

Supporting Information

Acidochromism-Enabled Aerobic Oxidative Cross-coupling of Quinoxalinones with Indoles and Fluorescence of Products

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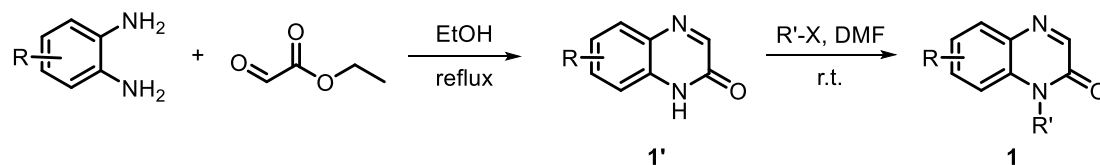
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1. General experimental information

^1H NMR and ^{13}C NMR spectra were recorded on an Agilent DD2 400-MR spectrometer in CDCl_3 or $\text{DMSO}-d_6$ with tetramethylsilane (TMS) as the internal standard; Chemical shifts (δ) are expressed in ppm and J -values are in Hz. UV-Vis absorption spectra were recorded by using Shimadzu UV-2600 UV/Vis spectrometer. Fluorescence Spectra were recorder by using RF-5301PC for all experiments. HRMS was measured on a TOF-Q mass spectrometer equipped with an ESI source. Melting point was measured with SGWX-4 Microscopic Melting Point Tester. The solvents and chemicals were purchased and used as received. All reactions were monitored by TLC with Huanghai GF254 silica gel coated plates. Flash column chromatography was carried out using 300-400 mesh silica gel at increased pressure.

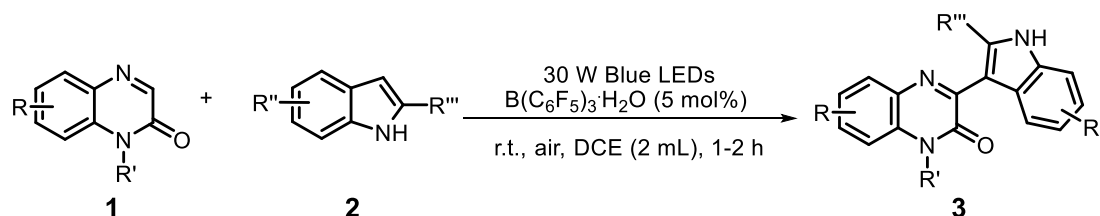
2. Preparation of starting materials

2.1 General procedure for the synthesis of quinoxalin-2-ones¹



To ethanol (1 mol/L) were added *o*-arylenediamine (1 equiv.) and ethyl 2-oxoacetate (1.1 equiv.). The reaction mixture was stirred at reflux for 1h, then at room temperature overnight. The precipitate was filtered and washed with ethanol, then dried to give quinoxalinone **1'**. To a suspension of quinoxalinone **1'** (1 equiv.) in DMF was added potassium carbonate (1.2 equiv.) and the corresponding halides (R'-X) (1.6 equiv.). The mixture was stirred at room temperature overnight. Ethyl acetate and water were added. The aqueous layer was extracted twice with EtOAc. The combined organic layers were washed with a saturated solution of NH₄Cl then brine, dried over MgSO₄, filtered and evaporated under reduced pressure. The residue is purified by flash chromatography over silica gel to afford the desired product **1**.

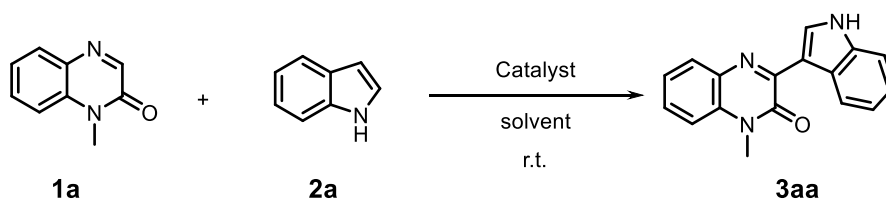
2.2 General procedure for the synthesis of methylquinoxalin-2(1H)-one with Indoles



To a mixture of **1** (0.2 mmol) and **2** (0.3 mmol) in DCE (2.0 mL) was added B(C₆F₅)₃·H₂O (5 mol%, 5.1 mg) at room temperature, the reaction mixture was irradiated by a 30 W blue LEDs lamp (approximately 1 cm away from the reaction vessel). After completion (checked by TLC), the mixture was concentrated under reduced pressure and the crude product was purified by silica gel column chromatography using petroleum ether and ethyl acetate (PE: EA= 2:1) as eluent to afford the corresponding products **3**.

3. Optimization of reaction conditions

Table S1 Optimization of experimental conditions ^a



Entry	Catalyst (5 mol %)	Indole (equiv.)	Solvent	Yield (%) ^b
1	B(C ₆ F ₅) ₃ ·H ₂ O + EosinY	1.5	THF	50
2	B(C ₆ F ₅) ₃ ·H ₂ O	1.5	THF	55
3	---	1.5	THF	Trace
4	B(C ₆ F ₅) ₃ ·H ₂ O	1.5	DCM	90
5	B(C₆F₅)₃·H₂O	1.5	DCE	94
6	B(C ₆ F ₅) ₃ ·H ₂ O	1.5	CH ₃ CN	72
7	B(C ₆ F ₅) ₃ ·H ₂ O	1.5	Toluene	91
8	B(C ₆ F ₅) ₃ ·H ₂ O	1.5	EA	55
9	B(C ₆ F ₅) ₃ ·H ₂ O	1.0	DCE	62
10	B(C ₆ F ₅) ₃ ·H ₂ O	1.2	DCE	87
11	TsOH	1.5	DCE	67
12	HCl	1.5	DCE	72
13	Yb(OTf) ₃	1.5	DCE	82
14	Sc(OTf) ₃	1.5	DCE	78
15 ^c	B(C ₆ F ₅) ₃ ·H ₂ O	1.5	DCE	89
16 ^d	B(C ₆ F ₅) ₃ ·H ₂ O	1.5	DCE	Trace
17 ^e	B(C ₆ F ₅) ₃ ·H ₂ O	1.5	DCE	Trace

^aReaction conditions: 0.2 mmol scale, catalyst (5.0 mol%), solvent (2.0 mL), r.t., air, Blue LEDs (455-460 nm, 30W) for 1 h. ^bIsolated yield. ^cOxygen atmosphere. ^dNitrogen atmosphere. ^eIn darkness.

4. Control experiments

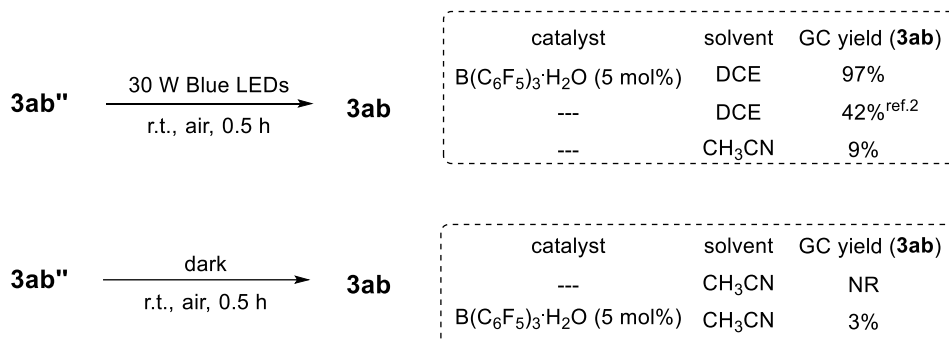
4.1 To get the intermediate 3ab' in the nitrogen atmosphere

To a mixture of **1a** (0.2 mmol) and **2b** (0.3 mmol) in DCE (2.0 mL) was added B(C₆F₅)₃·H₂O (5 mol%, 5.1 mg) at room temperature in the nitrogen atmosphere. The reaction mixture was irradiated by a 30 W blue LEDs lamp (approximately 1 cm away from the reaction vessel). After completion (checked by TLC), the mixture was concentrated under reduced pressure and the crude product was purified by silica gel column chromatography petroleum ether and ethyl acetate (PE: EA= 2:1) as eluent to afford the corresponding product **3ab'**.

The following reaction was carried out in general procedure: To a mixture of **3ab'** (0.2 mmol) in solvent (2.0 mL) was added catalyst (5 mol%) at room temperature. The

reaction mixture was irradiated by a 30 W blue LEDs lamp (approximately 1 cm away from the reaction vessel). After completion, the yields of **3ab** were determined by GC.

Scheme S1 Control experiments

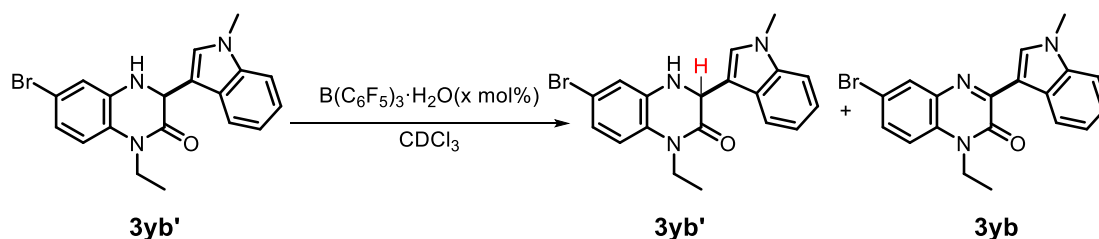


4.2 NMR verification of intermediate **3yb'**

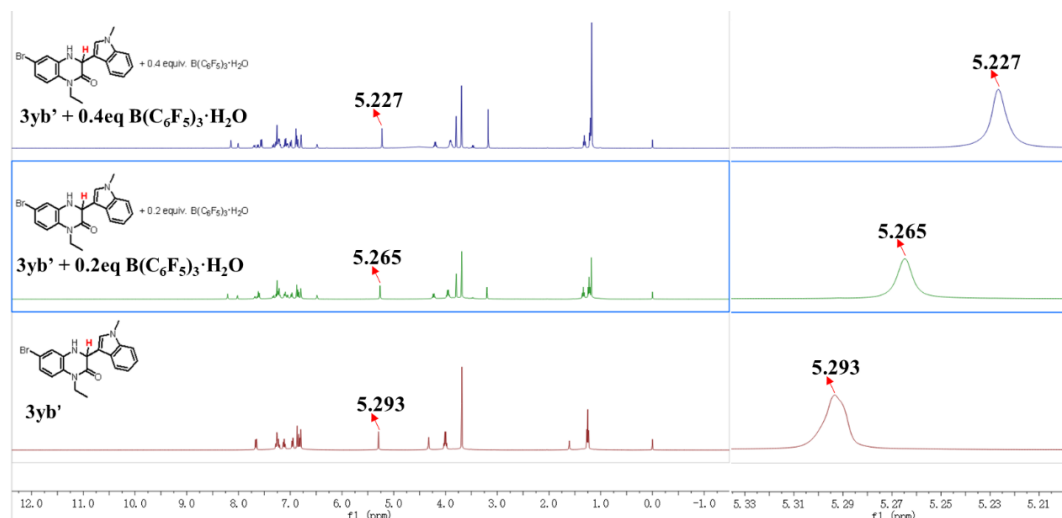
To a mixture of **3y** (0.2 mmol) and **2b** (0.3 mmol) in DCE (2.0 mL) was added $\text{B}(\text{C}_6\text{F}_5)_3 \cdot \text{H}_2\text{O}$ (5 mol%, 5.1 mg) at room temperature in the nitrogen atmosphere. The reaction mixture was irradiated by a 30 W blue LEDs lamp (approximately 1 cm away from the reaction vessel). After completion, the mixture was concentrated under reduced pressure and the crude product was purified by column chromatography (neutral Al_2O_3) using petroleum ether and ethyl acetate (PE: EA= 2:1) as eluent to afford the corresponding product **3yb'**.



The following reaction was carried out in general procedure: To a mixture of **3yb'** (0.1 mmol) in CDCl_3 (0.7 mL) at room temperature was added $\text{B}(\text{C}_6\text{F}_5)_3 \cdot \text{H}_2\text{O}$ (20 mol%, 10.2 mg). There are two compounds **3yb'** and **3yb**. And it was finally added $\text{B}(\text{C}_6\text{F}_5)_3 \cdot \text{H}_2\text{O}$ (20 mol%, 10.2 mg) to test $^1\text{HNMR}$. There are also two compounds **3yb'** and **3yb**.

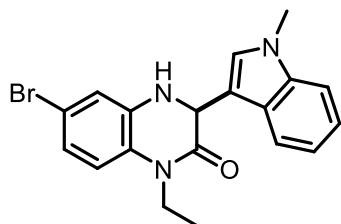


The C'-H chemical shift of intermediate **3yb'** is 5.293 ppm, then 5.265 ppm and 5.227 ppm with the addition of 0.2 equiv. $B(C_6F_5)_3 \cdot H_2O$ and another 0.2 equiv.



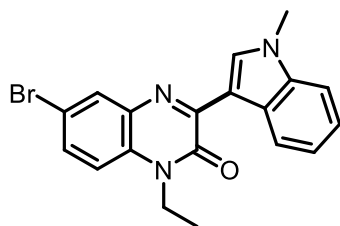
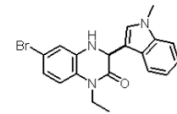
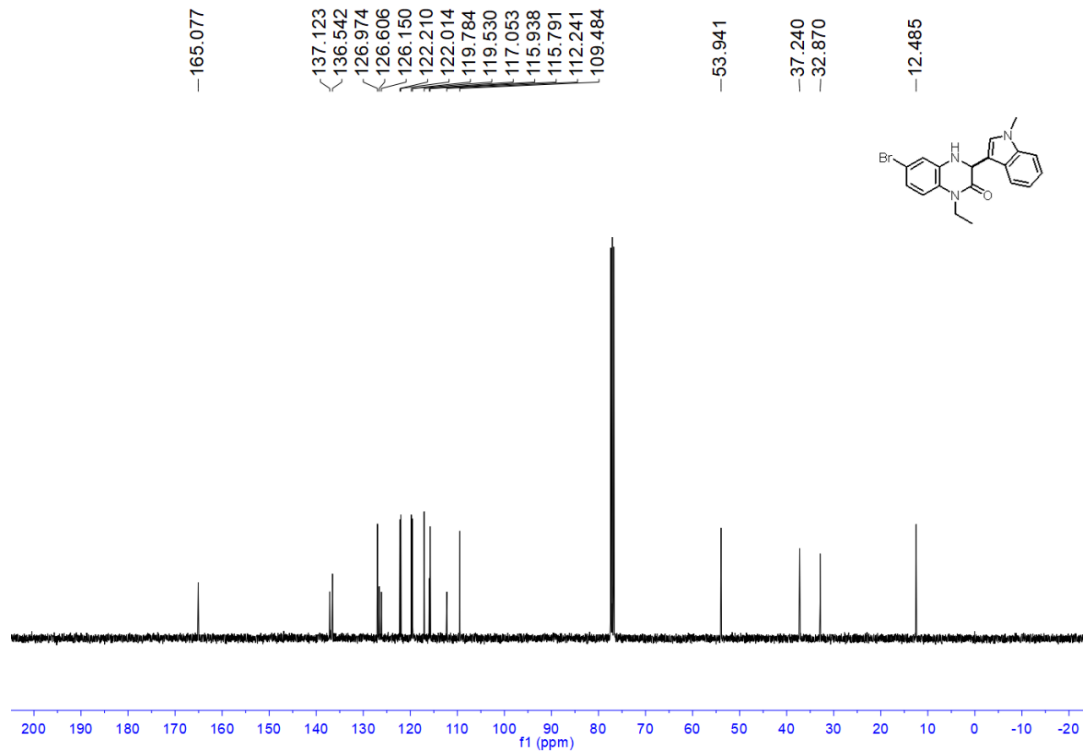
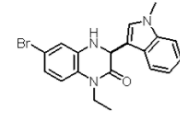
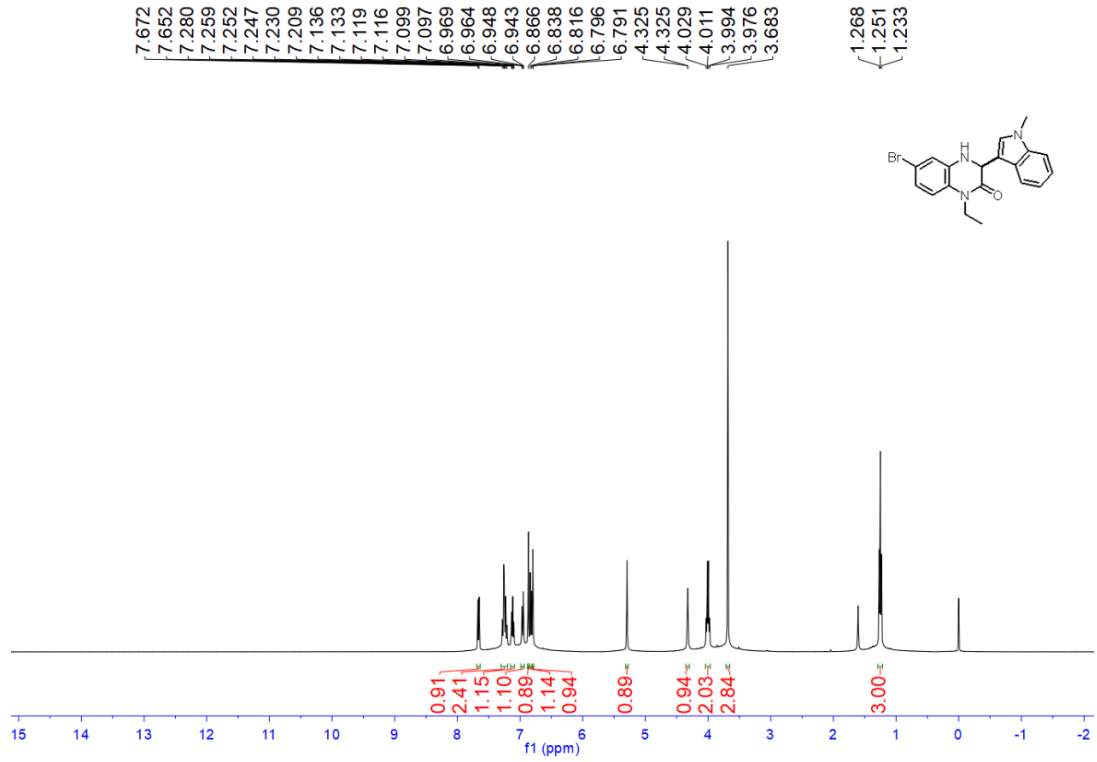
$B(C_6F_5)_3 \cdot H_2O$, indicating that the C-H is more electron rich to be oxidized in the presence of $B(C_6F_5)_3 \cdot H_2O$.

Figure S1 1H NMR spectra of **3yb'**, **3yb**+ $B(C_6F_5)_3 \cdot H_2O$ in $CDCl_3$



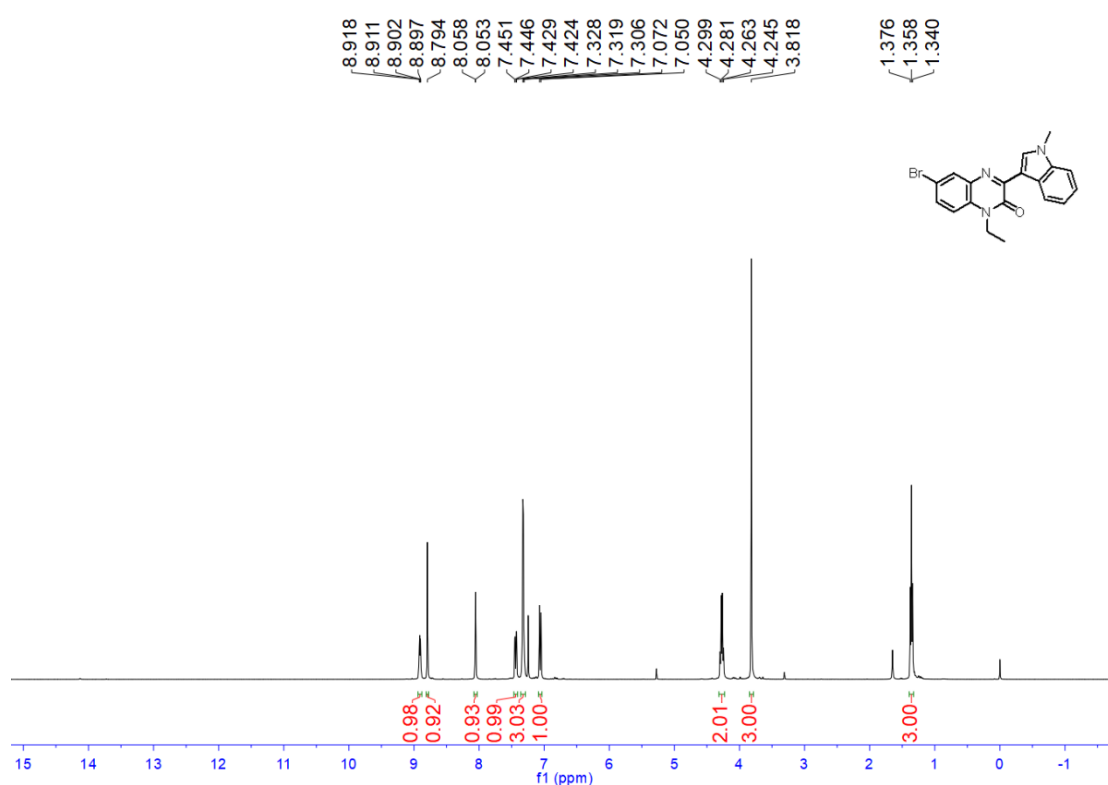
6-bromo-1-ethyl-3-(1-methyl-1H-indol-3-yl)-

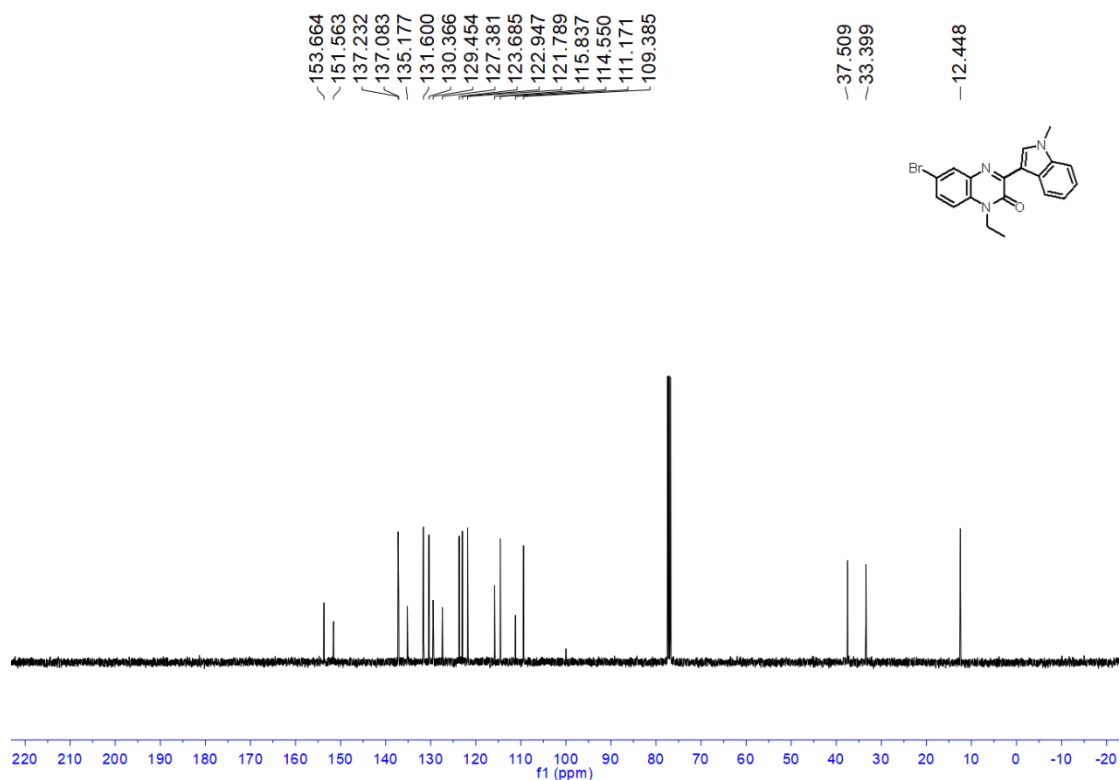
3,4-dihydroquinoxalin-2(1H)-one (3yb'). White solid, 42.5 mg, yield 22%. m.p.: 173.4-174.1 °C. 1H NMR (400 MHz, $CDCl_3$, TMS) δ 7.66 (d, $J = 8.0$ Hz, 1H), 7.30 – 7.19 (m, 2H), 7.15 – 7.09 (m, 1H), 6.99 – 6.93 (m, 1H), 6.87 (s, 1H), 6.83 (d, $J = 8.6$ Hz, 1H), 6.81 – 6.78 (m, 1H), 5.29 (br, 1H), 4.33 (s, 1H), 4.00 (q, $J = 7.1$ Hz, 2H), 3.68 (s, 3H), 1.25 (t, $J = 7.1$ Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$, TMS) δ 165.1, 137.1, 136.5, 127.0, 126.6, 126.2, 122.2, 122.0, 119.8, 119.5, 117.1, 115.9, 115.8, 112.2, 109.5, 53.9, 37.2, 32.9, 12.5. HRMS (ESI, m/z) calcd for $C_{19}H_{19}BrN_3O^+$ $[M+H]^+$: 384.0706, found 384.0709.



6-bromo-1-ethyl-3-(1-methyl-1H-indol-3-

yl)quinoxalin-2(1H)-one (3yb). Yellow solid, 69.0 mg, yield 90%. m.p.: 208.5-208.9 °C. ¹H NMR (400 MHz, CDCl₃, TMS) δ 8.94 – 8.88 (m, 1H), 8.79 (s, 1H), 8.06 (d, *J* = 2.1 Hz, 1H), 7.47 – 7.41 (m, 1H), 7.36 – 7.29 (m, 3H), 7.06 (d, *J* = 8.9 Hz, 1H), 4.27 (q, *J* = 7.1 Hz, 2H), 3.82 (s, 3H), 1.36 (t, *J* = 7.2 Hz, 3H). ¹³C NMR (101 MHz, CDCl₃, TMS) δ 153.7, 151.6, 137.2, 137.1, 135.2, 131.6, 130.4, 129.5, 127.4, 123.7, 123.0, 121.8, 115.8, 114.6, 111.2, 109.4, 37.5, 33.4, 12.5. HRMS (ESI, *m/z*) calcd for C₁₉H₁₇BrN₃O⁺ [M+H]⁺: 382.0550, found 382.0555.





4.3 Emission quenching experiments under nitrogen and oxygen atmosphere

Emission intensities were recorded using a SHIMADZU RF-5301PC luminescence spectrophotometer. **PC** solutions were excited at 390 nm and the emission intensity was collected at 460 nm. In a typical experiment, to a 2×10^{-6} M solution of **PC** in DCE under nitrogen (black line) and oxygen atmosphere of a quencher (red line) in a quartz cuvette. The relative luminescence intensity was quenched by oxygen.

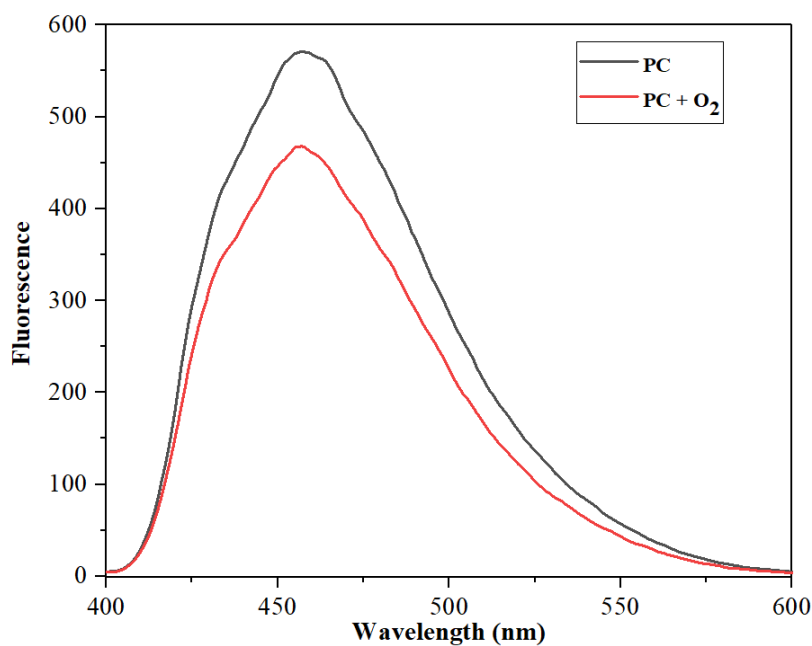


Figure S2 Fluorescence quenching under nitrogen and oxygen atmosphere.
4.4 UV/visible absorption spectra of 3ab'

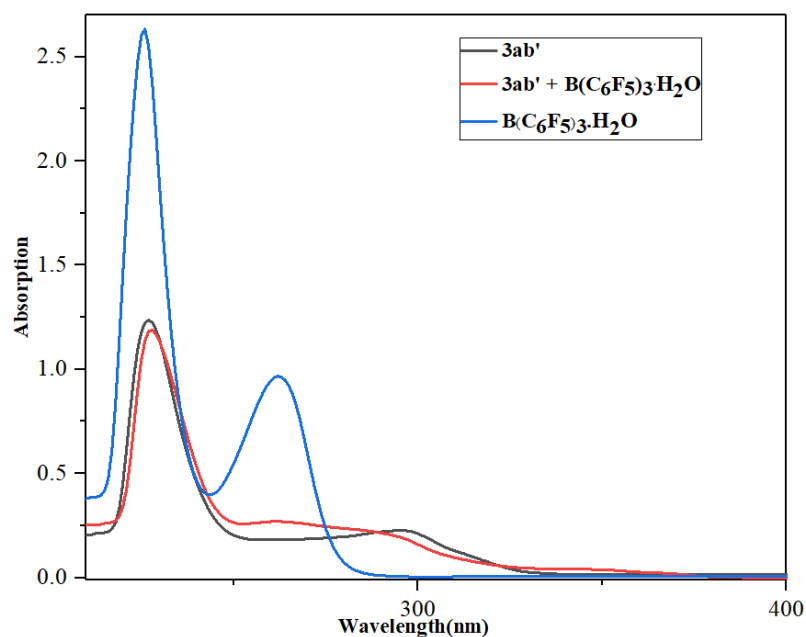


Figure S3 UV/visible absorption spectra of **3ab'**, **B(C₆F₅)₃·H₂O** and **3ab' + B(C₆F₅)₃·H₂O** in DCE at the concentration 2×10^{-5} M.

4.5 Cyclic voltammogram experiment and the estimation of excited state reduction potential of 3ab and PC

Cyclic voltammogram was recorded using a Gamry Interface 5000E potentiostat. Cyclic voltammogram measurement was performed with a glassy carbon working electrode, an Ag/AgCl, KCl (saturated) reference electrode and a Pt sheet auxiliary electrode at room temperature in nitrogen degassed MeCN solution (10 mL) of

tetrabutylammonium hexafluorophosphate (0.1 M), containing **3ab** (0.025 M), scan rate = 50 mV·s⁻¹.

Cyclic voltammogram was recorded using a Gamry Interface 5000E potentiostat. Cyclic voltammogram measurement was performed with a glassy carbon working electrode, an Ag/AgCl, KCl (saturated) reference electrode and a Pt sheet auxiliary electrode at room temperature in nitrogen degassed MeCN solution (10 mL) of tetrabutylammonium hexafluorophosphate (0.1 M), containing **PC** (**3ab** + **B(C₆F₅)₃·H₂O**) (0.025 M), scan rate = 50 mV·s⁻¹.

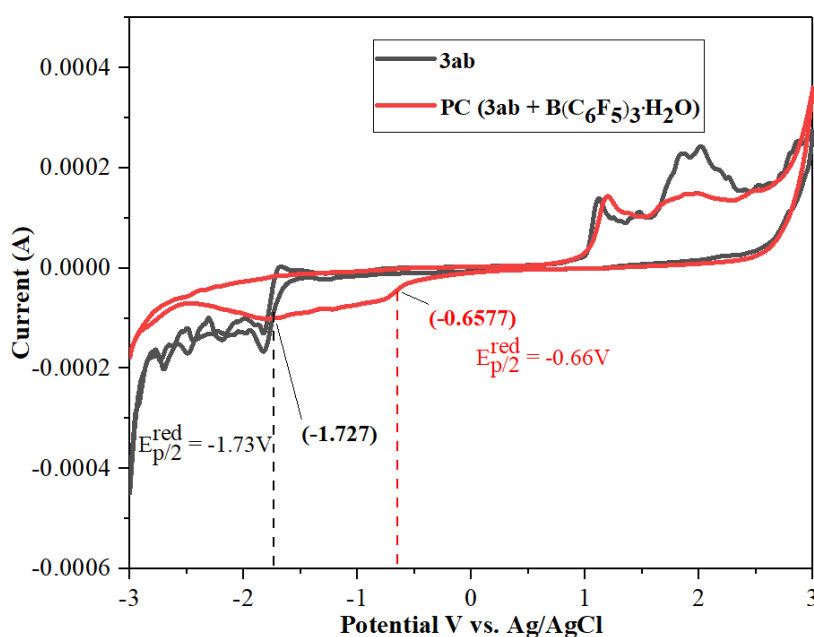


Figure S4: Cyclic voltammetry of **3ab** (black line) and **PC** (red line).

3ab (black line): $E_{1/2}^{\text{red}} = -1.73 \text{ V vs Ag/AgCl, KCl (sat'd)}$

$$E_{0,0}^{\text{S}1} = (3.24 \text{ eV (383 nm)} + 2.70 \text{ eV (449 nm)})/2 = 3.00 \text{ eV}$$

$$E_{1/2}^{\text{red}*} = -1.73 \text{ V} + 3.00 \text{ eV} = 1.27 \text{ V vs Ag/AgCl, KCl (sat'd)}$$

$$E_{1/2}^{\text{red}*} = 1.27 \text{ V} - 0.045 \text{ V} = 1.23 \text{ V vs SCE}$$

PC (red line): $E_{1/2}^{\text{red}} = -0.66 \text{ V vs Ag/AgCl, KCl (sat'd)}$

$$E_{0,0}^{\text{S}1} = (2.59 \text{ eV (479 nm)} + 2.76 \text{ eV (458 nm)})/2 = 2.65 \text{ eV}$$

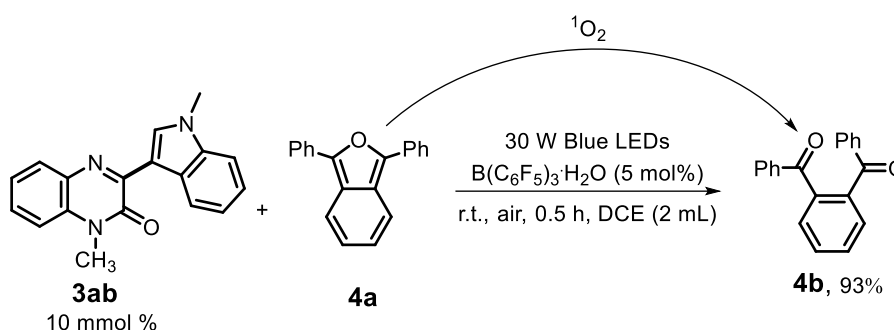
$$E_{1/2}^{\text{red}*} = -0.66 \text{ V} + 2.65 \text{ eV} = 1.99 \text{ V vs Ag/AgCl, KCl (sat'd)}$$

$$E_{1/2}^{\text{red}*} = 1.99 \text{ V} - 0.045 \text{ V} = 1.95 \text{ V vs SCE}$$

5. Determination of singlet oxygen species³

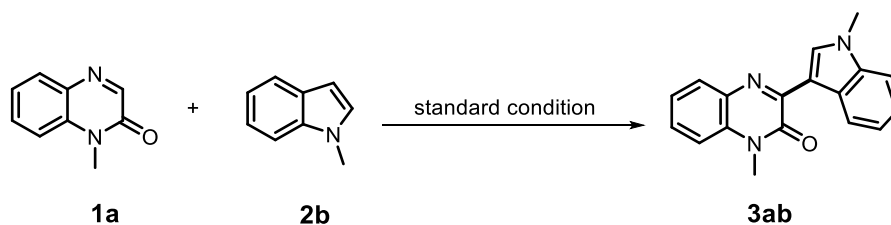
1,3-Diphenylbenzo[*c*]furan (DPBF, 0.2 mmol, 54.0 mg), B(C₆F₅)₃·H₂O (5 mol%, 5.1 mg), and 1-methyl-3-(1-methyl-1H-indol-3-yl)quinoxalin-2(1H)-one (**3ab**, 10mol%), were added into 2.0 mL 1,2-dichloroethane. The resulting solution was stirred at room temperature under air and blue LEDs for 0.5 h. Then, the reaction mixture was filtered, and the solvent was evaporated in vacuum. The crude product was purified by flash column chromatography on silica gel using petroleum ether and ethyl acetate (PE: EA= 20:1) as eluent.

Scheme S2 Determination of singlet oxygen species



6. Light on/off experiments

The light on/off experiment following the standard condition: A 10 mL reaction vial equipped with a stir bar was charged with **1a** (32.0 mg, 0.2 mmol), indole **2b** (39.4 mg, 0.3 mmol), B(C₆F₅)₃·H₂O (5.1 mg, 5mol%), and DCE (2 mL). The reaction mixture was irradiated by a 30 W blue LED lamp (approximately 1 cm away from the reaction vessel) at room temperature for corresponding time. Afterwards, the product **3ab** was detected by GC. These results demonstrated that light is necessary for the reaction.



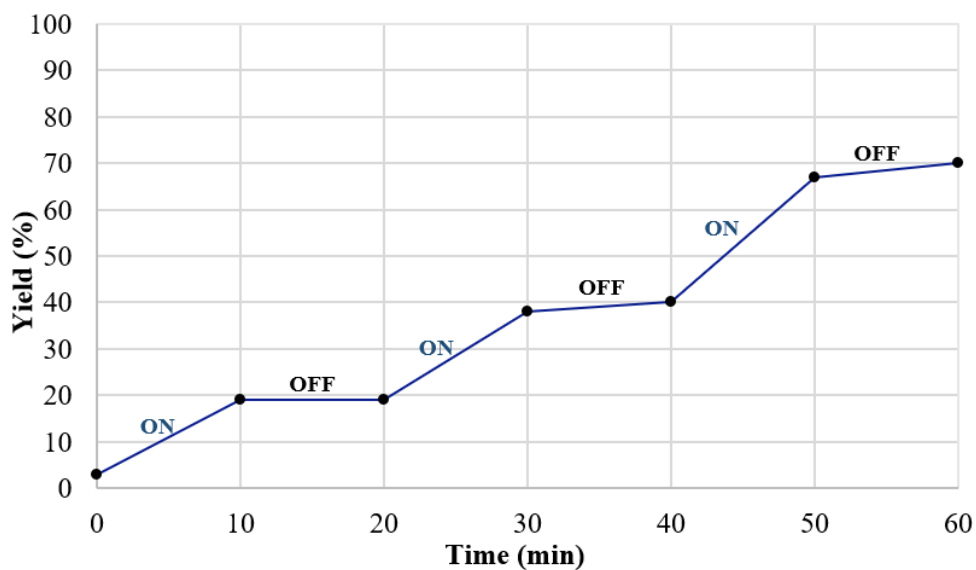
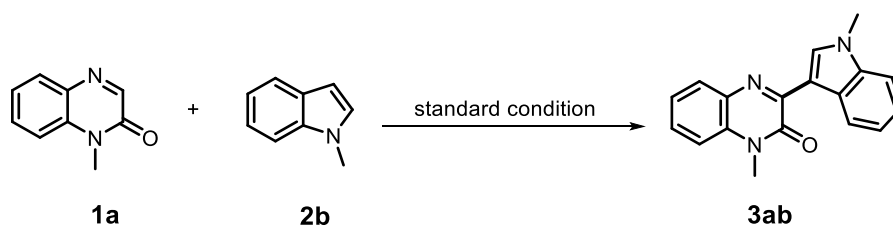


Figure S5 Light on/off experiment with $B(C_6F_5)_3 \cdot H_2O$ -catalyzed photoredox coupling reaction of **1a** and **2b**.

7. Reaction profiles

The experimental time plot following the standard condition: A 10 mL reaction vial equipped with a stir bar was charged with **1a** (32.0 mg, 0.2 mmol), indole **2b** (39.4 mg, 0.3 mmol), $B(C_6F_5)_3 \cdot H_2O$ (5.1 mg, 5 mol%), and DCE (2 mL). The reaction mixture was irradiated by a 30 W blue LED lamp (approximately 1 cm away from the reaction vessel) at room temperature for corresponding time. Afterwards, the product **3ab** was detected by GC. As the reaction time proceeds, the reaction rate is gradually accelerated. These results demonstrated that product **3** was able to catalyze the reaction under standard conditions. (for example: **1a** and **2b** in figure S3)



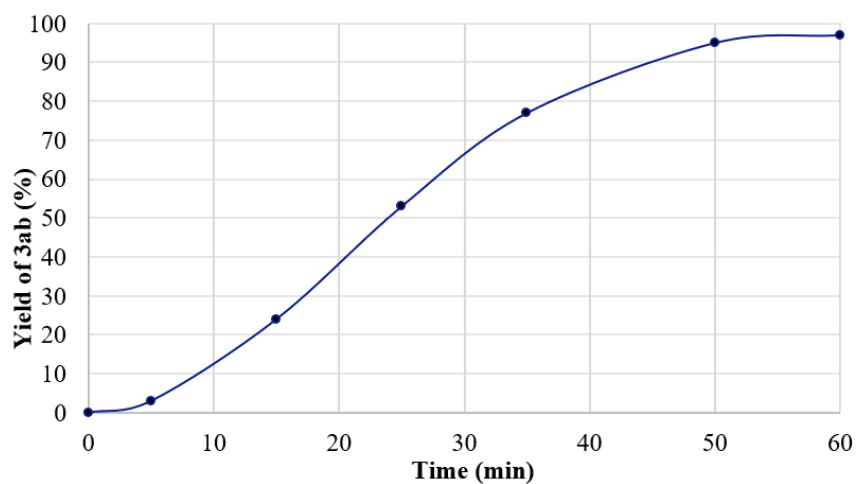


Figure S6 Reaction profiles of $B(C_6F_5)_3 \cdot H_2O$ -catalyzed photoredox coupling reaction of **1a** and **2b**.

8. UV-Vis absorption spectra

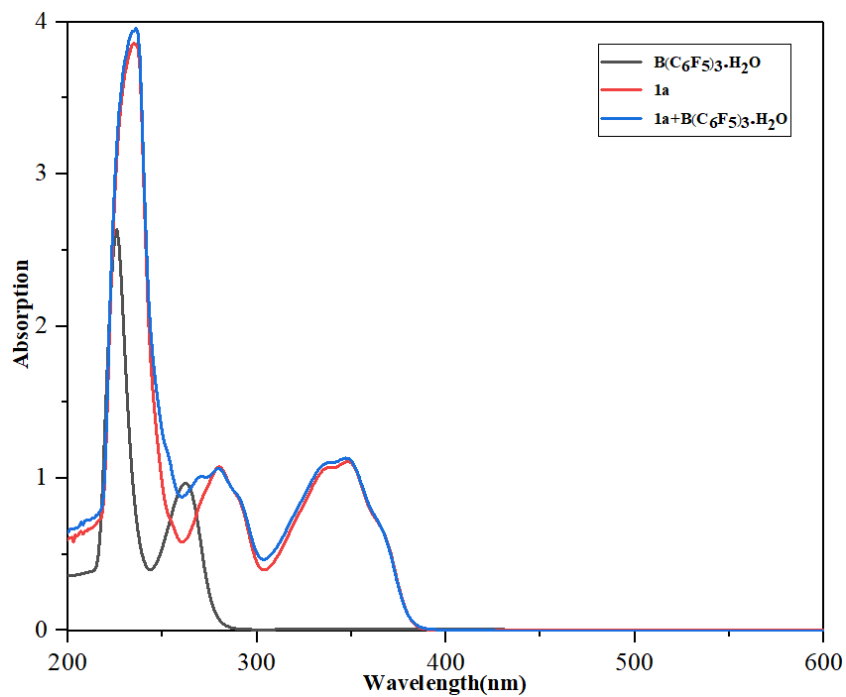


Figure S7 Absorption spectra of **1a**, $B(C_6F_5)_3 \cdot H_2O$, and **1a**+ $B(C_6F_5)_3 \cdot H_2O$ in DCE

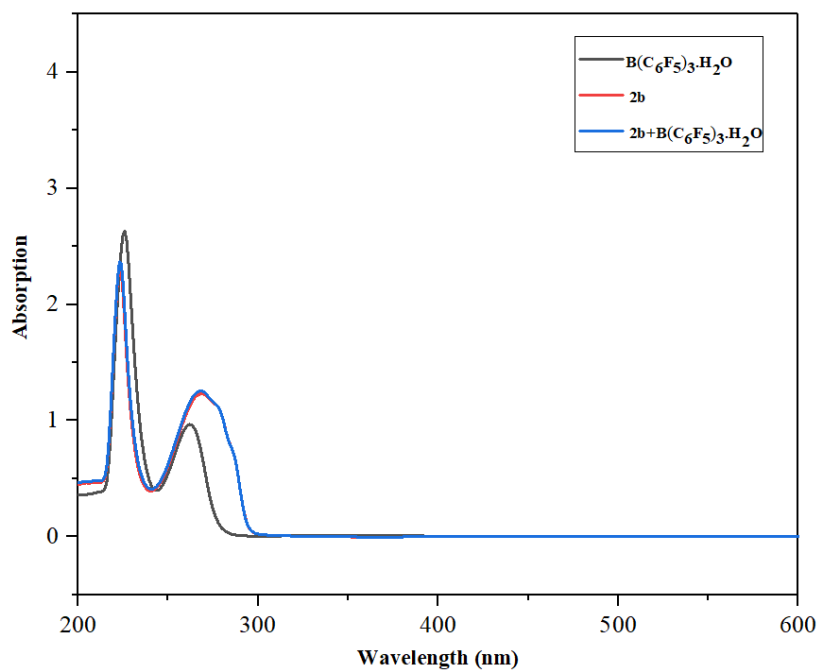


Figure S8 Absorption spectra of **2b**, $B(C_6F_5)_3 \cdot H_2O$, and **2b** + $B(C_6F_5)_3 \cdot H_2O$ in DCE

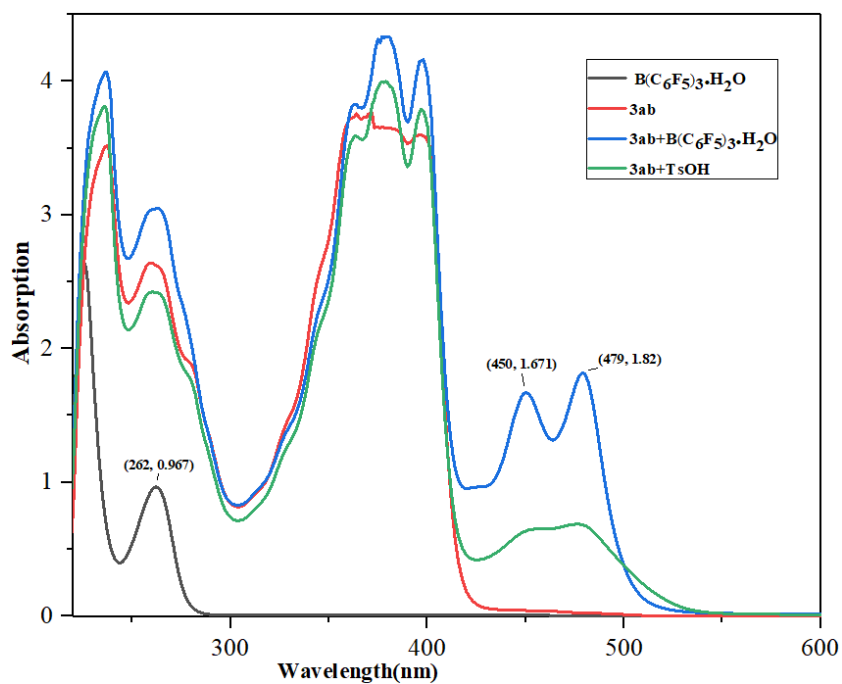


Figure S9 Absorption spectra of **3ab**, $B(C_6F_5)_3 \cdot H_2O$, **3ab** + $B(C_6F_5)_3 \cdot H_2O$ and **3ab** + TsOH in DCE

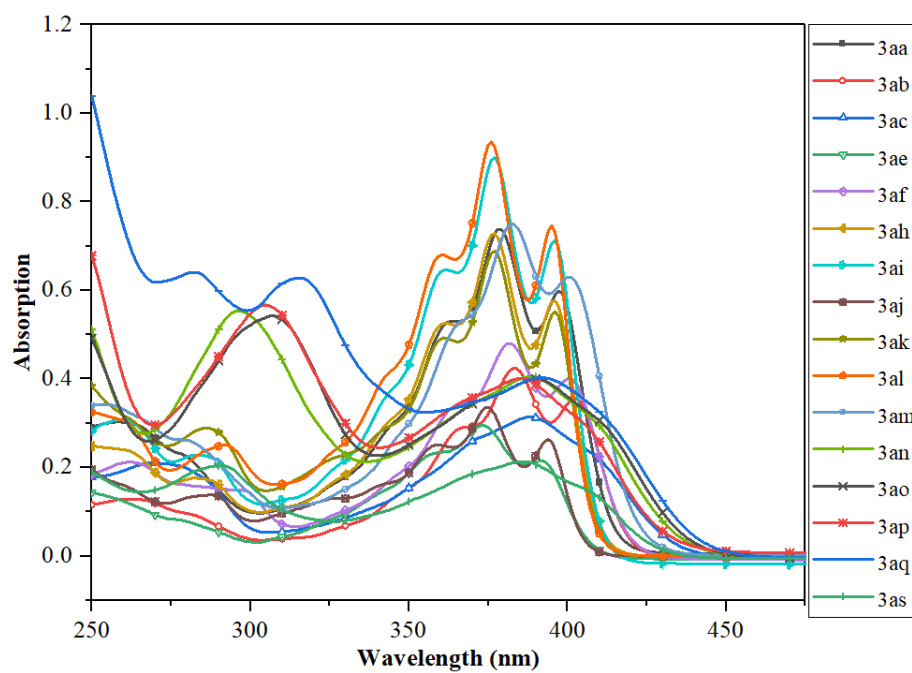


Figure S10 Absorption spectra of **3ab-3as** in EA at the concentration 2×10^{-5} M

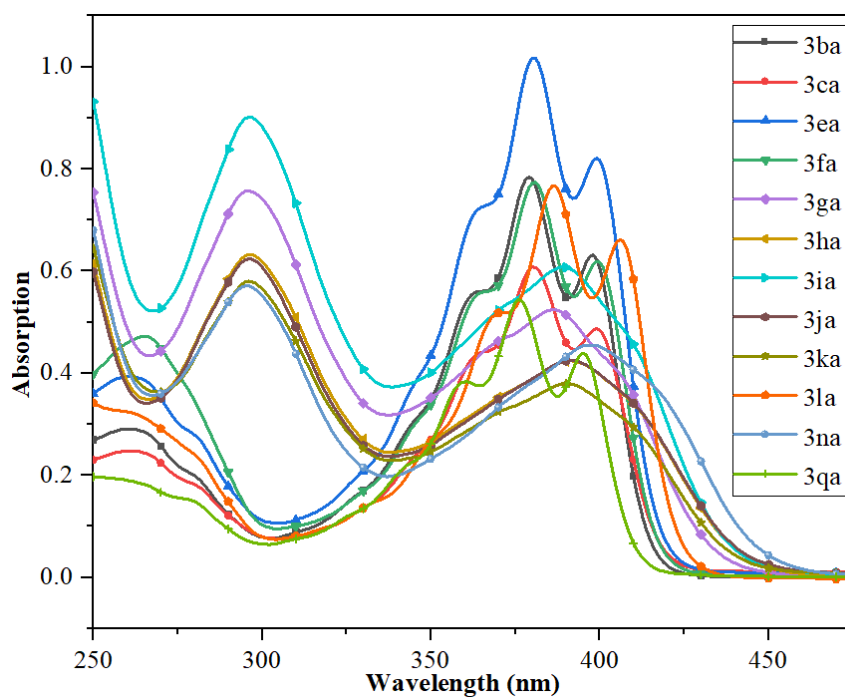


Figure S11 Absorption spectra of **3ba-3na** in EA at the concentration 2×10^{-5} M

9. Fluorescence spectra

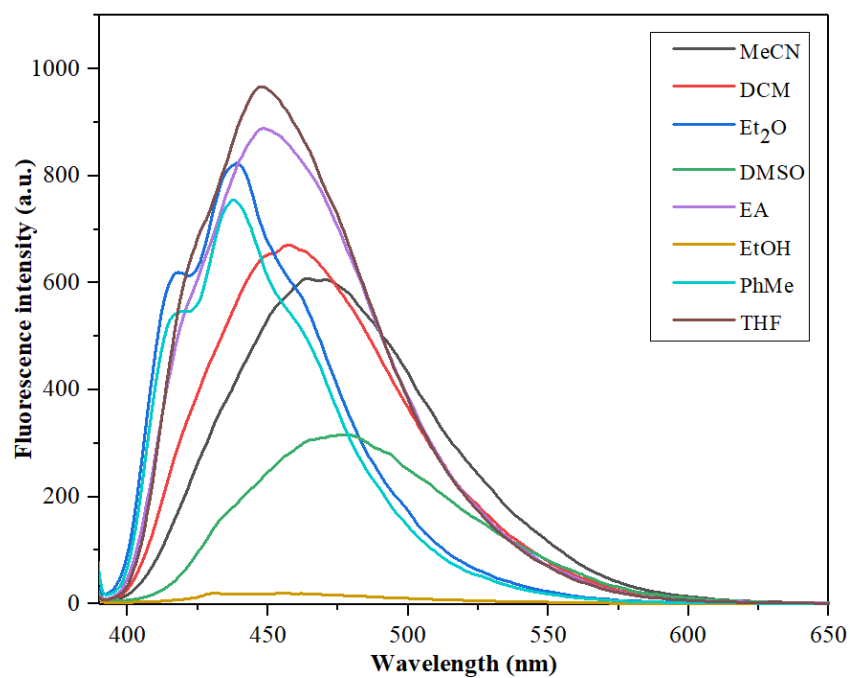


Figure S12 Fluorescence spectra of **3aa** in different solvents at the concentration 2×10^{-7} M

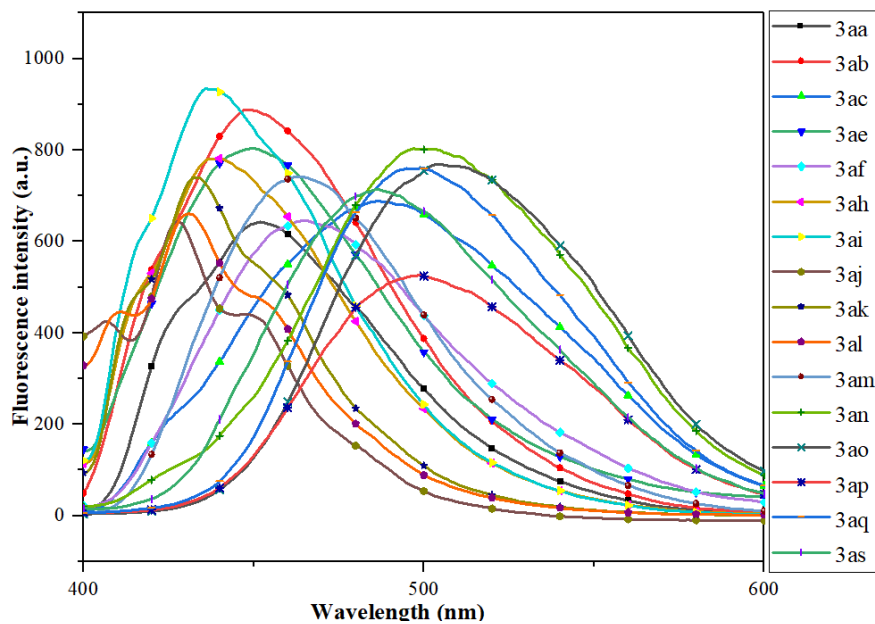


Figure S13 Fluorescence spectra of **3aa-3as** in EA at the concentration 2×10^{-6} M

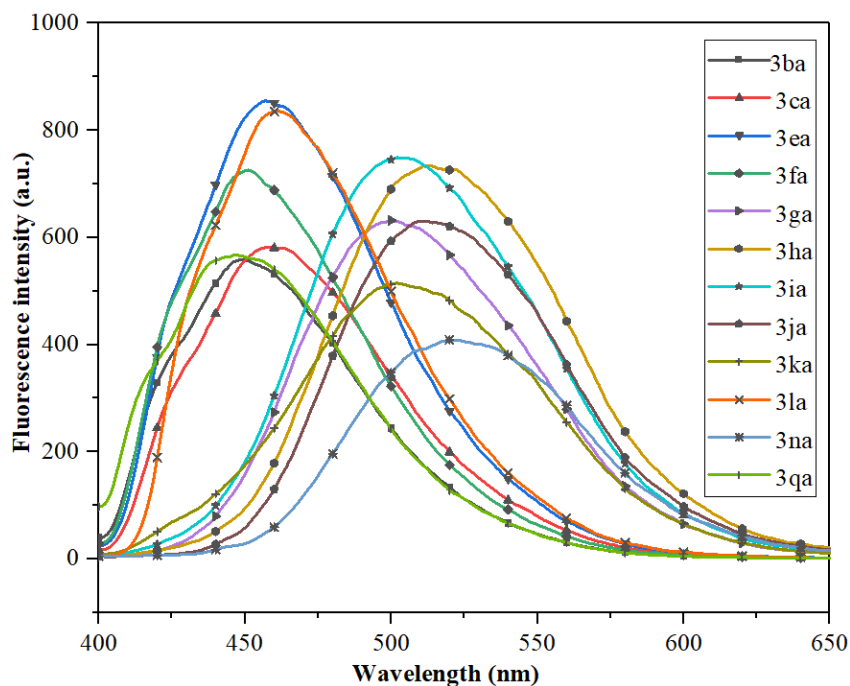


Figure S14 Fluorescence spectra of **3ba-3qa** in EA at the concentration 2×10^{-6} M.

10. Spectroscopic properties of fluorophores **3**⁶

Table S2 Summary of the measured photophysical properties of selected **3**

entry	product	λ_{abs}^a (nm)	λ_{em}^b (nm)	stokes shift (nm/cm ⁻¹)	Φ_F^c (%)
1	3aa	379	449	70/4113	28
2	3ab	383	452	69/3986	46
3	3ae	373	449	76/4538	10
4	3ai	377	436	59/3589	32
5	3ak	377	432	55/3377	20
6	3al	376	431	55/3394	30
7	3an	391	499	108/5535	3
8	3ba	379	450	71/4163	38
9	3ca	380	459	79/4530	51
10	3ea	380	456	76/4386	48
11	3fa	381	451	70/4074	44
12	3ga	386	500	114/5907	2
13	3la	386	460	74/4168	29
14	3na	398	519	121/5858	2

^aAbsorption maximum. ^bEmission maximum. ^cRelative quantum yields determined by an integrating sphere system in ethyl acetate.

The calculation formula of quantum yield was adopted as follows:

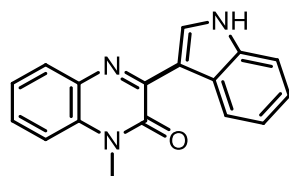
$$\Phi_s = \frac{F_s}{F_r} \times \frac{A_r}{A_s} \times \frac{n_s^2}{n_r^2} \times \Phi_r$$

Where, s and r represent sample and reference respectively. A is the absorbance. F is the relative integrated fluorescence intensity, and n is the refractive index of the solvent. The reference material in this paper is quinine, whose luminescence quantum yield in aqueous 0.5 M H₂SO₄ solution is 0.546.⁷

11. References

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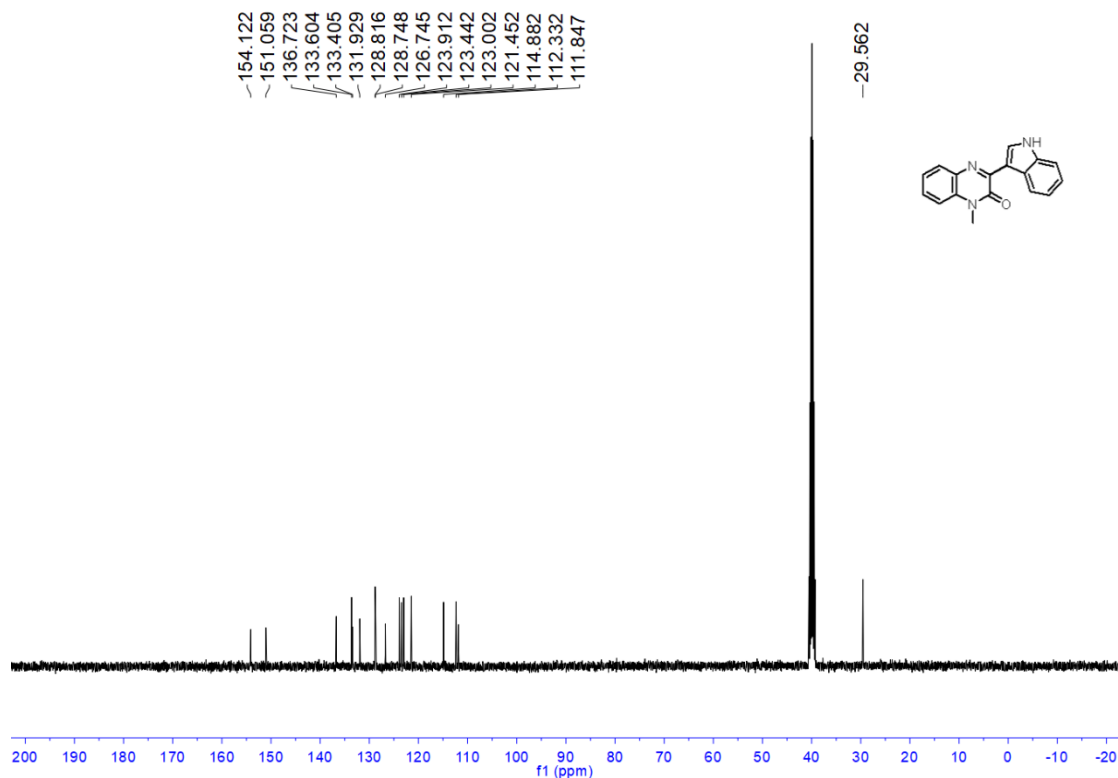
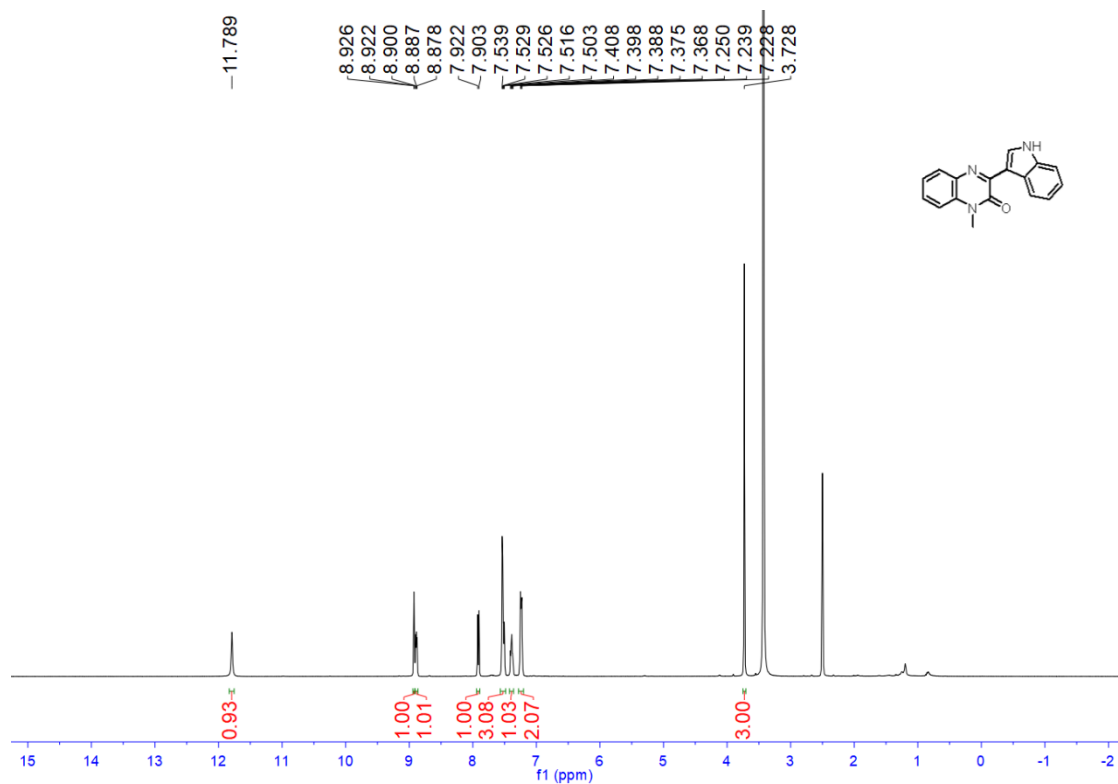
12. Characterization data for the products

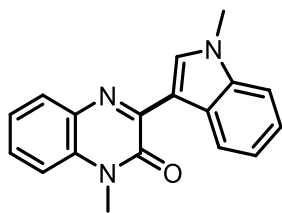


3-(1H-indol-3-yl)-1-methylquinoxalin-2-one (3aa). A known

compound.⁴ Orange solid, 51.7 mg, yield 94%. ¹H NMR (400 MHz, DMSO-*d*₆): δ 11.79

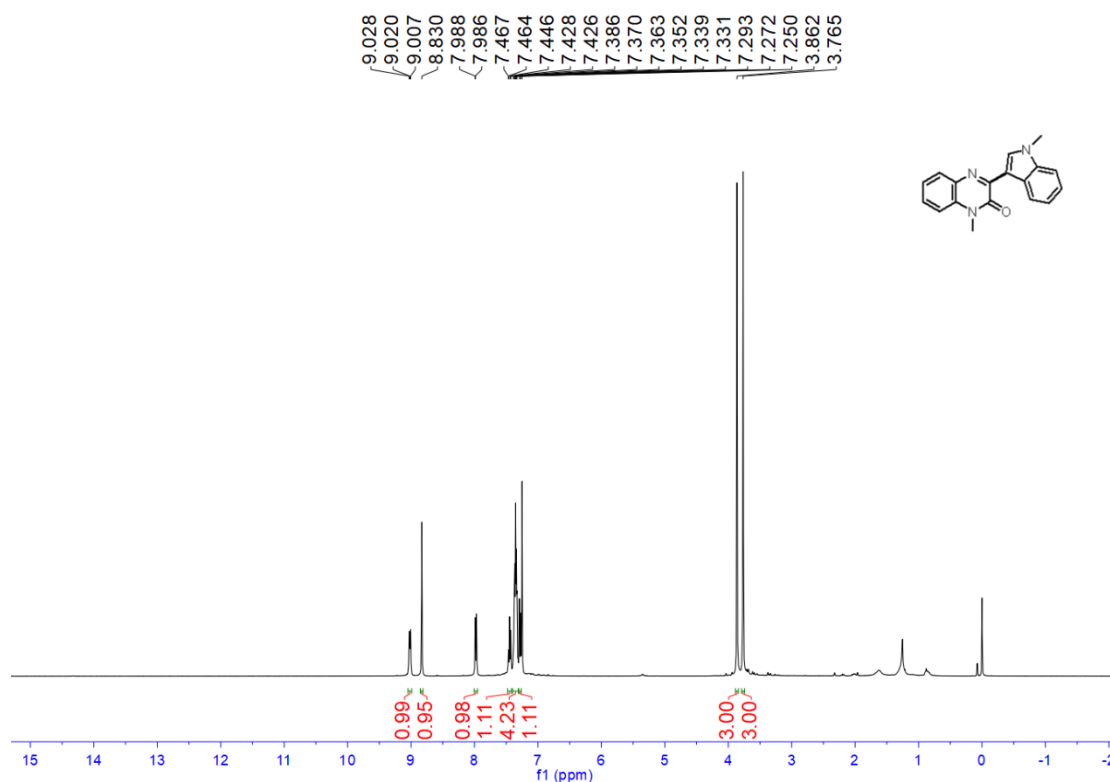
(s, 1H), 8.95 – 8.86 (m, 3H), 7.91 (d, $J = 7.9$ Hz, 1H), 7.59 – 7.47 (m, 3H), 7.44 – 7.35 (m, 1H), 7.29 – 7.19 (m, 2H), 3.73 (s, 3H); ^{13}C NMR (101 MHz, $\text{DMSO-}d_6$) δ 154.1, 151.1, 136.7, 133.6, 133.4, 131.9, 128.8, 128.7, 126.7, 123.9, 123.4, 123.0, 121.4, 114.8, 112.3, 111.9, 29.6.

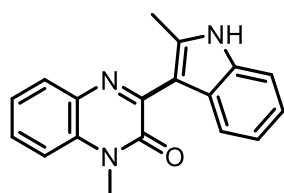
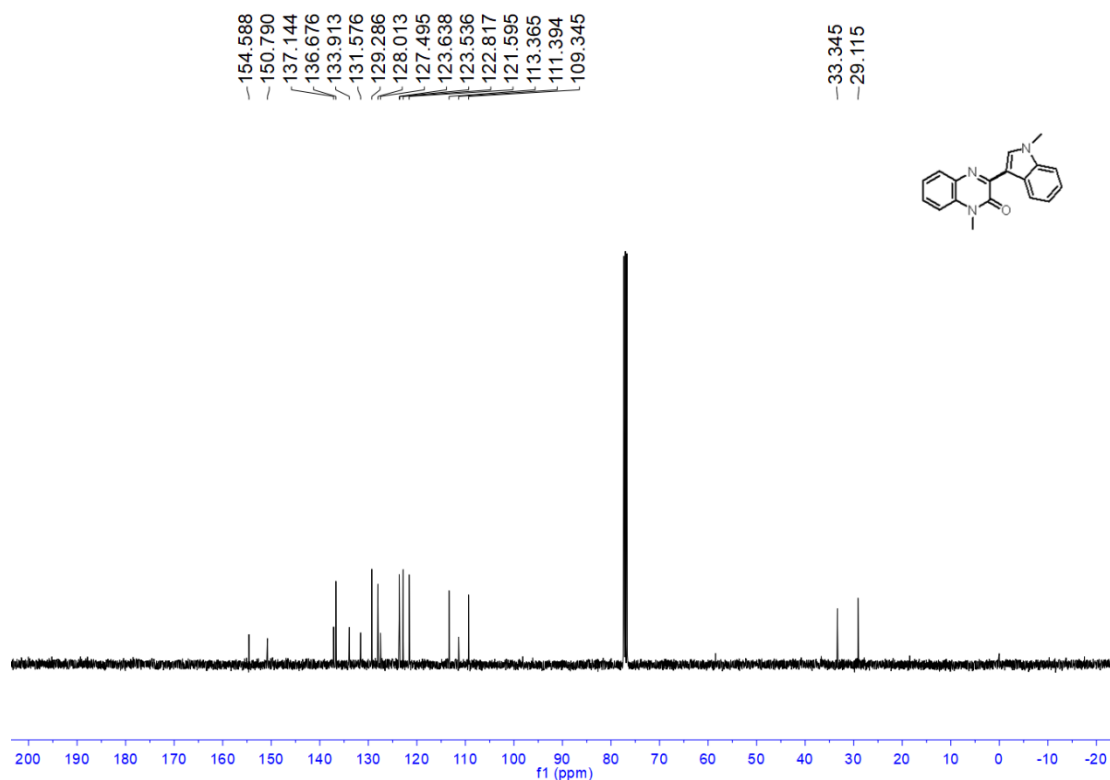




1-methyl-3-(1-methyl-1*H*-indol-3-yl)quinoxalin-2(1*H*)-one

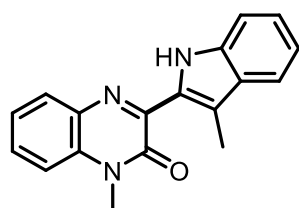
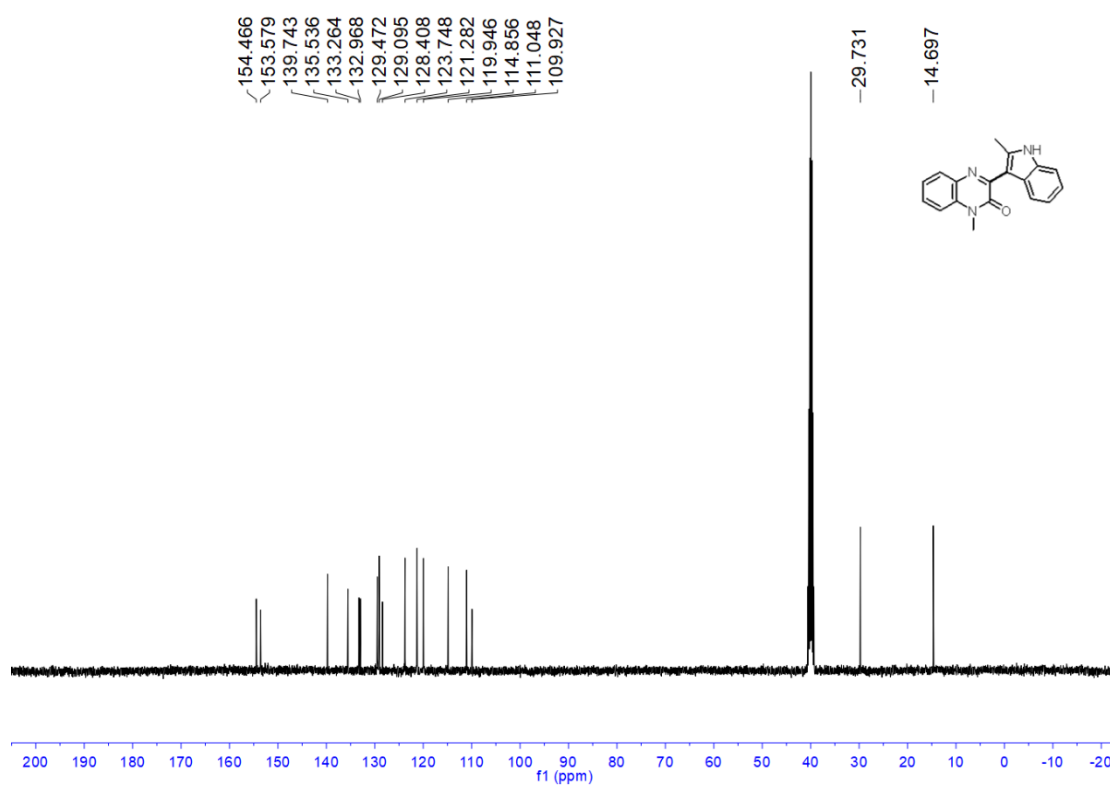
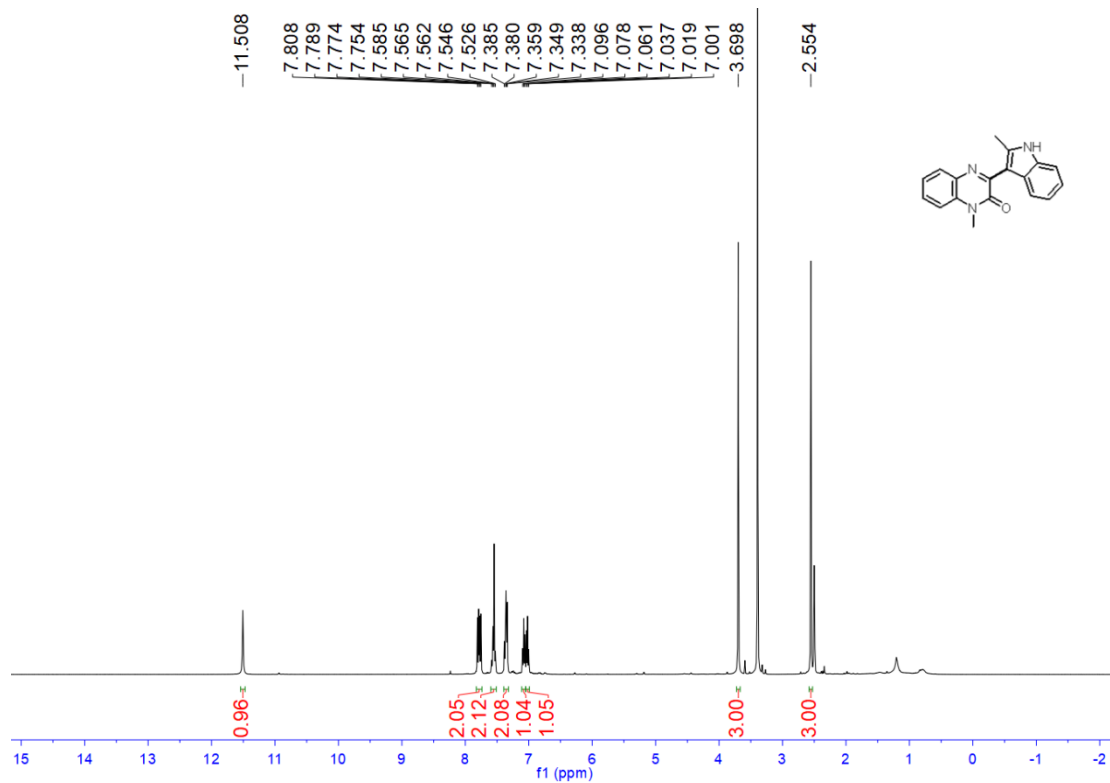
(3ab). Orange solid, 52.6 mg, yield 91%. m.p.: 232.9-233.8 °C. ¹H NMR (400 MHz, CDCl₃, TMS): δ 9.05 – 8.99 (m, 1H), 8.83 (s, 1H), 8.00 – 7.95 (m, 1H), 7.48 – 7.42 (m, 1H), 7.40 – 7.31 (m, 4H), 7.30 – 7.26 (d, *J* = 8.2 Hz, 1H), 3.86 (s, 3H), 3.77 (s, 3H). ¹³C NMR (101 MHz, CDCl₃, TMS): δ 154.6, 150.8, 137.1, 136.7, 133.9, 131.6, 129.3, 128.0, 127.5, 123.64, 123.5, 122.8, 121.5, 33.3, 29.1. HRMS (ESI, *m/z*) calcd for C₁₈H₁₆N₃O⁺ [M+H]⁺: 290.1288, found 290.1288.





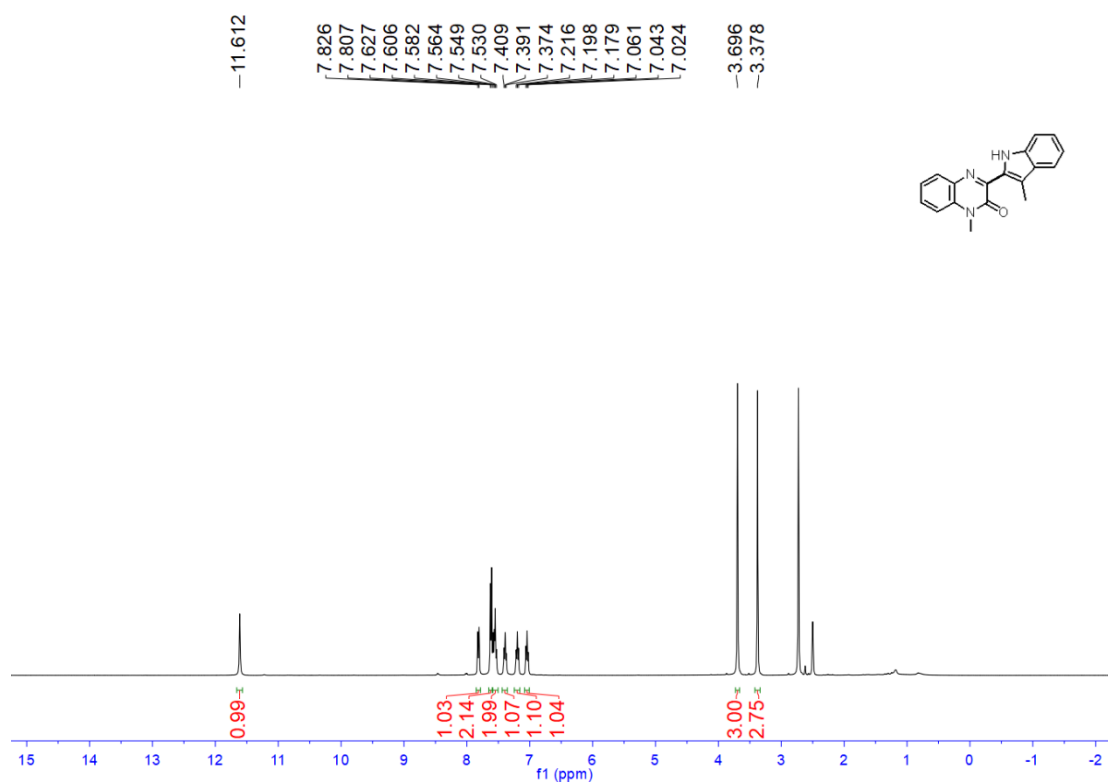
1-methyl-3-(2-methyl-1H-indol-3-yl)quinoxalin-2(1H)-one

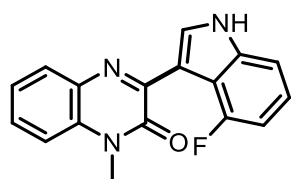
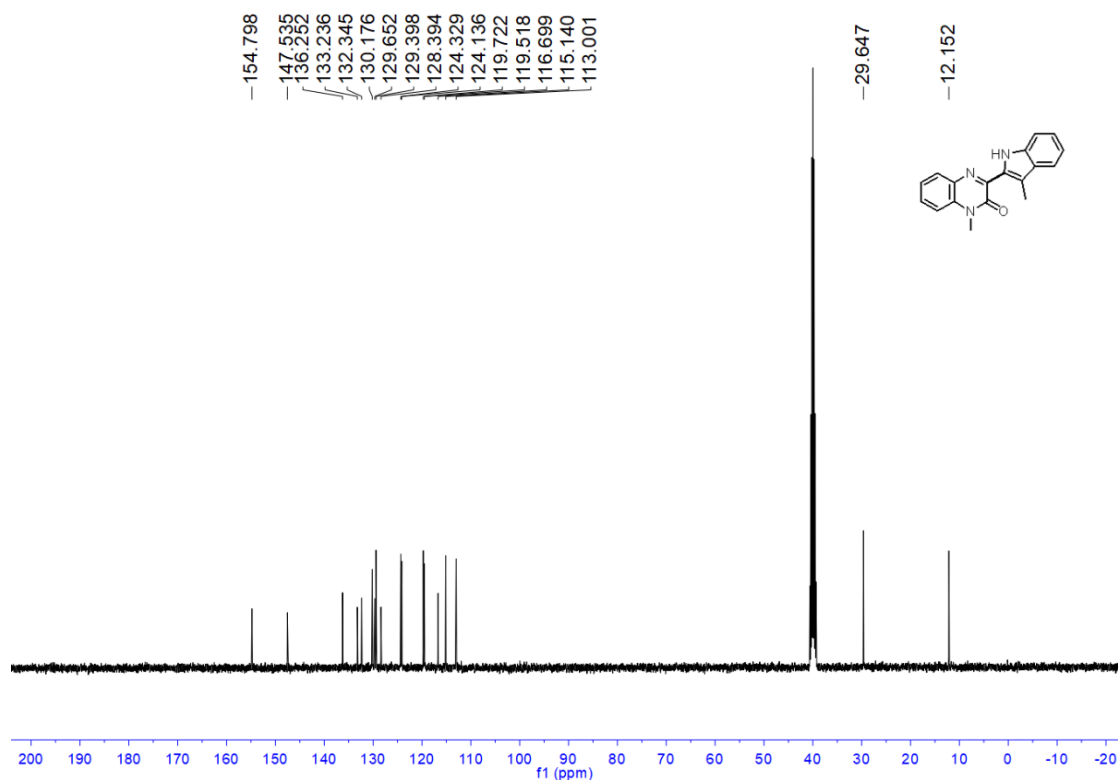
(3ac). A known compound.⁴ Orange solid, 54.7 mg, yield 94%. ¹H NMR (400 MHz, DMSO-*d*₆) δ 11.51 (s, 1H), 7.83 – 7.74 (m, 2H), 7.61 – 7.50 (m, 2H), 7.40 – 7.32 (m, 2H), 7.11 – 7.05 (m, 1H), 7.05 – 6.99 (m, 1H), 3.70 (s, 3H), 2.55 (s, 3H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 154.5, 153.6, 139.7, 135.5, 133.3, 133.0, 129.5, 129.1, 128.4, 123.8, 121.3, 120.0, 114.9, 111.1, 109.9, 29.7, 14.7.



1-methyl-3-(3-methyl-1H-indol-2-yl)quinoxalin-2(1H)-one

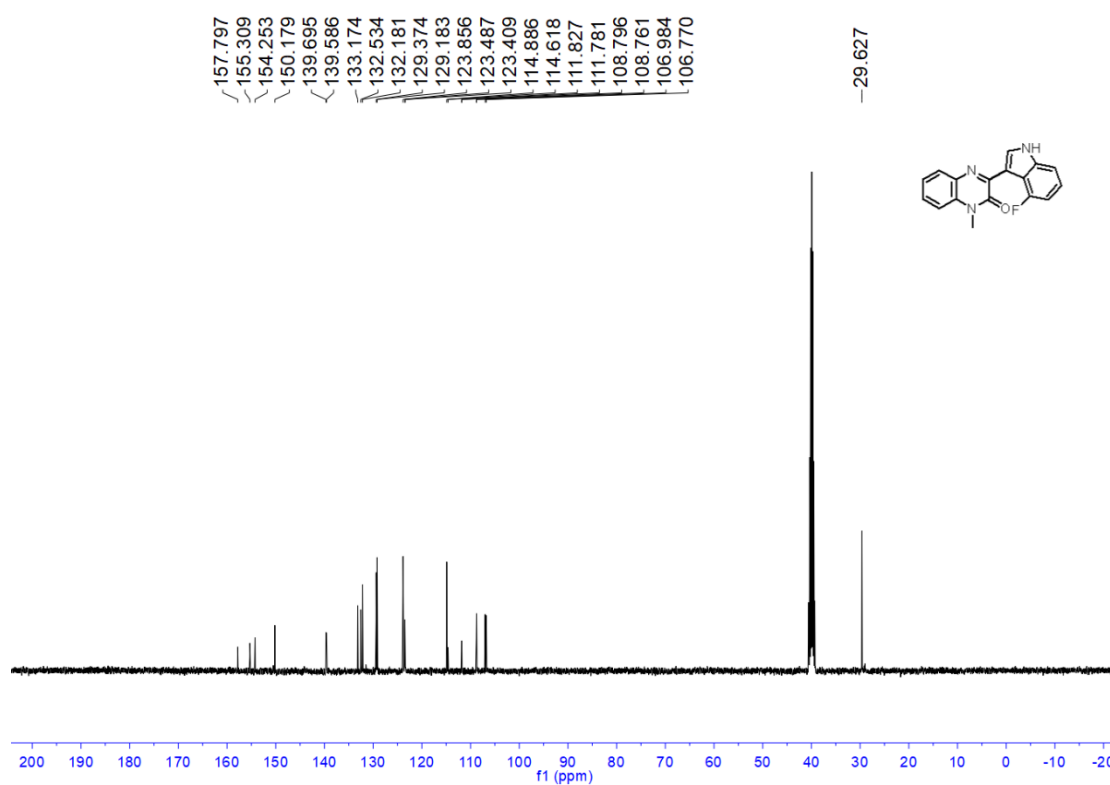
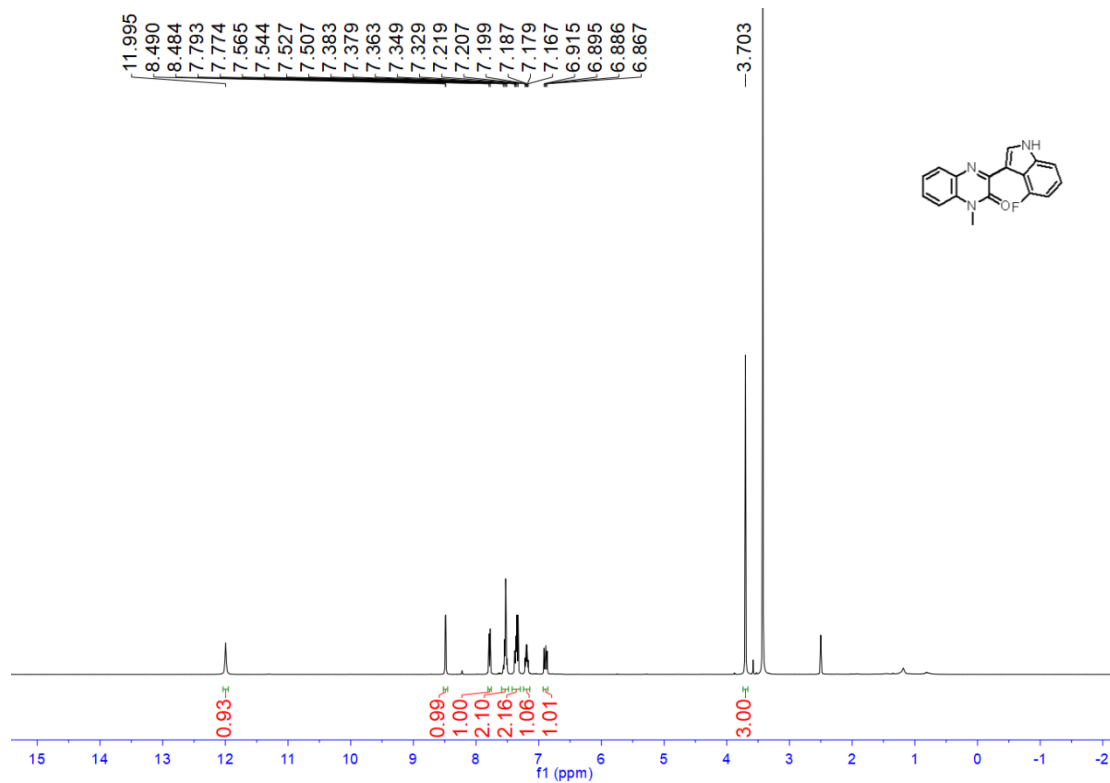
(3ad). Yellow solid, 55.6 mg, yield 96%. m.p.: 281.3-281.9 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ 11.61 (s, 1H), 7.82 (d, *J* = 7.8 Hz, 1H), 7.65 – 7.60 (m, 2H), 7.59 – 7.51 (m, 2H), 7.39 (dd, *J*₁ = *J*₂ = 7.1 Hz, 1H), 7.20 (dd, *J*₁ = *J*₂ = 7Hz, 1H), 7.04 (dd, *J*₁ = *J*₂ = 7.5 Hz, 1H), 3.70 (s, 3H), 3.38 (s, 3H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 154.8, 147.5, 136.3, 133.2, 132.4, 130.2, 129.7, 129.40, 128.39, 124.3, 124.1, 119.7, 119.5, 116.7, 115.1, 113.0, 29.7, 12.2. HRMS (ESI, *m/z*) calcd for C₁₈H₁₆N₃O⁺ [M+H]⁺: 290.1288, found 290.1290.

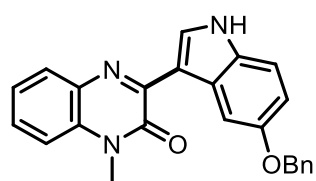
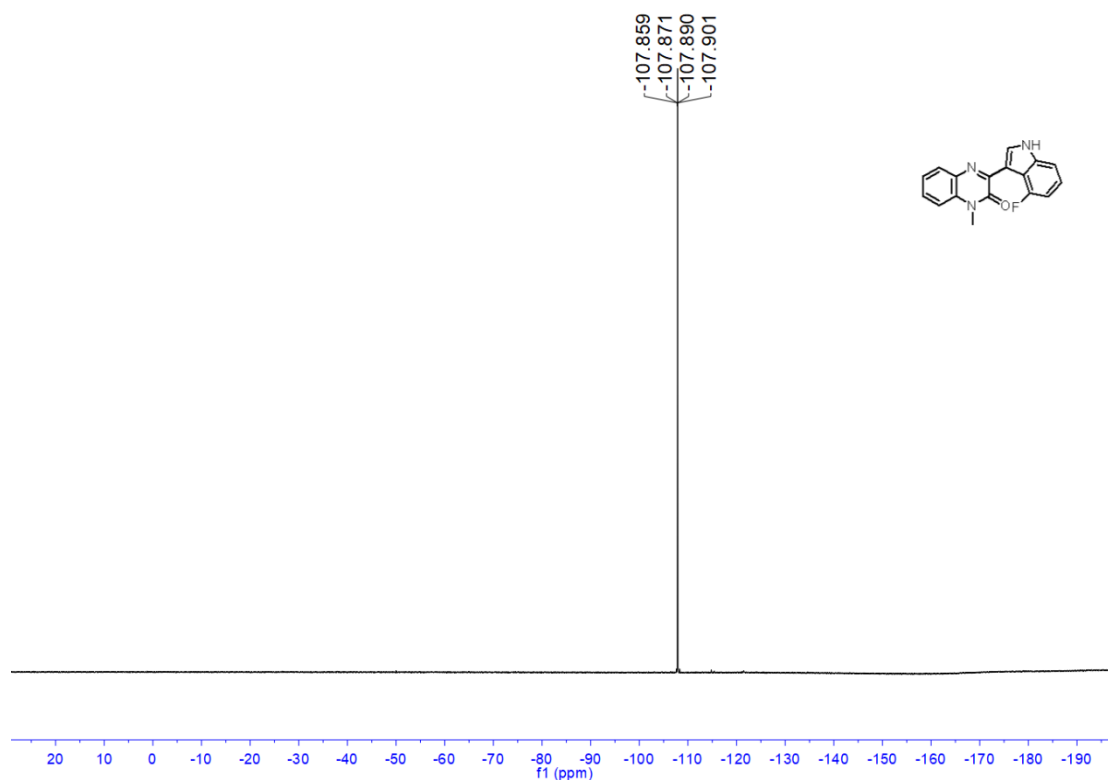




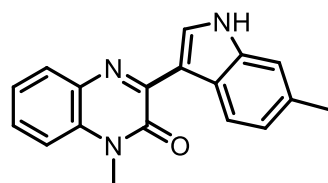
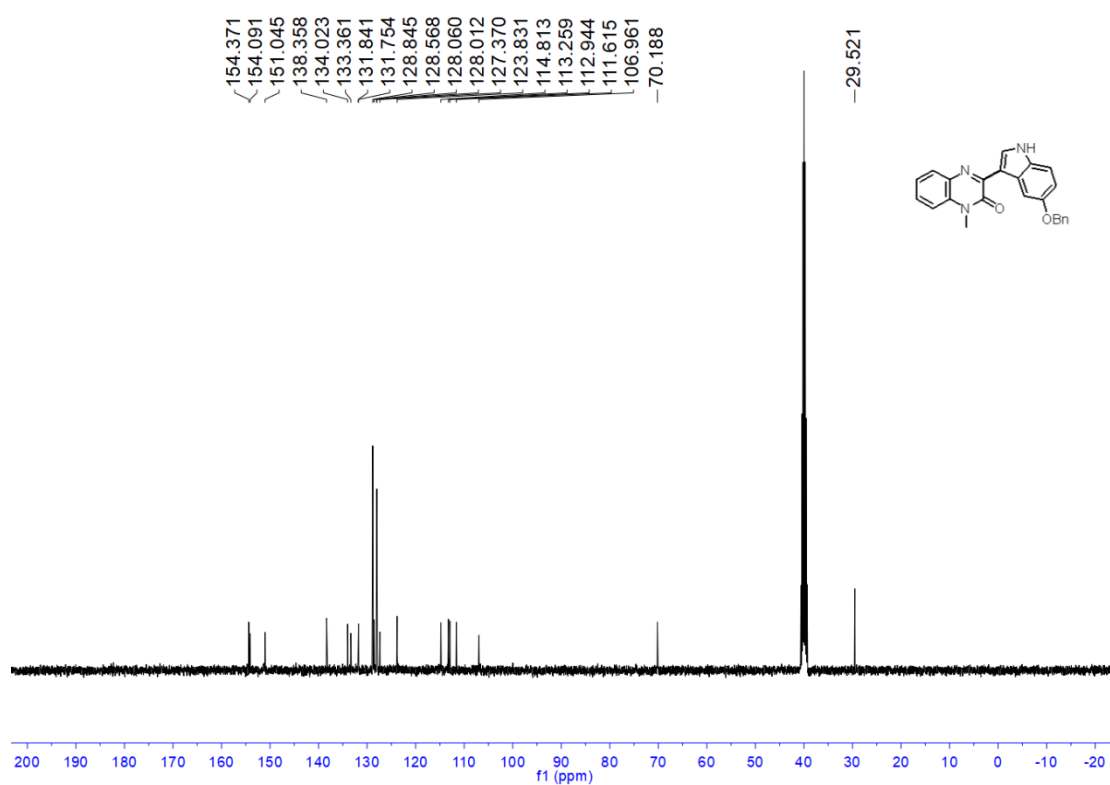
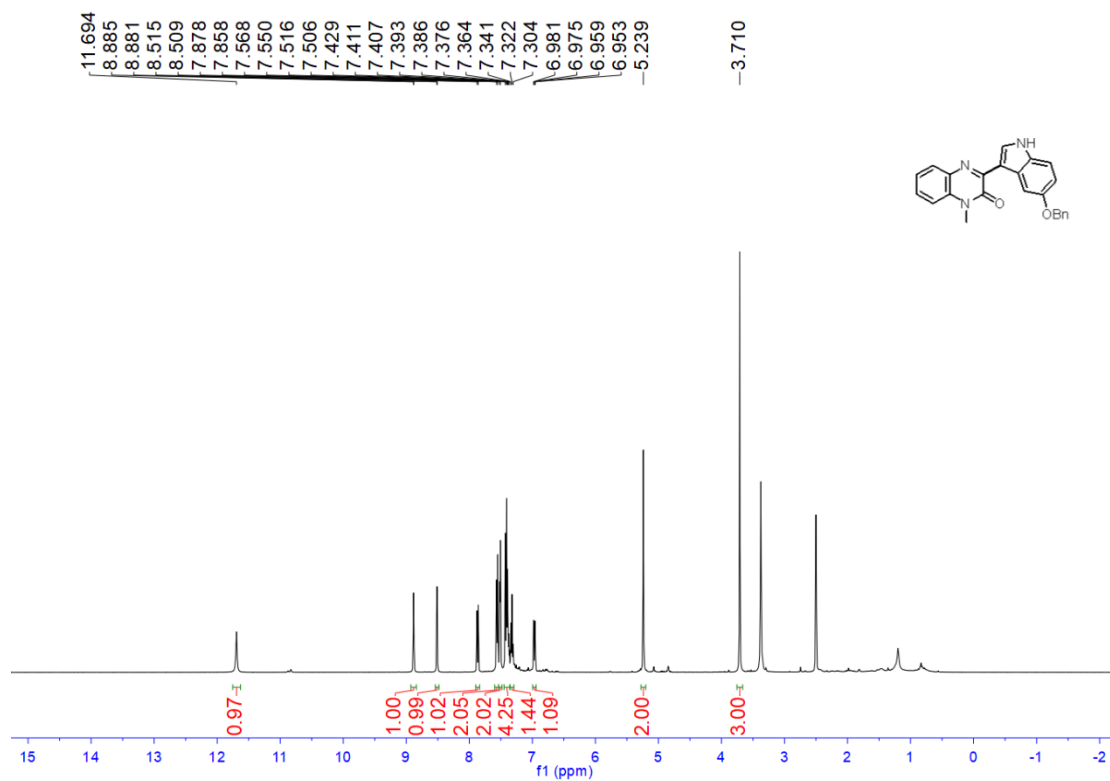
3-(4-fluoro-1H-indol-3-yl)-1-methylquinoxalin-2(1H)-one

(**3ae**). Orange solid, 49.7 mg, yield 85%. m.p.: 237.9-238.6 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ 11.99 (s, 1H), 8.49 (d, *J* = 2.4 Hz, 1H), 7.78 (d, *J* = 7.7 Hz, 1H), 7.58 – 7.49 (m, 2H), 7.40 – 7.31 (m, 2H), 7.23 – 7.16 (m, 1H), 6.93 – 6.86 (m, 1H), 3.70 (s, 3H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 156.6 (d, *J* = 250.7 Hz), 154.3 (d, *J* = 1.7 Hz), 150.2, 139.6 (d, *J* = 10.9 Hz), 133.2, 132.5, 132.2, 129.4, 129.2, 123.9, 123.5 (d, *J* = 7.8 Hz), 114.9, 114.7 (d, *J* = 19.1 Hz), 111.8 (d, *J* = 4.6 Hz), 108.8 (d, *J* = 3.6 Hz), 106.9 (d, *J* = 21.5 Hz), 29.6. ¹⁹F NMR (376 MHz, DMSO-*d*₆) δ -107.86 to -107.90. HRMS (ESI, *m/z*) calcd for C₁₇H₁₃FN₃O⁺ [M+H]⁺: 294.1037, found 294.1040.



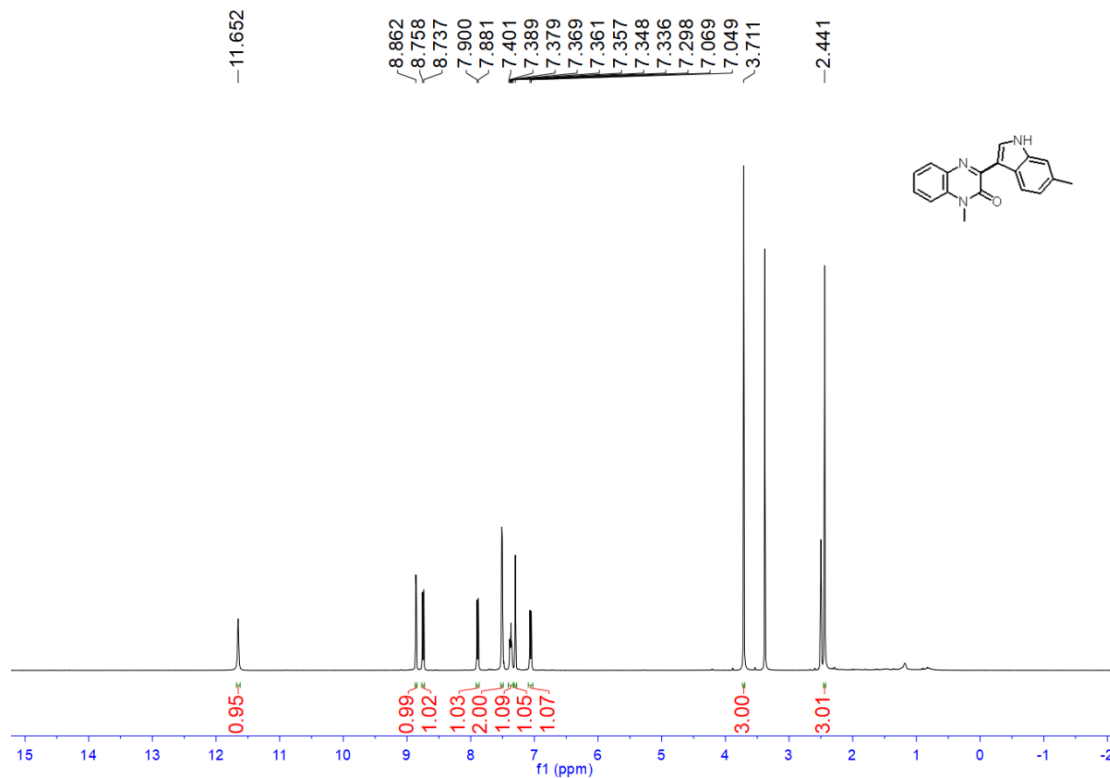


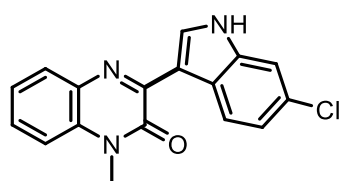
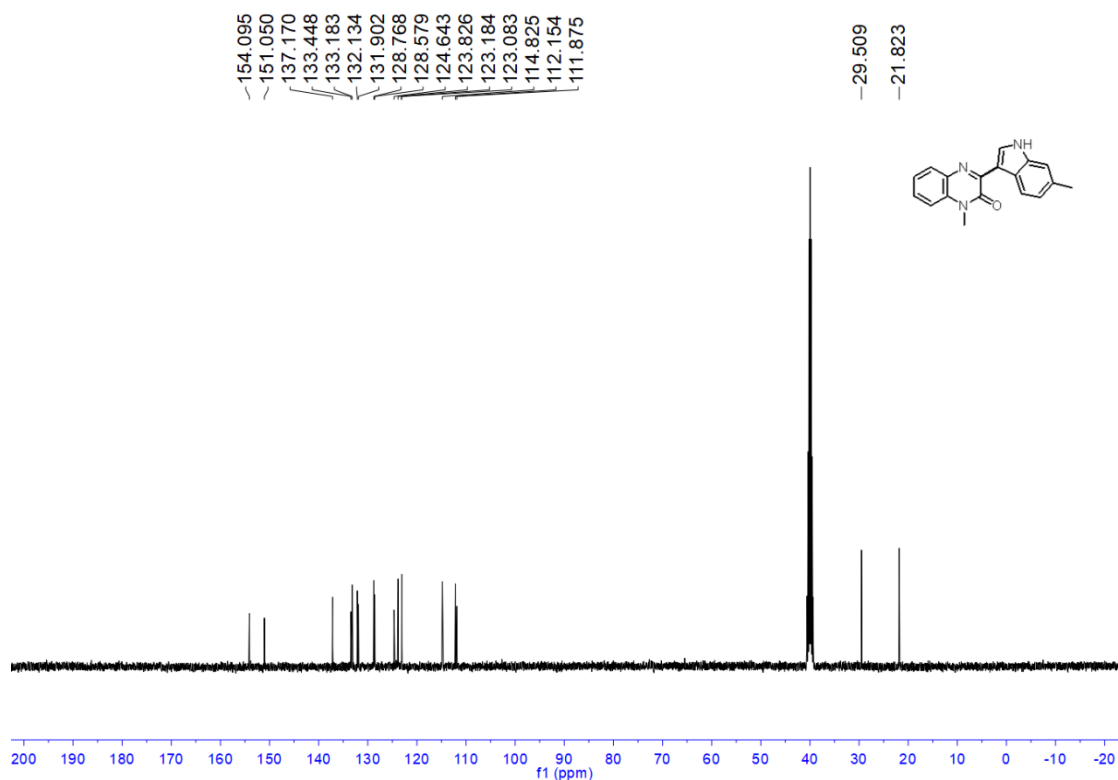
3-(5-(benzyloxy)-1H-pyrrolo[2,3-b]pyridin-3-yl)-1-methylquinoxalin-2(1H)-one (3af). A known compound.⁴ Orange solid, 72.8 mg, yield 95%. ¹H NMR (400 MHz, DMSO-*d*₆) δ 11.69 (s, 1H), 8.99 – 8.74 (m, 1H), 8.51 (d, *J* = 2.4 Hz, 1H), 7.87 (d, *J* = 7.8 Hz, 1H), 7.56 (d, *J* = 7.3 Hz, 2H), 7.51 (d, *J* = 3.8 Hz, 2H), 7.46 – 7.36 (m, 4H), 7.32 (t, *J* = 7.3 Hz, 2H), 6.97 (dd, *J* = 8.7, 2.5 Hz, 1H), 5.24 (s, 2H), 3.71 (s, 3H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 154.4, 154.1, 151.1, 138.4, 134.0, 133.3, 131.8, 131.8, 128.9, 128.6, 128.1, 128.0, 127.4, 123.8, 114.8, 113.3, 112.9, 111.6, 107.0, 70.2, 29.5.



1-methyl-3-(6-methyl-1H-indol-3-yl)quinoxalin-2(1H)-one (3ag). Orange solid, 54.2 mg, yield 94%. m.p.: 241.7-242.3 °C. ¹H NMR (400 MHz,

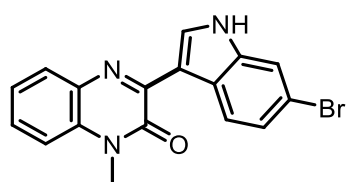
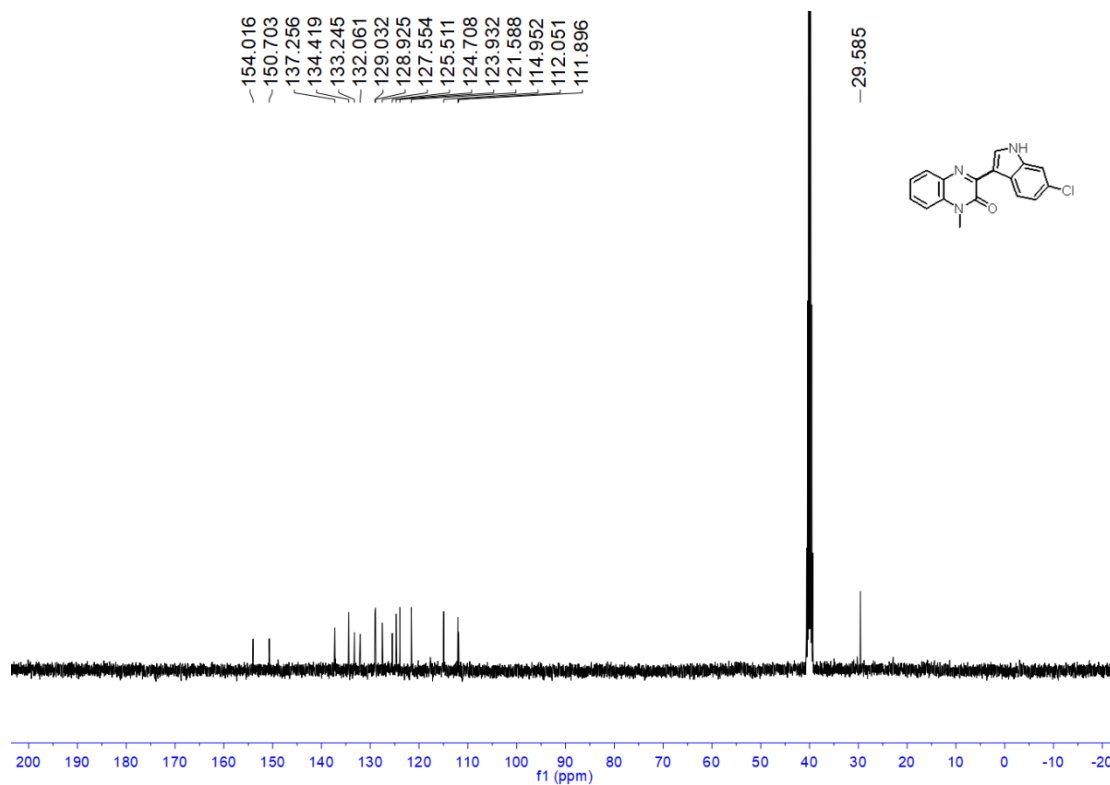
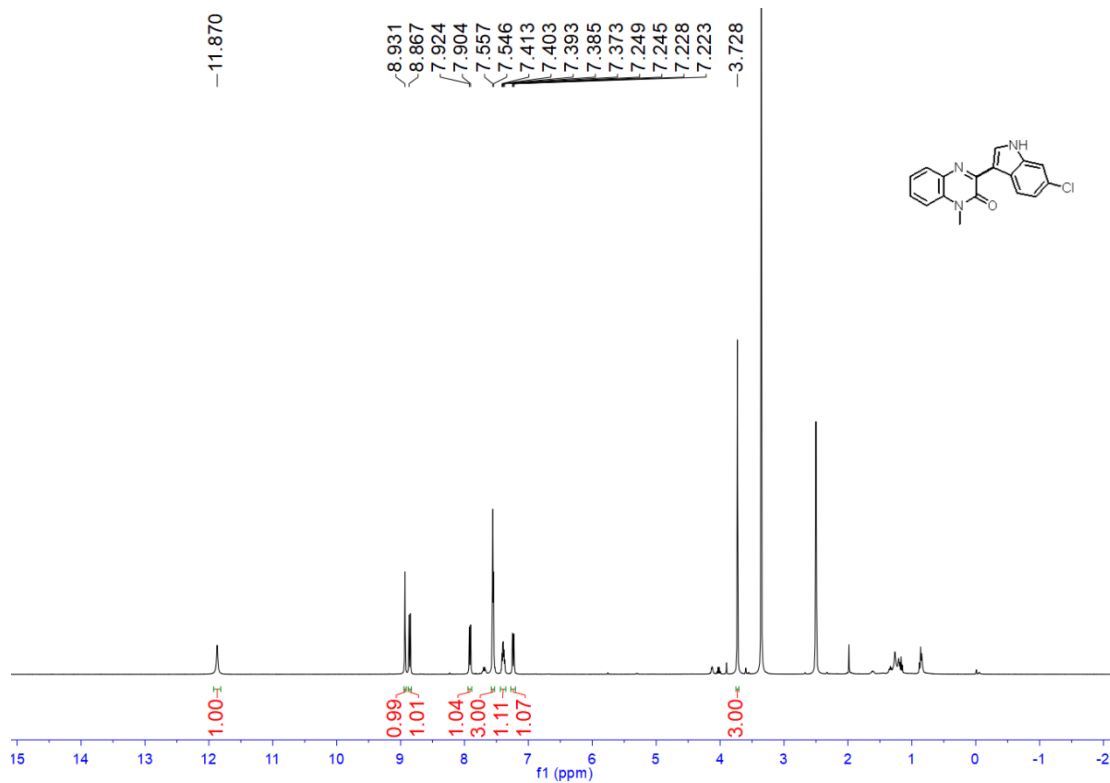
DMSO-*d*₆): δ 11.65 (s, 1H), 8.86 (d, *J* = 2.7 Hz, 1H), 8.75 (d, *J* = 8.1 Hz, 1H), 7.89 (d, *J* = 7.8 Hz, 1H), 7.54 – 7.48 (m, 2H), 7.41 – 7.33 (m, 1H), 7.30 (s, 1H), 7.06 (d, *J* = 8.1 Hz, 1H), 3.71 (s, 3H), 2.44 (s, 3H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ: 154.1, 151.0, 137.2, 133.5, 133.2, 132.1, 131.9, 128.8, 128.6, 124.6, 123.8, 123.2, 123.1, 29.5, 21.8. HRMS (ESI, *m/z*) calcd for C₁₈H₁₆N₃O⁺ [M+H]⁺: 290.1288, found 290.1290.





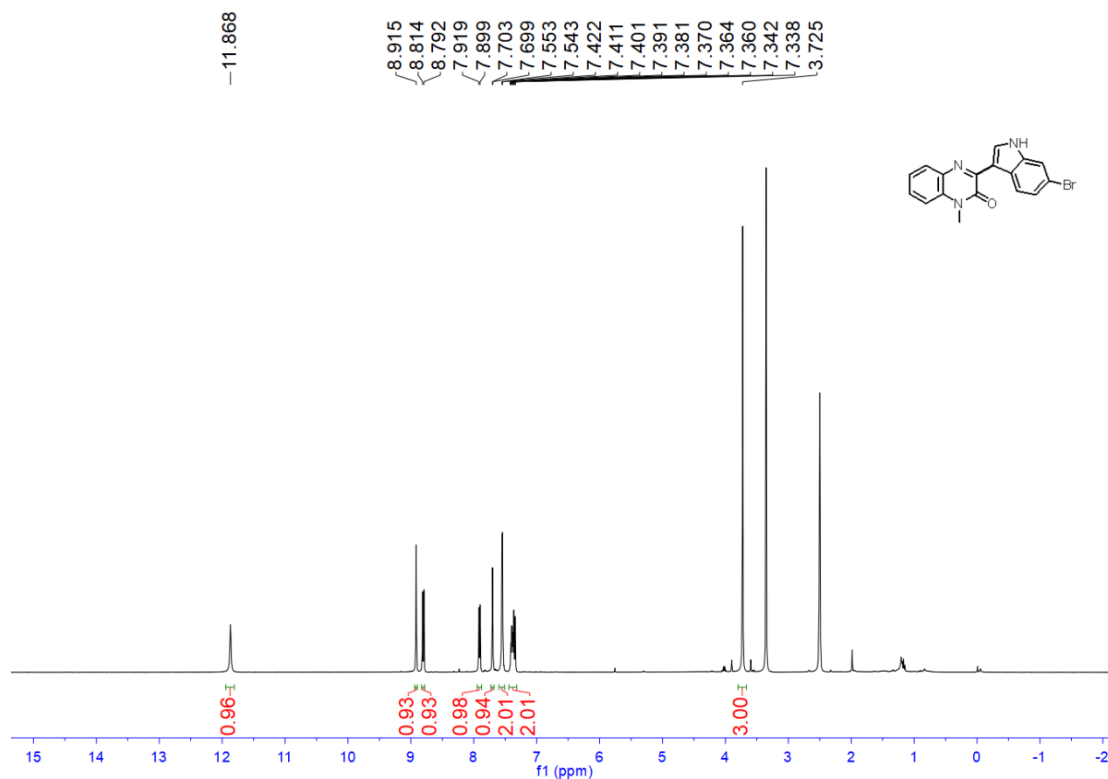
3-(6-chloro-1H-indol-3-yl)-1-methylquinoxalin-2(1H)-

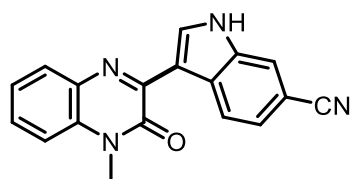
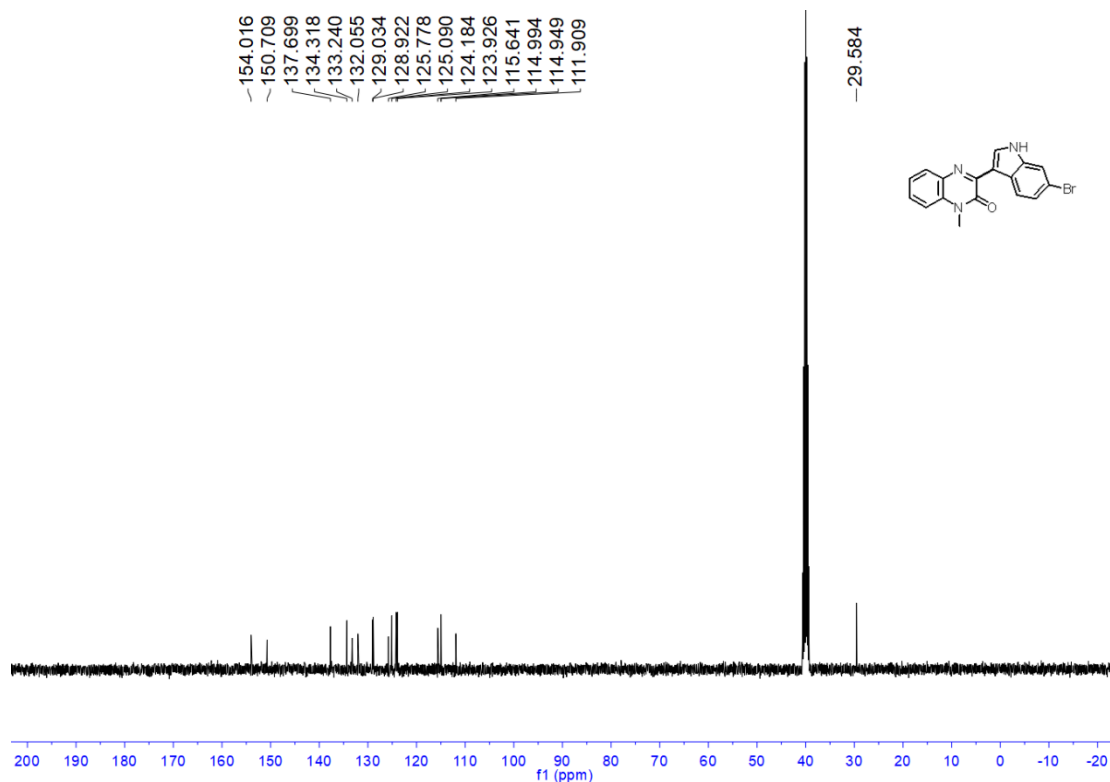
one (3ah). Yellow solid, 60.3 mg, yield 97%. m.p.: 270.0-271.5 °C. ¹H NMR (400 MHz, DMSO-*d*₆): δ 11.87 (s, 1H), 8.93 (s, 1H), 8.86 (d, *J* = 8.6 Hz, 1H), 7.91 (d, *J* = 7.9 Hz, 1H), 7.60 – 7.52 (m, 3H), 7.44 – 7.35 (m, 1H), 7.24 (dd, *J* = 8.6, 1.8 Hz, 1H), 3.73 (s, 3H). ¹³C NMR (101 MHz, DMSO-*d*₆): δ 154.0, 150.7, 137.3, 134.4, 133.2, 132.1, 129.0, 128.9, 127.6, 125.5, 124.7, 123.9, 121.6, 115.0, 112.1, 111.9, 29.6. HRMS (ESI, *m/z*) calcd for C₁₇H₁₂ClN₃NaO⁺ [M+Na]⁺: 332.0561, found 332.0565.



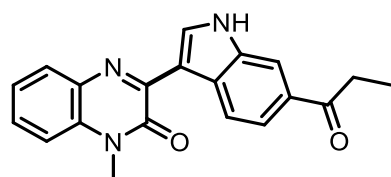
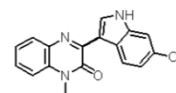
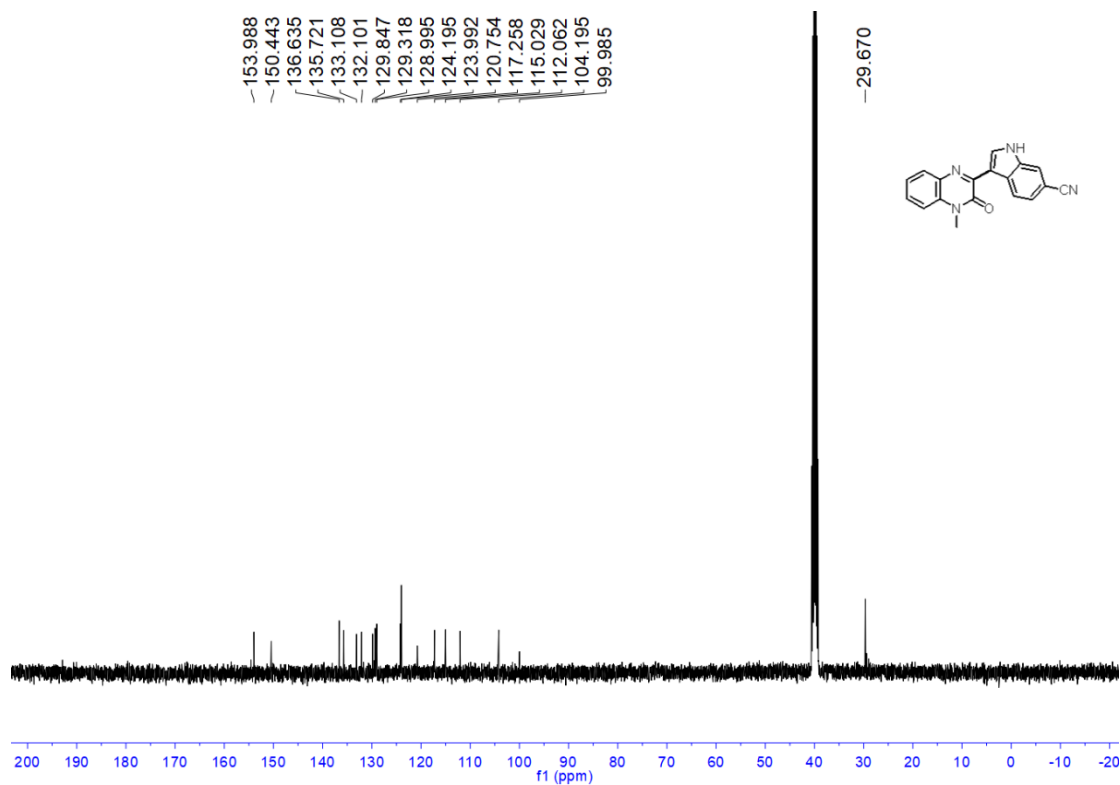
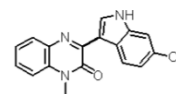
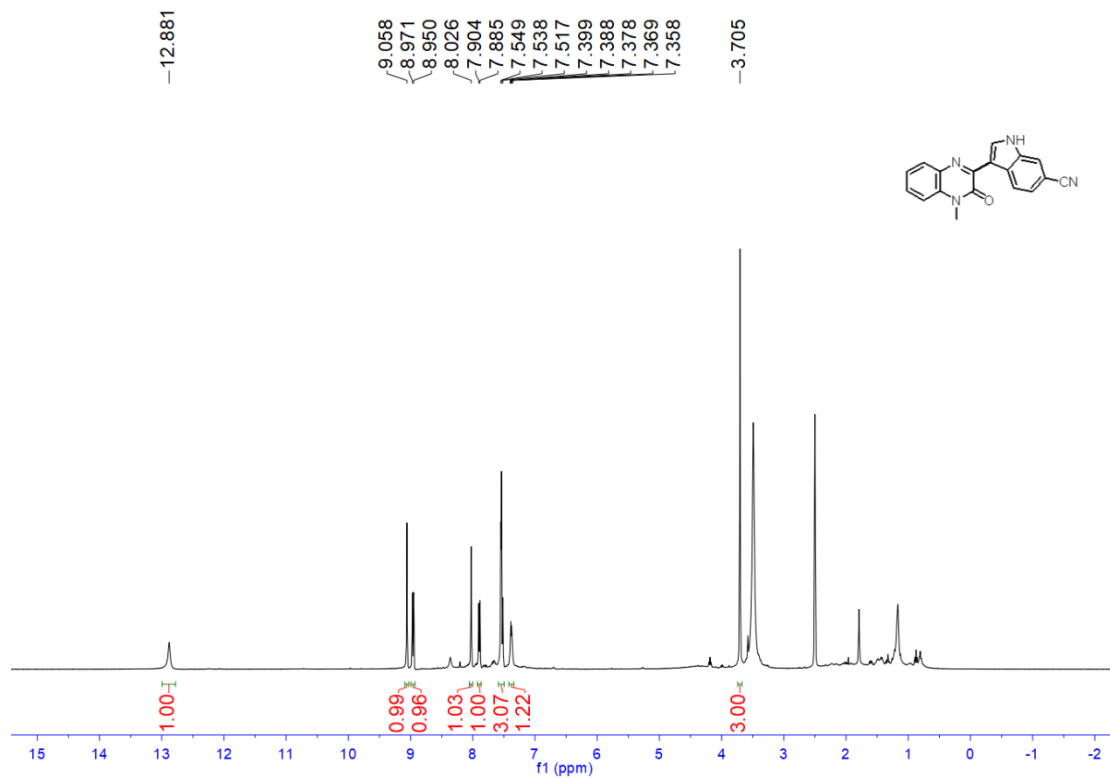
3-(6-bromo-1H-indol-3-yl)-1-methylquinoxalin-2(1H)-

one (3ai). Yellow solid, 63.0 mg, yield 89%. m.p.: 286.7-287.4 °C. ^1H NMR (400 MHz, $\text{DMSO-}d_6$): δ 11.87 (s, 1H), 8.92 (s, 1H), 8.80 (d, $J = 8.6$ Hz, 1H), 7.91 (d, $J = 7.9$ Hz, 1H), 7.70 (d, $J = 1.4$ Hz, 1H), 7.55 (d, $J = 3.8$ Hz, 2H), 7.44 – 7.32 (m, 2H), 3.73 (s, 3H). ^{13}C NMR (101 MHz, $\text{DMSO-}d_6$): δ 154.0, 150.7, 137.7, 134.3, 133.2, 132.1, 129.0, 128.9, 125.8, 125.1, 124.2, 123.9, 115.6, 115.0, 114.95, 111.9, 29.6. HRMS (ESI, m/z) calcd for $\text{C}_{17}\text{H}_{12}\text{BrN}_3\text{NaO}^+$ $[\text{M}+\text{Na}]^+$: 376.0056, found 376.0060.



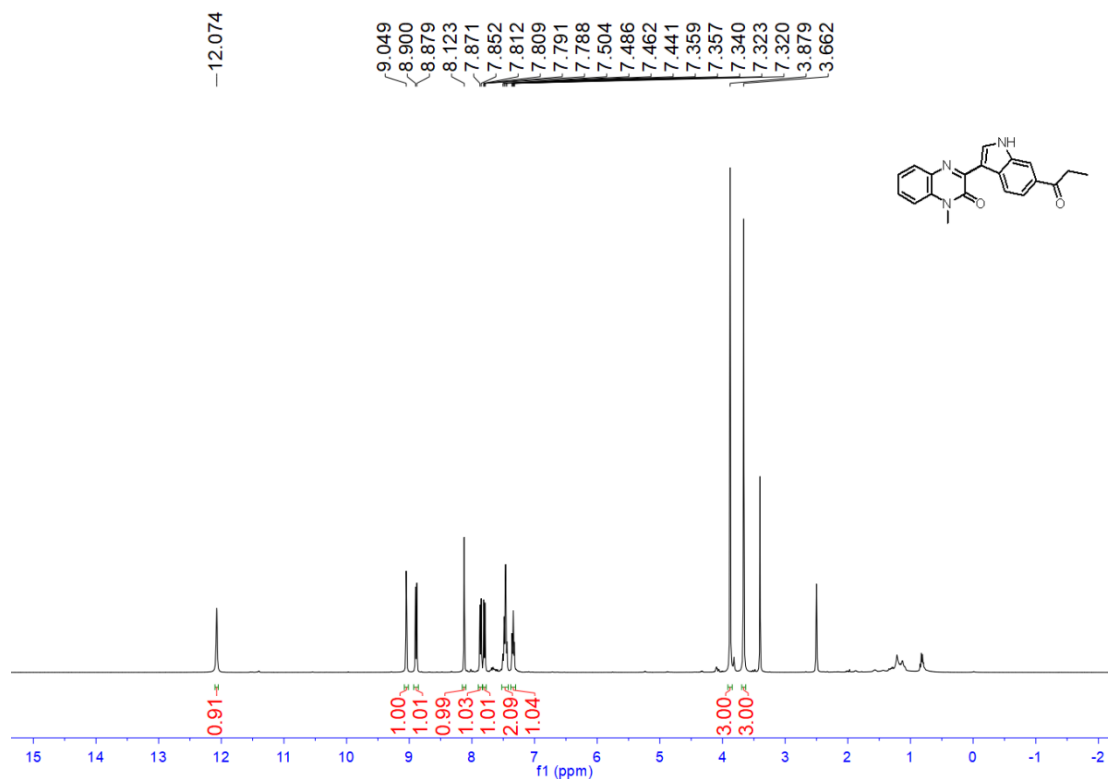


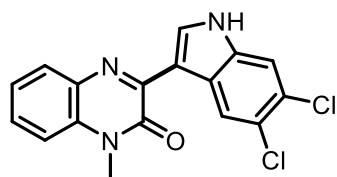
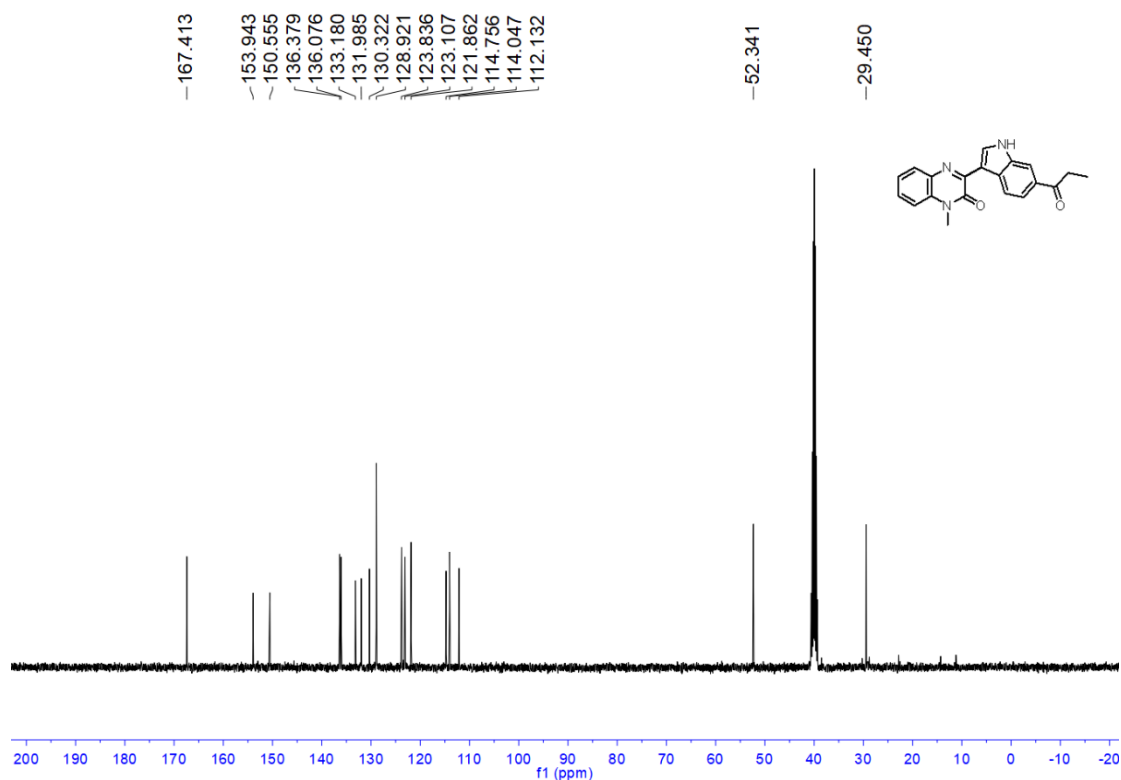
3-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)-1H-indole-6-carbonitrile (3aj). Brown solid, 42.7 mg, yield 71%. m.p.: 321.4-323.7 °C. ^1H NMR (400 MHz, DMSO- d_6) δ 12.88 (s, 1H), 9.06 (s, 1H), 8.96 (d, $J = 8.3$ Hz, 1H), 8.03 (s, 1H), 7.89 (d, $J = 7.8$ Hz, 1H), 7.60 – 7.49 (m, 3H), 7.42 – 7.34 (m, 1H), 3.70 (s, 3H). ^{13}C NMR (101 MHz, DMSO- d_6) δ 154.0, 150.4, 136.6, 135.7, 133.1, 132.1, 129.9, 129.3, 129.0, 124.2, 124.0, 120.8, 117.3, 115.0, 112.1, 104.1, 100.0, 29.7. HRMS (ESI, m/z) calcd for $\text{C}_{18}\text{H}_{12}\text{N}_4\text{NaO}^+$ $[\text{M}+\text{Na}]^+$: 323.0903, found 323.0903.



Methyl 3-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)-1H-indole-6-carboxylate (3ak). Yellow solid, 64.6 mg, yield 97%. m.p.: 238.6-

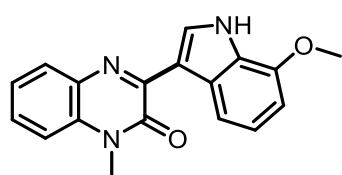
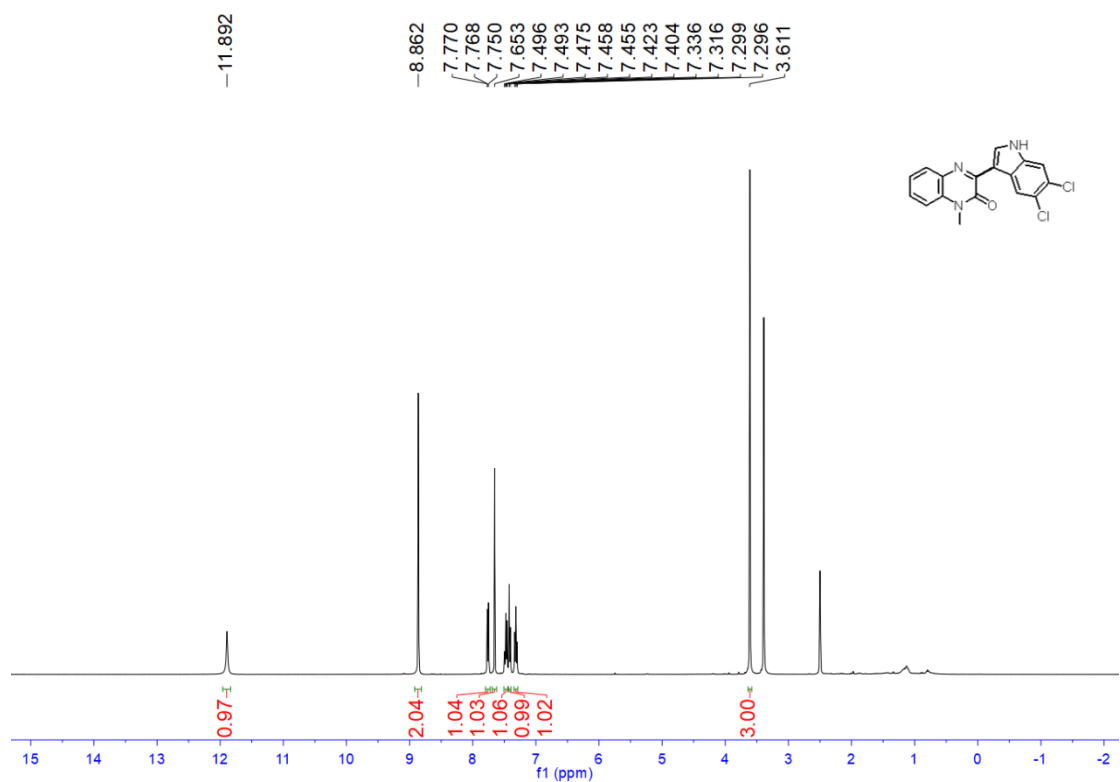
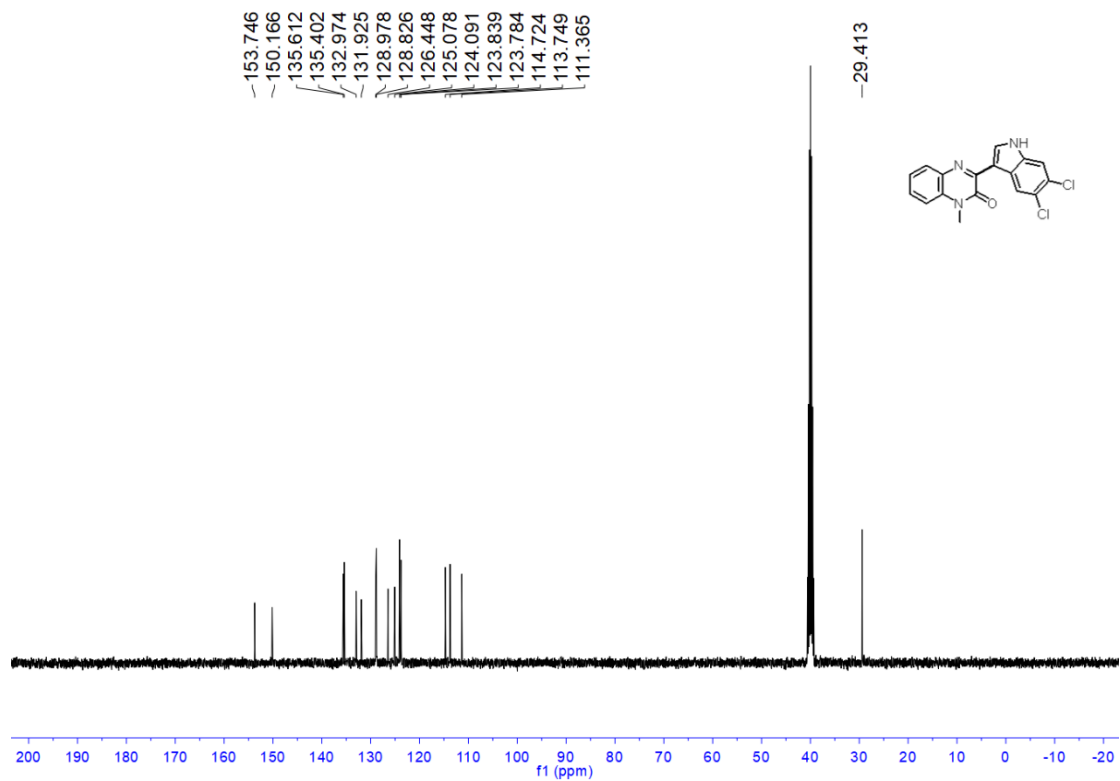
269.6 °C. ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 12.07 (s, 1H), 9.05 (d, $J = 2.0$ Hz, 1H), 8.89 (d, $J = 8.5$ Hz, 1H), 8.12 (s, 1H), 7.86 (d, $J = 7.7$ Hz, 1H), 7.83 – 7.77 (m, 1H), 7.52 – 7.42 (m, 2H), 7.38 – 7.30 (m, 1H), 3.88 (s, 3H), 3.66 (s, 3H). ^{13}C NMR (101 MHz, $\text{DMSO-}d_6$) δ 167.4, 153.9, 150.6, 136.4, 136.1, 133.2, 132.0, 130.3, 128.9, 123.84, 123.78, 123.1, 121.9, 114.8, 114.1, 112.1, 52.3, 29.5. HRMS (ESI, m/z) calcd for $\text{C}_{19}\text{H}_{16}\text{N}_3\text{O}_3^+$ $[\text{M}+\text{H}]^+$: 334.1186, found 334.1189.





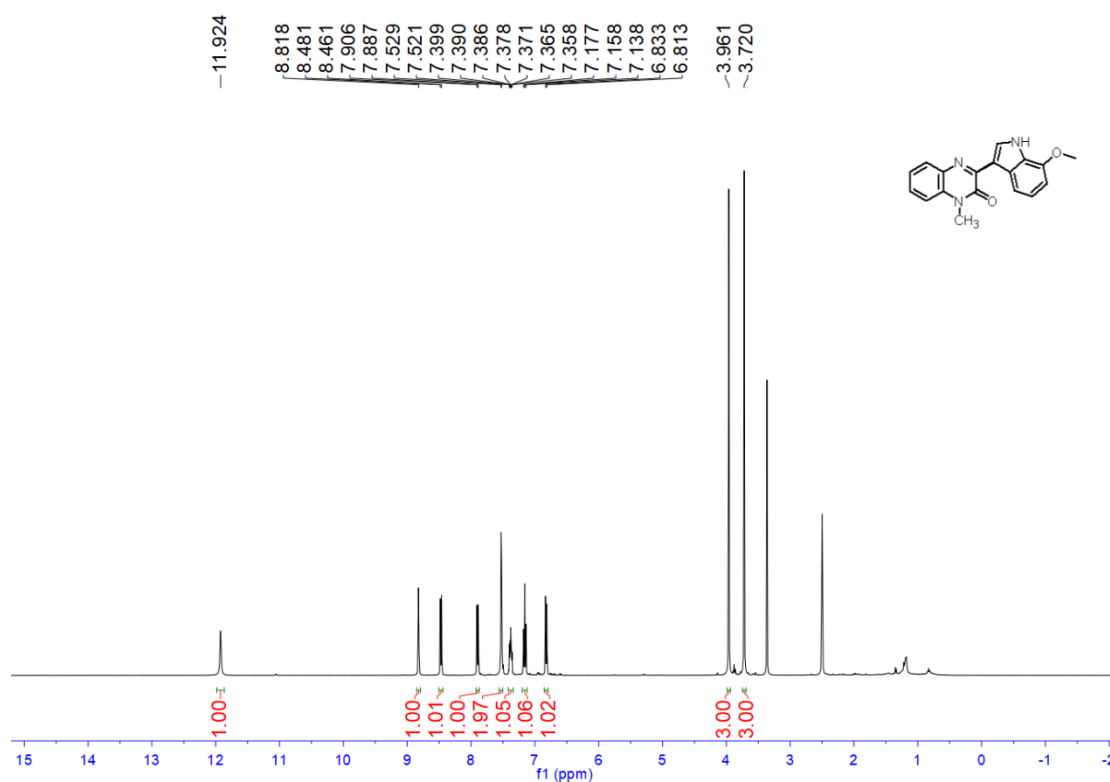
3-(5,6-dichloro-1H-indol-3-yl)-1-methylquinoxalin-

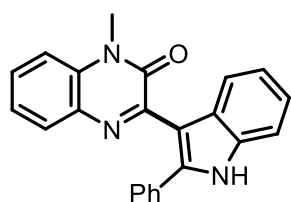
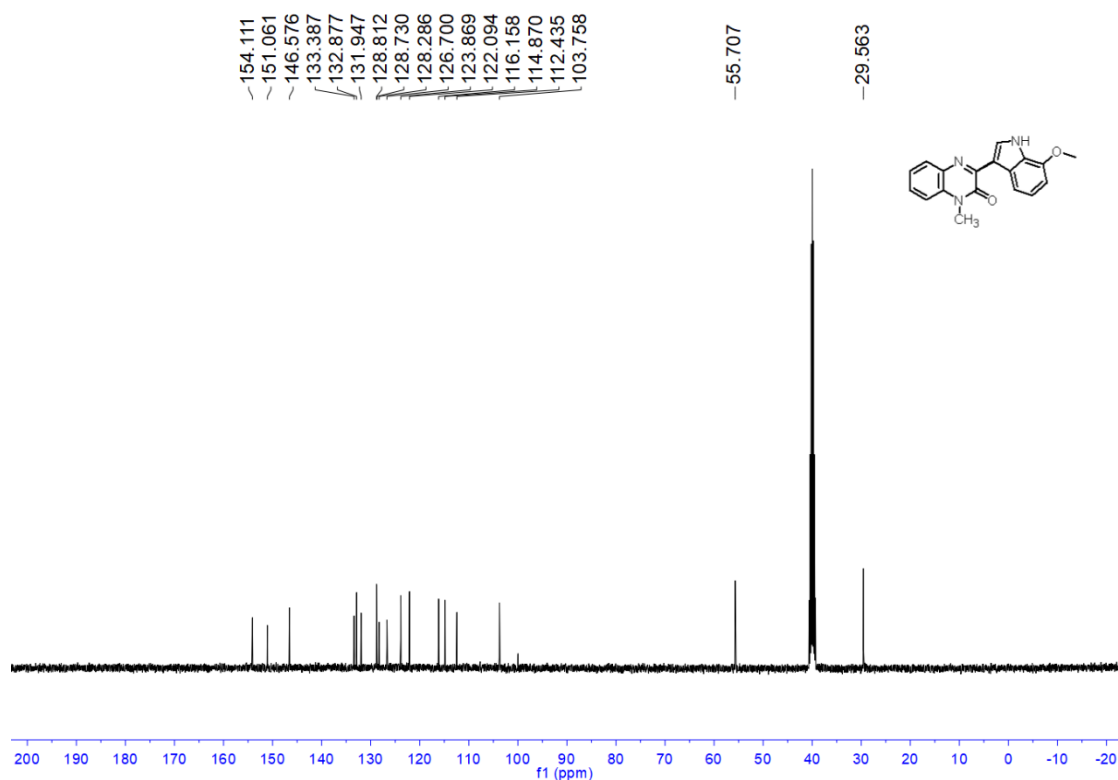
2(1H)-one (3a). Orange solid, 67.4 mg, yield 98%. m.p.: 256.3-257.6 °C. ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 11.89 (s, 1H), 8.86 (s, 2H), 7.79 – 7.73 (m, 1H), 7.65 (s, 1H), 7.51 – 7.44 (m, 1H), 7.44 – 7.39 (m, 1H), 7.36 – 7.28 (m, 1H), 3.61 (s, 3H). ^{13}C NMR (101 MHz, $\text{DMSO-}d_6$) δ 153.8, 150.2, 135.6, 135.4, 133.0, 131.9, 129.0, 128.8, 126.5, 125.1, 124.1, 123.8, 123.8, 114.7, 113.8, 111.4, 29.4. HRMS (ESI, m/z) calcd for $\text{C}_{17}\text{H}_{11}\text{Cl}_2\text{N}_3\text{NaO}^+$ $[\text{M}+\text{Na}]^+$: 366.0171, found 366.0175.



3-(7-methoxy-1H-indol-3-yl)-1-methylquinoxalin-2(1H)-

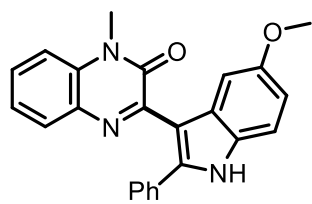
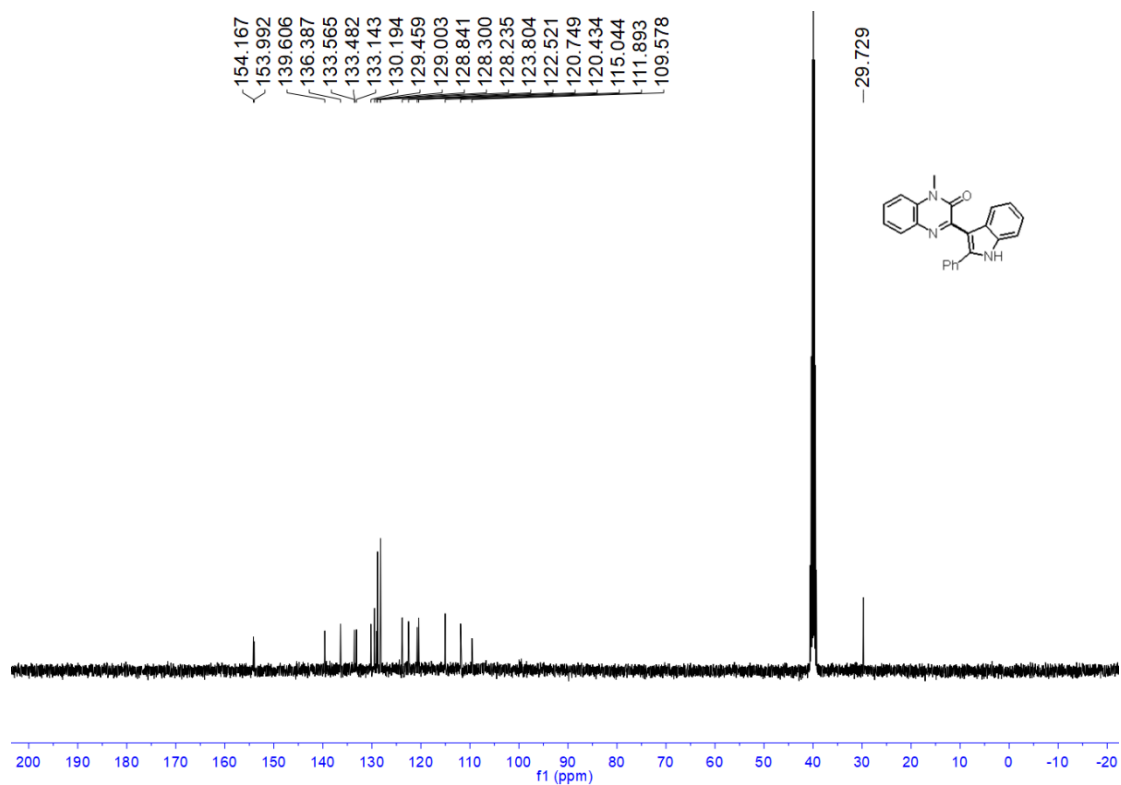
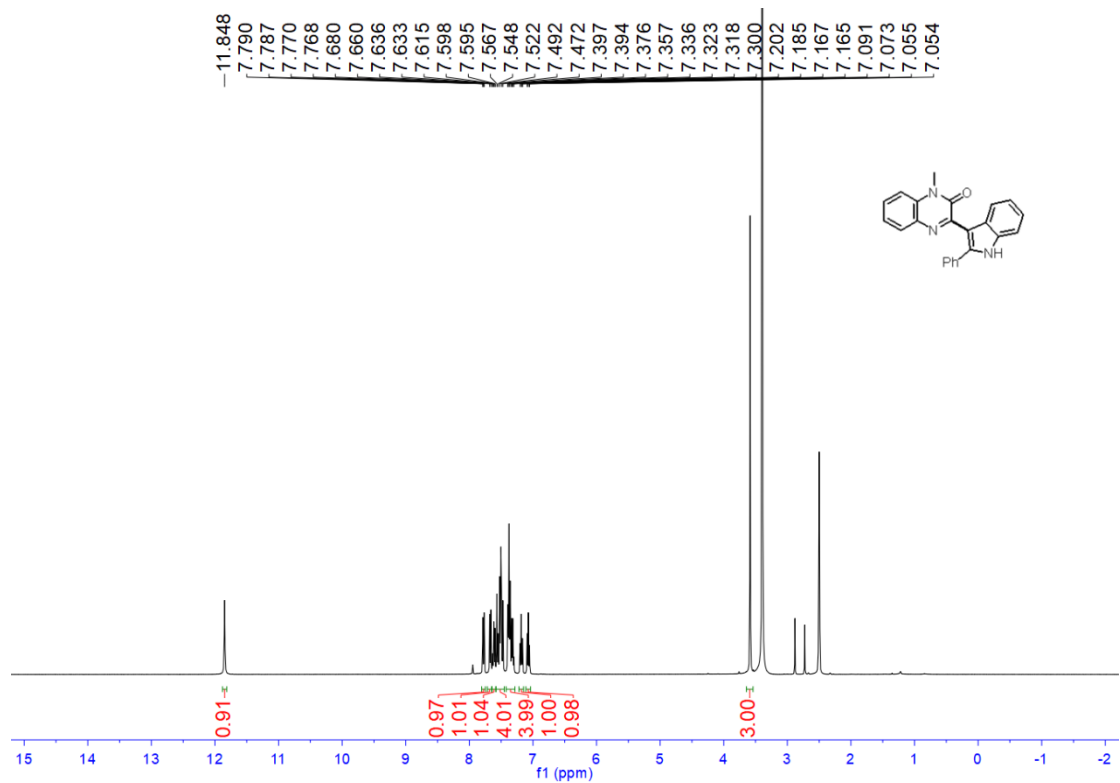
one (3am). Yellow solid, 59.9 mg, yield 98%. m.p.: 266.7-267.2 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ 11.92 (s, 1H), 8.82 (d, *J* = 2.3 Hz, 1H), 8.47 (d, *J* = 8.0 Hz, 1H), 7.90 (d, *J* = 7.8 Hz, 1H), 7.56 – 7.50 (m, 2H), 7.42 – 7.35 (m, 1H), 7.16 (dd, *J*₁ = *J*₂ = 7.9 Hz, 1H), 6.82 (d, *J* = 7.7 Hz, 1H), 3.96 (s, 3H), 3.72 (s, 3H). ¹³C NMR (101 MHz, DMSO-*d*₆): δ 154.1, 151.1, 146.6, 133.4, 132.9, 132.0, 128.8, 128.7, 128.3, 126.7, 123.9, 122.1, 116.2, 114.9, 112.4, 103.8, 55.7, 29.6. HRMS (ESI, *m/z*) calcd for C₁₈H₁₆N₃O₂⁺ [M+H]⁺: 306.1237, found 306.1239.





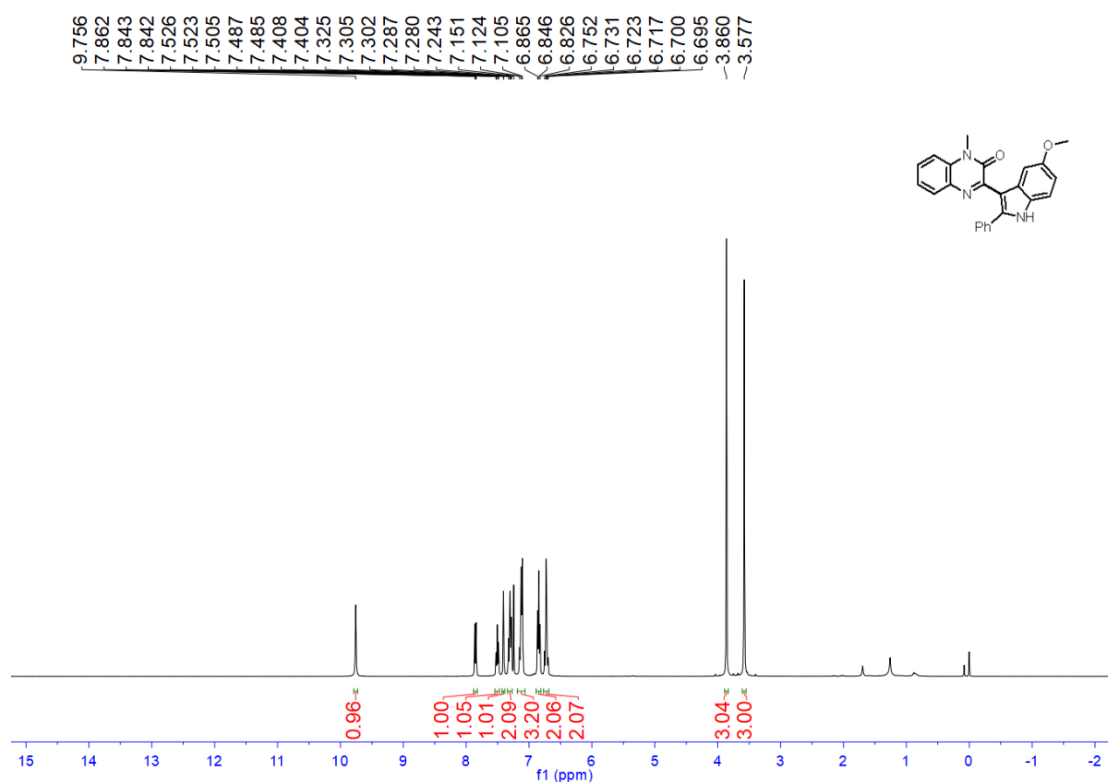
1-methyl-3-(2-phenyl-1H-indol-3-yl)quinoxalin-

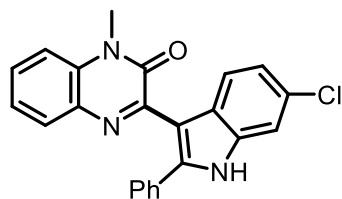
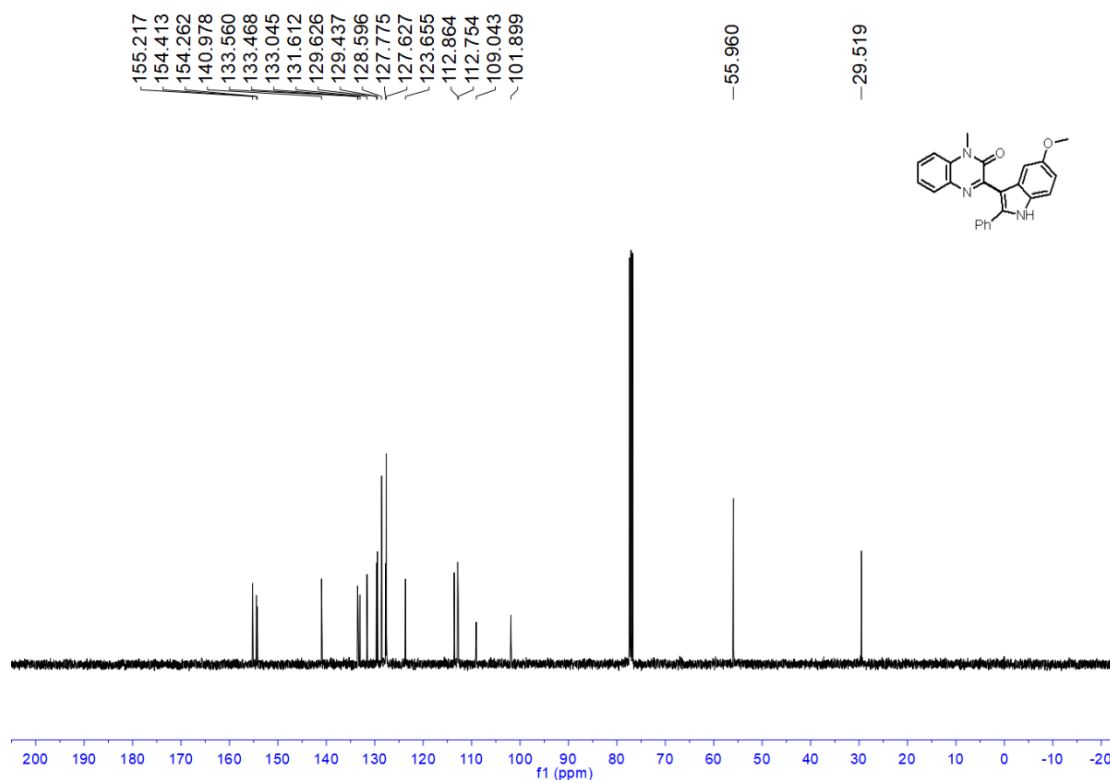
2(1H)-one (3an). Yellow solid, 68.9 mg, yield 98%. m.p.: 210.3-211.4 °C. ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 11.85 (s, 1H), 7.81 – 7.75 (m, 1H), 7.67 (d, $J = 8.0$ Hz, 1H), 7.65 – 7.59 (m, 1H), 7.59 – 7.45 (m, 4H), 7.42 – 7.28 (m, 4H), 7.23 – 7.15 (m, 1H), 7.11 – 7.04 (m, 1H), 3.59 (s, 3H). ^{13}C NMR (101 MHz, $\text{DMSO-}d_6$) δ 154.2, 154.0, 139.6, 136.4, 133.6, 133.5, 133.1, 130.2, 129.5, 129.0, 128.8, 128.3, 128.2, 123.8, 122.5, 120.8, 120.4, 115.0, 111.9, 109.6, 29.7. HRMS (ESI, m/z) calcd for $\text{C}_{23}\text{H}_{18}\text{N}_3\text{O}^+$ $[\text{M}+\text{H}]^+$: 352.1444, found 352.1447.



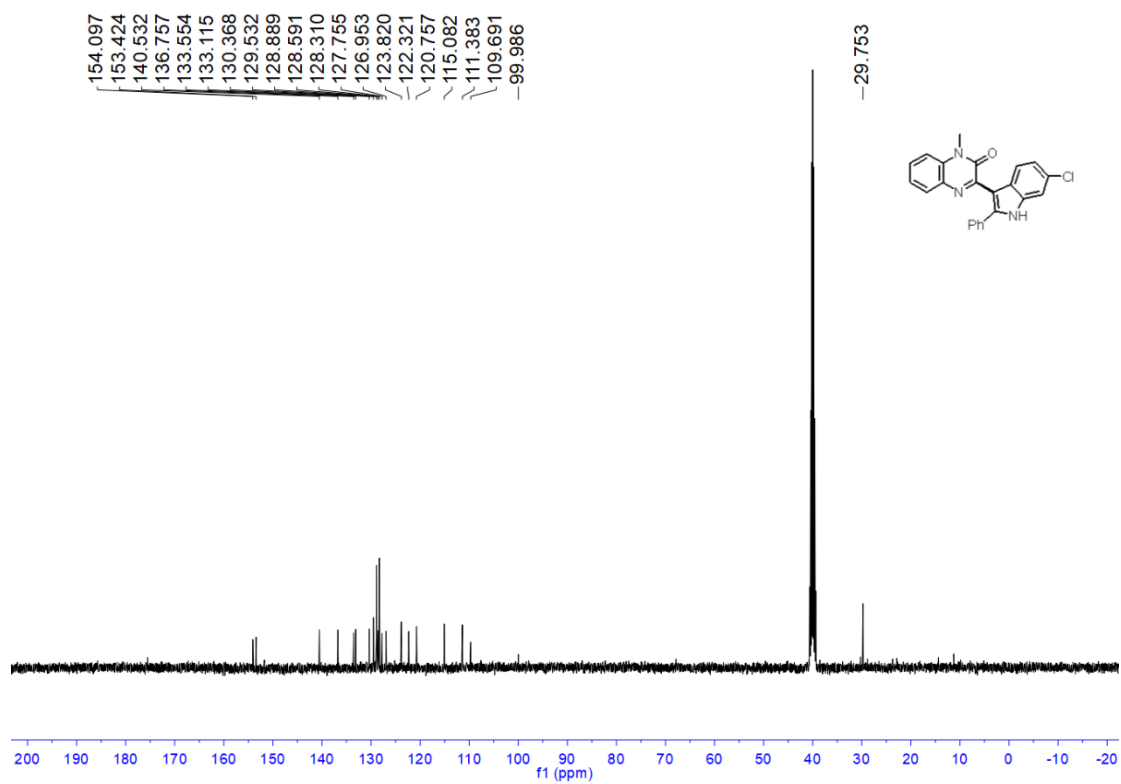
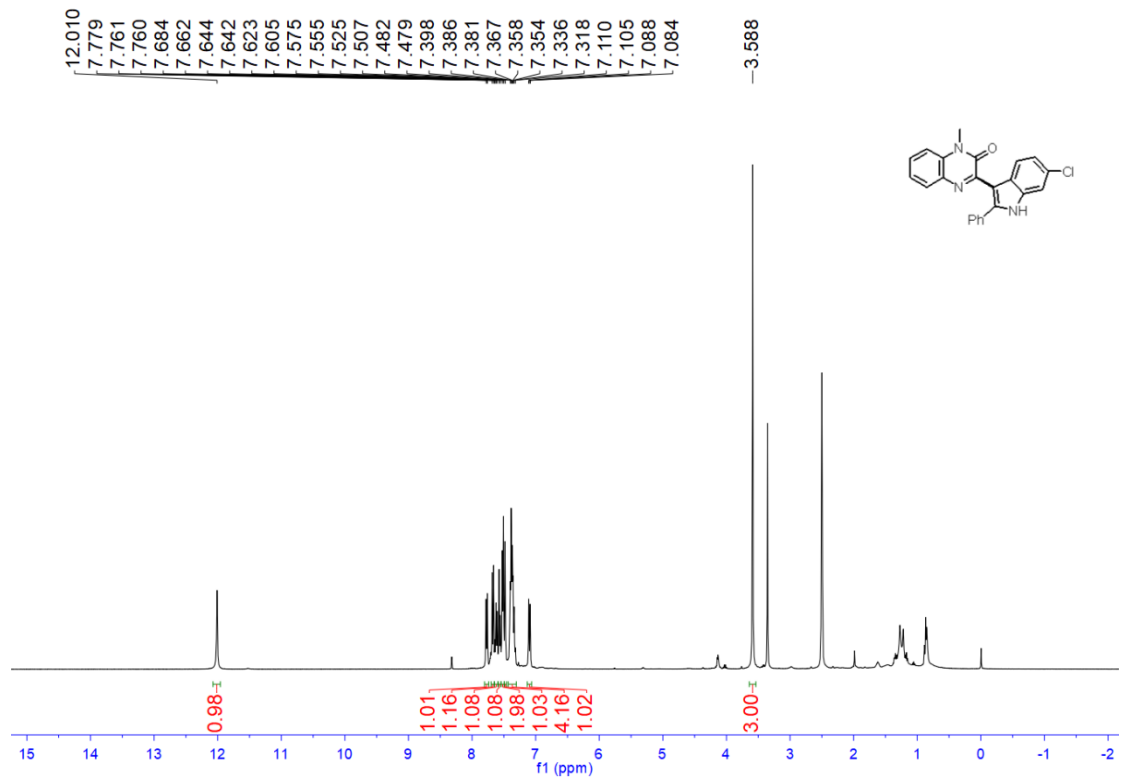
3-(5-methoxy-2-phenyl-1H-indol-3-yl)-1-

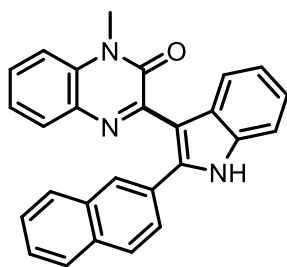
methylquinoxalin-2(1*H*)-one (3ao). Yellow solid, 65.9 mg, yield 86%. m.p.: 146.4-147.3 °C. ¹H NMR (400 MHz, CDCl₃, TMS) δ 9.76 (s, 1H), 7.88 – 7.82 (m, H), 7.55 – 7.47 (m, 1H), 7.44 – 7.38 (m, 1H), 7.34 – 7.27 (m, 2H), 7.19 – 7.10 (m, 3H), 6.85 (dd, *J*₁ = *J*₂ = 7.7 Hz, 2H), 6.78 – 6.68 (m, 2H), 3.86 (s, 3H), 3.58 (s, 3H). ¹³C NMR (101 MHz, CDCl₃, TMS) δ 155.2, 154.4, 154.3, 141.0, 133.6, 133.5, 133.1, 131.6, 129.6, 129.4, 128.6, 127.8, 127.6, 123.7, 113.6, 112.9, 112.8, 109.0, 101.9, 56.0, 29.5. HRMS (ESI, *m/z*) calcd for C₂₄H₂₀N₃O₂⁺ [M+H]⁺: 382.1550, found 382.1553.



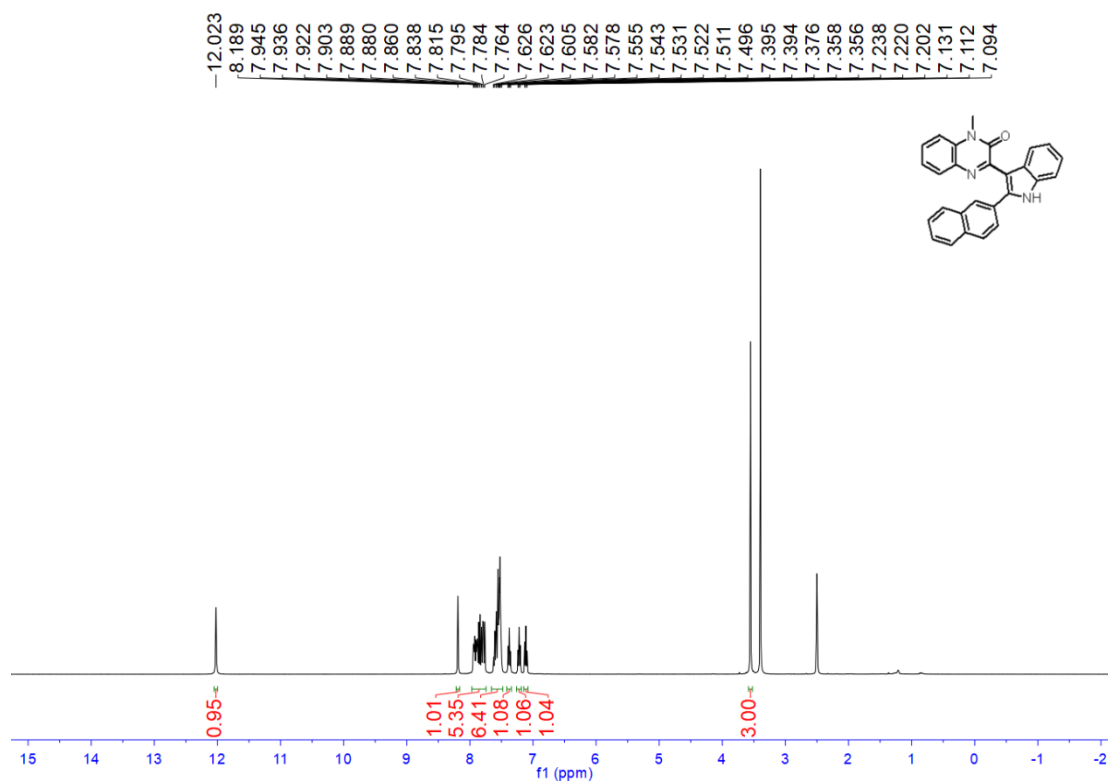


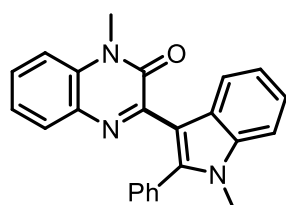
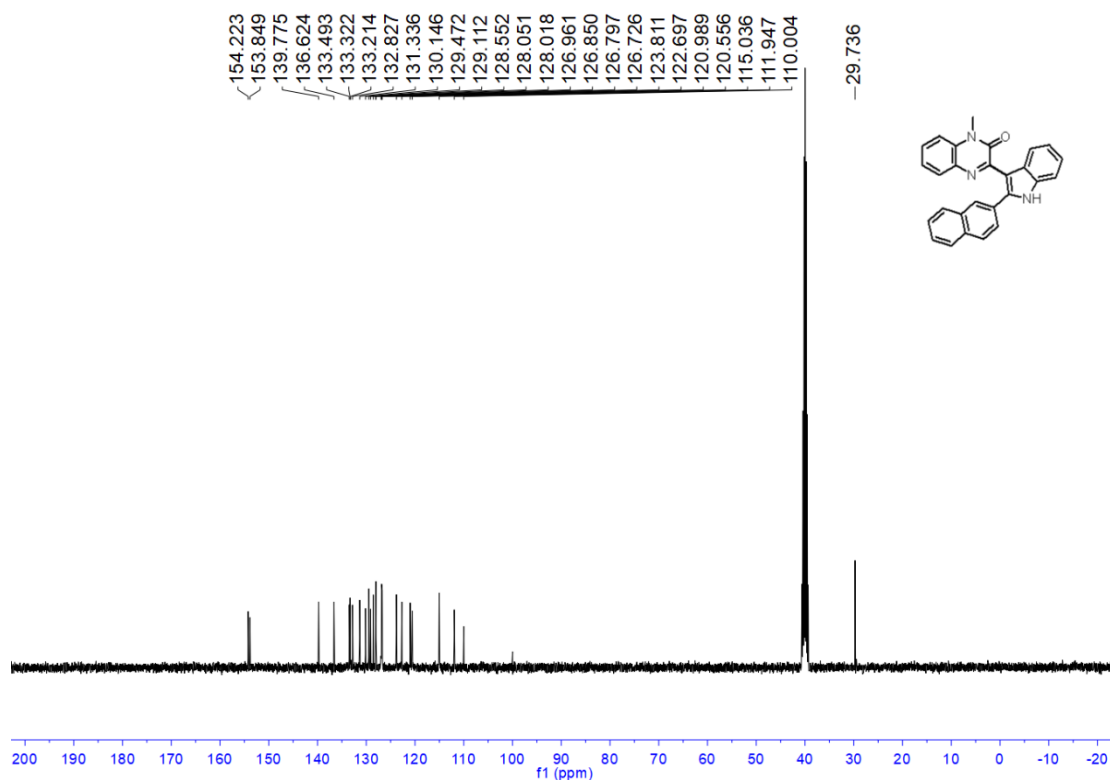
3-(6-chloro-2-phenyl-1*H*-indol-3-yl)-1-methylquinoxalin-2(1*H*)-one (3ap). Yellow solid, 61.0 mg, yield 79%. m.p.: 246.6-247.8 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ 12.01 (s, 1H), 7.81 – 7.74 (m, 1H), 7.67 (d, *J* = 8.5 Hz, 1H), 7.65 – 7.59 (m, 1H), 7.59-7.54(m, 1H), 7.54 – 7.49 (m, 2H), 7.48 (d, *J* = 1.5 Hz, 2H), 7.43 – 7.31 (m, 4H), 7.10 (dd, *J* = 8.6, 1.7 Hz, 1H), 3.59 (s, 3H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 154.1, 153.4, 140.5, 136.8, 133.6, 133.1, 130.4, 129.5, 128.9, 128.6, 128.3, 127.8, 127.0, 123.8, 122.3, 120.8, 115.1, 111.4, 109.7, 100.0, 29.8. HRMS (ESI, *m/z*) calcd for C₂₃H₁₇ClN₃NaO⁺ [M+Na]⁺: 408.0874, found 408.0876.





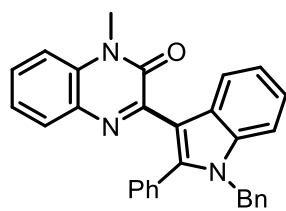
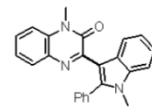
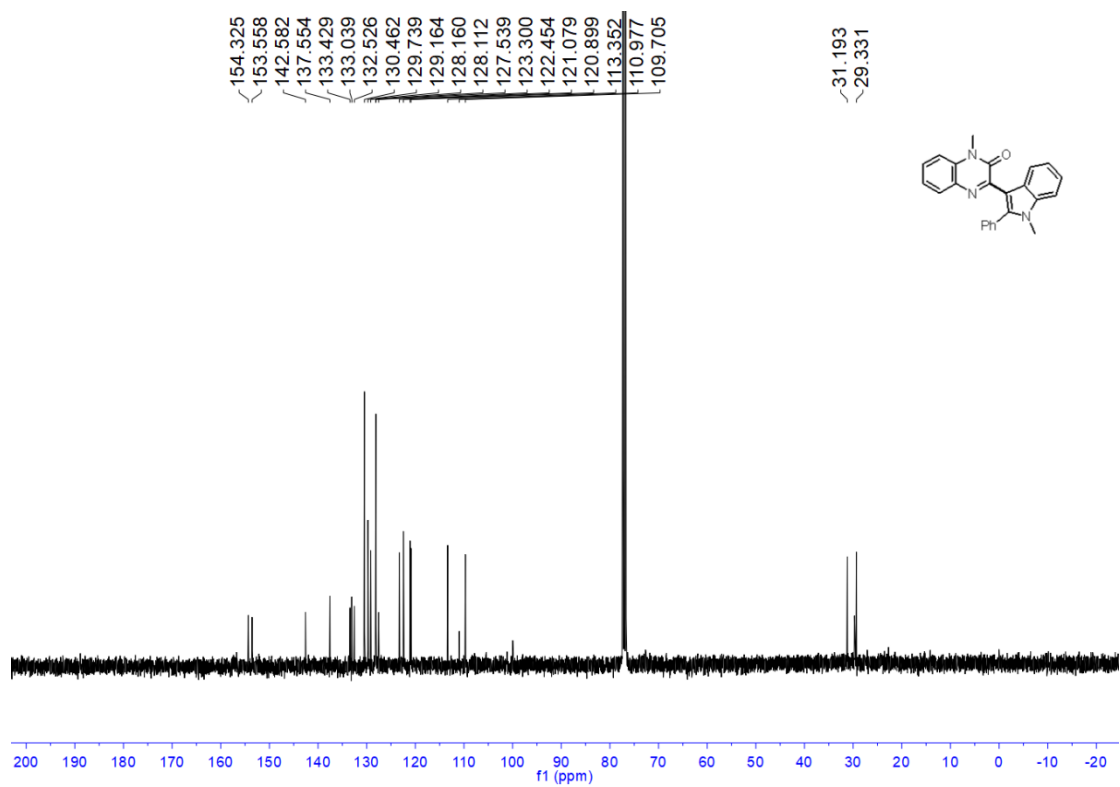
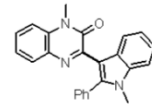
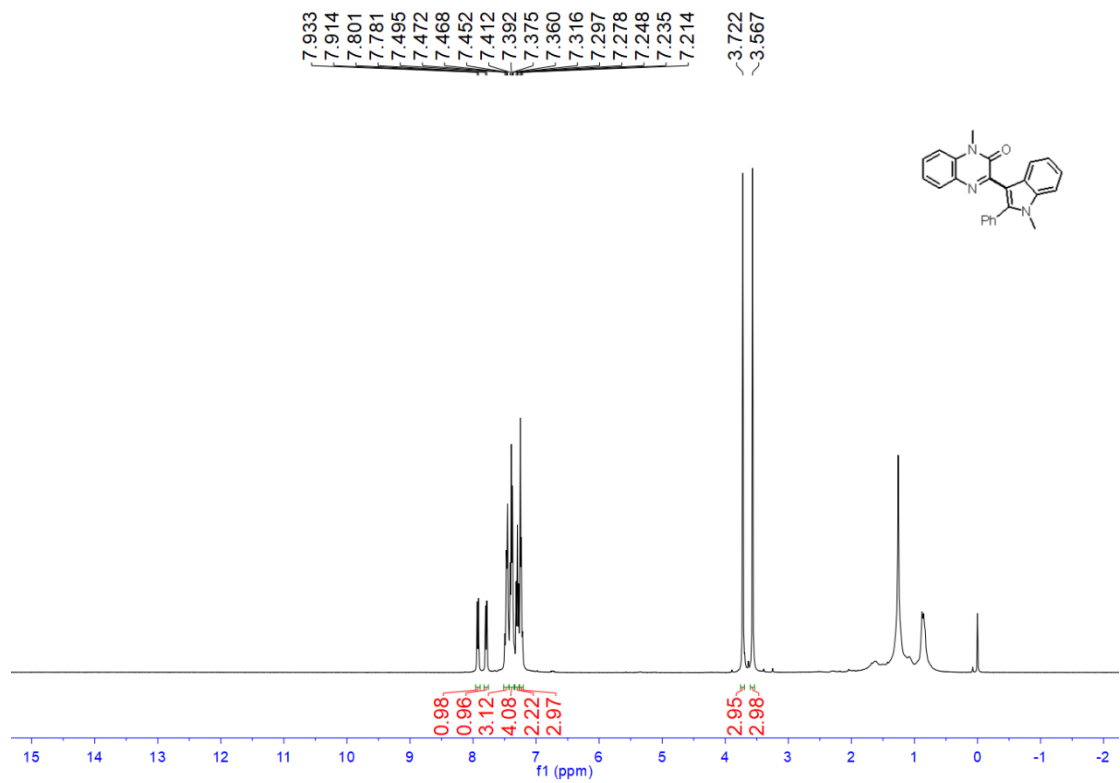
1-methyl-3-(2-(naphthalen-2-yl)-1H-indol-3-yl)quinoxalin-2(1H)-one (3aq). Yellow solid, 78.3 mg, yield 98%, m.p.: 193.3-194.6°C. ^1H NMR (400 MHz, DMSO- d_6) δ 12.02 (s, 1H), 8.19 (s, 1H), 7.98 – 7.74 (m, 5H), 7.65 – 7.48 (m, 6H), 7.42 – 7.34 (m, 1H), 7.22 (dd, $J_1 = J_2 = 7.2$ Hz, 1H), 7.11 (dd, $J_1 = J_2 = 7.4$ Hz, 1H), 3.55 (s, 3H). ^{13}C NMR (101 MHz, DMSO- d_6) δ 154.2, 153.9, 139.8, 136.6, 133.5, 133.3, 133.2, 132.8, 131.3, 130.2, 129.5, 129.1, 128.6, 128.1, 128.0, 127.0, 126.9, 126.8, 126.7, 123.8, 122.7, 121.0, 120.6, 115.0, 112.0, 110.0, 29.7. HRMS (ESI, m/z) calcd for $\text{C}_{27}\text{H}_{20}\text{N}_3\text{O}^+$ $[\text{M}+\text{H}]^+$: 402.1601, found 402.1602.





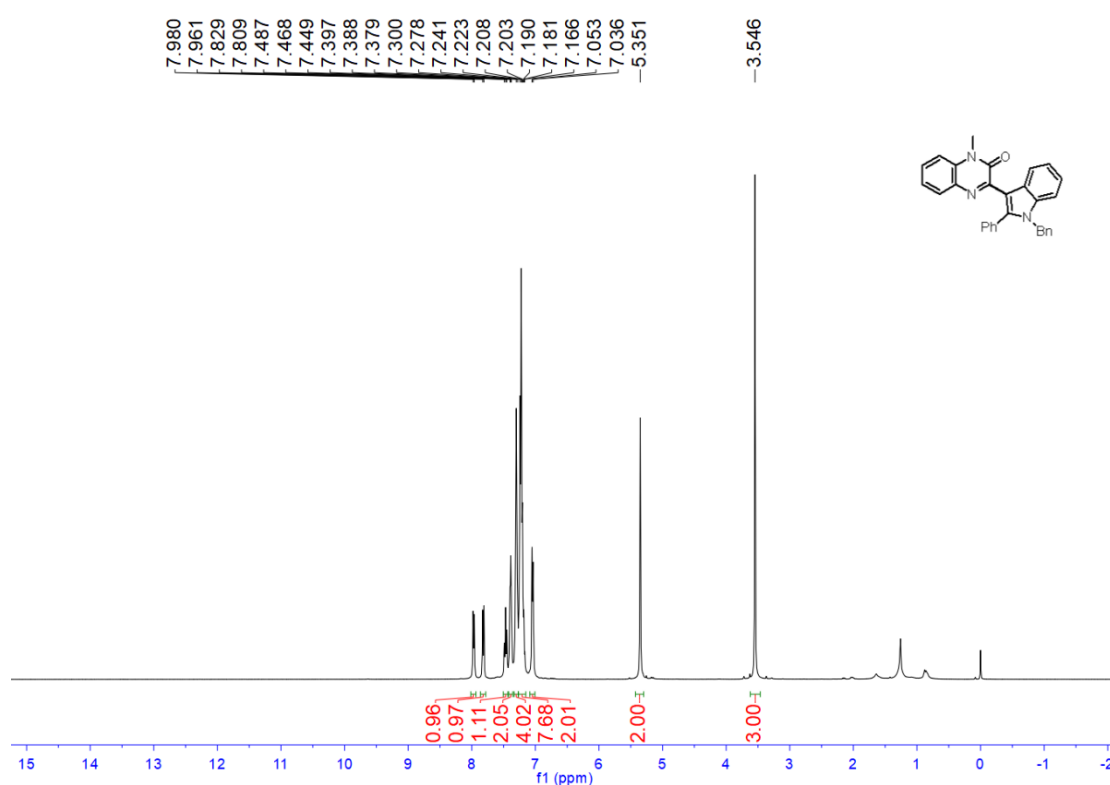
1-methyl-3-(1-methyl-2-phenyl-1H-indol-3-

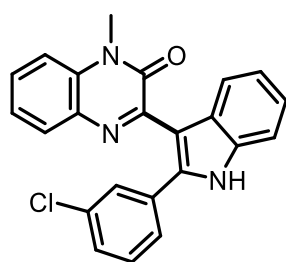
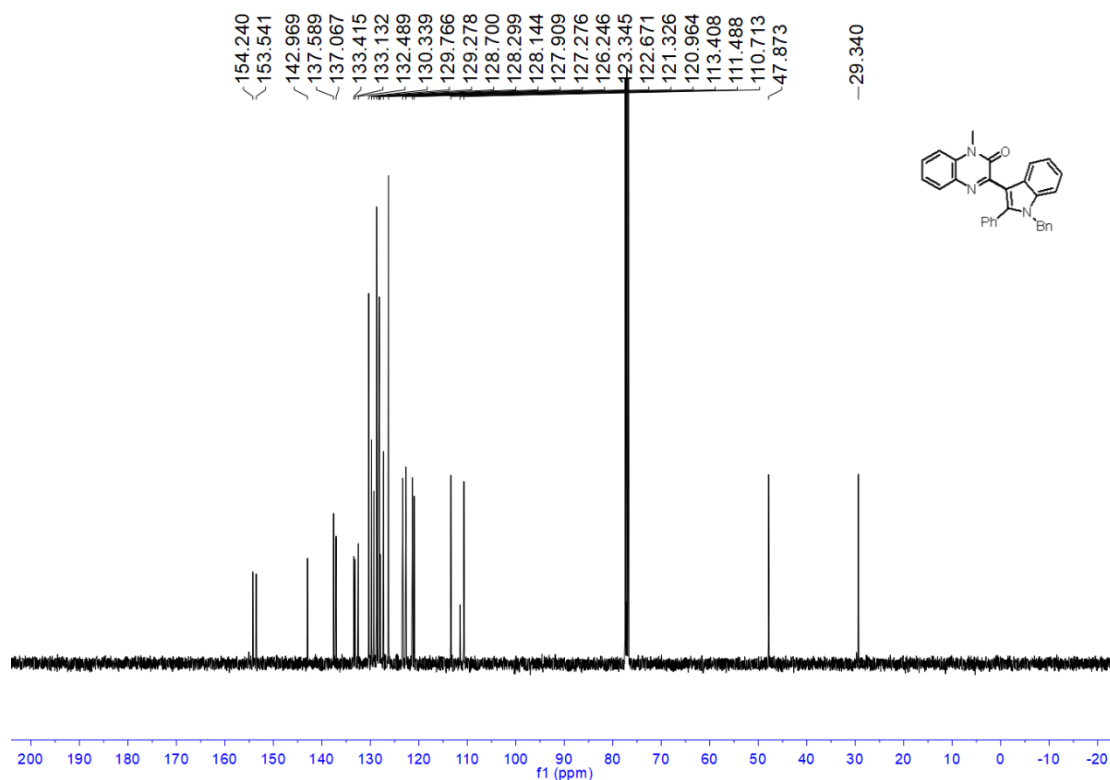
yl)quinoxalin-2(1H)-one (3ar). Orange solid, 60.3 mg, yield 82%. m.p.: 221.5-222.7 °C. ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.92 (d, *J* = 7.8 Hz, 1H), 7.79 (d, *J* = 7.8 Hz, 1H), 7.51-7.43(m, 3H), 7.43 – 7.35 (m, 4H), 7.30 (t, *J* = 7.5 Hz, 2H), 7.5 – 7.20 (m, 2H), 3.72 (s, 3H), 3.57 (s, 3H). ¹³C NMR (101 MHz, CDCl₃, TMS) δ 154.3, 153.6, 142.6, 137.6, 133.4, 133.1, 132.5, 130.5, 129.7, 129.2, 128.1, 128.2, 127.5, 123.3, 122.5, 121.1, 120.9, 113.4, 111.0, 109.7, 31.2, 29.3. HRMS (ESI, *m/z*) calcd for C₂₄H₂₀N₃O⁺ [M+H]⁺: 366.1601, found 366.1605.



3-(1-benzyl-2-phenyl-1H-indol-3-yl)-1-

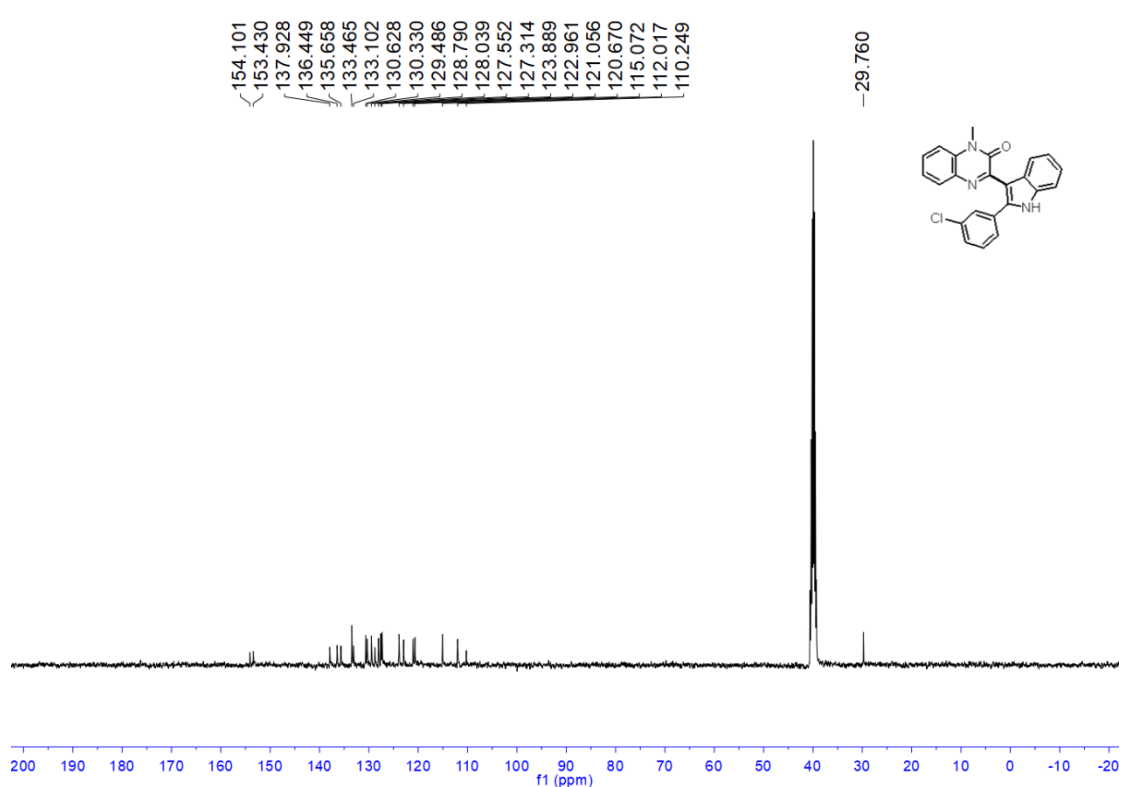
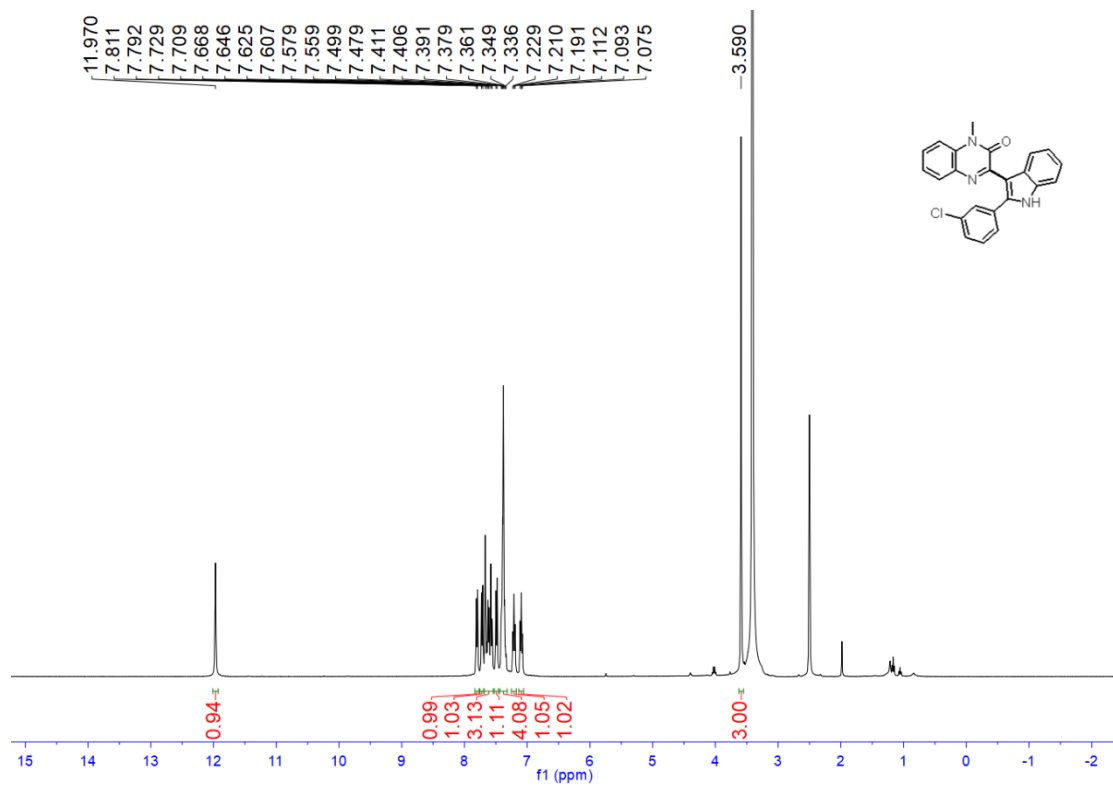
methylquinoxalin-2(1*H*)-one (3as). Yellow solid, 83.7 mg, yield 95%, m.p.: 244.2-245.1 °C. ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.97 (d, *J* = 7.4 Hz, 1H), 7.82 (d, *J* = 7.7 Hz, 1H), 7.47 (t, *J* = 7.5 Hz, 1H), 7.42 – 7.36 (m, 3H), 7.29 (d, *J* = 9.0 Hz, 4H), 7.27 – 7.16 (m, 9H), 7.04 (d, *J* = 6.8 Hz, 2H), 5.35 (s, 2H), 3.55 (s, 2H). ¹³C NMR (101 MHz, CDCl₃, TMS) δ 154.2, 153.5, 143.0, 137.6, 137.1, 133.4, 133.1, 132.5, 130.3, 129.8, 129.3, 128.7, 128.3, 128.1, 127.9, 127.3, 126.3, 123.3, 122.7, 121.3, 121.0, 113.4, 111.5, 110.7, 47.9, 29.3. HRMS (ESI, *m/z*) calcd for C₃₀H₂₄N₃O⁺ [M+H]⁺: 442.1914, found 442.1915.

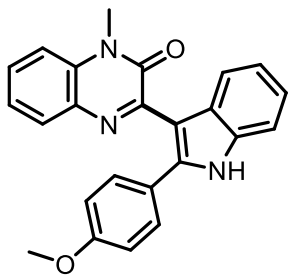




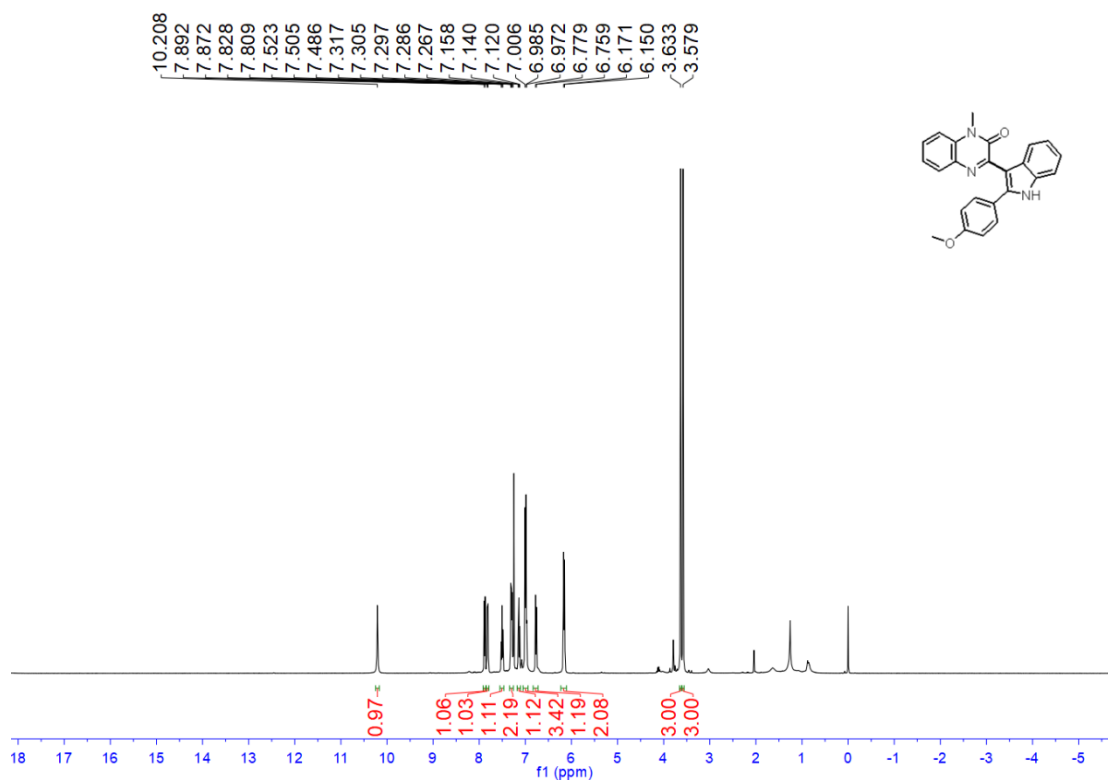
3-(2-(3-chlorophenyl)-1H-indol-3-yl)-1-

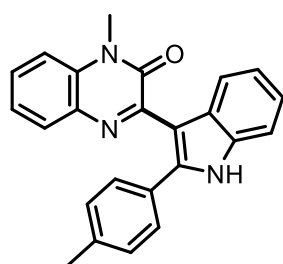
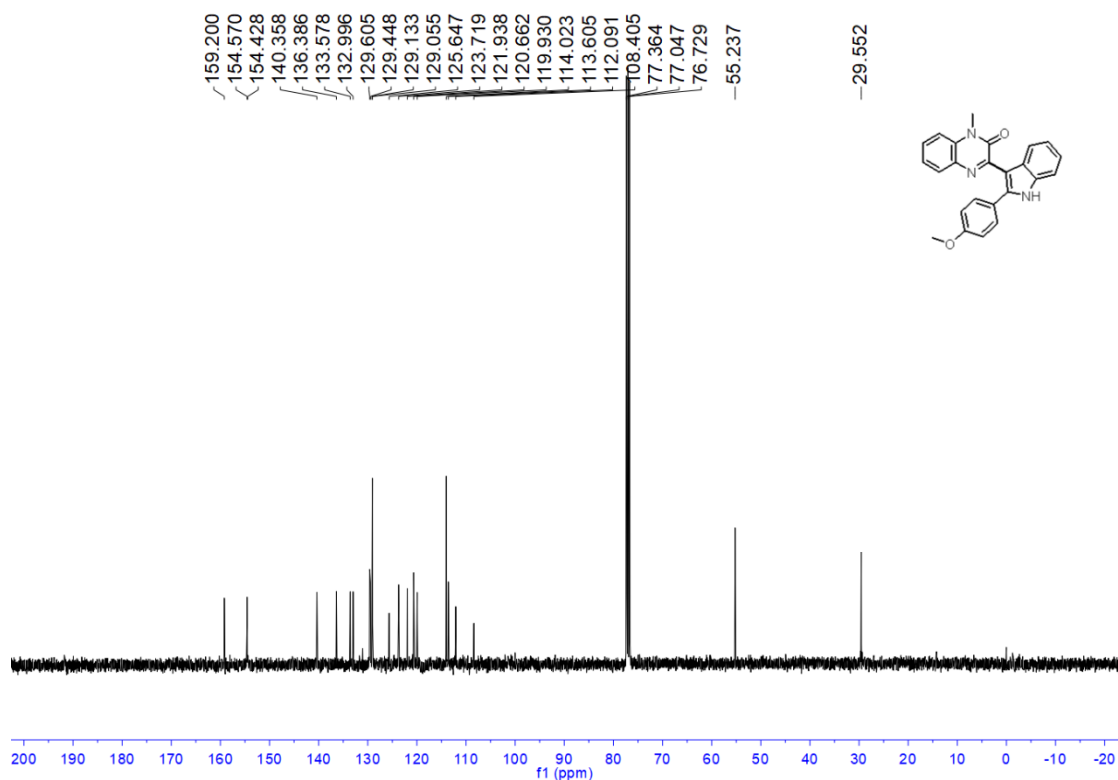
methylquinoxalin-2(1H)-one (3at). Yellow solid, 64.1 mg, yield 83%. m.p.: 270.0-271.9 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ 11.97 (s, 1H), 7.80 (d, *J* = 7.4 Hz, 1H), 7.72 (d, *J* = 8.0 Hz, 1H), 7.67 – 7.54 (m, 3H), 7.49 (d, *J* = 8.1 Hz, 1H), 7.44 – 7.32 (m, 4H), 7.21 (t, *J* = 7.5 Hz, 1H), 7.09 (t, *J* = 7.5 Hz, 1H), 3.59 (s, 3H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 154.1, 153.5, 138.0, 136.5, 135.7, 133.5, 133.1, 130.6, 130.3, 129.5, 128.8, 128.0, 127.6, 127.4, 123.9, 123.0, 121.1, 120.7, 115.1, 112.0, 110.3, 29.8. HRMS (ESI, *m/z*) calcd for C₂₃H₁₆ClN₃NaO⁺ [M+Na]⁺: 408.0874, found 408.0876.





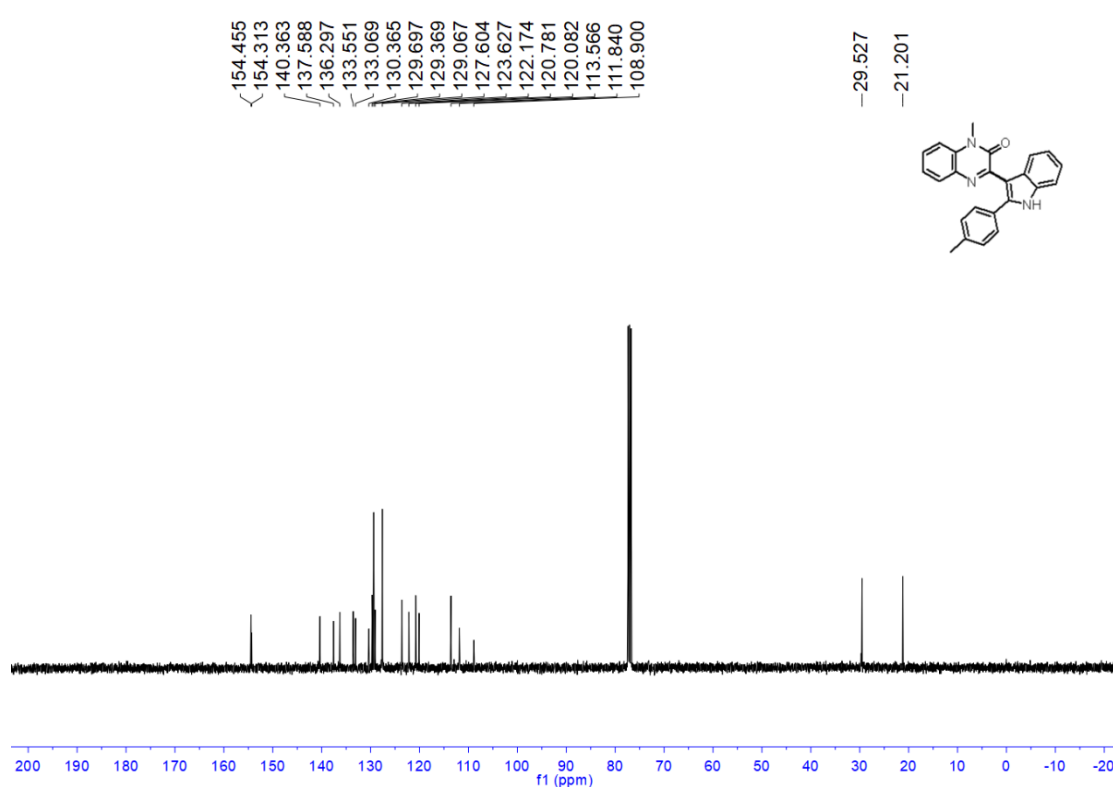
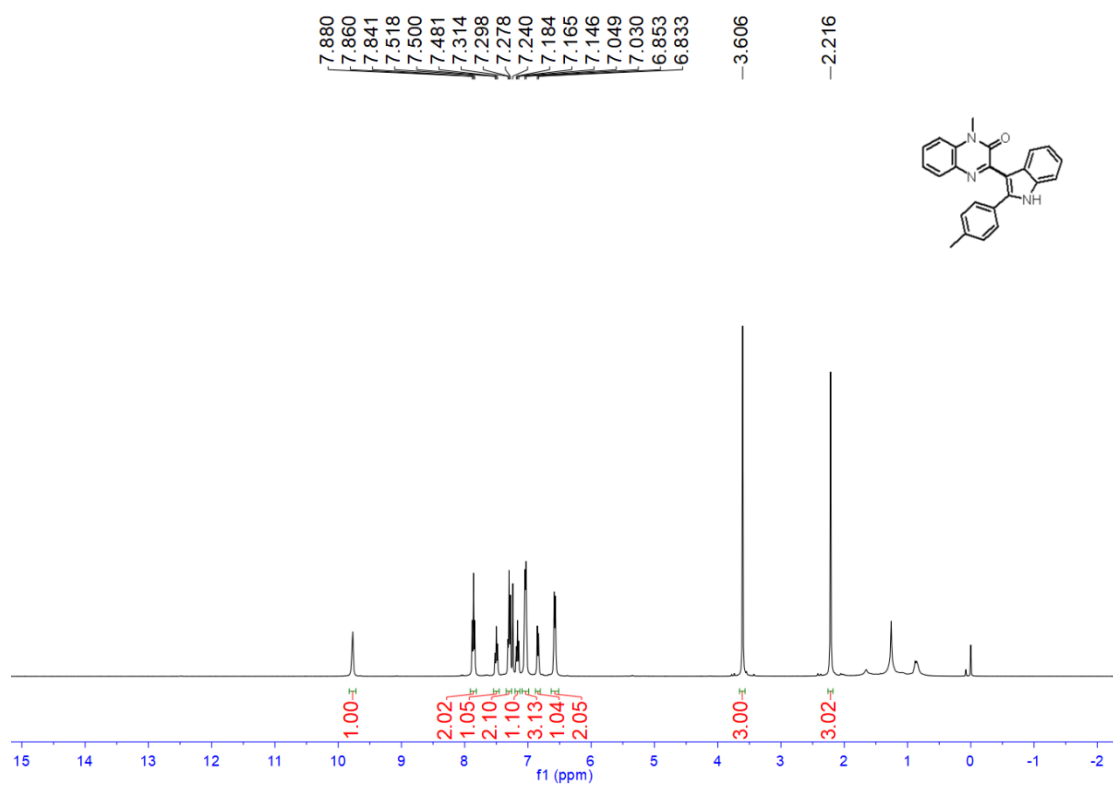
3-(2-(4-methoxyphenyl)-1H-indol-3-yl)-1-methylquinoxalin-2(1H)-one (3au). Yellow solid, 68.7 mg, yield 90%. m.p.: 218.4-218.7 °C. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 10.21 (s, 1H), 7.88 (d, $J = 8.0$ Hz, 1H), 7.82 (d, $J = 7.8$ Hz, 1H), 7.55 – 7.47 (m, 1H), 7.35 – 7.26 (m, 2H), 7.14 (dd, $J_1 = J_2 = 7.5$ Hz, 1H), 7.04 – 6.95 (m, 3H), 6.77 (d, $J = 8.1$ Hz, 1H), 6.16 (d, $J = 8.5$ Hz, 2H), 3.63 (s, 3H), 3.58 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3 , TMS) δ 159.2, 154.6, 154.4, 140.4, 136.4, 133.6, 133.0, 129.6, 129.5, 129.1, 129.1, 125.7, 123.7, 121.9, 120.7, 119.9, 114.0, 113.6, 112.1, 108.4, 55.2, 29.6. HRMS (ESI, m/z) calcd for $\text{C}_{24}\text{H}_{20}\text{N}_3\text{O}_2^+$ $[\text{M}+\text{H}]^+$: 382.1550, found 382.1552.

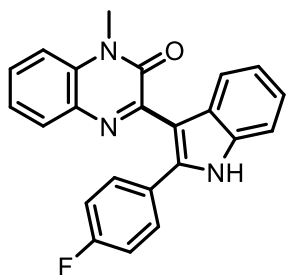




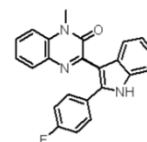
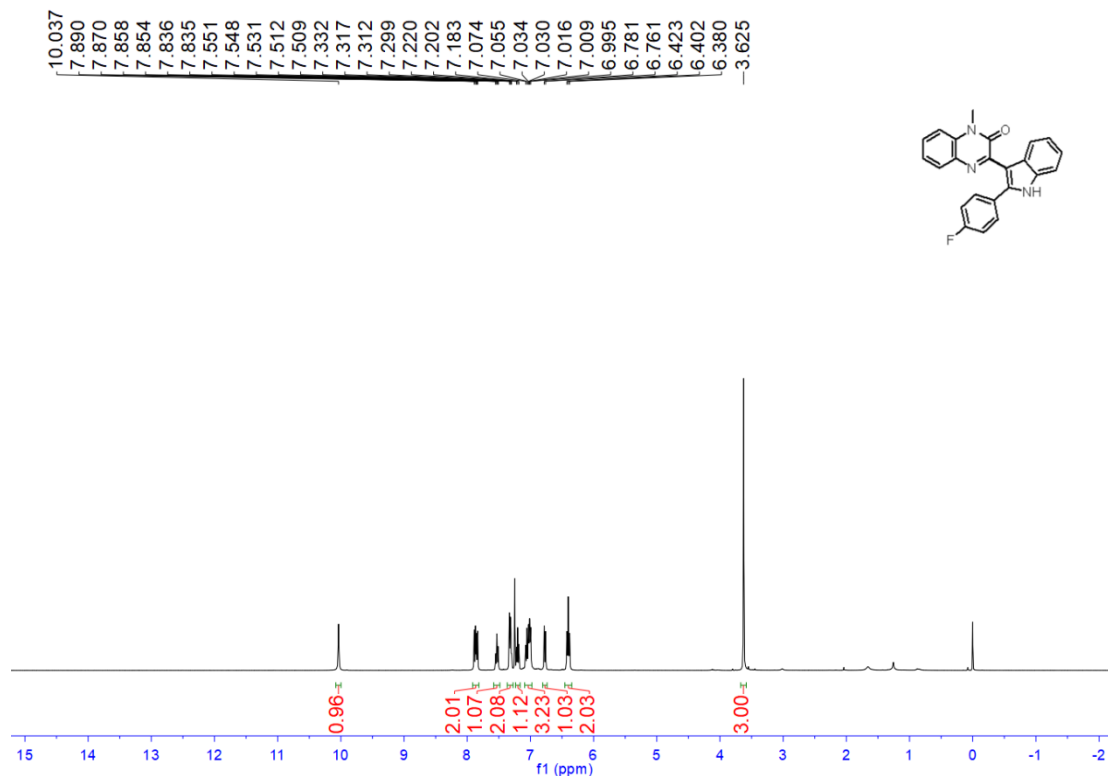
1-methyl-3-(2-(*p*-tolyl)-1*H*-indol-3-yl)quinoxalin-

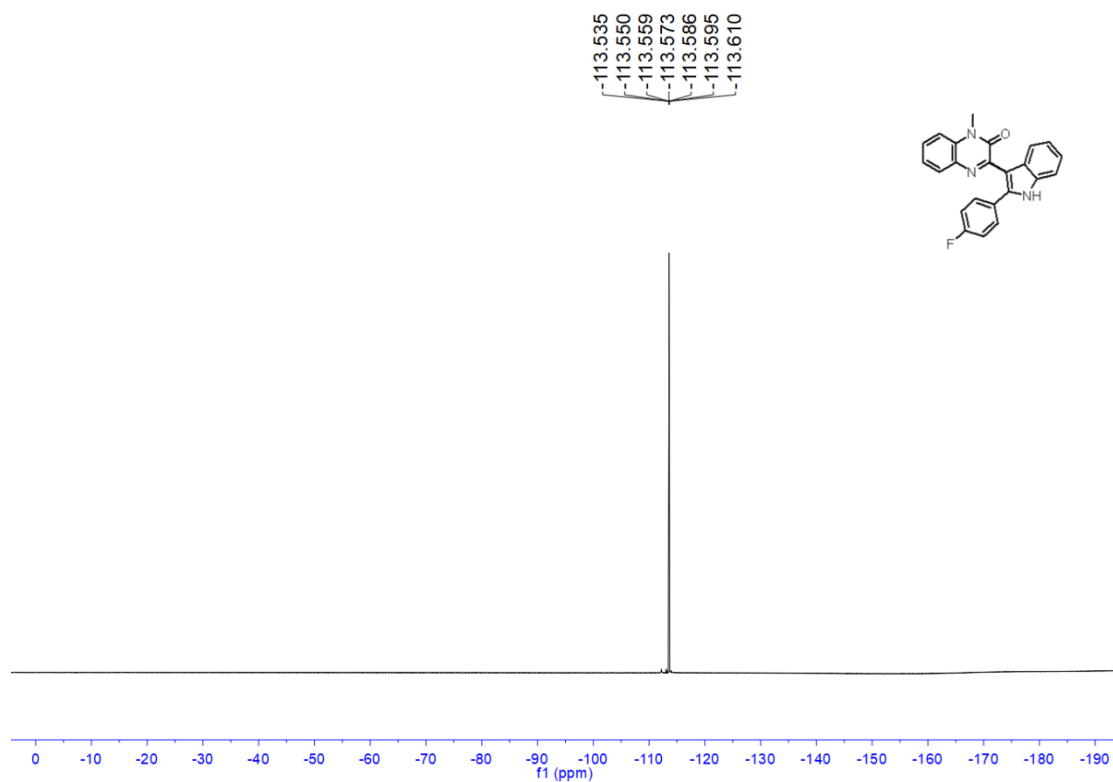
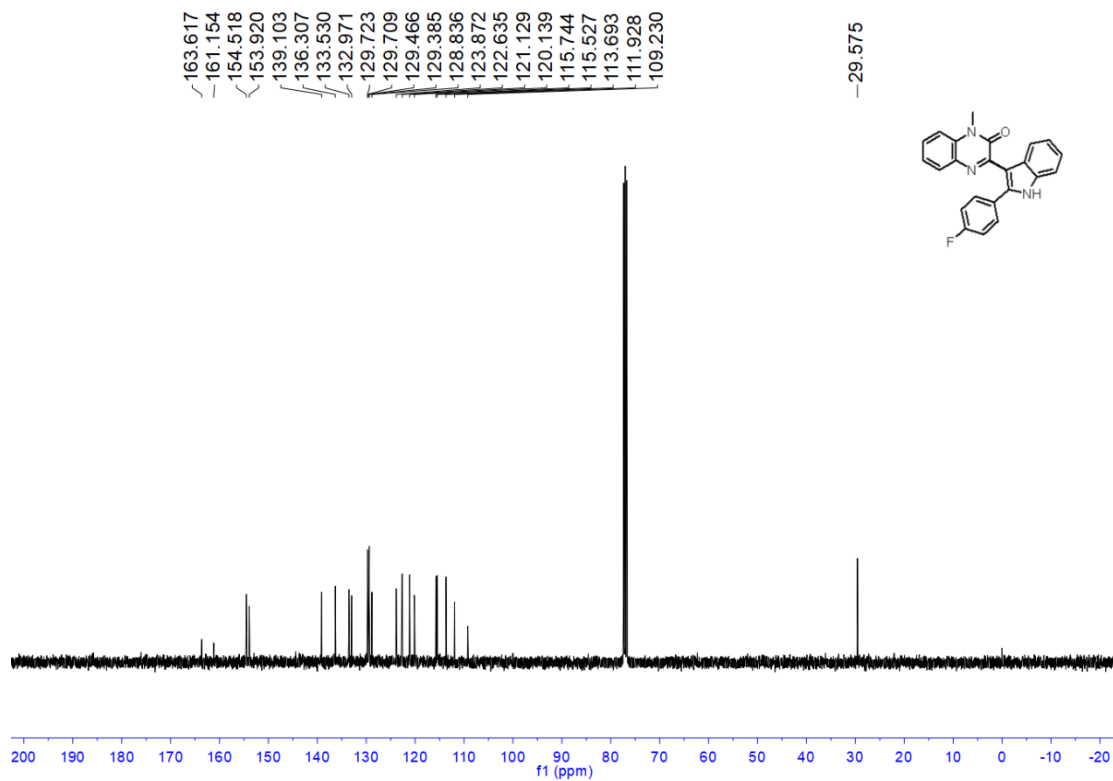
2(1*H*)-one (3av). Yellow solid, 65.1 mg, yield 89%. m.p.: 198.7-199.2 °C. ¹H NMR (400 MHz, CDCl₃, TMS) δ 9.78 (br, 1H), 7.86 (dd, $J_1 = J_2 = 7.8$ Hz, 2H), 7.50 (dd, $J_1 = J_2 = 7.5$ Hz, 1H), 7.34 – 7.26 (m, 2H), 7.17 (dd, $J_1 = J_2 = 7.5$ Hz, 1H), 7.0 – 6.99 (m, 3H), 6.84 (d, $J = 8.0$ Hz, 1H), 6.58 (d, $J = 7.7$ Hz, 2H), 3.61 (s, 3H), 2.22 (s, 3H). ¹³C NMR (101 MHz, CDCl₃, TMS) δ 154.5, 154.3, 140.4, 137.6, 136.3, 133.6, 133.1, 130.4, 129.7, 129.43, 129.37, 129.1, 127.6, 123.6, 122.2, 120.8, 120.1, 113.6, 111.8, 108.9, 29.5, 21.2. HRMS (ESI, m/z) calcd for C₂₄H₂₀N₃O⁺ [M+H]⁺: 366.1601, found 366.1604.

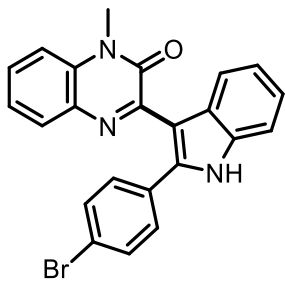




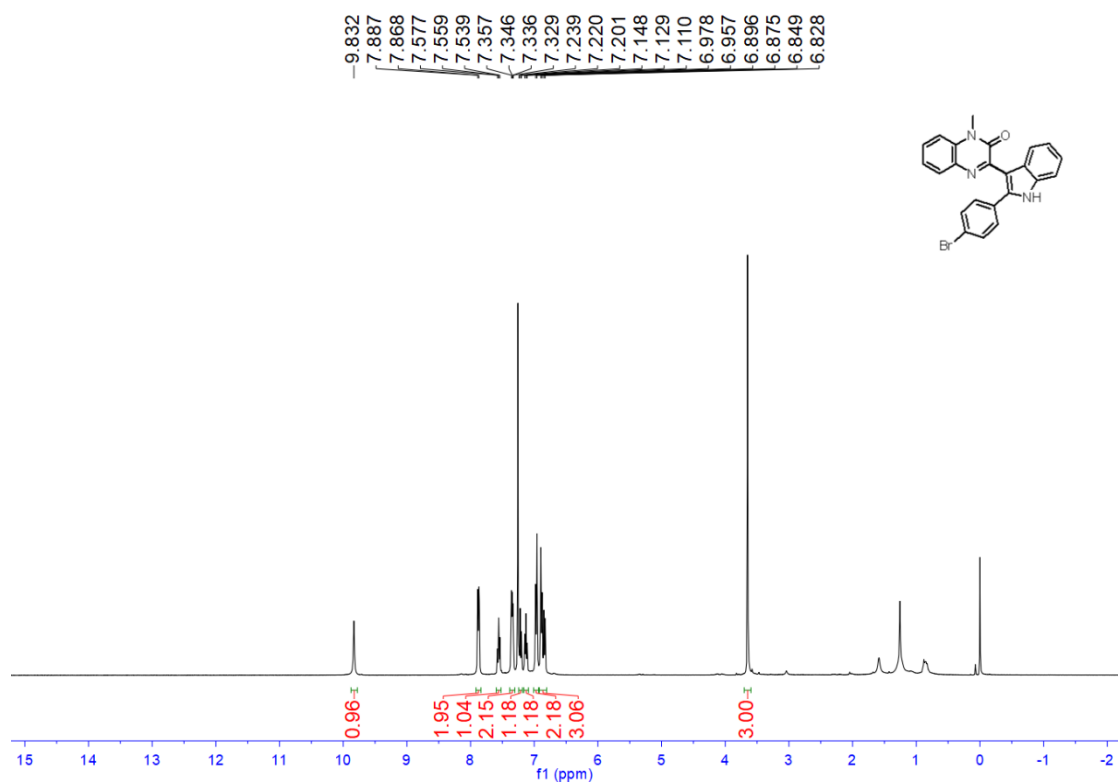
3-(2-(4-fluorophenyl)-1H-indol-3-yl)-1-methylquinoxalin-2(1H)-one (3aw). Yellow solid, 69.4 mg, yield 94%. m.p.: 218.8-220.4 °C. ^1H NMR (400 MHz, CDCl_3 , TMS) δ 10.04 (s, 1H), 7.92 – 7.81 (m, 2H), 7.58 – 7.48 (m, 1H), 7.36 – 7.28 (m, 2H), 7.20 (dd, $J_1 = J_2 = 7.5$ Hz, 1H), 7.10 – 6.97 (m, 3H), 6.77 (d, $J = 8.1$ Hz, 1H), 6.40 (dd, $J_1 = J_2 = 8.6$ Hz, 2H), 3.62 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3 , TMS) δ 162.4(d, $J = 247.8$ Hz), 154.5, 153.9, 139.1, 136.3, 133.5, 133.0, 129.72, 129.71, 129.43 (d, $J = 8.2$ Hz), 129.39 (br), 128.8, 123.9, 122.6, 121.1, 120.1, 115.6 (d, $J = 21.8$ Hz), 113.7, 111.9, 109.2, 29.6. ^{19}F NMR (376 MHz, CDCl_3 , TMS) δ -113.52 to -113.63 (m). HRMS (ESI, m/z) calcd for $\text{C}_{23}\text{H}_{17}\text{FN}_3\text{O}^+$ $[\text{M}+\text{H}]^+$: 370.1350, found 370.1353.

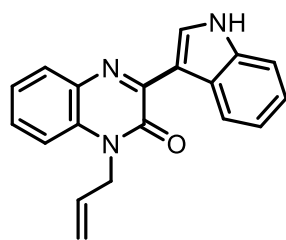
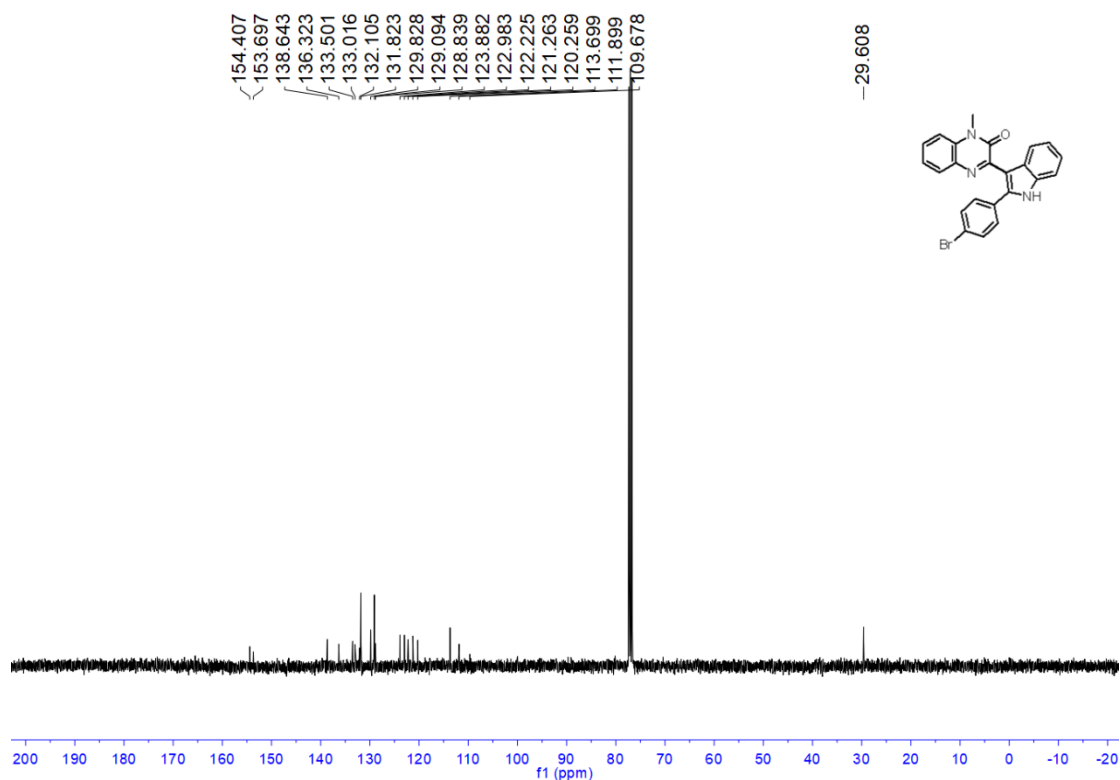




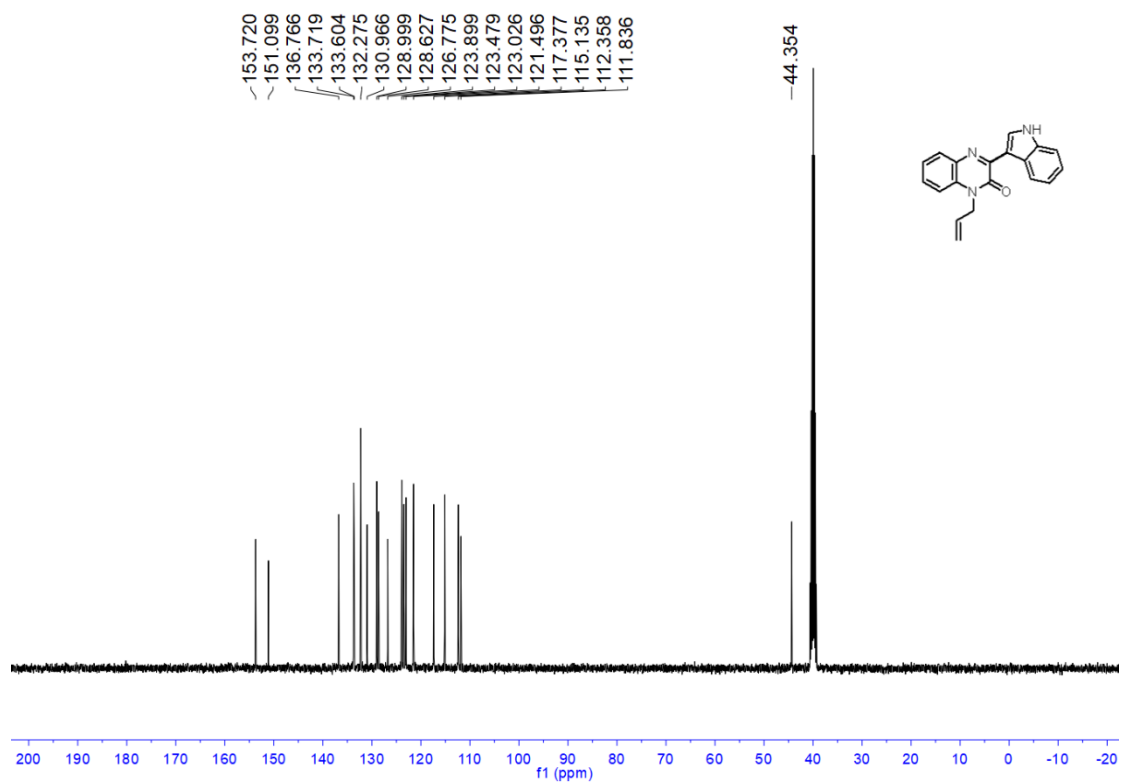
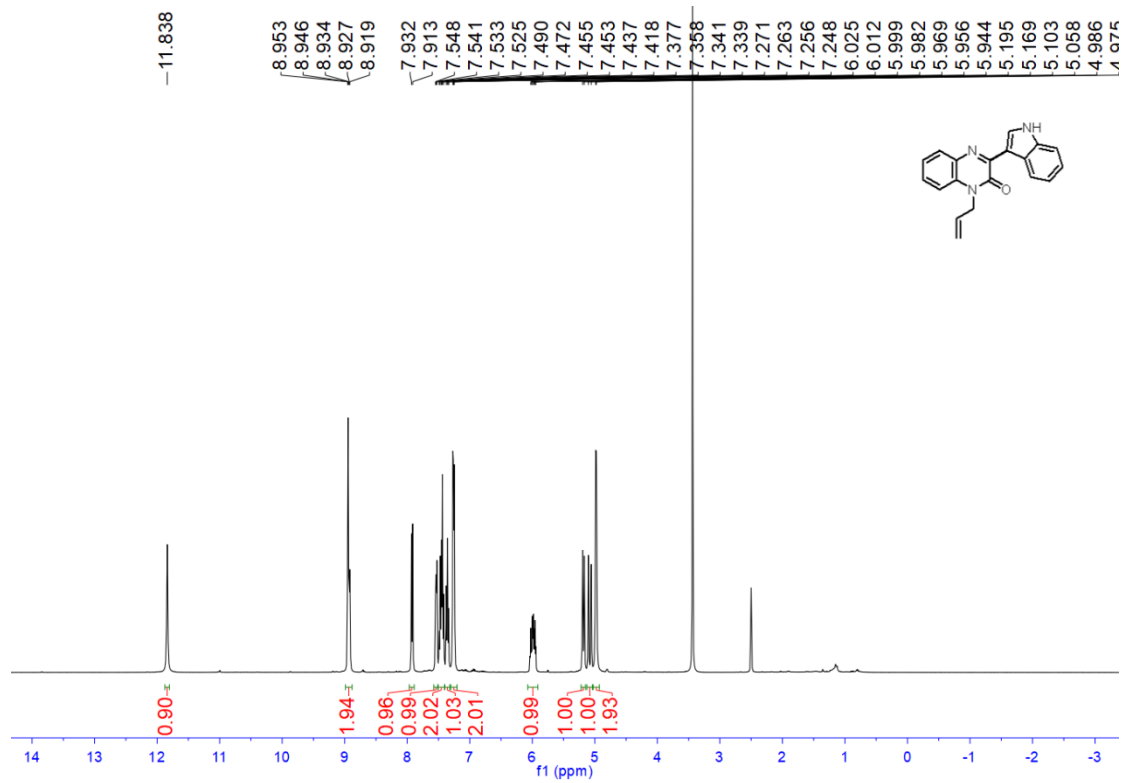


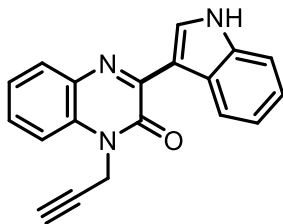
3-(2-(4-bromophenyl)-1H-indol-3-yl)-1-methylquinoxalin-2(1H)-one (3ax). Yellow solid, 82.7 mg, yield 96%, m.p.: 251.3-252.4 °C. ¹H NMR (400 MHz, CDCl₃, TMS) δ 9.83 (s, 1H), 7.88 (d, *J* = 7.4 Hz, 2H), 7.56 (t, *J* = 7.5 Hz, 1H), 7.39 – 7.31 (m, 2H), 7.22 (t, *J* = 7.6 Hz, 1H), 7.13 (dd, *J*₁ = *J*₂ = 7.5 Hz, 1H), 6.97 (d, *J* = 8.3 Hz, 2H), 6.89 (d, *J* = 8.2 Hz, 2H), 6.84 (d, *J* = 8.1 Hz, 1H), 3.65 (s, 3H). ¹³C NMR (101 MHz, CDCl₃, TMS) δ 154.4, 153.7, 138.6, 136.3, 133.5, 133.0, 132.1, 131.8, 129.83, 129.80, 129.1, 128.8, 123.9, 123.0, 122.2, 121.3, 120.3, 113.7, 111.9, 109.7, 29.6. HRMS (ESI, *m/z*) calcd for C₂₃H₁₆BrN₃NaO⁺ [M+Na]⁺: 452.0369, found 452.0373.





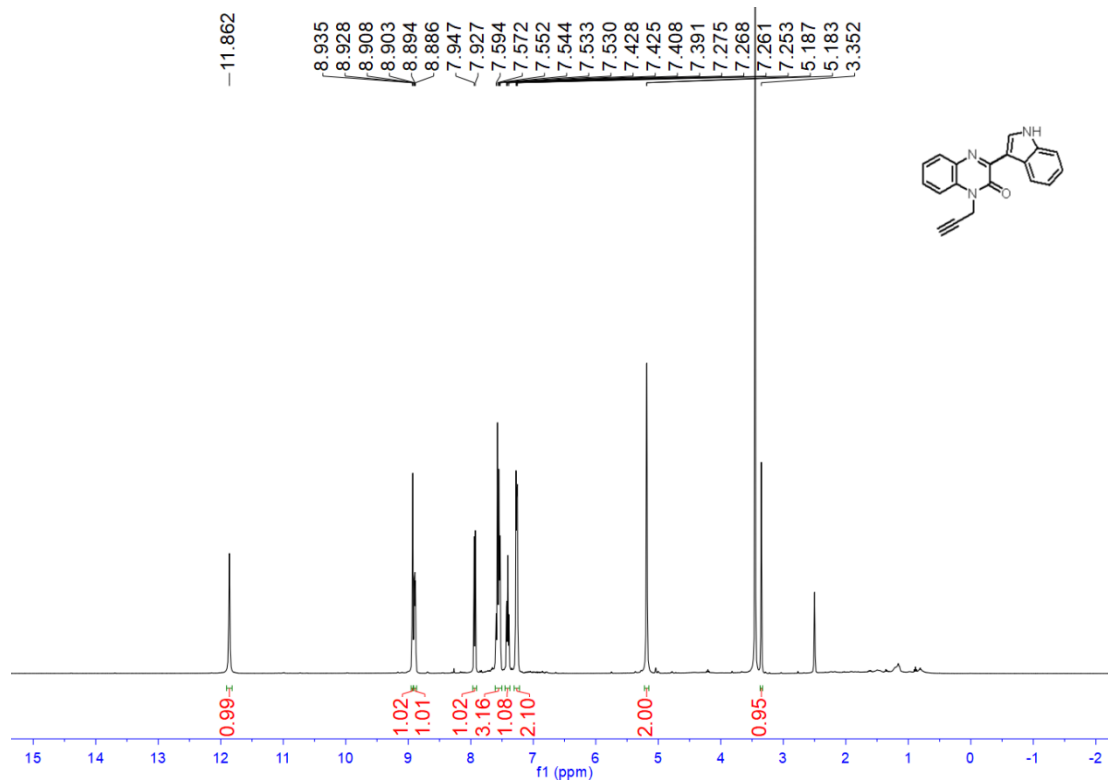
1-allyl-3-(1H-indol-3-yl)quinoxalin-2(1H)-one (3ba). A known compound.⁴ Yellow solid, 53.9 mg, yield 89%. ¹H NMR (400 MHz, DMSO-*d*₆) δ 11.84 (s, 1H), 9.00 – 8.89 (m, 2H), 7.92 (d, *J* = 7.6 Hz, 1H), 7.54 (dd, *J* = 5.9, 2.9 Hz, 1H), 7.51 – 7.40 (m, 2H), 7.39 – 7.33 (m, 1H), 7.26 (dd, *J* = 6.0, 3.2 Hz, 2H), 6.06 – 5.93 (m, 1H), 5.18 (d, *J* = 10.4 Hz, 1H), 5.08 (d, *J* = 17.9 Hz, 1H), 4.98 (d, *J* = 4.2 Hz, 2H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 153.7, 151.1, 136.8, 133.7, 133.6, 132.3, 131.0, 129.0, 128.6, 126.8, 123.9, 123.5, 123.0, 121.5, 117.4, 115.1, 112.4, 111.8, 44.4.

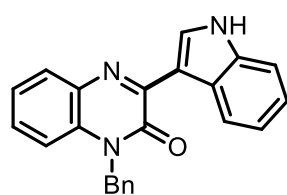
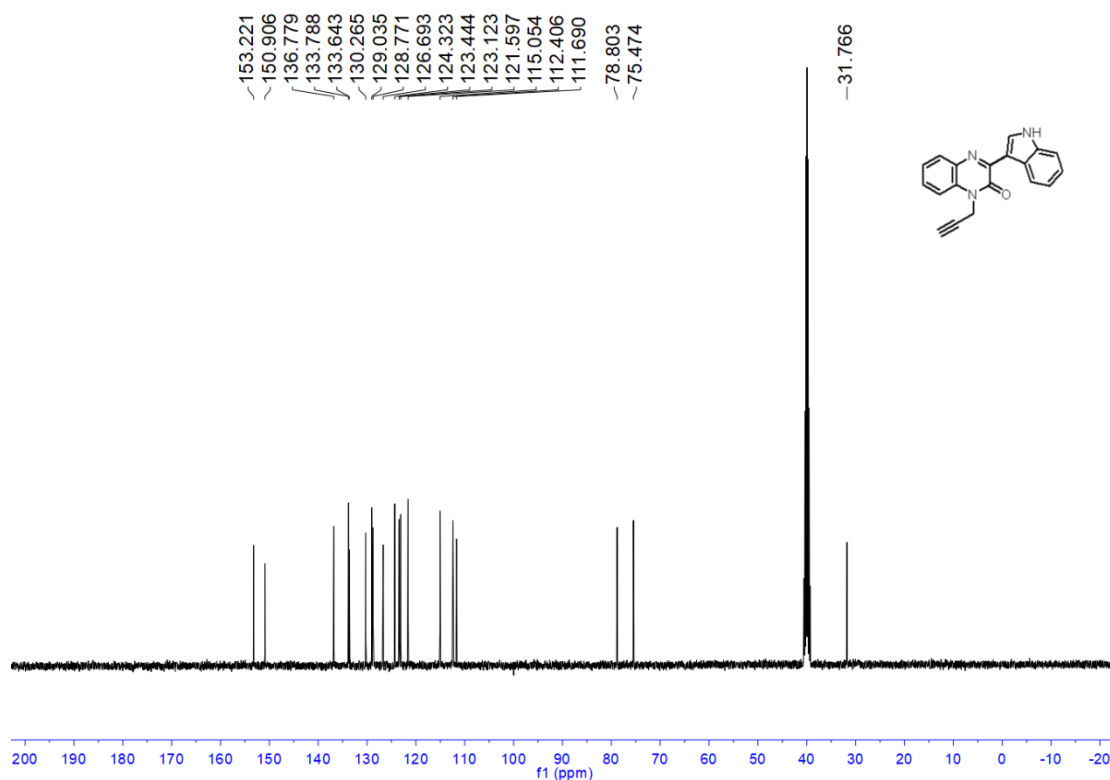




3-(1*H*-indol-3-yl)-1-(prop-2-yn-1-yl)quinoxalin-2(1*H*)-one

(3ca). Brown solid, 53.5 mg, yield 89%, m.p.: 228.1-228.7 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ 11.86 (s, 1H), 8.93 (d, *J* = 2.7 Hz, 1H), 8.92 – 8.86 (m, 1H), 7.94 (d, *J* = 7.8 Hz, 1H), 7.62 – 7.50 (m, 3H), 7.45 – 7.38 (m, 1H), 7.31 – 7.23 (m, 2H), 5.18 (d, *J* = 1.6 Hz, 2H), 3.35 (s, 1H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 153.2, 150.9, 136.8, 133.8, 133.6, 130.3, 129.0, 128.8, 126.7, 124.3, 123.4, 123.1, 121.6, 115.1, 112.4, 111.7, 78.8, 75.5, 31.8. HRMS (ESI, *m/z*) calcd for C₁₉H₁₄N₃O⁺ [M+H]⁺: 300.1131, found 300.1134.

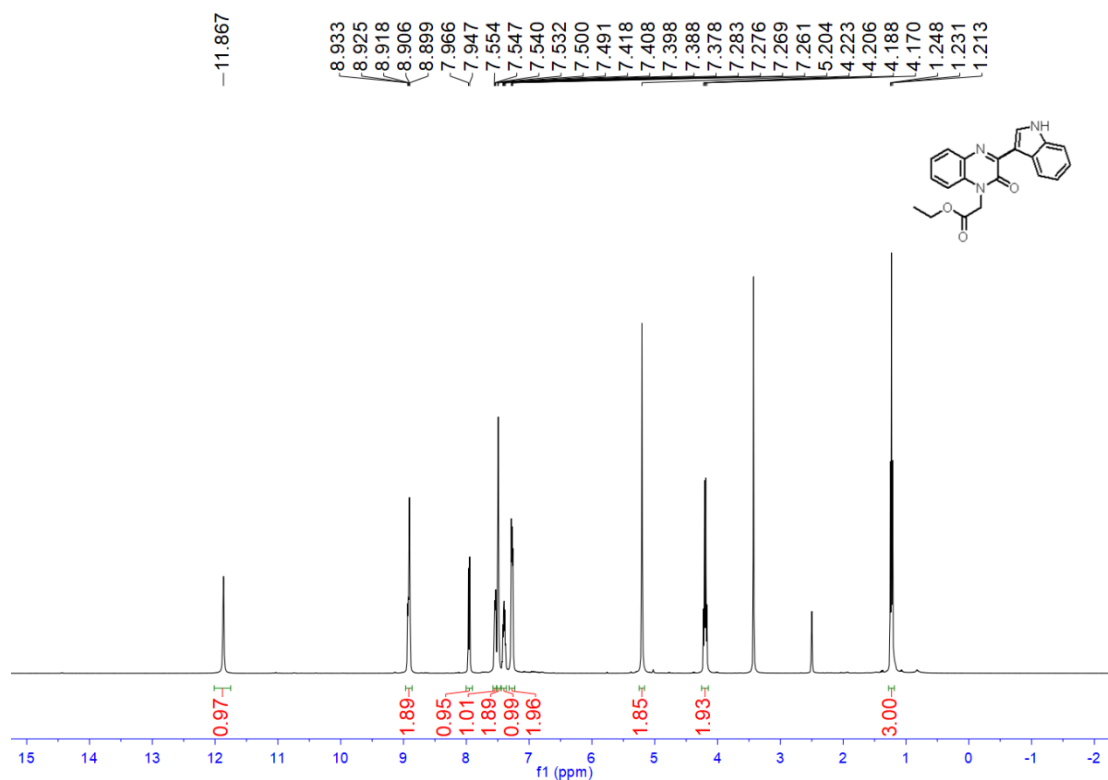


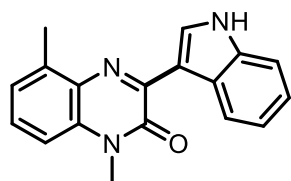
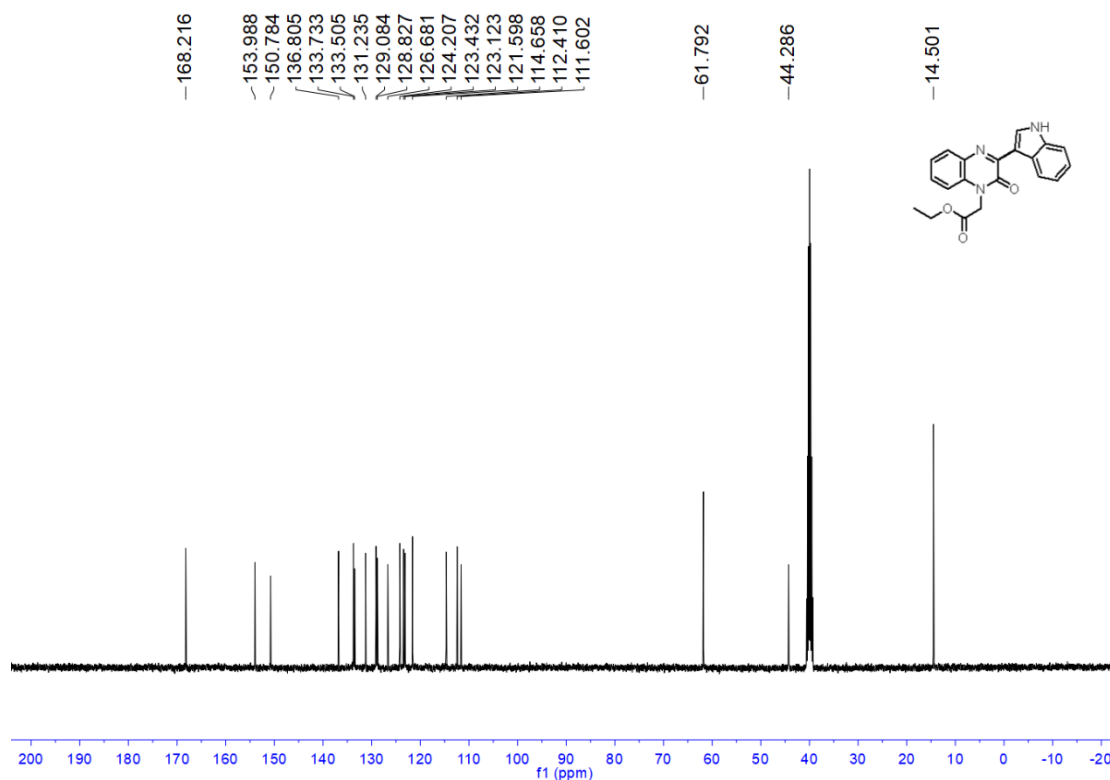


1-benzyl-3-(1H-indol-3-yl)quinoxalin-2(1H)-one (3da). A

known compound.⁴ Yellow solid, 69.4 mg, yield 99%. ¹H NMR (400 MHz, DMSO-*d*₆) δ 11.88 (s, 1H), 8.99 (d, *J* = 2.4 Hz, 1H), 8.98 – 8.93 (m, 1H), 7.94 (d, *J* = 7.7 Hz, 1H), 7.60 – 7.51 (m, 1H), 7.40 (d, *J* = 3.7 Hz, 2H), 7.37 – 7.19 (m, 8H), 5.61 (s, 2H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 154.3, 151.2, 136.8, 136.6, 133.9, 133.8, 131.1, 129.2, 129.1, 128.7, 127.7, 127.2, 126.8, 124.0, 123.5, 123.1, 121.6, 115.2, 112.4, 111.9, 45.4.

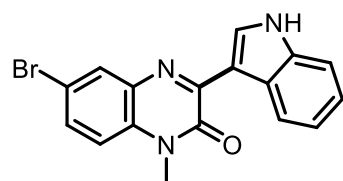
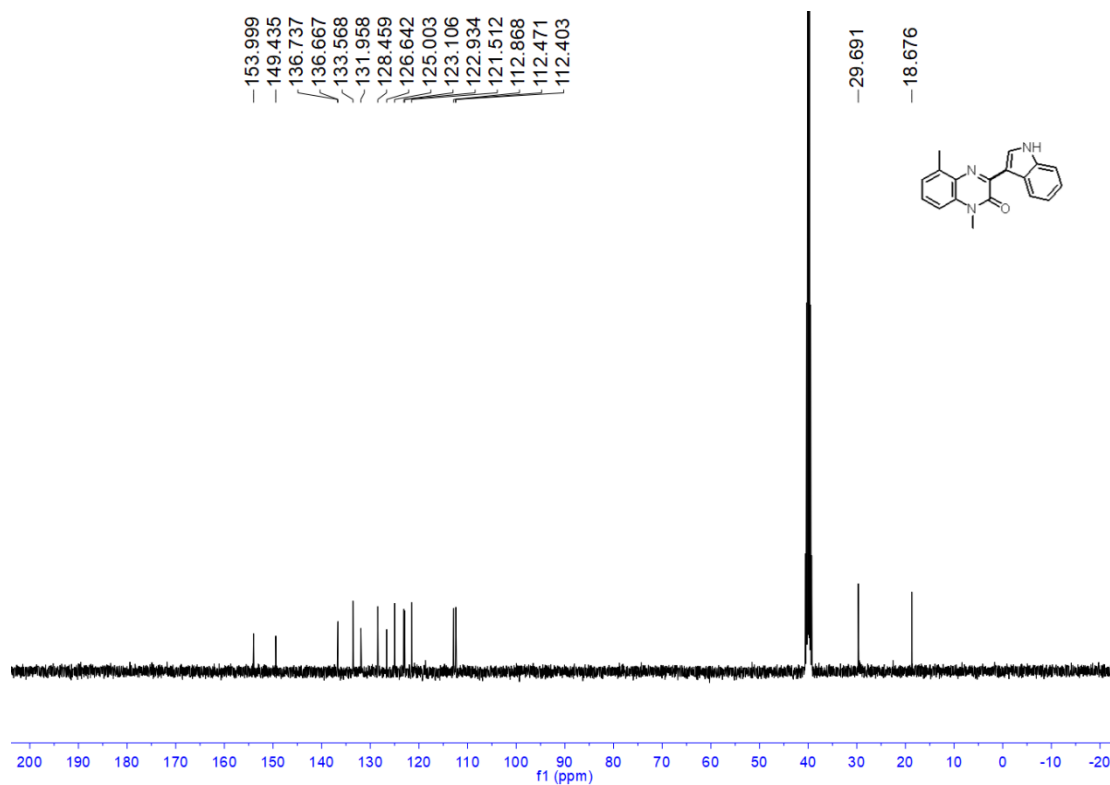
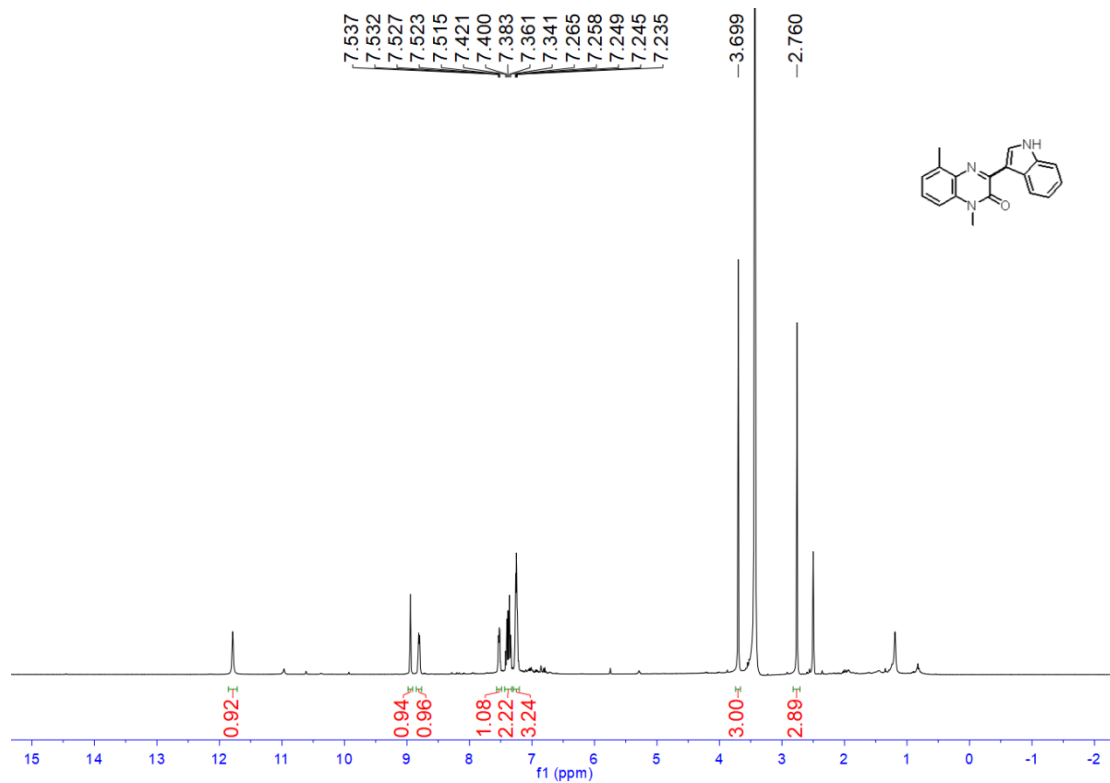
y)acetate (3ea). Orange solid, 64.4 mg, yield 93%. m.p.: 214.1-215.6 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ 11.87 (s, 1H), 9.00 – 8.86 (m, 2H), 7.96 (d, *J* = 7.9 Hz, 1H), 7.54 (dd, *J* = 5.9, 3.0 Hz, 1H), 7.50 (d, *J* = 3.7 Hz, 2H), 7.40 (dt, *J* = 8.1, 4.1 Hz, 1H), 7.27 (dd, *J* = 6.0, 3.1 Hz, 2H), 5.20 (s, 2H), 4.20 (q, *J* = 7.1 Hz, 2H), 1.23 (t, *J* = 7.1 Hz, 3H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 168.2, 154.0, 150.8, 136.8, 133.7, 133.5, 131.2, 129.1, 128.8, 126.7, 124.2, 123.4, 123.1, 121.6, 114.7, 112.4, 111.6, 61.8, 44.3, 14.5. HRMS (ESI, *m/z*) calcd for C₂₀H₁₇N₃NaO₃⁺ [M+Na]⁺: 370.1162, found 370.1163.





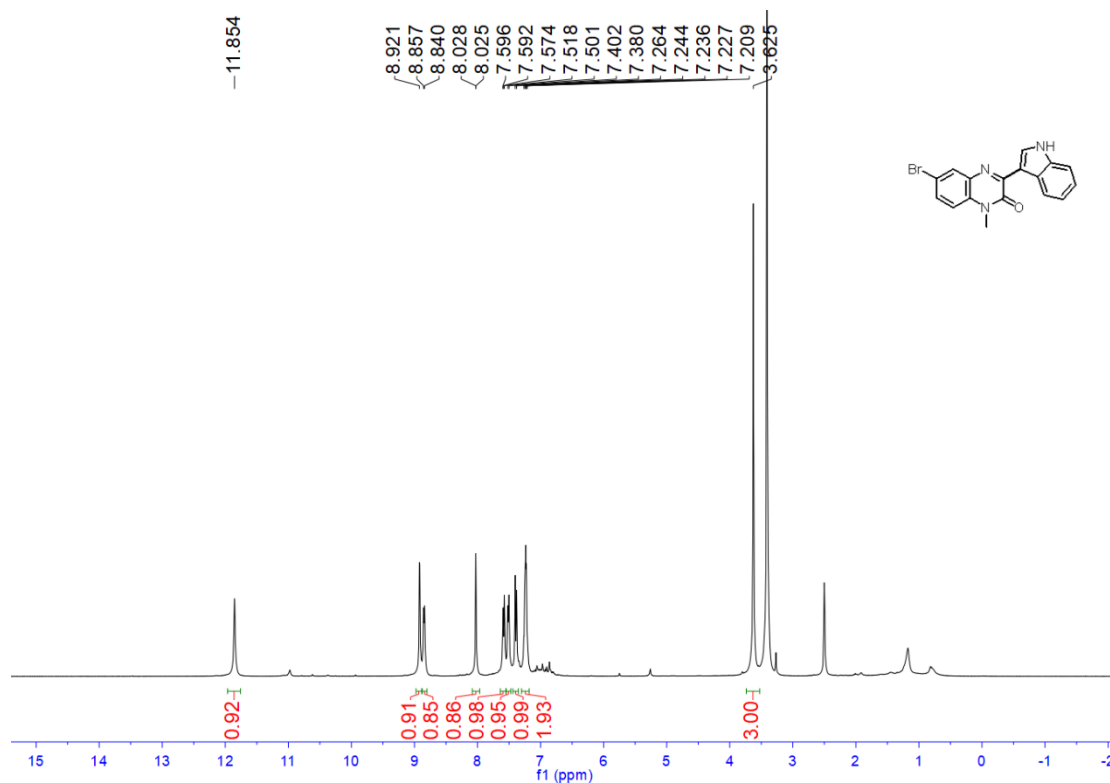
3-(1H-indol-3-yl)-1,6-dimethylquinoxalin-2(1H)-one (3fa).

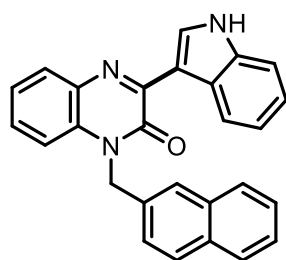
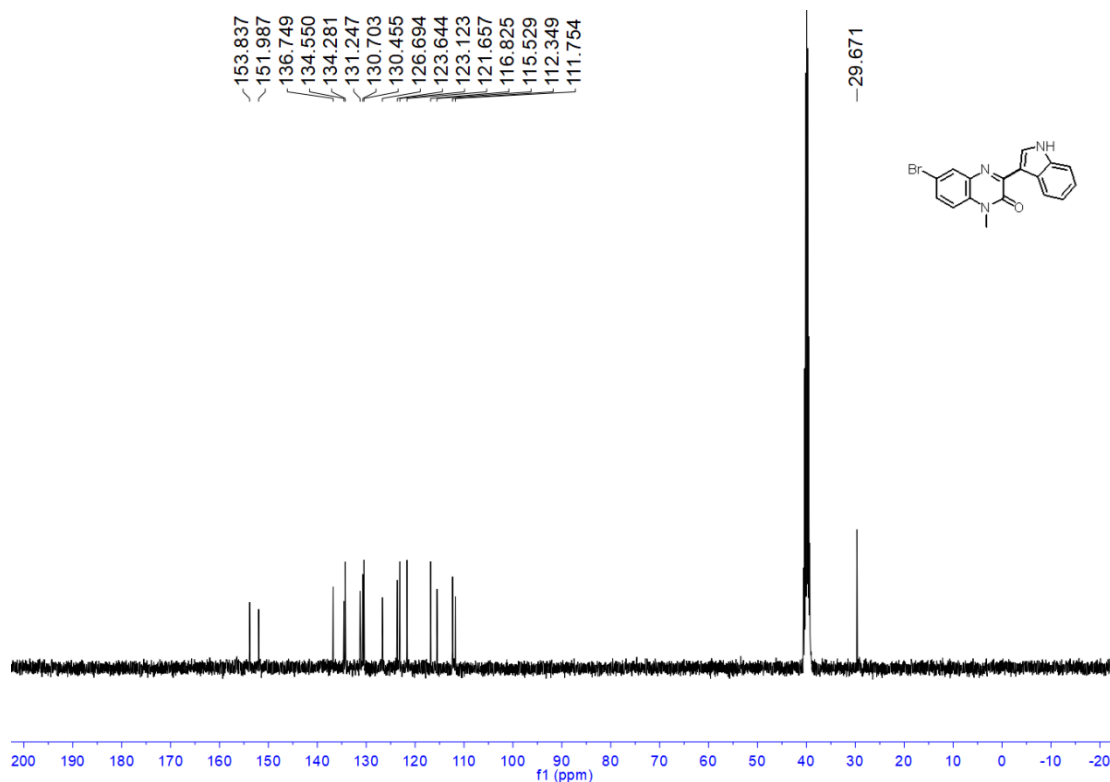
Orange solid, 54.7 mg, yield 94%, m.p.: 284.5-285.7 °C. ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 11.91 – 11.69 (m, 1H), 8.95 (d, $J = 2.7$ Hz, 1H), 8.86 – 8.77 (m, 1H), 7.56 – 7.49 (m, 1H), 7.44 – 7.32 (m, 2H), 7.29 – 7.21 (m, 3H), 3.70 (s, 3H), 2.76 (s, 3H). ^{13}C NMR (101 MHz, $\text{DMSO-}d_6$) δ 154.0, 149.4, 136.74, 136.67, 133.6, 132.0, 128.5, 126.6, 125.0, 123.1, 122.9, 121.5, 112.9, 112.5, 112.4, 29.7, 18.7. HRMS (ESI, m/z) calcd for $\text{C}_{18}\text{H}_{16}\text{N}_3\text{O}^+$ $[\text{M}+\text{H}]^+$: 290.1288, found 290.1289.



6-bromo-3-(1H-indol-3-yl)-1-methylquinoxalin-2(1H)-one (3ga). Orange solid, 68.4 mg, yield 97%. m.p.: 289.2-290.1 °C. ¹H NMR (400 MHz,

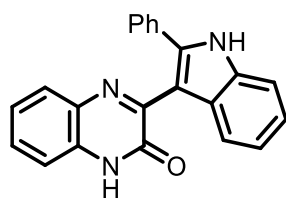
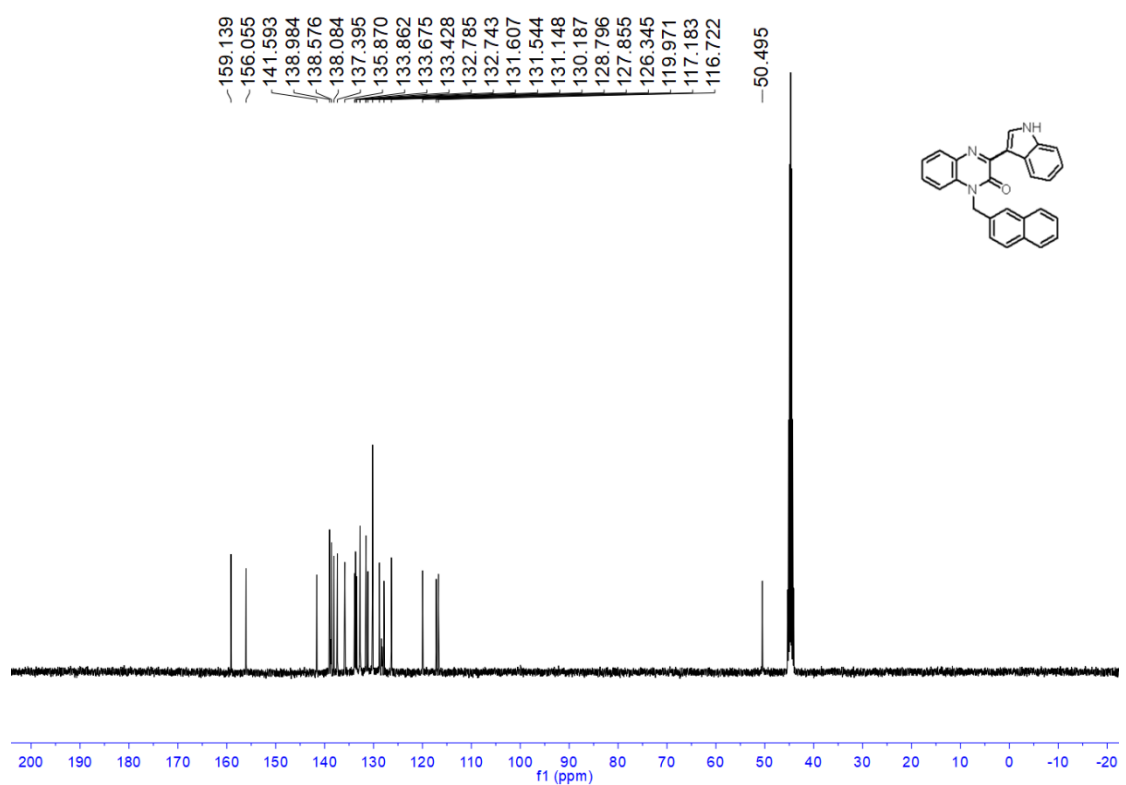
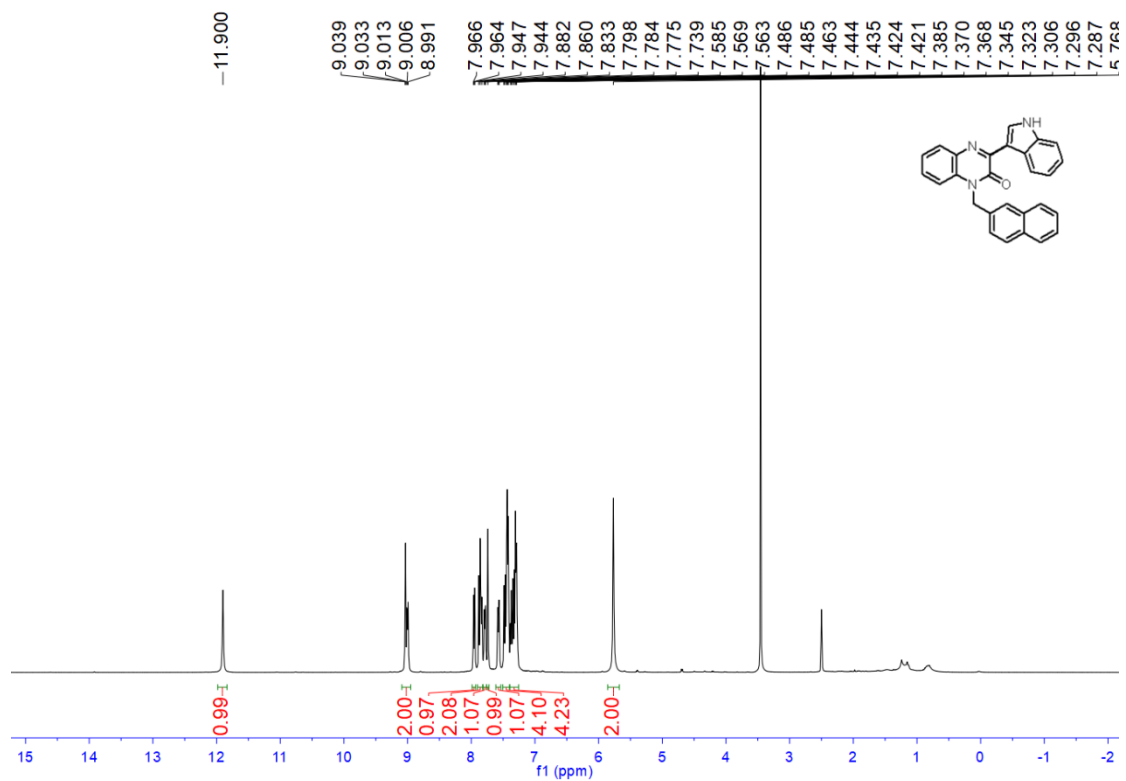
DMSO-*d*₆) δ 11.85 (s, 1H), 8.92 (d, *J* = 2.4 Hz, 1H), 8.85 (d, *J* = 6.7 Hz, 1H), 8.11 – 7.96 (m, 1H), 7.65 – 7.55 (m, 1H), 7.51 (d, *J* = 6.7 Hz, 1H), 7.39 (d, *J* = 8.9 Hz, 1H), 7.29 – 7.17 (m, 2H), 3.63 (s, 3H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 153.8, 152.0, 136.8, 134.6, 134.3, 131.3, 130.7, 130.5, 126.7, 123.6, 123.1, 121.7, 116.8, 115.5, 112.4, 111.8, 29.7. HRMS (ESI, *m/z*) calcd for C₁₇H₁₂BrN₃NaO⁺ [M+Na]⁺: 376.0056, found 376.0060.





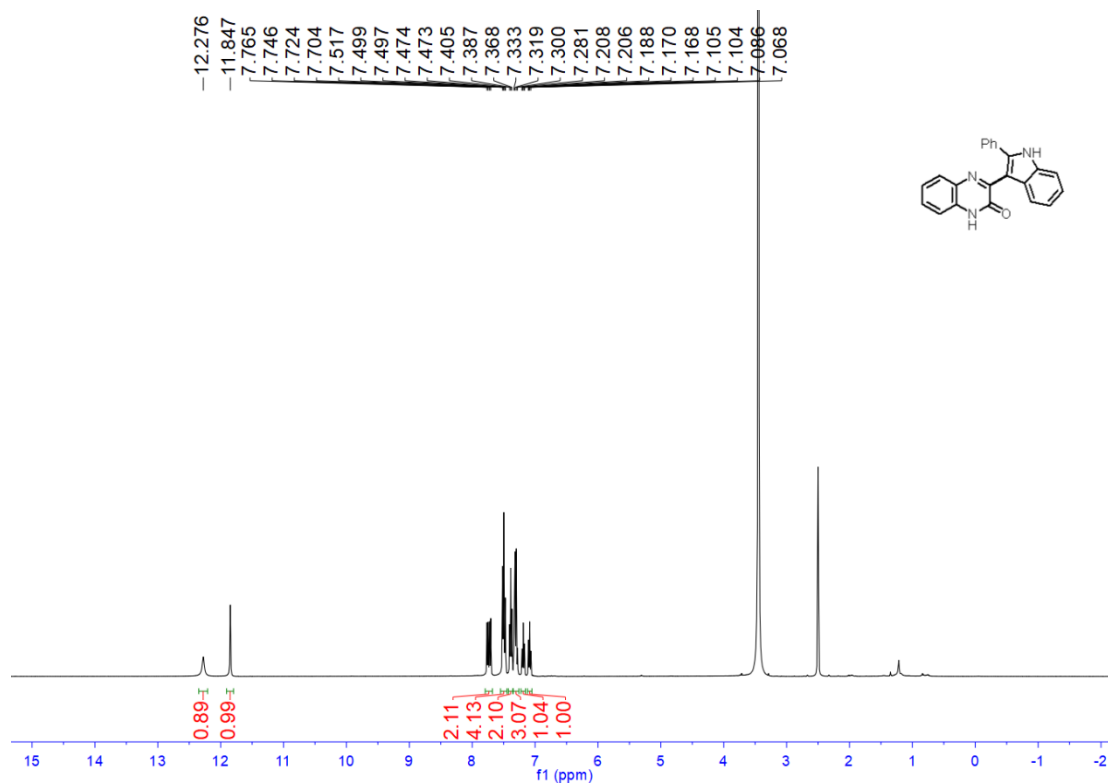
3-(1H-indol-3-yl)-1-(naphthalen-2-ylmethyl)quinoxalin-

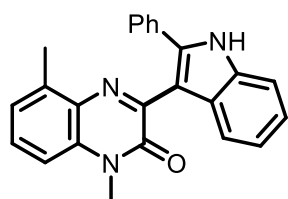
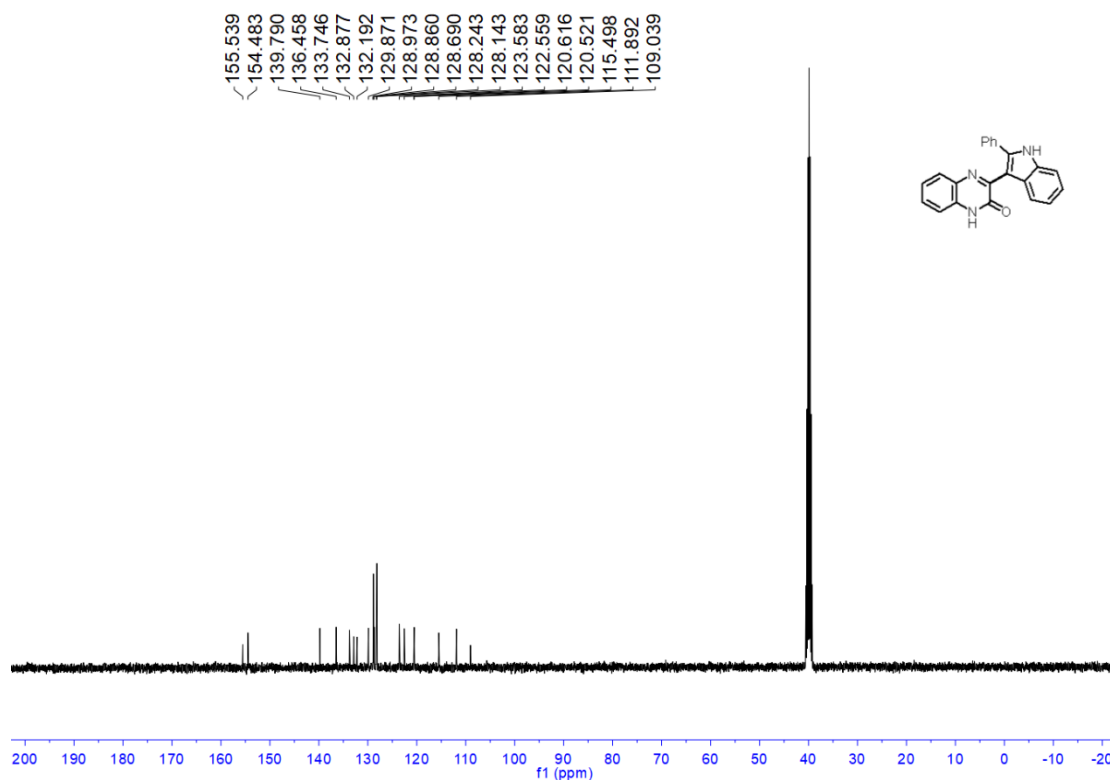
2(1H)-one (3ha). Yellow solid, 73.8 mg, yield 92%. m.p.: 191.3-192.7 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ 11.90 (s, 1H), 9.04 (d, *J* = 2.4 Hz, 1H), 9.02 – 8.97 (m, 1H), 7.96 (*J* = 7.6, 1.2 Hz, 1H), 7.90 – 7.82 (m, 2H), 7.81 – 7.76 (m, 1H), 7.74 (s, 1H), 7.61 – 7.54 (m, 1H), 7.50 – 7.40 (m, 4H), 7.40 – 7.25 (m, 4H), 5.77 (s, 2H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 159.1, 156.1, 141.6, 139.0, 138.8, 138.6, 138.1, 137.4, 135.9, 133.9, 133.7, 133.4, 132.8, 132.7, 131.6, 131.5, 131.2, 130.2, 128.8, 128.4, 128.2, 127.9, 126.3, 120.0, 117.2, 116.7, 50.5. HRMS (ESI, *m/z*) calcd for C₂₇H₂₀N₃O⁺ [M+H]⁺: 402.1601, found 402.1603.



3-(2-phenyl-1H-indol-3-yl)quinoxalin-2(1H)-one

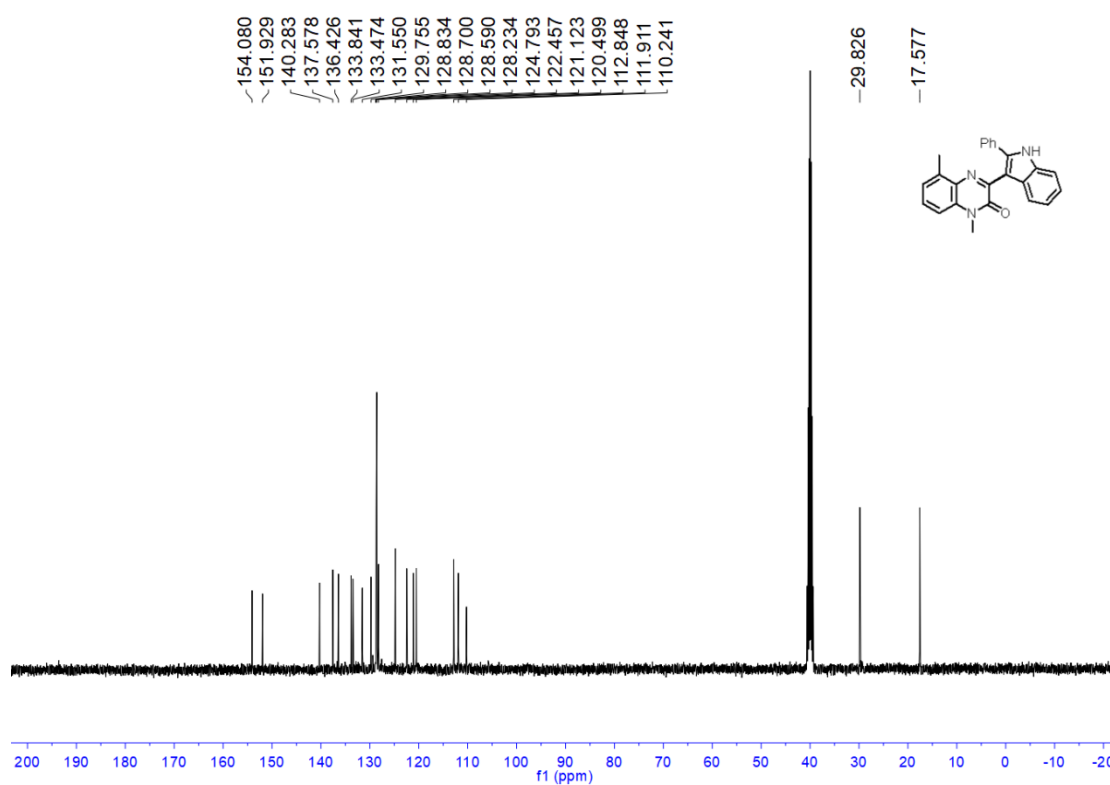
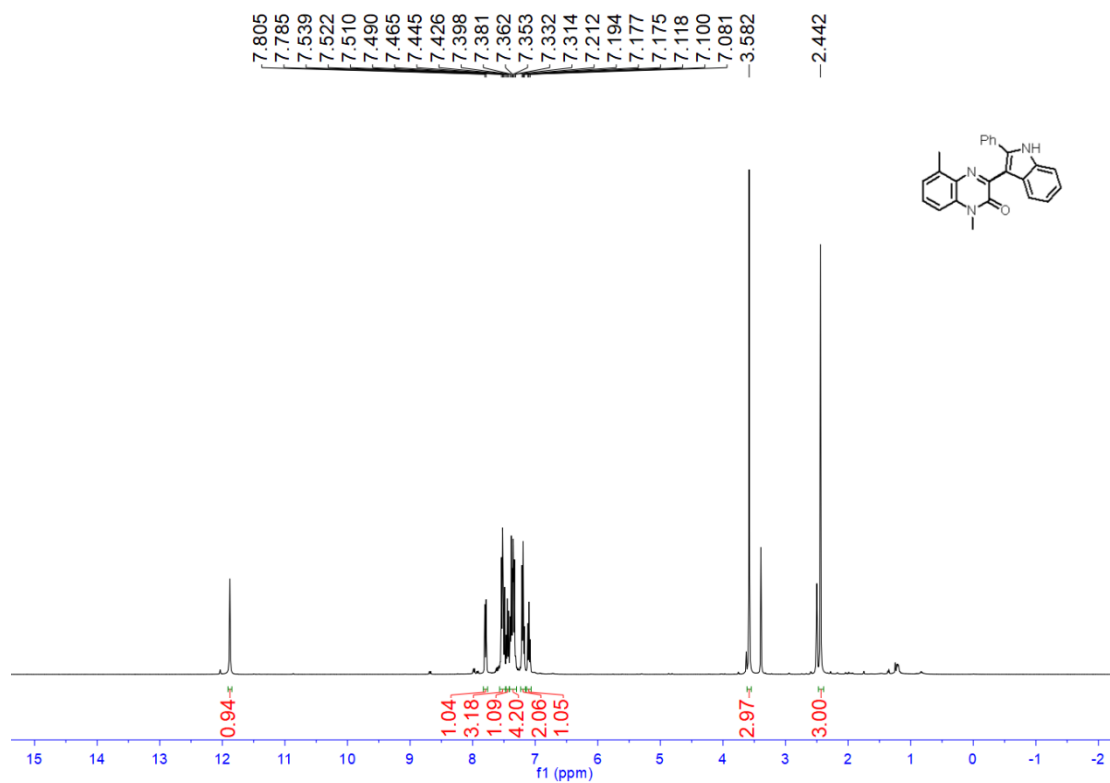
(3ia). Yellow solid, 46.3 mg, yield 69%. m.p.: 167.2-168.9 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ 12.28 (br, 1H), 11.85 (s, 1H), 7.79 – 6.69 (m, 2H), 7.57 – 7.44 (m, 4H), 7.43 – 7.35 (m, 2H), 7.35 – 7.25 (m, 3H), 7.23 – 7.15 (m, 1H), 7.13 – 7.05 (m, 1H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 155.5, 154.5, 139.8, 136.5, 133.8, 132.9, 132.2, 129.9, 129.0, 128.9, 128.7, 128.2, 128.1, 123.6, 122.6, 120.6, 120.5, 115.5, 111.9, 109.0. HRMS (ESI, *m/z*) calcd for C₂₂H₁₅N₃NaO⁺ [M+Na]⁺: 360.1107, found 360.1108.

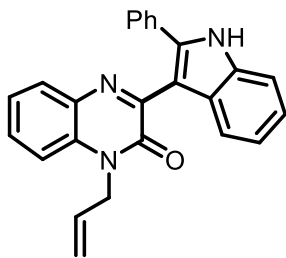




1,6-dimethyl-3-(2-phenyl-1*H*-indol-3-yl)quinoxalin-

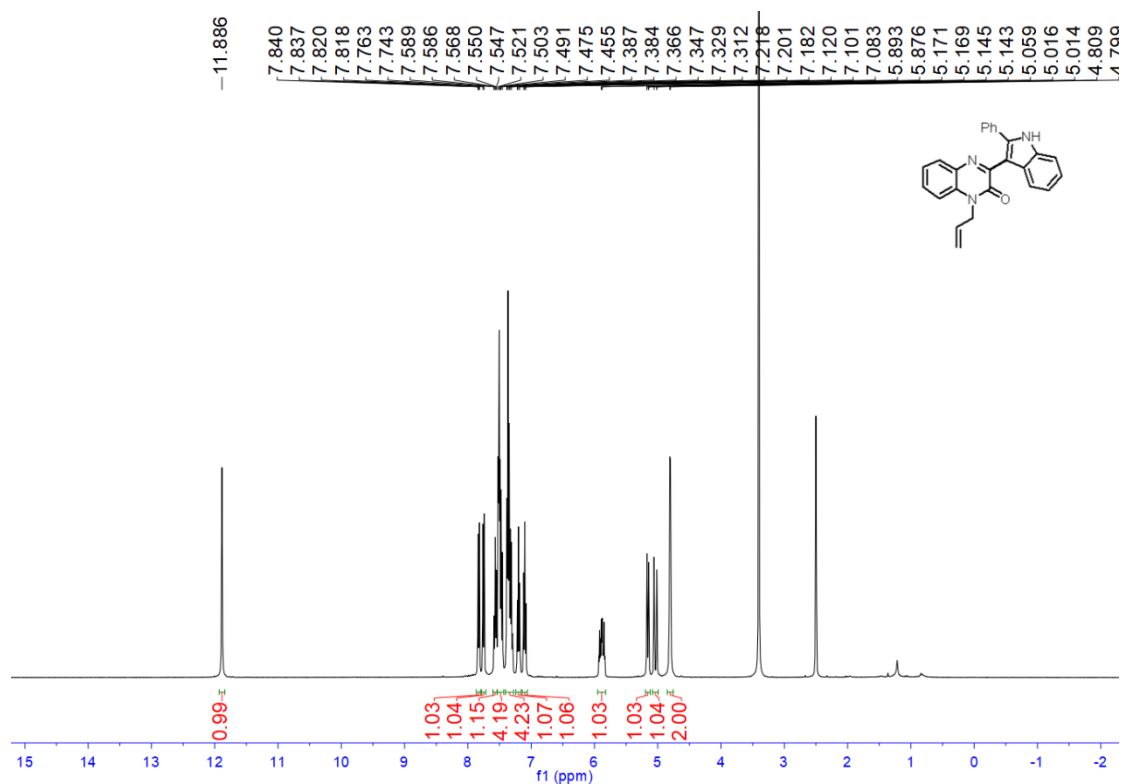
2(1*H*)-one (3ja). Yellow solid, 68.7 mg, yield 94%. m.p.: 252.3-253.1 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ 11.88 (s, 1H), 7.79 (d, *J* = 7.9 Hz, 1H), 7.56 – 7.48 (m, 3H), 7.47 – 7.42 (m, 1H), 7.41 – 7.30 (m, 4H), 7.24 – 7.16 (m, 2H), 7.14 – 7.07 (m, 1H), 3.58 (s, 3H), 2.44 (s, 3H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 154.1, 151.9, 140.3, 137.6, 136.4, 133.8, 133.5, 131.6, 129.8, 128.8, 128.7, 128.6, 128.2, 124.8, 122.5, 121.1, 120.5, 112.9, 111.9, 110.2, 29.8, 17.6. HRMS (ESI, *m/z*) calcd for C₂₄H₂₀N₃O⁺ [M+H]⁺: 366.1601, found 366.1602.

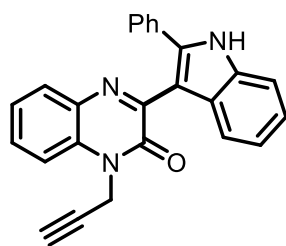
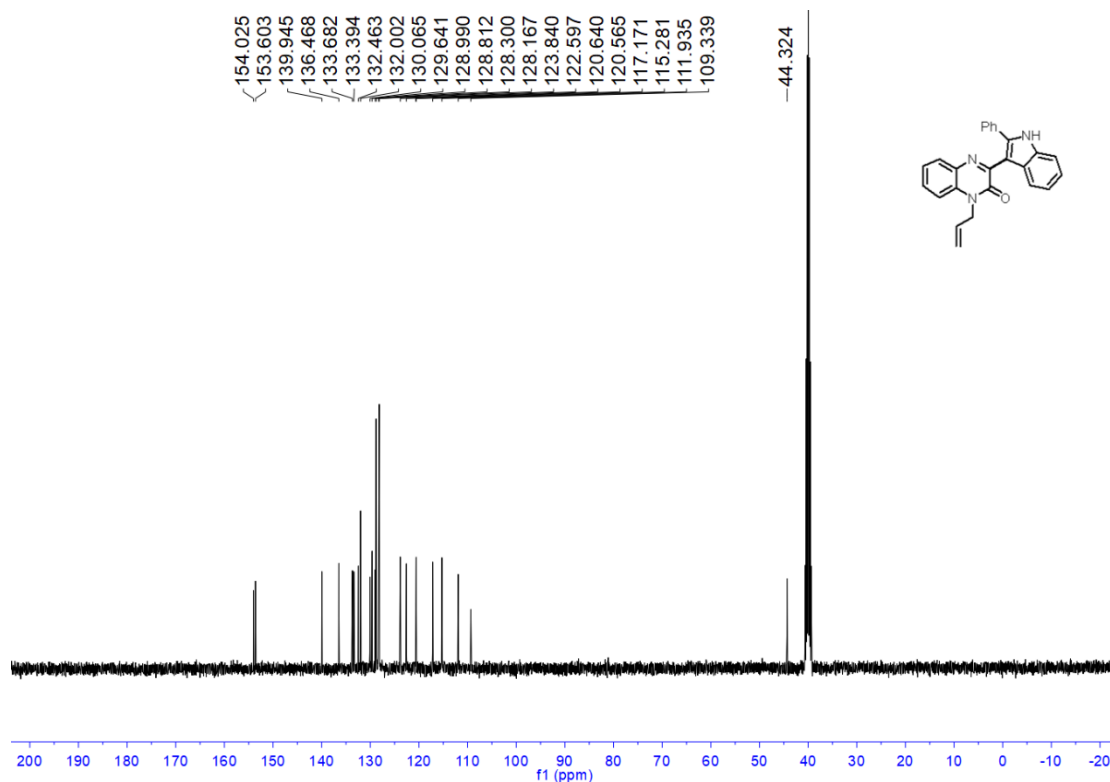




1-allyl-3-(2-phenyl-1H-indol-3-yl)quinoxalin-

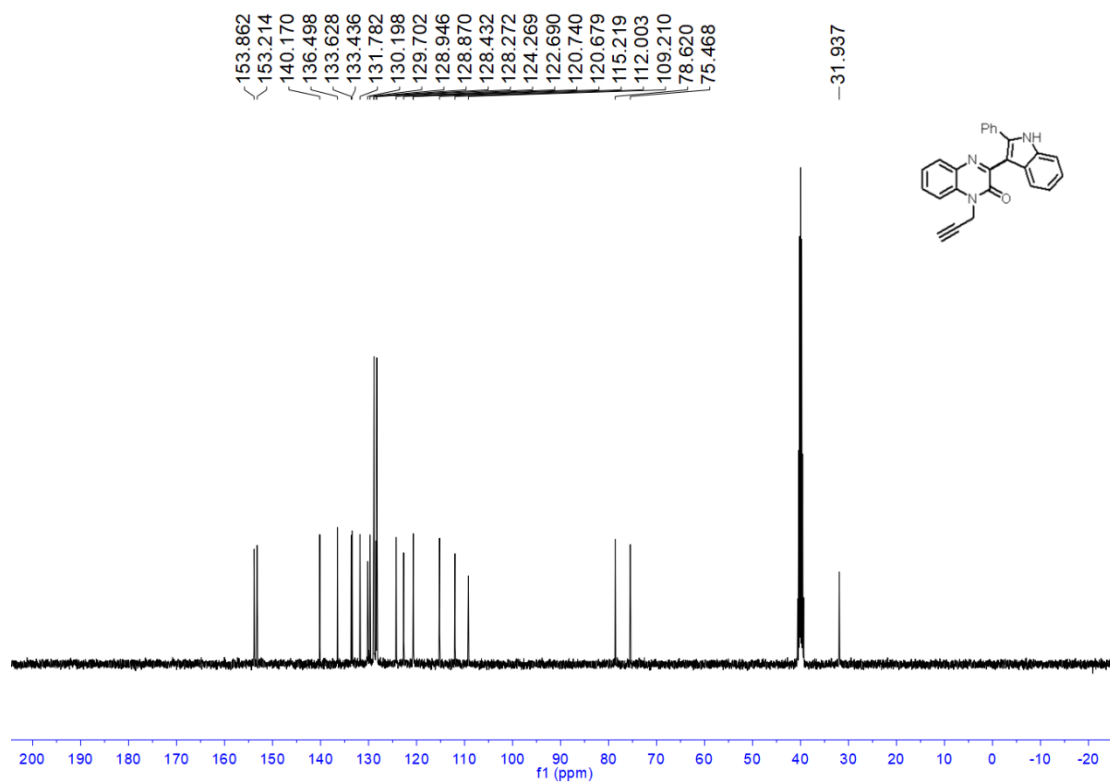
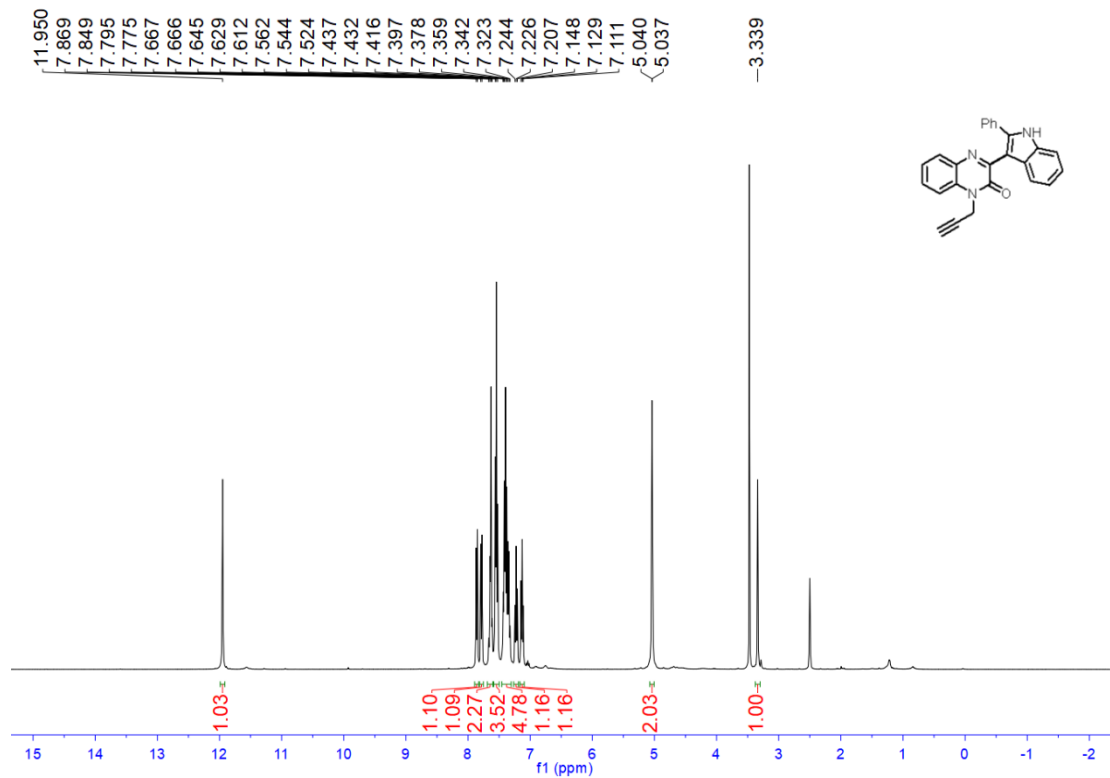
2(1H)-one (3ka). Yellow solid, 74.0 mg, yield 98%. m.p.: 233.6-234.0 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ 11.89 (s, 1H), 7.86 – 7.80 (m, 1H), 7.75 (d, *J* = 7.9 Hz, 1H), 7.60 – 7.54 (m, 1H), 7.54 – 7.43 (m, 4H), 7.41 – 7.28 (m, 4H), 7.24 – 7.16 (m, 1H), 7.14 – 7.07 (m, 1H), 5.95 – 5.82 (m, 1H), 5.19 – 5.12 (m, 1H), 5.08 – 4.99 (m, 1H), 4.85 – 4.76 (m, 2H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 154.0, 153.6, 139.9, 136.5, 133.7, 133.4, 132.5, 132.0, 130.1, 129.6, 129.0, 128.8, 128.3, 128.2, 123.8, 122.6, 120.64, 120.57, 117.2, 115.3, 111.9, 109.3, 44.3. HRMS (ESI, *m/z*) calcd for C₂₅H₂₀N₃O⁺ [M+H]⁺: 378.1601, found 378.1604.

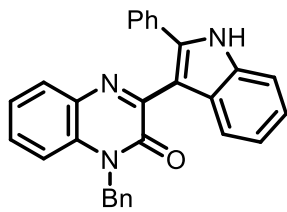




3-(2-phenyl-1*H*-indol-3-yl)-1-(prop-2-yn-1-

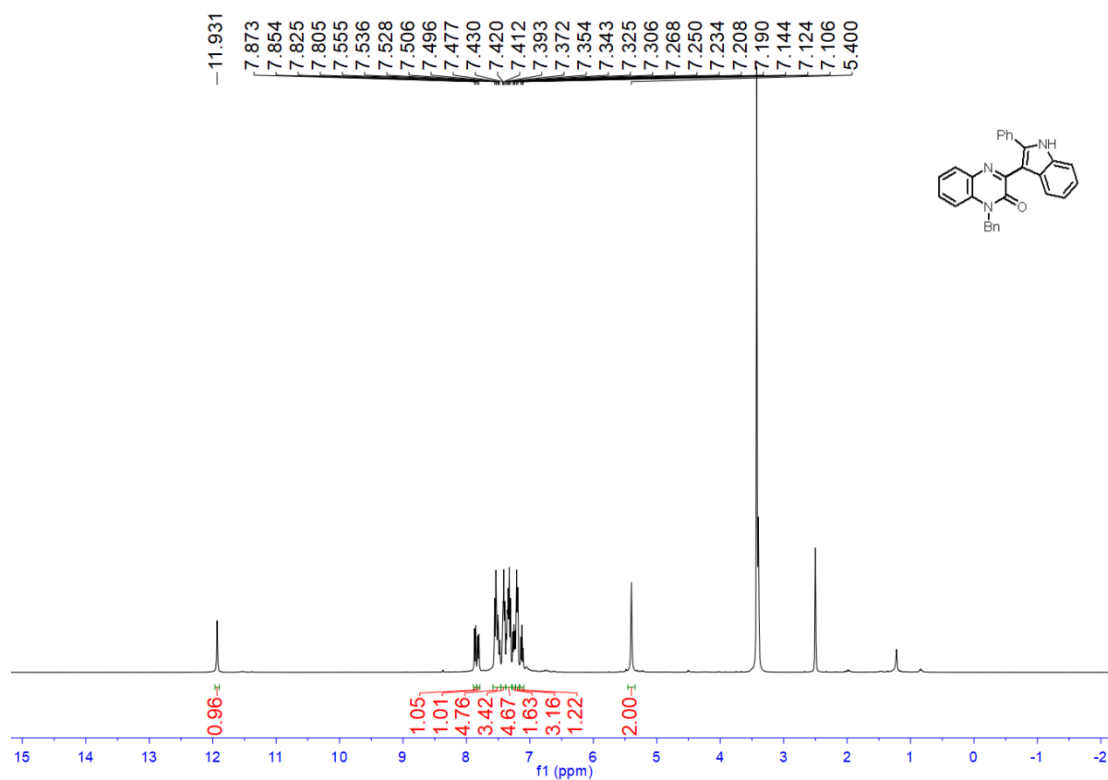
yl)quinoxalin-2(1*H*)-one (3la). Yellow solid, 74.5 mg, yield 99%. m.p.: 203.1-204.3 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ 11.95 (s, 1H), 7.86 (d, *J* = 7.8 Hz, 1H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.69 – 7.60 (m, 2H), 7.58 – 7.51 (m, 3H), 7.46 – 7.31 (m, 4H), 7.27 – 7.19 (m, 1H), 7.16 – 7.10 (m, 1H), 5.08 – 5.00 (m, 2H), 3.36 – 3.2 (m, 1H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 153.9, 153.2, 140.2, 136.5, 133.6, 133.4, 131.8, 130.2, 129.7, 129.0, 128.9, 128.4, 128.3, 124.3, 122.7, 120.74, 120.68, 115.2, 112.0, 109.2, 78.6, 75.4, 31.9. HRMS (ESI, *m/z*) calcd for C₂₅H₁₇N₃NaO⁺ [M+Na]⁺: 398.1264, found 398.1265.

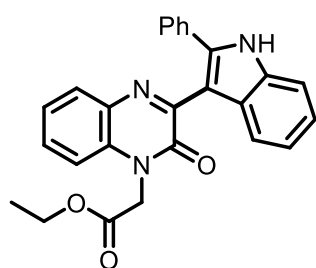
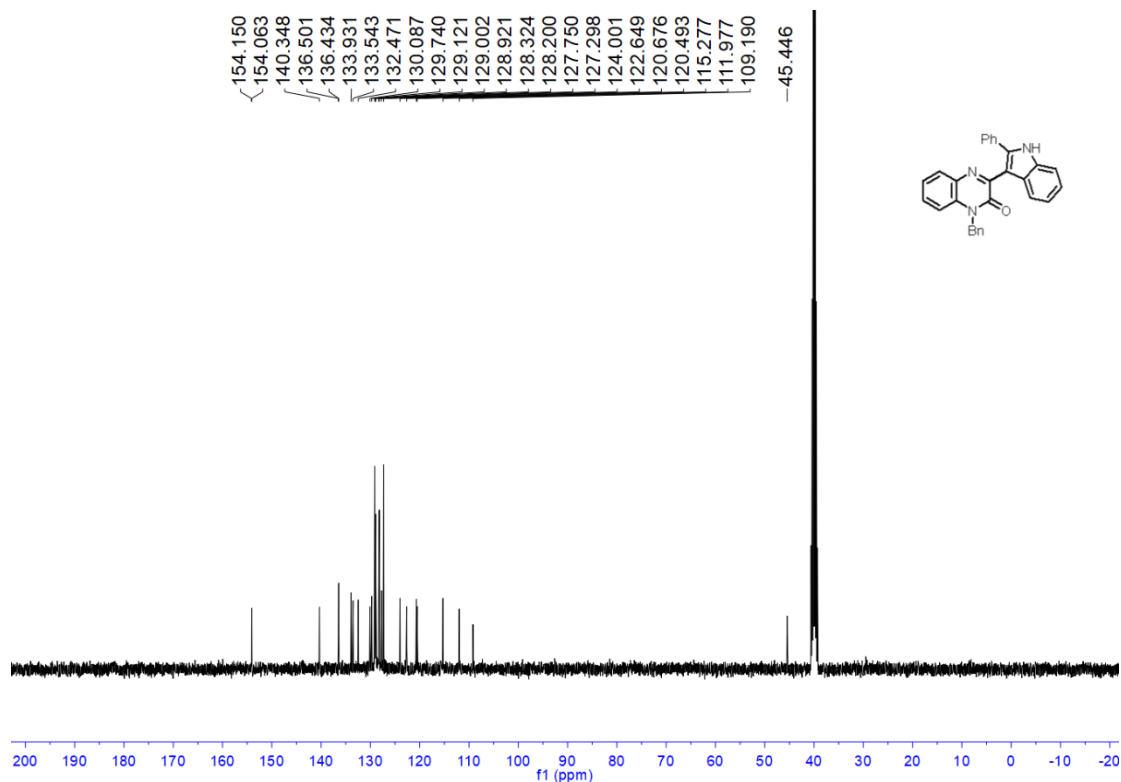




1-benzyl-3-(2-phenyl-1*H*-indol-3-yl)quinoxalin-

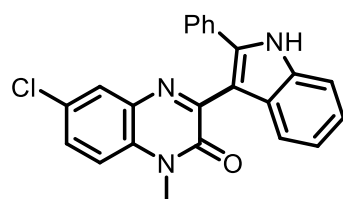
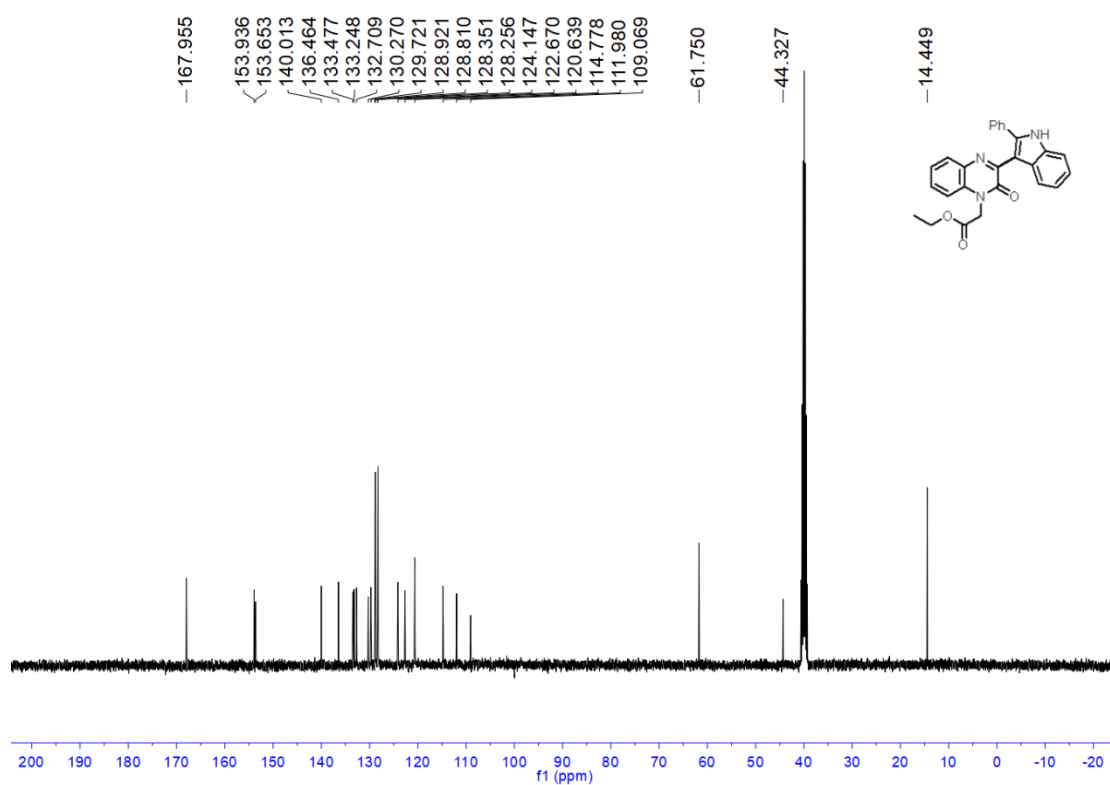
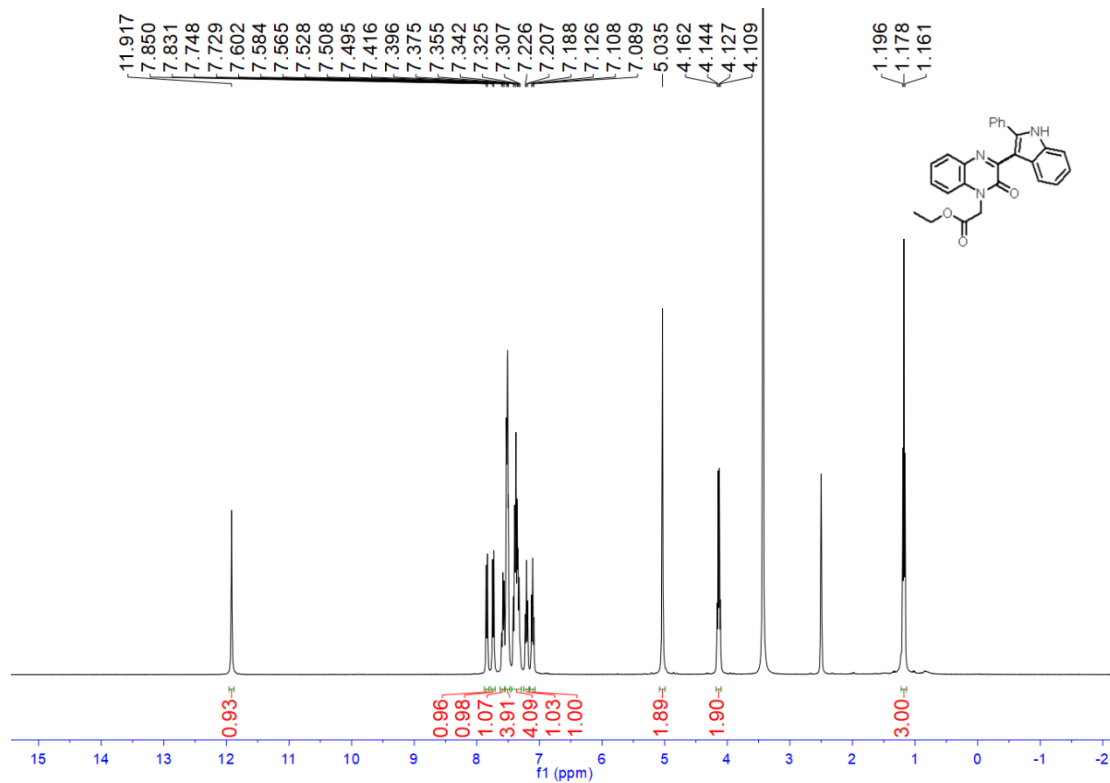
2(1*H*)-one (3ma). Yellow solid, 72.3 mg, yield 85%. m.p.: 194.1-194.9 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ 11.93 (s, 1H), 7.86 (d, *J* = 7.8 Hz, 1H), 7.81 (d, *J* = 7.9 Hz, 1H), 7.56 – 7.47 (m, 4H), 7.45 – 7.38 (m, 3H), 7.38 – 7.29 (m, 4H), 7.28 – 7.22 (m, 1H), 7.22 – 7.18 (m, 3H), 7.15 – 7.10 (m, 1H), 5.40 (s, 2H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 154.2, 154.1, 140.4, 136.5, 136.4, 133.9, 133.5, 132.5, 130.1, 129.7, 129.1, 129.0, 128.9, 128.3, 128.2, 127.8, 127.3, 124.0, 122.7, 120.7, 120.5, 115.3, 112.0, 109.2, 45.5. HRMS (ESI, *m/z*) calcd for C₂₉H₂₁N₃NaO⁺ [M+Na]⁺: 450.1577, found 450.1577.





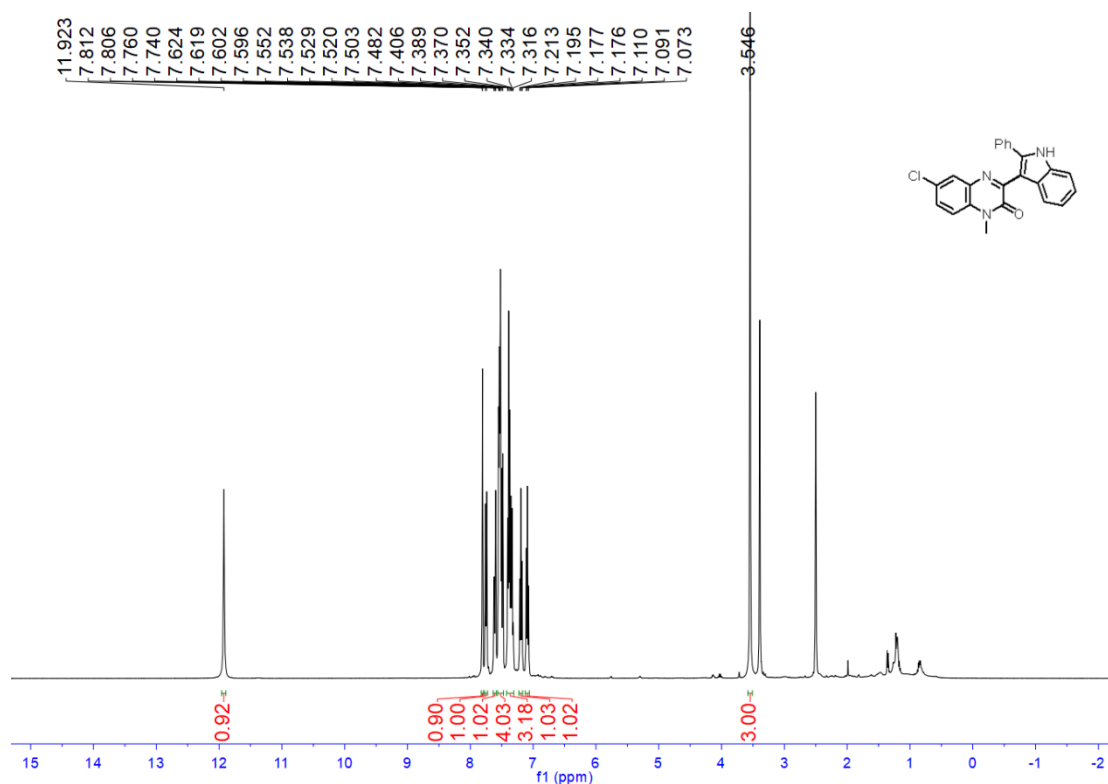
Ethyl 2-(2-oxo-3-(2-phenyl-1H-indol-3-

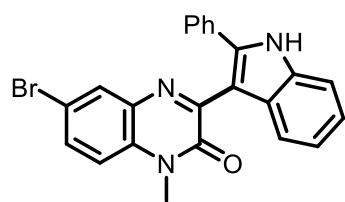
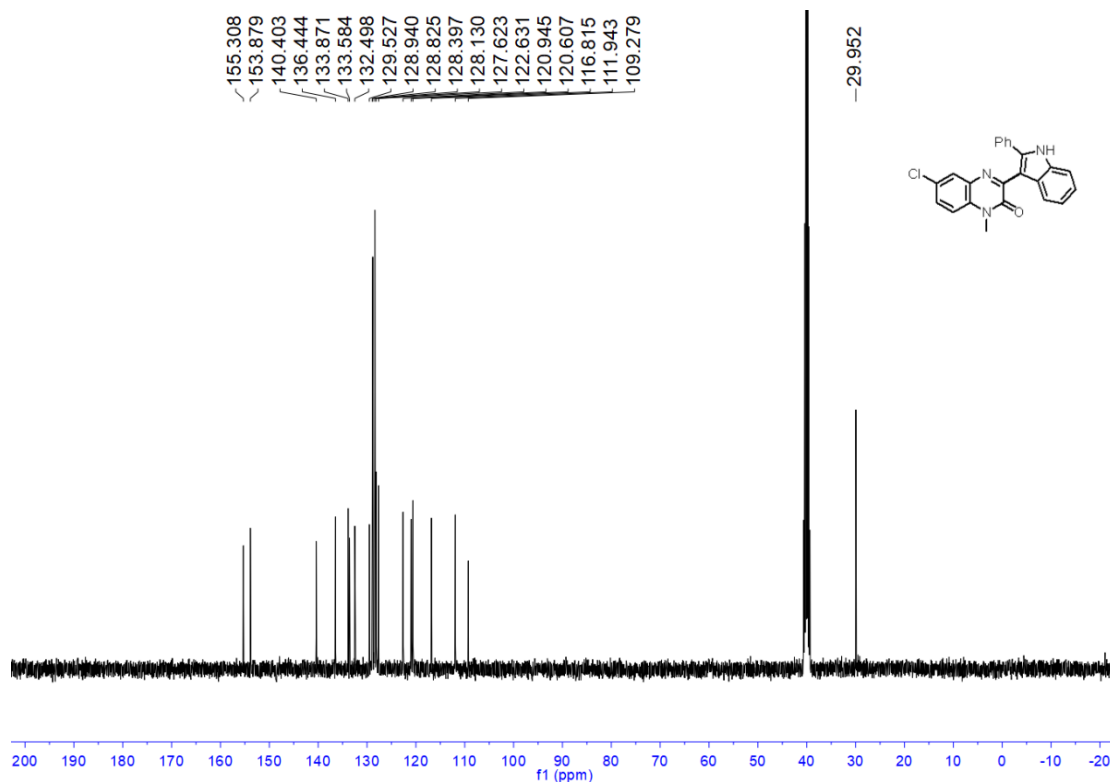
yl)quinoxalin-1(2H)-yl)acetate (3na). Yellow solid, 83.8 mg, yield 99%. m.p.: 208.7-209.2 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ 11.92 (s, 1H), 7.84 (d, *J* = 7.7 Hz, 1H), 7.74 (d, *J* = 7.9 Hz, 1H), 7.62 – 7.55 (m, 1H), 7.55 – 7.47 (m, 4H), 7.44 – 7.29 (m, 4H), 7.21 (dd, *J*₁ = *J*₂ = 7.4 Hz, 1H), 7.11 (dd, *J*₁ = *J*₂ = 7.4 Hz, 1H), 5.04 (s, 2H), 4.14 (q, *J* = 7.0 Hz, 2H), 1.18 (t, *J* = 7.0 Hz, 3H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 168.0, 153.9, 153.7, 140.0, 136.5, 133.5, 133.3, 132.7, 130.3, 129.7, 128.9, 128.8, 128.4, 128.3, 124.2, 122.7, 120.6, 114.8, 112.0, 109.1, 61.8, 44.3, 14.5. HRMS (ESI, *m/z*) calcd for C₂₆H₂₁N₃NaO₃⁺ [M+Na]⁺: 446.1475, found 446.1475.



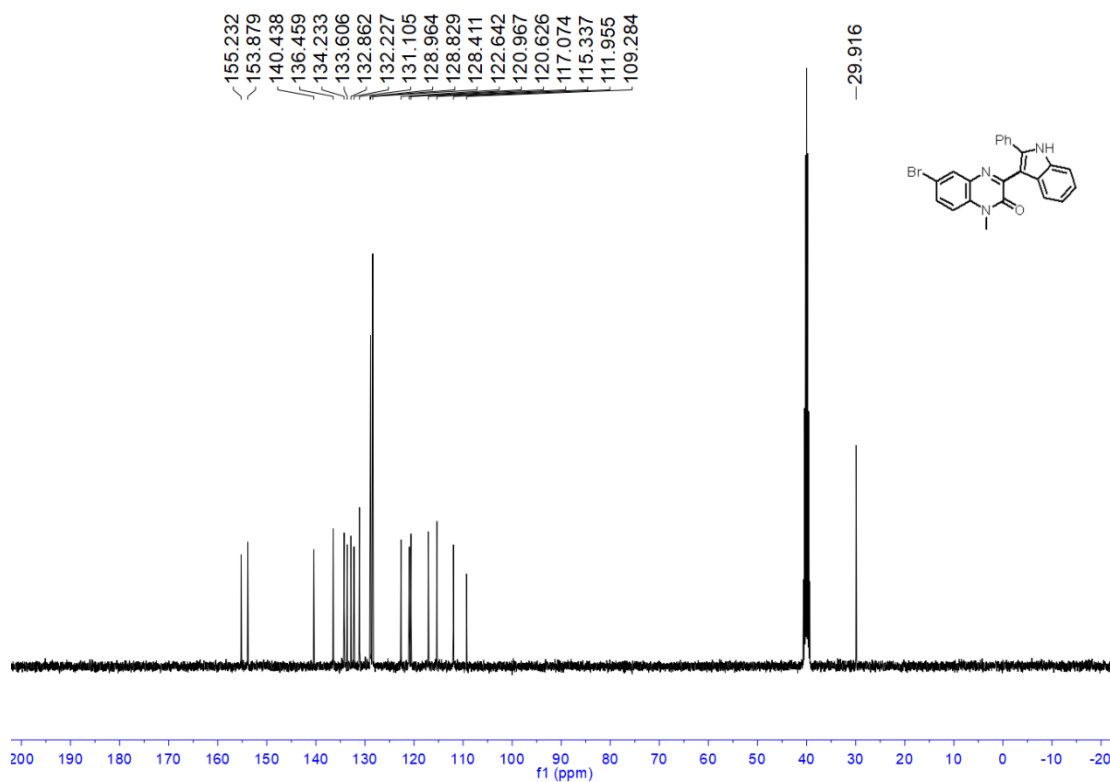
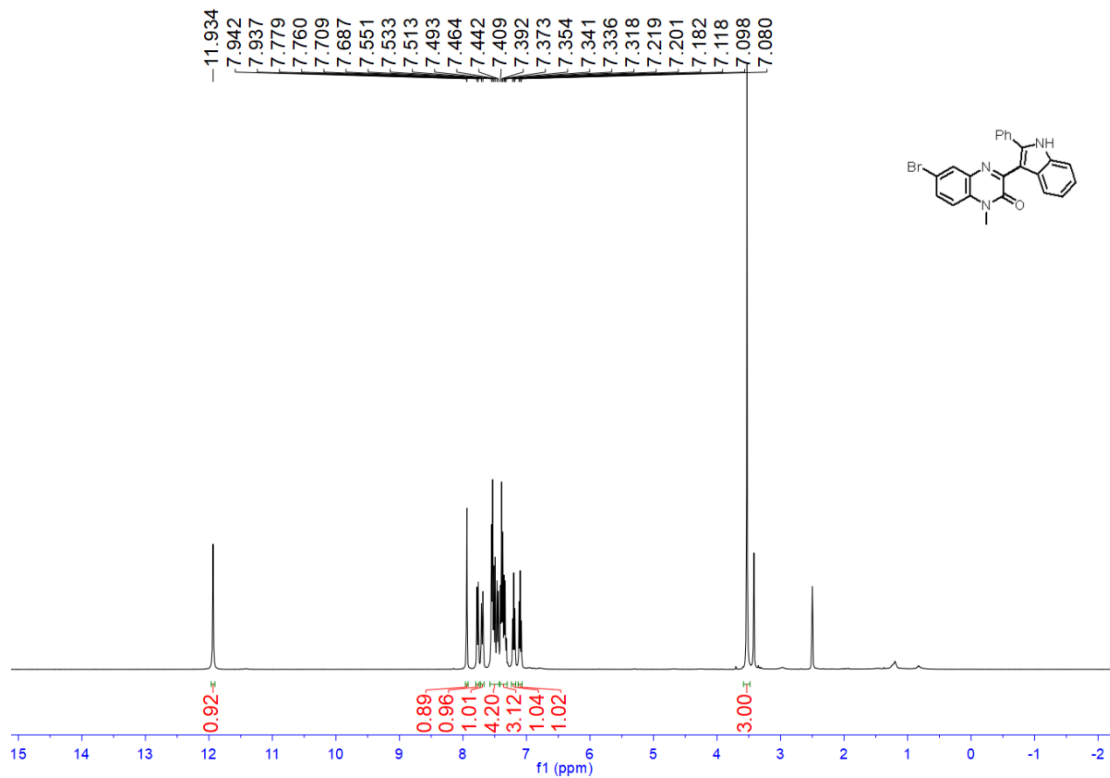
6-chloro-1-methyl-3-(2-phenyl-1H-indol-3-

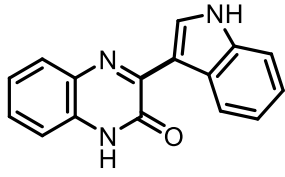
yl)quinoxalin-2(1H)-one (3oa). Yellow solid, 71.8 mg, yield 93%. m.p.: 253.4-254.1 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ 11.92 (s, 1H), 7.81 (d, *J* = 2.3 Hz, 1H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.64 – 7.58 (m, 1H), 7.57 – 7.47 (m, 4H), 7.43 – 7.30 (m, 3H), 7.23 – 7.16 (m, 1H), 7.13 – 7.06 (m, 1H), 3.55 (s, 3H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 155.3, 153.9, 140.4, 136.4, 133.9, 133.6, 132.5, 129.5, 128.9, 128.8, 128.4, 128.1, 127.6, 122.6, 120.9, 120.6, 116.8, 111.9, 109.3, 30.0. HRMS (ESI, *m/z*) calcd for C₂₃H₁₆ClN₃NaO⁺ [M+Na]⁺: 408.0874, found 408.0875.





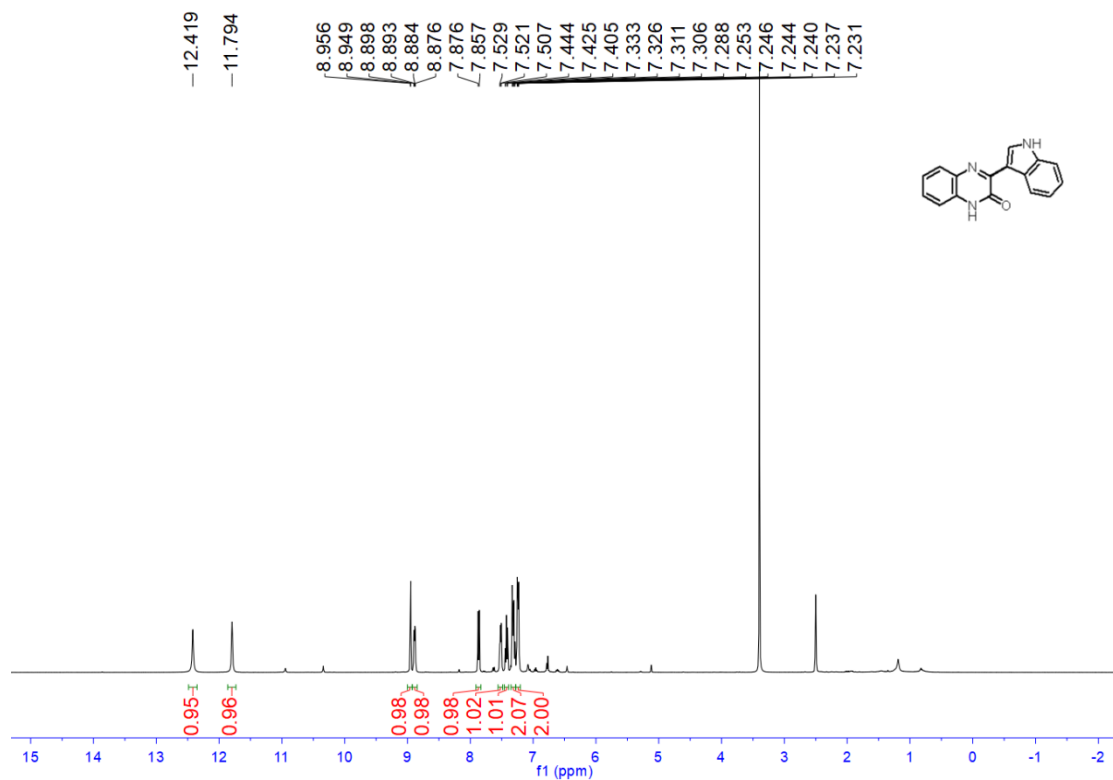
6-bromo-1-methyl-3-(2-phenyl-1H-indol-3-yl)quinoxalin-2(1H)-one (3pa). Yellow solid, 83.5 mg, yield 97%. m.p.: 271.2-273.7 °C. ^1H NMR (400 MHz, DMSO- d_6) δ 11.93 (s, 1H), 7.94 (d, $J = 2.2$ Hz, 1H), 7.77 (d, $J = 8.0$ Hz, 1H), 7.73 – 7.67 (m, 1H), 7.57 – 7.43 (m, 4H), 7.43 – 7.30 (m, 3H), 7.20 (dd, $J_1 = J_2 = 7.2$ Hz, 1H), 7.10 (dd, $J_1 = J_2 = 7.5$ Hz, 1H), 3.53 (s, 3H). ^{13}C NMR (101 MHz, DMSO- d_6) δ 155.2, 153.9, 140.4, 136.5, 134.2, 133.6, 132.9, 132.2, 131.1, 129.0, 128.8, 128.4, 122.6, 121.0, 120.6, 117.1, 115.3, 112.0, 109.3, 29.9. HRMS (ESI, m/z) calcd for $\text{C}_{23}\text{H}_{16}\text{BrN}_3\text{NaO}^+ [\text{M}+\text{Na}]^+$: 452.0369, found 452.0372.

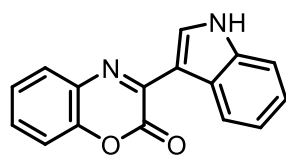
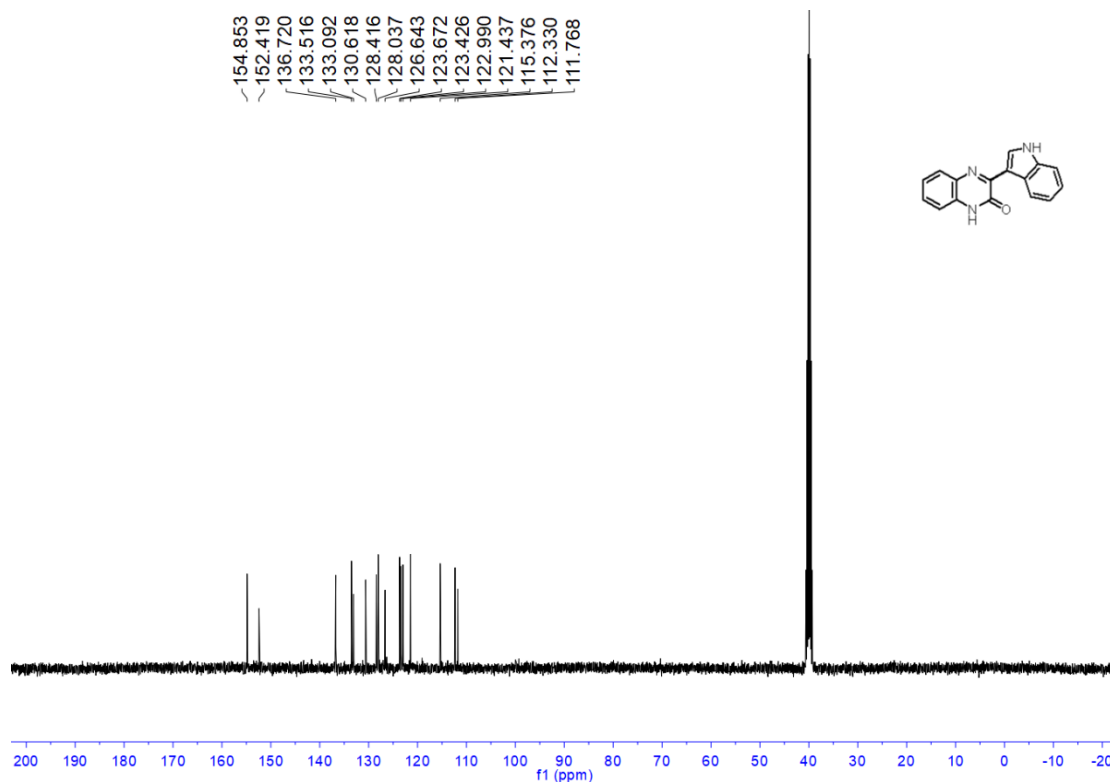




3-(1*H*-indol-3-yl)quinoxalin-2(1*H*)-one (3qa). A known

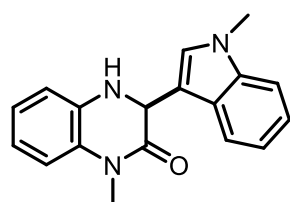
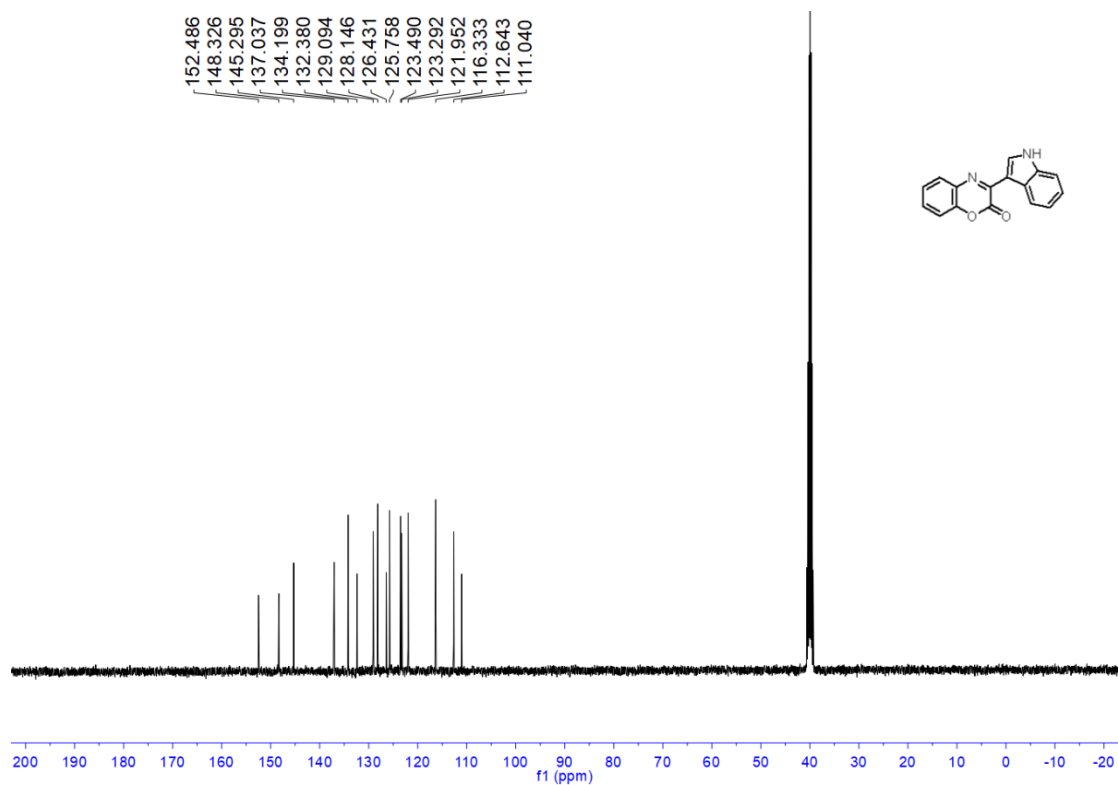
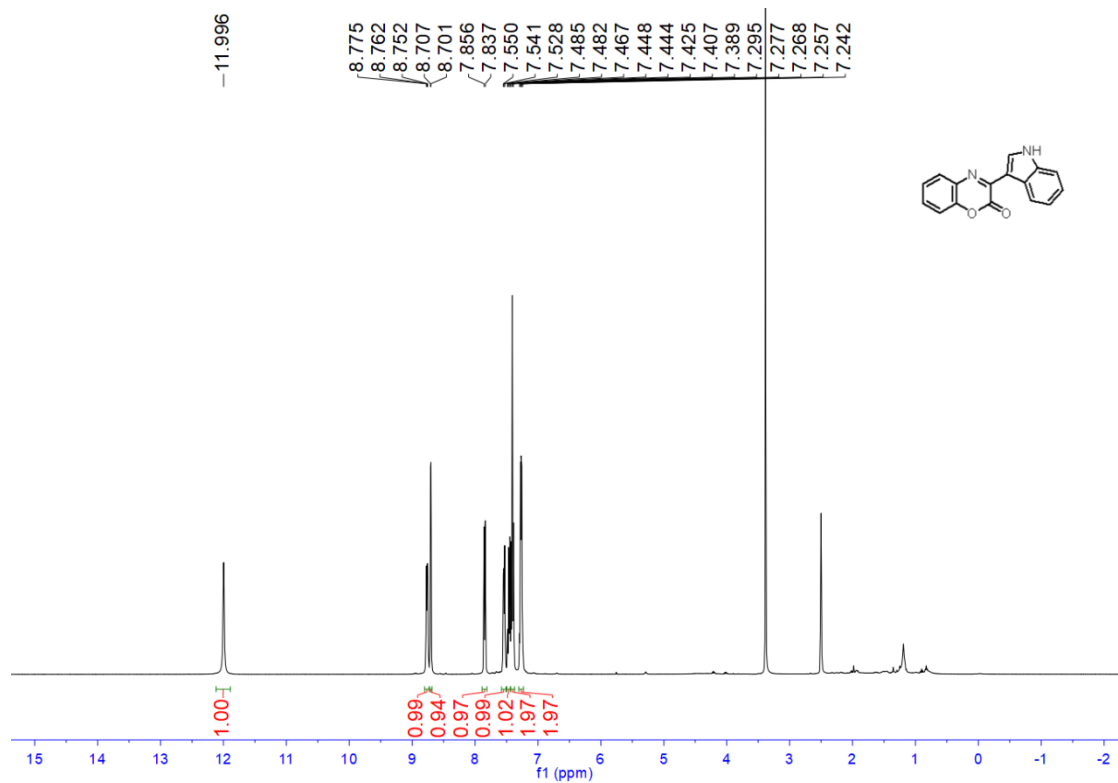
compound.⁵ Orange solid, 30.1 mg, yield 58%. ¹H NMR (400 MHz, DMSO-*d*₆) δ 12.42 (s, 1H), 11.79 (s, 1H), 8.95 (d, *J* = 2.7 Hz, 1H), 8.92 – 8.85 (m, 1H), 7.87 (d, *J* = 7.9 Hz, 1H), 7.56 – 7.48 (m, 1H), 7.46 – 7.39 (m, 1H), 7.36 – 7.28 (m, 2H), 7.27 – 7.21 (m, 2H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 154.9, 152.4, 136.7, 133.5, 133.1, 130.6, 128.4, 128.0, 126.6, 123.7, 123.4, 123.0, 121.4, 115.4, 112.3, 111.8.





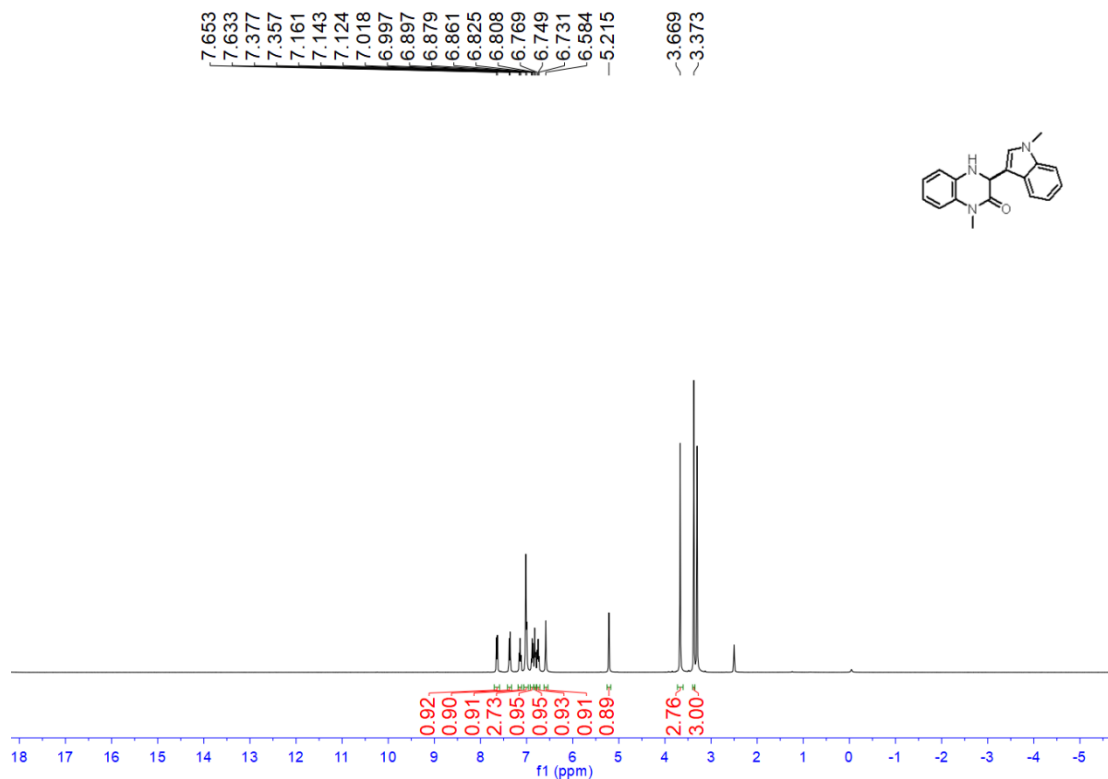
3-(1*H*-indol-3-yl)-2*H*-benzo[*b*][1,4]oxazin-2-one (3ra). A

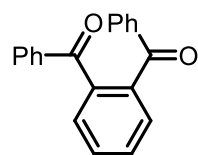
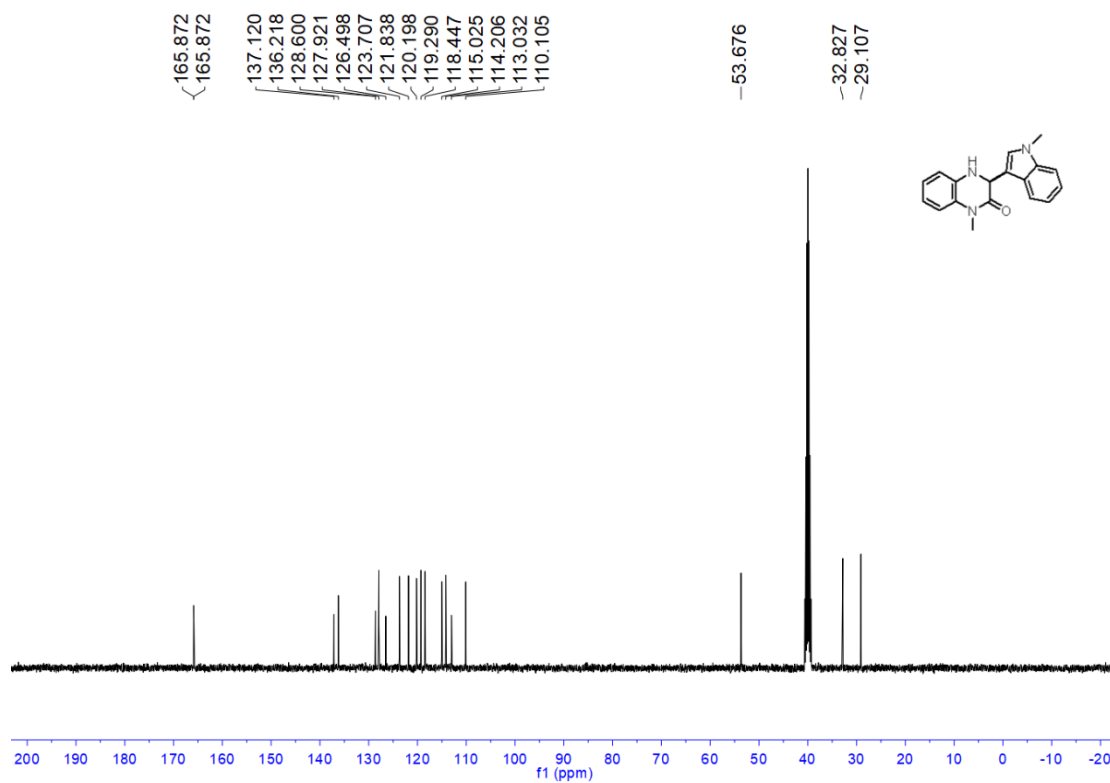
known compound.⁵ Yellow solid, 43.6 mg, yield 83%. ¹H NMR (400 MHz, DMSO-*d*₆) δ 12.00 (s, 1H), 8.80 – 8.73 (m, 1H), 8.70 (d, *J* = 2.3 Hz, 1H), 7.88 – 7.82 (m, 1H), 7.58 – 7.51 (m, 1H), 7.50 – 7.44 (m, 1H), 7.44 – 7.37 (m, 2H), 7.31 – 7.23 (m, 2H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 152.5, 148.3, 145.3, 137.0, 134.2, 132.4, 129.1, 128.2, 126.4, 125.8, 123.5, 123.3, 122.0, 116.3, 112.6, 111.0.



1-methyl-3-(1-methyl-1H-indol-3-yl)-3,4-dihydroquinoxalin-2(1H)-one (3ab'). White solid, 55.4 mg, yield 95%. m.p.: 208.3-

209.1 °C. ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 7.64 (d, $J = 7.9$ Hz, 1H), 7.37 (d, $J = 8.2$ Hz, 1H), 7.14 (t, $J = 7.5$ Hz, 1H), 7.06 – 6.97 (m, 2H), 6.92 – 6.85 (m, 1H), 6.84 – 6.80 (m, 1H), 6.78 – 6.71 (m, 1H), 6.58 (s, 1H), 5.22 (s, 1H), 3.67 (s, 3H), 3.37 (s, 3H). ^{13}C NMR (101 MHz, $\text{DMSO-}d_6$) δ 165.9, 137.1, 136.2, 128.6, 127.9, 126.5, 123.7, 121.8, 120.2, 119.3, 118.5, 115.0, 114.2, 113.0, 110.1, 53.7, 32.8, 29.1. HRMS (ESI, m/z) calcd for $\text{C}_{18}\text{H}_{17}\text{N}_3\text{ONa}^+$ $[\text{M}+\text{Na}]^+$: 314.1264, found 314.1268.





Cyclohexa-3,5-diene-1,2-diylbis(phenylmethanone) (4b) A known compound.² Yellow solid, 53.7 mg, yield 93%. ¹H NMR (400 MHz, CDCl₃, TMS) δ 7.70 (d, *J* = 7.6 Hz, 4H), 7.61 (s, 4H), 7.67 – 7.54 (m, 2H), 7.41 – 7.33 (m, 4H). ¹³C NMR (101 MHz, CDCl₃, TMS) δ 196.6, 140.0, 137.2, 133.0, 130.4, 129.8, 129.7, 128.3.

