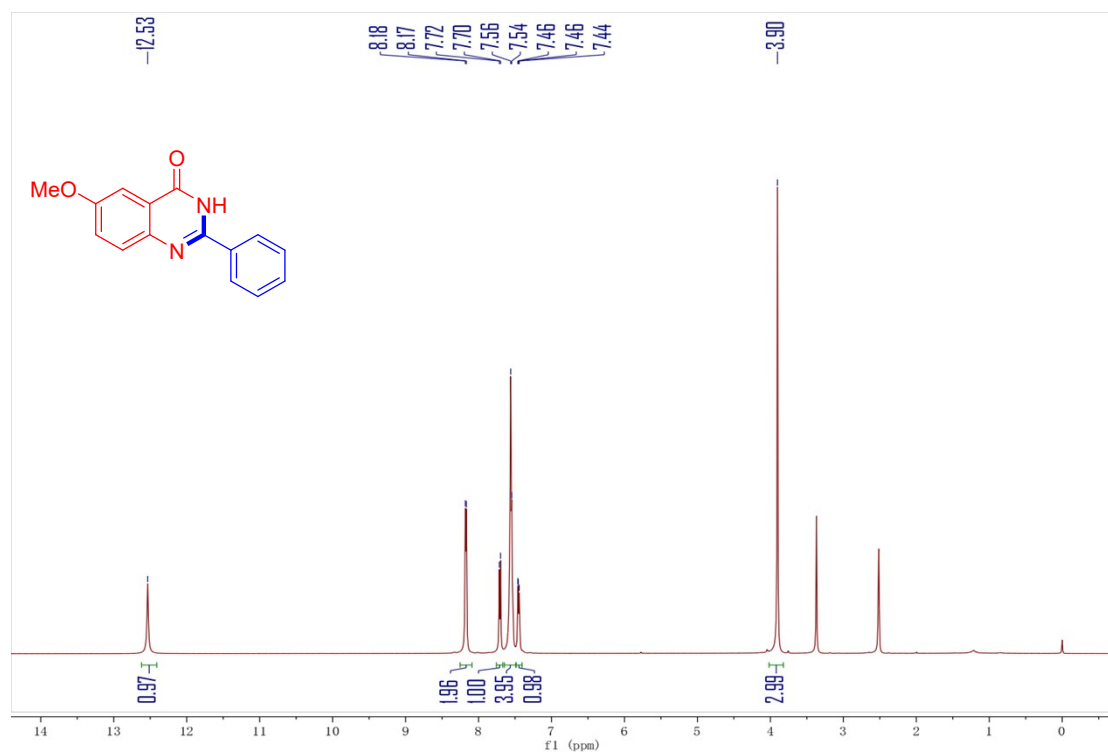
¹H NMR spectra of compound 3n



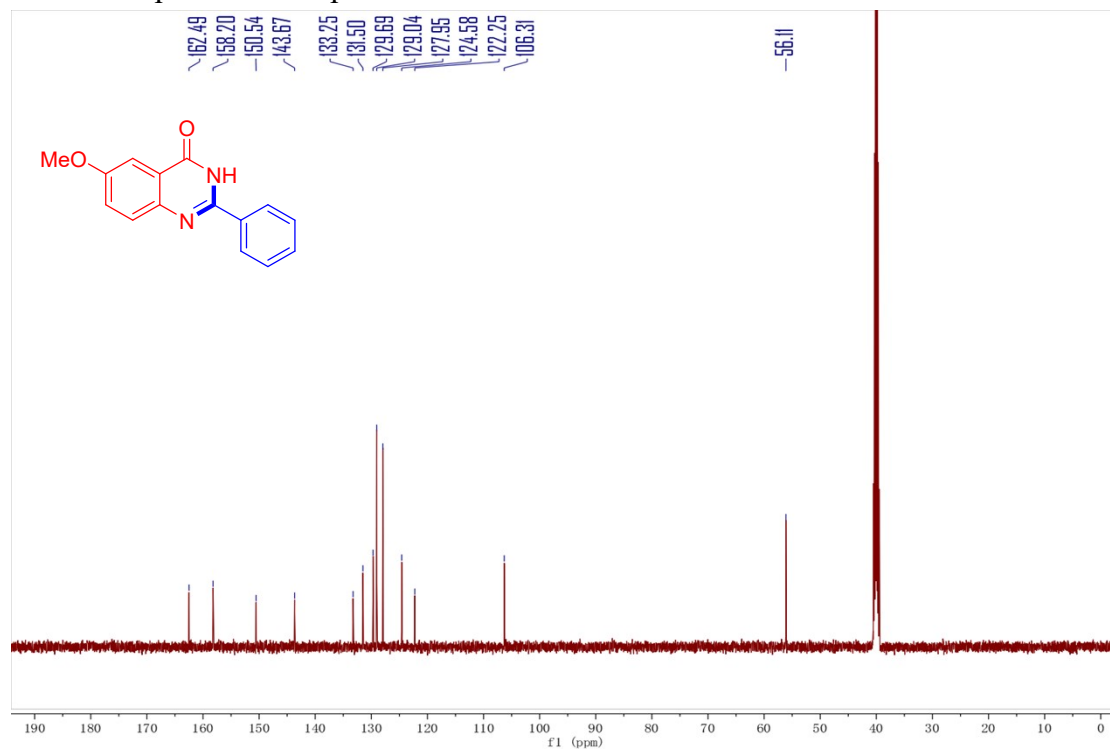
¹³C NMR spectra of compound **3n**



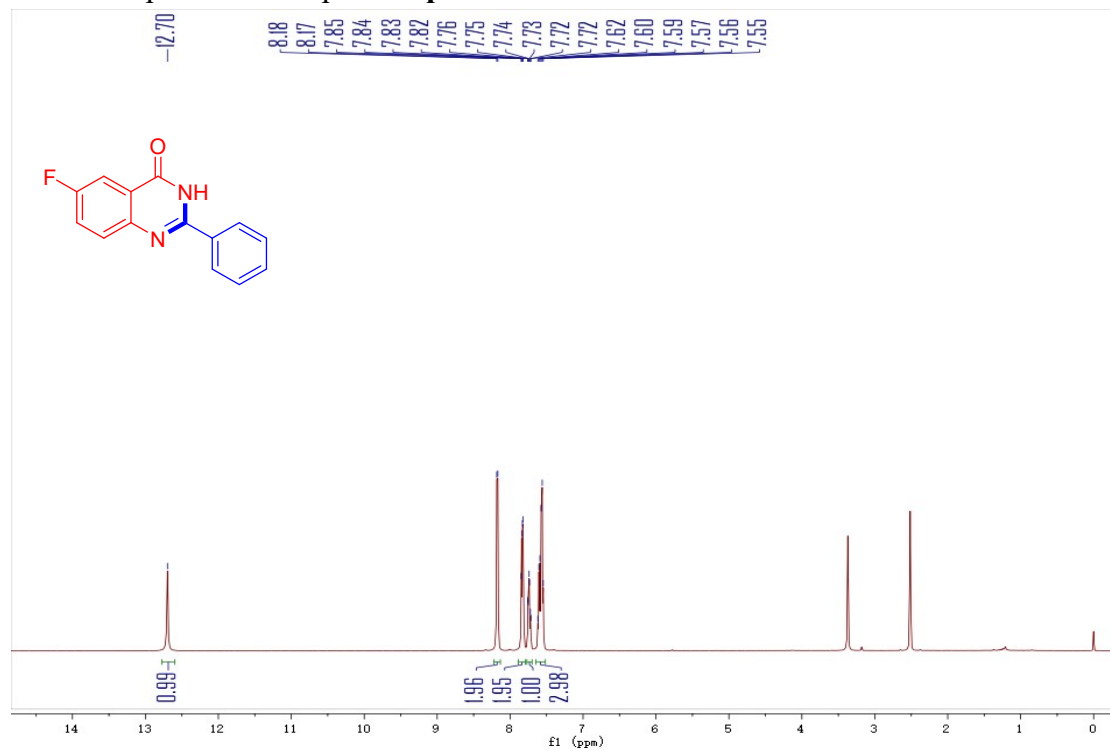
¹H NMR spectra of compound **3o**



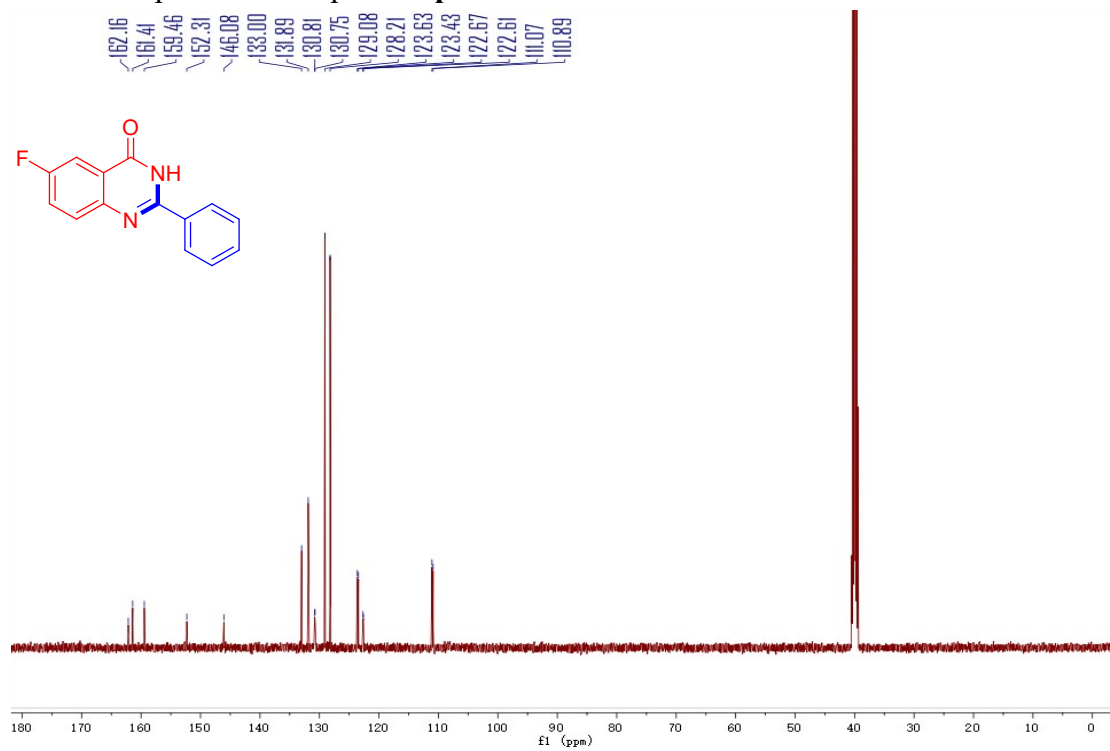
¹³C NMR spectra of compound **3o**



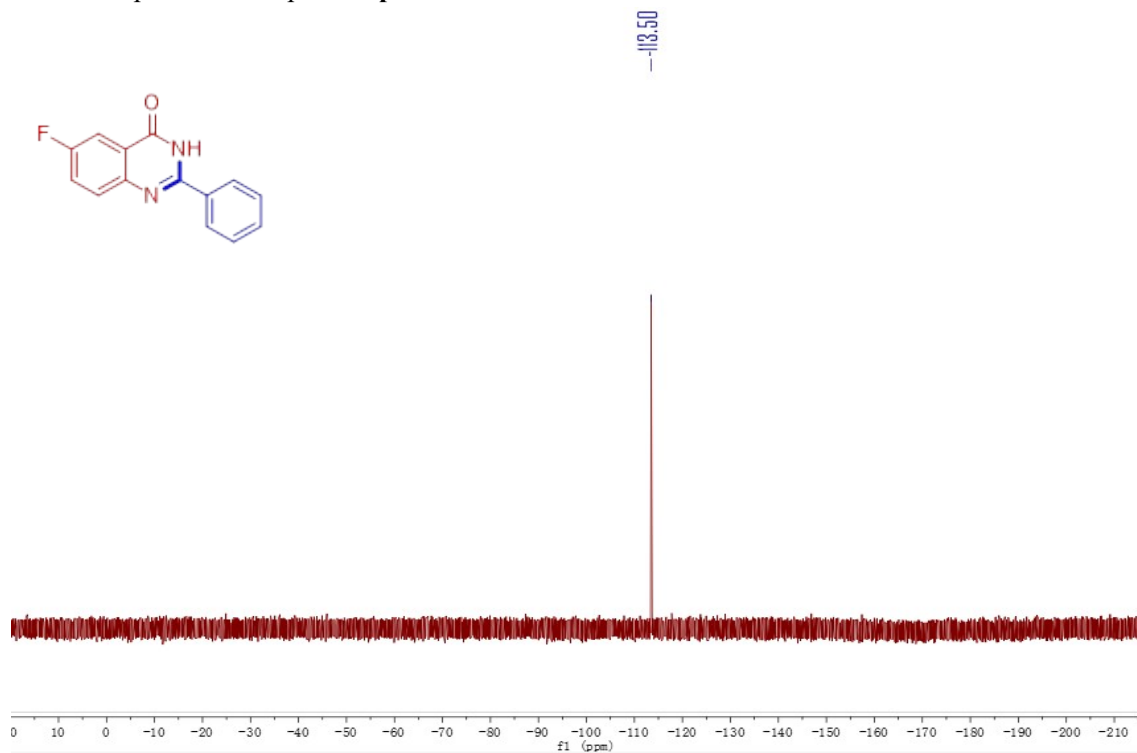
¹H NMR spectra of compound **3p**



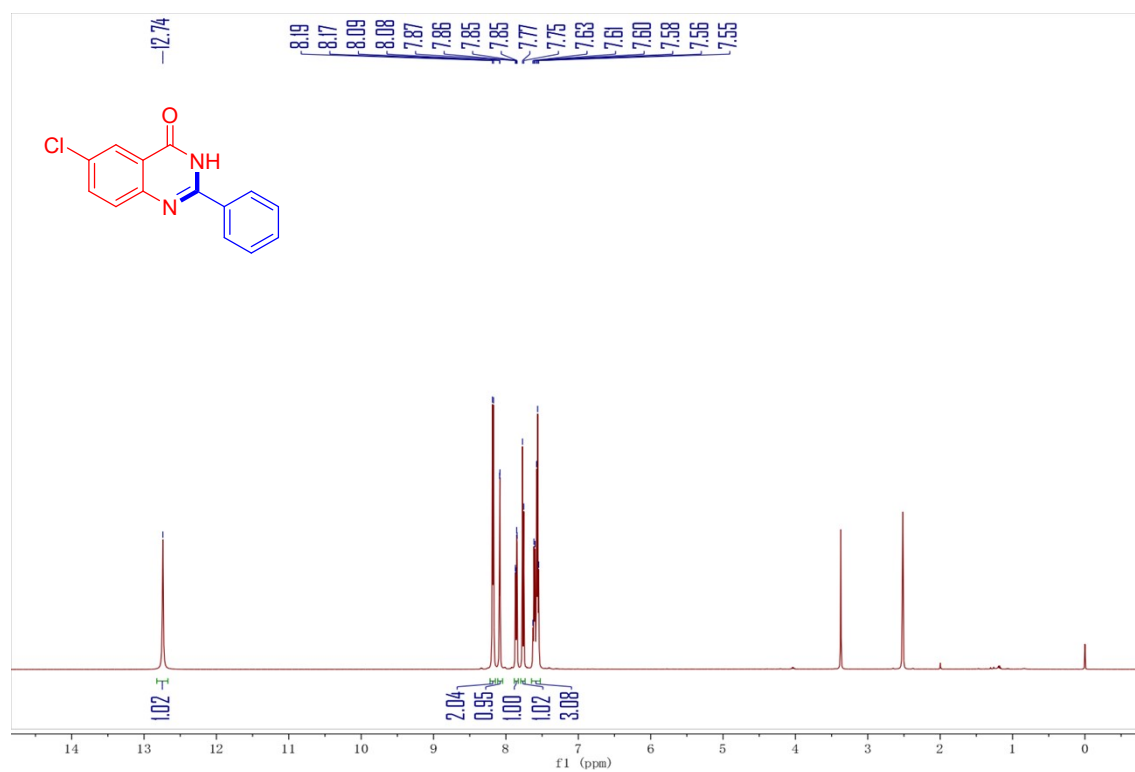
¹³C NMR spectra of compound **3p**



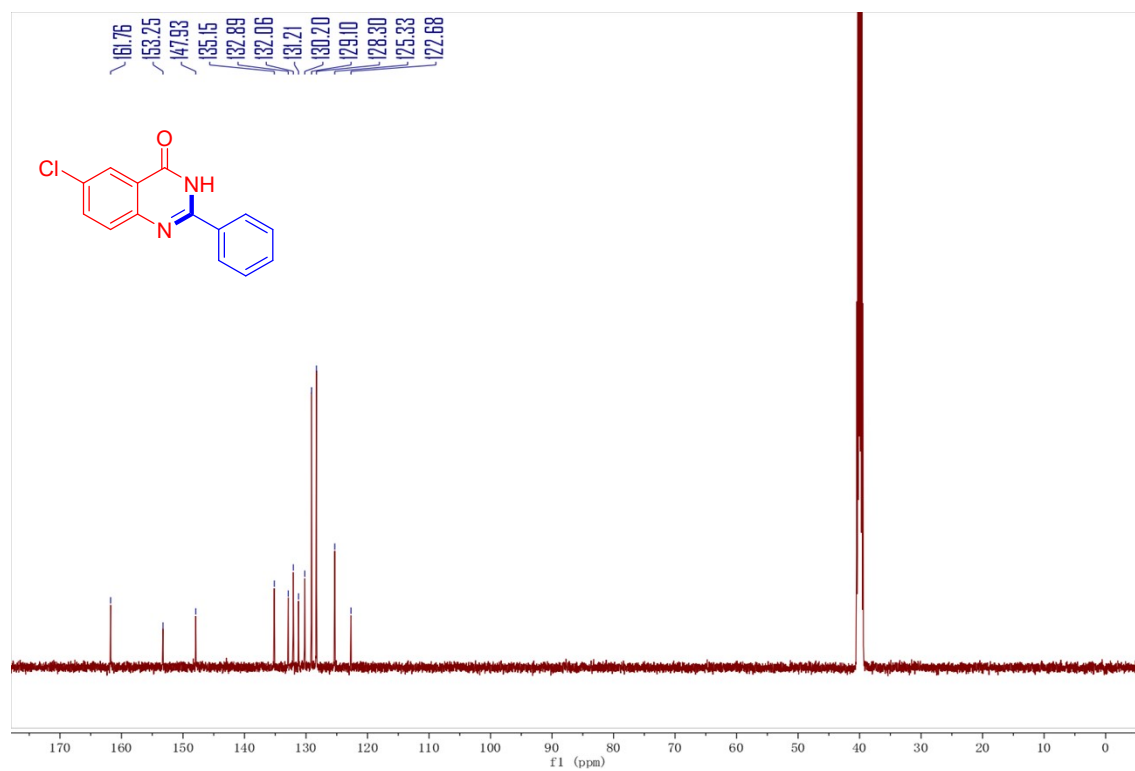
¹⁹F NMR spectra of compound **3p**



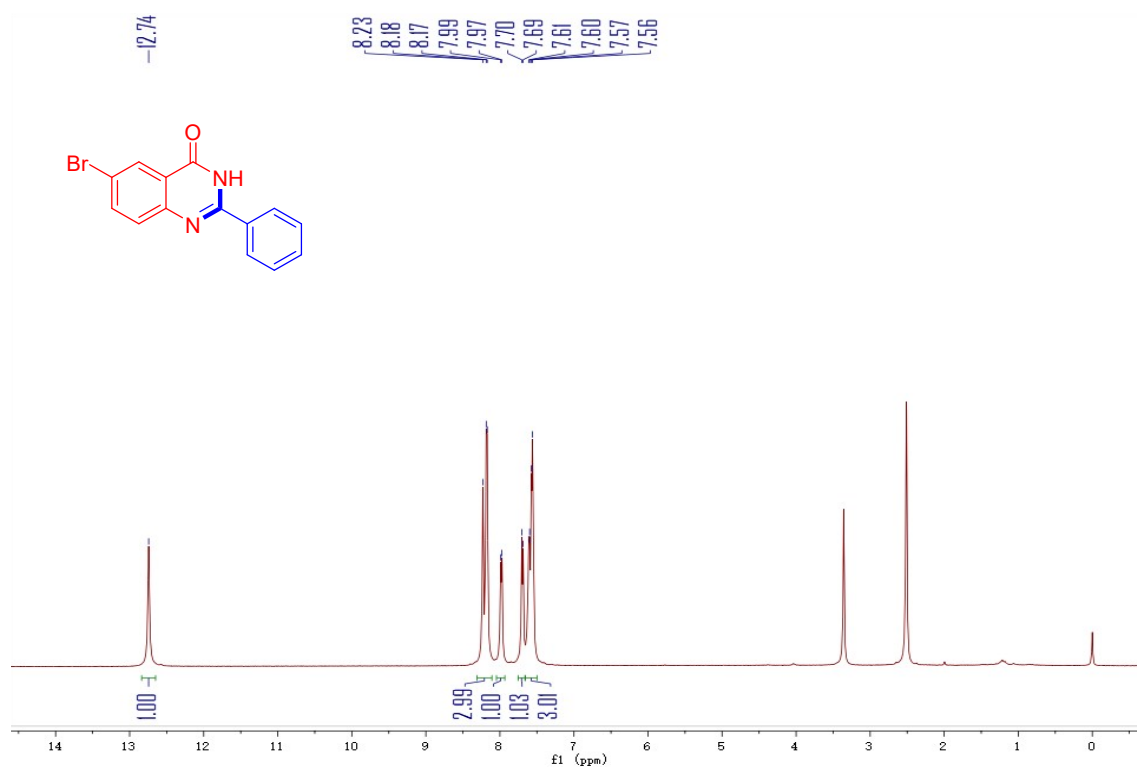
^1H NMR spectra of compound **3q**



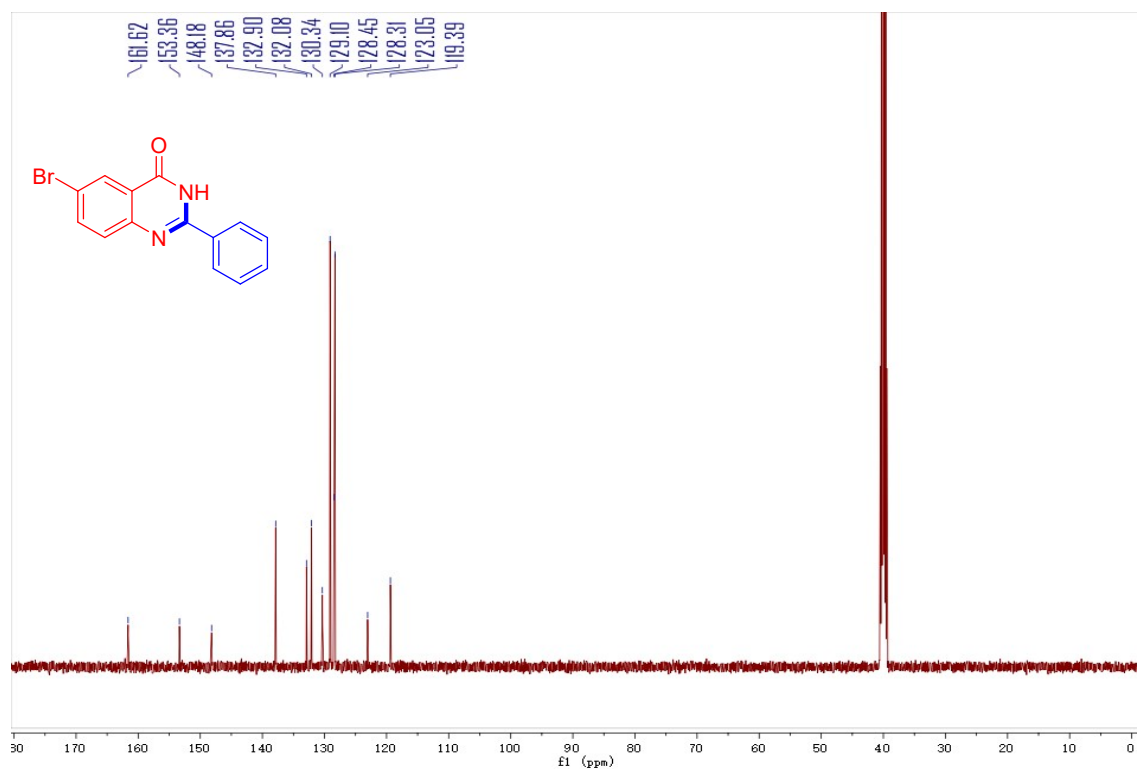
^{13}C NMR spectra of compound **3q**



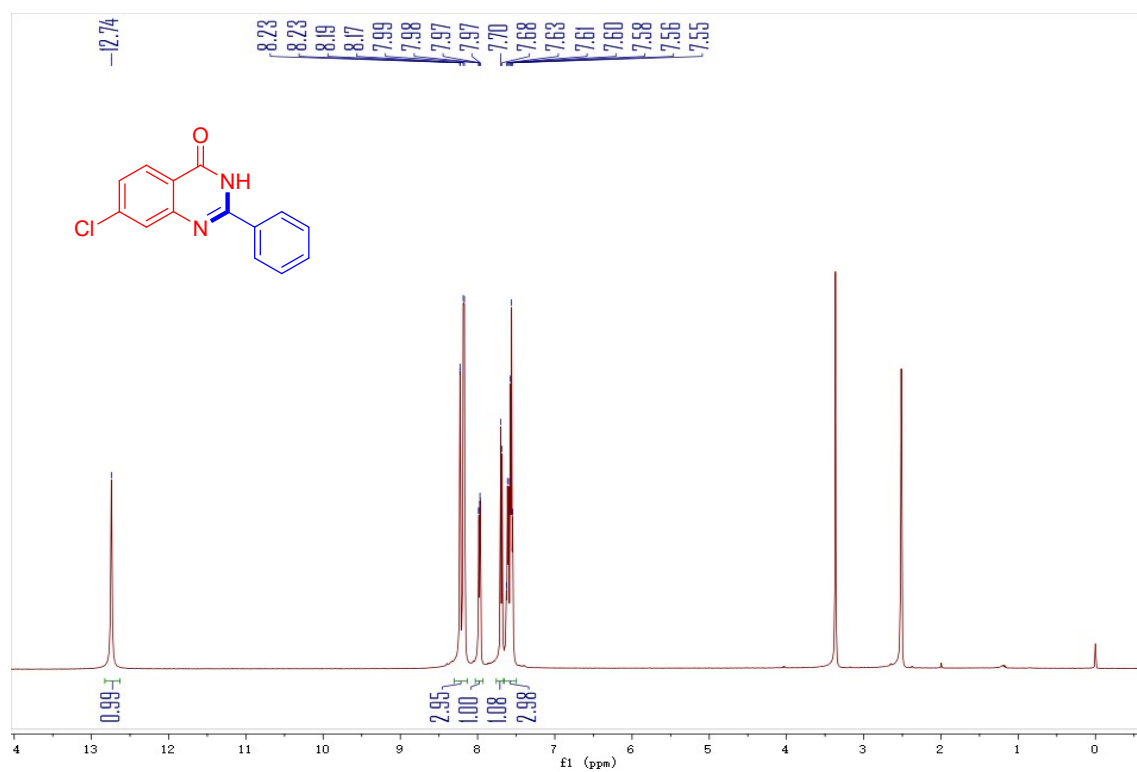
^1H NMR spectra of compound **3r**



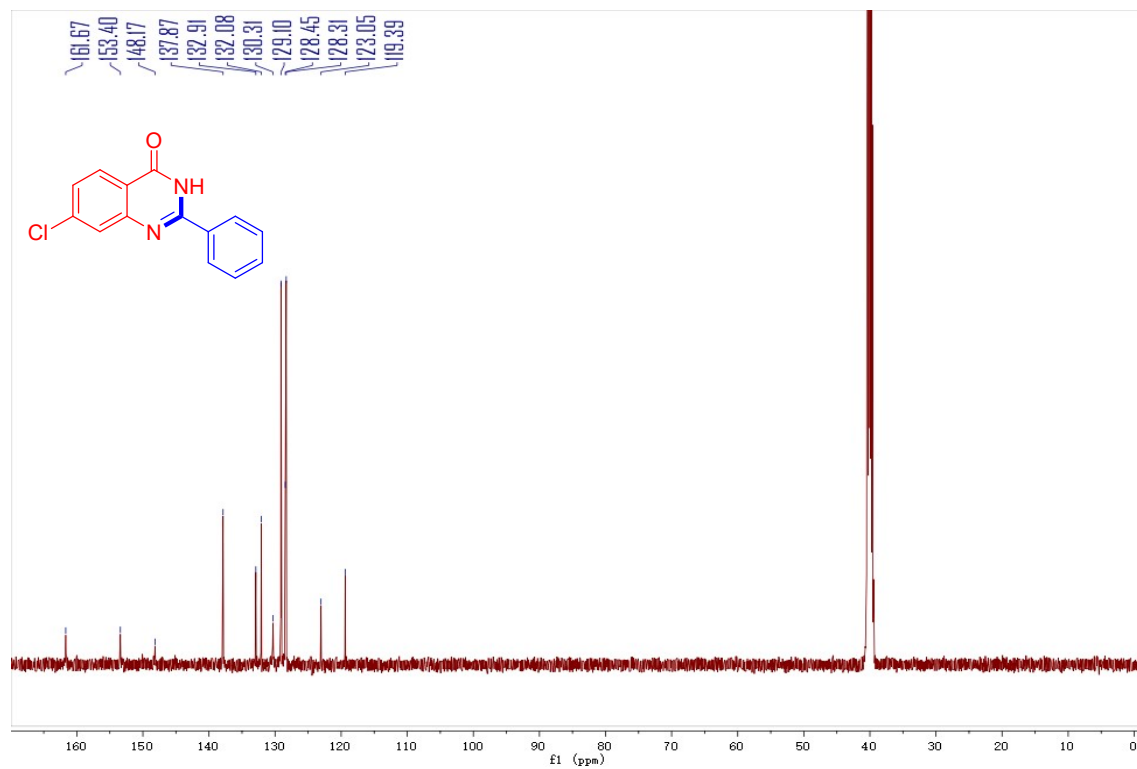
^{13}C NMR spectra of compound **3r**

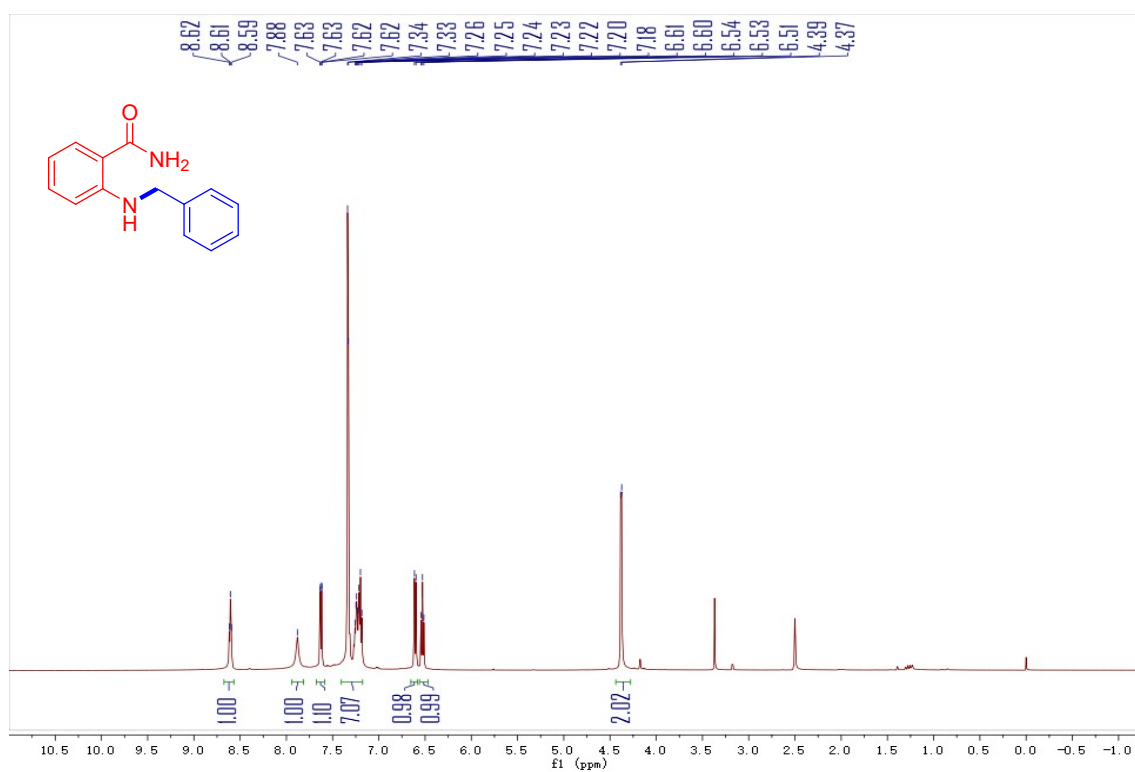


^1H NMR spectra of compound **3s**



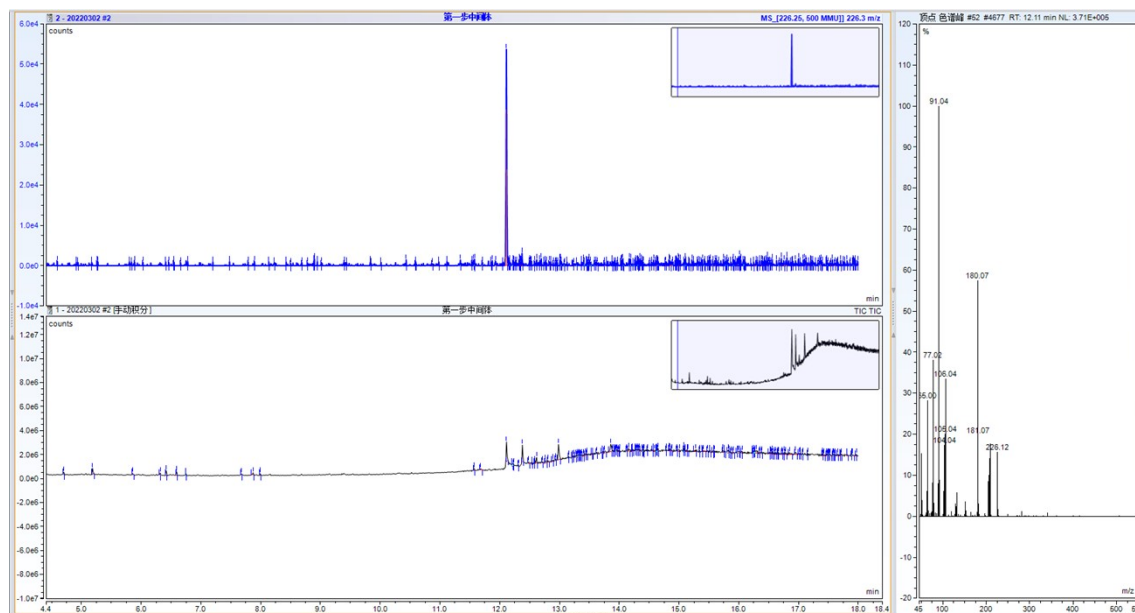
^{13}C NMR spectra of compound **3s**





^1H NMR spectra of compound A

GC-MS of compound A



4. Reference

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