

Supporting information

Photocatalytic cyclization of 3-(2-isocyanophenyl)quinazolin-4(3H)-ones for the construction of quinoxalino[2,1-*b*]quinazolinones

Xian Wu, Lingli Liu, Chengli Xiang, Jin-Tao Yu* and Changduo Pan*

Email: yujintao@cczu.edu.cn; panchangduo@jsut.edu.cn

Table of Contents

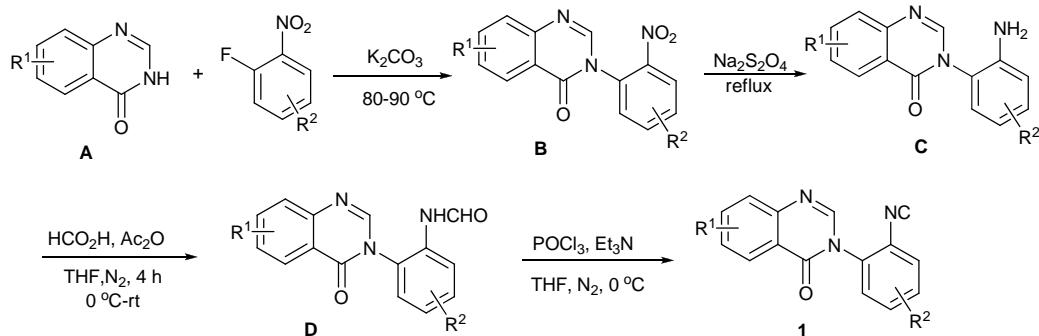
1. General Considerations	S2
2. General Synthetic Procedures	S2
3. Mechanism Studies	S3
4. Characterization Data for the Substrates and Products	S7
5. References	S23
6. Copies of the ^1H NMR and ^{13}C NMR Spectra	S24

1. General Considerations

General Information: Unless otherwise noted, all chemicals were purchased and used without further purification. ^1H NMR and ^{13}C NMR spectra were recorded at ambient temperature on a 400 MHz NMR spectrometer (101 MHz for ^{13}C). NMR experiments are reported in δ units, parts per million (ppm), and were referenced to CDCl_3 (δ 7.26 or 77.0) as the internal standard. The coupling constants J are given in Hz. Column chromatography was performed using EM Silica gel 60 (300-400 mesh).

2. General Synthetic Procedures

2.1 General procedure for the synthesis of substrates 1:



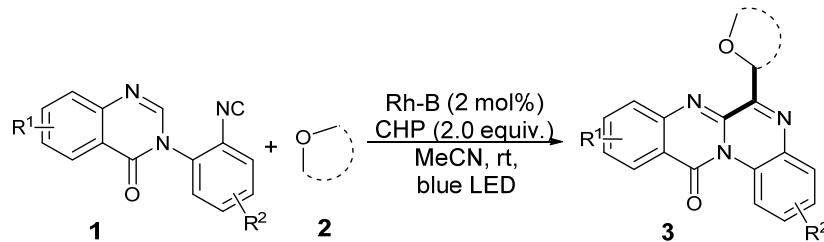
First, to a mixture of quinazolin-4(*3H*)-one **A** (10.0 mmol) in 25 mL of *N,N*-dimethylformamide (DMF) were added K_2CO_3 (15.0 mmol, 1.5 equiv) and 1-fluoro-2-nitrobenzene (12 mmol, 1.2 equiv) sequentially. The mixture was refluxed at 80-90 °C for 8 h in a flask equipped with a guard tube. The reaction was quenched with H_2O and extracted with ethyl acetate (3×25 mL). The combined organic layers were washed several times with H_2O and finally with brine solution, dried over anhydrous Na_2SO_4 , and concentrated under vacuum. Crude product was recrystallized from ethyl acetate to obtain **B**.¹

Then, a solution of $\text{Na}_2\text{S}_2\text{O}_4$ (40.0 mmol, 5.0 equiv) in H_2O (80 mL) was added to the solution of **B** (8.0 mmol) in dioxane (80 mL). The reaction mixture was stirred at reflux temperature for 3 h then cooled to room temperature and was poured into water. The resulting precipitate was filtered off, washed with water (2×50 mL) and dried in air to give **C**.²

Next, acetic formic anhydride (24.0 mmol), which was newly prepared from the reaction of acetic anhydride (2.3 mL, 24.0 mmol) with formic acid (1.1 mL, 27 mmol) at 55 °C for 2 h, was added dropwise to a mixture of **C** (4.0 mmol) in 6.0 mL THF at 0 °C. The mixture was warmed to room temperature and stirred for 3 h. Then, the reaction was quenched by saturated NaHCO_3 and extracted with EtOAc . The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4 and concentrated in vacuum to give the products **D**. These formamides were used for the subsequent dehydration reaction without further purification. POCl_3 (1.1 mL, 12.0 mmol) was added via syringe pump to a mixture of Et_3N (5.1 mL, 36.0 mmol) and **D** (4.0 mmol) in THF (6 mL) at 0 °C within 2 hours. After that, the resulting mixture was stirred at 0 °C for another 2 hours. Then, the mixture was quenched with Sat.

NaHCO_3 and extracted with CH_2Cl_2 . The combined organic layer was washed with brine, dried over anhydrous Na_2SO_4 and concentrated in vacuum. The residue was purified by chromatography on silica gel using petroleum ether/ethyl acetate as eluent to afford the products **1** in 30-70% yield.³

2.2 General procedure for the synthesis of products **3**.



The mixture of 3-(2-Isocyanophenyl)quinazolin-4(3*H*)-ones **1** (0.2 mmol), Rhodamine B (2 mol%, 1.9 mg), CHP (2.0 equiv, 60.9 mg), THF (1 mL) and MeCN (1 mL) was added into a Schlenk tube and sealed. The tube was evacuated and backfilled with nitrogen (repeated five times). The mixture was stirred at room temperature for 12 hours under the irradiation of 10 W blue LED. Then, the solvent was evaporated under reduced pressure, and purified by silica gel flash column chromatography to give the products **3**.

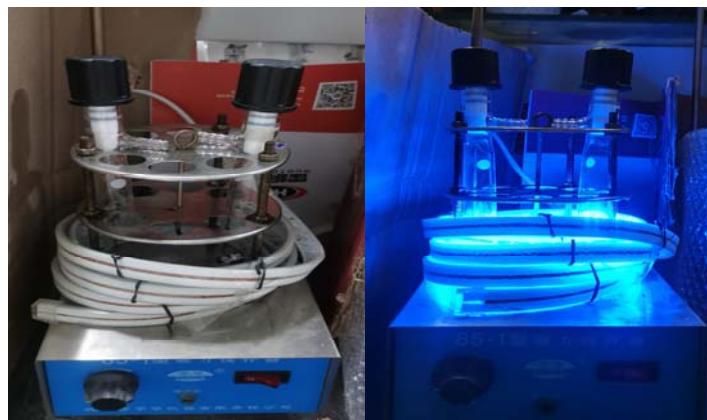
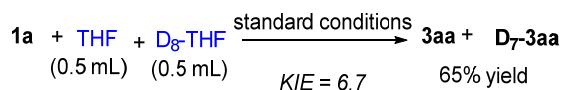


Figure S1 Photoreactor used in this work.

3. Mechanism Studies

3.1 The KIE experiment:



The mixture of **1a** (0.2 mmol), Rhodamine B (2 mol%, 1.9 mg), CHP (2.0 equiv, 60.9 mg), THF (0.5 mL), $\text{D}_8\text{-THF}$ (0.5 mL) and MeCN (1 mL) was added into a Schlenk tube and sealed. The tube was evacuated and backfilled with nitrogen (repeated for five times). The mixture was stirred at room temperature for 8 hours under the irradiation of 10 W blue LEDs. Then, the solvent was evaporated under reduced pressure, and purified by silica gel flash column chromatography to give product **3aa** and **D₇-3aa** in 65% total yield. A KIE value of

6.7 was observed from ^1H NMR spectrum.

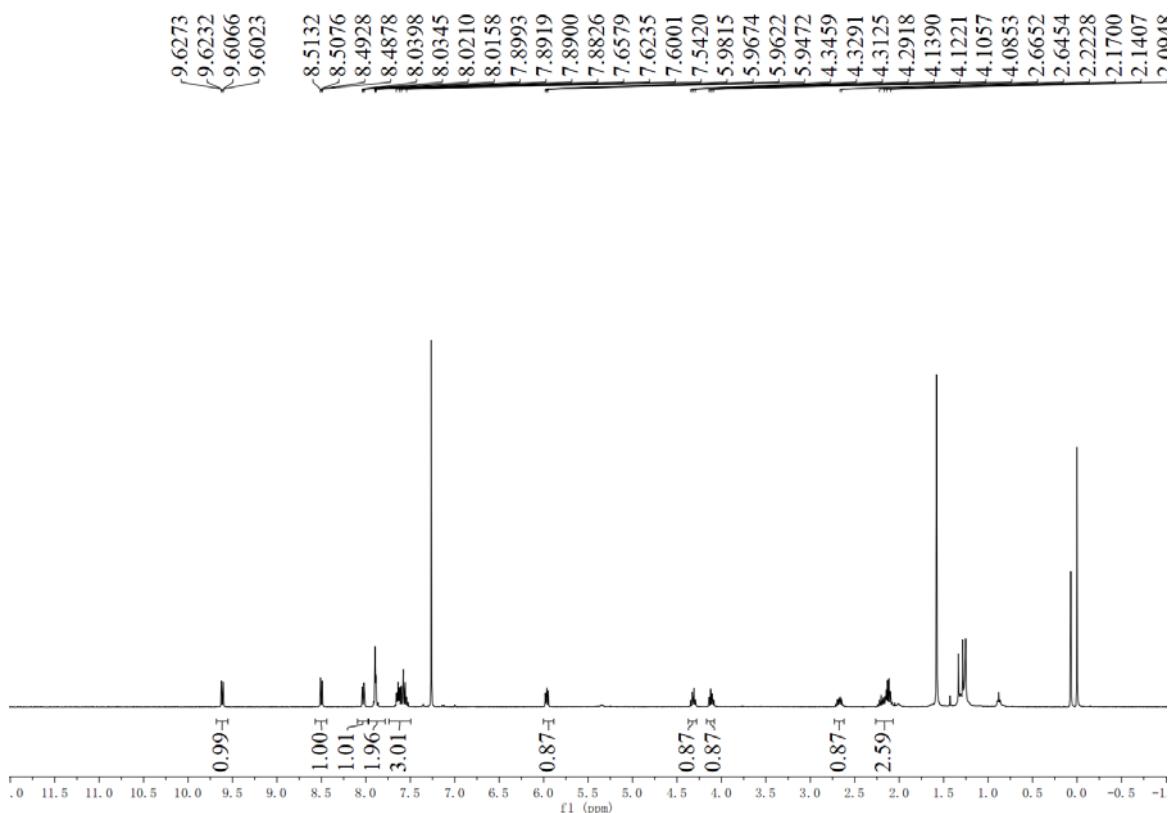
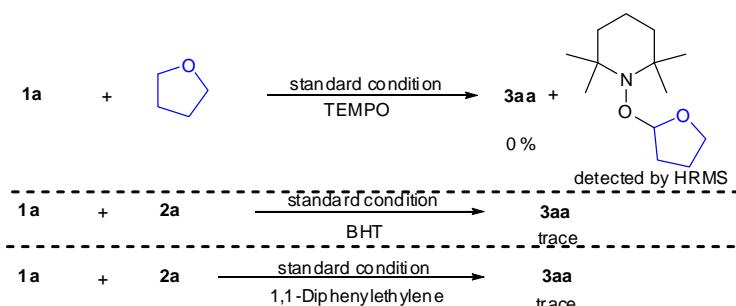


Figure S2. ^1H NMR spectrum of the KIE experiment

3.2 Radical inhibiting and trapping experiment



Under standard conditions, TEMPO (2.0 equiv., 0.4 mmol, 62.5 mg; or 1 equiv., 0.2 mmol, 31.2 mg), BHT (2.0 equiv, 0.4 mmol, 88.1 mg; or 1 equiv, 0.2 mmol, 44 mg) or 1,1-diphenylethylene (2.0 equiv, 0.4 mmol, 72.0 mg; or 1 equiv., 0.2 mmol, 36 mg) was added into a Schlenk tube and sealed. The tube was evacuated and backfilled with nitrogen (repeated five times). The mixture was stirred at room temperature for 12 hours under the irradiation of 10 W blue LEDs.

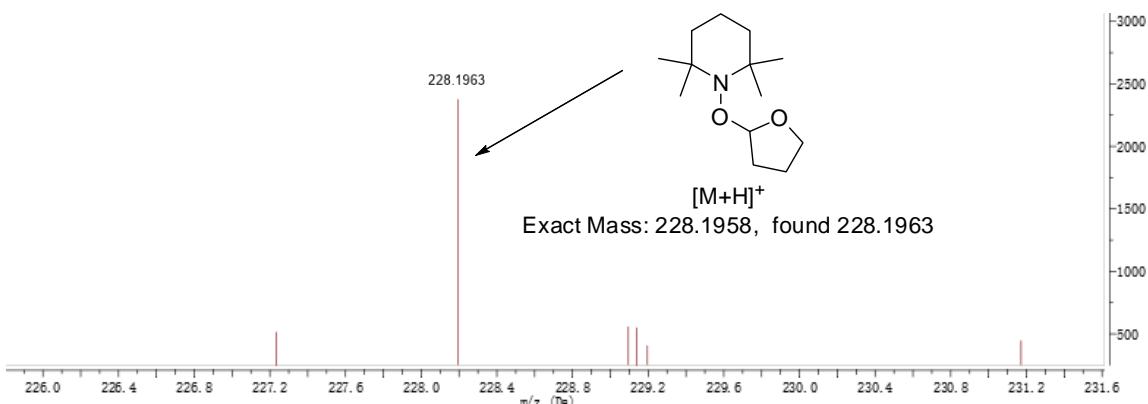


Figure S3. The adduct of TEMPO and tetrahydrofuran-2-yl radical detected by HRMS.

3.3 Cyclic voltammetry study

Cyclic voltammetry measurements were performed in a three-electrode cell (volume 5 mL) with glassy carbon as the working electrode, Pt wire as the auxiliary electrode, and SCE (saturated calomel electrode) as the reference electrode. The electrodes are first polished with sandpaper, then with alumina powder until the surface of the electrodes is mirror-like. Finally, the electrodes are washed with distilled water and ultrasonication. The solvent (MeCN) exhaust employs a nitrogen blast for 30 min. CHP (1 mM) was tested with tetrabutylammonium hexafluorophosphate (0.1 M) as the supporting electrolyte in 30 mL MeCN, respectively. Solutions were kept under positive pressure of nitrogen during the measurements. Cyclic voltammetry (CV) with the following settings: Scan Rates = 0.1 V/s, Sweep Segments = 10, Sample Interval = 0.001 V, Quiet Time = 2 sec. The redox potentials of CHP is $E_{1/2}^{\text{red}} = -0.89$ V vs SCE.

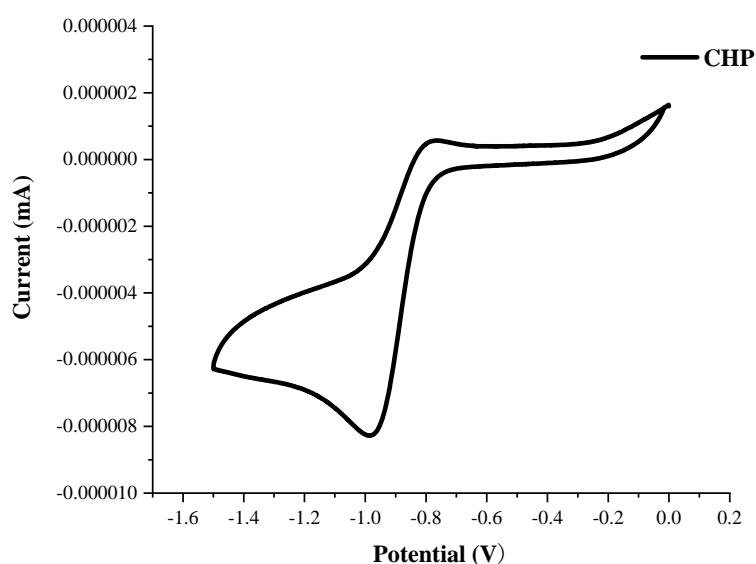
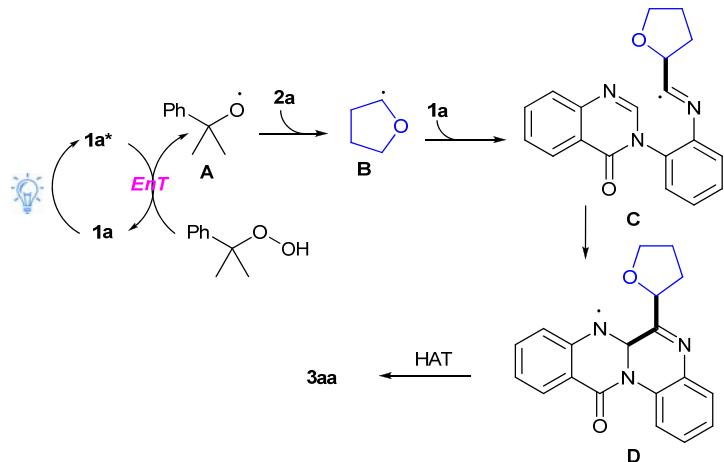


Figure S4. Cyclic voltammetry plots of CHP. Scan direction: from 0 V to -1.5 V, then back to 0 V

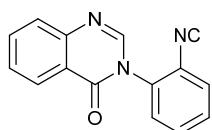
3.4 Alternative mechanism

Control experiments indicated that 23% yield of **3aa** was obtained in the absence of photocatalyst, and no reaction occurred in the absence of both photocatalyst and light irradiation. Moreover, the reaction did not occur in the presence of ambient oxygen or (*E*)-stilbene. Those results indicated that an energy transfer process maybe involved as proposed in Scheme S1.

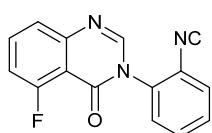


Scheme S1. Alternative mechanism involving the EnT process.

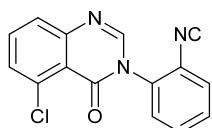
4. Characterization Data for the Substrates and Products



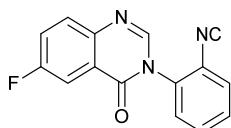
3-(2-Isocyanophenyl)quinazolin-4(3H)-one (1a) (692.3 mg, 70% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 2/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): δ = 8.37-8.34 (m, 1H), 7.99 (s, 1H), 7.85-7.77 (m, 2H), 7.62-7.54 (m, 4H), 7.49-7.47 (m, 1H); ^{13}C NMR (101 MHz, CDCl_3): δ = 170.3, 156.0, 147.8, 144.9, 135.1, 133.8, 130.7, 130.6, 129.3, 128.2, 128.1, 127.9, 127.3, 124.9, 122.1; HRMS (ESI) m/z calcd for $\text{C}_{15}\text{H}_{10}\text{N}_3\text{O} [\text{M}+\text{H}]^+$ 248.0818, found 248.0811.



5-Fluoro-3-(2-isocyanophenyl)quinazolin-4(3H)-one (1b) (689.6 mg, 65% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 2/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): δ = 7.97 (s, 1H), 7.79-7.74 (m, 1H), 7.63-7.57 (m, 4H), 7.49-7.47 (m, 1H), 7.24-7.19 (m, 1H); ^{13}C NMR (101 MHz, CDCl_3): δ = 170.5, 161.6 (d, $J_{\text{C}-\text{F}} = 268.7$ Hz), 156.9 (d, $J_{\text{C}-\text{F}} = 4.1$ Hz), 149.8, 145.7, 135.7, 135.6 (d, $J_{\text{C}-\text{F}} = 10.4$ Hz), 133.4, 130.8, 130.7, 129.4, 128.1, 123.8 (d, $J_{\text{C}-\text{F}} = 4.2$ Hz), 114.9 (d, $J_{\text{C}-\text{F}} = 20.8$ Hz), 111.9 (d, $J_{\text{C}-\text{F}} = 6.1$ Hz); HRMS (ESI) m/z calcd for $\text{C}_{15}\text{H}_8\text{FN}_3\text{O} [\text{M}+\text{Na}]^+$ 288.0544, found 288.0556.

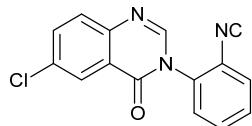


5-Chloro-3-(2-isocyanophenyl)quinazolin-4(3H)-one (1c) (709.9 mg, 63% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 2/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): δ = 7.98 (s, 1H), 7.68-7.67 (m, 2H), 7.61-7.54 (m, 4H), 7.50-7.48 (m, 1H); ^{13}C NMR (101 MHz, CDCl_3): δ = 170.4, 158.1, 150.2, 145.5, 134.9, 134.5, 133.5, 130.9, 130.8, 130.7, 129.4, 128.1, 127.2, 124.9, 119.4; HRMS (ESI) m/z calcd for $\text{C}_{15}\text{H}_8\text{ClN}_3\text{O} [\text{M}+\text{H}]^+$ 282.0429, found 282.0417.

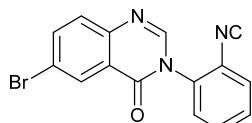


6-Fluoro-3-(2-isocyanophenyl)quinazolin-4(3H)-one (1d) (647.2 mg, 61% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 2/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): δ = 8.00-7.96 (m, 2H), 7.82-7.79 (m, 1H), 7.64-7.52 (m, 4H),

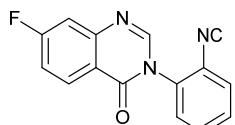
7.50-7.47 (m, 1H); ^{13}C NMR (101 MHz, CDCl_3): δ = 170.4, 161.6 (d, $J_{\text{C-F}} = 251.1$ Hz), 159.3 (d, $J_{\text{C-F}} = 3.2$ Hz), 144.4 (d, $J_{\text{C-F}} = 2.1$ Hz), 144.2 (d, $J_{\text{C-F}} = 2.5$ Hz), 133.6, 130.8, 130.7, 130.4 (d, $J_{\text{C-F}} = 8.2$ Hz), 129.2, 128.2, 123.6 (d, $J_{\text{C-F}} = 24.0$ Hz), 123.5, 112.4 (d, $J_{\text{C-F}} = 24.1$ Hz); HRMS (ESI) m/z calcd for $\text{C}_{15}\text{H}_8\text{FN}_3\text{O} [\text{M}+\text{H}]^+$ 266.0724, found 266.0715.



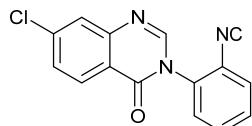
6-Chloro-3-(2-isocyanophenyl)quinazolin-4(3H)-one (1e) (619.7 mg, 55% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 2/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): δ = 8.31 (m, 1H), 7.98 (s, 1H), 7.78-7.72 (m, 2H), 7.63-7.58 (m, 3H), 7.49-7.47 (m, 1H); ^{13}C NMR (101 MHz, CDCl_3): δ = 170.5, 159.0, 146.3, 145.0, 135.5, 134.0, 133.5, 130.9, 130.8, 129.6, 129.1, 128.2, 126.7, 124.8, 123.2; HRMS (ESI) m/z calcd for $\text{C}_{15}\text{H}_8\text{ClN}_3\text{O} [\text{M}+\text{H}]^+$ 282.0429, found 282.0421.



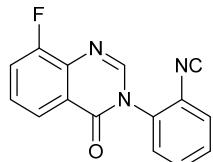
6-Bromo-3-(2-isocyanophenyl)quinazolin-4(3H)-one (1f) (769.7 mg, 59% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 2/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): δ = 8.46 (d, $J = 2.3$ Hz, 1H), 7.99 (s, 1H), 7.90 (m, 1H), 7.67-7.58 (m, 4H), 7.52-7.43 (m, 1H); ^{13}C NMR (101 MHz, CDCl_3): δ = 170.5, 158.8, 146.6, 145.2, 138.3, 133.5, 130.9, 130.8, 129.8, 129.7, 129.1, 128.2, 127.2, 123.5, 121.8; HRMS (ESI) m/z calcd for $\text{C}_{15}\text{H}_8\text{BrN}_3\text{O} [\text{M}+\text{H}]^+$ 325.9924, found 325.9929.



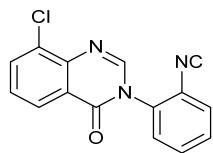
7-Fluoro-3-(2-isocyanophenyl)quinazolin-4(3H)-one (1g) (498.7 mg, 47% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 2/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): δ = 8.39 (m, 1H), 8.02 (s, 1H), 7.65-7.59 (m, 3H), 7.51-7.43 (m, 2H), 7.32-7.27 (m, 1H); ^{13}C NMR (101 MHz, CDCl_3): δ = 170.4, 166.8 (d, $J_{\text{C-F}} = 256.9$ Hz), 159.2, 150.0 (d, $J_{\text{C-F}} = 12.9$ Hz), 146.1, 133.5, 130.8, 130.7, 130.1 (d, $J_{\text{C-F}} = 10.8$ Hz), 129.2, 128.2, 118.8 (d, $J_{\text{C-F}} = 2.2$ Hz), 116.8 (d, $J_{\text{C-F}} = 23.6$ Hz), 113.5 (d, $J_{\text{C-F}} = 22.3$ Hz); HRMS (ESI) m/z calcd for $\text{C}_{15}\text{H}_8\text{FN}_3\text{O} [\text{M}+\text{H}]^+$ 266.0724, found 266.0719.



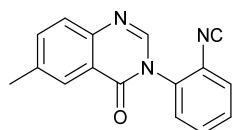
7-Chloro-3-(2-isocyanophenyl)quinazolin-4(3*H*)-one (1h**, 439.5 mg, 39% yield),** flash column chromatography on silica gel (petroleum ether/ethyl acetate 2/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): δ = 8.28 (d, J = 8.5 Hz, 1H), 8.00 (s, 1H), 7.77 (d, J = 2.0 Hz, 1H), 7.63-7.57 (m, 3H), 7.53-7.46 (m, 2H); ^{13}C NMR (101 MHz, CDCl_3): δ = 170.5, 159.4, 148.7, 146.1, 141.4, 133.5, 130.9, 130.8, 129.2, 128.8, 128.7, 128.2, 127.5, 124.8, 120.6; HRMS (ESI) m/z calcd for $\text{C}_{15}\text{H}_8\text{ClN}_3\text{NaO} [\text{M}+\text{Na}]^+$ 304.0248, found 304.0241.



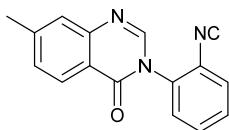
8-Fluoro-3-(2-isocyanophenyl)quinazolin-4(3*H*)-one (1i**, 424.4 mg, 40% yield),** flash column chromatography on silica gel (petroleum ether/ethyl acetate 2/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): δ = 8.15-8.12 (m, 1H), 8.03 (s, 1H), 7.64-7.48 (m, 6H); ^{13}C NMR (101 MHz, CDCl_3): δ = 170.5, 159.0 (d, $J_{\text{C}-\text{F}}$ = 3.1 Hz), 157.2 (d, $J_{\text{C}-\text{F}}$ = 257.8 Hz), 145.4, 137.1 (d, $J_{\text{C}-\text{F}}$ = 12.2 Hz), 133.5, 130.9, 130.8, 129.1, 128.4 (d, $J_{\text{C}-\text{F}}$ = 7.8 Hz), 128.2, 123.9, 122.8 (d, $J_{\text{C}-\text{F}}$ = 4.3 Hz), 120.7 (d, $J_{\text{C}-\text{F}}$ = 19.0 Hz); HRMS (ESI) m/z calcd for $\text{C}_{15}\text{H}_8\text{FN}_3\text{NaO} [\text{M}+\text{Na}]^+$ 288.0544, found 288.0546.



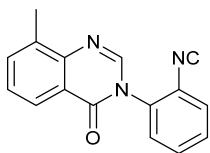
8-Chloro-3-(2-isocyanophenyl)quinazolin-4(3*H*)-one (1j**, 473.3 mg, 42% yield),** flash column chromatography on silica gel (petroleum ether/ethyl acetate 2/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): δ = 8.28-8.25 (m, 1H), 8.10 (s, 1H), 7.91-7.89 (m, 1H), 7.64-7.56 (m, 3H), 7.51-7.47 (m, 2H); ^{13}C NMR (101 MHz, CDCl_3): δ = 170.6, 159.4, 145.6, 144.5, 135.4, 133.4, 132.2, 131.0, 130.8, 129.1, 128.3, 128.2, 126.2, 124.8, 123.7; HRMS (ESI) m/z calcd for $\text{C}_{15}\text{H}_8\text{ClN}_3\text{O} [\text{M}+\text{H}]^+$ 282.0429, found 282.0417.



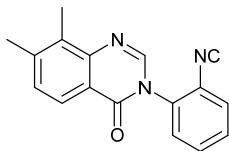
3-(2-Isocyanophenyl)-6-methylquinazolin-4(3*H*)-one (1k**, 606.2 mg, 58% yield),** flash column chromatography on silica gel (petroleum ether/ethyl acetate 2/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): δ = 8.14 (s, 1H), 7.94 (s, 1H), 7.68-7.53 (m, 5H), 7.48-7.46 (m, 1H), 2.50 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3): δ = 170.2, 160.0, 145.7, 144.1, 138.5, 136.7, 134.0, 130.7, 130.6, 129.2, 128.1, 127.7, 126.7, 124.9, 121.8, 21.4; HRMS (ESI) m/z calcd for $\text{C}_{16}\text{H}_{11}\text{N}_3\text{O} [\text{M}+\text{H}]^+$ 262.0975, found 262.0975.



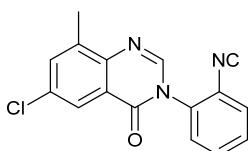
3-(2-Isocyanophenyl)-7-methylquinazolin-4(3H)-one (1l, 459.9 mg, 44% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 2/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): δ = 8.24 (d, J = 8.1 Hz, 1H), 7.97 (s, 1H), 7.62-7.54 (m, 4H), 7.49-7.47 (m, 1H), 7.38 (d, J = 8.1 Hz, 1H), 2.53 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3): δ = 170.2, 160.0, 147.9, 146.3, 144.9, 133.9, 130.7, 130.6, 129.6, 129.3, 128.1, 127.7, 127.1, 125.0, 119.6, 22.0; HRMS (ESI) m/z calcd for $\text{C}_{16}\text{H}_{11}\text{N}_3\text{O} [\text{M}+\text{H}]^+$ 262.0975, found 262.0979.



3-(2-Isocyanophenyl)-8-methylquinazolin-4(3H)-one (1m, 658.4 mg, 63% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 2/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): δ = 8.22-8.19 (m, 1H), 8.01 (s, 1H), 7.67 (d, J = 7.4 Hz, 1H), 7.62-7.53 (m, 3H), 7.49-7.42 (m, 2H), 2.65 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3): δ = 170.2, 160.4, 146.3, 143.6, 136.4, 135.8, 134.0, 130.7, 130.6, 129.3, 128.1, 127.6, 125.0, 123.8, 122.1, 17.6; HRMS (ESI) m/z calcd for $\text{C}_{16}\text{H}_{11}\text{N}_3\text{O} [\text{M}+\text{H}]^+$ 262.0975, found 262.0968.

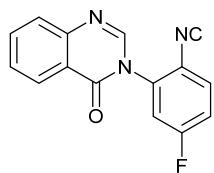


3-(2-Isocyanophenyl)-7,8-dimethylquinazolin-4(3H)-one (1n, 649.7 mg, 59% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 2/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): δ = 8.12 (d, J = 8.1 Hz, 1H), 7.98 (s, 1H), 7.62-7.54 (m, 3H), 7.49-7.47 (m, 1H), 7.37 (d, J = 8.1 Hz, 1H), 2.59 (s, 3H), 2.47 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3): δ = 170.1, 160.5, 146.1, 144.4, 143.3, 134.5, 134.1, 130.6, 130.5, 129.9, 129.3, 128.1, 124.9, 124.1, 120.0, 21.2, 13.3; HRMS (ESI) m/z calcd for $\text{C}_{17}\text{H}_{13}\text{N}_3\text{O} [\text{M}+\text{H}]^+$ 276.1131, found 276.1120.

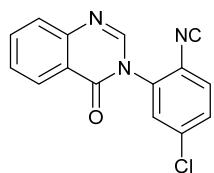


6-Chloro-3-(2-isocyanophenyl)-8-methylquinazolin-4(3H)-one (1o, 674.3 mg, 57% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 2/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): δ = 8.15 (d, J = 2.5 Hz, 1H), 7.98 (s, 1H), 7.62-7.57 (m, 4H), 7.48-7.46 (m, 1H), 2.63 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3): δ = 170.4, 159.4, 145.0,

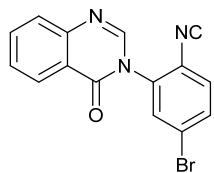
143.8, 138.8, 135.8, 133.6, 133.4, 130.78, 130.75, 129.1, 128.2, 124.8, 124.2, 123.2, 17.5; HRMS (ESI) m/z calcd for $C_{16}H_{10}ClN_3O$ [M+H]⁺ 296.0585, found 296.0593.



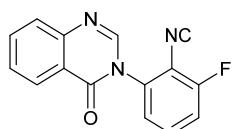
3-(5-Fluoro-2-isocyanophenyl)quinazolin-4(3H)-one (1p) (456.2 mg, 43% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 2/1) gave yellow solid; ¹H NMR (400 MHz, CDCl₃): δ = 8.38-8.36 (m, 1H), 7.99 (s, 1H), 7.88-7.79 (m, 2H), 7.65-7.58 (m, 2H), 7.33-7.26 (m, 2H); ¹³C NMR (101 MHz, CDCl₃): δ = 170.6, 162.2 (d, J_{C-F} = 256.9 Hz), 159.7, 147.6, 144.2, 135.4, 135.3, 129.7 (d, J_{C-F} = 9.5 Hz), 128.3, 128.0, 127.3, 122.0, 118.0 (d, J_{C-F} = 23.1 Hz), 117.3 (d, J_{C-F} = 25.2 Hz); HRMS (ESI) m/z calcd for $C_{15}H_8FN_3O$ [M+H]⁺ 266.0724, found 266.0715.



3-(5-Chloro-2-isocyanophenyl)quinazolin-4(3H)-one (1q) (450.7 mg, 40% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 2/1) gave yellow solid; ¹H NMR (400 MHz, CDCl₃): δ = 8.38-8.35 (m, 1H), 7.97 (s, 1H), 7.87-7.79 (m, 2H), 7.61-7.52 (m, 4H); ¹³C NMR (101 MHz, CDCl₃): δ = 171.7, 159.8, 147.6, 144.2, 136.4, 135.3, 134.8, 131.0, 129.7, 129.0, 128.3, 128.0, 127.3, 124.4, 122.0; HRMS (ESI) m/z calcd for $C_{15}H_8ClN_3O$ [M+H]⁺ 282.0429, found 282.0418.

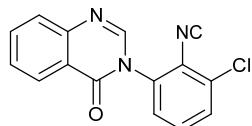


3-(5-Bromo-2-isocyanophenyl)quinazolin-4(3H)-one (1r) (587.1 mg, 45% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 2/1) gave yellow solid; ¹H NMR (400 MHz, CDCl₃): δ = 8.36-8.34 (m, 1H), 7.97 (s, 1H), 7.86-7.82 (m, 1H), 7.80-7.77 (m, 1H), 7.72-7.66 (m, 2H), 7.60-7.56 (m, 1H), 7.48 (d, J = 8.5 Hz, 1H); ¹³C NMR (101 MHz, CDCl₃): δ = 171.9, 159.8, 147.6, 144.2, 135.3, 134.8, 133.9, 132.5, 129.1, 128.3, 128.0, 127.3, 124.0, 123.9, 121.9; HRMS (ESI) m/z calcd for $C_{15}H_8BrN_3O$ [M+H]⁺ 325.9924, found 325.9917.

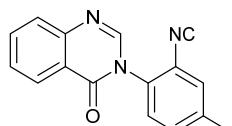


3-(3-Fluoro-2-isocyanophenyl)quinazolin-4(3H)-one (1s) (318.3 mg, 30% yield), flash

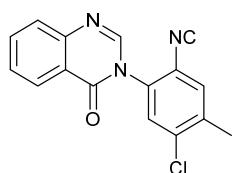
column chromatography on silica gel (petroleum ether/ethyl acetate 2/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): $\delta = 8.36$ (d, $J = 8.0$ Hz, 1H), 7.99 (s, 1H), 7.86-7.78 (m, 2H), 7.61-7.56 (m, 2H), 7.41 (t, $J = 8.5$ Hz, 1H), 7.30 (d, $J = 8.1$ Hz, 1H); ^{13}C NMR (101 MHz, CDCl_3): $\delta = 176.3, 159.7, 158.2$ (d, $J_{\text{C}-\text{F}} = 261.2$ Hz), 147.6, 144.3, 135.3, 135.2, 131.0 (d, $J_{\text{C}-\text{F}} = 8.9$ Hz), 128.3, 128.0, 127.4, 124.5 (d, $J_{\text{C}-\text{F}} = 3.6$ Hz), 121.9, 117.9 (d, $J_{\text{C}-\text{F}} = 18.9$ Hz); HRMS (ESI) m/z calcd for $\text{C}_{15}\text{H}_8\text{FN}_3\text{O} [\text{M}+\text{H}]^+$ 266.0724, found 266.0717.



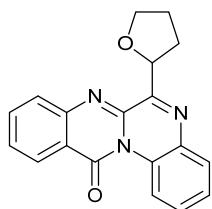
3-(3-Chloro-2-isocyanophenyl)quinazolin-4(3H)-one (1t) (428.2 mg, 38% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 2/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): $\delta = 8.38-7.36$ (m, 1H), 7.99 (s, 1H), 7.88-7.79 (m, 2H), 7.70-7.67 (m, 1H), 7.61-7.53 (m, 2H), 7.42-7.40 (m, 1H); ^{13}C NMR (101 MHz, CDCl_3): $\delta = 175.3, 159.8, 147.7, 144.3, 135.3, 135.2, 132.8, 131.3, 130.5, 128.3, 128.0, 127.5, 127.4, 125.5, 122.0$; HRMS (ESI) m/z calcd for $\text{C}_{15}\text{H}_8\text{ClN}_3\text{O} [\text{M}+\text{H}]^+$ 282.0429, found 282.0422.



3-(2-Isocyano-4-methylphenyl)quinazolin-4(3H)-one (1u) (480.8 mg, 46% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 2/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): $\delta = 8.37-8.34$ (m, 1H), 7.98 (s, 1H), 7.84-7.76 (m, 2H), 7.58-7.54 (m, 1H), 7.41-7.33 (m, 3H), 2.45 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3): $\delta = 169.7, 160.1, 147.8, 145.1, 141.5, 135.0, 131.4, 131.2, 128.8, 128.5, 128.0, 127.9, 127.3, 124.5, 122.2, 21.1$; HRMS (ESI) m/z calcd for $\text{C}_{16}\text{H}_{11}\text{N}_3\text{O} [\text{M}+\text{H}]^+$ 262.0975, found 262.0983.



3-(5-Chloro-2-isocyano-4-methylphenyl)quinazolin-4(3H)-one (1v) (508.7 mg, 43% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 2/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): $\delta = 8.36-8.33$ (m, 1H), 7.96 (s, 1H), 7.85-7.76 (m, 2H), 7.59-7.55 (m, 1H), 7.48 (d, $J = 1.9$ Hz, 2H), 2.45 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3): $\delta = 171.0, 159.9, 147.7, 144.5, 139.8, 136.3, 135.2, 132.1, 129.7, 128.2, 128.0, 127.6, 127.3, 123.1, 122.0, 20.0$; HRMS (ESI) m/z calcd for $\text{C}_{16}\text{H}_{10}\text{ClN}_3\text{O} [\text{M}+\text{H}]^+$ 296.0585, found 296.0595.



6-(Tetrahydrofuran-2-yl)-12*H*-quinoxalino[2,1-*b*]quinazolin-12-one (3aa, 45.7 mg, 72% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): δ = 9.59-9.56 (m, 1H), 8.46-8.44 (m, 1H), 8.01-7.99 (m, 1H), 7.87-7.81 (m, 2H), 7.61-7.51 (m, 3H), 5.95-5.91 (m, 1H), 4.33-4.28 (m, 1H), 4.12-4.07 (m, 1H), 2.70-2.62 (m, 1H), 2.20-2.06 (m, 3H); ^{13}C NMR (101 MHz, CDCl_3): δ = 161.9, 161.5, 145.4, 138.5, 135.0, 134.8, 130.2, 129.3, 128.1, 128.0, 127.9, 127.3, 127.2, 121.3, 120.4, 77.3, 69.4, 31.5, 25.7; HRMS (ESI) m/z calcd for $\text{C}_{19}\text{H}_{15}\text{N}_3\text{O}_2$ [$\text{M}+\text{H}]^+$ 318.1237, found 318.1224.

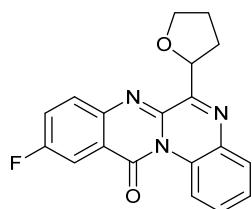


11-Fluoro-6-(tetrahydrofuran-2-yl)-12*H*-quinoxalino[2,1-*b*]quinazolin-12-one (3ba, 44.9 mg, 67% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): δ = 9.41-9.39 (m, 1H), 7.99-7.97 (m, 1H), 7.78-7.73 (m, 1H), 7.65-7.62 (m, 1H), 7.57-7.50 (m, 2H), 7.24-7.19 (m, 1H), 5.89-5.85 (m, 1H), 4.30-4.24 (m, 1H), 4.10-4.05 (m, 1H), 2.65-2.58 (m, 1H), 2.20-2.05 (m, 3H); ^{13}C NMR (101 MHz, CDCl_3): δ = 161.3 (d, $J_{\text{C}-\text{F}} = 268.4$ Hz), 161.1, 158.9 (d, $J_{\text{C}-\text{F}} = 4.8$ Hz), 147.4, 139.1, 135.1 (d, $J_{\text{C}-\text{F}} = 10.5$ Hz), 135.0, 130.2, 129.5, 127.5, 127.4, 123.9 (d, $J_{\text{C}-\text{F}} = 4.4$ Hz), 120.1, 114.2 (d, $J_{\text{C}-\text{F}} = 20.9$ Hz), 110.8 (d, $J_{\text{C}-\text{F}} = 5.1$ Hz), 77.2, 69.4, 31.4, 25.7; HRMS (ESI) m/z calcd for $\text{C}_{19}\text{H}_{14}\text{FN}_3\text{O}_2$ [$\text{M}+\text{H}]^+$ 336.1143, found 336.1143.

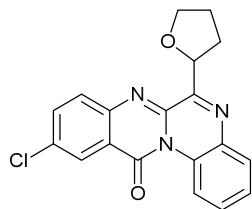


11-Chloro-6-(tetrahydrofuran-2-yl)-12*H*-quinoxalino[2,1-*b*]quinazolin-12-one (3ca, 52.1 mg, 74% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): δ = 9.30-9.28 (m, 1H), 7.99-7.97 (m, 1H), 7.75-7.72 (m, 1H), 7.66 (t, $J = 7.9$ Hz, 1H), 7.56-7.51 (m, 3H), 5.88-5.85 (m, 1H), 4.31-4.25 (m, 1H), 4.10-4.05 (m, 1H), 2.65-2.57 (m, 1H), 2.20-2.05 (m, 3H); ^{13}C NMR (101 MHz, CDCl_3): δ = 161.1, 159.8, 147.8, 138.9, 135.1, 134.3, 134.0, 130.4, 130.2, 129.4, 127.4, 127.3, 127.2, 120.0, 118.2, 77.1, 69.4, 31.4, 25.8; HRMS (ESI) m/z calcd for $\text{C}_{19}\text{H}_{14}\text{ClN}_3\text{O}_2$ [$\text{M}+\text{H}]^+$

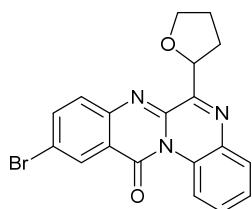
352.0847, found 352.0842.



10-Fluoro-6-(tetrahydrofuran-2-yl)-12*H*-quinoxalino[2,1-*b*]quinazolin-12-one (3da, 41.6 mg, 62% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): δ = 9.58-9.55 (m, 1H), 8.09-8.06 (m, 1H), 8.01-7.99 (m, 1H), 7.90-7.87 (m, 1H), 7.61-7.56 (m, 3H), 5.93-5.90 (m, 1H), 4.32-4.26 (m, 1H), 4.12-4.07 (m, 1H), 2.67-2.59 (m, 1H), 2.22-2.06 (m, 3H); ^{13}C NMR (101 MHz, CDCl_3): δ = 161.6 (d, $J_{\text{C}-\text{F}} = 251.8$ Hz), 161.3, 161.2 (d, $J_{\text{C}-\text{F}} = 3.8$ Hz), 142.1 (d, $J_{\text{C}-\text{F}} = 2.0$ Hz), 137.9 (d, $J_{\text{C}-\text{F}} = 2.2$ Hz), 135.1, 130.6 (d, $J_{\text{C}-\text{F}} = 8.2$ Hz), 130.2, 129.4, 127.9, 127.5, 123.8 (d, $J_{\text{C}-\text{F}} = 24.4$ Hz), 122.5 (d, $J_{\text{C}-\text{F}} = 8.8$ Hz), 120.4, 112.1 (d, $J_{\text{C}-\text{F}} = 24.2$ Hz), 77.3, 69.4, 31.4, 25.8; HRMS (ESI) m/z calcd for $\text{C}_{19}\text{H}_{14}\text{FN}_3\text{O}_2$ [$\text{M}+\text{H}]^+$ 336.1143, found 336.1140.

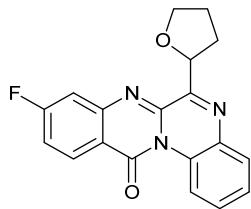


10-Chloro-6-(tetrahydrofuran-2-yl)-12*H*-quinoxalino[2,1-*b*]quinazolin-12-one (3ea, 47.8 mg, 68% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): δ = 9.54-9.51 (m, 1H), 8.38-8.38 (m, 1H), 8.01-7.98 (m, 1H), 7.81-7.74 (m, 2H), 7.59-7.52 (m, 2H), 5.92-5.88 (m, 1H), 4.31-4.26 (m, 1H), 4.11-4.06 (m, 1H), 2.66-2.58 (m, 1H), 2.21-2.06 (m, 3H); ^{13}C NMR (101 MHz, CDCl_3): δ = 161.3, 160.8, 143.9, 138.5, 135.3, 135.0, 133.9, 130.2, 129.7, 129.5, 127.9, 127.6, 126.6, 122.1, 120.3, 77.3, 69.4, 31.4, 25.8; HRMS (ESI) m/z calcd for $\text{C}_{19}\text{H}_{14}\text{ClN}_3\text{O}_2$ [$\text{M}+\text{Na}]^+$ 374.0667, found 374.0665.

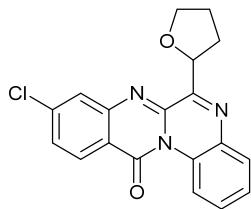


10-Bromo-6-(tetrahydrofuran-2-yl)-12*H*-quinoxalino[2,1-*b*]quinazolin-12-one (3fa, 58.6 mg, 74% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): δ = 9.51-9.49 (m, 1H), 8.53 (d, $J = 2.3$ Hz, 1H), 7.99-7.97 (m, 1H), 7.89-7.87 (m, 1H), 7.70 (d, $J = 8.7$ Hz, 1H), 7.58-7.50 (m, 2H), 5.91-5.87 (m, 1H), 4.30-4.25 (m, 1H), 4.11-4.05 (m, 1H), 2.65-2.57 (m, 1H), 2.20-2.03 (m, 3H); ^{13}C NMR (101 MHz, CDCl_3): δ = 161.3, 160.7, 144.2, 138.6, 138.0, 135.0, 130.2, 129.8,

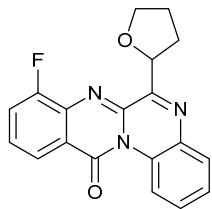
129.7, 129.5, 127.9, 127.5, 122.4, 121.7, 120.3, 77.3, 69.4, 31.4, 25.8; HRMS (ESI) m/z calcd for C₁₉H₁₄BrN₃O₂ [M+H]⁺ 396.0342, found 396.0328.



9-Fluoro-6-(tetrahydrofuran-2-yl)-12*H*-quinoxalino[2,1-*b*]quinazolin-12-one (3ga, 42.9 mg, 64% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave yellow solid; ¹H NMR (400 MHz, CDCl₃): δ = 9.55-9.53 (m, 1H), 8.47-8.43 (m, 1H), 8.02-7.99 (m, 1H), 7.59-7.52 (m, 2H), 7.50-7.47 (m, 1H), 7.33-7.28 (m, 1H), 5.91-5.88 (m, 1H), 4.32-4.26 (m, 1H), 4.12-4.06 (m, 1H), 2.67-2.59 (m, 1H), 2.20-2.06 (m, 3H); ¹³C NMR (101 MHz, CDCl₃): δ = 166.7 (d, J_{C-F} = 257.0 Hz), 161.2, 161.1, 147.5 (d, J_{C-F} = 13.4 Hz), 139.4, 135.0, 130.25, 130.23 (d, J_{C-F} = 10.8 Hz), 129.5, 127.9, 127.4, 120.3, 117.97 (d, J_{C-F} = 1.8 Hz), 117.0 (d, J_{C-F} = 23.9 Hz), 112.9 (d, J_{C-F} = 21.8 Hz), 77.3, 69.4, 31.5, 25.7; HRMS (ESI) m/z calcd for C₁₉H₁₄FN₃O₂ [M+H]⁺ 336.1143, found 336.1142.

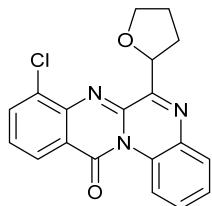


9-Chloro-6-(tetrahydrofuran-2-yl)-12*H*-quinoxalino[2,1-*b*]quinazolin-12-one (3ha, 49.3 mg, 70% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave yellow solid; ¹H NMR (400 MHz, CDCl₃): δ = 9.55-9.53 (m, 1H), 8.36 (d, J = 8.6 Hz, 1H), 8.02-8.00 (m, 1H), 7.86 (d, J = 2.0 Hz, 1H), 7.60-7.51 (m, 3H), 5.90-5.87 (m, 1H), 4.32-4.27 (m, 1H), 4.12-4.07 (m, 1H), 2.68-2.60 (m, 1H), 2.18-2.06 (m, 3H); ¹³C NMR (101 MHz, CDCl₃): δ = 161.4, 161.3, 146.3, 141.2, 139.3, 135.0, 130.3, 129.6, 128.9, 128.6, 127.9, 127.5, 127.3, 120.3, 119.6, 77.3, 69.4, 31.5, 25.7; HRMS (ESI) m/z calcd for C₁₉H₁₄ClN₃O₂ [M+H]⁺ 352.0847, found 352.0852.

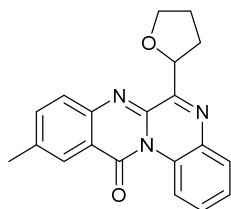


8-Fluoro-6-(tetrahydrofuran-2-yl)-12*H*-quinoxalino[2,1-*b*]quinazolin-12-one (3ia, 53.7 mg, 80% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave yellow solid; ¹H NMR (400 MHz, CDCl₃): δ = 9.54-9.51 (m, 1H), 8.22-8.19 (m, 1H), 8.03-8.00 (m, 1H), 7.59-7.49 (m, 4H), 5.91-5.88 (m, 1H), 4.33-4.27 (m, 1H), 4.11-4.06 (m, 1H), 2.76-2.69 (m, 1H), 2.17-2.07 (m, 3H); ¹³C NMR (101 MHz, CDCl₃): δ = 161.6, 161.0 (d,

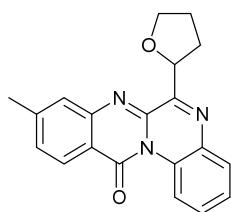
$J_{C-F} = 3.2$ Hz), 157.3 (d, $J_{C-F} = 259.9$ Hz), 138.5, 135.3, 135.1, 130.3, 129.5, 128.0 (d, $J_{C-F} = 7.6$ Hz), 127.8, 127.6, 123.0, 122.8 (d, $J_{C-F} = 4.6$ Hz), 120.3, 120.0 (d, $J_{C-F} = 18.4$ Hz), 77.7, 69.4, 31.7, 25.8; HRMS (ESI) m/z calcd for $C_{19}H_{14}FN_3O_2 [M+H]^+$ 336.1143, found 336.1138.



8-Chloro-6-(tetrahydrofuran-2-yl)-12H-quinoxalino[2,1-b]quinazolin-12-one (3ja, 51.4 mg, 73% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave yellow solid; 1H NMR (400 MHz, $CDCl_3$): $\delta = 9.52\text{-}9.48$ (m, 1H), 8.29-8.27 (m, 1H), 8.03-8.00 (m, 1H), 7.87-7.84 (m, 1H), 7.57-7.51 (m, 2H), 7.44 (t, $J = 7.9$ Hz, 1H), 5.90-5.87 (m, 1H), 4.33-4.27 (m, 1H), 4.12-4.07 (m, 1H), 2.86-2.80 (m, 1H), 2.14-2.05 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): $\delta = 161.8, 161.3, 142.1, 138.4, 135.1, 134.8, 132.6, 130.3, 129.5, 127.8, 127.7, 127.6, 126.0, 122.6, 120.2, 77.9, 69.4, 32.0, 25.8$; HRMS (ESI) m/z calcd for $C_{19}H_{14}ClN_3O_2 [M+H]^+$ 352.0847, found 352.0854.

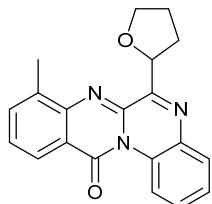


10-Methyl-6-(tetrahydrofuran-2-yl)-12H-quinoxalino[2,1-b]quinazolin-12-one (3ka, 45.1 mg, 68% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave yellow solid; 1H NMR (400 MHz, $CDCl_3$): $\delta = 9.59\text{-}9.56$ (m, 1H), 8.24-8.22 (m, 1H), 8.00-7.98 (m, 1H), 7.76-7.74 (m, 1H), 7.67-7.63 (m, 1H), 7.58-7.50 (m, 2H), 5.94-5.90 (m, 1H), 4.33-4.27 (m, 1H), 4.12-4.06 (m, 1H), 2.67-2.62 (m, 1H), 2.54 (s, 3H), 2.20-2.04 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): $\delta = 161.9, 161.5, 143.4, 138.9, 137.9, 136.4, 135.0, 130.1, 129.2, 128.3, 127.9, 127.2, 126.6, 121.0, 120.4, 77.3, 69.4, 31.5, 25.7, 21.7$; HRMS (ESI) m/z calcd for $C_{20}H_{17}N_3O_2 [M+H]^+$ 332.1394, found 332.1389.

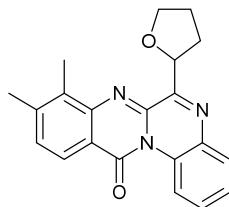


9-Methyl-6-(tetrahydrofuran-2-yl)-12H-quinoxalino[2,1-b]quinazolin-12-one (3la, 48.3 mg, 73% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave yellow solid; 1H NMR (400 MHz, $CDCl_3$): $\delta = 9.59\text{-}9.56$ (m, 1H), 8.31 (d, $J = 8.2$ Hz, 1H), 8.00-7.97 (m, 1H), 7.63 (s, 1H), 7.57-7.49 (m, 2H), 7.39-7.37 (m, 1H), 5.92-5.89 (m, 1H), 4.33-4.27 (m, 1H), 4.12-4.06 (m, 1H), 2.69-2.61 (m, 1H), 2.52 (s, 3H), 2.17-2.07 (m,

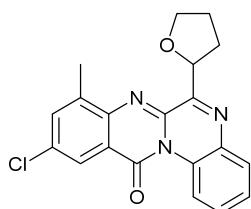
3H); ^{13}C NMR (101 MHz, CDCl_3): δ = 161.9, 161.5, 146.0, 145.5, 138.6, 135.0, 130.1, 129.7, 129.3, 128.3, 127.6, 127.1, 120.4, 118.9, 77.4, 69.4, 31.6, 25.7, 22.0; HRMS (ESI) m/z calcd for $\text{C}_{20}\text{H}_{17}\text{N}_3\text{O}_2$ [$\text{M}+\text{H}]^+$ 332.1394, found 332.1384.



8-Methyl-6-(tetrahydrofuran-2-yl)-12H-quinoxalino[2,1-b]quinazolin-12-one (3ma, 45.1 mg, 68% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): δ = 9.57-9.55 (m, 1H), 8.23-8.21 (m, 1H), 8.00-7.98 (m, 1H), 7.63-7.60 (m, 1H), 7.54-7.50 (m, 2H), 7.41 (t, J = 7.7 Hz, 1H), 5.92-5.89 (m, 1H), 4.34-4.29 (m, 1H), 4.11-4.06 (m, 1H), 2.73-2.67 (m, 1H), 2.65 (s, 3H), 2.14-2.03 (m, 3H); ^{13}C NMR (101 MHz, CDCl_3): δ = 162.1, 161.9, 143.8, 137.2, 136.5, 135.1, 135.0, 130.1, 129.2, 128.1, 127.7, 127.2, 124.9, 121.2, 120.4, 77.6, 69.4, 32.0, 25.6, 17.3; HRMS (ESI) m/z calcd for $\text{C}_{20}\text{H}_{17}\text{N}_3\text{O}_2$ [$\text{M}+\text{H}]^+$ 332.1394, found 332.1387.

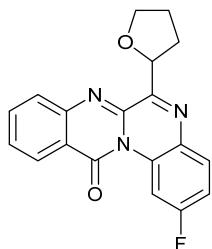


8,9-Dimethyl-6-(tetrahydrofuran-2-yl)-12H-quinoxalino[2,1-b]quinazolin-12-one (3na, 51.1 mg, 74% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): δ = 9.61-9.58 (m, 1H), 8.16 (d, J = 8.2 Hz, 1H), 8.01-7.98 (m, 1H), 7.57-7.49 (m, 2H), 7.35 (d, J = 8.2 Hz, 1H), 5.96-5.93 (m, 1H), 4.36-4.30 (m, 1H), 4.14-4.08 (m, 1H), 2.74-2.69 (m, 1H), 2.60 (s, 3H), 2.43 (s, 3H), 2.15-2.04 (m, 3H); ^{13}C NMR (101 MHz, CDCl_3): δ = 162.2, 162.0, 143.9, 143.5, 137.2, 135.0, 134.4, 130.2, 130.1, 129.2, 128.2, 127.1, 124.1, 120.4, 119.2, 77.6, 69.4, 32.0, 25.6, 20.9, 13.1; HRMS (ESI) m/z calcd for $\text{C}_{21}\text{H}_{19}\text{N}_3\text{O}_2$ [$\text{M}+\text{H}]^+$ 346.1550, found 346.1558.

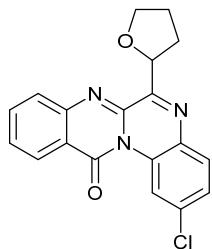


10-Chloro-8-methyl-6-(tetrahydrofuran-2-yl)-12H-quinoxalino[2,1-b]quinazolin-12-one (3oa, 52.0 mg, 71% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): δ = 9.52-9.50 (m, 1H), 8.16 (d, J = 2.3 Hz, 1H), 8.00-7.97 (m, 1H), 7.58 (d, J = 2.4 Hz, 1H), 7.54-7.51 (m, 2H), 5.92-5.88 (m, 1H), 4.33-4.28 (m, 1H), 4.12-4.06 (m, 1H), 2.72-2.67 (m, 1H), 2.64 (s, 3H), 2.14-2.06 (m,

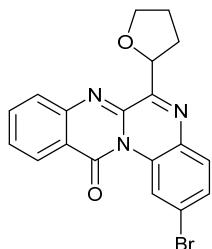
3H); ^{13}C NMR (101 MHz, CDCl_3): δ = 161.7, 161.0, 142.5, 138.8, 137.4, 135.3, 135.1, 133.4, 130.2, 129.4, 127.8, 127.5, 124.1, 122.0, 120.3, 77.4, 69.4, 31.9, 25.7, 17.2; HRMS (ESI) m/z calcd for $\text{C}_{20}\text{H}_{16}\text{ClN}_3\text{O}_2$ [$\text{M}+\text{H}]^+$ 366.1004, found 366.1004.



2-Fluoro-6-(tetrahydrofuran-2-yl)-12H-quinoxalino[2,1-b]quinazolin-12-one (3pa, 49.0 mg, 73% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): δ = 9.44-9.40 (m, 1H), 8.43-8.40 (m, 1H), 7.99-7.95 (m, 1H), 7.84 (d, J = 3.9 Hz, 2H), 7.61-7.57 (m, 1H), 7.27-7.23 (m, 1H), 5.92-5.88 (m, 1H), 4.31-4.26 (m, 1H), 4.12-4.06 (m, 1H), 2.69-2.61 (m, 1H), 2.21-2.04 (m, 3H); ^{13}C NMR (101 MHz, CDCl_3): δ = 161.9 (d, $J_{\text{C}-\text{F}}$ = 248.9 Hz), 161.8, 160.6, 145.3, 138.0, 135.0, 131.7, 131.4 (d, $J_{\text{C}-\text{F}}$ = 9.9 Hz), 128.9 (d, $J_{\text{C}-\text{F}}$ = 12.5 Hz), 128.2, 128.1, 127.3, 120.9, 114.8 (d, $J_{\text{C}-\text{F}}$ = 23.2 Hz), 108.1 (d, $J_{\text{C}-\text{F}}$ = 32.0 Hz), 77.3, 69.4, 31.5, 25.7; HRMS (ESI) m/z calcd for $\text{C}_{19}\text{H}_{14}\text{FN}_3\text{O}_2$ [$\text{M}+\text{H}]^+$ 336.1143, found 336.1138.

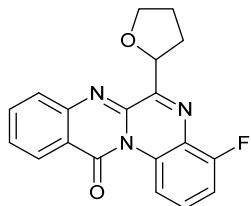


2-Chloro-6-(tetrahydrofuran-2-yl)-12H-quinoxalino[2,1-b]quinazolin-12-one (3qa, 49.3 mg, 78% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): δ = 9.68 (d, J = 2.2 Hz, 1H), 8.44-8.42 (m, 1H), 7.91 (d, J = 8.5 Hz, 1H), 7.87-7.85 (m, 2H), 7.63-7.59 (m, 1H), 7.51-7.48 (m, 1H), 5.92-5.89 (m, 1H), 4.31-4.26 (m, 1H), 4.12-4.06 (m, 1H), 2.70-2.62 (m, 1H), 2.16-2.6 (m, 3H); ^{13}C NMR (101 MHz, CDCl_3): δ = 161.78, 161.77, 145.2, 138.0, 135.09, 135.06, 133.6, 130.9, 128.6, 128.3, 128.1, 127.6, 127.4, 121.1, 120.5, 77.3, 69.4, 31.6, 25.8; HRMS (ESI) m/z calcd for $\text{C}_{19}\text{H}_{14}\text{ClN}_3\text{O}_2$ [$\text{M}+\text{H}]^+$ 352.0847, found 352.0841.

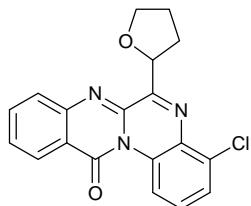


2-Bromo-6-(tetrahydrofuran-2-yl)-12H-quinoxalino[2,1-b]quinazolin-12-one (3ra, 60.2

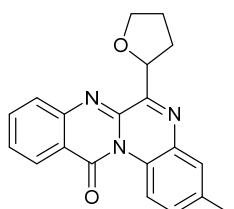
mg, 76% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): δ = 9.85 (t, J = 1.9 Hz, 1H), 8.47-8.44 (m, 1H), 7.88-7.84 (m, 3H), 7.67-7.61 (m, 2H), 5.93-7.89 (m, 1H), 4.31-4.26 (m, 1H), 4.12-4.07 (m, 1H), 2.70-2.63 (m, 1H), 2.20-2.06 (m, 3H); ^{13}C NMR (101 MHz, CDCl_3): δ = 162.0, 161.8, 145.3, 138.0, 135.1, 134.0, 131.1, 130.6, 128.8, 128.4, 128.2, 127.4, 123.4, 123.3, 121.1, 77.3, 69.5, 31.6, 25.8; HRMS (ESI) m/z calcd for $\text{C}_{19}\text{H}_{14}\text{BrN}_3\text{O}_2$ [M+Na] $^+$ 418.0162, found 418.0168.



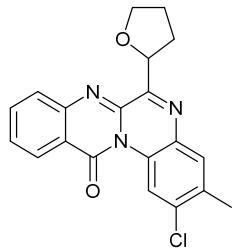
4-Fluoro-6-(tetrahydrofuran-2-yl)-12H-quinoxalino[2,1-b]quinazolin-12-one (3sa, 40.2 mg, 60% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): δ = 9.37-9.34 (m, 1H), 8.45-8.42 (m, 1H), 7.89-7.84 (m, 2H), 7.63-7.59 (m, 1H), 7.54-7.48 (m, 1H), 7.31-7.28 (m, 1H), 6.00-5.96 (m, 1H), 4.33-4.27 (m, 1H), 4.13-4.08 (m, 1H), 2.62-2.53 (m, 1H), 2.32-2.24 (m, 1H), 2.19-2.06 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ = 161.88 (d, $J_{\text{C}-\text{F}} = 2.1$ Hz), 161.81, 157.8 (d, $J_{\text{C}-\text{F}} = 256.9$ Hz), 145.3, 138.2, 135.0, 129.4 (d, $J_{\text{C}-\text{F}} = 8.9$ Hz), 129.3, 128.3, 128.2, 127.4, 125.1 (d, $J_{\text{C}-\text{F}} = 12.8$ Hz), 121.3, 116.0 (d, $J_{\text{C}-\text{F}} = 4.3$ Hz), 113.8 (d, $J_{\text{C}-\text{F}} = 19.3$ Hz), 77.3, 69.4, 31.1, 25.8; HRMS (ESI) m/z calcd for $\text{C}_{19}\text{H}_{14}\text{FN}_3\text{O}_2$ [M+H] $^+$ 336.1143, found 336.1140.



4-Chloro-6-(tetrahydrofuran-2-yl)-12H-quinoxalino[2,1-b]quinazolin-12-one (3ta, 50.0 mg, 71% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): δ = 9.48-9.45 (m, 1H), 8.43-8.40 (m, 1H), 7.89-7.83 (m, 2H), 7.62-7.57 (m, 2H), 7.47-7.43 (m, 1H), 6.08-6.05 (m, 1H), 4.37-4.31 (m, 1H), 4.15-4.09 (m, 1H), 2.54-2.45 (m, 1H), 2.40-2.32 (m, 1H), 2.27-2.17 (m, 1H), 2.14-2.06 (m, 1H); ^{13}C NMR (101 MHz, CDCl_3): δ = 162.2, 161.9, 145.4, 138.1, 135.0, 134.5, 131.9, 129.6, 129.1, 128.3, 128.2, 128.1, 127.4, 121.2, 119.0, 76.8, 69.4, 30.7, 25.5; HRMS (ESI) m/z calcd for $\text{C}_{19}\text{H}_{14}\text{ClN}_3\text{O}_2$ [M+H] $^+$ 352.0847, found 352.0845.

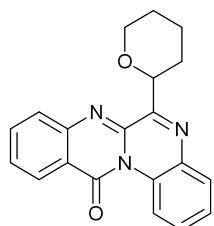


3-Methyl-6-(tetrahydrofuran-2-yl)-12*H*-quinoxalino[2,1-*b*]quinazolin-12-one (3ua, 47.1 mg, 71% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): δ = 9.46-9.43 (m, 1H), 8.43-8.40 (m, 1H), 7.84-7.78 (m, 3H), 7.58-7.53 (m, 1H), 7.36-7.33 (m, 1H), 5.94-5.90 (m, 1H), 4.31-4.26 (m, 1H), 4.11-4.06 (m, 1H), 2.68-2.59 (m, 1H), 2.46 (s, 3H), 2.19-2.05 (m, 3H); ^{13}C NMR (101 MHz, CDCl_3): δ = 161.8, 161.3, 145.4, 138.5, 137.3, 134.9, 134.6, 130.3, 130.1, 128.0, 127.8, 127.2, 125.8, 121.2, 120.1, 77.3, 69.4, 31.5, 25.8, 20.8; HRMS (ESI) m/z calcd for $\text{C}_{20}\text{H}_{17}\text{N}_3\text{O}_2$ [M+H] $^+$ 332.1394, found 332.1391.

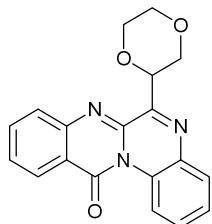


2-Chloro-3-methyl-6-(tetrahydrofuran-2-yl)-12*H*-quinoxalino[2,1-*b*]quinazolin-12-one (3va, 57.8 mg, 79% yield),

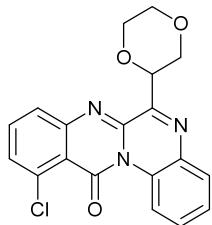
flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): δ = 9.65 (s, 1H), 8.41-8.35 (m, 1H), 7.83-7.81 (m, 3H), 7.60-7.54 (m, 1H), 5.91-5.87 (m, 1H), 4.30-4.25 (m, 1H), 4.11-4.05 (m, 1H), 2.69-2.60 (m, 1H), 2.45 (s, 3H), 2.17-2.06 (m, 3H); ^{13}C NMR (101 MHz, CDCl_3): δ = 161.6, 145.3, 138.0, 135.5, 135.4, 134.9, 133.6, 131.3, 128.1, 128.0, 127.3, 126.4, 121.0, 120.7, 77.3, 69.4, 31.5, 25.8, 19.8; HRMS (ESI) m/z calcd for $\text{C}_{20}\text{H}_{16}\text{ClN}_3\text{O}_2$ [M+H] $^+$ 366.1004, found 366.1010.



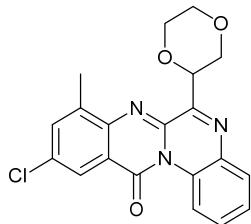
6-(Tetrahydro-2*H*-pyran-2-yl)-12*H*-quinoxalino[2,1-*b*]quinazolin-12-one (3ab, 42.4 mg, 64% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): δ = 9.57-9.55 (m, 1H), 8.46-8.44 (m, 1H), 8.11-8.09 (m, 1H), 7.87-7.82 (m, 2H), 7.62-7.51 (m, 3H), 5.58-5.55 (m, 1H), 4.37-4.32 (m, 1H), 3.84-3.77 (m, 1H), 2.29-2.25 (m, 1H), 2.06-1.99 (m, 1H), 1.94-1.86 (m, 2H), 1.80-1.62 (m, 3H); ^{13}C NMR (101 MHz, CDCl_3): δ = 161.9, 160.7, 145.3, 138.0, 135.1, 134.8, 130.2, 129.4, 127.98, 127.93, 127.90, 127.3, 127.2, 121.2, 120.3, 76.4, 69.6, 31.0, 25.7, 23.9; HRMS (ESI) m/z calcd for $\text{C}_{20}\text{H}_{17}\text{N}_3\text{O}_2$ [M+H] $^+$ 332.1394, found 332.1389.



6-(1,4-Dioxan-2-yl)-12*H*-quinoxalino[2,1-*b*]quinazolin-12-one (3ac, 38.7 mg, 58% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): δ = 9.58-9.55 (m, 1H), 8.45-8.43 (m, 1H), 8.09-8.07 (m, 1H), 7.88-7.83 (m, 2H), 7.62-7.52 (m, 3H), 5.87-5.84 (m, 1H), 4.48-4.45 (m, 1H), 4.21-4.17 (m, 1H), 4.12-4.06 (m, 1H), 3.95-3.86 (m, 2H), 3.75-3.70 (m, 1H); ^{13}C NMR (101 MHz, CDCl_3): δ = 161.8, 157.1, 145.2, 138.1, 135.0, 134.9, 130.3, 130.0, 128.3, 128.0, 127.4, 127.3, 121.2, 120.4, 74.9, 70.4, 67.7, 66.5; HRMS (ESI) m/z calcd for $\text{C}_{19}\text{H}_{15}\text{N}_3\text{O}_3$ [$\text{M}+\text{H}]^+$ 334.1186, found 334.1192.

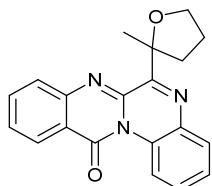


11-Chloro-6-(1,4-dioxan-2-yl)-12*H*-quinoxalino[2,1-*b*]quinazolin-12-one (3cc, 44.1 mg, 60% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): δ = 9.32-9.30 (m, 1H), 8.10-8.07 (m, 1H), 7.80-7.77 (m, 1H), 7.72 (t, J = 7.9 Hz, 1H), 7.61-7.53 (m, 3H), 5.82-5.79 (m, 1H), 4.44-4.41 (m, 1H), 4.20-4.16 (m, 1H), 4.11-4.05 (m, 1H), 3.95-3.86 (m, 2H), 3.75-3.70 (m, 1H); ^{13}C NMR (101 MHz, CDCl_3): δ = 159.6, 156.7, 147.7, 138.5, 135.0, 134.4, 134.3, 130.7, 130.5, 130.1, 127.6, 127.2, 120.0, 118.2, 74.7, 70.3, 67.7, 66.4; HRMS (ESI) m/z calcd for $\text{C}_{19}\text{H}_{14}\text{ClN}_3\text{O}_3$ [$\text{M}+\text{H}]^+$ 368.0796, found 368.0813.

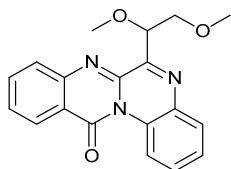


10-Chloro-6-(1,4-dioxan-2-yl)-8-methyl-12*H*-quinoxalino[2,1-*b*]quinazolin-12-one (3oc, 44.3 mg, 58% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): δ = 9.56-9.53 (m, 1H), 8.22 (d, J = 2.4 Hz, 1H), 8.09-8.07 (m, 1H), 7.64-7.54 (m, 3H), 5.80-5.77 (m, 1H), 4.47-4.44 (m, 1H), 4.21-4.17 (m, 1H), 4.11-4.05 (m, 1H), 3.95-3.87 (m, 2H), 3.80-3.75 (m, 1H), 2.70 (s, 3H); ^{13}C

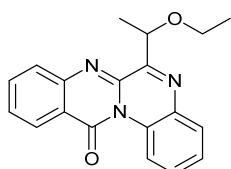
NMR (101 MHz, CDCl₃): δ = 161.0, 157.0, 142.3, 138.9, 137.1, 135.6, 135.0, 133.7, 130.4, 130.1, 127.8, 127.7, 124.2, 122.1, 120.4, 75.1, 70.4, 67.7, 66.5, 17.3; HRMS (ESI) m/z calcd for C₂₀H₁₆ClN₃O₃ [M+H]⁺ 382.0953, found 382.0945.



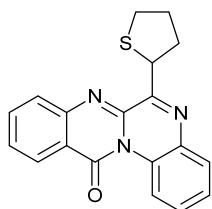
6-(2-Methyltetrahydrofuran-2-yl)-12H-quinoxalino[2,1-b]quinazolin-12-one (3ad, 45.1 mg, 68% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave yellow solid; ¹H NMR (400 MHz, CDCl₃): δ = 9.53-9.50 (m, 1H), 8.47-8.45 (m, 1H), 8.06-8.03 (m, 1H), 7.88-7.84 (m, 2H), 7.63-7.50 (m, 3H), 4.18-4.07 (m, 2H), 2.79-2.71 (m, 1H), 2.49-2.42 (m, 1H), 2.14-2.04 (m, 1H), 1.95 (s, 3H), 1.92-1.87 (m, 1H); ¹³C NMR (101 MHz, CDCl₃): δ = 163.4, 162.1, 144.9, 137.7, 134.8, 134.7, 130.4, 129.3, 128.1, 128.0, 127.8, 127.3, 127.2, 121.1, 120.1, 86.1, 67.7, 37.9, 26.6, 25.6; HRMS (ESI) m/z calcd for C₂₀H₁₇N₃O₂ [M+H]⁺ 332.1394, found 332.1386.



6-(1,2-Dimethoxyethyl)-12H-quinoxalino[2,1-b]quinazolin-12-one (3ae, 23.5 mg, 35% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave yellow solid; ¹H NMR (400 MHz, CDCl₃): δ = 9.62-9.60 (m, 1H), 8.50-8.47 (m, 1H), 8.09-8.06 (m, 1H), 7.91-7.86 (m, 2H), 7.66-7.55 (m, 3H), 5.76 (t, J = 5.0 Hz, 1H), 3.94 (d, J = 5.0 Hz, 2H), 3.58 (s, 3H), 3.47 (s, 3H); ¹³C NMR (101 MHz, CDCl₃): δ = 162.0, 158.2, 145.4, 138.9, 135.1, 135.0, 130.4, 129.8, 128.2, 128.1, 128.0, 127.4, 121.3, 120.4, 78.4, 74.4, 59.5, 58.4; HRMS (ESI) m/z calcd for C₁₉H₁₇N₃O₂ [M+H]⁺ 336.1343, found 336.1355.



6-(1-Ethoxyethyl)-12H-quinoxalino[2,1-b]quinazolin-12-one (3af, 19.2 mg, 30% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave yellow solid; ¹H NMR (400 MHz, CDCl₃): δ = 9.58-9.56 (m, 1H), 8.46-8.44 (m, 1H), 8.05-8.03 (m, 1H), 7.87-7.82 (m, 2H), 7.61-7.52 (m, 3H), 5.73-5.68 (m, 1H), 3.75-3.59 (m, 2H), 1.66 (d, J = 6.5 Hz, 3H), 1.30 (t, J = 7.0 Hz, 3H); ¹³C NMR (101 MHz, CDCl₃): δ = 162.1, 162.0, 145.4, 138.7, 135.2, 134.8, 130.2, 129.4, 128.1, 128.0, 127.9, 127.4, 127.3, 121.2, 120.4, 73.2, 65.3, 20.3, 15.6; HRMS (ESI) m/z calcd for C₁₉H₁₅N₃O₂ [M+Na]⁺ 320.1394, found 320.1386.

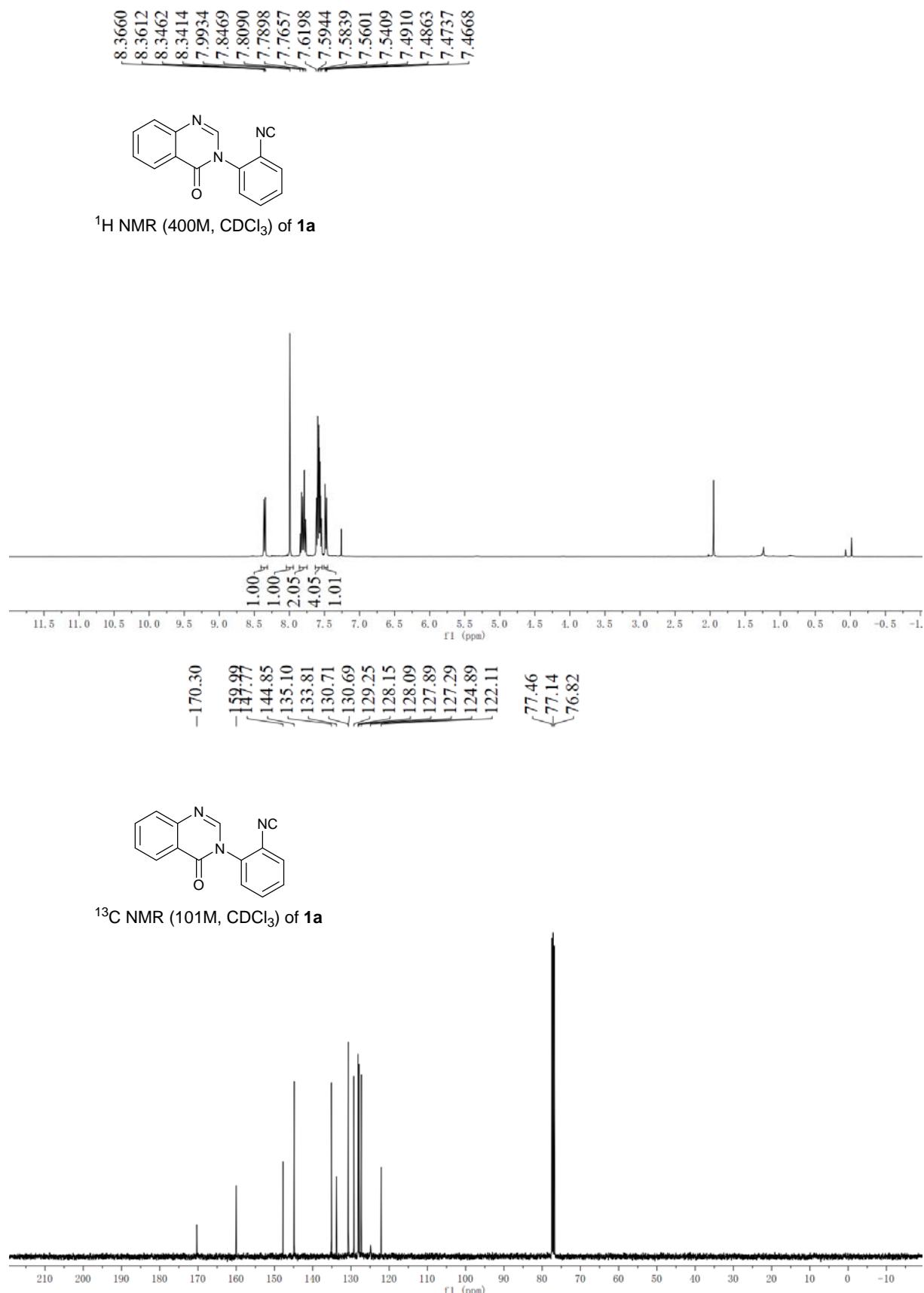


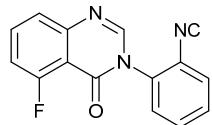
6-(Tetrahydrothiophen-2-yl)-12H-quinoxalino[2,1-b]quinazolin-12-one (3ag, 34.0 mg, 51% yield), flash column chromatography on silica gel (petroleum ether/ethyl acetate 5/1) gave yellow solid; ^1H NMR (400 MHz, CDCl_3): δ = 9.58-9.56 (m, 1H), 8.46-8.43 (m, 1H), 7.92-7.83 (m, 3H), 7.61-7.49 (m, 3H), 5.43-5.40 (m, 1H), 2.99-2.90 (m, 3H), 2.52-2.42 (m, 1H), 2.31-2.14 (m, 2H); ^{13}C NMR (101 MHz, CDCl_3): δ = 162.1, 161.6, 145.3, 139.2, 135.0, 134.8, 129.8, 129.1, 128.2, 128.1, 127.9, 127.3, 127.2, 121.2, 120.5, 47.8, 33.2, 32.1, 31.3; HRMS (ESI) m/z calcd for $\text{C}_{19}\text{H}_{15}\text{N}_3\text{OS} [\text{M}+\text{H}]^+$ 334.1009, found 334.1019.

5. References

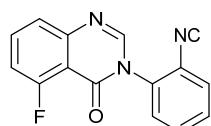
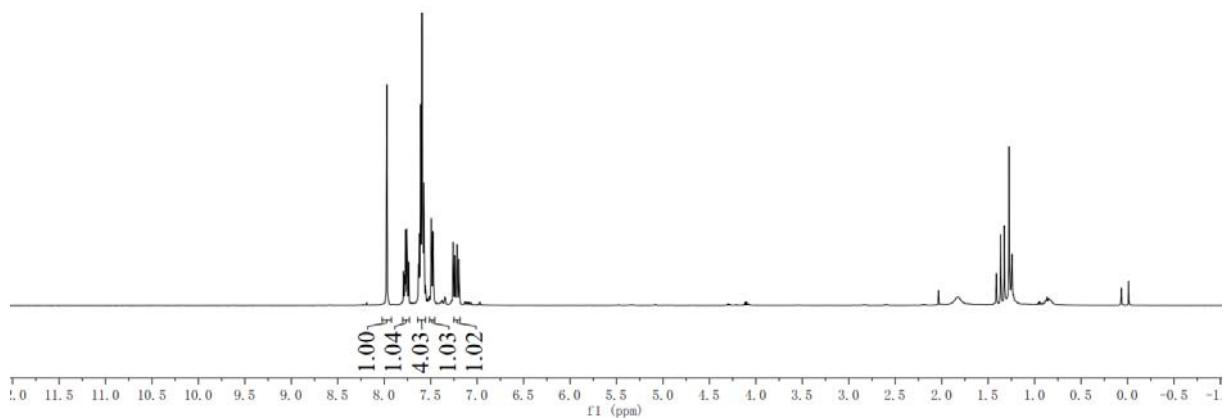
1. A. Banerjee, P. Subramanian and K. P. Kaliappan, *J. Org. Chem.*, 2016, **81**, 10424.
2. V. A. Mamedov, V. L. Mamedova, V. V. Syakaev, D. E. Korshin, G. Z. Khikmatova, E. V. Mironova, O. B. Bazanova, I. Kh. Rizvanov and S. K. Latypov, *Tetrahedron.*, 2017, **73**, 5082.
3. Y. Liu, X.-L. Chen, X.-Y. Li, S.-S. Zhu, S.-J. Li, Y. Song, L.-B. Qu and B. Yu, *J. Am. Chem. Soc.*, 2021, **143**, 964.

6. Copies of the ^1H NMR and ^{13}C NMR Spectra

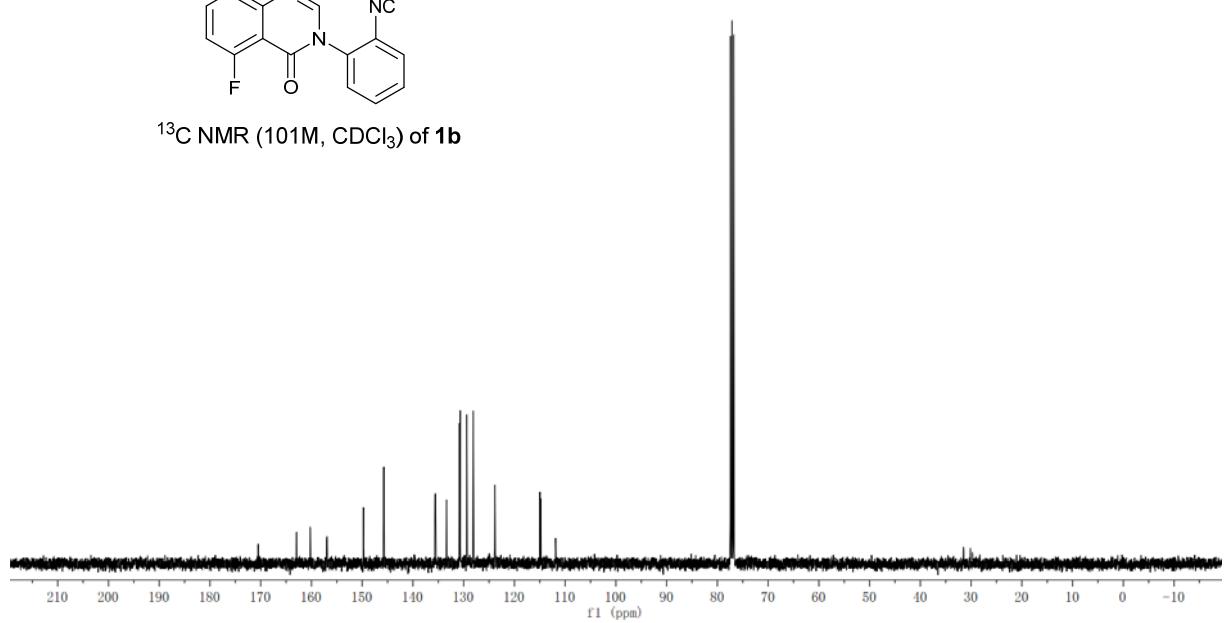




¹H NMR (400M, CDCl₃) of **1b**

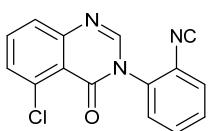
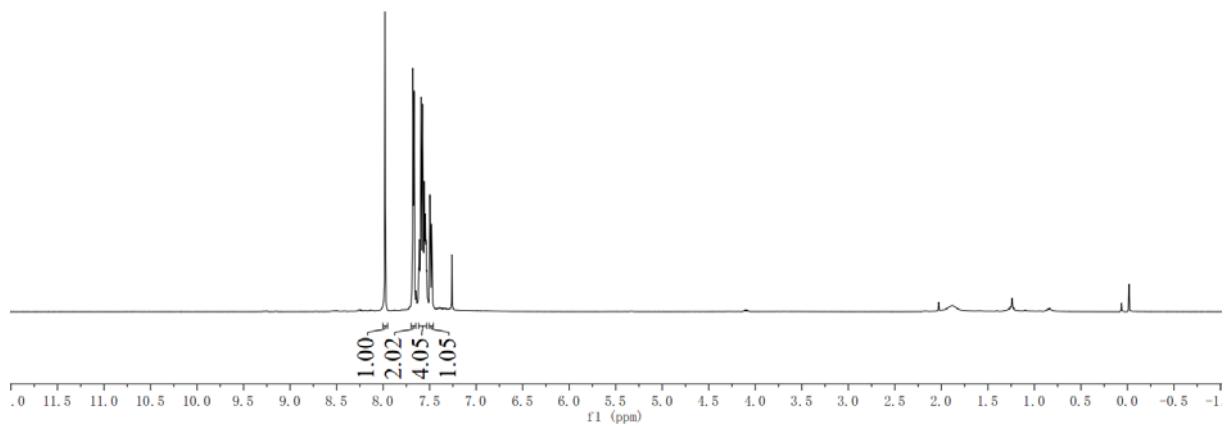


¹³C NMR (101M, CDCl₃) of 1b

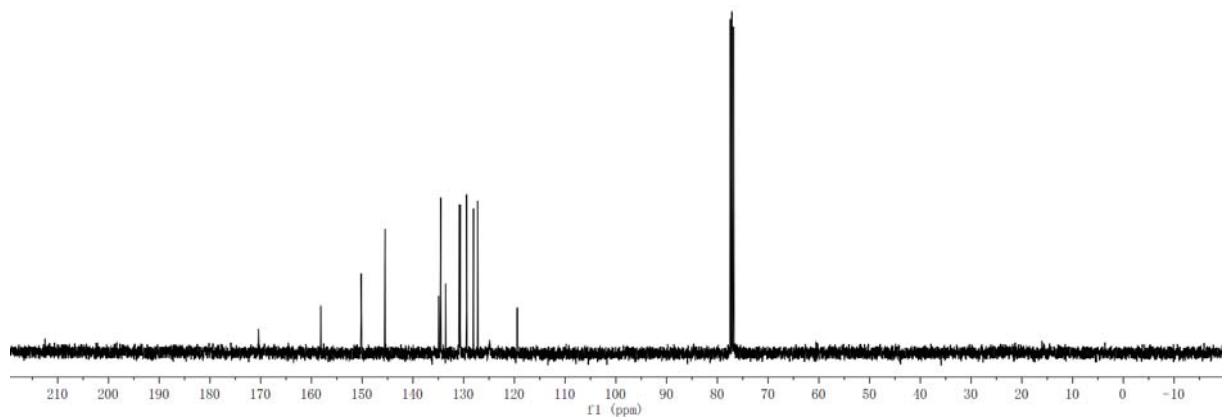


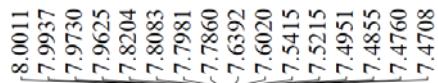


¹H NMR (400M, CDCl₃) of **1c**

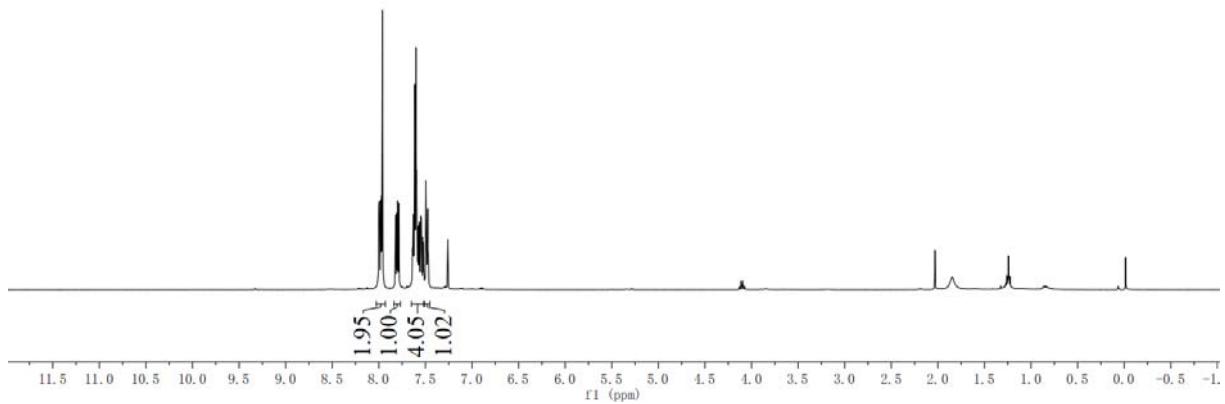


¹³C NMR (101M, CDCl₃) of **1c**

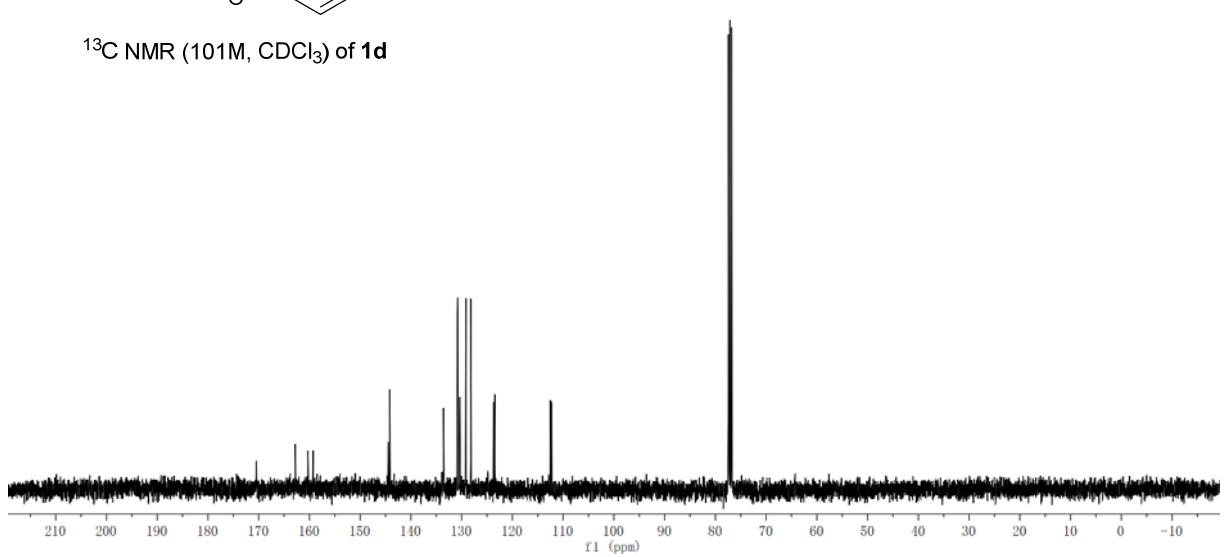
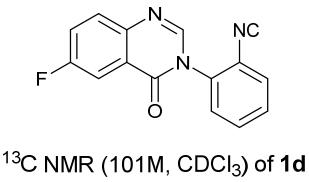


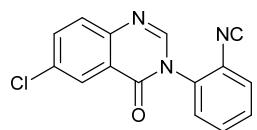


¹H NMR (400M, CDCl₃) of **1d**

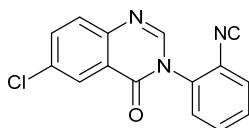
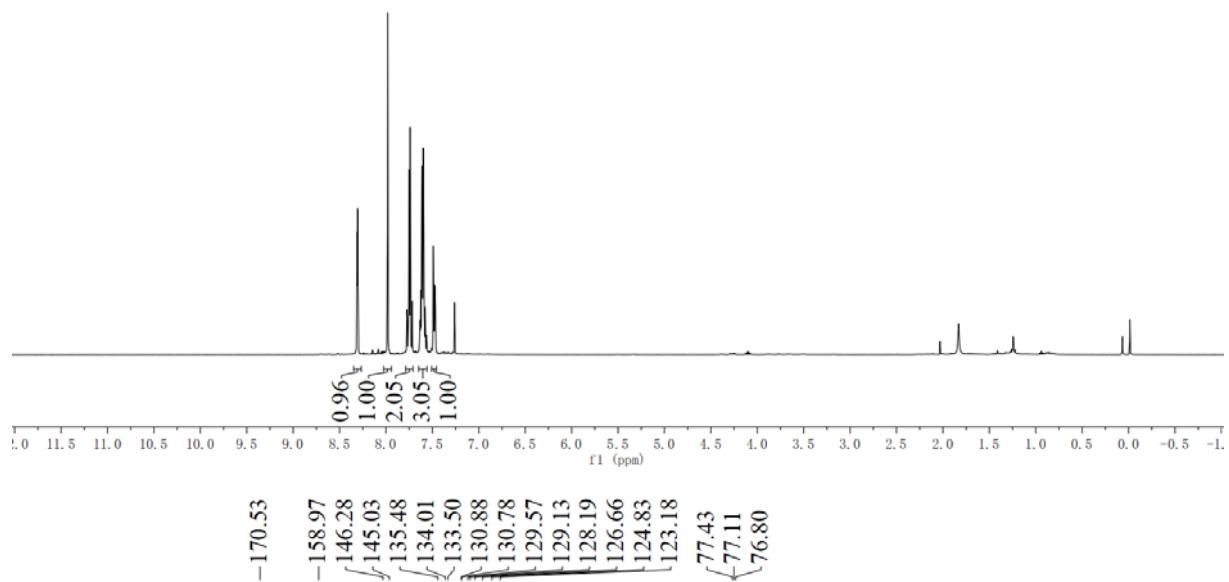


170.449	162.799	160.313	159.301	159.269	144.469	144.448	144.167	144.143	133.570	130.841	130.764	130.440	130.358	129.164	128.185	123.691	123.556	123.453	112.514	112.275
---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------	---------

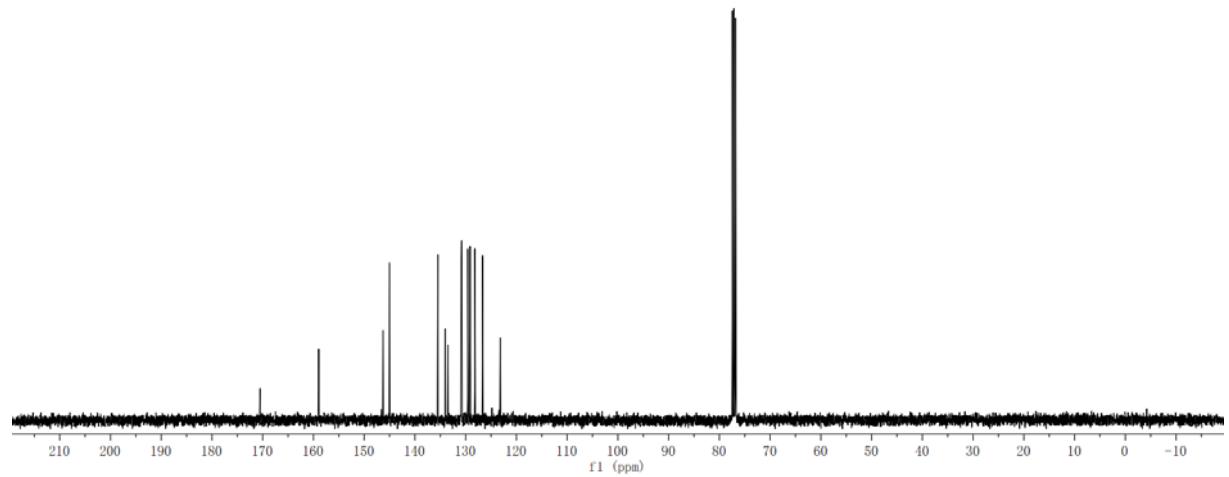




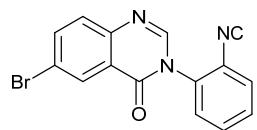
¹H NMR (400M, CDCl₃) of **1e**



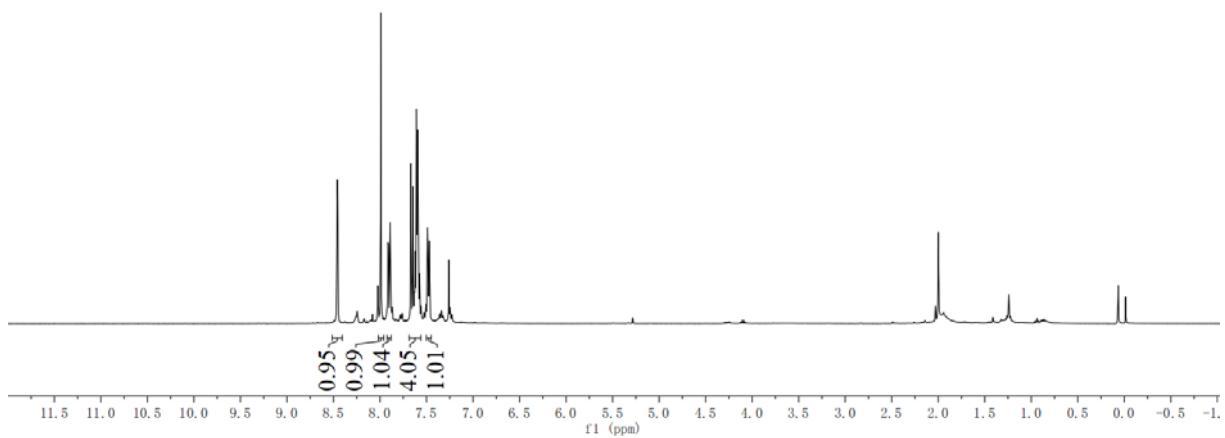
¹³C NMR (101M, CDCl₃) of **1e**



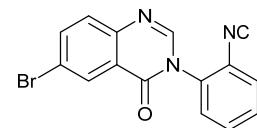
8.4602
 8.4545
 7.9913
 7.9138
 7.9080
 7.8923
 7.8865
 7.6681
 7.6466
 7.6216
 7.5753
 7.4902
 7.4898
 7.4706
 7.4656



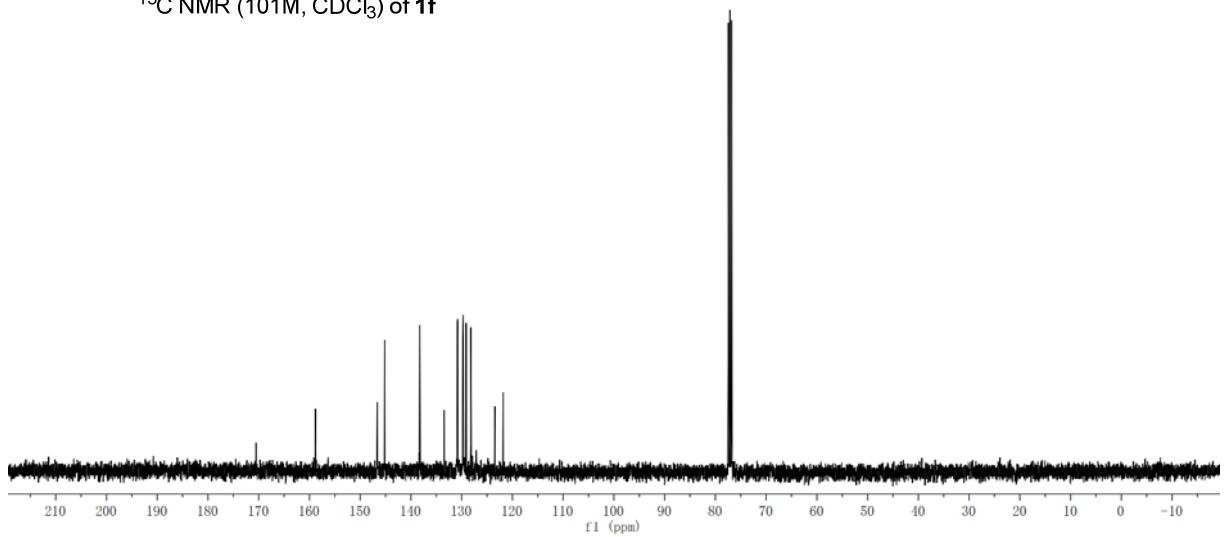
¹H NMR (400M, CDCl₃) of **1f**

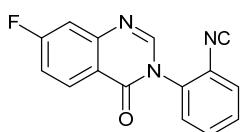
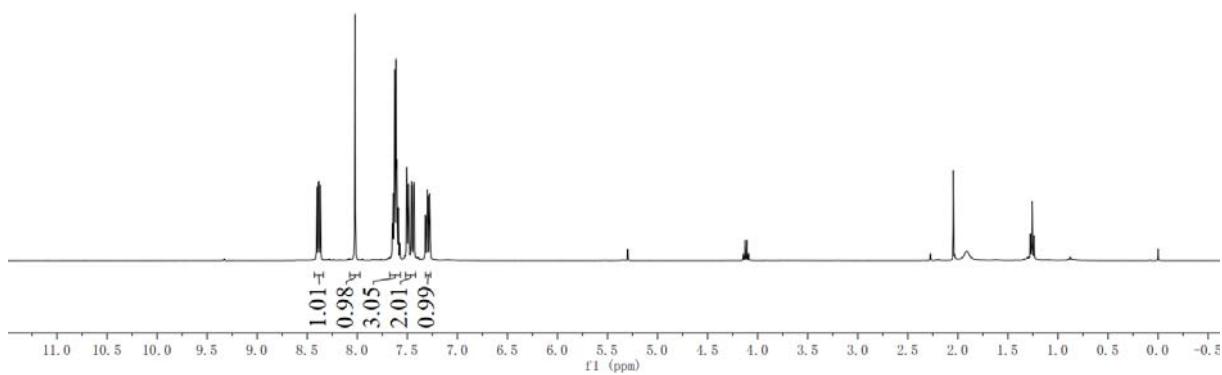
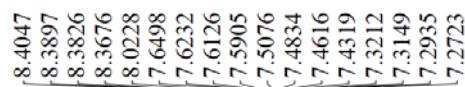


-170.54
 -158.82
 -146.61
 /145.18
 /138.28
 /133.48
 /130.88
 /130.79
 129.81
 129.68
 129.13
 128.19
 127.16
 123.45
 121.82
 77.43
 77.11
 76.79

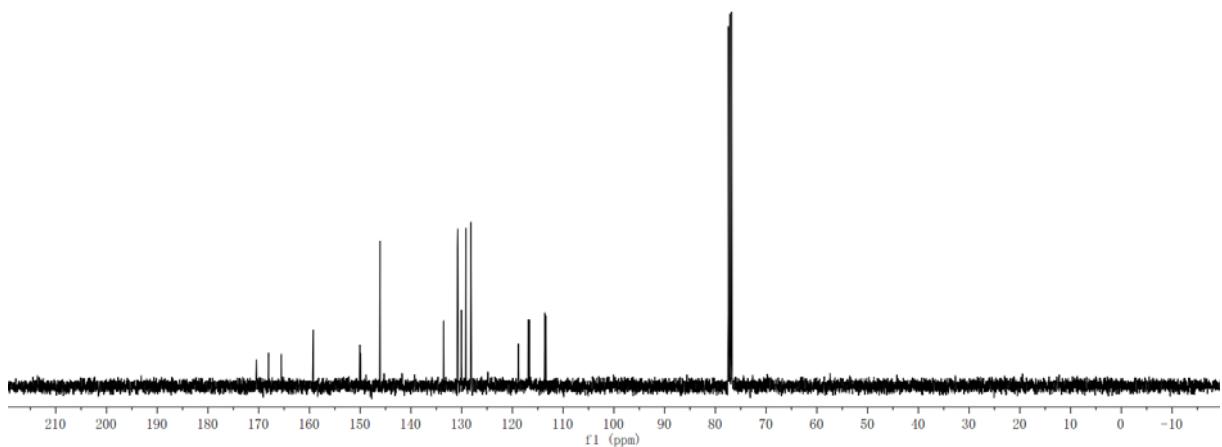


¹³C NMR (101M, CDCl₃) of **1f**

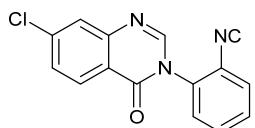




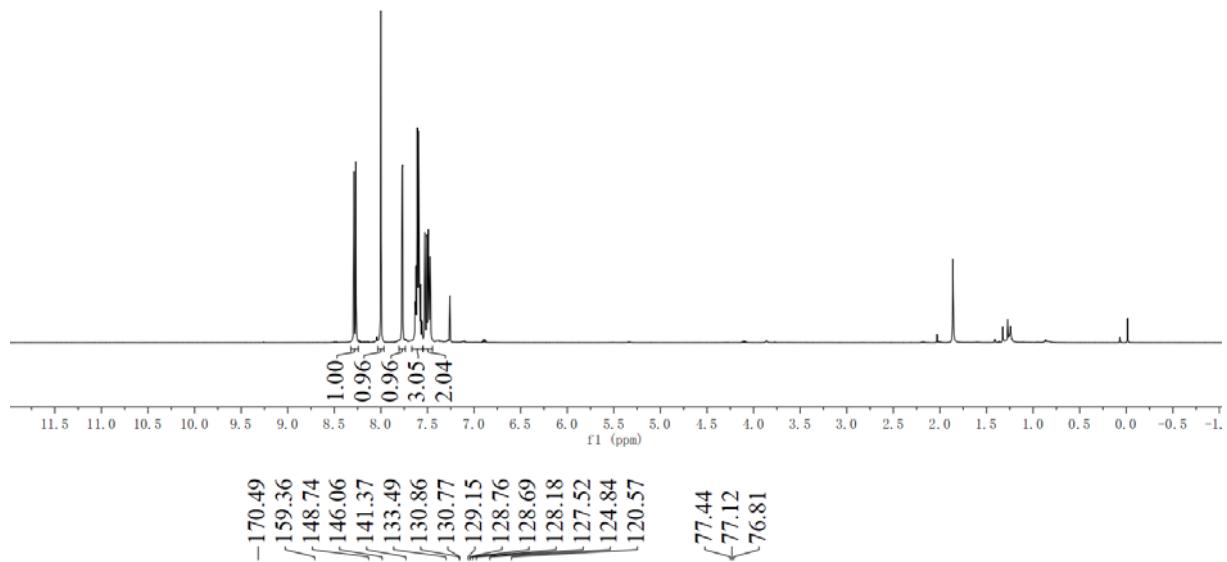
¹³C NMR (101M, CDCl₃) of **1g**



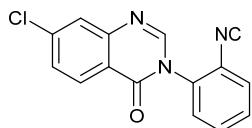
8.2899
 8.2686
 8.0000
 7.7729
 7.7680
 7.6327
 7.6087
 7.5959
 7.5743
 7.5286
 7.5072
 7.4912
 7.4640



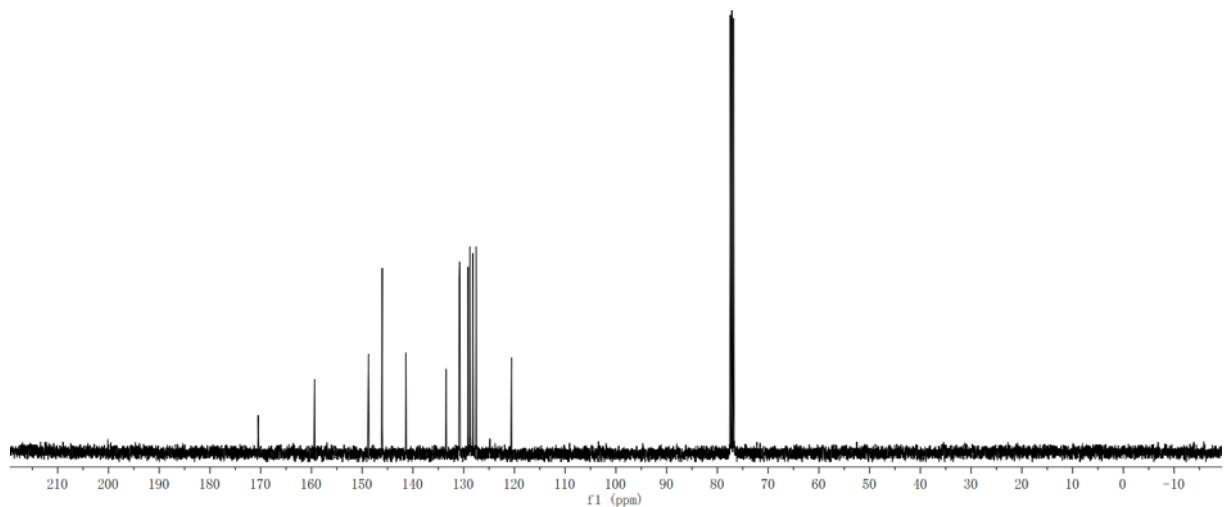
¹H NMR (400M, CDCl₃) of **1h**



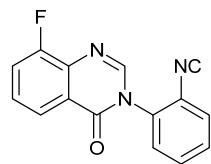
-170.49
 -159.36
 /148.74
 /146.06
 141.37
 /133.49
 /130.86
 130.77
 129.15
 128.76
 128.69
 128.18
 127.52
 124.84
 120.57
 77.44
 77.12
 76.81



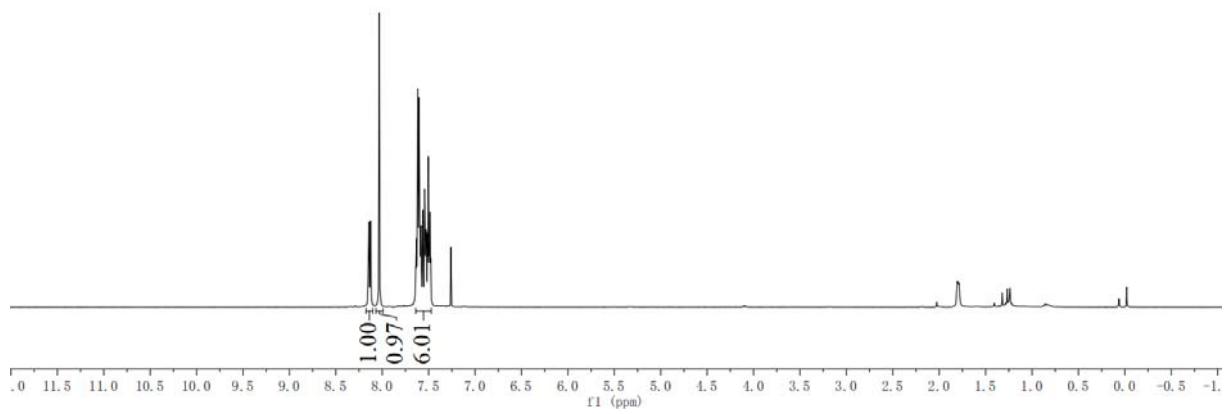
¹³C NMR (101M, CDCl₃) of **1h**



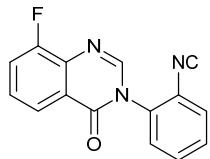
8.1494
 8.1411
 8.1317
 8.1242
 8.0318
 7.6422
 7.6045
 7.5385
 7.4785



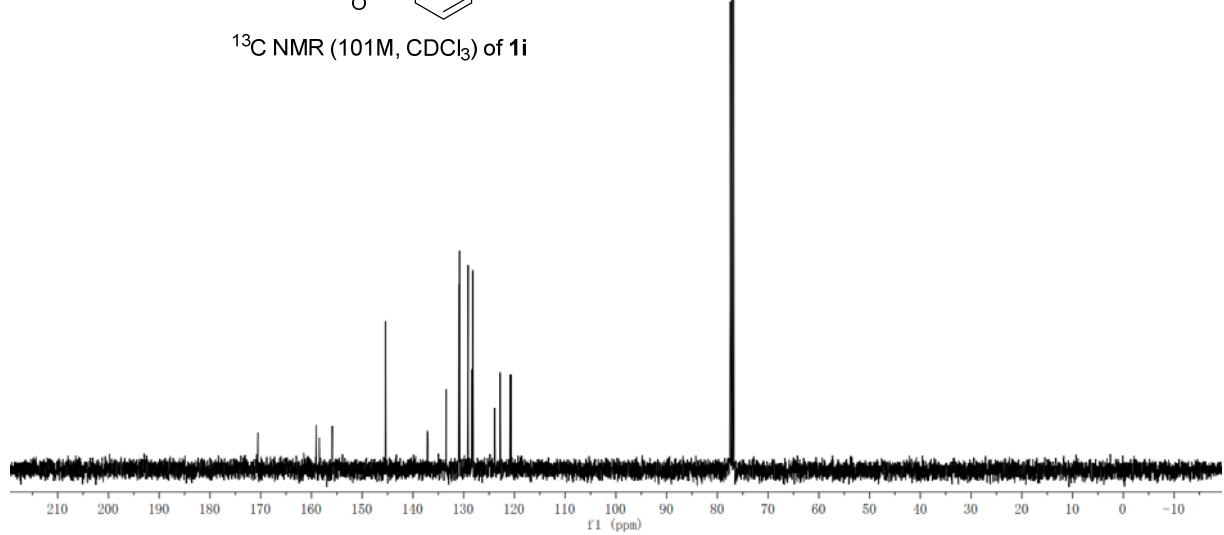
¹H NMR (400M, CDCl₃) of **1i**



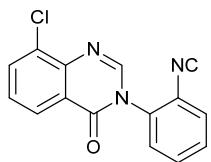
-170.561
 -159.047
 -159.016
 -158.451
 -155.898
 -145.386
 -137.160
 -137.039
 -133.471
 -130.922
 -129.137
 -128.427
 -128.350
 -128.199
 -123.900
 -122.851
 -122.808
 -120.861
 -120.673
 -77.434
 -77.117
 76.798



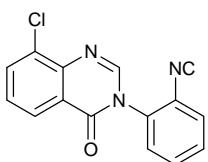
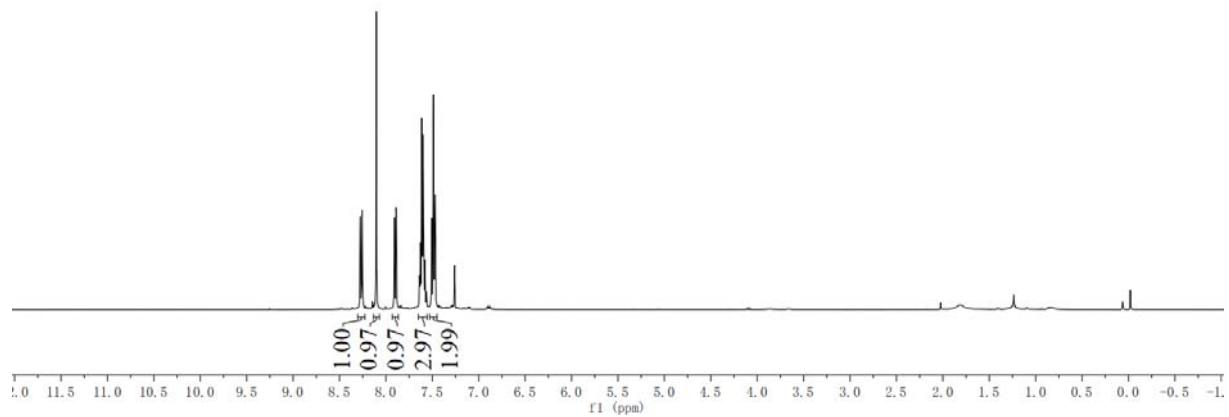
¹³C NMR (101M, CDCl₃) of **1i**



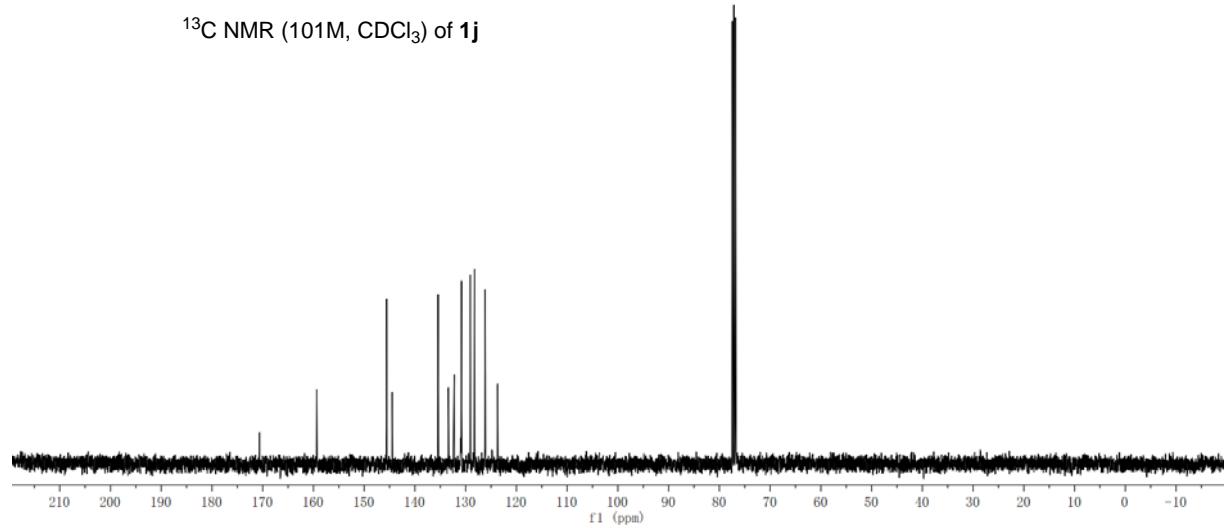
8.2770
 8.2734
 8.2570
 8.2534
 8.1034
 7.9103
 7.9067
 7.8907
 7.8871
 7.6380
 7.6150
 7.6006
 7.5618
 7.5070
 7.4926
 7.4872
 7.4677



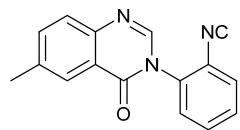
¹H NMR (400M, CDCl₃) of **1j**



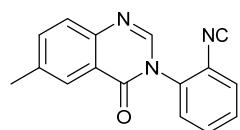
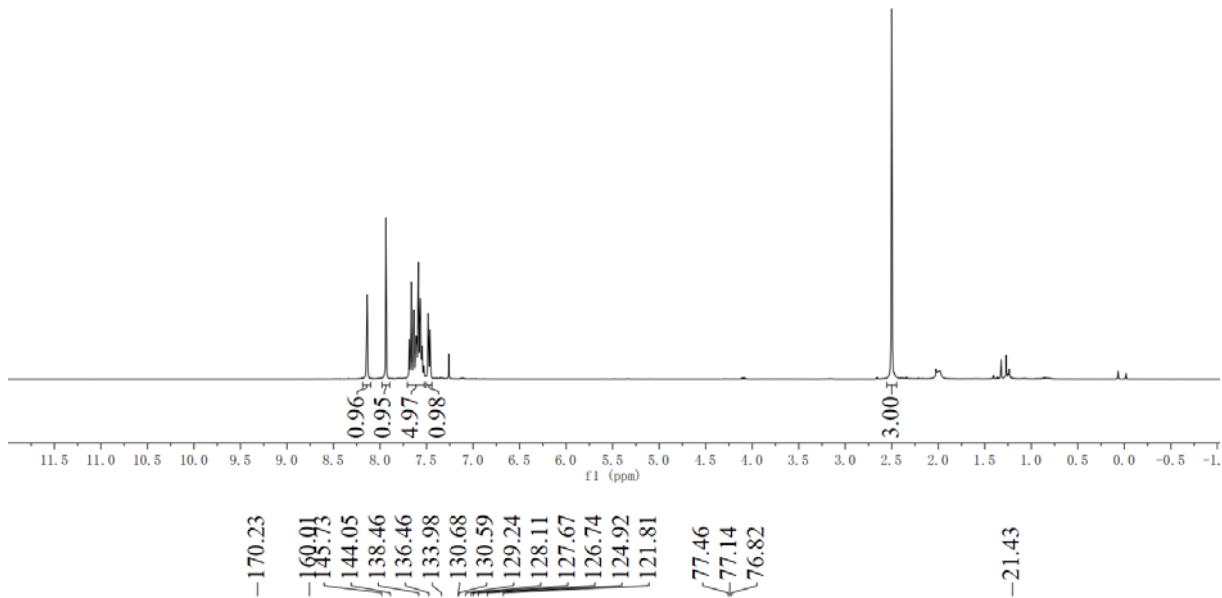
¹³C NMR (101M, CDCl₃) of **1j**



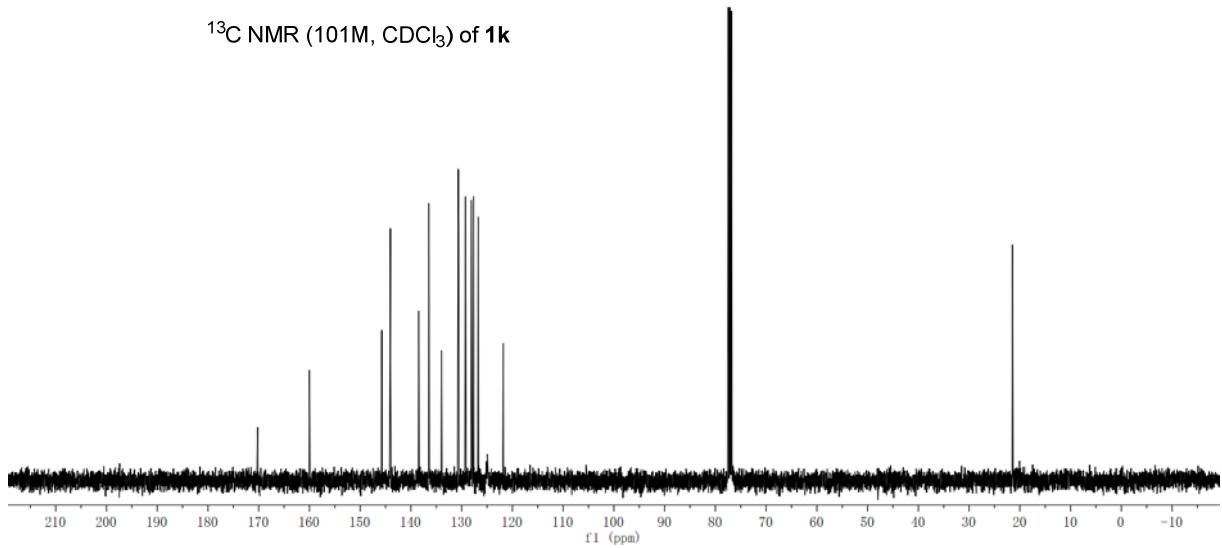
8.1384
 7.9362
 7.6844
 7.6638
 7.5916
 7.5293
 7.4831
 7.4747
 7.4643
 7.4587



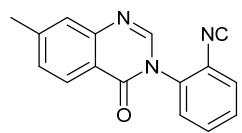
¹H NMR (400M, CDCl₃) of **1k**



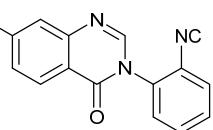
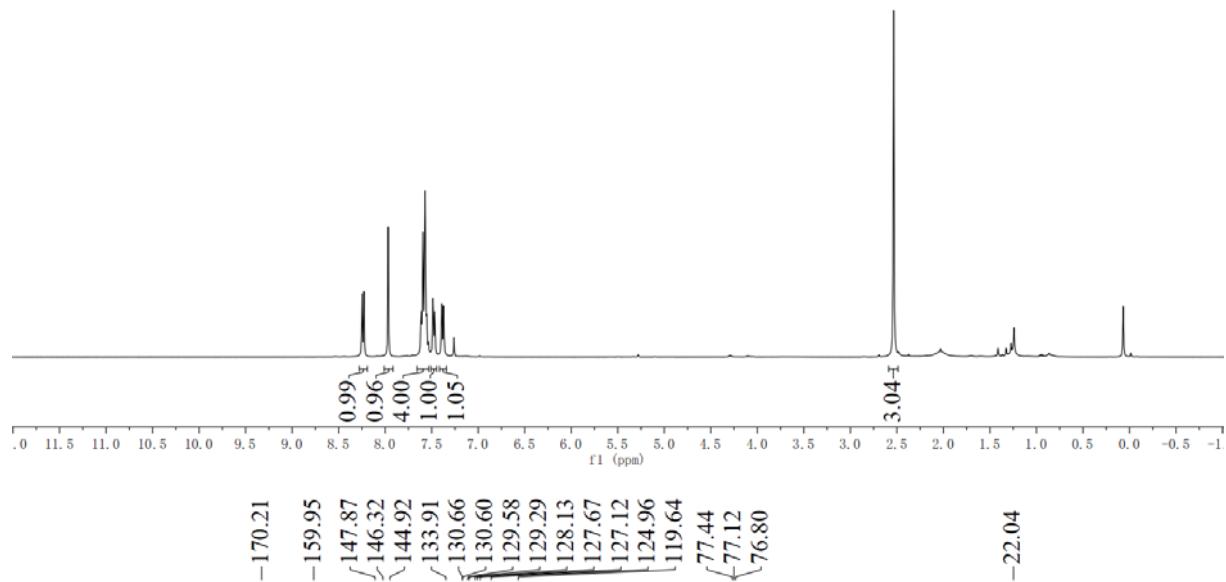
¹³C NMR (101M, CDCl₃) of **1k**



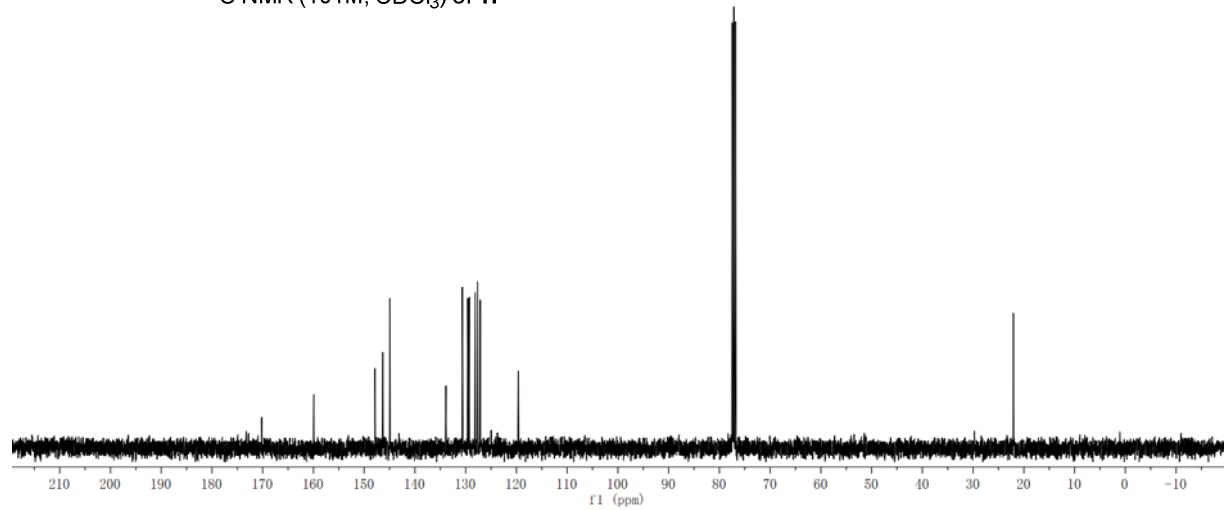
8.2488
 8.2285
 7.9671
 7.6168
 7.5945
 7.5703
 7.5360
 7.4876
 7.4824
 7.4685
 7.3917
 7.3715

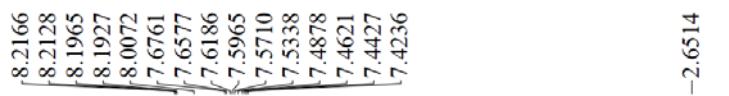


¹H NMR (400M, CDCl₃) of **1I**

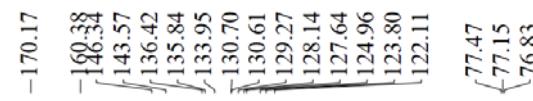
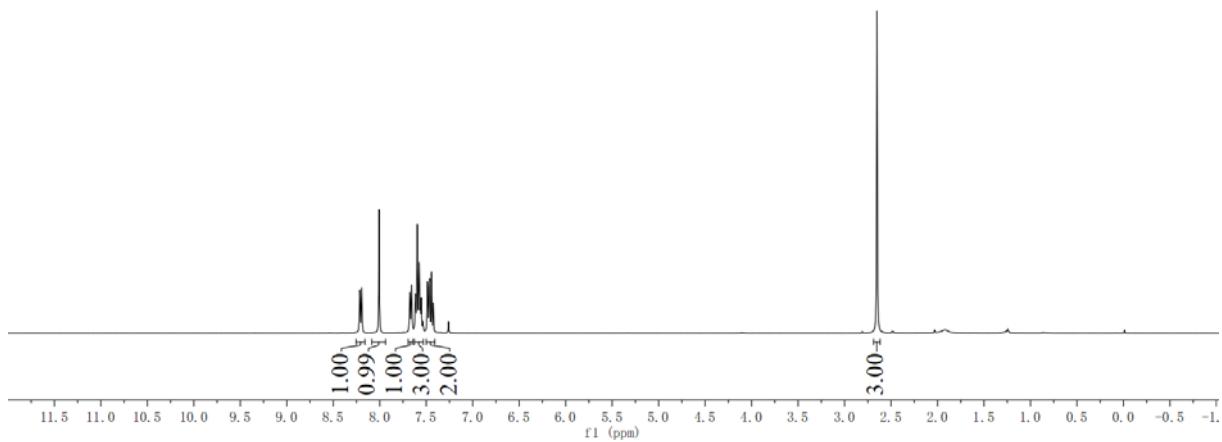


¹³C NMR (101M, CDCl₃) of **1I**

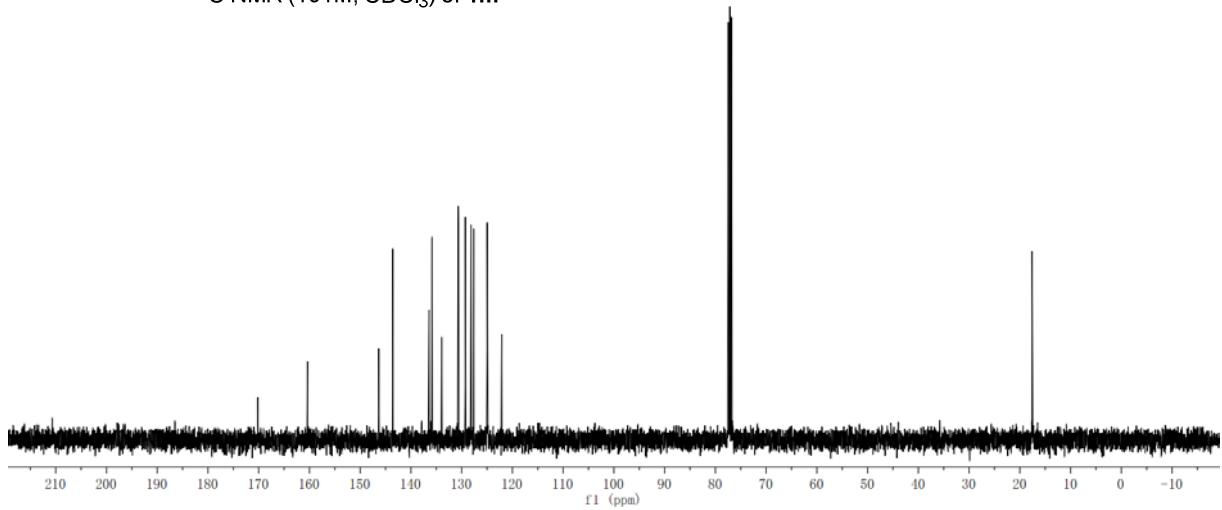


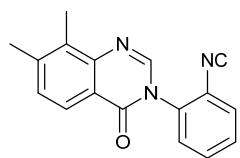


^1H NMR (400M, CDCl_3) of **1m**

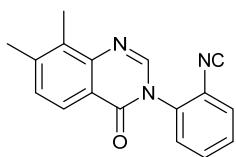
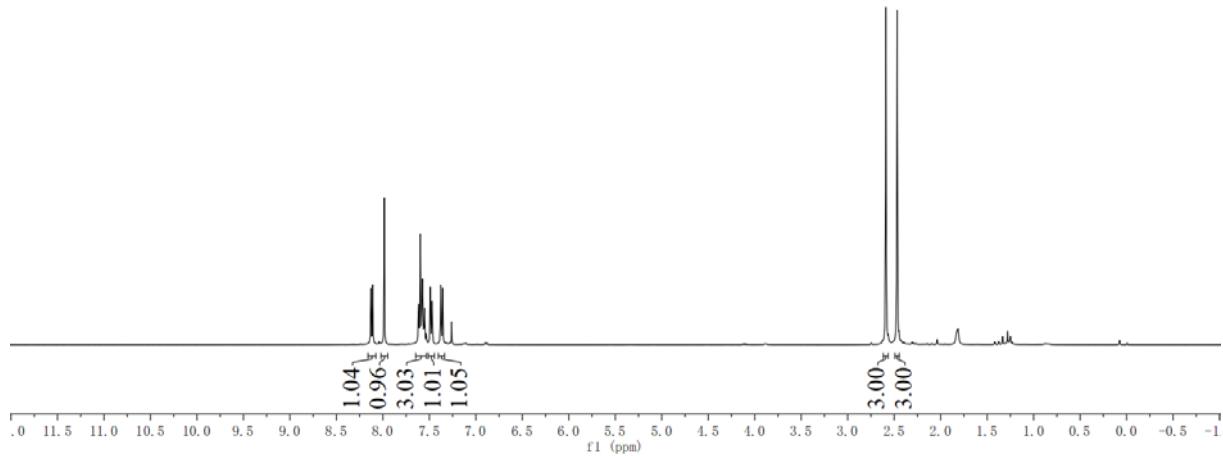


^{13}C NMR (101M, CDCl_3) of **1m**

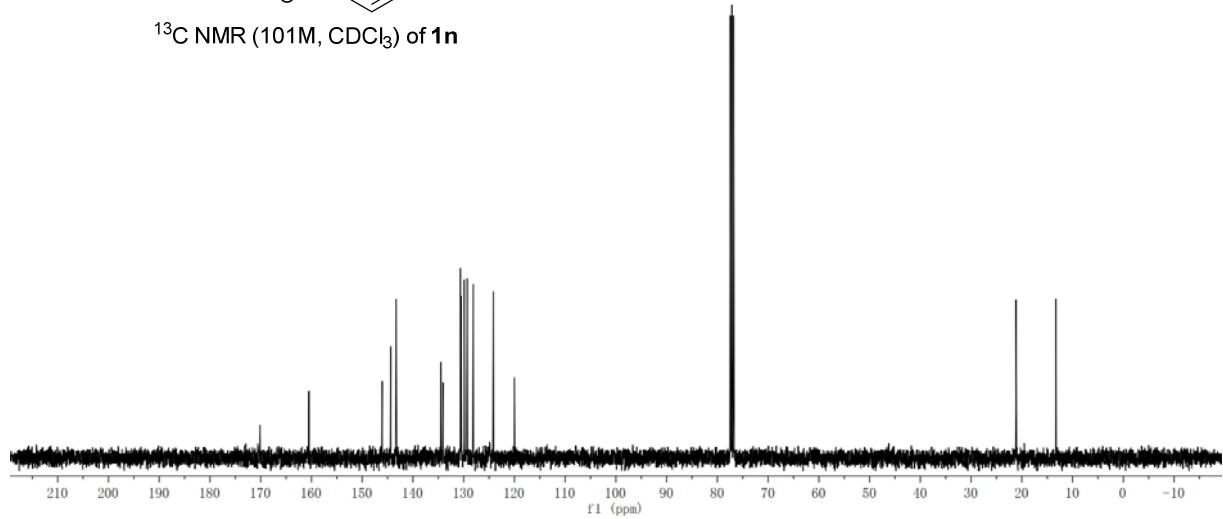




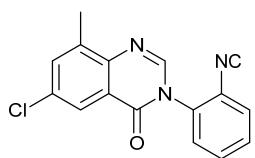
¹H NMR (400M, CDCl₃) of **1n**



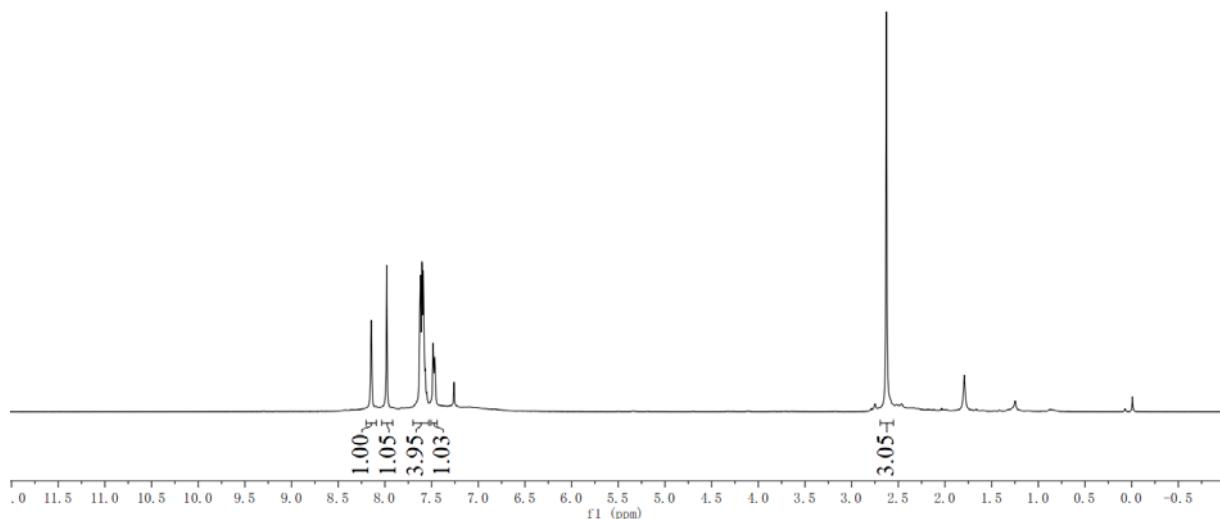
¹³C NMR (101M, CDCl₃) of **1n**



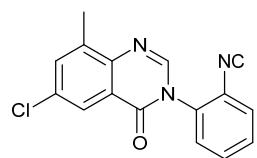
8.1496
8.1433
7.9811
7.6248
7.6031
7.5895
7.5672
7.4843
7.4792
7.4659
7.4596



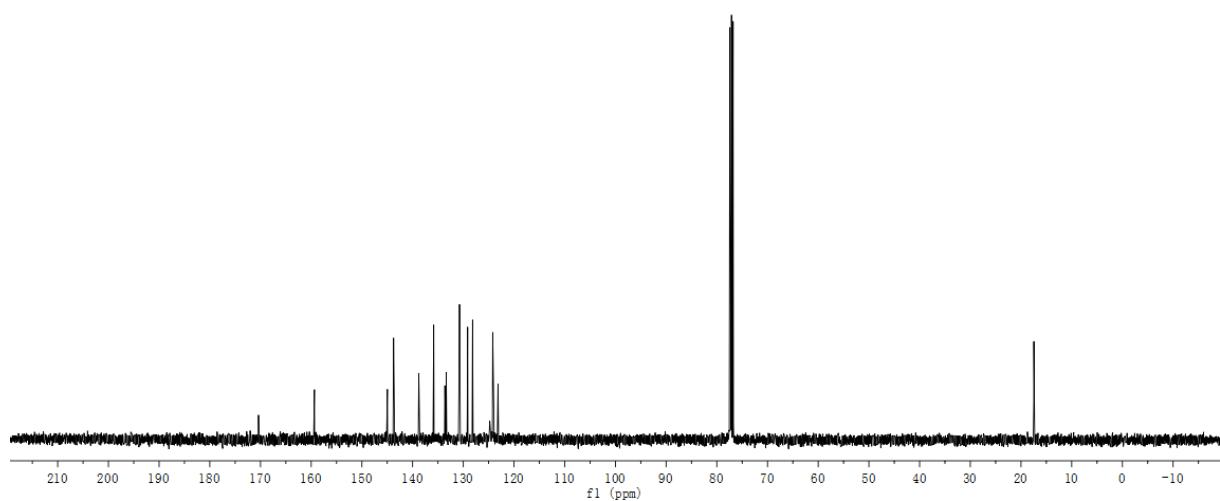
¹H NMR (400M, CDCl₃) of **1o**

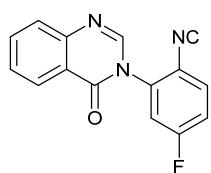
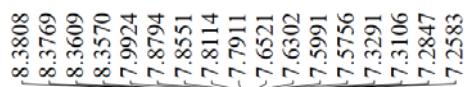


-170.39
-159.36
-144.97
143.75
138.78
135.83
133.63
133.36
130.78
130.75
129.14
128.17
124.78
124.20
123.15
77.42
77.10
76.79

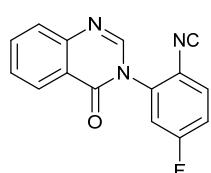
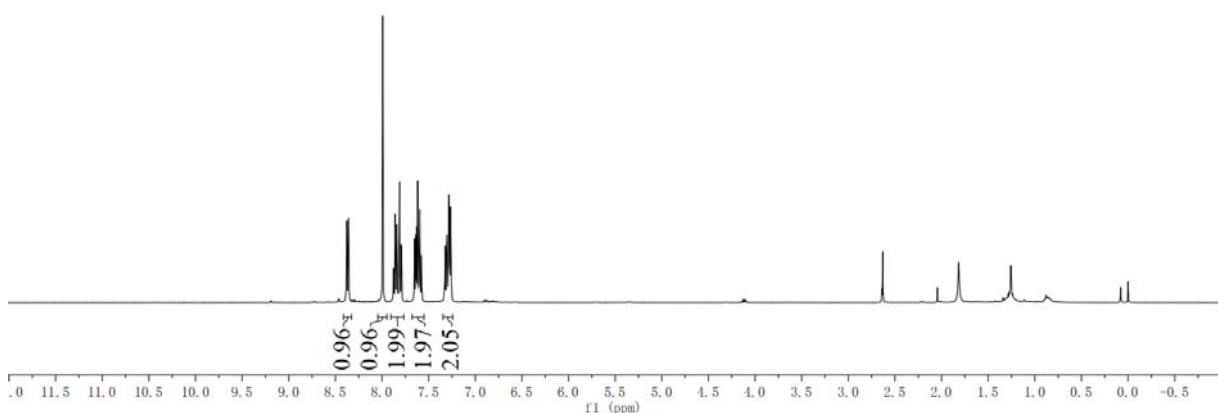


¹³C NMR (101M, CDCl₃) of **1o**

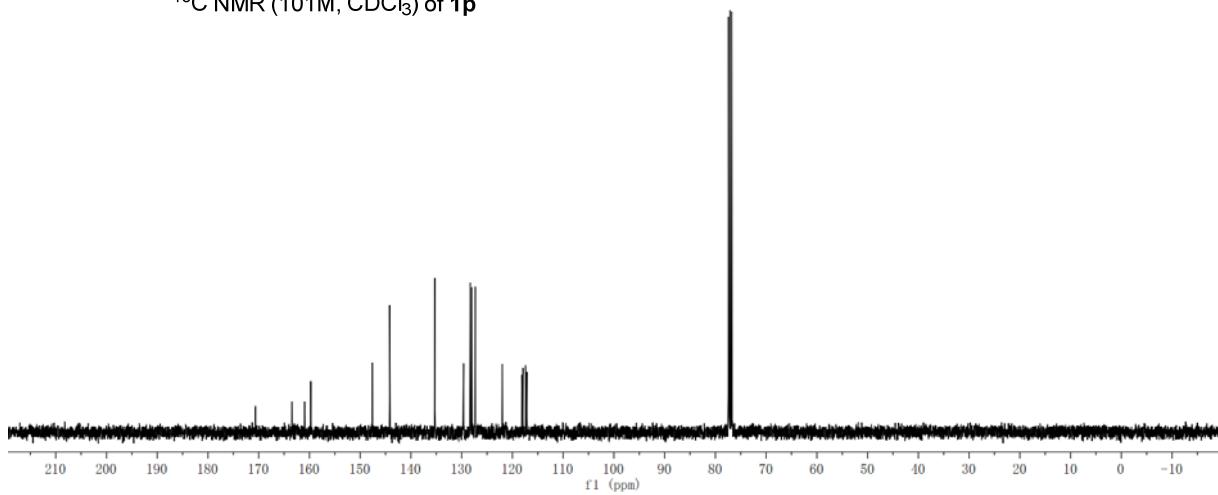


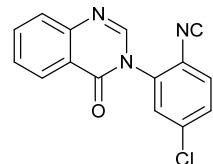
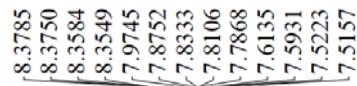


¹H NMR (400M, CDCl₃) of 1p

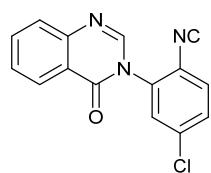
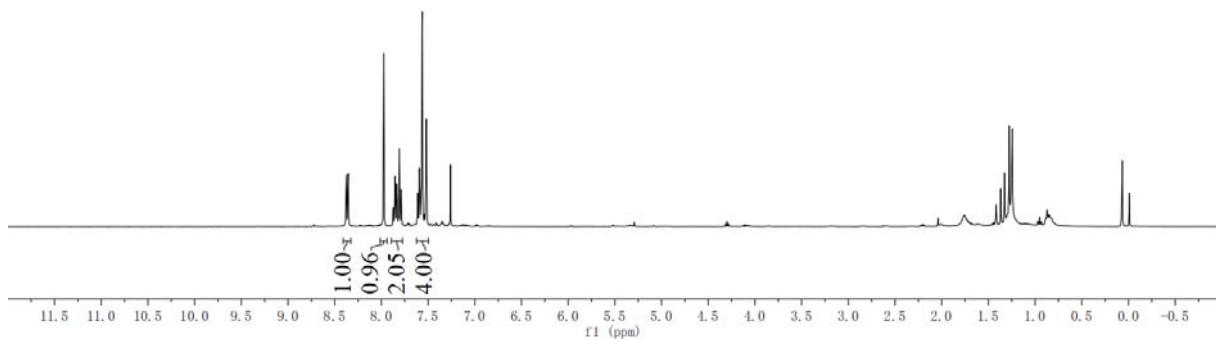


¹³C NMR (101M, CDCl₃) of **1p**

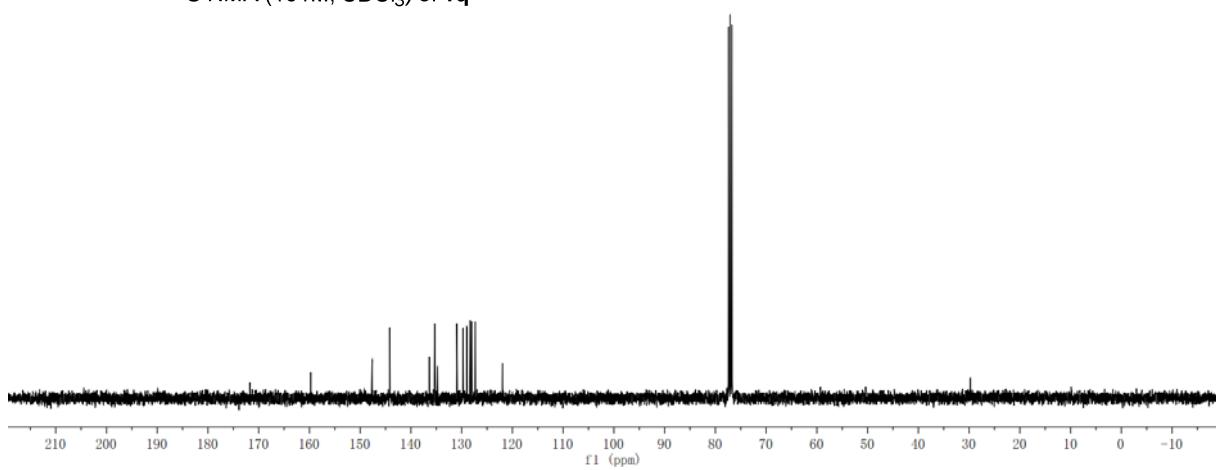




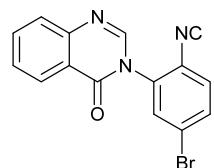
¹H NMR (400M, CDCl₃) of **1q**



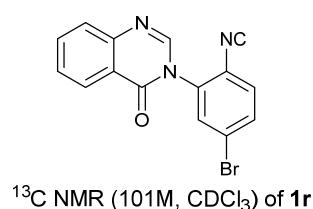
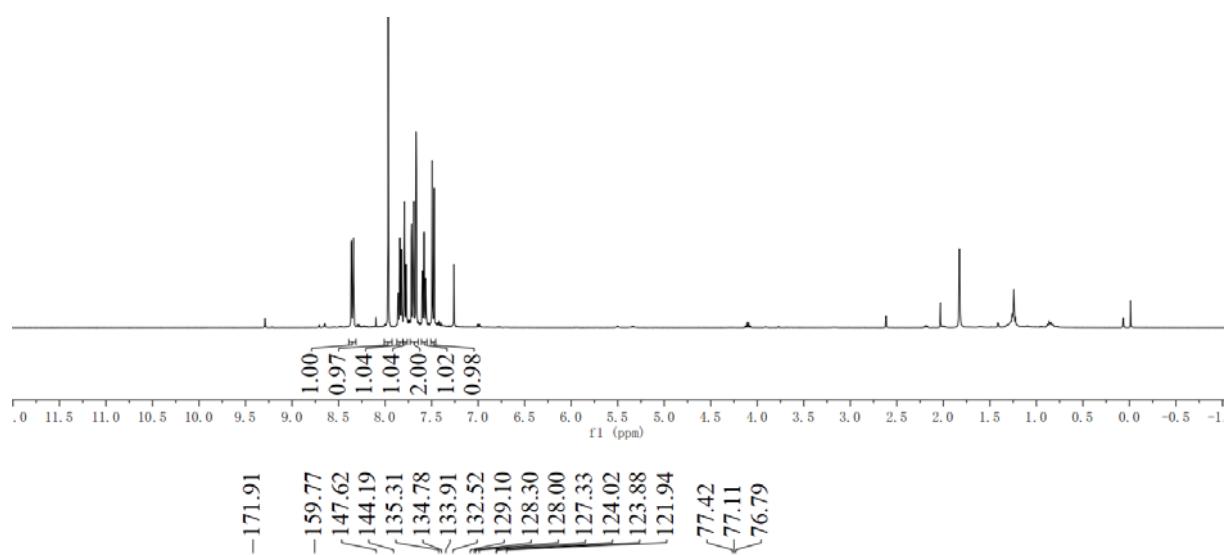
¹³C NMR (101M, CDCl₃) of 1q



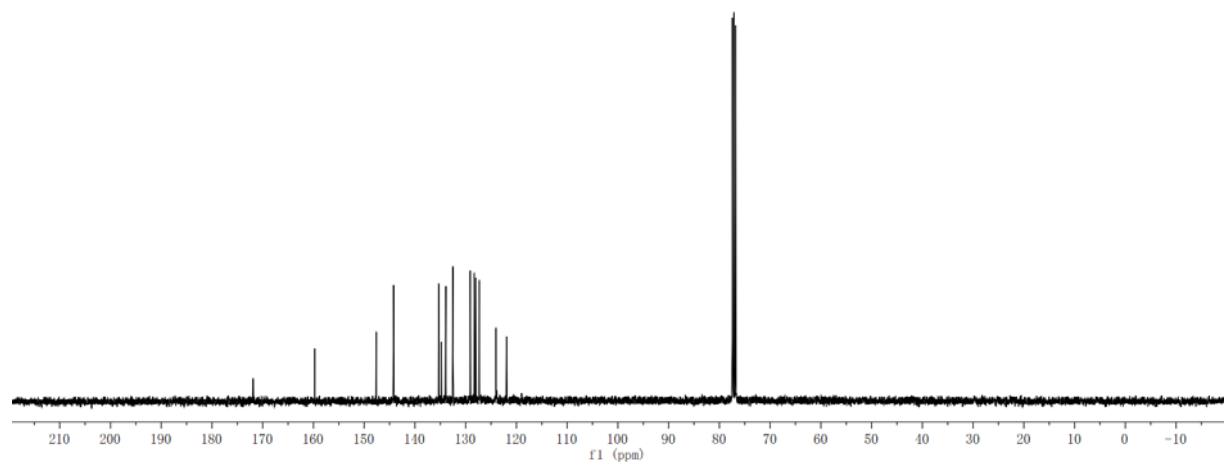
8.3627
8.3587
8.3428
8.3391
7.9657
7.8628
7.8453
7.8247
7.8209
7.7961
7.7929
7.7758
7.7726
7.7184
7.6971
7.6919
7.6632
7.6005
7.5971
7.5632
7.5597
7.4937
7.4725



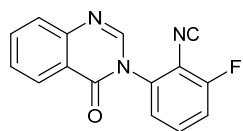
¹H NMR (400M, CDCl₃) of **1r**



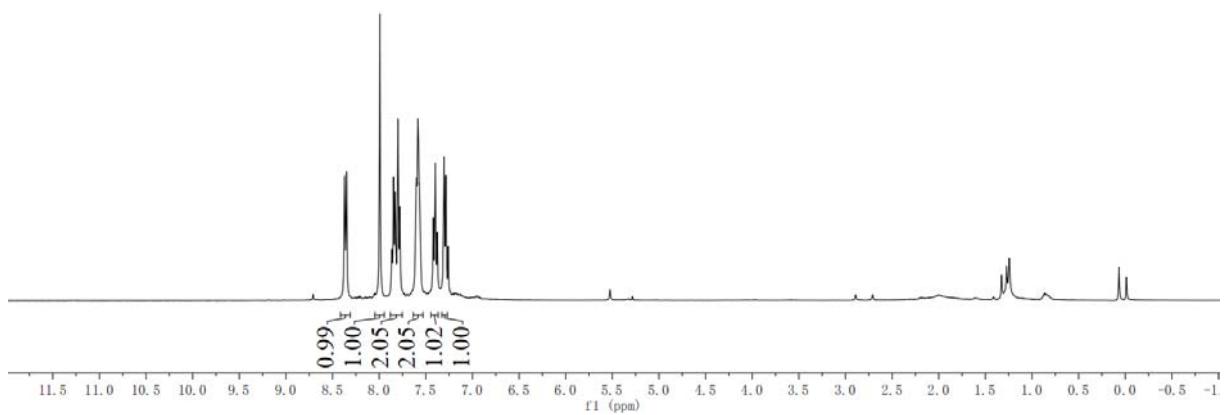
¹³C NMR (101M, CDCl₃) of **1r**



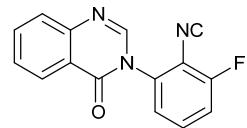
8.3705
 8.3506
 7.9929
 7.8652
 7.8455
 7.7992
 7.7790
 7.6127
 7.5919
 7.5785
 7.5568
 7.4197
 7.3984
 7.3772
 7.3056
 7.2854



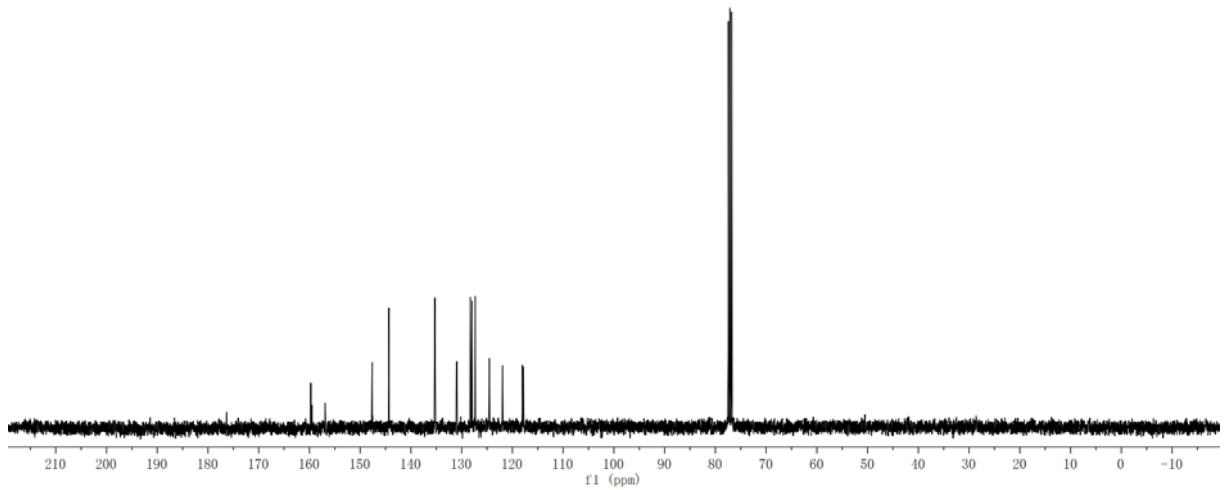
¹H NMR (400M, CDCl₃) of **1s**



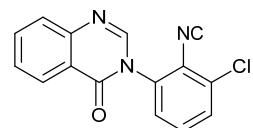
-176.290
 159.735
 159.491
 156.905
 147.643
 144.341
 135.287
 135.178
 131.031
 130.943
 128.282
 127.958
 127.346
 124.561
 124.525
 121.961
 118.026
 117.839
 77.419
 77.100
 76.783



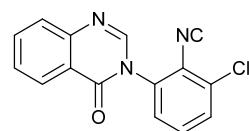
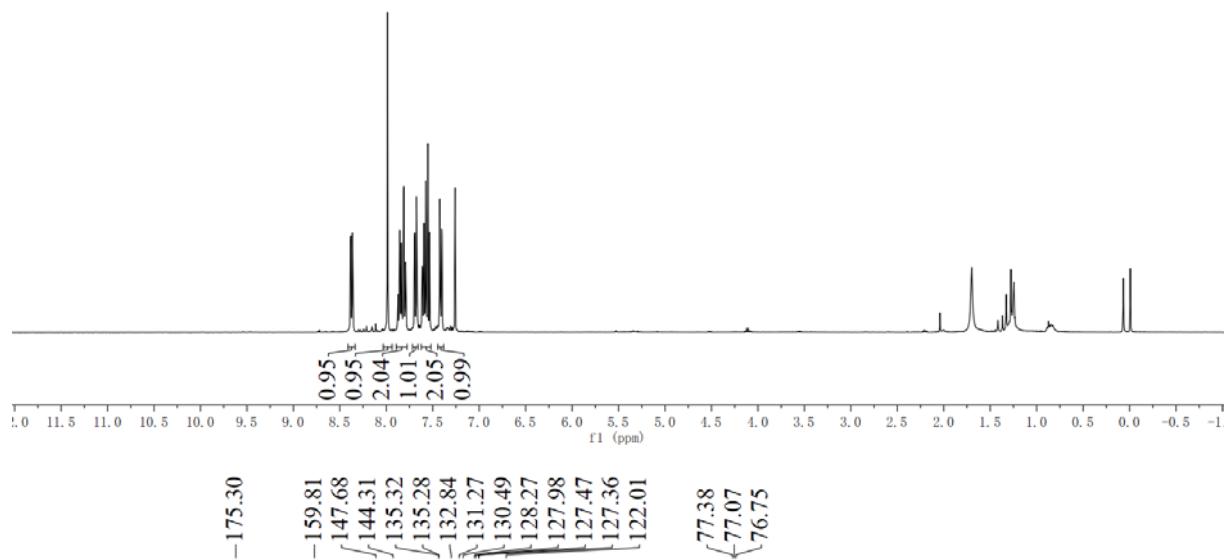
¹³C NMR (101M, CDCl₃) of **1s**



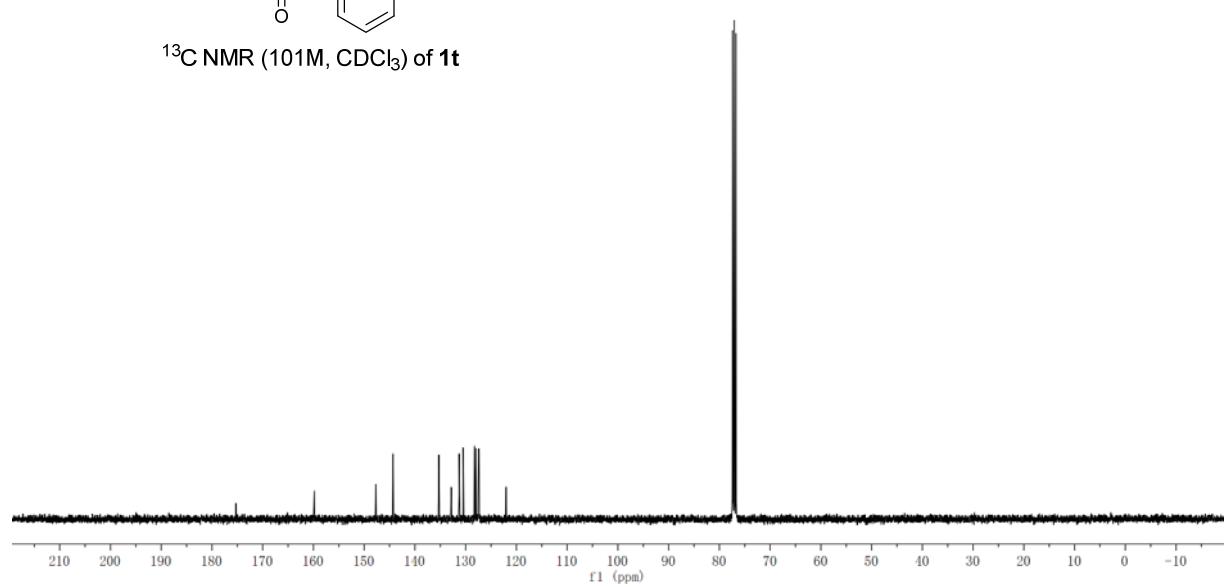
8.3848
8.3810
8.3648
8.3609
7.9860
7.8767
7.8387
7.8103
7.7901
7.6961
7.6927
7.6754
7.6720
7.6148
7.5973
7.5535
7.5330
7.4245
7.4212
7.4045
7.4013

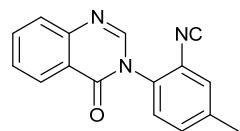


^1H NMR (400M, CDCl_3) of **1t**

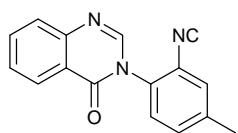
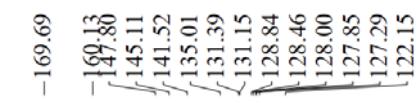
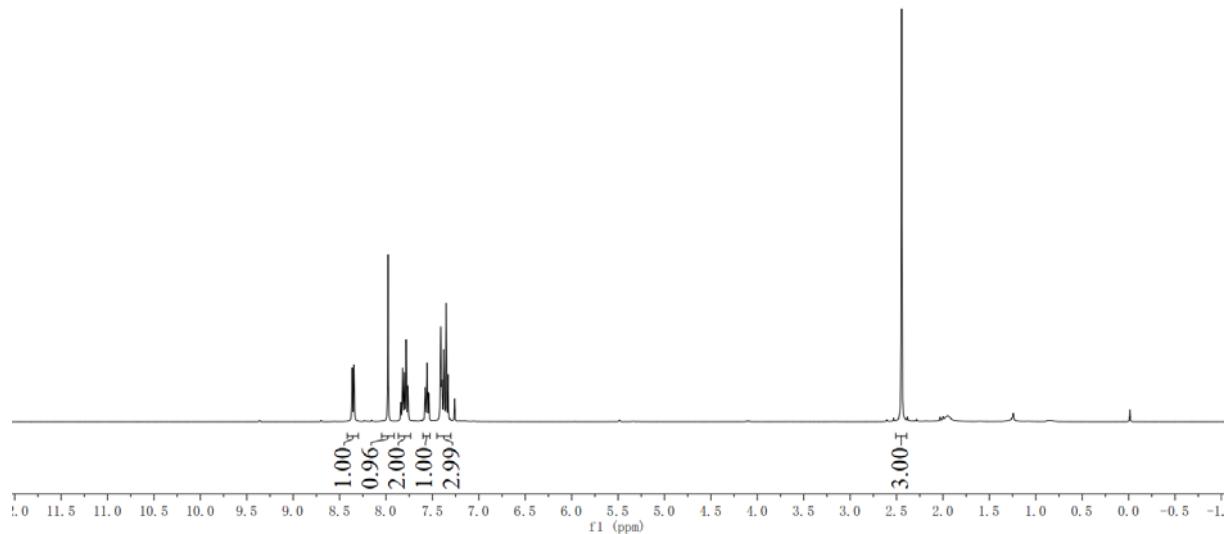


^{13}C NMR (101M, CDCl_3) of **1t**

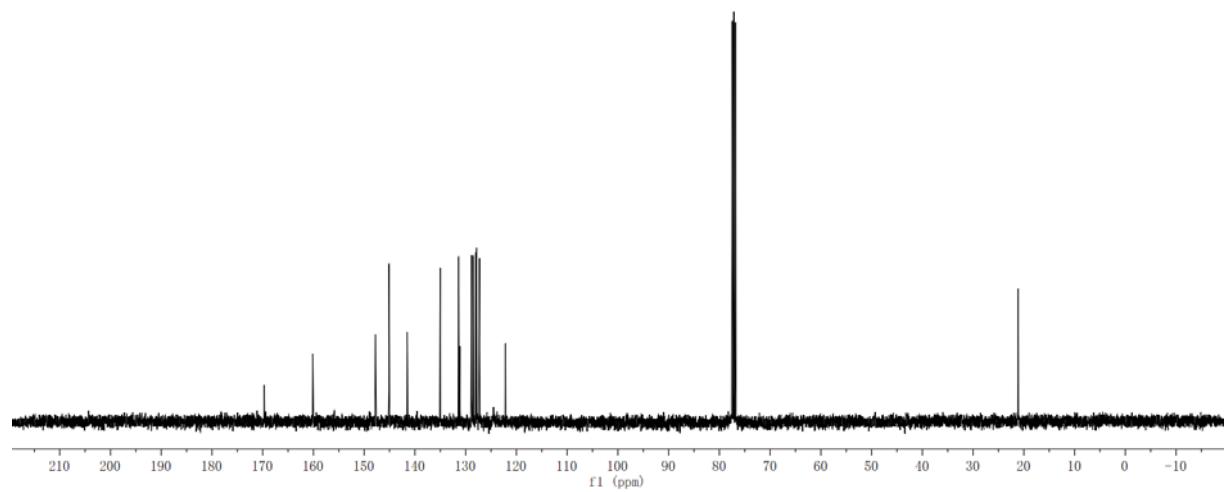




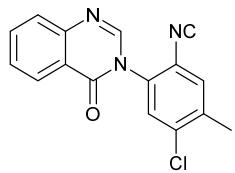
¹H NMR (400M, CDCl₃) of **1u**



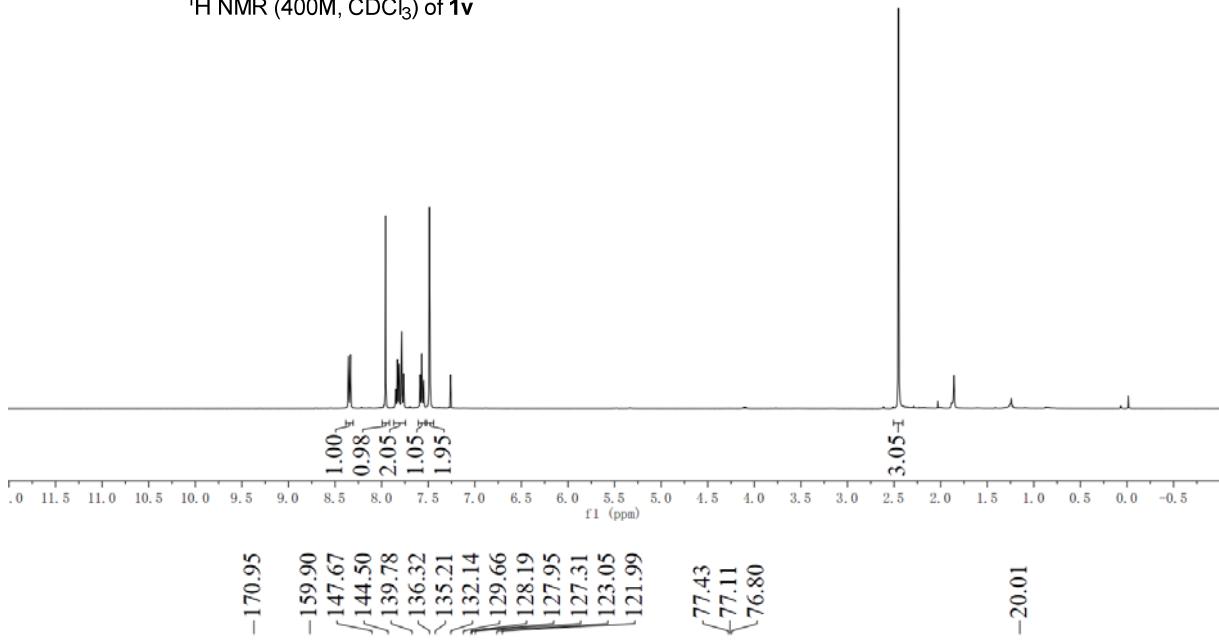
¹³C NMR (101M, CDCl₃) of **1u**



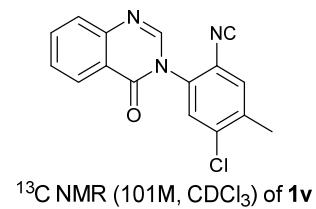
8.3583
 8.3544
 8.3382
 8.3346
 7.9584
 7.8523
 7.8281
 7.7876
 7.7637
 7.5899
 7.5865
 7.5523
 7.5489
 7.4877
 7.4830



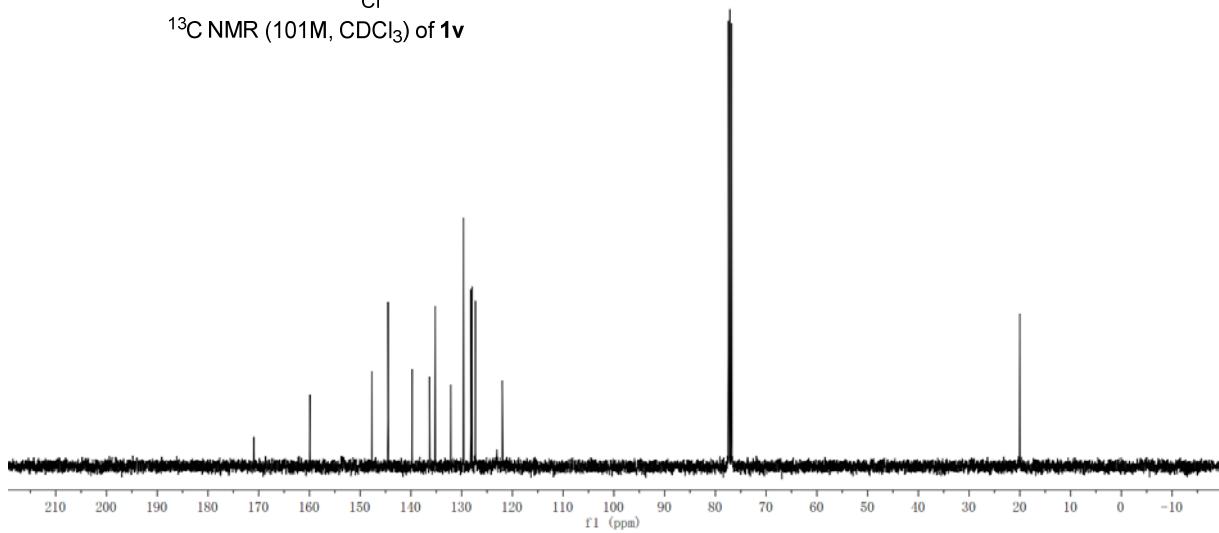
¹H NMR (400M, CDCl₃) of **1v**

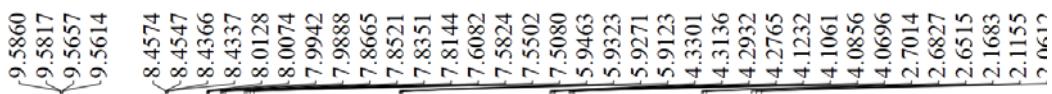


-170.95
 -159.90
 -147.67
 /-144.50
 /-139.78
 /-136.32
 /-135.21
 /-132.14
 /-129.66
 /-128.19
 /-127.95
 /-127.31
 /-123.05
 /-121.99

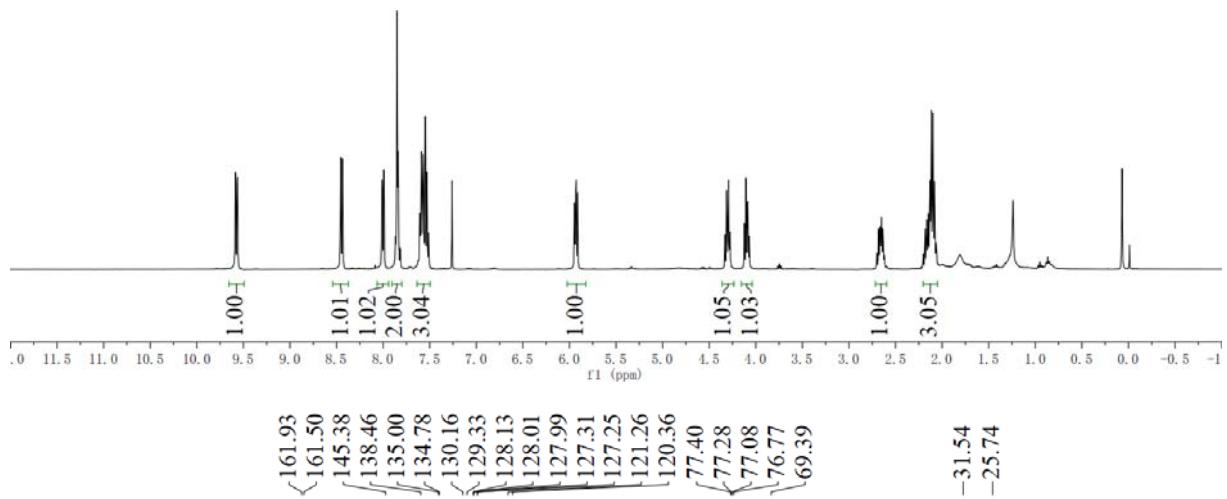


¹³C NMR (101M, CDCl₃) of **1v**

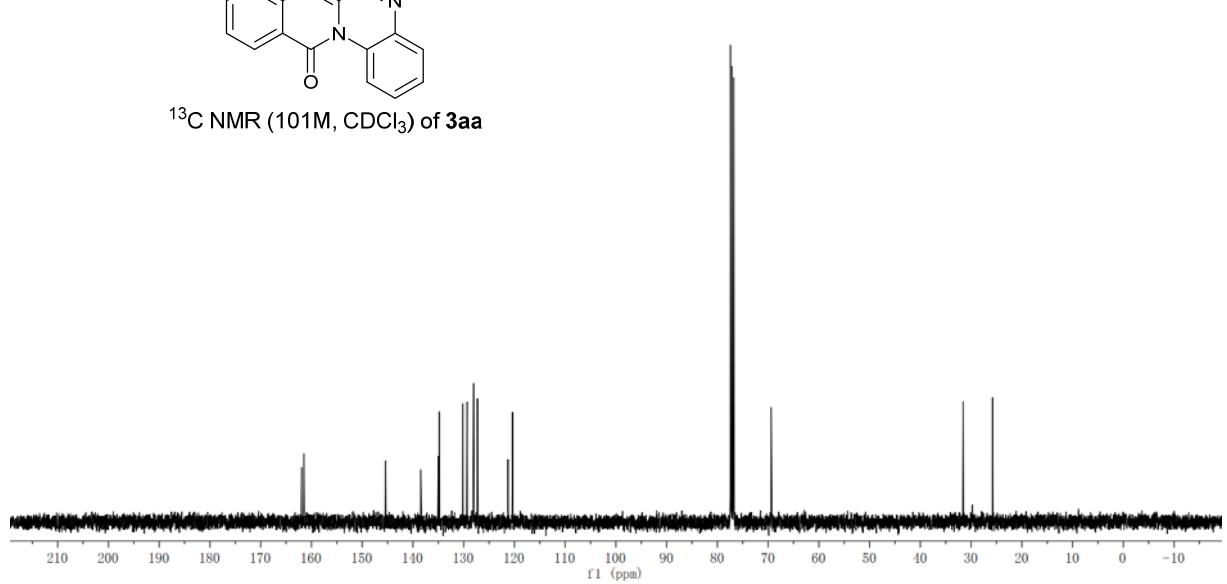


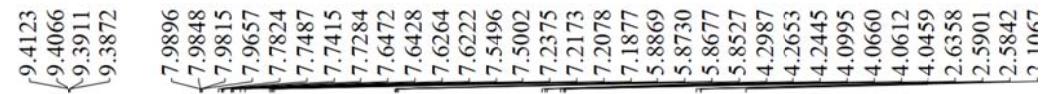


¹H NMR (400M, CDCl₃) of 3aa

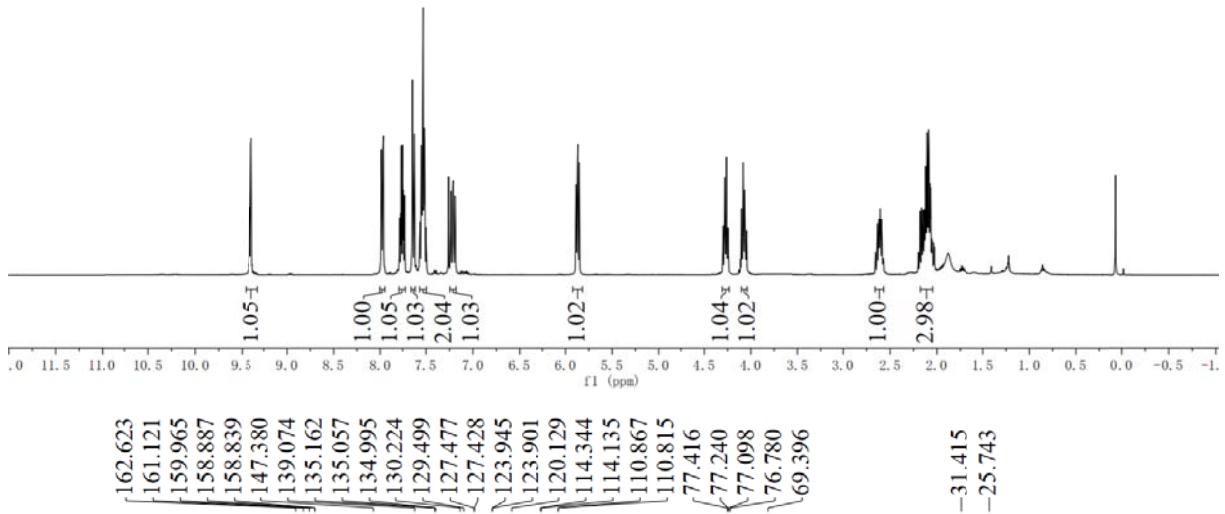


¹³C NMR (101M, CDCl₃) of 3aa

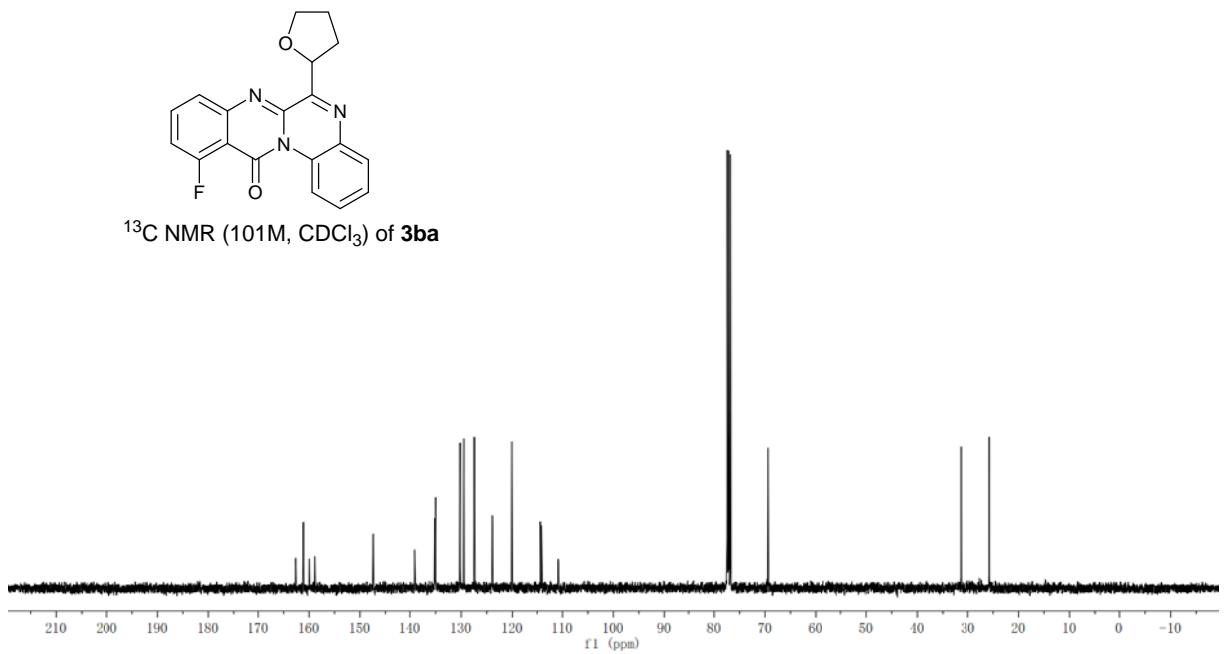


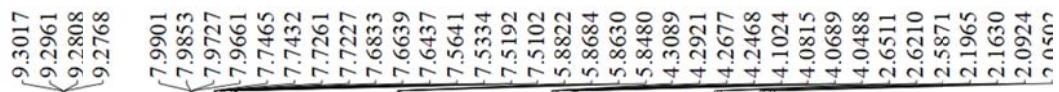


^1H NMR (400M , CDCl_3) of 3ba

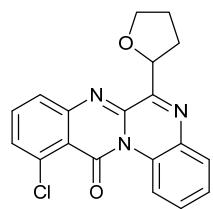
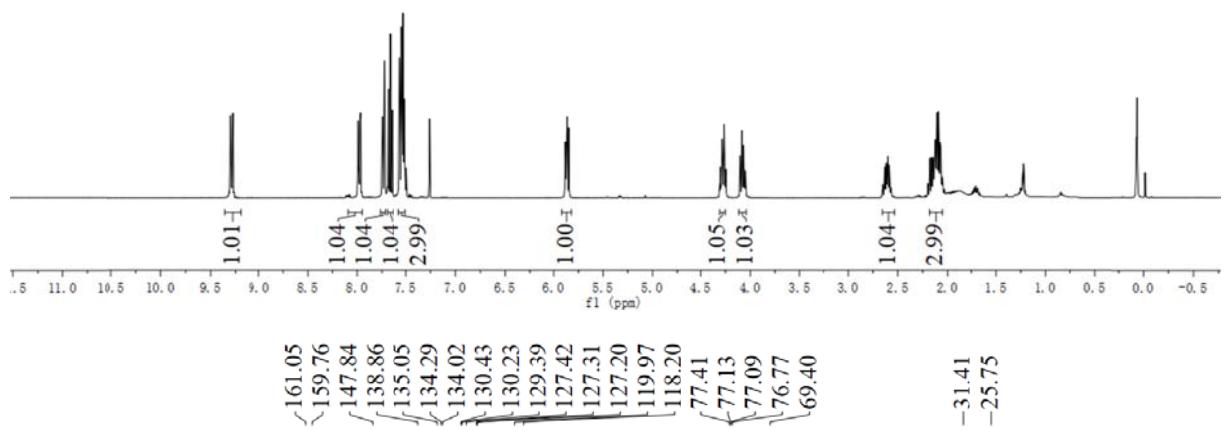


^{13}C NMR (101M , CDCl_3) of 3ba

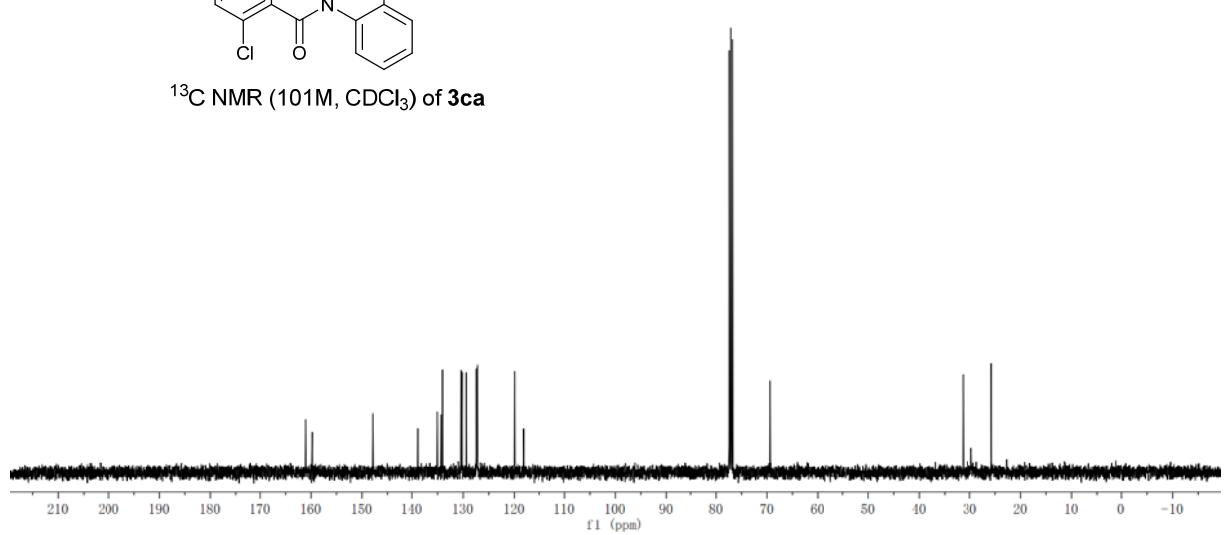




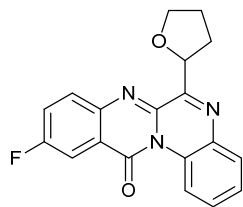
¹H NMR (400M, CDCl₃) of 3ca



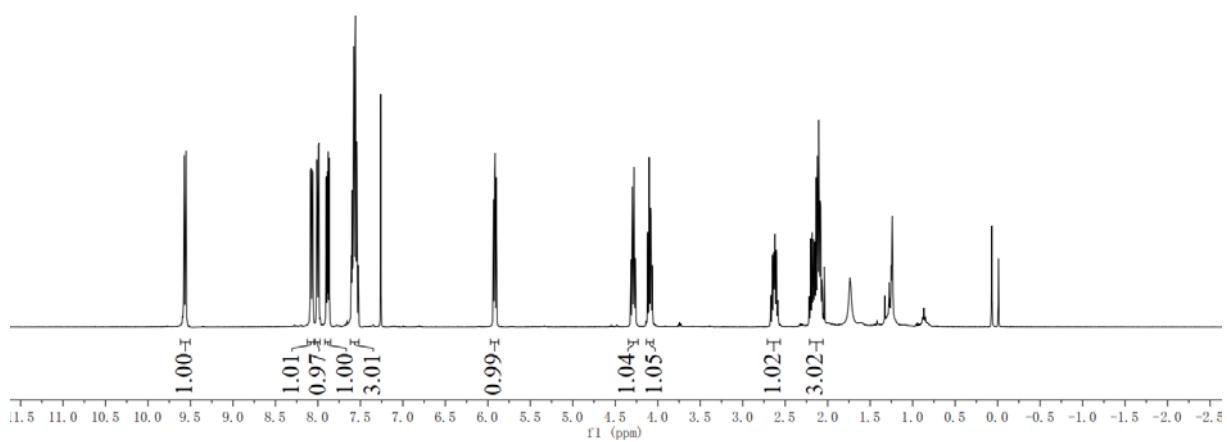
¹³C NMR (101M, CDCl₃) of 3ca



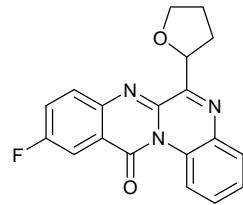
9.5776	9.5724
9.5565	9.5524
9.5524	8.0887
8.0887	8.0814
8.0674	8.0600
8.0600	8.0124
8.0124	7.9945
7.9945	7.9883
7.9883	7.9021
7.9021	7.8898
7.8898	7.8797
7.8797	7.5584
7.5584	7.5270
7.5270	7.6056
7.6056	7.5859
7.5859	7.4300
7.4300	-4.3167
-4.3167	-4.0851
-4.0851	-31.408
-31.408	-25.759
-25.759	2.0639



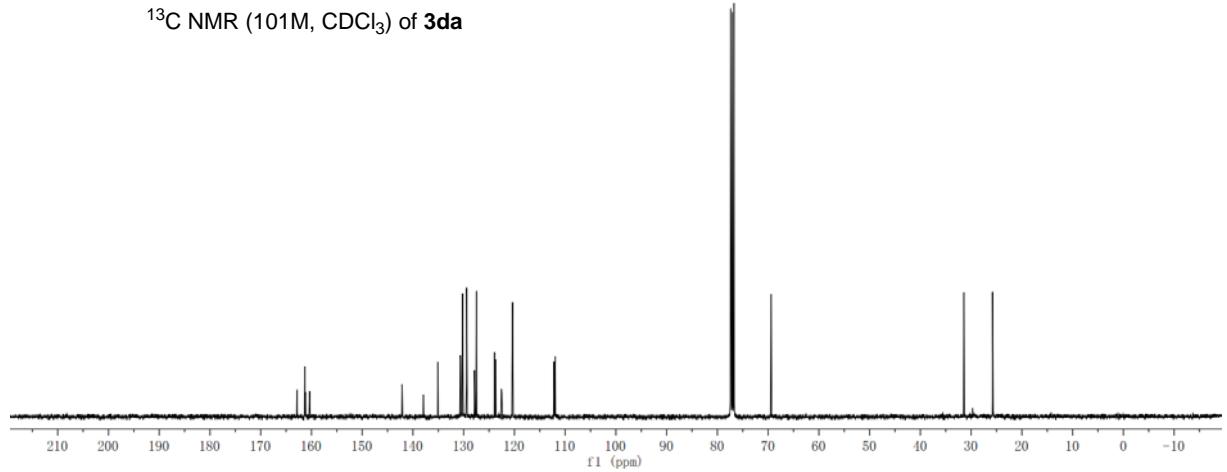
¹H NMR (400M, CDCl₃) of 3da

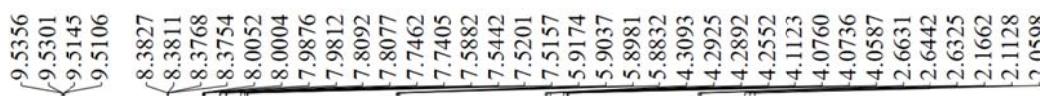


162.860
161.329
161.177
161.139
160.367
142.135
142.115
137.959
137.937
135.071
130.670
130.588
130.210
129.424
127.884
127.485
123.934
123.692
122.584
122.497
120.369
112.211
111.971
77.377
77.281
77.062
76.742
69.394

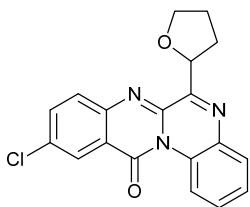
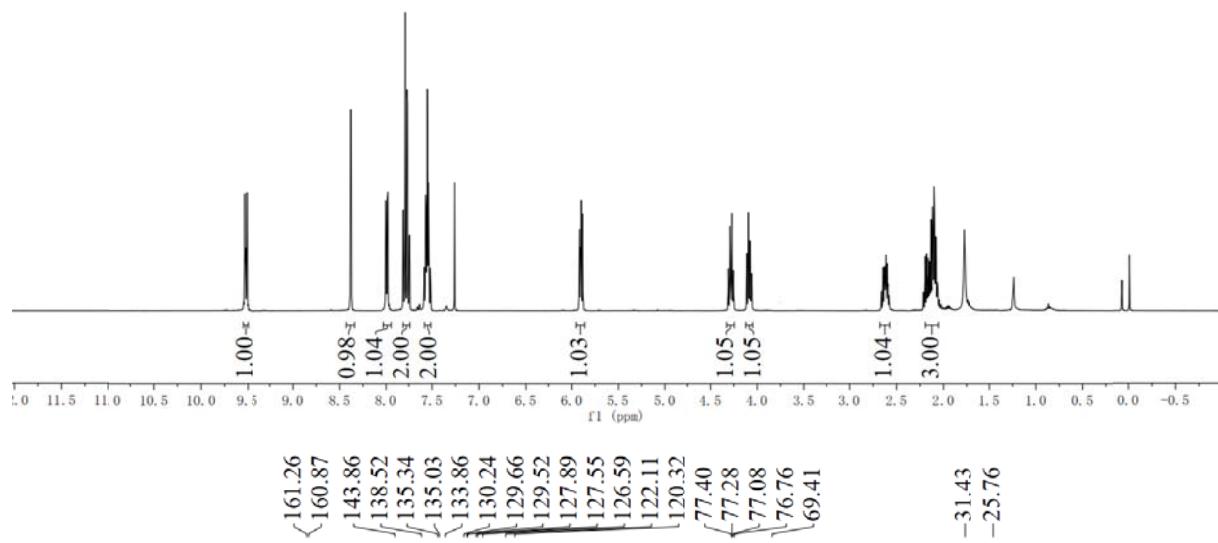


¹³C NMR (101M, CDCl₃) of 3da

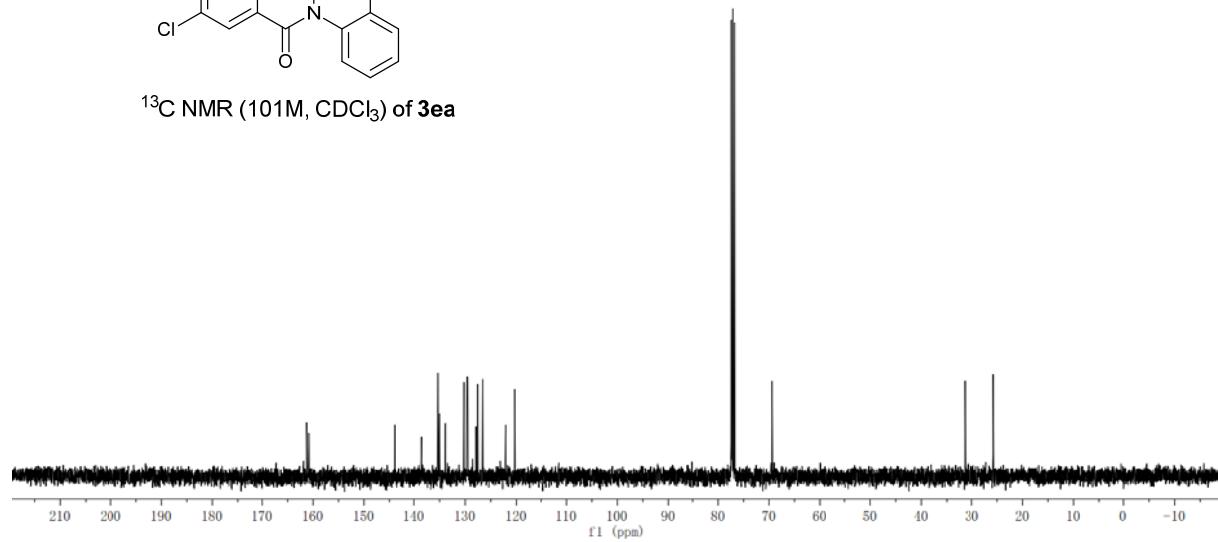


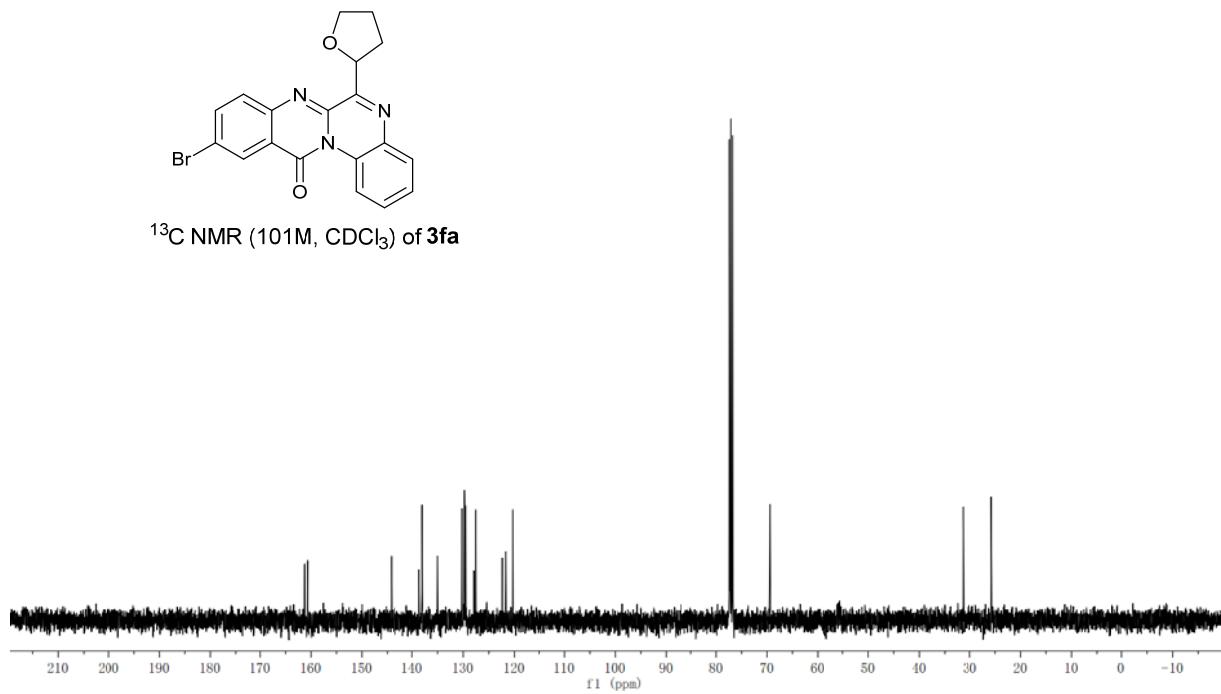
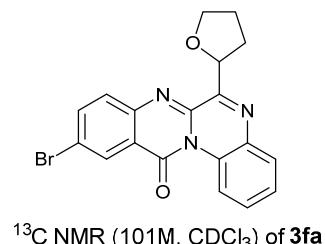
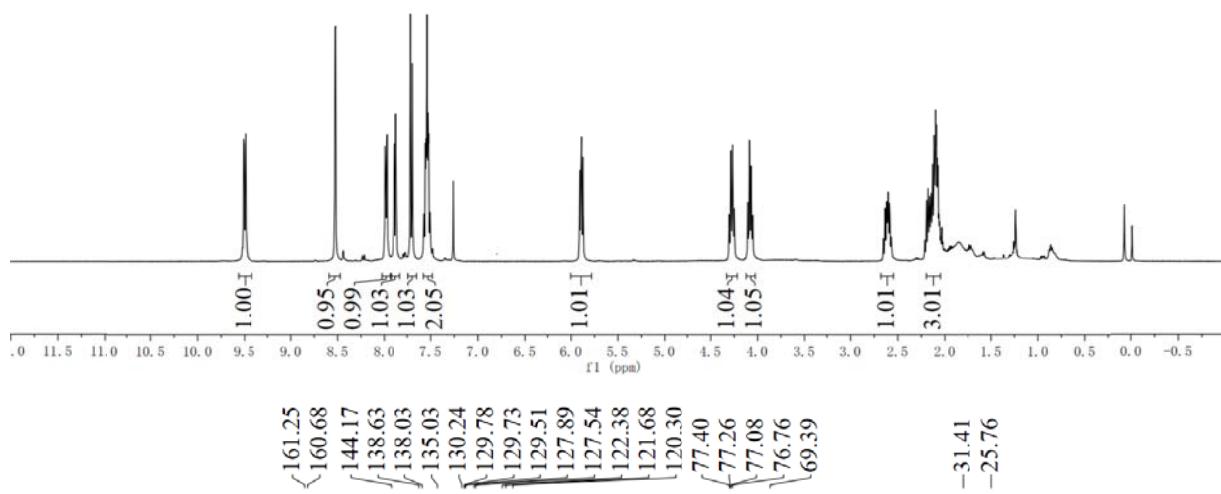
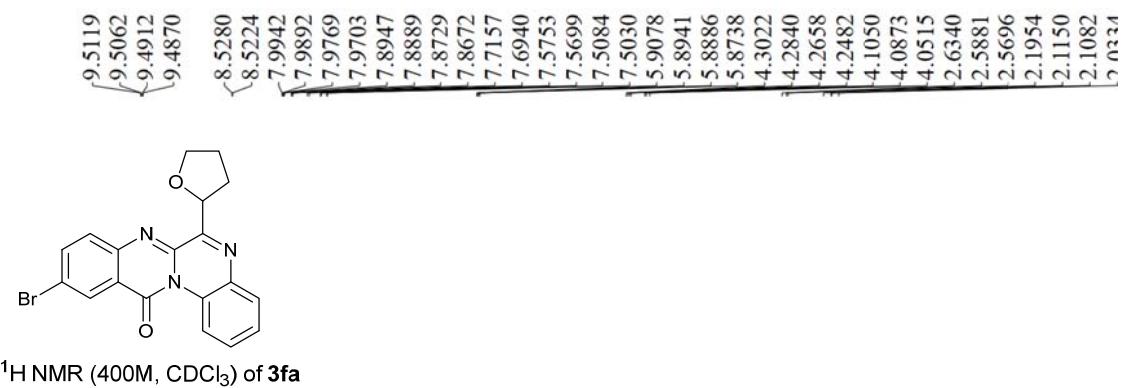


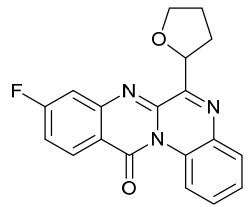
^1H NMR (400M, CDCl_3) of 3ea



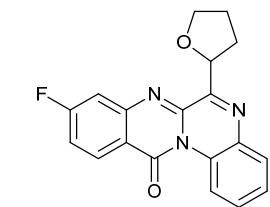
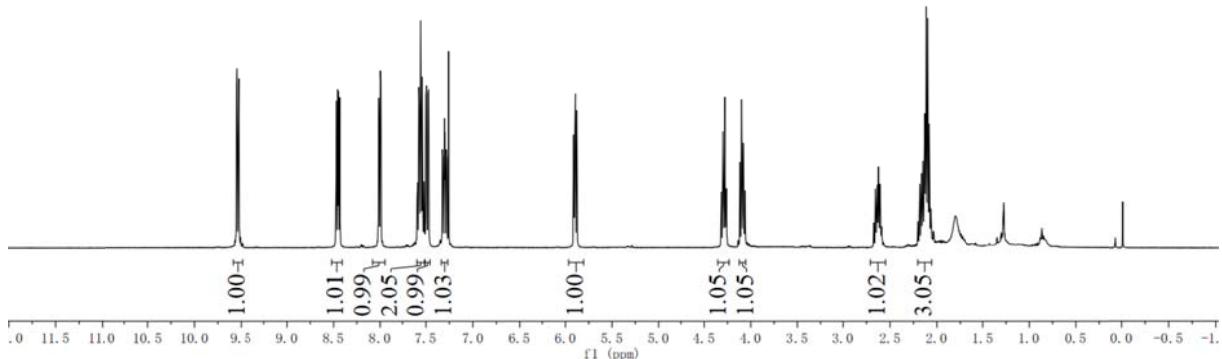
^{13}C NMR (101M, CDCl_3) of 3ea



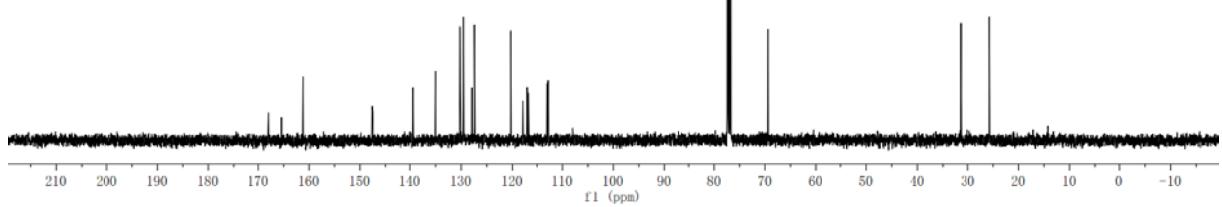


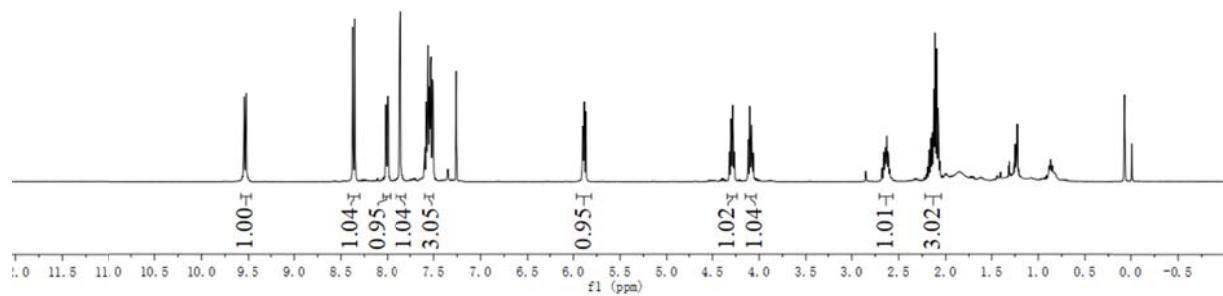
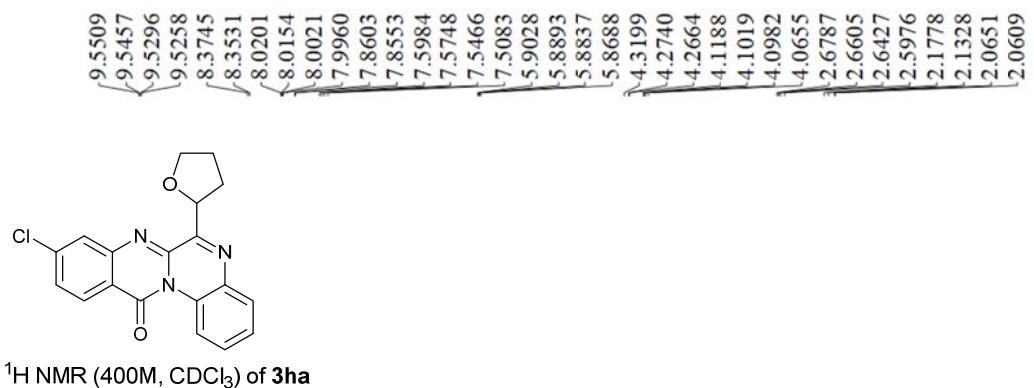


^1H NMR (400M, CDCl_3) of 3ga

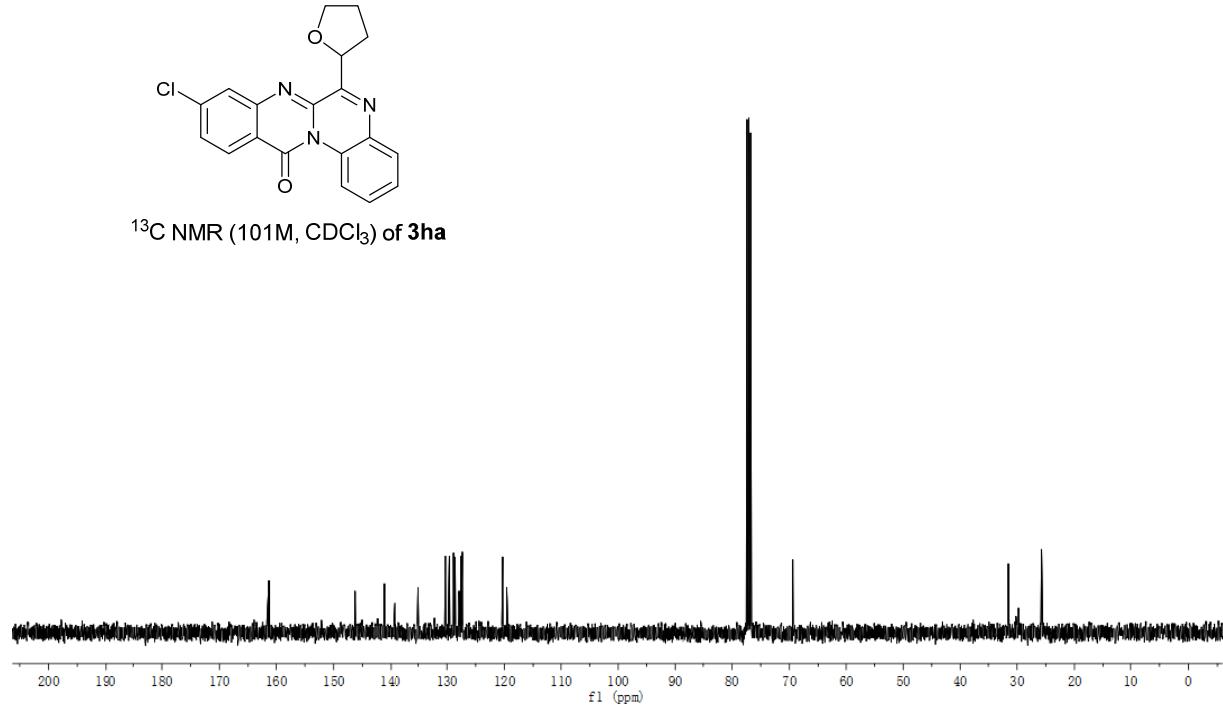


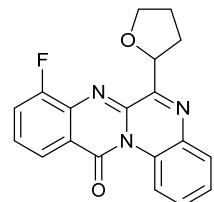
¹³C NMR (101M, CDCl₃) of 3ga



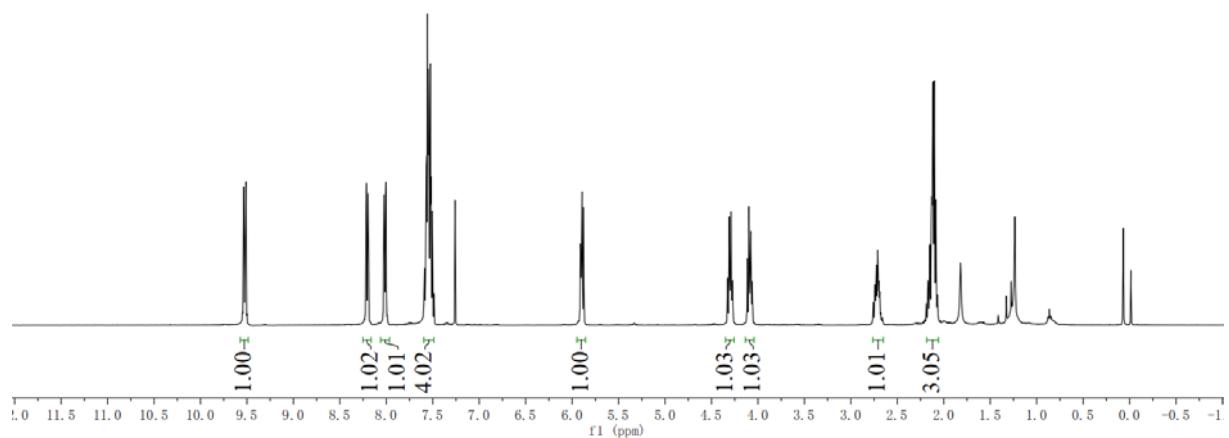


¹³C NMR (101M, CDCl₃) of **3ha**

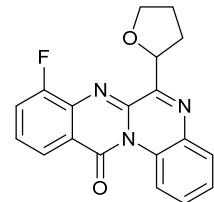




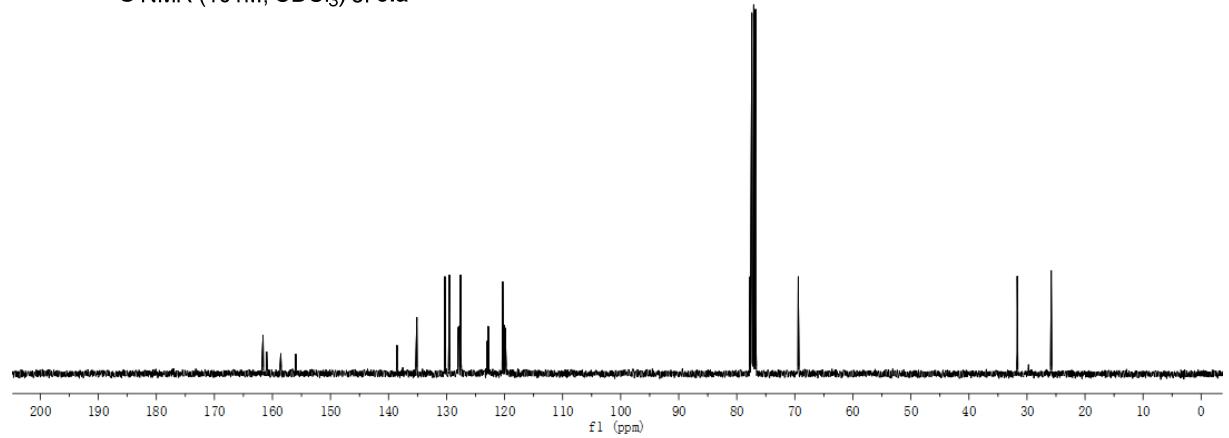
¹H NMR (400M, CDCl₃) of 3ia

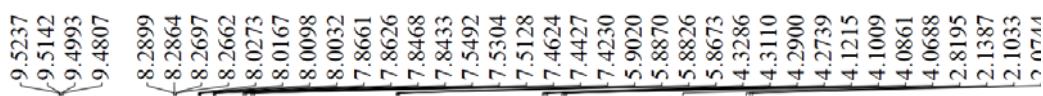


161.613
 161.036
 161.004
 158.560
 155.986
 135.126
 130.289
 129.515
 128.008
 127.933
 127.822
 127.575
 122.994
 122.814
 122.768
 120.328
 120.068
 119.886
 117.08
 77.404
 77.086
 76.768
 69.413
 -31.663
 -25.828

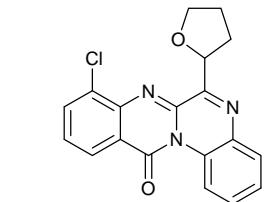
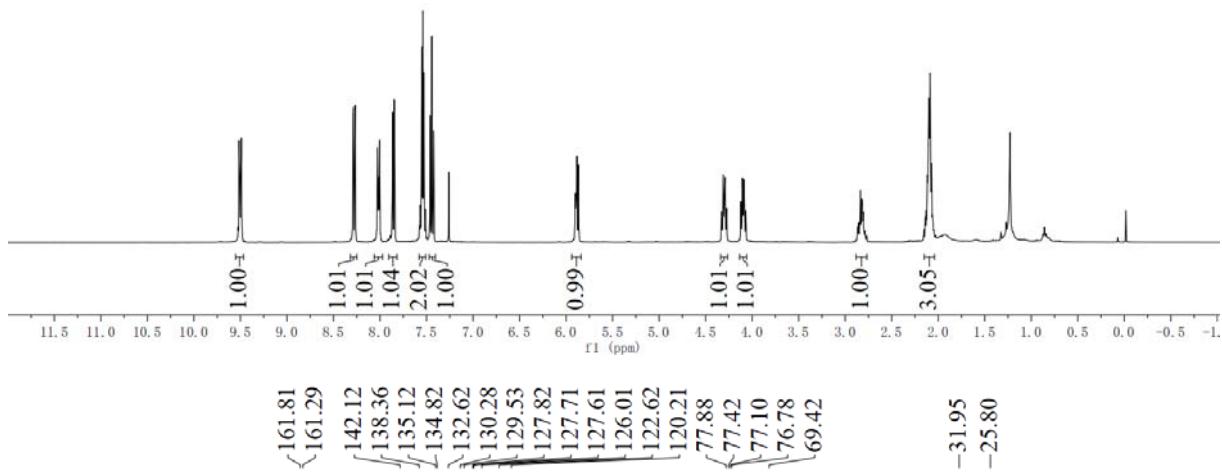


¹³C NMR (101M, CDCl₃) of 3ia

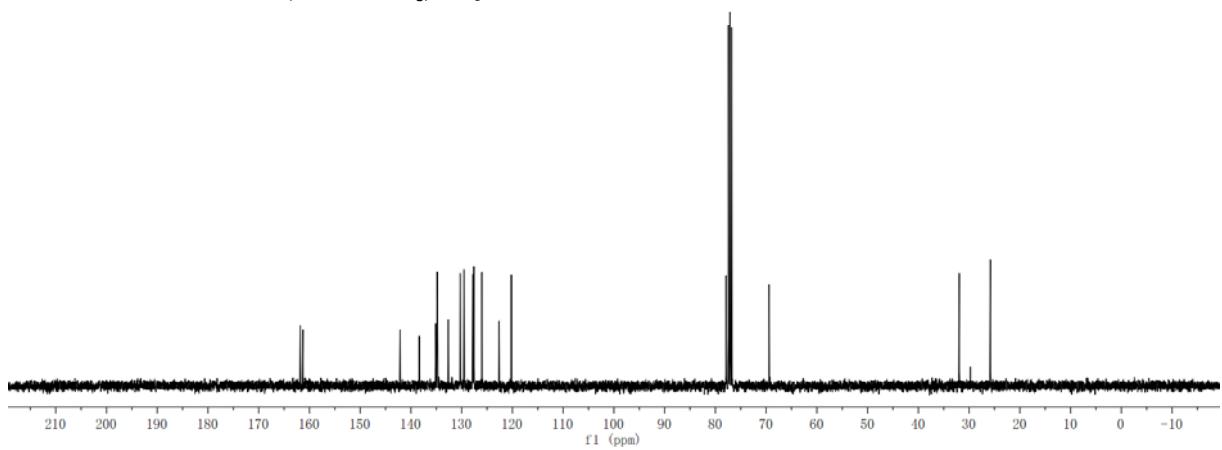




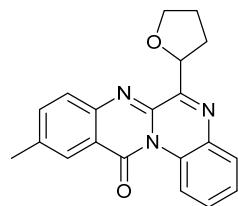
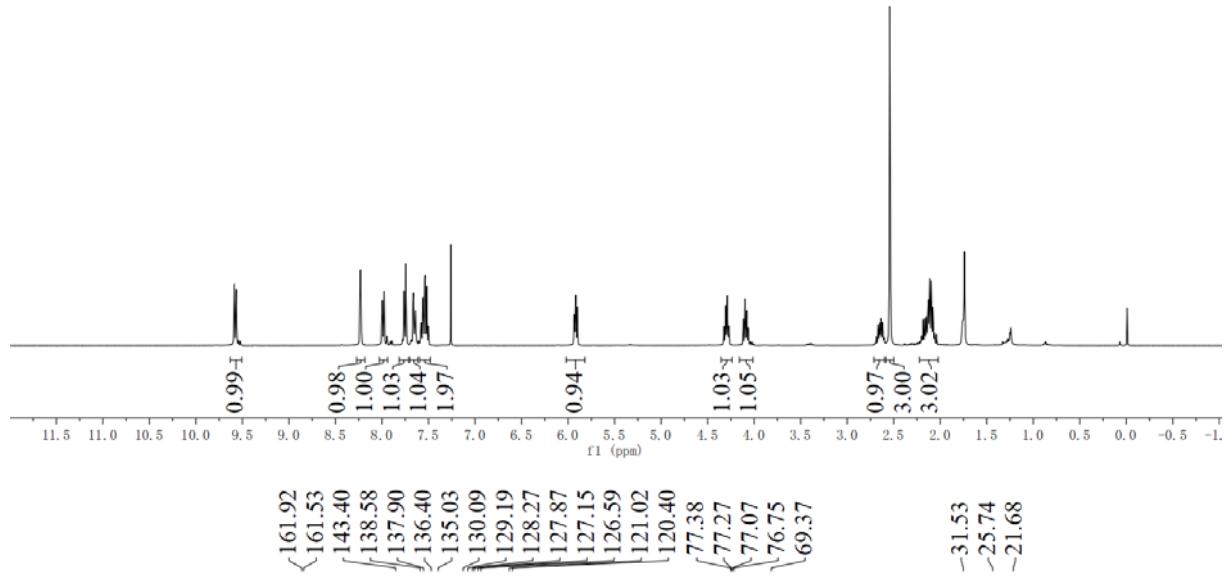
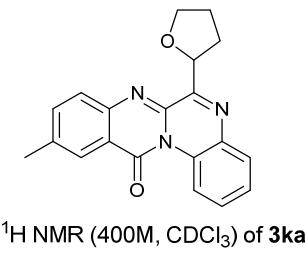
¹H NMR (400M, CDCl₃) of **3ja**



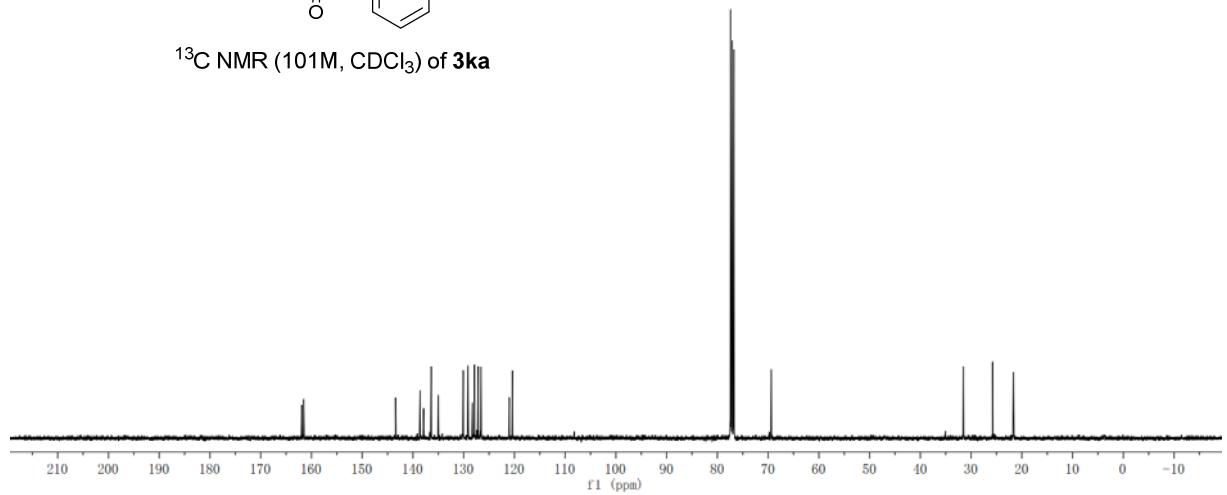
¹³C NMR (101M, CDCl₃) of **3ja**

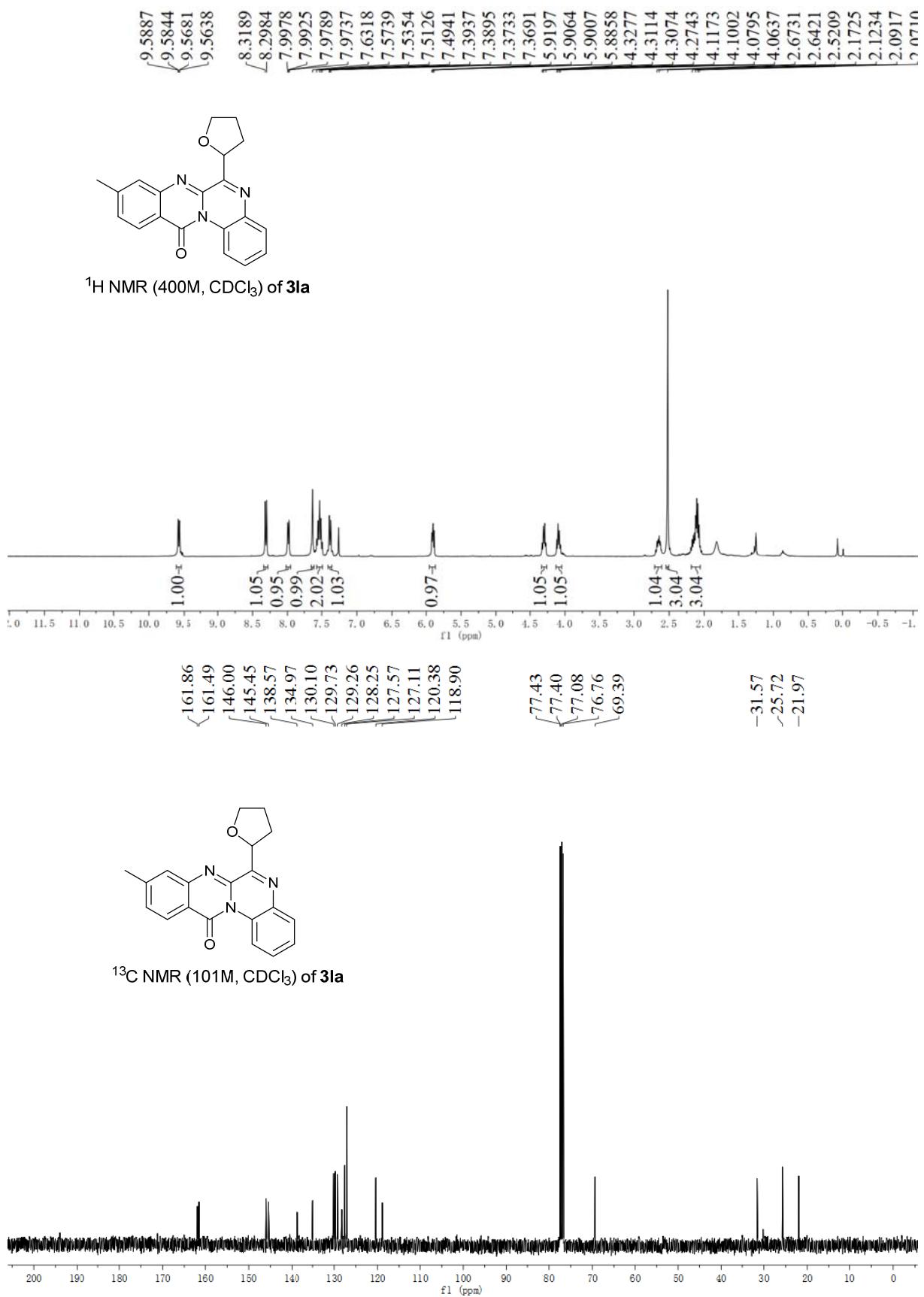


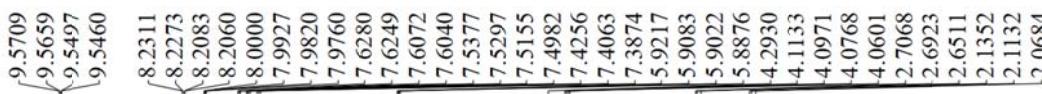
9.5916
9.5829
9.5710
9.5620
8.2366
8.2335
8.2301
8.2240
8.0006
7.9944
7.9820
7.9767
7.7644
7.7587
7.7436
7.7374
7.6667
7.5828
7.5598
7.5356
7.4993
5.9358
5.9217
5.9166
5.9014
4.3250
4.3051
4.2883
4.2709
4.1168
4.0961
4.0790
4.0629
2.6160
2.6560
2.6410
2.2010
-2.1340
-2.0911
2.0392



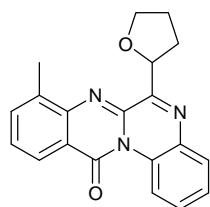
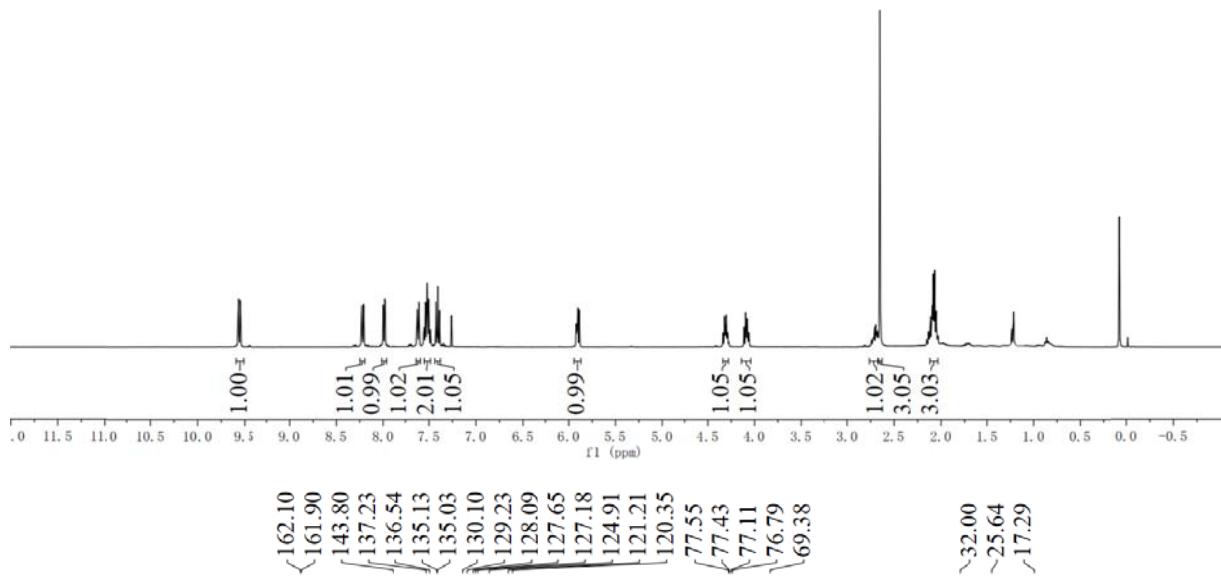
¹³C NMR (101M, CDCl₃) of **3ka**



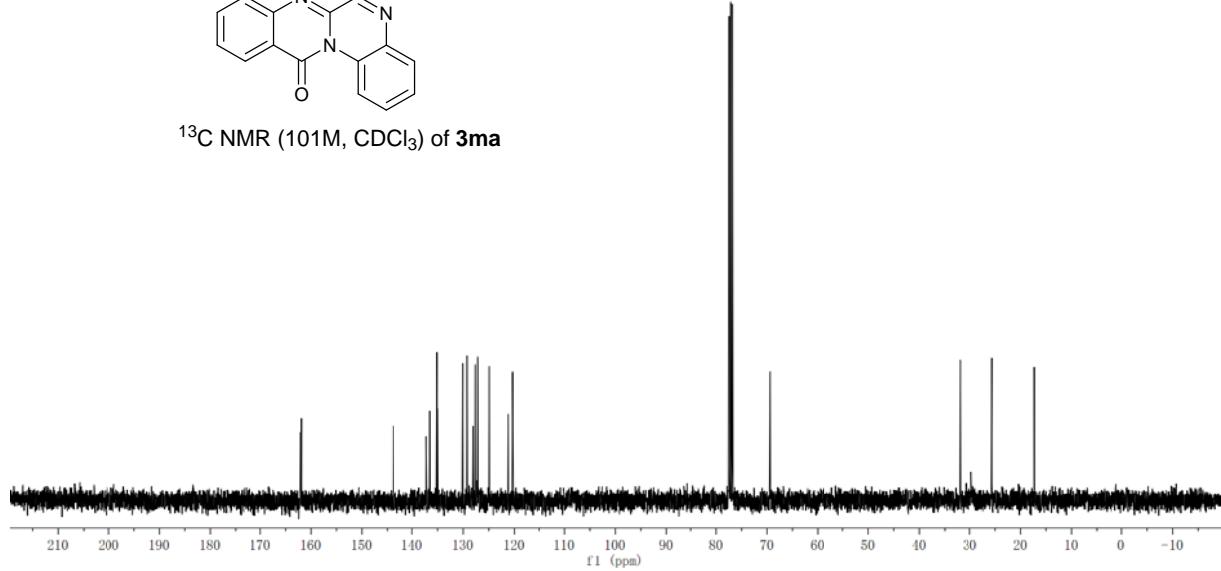




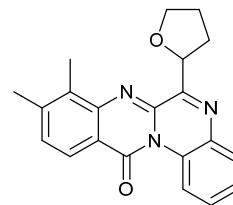
¹H NMR (400M, CDCl₃) of **3ma**



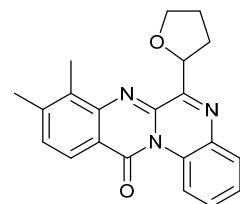
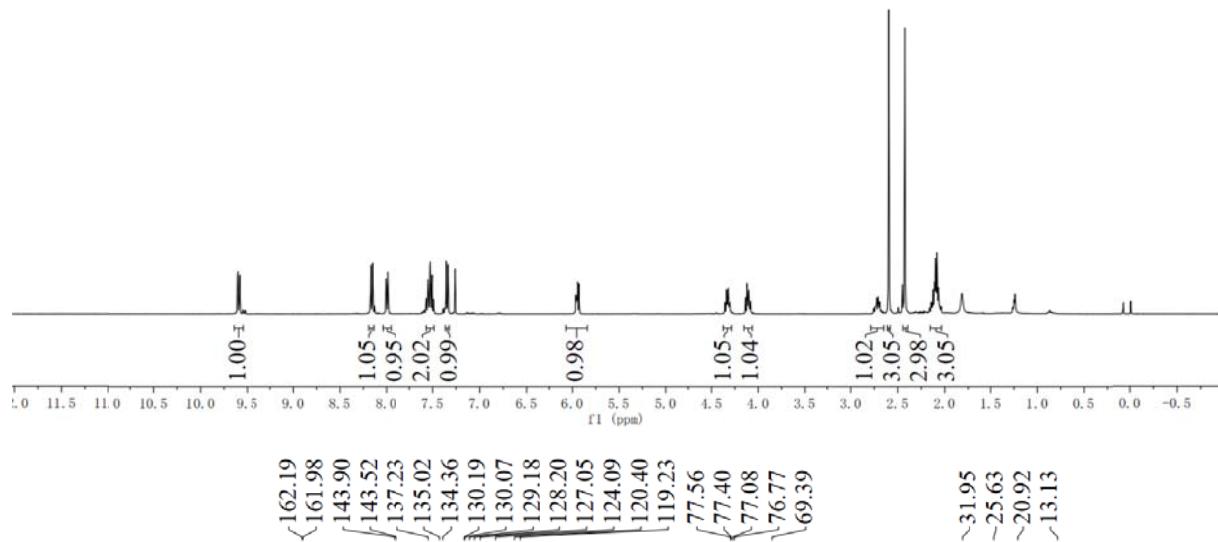
¹³C NMR (101M, CDCl₃) of **3ma**



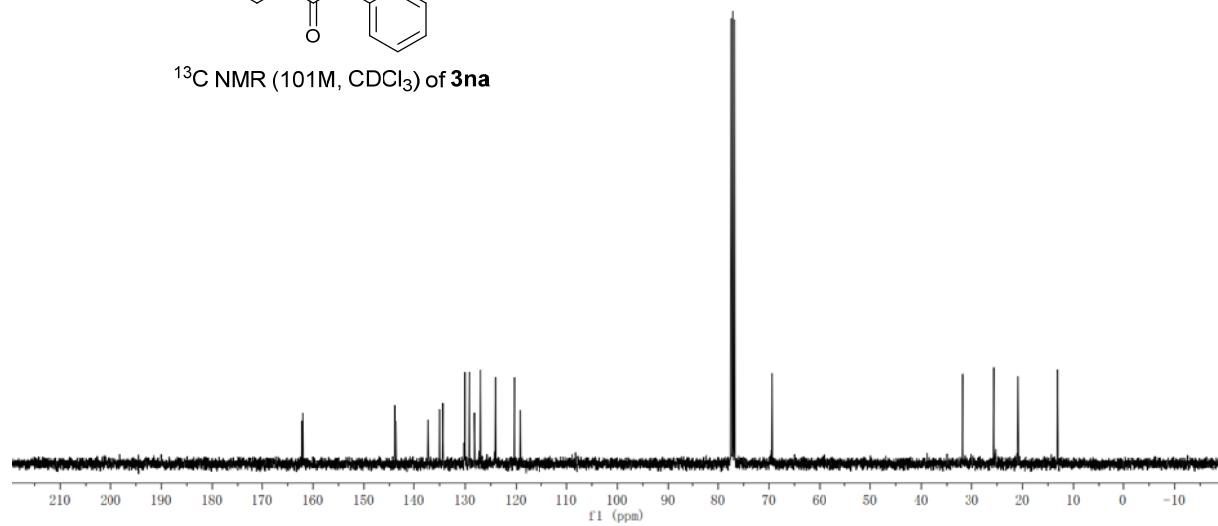
9.6063
9.6019
9.5847
9.5812
8.1697
8.1493
8.0061
7.9998
7.9874
7.9821
7.5697
7.5435
7.5099
7.4874
7.3564
7.3359
5.9638
5.9510
5.9444
5.9302
4.3574
4.3402
4.3101
4.3034
4.1354
4.1193
4.0992
4.0823
2.7420
2.7218
2.7099
2.6902
2.5952
2.4246
2.1473
2.0967
2.0672
2.0377



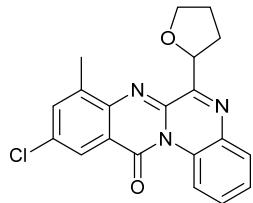
¹H NMR (400M, CDCl₃) of 3na



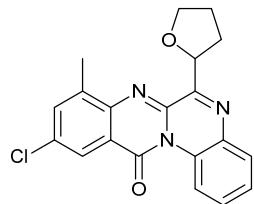
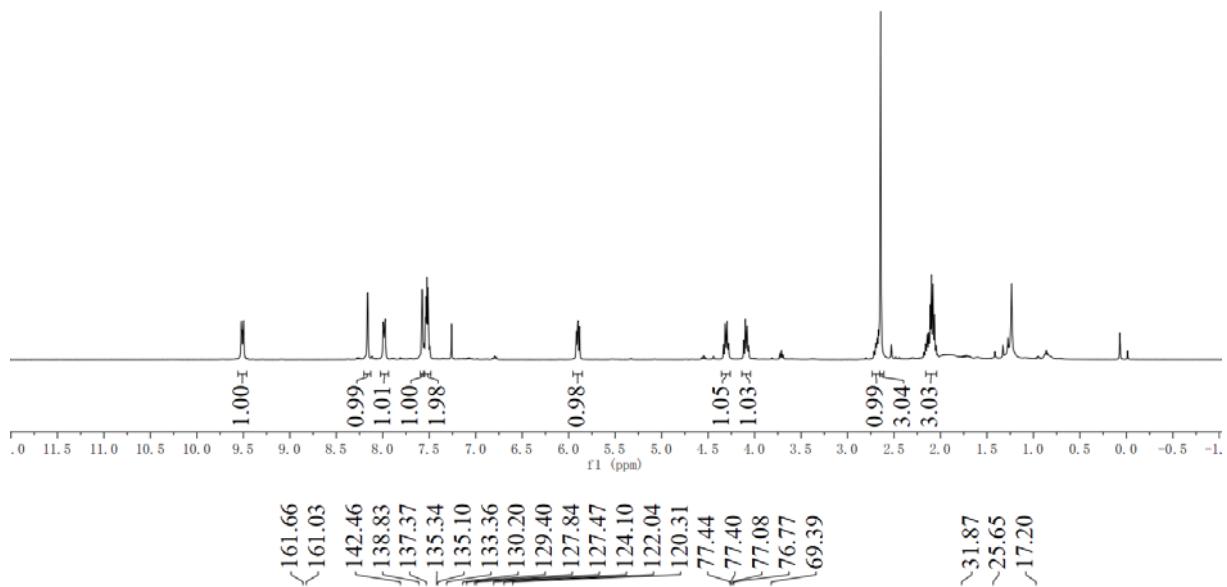
¹³C NMR (101M, CDCl₃) of 3na



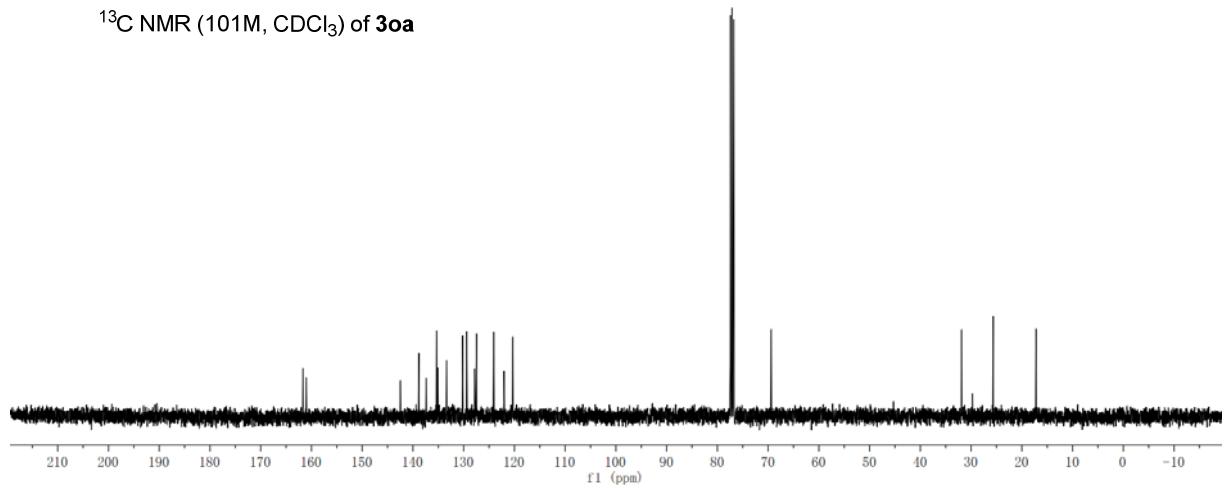
9.5217
9.5151
9.5058
9.4968
8.1657
8.1599
7.9966
7.9914
7.9799
7.9726
7.5785
7.5726
7.5406
7.5333
7.5239
7.5089
5.9174
5.9044
5.8981
5.8835
4.3337
4.3155
4.2974
4.2801
4.1169
4.0963
4.0799
4.0636
2.7156
2.6954
2.6800
2.6668
2.6443
2.1414
2.1110
2.0820
2.0612

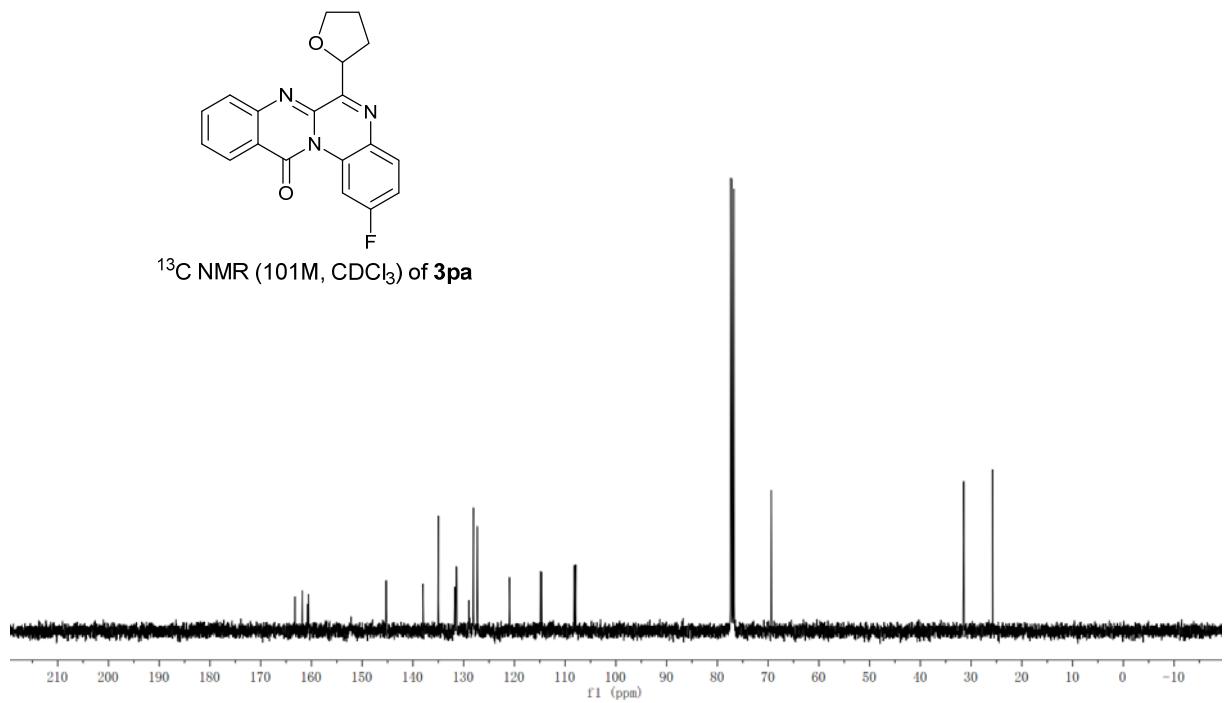
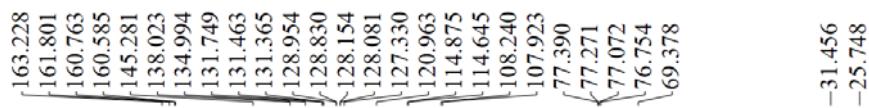
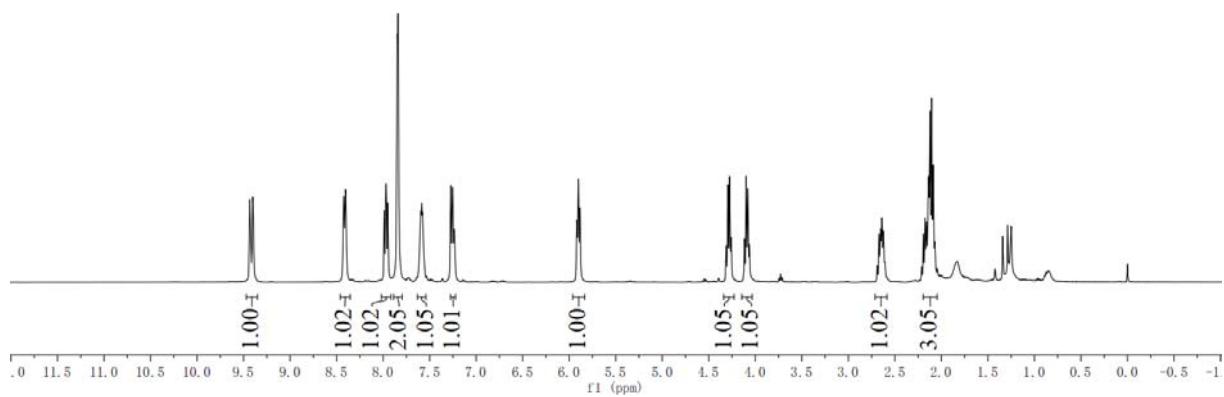
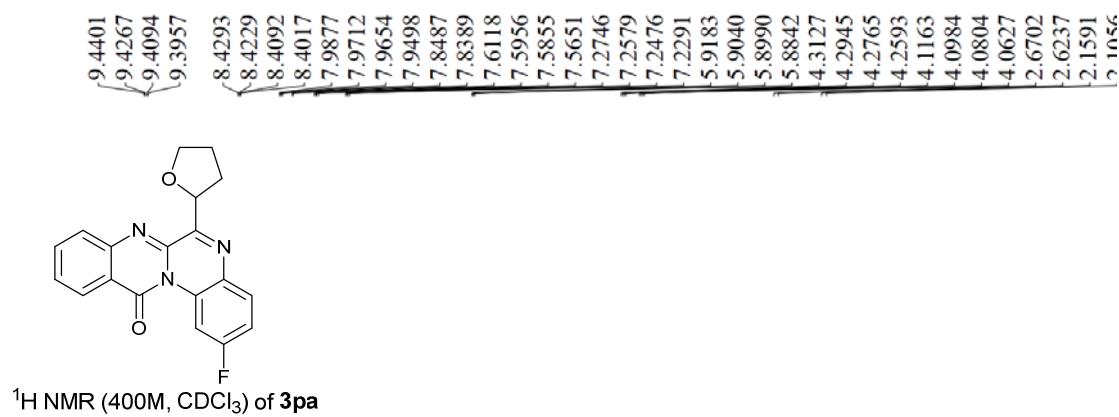


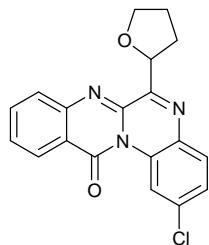
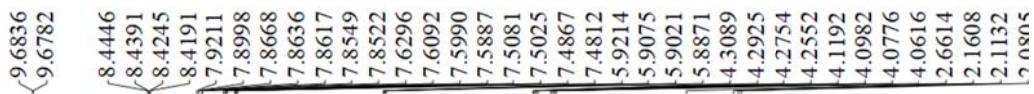
¹H NMR (400M, CDCl₃) of 3oa



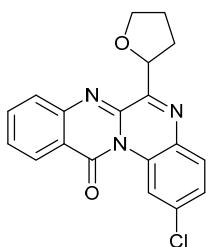
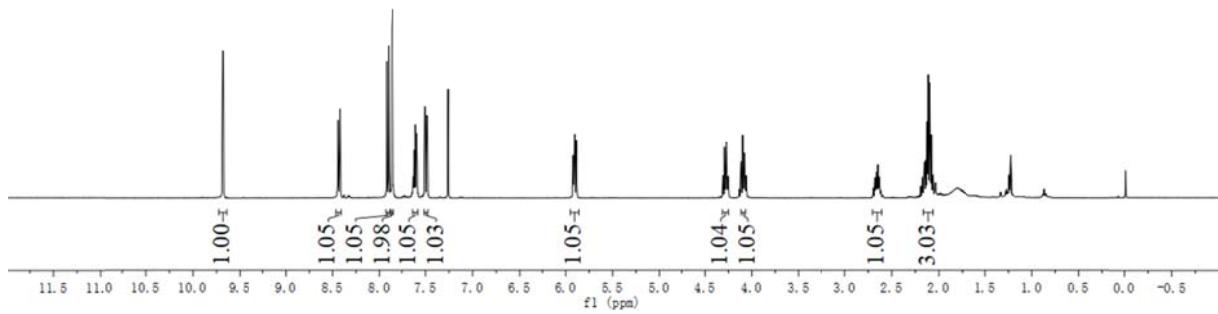
¹³C NMR (101M, CDCl₃) of 3oa



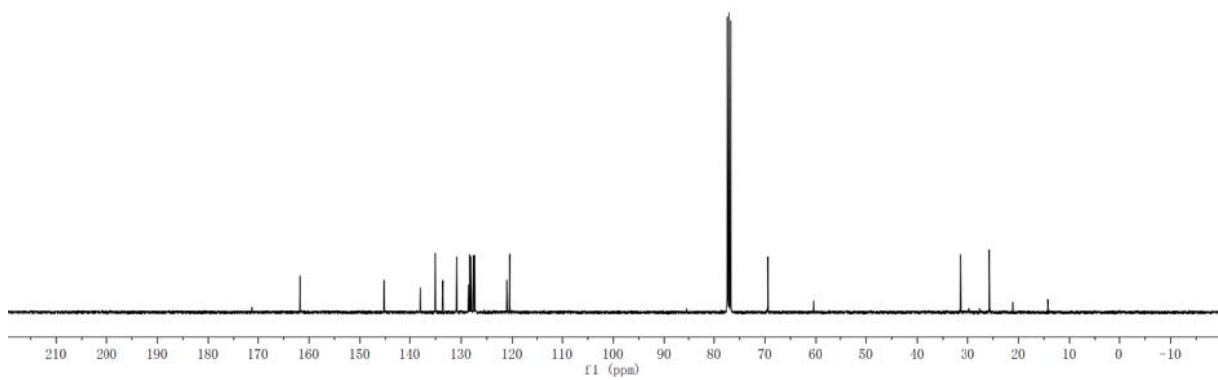




¹H NMR (400M, CDCl₃) of **3qa**

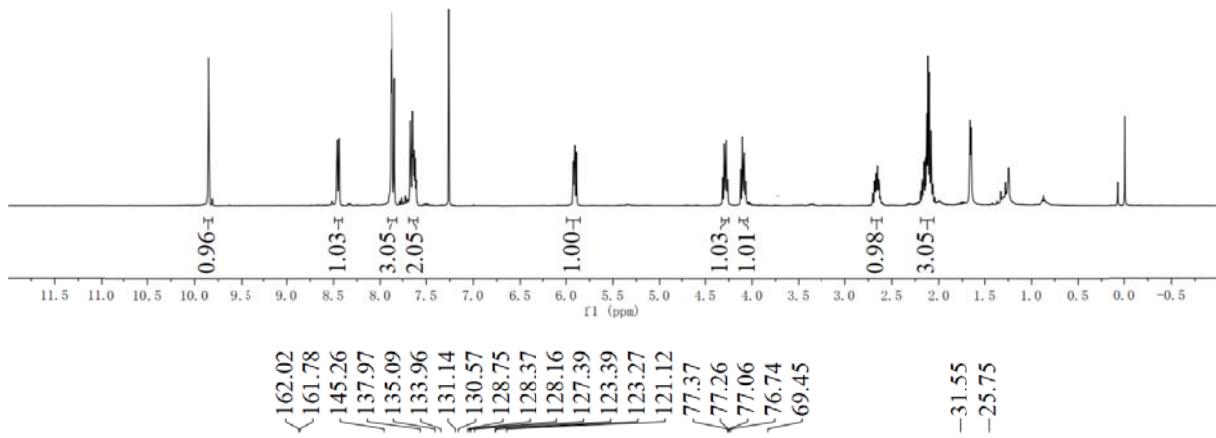


¹³C NMR (101M, CDCl₃) of 3qa

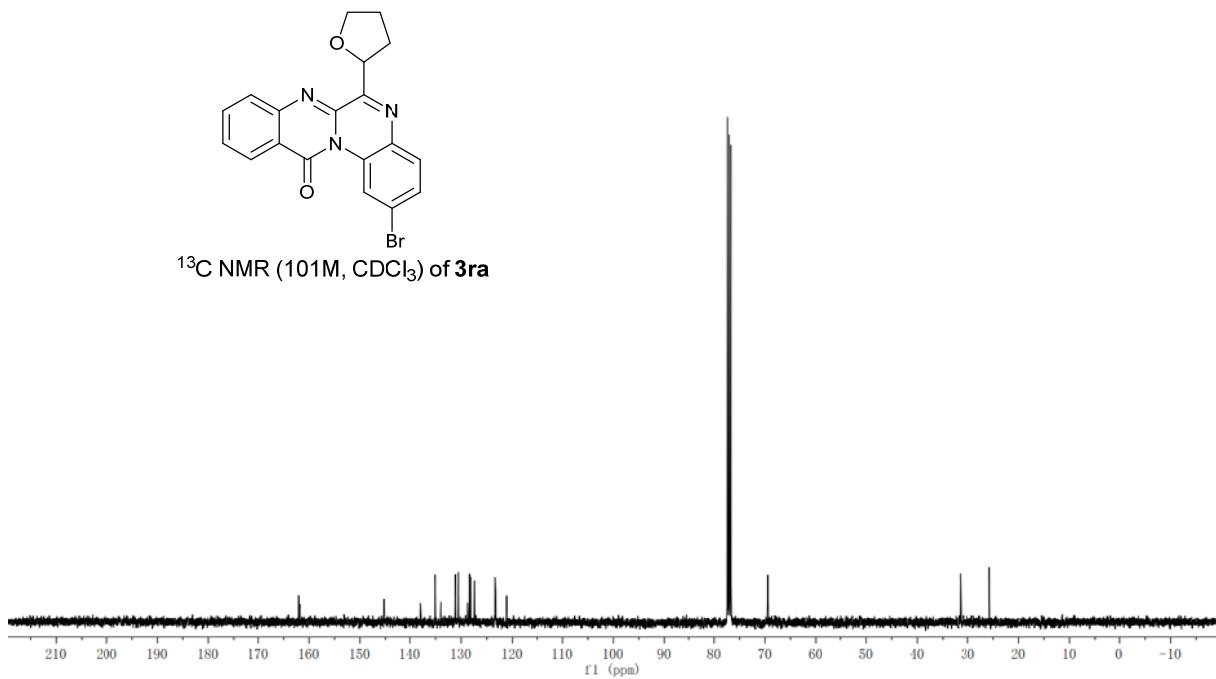




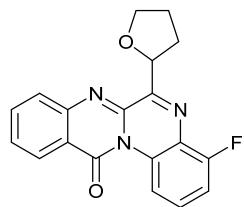
¹H NMR (400M, CDCl₃) of 3ra



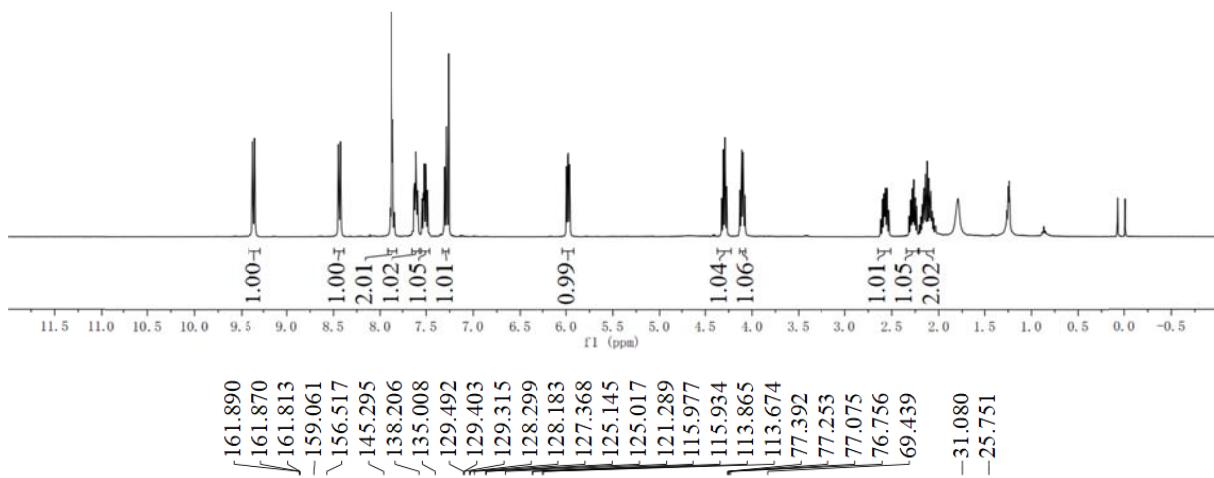
¹³C NMR (101M, CDCl₃) of 3ra

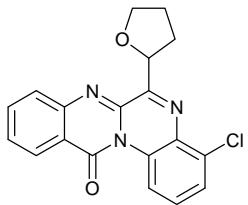
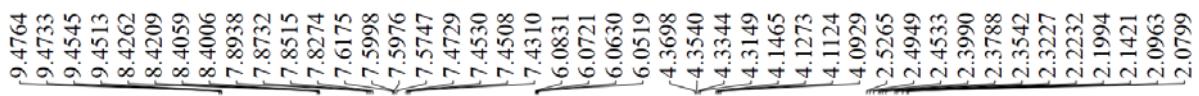


9.3707	-9.3639
9.3484	-9.3484
9.3415	-9.3415
8.4506	-8.4506
8.4419	-8.4419
8.4302	-8.4302
8.4242	-8.4242
7.8897	-7.8897
7.8697	-7.8697
7.8588	-7.8588
7.8384	-7.8384
7.6304	-7.6304
7.6045	-7.6045
7.5954	-7.5954
7.5436	-7.5436
7.5284	-7.5284
7.4854	-7.4854
7.4826	-7.4826
7.3072	-7.3072
7.2867	-7.2867
7.2842	-7.2842
7.2816	-7.2816
5.9962	-5.9962
5.9828	-5.9828
5.9767	-5.9767
5.9625	-5.9625
4.3260	-4.3260
4.3090	-4.3090
4.3063	-4.3063
4.2711	-4.2711
4.1293	-4.1293
4.1100	-4.1100
4.0953	-4.0953
4.0759	-4.0759
2.5981	-2.5981
2.5513	-2.5513
2.5310	-2.5310
2.3168	-2.3168
2.2965	-2.2965
2.2659	-2.2659
2.2352	-2.2352
2.1405	-2.1405
2.1010	-2.1010

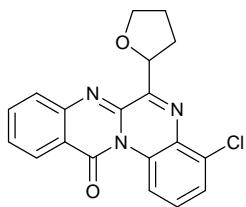
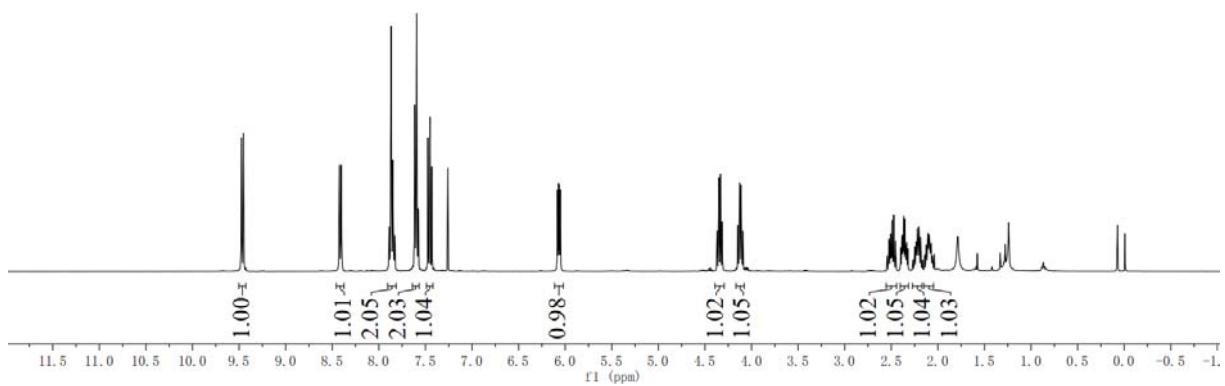


¹H NMR (400M, CDCl₃) of 3sa

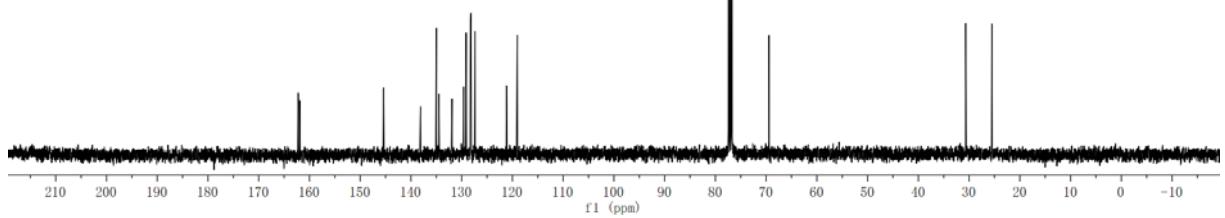


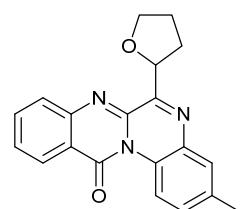
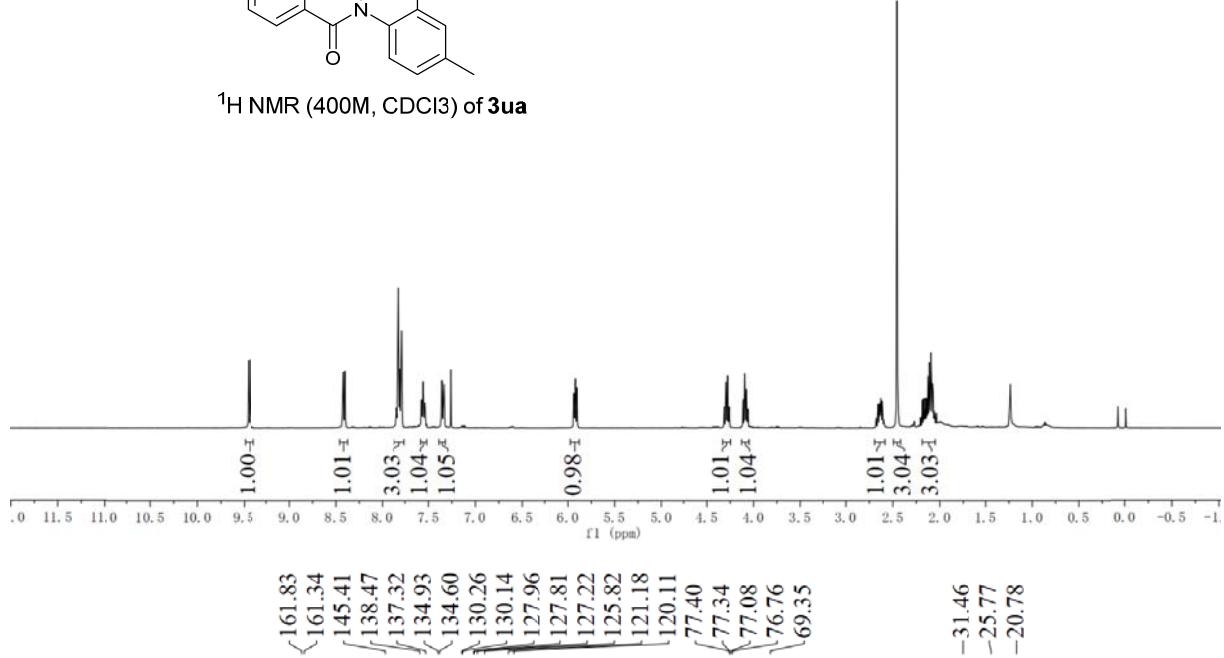
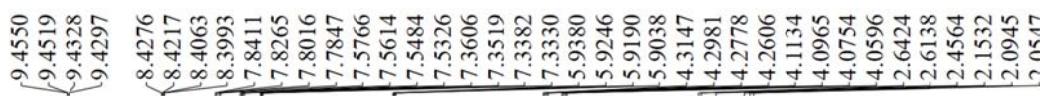


¹H NMR (400M, CDCl₃) of 3ta

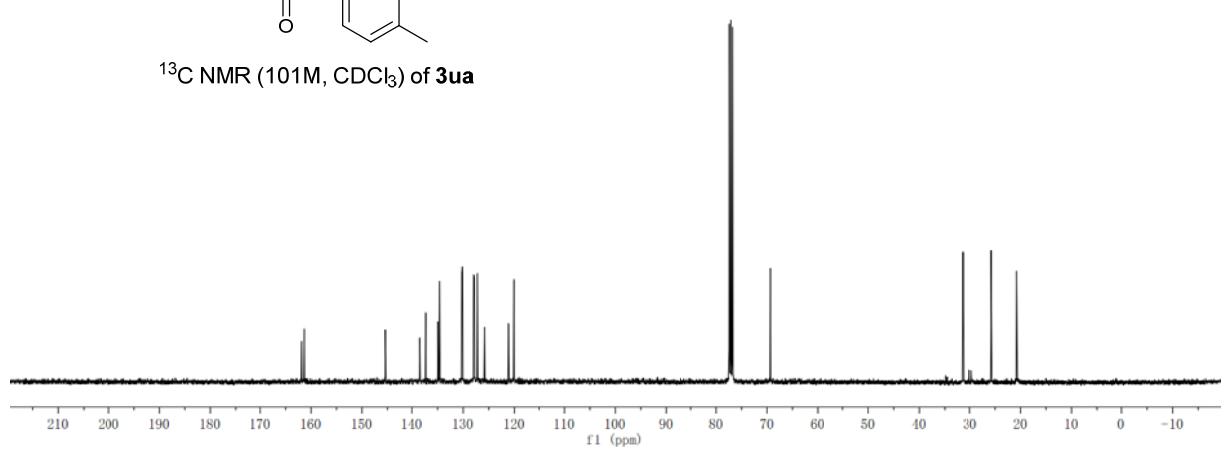


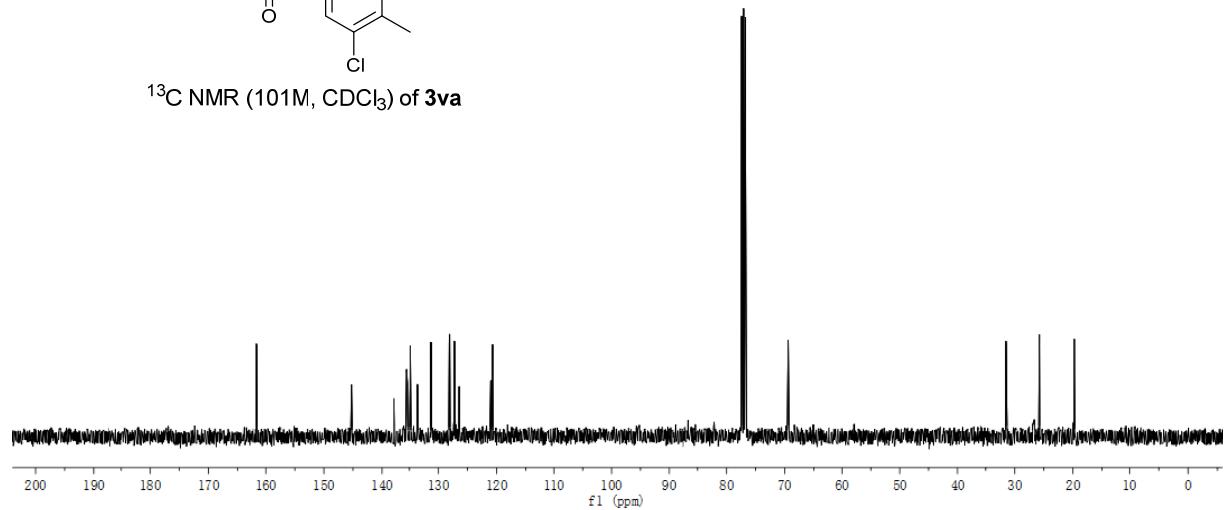
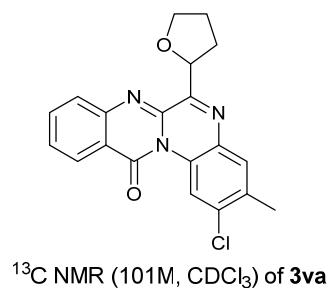
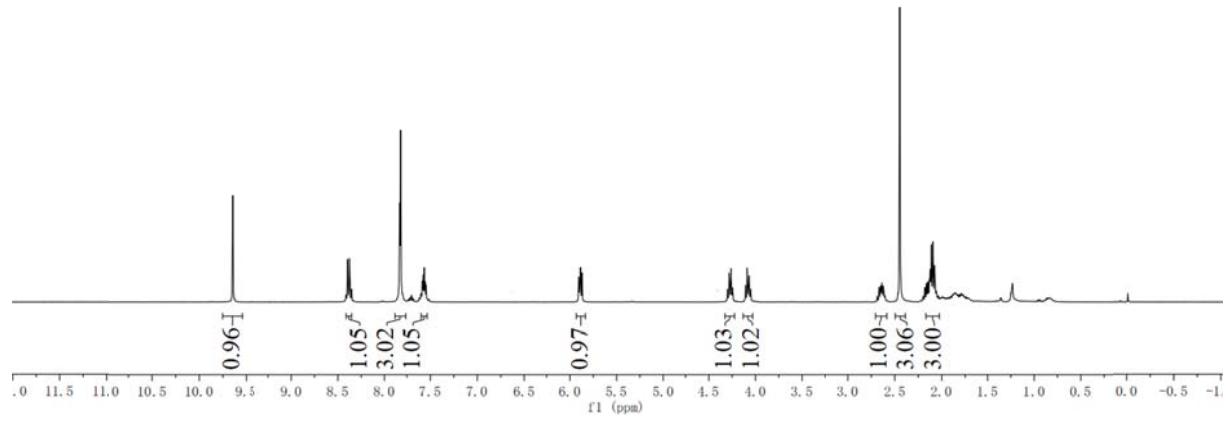
¹³C NMR (101M, CDCl₃) of 3ta



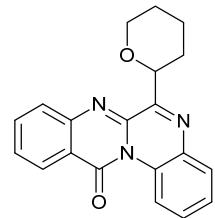


¹³C NMR (101M, CDCl₃) of 3ua

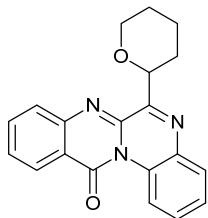
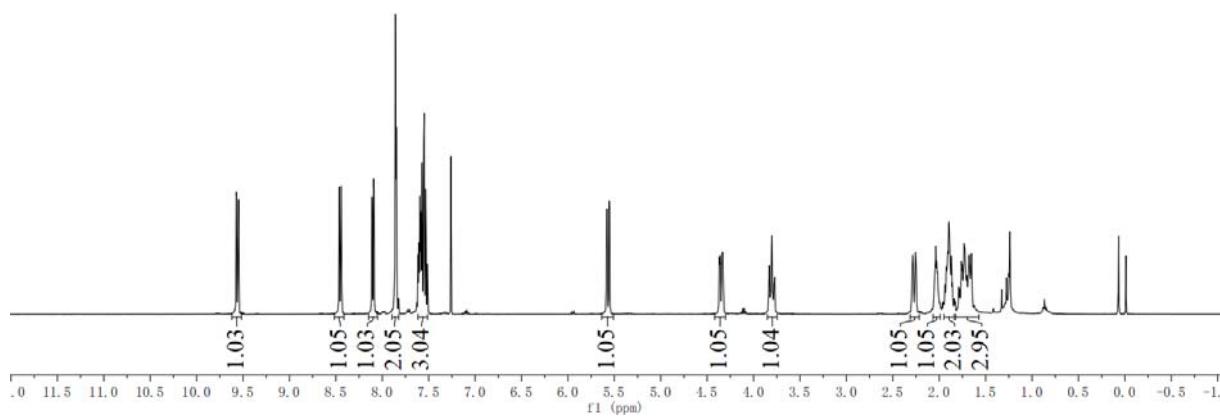




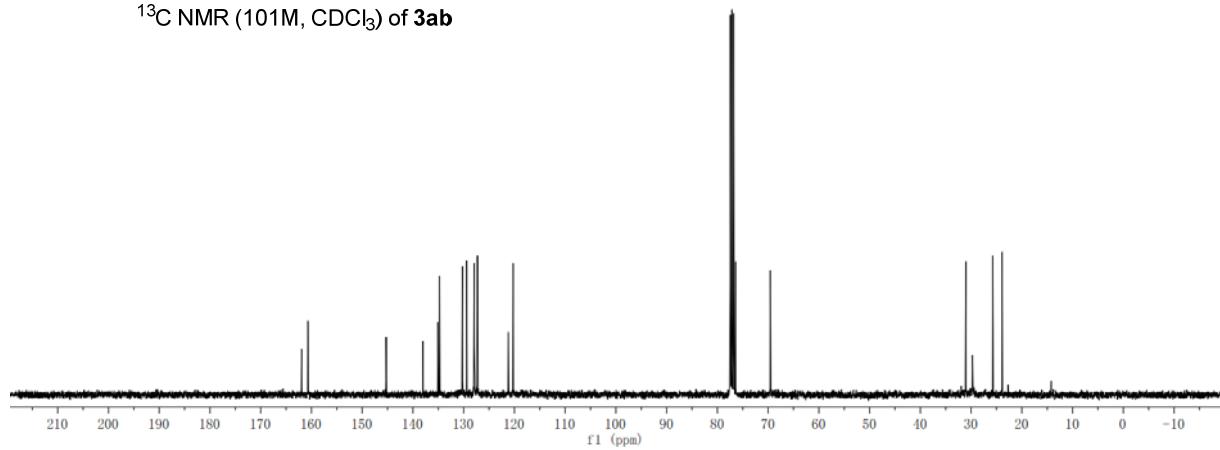
9.5722	9.5679
9.5519	9.5476
8.4636	8.4580
8.4432	8.4384
8.1121	8.1057
8.0934	8.0880
7.8712	7.8594
7.8507	7.6151
7.5742	7.5478
7.5112	7.5112
5.5773	5.5555
5.5505	4.3688
4.3579	4.3408
4.3251	4.3251
3.8070	3.8070
3.8011	3.7720
2.2899	2.2899
2.2598	2.2492
2.0368	2.0368
2.0224	2.0224
1.9368	1.9368
1.8584	1.8584
1.7911	1.7911
1.7599	1.7599
1.7329	1.7329

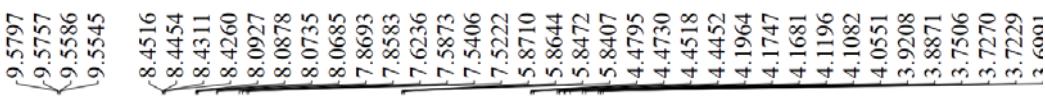


¹H NMR (400M, CDCl₃) of 3ab

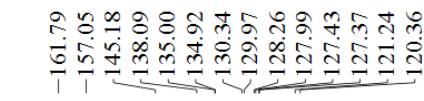
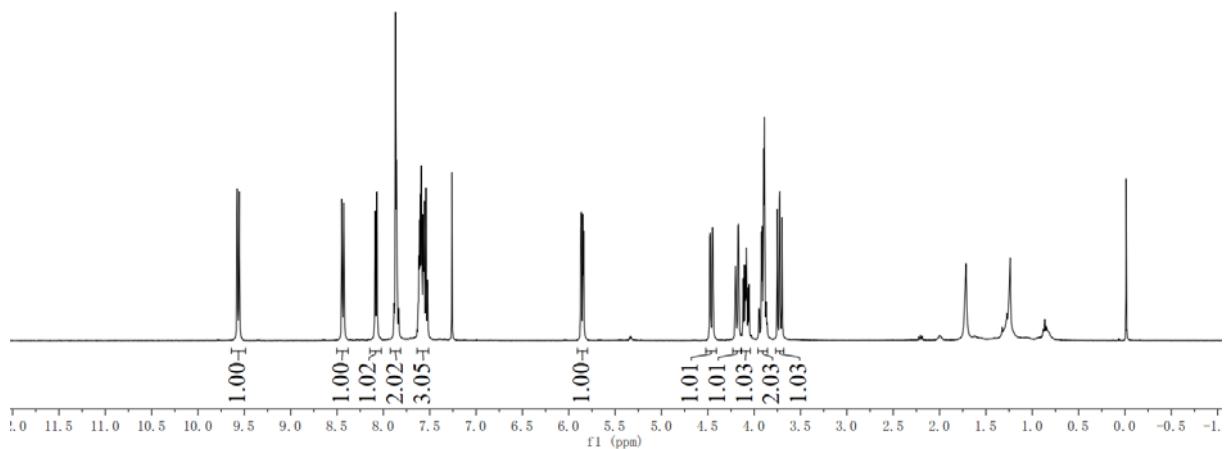


¹³C NMR (101M, CDCl₃) of 3ab

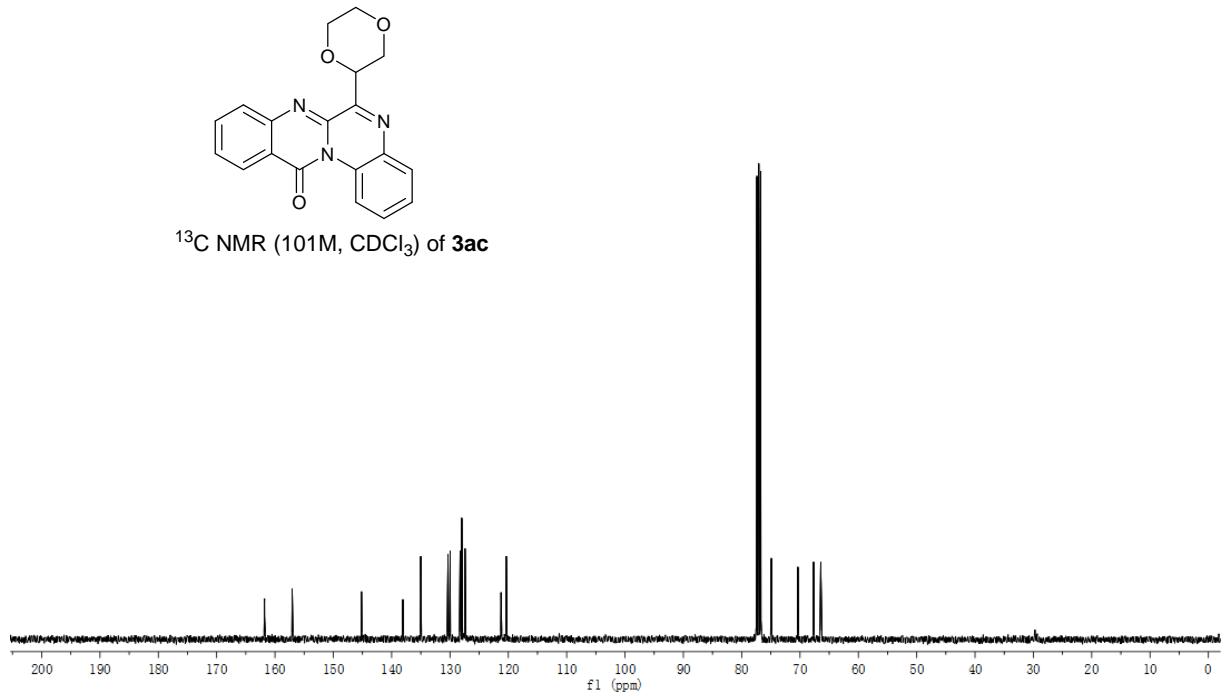


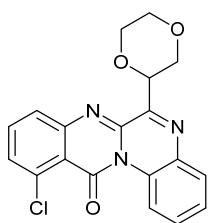
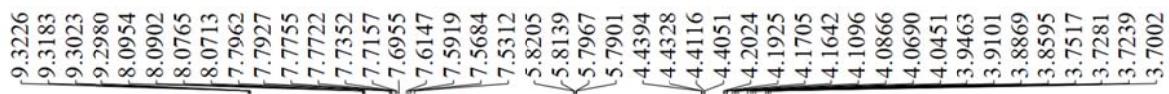


¹H NMR (400M, CDCl₃) of 3ac

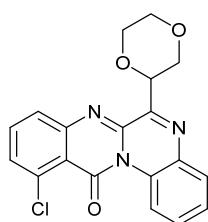
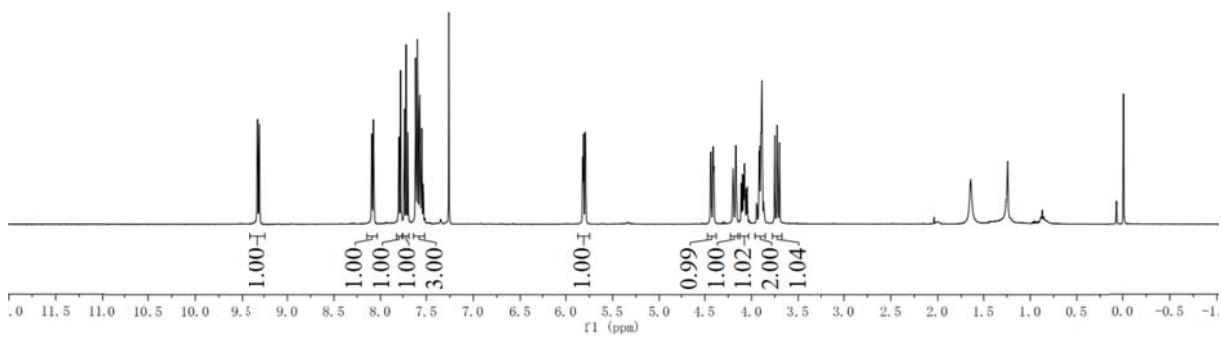


¹³C NMR (101M, CDCl₃) of 3ac

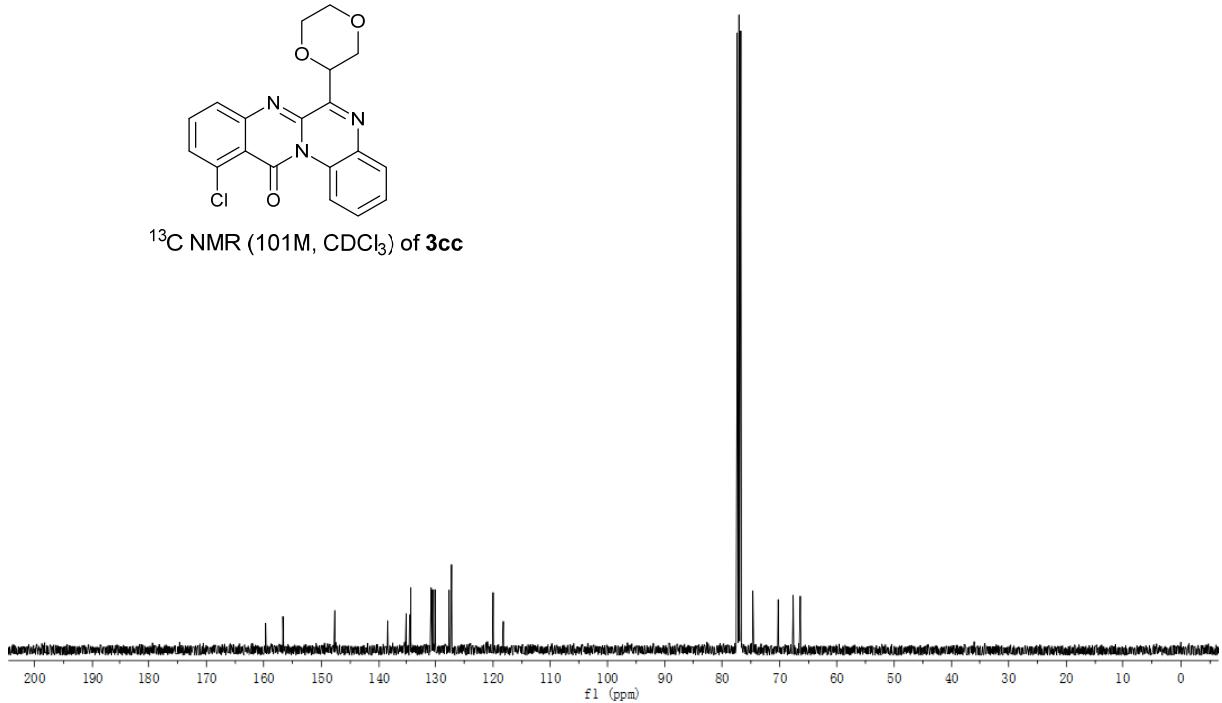


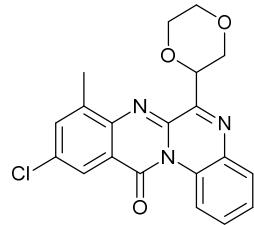
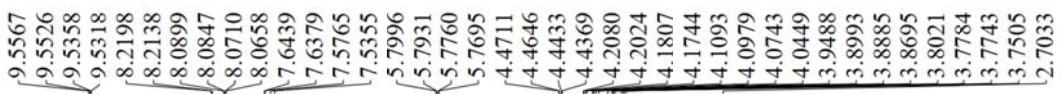


¹H NMR (400M, CDCl₃) of 3cc

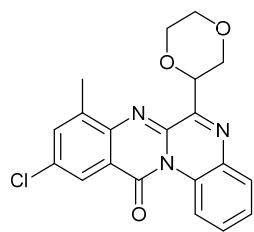
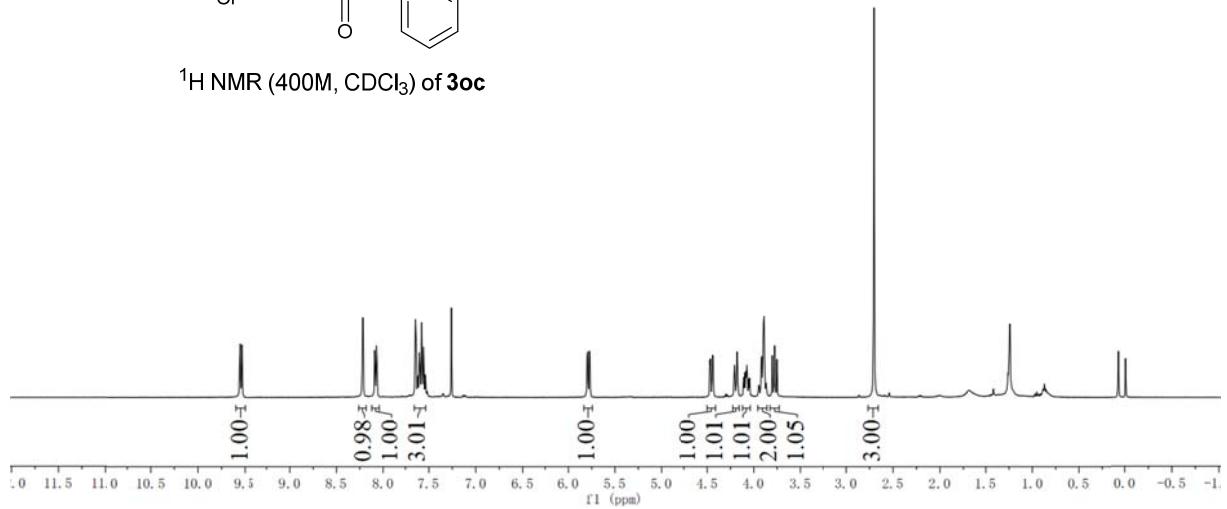


¹³C NMR (101M, CDCl₃) of 3cc

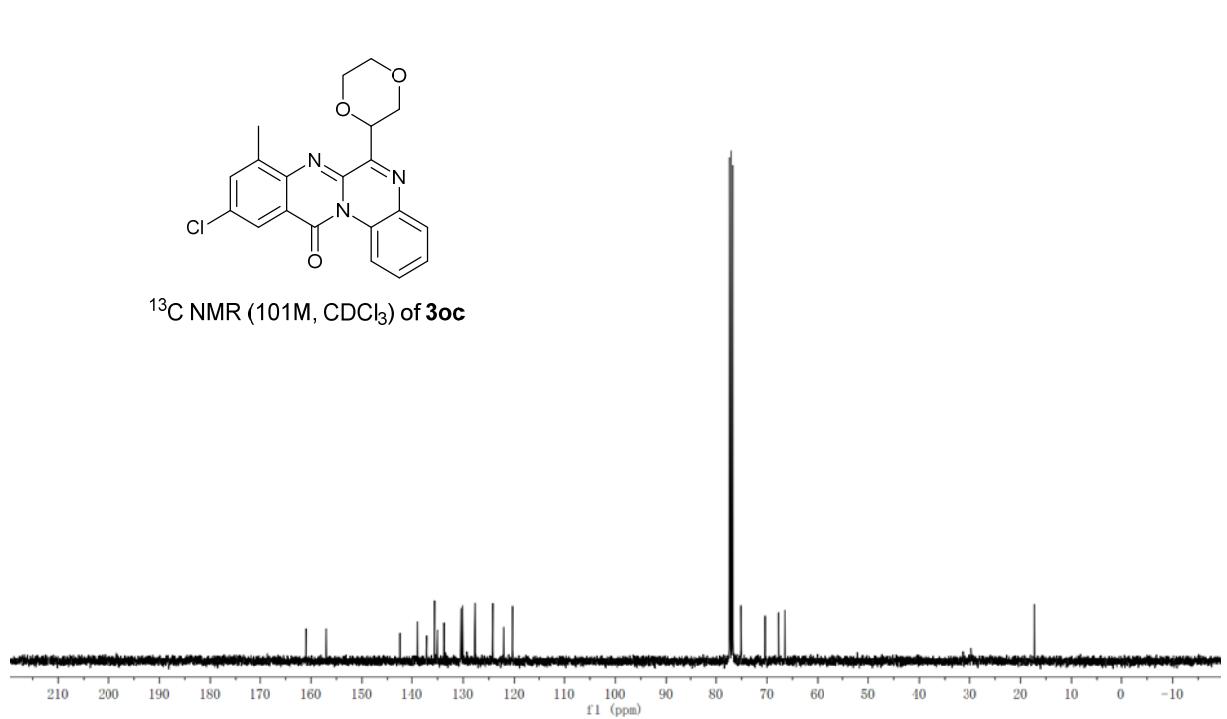


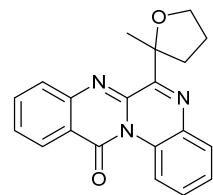
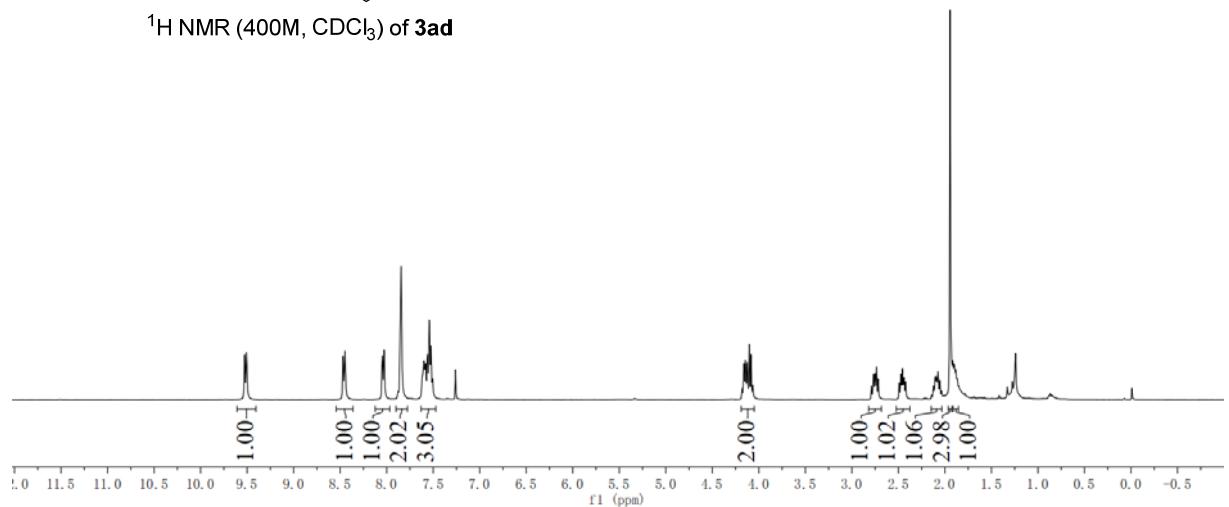
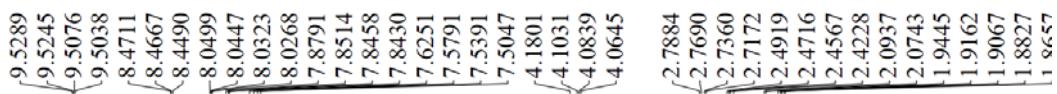


¹H NMR (400M, CDCl₃) of **3oc**

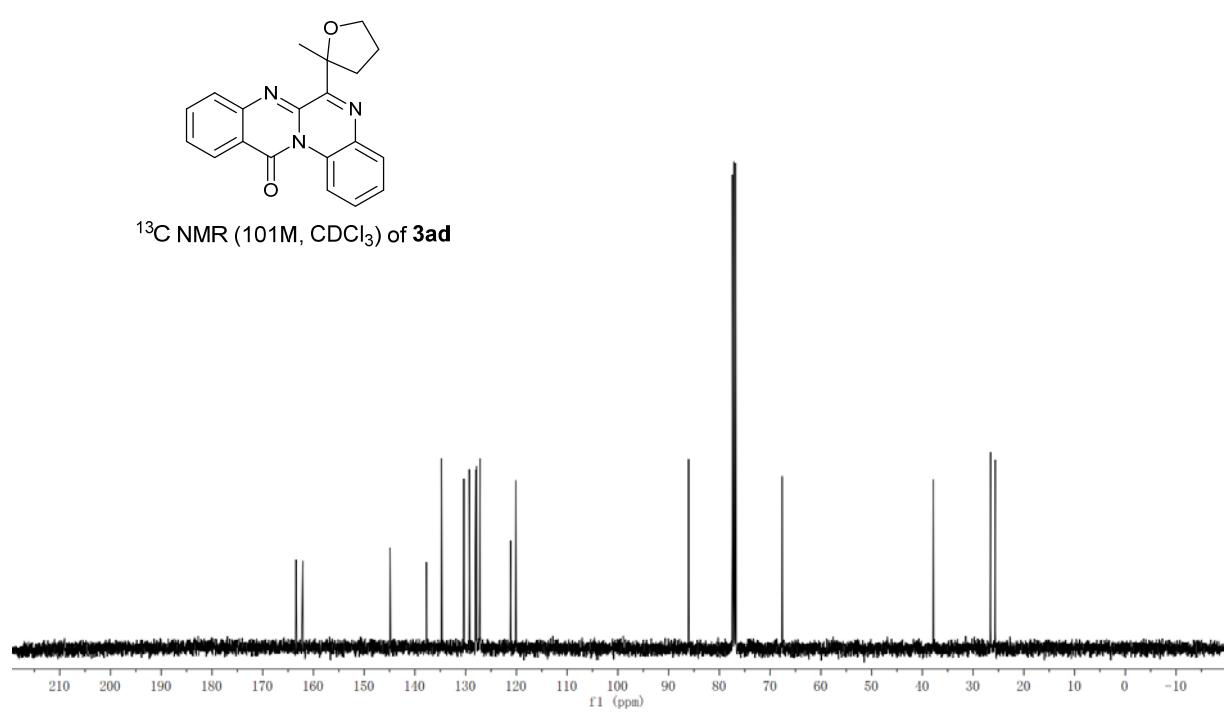


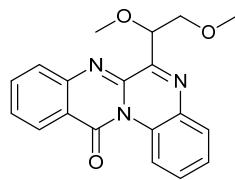
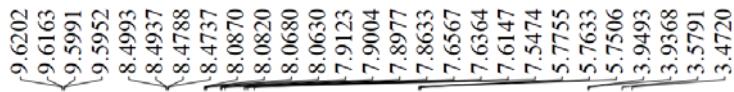
¹³C NMR (101M, CDCl₃) of **3oc**



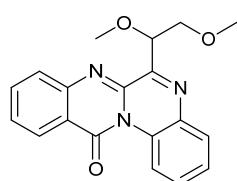
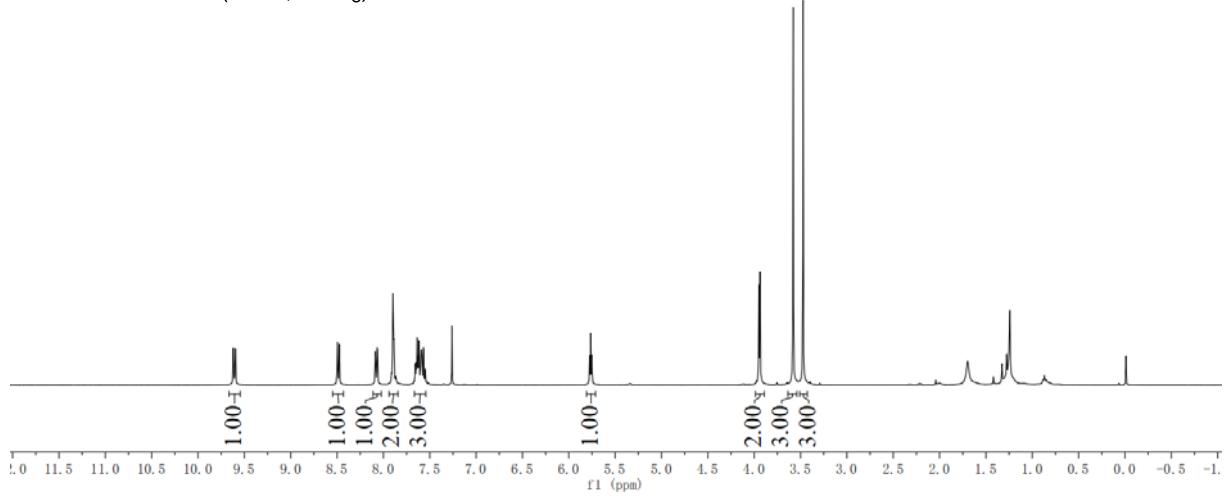


¹³C NMR (101M, CDCl₃) of **3ad**

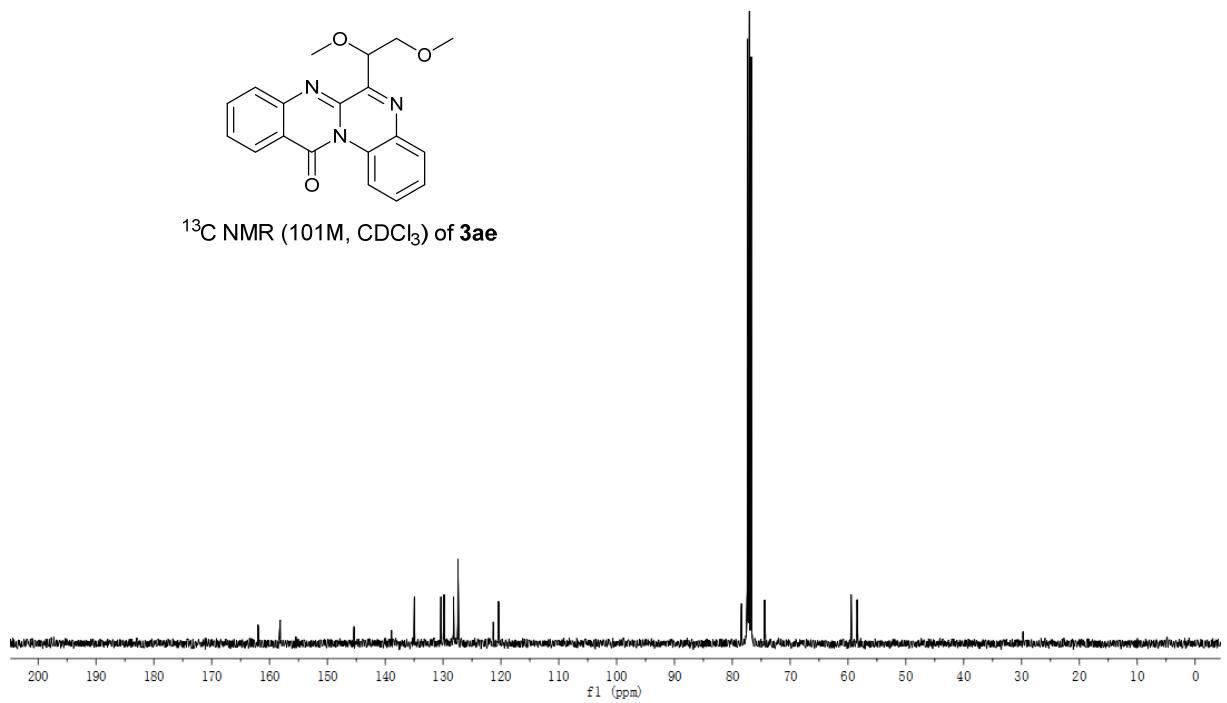


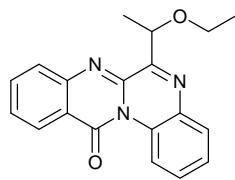
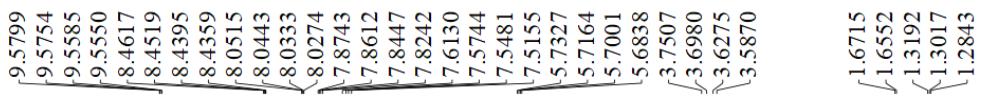


^1H NMR (400M, CDCl_3) of 3ae

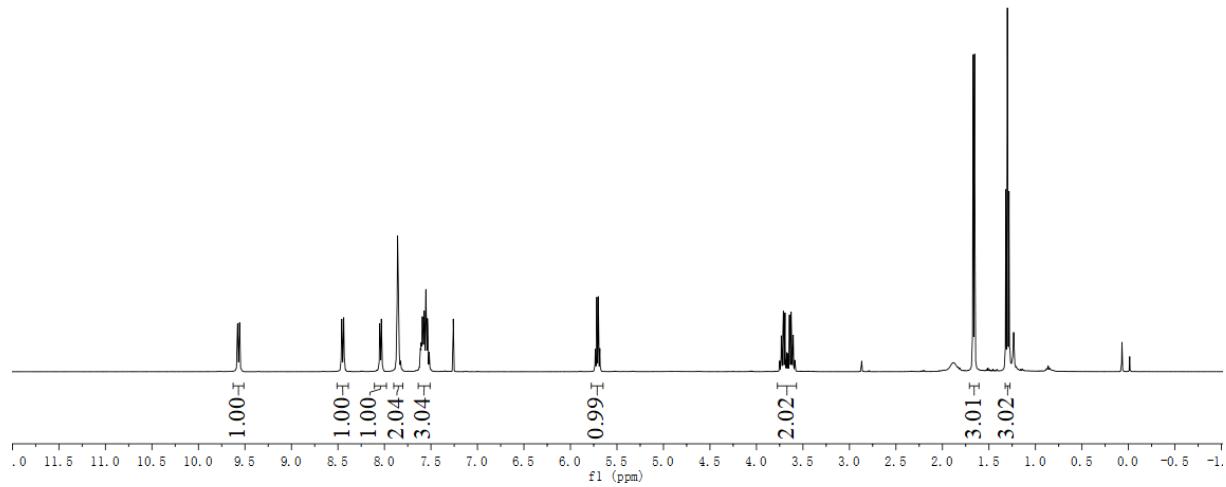


¹³C NMR (101M, CDCl₃) of 3ae

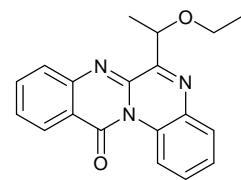




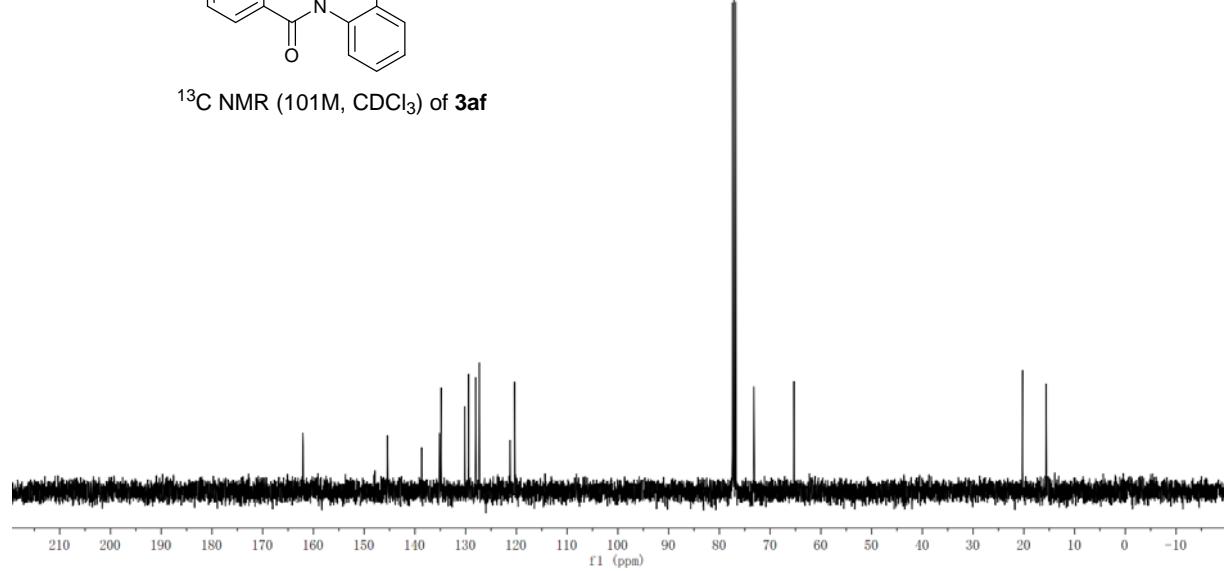
¹H NMR (400M, CDCl₃) of 3af



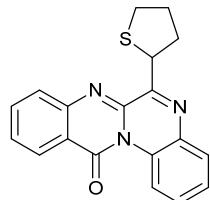
162.12
 162.02
 145.40
 138.66
 135.18
 134.83
 130.15
 129.42
 128.05
 128.02
 127.97
 127.35
 127.33
 121.24
 120.35
 77.40
 77.08
 76.77
 73.22
 65.29



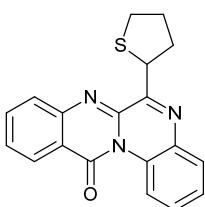
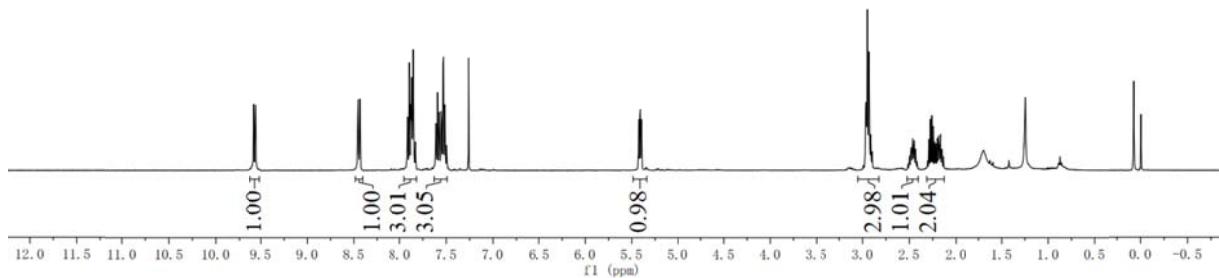
¹³C NMR (101M, CDCl₃) of 3af



9.5804
 9.5760
 9.5600
 9.5556
 8.4571
 8.4536
 8.4369
 8.4334
 7.9162
 7.8923
 7.8493
 7.8289
 7.6136
 7.5346
 7.5289
 7.4926
 5.4139
 5.4081
 5.4260
 5.3963
 2.9920
 2.9469
 2.9312
 2.8986
 2.5150
 2.4836
 2.4634
 2.4173
 2.3056
 2.2751
 2.2599
 2.1361



¹H NMR (400M, CDCl₃) of 3ag



¹³C NMR (101M, CDCl₃) of 3ag

