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Supporting Information

TBAI-mediated electrochemical oxidative synthesis of quinazolin-4(3*H*)-one from 2-aminobenzamides and isothiocyanates

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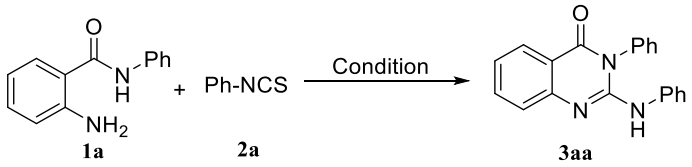
1. General remark

All of the electrochemical reactions were performed in an undivided cell unless otherwise noted.

^{1}H NMR, ^{13}C NMR, and ^{19}F NMR spectra were recorded on a Bruker 400 M and in $CDCl_3$ or DMSO-d_6. All ^{1}H NMR, ^{13}C NMR, and ^{19}F NMR chemical shifts were given as δ values (ppm) with reference to tetramethylsilane (TMS) as an internal standard. The NMR peak multiplicities identified as s = singlet, br s = broad singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, m = multiplet; coupling constants (*J*) were reported in Hz. All compounds were further characterized by HRMS ESI-mass data were recorded on the Thermo Scientific Q Exactive Focus Orbitrap LCMS/MS System (U3000-Q-Exactive instrument); copies of their ^{1}H NMR, ^{13}C NMR, and ^{19}F NMR spectra were provided. Cyclic voltammograms were obtained on a CHI 660C potentiostat (CH Instruments, Inc.). The DC regulated power supply was manufactured by WANPTEK (Model: GPS305D).

Products were purified by flash chromatography on 200–300 mesh silica gels (Leyan). Yields refer to chromatographically and spectroscopically pure materials unless otherwise stated. Analytical thin-layer chromatography was performed on 0.20 mm silica gel GF-254 plates (Energy Chemical). All melting points were determined without a correction. All reactions were carried out under air in oven-dried glassware, unless otherwise noted. All reagents were purchased commercially and used as received, unless otherwise noted.

2. Development of the reaction condition



1a **2a** **3aa**

An undivided test column-type electrolysis cell (20 mL) was charged with a stir bar, **1a** (0.2 mmol, 1.0 equiv.), electrolyte (0.4 mmol), solvent (5 mL), then, add **2a** (0.4 mmol), base (0.4 mmol), and the resulting suspension was stirred for a minute. Then the anode and the cathode were placed into reaction system. The distance between the two electrodes was 1.5 cm. The mixture was electrolyzed under a constant current at room temperature until the reagent and its intermediate were consumed entirely (monitored by TLC). The reaction electrodes were taken out, washed twice with ethyl acetate (10 mL) ultrasonically, and the ethyl acetate was combined with the reaction

mixture. The combined mixture was washed with H_2O and extracted with ethyl acetate (20 mL × 3), brine, dried over anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The resulting crude product was purified by silica gel column chromatography with petroleum ether and ethyl acetate as eluents to afford the desired product **3aa**.

(a) Table S1. Survey of solvent[a]

Entry	Solvent	Yield of 3aa (%)
1	**CH_3CN : CH_3OH = 1 : 1**	**82**
2	CH_3OH	47
3	CH_3CN : CH_2Cl_2 = 1 : 1	37
4	CH_3CN : H_2O = 1 : 1	trace

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), *n*Bu_4NI (0.4 mmol), 1,10-phen (0.4 mmol) in an undivided cell equipped with carbon rod (*Φ* 6 mm) as anode and Ni foam (1.0 cm × 1.0 cm × 0.3 cm) as cathode at a constant current of 7 mA in selected solvent (5 mL), the distance between the two electrodes was 1.5 cm, rt, 10 h, air.

(b) Table S2. Survey of base[a]

Entry	Base	Yield of 3aa (%)
1	**1,10-phen**	**82**
2	$NaHCO_3$	56
3	DABCO	63
4	pyridine	50
5	DIPEA	44
6	Me_3N	71

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), *n*Bu_4NI (0.4 mmol), Base (0.4 mmol) in an undivided cell equipped with carbon rod (*Φ* 6 mm) as anode and Ni foam (1.0 cm × 1.0 cm × 0.3 cm) as cathode at a constant current of 7 mA in CH_3OH/CH_3CN (1:1, 5 mL), the distance between the two electrodes was 1.5 cm, rt, 10 h, air.

(c) Table S3. Survey of electrodes[a]

Entry	Electrodes	Yield of 3aa (%)
1	**C(+)/Ni foam (−)**	**82**
2	C(+)/C(−)	57
3	Pt(+)/Pt(−)	64
4	C(+)/Pt(−)	66

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), *n*Bu_4NI (0.4 mmol), 1,10-phen (0.4 mmol) in an undivided cell equipped with selected electrodes at a constant current of 7 mA in CH_3OH/CH_3CN (1:1, 5 mL), the distance between the two electrodes was 1.5 cm, rt, 10 h, air.

(d) Table S4. Survey of electrolyte[a]

Entry	Electrolyte	Yield of 3aa (%)
1	***n*Bu$_4$NI**	**82**
2	NH_4I	35
3	KI	10
4	*n*Bu$_4$NBr/*n*Bu$_4$NPF$_6$/*n*Bu$_4$NBF$_4$/*n*Bu$_4$NClO$_4$	trace

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), electrolyte (0.4 mmol), 1,10-phen (0.4 mmol) in an undivided cell equipped with carbon rod (*Φ* 6 mm) as anode and Ni foam (1.0 cm × 1.0 cm × 0.3 cm) as cathode at a constant current of 7 mA in CH_3OH/CH_3CN (1:1, 5 mL), the distance between the two electrodes was 1.5 cm, rt, 10 h, air.

(f) Table S5. Survey of current intensity and reaction time[a]

Entry	Reaction current and time	Yield of 3aa (%)
1	**7 mA for 10 h**	**82**
2	10 mA for 7 h	43
3	5 mA for 14 h	65
4	3 mA for 10 h	62
5	7 mA for 5 h	77

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), *n*Bu$_4$NI (0.4 mmol), 1,10-phen (0.4 mmol) in an undivided cell equipped with carbon rod (*Φ* 6 mm) as anode and Ni foam (1.0 cm × 1.0 cm × 0.3 cm) as cathode at a constant current of *x* mA in CH_3OH/CH_3CN (1:1, 5 mL), the distance between the two electrodes was 1.5 cm, rt, *x* h, air.

3. General procedures for the electrolysis

(a) The materials used to make the electrolytic cell

All the materials used to make the electrolytic cell were commercially available (Figure S1). The anode and the cathode were carbon rod (*Φ* 6 mm) and Ni foam (1.0 cm × 1.0 cm × 0.3 cm) (Shanghai yueci).

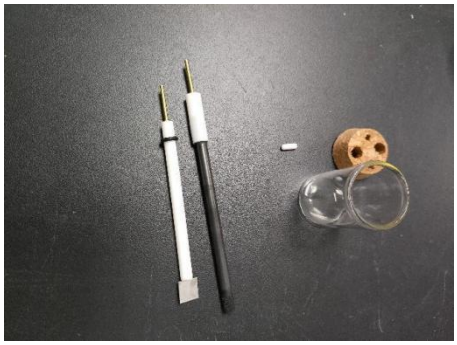
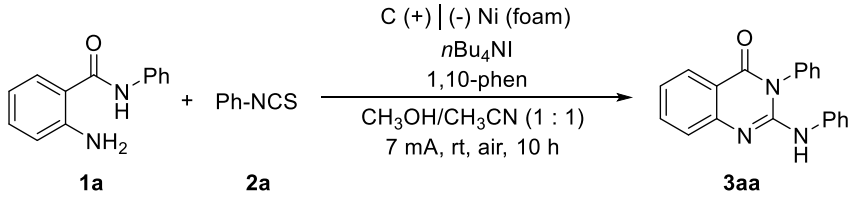


Figure S1. The materials used to make the electrolytic cell for the synthesis of quinazolin-4(3*H*)-one

(b) General procedure for the electrosynthesis of quinazolin-4(3*H*)-one



An undivided test column-type electrolysis cell (20 mL) was charged with a stir bar, **1a** (0.2 mmol, 1.0 equiv.), *n*Bu$_4$NI (0.4 mmol, 2 equiv.), CH_3OH/CH_3CN (1:1, 5 mL), then, add **2a** (0.4 mmol, 2 equiv.), 1,10-phen (0.4 mmol, 2 equiv.), and the resulting suspension was stirred for a minute. Then the prepared electrodes were placed into the reaction mixture. The anode was a carbon rod (Φ 6 mm), and the cathode was Ni foam (1.0 cm × 1.0 cm × 0.3 cm). The distance between the two electrodes was 1.5 cm, and the immersion depth of both electrodes into the solvent was 1 cm. The mixture was electrolyzed at a constant current of 7 mA at room temperature until the reagent and its intermediate were consumed entirely (monitored by TLC). The reaction electrodes were taken out, washed twice with ethyl acetate (10 mL) ultrasonically, and the ethyl acetate was combined with the reaction mixture. The combined mixture was washed with H_2O and extracted with ethyl acetate (20 mL × 3), brine, dried over anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The resulting crude product was purified by silica gel column chromatography with petroleum ether and ethyl acetate (4:1) as eluents to afford the desired product **3aa**.

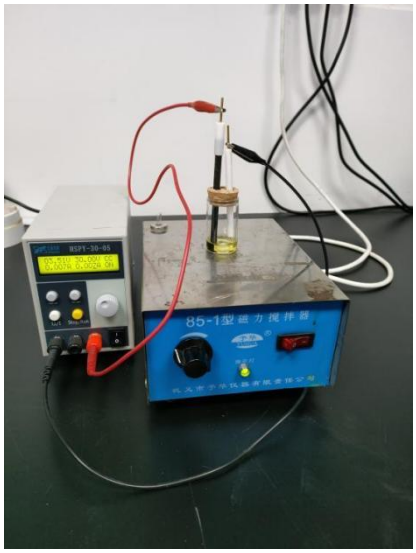


Figure S2. Reaction setup.

4. Scale-up experiment

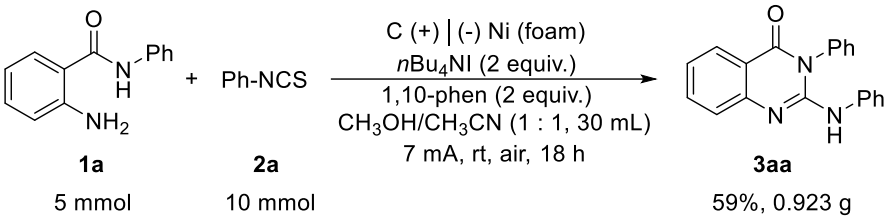


Figure S3. Reaction setup.

An electrolysis cell (40 mL) was charged with a stir bar, **1a** (5 mmol, 1.060 g), *n*Bu$_4$NI (10 mmol, 2 equiv.), CH$_3$OH/CH$_3$CN (1:1, 30 mL) then, add **2a** (10 mmol, 2 equiv.), 1,10-phen (10 mmol, 2 equiv.), and the resulting suspension was stirred for a minute. Then the prepared electrodes were placed into the reaction mixture. The anode and the cathode were carbon rod (Φ 6 mm), Ni foam (1.0 cm × 1.0 cm × 0.3 cm). The distance between the two electrodes was 1.25 cm. The mixture was electrolyzed at a constant current of 7 mA at room temperature for 18 h. After the reaction, the electrodes were taken out, washed twice with ethyl acetate (10 mL) ultrasonically, and the ethyl acetate was combined with the reaction mixture. The combined mixture dried over anhydrous Na$_2$SO$_4$, filtered, and concentrated under reduced pressure. The resulting crude product was purified by silica gel column chromatography with petroleum ether and ethyl acetate (4 : 1) as eluents to afford the desired product **3aa**.

5. Cyclic voltammetry experiments

The cyclic voltammetry experiments were carried out with a computer-controlled electrochemical analyzer for electrochemical measurements. The experiment was performed in a three-electrode cell (volume 20 mL, height 5.5 cm, inner diameter 3 cm.) with CH$_3$OH/CH$_3$CN (1:1, 6 mL) as the solvent, *n*Bu$_4$NPF$_6$ (5 mM) as the supporting electrolyte, the tested compound was added respectively, glassy carbon (diameter 3 mm,

area 7.065 mm^2 disc-shaped, embedded at the end of a polytetrafluoroethylene rod) as the working electrode, Pt plate (1.0 cm × 1.0 cm × 0.1 mm) as the auxiliary electrode, the distance between the two electrodes was 1.25 cm, and Ag/AgCl (saturated aqueous KCl) as the reference electrode. The working electrode, counter electrode, and reference electrode are all from Shanghai Yueci. Before each use, take 10 mg of 50 nm alumina powder on a wool buffing wheel, add 0.25 mL of distilled water dropwise onto it, vertically press the glassy carbon electrode lightly onto the water-moistened alumina powder with consistent pressure, grind clockwise for 30 rotations followed by counterclockwise for 30 rotations, and finally rinse the electrode with distilled water, dry it, and use. Electrochemical measurements were conducted with the following parameters: scan speed of 50 mV/s, sample interval of 0.001 V, quiet time of 2 s, and sensitivity of $1e^{-5}$ A/V. Potential ranges investigated spanned from 0 V to + 1.8 V, with initial scan polarity set to positive, total scan time was 36 s. All experiments were performed at room temperature.

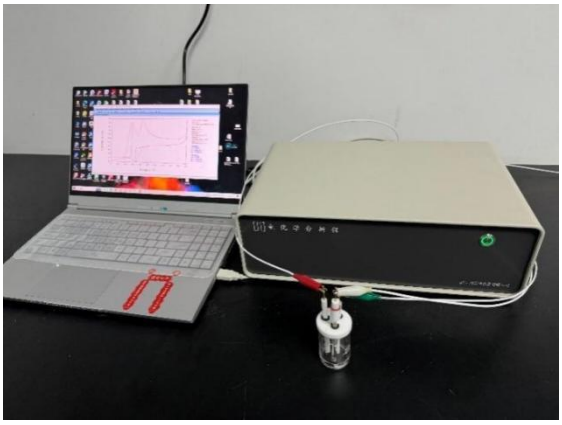


Figure S4. Cyclic voltammograms experiments setup

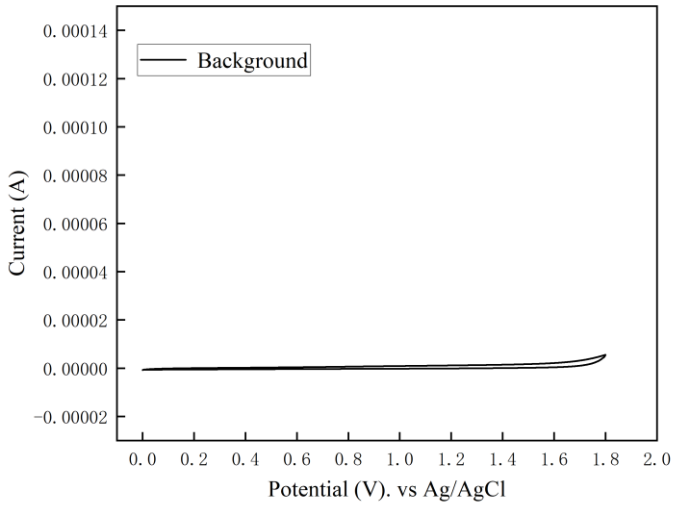


Figure S5. Cyclic voltammogram of nBu$_4$NPF$_6$ (5 mM) as an electrolyte in CH$_3$OH/CH$_3$CN (1:1, 6 mL).

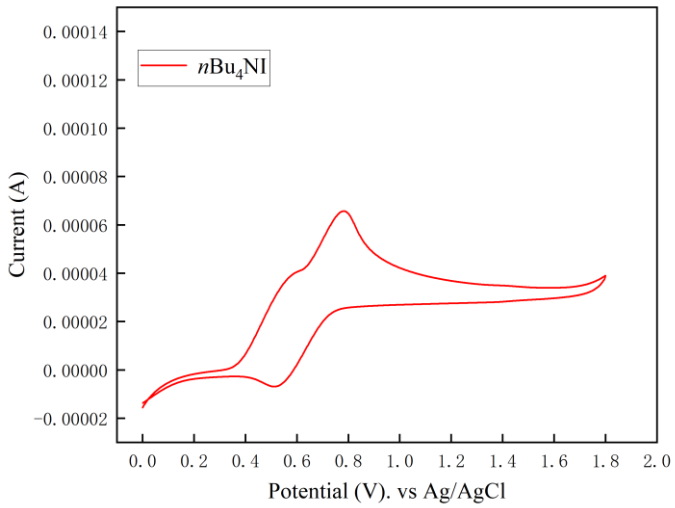


Figure S6. Cyclic voltammogram of nBu$_4$NPF$_6$ (5 mM) and nBu$_4$NI (5 mM) in CH$_3$OH/CH$_3$CN (1:1, 6 mL).

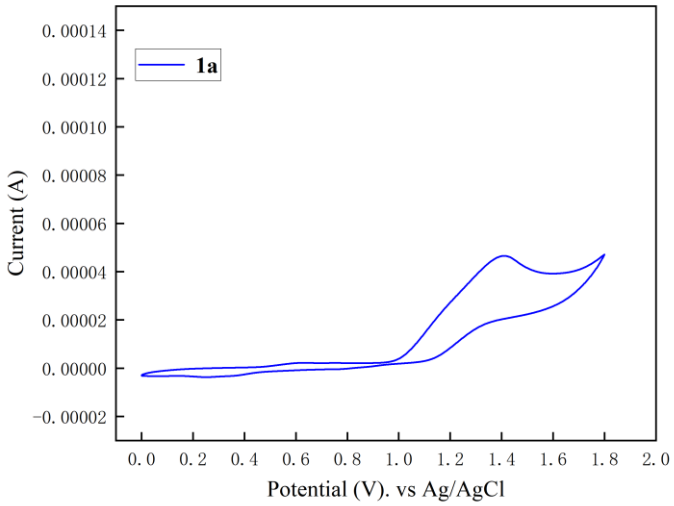


Figure S7. Cyclic voltammogram of nBu$_4$NPF$_6$ (5 mM) and **1a** (2.5 mM) in CH$_3$OH/CH$_3$CN (1:1, 6 mL).

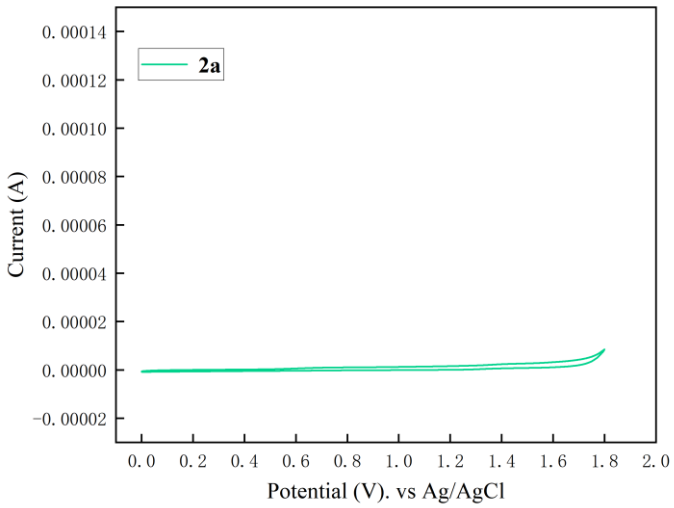


Figure S8. Cyclic voltammogram of nBu$_4$NPF$_6$ (5 mM) and **2a** (5 mM) in CH$_3$OH/CH$_3$CN (1:1, 6 ml).

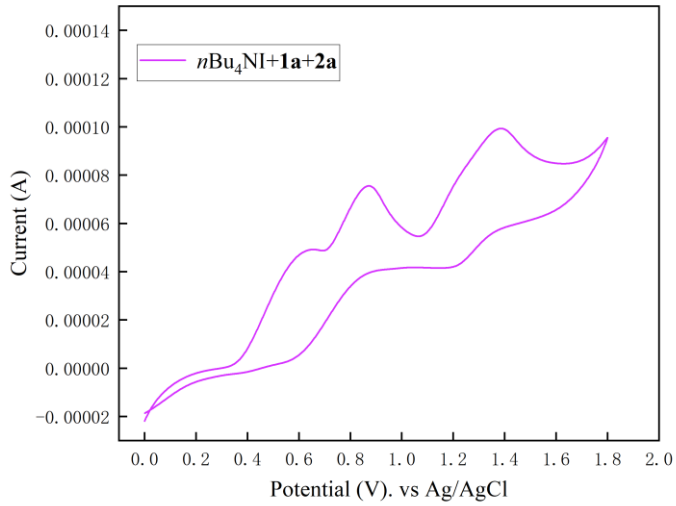


Figure S9. Cyclic voltammogram of nBu$_4$NPF$_6$ (5 mM), nBu$_4$NI (5 mM), **1a** (2.5 mM), and **2a** (5 mM) in CH$_3$OH/CH$_3$CN (1:1, 6 mL).

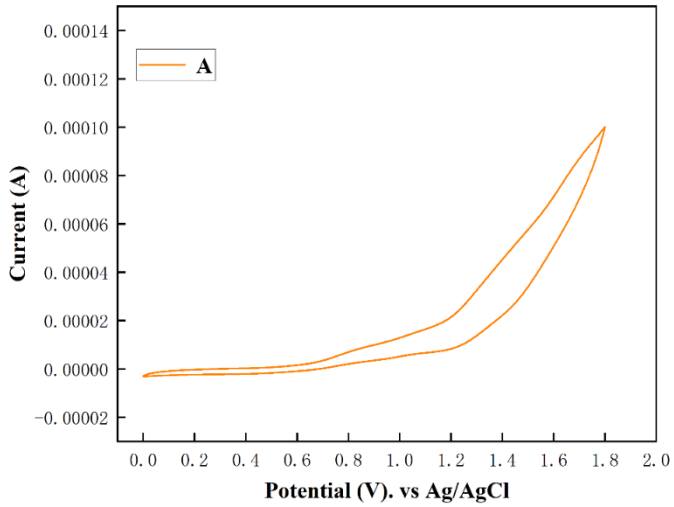


Figure S10. Cyclic voltammogram of nBu$_4$NPF$_6$ (5 mM) and **A** (2.5 mM) in CH$_3$OH/CH$_3$CN (1:1, 6 mL).

6. Mechanistic experiments

(a) Intermediate trapping experiments

In order to confirm if a thiourea intermediate exists in the reaction process, we further characterized by HRMS to detect. As result, the possible product and intermediate were detected.

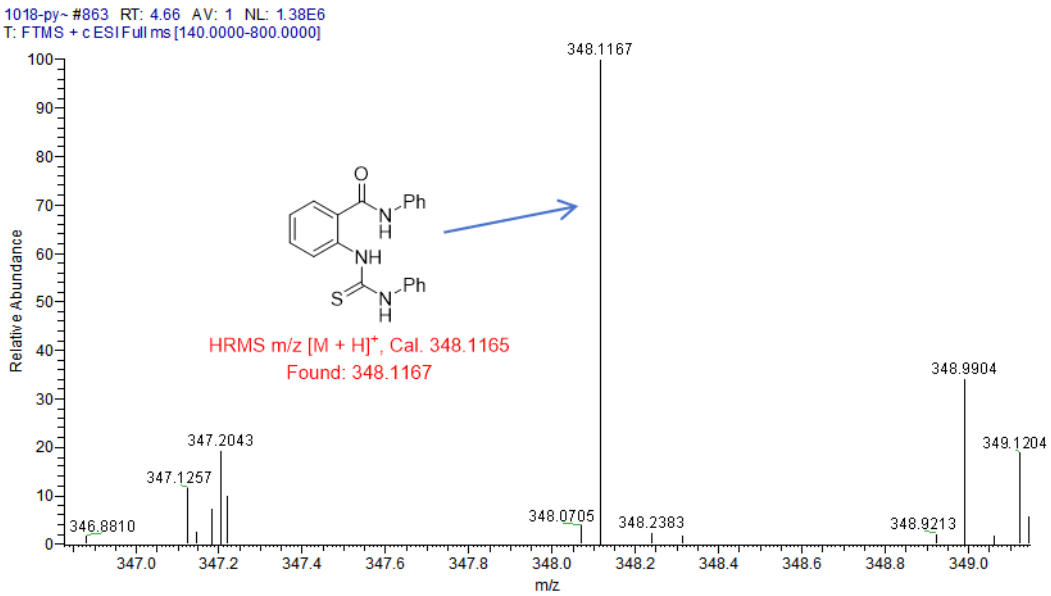


Figure S11. Mass spectrometry (HRMS) data of compound **A**

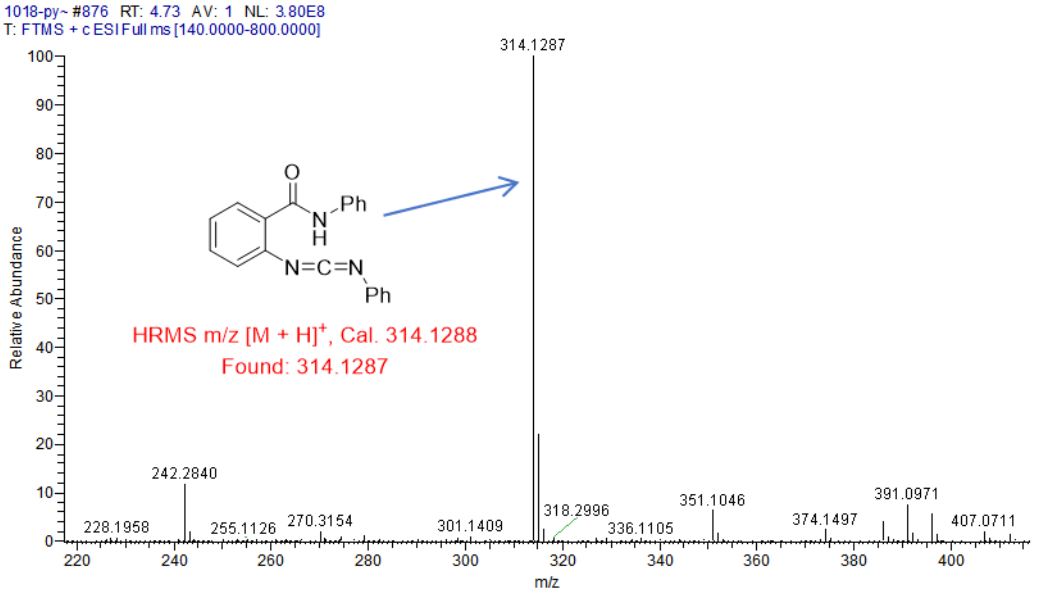


Figure S12 Mass spectrometry (HRMS) data of compound **B**

(b) Detection of H_2S and S_8

In order to detect the existence of H_2S or S_8, a series of experiments were carried out. A solution of $Pb(OAc)_2$ was added to the reaction mixture, however, no black sediment was observed. Then, a drop of reaction solution was added to the $Pb(OAc)_2$ test paper, and no significant changes were observed. This indicates that no hydrogen sulfide is produced during the reaction process.

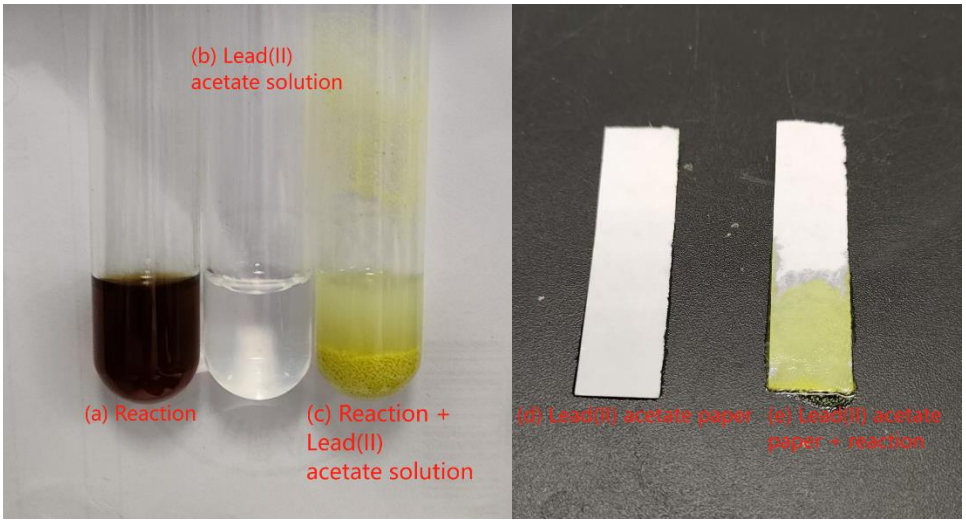


Figure S13. Detection of H_2S

Besides, we detected the by-produet of demental sulfur during the reaction process using thin-layer chromatography (Petroleum ether).

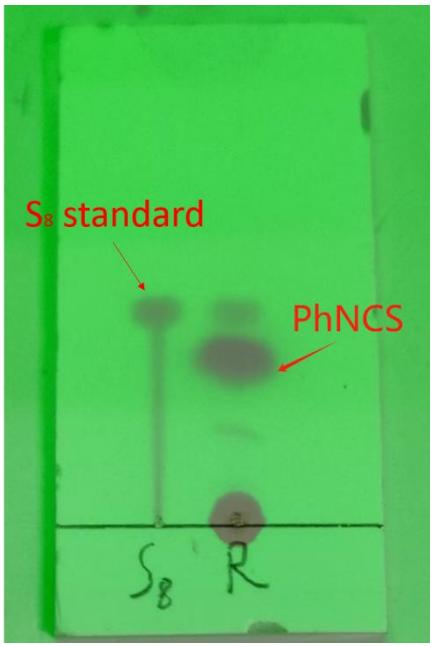
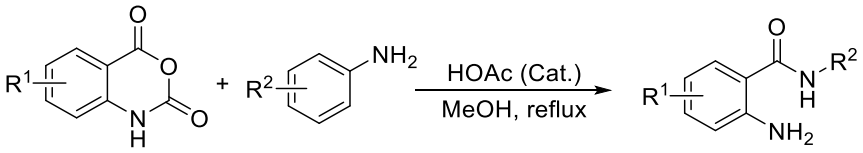


Figure S14. Detection of S_8

7. General procedure for the synthesis of 1a-1p

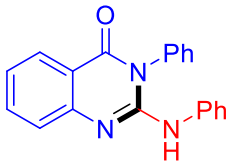


A suspension of isatoic anhydride, 1.1 equivalent of aryl- or benzyl-amine and 1% AcOH in MeOH was stirred at 75 ºC for 10 h. After the reaction was completed, as

indicated by TLC (PE:EA = 3:2), the brown solution was filtered in a buchner funnel that had been packed with a layer of celite and activated charcoal; the colorless solution was then evaporated under reduced pressure. Recrystallization from Et_2O afforded benzamide.

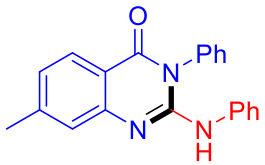
8. Characterization of data for the electrolysis products

3-Phenyl-2-(phenylamino)quinazolin-4(3*H*)-one (3aa).



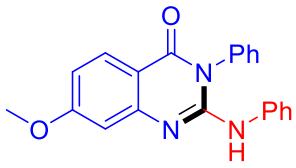
The product was purified by column chromatography (petroleum ether/EtOAc = 4:1). White solid (51.3 mg, 82% yield), melting point: 106–108 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (dd, *J* = 8.0 Hz, *J* = 1.6 Hz, 1 H), 7.68–7.57 (m, 4 H), 7.52 (t, *J* = 8.4 Hz, 3 H), 7.42–7.40 (m, 2 H), 7.33–7.23 (m, 3 H), 7.08 (t, *J* = 7.4 Hz, 1 H), 5.96 (br s, 1 H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 162.6, 148.6, 146.4, 137.9, 134.8, 134.6, 130.9, 130.4, 129.1, 129.0, 127.3, 125.7, 124.1, 123.8, 120.9, 118.5; HRMS (ESI) *m*/*z* calcd for $C_{20}H_{16}N_3O$ $[M + H]^+$ 314.1288, found: 314.1287.

7-Methyl-3-phenyl-2-(phenylamino)quinazolin-4(3*H*)-one (3ba).



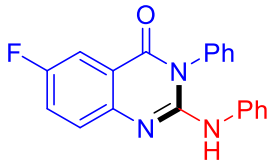
The product was purified by column chromatography (petroleum ether/EtOAc = 4:1). Yellow solid (51.7 mg, 79% yield), melting point: 126–128 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (s, 1 H), 7.67–7.58 (m, 3 H), 7.52–7.40 (m, 6 H), 7.31 (t, *J* = 7.6 Hz, 2 H), 7.09 (t, *J* = 7.6 Hz, 1 H), 5.96 (br s, 1 H), 2.44 (s, 3 H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 162.6, 146.4, 145.9, 138.1, 136.3, 134.8, 133.6, 130.9, 130.3, 129.2, 129.0, 126.7, 125.5, 124.0, 120.8, 118.2, 21.1; HRMS (ESI) *m*/*z* calcd for $C_{21}H_{18}N_3O$ $[M + H]^+$ 328.1444, found: 328.1443.

7-Methoxy-3-phenyl-2-(phenylamino)quinazolin-4(3*H*)-one (3ca).



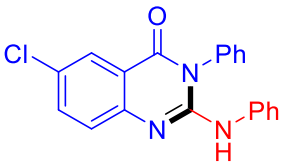
The product was purified by column chromatography (petroleum ether/EtOAc = 3:1). Yellow solid (55.6 mg, 81% yield), melting point: 157–159 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60–7.49 (m, 4 H), 7.43–7.40 (m, 3 H), 7.34 (d, *J* = 8.0 Hz, 2 H), 7.23 (t, *J* = 7.4 Hz, 3 H), 7.00 (t, *J* = 7.4 Hz, 1 H), 5.81 (br s, 1 H), 3.80 (s, 3 H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 162.5, 156.3, 145.0, 143.1, 138.1, 134.8, 131.0, 130.4, 129.1, 129.0, 127.3, 125.1, 123.9, 120.6, 118.8, 106.9, 55.9; HRMS (ESI) *m*/*z* calcd for $C_{21}H_{18}N_3O_2$ $[M + H]^+$ 344.1394, found: 344.1392.

6-Fluoro-3-phenyl-2-(phenylamino)quinazolin-4(3*H*)-one (3da).



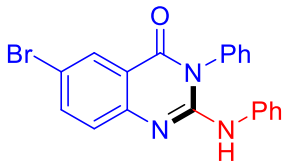
The product was purified by column chromatography (petroleum ether/EtOAc = 4:1). Yellow solid (49.0 mg, 74% yield). melting point: 189–191 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (dd, *J* = 8.4 Hz, *J* = 3.2 Hz, 1 H), 7.68–7.59 (m, 3 H), 7.53–7.47 (m, 3 H), 7.42–7.36 (m, 3 H), 7.31 (t, *J* = 8.0 Hz, 2 H), 7.16 (t, *J* = 7.6 Hz, 1 H), 5.96 (br s, 1 H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 161.9 (d, *J* = 3.3 Hz, 1 C), 159.1 (d, *J* = 242.5 Hz, 1 C), 146.1, 145.2, 137.8, 134.5, 131.0, 130.5, 129.1, 129.0, 127.8 (d, *J* = 7.7 Hz, 1 C), 124.3, 123.3 (d, *J* = 23.9 Hz, 1 C), 121.0, 119.2 (d, *J* = 8.5 Hz, 1 C), 112.0 (d, *J* = 23.4 Hz, 1 C); ^{19}F NMR (377 MHz, $CDCl_3$) δ –117.6; HRMS (ESI) *m*/*z* calcd for $C_{20}H_{15}FN_3O$ $[M + H]^+$ 332.1194, found: 332.1194.

6-Chloro-3-phenyl-2-(phenylamino)quinazolin-4(3*H*)-one (3ea).



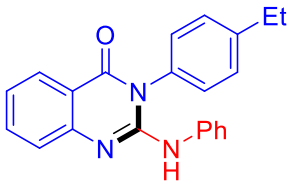
The product was purified by column chromatography (petroleum ether/EtOAc = 4:1). White solid (48.6 mg, 70% yield), melting point: 200–202 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, *J* = 2.4 Hz, 1 H), 7.67–7.64 (m, 2 H), 7.62–7.56 (m, 2 H), 7.48–7.45 (m, 3 H), 7.41–7.39 (m, 2 H), 7.31 (t, *J* = 7.8 Hz, 2 H), 7.10 (t, *J* = 7.4 Hz, 1 H), 6.01 (br s, 1 H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 161.6, 147.1, 146.7, 137.6, 135.2, 134.3, 131.1, 130.6, 129.2, 129.1, 127.3, 126.5, 124.5, 121.2, 119.5; HRMS (ESI) *m*/*z* calcd for $C_{20}H_{15}ClN_3O$ $[M + H]^+$ 348.0898, found: 348.0898.

6-Bromo-3-phenyl-2-(phenylamino)quinazolin-4(3*H*)-one (3fa).



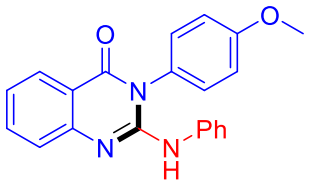
The product was purified by column chromatography (petroleum ether/EtOAc = 4:1). White solid (55.5 mg, 71% yield), melting point: 221–223 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, *J* = 2.4 Hz, 1 H), 7.73–7.70 (m, 1 H), 7.68–7.59 (m, 3 H), 7.48–7.46 (m, 2 H), 7.41–7.38 (m, 3 H), 7.31 (t, *J* = 8.0 Hz, 2 H), 7.12 (t, *J* = 7.4 Hz, 1 H), 6.01 (br s, 1 H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 161.4, 147.5, 146.8, 137.9, 137.6, 134.3, 131.1, 130.6, 129.7, 129.1, 127.6, 124.5, 121.2, 119.9, 116.6; HRMS (ESI) *m*/*z* calcd for $C_{20}H_{15}BrN_3O$ $[M + H]^+$ 392.0393, found: 392.0390.

3-(4-Ethylphenyl)-2-(phenylamino)quinazolin-4(3*H*)-one (3ga).



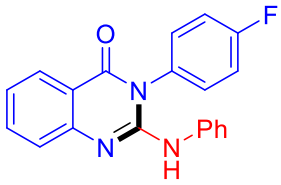
The product was purified by column chromatography (petroleum ether/EtOAc = 4:1). Yellow solid (50.5 mg, 74% yield), melting point: 151–153 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (dd, *J* = 8.0 Hz, *J* = 1.6 Hz, 1 H), 7.67–7.63 (m, 1 H), 7.53–7.51 (m, 3 H), 7.46 (d, *J* = 8.4 Hz, 2 H), 7.32–7.29 (m, 4 H), 7.26–7.22 (m, 1 H), 7.09 (t, *J* = 7.4 Hz, 1 H), 6.03 (br s, 1 H), 2.78 (q, *J* = 7.6 Hz, 2 H), 1.33 (t, *J* = 7.6 Hz, 3 H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 162.7, 148.6, 146.7, 146.7, 138.0, 134.8, 132.0, 130.4, 129.0, 128.9, 127.3, 125.7, 124.1, 123.7, 121.0, 118.6, 28.8, 15.3; HRMS (ESI) *m*/*z* calcd for $C_{22}H_{20}N_3O$ $[M + H]^+$ 342.1601, found: 342.1601.

3-(4-Methoxyphenyl)-2-(phenylamino)quinazolin-4(3*H*)-one (3ha).



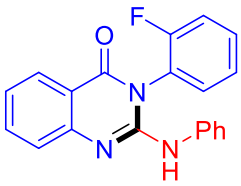
The product was purified by column chromatography (petroleum ether/EtOAc = 3:1). Yellow solid (41.9 mg, 61% yield), melting point: 203–205 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (dd, *J* = 8.0 Hz, *J* = 1.6 Hz, 1 H), 7.68–7.63 (m, 1 H), 7.54–7.52 (m, 3 H), 7.34–7.30 (m, 4 H), 7.27–7.23 (m, 1 H), 7.15–7.07 (m, 3 H), 6.10 (br s, 1 H), 3.90 (s, 3 H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 162.9, 160.8, 148.6, 146.8, 138.0, 134.8, 130.3, 129.0, 127.3, 126.7, 125.7, 124.0, 123.7, 120.8, 118.6, 116.2, 55.8; HRMS (ESI) *m*/*z* calcd for $C_{21}H_{18}N_3O_2$ $[M + H]^+$ 344.1394, found: 344.1395.

3-(4-Fluorophenyl)-2-(phenylamino)quinazolin-4(3*H*)-one (3ia).



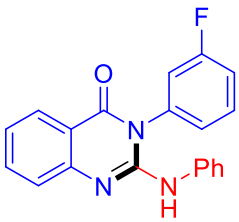
The product was purified by column chromatography (petroleum ether/EtOAc = 4:1). White solid (42.4 mg, 64% yield), melting point: 144–146 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (dd, *J* = 8.0 Hz, *J* = 1.6 Hz, 1 H), 7.68–7.64 (m, 1 H), 7.53 (d, *J* = 8.8 Hz, 3 H), 7.42–7.39 (m, 2 H), 7.36–7.30 (m, 4 H), 7.28–7.24 (m, 1 H), 7.12–7.08 (m, 1 H), 5.90 (s, 1 H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 163.4 (d, *J* = 249.9 Hz, 1 C), 162.7, 148.5, 146.3, 137.8, 135.0, 131.2 (d, *J* = 8.9 Hz, 1 C), 130.4 (d, *J* = 3.4 Hz, 1 C), 129.1, 127.3, 125.8, 124.3, 124.0, 121.0, 118.4, 118.1 (d, *J* = 23.0 Hz, 1 C); ^{19}F NMR (377 MHz, $CDCl_3$) δ –109.6; HRMS (ESI) *m*/*z* calcd for $C_{20}H_{15}FN_3O$ $[M + H]^+$ 332.1194, found: 332.1190.

3-(2-Fluorophenyl)-2-(phenylamino)quinazolin-4(3*H*)-one (3ja).



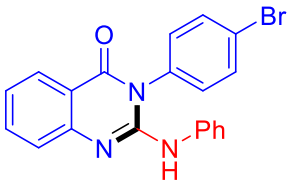
The product was purified by column chromatography (petroleum ether/EtOAc = 4:1). Yellow solid (40.4 mg, 61% yield), melting point: 118–120 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (dd, J = 8.0 Hz, J = 1.6 Hz, 1 H), 7.69–7.64 (m, 1 H), 7.63–7.57 (m, 1 H), 7.53–7.50 (m, 3 H), 7.46–7.36 (m, 3 H), 7.34–7.30 (m, 2 H), 7.28–7.24 (m, 1 H), 7.11 (t, J = 7.4 Hz, 1 H), 5.97 (s, 1 H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 162.0, 158.5 (d, J = 252.7 Hz, 1 C), 148.7, 146.0, 137.8, 135.1, 132.6 (d, J = 7.9 Hz, 1 C), 130.9, 129.0, 127.4, 126.1 (d, J = 4.0 Hz, 1 C), 125.9, 124.4, 124.0, 122.2 (d, J = 13.5 Hz, 1 C), 121.4, 118.3, 118.0 (d, J = 19.2 Hz, 1 C); ^{19}F NMR (377 MHz, $CDCl_3$) δ –118.3; HRMS (ESI) *m/z* calcd for $C_{20}H_{15}FN_3O$ $[M + H]^+$ 332.1194, found: 332.1189.

3-(3-Fluorophenyl)-2-(phenylamino)quinazolin-4(3*H*)-one (3ka).



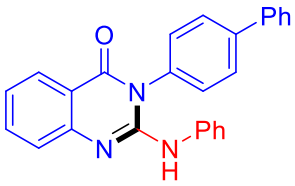
The product was purified by column chromatography (petroleum ether/EtOAc = 4:1). Light Yellow liquid (41.7 mg, 63% yield), melting point: 129–131 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (dd, J = 8.0 Hz, J = 1.6 Hz, 1 H), 7.68–7.60 (m, 2 H), 7.53–7.50 (m, 3 H), 7.34–7.29 (m, 3 H), 7.28–7.22 (m, 2 H), 7.19–7.16 (m, 1 H), 7.13–7.09 (m, 1 H), 5.90 (s, 1 H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 163.7 (d, J = 249.6 Hz, 1 C), 162.4, 148.5, 146.0, 137.8, 136.1 (d, J = 9.5 Hz, 1 C), 135.0, 132.2 (d, J = 8.9 Hz, 1 C), 129.1, 127.3, 125.8, 125.0 (d, J = 3.5 Hz, 1 C), 124.2, 124.0, 121.2, 118.4, 117.8 (d, J = 20.8 Hz, 1 C), 117.1 (d, J = 22.8 Hz, 1 C); ^{19}F NMR (377 MHz, $CDCl_3$) δ –108.3; HRMS (ESI) *m/z* calcd for $C_{20}H_{15}FN_3O$ $[M + H]^+$ 332.1194, found: 332.1189.

3-(4-Bromophenyl)-2-(phenylamino)quinazolin-4(3*H*)-one (3la).



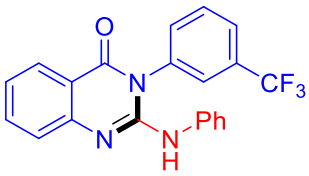
The product was purified by column chromatography (petroleum ether/EtOAc = 4:1). Yellow solid (55.5 mg, 71% yield), melting point: 158–160 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (dd, J = 8.0 Hz, J = 1.6 Hz, 1 H), 7.79–7.75 (m, 2 H), 7.68–7.64 (m, 1 H), 7.52–7.50 (m, 3 H), 7.34–7.28 (m, 4 H), 7.27–7.23 (m, 1 H), 7.13–7.08 (m, 1 H), 5.88 (s, 1 H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 162.5, 148.5, 146.0, 137.8, 135.0, 134.2, 133.7, 130.9, 129.1, 127.3, 125.8, 124.7, 124.4, 124.0, 121.1, 118.4; HRMS (ESI) *m/z* calcd for $C_{20}H_{15}BrN_3O$ $[M + H]^+$ 392.0393, found: 392.0391.

3-([1,1'-Biphenyl]-4-yl)-2-(phenylamino)quinazolin-4(3*H*)-one (3ma).



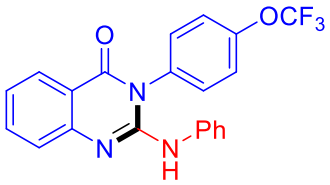
The product was purified by column chromatography (petroleum ether/EtOAc = 2:1). Yellow solid (52.1 mg, 67% yield), melting point: 218–220 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (dd, *J* = 8.0 Hz, *J* = 1.6 Hz, 1 H), 7.86–7.83 (m, 2 H), 7.69–7.65 (m, 3 H), 7.55–7.41 (m, 8 H), 7.35–7.27 (m, 3 H), 7.12–7.08 (m, 1 H), 6.11 (br s, 1 H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 162.7, 148.6, 146.5, 143.4, 139.7, 137.9, 134.9, 133.6, 129.6, 129.5, 129.2, 129.0, 128.3, 127.4, 127.3, 125.8, 124.2, 123.8, 121.1, 118.5; HRMS (ESI) *m*/*z* calcd for $C_{26}H_{20}N_3O$ $[M + H]^+$ 390.1601, found: 390.1601.

2-(Phenylamino)-3-(3-(trifluoromethyl)phenyl)quinazolin-4(3*H*)-one (3na).



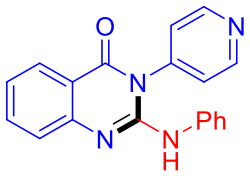
The product was purified by column chromatography (petroleum ether/EtOAc = 2:1). Yellow solid (55.6 mg, 73% yield), melting point: 142–144 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (dd, *J* = 8.0 Hz, *J* = 1.6 Hz, 1 H), 7.87–7.77 (m, 2 H), 7.71–7.62 (m, 3 H), 7.53–7.47 (m, 3 H), 7.35–7.25 (m, 3 H), 7.12 (t, *J* = 7.4 Hz, 1 H), 5.83 (br s, 1 H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 162.5, 148.5, 145.9, 137.6, 135.4, 135.2, 133.5 (q, *J* = 33.2 Hz, 1 C), 132.9, 131.6, 129.1, 127.3 (q, *J* = 3.4 Hz, 1 C), 127.3, 126.6 (q, *J* = 3.8 Hz, 1 C), 125.9, 124.6, 124.1, 123.3 (q, *J* = 271.3 Hz, 1 C),121.3, 118.3; ^{19}F NMR (377 MHz, $CDCl_3$) δ –62.6; HRMS (ESI) *m*/*z* calcd for $C_{21}H_{15}F_3N_3O$ $[M + H]^+$ 382.1162, found: 382.1160.

2-(Phenylamino)-3-(4-(trifluoromethoxy)phenyl)quinazolin-4(3*H*)-one (3oa).



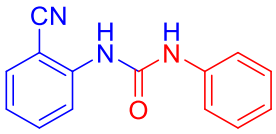
The product was purified by column chromatography (petroleum ether/EtOAc = 2:1). White solid (52.4 mg, 66% yield), melting point: 168–170 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (dd, *J* = 8.0 Hz, *J* = 1.6 Hz, 1 H), 7.69–7.64 (m, 1 H), 7.53–7.45 (m, 7 H), 7.35–7.31 (m, 2 H), 7.28–7.24 (m, 1 H), 7.14–7.09 (m, 1 H), 5.84 (s, 1 H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 162.6, 150.3 (q, *J* = 1.9 Hz, 1 C), 148.5, 146.1, 137.7, 135.1, 132.9, 131.1, 129.1, 127.3, 125.9, 124.5, 124.0, 123.1, 121.2, 120.5 (q, *J* = 257.2 Hz, 1 C), 118.4; ^{19}F NMR (377 MHz, $CDCl_3$) δ –57.7; HRMS (ESI) *m*/*z* calcd for $C_{21}H_{15}F_3N_3O_2$ $[M + H]^+$ 398.1111, found: 398.1109.

2-(Phenylamino)-3-(pyridin-4-yl)quinazolin-4(3*H*)-one (3pa).



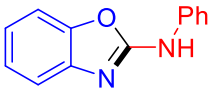
The product was purified by column chromatography (petroleum ether/EtOAc = 1:2). White solid (47.7 mg, 76% yield), melting point: 203–205 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.82 (d, J = 6.4 Hz, 2 H), 7.98 (d, J = 7.6 Hz, 1 H), 7.80 (s, 1 H), 7.67 (t, J = 7.4 Hz, 1 H), 7.61 (d, J = 6.0 Hz, 2 H), 7.50 (d, J = 6.0 Hz, 2 H), 7.31 (t, J = 8.2 Hz, 3 H), 7.25 (t, J = 7.4 Hz, 1 H), 7.09 (t, J = 7.4 Hz, 1 H); ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 161.4, 151.5, 148.7, 147.4, 142.9, 138.8, 134.8, 128.1, 126.5, 125.1, 124.9, 123.9, 123.7, 123.1, 117.7; HRMS (ESI) *m/z* calcd for $C_{19}H_{15}N_4O$ $[M + H]^+$ 315.1240, found: 315.1239.

1-(2-cyanophenyl)-3-phenylurea (3qa).[1]



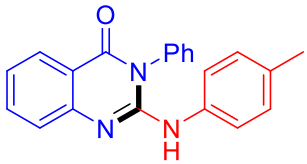
The product was purified by column chromatography (petroleum ether/EtOAc = 4:1). White solid (21.3 mg, 45% yield), melting point: 161–163 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.39 (s, 1 H), 8.74 (s, 1 H), 8.09 (d, J = 8.4 Hz, 1 H), 7.75 (dd, J = 7.6 Hz, J = 1.6 Hz, 1 H), 7.66–7.62 (m, 1 H), 7.49–7.46 (m, 2 H), 7.33–7.29 (m, 2 H), 7.20–7.16 (m, 1 H), 7.01(t, J = 7.4 Hz, 1 H); ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 152.0, 142.0, 139.2, 134.0, 133.1, 128.9, 123.0, 122.4, 121.3, 118.4, 117.0, 102.0; HRMS (ESI) *m/z* calcd for $C_{14}H_{12}N_3O$ $[M + H]^+$ 238.0975, found: 238.0973.

***N*-phenylbenzo[*d*]oxazol-2-amine (3sa).**



The product was purified by column chromatography (petroleum ether/EtOAc = 4:1). White solid (21.4 mg, 51% yield), melting point: 168–170 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.60 (s, 1 H), 7.77 (d, J = 8.0 Hz, 2 H), 7.47 (t, J = 8.8 Hz, 2 H), 7.37 (t, J = 7.8 Hz, 2 H), 7.22 (t, J = 7.6 Hz, 1 H), 7.12 (t, J = 7.6 Hz, 1 H), 7.03 (t, J = 7.4 Hz, 1 H); ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 158.0, 147.0, 142.4, 138.7, 129.0, 124.0, 122.1, 121.6, 117.6, 116.6, 108.9; HRMS (ESI) *m/z* calcd for $C_{13}H_{11}N_2O$ $[M + H]^+$ 211.0866, found: 211.0866.

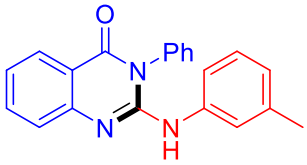
3-Phenyl-2-(*p*-tolylamino)quinazolin-4(3*H*)-one (3ab).



The product was purified by column chromatography (petroleum ether/EtOAc = 4:1). White solid (53.0 mg, 81% yield), melting point: 145–147 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (d, J = 7.6 Hz, 1 H), 7.66–7.56 (m, 4 H), 7.50 (d, J = 8.4 Hz, 1 H), 7.41–7.36 (m, 4 H), 7.25–7.21 (m, 1 H), 7.11 (d, J = 8.0 Hz, 2 H), 5.87 (s, 1

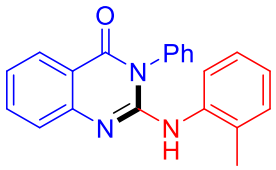
H), 2.31 (s, 3 H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 162.7, 148.8, 146.7, 135.3, 134.8, 134.7, 133.9, 130.9, 130.3, 129.5, 129.1, 127.3, 125.7, 123.6, 121.3, 118.4, 21.0; HRMS (ESI) *m/z* calcd for $C_{21}H_{18}N_3O$ $[M + H]^+$ 328.1444, found: 328.1444.

3-Phenyl-2-(*m*-tolylamino)quinazolin-4(3*H*)-one (3ac).



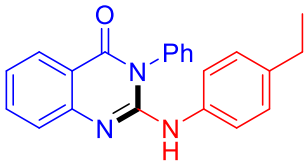
The product was purified by column chromatography (petroleum ether/EtOAc = 4:1). White solid (48.4 mg, 74% yield), melting point: 127–129 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.0 Hz, 1 H), 7.66–7.57 (m, 4 H), 7.52 (d, *J* = 8.0 Hz, 1 H), 7.41–7.37 (m, 3 H), 7.24–7.18 (m, 3 H), 6.90 (d, *J* = 7.6 Hz, 1 H), 5.90 (s, 1 H), 2.32(s, 3 H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 162.6, 148.7, 146.5, 138.9, 137.8, 134.8, 134.7, 130.9, 130.3, 129.1, 128.8, 127.3, 125.7, 125.0, 123.7, 121.6, 118.5, 118.2, 21.6; HRMS (ESI) *m/z* calcd for $C_{21}H_{18}N_3O$ $[M + H]^+$ 328.1444, found: 328.1443.

3-Phenyl-2-(*o*-tolylamino)quinazolin-4(3*H*)-one (3ad).



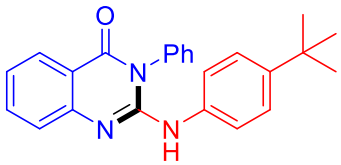
The product was purified by column chromatography (petroleum ether/EtOAc = 4:1). White solid (32.7 mg, 50% yield), melting point: 87–89 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21–8.17 (m, 2 H), 7.68–7.58 (m, 4 H), 7.50–7.44 (m, 3 H), 7.28–7.22 (m, 2 H), 7.12–7.02 (m, 2 H), 5.84 (br s, 1 H), 1.86 (s, 3 H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 162.7, 148.8, 146.7, 136.3, 134.9, 134.8, 131.0, 130.5, 130.4, 129.1, 128.8, 127.3, 126.9, 125.8, 124.6, 123.7, 122.4, 118.5, 17.4; HRMS (ESI) *m/z* calcd for $C_{21}H_{18}N_3O$ $[M + H]^+$ 328.1444, found: 328.1443.

2-((4-Ethylphenyl)amino)-3-phenylquinazolin-4(3*H*)-one (3ae).



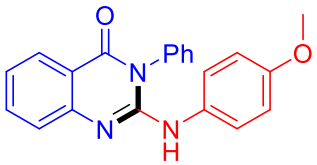
The product was purified by column chromatography (petroleum ether/EtOAc = 4:1). White solid (57.3 mg, 84% yield), melting point: 147–149 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (dd, *J* = 8.0 Hz, *J* = 1.2 Hz, 1 H), 7.66–7.56 (m, 4 H), 7.50 (d, *J* = 8.0 Hz, 1 H), 7.41–7.38 (m, 4 H), 7.25–7.21 (m, 1 H), 7.13 (d, *J* = 8.4 Hz, 2 H), 5.89 (s, 1 H), 2.61 (q, *J* = 7.6 Hz, 2 H), 1.20 (t, *J* = 7.4 Hz, 3 H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 162.6, 148.7, 146.7, 140.3, 135.4, 134.8, 134.7, 130.9, 130.3, 129.1, 128.3, 127.2, 125.7, 123.6, 121.3, 118.4, 28.4, 15.8; HRMS (ESI) *m/z* calcd for $C_{22}H_{20}N_3O$ $[M + H]^+$ 342.1601, found: 342.1601.

2-((4-(*tert*-Butyl)phenyl)amino)-3-phenylquinazolin-4(3*H*)-one (3af).



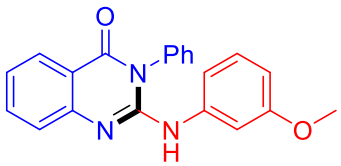
The product was purified by column chromatography (petroleum ether/EtOAc = 4:1). White solid (58.3 mg, 79% yield), melting point: 88–90 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (dd, *J* = 8.0 Hz, *J* = 1.6 Hz, 1 H), 7.67–7.56 (m, 4 H), 7.51 (d, *J* = 8.4 Hz, 1 H), 7.42–7.39 (m, 4 H), 7.34–7.32 (m, 2 H), 7.26–7.22 (m, 1 H), 5.89 (s, 1 H), 1.30 (s, 9 H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 162.6, 148.7, 147.2, 146.6, 135.2, 134.8, 134.7, 130.9, 130.3, 129.1, 127.3, 125.8, 125.7, 123.6, 120.8, 118.5, 34.4, 31.5; HRMS (ESI) *m/z* calcd for $C_{24}H_{24}N_3O$ $[M + H]^+$ 370.1914, found: 370.1913.

2-((4-Methoxyphenyl)amino)-3-phenylquinazolin-4(3*H*)-one (3ag).



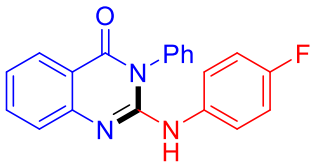
The product was purified by column chromatography (petroleum ether/EtOAc = 3:1). White solid (46.0 mg, 67% yield), melting point: 162–164 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (dd, *J* = 8.0 Hz, *J* = 1.6 Hz, 1 H), 7.65–7.56 (m, 4 H), 7.46 (d, *J* = 8.0 Hz, 1 H), 7.42–7.36 (m, 4 H), 7.22 (t, *J* = 7.4 Hz, 1 H), 6.87–6.83 (m, 2 H), 5.81 (s, 1 H), 3.78 (s, 3 H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 162.7, 156.6, 148.9, 147.1, 134.7, 134.7, 130.9, 130.8, 130.3, 129.1, 127.2, 125.6, 123.5, 123.4, 118.3, 114.2, 55.6; HRMS (ESI) *m/z* calcd for $C_{21}H_{18}N_3O_2$ $[M + H]^+$ 344.1394, found: 344.1393.

2-((3-Methoxyphenyl)amino)-3-phenylquinazolin-4(3*H*)-one (3ah).



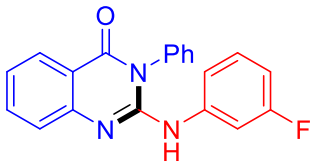
The product was purified by column chromatography (petroleum ether/EtOAc = 3:1). White solid (43.2 mg, 63% yield), melting point: 146–148 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (dd, *J* = 8.0 Hz, *J* = 1.6 Hz, 1 H), 7.68–7.57 (m, 4 H), 7.53 (d, *J* = 8.0 Hz, 1 H), 7.44–7.39 (m, 3 H), 7.28–7.24 (m, 1 H), 7.17 (t, *J* = 8.0 Hz, 1 H), 6.84 (d, *J* = 8.8 Hz, 1 H), 6.63 (dd, *J* = 8.0 Hz, *J* = 2.4 Hz, 1 H), 5.96 (s, 1 H), 3.82 (s, 3 H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 162.6, 160.2, 148.5, 146.2, 139.1, 134.8, 134.6, 131.0, 130.4, 129.6, 129.1, 127.3, 125.8, 123.9, 118.5, 112.9, 109.5, 106.8, 55.4; HRMS (ESI) *m/z* calcd for $C_{21}H_{18}N_3O_2$ $[M + H]^+$ 344.1394, found: 344.1393.

2-((4-Fluorophenyl)amino)-3-phenylquinazolin-4(3*H*)-one (3ai).



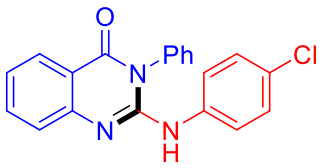
The product was purified by column chromatography (petroleum ether/EtOAc = 4:1). White solid (48.3 mg, 73% yield), melting point: 123–125 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (dd, *J* = 8.0 Hz, *J* = 1.6 Hz, 1 H), 7.67–7.57 (m, 4 H), 7.50–7.40 (m, 5 H), 7.27–7.23 (m, 1 H), 7.02–6.98 (m, 2 H), 5.89 (s, 1 H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 162.6, 159.5 (d, *J* = 242.0 Hz, 1 C), 148.5, 146.7, 134.9, 134.6, 133.8 (d, *J* = 2.7 Hz, 1 C), 131.0, 130.4, 129.1, 127.3, 125.7, 123.8, 123.1 (d, *J* = 7.8 Hz, 1 C), 118.5, 115.6 (d, *J* = 22.4 Hz, 1 C); ^{19}F NMR (377 MHz, $CDCl_3$) δ –118.3; HRMS (ESI) *m/z* calcd for $C_{20}H_{15}FN_3O$ $[M + H]^+$ 332.1194, found: 332.1192.

2-((3-Fluorophenyl)amino)-3-phenylquinazolin-4(3*H*)-one (3aj).



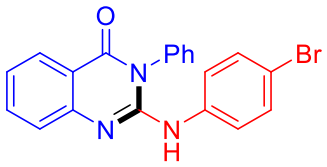
The product was purified by column chromatography (petroleum ether/EtOAc = 4:1). White solid (51.0 mg, 77% yield), melting point: 111–113 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (d, *J* = 8.0 Hz, 1 H), 7.74–7.57 (m, 6 H), 7.41 (m, 2 H), 7.31–7.28 (m, 1 H), 7.24–7.18 (m, 1 H), 6.96 (d, *J* = 8.0 Hz, 1 H), 6.78 (t, *J* = 8.2 Hz, 1 H), 6.05 (br s, 1 H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 163.1 (d, *J* = 243.0 Hz, 1 C), 162.5, 148.2, 145.9, 139.5 (d, *J* = 11.1 Hz, 1 C), 135.0, 134.4, 131.1, 130.6, 130.0 (d, *J* = 9.5 Hz, 1 C), 129.1, 127.4, 125.8, 124.2, 118.6, 115.8, 110.6 (d, *J* = 21.3 Hz, 1 C), 108.1 (d, *J* = 26.6 Hz, 1 C); ^{19}F NMR (377 MHz, $CDCl_3$) δ –111.3; HRMS (ESI) *m/z* calcd for $C_{20}H_{15}FN_3O$ $[M + H]^+$ 332.1194, found: 332.1192.

2-((4-Chlorophenyl)amino)-3-phenylquinazolin-4(3*H*)-one (3ak).



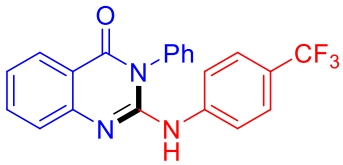
The product was purified by column chromatography (petroleum ether/EtOAc = 4:1). Light yellow solid (49.3 mg, 71% yield), melting point: 130–132 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (dd, *J* = 8.0 Hz, *J* = 1.6 Hz, 1 H), 7.68–7.57 (m, 4 H), 7.52–7.45 (m, 3 H), 7.41–7.38 (m, 2 H), 7.28–7.24 (m, 3 H), 5.94 (s, 1 H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 162.5, 148.3, 146.2, 136.5, 134.9, 134.5, 131.0, 130.5, 129.1, 129.0, 128.9, 127.3, 125.7, 124.0, 122.2, 118.6; HRMS (ESI) *m/z* calcd for $C_{20}H_{15}ClN_3O$ $[M + H]^+$ 348.0898, found: 348.0898.

2-((4-Bromophenyl)amino)-3-phenylquinazolin-4(3*H*)-one (3al).



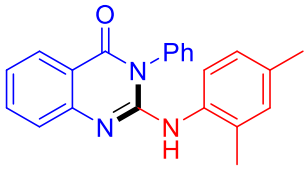
The product was purified by column chromatography (petroleum ether/EtOAc = 4:1). Light Yellow solid (56.3 mg, 72% yield), melting point: 141–143 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.4 Hz, 1 H), 7.69–7.58 (m, 4 H), 7.52 (d, *J* = 8.4 Hz, 1 H), 7.41–7.39 (m, 6 H), 7.27 (t, *J* = 7.4 Hz, 1 H), 5.94 (s, 1 H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 162.5, 148.3, 146.1, 137.0, 135.0, 134.5, 131.9, 131.0, 130.5, 129.1, 127.3, 125.7, 124.1, 122.5, 118.6, 116.7; HRMS (ESI) *m/z* calcd for $C_{20}H_{15}BrN_3O$ $[M + H]^+$ 392.0393, found: 392.0390.

3-Phenyl-2-((4-(trifluoromethyl)phenyl)amino)quinazolin-4(3*H*)-one (3am).



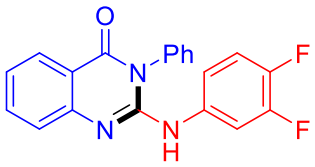
The product was purified by column chromatography (petroleum ether/EtOAc = 4:1). White solid (51.1 mg, 67% yield), melting point: 168–170 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (dd, *J* = 8.0 Hz, *J* = 1.6 Hz, 1 H), 7.71–7.61 (m, 6 H), 7.57–7.54 (m, 3 H), 7.42–7.40 (m, 2 H), 7.30 (t, *J* = 7.4 Hz, 1 H), 6.13 (s, 1 H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 162.4, 148.1, 145.7, 141.1, 135.0, 134.3, 131.1, 130.6, 129.1, 127.4, 126.2 (q, *J* = 3.7 Hz, 1 C), 125.5 (q, *J* = 32.7 Hz, 1 C), 124.4, 124.2 (q, *J* = 269.8 Hz, 1 C), 122.9, 120.1, 118.8; ^{19}F NMR (377 MHz, $CDCl_3$) δ –61.9; HRMS (ESI) *m/z* calcd for $C_{21}H_{15}F_3N_3O$ $[M + H]^+$ 382.1162, found: 382.1159.

2-((2,4-Dimethylphenyl)amino)-3-phenylquinazolin-4(3*H*)-one (3an).



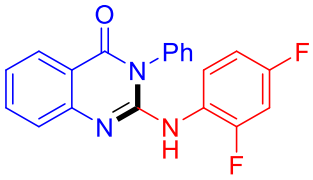
The product was purified by column chromatography (petroleum ether/EtOAc = 4:1). White solid (52.5 mg, 77% yield), melting point: 156–158 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (dd, *J* = 8.0 Hz, *J* = 1.6 Hz, 1 H), 7.91 (d, *J* = 8.4 Hz, 1 H), 7.67–7.57 (m, 4 H), 7.45 (t, *J* = 8.4 Hz, 3 H), 7.25–7.21 (m, 1 H), 7.05 (d, *J* = 8.4 Hz, 1 H), 6.95 (s, 1 H), 5.72 (s, 1 H), 2.29 (s, 3 H), 1.88 (s, 3 H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 162.7, 149.0, 147.1, 135.0, 134.7, 134.6, 133.6, 131.2, 131.0, 130.3, 129.6, 129.1, 127.4, 127.2, 125.7, 123.5, 123.2, 118.4, 21.0, 17.5.; HRMS (ESI) *m/z* calcd for $C_{22}H_{20}N_3O$ $[M + H]^+$ 342.1601, found: 342.1601.

2-((3,4-Difluorophenyl)amino)-3-phenylquinazolin-4(3*H*)-one (3ao).



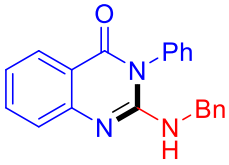
The product was purified by column chromatography (petroleum ether/EtOAc = 4:1). White solid (54.5 mg, 78% yield), melting point: 204–206 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, *J* = 8.0 Hz, 1 H), 7.84–7.79 (m, 1 H), 7.71–7.60 (m, 4 H), 7.54 (d, *J* = 8.4 Hz, 1 H), 7.40 (d, *J* = 7.2 Hz, 2 H), 7.31–7.26 (m, 1 H), 7.05 (q, *J* = 9.2 Hz, 1 H), 6.93–6.89 (m, 1 H), 5.94 (s, 1 H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 162.4, 150.1 (dd, *J* = 245.2 Hz, *J* = 13.2 Hz, 1 C), 148.2, 146.9 (dd, *J* = 243.8 Hz, *J* = 12.9 Hz, 1 C), 146.0, 135.0, 134.4 (dd, *J* = 9.0 Hz, *J* = 3.0 Hz, 1 C), 134.3, 131.1, 130.6, 129.1, 127.3, 125.7, 124.2, 118.6, 117.1 (dd, *J* = 18.0 Hz, *J* = 1.5 Hz, 1 C), 116.5 (dd, *J* = 5.9 Hz, *J* = 3.4 Hz, 1 C), 110.7 (d, *J* = 21.9 Hz, 1 C); ^{19}F NMR (377 MHz, $CDCl_3$) δ –135.6, –143.1; HRMS (ESI) *m/z* calcd for $C_{20}H_{14}F_2N_3O$ $[M + H]^+$ 350.1099, found: 350.1097.

2-((2,4-Difluorophenyl)amino)-3-phenylquinazolin-4(3*H*)-one (3ap).



The product was purified by column chromatography (petroleum ether/EtOAc = 4:1). White solid (42.6 mg, 61% yield), melting point: 197–199 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53–8.47 (m, 1 H), 8.20 (dd, *J* = 8.0 Hz, *J* = 1.6 Hz, 1 H), 7.69–7.58 (m, 4 H), 7.51 (d, *J* = 8.4 Hz, 1 H), 7.43–7.41 (m, 2 H), 7.30–7.25 (m, 1 H), 6.95–6.90 (m, 1 H), 6.8–6.76 (m, 1 H), 6.12 (br s, 1 H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 162.4, 158.5 (dd, *J* = 244.4 Hz, *J* = 11.4 Hz, 1 C), 153.3 (dd, *J* = 245.1 Hz, *J* = 12.0 Hz, 1 C), 148.2, 146.2, 135.0, 134.3, 131.0, 130.5, 129.0, 127.4, 125.7, 124.2, 123.6 (d, *J* = 8.6 Hz, 1 C), 122.9 (d, *J* = 10.1 Hz, 1 C), 118.7, 111.1 (dd, *J* = 18.0 Hz, *J* = 3.6 Hz, 1 C), 103.8 (dd, *J* = 23.1 Hz, *J* = 3.4 Hz, 1 C); ^{19}F NMR (377 MHz, $CDCl_3$) δ –107.5, –115.5, –116.1, –126.5; HRMS (ESI) *m/z* calcd for $C_{20}H_{14}F_2N_3O$ $[M + H]^+$ 350.1099, found: 350.1097.

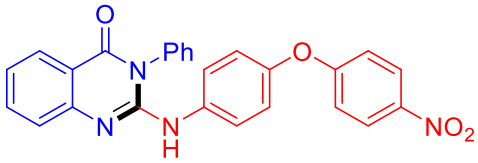
2-(Benzylamino)-3-phenylquinazolin-4(3*H*)-one (3aq).



The product was purified by column chromatography (petroleum ether/EtOAc = 4:1). White solid (34.7 mg, 53% yield), melting point: 171–173 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (dd, *J* = 8.0 Hz, *J* = 1.6 Hz, 1 H), 7.64–7.60 (m, 1 H), 7.58–7.54 (m, 2 H), 7.51–7.43 (m, 2 H), 7.32–7.28 (m, 4 H), 7.25–7.23 (m, 3 H), 7.18 (t, *J* = 7.4 Hz, 1 H), 4.66 (d, *J* = 5.6

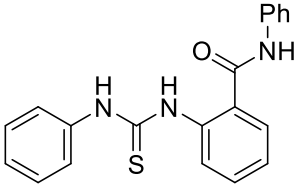
Hz, 2 H), 4.40 (t, J = 5.4 Hz, 1 H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 162.8, 149.5, 149.5, 138.5, 134.8, 130.7, 130.0, 128.9, 128.8, 127.6, 127.5, 127.4, 125.2, 122.9, 117.9, 45.6; HRMS (ESI) *m/z* calcd for $C_{21}H_{18}N_3O$ $[M + H]^+$ 328.1444, found: 328.1444.

2-((4-(4-Nitrophenoxy)phenyl)amino)-3-phenylquinazolin-4(3*H*)-one (3ar).



The product was purified by column chromatography (petroleum ether/EtOAc = 1:4). Light pink solid (44.1 mg, 49% yield), melting point: 237–239 °C. ^{1}H NMR (400 MHz, DMSO–d_6) δ 8.26–8.22 (m, 2 H), 7.98 (dd, J = 8.0 Hz, J = 1.6 Hz, 1 H), 7.70–7.57 (m, 7 H), 7.52–7.49 (m, 2 H), 7.36 (d, J = 8.4 Hz, 1 H), 7.25 (t, J = 7.4 Hz, 1 H), 7.14–7.10 (m, 4 H); $^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO–d_6) δ 163.3, 161.8, 149.9, 148.5, 148.0, 142.1, 136.3, 134.8, 134.6, 130.0, 129.5, 129.4, 126.5, 126.2, 125.1, 124.9, 123.1, 120.3, 118.0, 117.0.; HRMS (ESI) *m/z* calcd for $C_{26}H_{19}N_4O_4$ $[M + H]^+$ 451.1401, found: 451.1401.

***N*-phenyl-2-(3-phenylthioureido)benzamide (A).**



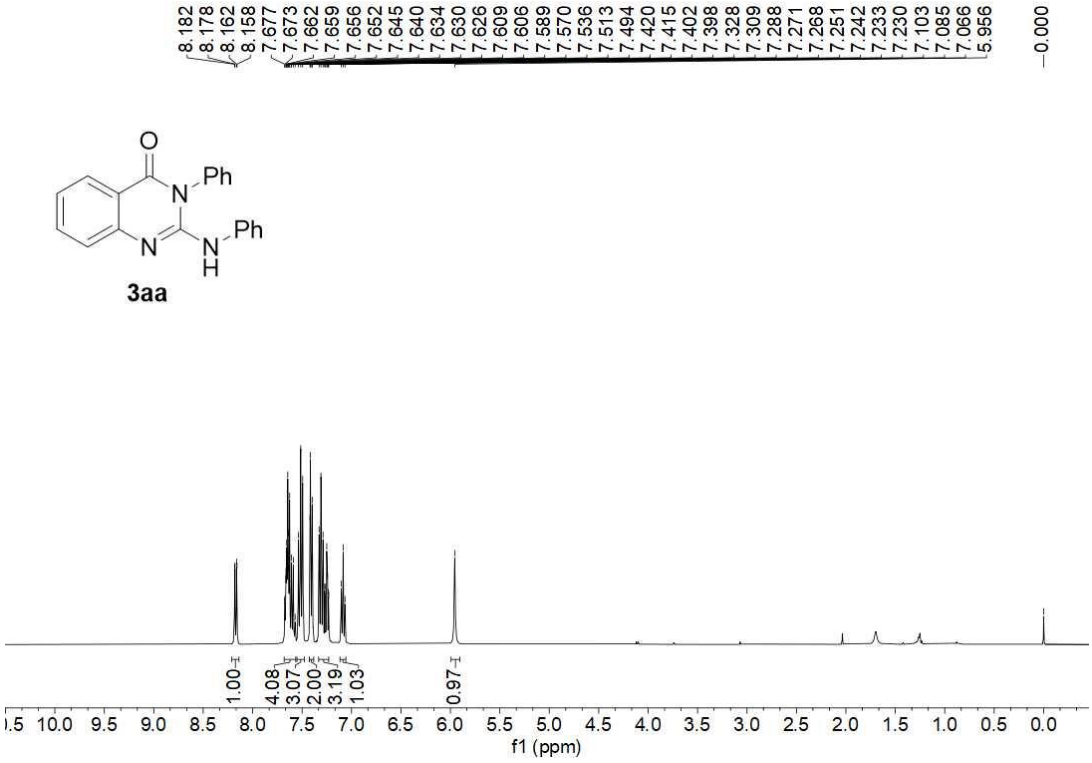
The product was purified by column chromatography (petroleum ether/EtOAc = 3:1). White solid, melting point: 256–258 °C. ^{1}H NMR (400 MHz, DMSO–d_6) δ 10.49 (s, 1 H), 10.45 (s, 1 H), 10.11 (s, 1 H), 8.02–8.00 (m, 1 H), 7.72–7.68 (m, 3 H), 7.54–7.47 (m, 3 H), 7.37–7.27 (m, 5 H), 7.19–7.10 (m, 2 H); $^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO–d_6) δ 179.6, 166.6, 138.9, 138.9, 138.2, 130.5, 128.9, 128.8, 128.4, 127.0, 125.1, 124.5, 124.1, 124.0, 120.4.; HRMS (ESI) *m/z* calcd for $C_{20}H_{18}N_3OS$ $[M + H]^+$ 348.1165, found: 348.1167.

References

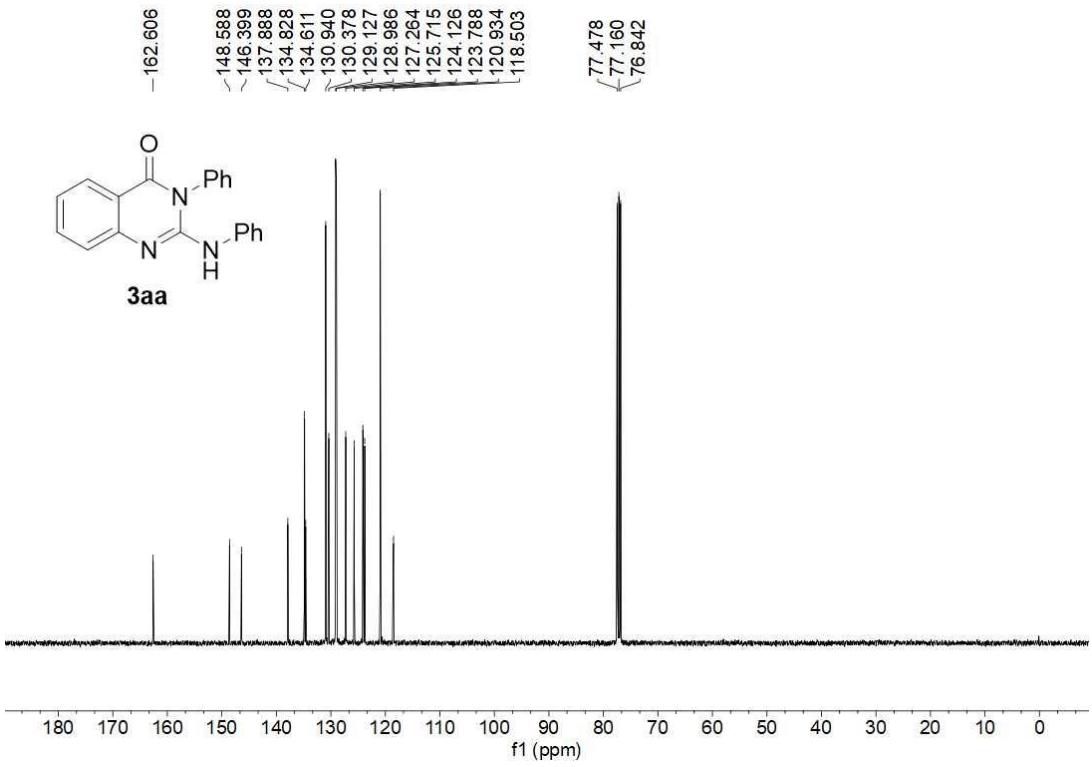
1 S. Shamanth, N. Chaithra, M. Gurukiran, M. Mamatha, N. Lokanath, K. S. Rangappa and K. Mantelingu, *Org. Biomol. Chem.*, 2020, **18**, 2678-2684.

9. NMR spectra for electrolysis products

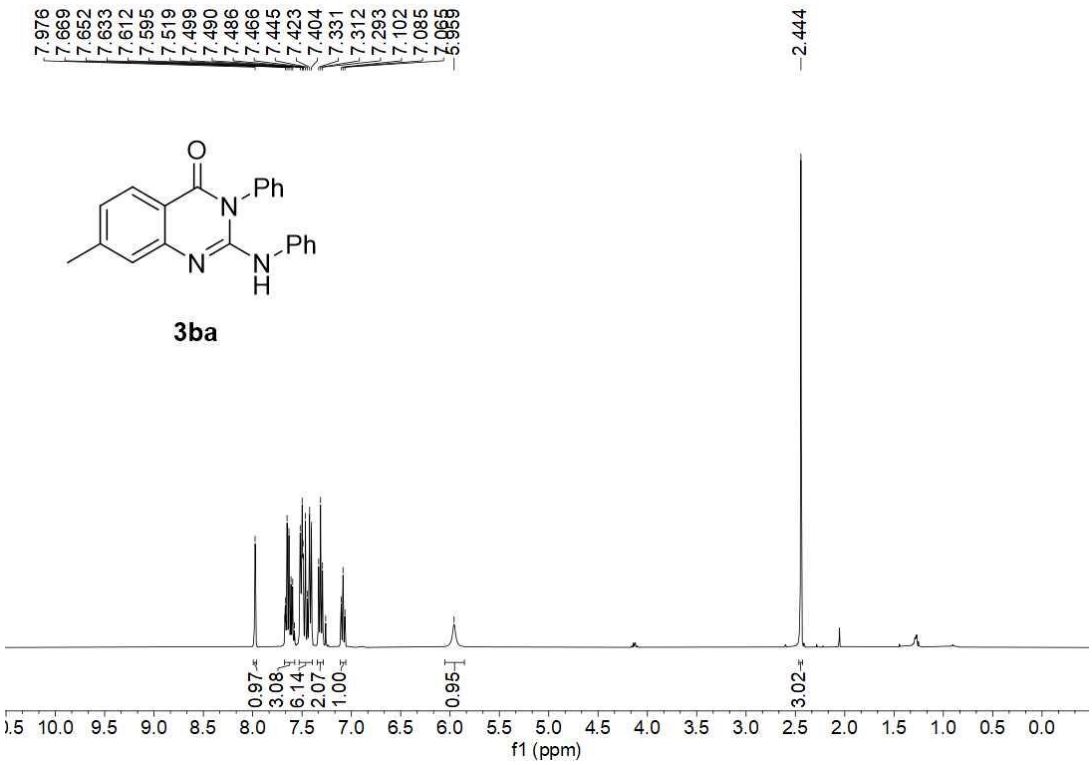
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3aa**



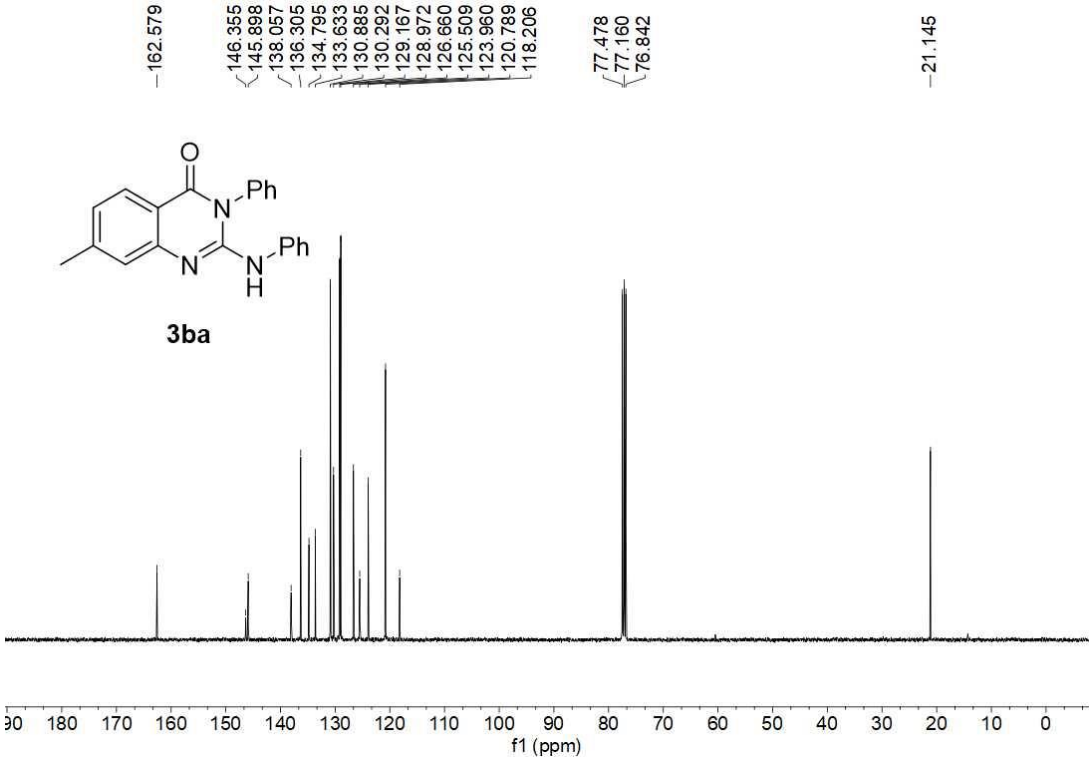
^{13}C{^{1}H} NMR spectrum (100 MHz, $CDCl_3$) of **3aa**



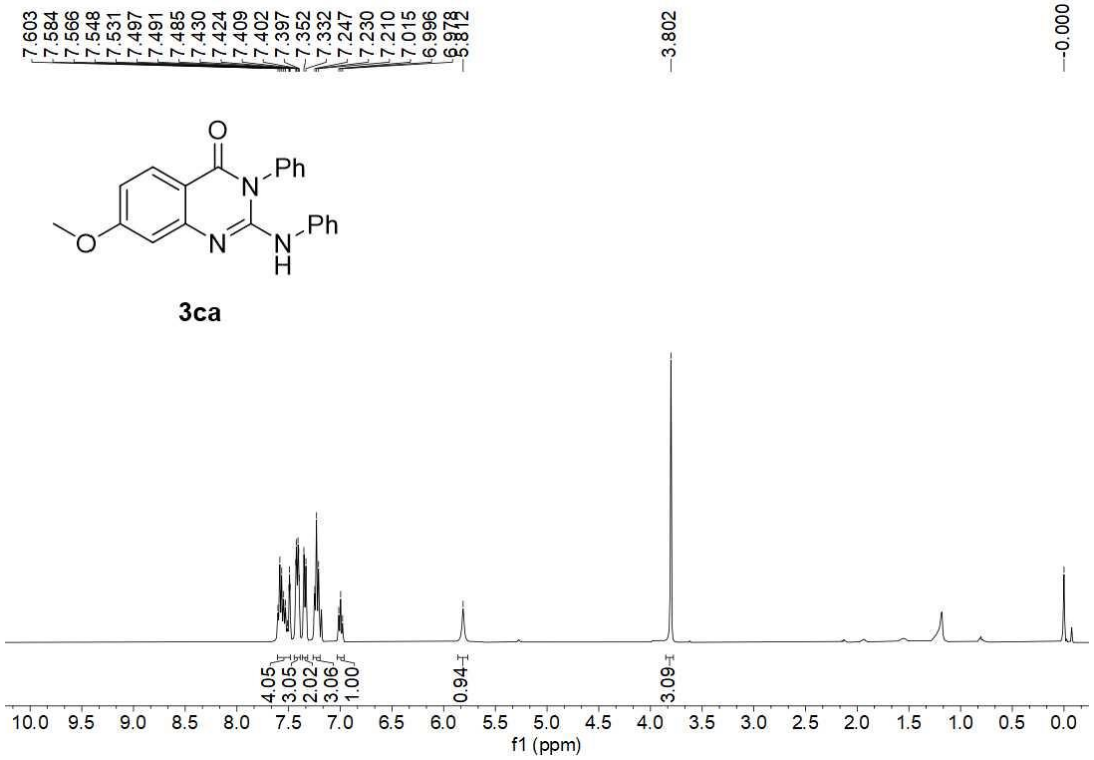
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3ba**



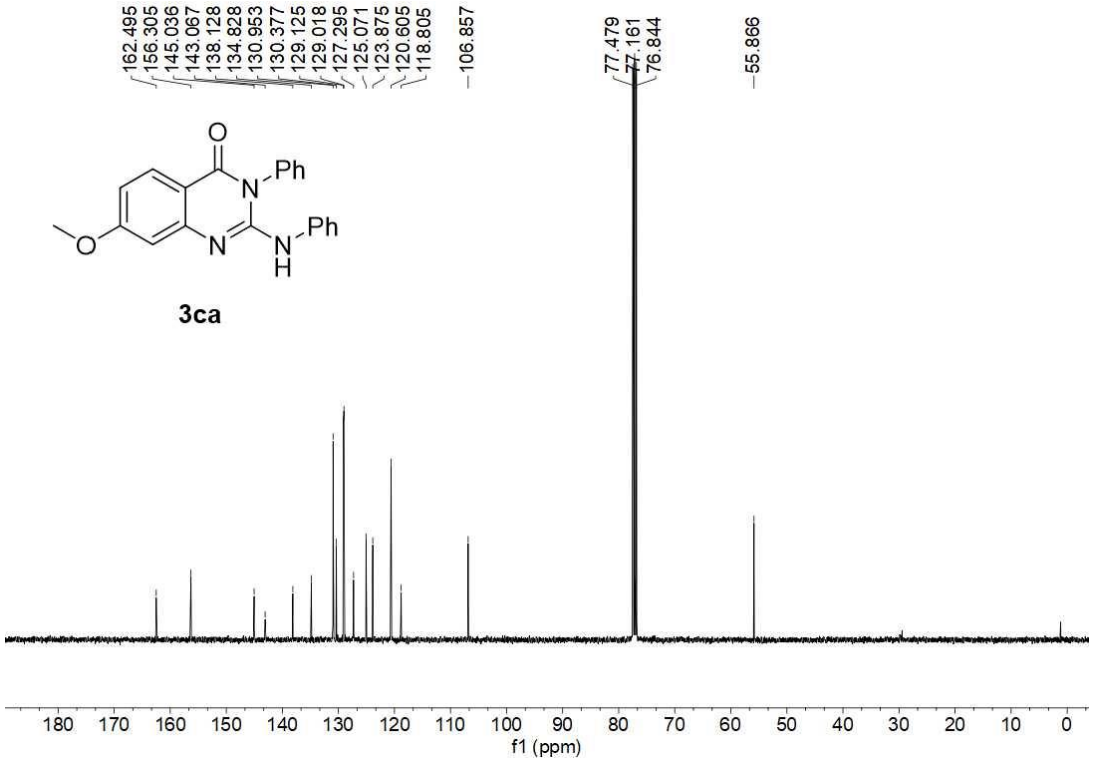
^{13}C{^{1}H} NMR spectrum (100 MHz, $CDCl_3$) of **3ba**



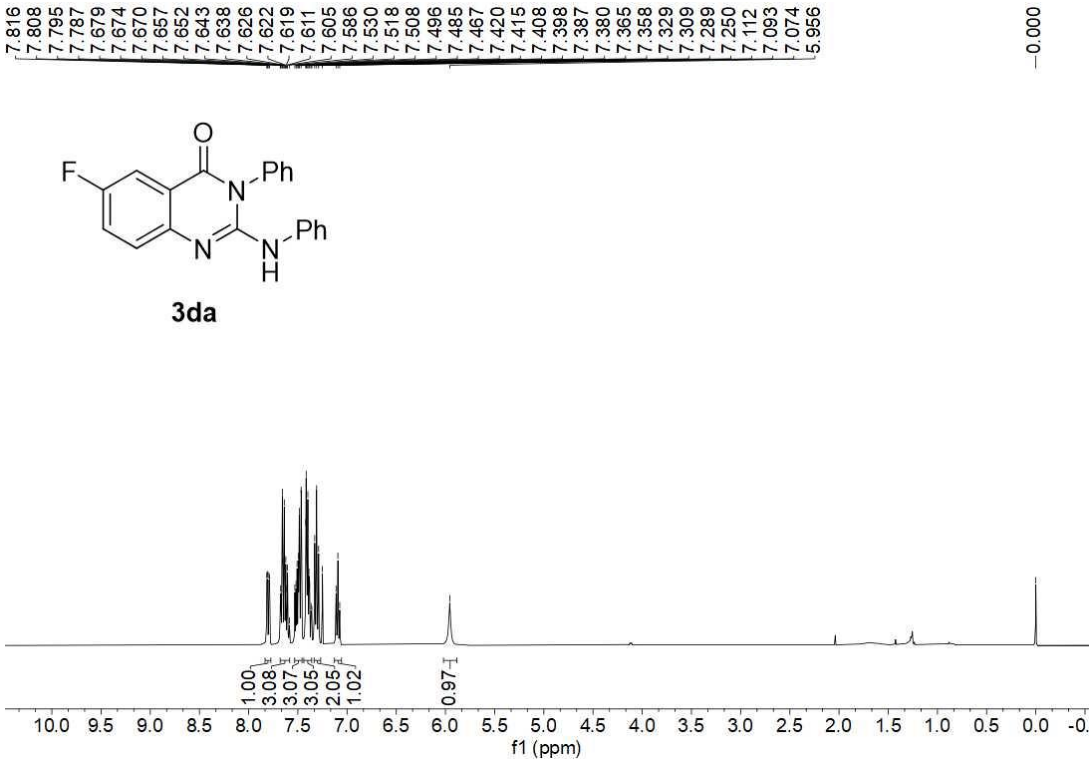
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3ca**



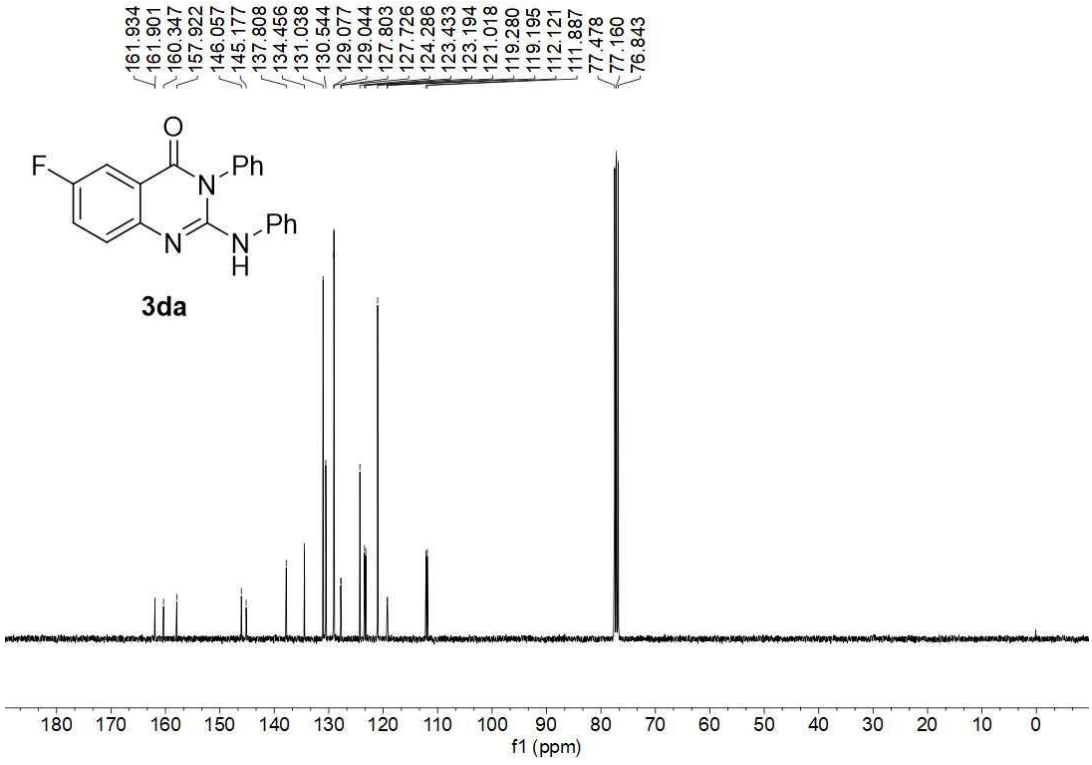
^{13}C{^{1}H} NMR spectrum (100 MHz, $CDCl_3$) of **3ca**



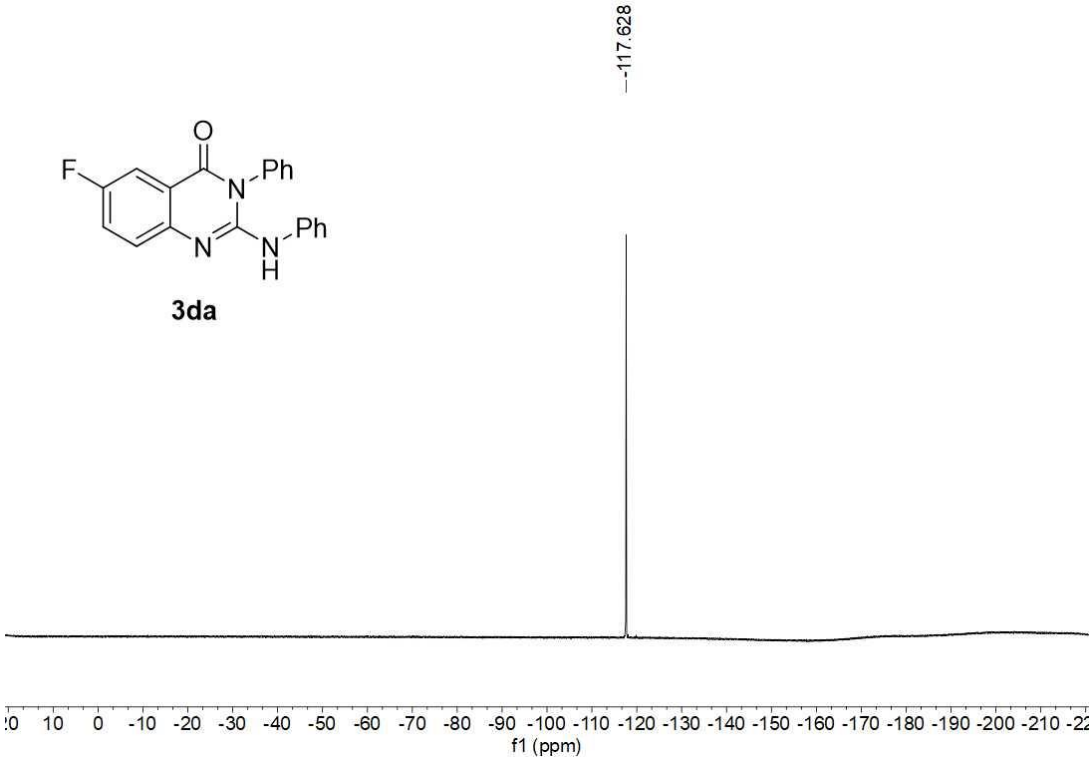
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3da**



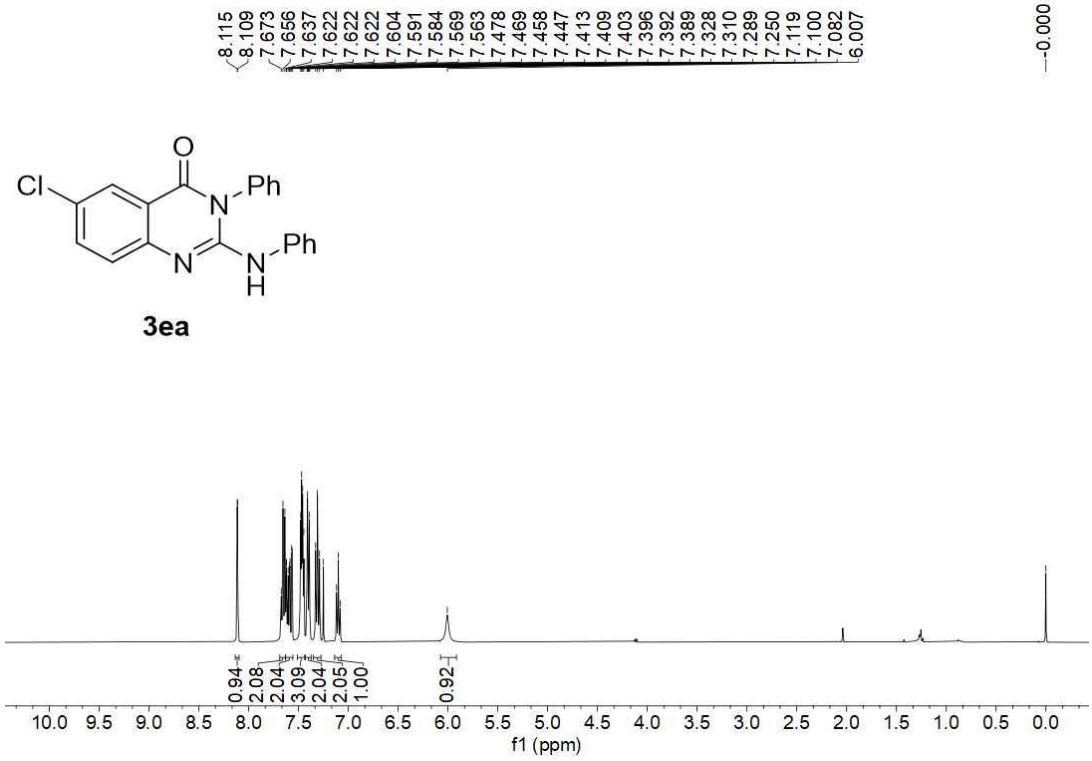
^{13}C{^{1}H} NMR spectrum (100 MHz, $CDCl_3$) of **3da**



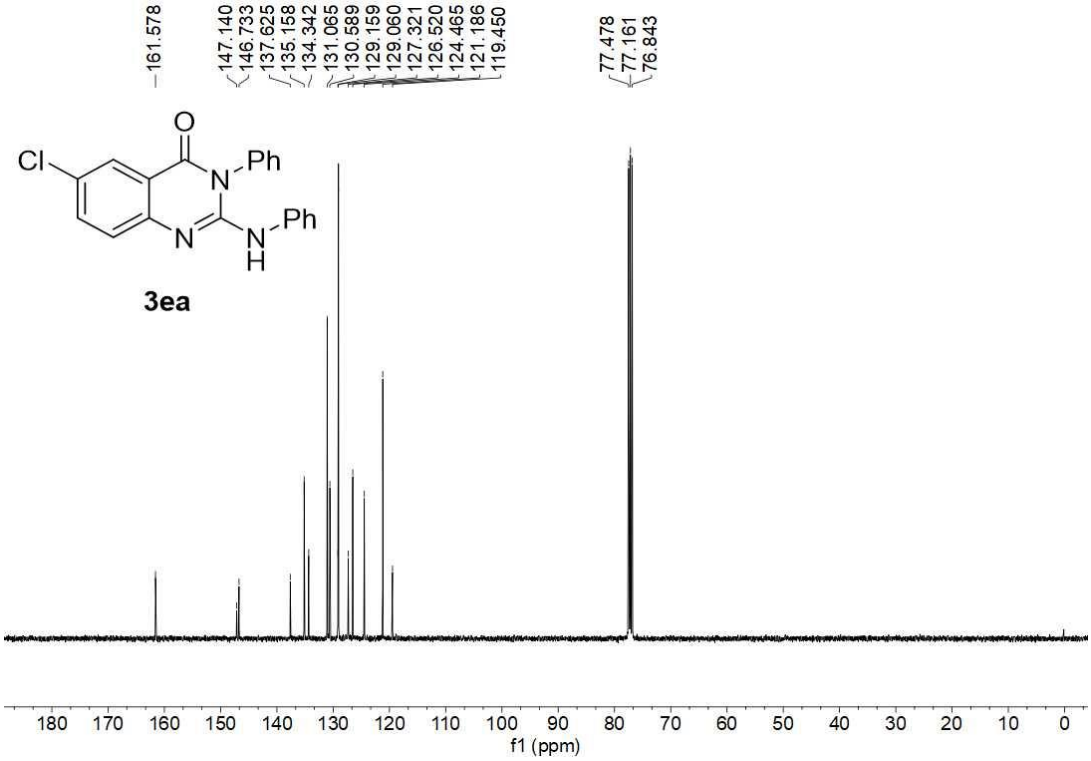
^{19}F NMR spectrum (377 MHz, $CDCl_3$) of **3da**



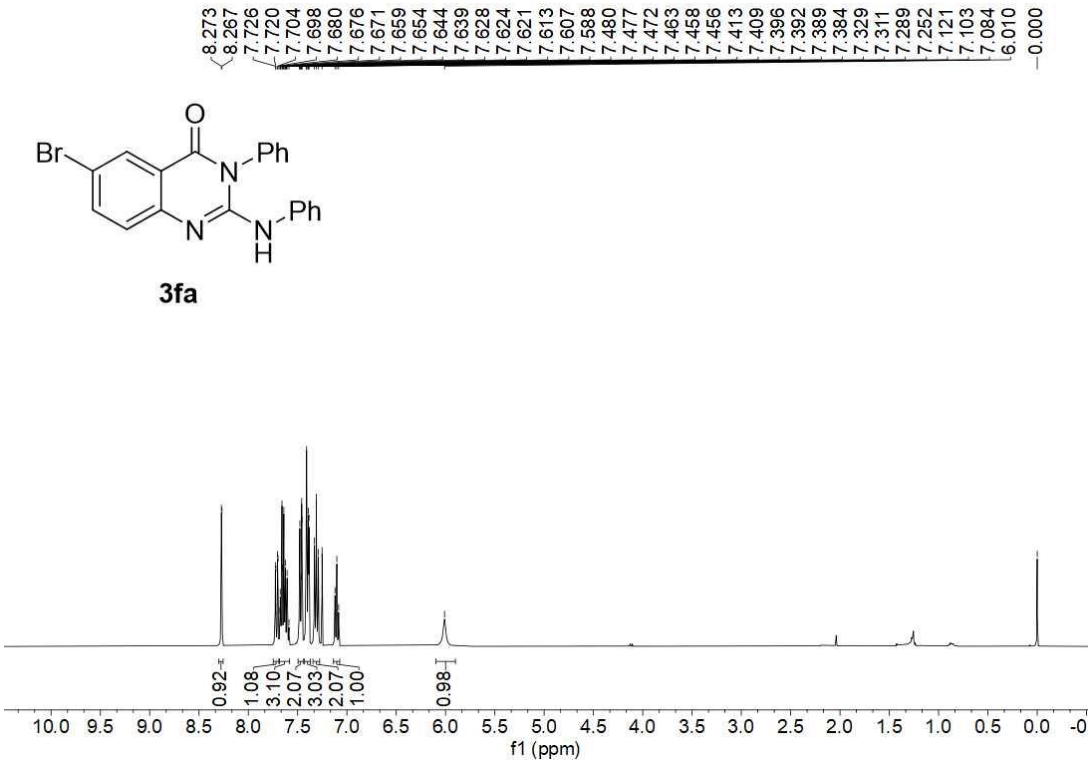
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3ea**



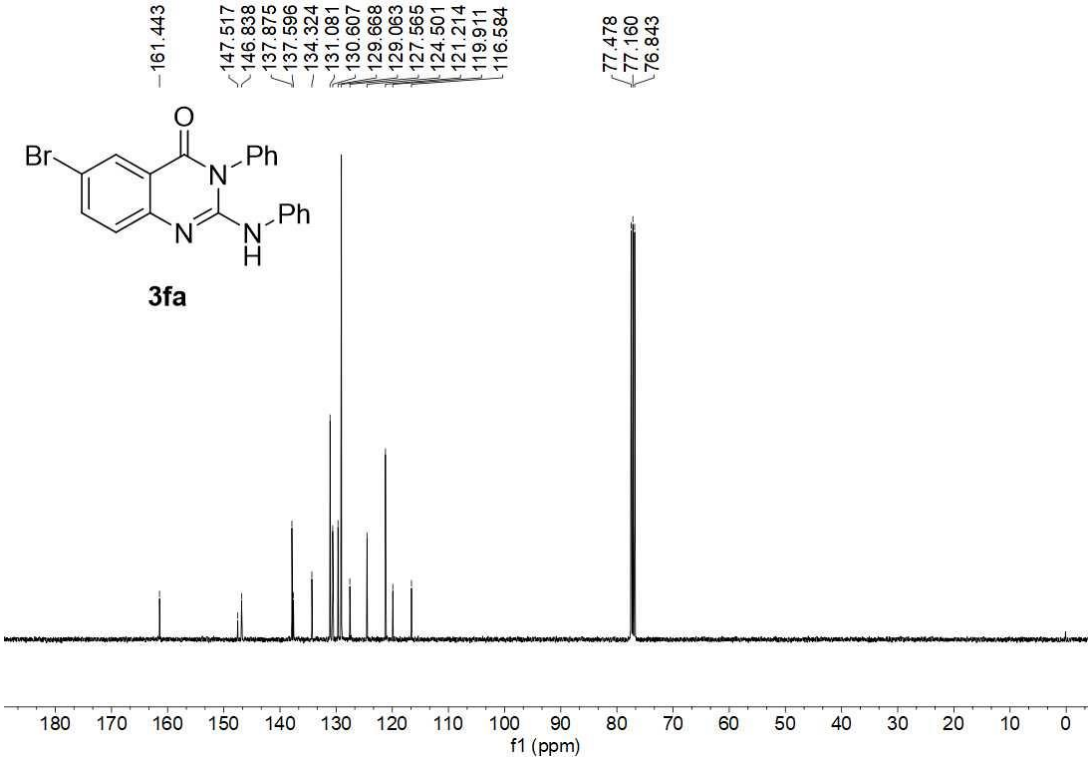
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of **3ea**



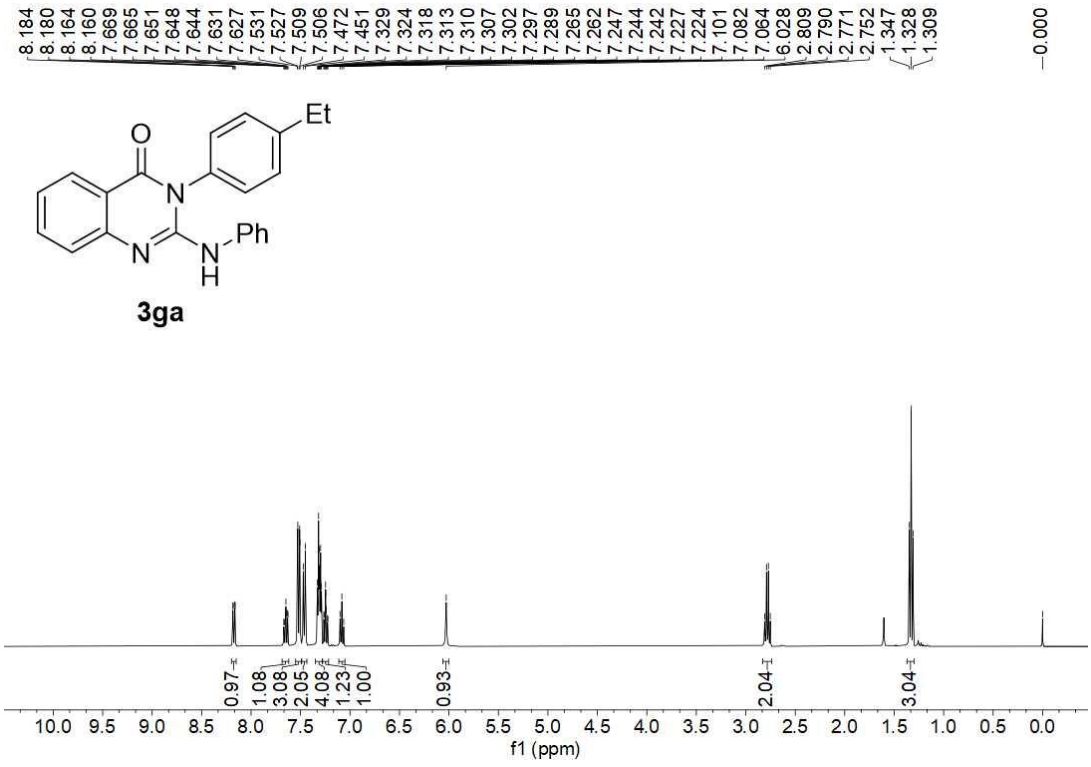
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3fa**



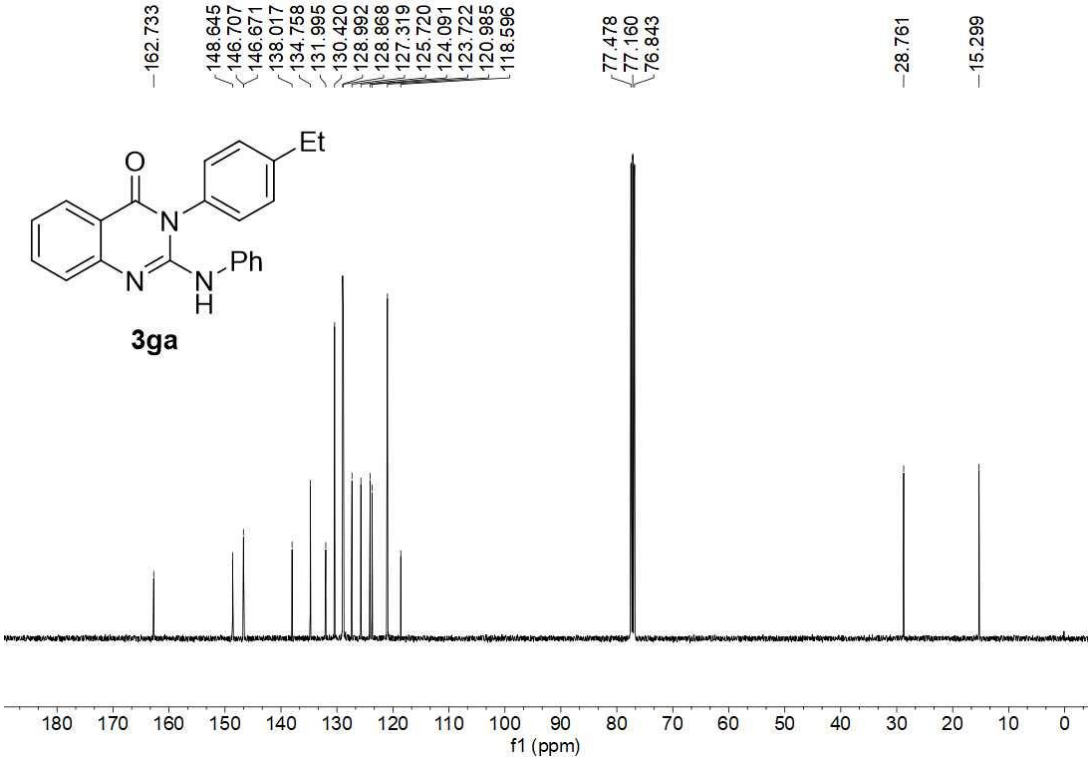
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of **3fa**



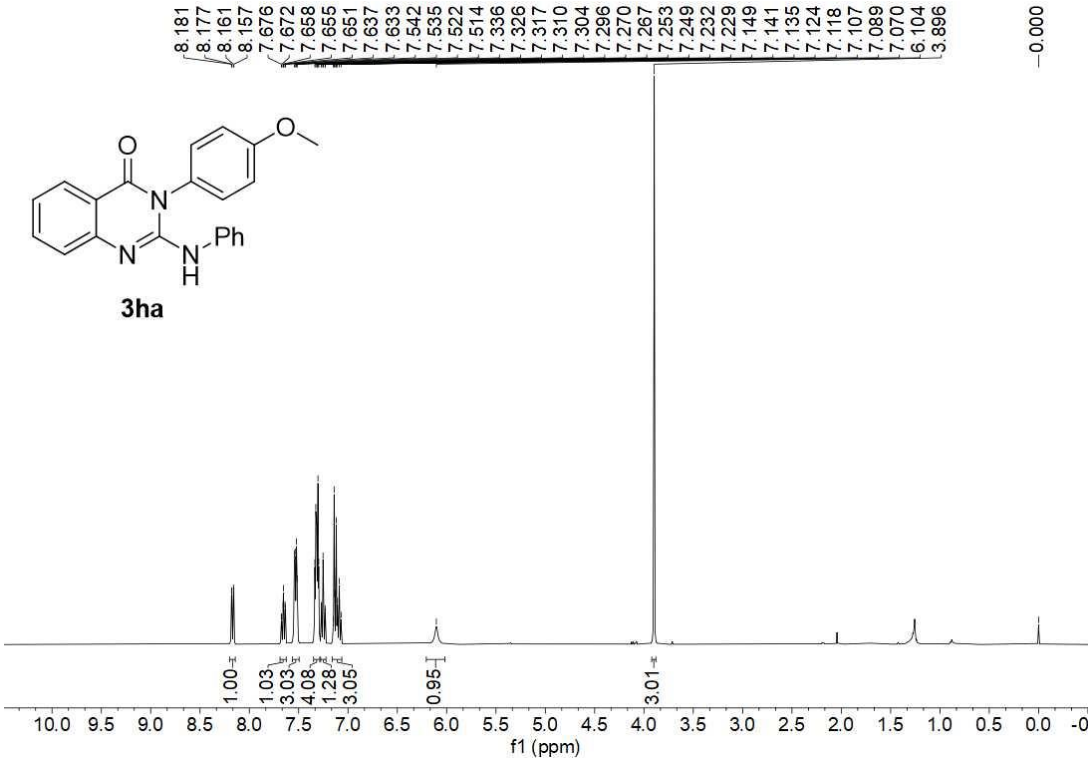
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3ga**



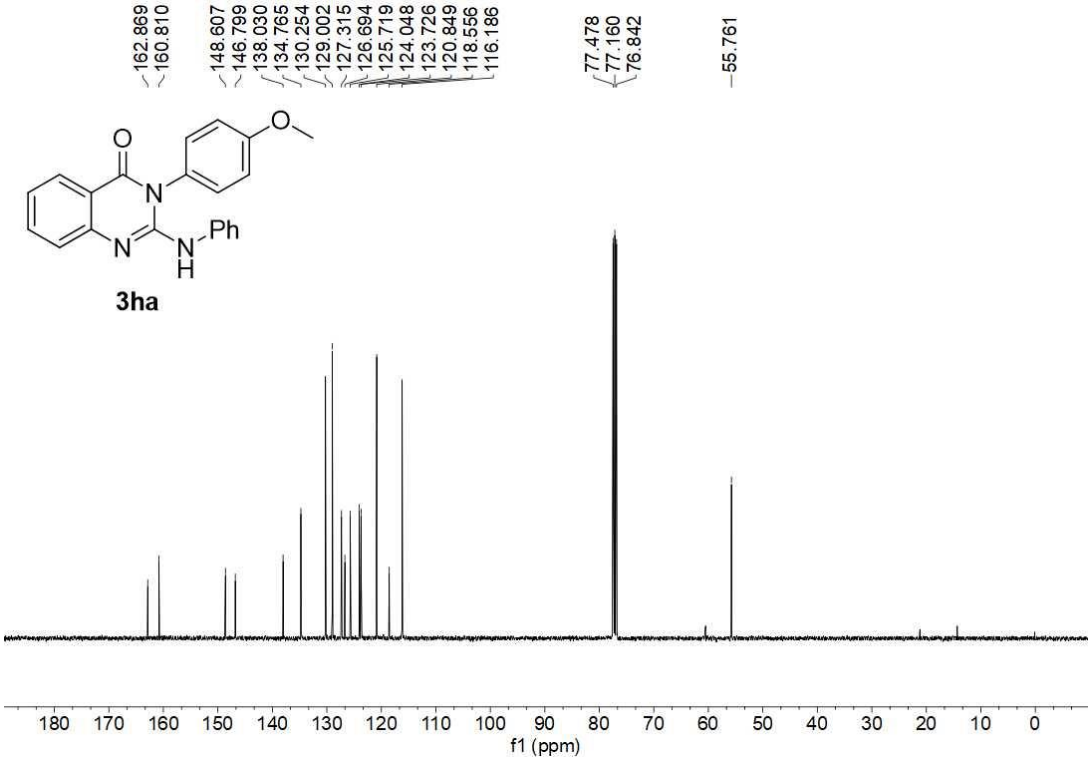
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of **3ga**



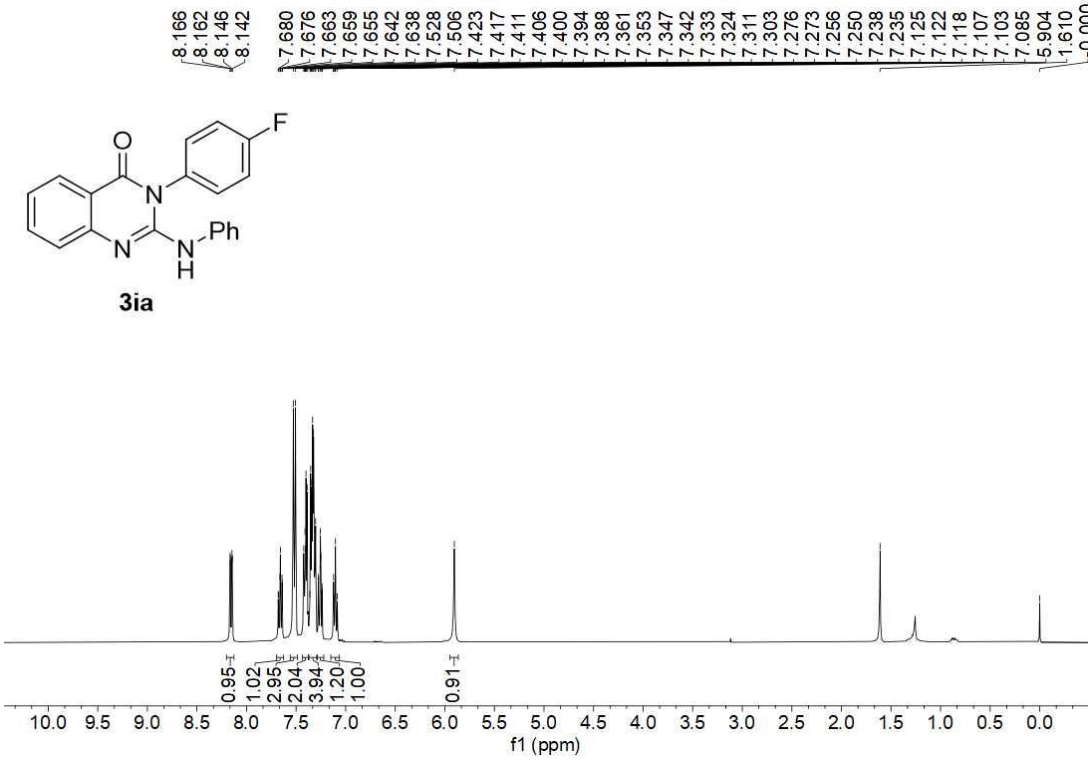
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3ha**



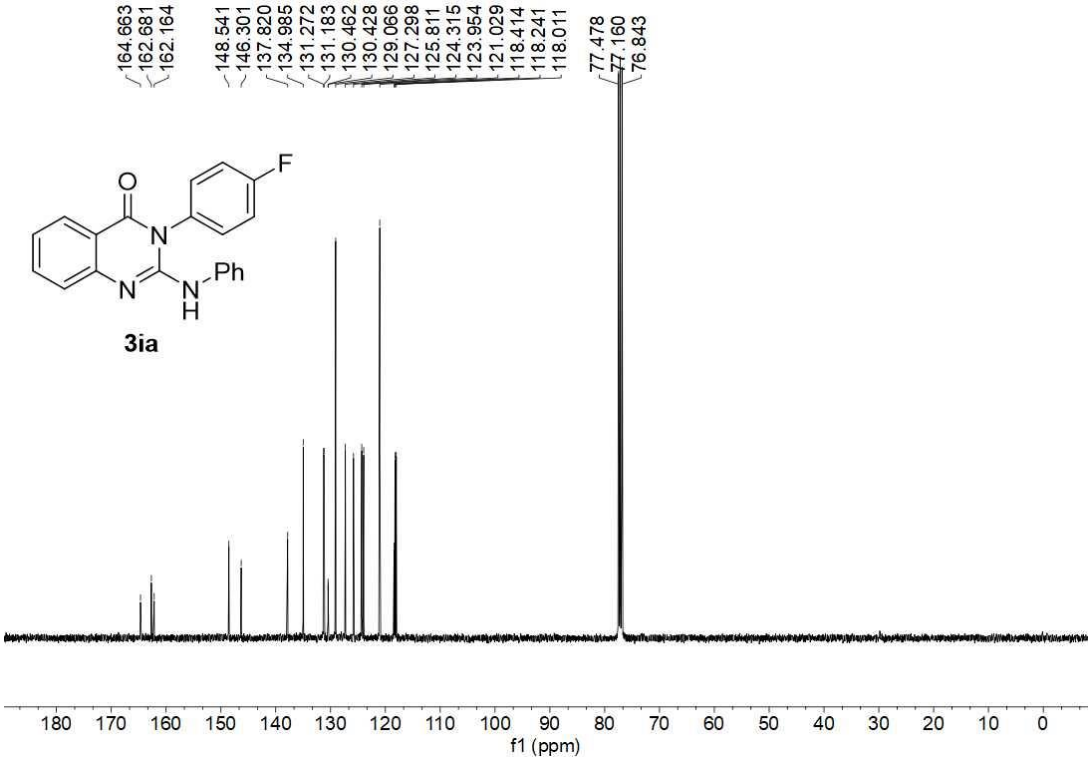
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of **3ha**



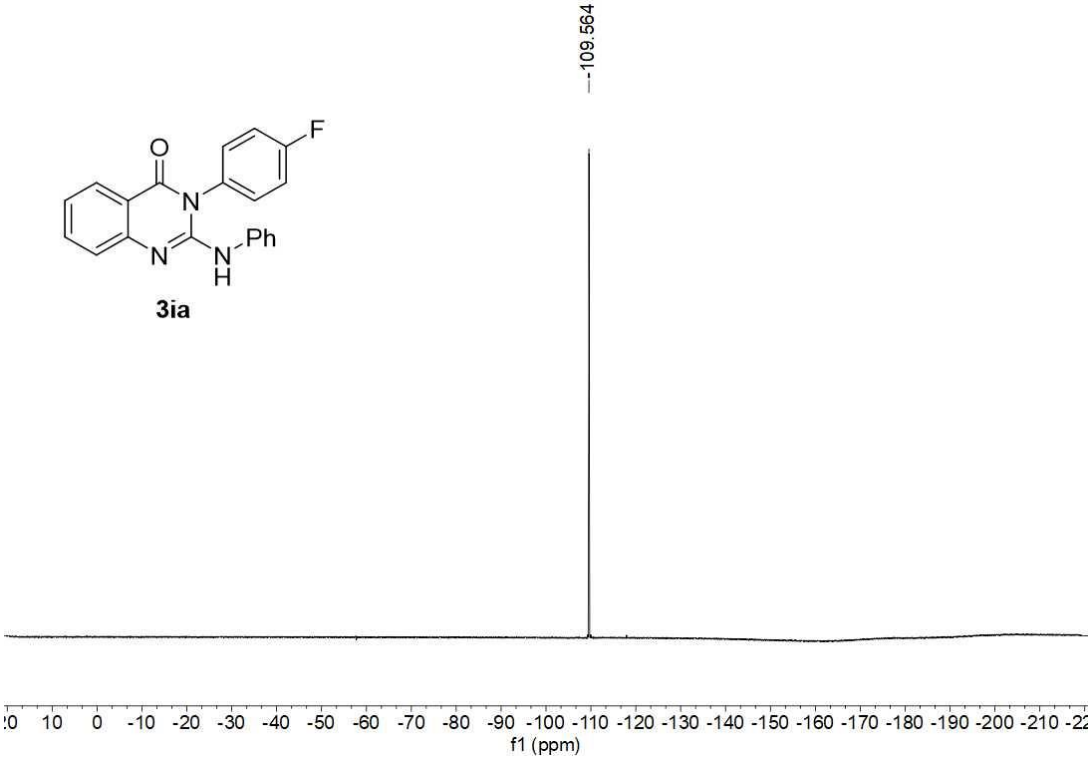
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3ia**



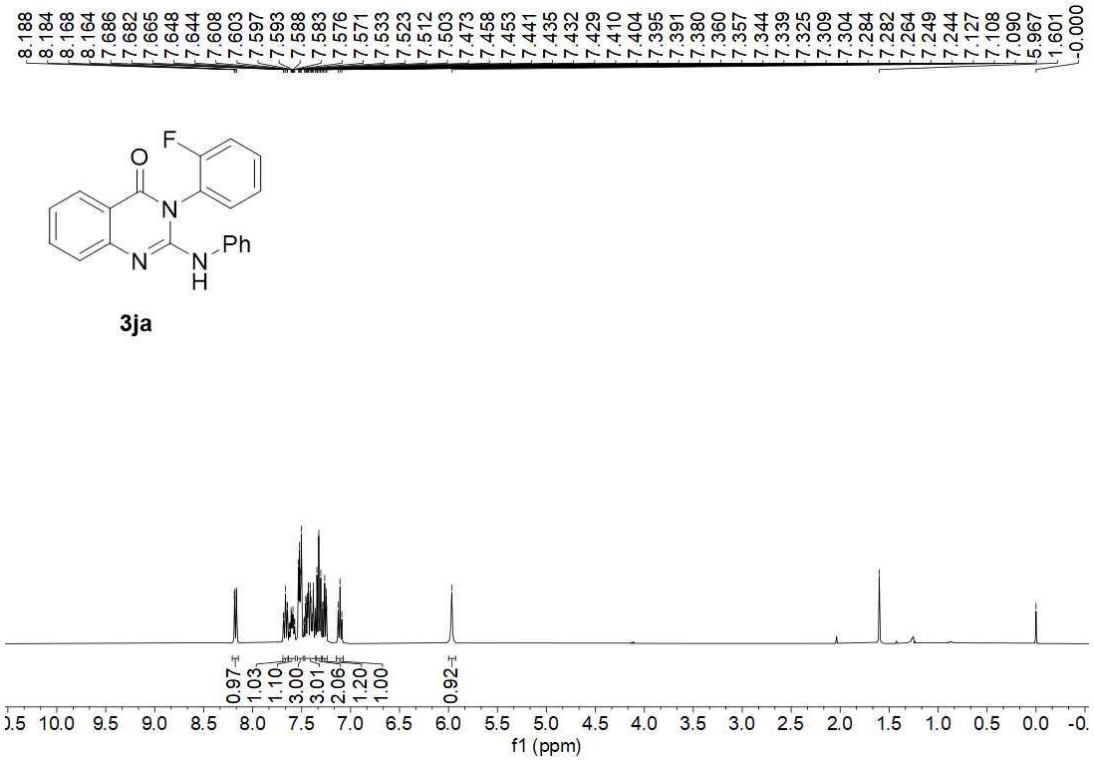
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of **3ia**



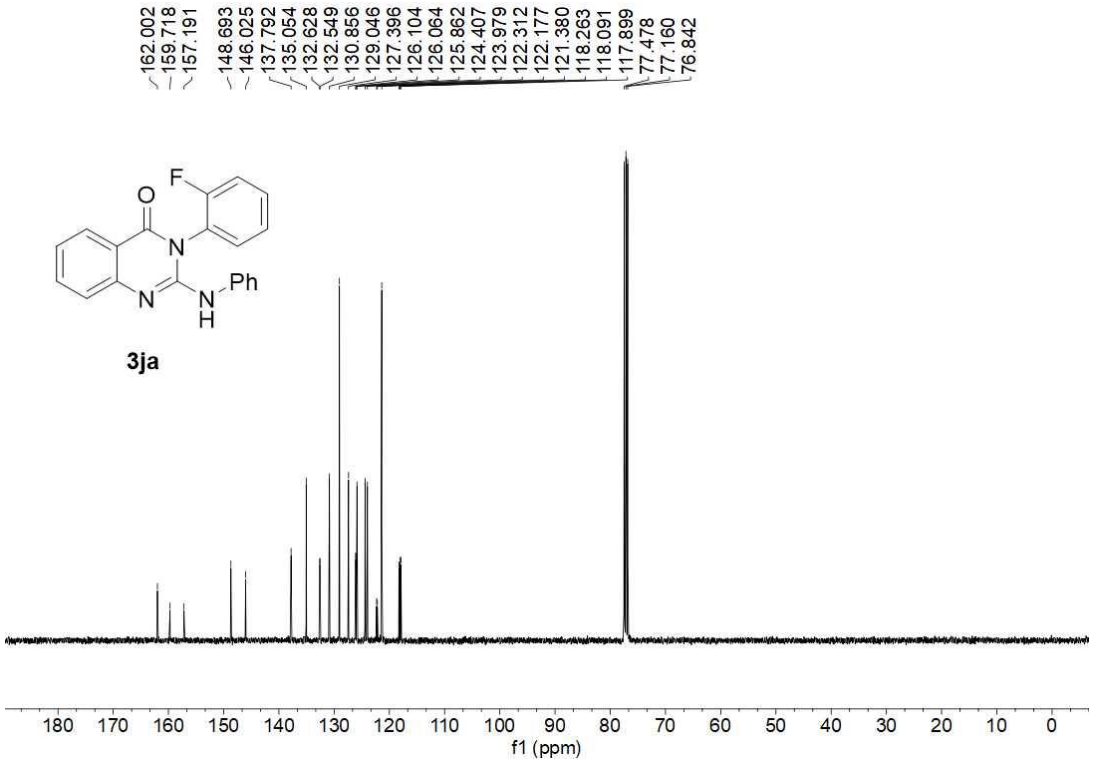
^{19}F NMR spectrum (377 MHz, $CDCl_3$) of **3ia**



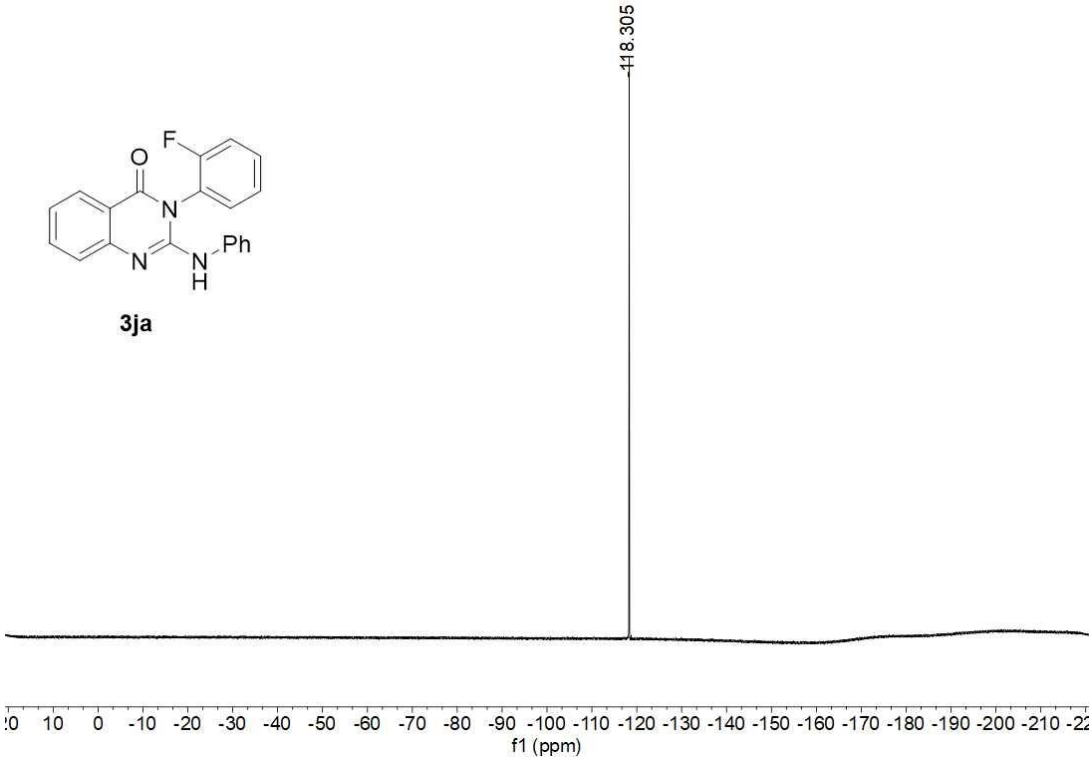
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3ja**



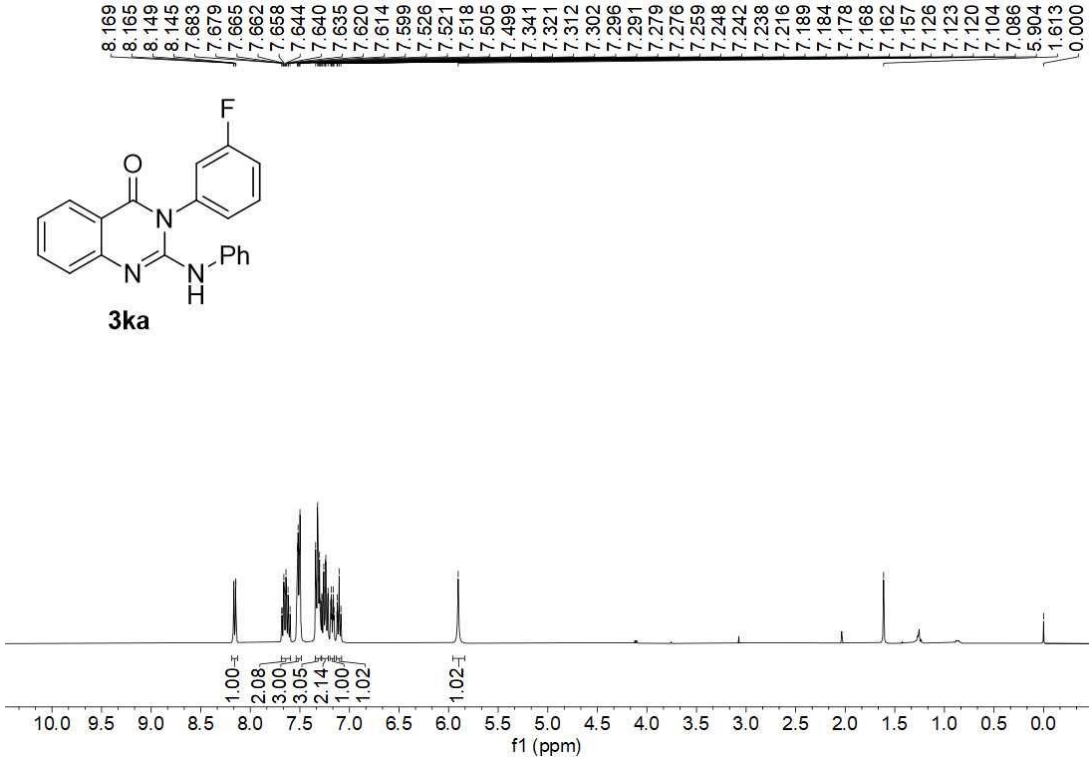
^{13}C{^{1}H} NMR spectrum (100 MHz, $CDCl_3$) of **3ja**



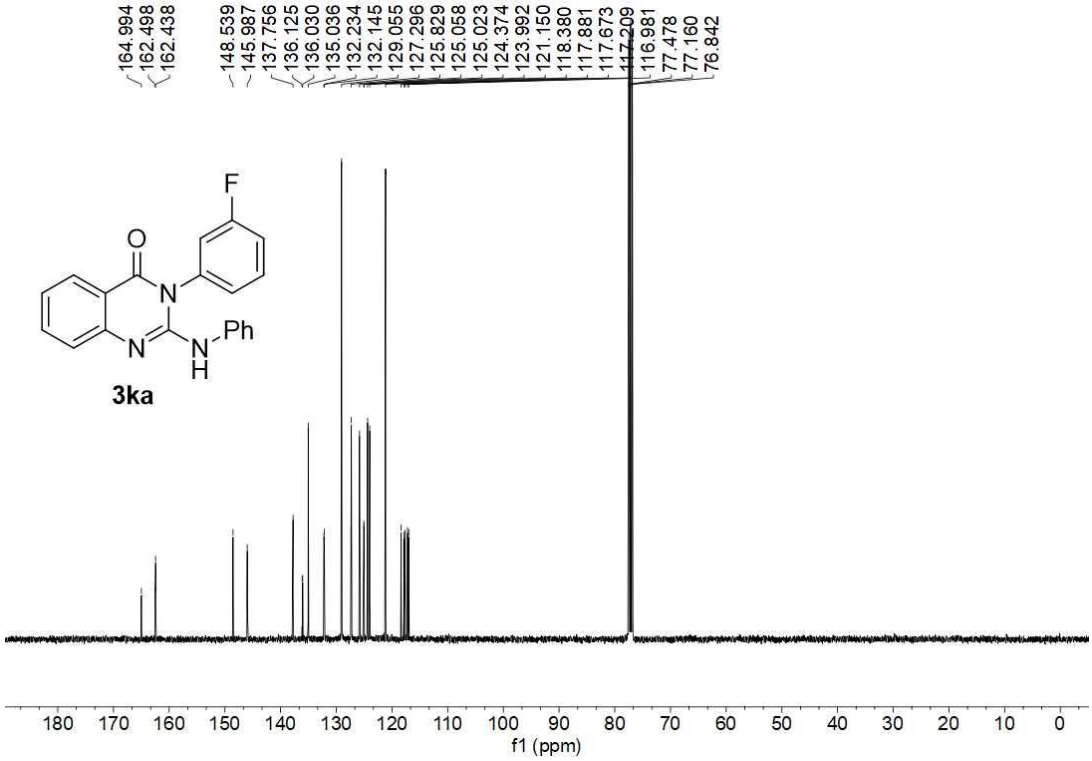
^{19}F NMR spectrum (377 MHz, $CDCl_3$) of **3ja**



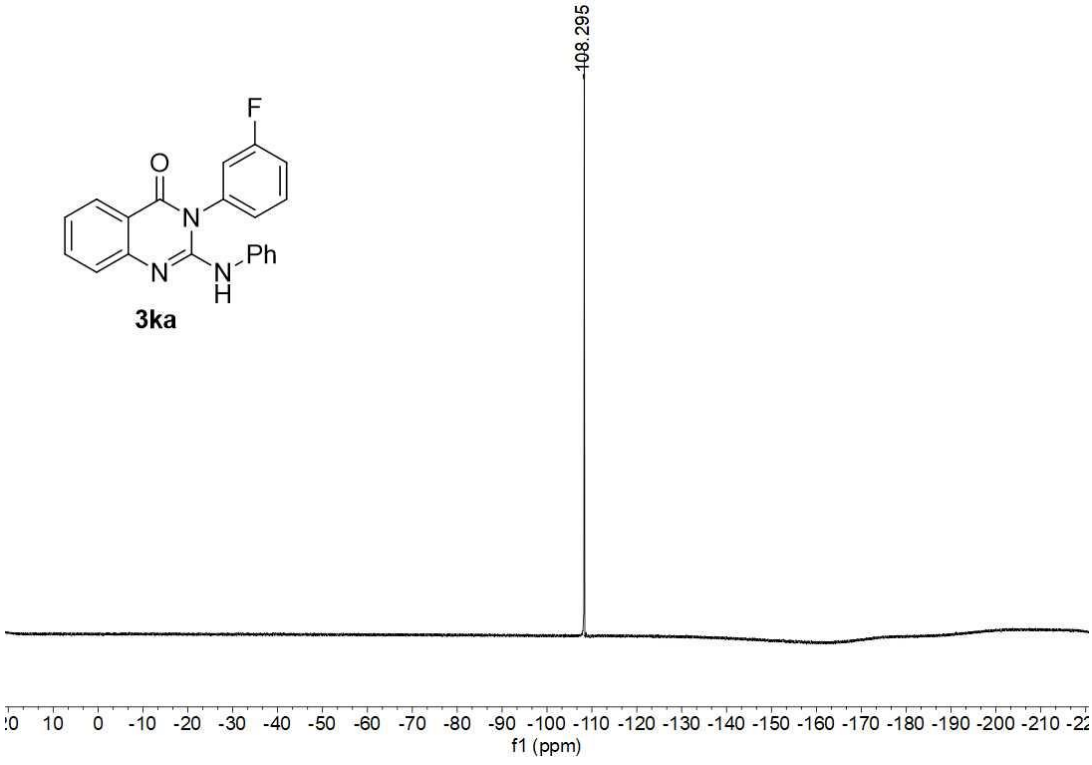
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3ka**



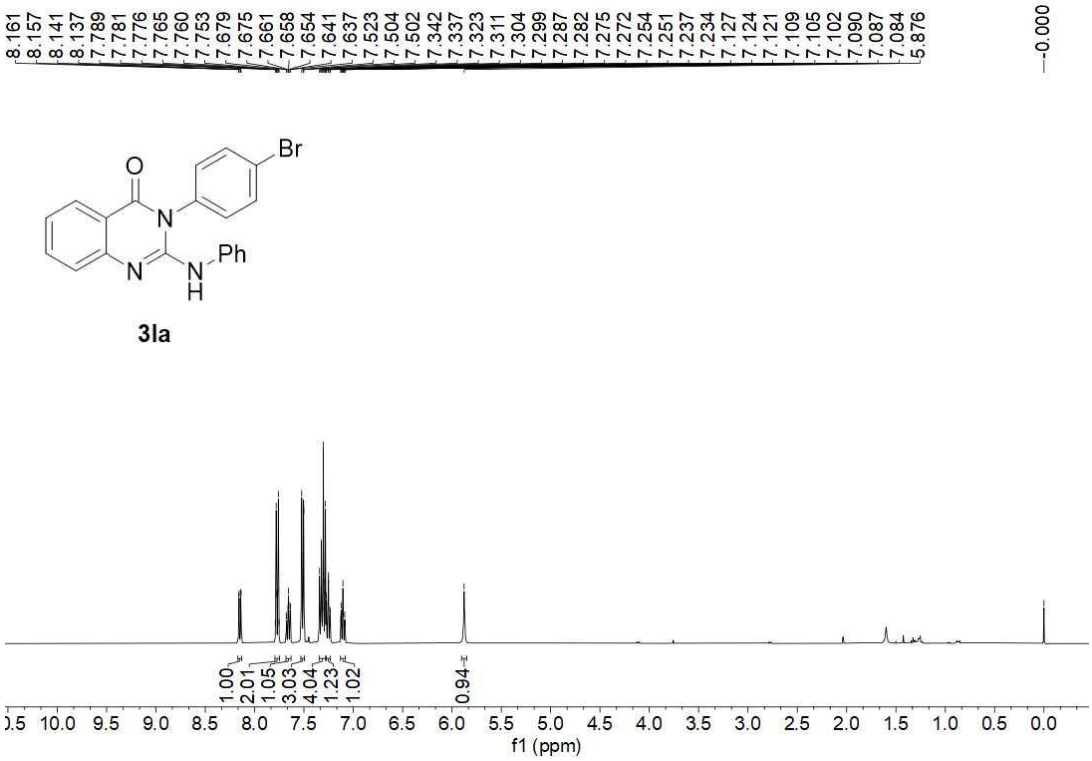
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of **3ka**



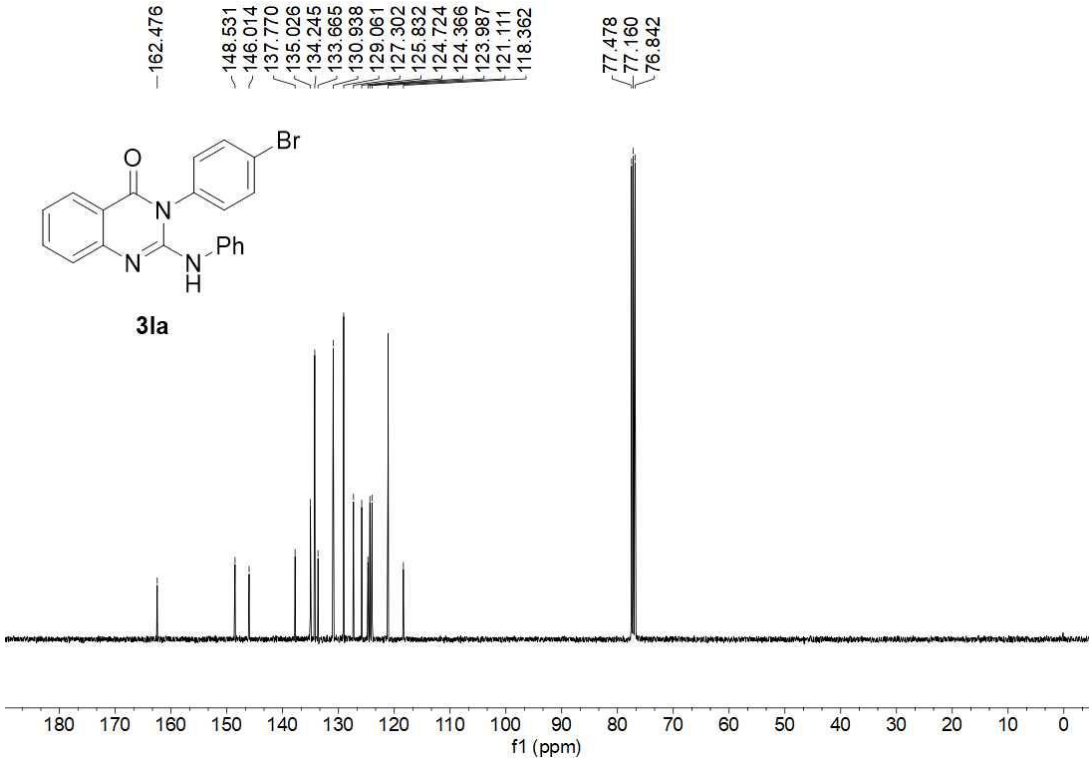
^{19}F NMR spectrum (377 MHz, $CDCl_3$) of **3ka**



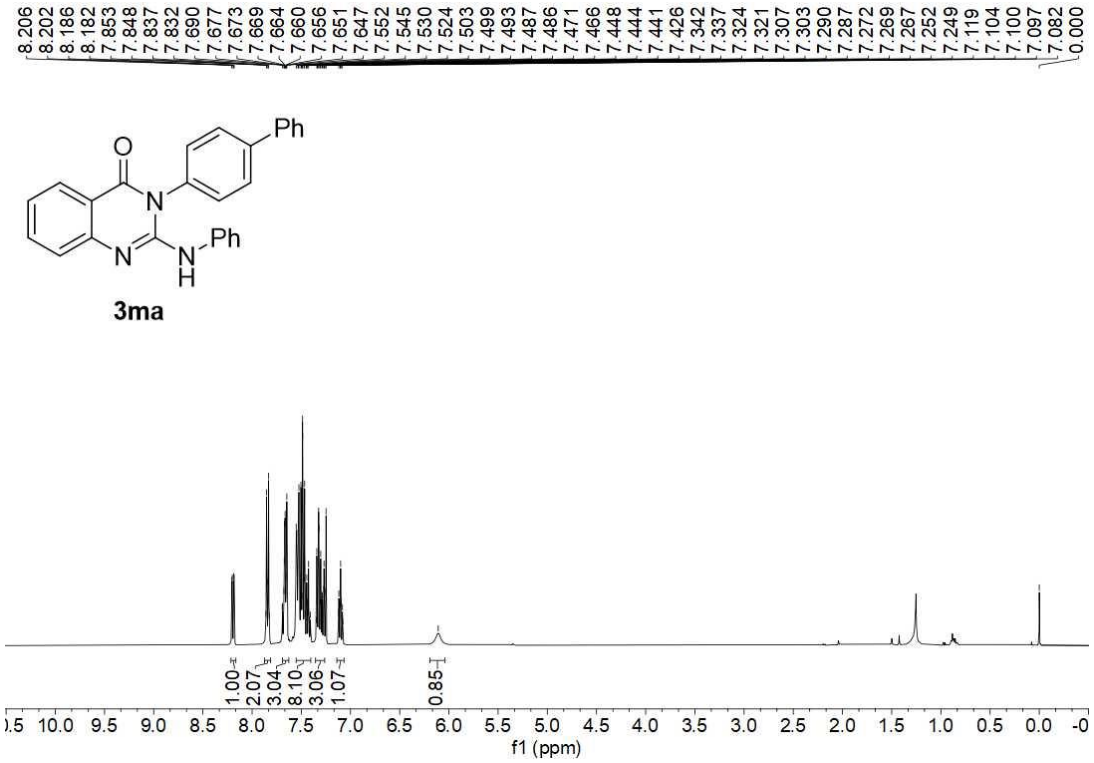
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3la**



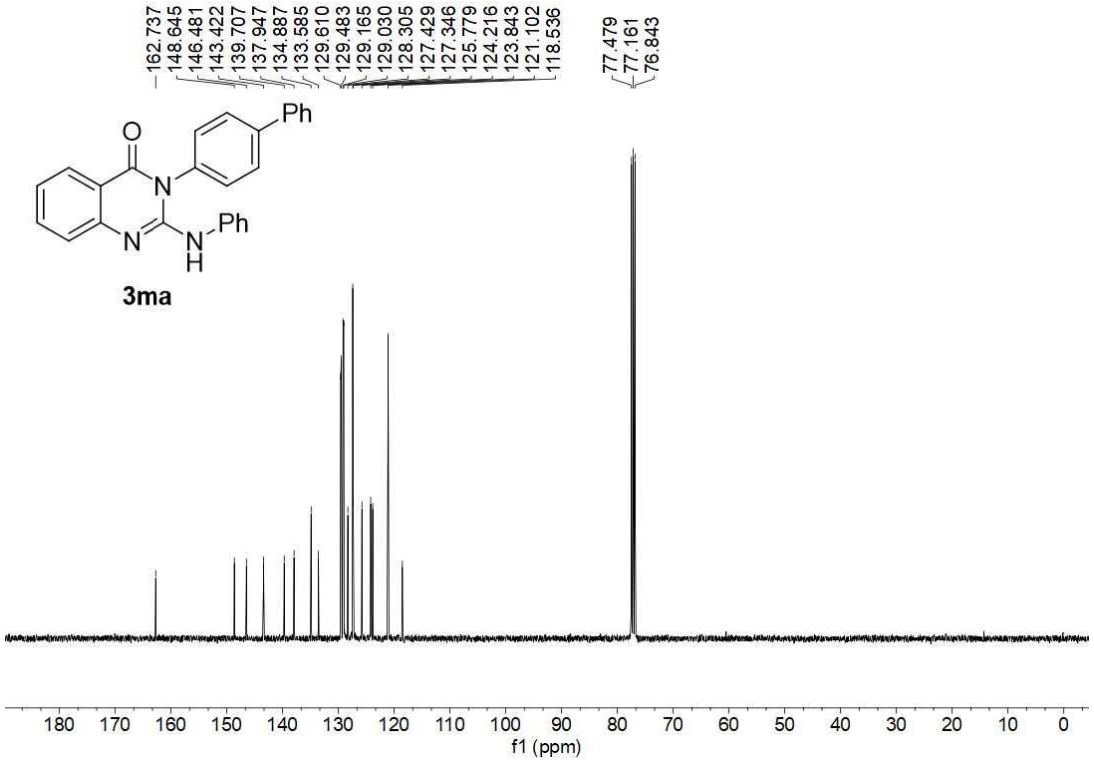
^{13}C{^{1}H} NMR spectrum (100 MHz, $CDCl_3$) of **3la**



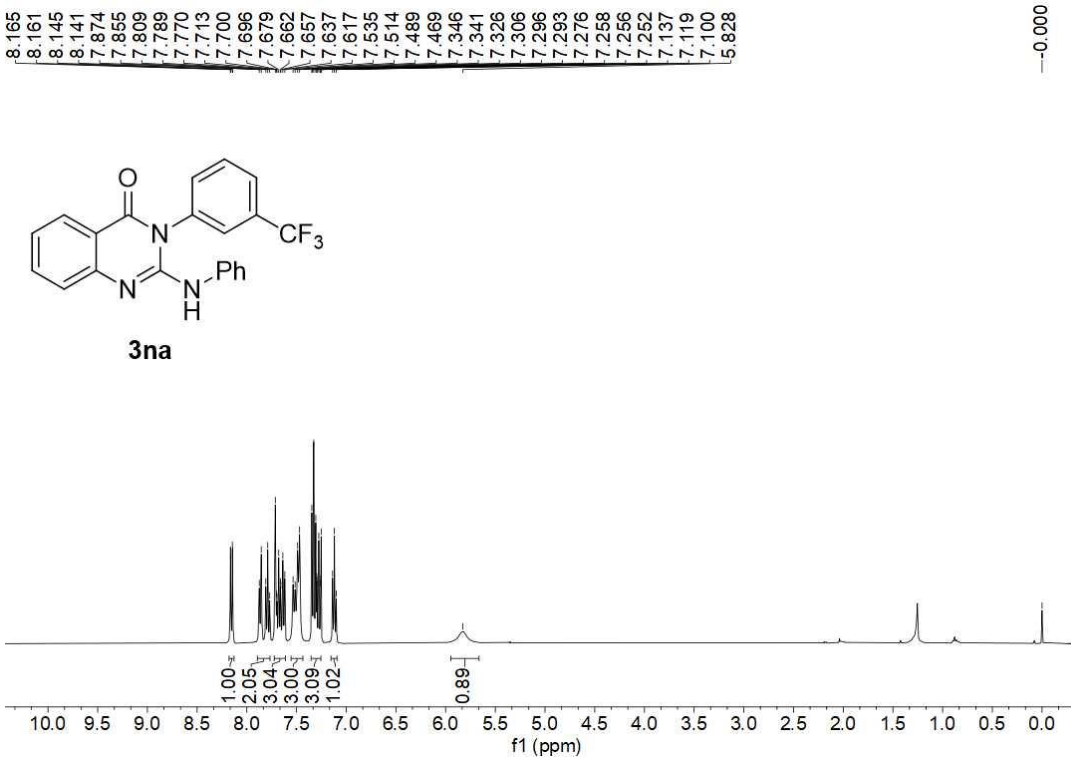
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3ma**



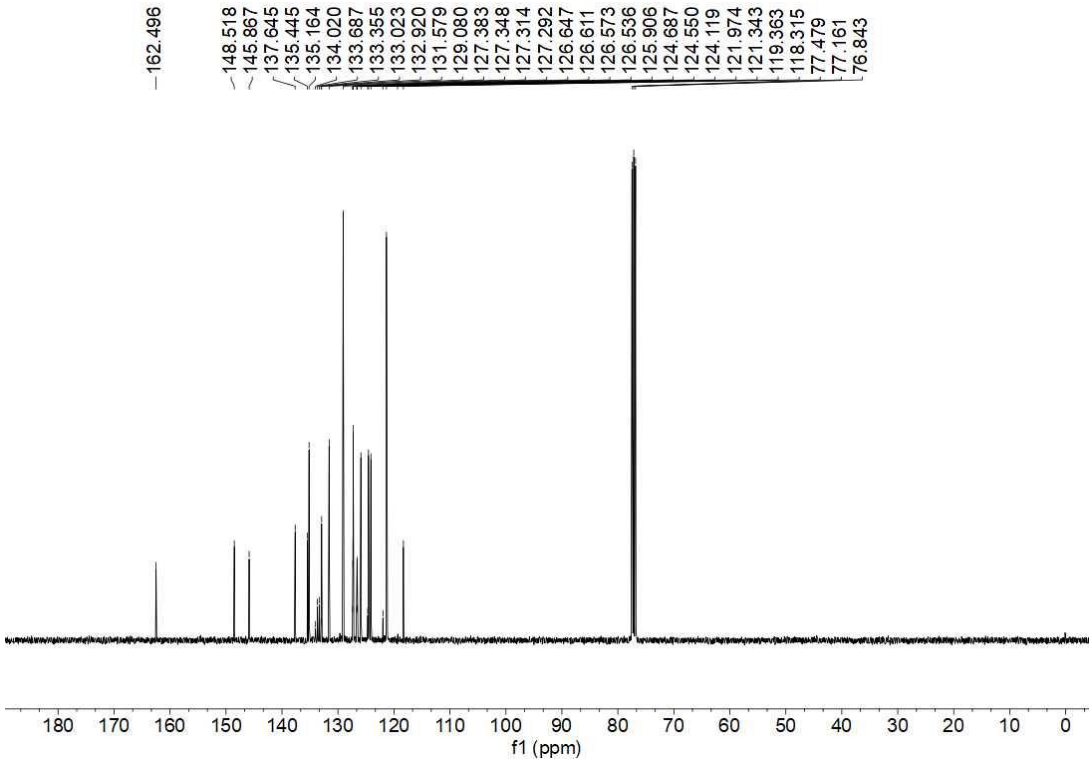
^{13}C{^{1}H} NMR spectrum (100 MHz, $CDCl_3$) of **3ma**



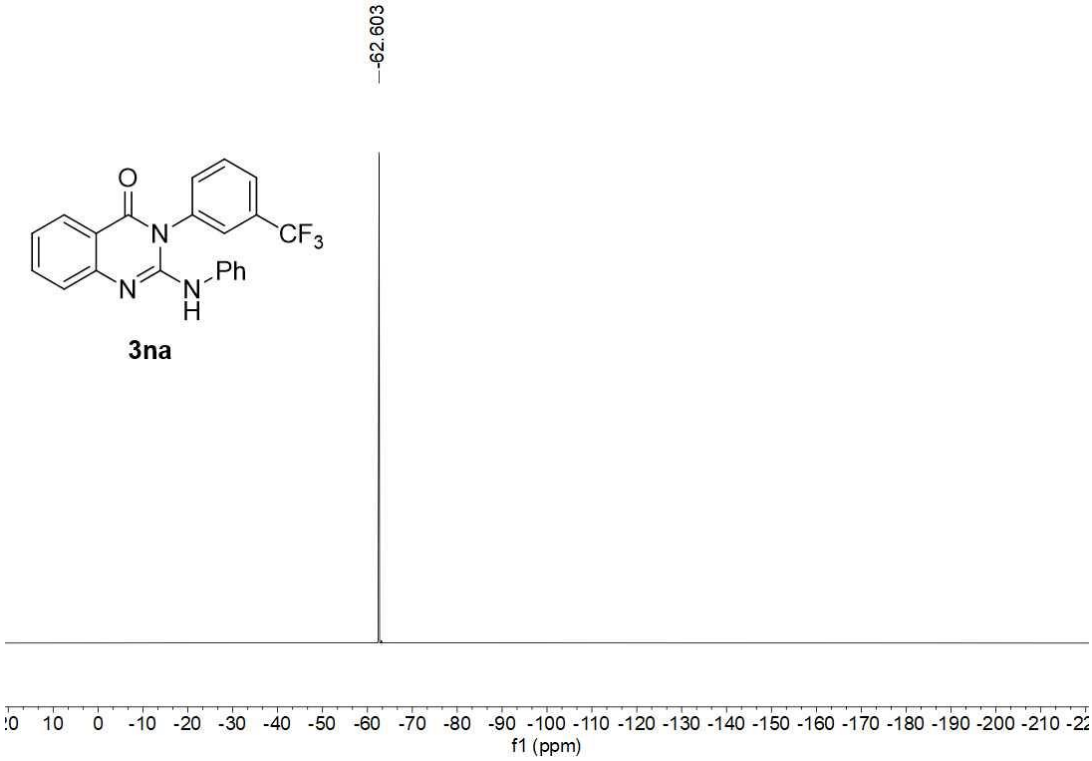
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3na**



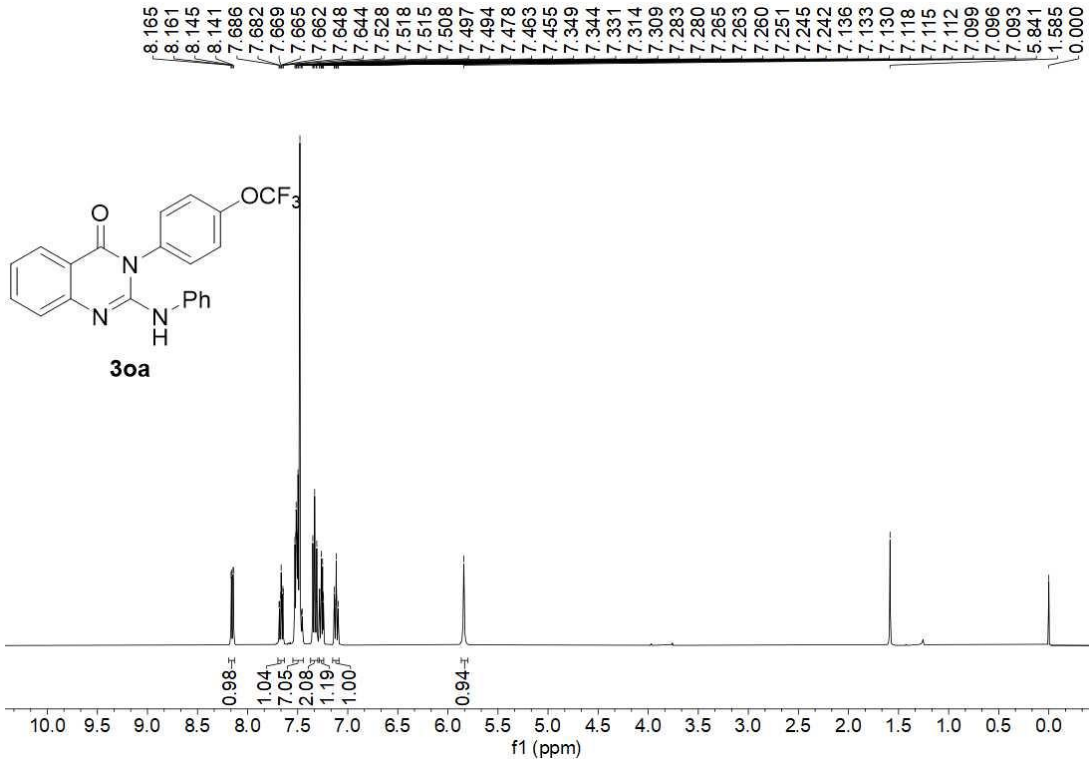
^{13}C{^{1}H} NMR spectrum (100 MHz, $CDCl_3$) of **3na**



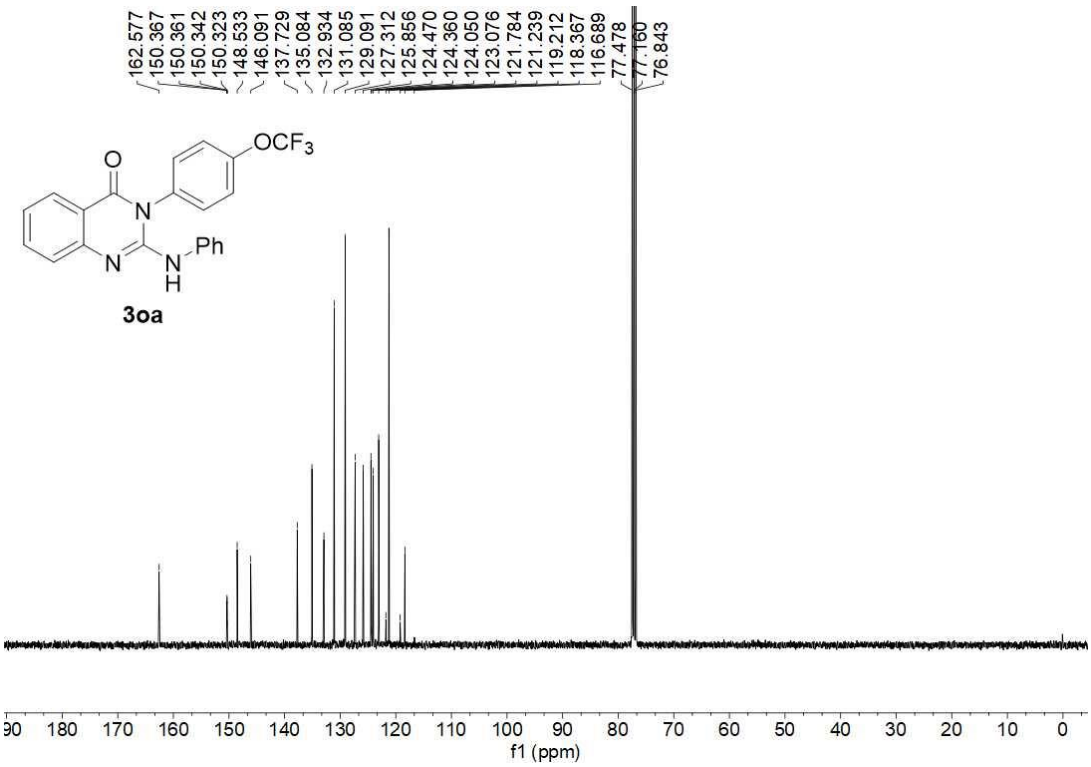
^{19}F NMR spectrum (377 MHz, $CDCl_3$) of **3na**



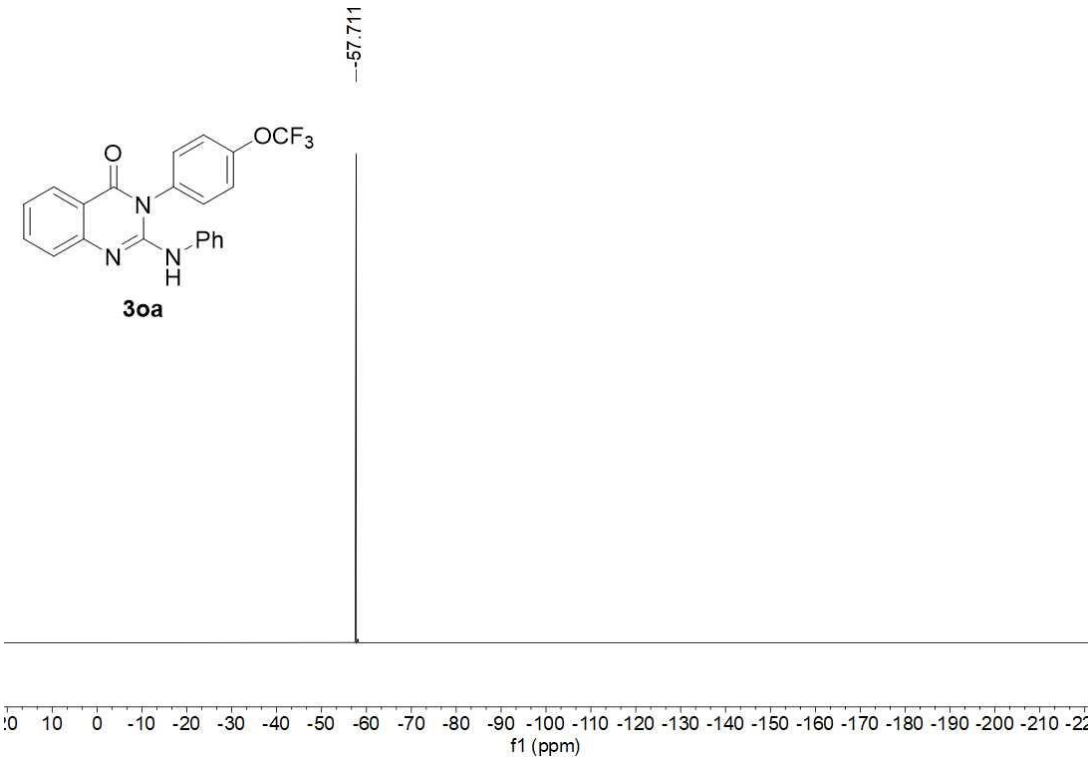
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3oa**



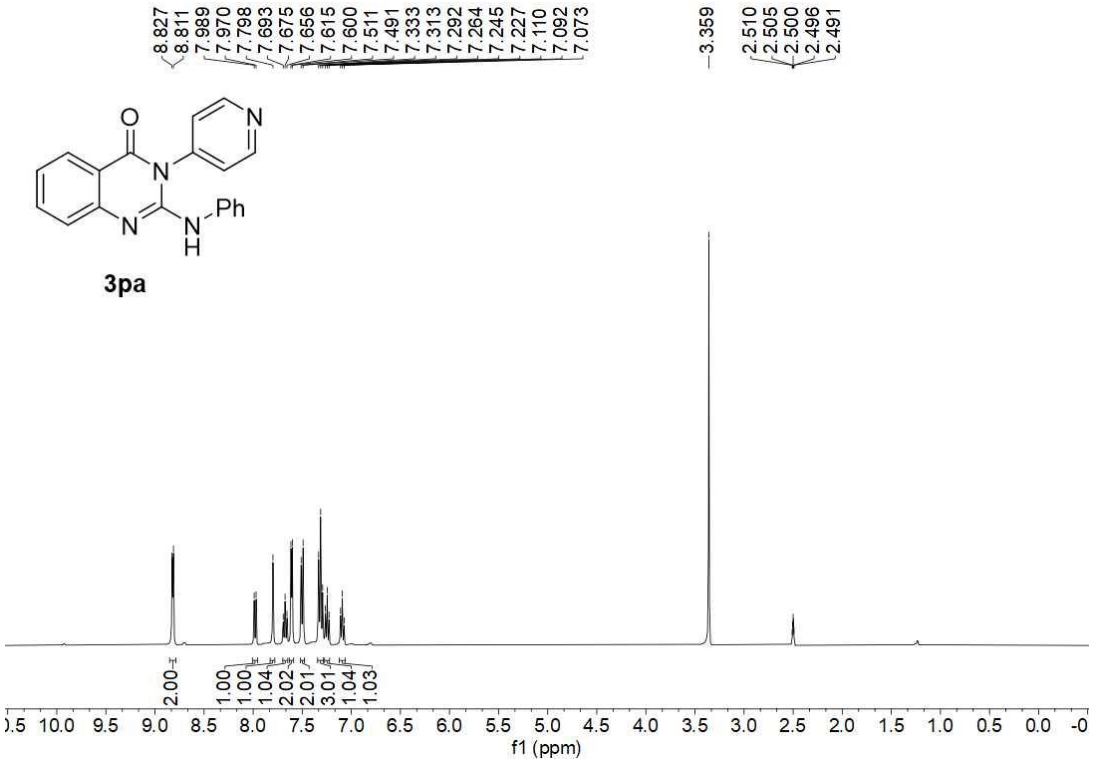
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of **3oa**



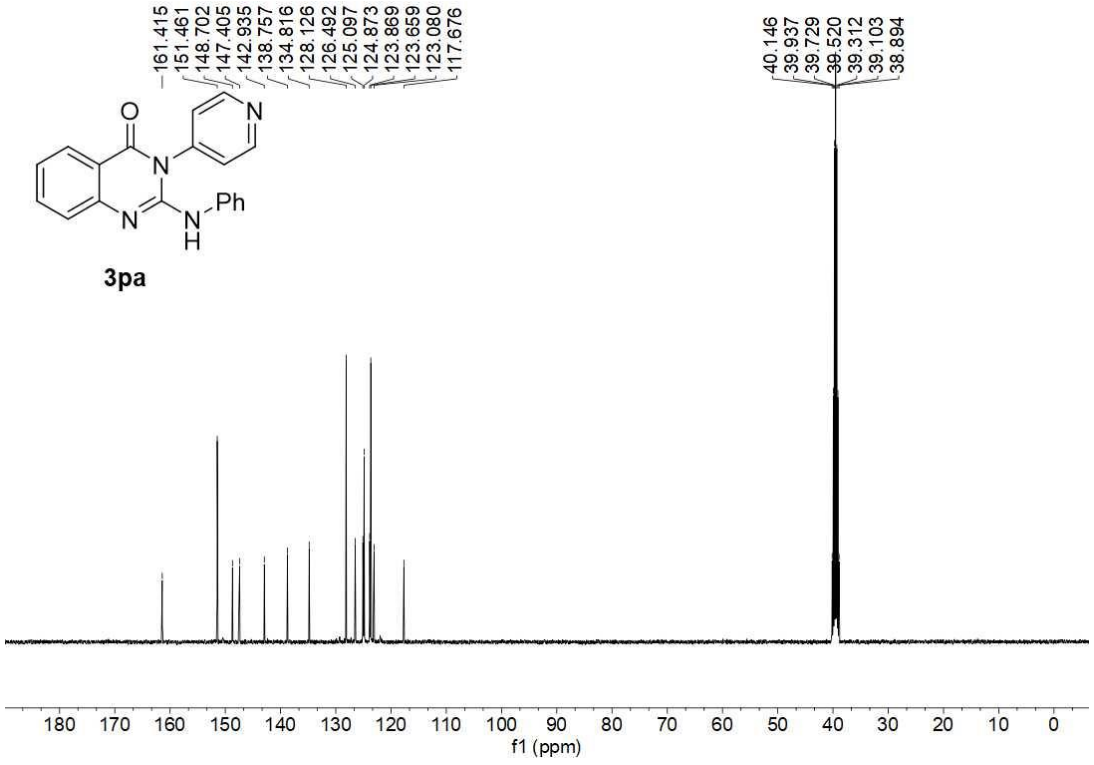
^{19}F NMR spectrum (377 MHz, $CDCl_3$) of **3oa**



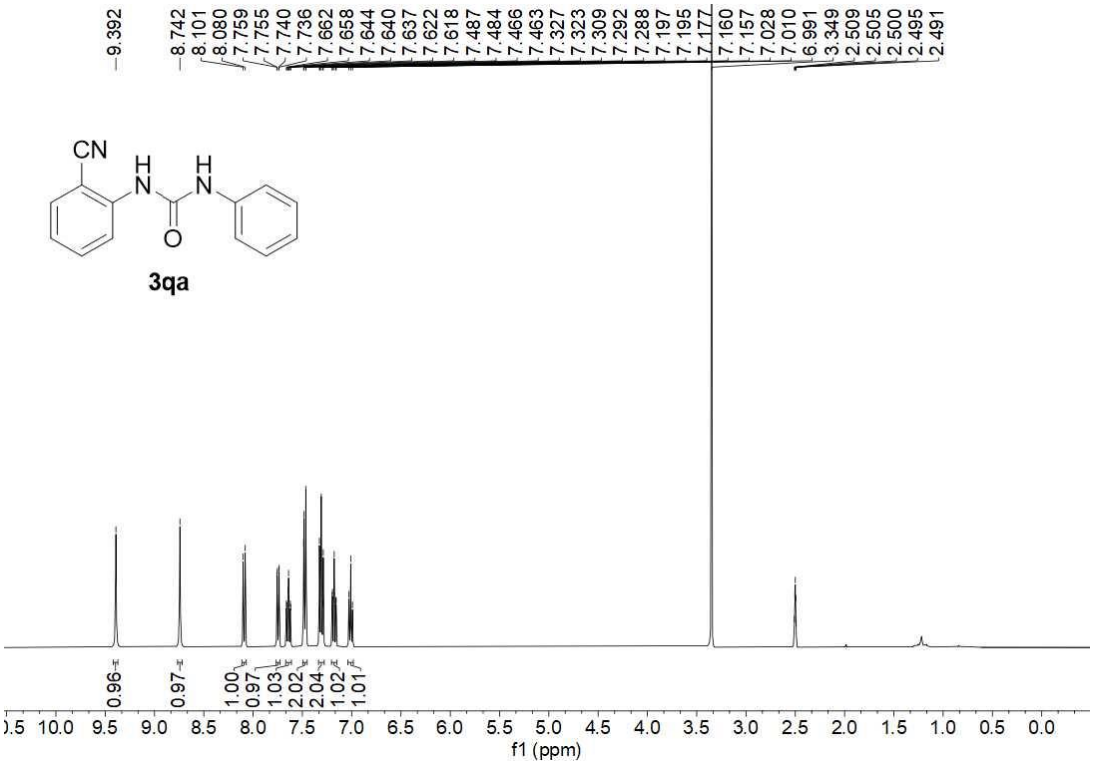
^{1}H NMR spectrum (400 MHz, DMSO-d_6) of **3pa**



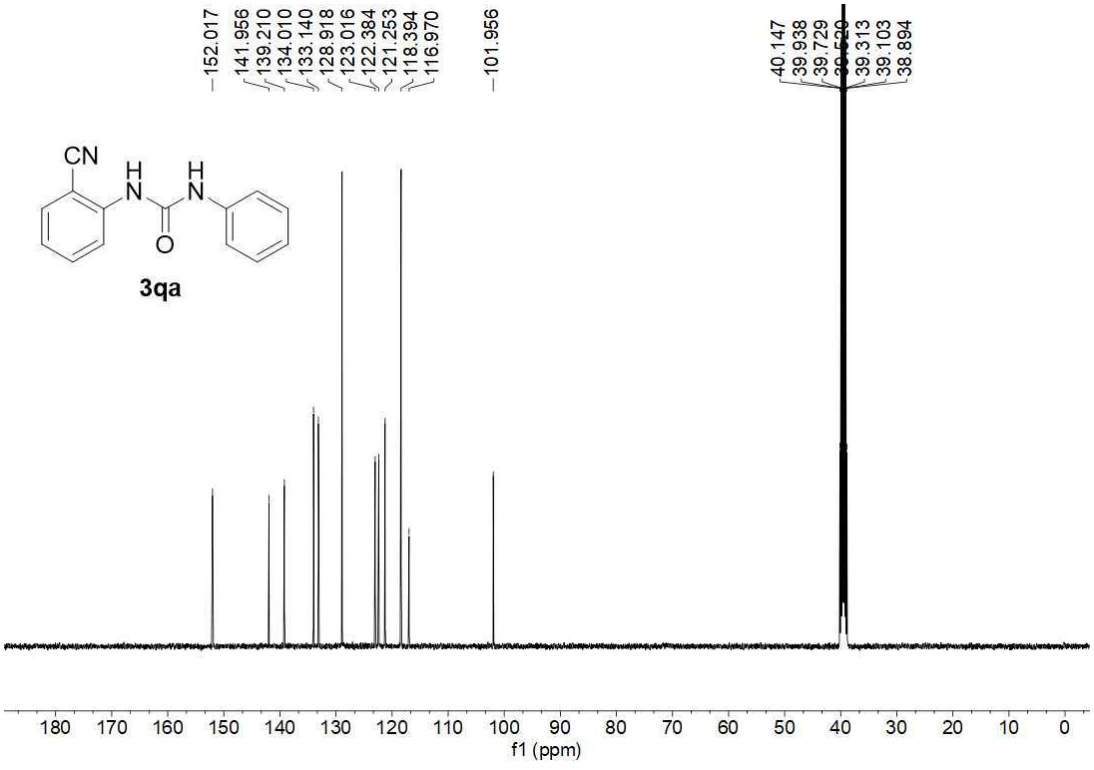
^{13}C{^{1}H} NMR spectrum (100 MHz, DMSO-d_6) of **3pa**



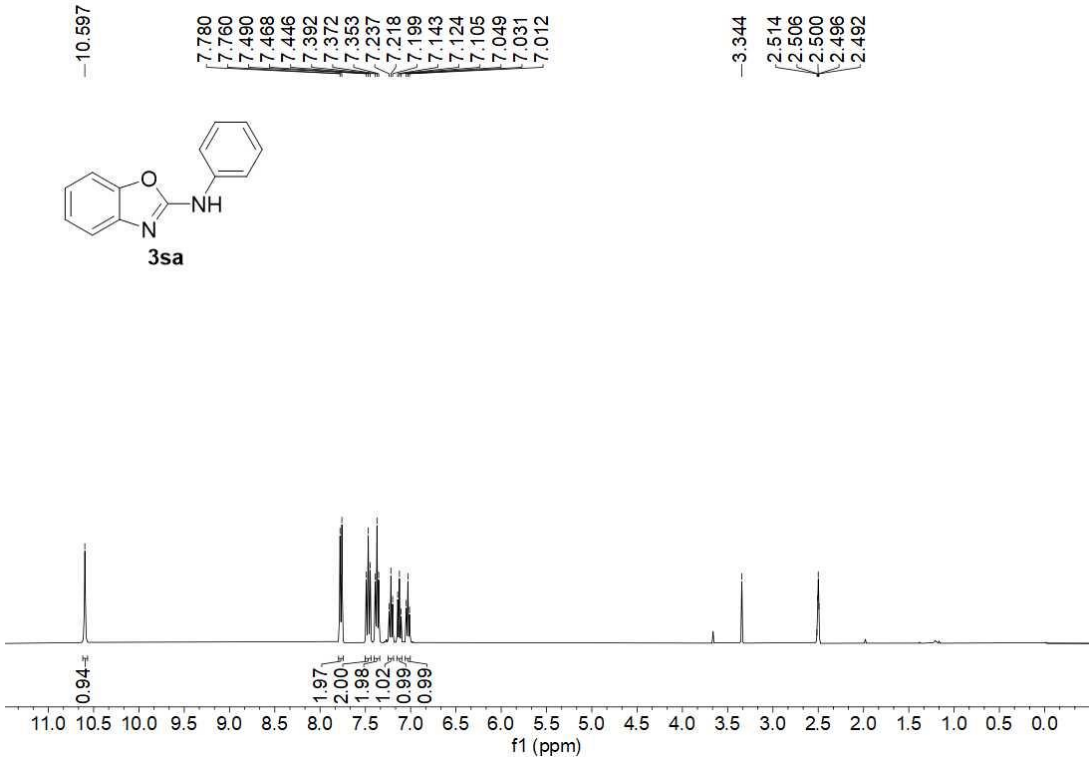
^{1}H NMR spectrum (400 MHz, DMSO-d_6) of **3qa**



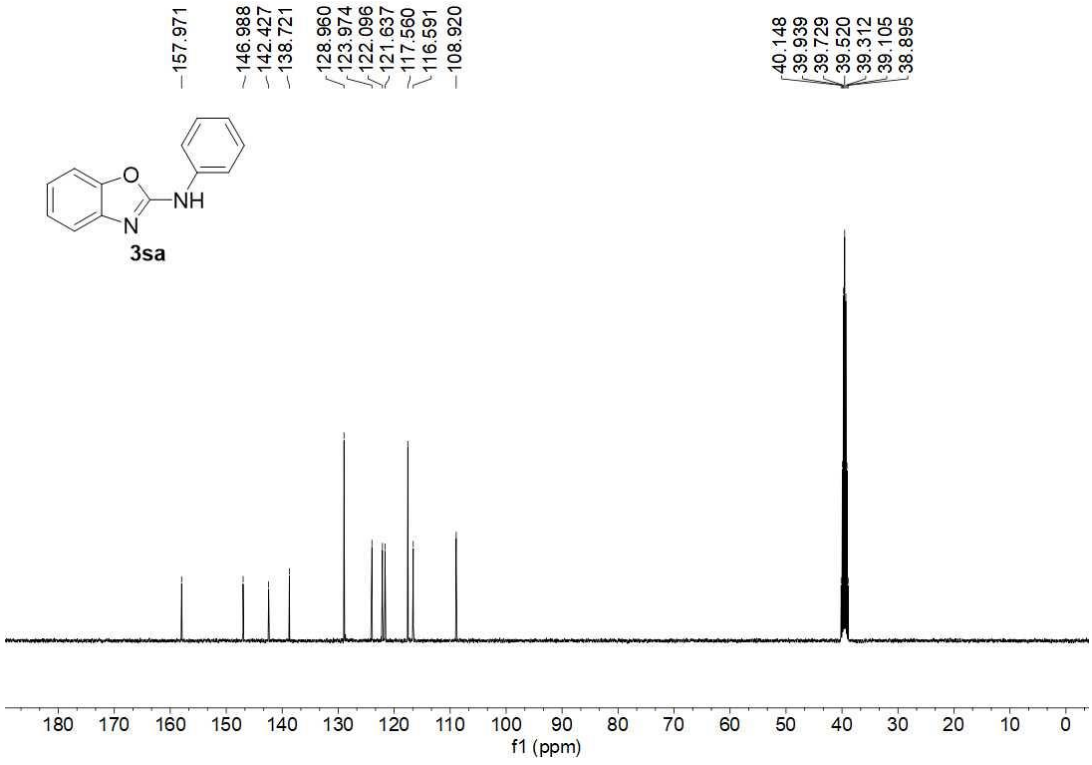
^{13}C{^{1}H} NMR spectrum (100 MHz, DMSO-d_6) of **3qa**



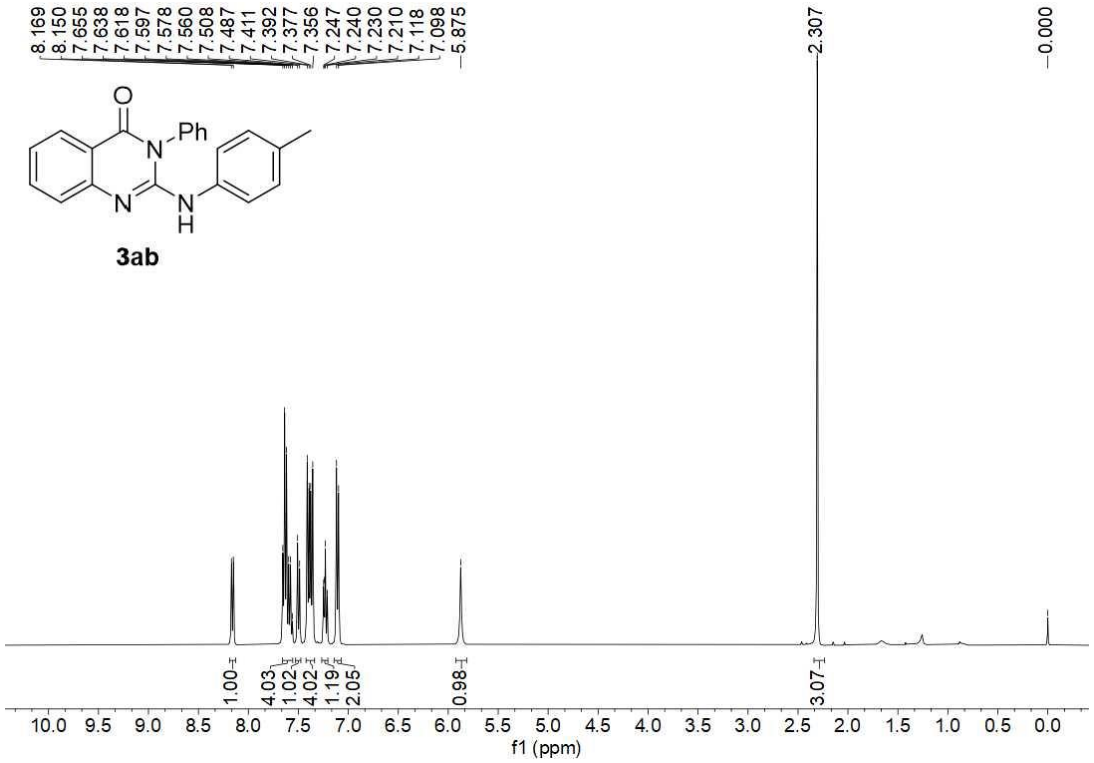
^{1}H NMR spectrum (400 MHz, DMSO-d_6) of **3sa**



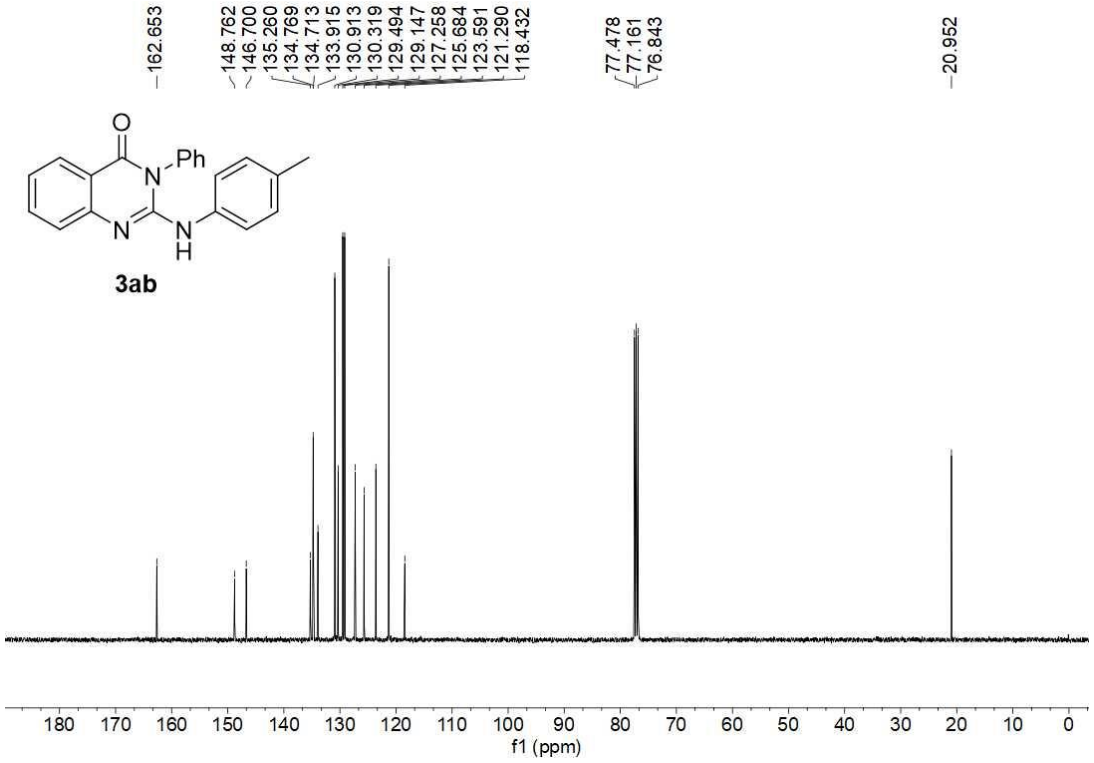
^{13}C{^{1}H} NMR spectrum (100 MHz, DMSO-d_6) of **3sa**



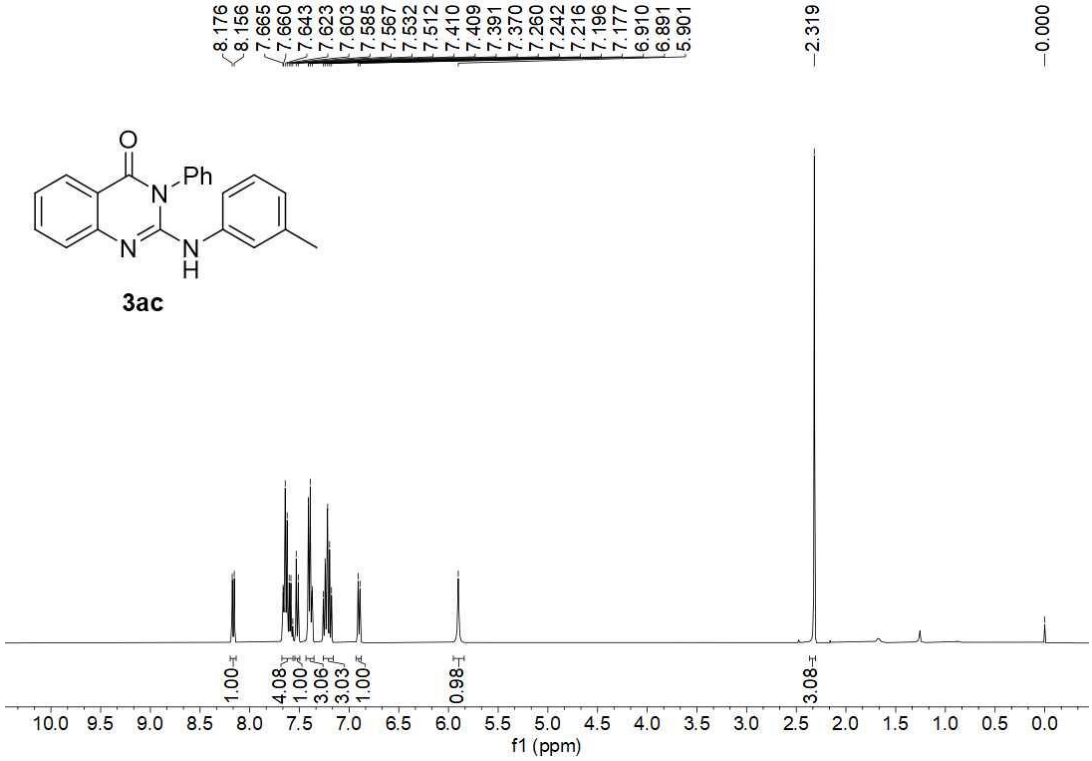
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3ab**



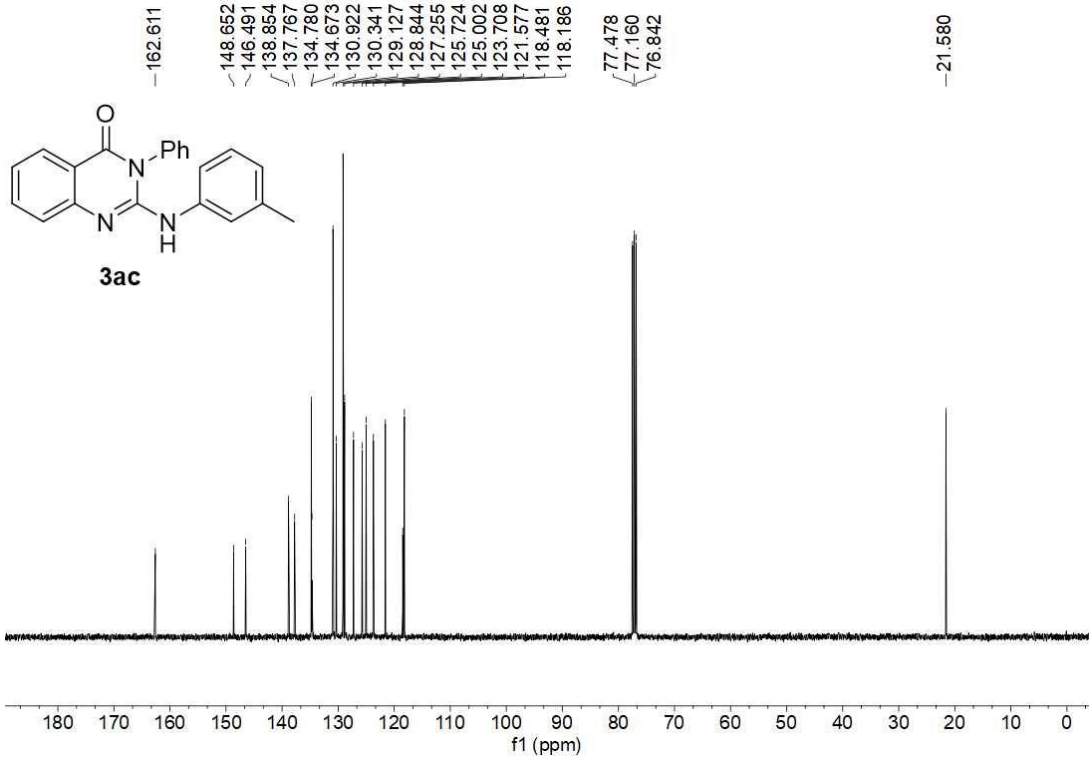
^{13}C{^{1}H} NMR spectrum (100 MHz, $CDCl_3$) of **3ab**



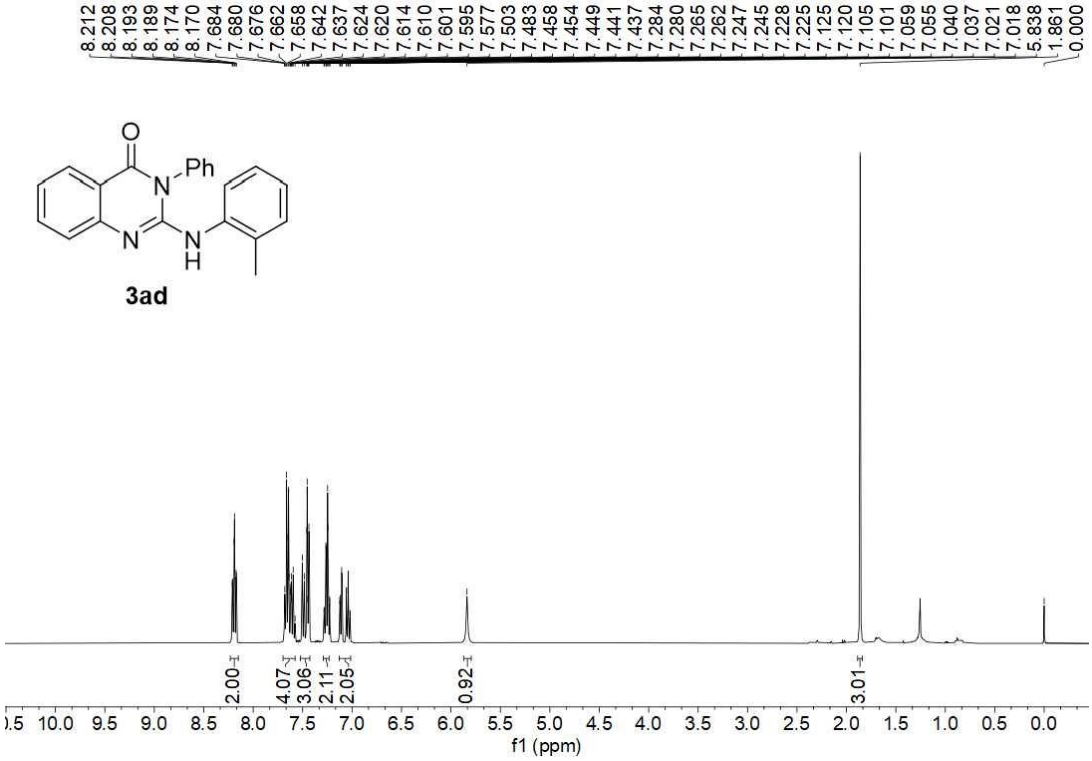
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3ac**



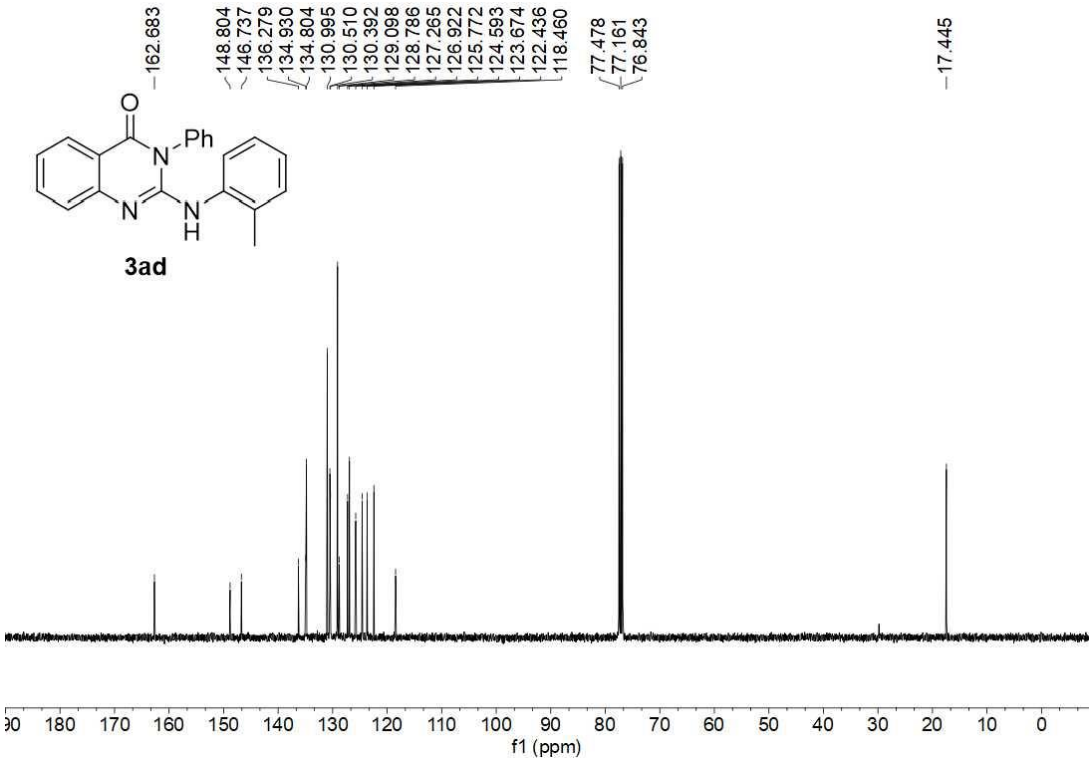
^{13}C{^{1}H} NMR spectrum (100 MHz, $CDCl_3$) of **3ac**



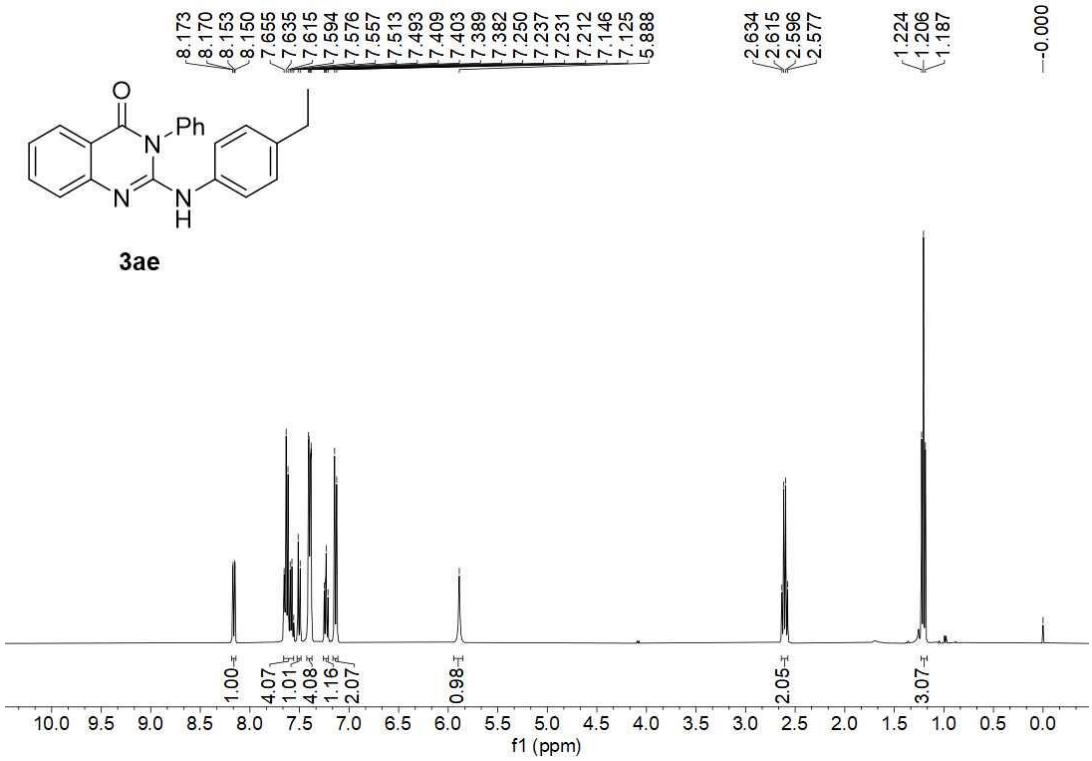
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3ad**



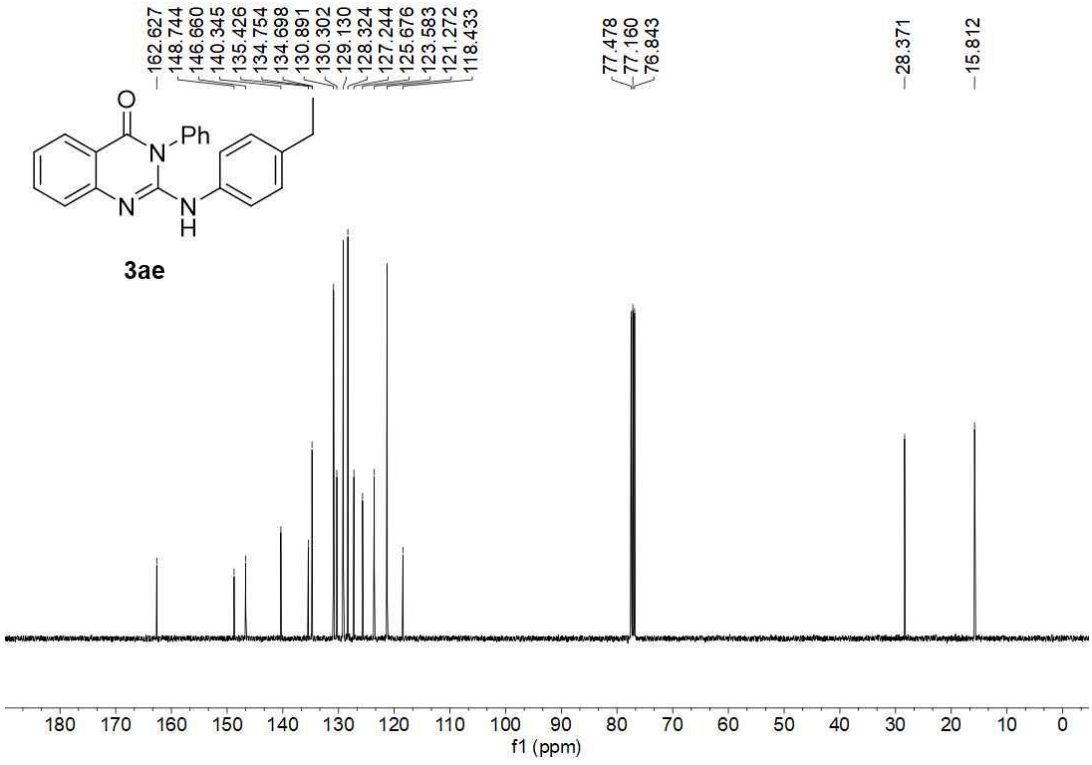
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of **3ad**



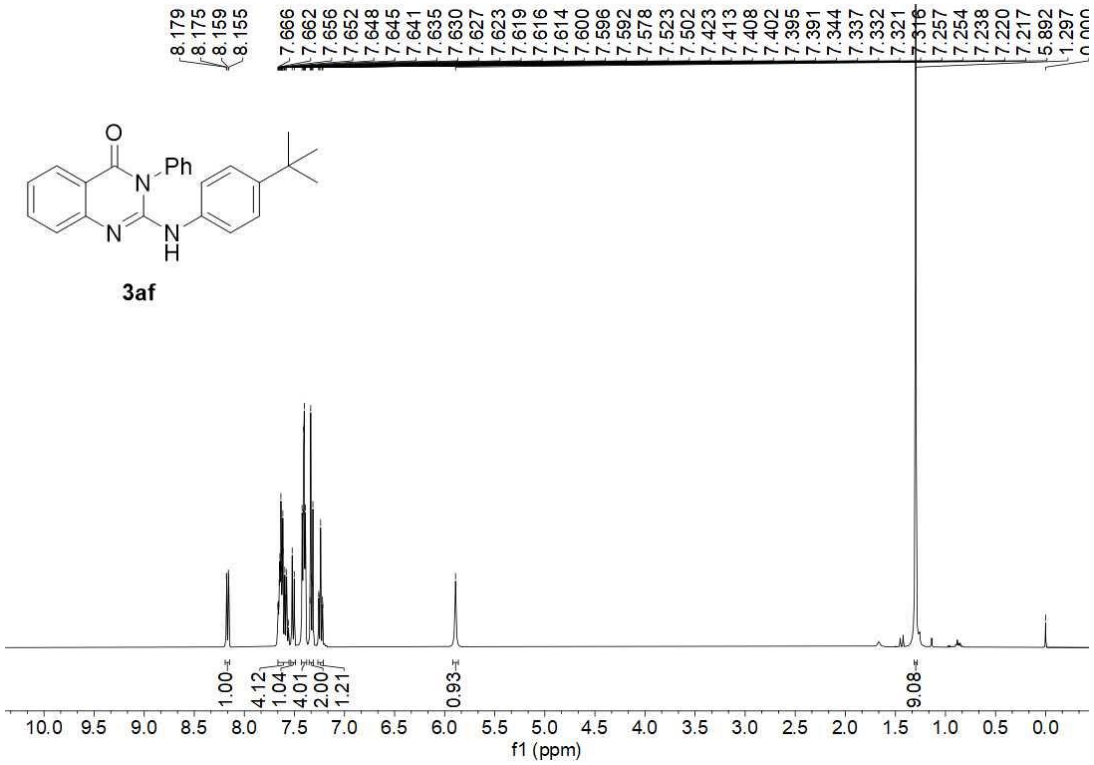
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3ae**



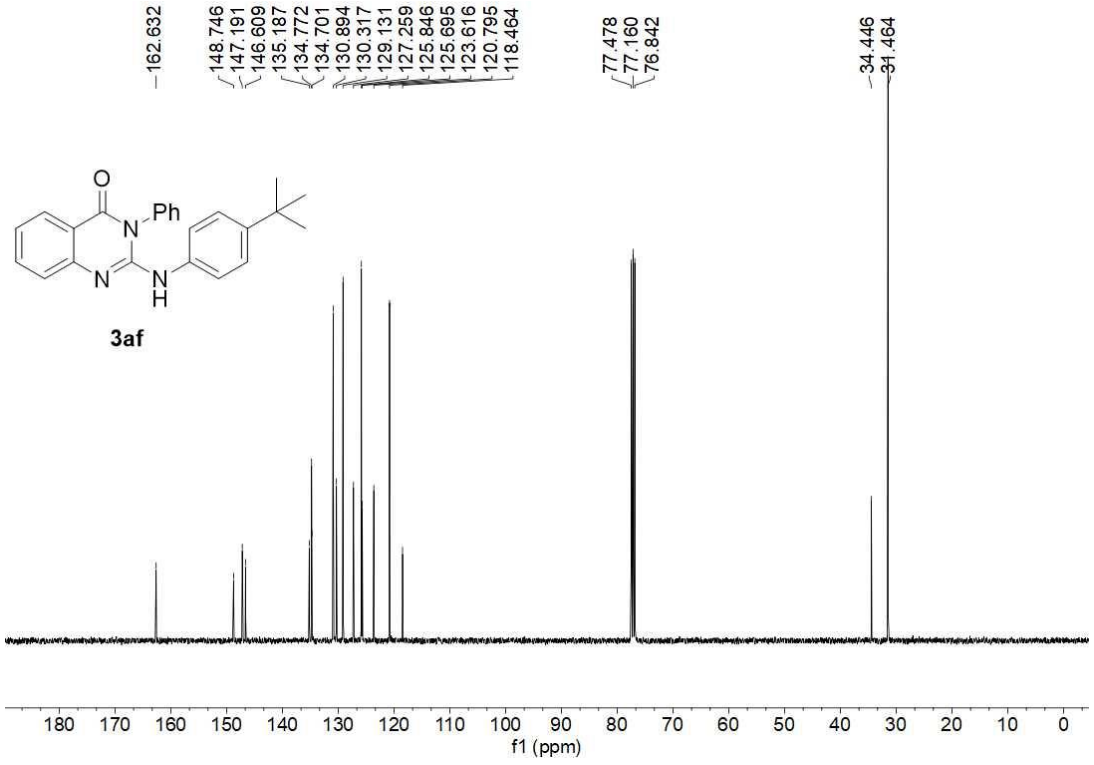
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of **3ae**



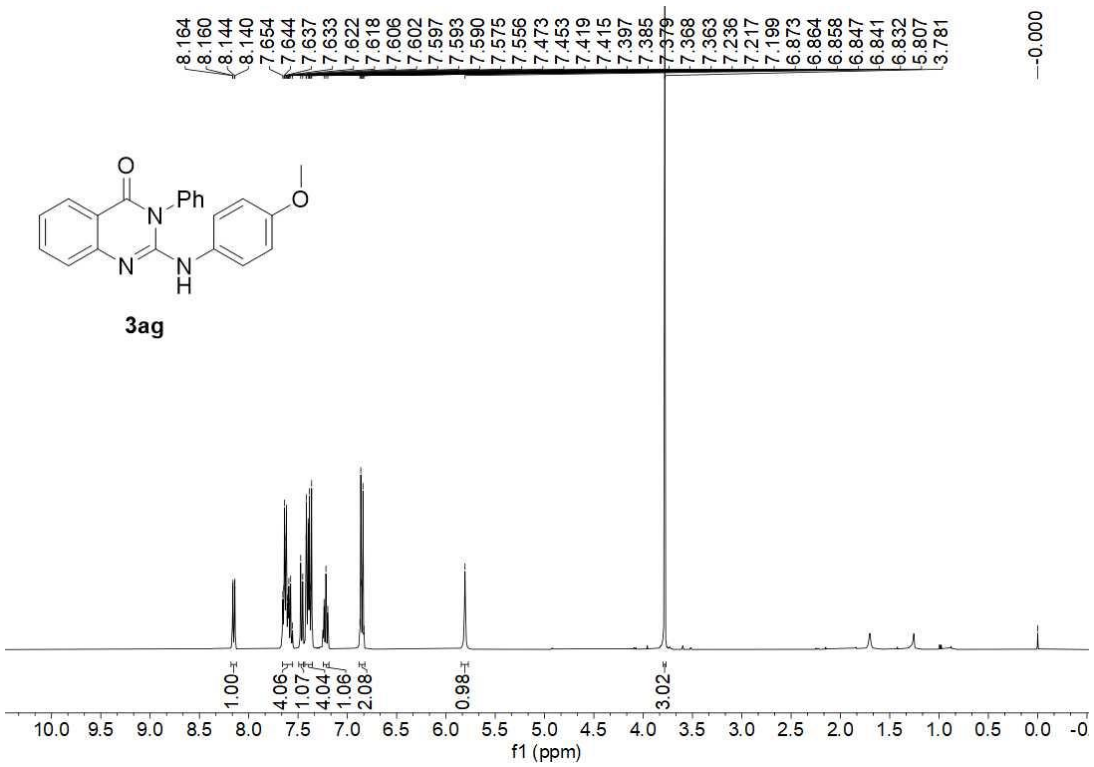
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3af**



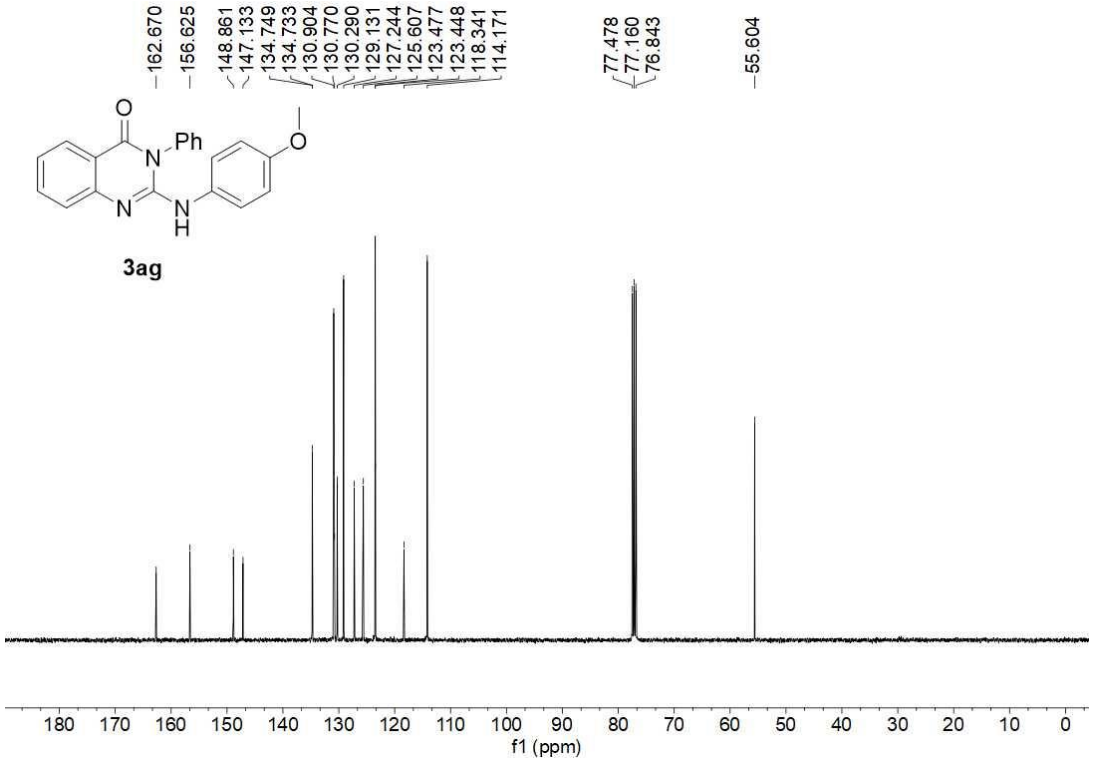
^{13}C{^{1}H} NMR spectrum (100 MHz, $CDCl_3$) of **3af**



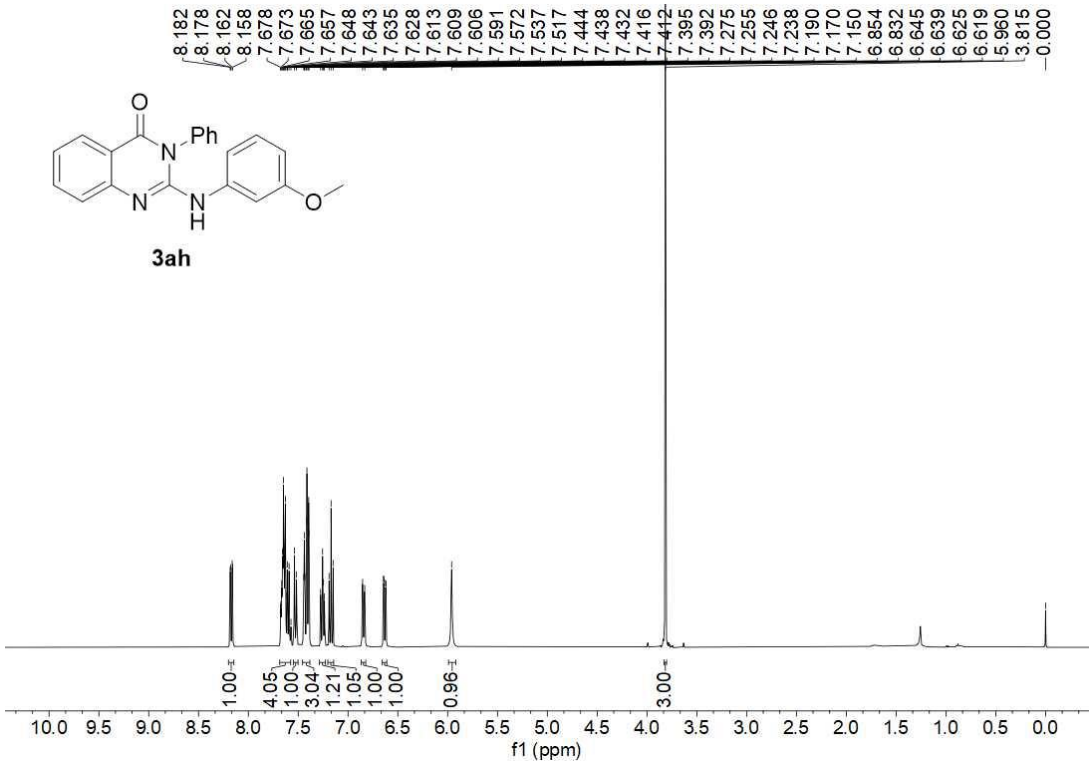
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3ag**



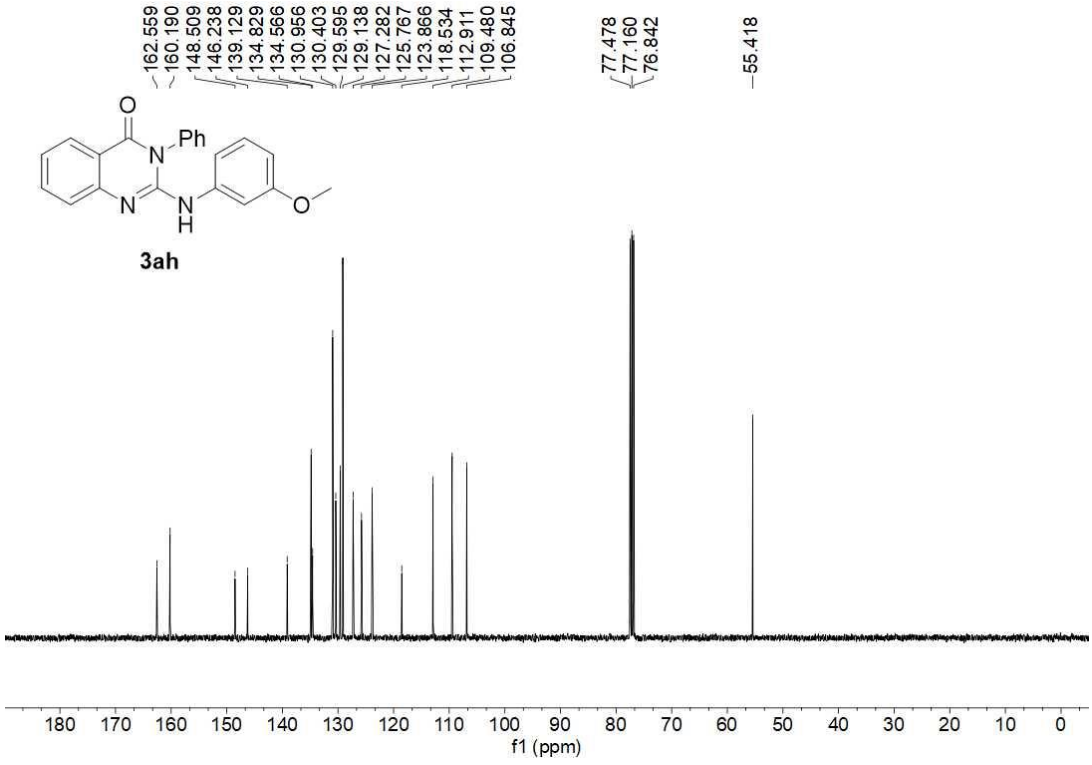
^{13}C{^{1}H} NMR spectrum (100 MHz, $CDCl_3$) of **3ag**



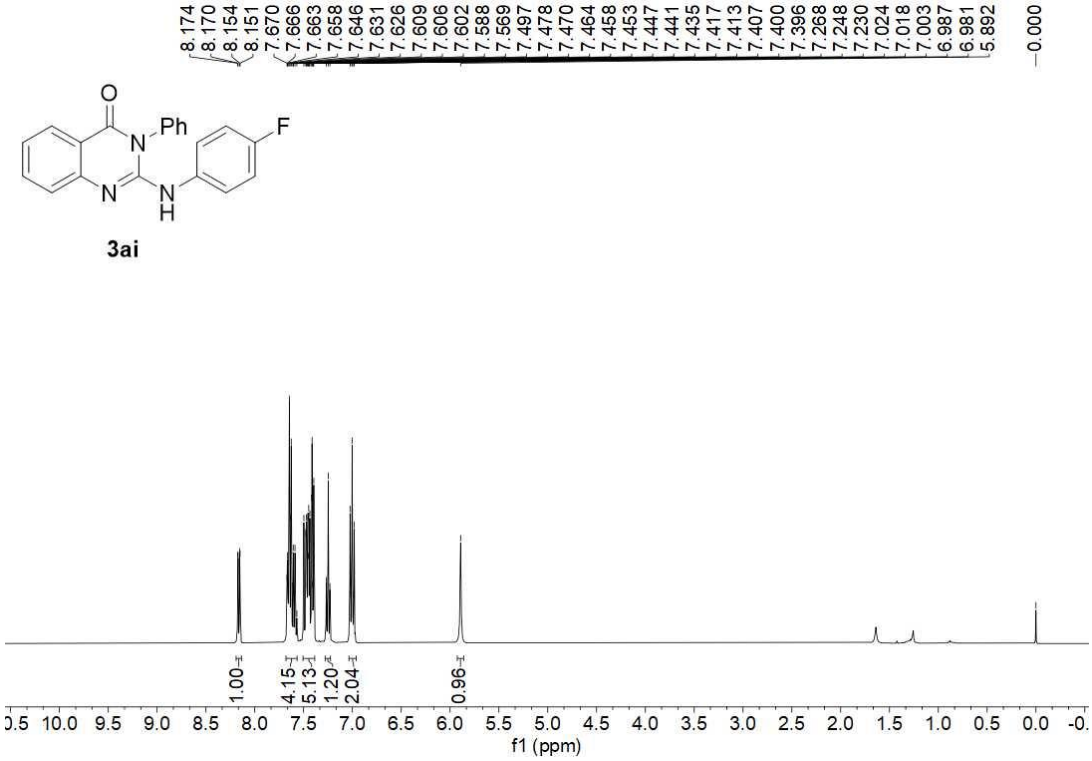
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3ah**



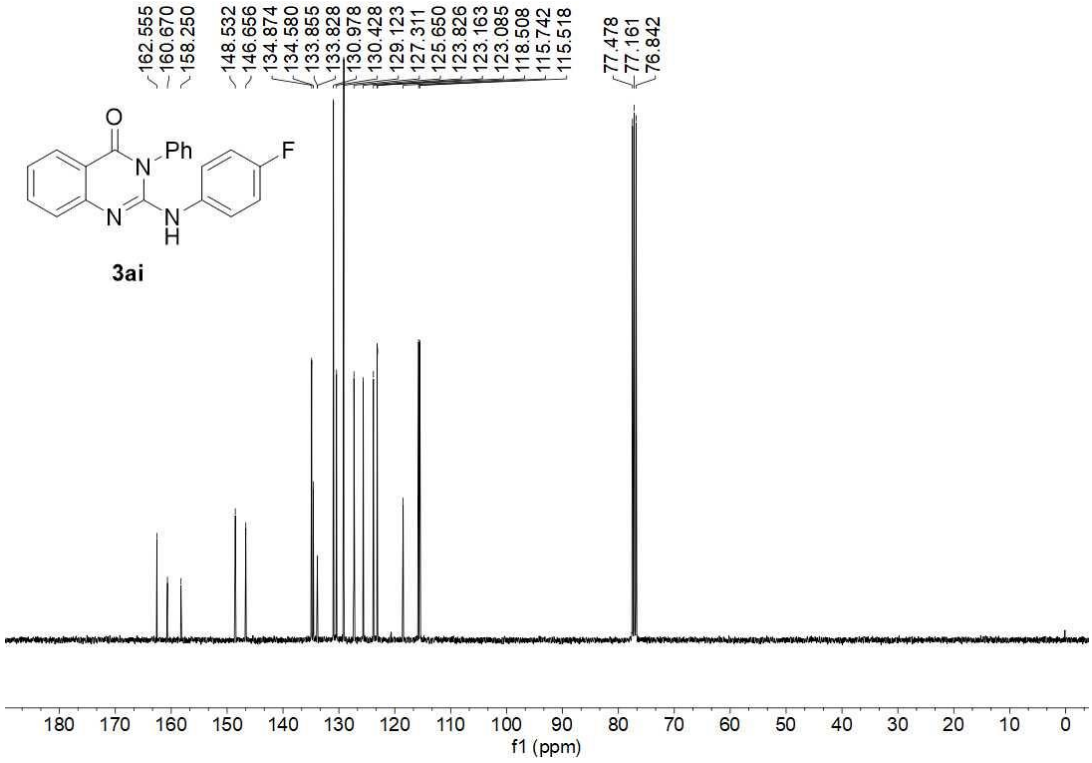
^{13}C{^{1}H} NMR spectrum (100 MHz, $CDCl_3$) of **3ah**



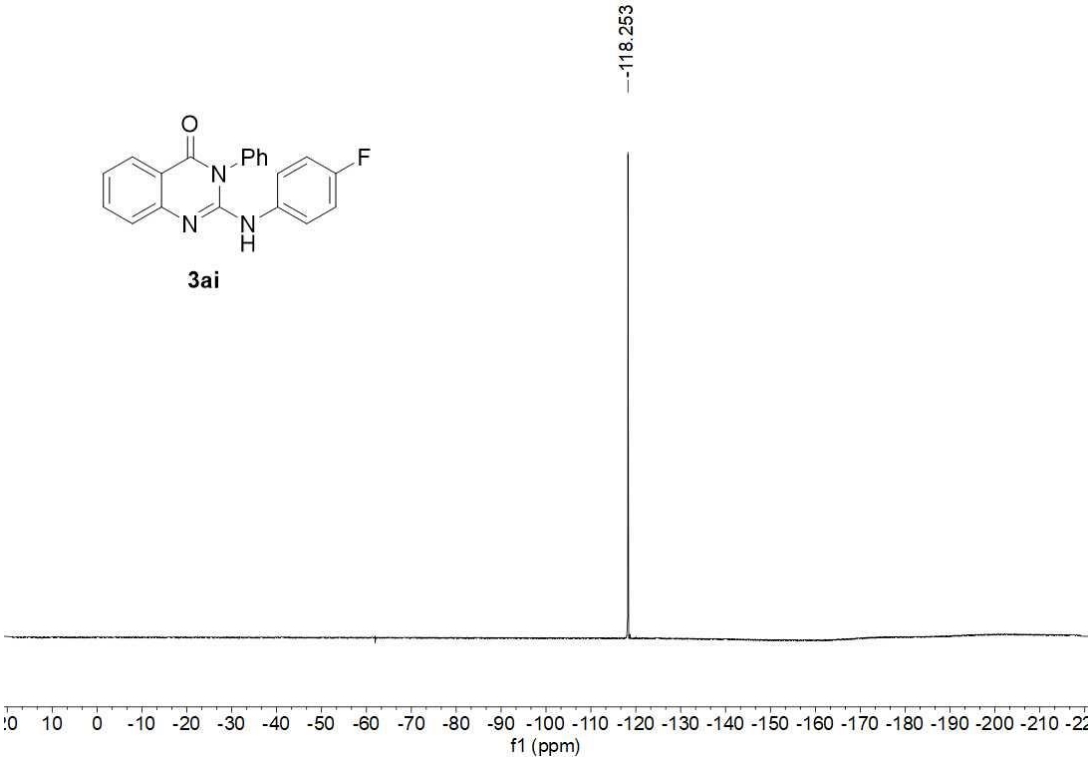
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3ai**



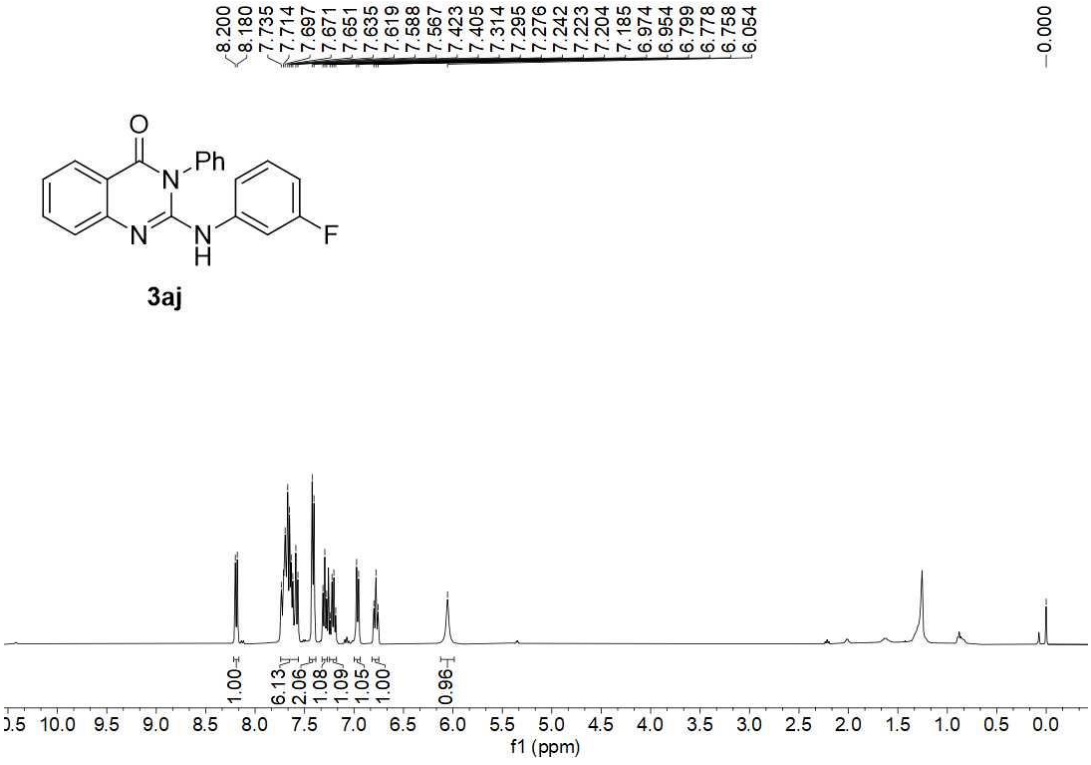
^{13}C{^{1}H} NMR spectrum (100 MHz, $CDCl_3$) of **3ai**



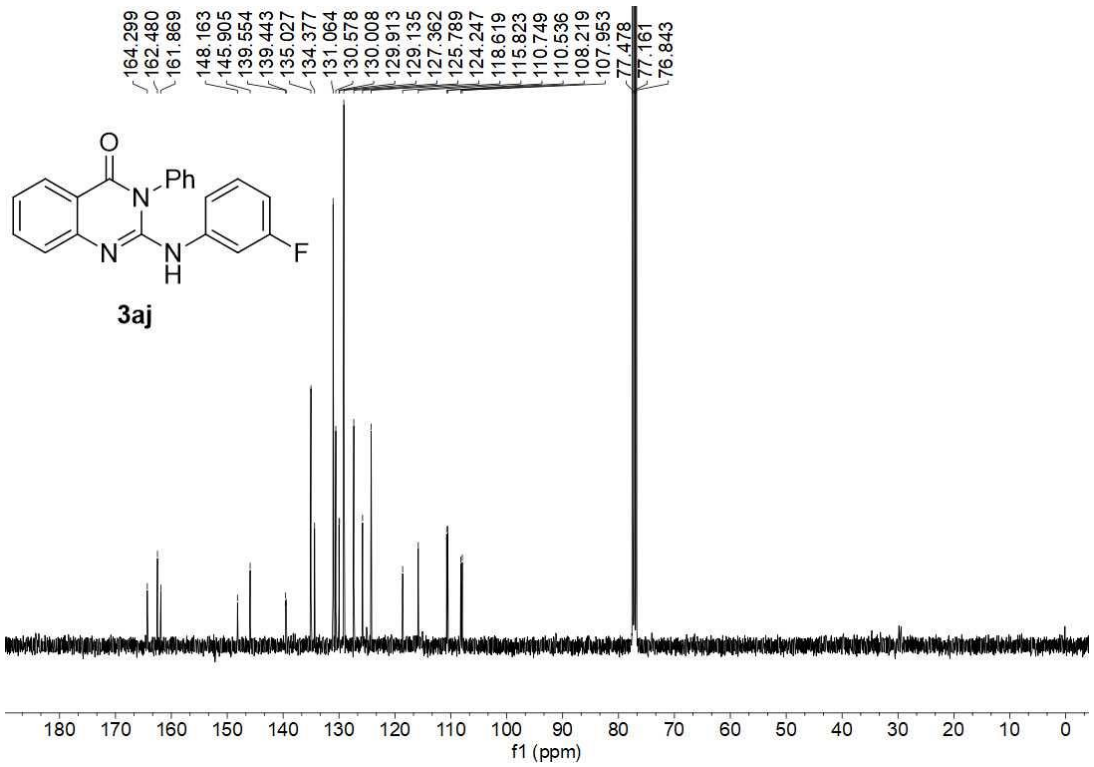
^{19}F NMR spectrum (377 MHz, $CDCl_3$) of **3ai**



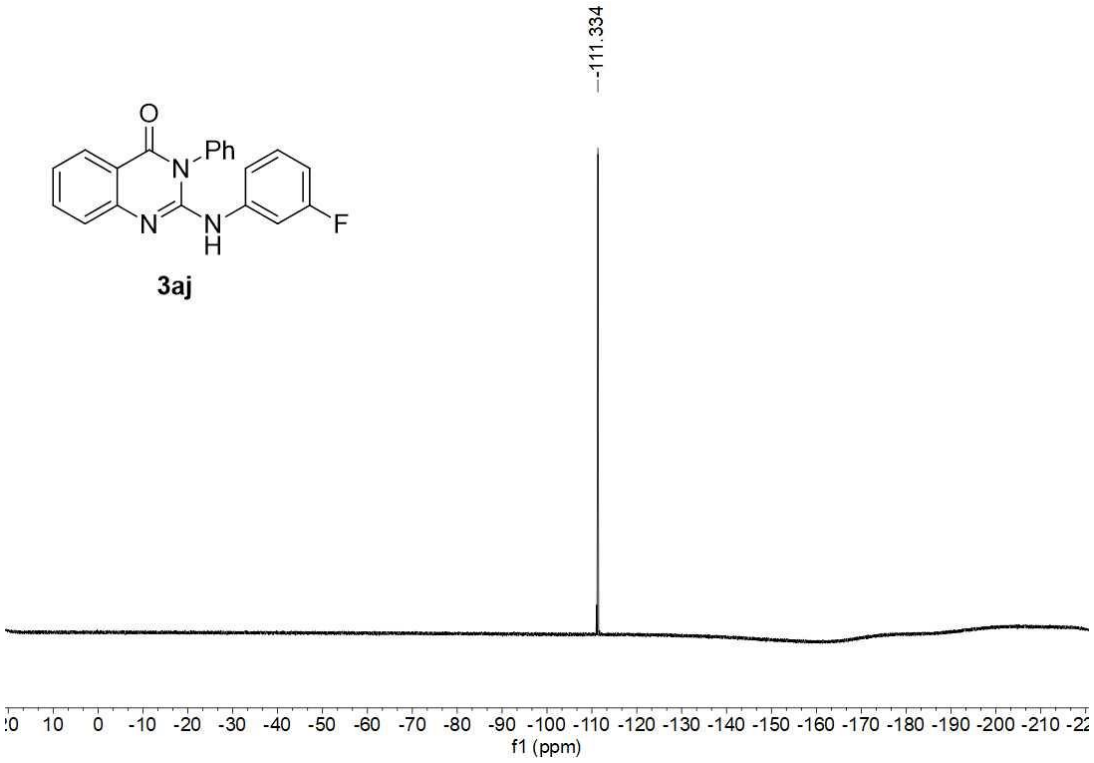
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3aj**



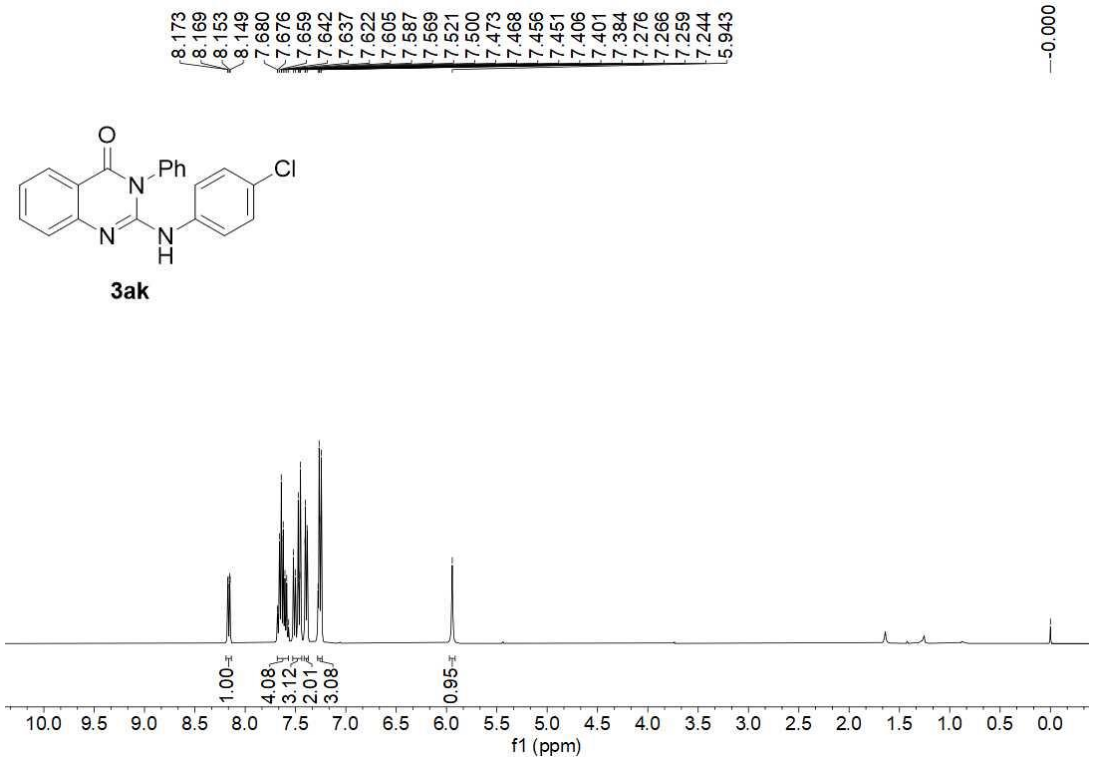
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of **3aj**



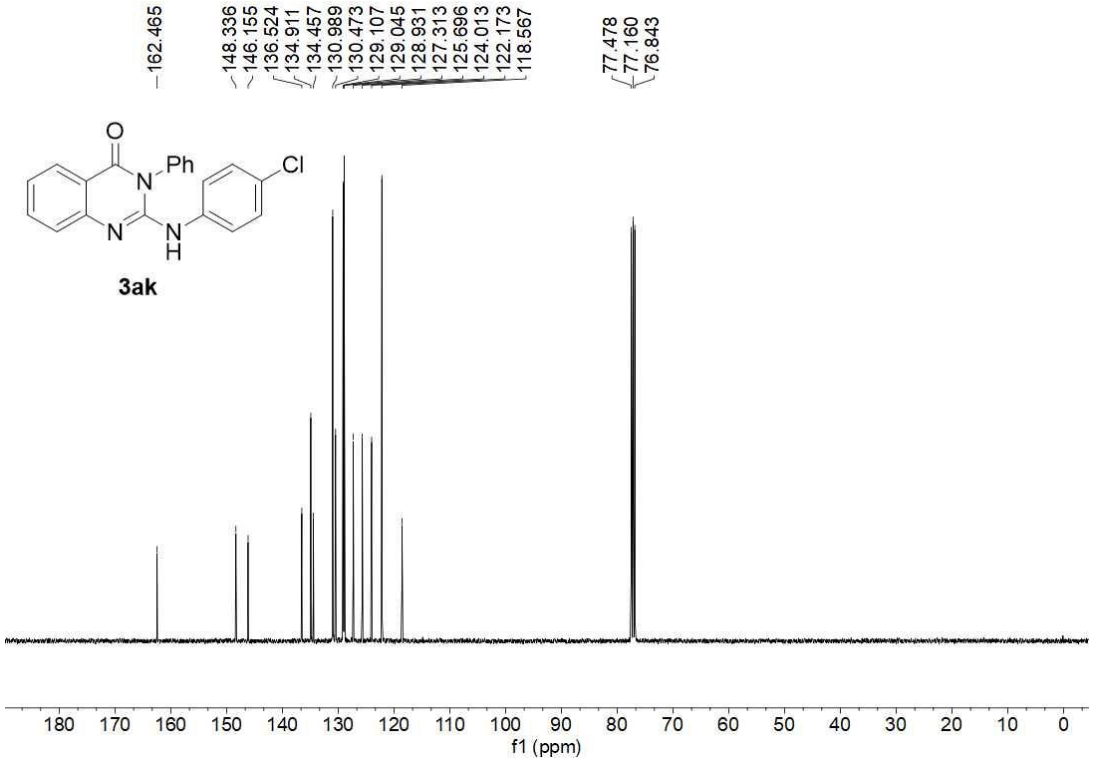
^{19}F NMR spectrum (377 MHz, $CDCl_3$) of **3aj**



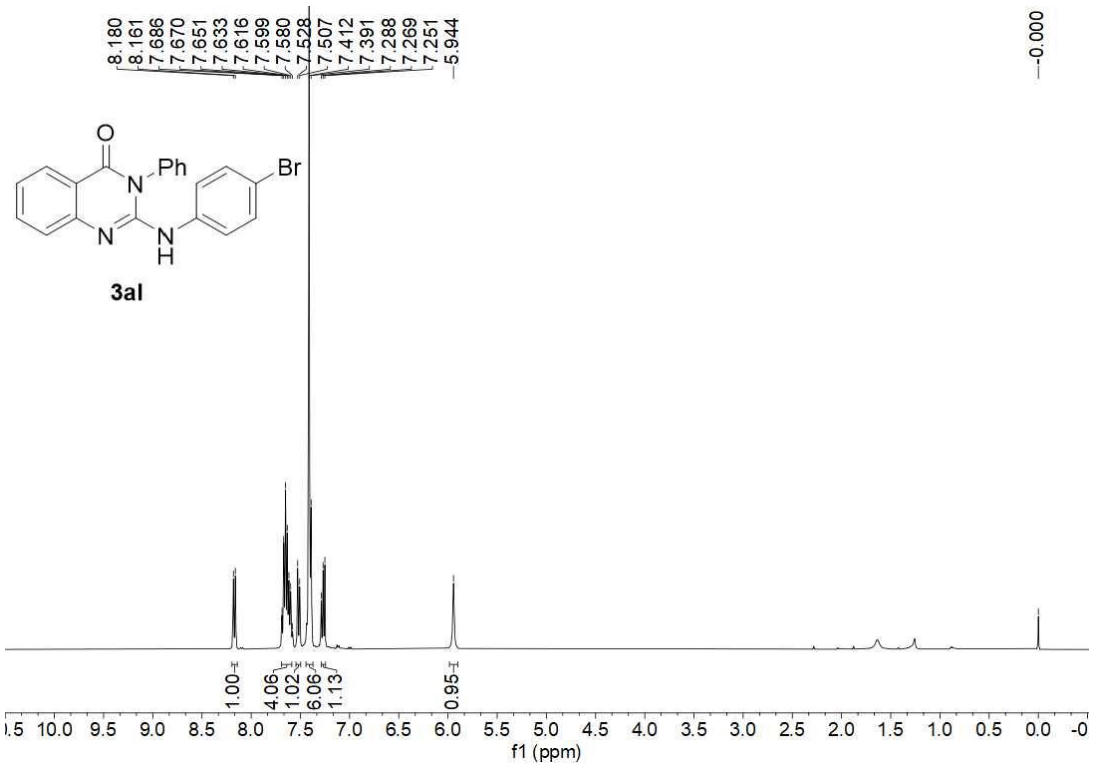
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3ak**



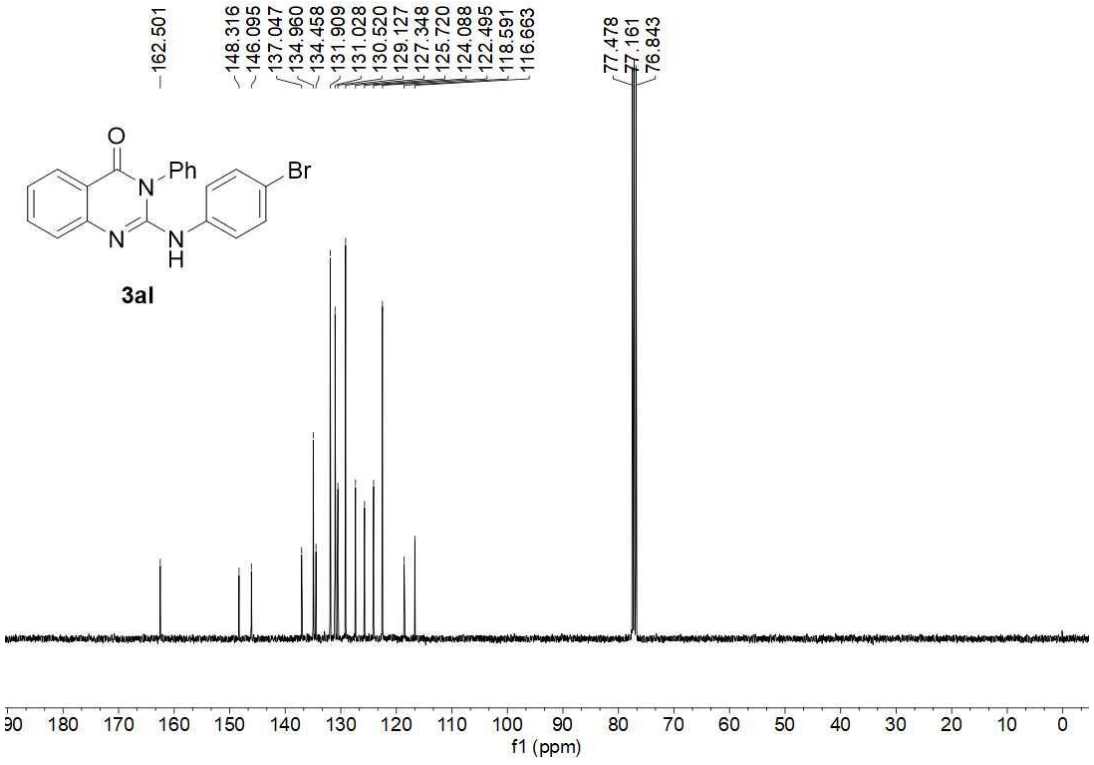
^{13}C{^{1}H} NMR spectrum (100 MHz, $CDCl_3$) of **3ak**



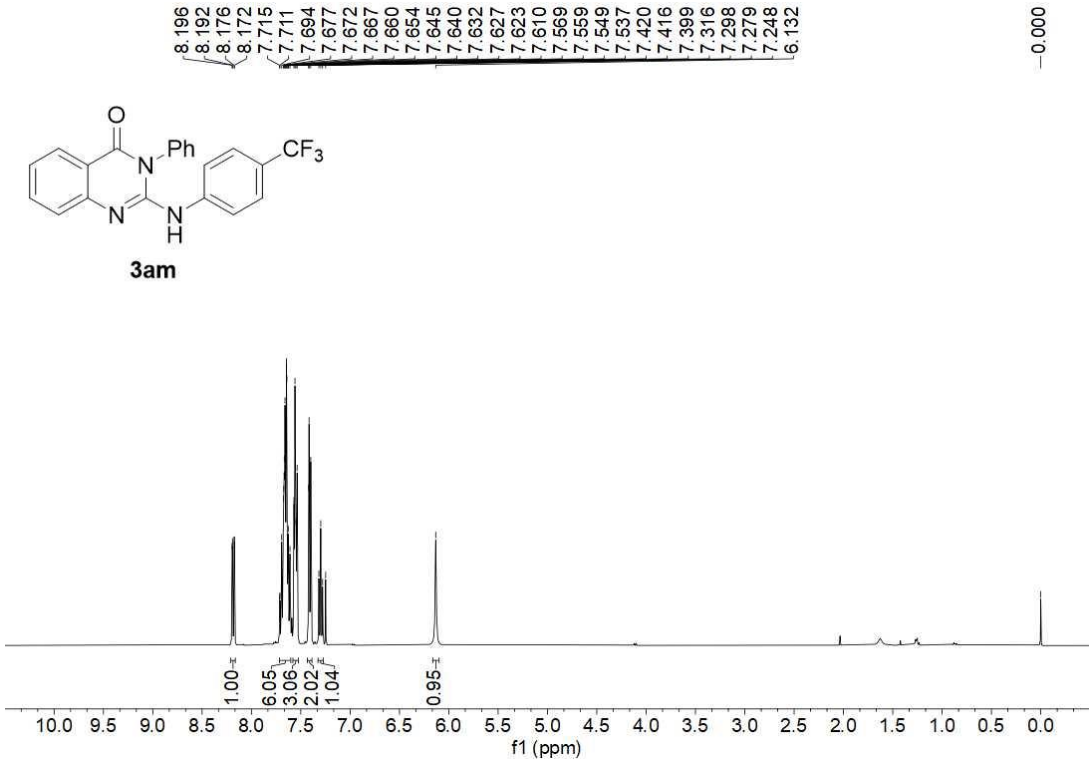
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3al**



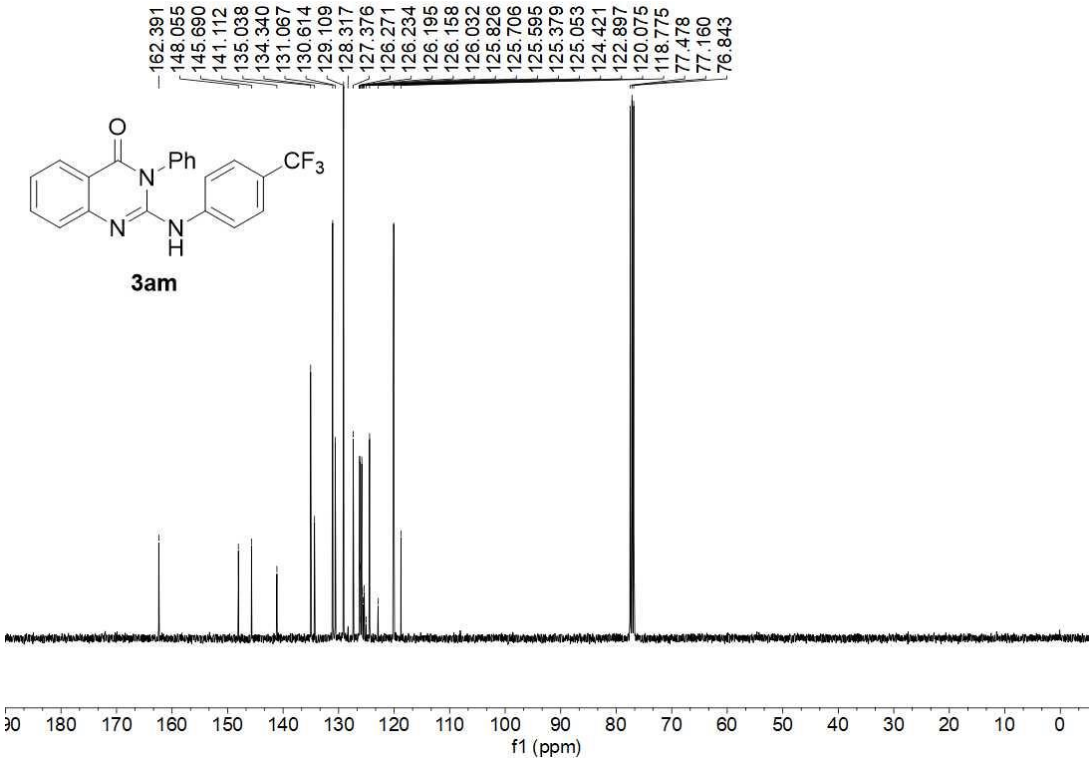
^{13}C{^{1}H} NMR spectrum (100 MHz, $CDCl_3$) of **3al**



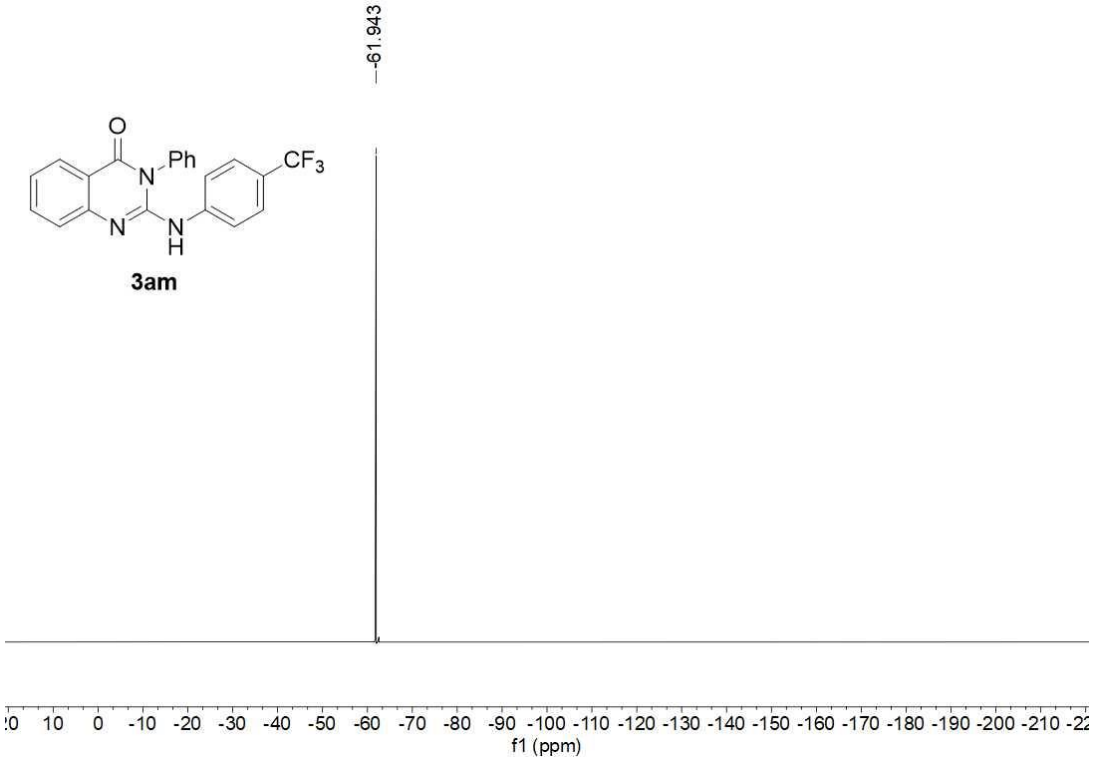
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3am**



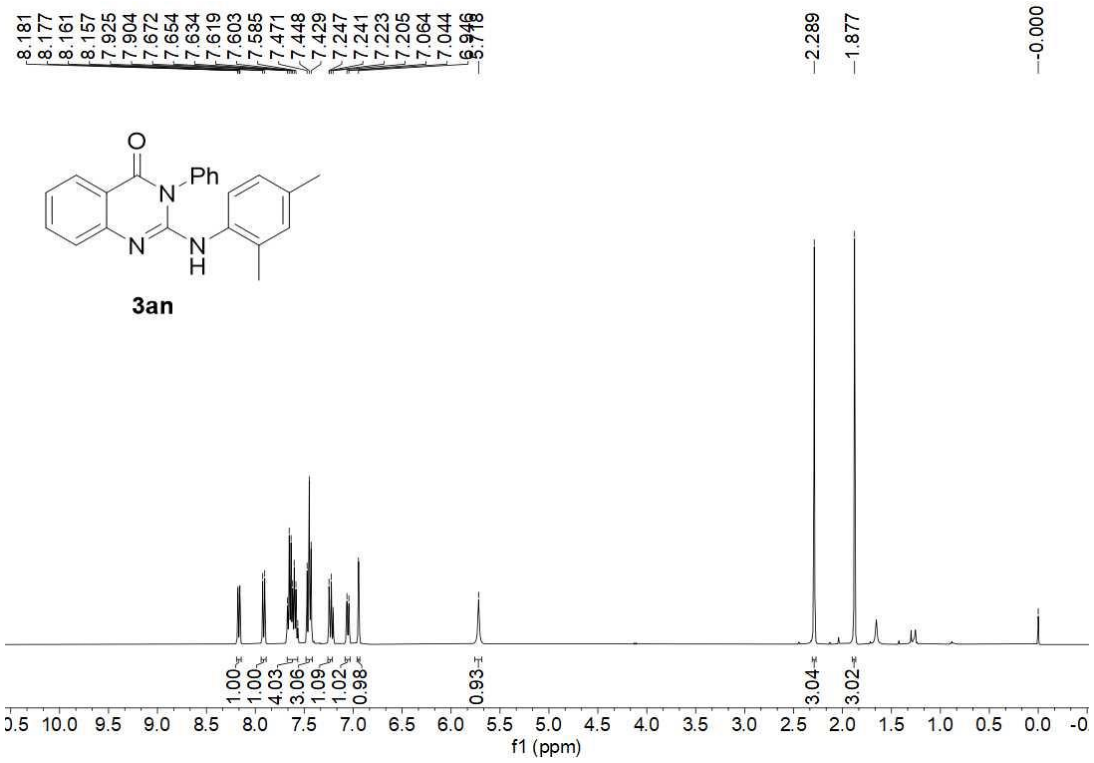
^{13}C{^{1}H} NMR spectrum (100 MHz, $CDCl_3$) of **3am**



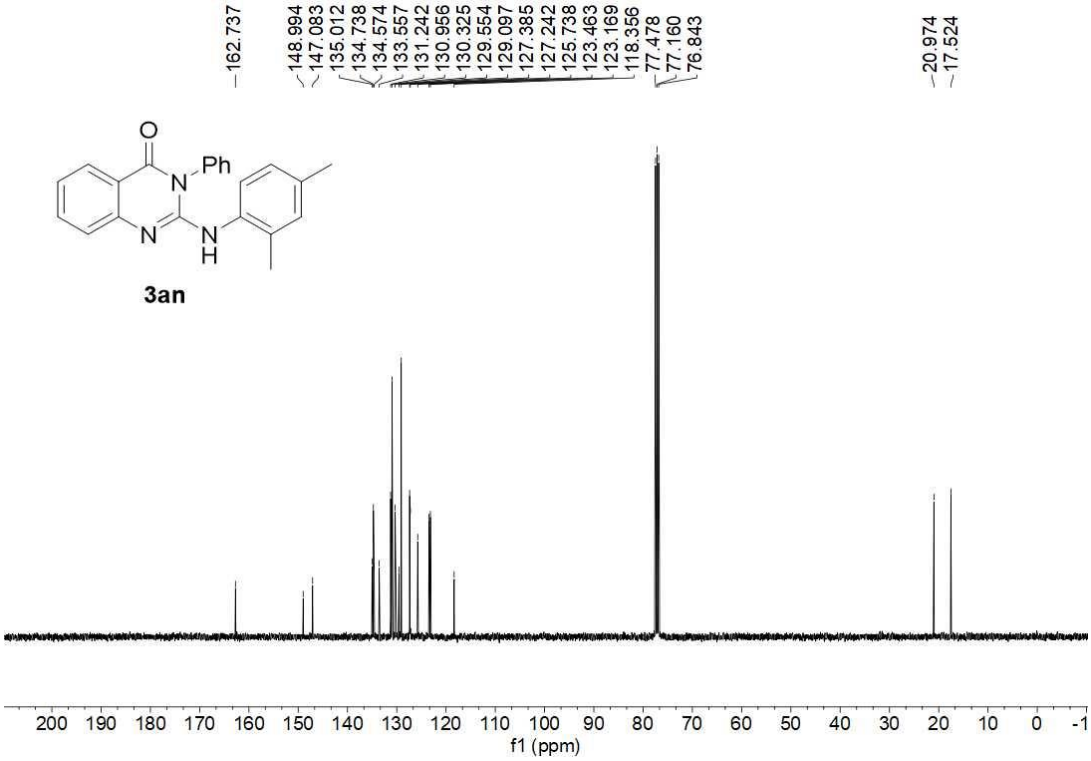
^{19}F NMR spectrum (377 MHz, $CDCl_3$) of **3am**



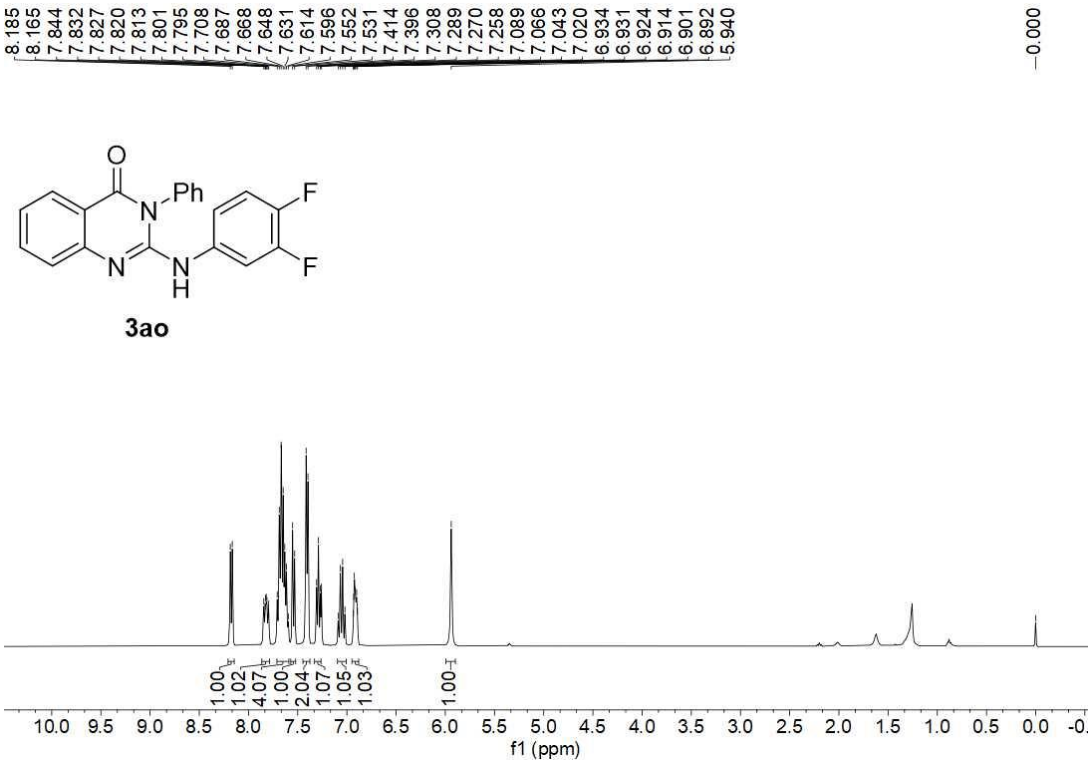
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3an**



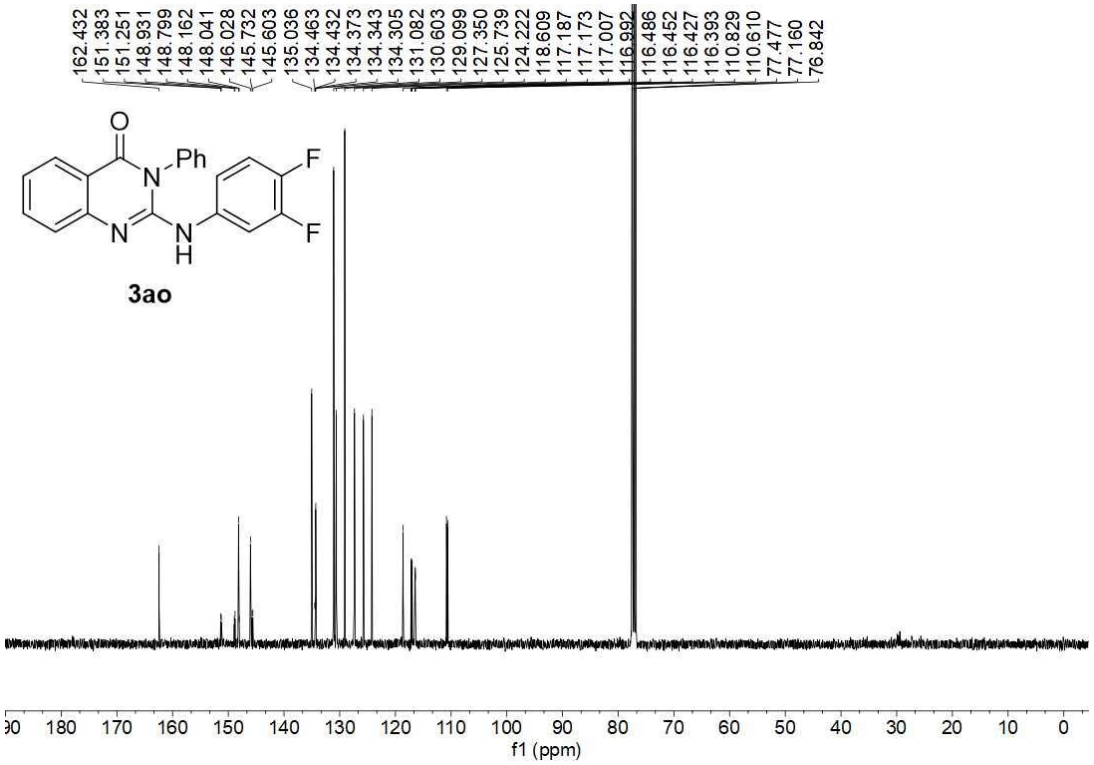
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of **3an**



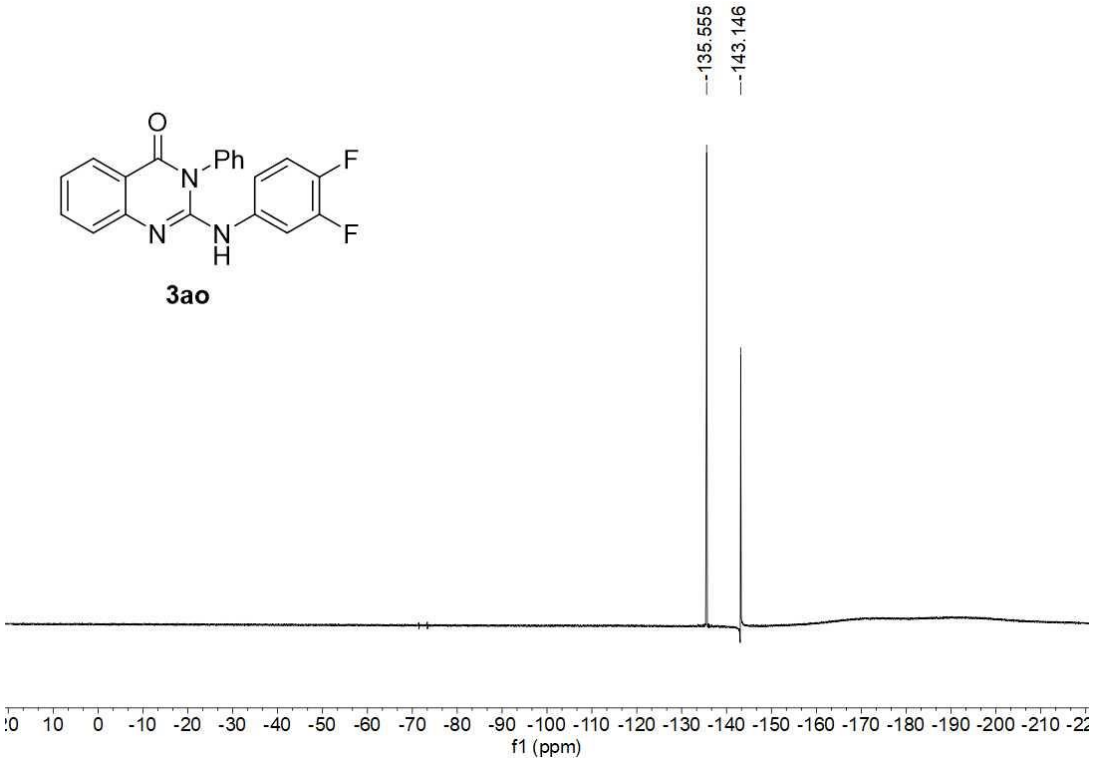
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3ao**



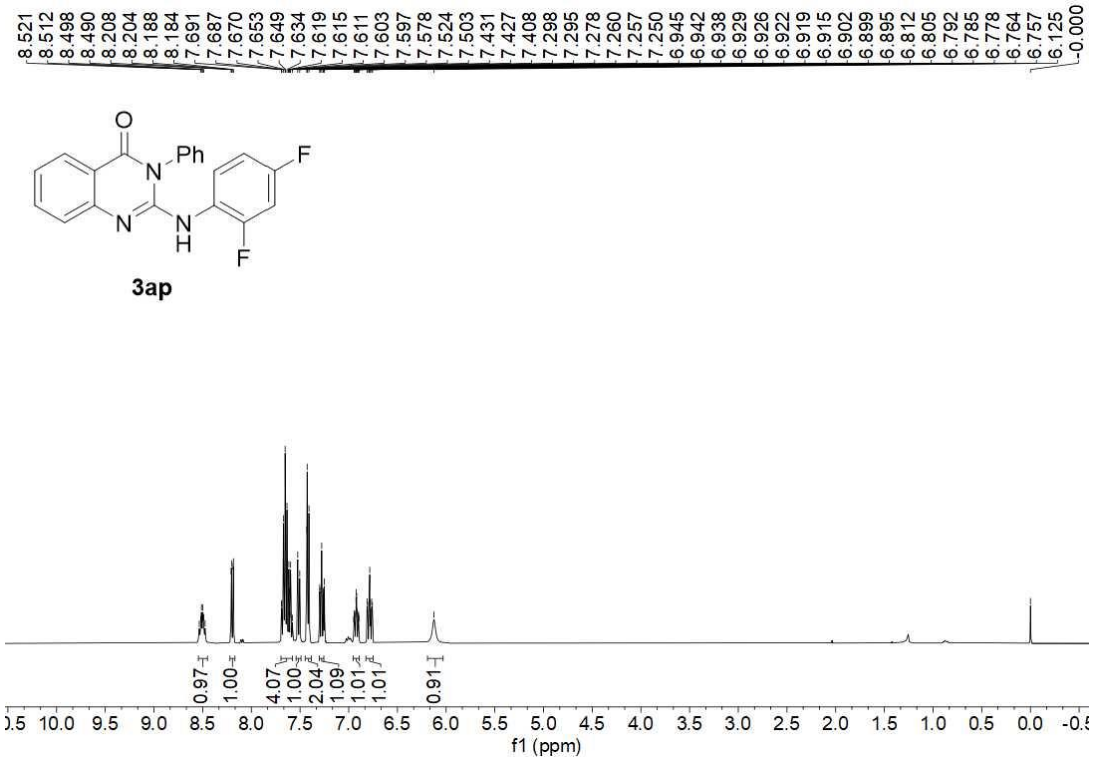
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of **3ao**



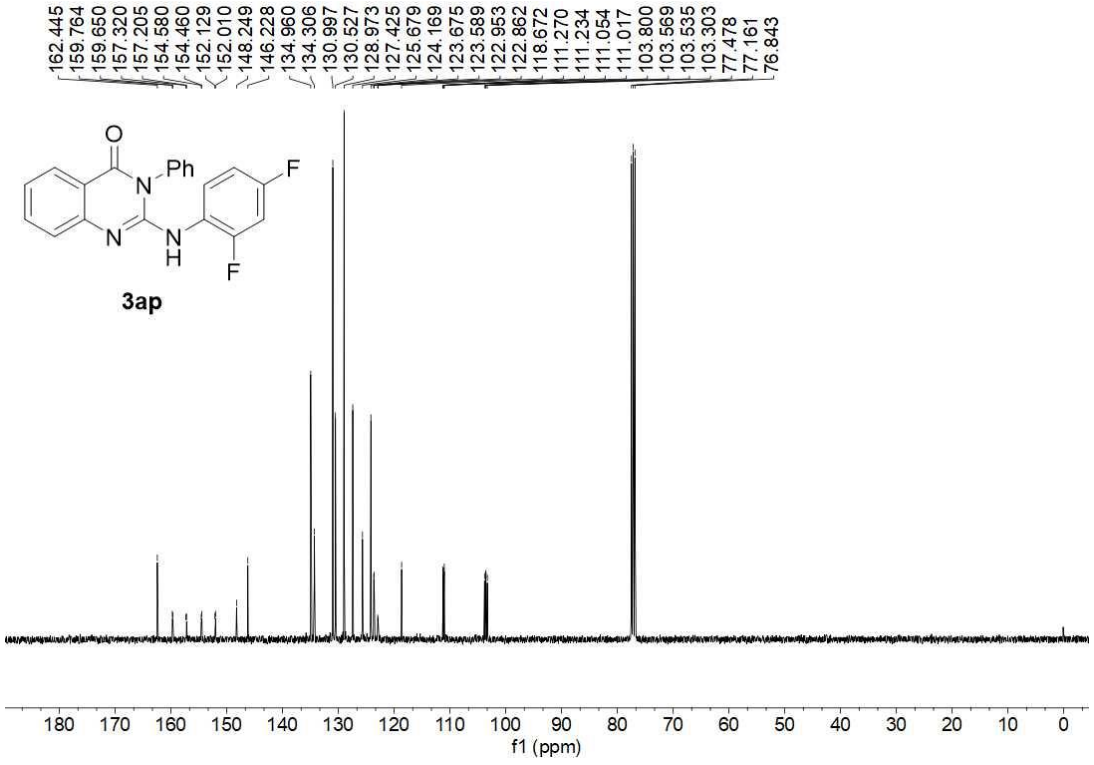
^{19}F NMR spectrum (377 MHz, $CDCl_3$) of **3ao**



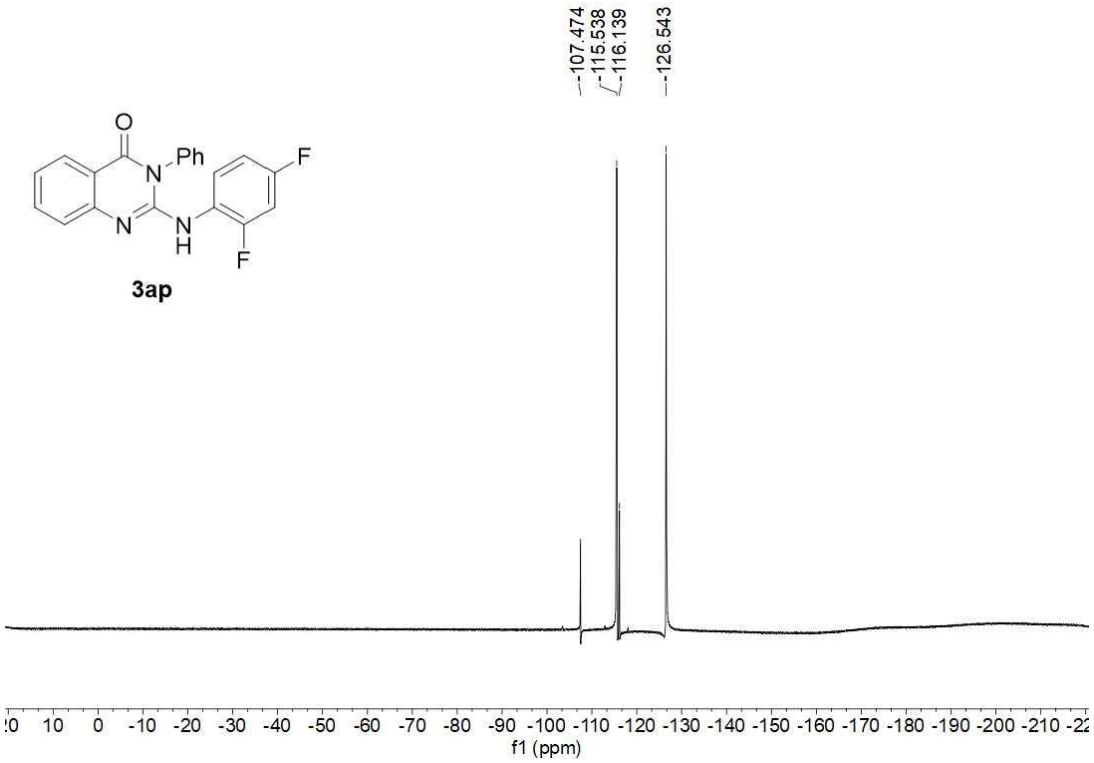
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3ap**



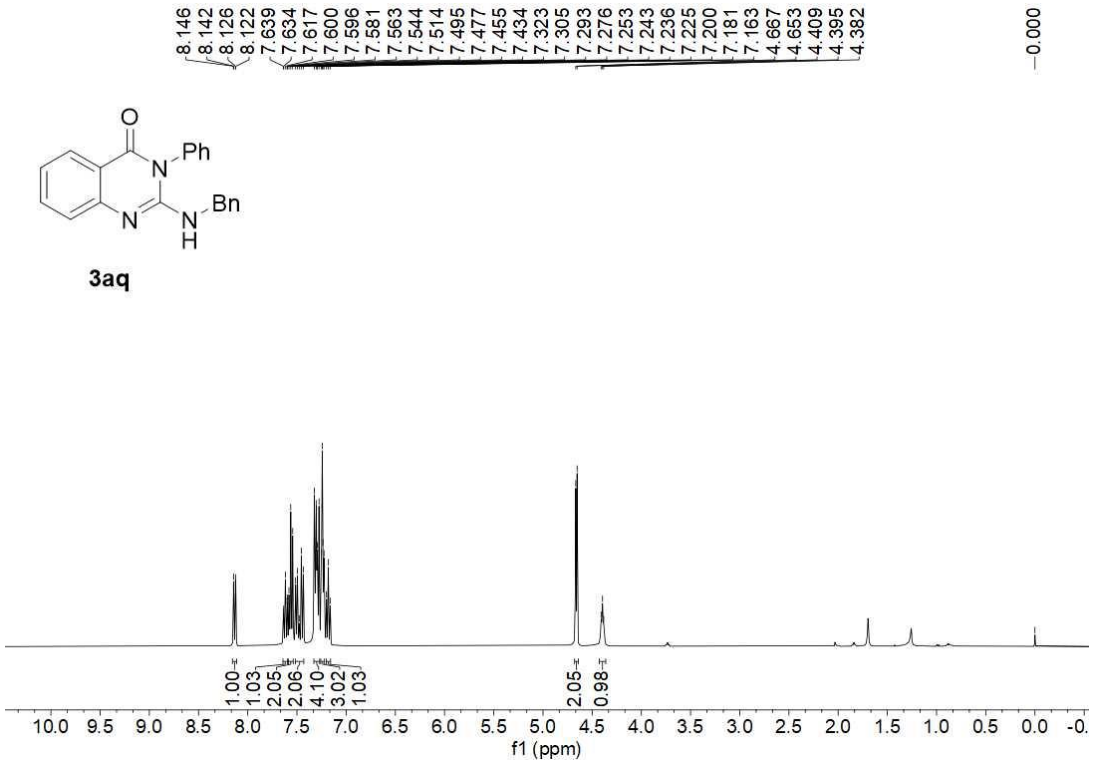
^{13}C{^{1}H} NMR spectrum (100 MHz, $CDCl_3$) of **3ap**



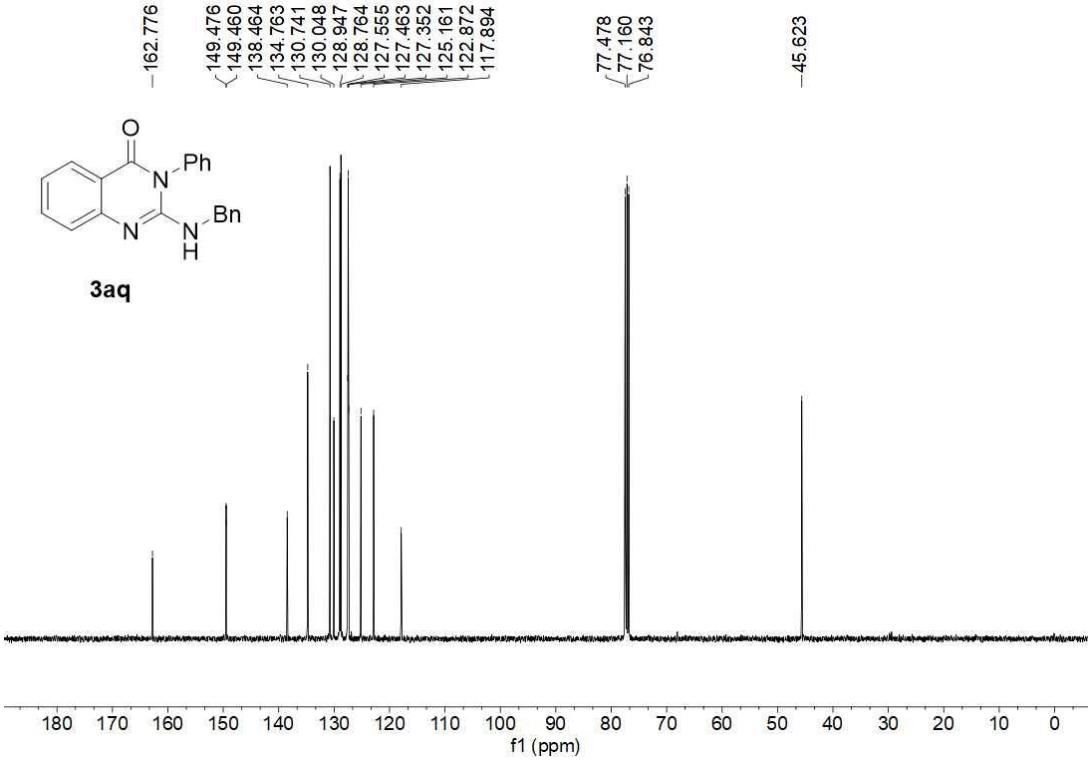
^{19}F NMR spectrum (377 MHz, $CDCl_3$) of **3ap**



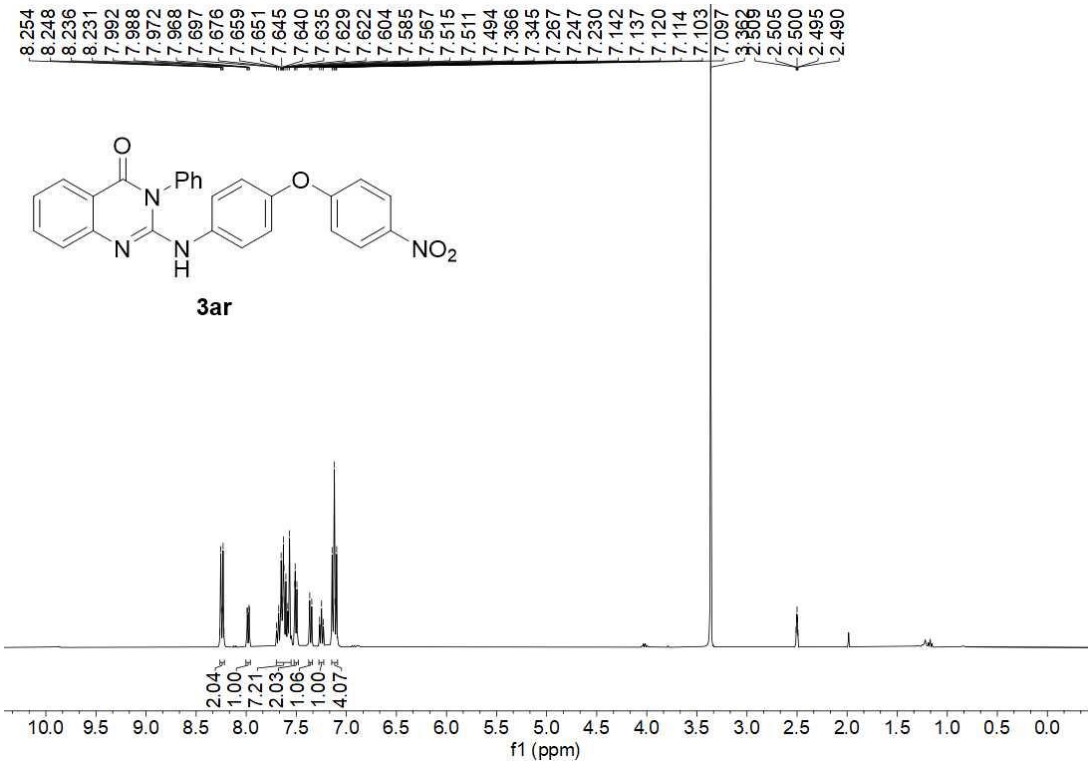
^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3aq**



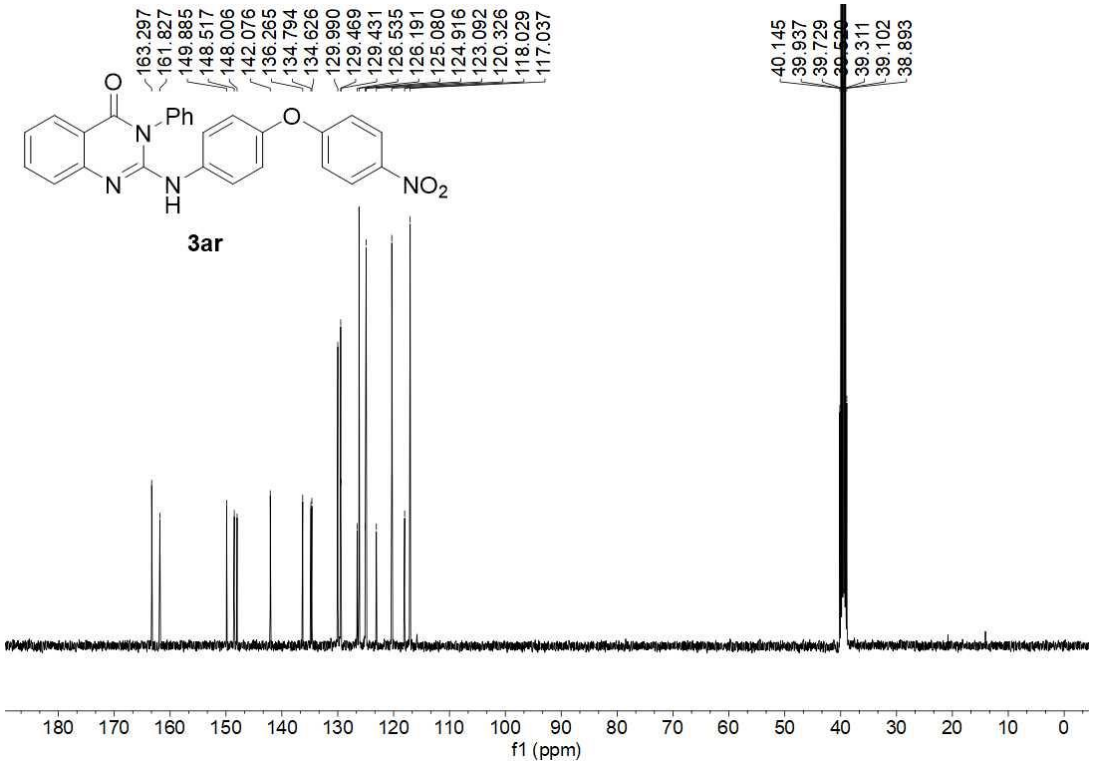
$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, $CDCl_3$) of **3aq**



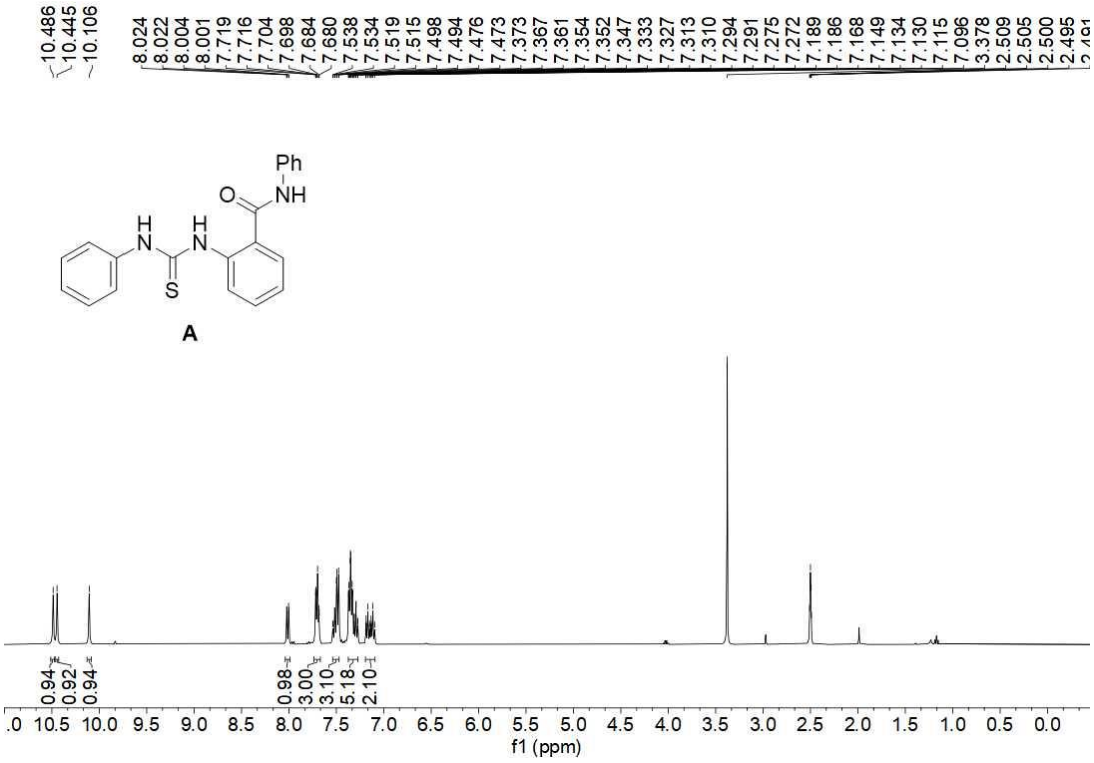
^{1}H NMR spectrum (400 MHz, DMSO-d_6) of **3ar**



$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, DMSO-d_6) of **3ar**



^{1}H NMR spectrum (400 MHz, DMSO-d_6) of **A**



$^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, DMSO-d_6) of **A**