Electronic Supplementary Material (ESI) for Green Chemistry.

Direct *para*-C-H heteroarylation of anilines with quinoxalinones by metal-free cross-dehydrogenative coupling under aerobic atmosphere

Jun Xu, Lin Huang, Lei He, Chenfeng Liang, Yani Ouyang, Jiabin Shen, Min Jiang, and Wanmei Li*

College of Material, Chemistry and Chemical Engineering, Hangzhou Normal University, Hangzhou 311121, China. Email: liwanmei@hznu.edu.cn.

Supporting Information

Table of contents

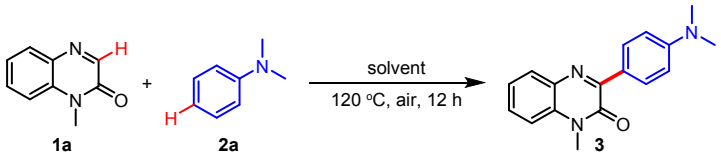
General Information

All reagents and deuterated solvents were commercially available and used without further purification. All products were separated by silica gel (200-300 mesh) column chromatography with petroleum ether (PE) (60-90°C) and ethyl acetate (EA). ^{1}H, ^{13}C and ^{19}F NMR spectra were recorded on a Bruker Advance 500 spectrometer at ambient temperature with $CDCl_3$ or CD_3SOCD_3 as solvent and tetramethylsilane (TMS) as the internal standard. Analytical thin layer chromatography (TLC) was performed on Merk precoated TLC (silica gel 60 F254) plates. Compounds for HRMS were analyzed by positive mode electrospray ionization (ESI) using Agilent 6530 QTOF mass spectrometer. The Electron Spin Resonance (ESR) spectrum was recorded by a JES X320 (JEOL Co.).

1. Experimental Section

1.1 Optimization of reaction conditions

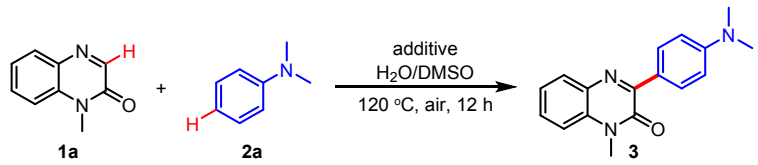
Table S1 Optimization of solvent [a]



Entry	Solvent	Temp. (°C)	Yield (%) [b]
1	acetone	120	trace
2	THF	120	25
3	MeCN	120	27
4	DMF	120	trace
5	DMC	120	trace
6	NMP	120	trace
7	DMPU	120	trace
8	PEG-200	120	trace
9	C_2H_5OH	120	15
10	1,4-dioxane	120	30
11	Cyrene	120	18
12	H_2O	120	28
13	DMSO	120	66
14	H_2O/DMSO (*v*/*v* = 1:1)	120	71
15	H_2O/DMSO (*v*/*v* = 2:1)	120	77
16	H_2O/DMSO (*v*/*v* = 3:1)	120	56
17	H_2O/THF (*v*/*v* = 2:1)	120	32
18	H_2O/C_2H_5OH (*v*/*v* = 2:1)	120	20
19	H_2O/1,4-dioxane (*v*/*v* = 2:1)	120	16
20	H_2O/Cyrene (*v*/*v* = 2:1)	120	25

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (0.3 mmol), solvent, 120 °C, air, 12 h. [b] Isolated yields. Note: THF = Tetrahydrofuran. DMF = *N, N*-Dimethyl formamide. DMC = Dimethyl carbonate. NMP = *N*-Methylpyrrolidone. DMPU = 1,3-Dimethyl-3,4,5,6-tetrahydro-2(1H)-pyrimidinone. PEG = Polyethylene glycol. DMSO = Dimethylsulfoxide.

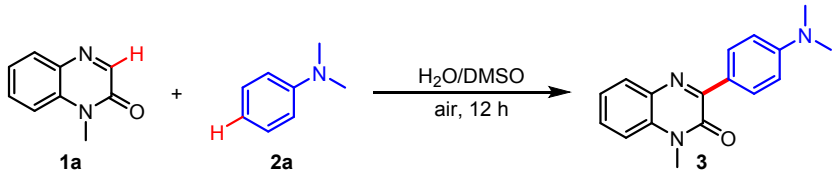
Table S2 Optimization of additive [a]



Entry	Additive	Temp. (°C)	Yield (%)[b]
1	-	120	77
2	$(NH_4)_2S_2O_8$	120	61
3	$Na_2S_2O_8$	120	66
4	$Na_2S_2O_4$	120	68
5	Na_2CO_3	120	67
6	NaCl	120	73

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (0.3 mmol), additive (1.5 equiv), H_2O/DMSO (1.0 mL, *v*/*v* = 2:1), 120 °C, air, 12 h. [b] Isolated yields.

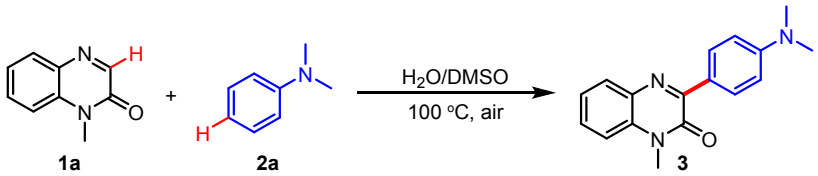
Table S3 Optimization of reaction temperature [a]



Entry	Temp. (°C)	Time (h)	Yield (%) [b]
1	rt	12	0
2	40	12	0
3	60	12	trace
4	80	12	51
5	100	12	82
6	120	12	77

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (0.3 mmol), H_2O/DMSO (1.0 mL, *v*/*v* = 2:1), reaction temperature, air, 12 h. [b] Isolated yields.

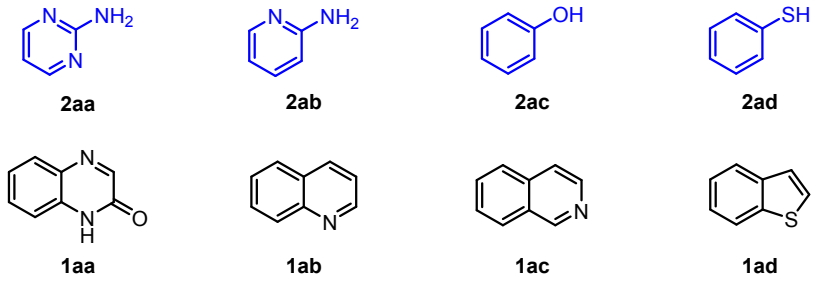
Table S4 Optimization of reaction time [a]



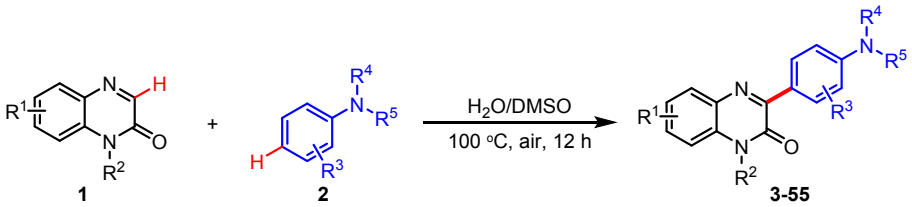
Entry	Time (h)	Yield (%)[b]
1	6	42
2	8	60
3	10	73
4	12	82
5	14	81
6	16	78

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (0.3 mmol), H_2O/DMSO (1.0 mL, *v*/*v* = 2:1), 100 °C, air, reaction time. [b] Isolated yields.

Table S5 Ineffective substrates for the metal-free cross-dehydrogenative coupling

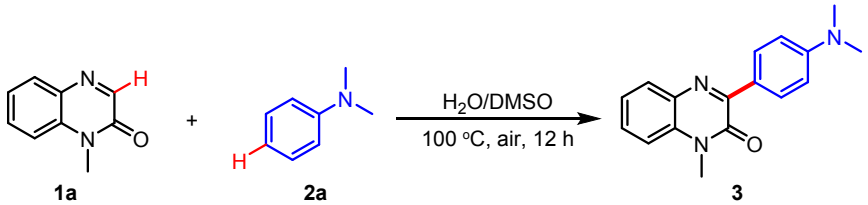


1.2 General procedure for C-H heteroarylation of anilines with quinoxalinones



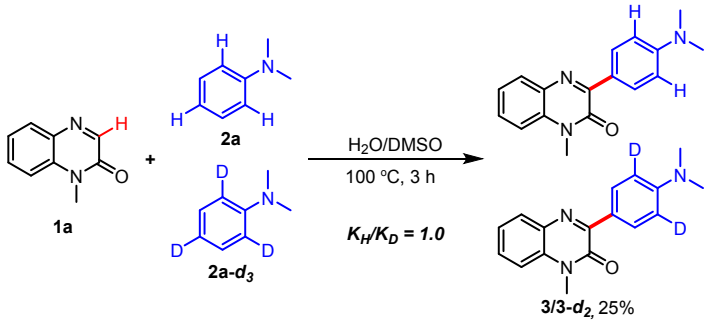
To a 15 mL tube was added quinoxalinones (**1**) (0.2 mmol), anilines (**2**) (0.3 mmol), and H_2O/DMSO (1.0 mL, *v*/*v* = 2:1). The above mixture was vigorous stirred at 100 °C for 12 hours. After completion, the reaction mixture was cooled down to room temperature and diluted with water. The resulting mixture was extracted with ethyl acetate and the collected organic layer was washed with brine, dried with $MgSO_4$. After the solvent was removed under reduced pressure, the crude product was further purified by silica gel column chromatography (200-300 mesh silica gel, PE(*v*)/EA(*v*) = 3:1, 200 mL) to afford the target product. Of note, during the purification of products, the eluent was recycled through vacuum distillation and was reused for further purification.

1.3 General procedure for gram-scale C-H heteroarylation of anilines with quinoxalinones



To a 100 mL flask was added quinoxalinone (**1a**) (5.0 mmol), aniline (**2a**) (7.5 mmol), and H_2O/DMSO (25.0 mL, *v*/*v* = 2:1). The above mixture was vigorous stirred at 100 °C for 12 hours. After completion, the reaction mixture was cooled down to room temperature and diluted with water. The resulting mixture was extracted with ethyl acetate and the collected organic layer was washed with brine, dried with $MgSO_4$. After the solvent was removed under reduced pressure, and the crude product was further purified by silica gel column chromatography (200-300 mesh silica gel, PE(*v*)/EA(*v*) = 3:1, 600 mL) to afford the target product. Of note, during the purification of products, the eluent was recycled through vacuum distillation and was reused for further purification.

1.4 Competing kinetic isotope effect (KIE) experiment.



To a 15 mL tube was added quinoxalinone (**1a**) (0.2 mmol), aniline (**2a**) (0.15 mmol), deuterated aniline (**2a-*d*$_3$**) (0.15 mmol), and H_2O/DMSO (1.0 mL, *v*/*v* = 2:1). The above mixture was vigorous stirred at 100 °C for 3 hours. The resulting mixture was extracted with ethyl acetate and the collected organic layer was washed with brine, dried with $MgSO_4$. After the solvent was removed under reduced pressure, and the crude product was further purified by silica gel column chromatography (200-300 mesh silica gel, PE(*v*)/EA(*v*) = 3:1, 200 mL) to afford a mixture of **3** and **3-*d*$_2$**. The distribution was then measured via ^{1}H NMR spectra. Of note, during the purification of products, the eluent was recycled through vacuum distillation and was reused for further purification.

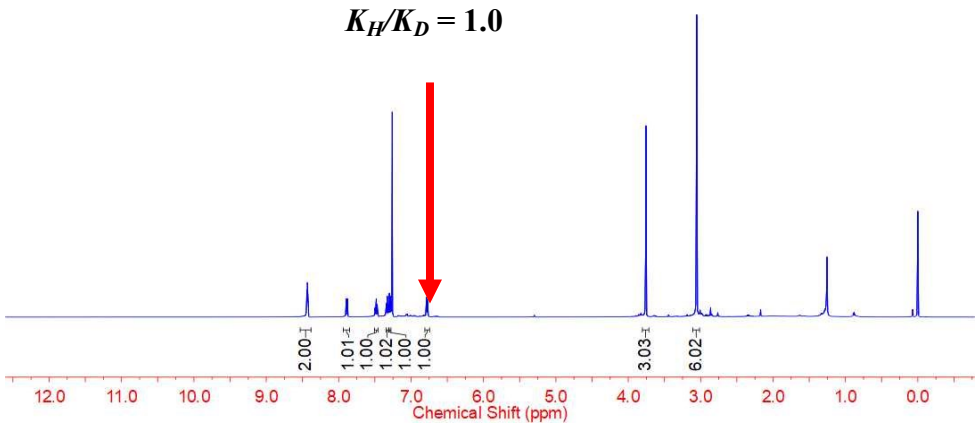
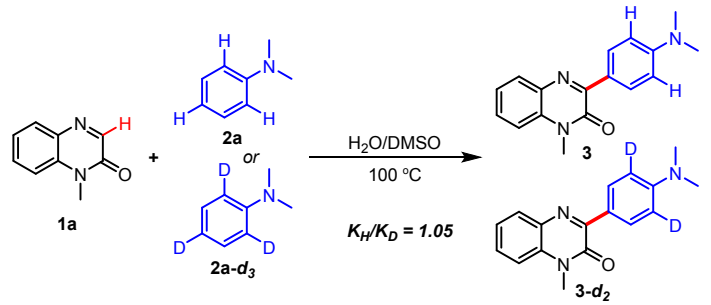


Figure S1 ^{1}H NMR spectrum of mixture compounds **3/3-*d*$_2$**

1.5 Parallel kinetic isotope effect (KIE) experiment.



To a 15 mL tube was added quinoxalinone (**1a**) (0.2 mmol), aniline (**2a**) or deuterated aniline (**2a-*d*$_3$**) (0.3 mmol), and H_2O/DMSO (1.0 mL, *v*/*v* = 2:1). The above mixture was vigorous stirred at 100 °C. Upon an indicated time, the resulting mixture was extracted with ethyl acetate and the collected organic layer was washed with brine, dried with $MgSO_4$. After the solvent was removed under

reduced pressure, and the crude product was further purified by silica gel column chromatography (200-300 mesh silica gel, PE(*v*)/EA(*v*) = 3:1, 200 mL) to afford the product **3** or **3-*d*$_2$**. Of note, during the purification of products, the eluent was recycled through vacuum distillation and was reused for further purification.

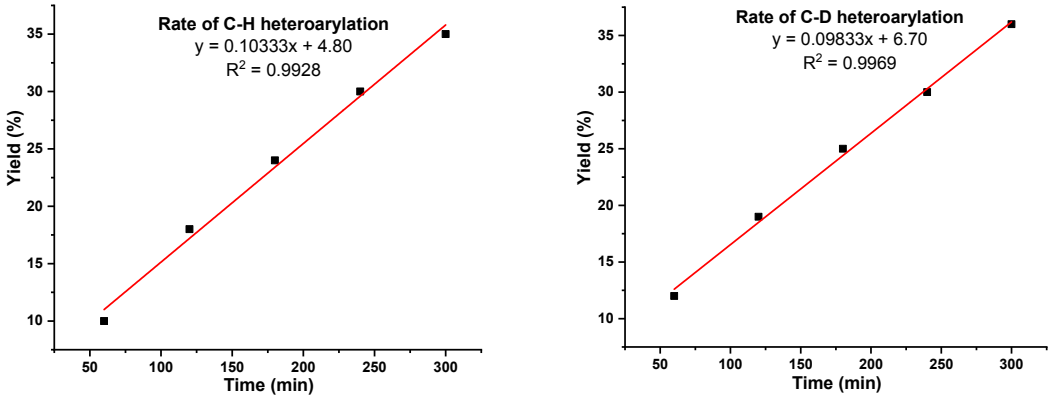


Figure S2 Time-yield curves of **3** and **3-*d*$_2$**

1.6 Determination of singlet oxygen by electron spin resonance (ESR) spectroscopy.

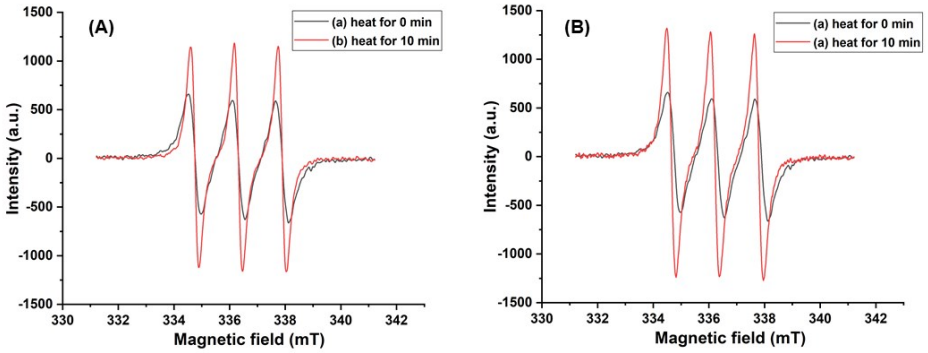
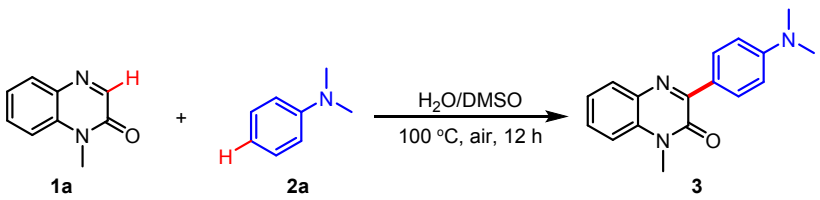


Figure S3 ESR spectra of singlet oxygen captured by TEMP. (A) (a) Solution of **1a**, **2a** and TEMP in air-saturated H_2O/DMSO without heating. (b) Solution of **1a**, **2a** and TEMP in air-saturated H_2O/DMSO with heating for 10 min; (B) (a) Solution of TEMP in air-saturated H_2O/DMSO without heating. (b) Solution of TEMP in air-saturated H_2O/DMSO with heating for 10 min. These two experimental results have no significant difference, which demonstrate that there is no singlet oxygen involved in this reaction.

1.7 Testing of the recyclability of the reaction system.



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

To a 150 mL flask was added quinoxalinone (**1a**) (10.0 mmol), aniline (**2a**) (15.0 mmol), and H_2O/DMSO (50.0 mL, *v*/*v* = 2:1). The above mixture was vigorous stirred at 100 °C for 12 hours. After completion, the reaction mixture was cooled down to room temperature, and the mixed solvent (H_2O/DMSO) was recycled through vacuum distillation and was reused for the next cross-dehydrogenative coupling. The crude product was further purified by silica gel column

chromatography (200-300 mesh silica gel, PE(*v*)/EA(*v*) = 3:1, 800 mL) to afford the target product. Of note, during the purification of products, the eluent was recycled through vacuum distillation and was reused for further purification.

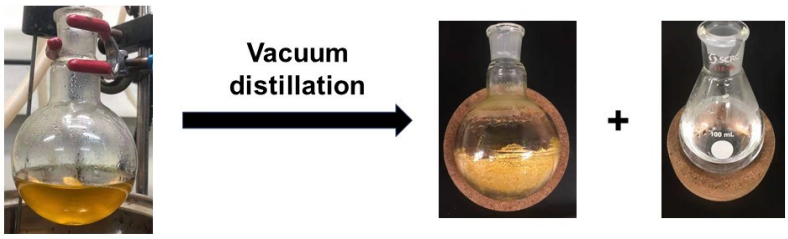


Figure S4 The schematic of recovering mixed solvent

Table S6 Calculation of green chemistry metrics

Steps	Reagent 1	Reagent 2	Solvent	Oxidant	Yield	Product
1	Quinoxalinone (**1a**), 10 mmol, MW: 160.2, 1602 mg	Aniline (**2a**), 15 mmol, MW: 121.2, 1818 mg	Water, 33.3 mL	DMSO, 234.7 mmol, MW: 78.1, 18333.3 mg	O_2, MW: 32.0	76%	**3**, 7.6 mmol, MW: 279.3, 2122.7 mg

$$Atom\ Economy = \frac{279.3}{160.2 + 121.2 + 32.0}\ X\ 100\% = 89.1\%$$

With solvent recycling

$$E - factor = \frac{\sum 1602 + 1818 - 2122.7}{2122.7} = 0.6$$

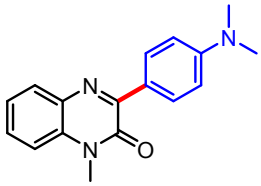
Without solvent recycling

$$E - factor = \frac{\sum 1602 + 1818 + 18333.3 - 2122.7}{2122.7} = 9.2$$

Parameter	Detail of parameters	Penalty points
1. Yield	76%	12
2. Cost of reactants to obtain	10 mmol of product	0
	Quinoxalinone (**1a**)	0
	Aniline (**2a**)	0
	H_2O	0
	DMSO	0
	O_2	0
3. Safety	DMSO	10 (N, T)
4. Technical setup	Common setup	0
5. Temperature/time	Heating, > 1 h	3
6. Workup and purification	Classical chromatography	10
Eco-scale score		65

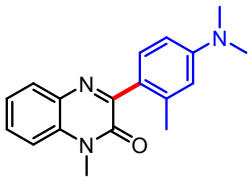
2. Characterization of Products

3-(4-(Dimethylamino)phenyl)-1-methylquinoxalin-2(1*H*)-one (3)



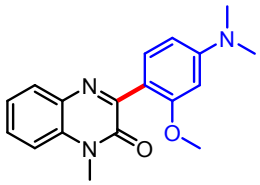
Obtained as a yellow liquid (46 mg, 82% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.43 (d, J = 9.1 Hz, 2H), 7.88 (dd, J = 8.0, 1.2 Hz, 1H), 7.49 – 7.46 (m, 1H), 7.33 (d, J = 7.2 Hz, 1H), 7.28 (d, J = 8.3 Hz, 1H), 6.80 (d, J = 8.4 Hz, 2H), 3.75 (s, 3H), 3.05 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.09, 153.05, 151.56, 133.43, 132.89, 131.19, 129.73, 128.97, 123.52, 123.28, 113.40, 111.63, 40.49, 29.21; HRMS (ESI+): Calculated for $C_{17}H_{17}N_3O$: $[M+Na]^+$ 302.1264, Found 302.1260.

3-(4-(Dimethylamino)-2-methylphenyl)-1-methylquinoxalin-2(1*H*)-one (4)



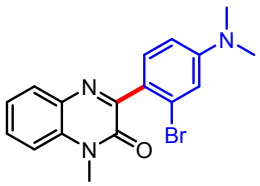
Obtained as a yellow liquid (42 mg, 72% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.81 (dd, J = 7.9, 1.3 Hz, 1H), 7.46 (ddd, J = 8.7, 7.4, 1.5 Hz, 1H), 7.42 (d, J = 8.3 Hz, 1H), 7.27 (d, J = 7.4 Hz, 1H), 7.24 (s, 1H), 6.56 (d, J = 8.3 Hz, 2H), 3.68 (s, 3H), 2.92 (s, 6H), 2.31 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.96, 155.09, 151.32, 138.41, 133.31, 133.12, 131.02, 130.04, 129.66, 124.19, 123.51, 114.50, 113.53, 109.52, 40.44, 29.39, 20.98; HRMS (ESI+): Calculated for $C_{18}H_{19}N_3O$: $[M+Na]^+$ 316.1420, Found 316.1428.

3-(4-(Dimethylamino)-2-methoxyphenyl)-1-methylquinoxalin-2(1*H*)-one (5)



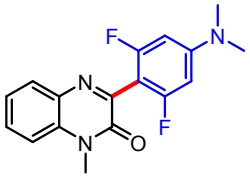
Obtained as a yellow liquid (46 mg, 74% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (dd, J = 7.9, 1.3 Hz, 1H), 7.46 – 7.42 (m, 1H), 7.30 (d, J = 8.5 Hz, 1H), 7.26 – 7.21 (m, 2H), 6.32 (d, J = 32.1 Hz, 2H), 3.76 (s, 3H), 3.65 (s, 3H), 2.94 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.33, 157.17, 154.75, 152.89, 133.53, 133.23, 131.09, 130.05, 129.61, 123.40, 123.32, 113.50, 105.19, 96.58, 55.92, 40.82, 29.36; HRMS (ESI+): Calculated for $C_{18}H_{19}N_3O_2$: $[M+Na]^+$ 332.1369, Found 332.1369.

3-(2-Bromo-4-(dimethylamino)phenyl)-1-methylquinoxalin-2(1*H*)-one (6)



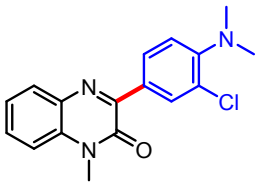
Obtained as a yellow liquid (47 mg, 66% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.92 (d, J = 8.0 Hz, 1H), 7.57 (t, J = 7.2 Hz, 1H), 7.40 (d, J = 8.6 Hz, 1H), 7.35 (d, J = 5.5 Hz, 2H), 6.97 (d, J = 2.4 Hz, 1H), 6.72 (d, J = 11.1 Hz, 1H), 3.75 (s, 3H), 2.99 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.26, 154.48, 151.81, 133.81, 133.67, 132.90, 131.34, 130.33, 124.84, 123.65, 123.49, 116.25, 113.70, 110.89, 40.34, 29.46; HRMS (ESI+): Calculated for $C_{17}H_{16}BrN_3O$: $[M+Na]^+$ 380.0369, Found 380.0368.

3-(4-(Dimethylamino)-2,6-difluorophenyl)-1-methylquinoxalin-2(1*H*)-one (7)



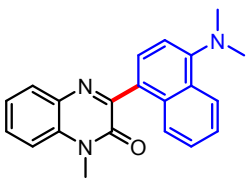
Obtained as a yellow liquid (36 mg, 57% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.94 (d, J = 8.0 Hz, 1H), 7.59 (t, J = 7.9 Hz, 1H), 7.38 (d, J = 7.3 Hz, 1H), 7.35 (d, J = 8.1 Hz, 1H), 6.28 (d, J = 11.6 Hz, 2H), 3.76 (s, 3H), 3.00 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.01 (dd, J = 246.2, 10.8 Hz), 154.37, 152.50, 150.45, 142.10, 133.51, 133.06, 130.60 (d, J = 19.3 Hz), 123.69, 113.67, 99.99, 95.10 (d, J = 28.9 Hz), 40.22, 29.49; ^{19}F NMR (471 MHz, $CDCl_3$) δ -69.87; HRMS (ESI+): Calculated for $C_{17}H_{15}F_2N_3O$: $[M+Na]^+$ 338.1075, Found 338.1071.

3-(3-Chloro-4-(dimethylamino)phenyl)-1-methylquinoxalin-2(1*H*)-one (8)



Obtained as a yellow liquid (39 mg, 62% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.52 (s, 1H), 8.44 (d, J = 8.7 Hz, 1H), 7.90 (d, J = 8.0 Hz, 1H), 7.51 (t, J = 7.8 Hz, 1H), 7.35 (t, J = 7.6 Hz, 1H), 7.30 (d, J = 8.4 Hz, 1H), 6.70 (d, J = 8.7 Hz, 1H), 3.76 (s, 3H), 2.98 (s, 3H), 1.25 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.88, 151.83, 146.67, 133.22, 132.93, 130.43, 130.09, 129.88, 129.38, 125.01, 123.67, 118.61, 113.46, 109.47 , 30.23, 29.71, 29.24; HRMS (ESI+): Calculated for $C_{17}H_{16}ClN_3O$: $[M+Na]^+$ 336.0874, Found 336.0876.

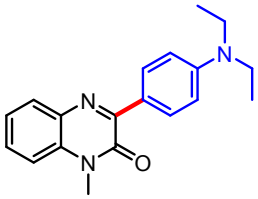
3-(4-(Dimethylamino)naphthalen-1-yl)-1-methylquinoxalin-2(1*H*)-one (9)



Obtained as a yellow liquid (46 mg, 70% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.29 (d, J = 8.4 Hz, 1H), 7.98 – 7.91 (m, 2H), 7.73 (d, J = 7.8 Hz, 1H), 7.60 (t, J = 7.2 Hz, 1H), 7.50 – 7.46 (m, 1H), 7.45

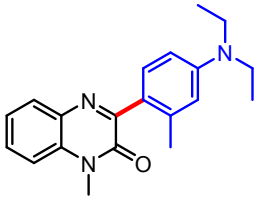
– 7.37 (m, 3H), 7.14 (d, J = 7.8 Hz, 1H), 3.80 (s, 3H), 2.95 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.37, 155.21, 152.56, 144.87, 133.53, 133.12, 132.96, 132.88, 130.44, 128.84, 128.30, 126.32, 125.87, 125.12, 124.69, 123.80, 113.72, 113.01, 45.12, 29.55; HRMS (ESI+): Calculated for $C_{21}H_{19}N_3O$: $[M+Na]^+$ 352.1420, Found 352.1420.

3-(4-(Diethylamino)phenyl)-1-methylquinoxalin-2(1*H*)-one (10)



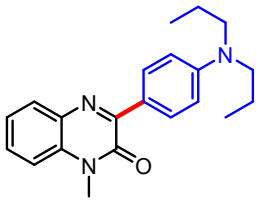
Obtained as a yellow liquid (50 mg, 81% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.33 (d, J = 9.0 Hz, 2H), 7.78 (d, J = 7.3 Hz, 1H), 7.37 (t, J = 7.5 Hz, 1H), 7.23 (t, J = 7.5 Hz, 1H), 7.18 (d, J = 8.2 Hz, 1H), 6.65 (s, 2H), 3.65 (s, 3H), 3.35 (d, J = 7.0 Hz, 4H), 1.13 (t, J = 7.1 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.12, 153.04, 149.37, 133.53, 132.81, 131.42, 129.60, 128.65, 123.45, 123.03, 113.36, 110.71, 44.48, 29.17, 12.69; HRMS (ESI+): Calculated for $C_{19}H_{21}N_3O$: $[M+Na]^+$ 330.1577, Found 330.1577.

3-(4-(Diethylamino)-2-methylphenyl)-1-methylquinoxalin-2(1*H*)-one (11)



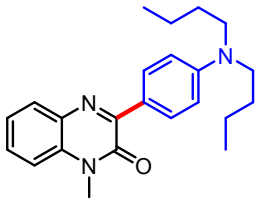
Obtained as a yellow liquid (45 mg, 70% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.88 (d, J = 7.8 Hz, 1H), 7.55 – 7.48 (m, 2H), 7.33 (t, J = 10.0 Hz, 2H), 6.57 (d, J = 8.0 Hz, 2H), 3.75 (s, 3H), 3.41 – 3.37 (m, 4H), 2.39 (s, 3H), 1.18 (t, J = 6.9 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.88, 155.15, 148.59, 138.67, 133.27, 133.19, 131.38, 129.98, 129.45, 123.46, 122.98, 113.70, 113.48, 108.73, 44.37, 29.37, 21.16, 12.71; HRMS (ESI+): Calculated for $C_{20}H_{23}N_3O$: $[M+Na]^+$ 344.1733, Found 344.1734.

3-(4-(Dipropylamino)phenyl)-1-methylquinoxalin-2(1*H*)-one (12)



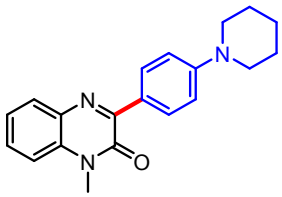
Obtained as a yellow liquid (54 mg, 80% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.40 (d, J = 9.1 Hz, 2H), 7.79 (dd, J = 7.9, 1.1 Hz, 1H), 7.35 (t, J = 7.7 Hz, 1H), 7.22 (t, J = 7.6 Hz, 1H), 7.14 (d, J = 8.3 Hz, 1H), 6.67 (d, J = 8.9 Hz, 2H), 3.63 (s, 3H), 3.31 – 3.25 (m, 4H), 1.63 (dq, J = 14.9, 7.4 Hz, 4H), 0.92 (t, J = 7.4 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.02, 152.86, 149.81, 133.47, 132.71, 131.37, 129.46, 128.57, 123.33, 123.01, 113.34, 110.77, 52.77, 29.09, 20.58, 11.47; HRMS (ESI+): Calculated for $C_{21}H_{25}N_3O$: $[M+Na]^+$ 358.1890, Found 358.1891.

3-(4-(Dibutylamino)phenyl)-1-methylquinoxalin-2(1*H*)-one (13)



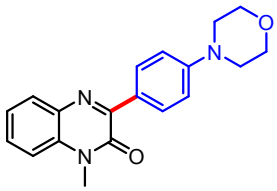
Obtained as a yellow liquid (54 mg, 75% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.40 (d, J = 9.0 Hz, 2H), 7.82 (d, J = 9.0 Hz, 1H), 7.39 (t, J = 7.7 Hz, 1H), 7.28 – 7.24 (m, 1H), 7.20 (d, J = 8.3 Hz, 1H), 6.68 (d, J = 8.7 Hz, 2H), 3.68 (s, 3H), 3.37 – 3.28 (m, 4H), 1.64 – 1.55 (m, 4H), 1.37 (dt, J = 15.0, 7.4 Hz, 4H), 0.95 (t, J = 7.4 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.07, 152.96, 149.79, 133.52, 132.75, 131.34, 129.52, 128.58, 123.38, 122.91, 113.34, 110.78, 50.76, 29.52, 29.13, 20.35, 14.04; HRMS (ESI+): Calculated for $C_{23}H_{29}N_3O$: $[M+Na]^+$ 386.2203, Found 386.2200.

1-Methyl-3-(4-(piperidin-1-yl)phenyl)quinoxalin-2(1*H*)-one (14)



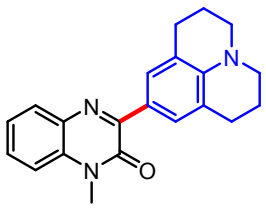
Obtained as a yellow liquid (51 mg, 80% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.39 (d, J = 9.0 Hz, 2H), 7.87 (d, J = 7.9 Hz, 1H), 7.46 (t, J = 7.8 Hz, 1H), 7.31 (t, J = 7.6 Hz, 1H), 7.26 (d, J = 8.3 Hz, 1H), 6.96 (d, J = 8.9 Hz, 2H), 3.72 (s, 3H), 3.34 – 3.30 (m, 4H), 1.70 (s, 4H), 1.63 (s, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.00, 153.11, 153.05, 133.39, 132.93, 131.05, 129.82, 129.11, 125.84, 123.51, 114.39, 113.41, 49.37, 29.19, 25.48, 24.45; HRMS (ESI+): Calculated for $C_{20}H_{21}N_3O$: $[M+Na]^+$ 342.1577, Found 342.1575.

1-Methyl-3-(4-morpholinophenyl)quinoxalin-2(1*H*)-one (15)



Obtained as a yellow liquid (52 mg, 81% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.41 (d, J = 9.0 Hz, 2H), 7.87 (d, J = 9.3 Hz, 1H), 7.47 (t, J = 8.5 Hz, 1H), 7.32 (d, J = 8.2 Hz, 1H), 7.26 (d, J = 8.3 Hz, 1H), 6.95 (d, J = 9.0 Hz, 2H), 3.87 – 3.85 (m, 4H), 3.72 (s, 3H), 3.28 – 3.26 (m, 4H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.90, 152.90, 152.54, 133.28, 133.00, 131.04, 129.92, 129.40, 127.15, 123.56, 114.06, 113.46, 66.72, 48.25, 29.21; HRMS (ESI+): Calculated for $C_{19}H_{19}N_3O$: $[M+Na]^+$ 344.1369, Found 344.1365.

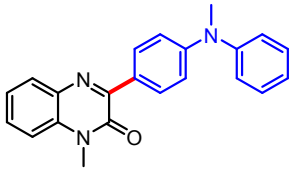
1-Methyl-3-(2,3,6,7-tetrahydro-1*H*,5*H*-pyrido[3,2,1-ij]quinolin-9-yl)quinoxalin-2(1*H*)-one (16)



Obtained as a yellow liquid (56 mg, 84% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.00 (s, 2H), 7.84 (d, J = 7.9 Hz, 1H), 7.42 (t, J = 7.7 Hz, 1H), 7.29 (t, J = 7.6 Hz, 1H), 7.24 (d, J = 8.3 Hz, 1H), 3.71 (s,

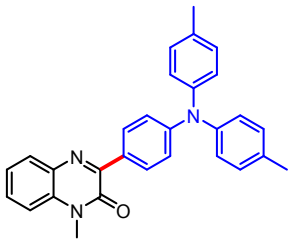
3H), 3.25 – 3.21 (m, 4H), 2.82 (t, J = 6.3 Hz, 4H), 2.00 – 1.94 (m, 4H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.16, 153.10, 144.96, 133.60, 132.69, 129.45, 128.76, 128.42, 123.39, 122.75, 120.27, 113.31, 50.02, 29.12, 27.92, 21.88; HRMS (ESI+): Calculated for $C_{21}H_{21}N_3O$: $[M+H]^+$ 332.1757, Found 332.1749.

1-Methyl-3-(4-(methyl(phenyl)amino)phenyl)quinoxalin-2(1*H*)-one (17)



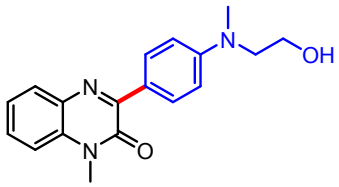
Obtained as a yellow liquid (57 mg, 83% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.34 (d, J = 9.0 Hz, 2H), 7.86 (d, J = 8.0 Hz, 1H), 7.45 (d, J = 6.9 Hz, 1H), 7.34 (t, J = 7.9 Hz, 2H), 7.29 (d, J = 7.9 Hz, 1H), 7.24 (d, J = 7.5 Hz, 1H), 7.20 (d, J = 8.4 Hz, 2H), 7.11 (t, J = 7.4 Hz, 1H), 6.94 (d, J = 9.0 Hz, 2H), 3.71 (s, 3H), 3.38 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.97, 153.09, 150.75, 148.09, 133.33, 132.98, 130.92, 129.87, 129.54, 129.28, 126.78, 124.34, 123.98, 123.56, 115.82, 113.46, 40.23, 29.24; HRMS (ESI+): Calculated for $C_{22}H_{19}N_3O$: $[M+Na]^+$ 364.1420, Found 364.1416.

3-(4-(Di-*p*-tolylamino)phenyl)-1-methylquinoxalin-2(1*H*)-one (18)



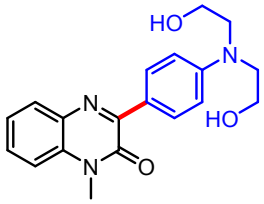
Obtained as a yellow liquid (71 mg, 82% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.24 (d, J = 8.8 Hz, 2H), 7.89 (d, J = 8.0 Hz, 1H), 7.49 (dd, J = 11.4, 4.1 Hz, 1H), 7.33 (d, J = 7.5 Hz, 1H), 7.29 (d, J = 8.4 Hz, 1H), 7.10 (s, 1H), 7.08 (s, 3H), 7.06 (d, J = 2.7 Hz, 4H), 7.04 (d, J = 3.3 Hz, 2H), 3.74 (s, 3H), 2.33 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.95, 153.24, 150.29, 144.63, 133.46, 133.29, 133.07, 130.74, 130.02, 129.99, 129.52, 128.37, 125.49, 123.66, 120.34, 113.49, 29.28, 20.92; HRMS (ESI+): Calculated for $C_{29}H_{25}N_3O$: $[M+Na]^+$ 454.1890, Found 454.1883.

3-(4-((2-Hydroxyethyl)(methyl)amino)phenyl)-1-methylquinoxalin-2(1*H*)-one (19)



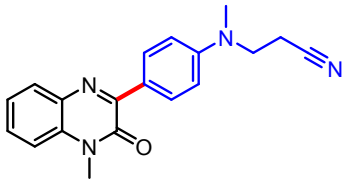
Obtained as a yellow liquid (44 mg, 71% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.31 (d, J = 9.0 Hz, 2H), 7.81 (d, J = 7.9 Hz, 1H), 7.42 – 7.37 (m, 1H), 7.24 (t, J = 7.6 Hz, 1H), 7.20 (d, J = 5.6 Hz, 1H), 6.89 (s, 2H), 3.76 (t, J = 5.6 Hz, 2H), 3.64 (s, 3H), 3.50 (t, J = 5.5 Hz, 2H), 3.02 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.93, 152.62, 149.75, 133.12, 132.90, 131.44, 129.69, 129.38, 123.67, 113.50, 113.16, 111.21, 59.45, 56.13, 40.24, 29.28; HRMS (ESI+): Calculated for $C_{18}H_{19}N_3O_2$: $[M+Na]^+$ 332.1369, Found 332.1370.

3-(4-(Bis(2-hydroxyethyl)amino)phenyl)-1-methylquinoxalin-2(1*H*)-one (20)



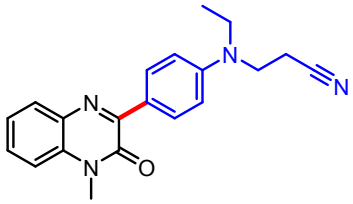
Obtained as a yellow liquid (50 mg, 74% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.11 (d, J = 8.8 Hz, 2H), 7.67 (d, J = 7.9 Hz, 1H), 7.24 (t, J = 7.7 Hz, 1H), 7.11 (t, J = 7.6 Hz, 1H), 7.06 (d, J = 8.3 Hz, 1H), 6.54 (d, J = 8.9 Hz, 2H), 4.67 (s, 2H), 3.66 (t, J = 4.7 Hz, 4H), 3.52 (s, 3H), 3.44 (t, J = 4.6 Hz, 4H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.91, 152.79, 149.50, 133.28, 132.62, 131.13, 129.43, 128.88, 123.79, 123.54, 113.49, 111.36, 60.19, 54.83, 29.23; HRMS (ESI+): Calculated for $C_{19}H_{21}N_3O_3$: $[M+Na]^+$ 362.1475, Found 362.1470.

3-(Methyl(4-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)phenyl)amino)propanenitrile (21)



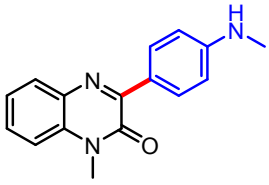
Obtained as a yellow liquid (44 mg, 70% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.42 (d, J = 9.0 Hz, 2H), 7.89 (d, J = 9.1 Hz, 1H), 7.48 (t, J = 8.4 Hz, 1H), 7.32 (t, J = 7.6 Hz, 1H), 7.28 (d, J = 8.4 Hz, 1H), 6.75 (d, J = 9.1 Hz, 2H), 3.78 (t, J = 6.9 Hz, 2H), 3.73 (s, 3H), 3.12 (s, 3H), 2.62 (t, J = 6.8 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.97, 152.83, 149.06, 133.25, 132.94, 131.51, 129.78, 129.28, 125.27, 123.59, 118.23, 113.48, 111.42, 48.62, 38.90, 29.24, 15.40; HRMS (ESI+): Calculated for $C_{19}H_{18}N_4O$: $[M+Na]^+$ 341.1373, Found 341.1375.

3-(Ethyl(4-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)phenyl)amino)propanenitrile (22)



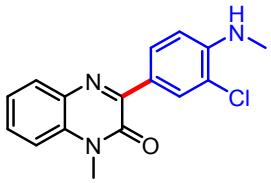
Obtained as a yellow liquid (48 mg, 72% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.40 (d, J = 9.1 Hz, 2H), 7.86 (d, J = 8.0 Hz, 1H), 7.46 (t, J = 7.8 Hz, 1H), 7.31 (t, J = 8.4 Hz, 1H), 7.26 (d, J = 8.2 Hz, 1H), 6.71 (d, J = 9.1 Hz, 2H), 3.71 (d, J = 8.9 Hz, 5H), 3.51 (q, J = 7.0 Hz, 2H), 2.63 (t, J = 6.9 Hz, 2H), 1.22 (t, J = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.96, 152.83, 147.96, 134.67, 134.12, 133.34, 132.91, 131.57, 129.78, 129.18, 124.93, 123.55, 118.25, 113.48, 111.23, 46.47, 45.65, 29.22, 16.19, 12.57; HRMS (ESI+): Calculated for $C_{20}H_{20}N_4O$: $[M+Na]^+$ 355.1529, Found 355.1523.

1-Methyl-3-(4-(methylamino)phenyl)quinoxalin-2(1*H*)-one (23)



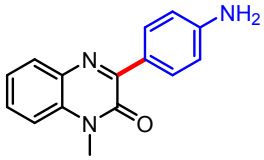
Obtained as a yellow liquid (37 mg, 70% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.38 (d, J = 8.7 Hz, 2H), 7.88 (d, J = 7.9 Hz, 1H), 7.48 (t, J = 7.7 Hz, 1H), 7.32 (t, J = 7.5 Hz, 1H), 7.28 (d, J = 8.3 Hz, 1H), 6.68 (d, J = 8.7 Hz, 2H), 3.75 (s, 3H), 2.91 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.06, 153.20, 151.10, 133.41, 132.90, 131.37, 129.76, 128.98, 125.11, 123.52, 113.39, 111.59, 30.45, 29.21; HRMS (ESI+): Calculated for $C_{16}H_{15}N_3O$: $[M+Na]^+$ 288.1107, Found 288.1108.

3-(3-Chloro-4-(methylamino)phenyl)-1-methylquinoxalin-2(1*H*)-one (24)



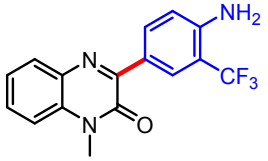
Obtained as a yellow liquid (38 mg, 63% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.52 (d, J = 1.9 Hz, 1H), 8.45 (dd, J = 8.7, 1.9 Hz, 1H), 7.93 (d, J = 7.9 Hz, 1H), 7.55 – 7.48 (m, 1H), 7.35 (t, J = 7.2 Hz, 1H), 7.31 (d, J = 8.3 Hz, 1H), 6.72 (d, J = 8.7 Hz, 1H), 3.76 (s, 3H), 2.99 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.88, 151.82, 146.68, 133.19, 132.93, 130.44, 130.10, 129.86, 129.39, 124.99, 123.68, 118.61, 113.46, 109.49, 30.24, 29.24; HRMS (ESI+): Calculated for $C_{16}H_{14}ClN_3O$: $[M+Na]^+$ 322.0718, Found 322.0716.

3-(4-Aminophenyl)-1-methylquinoxalin-2(1*H*)-one (25)



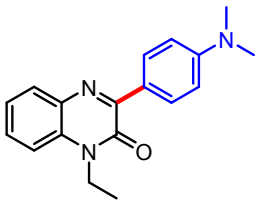
Obtained as a yellow liquid (26 mg, 52% yield); ^{1}H NMR (500 MHz, DMSO) δ 8.23 (d, J = 8.8 Hz, 2H), 7.78 (dd, J = 7.9, 1.0 Hz, 1H), 7.58 – 7.49 (m, 2H), 7.35 (ddd, J = 8.1, 6.8, 1.7 Hz, 1H), 6.62 (d, J = 8.8 Hz, 2H), 5.74 (s, 2H), 3.67 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 154.66, 152.43, 151.79, 133.03, 133.03, 131.53, 129.41, 129.18, 123.84, 123.55, 114.88, 113.12, 29.57; HRMS (ESI+): Calculated for $C_{15}H_{13}N_3O$: $[M+Na]^+$ 274.0951, Found 274.0952.

3-(4-Amino-3-(trifluoromethyl)phenyl)-1-methylquinoxalin-2(1*H*)-one (26)



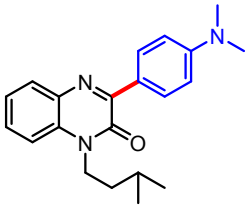
Obtained as a yellow liquid (29 mg, 45% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.62 (s, 1H), 8.41 (d, J = 10.0 Hz, 1H), 7.85 (d, J = 9.1 Hz, 1H), 7.47 (t, J = 7.8 Hz, 1H), 7.29 (t, J = 7.6 Hz, 1H), 7.25 (d, J = 8.3 Hz, 1H), 6.74 (d, J = 8.6 Hz, 1H), 3.70 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.80, 151.80, 146.27 (q, J = 1.3 Hz), 134.33, 133.05, 133.04, 130.05, 129.84, 128.84 (q, J = 5.0 Hz), 125.50, 124.91 (q, J = 272.2 Hz), 123.80, 116.37, 113.54, 113.10 (q, J = 30.2 Hz), 29.28; ^{19}F NMR (471 MHz, $CDCl_3$) δ -70.27; HRMS (ESI+): Calculated for $C_{16}H_{12}F_3N_3O$: $[M+Na]^+$ 342.0825, Found342.0825.

3-(4-(Dimethylamino)phenyl)-1-ethylquinoxalin-2(1*H*)-one (27)



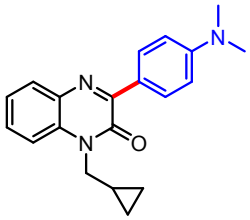
Obtained as a yellow liquid (47 mg, 79% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.37 (d, J = 9.2 Hz, 2H), 7.83 (d, J = 7.9 Hz, 1H), 7.42 – 7.38 (m, 1H), 7.23 (d, J = 7.8 Hz, 2H), 6.76 (d, J = 7.3 Hz, 2H), 4.30 (d, J = 7.2 Hz, 2H), 2.98 (s, 6H), 1.34 (d, J = 7.2 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.53, 152.98, 151.34, 133.69, 131.80, 131.25, 130.01, 129.05, 123.36, 121.02, 113.26, 111.97, 40.68, 37.45, 12.44; HRMS (ESI+): Calculated for $C_{18}H_{19}N_3O$: $[M+Na]^+$ 316.1420, Found 316.1420.

3-(4-(Dimethylamino)phenyl)-1-isopentylquinoxalin-2(1*H*)-one (28)



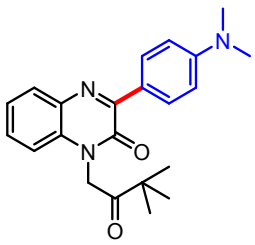
Obtained as a yellow liquid (57 mg, 78% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.43 (d, J = 9.1 Hz, 2H), 7.89 (d, J = 6.6 Hz, 1H), 7.47 (t, J = 7.1 Hz, 1H), 7.31 (t, J = 7.1 Hz, 1H), 7.27 (d, J = 8.4 Hz, 1H), 6.79 (d, J = 8.5 Hz, 2H), 4.33 – 4.29 (m, 2H), 3.05 (s, 6H), 1.82 (dt, J = 13.3, 6.7 Hz, 1H), 1.70 – 1.65 (m, 2H), 1.06 (d, J = 6.6 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.69, 153.02, 151.59, 133.75, 132.00, 131.19, 129.98, 128.90, 123.30, 122.17, 113.31, 111.57, 41.11, 40.43, 35.81, 26.66, 22.56; HRMS (ESI+): Calculated for $C_{21}H_{25}N_3O$: $[M+Na]^+$ 358.1890, Found 358.1891.

1-(Cyclopropylmethyl)-3-(4-(dimethylamino)phenyl)quinoxalin-2(1*H*)-one (29)



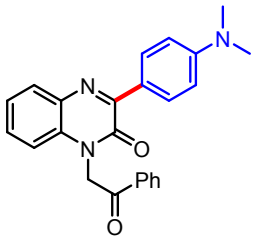
Obtained as a yellow liquid (49 mg, 72% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.33 (d, J = 8.9 Hz, 2H), 7.82 (dd, J = 8.0, 1.1 Hz, 1H), 7.41 – 7.38 (m, 1H), 7.33 (d, J = 8.1 Hz, 1H), 7.23 (t, J = 7.5 Hz, 1H), 6.73 (d, J = 7.9 Hz, 2H), 4.19 (d, J = 7.0 Hz, 2H), 2.97 (s, 6H), 1.24 (s, 1H), 0.52 (d, J = 3.8 Hz, 2H), 0.47 (d, J = 7.6 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.04, 153.32, 151.53, 133.64, 132.29, 131.18, 129.96, 128.88, 123.32, 123.21, 113.70, 111.70, 46.08, 40.50, 9.69, 4.16; HRMS (ESI+): Calculated for $C_{20}H_{21}N_3O$: $[M+H]^+$ 320.1757, Found 320.1757.

1-(3,3-Dimethyl-2-oxobutyl)-3-(4-(dimethylamino)phenyl)quinoxalin-2(1*H*)-one (30)



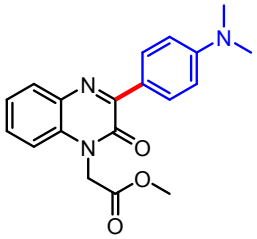
Obtained as a yellow liquid (48 mg, 78% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.31 (d, J = 9.1 Hz, 2H), 7.81 (dd, J = 8.0, 1.3 Hz, 1H), 7.32 – 7.28 (m, 1H), 7.22 – 7.19 (m, 1H), 6.75 (t, J = 8.3 Hz, 3H), 5.20 (s, 2H), 2.96 (s, 6H), 1.28 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 206.86, 154.61, 152.49, 150.88, 133.41, 132.37, 131.24, 129.99, 129.13, 123.61, 123.56, 112.84, 112.37, 47.09, 43.83, 40.95, 26.55; HRMS (ESI+): Calculated for $C_{22}H_{25}N_3O_2$: $[M+Na]^+$ 386.1839, Found 386.1839.

3-(4-(Dimethylamino)phenyl)-1-(2-oxo-2-phenylethyl)quinoxalin-2(1*H*)-one (31)



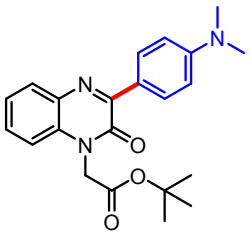
Obtained as a yellow liquid (60 mg, 70% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.37 (d, J = 9.1 Hz, 2H), 8.02 (d, J = 7.8 Hz, 2H), 7.85 (d, J = 6.6 Hz, 1H), 7.59 (t, J = 7.4 Hz, 1H), 7.47 (t, J = 7.7 Hz, 2H), 7.30 (t, J = 7.1 Hz, 1H), 7.23 (t, J = 7.6 Hz, 1H), 6.86 (d, J = 8.1 Hz, 1H), 6.75 (s, 2H), 5.70 (s, 2H), 2.98 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 191.51, 154.78, 152.62, 134.72, 134.22, 133.57, 132.30, 131.27, 130.01, 129.61, 129.38, 129.11, 129.04, 128.20, 123.73, 113.27, 111.95, 48.64, 40.66; HRMS (ESI+): Calculated for $C_{24}H_{21}N_3O_2$: $[M+Na]^+$ 406.1526, Found 406.1550.

Methyl 2-(3-(4-(dimethylamino)phenyl)-2-oxoquinoxalin-1(2*H*)-yl)acetate (32)



Obtained as a yellow liquid (52 mg, 77% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.44 (d, J = 9.1 Hz, 2H), 7.91 (dd, J = 8.0, 1.4 Hz, 1H), 7.47 – 7.43 (m, 1H), 7.35 – 7.32 (m, 1H), 7.06 (d, J = 7.7 Hz, 1H), 6.78 (d, J = 8.5 Hz, 2H), 5.10 (s, 2H), 3.78 (s, 3H), 3.06 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 167.94, 154.64, 152.66, 151.32, 149.93, 133.49, 132.00, 131.27, 130.10, 129.23, 123.92, 112.79, 112.05, 52.82, 46.19, 43.63, 40.76; HRMS (ESI+): Calculated for $C_{19}H_{19}N_3O_3$: $[M+Na]^+$ 360.1319, Found 360.1323.

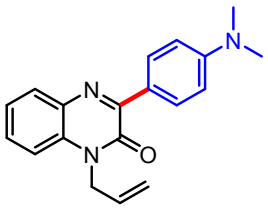
***Tert*-butyl 2-(3-(4-(dimethylamino)phenyl)-2-oxoquinoxalin-1(2*H*)-yl)acetate (33)**



Obtained as a yellow liquid (61 mg, 80% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.37 (d, J = 8.8 Hz, 2H), 7.85 (d, J = 7.8 Hz, 1H), 7.39 (t, J = 7.5 Hz, 1H), 7.26 (t, J = 7.5 Hz, 1H), 6.99 (d, J = 8.3 Hz,

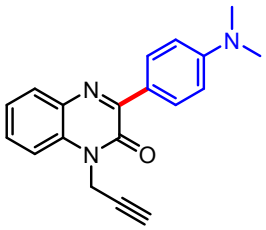
1H), 6.83 (s, 2H), 4.93 (s, 2H), 3.00 (s, 6H), 1.39 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.40, 154.60, 152.71, 151.85, 133.38, 132.17, 131.30, 130.06, 129.90, 129.21, 123.79, 112.93, 112.14, 83.03, 44.41, 29.72, 28.01; HRMS (ESI+): Calculated for $C_{22}H_{25}N_3O_3$: $[M+Na]^+$ 402.1788, Found 402.1784.

1-Allyl-3-(4-(dimethylamino)phenyl)quinoxalin-2(1*H*)-one (34)



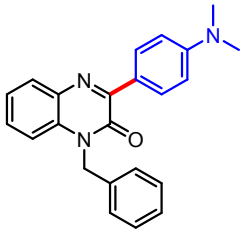
Obtained as a yellow liquid (46 mg, 75% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.39 (d, J = 9.1 Hz, 2H), 7.83 (d, J = 8.0 Hz, 1H), 7.37 (t, J = 7.8 Hz, 1H), 7.24 (t, J = 7.6 Hz, 1H), 7.18 (d, J = 8.4 Hz, 1H), 6.82 (s, 2H), 5.93 – 5.86 (m, 1H), 5.19 (d, J = 10.4 Hz, 1H), 5.12 (d, J = 17.2 Hz, 1H), 4.88 (d, J = 5.1 Hz, 2H), 2.99 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.56, 152.76, 152.72, 133.44, 132.14, 131.36, 130.97, 130.87, 129.86, 129.16, 123.61, 117.94, 113.99, 112.56, 44.67, 41.12; HRMS (ESI+): Calculated for $C_{19}H_{19}N_3O$: $[M+Na]^+$ 328.1420, Found 328.1431.

3-(4-(Dimethylamino)phenyl)-1-(prop-2-yn-1-yl)quinoxalin-2(1*H*)-one (35)



Obtained as a yellow liquid (47 mg, 77 % yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.44 (d, J = 9.2 Hz, 2H), 7.88 (dd, J = 8.0, 1.3 Hz, 1H), 7.49 (t, J = 7.8 Hz, 1H), 7.41 (d, J = 8.2 Hz, 1H), 7.35 – 7.32 (m, 1H), 6.77 (d, J = 8.8 Hz, 2H), 5.09 (d, J = 2.4 Hz, 2H), 3.05 (s, 6H), 2.28 (t, J = 2.5 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.08, 152.81, 151.79, 133.65, 131.32, 131.21, 129.81, 128.94, 123.88, 120.91, 113.82, 111.41, 77.29, 72.87, 40.29, 31.54; HRMS (ESI+): Calculated for $C_{19}H_{17}N_3O$: $[M+Na]^+$ 326.1264, Found 326.1265.

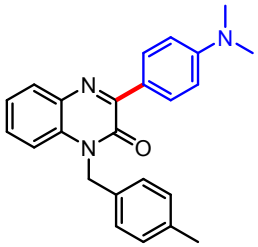
1-Benzyl-3-(4-(dimethylamino)phenyl)quinoxalin-2(1*H*)-one (36)



Obtained as a yellow liquid (57 mg, 79 % yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.42 (d, J = 9.1 Hz, 2H), 7.83 (d, J = 7.9 Hz, 1H), 7.28 (t, J = 7.8 Hz, 1H), 7.24 – 7.22 (m, 2H), 7.19 (dd, J = 13.4, 5.5 Hz, 4H), 7.15 (d, J = 8.3 Hz, 1H), 6.79 (s, 2H), 5.49 (s, 2H), 2.99 (s, 6H); ^{13}C NMR (126 MHz,

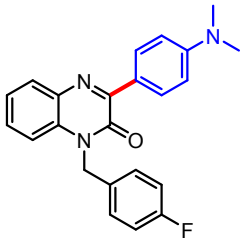
$CDCl_3$) δ 155.10, 153.00, 152.95, 135.58, 133.61, 132.27, 131.37, 129.87, 129.14, 129.02, 128.90, 127.58, 126.92, 123.66, 114.22, 112.42, 46.02, 40.89; HRMS (ESI+): Calculated for $C_{23}H_{21}N_3O$: $[M+Na]^+$ 378.1577, Found 378.1565.

3-(4-(Dimethylamino)phenyl)-1-(4-methylbenzyl)quinoxalin-2(1*H*)-one (37)



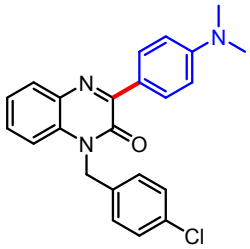
Obtained as a yellow liquid (47 mg, 71% yield); ^1H NMR (500 MHz, $CDCl_3$) δ 8.48 (d, J = 7.7 Hz, 2H), 7.87 (d, J = 6.7 Hz, 1H), 7.33 (t, J = 7.0 Hz, 1H), 7.26 (d, J = 7.7 Hz, 1H), 7.23 (s, 1H), 7.17 (d, J = 8.0 Hz, 2H), 7.09 (d, J = 8.0 Hz, 2H), 6.77 (d, J = 9.0 Hz, 2H), 5.50 (s, 2H), 3.04 (s, 6H), 2.28 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.16, 153.15, 151.84, 137.23, 133.74, 132.69, 132.23, 131.27, 129.78, 129.67, 129.55, 128.87, 126.98, 123.53, 114.23, 111.41, 45.76, 40.30, 21.13; HRMS (ESI+): Calculated for $C_{24}H_{23}N_3O$: $[M+Na]^+$ 392.1733, Found 392.1741.

3-(4-(Dimethylamino)phenyl)-1-(4-fluorobenzyl)quinoxalin-2(1*H*)-one (38)



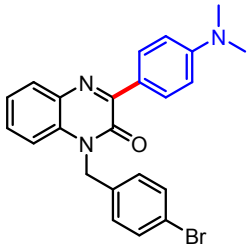
Obtained as a yellow liquid (55 mg, 77% yield); ^1H NMR (500 MHz, $CDCl_3$) δ 8.44 (d, J = 8.8 Hz, 2H), 7.88 (d, J = 7.9 Hz, 1H), 7.35 (t, J = 7.7 Hz, 1H), 7.25 (t, J = 7.6 Hz, 1H), 7.23 – 7.18 (m, 3H), 7.17 (d, J = 8.4 Hz, 1H), 7.04 (s, 1H), 6.93 (t, J = 8.6 Hz, 2H), 5.45 (s, 2H), 3.04 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.28 (d, J = 246.7 Hz), 154.71, 154.70, 151.84, 132.51, 132.48, 132.09, 132.01, 130.99, 130.85, 130.83, 130.41, 128.82 (d, J = 8.2 Hz), 124.28, 115.98 (d, J = 21.7 Hz), 114.25, 45.63, 29.71; ^{19}F NMR (471 MHz, $CDCl_3$) δ -118.38; HRMS (ESI+): Calculated for $C_{23}H_{20}FN_3O$: $[M+Na]^+$ 396.1483, Found 396.1489.

1-(4-Chlorobenzyl)-3-(4-(dimethylamino)phenyl)quinoxalin-2(1*H*)-one (39)



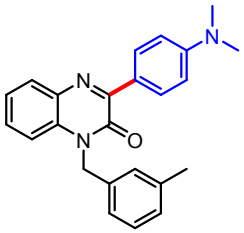
Obtained as a yellow liquid (58 mg, 75% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.40 (d, J = 9.1 Hz, 2H), 7.83 (dd, J = 7.9, 1.4 Hz, 1H), 7.29 (t, J = 7.0 Hz, 1H), 7.24 – 7.20 (m, 2H), 7.18 (d, J = 4.8 Hz, 1H), 7.14 (d, J = 8.5 Hz, 2H), 7.09 (d, J = 9.0 Hz, 1H), 6.77 (s, 2H), 5.43 (s, 2H), 2.99 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.04, 152.96, 151.48, 134.16, 133.67, 133.43, 132.05, 131.99, 131.31, 129.97, 129.24, 129.08, 128.42, 123.79, 113.94, 111.91, 45.41, 40.64, 29.73; HRMS (ESI+): Calculated for $C_{23}H_{20}ClN_3O$: $[M+Na]^+$ 412.1187, Found 412.1151.

1-(4-Bromobenzyl)-3-(4-(dimethylamino)phenyl)quinoxalin-2(1*H*)-one (40)



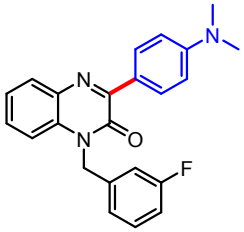
Obtained as a yellow liquid (62 mg, 72% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.47 (d, J = 9.1 Hz, 2H), 7.90 (dd, J = 7.9, 1.4 Hz, 1H), 7.43 (d, J = 8.4 Hz, 2H), 7.36 (t, J = 7.0 Hz, 1H), 7.30 (t, J = 7.0 Hz, 1H), 7.16 (d, J = 8.4 Hz, 3H), 6.81 (d, J = 7.3 Hz, 2H), 5.49 (s, 2H), 3.06 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.04, 152.98, 151.54, 134.71, 133.69, 132.02, 131.98, 131.30, 129.97, 129.05, 128.75, 128.20, 123.79, 121.50, 113.92, 111.86, 45.46, 40.58; HRMS (ESI+): Calculated for $C_{23}H_{20}BrN_3O$: $[M+Na]^+$ 456.0682, Found 456.0668.

3-(4-(Dimethylamino)phenyl)-1-(3-methylbenzyl)quinoxalin-2(1*H*)-one (41)



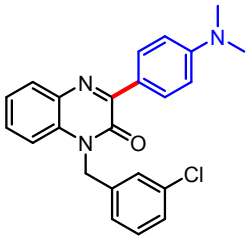
Obtained as a yellow liquid (52 mg, 70% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.43 (d, J = 9.1 Hz, 2H), 7.83 (d, J = 6.6 Hz, 1H), 7.29 (s, 1H), 7.21 (t, J = 7.6 Hz, 1H), 7.16 (d, J = 8.3 Hz, 1H), 7.13 – 7.10 (m, 1H), 7.01 – 6.97 (m, 3H), 6.81 (s, 2H), 5.45 (s, 2H), 3.00 (s, 6H), 2.21 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.11, 152.90, 150.87, 138.69, 135.50, 133.56, 132.34, 131.40, 129.83, 129.21, 128.76, 128.39, 128.18, 127.48, 123.95, 123.65, 114.31, 112.49, 46.07, 41.12, 21.47; HRMS (ESI+): Calculated for $C_{24}H_{23}N_3O$: $[M+Na]^+$ 392.1733, Found 392.1734.

3-(4-(Dimethylamino)phenyl)-1-(3-fluorobenzyl)quinoxalin-2(1*H*)-one (42)



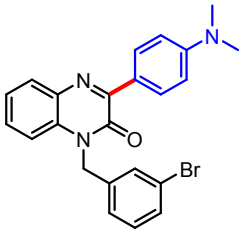
Obtained as a yellow liquid (50 mg, 70% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.48 (d, J = 9.1 Hz, 2H), 7.90 (d, J = 9.4 Hz, 1H), 7.35 (d, J = 6.9 Hz, 1H), 7.31 – 7.27 (m, 2H), 7.16 (d, J = 8.3 Hz, 1H), 7.06 (d, J = 7.7 Hz, 1H), 6.98 – 6.94 (m, 2H), 6.78 (d, J = 8.8 Hz, 2H), 5.53 (s, 2H), 3.06 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.15 (d, J = 246.7 Hz), 155.06, 153.06, 151.93, 138.25 (d, J = 7.2 Hz), 133.75, 132.00, 131.25, 130.52, 130.45, 129.93, 128.93, 123.74, 122.51 (d, J = 2.5 Hz), 114.59 (d, J = 21.1 Hz), 114.09, 113.91, 111.38, 45.53, 40.26; ^{19}F NMR (471 MHz, $CDCl_3$) δ -113.66; HRMS (ESI+): Calculated for $C_{23}H_{20}FN_3O$: $[M+Na]^+$ 396.1483, Found 396.1483.

1-(3-Chlorobenzyl)-3-(4-(dimethylamino)phenyl)quinoxalin-2(1*H*)-one(43)



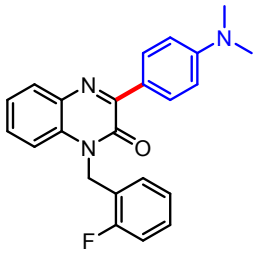
Obtained as a yellow liquid (55 mg, 71% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.44 (d, J = 8.9 Hz, 2H), 7.87 (d, J = 8.9 Hz, 1H), 7.34 (t, J = 8.3 Hz, 1H), 7.26 (d, J = 7.2 Hz, 1H), 7.19 (s, 1H), 7.17 (d, J = 4.7 Hz, 2H), 7.14 – 7.05 (m, 3H), 7.02 (s, 1H), 5.45 (s, 2H), 3.03 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.91, 152.56, 151.68, 137.52, 134.89, 133.41, 132.14, 131.61, 131.55, 130.25, 130.14, 129.72, 127.99, 127.03, 125.14, 125.09, 124.01, 114.02, 45.62, 29.72; HRMS (ESI+): Calculated for $C_{23}H_{20}ClN_3O$: $[M+Na]^+$ 412.1187, Found 412.1179.

1-(3-Bromobenzyl)-3-(4-(dimethylamino)phenyl)quinoxalin-2(1*H*)-one (44)



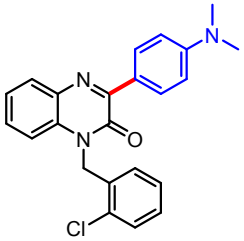
Obtained as a yellow liquid (60 mg, 69% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.48 (d, J = 9.1 Hz, 2H), 7.91 (dd, J = 7.9, 1.4 Hz, 1H), 7.44 (s, 1H), 7.37 (d, J = 8.5 Hz, 2H), 7.31 (t, J = 7.6 Hz, 1H), 7.20 – 7.15 (m, 3H), 6.80 (d, J = 8.7 Hz, 2H), 5.52 (s, 2H), 3.07 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.04, 152.98, 145.07, 137.97, 133.69, 131.99, 131.30, 130.85, 130.48, 129.99, 129.92, 129.13, 129.11, 125.55, 123.83, 123.03, 113.90, 111.92, 45.48, 40.60; HRMS (ESI+): Calculated for $C_{23}H_{20}BrN_3O$: $[M+Na]^+$ 456.0682, Found 456.0682.

3-(4-(Dimethylamino)phenyl)-1-(2-fluorobenzyl)quinoxalin-2(1*H*)-one (45)



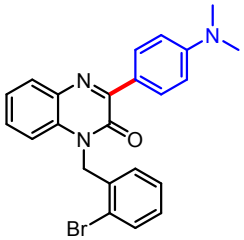
Obtained as a yellow liquid (48 mg, 64% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.49 (d, J = 9.1 Hz, 2H), 7.90 (dd, J = 7.9, 1.3 Hz, 1H), 7.38 (t, J = 7.8 Hz, 1H), 7.30 (t, J = 7.1 Hz, 1H), 7.20 (d, J = 8.5 Hz, 2H), 7.14 – 7.09 (m, 1H), 7.05 (t, J = 7.6 Hz, 1H), 7.00 (t, J = 7.2 Hz, 1H), 6.83 (d, J = 7.5 Hz, 2H), 5.62 (s, 2H), 3.07 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.39 (d, J = 245.6 Hz), 155.25, 152.90, 150.25, 133.64, 131.95, 131.32, 129.90, 129.31, 129.25, 128.46 (d, J = 3.6 Hz), 124.66 (d, J = 3.5 Hz), 123.79, 122.70, 122.59, 115.47 (d, J = 21.4 Hz), 113.79 (d, J = 1.8 Hz), 112.04, 40.66, 39.46 (d, J = 5.4 Hz); ^{19}F NMR (471 MHz, $CDCl_3$) δ -118.42; HRMS (ESI+): Calculated for $C_{23}H_{20}FN_3O$: $[M+Na]^+$ 396.1483, Found 396.1379.

1-(2-Chlorobenzyl)-3-(4-(dimethylamino)phenyl)quinoxalin-2(1*H*)-one (46)



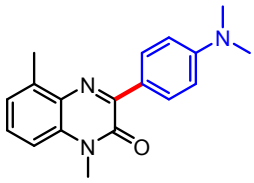
Obtained as a yellow liquid (52 mg, 67% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.54 (d, J = 8.0 Hz, 2H), 8.00 (d, J = 7.9 Hz, 1H), 7.65 (s, 2H), 7.41 (d, J = 8.1 Hz, 2H), 7.32 (t, J = 7.6 Hz, 1H), 7.17 (t, J = 7.7 Hz, 1H), 7.05 (t, J = 8.8 Hz, 2H), 6.73 (d, J = 7.7 Hz, 1H), 5.59 (s, 2H), 3.14 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.71, 153.44, 151.50, 132.72, 132.42, 132.15, 131.99, 131.21, 130.39, 130.36, 129.91, 129.00, 128.36, 127.42, 126.79, 124.47, 119.15, 114.42, 44.02, 29.70; HRMS (ESI+): Calculated for $C_{23}H_{20}ClN_3O$: $[M+Na]^+$ 412.1187, Found 412.1180.

1-(2-Bromobenzyl)-3-(4-(dimethylamino)phenyl)quinoxalin-2(1*H*)-one (47)



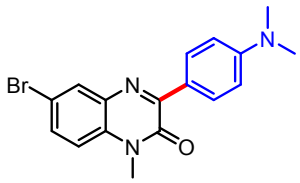
Obtained as a yellow liquid (52 mg, 60% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.51 (s, 2H), 7.93 (s, 1H), 7.64 (s, 1H), 7.34 (d, J = 26.8 Hz, 2H), 7.13 (s, 2H), 7.01 (s, 1H), 6.88 (s, 2H), 6.77 (s, 1H), 5.61 (s, 2H), 3.08 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.07, 153.04, 152.73, 133.97, 133.56, 133.02, 131.97, 131.51, 131.48, 130.70, 130.00, 129.41, 129.03, 127.96, 127.02, 123.95, 122.61, 114.21, 46.46, 46.31; HRMS (ESI+): Calculated for $C_{23}H_{20}BrN_3O$: $[M+Na]^+$ 456.0682, Found 456.0693.

3-(4-(Dimethylamino)phenyl)-1,5-dimethylquinoxalin-2(1*H*)-one (48)



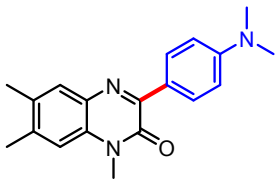
Obtained as a yellow liquid (40 mg, 74% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.45 (d, J = 9.1 Hz, 2H), 7.28 (t, J = 7.9 Hz, 1H), 7.11 (d, J = 7.4 Hz, 1H), 7.05 (d, J = 8.4 Hz, 1H), 6.79 (s, 2H), 3.66 (s, 3H), 2.99 (s, 6H), 2.67 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.93, 150.70, 150.34, 138.48, 132.96, 131.85, 131.22, 128.84, 124.76, 120.99, 112.42, 111.35, 40.81, 29.32, 17.63; HRMS (ESI+): Calculated for $C_{18}H_{19}N_3O$: $[M+Na]^+$ 316.1420, Found 316.1425.

6-Bromo-3-(4-(dimethylamino)phenyl)-1-methylquinoxalin-2(1*H*)-one (49)



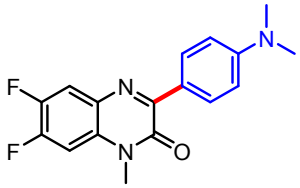
Obtained as a yellow liquid (59 mg, 75% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.43 (d, J = 9.1 Hz, 2H), 7.71 (d, J = 8.7 Hz, 1H), 7.43 – 7.40 (m, 2H), 6.81 (d, J = 8.9 Hz, 2H), 3.70 (s, 3H), 3.06 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.72, 153.01, 151.54, 133.84, 132.29, 131.26, 130.85, 126.74, 122.68, 116.40, 111.80, 111.78, 40.54, 29.31; HRMS (ESI+): Calculated for $C_{17}H_{16}BrN_3O$: $[M+Na]^+$ 380.0369, Found 380.0355.

3-(4-(Dimethylamino)phenyl)-1,6,7-trimethylquinoxalin-2(1*H*)-one (50)



Obtained as a yellow liquid (48 mg, 77% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.40 (d, J = 9.1 Hz, 2H), 7.63 (s, 1H), 7.02 (s, 1H), 6.77 (d, J = 8.9 Hz, 2H), 3.70 (s, 3H), 3.04 (s, 6H), 2.39 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.12, 151.99, 151.50, 138.68, 132.30, 131.81, 130.95, 130.89, 129.81, 124.56, 114.01, 111.47, 40.35, 29.09, 20.53, 19.21; HRMS (ESI+): Calculated for $C_{19}H_{21}N_3O$: $[M+Na]^+$ 330.1577, Found 330.1571.

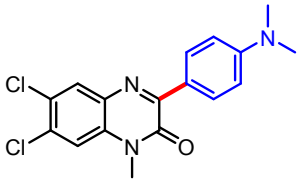
3-(4-(Dimethylamino)phenyl)-6,7-difluoro-1-methylquinoxalin-2(1*H*)-one (51)



Obtained as a yellow liquid (47 mg, 75% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.34 (d, J = 9.1 Hz, 2H), 7.59 (dd, J = 10.4, 8.3 Hz, 1H), 6.99 (dd, J = 11.4, 7.1 Hz, 1H), 6.80 (s, 2H), 3.61 (s, 3H), 3.00 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.67, 153.16 (d, J = 3.3 Hz), 152.02, 150.51 (dd, J = 251.6, 14.3 Hz), 146.70 (dd, J = 245.8, 14.1 Hz), 131.19, 129.82 (d, J = 9.8 Hz), 123.34, 116.94 (d, J = 19.6

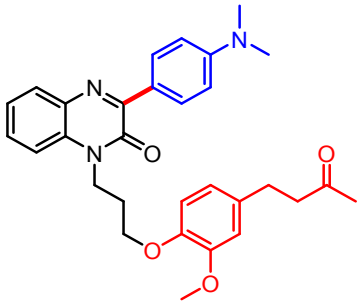
Hz), 111.46, 111.22, 101.92 (d, J = 23.0 Hz), 40.16, 29.69; ^{19}F NMR (471 MHz, $CDCl_3$) δ -83.82, 83.85; HRMS (ESI+): Calculated for $C_{17}H_{15}F_2N_3O$: $[M+Na]^+$ 338.1075, Found 338.1078.

6,7-Dichloro-3-(4-(dimethylamino)phenyl)-1-methylquinoxalin-2(1*H*)-one (52)



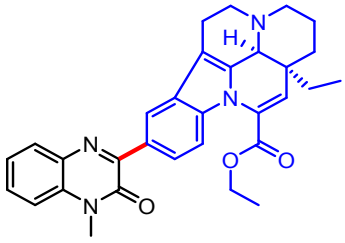
Obtained as a yellow liquid (56 mg, 81% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.36 (d, J = 9.1 Hz, 2H), 7.85 (s, 1H), 7.26 (s, 1H), 6.77 (s, 2H), 3.60 (s, 3H), 3.00 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.46, 153.57, 152.75, 132.64, 132.58, 132.22, 131.46, 130.37, 130.26, 127.17, 114.83, 112.12, 40.76, 29.45; HRMS (ESI+): Calculated for $C_{17}H_{15}Cl_2N_3O$: $[M+Na]^+$ 370.0484, Found 370.0479.

3-(4-(Dimethylamino)phenyl)-1-(3-(2-methoxy-4-(3-oxobutyl)phenoxy)propyl)quinoxalin-2(1*H*)-one (53)



Obtained as a yellow liquid (72 mg, 72% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.42 (d, J = 8.9 Hz, 2H), 7.89 (d, J = 7.7 Hz, 1H), 7.56 (d, J = 8.3 Hz, 1H), 7.42 (t, J = 7.5 Hz, 1H), 7.30 (t, J = 7.5 Hz, 1H), 6.83 (d, J = 8.1 Hz, 1H), 6.80 (d, J = 8.1 Hz, 1H), 6.74 (s, 1H), 6.69 (d, J = 10.1 Hz, 2H), 4.55 (t, J = 7.3 Hz, 2H), 4.14 (t, J = 5.8 Hz, 2H), 3.87 (s, 3H), 3.06 (s, 6H), 2.84 (dd, J = 15.4, 7.7 Hz, 2H), 2.76 – 2.73 (m, 2H), 2.32 (dd, J = 9.8, 4.3 Hz, 2H), 2.14 (d, J = 3.5 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 208.07, 154.94, 149.59, 149.47, 146.76, 146.50, 134.42, 134.01, 133.67, 132.16, 131.19, 129.83, 123.43, 120.21, 113.94, 113.79, 113.69, 112.30, 112.24, 66.75, 65.98, 55.97, 55.93, 45.42, 39.85, 30.17, 29.45, 27.41; HRMS (ESI+): Calculated for $C_{30}H_{33}N_3O_4$: $[M+Na]^+$ 522.2363, Found 522.2361.

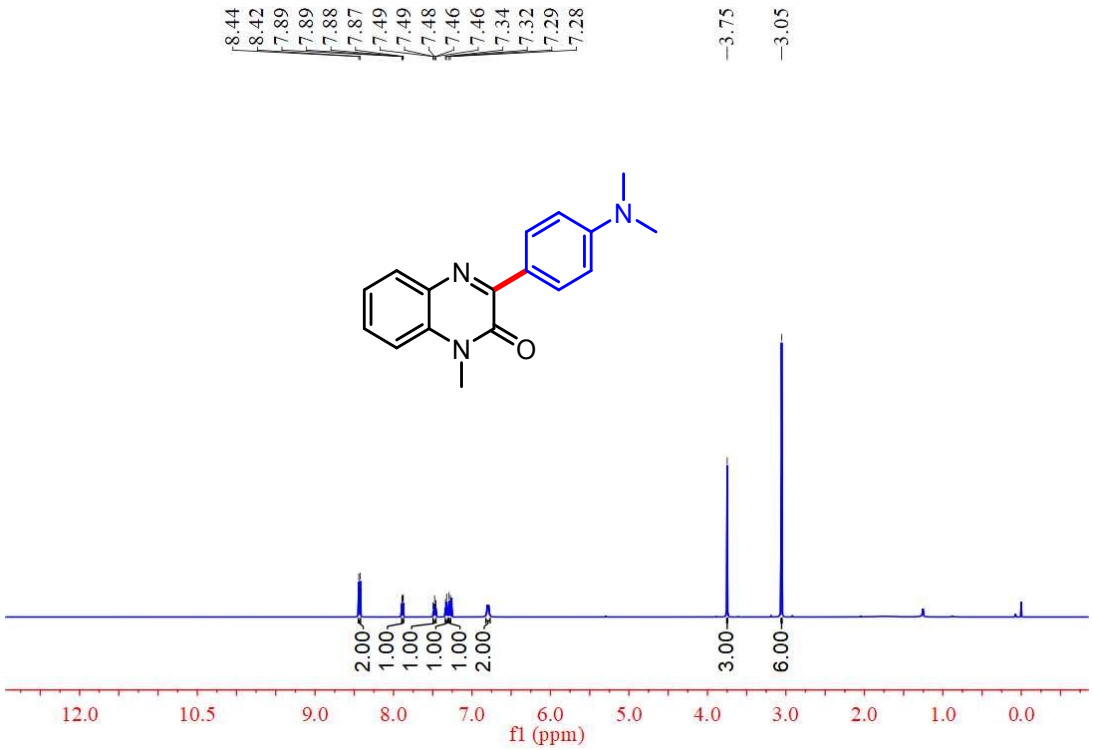
Ethyl(*41S*,*13aS*)-13a-ethyl-8-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)-2,3,41,5,6,13a-hexahydro-1*H*-indolo[3,2,1-de]pyrido[3,2,1-ij][1,5]naphthyridine-12-carboxylate (54)



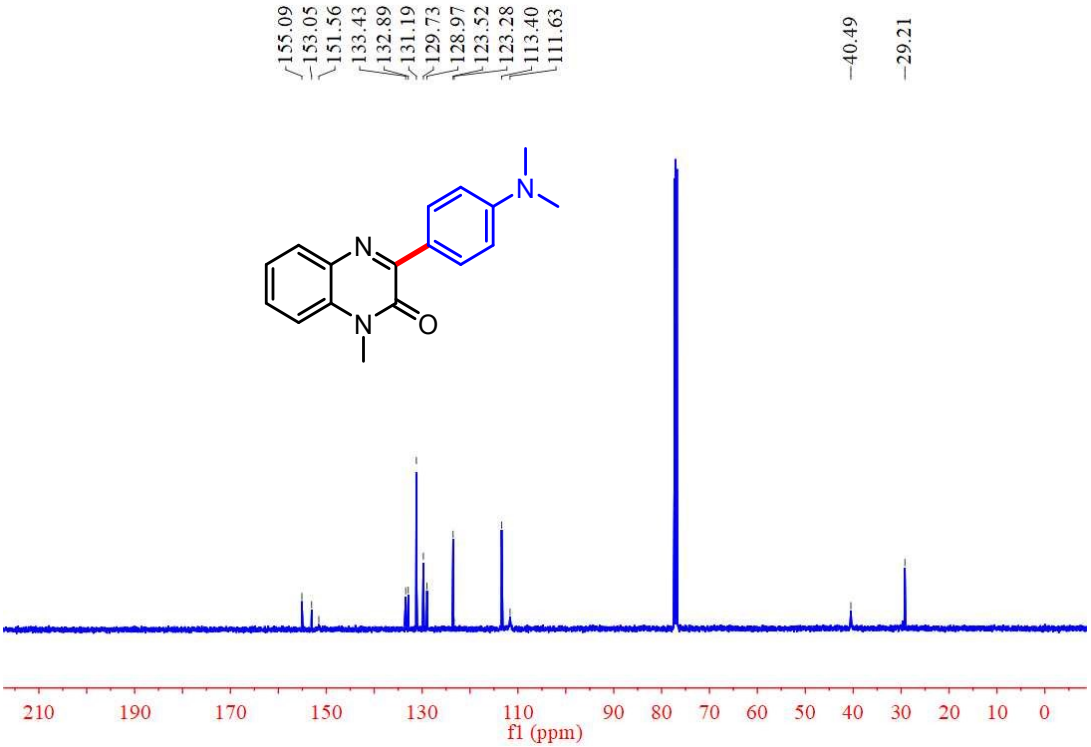
Obtained as a yellow liquid (65 mg, 64% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.74 (s, 1H), 7.58 (d, J = 7.8 Hz, 1H), 7.39 (d, J = 7.7 Hz, 1H), 7.30 (d, J = 7.2 Hz, 1H), 7.22 – 7.18 (m, 1H), 7.16 – 7.12 (m, 1H), 7.08 (t, J = 7.3 Hz, 1H), 6.41 (s, 1H), 4.43 (s, 3H), 3.94 (s, 1H), 3.66 (s, 3H), 3.09 (s, 2H), 3.03 (s, 1H), 2.93 (s, 1H), 2.73 (s, 1H), 1.80 (s, 1H), 1.74 (s, 1H), 1.46 (s, 2H), 1.42 (s, 3H), 1.26 (s, 2H), 1.03 (t, J = 7.4 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.28, 155.03, 151.23, 144.03, 134.70, 131.84, 131.07, 129.57, 128.97, 128.42, 127.76, 126.95, 123.39, 122.32, 120.49, 118.31, 113.14, 112.67, 109.99, 61.90, 53.64, 51.67, 45.80, 37.47, 29.71, 28.45, 27.56, 22.32, 14.26, 8.92, 8.63; HRMS (ESI+): Calculated for $C_{31}H_{32}N_4O_3$: $[M+H]^+$ 509.2547, Found 509.2539.

3. Copies of ^{1}H, ^{13}C and ^{19}F NMR Spectra

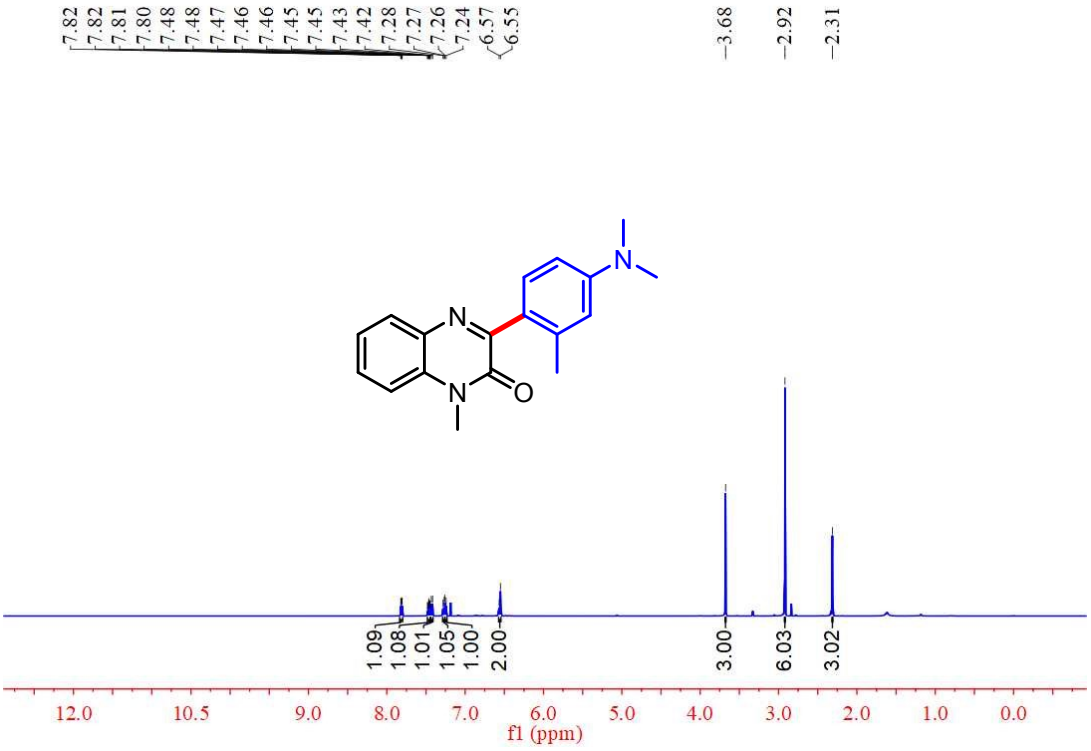
3 ^{1}H NMR (500 MHz, $CDCl_3$)



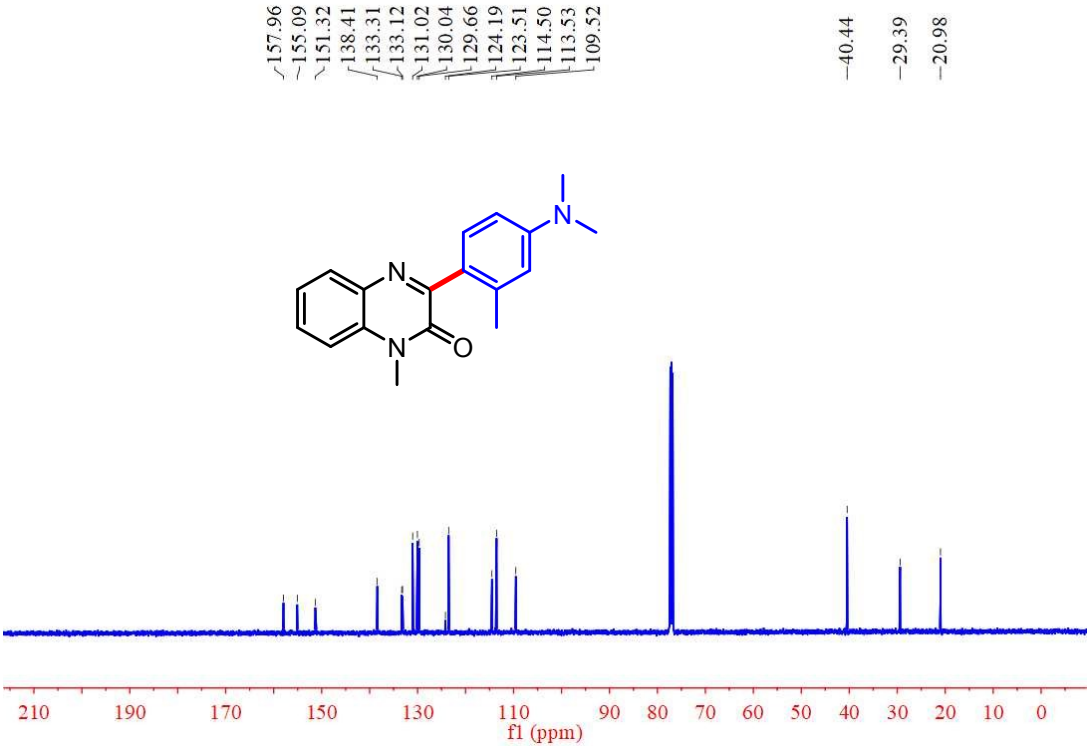
3 ^{13}C NMR (126 MHz, $CDCl_3$)



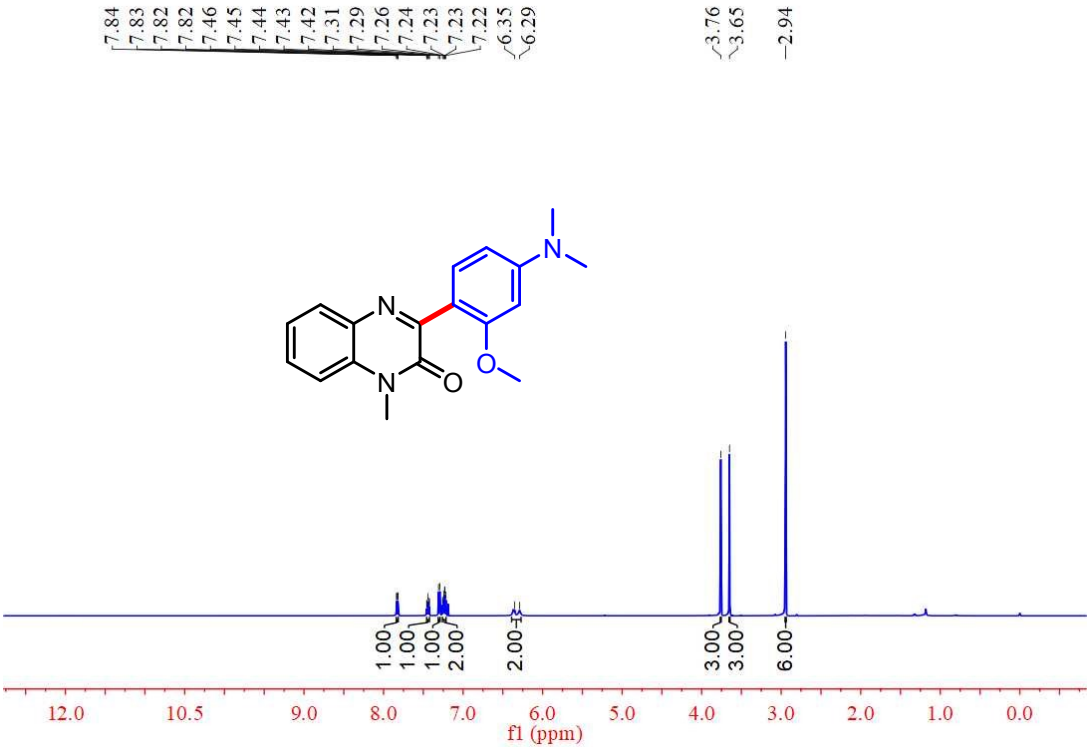
4 ^{1}H NMR (500 MHz, $CDCl_3$)



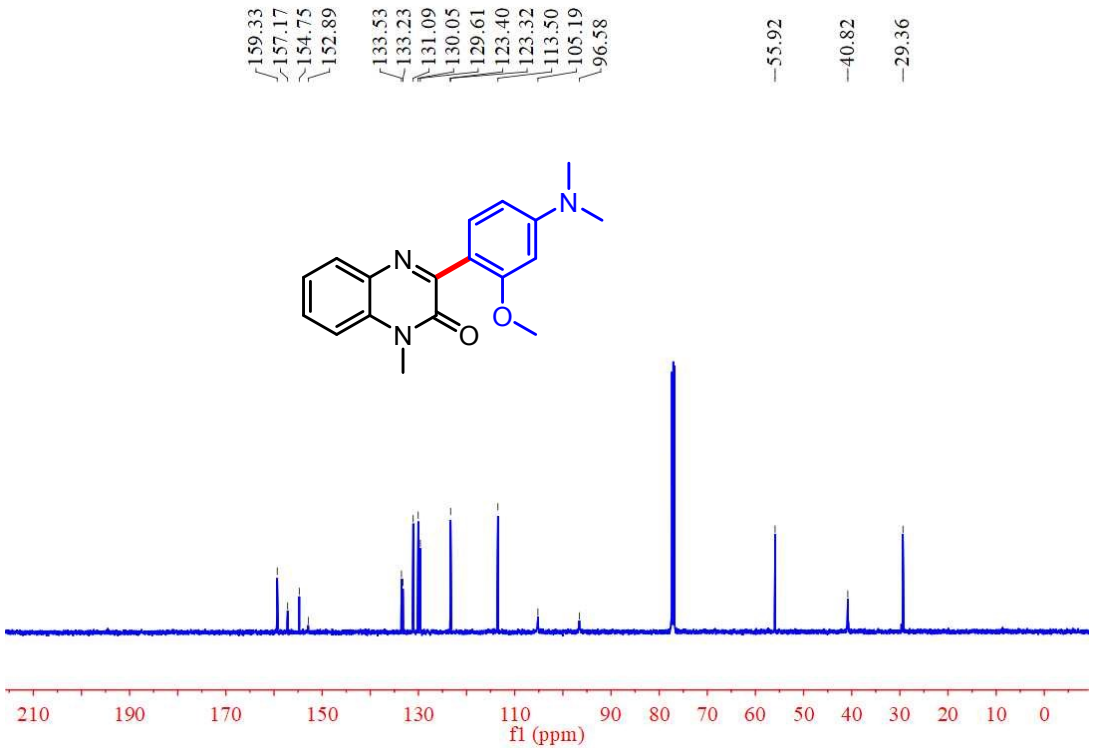
4 ^{13}C NMR (126 MHz, $CDCl_3$)



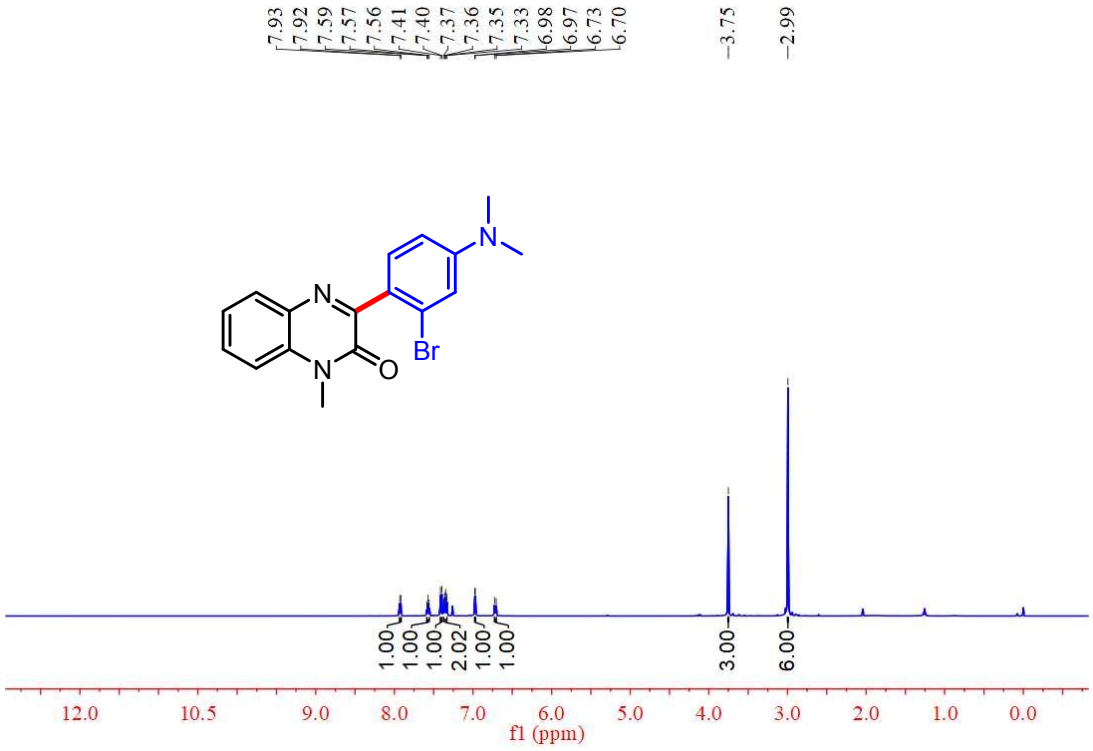
5 ^{1}H NMR (500 MHz, $CDCl_3$)



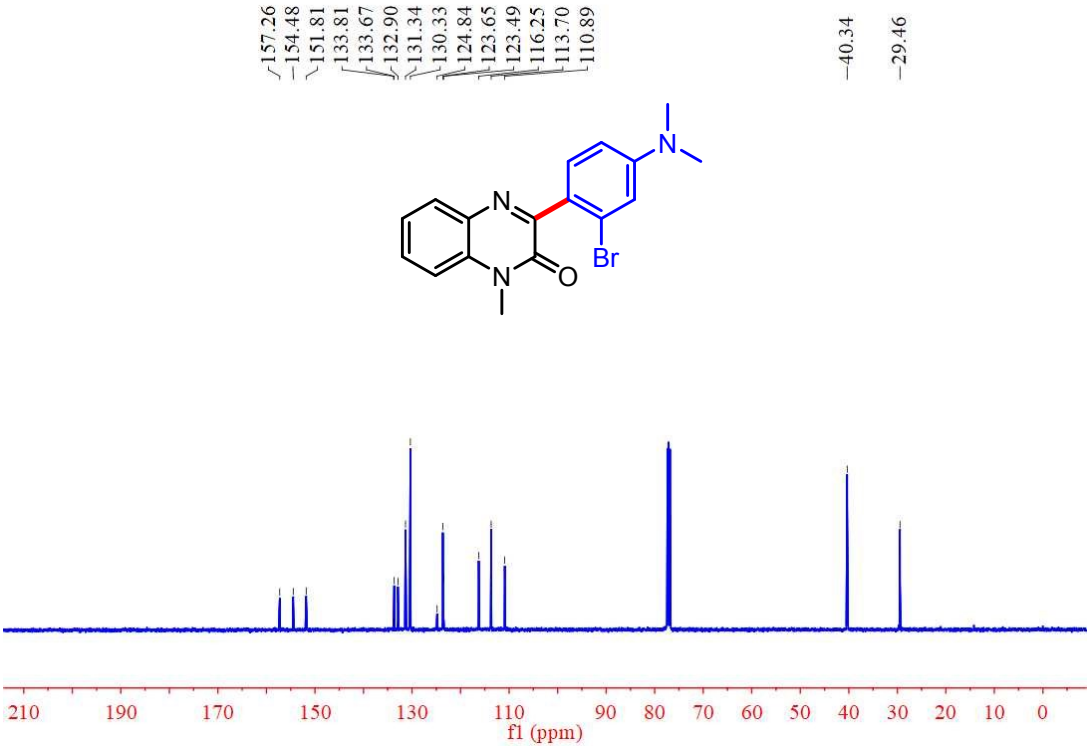
5 ^{13}C NMR (126 MHz, $CDCl_3$)



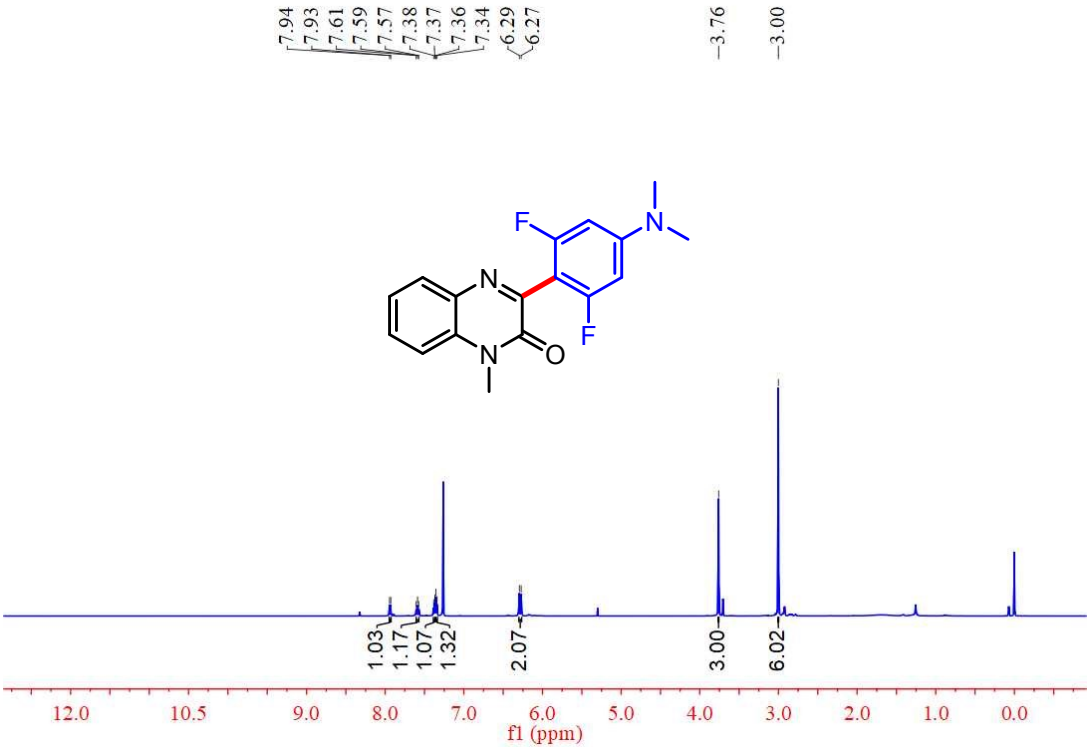
6 ^{1}H NMR (500 MHz, $CDCl_3$)



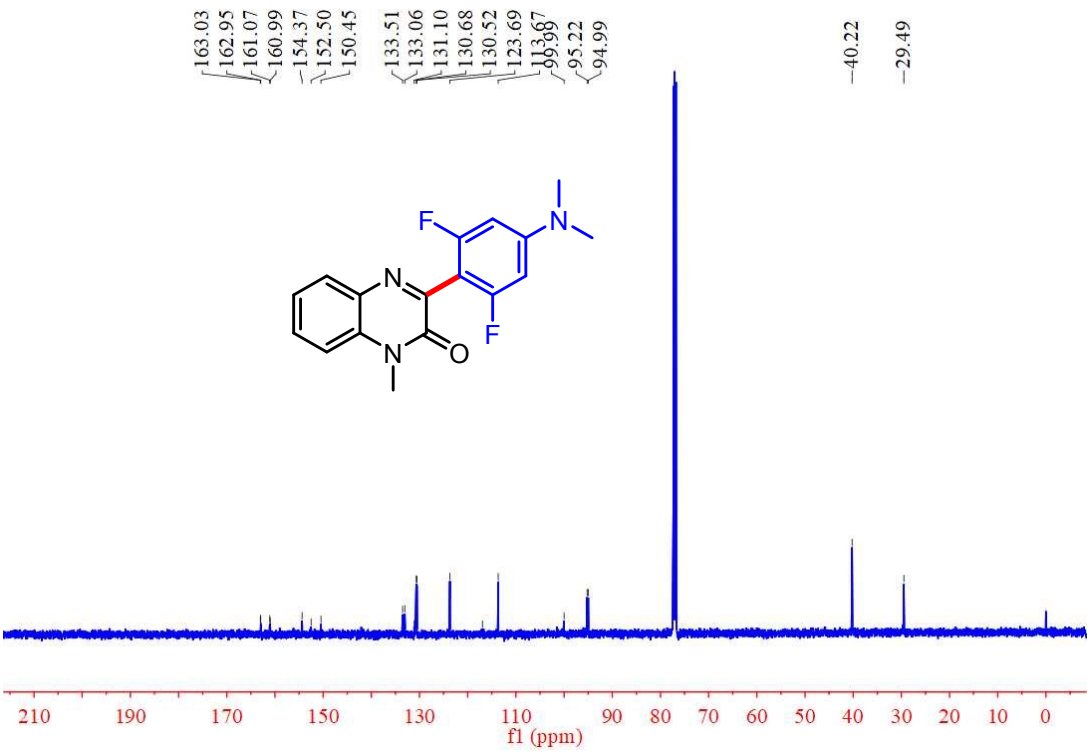
6 ^{13}C NMR (126 MHz, $CDCl_3$)



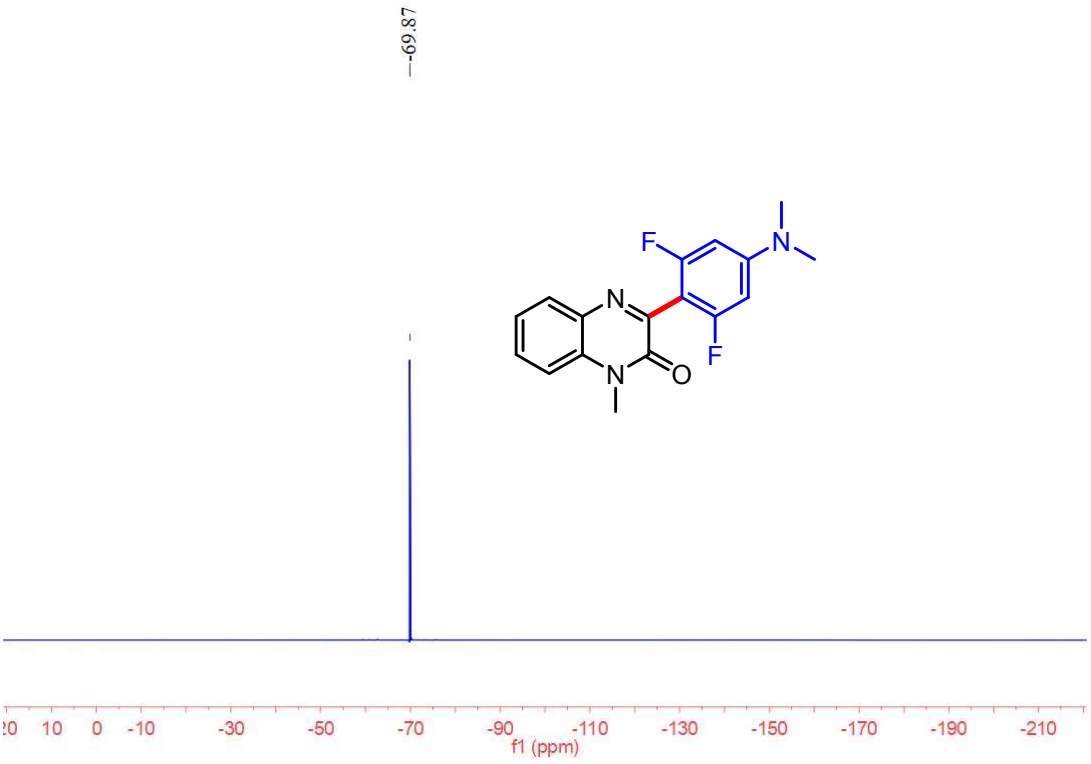
7 ^{1}H NMR (500 MHz, $CDCl_3$)



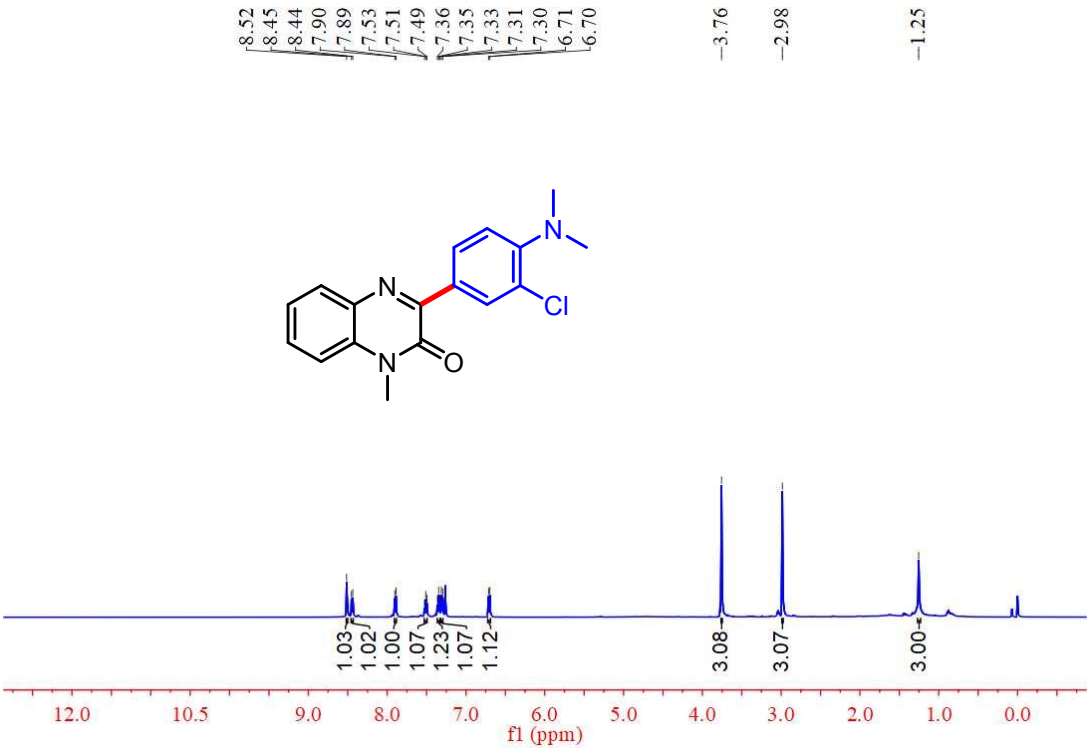
7 ^{13}C NMR (126 MHz, $CDCl_3$)



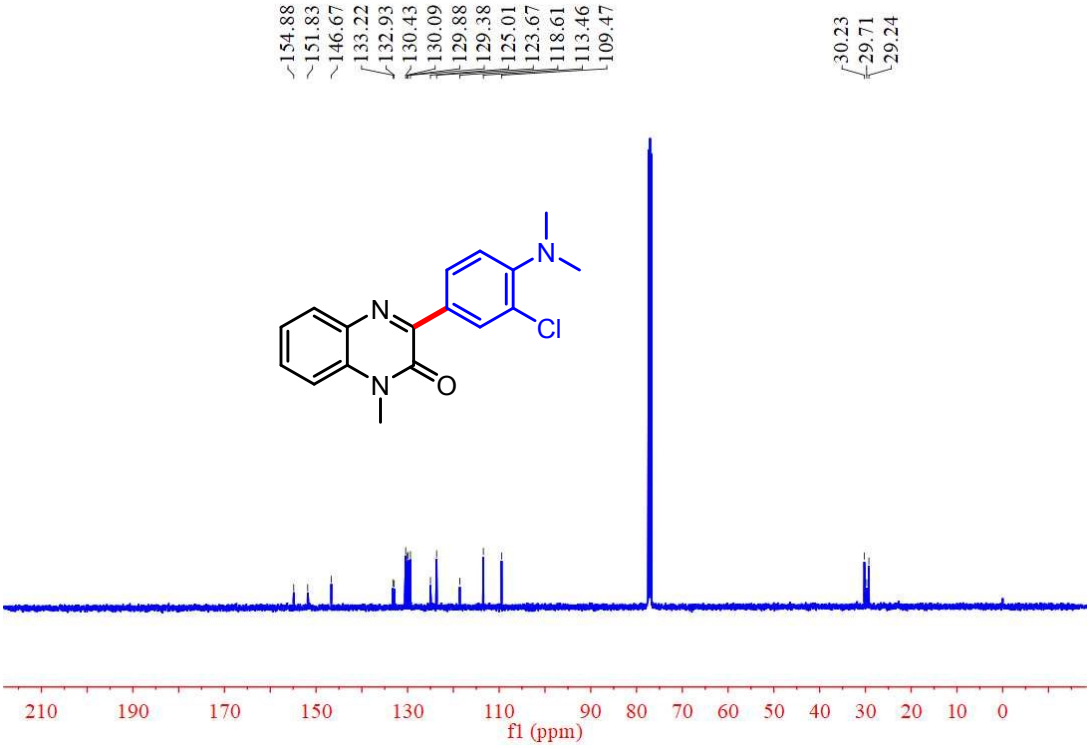
7 ^{19}F NMR (471 MHz, $CDCl_3$)



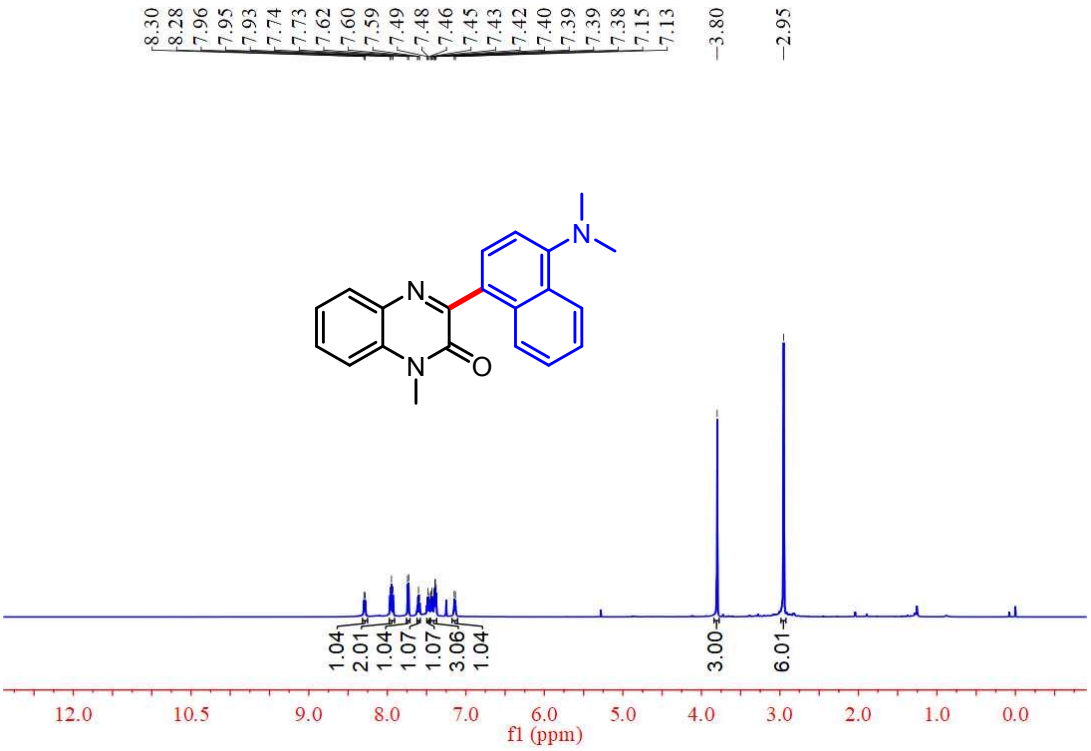
8 ^{1}H NMR (500 MHz, $CDCl_3$)



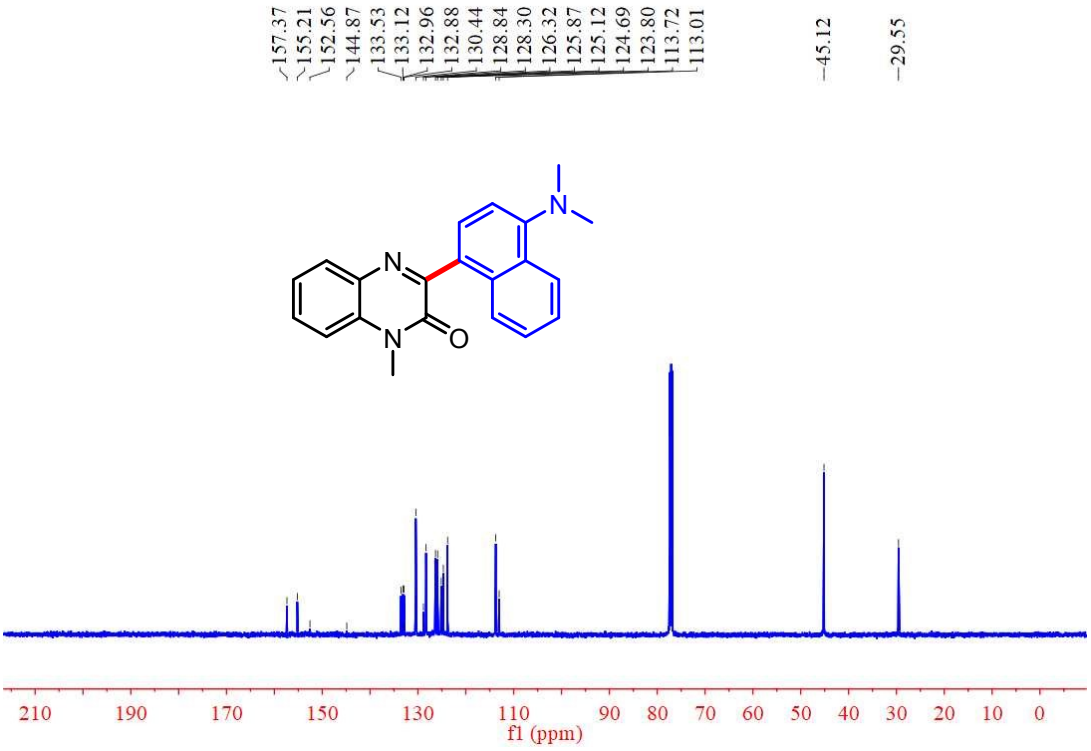
8 ^{13}C NMR (126 MHz, $CDCl_3$)



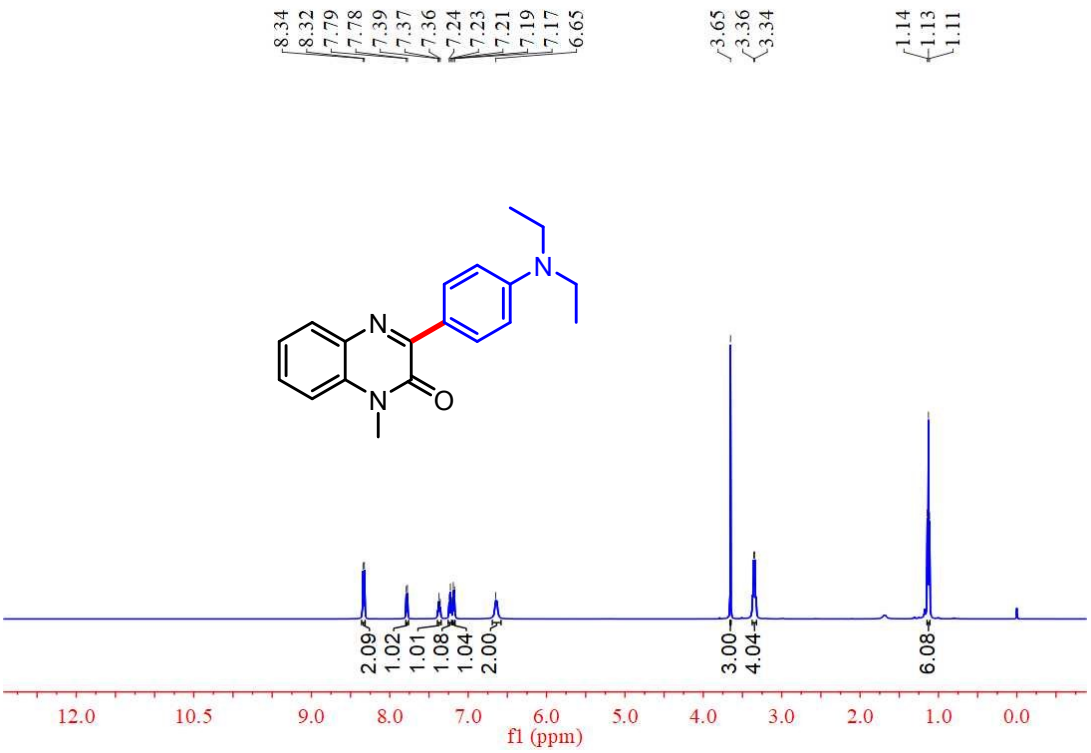
9 ^{1}H NMR (500 MHz, $CDCl_3$)



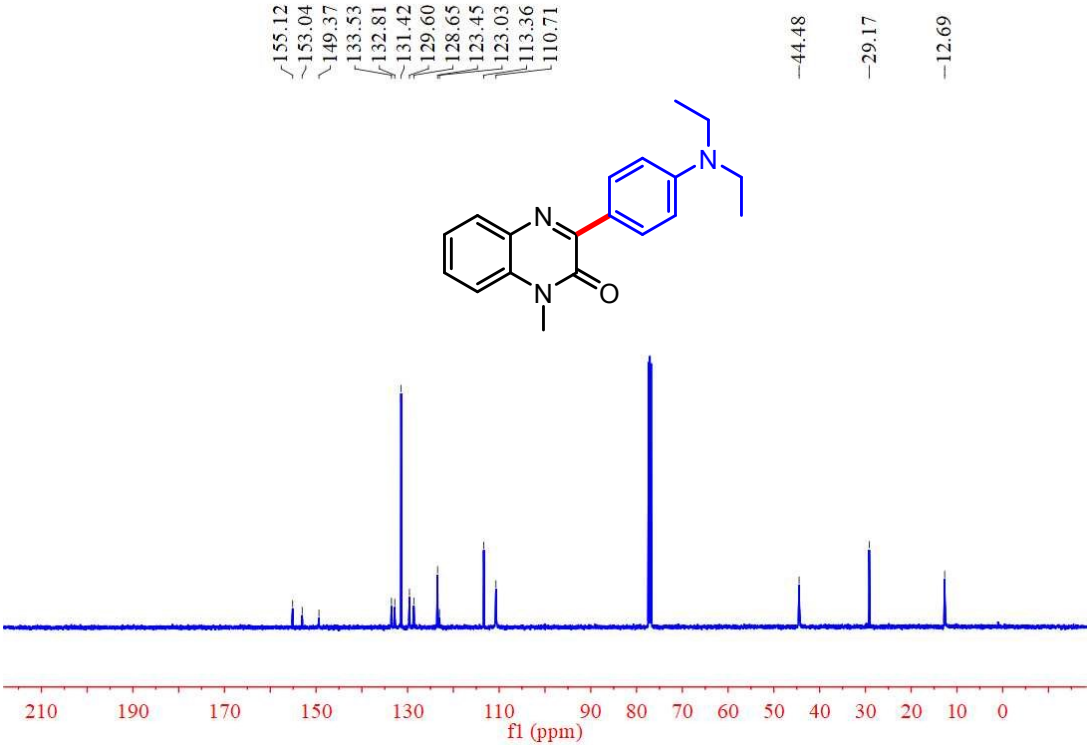
9 ^{13}C NMR (126 MHz, $CDCl_3$)



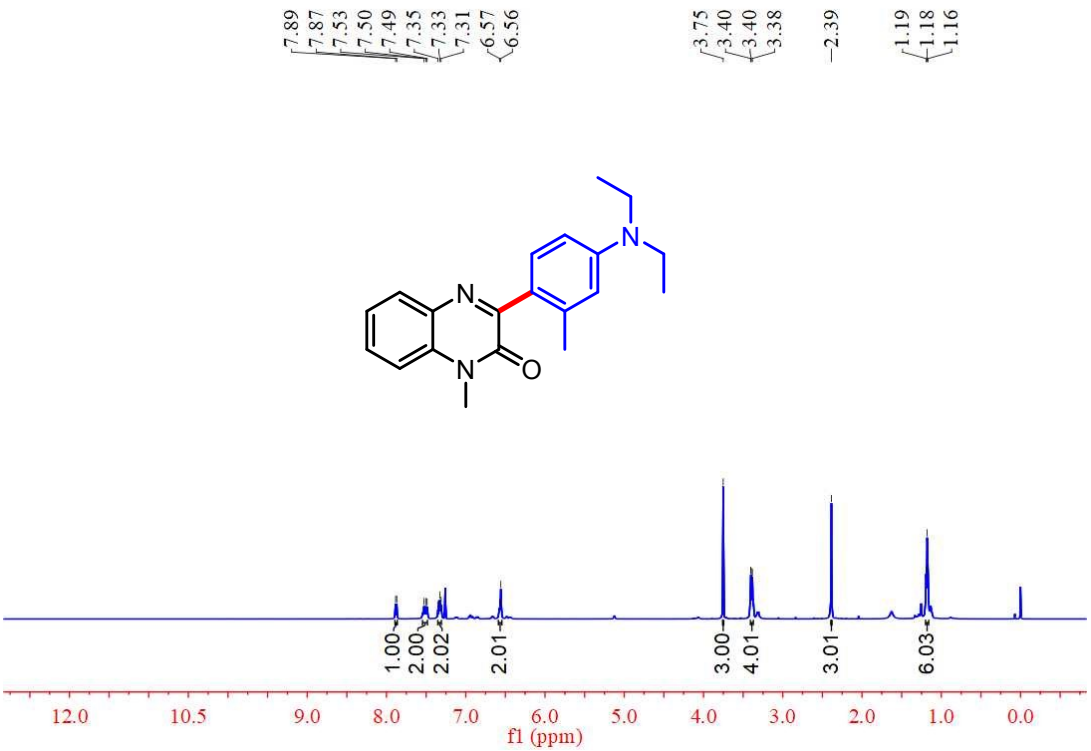
10 ^{1}H NMR (500 MHz, $CDCl_3$)



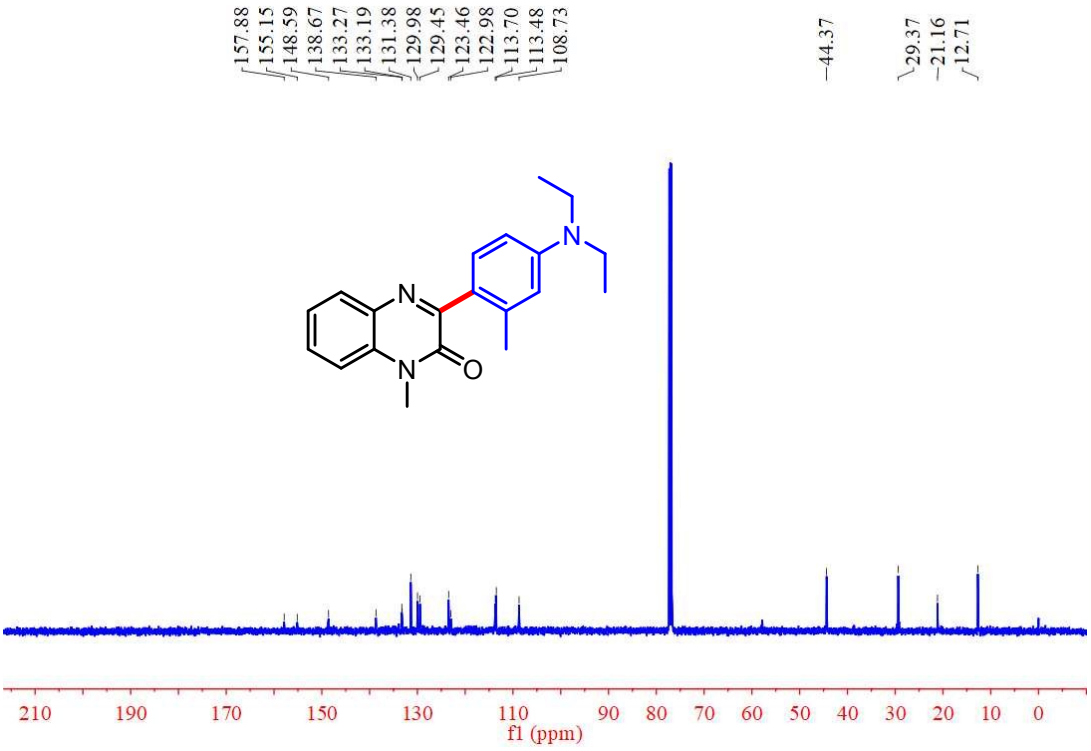
10 ^{13}C NMR (126 MHz, $CDCl_3$)



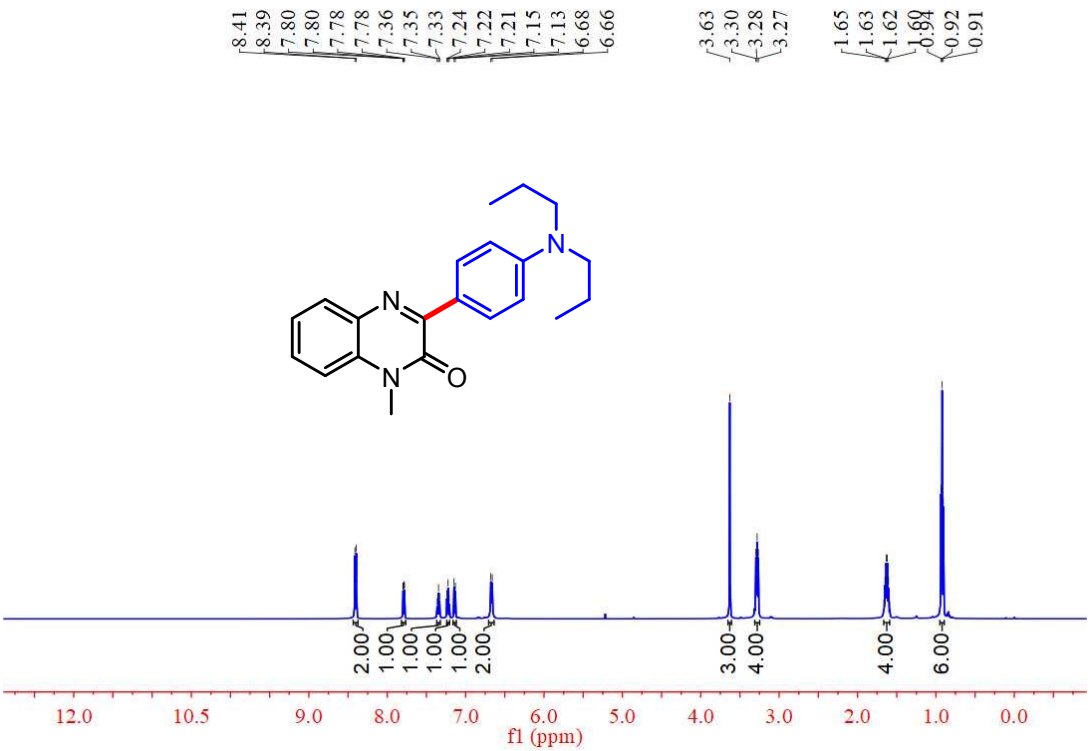
11 ^{1}H NMR (500 MHz, $CDCl_3$)



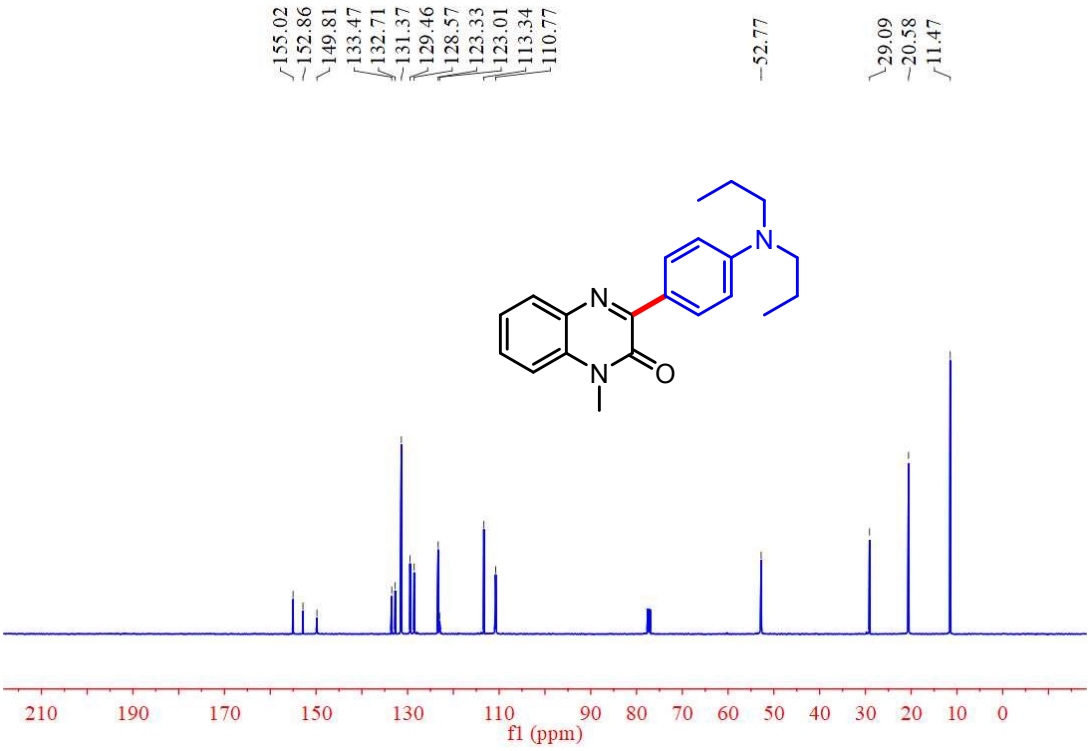
11 ^{13}C NMR (126 MHz, $CDCl_3$)



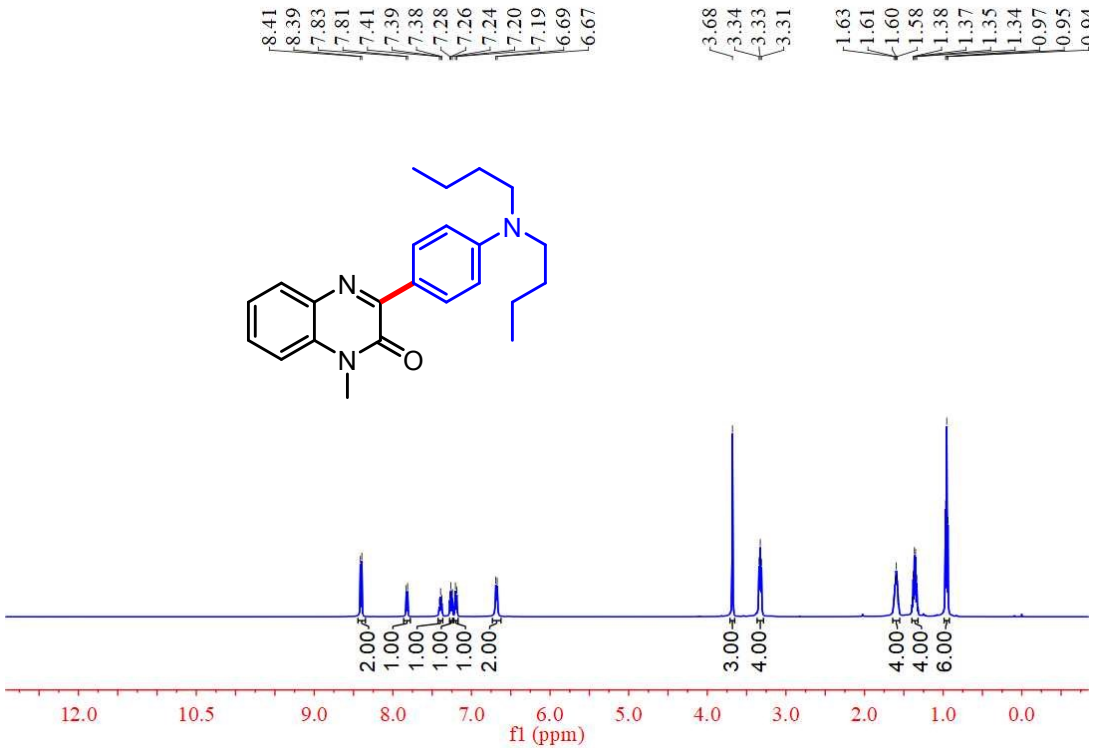
12 ^{1}H NMR (500 MHz, $CDCl_3$)



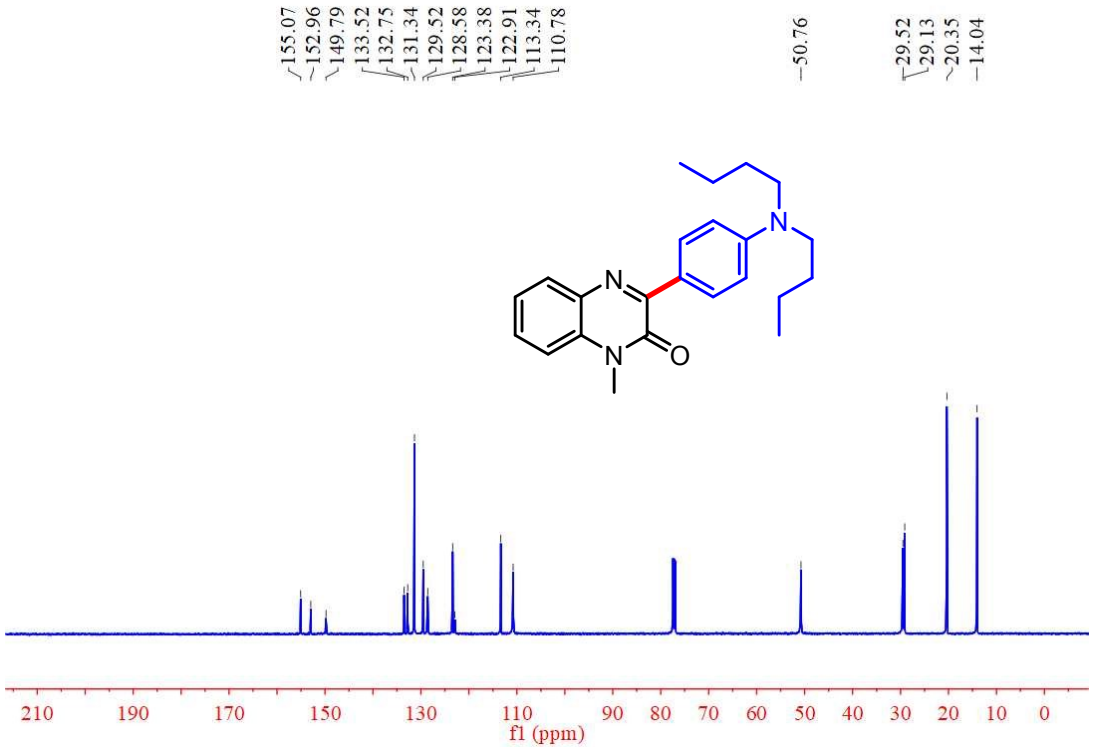
12 ^{13}C NMR (126 MHz, $CDCl_3$)



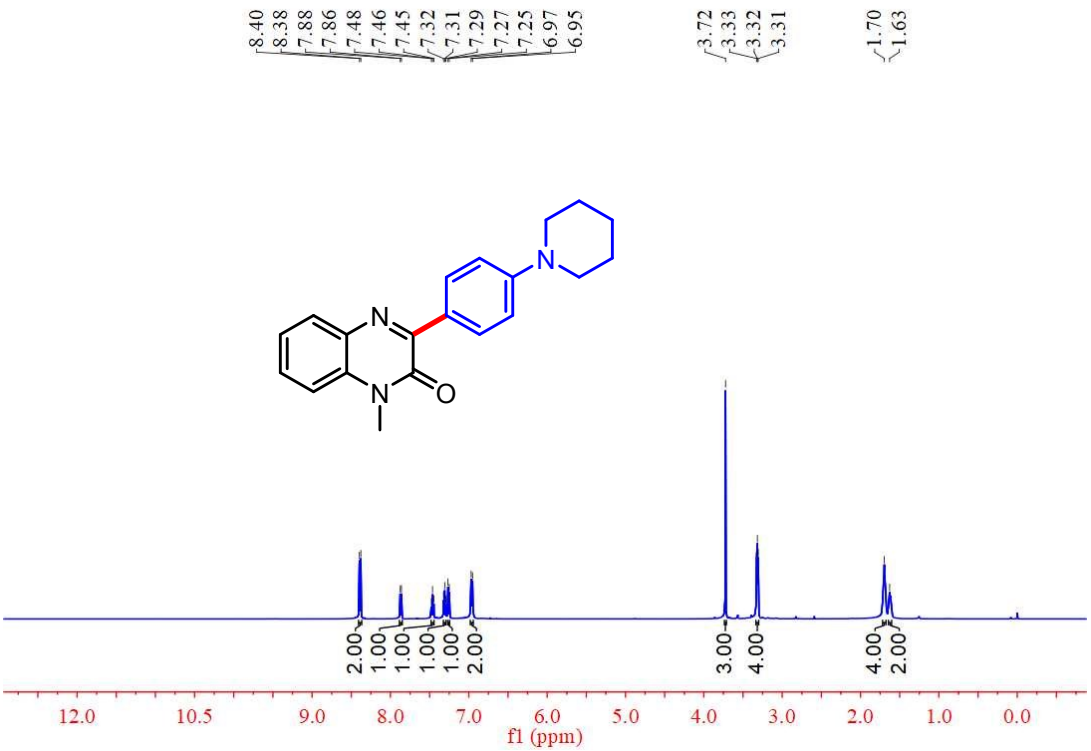
13 ^{1}H NMR (500 MHz, $CDCl_3$)



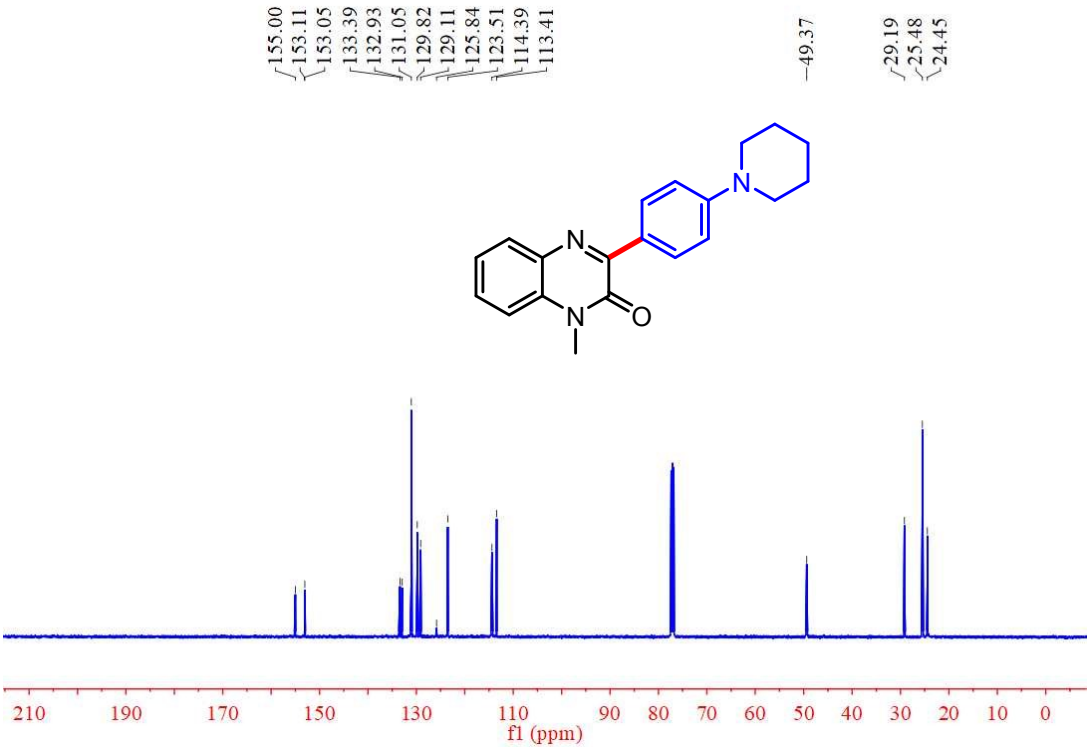
13 ^{13}C NMR (126 MHz, $CDCl_3$)



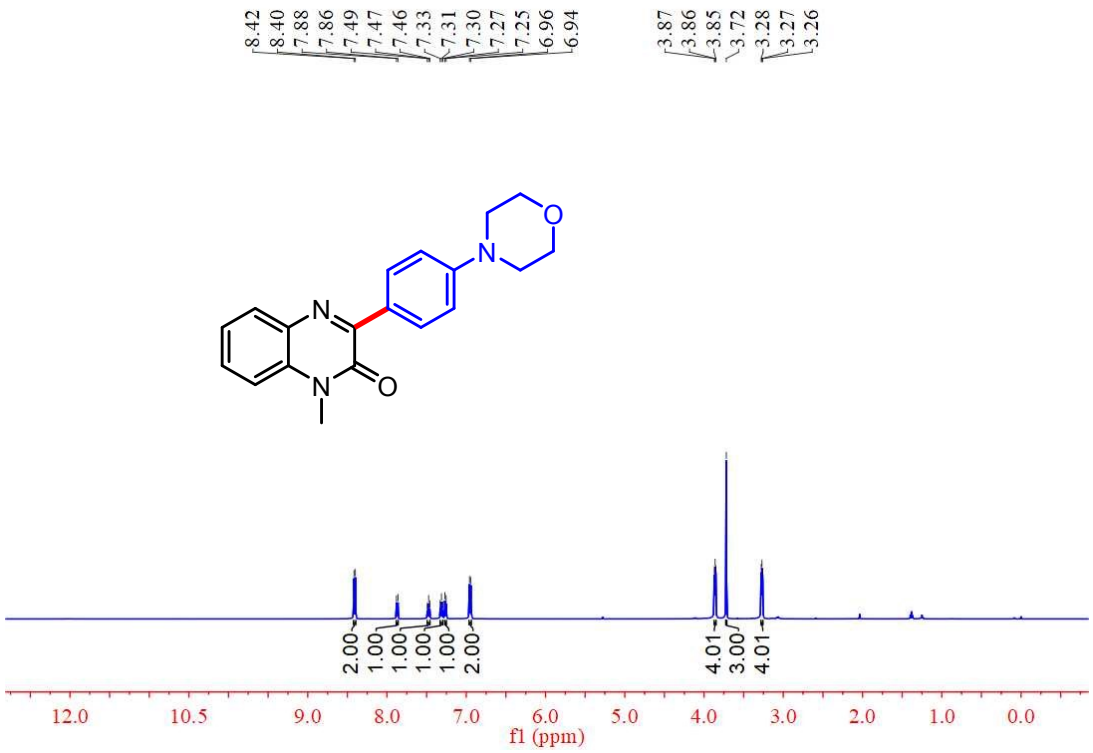
14 ^{1}H NMR (500 MHz, $CDCl_3$)



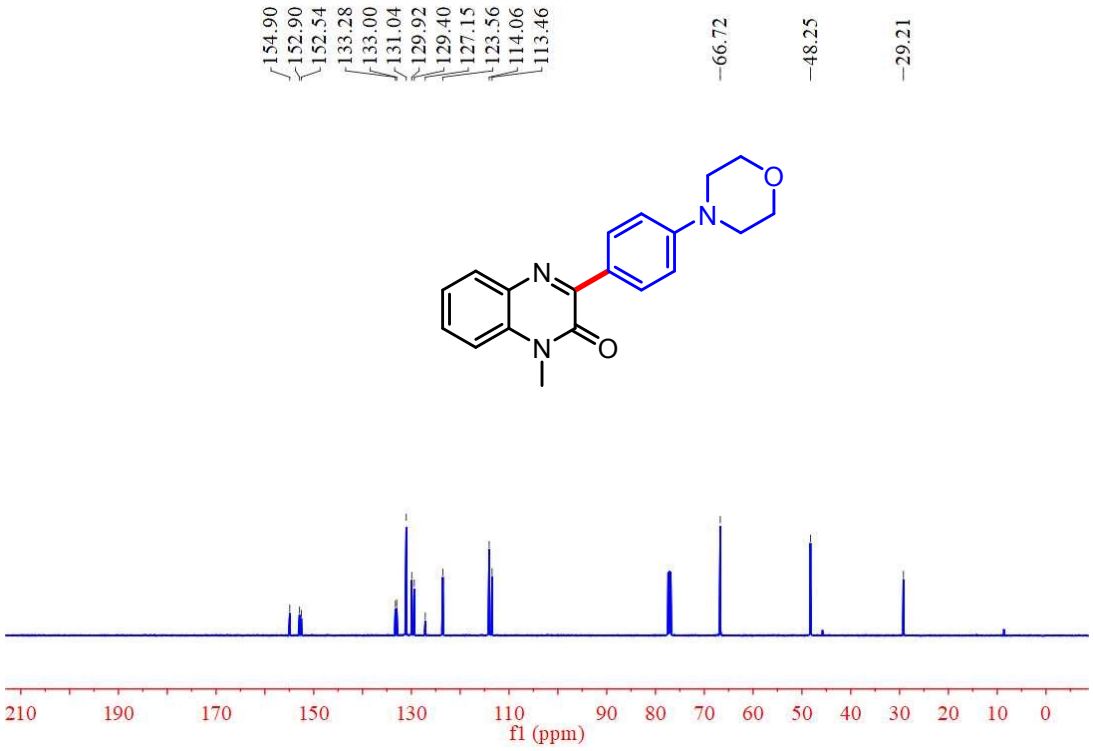
14 ^{13}C NMR (126 MHz, $CDCl_3$)



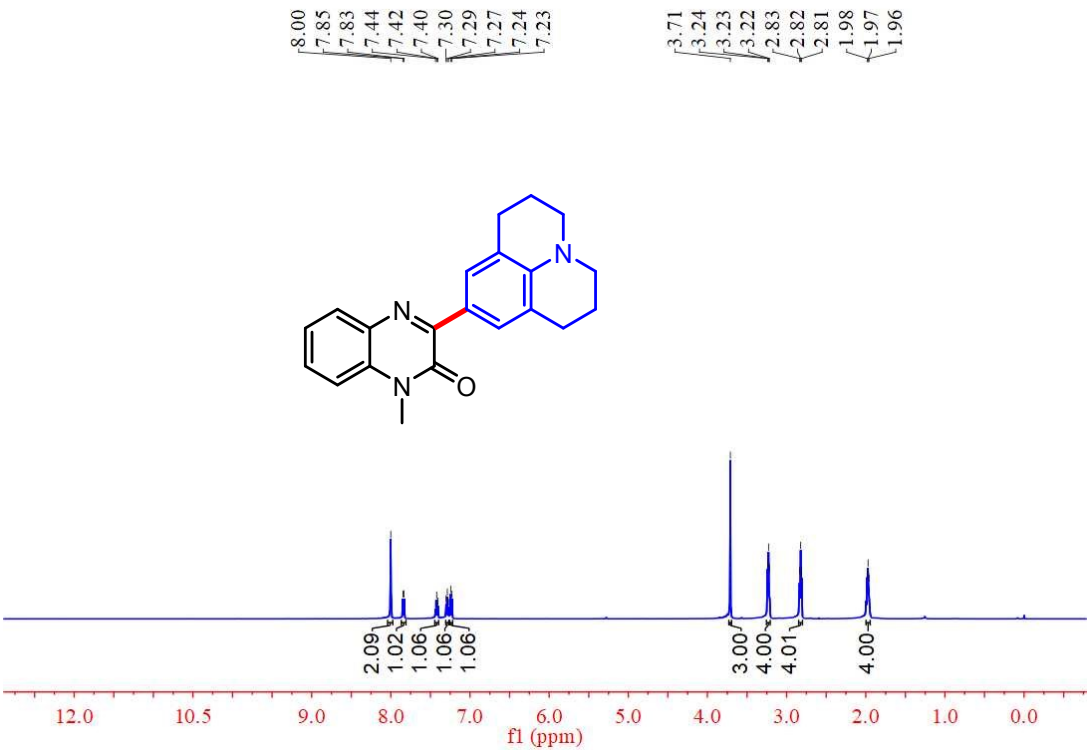
15 ^{1}H NMR (500 MHz, $CDCl_3$)



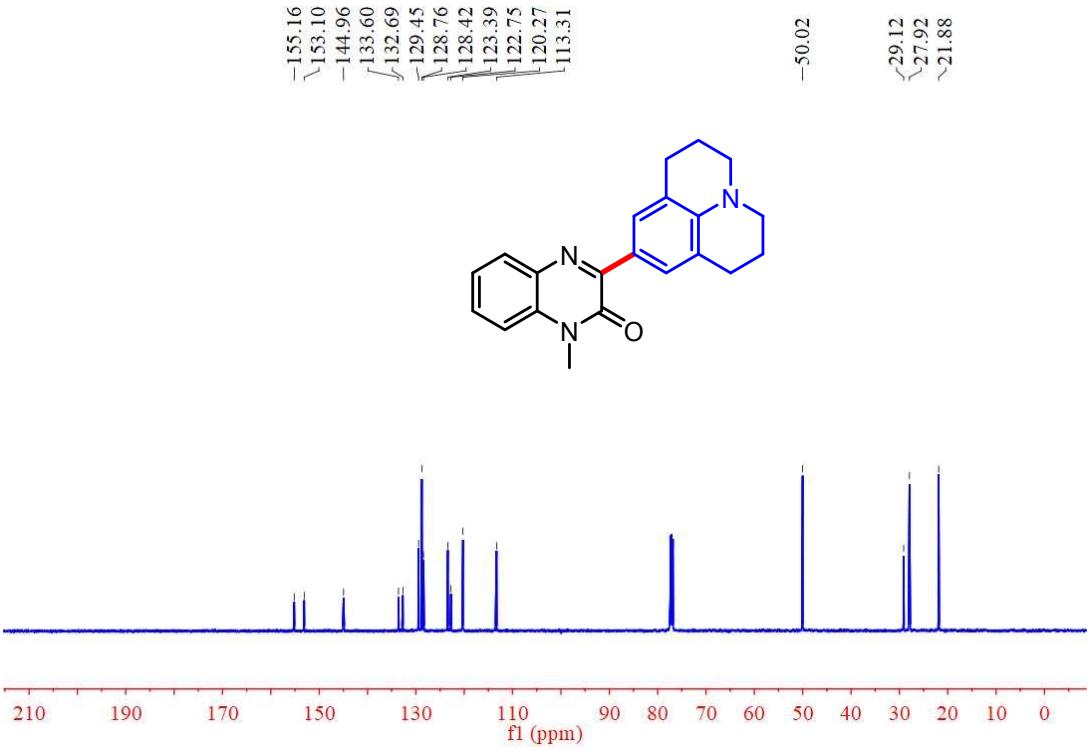
15 ^{13}C NMR (126 MHz, $CDCl_3$)



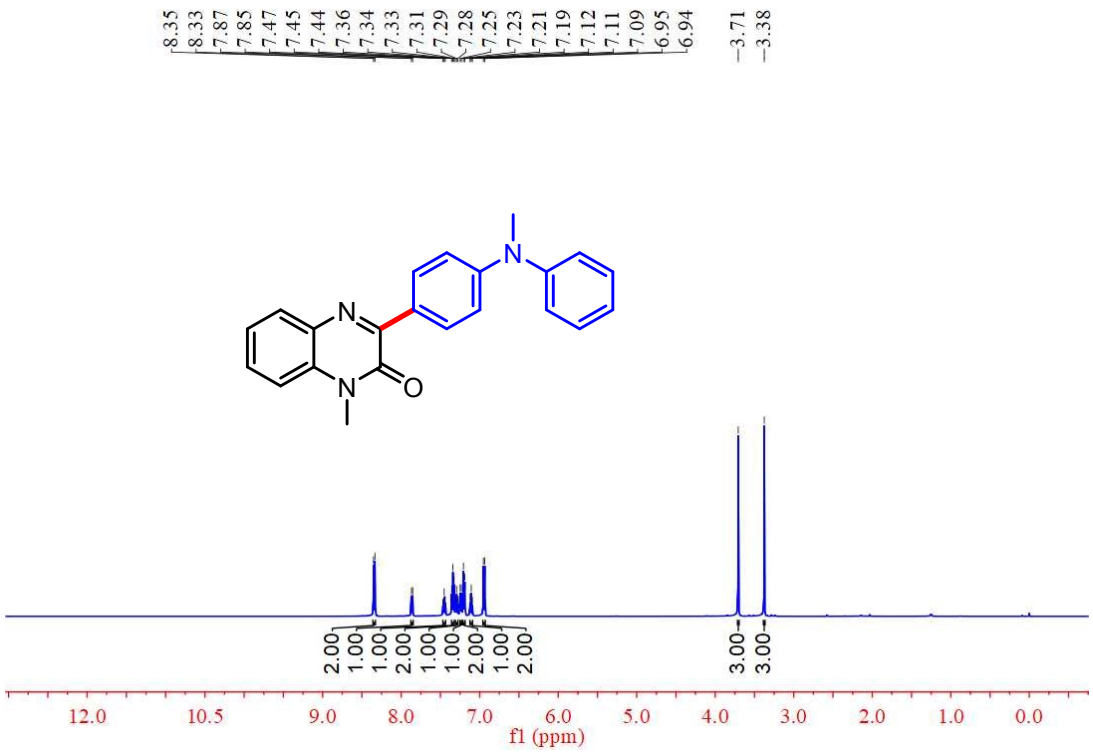
16 ^{1}H NMR (500 MHz, $CDCl_3$)



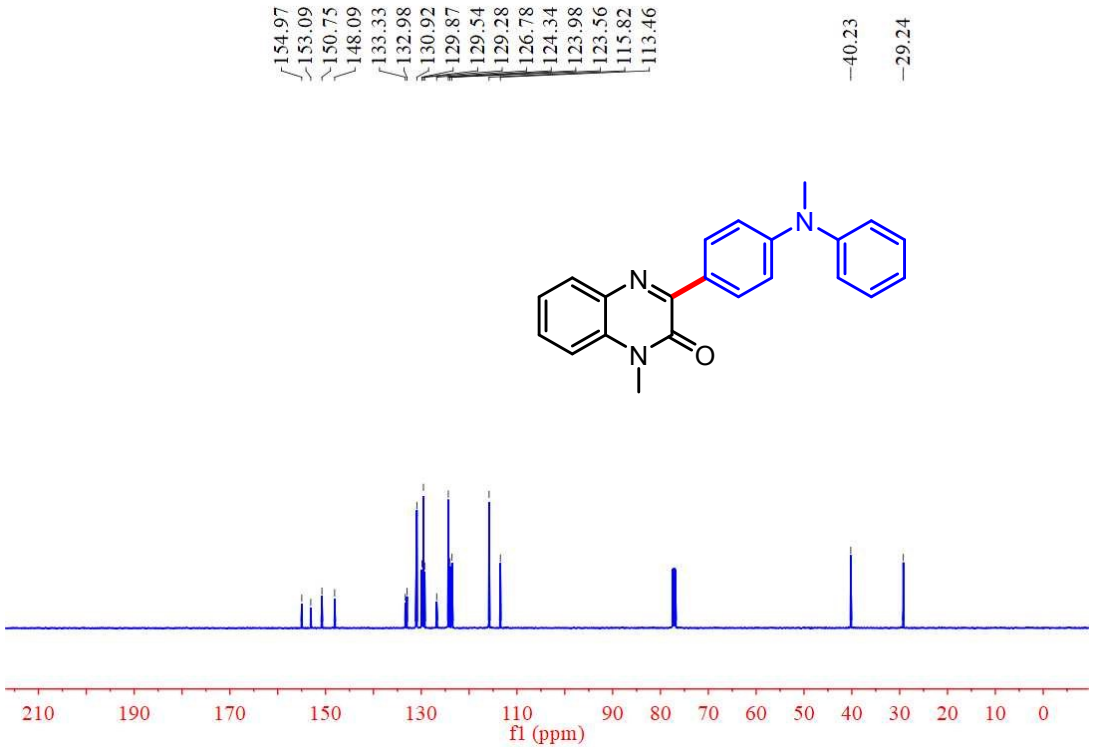
16 ^{13}C NMR (126 MHz, $CDCl_3$)



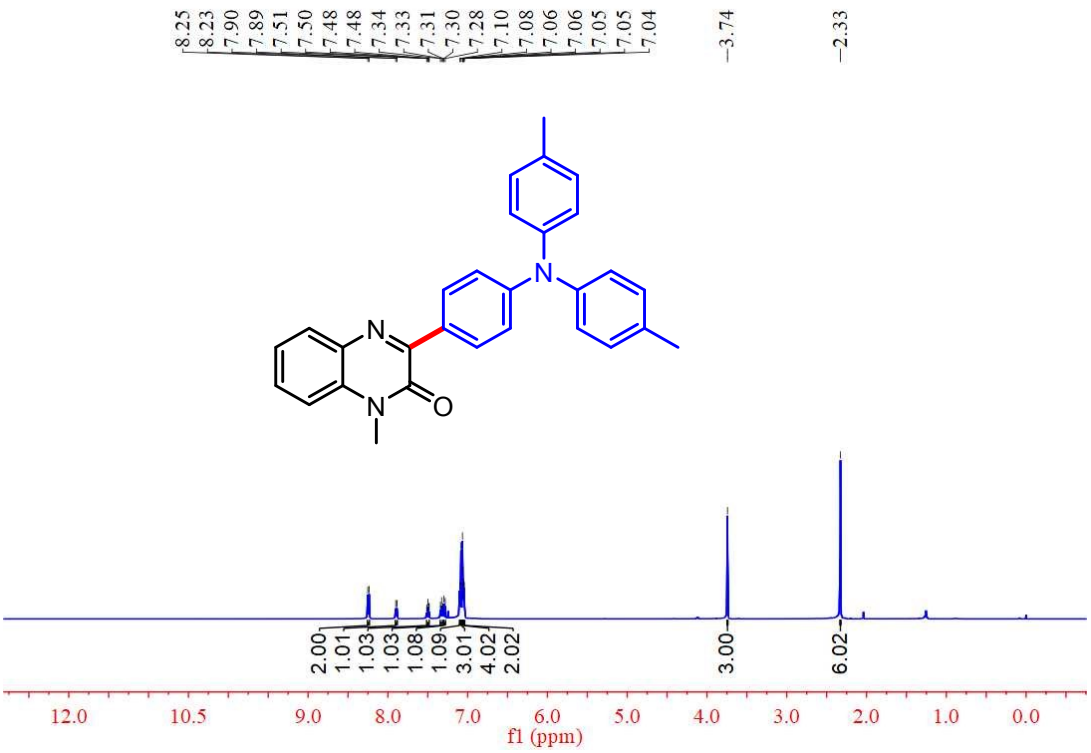
17 ^{1}H NMR (500 MHz, $CDCl_3$)



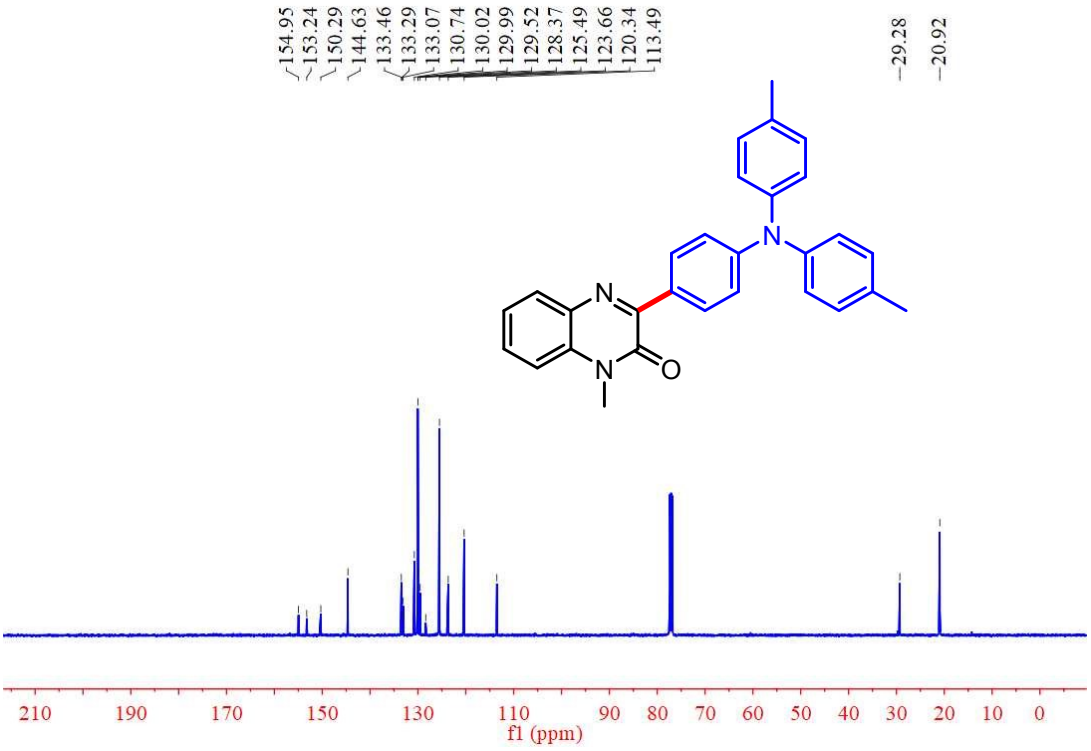
17 ^{13}C NMR (126 MHz, $CDCl_3$)



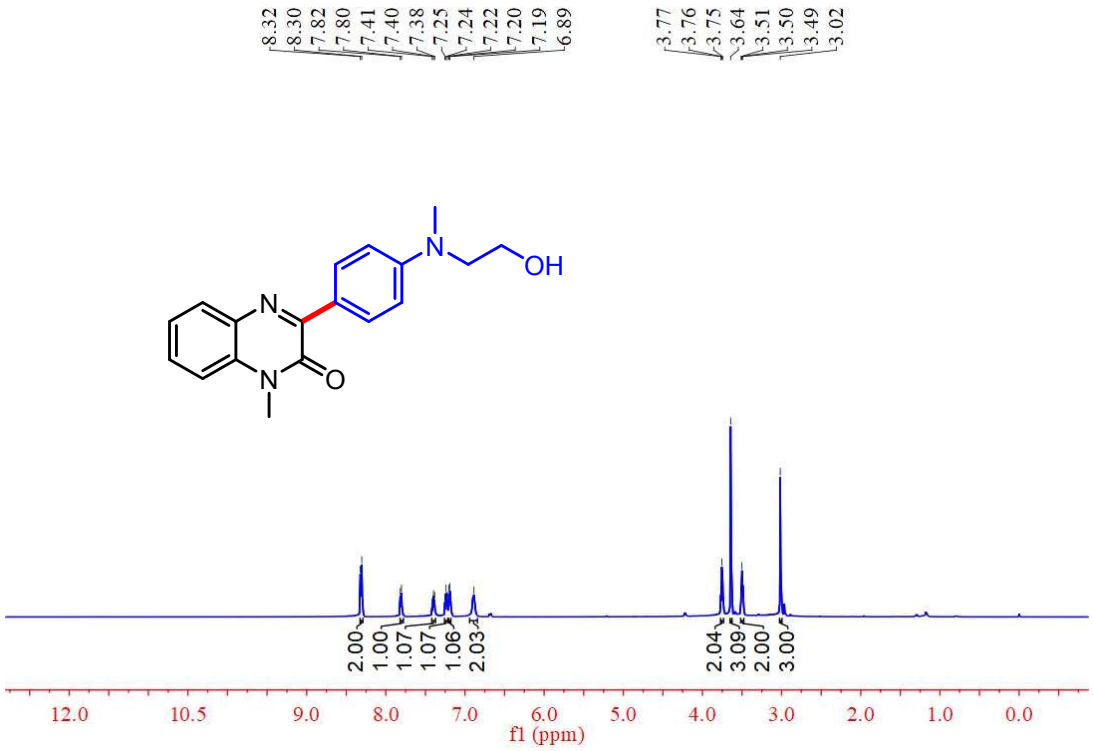
18 ^{1}H NMR (500 MHz, $CDCl_3$)



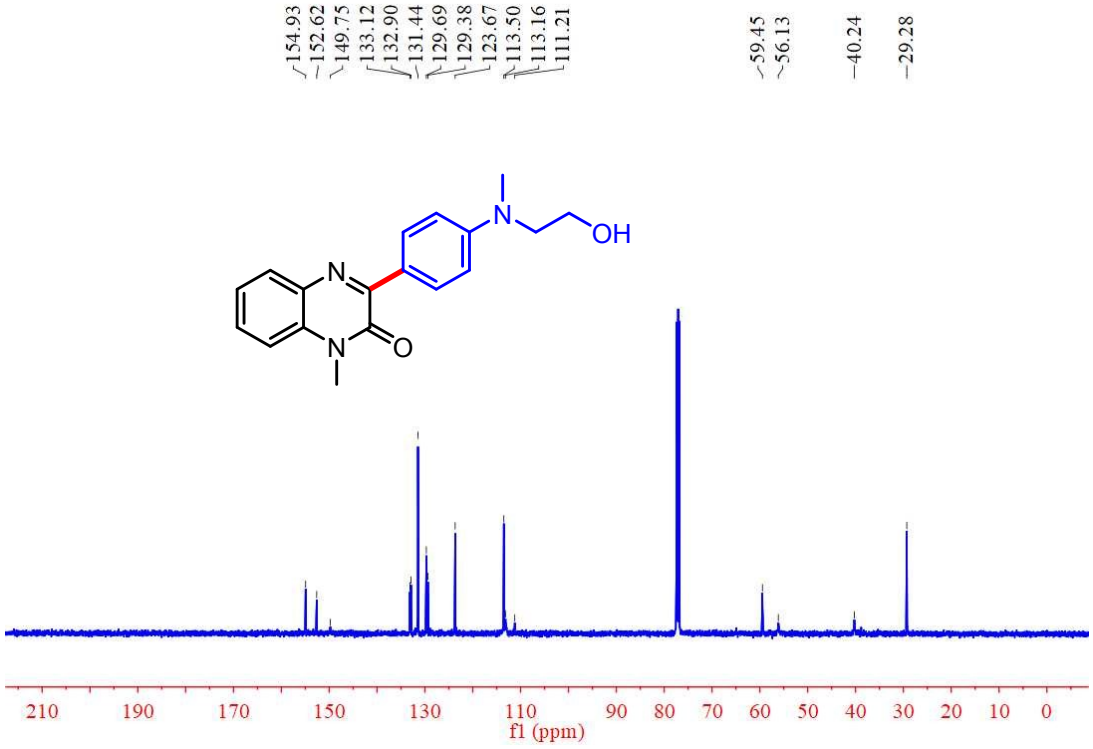
18 ^{13}C NMR (126 MHz, $CDCl_3$)



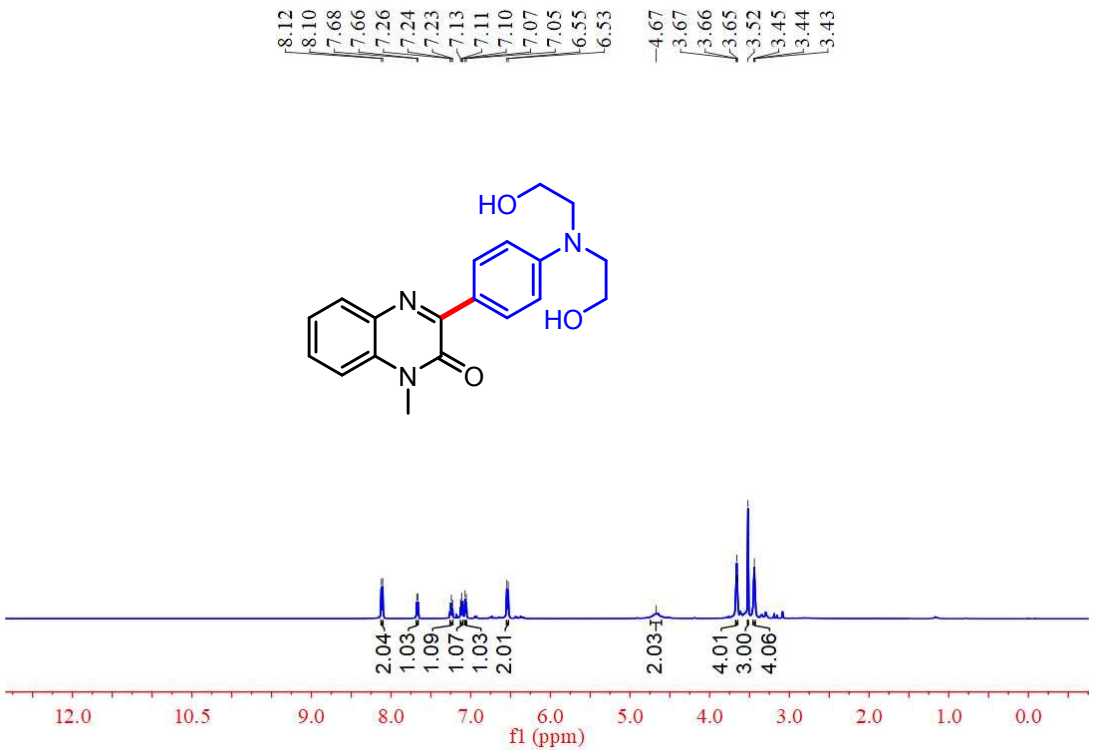
19 ^{1}H NMR (500 MHz, $CDCl_3$)



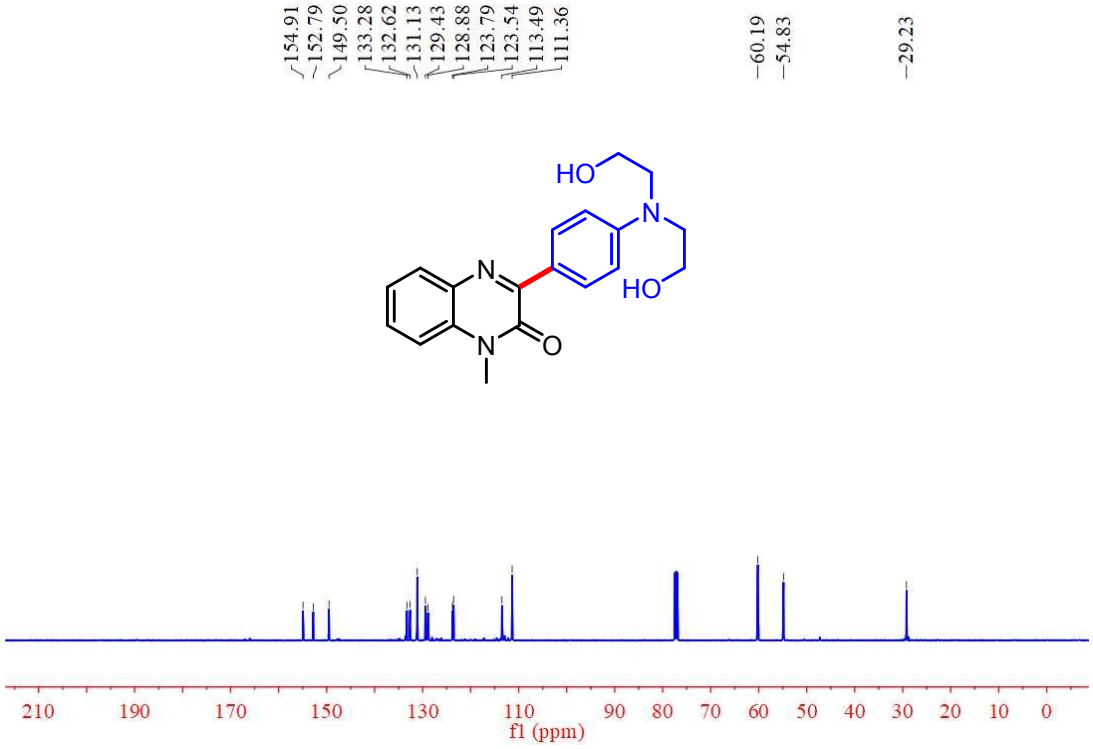
19 ^{13}C NMR (126 MHz, $CDCl_3$)



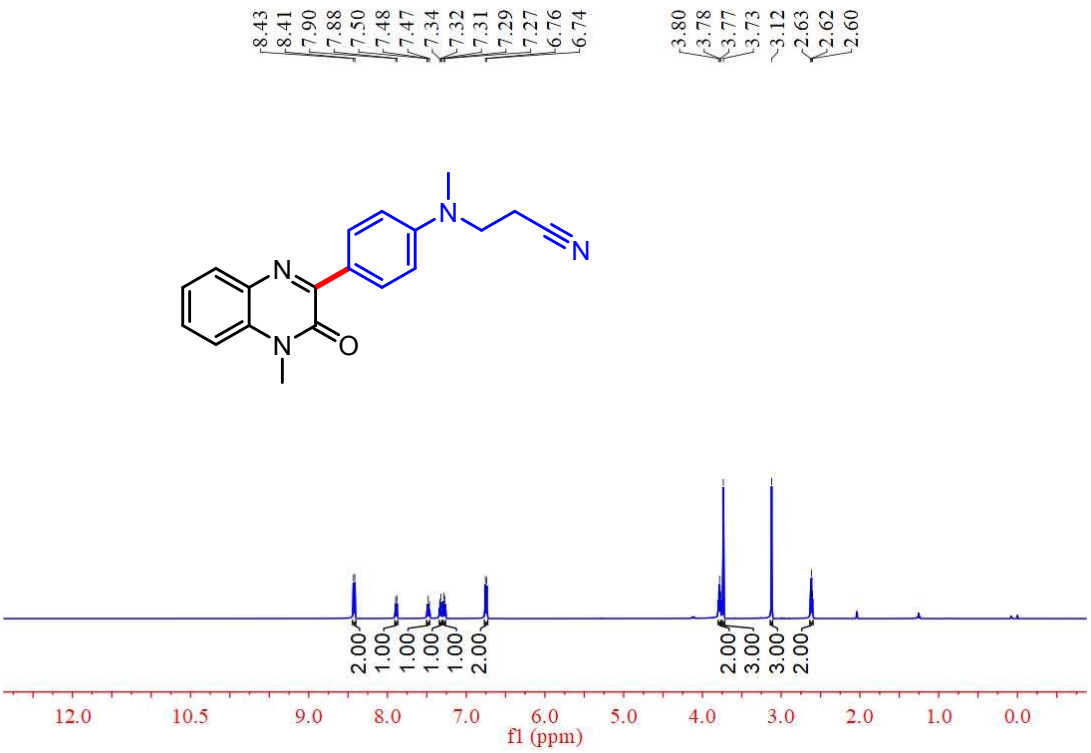
20 ^{1}H NMR (500 MHz, $CDCl_3$)



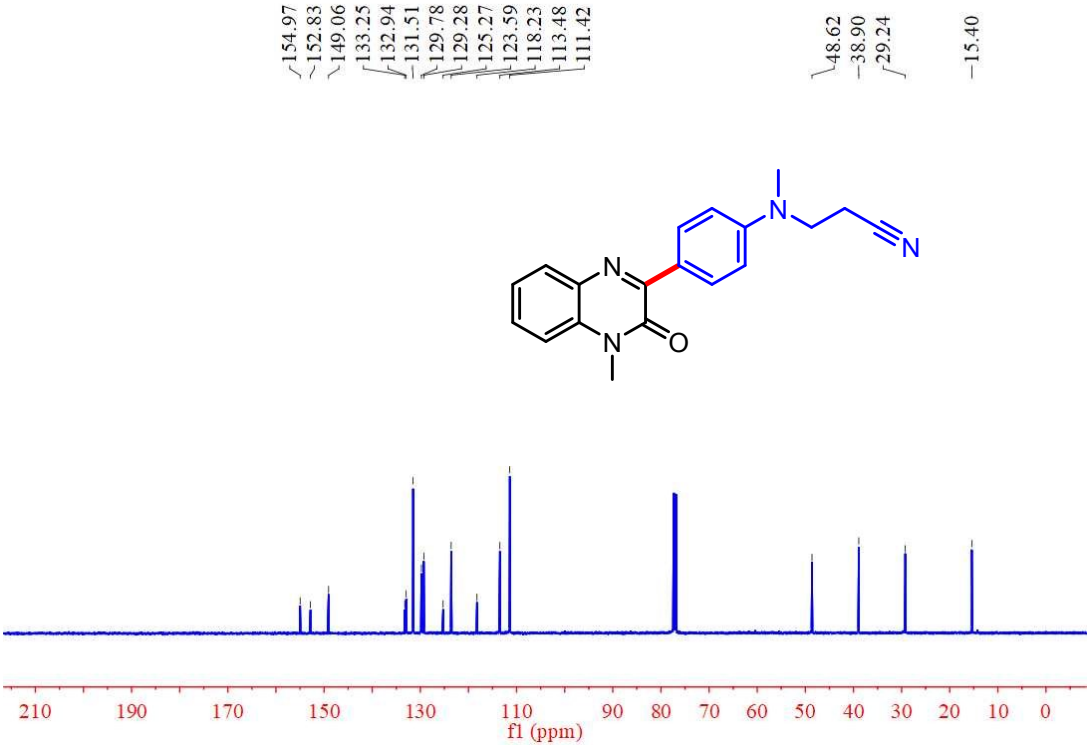
20 ^{13}C NMR (126 MHz, $CDCl_3$)



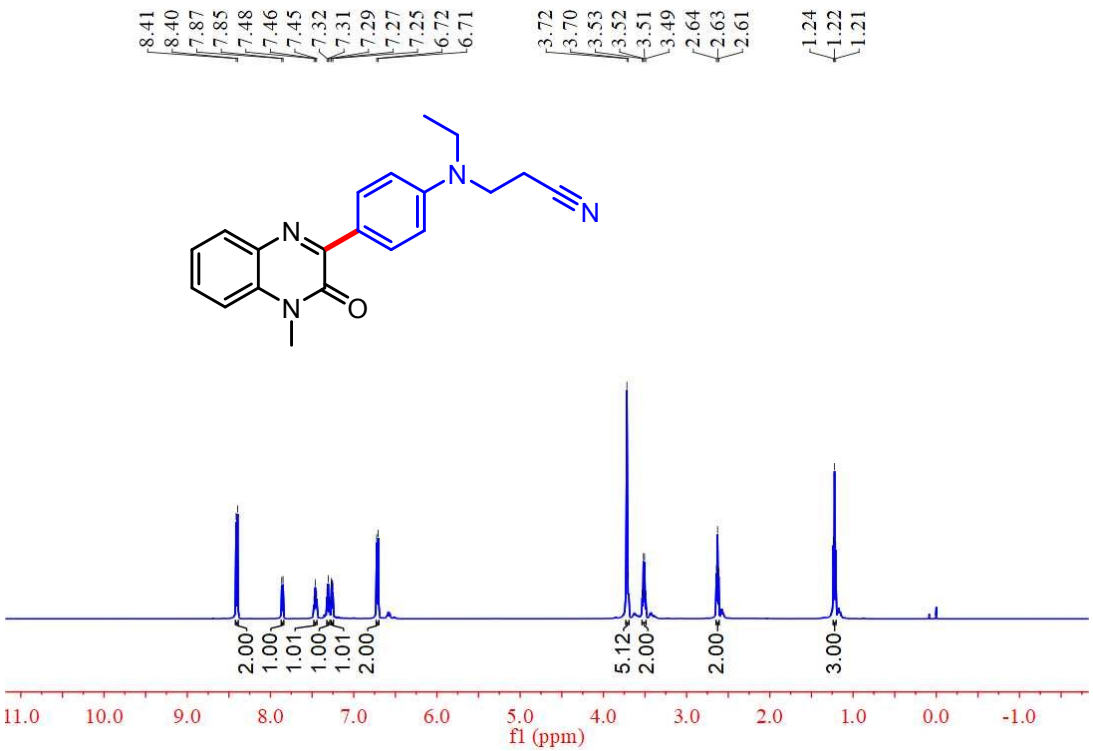
21 ^{1}H NMR (500 MHz, $CDCl_3$)



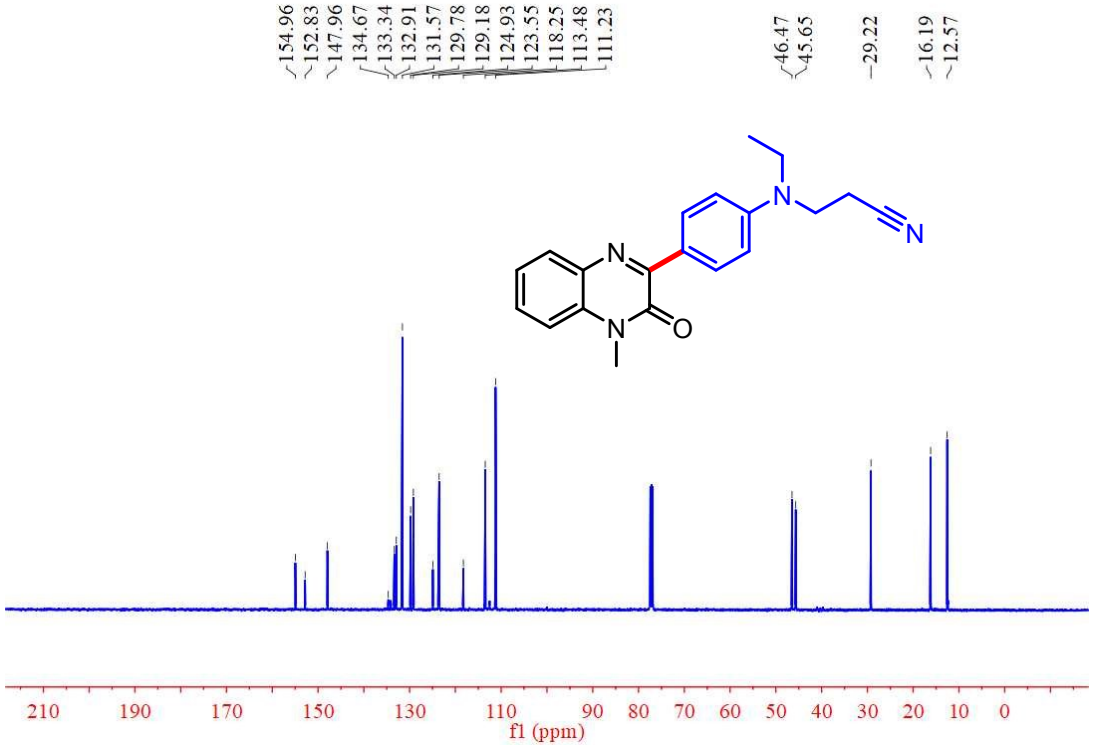
21 ^{13}C NMR (126 MHz, $CDCl_3$)



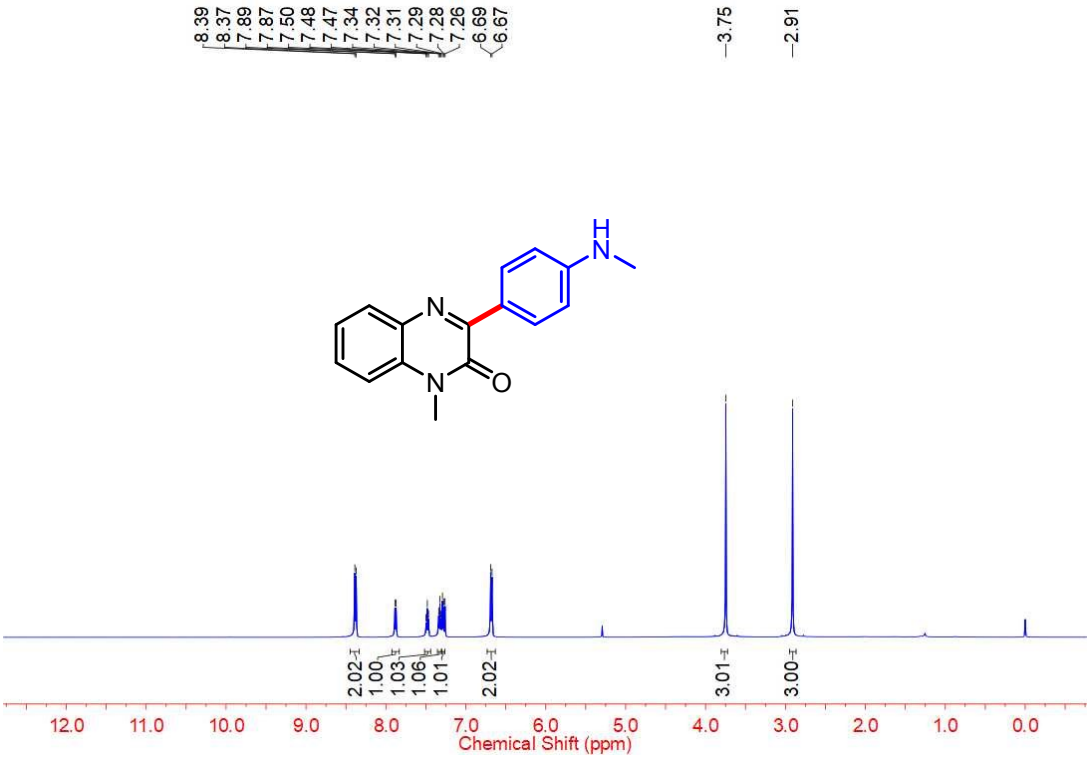
22 ^{1}H NMR (500 MHz, $CDCl_3$)



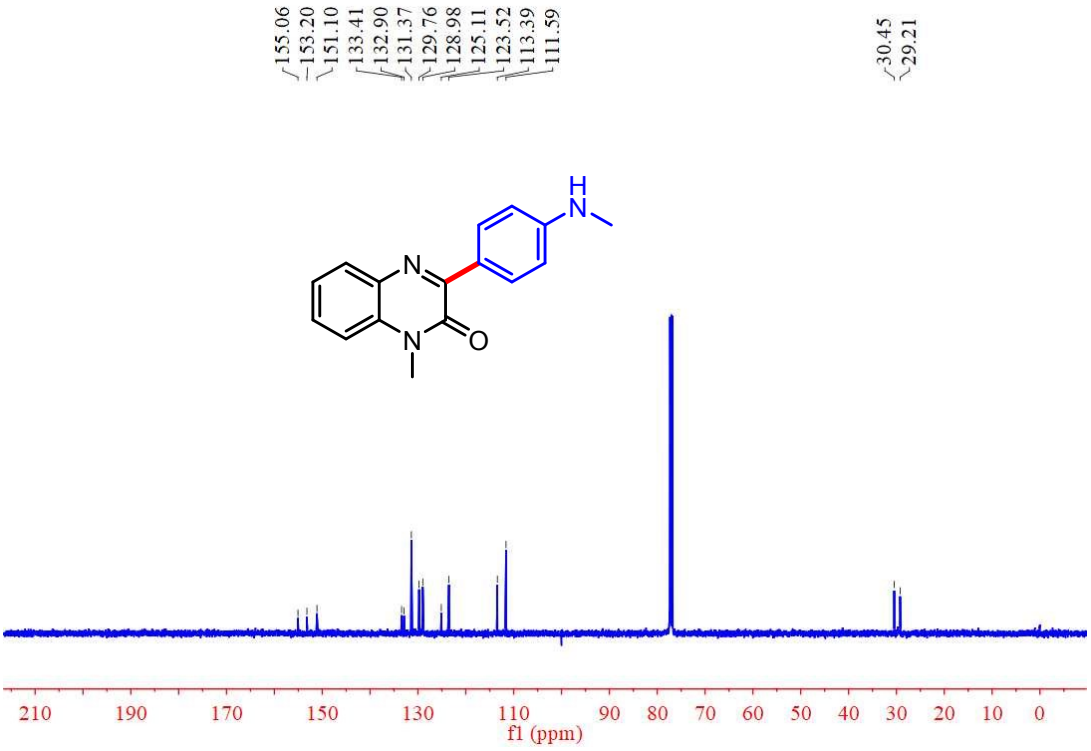
22 ^{13}C NMR (126 MHz, $CDCl_3$)



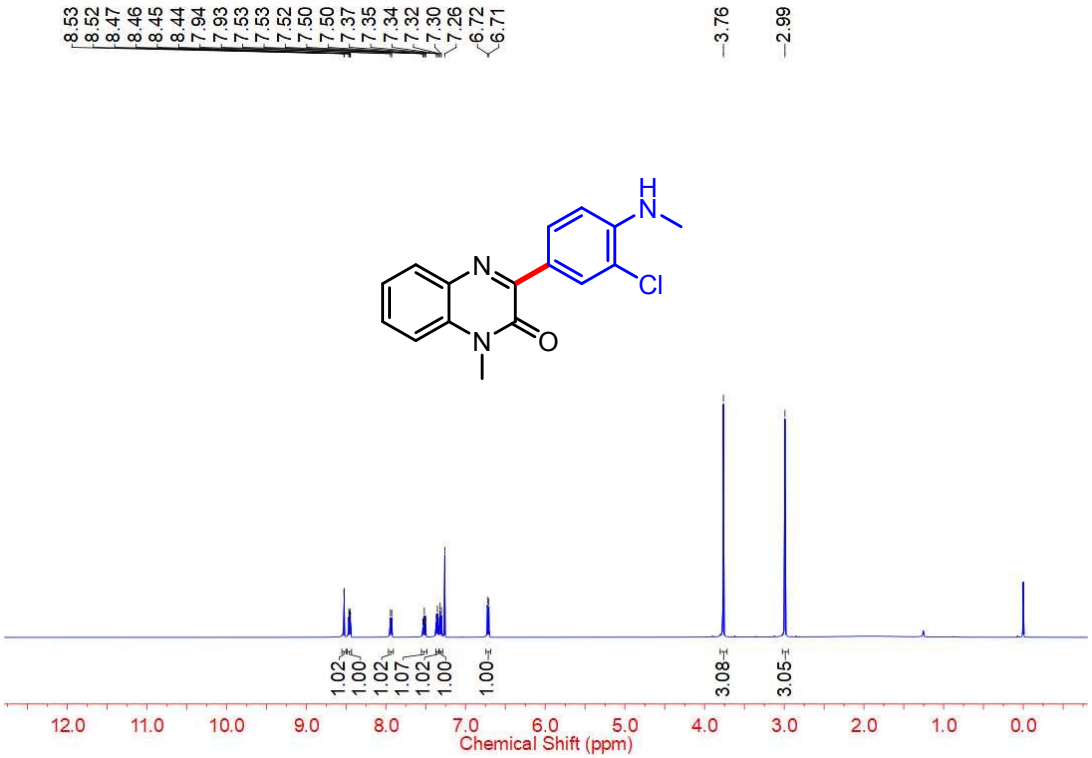
23 ^{1}H NMR (500 MHz, $CDCl_3$)



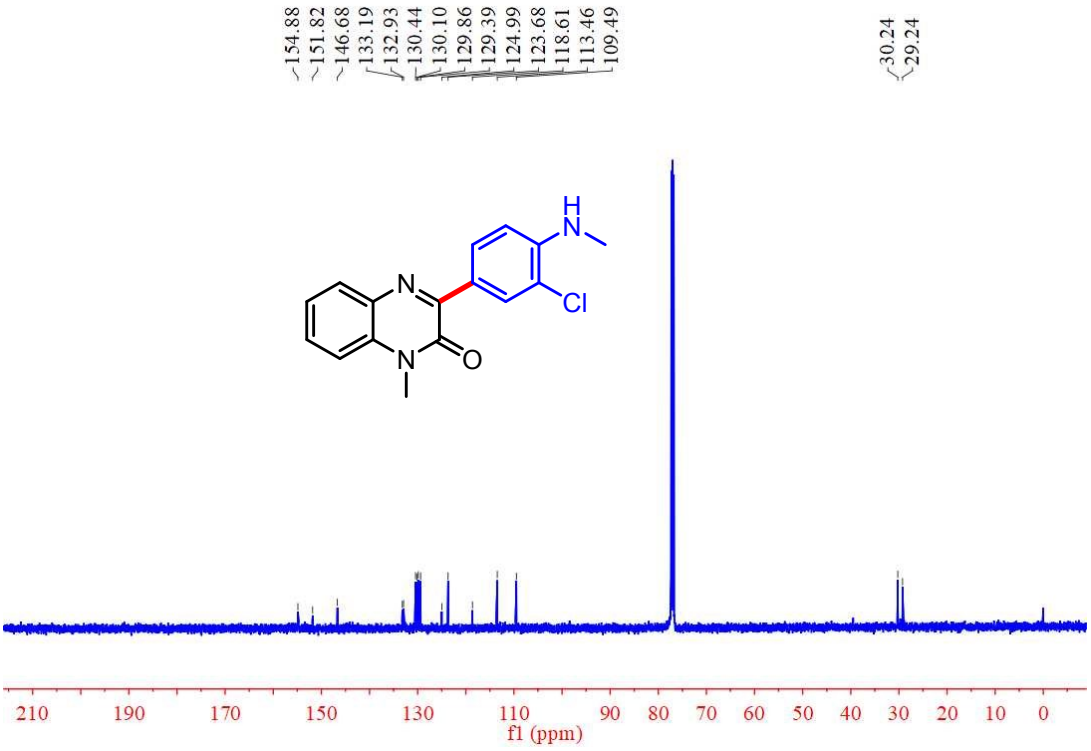
23 ^{13}C NMR (126 MHz, $CDCl_3$)



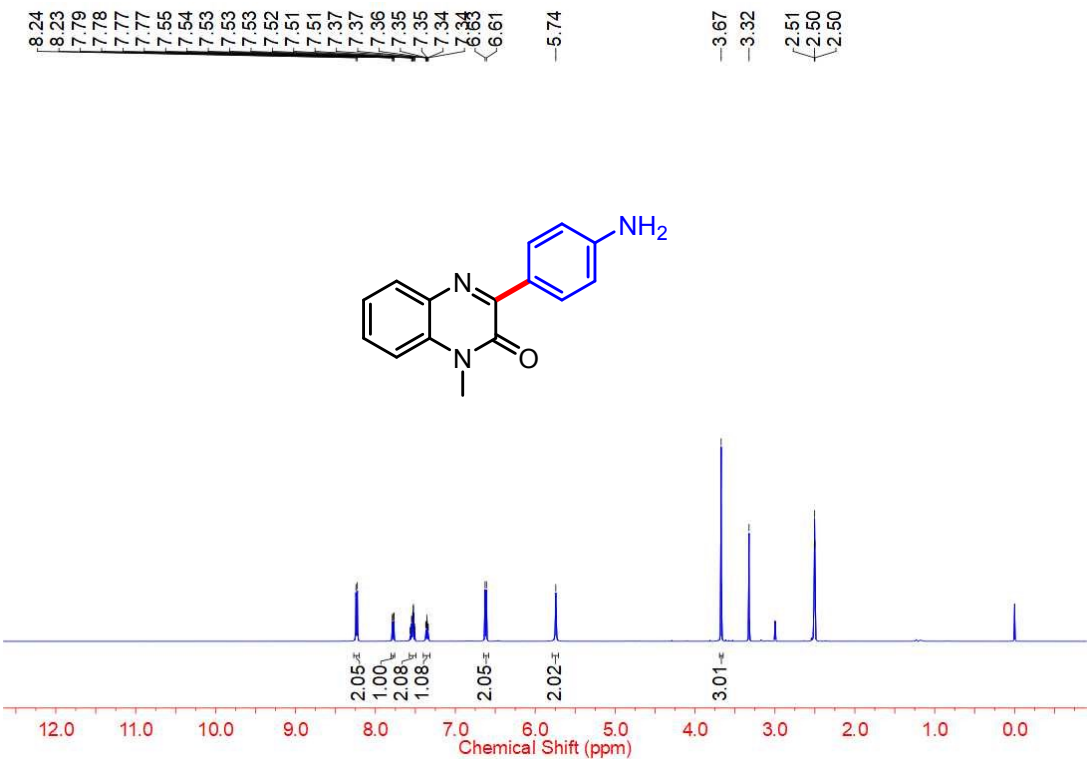
24 ^{1}H NMR (500 MHz, $CDCl_3$)



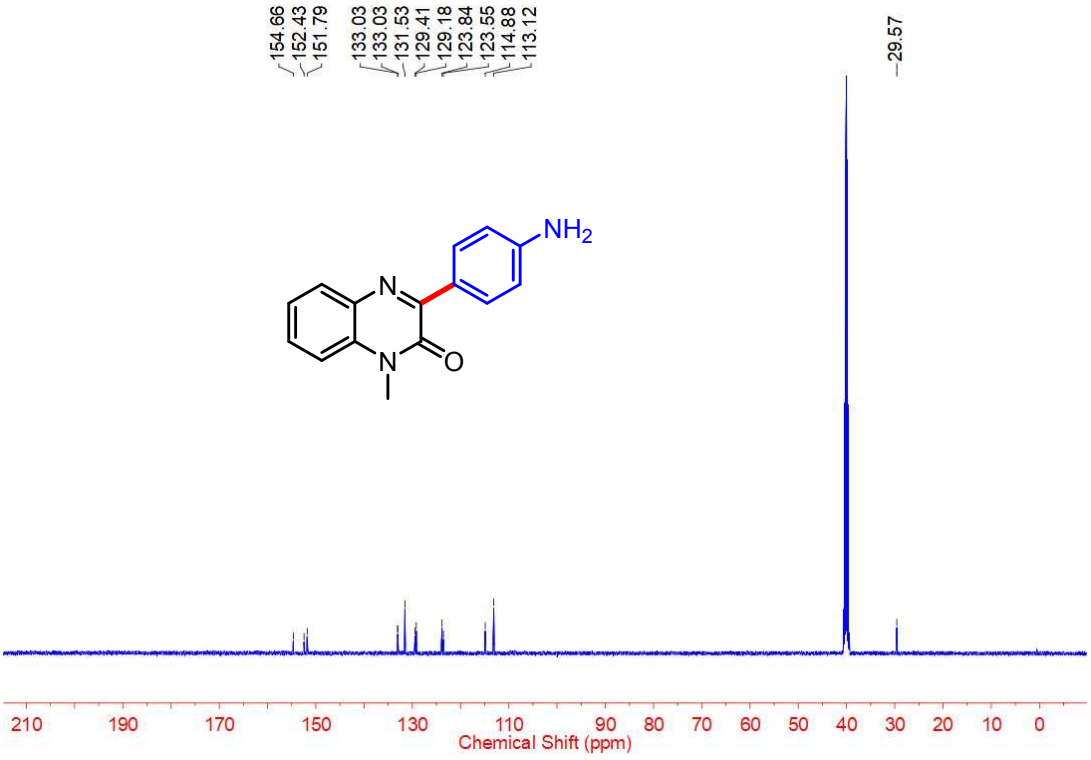
24 ^{13}C NMR (126 MHz, $CDCl_3$)



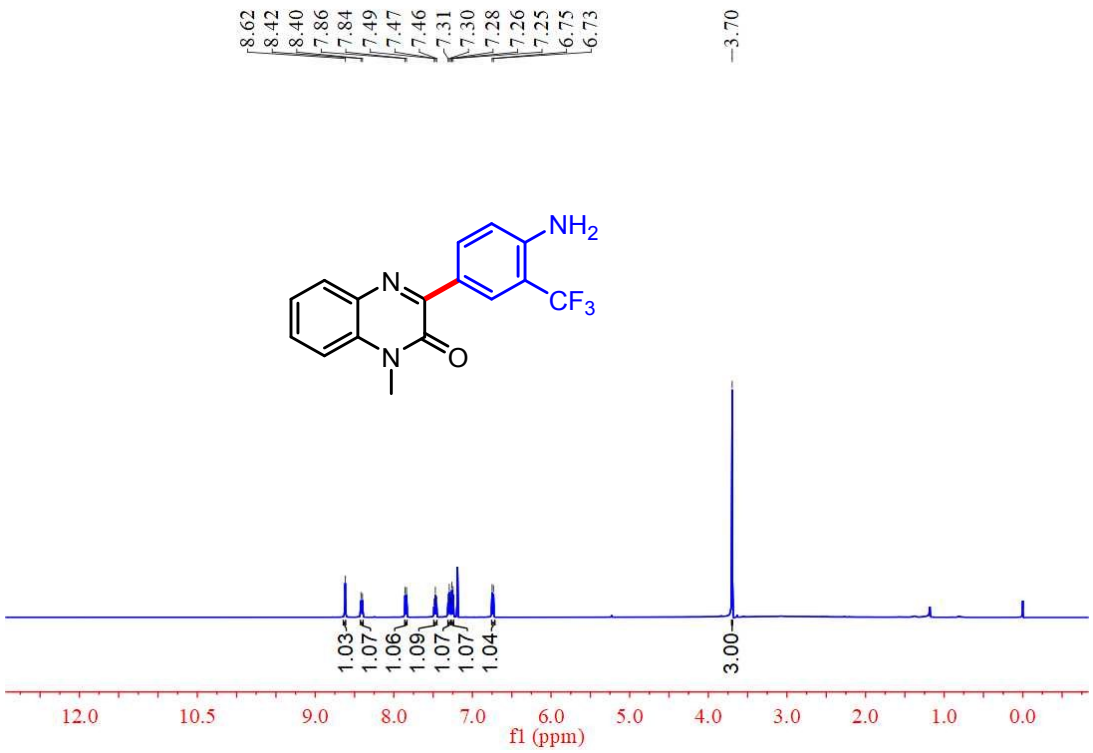
25 ^{1}H NMR (500 MHz, DMSO)



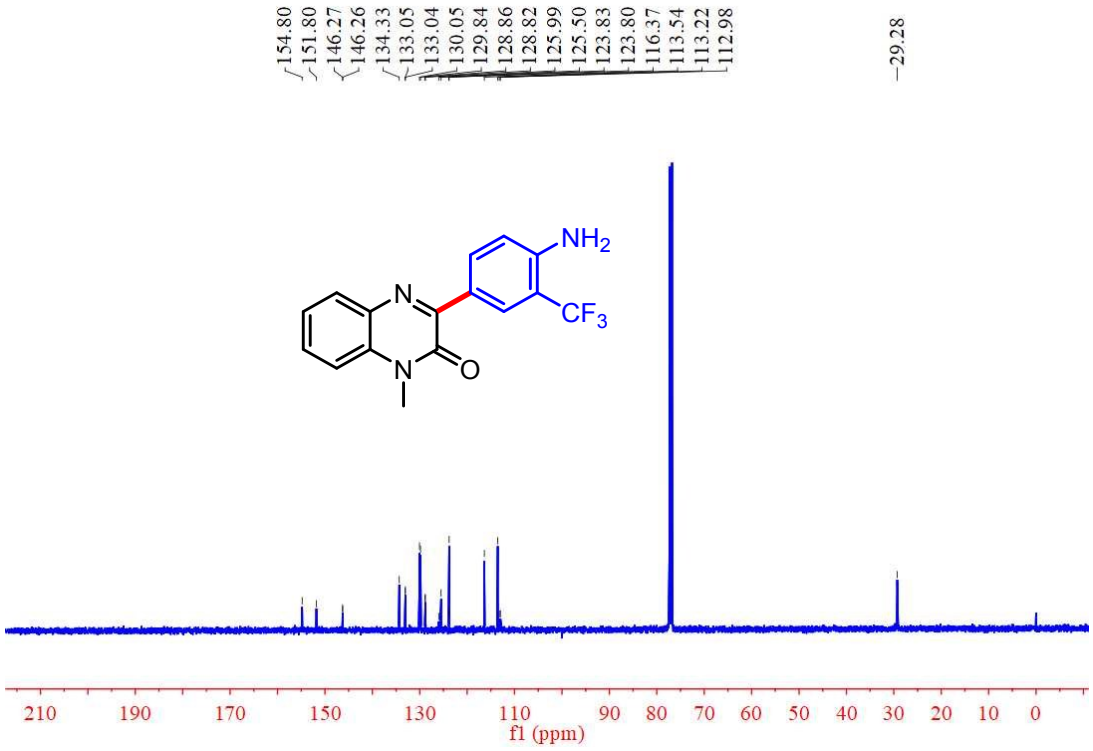
25 ^{13}C NMR (126 MHz, DMSO)



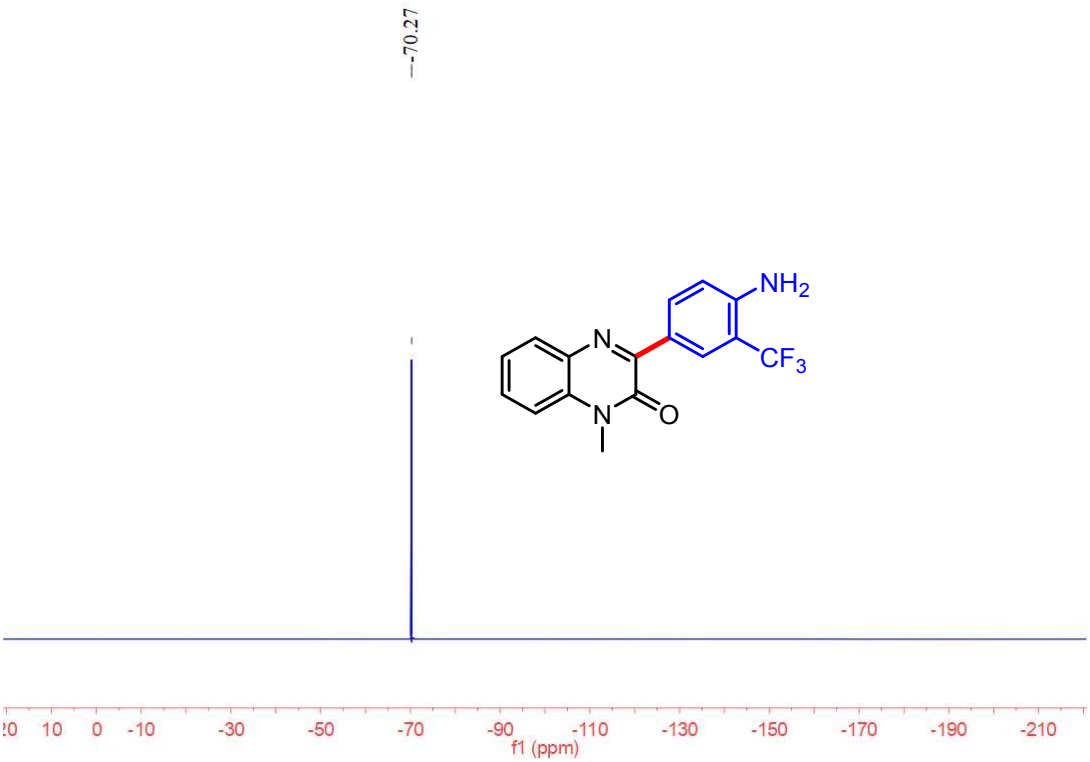
26 ^{1}H NMR (500 MHz, $CDCl_3$)



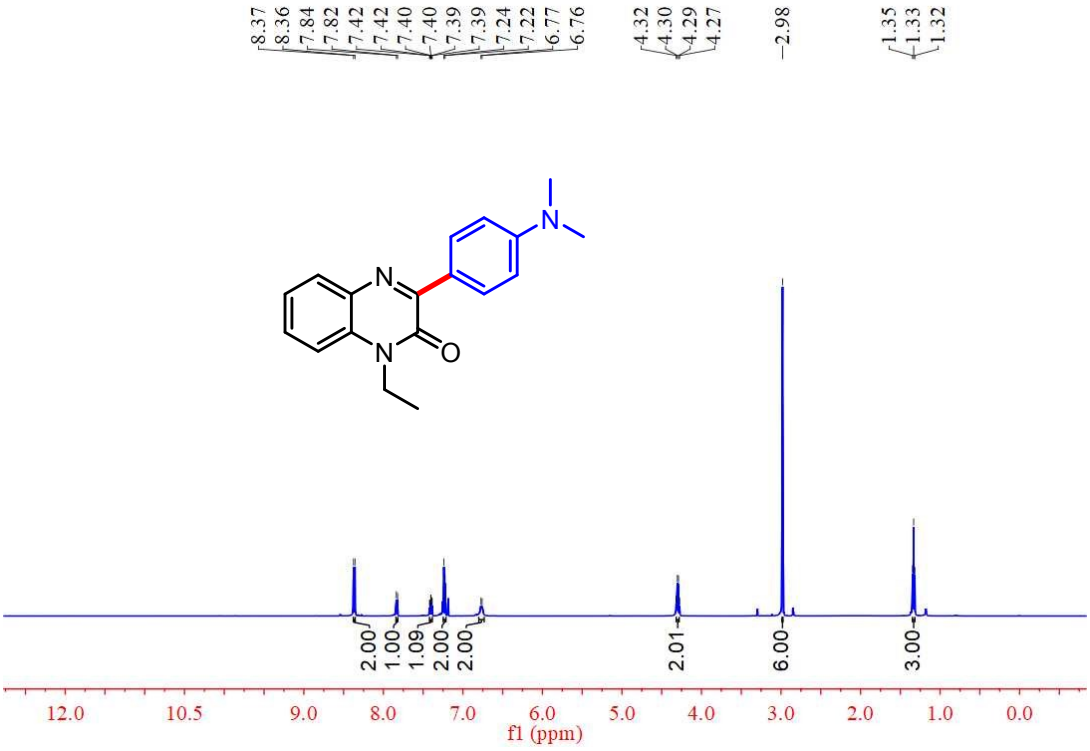
26 ^{13}C NMR (126 MHz, $CDCl_3$)



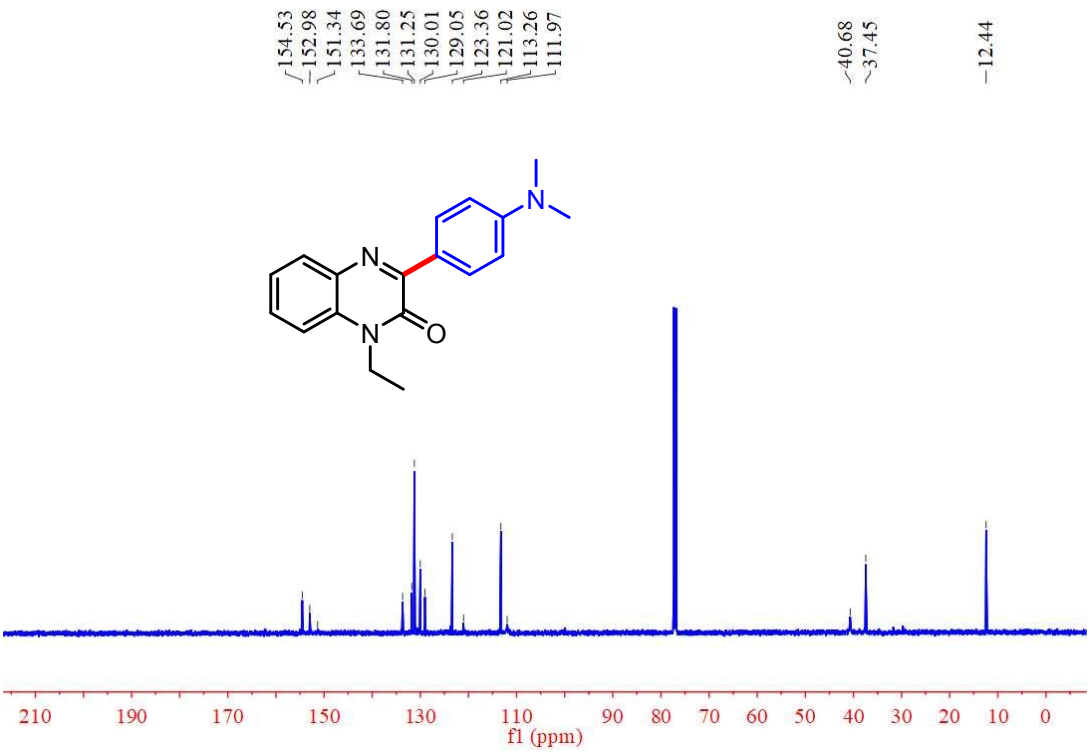
26 ^{19}F NMR (471 MHz, $CDCl_3$)



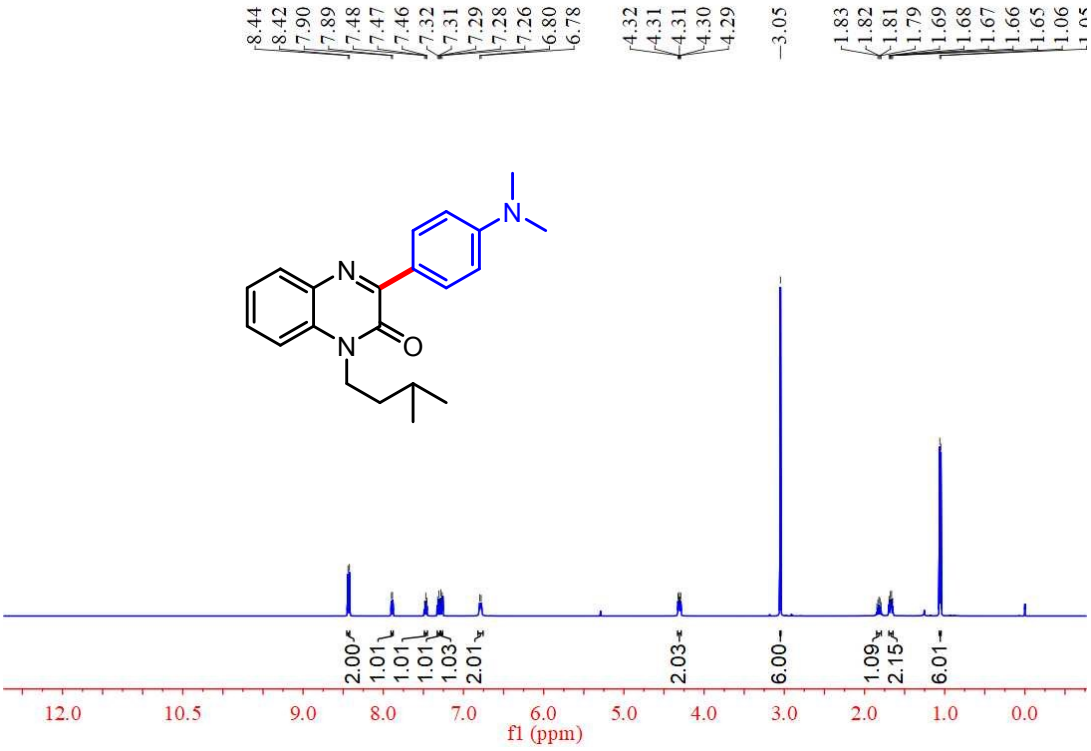
27 ^{1}H NMR (500 MHz, $CDCl_3$)



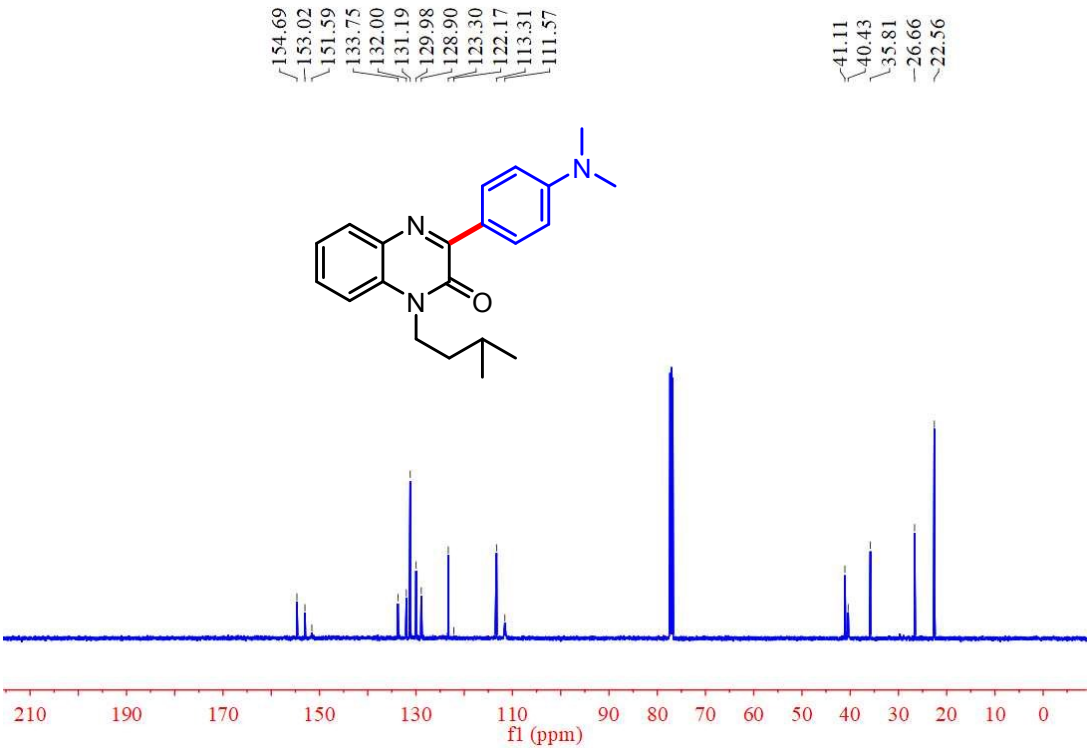
27 ^{13}C NMR (126 MHz, $CDCl_3$)



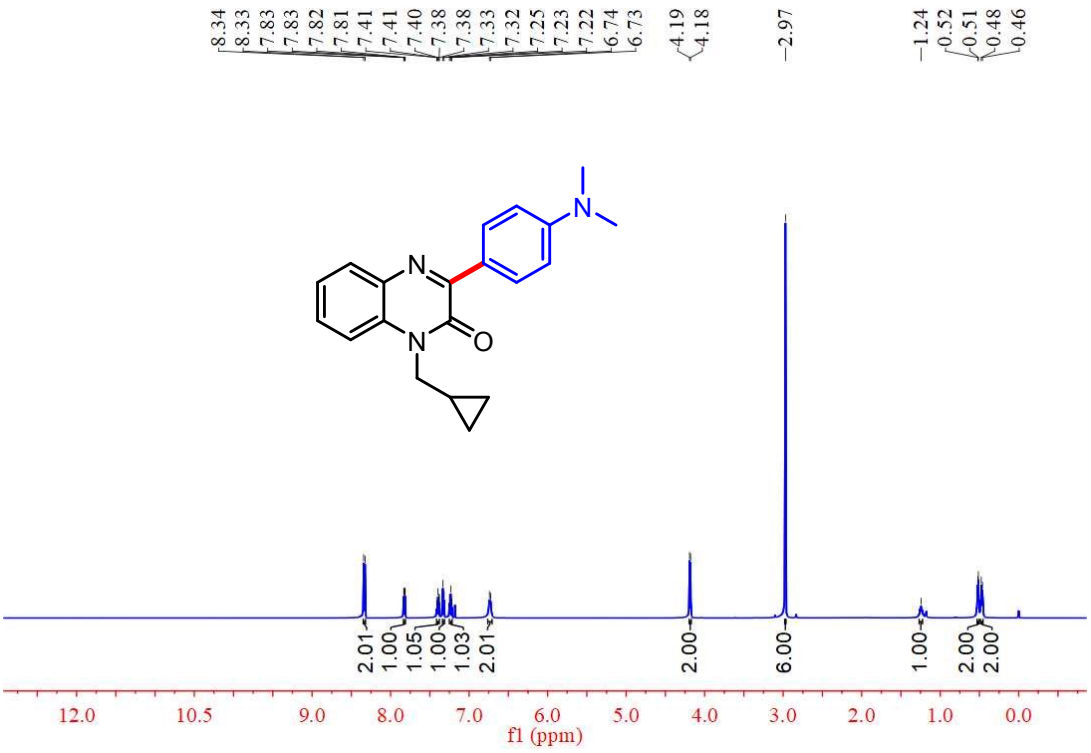
28 ^{1}H NMR (500 MHz, $CDCl_3$)



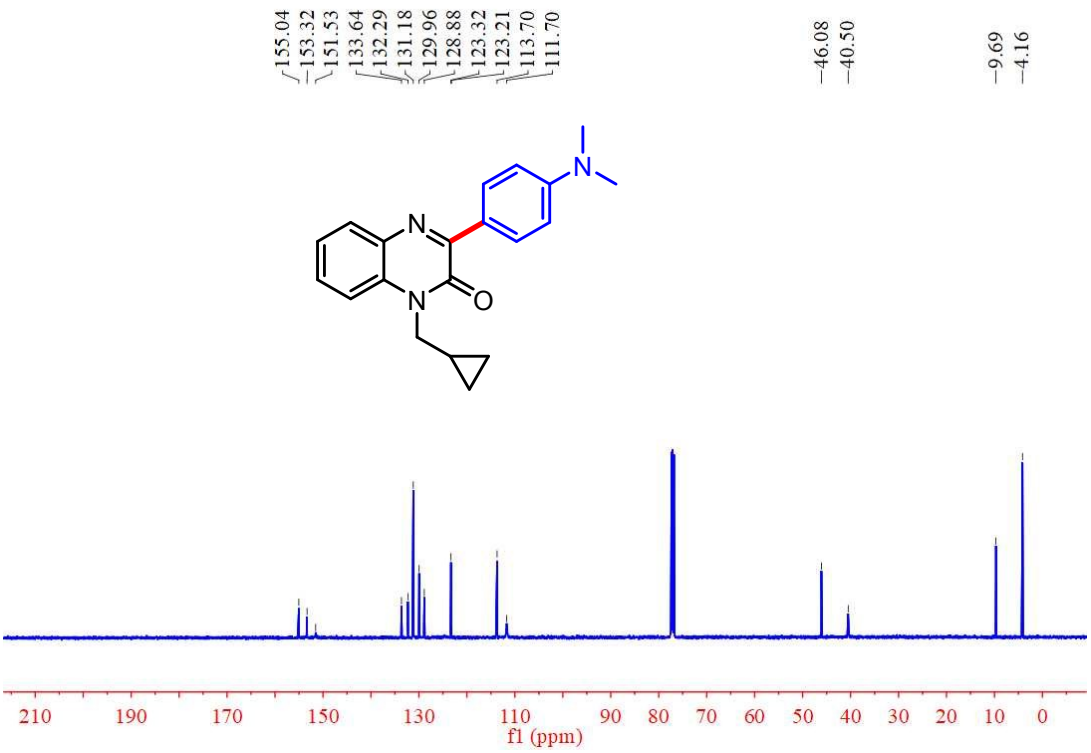
28 ^{13}C NMR (126 MHz, $CDCl_3$)



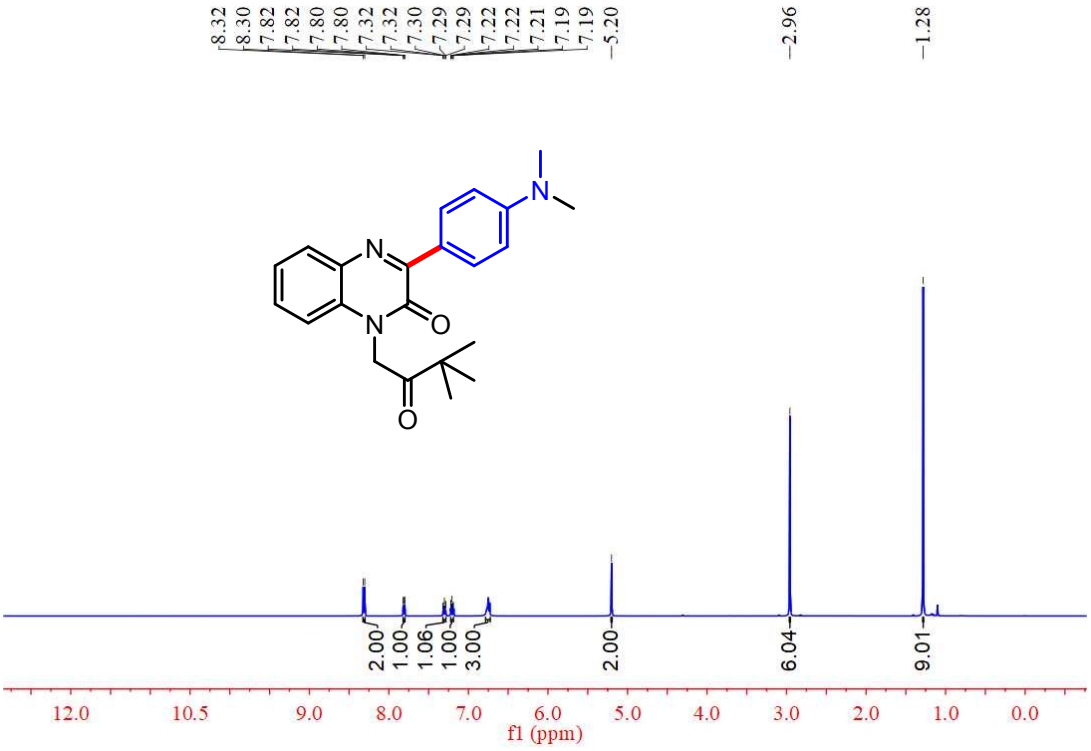
29 ^{1}H NMR (500 MHz, $CDCl_3$)



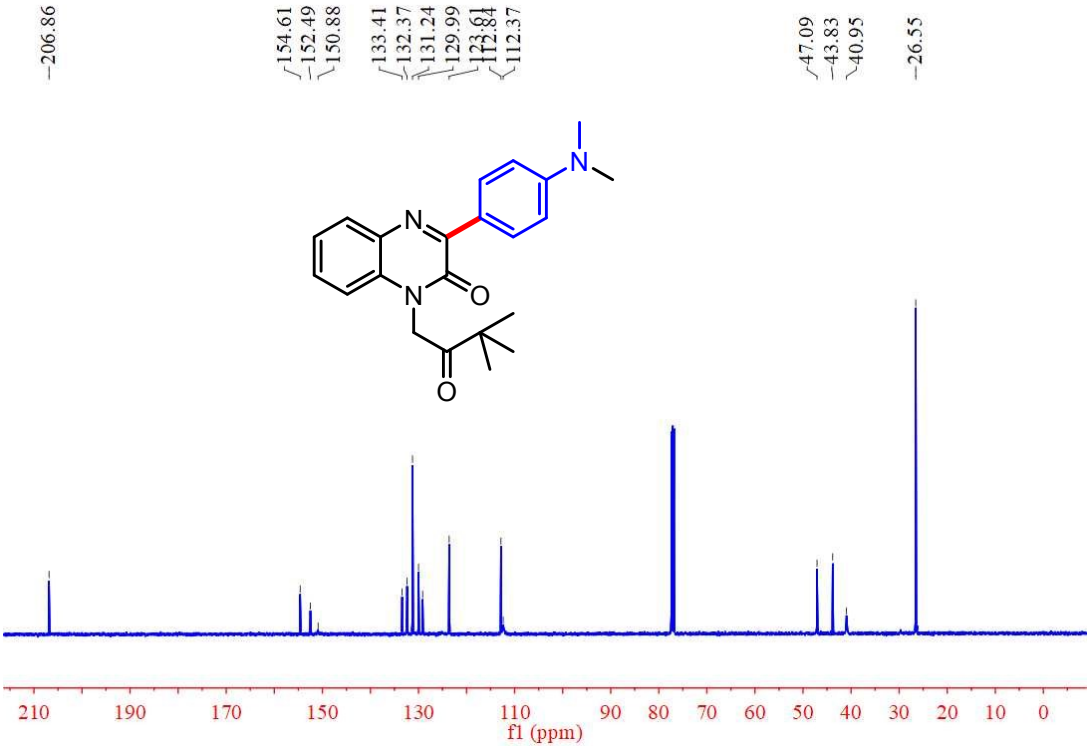
29 ^{13}C NMR (126 MHz, $CDCl_3$)



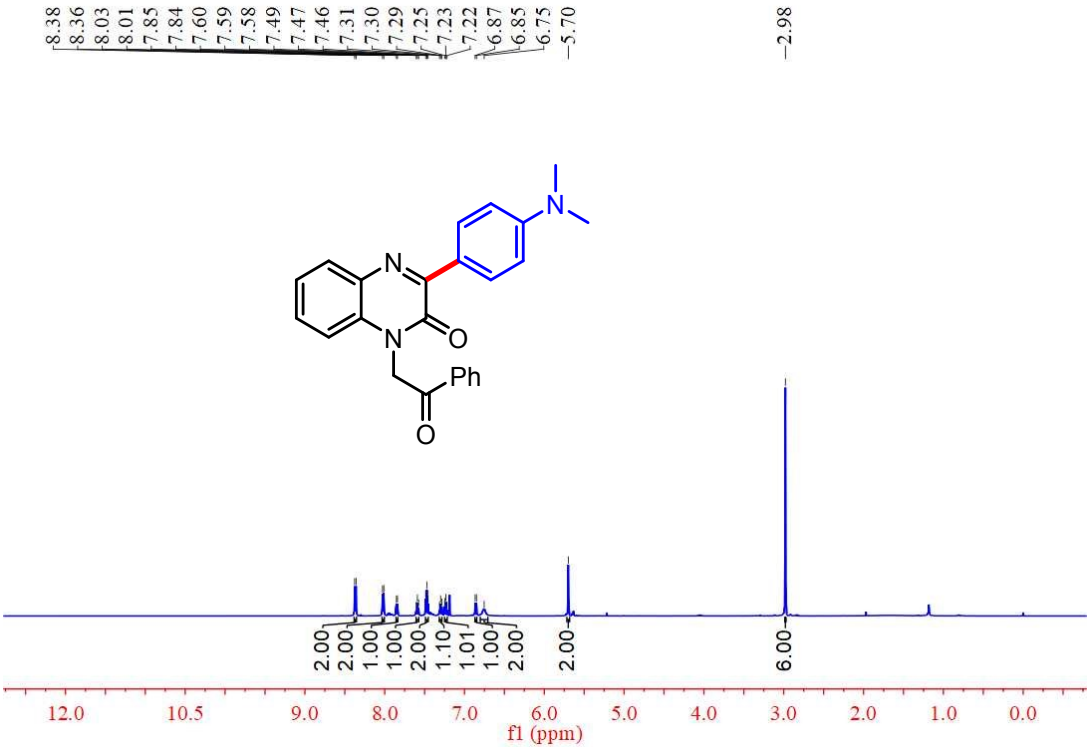
30 ^{1}H NMR (500 MHz, $CDCl_3$)



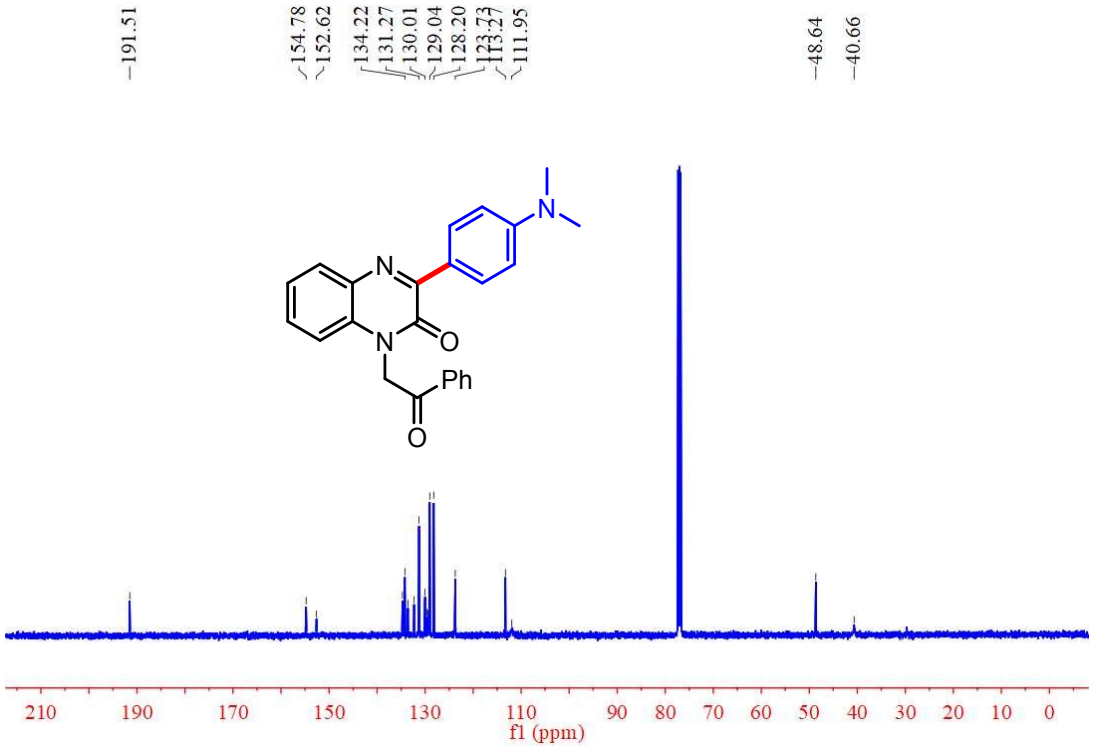
30 ^{13}C NMR (126 MHz, $CDCl_3$)



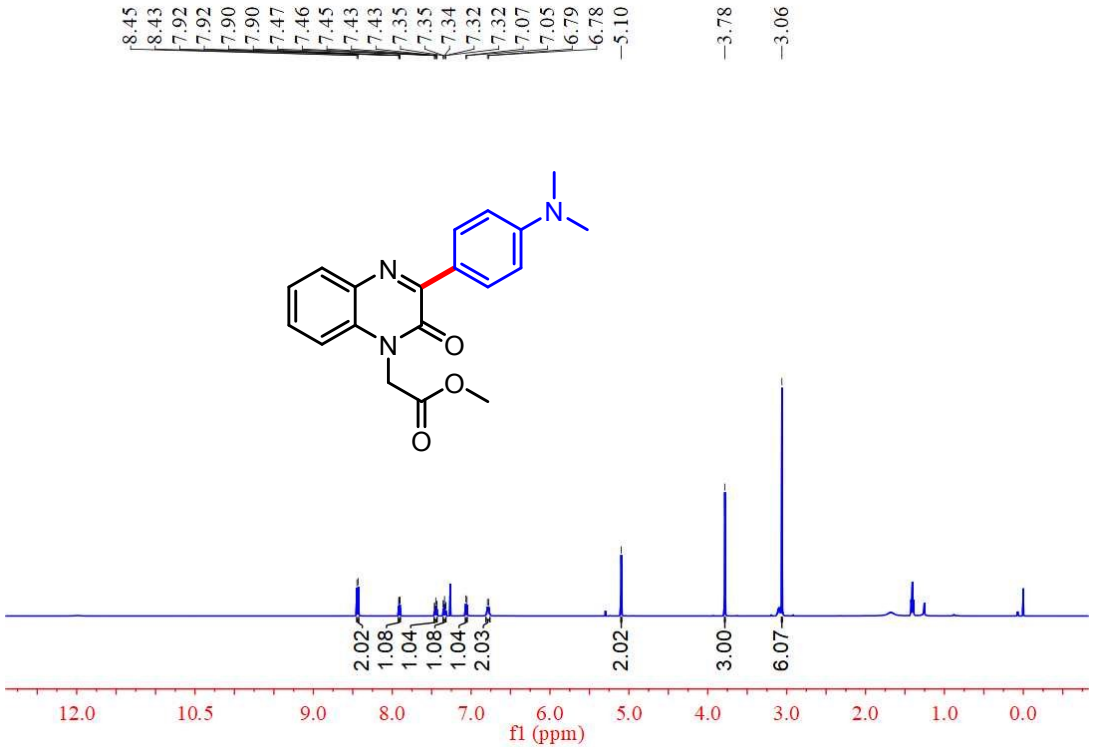
31 ^{1}H NMR (500 MHz, $CDCl_3$)



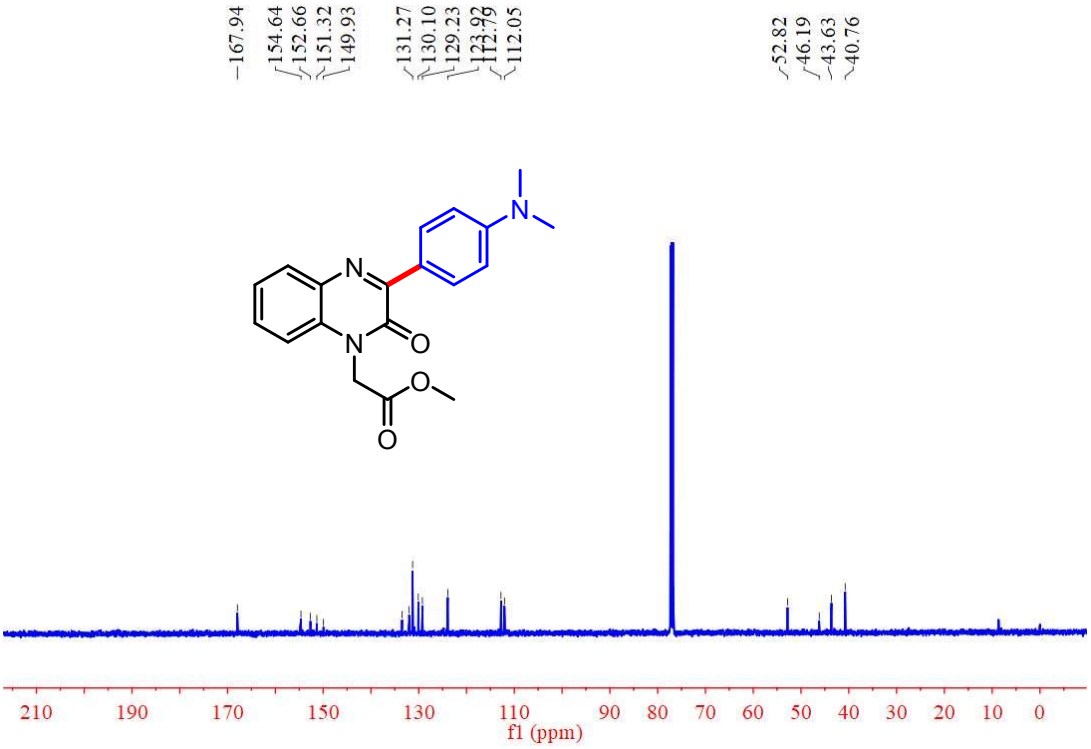
31 ^{13}C NMR (126 MHz, $CDCl_3$)



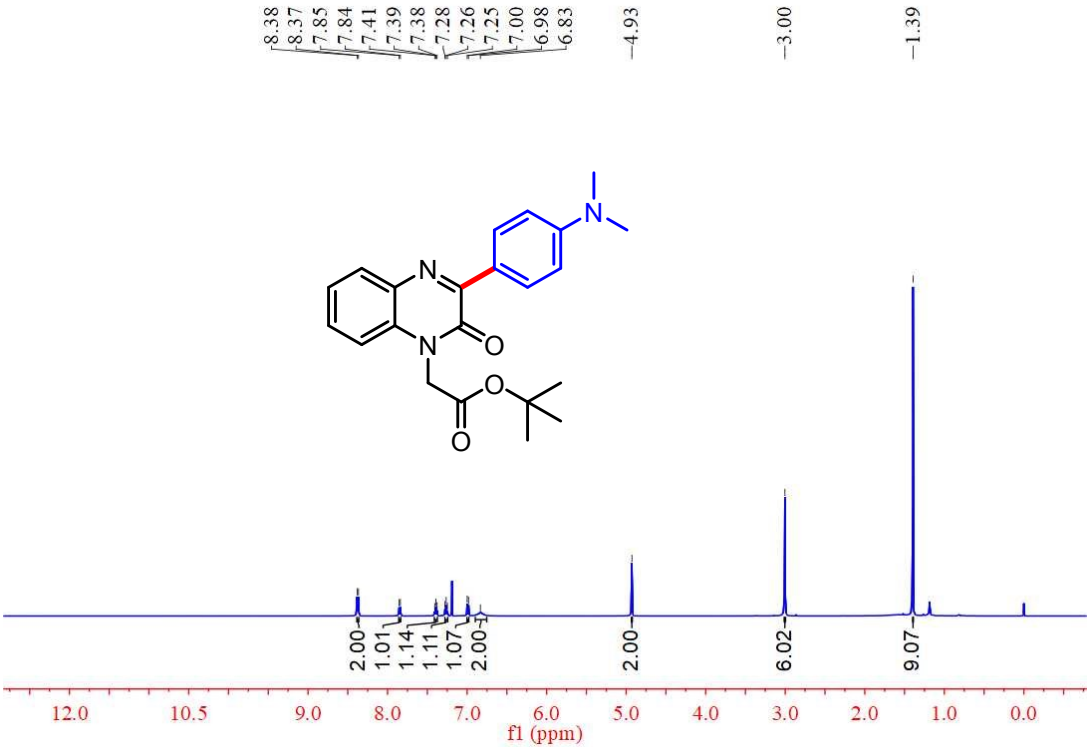
32 ^{1}H NMR (500 MHz, $CDCl_3$)



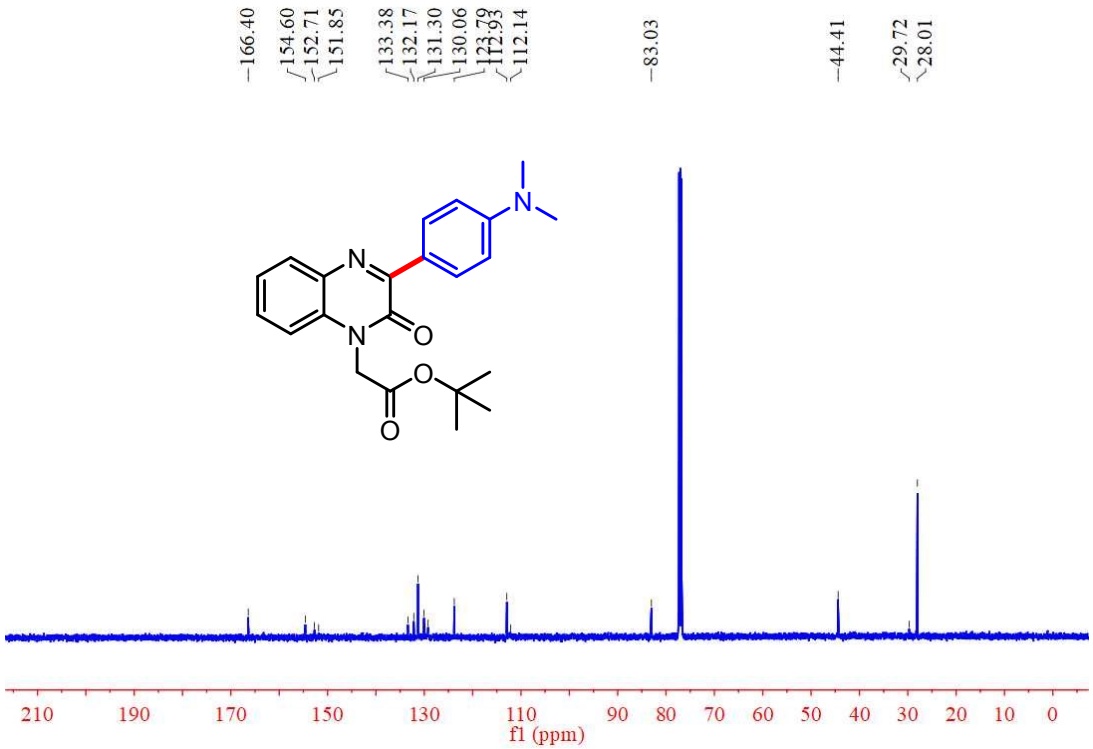
32 ^{13}C NMR (126 MHz, $CDCl_3$)



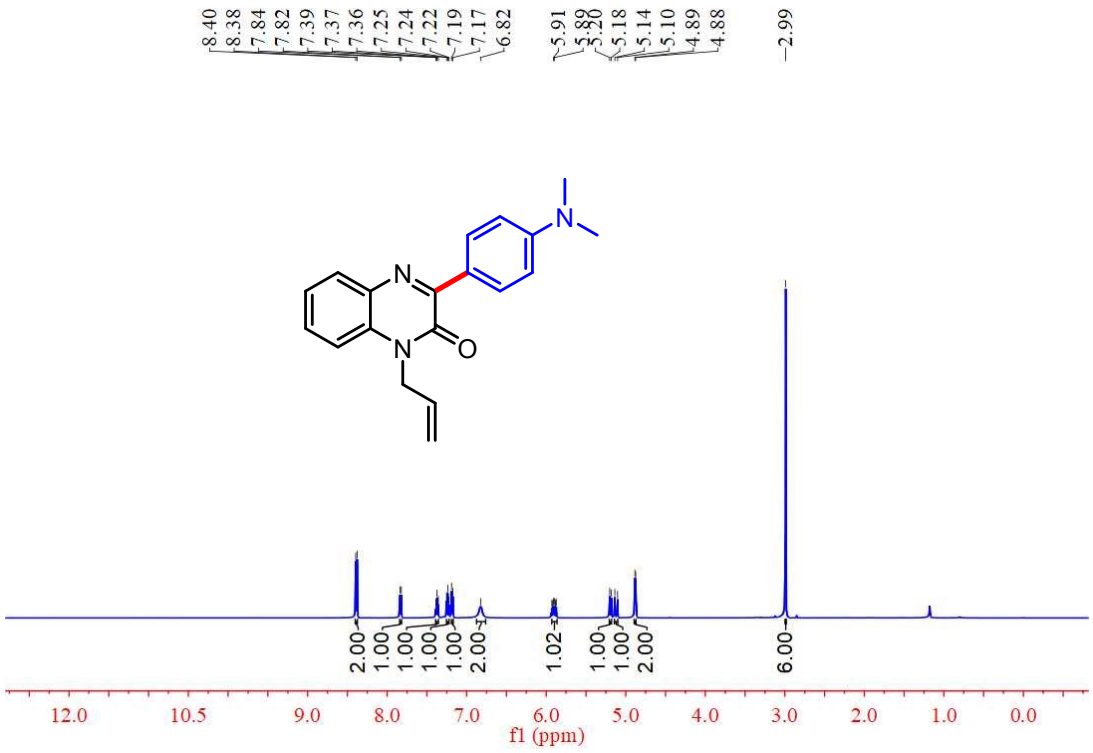
33 ^{1}H NMR (500 MHz, $CDCl_3$)



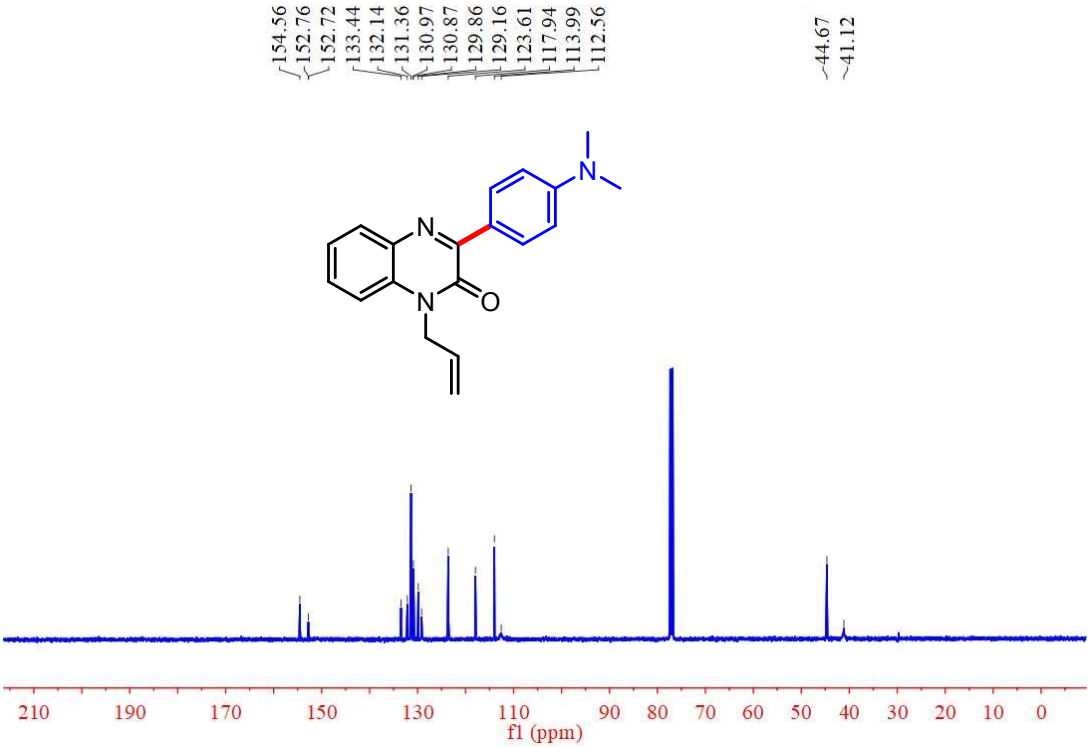
33 ^{13}C NMR (126 MHz, $CDCl_3$)



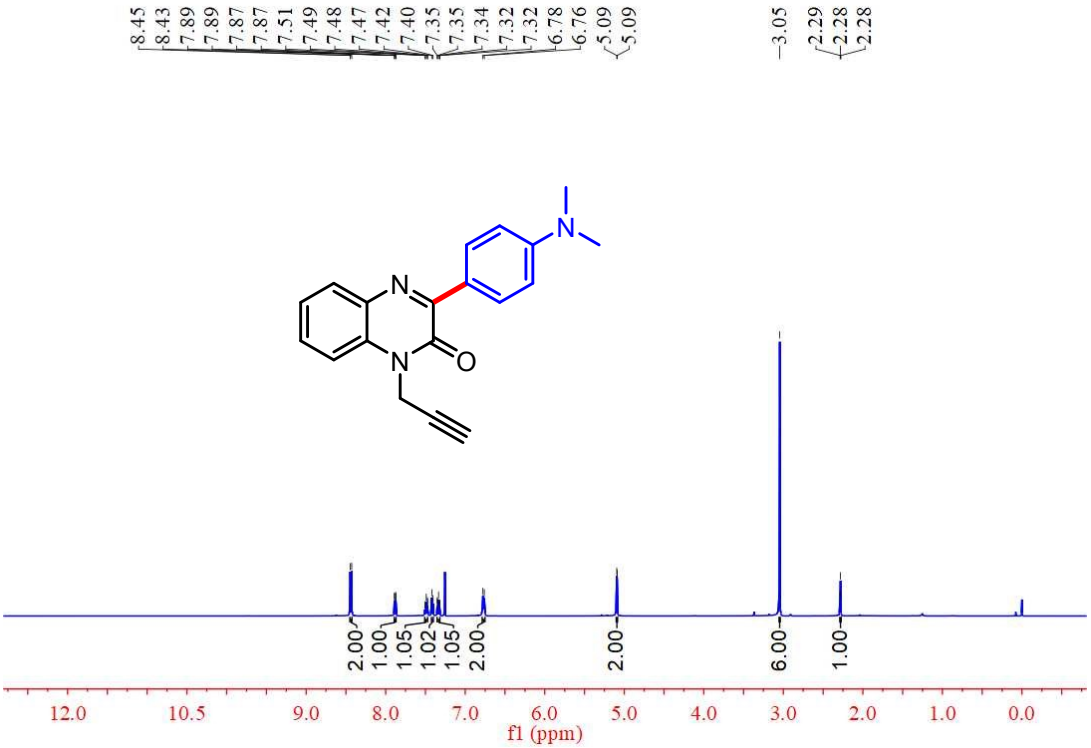
34 ^{1}H NMR (500 MHz, $CDCl_3$)



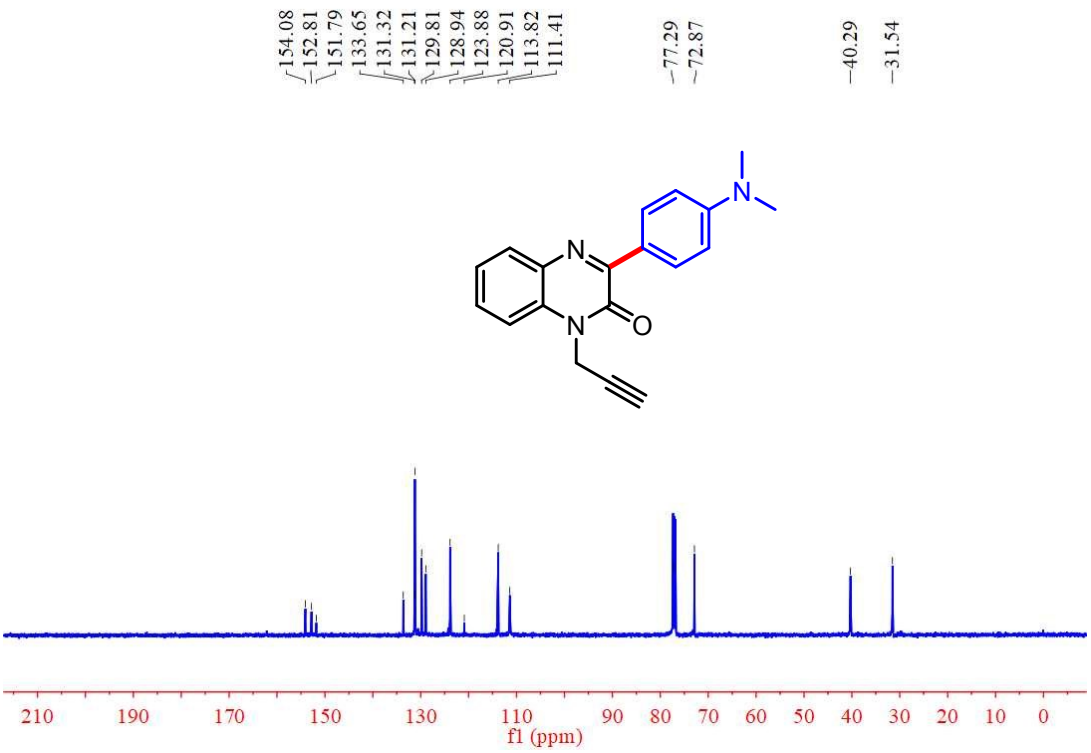
34 ^{13}C NMR (126 MHz, $CDCl_3$)



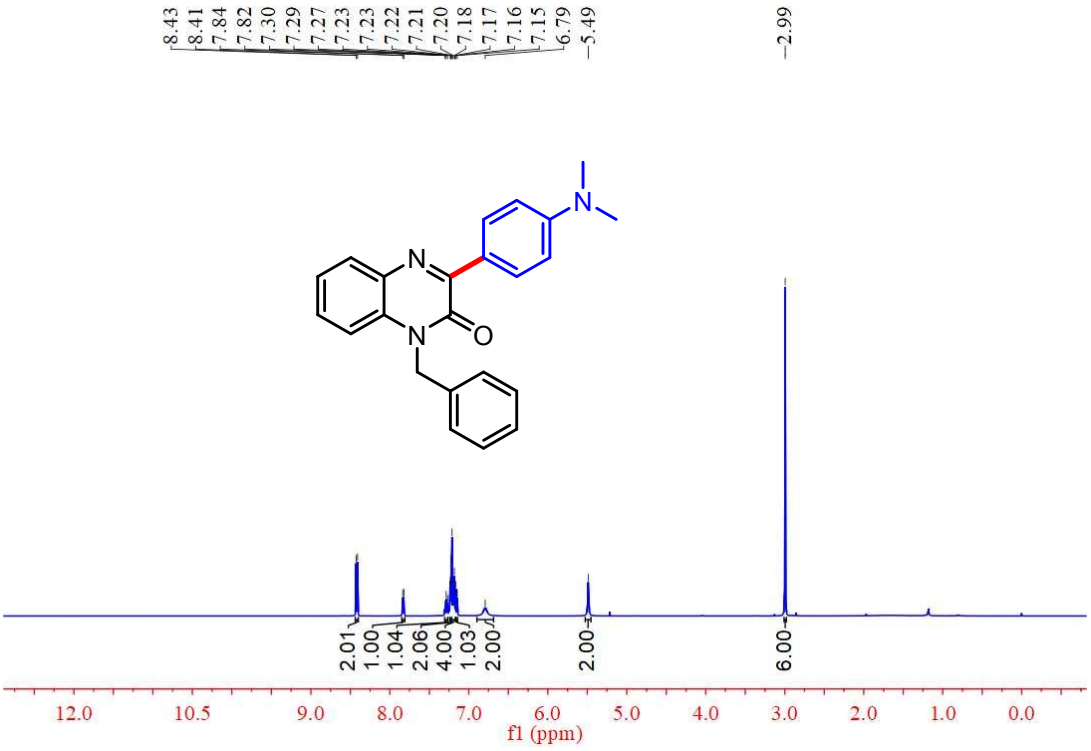
35 ^{1}H NMR (500 MHz, $CDCl_3$)



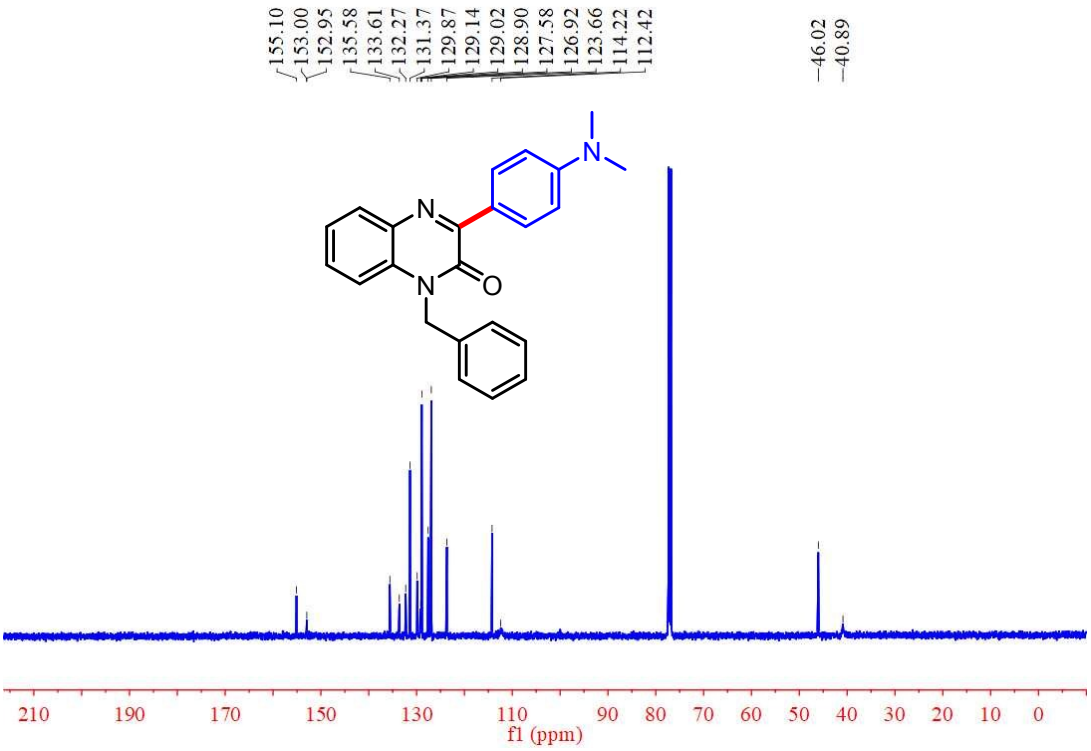
35 ^{13}C NMR (126 MHz, $CDCl_3$)



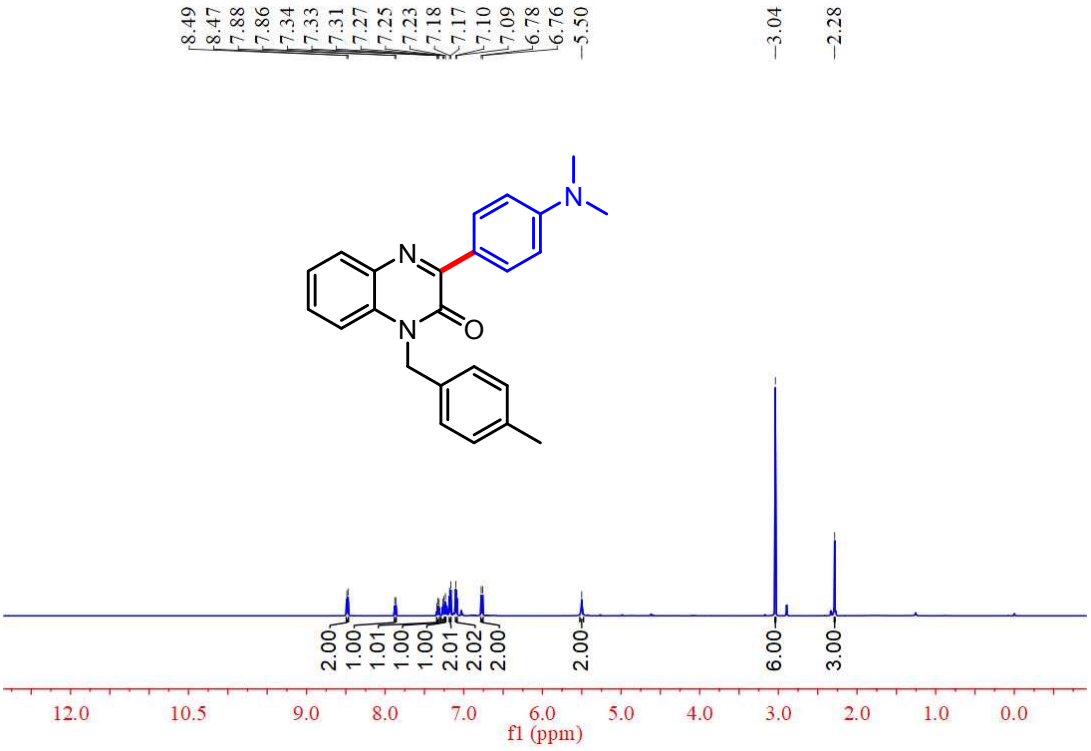
36 ^{1}H NMR (500 MHz, $CDCl_3$)



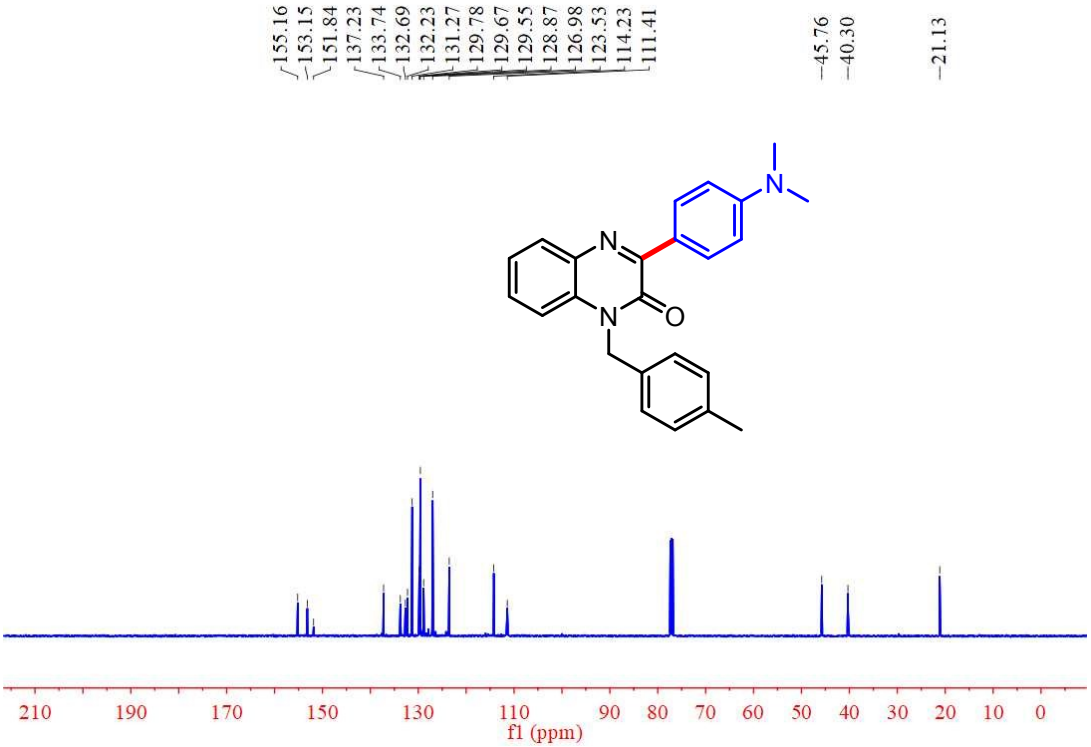
36 ^{13}C NMR (126 MHz, $CDCl_3$)



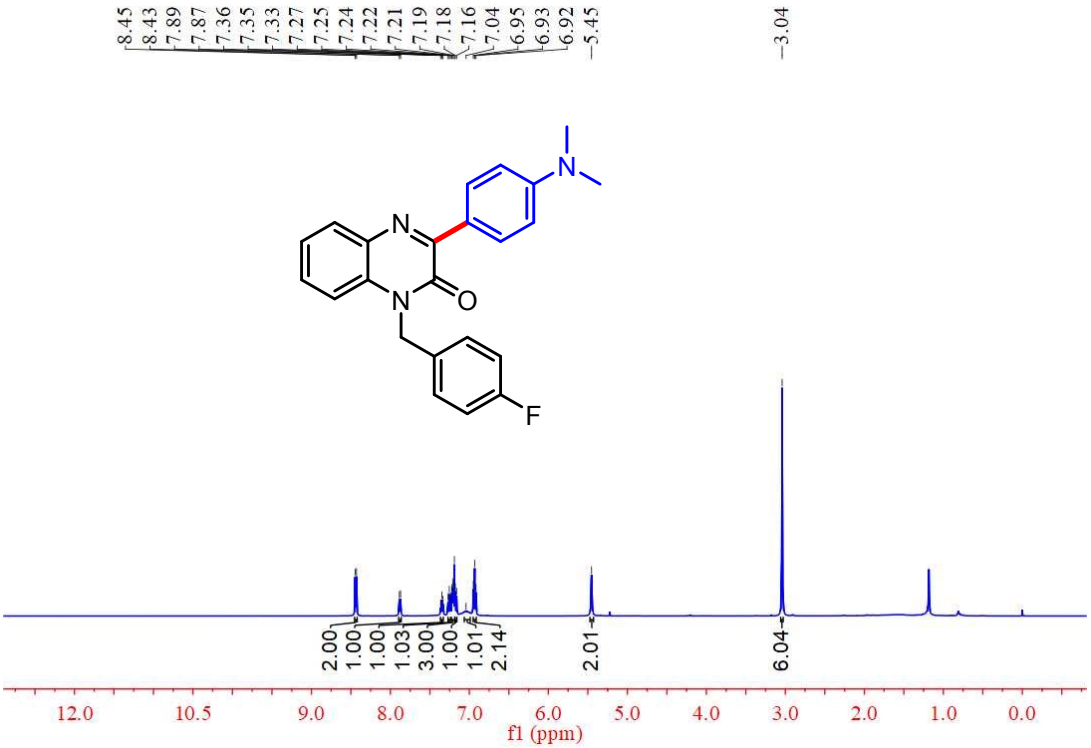
37 ^{1}H NMR (500 MHz, $CDCl_3$)



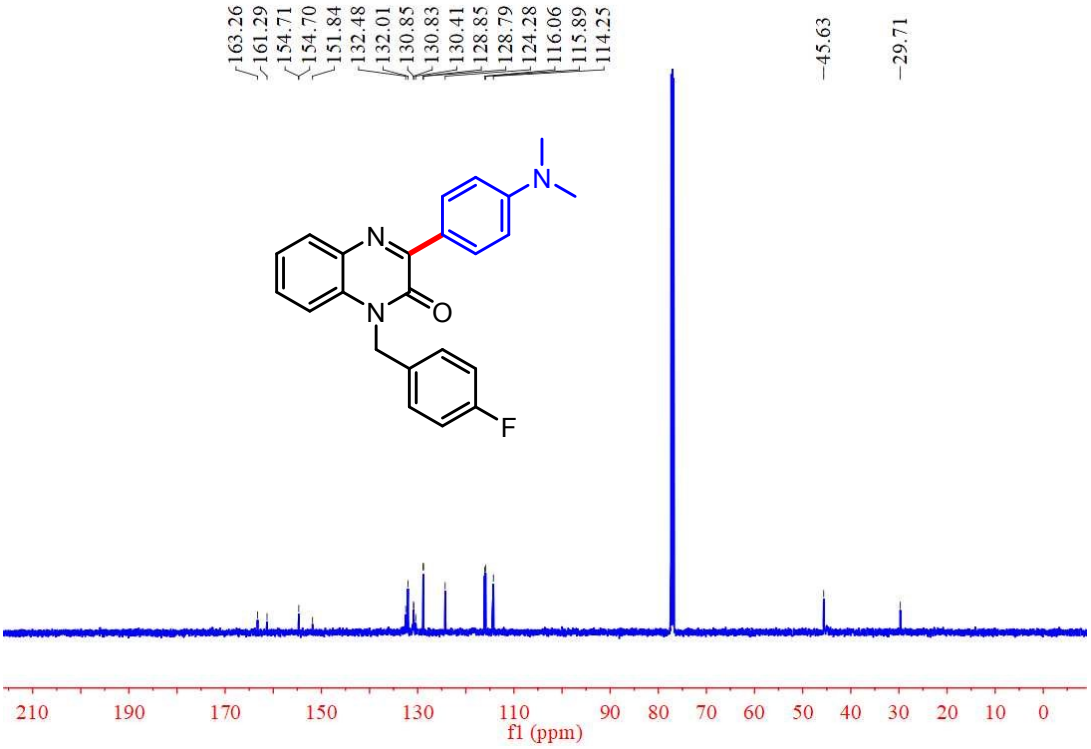
37 ^{13}C NMR (126 MHz, $CDCl_3$)



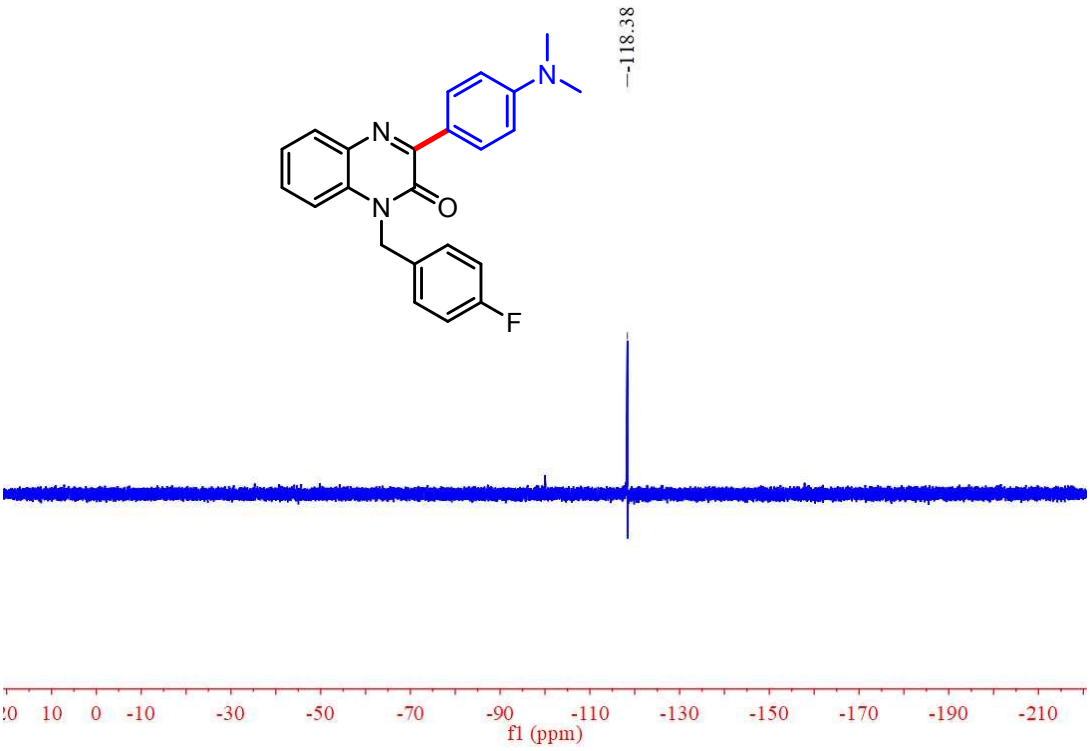
38 ^{1}H NMR (500 MHz, $CDCl_3$)



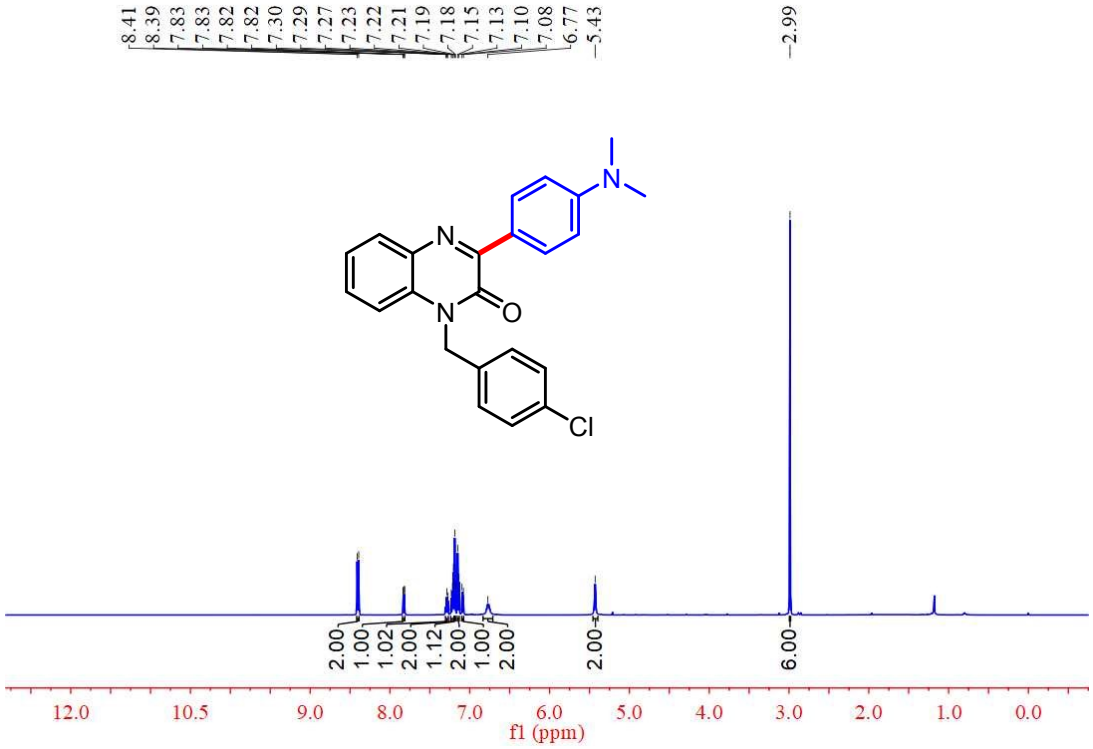
38 ^{13}C NMR (126 MHz, $CDCl_3$)



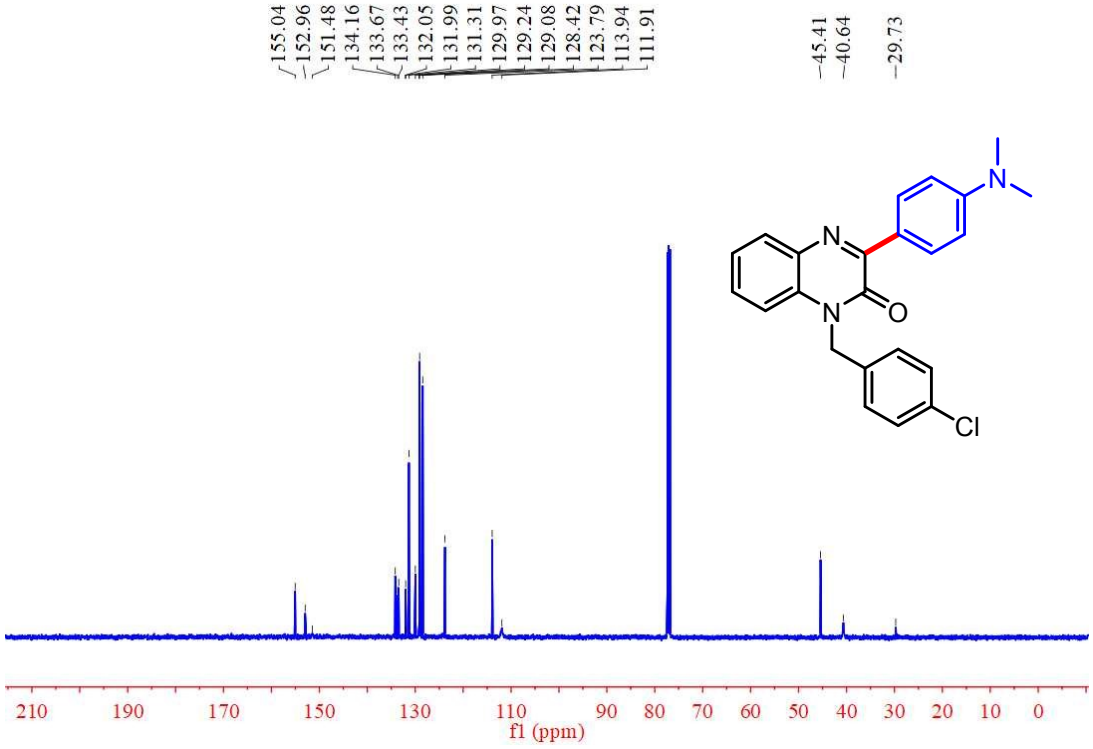
38 ^{19}F NMR (471 MHz, $CDCl_3$)



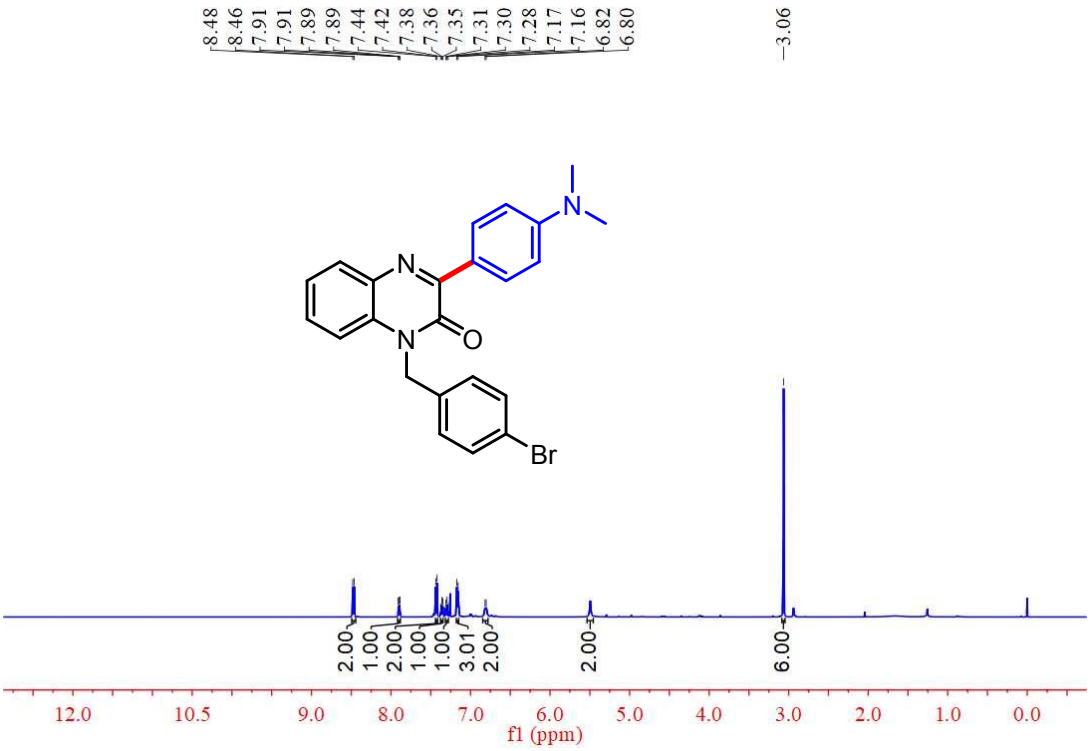
39 ^{1}H NMR (500 MHz, $CDCl_3$)



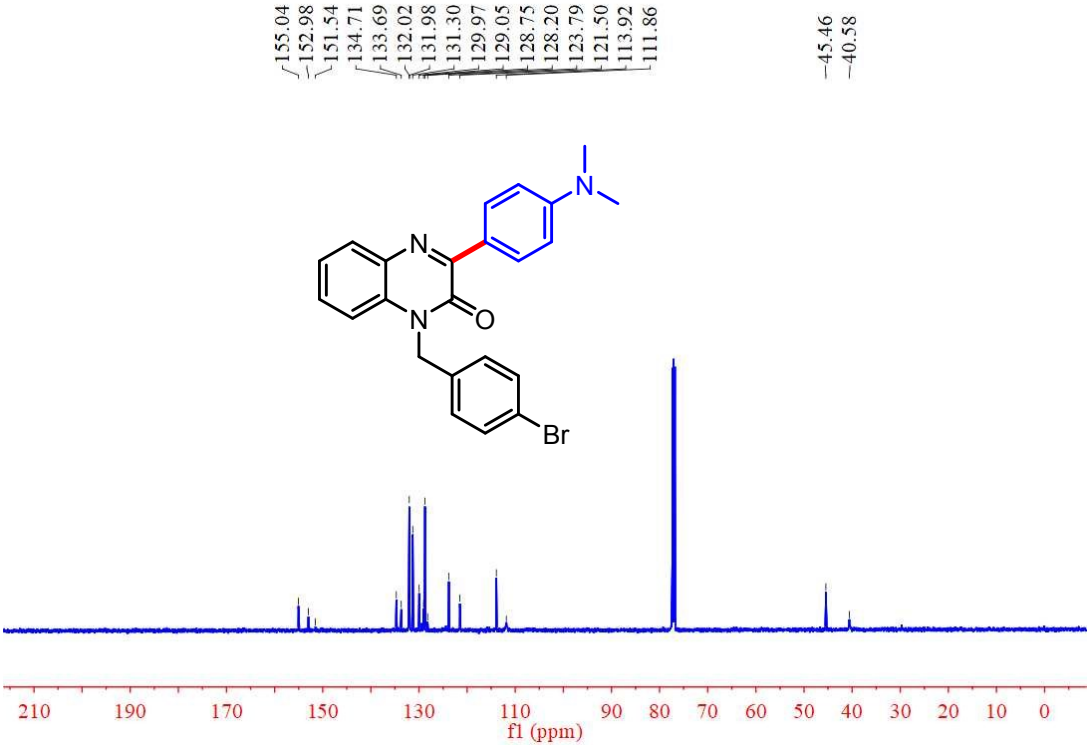
39 ^{13}C NMR (126 MHz, $CDCl_3$)



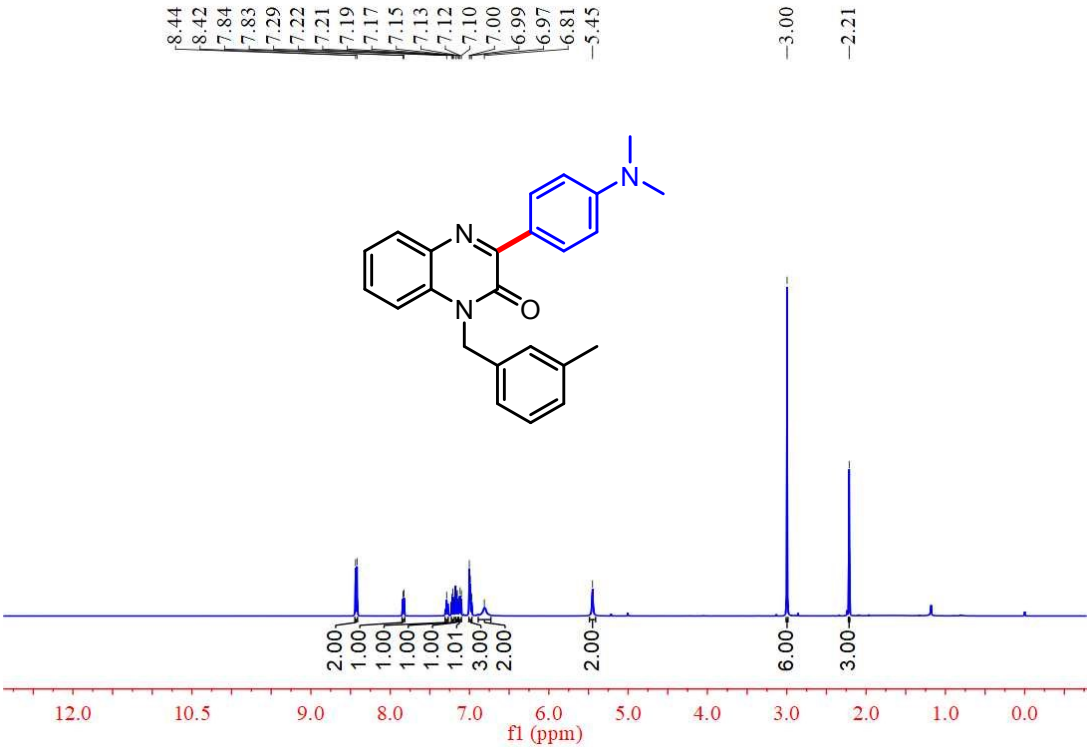
40 ^{1}H NMR (500 MHz, $CDCl_3$)



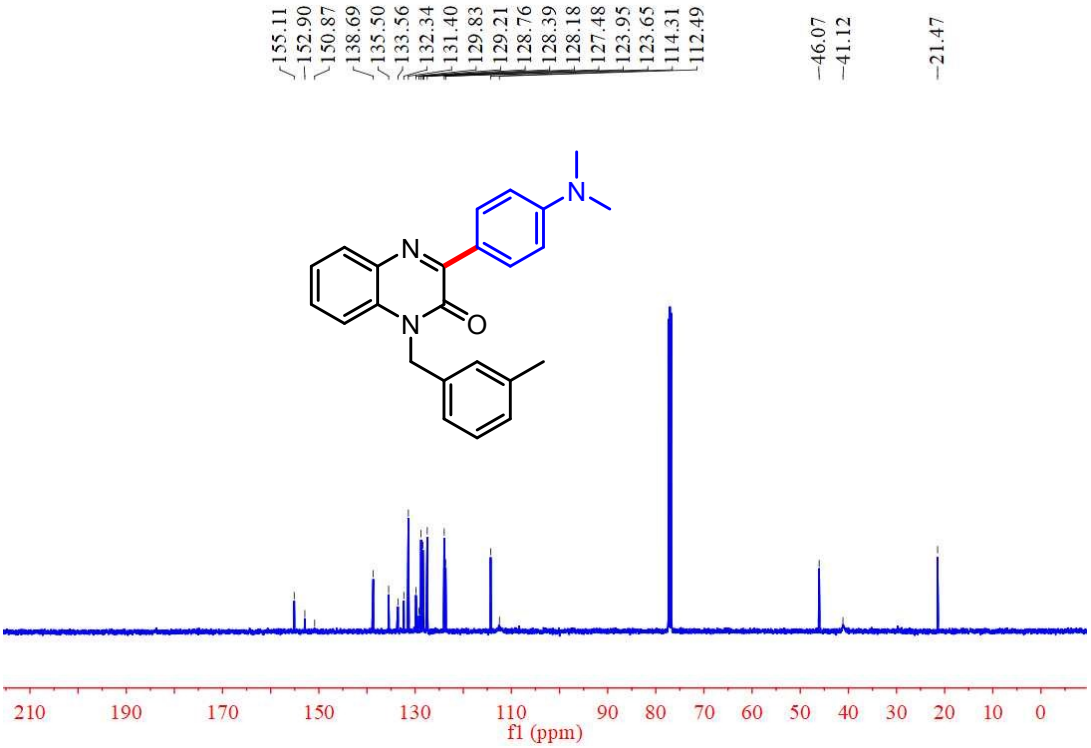
40 ^{13}C NMR (126 MHz, $CDCl_3$)



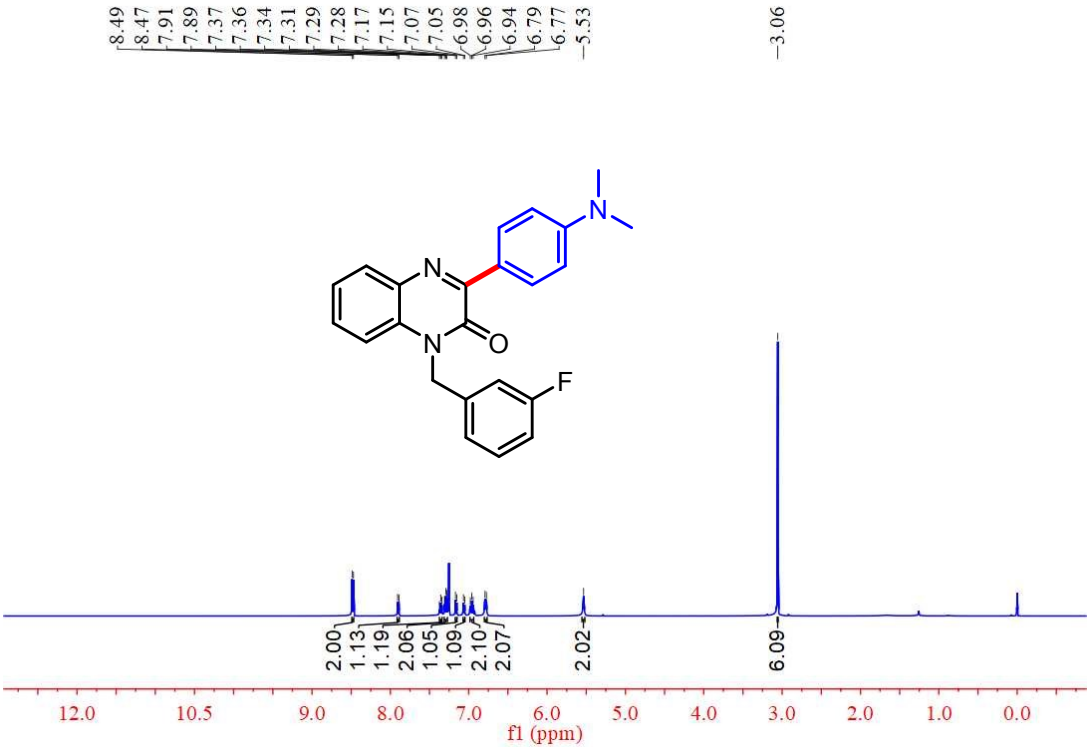
41 ^{1}H NMR (500 MHz, $CDCl_3$)



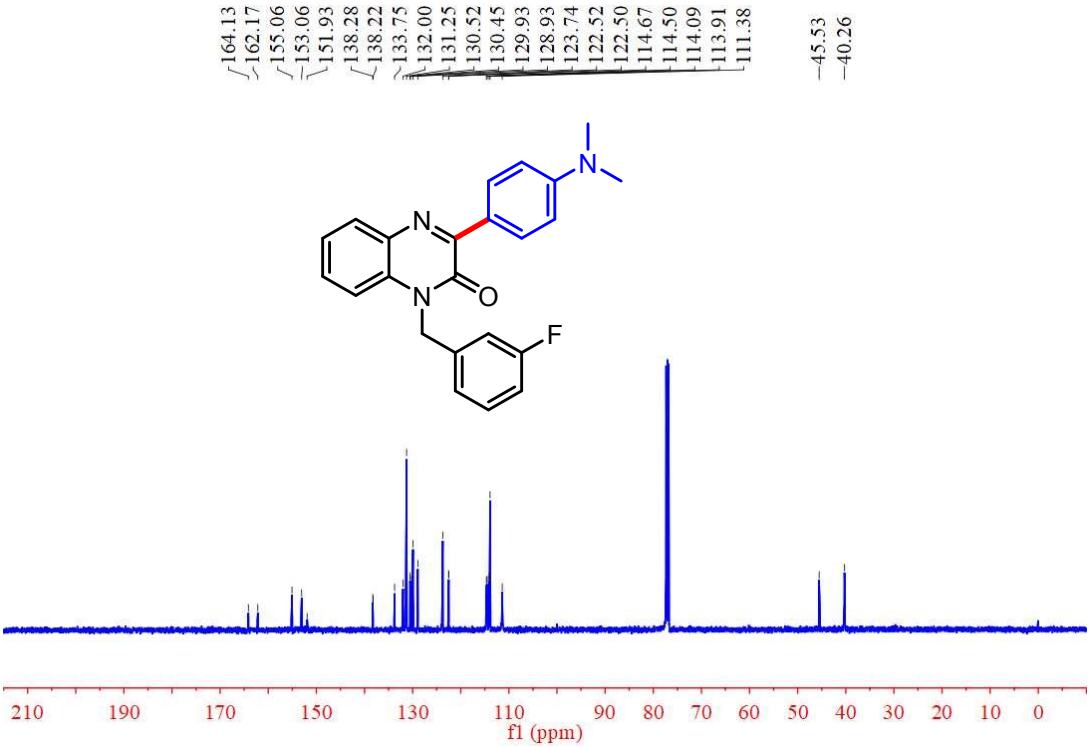
41 ^{13}C NMR (126 MHz, $CDCl_3$)



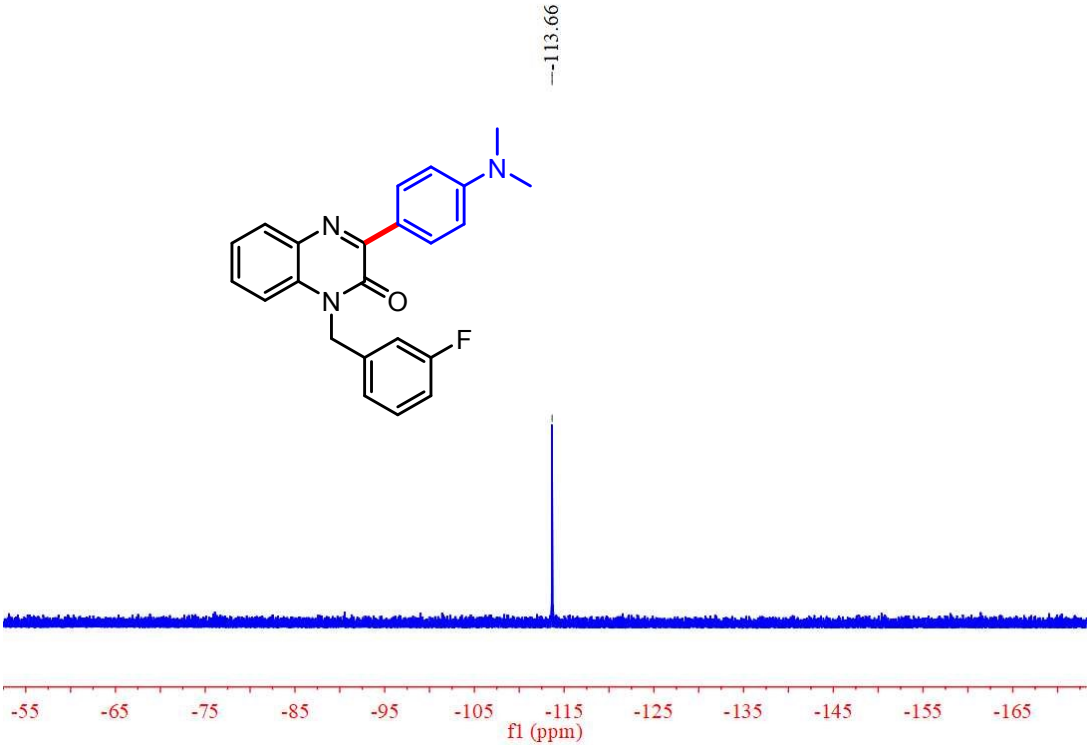
42 ^{1}H NMR (500 MHz, $CDCl_3$)



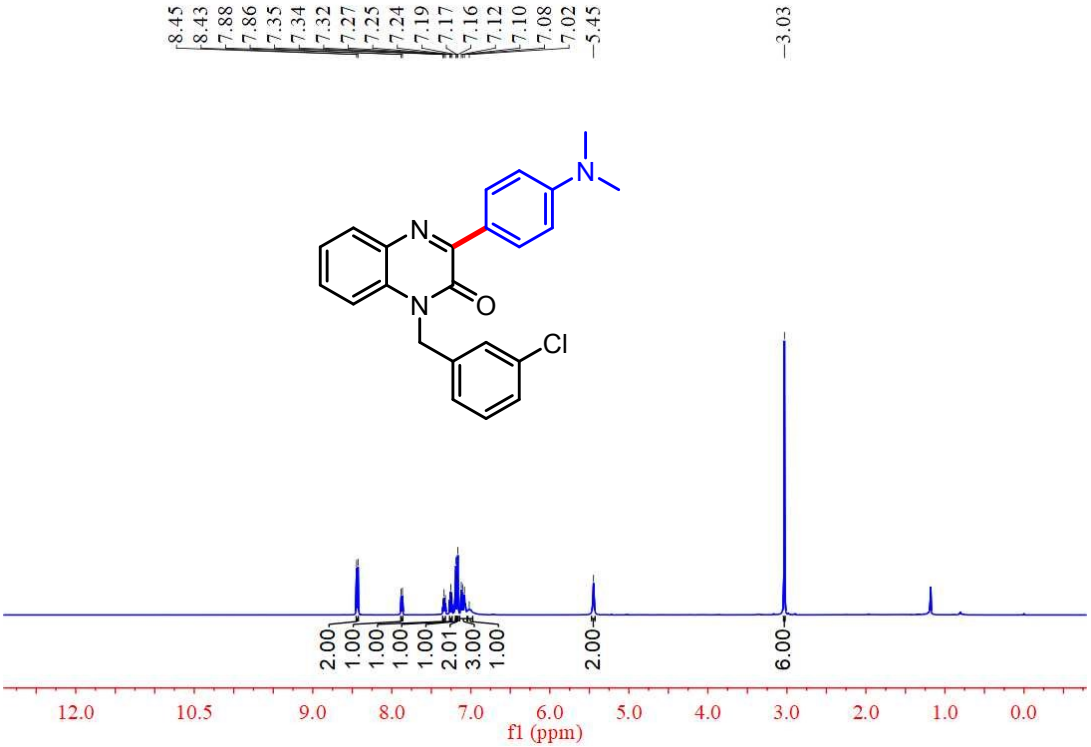
42 ^{13}C NMR (126 MHz, $CDCl_3$)



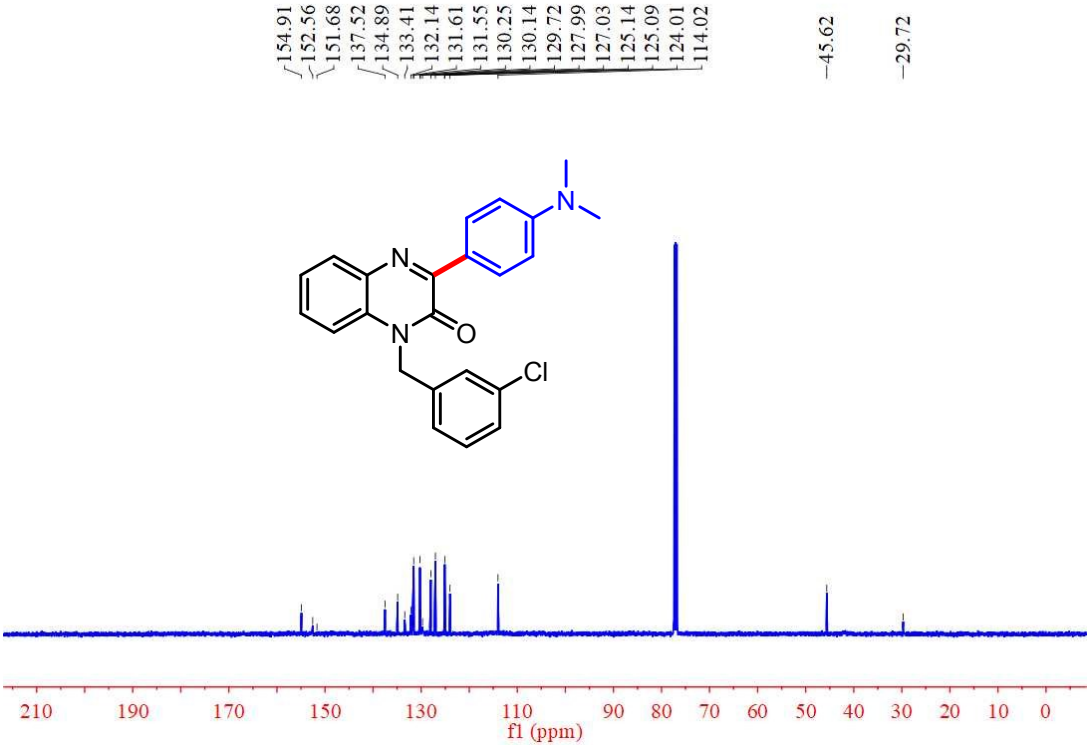
42 ^{19}F NMR (471 MHz, $CDCl_3$)



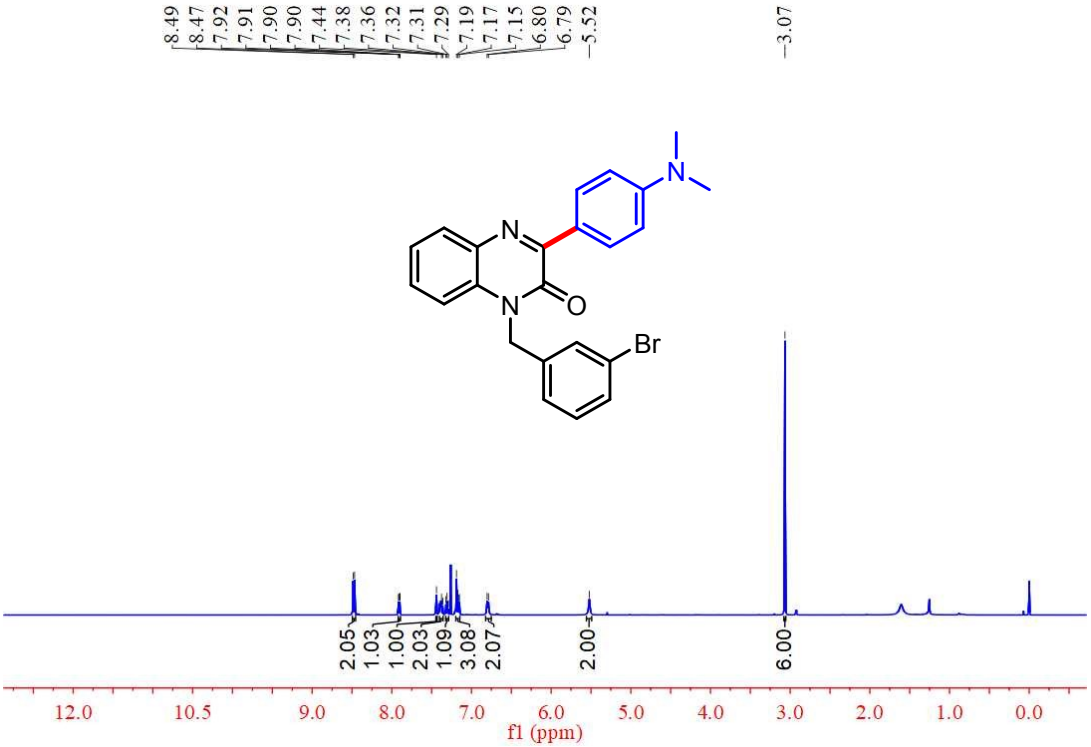
43 ^{1}H NMR (500 MHz, $CDCl_3$)



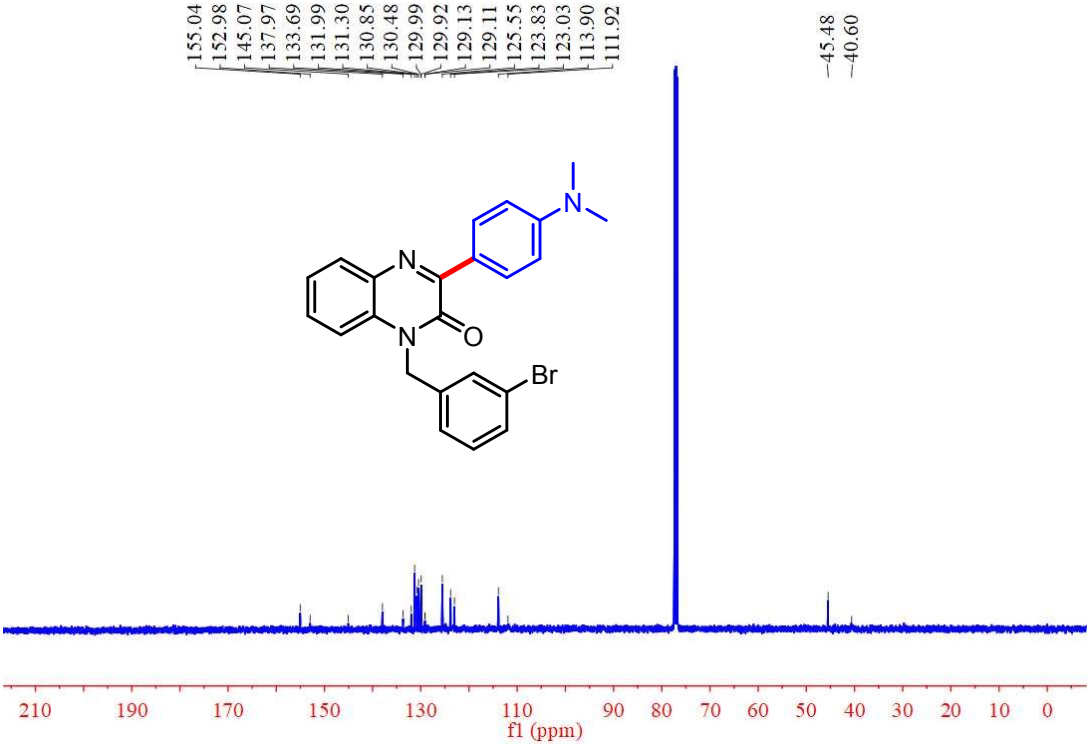
43 ^{13}C NMR (126 MHz, $CDCl_3$)



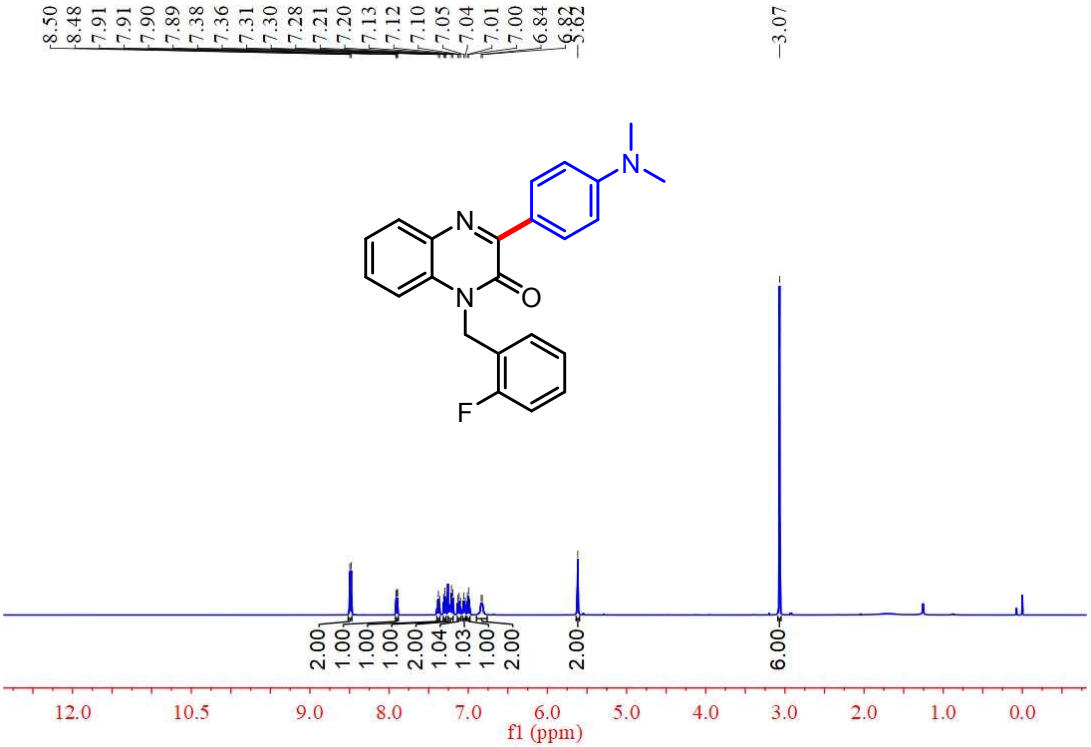
44 ^{1}H NMR (500 MHz, $CDCl_3$)



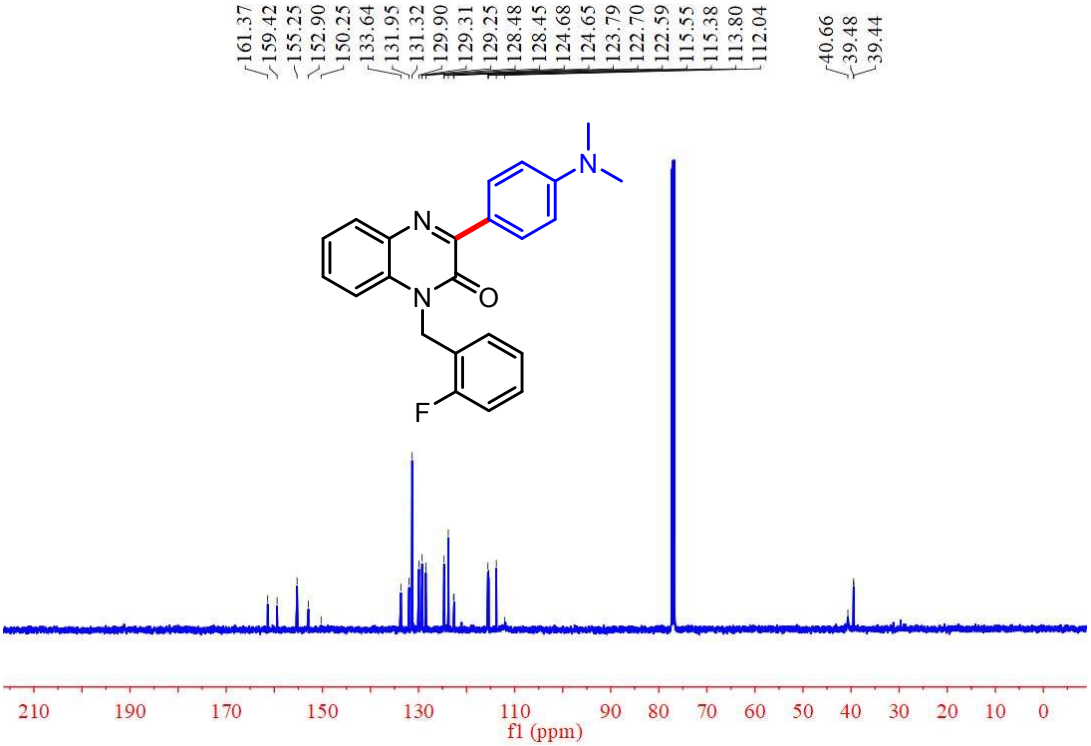
44 ^{13}C NMR (126 MHz, $CDCl_3$)



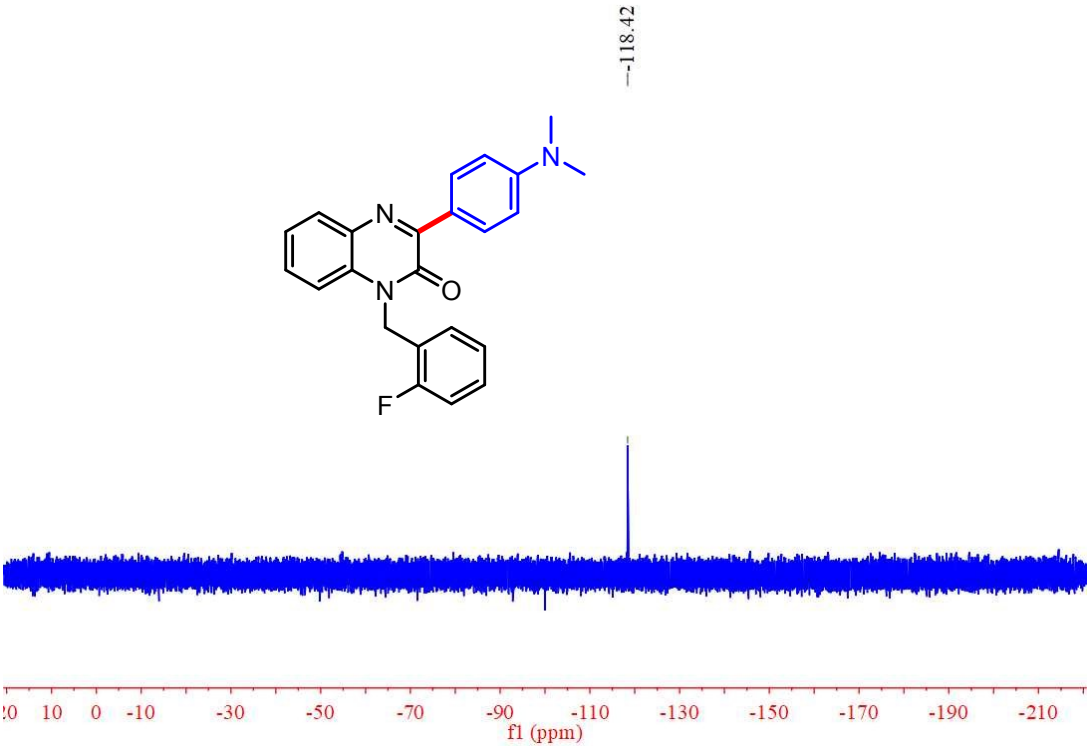
45 ^{1}H NMR (500 MHz, $CDCl_3$)



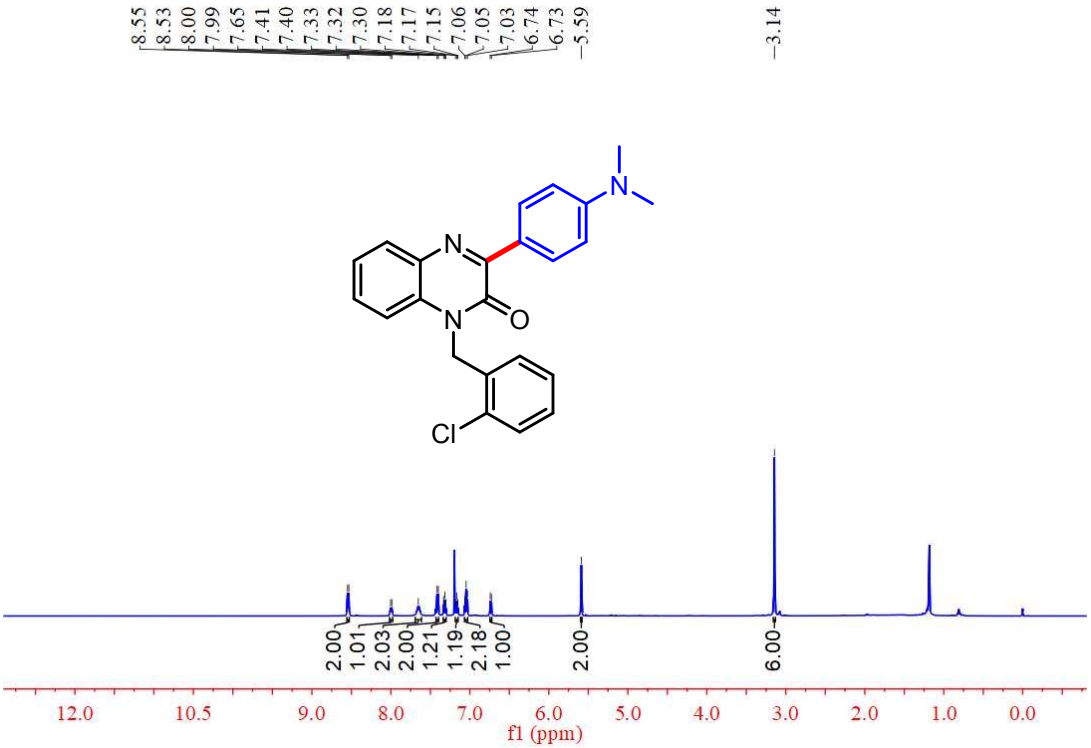
45 ^{13}C NMR (126 MHz, $CDCl_3$)



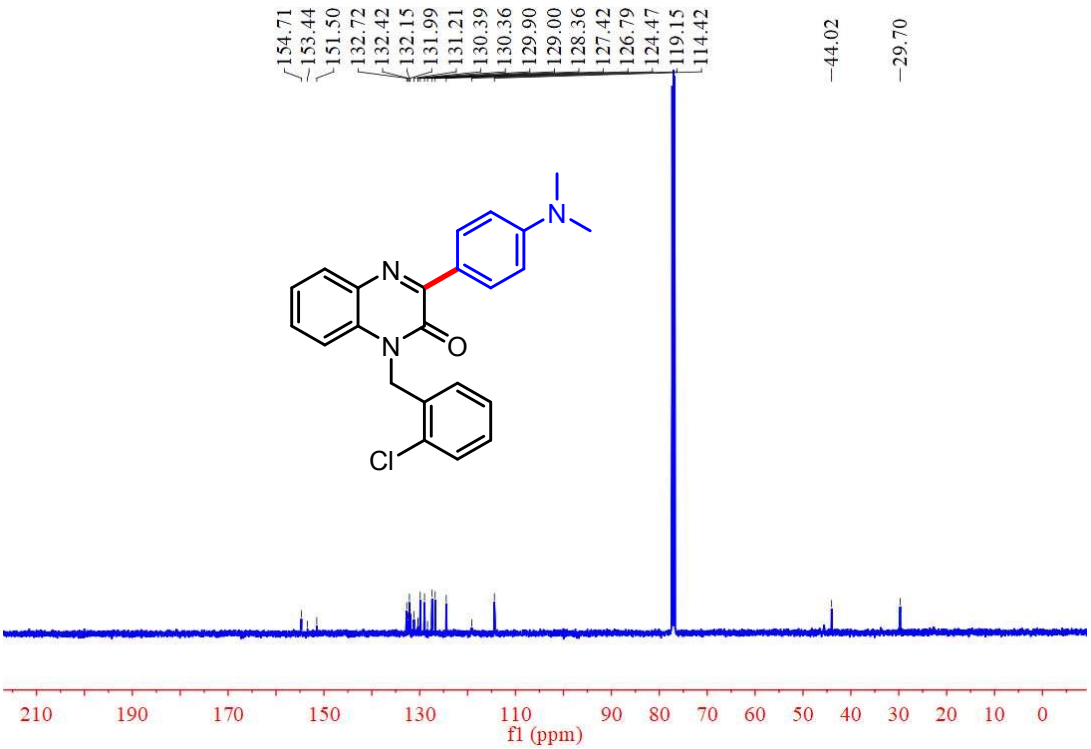
45 ^{19}F NMR (471 MHz, $CDCl_3$)



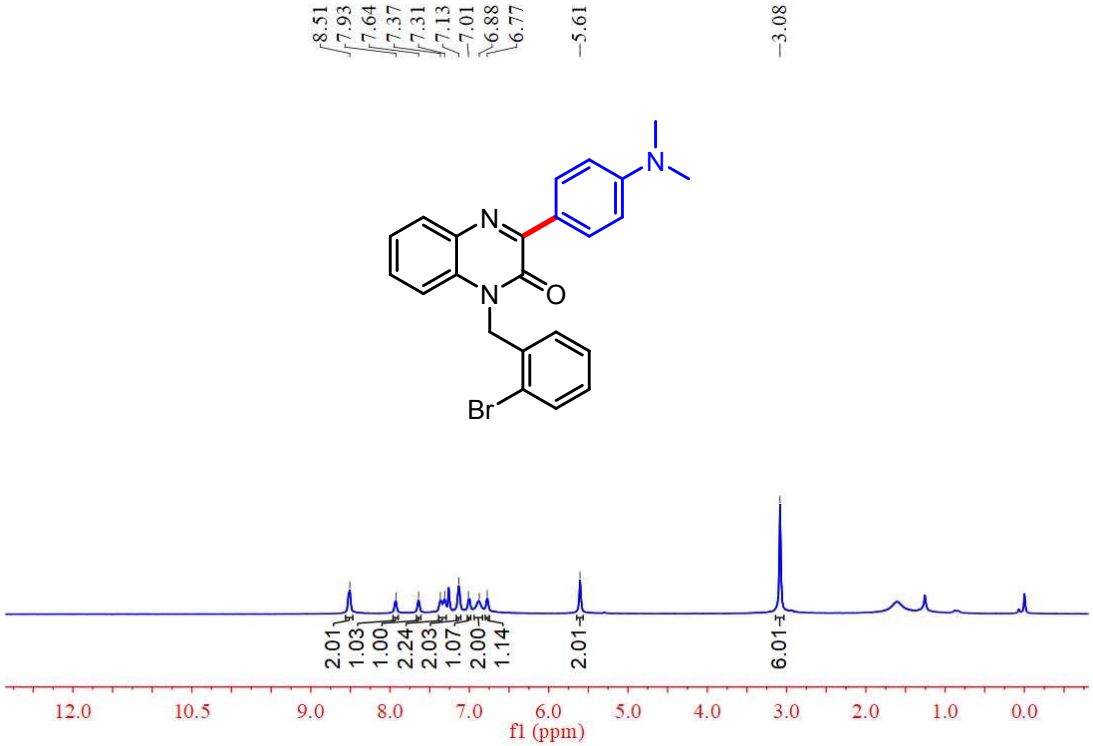
46 ^{1}H NMR (500 MHz, $CDCl_3$)



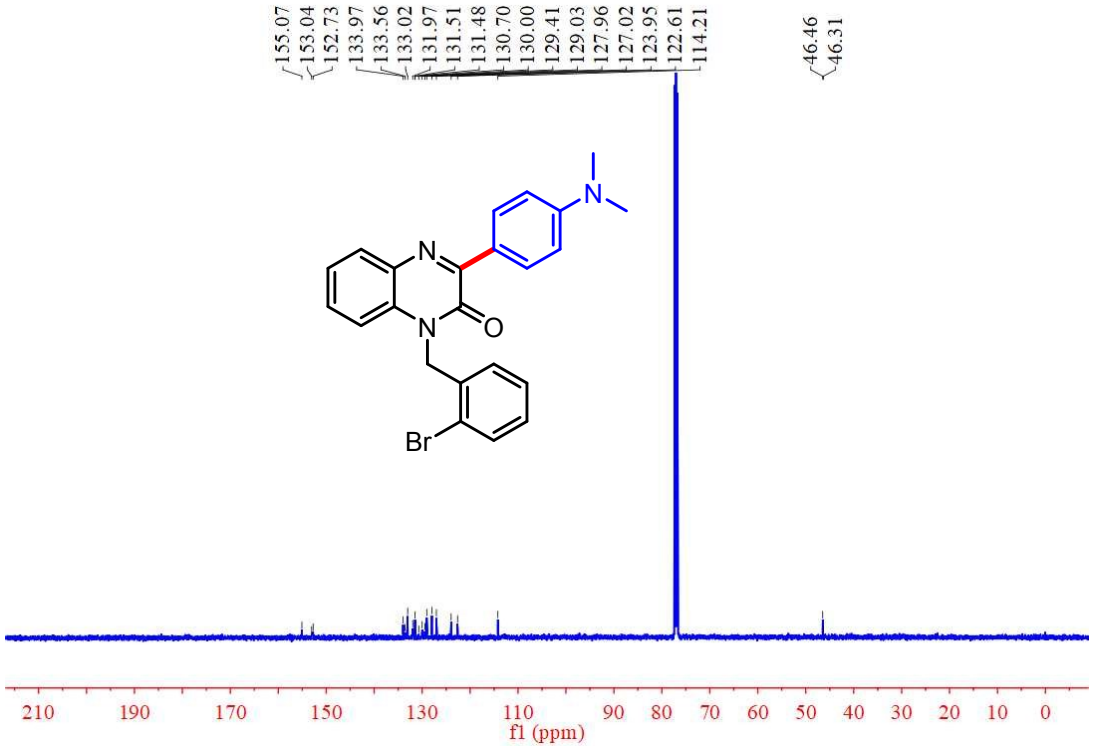
46 ^{13}C NMR (126 MHz, $CDCl_3$)



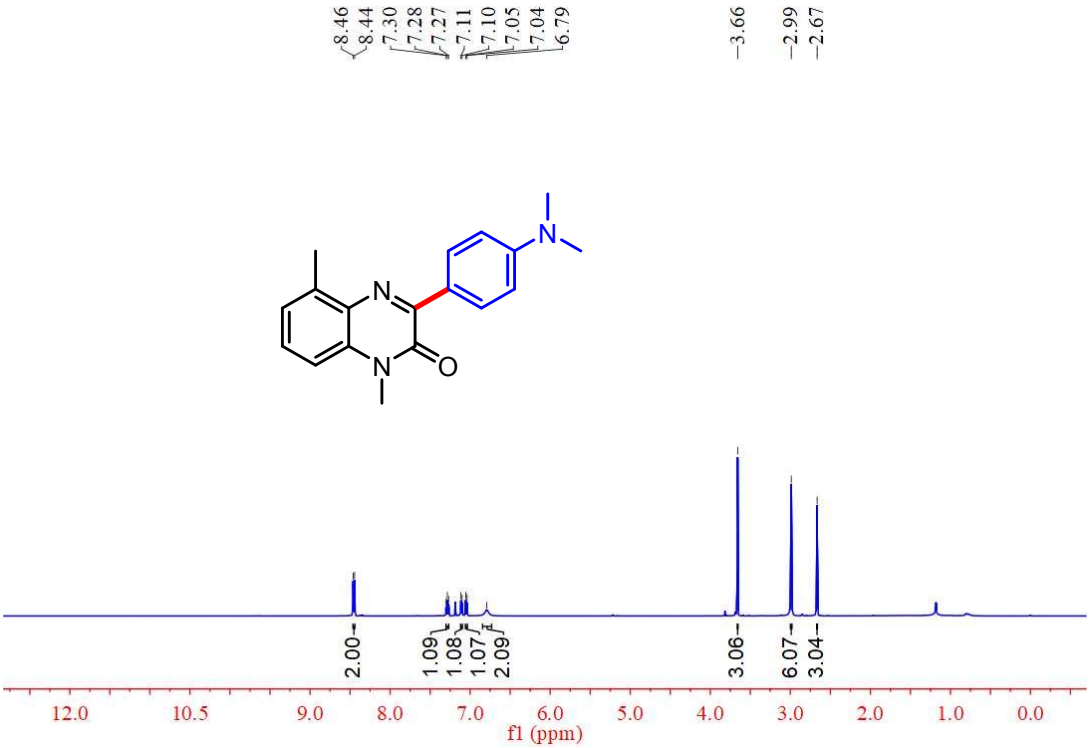
47 ^{1}H NMR (500 MHz, $CDCl_3$)



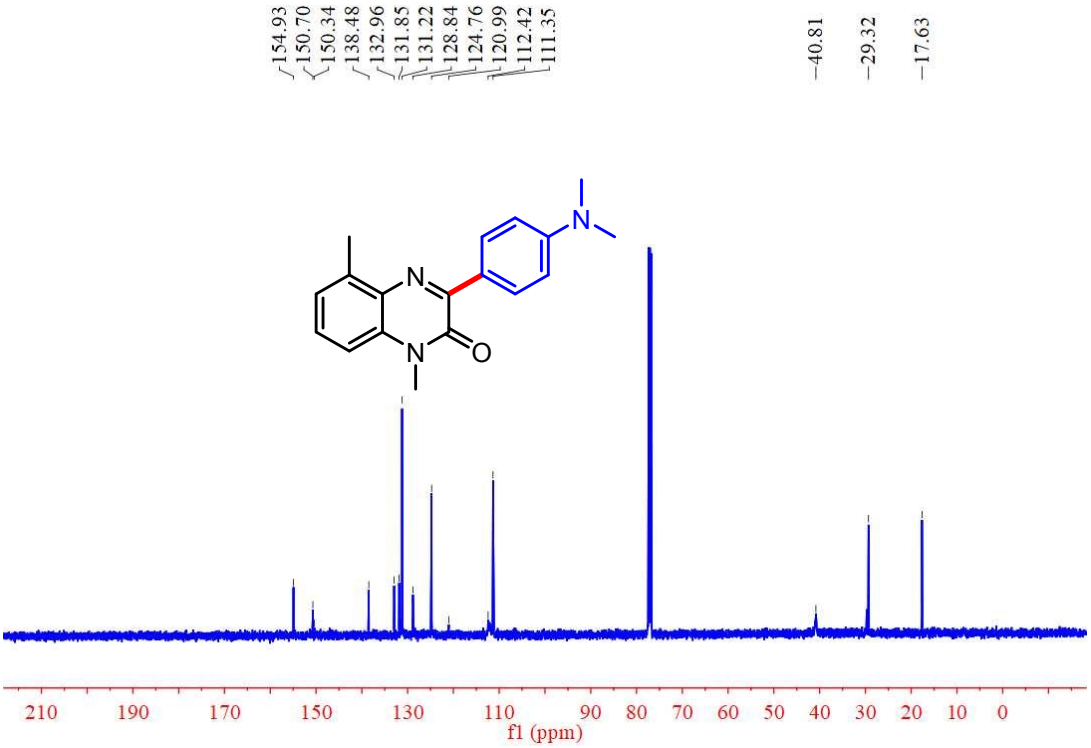
47 ^{13}C NMR (126 MHz, $CDCl_3$)



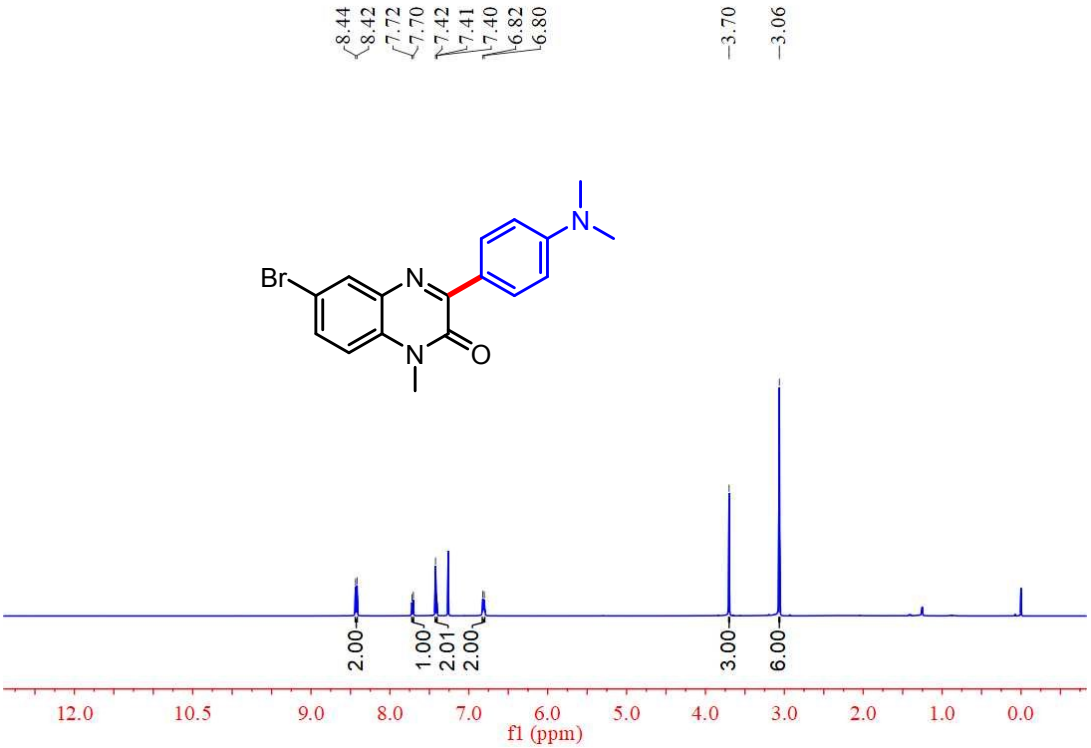
48 ^{1}H NMR (500 MHz, $CDCl_3$)



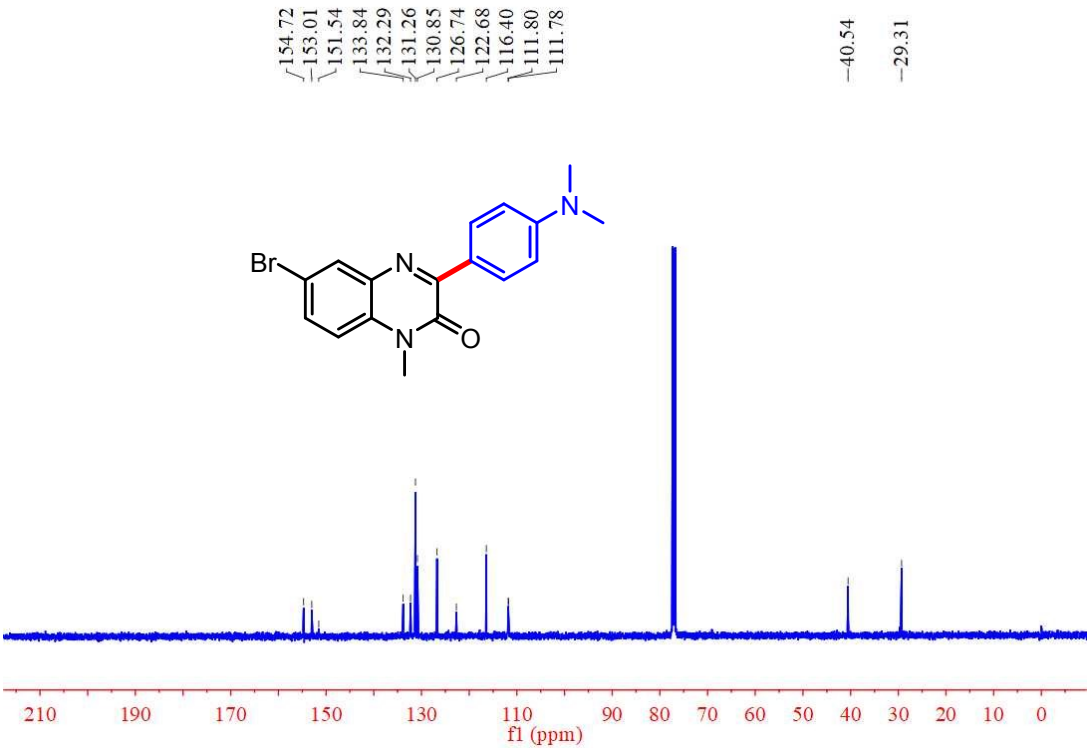
48 ^{13}C NMR (126 MHz, $CDCl_3$)



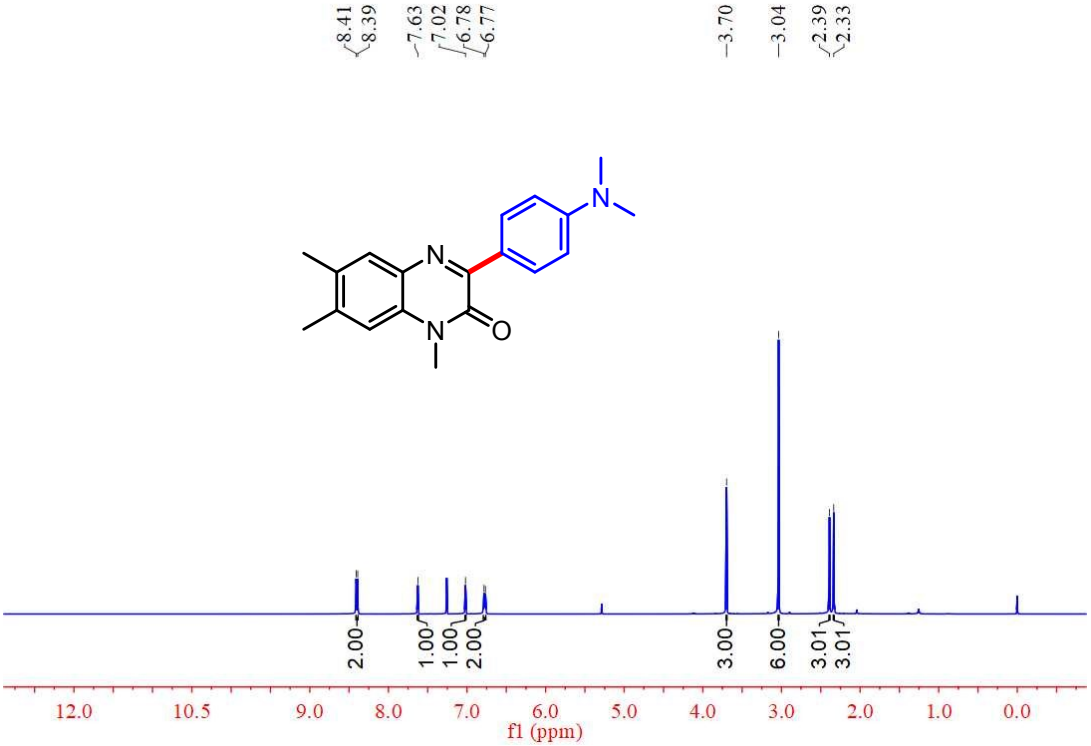
49 ^{1}H NMR (500 MHz, $CDCl_3$)



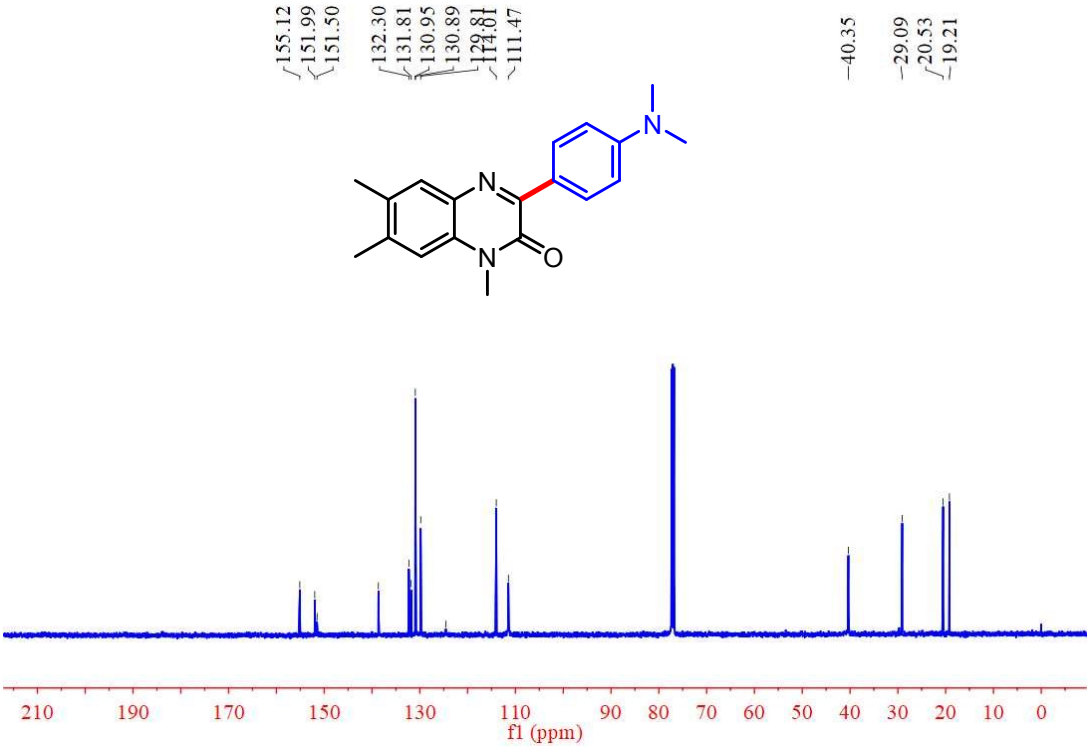
49 ^{13}C NMR (126 MHz, $CDCl_3$)



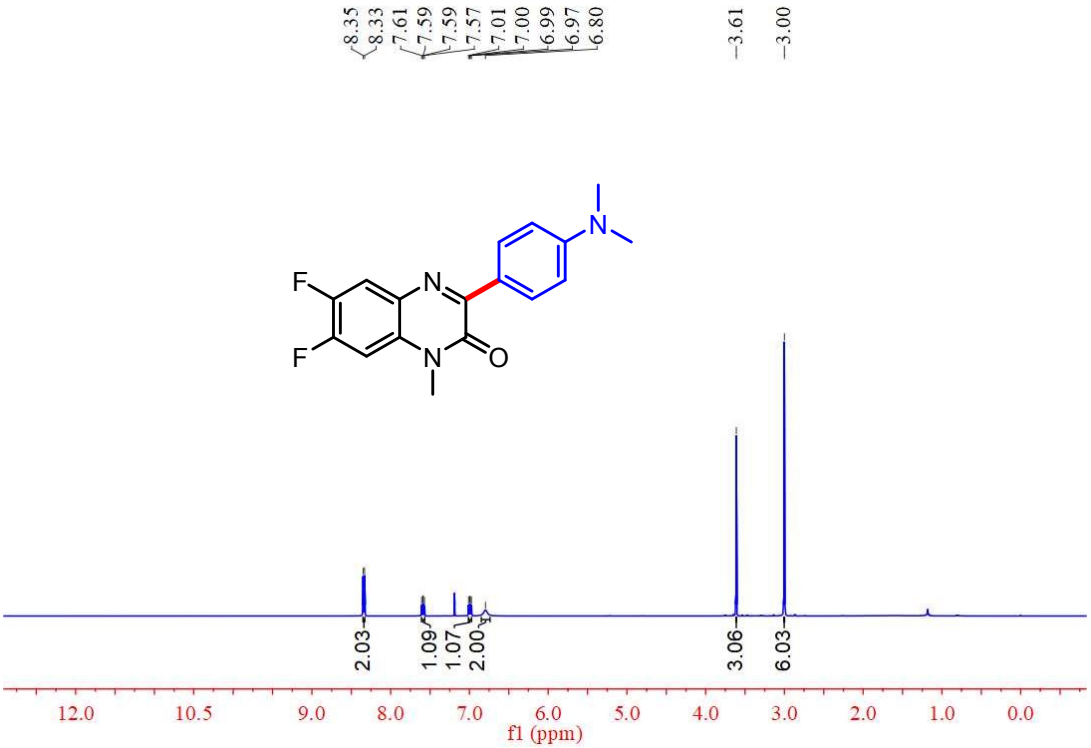
50 ^{1}H NMR (500 MHz, $CDCl_3$)



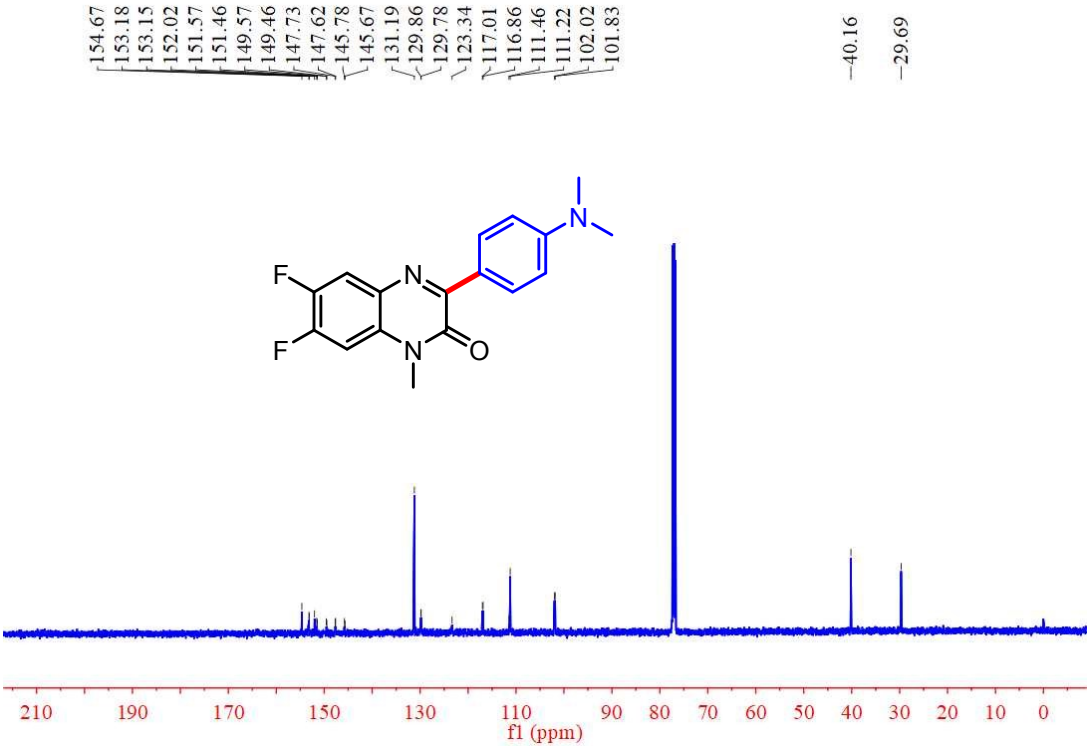
50 ^{13}C NMR (126 MHz, $CDCl_3$)



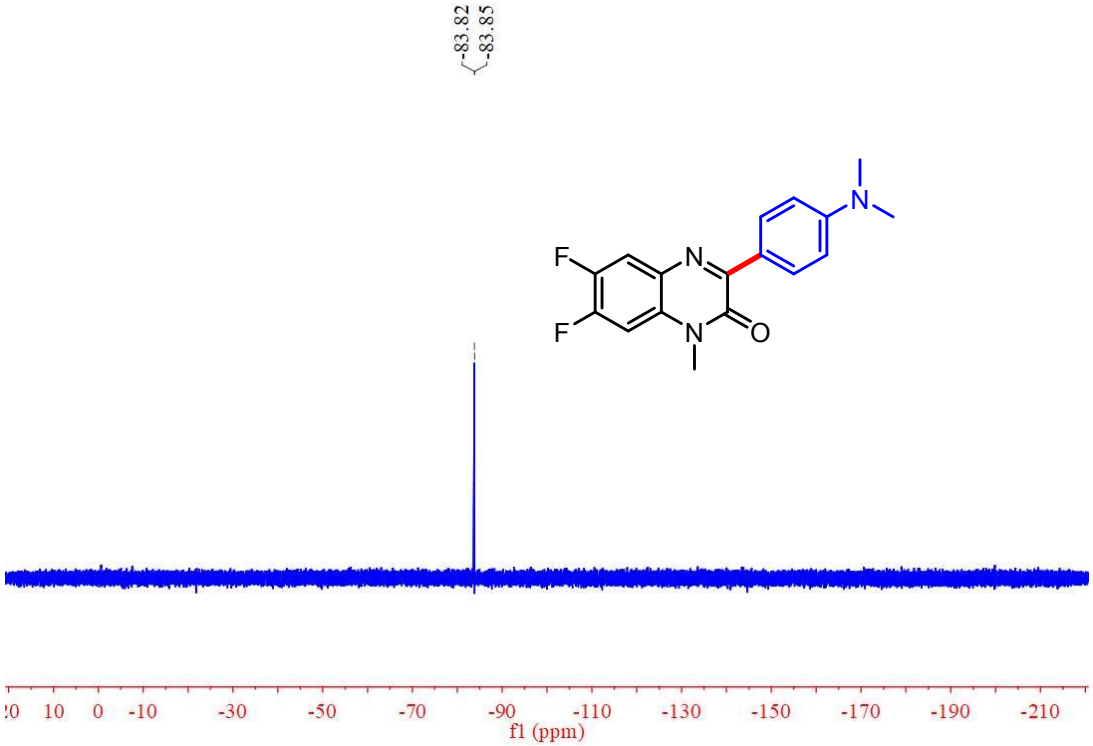
51 ^{1}H NMR (500 MHz, $CDCl_3$)



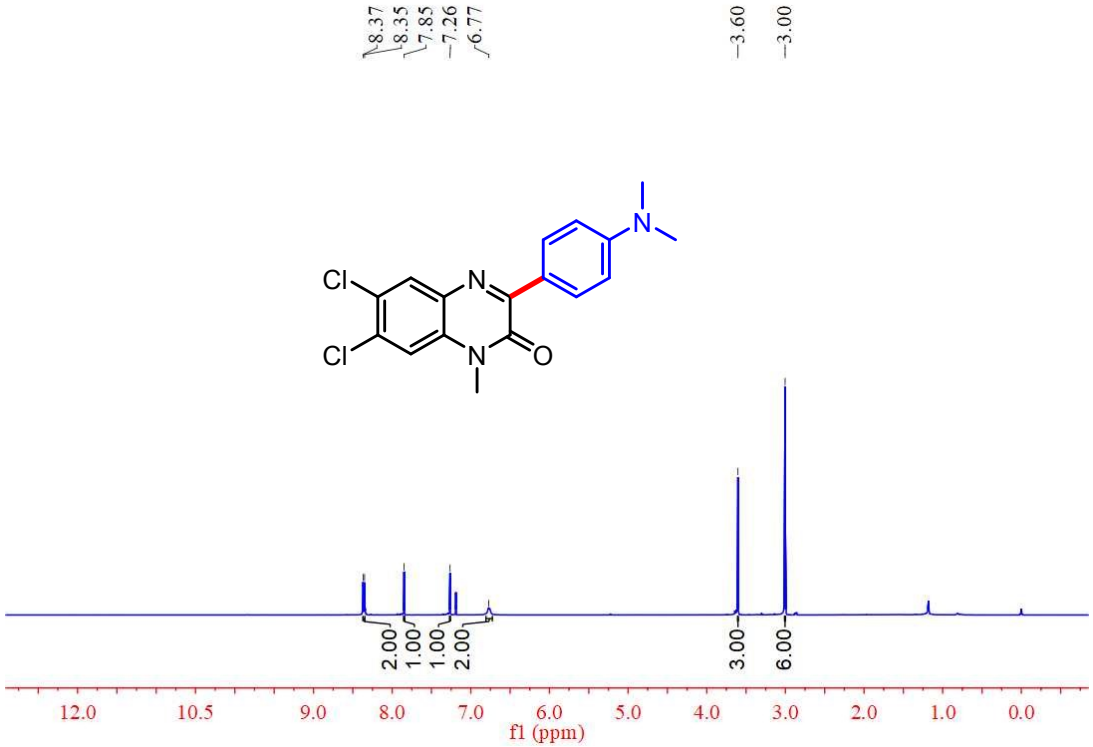
51 ^{13}C NMR (126 MHz, $CDCl_3$)



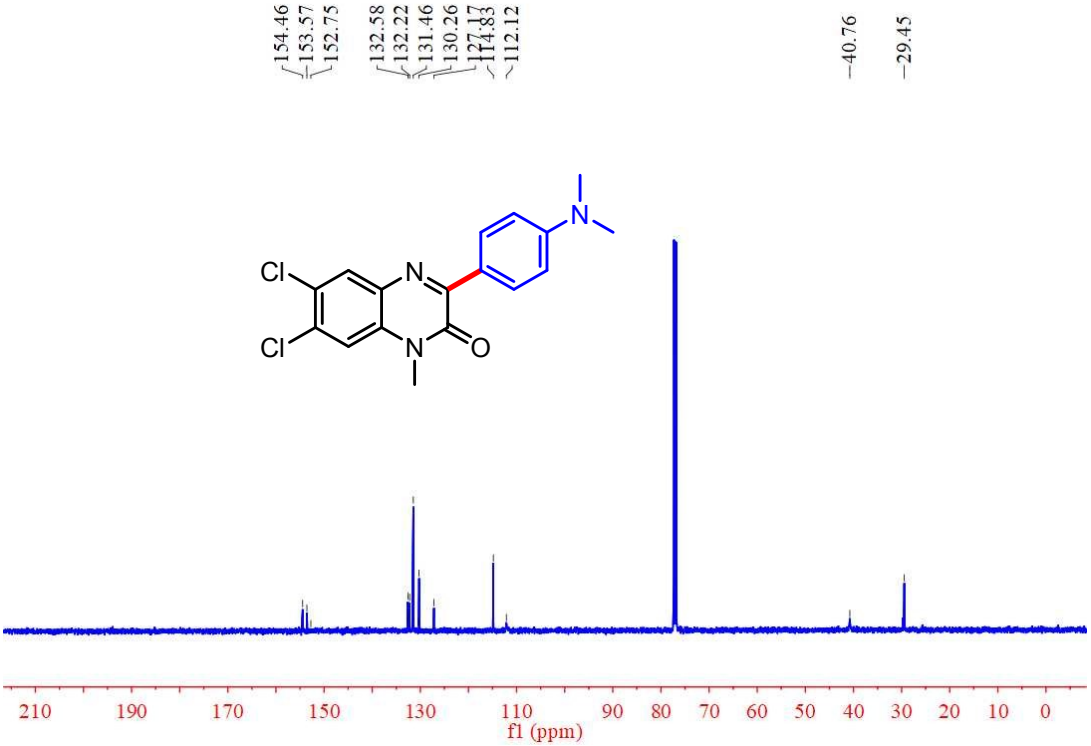
51 ^{19}F NMR (471 MHz, $CDCl_3$)



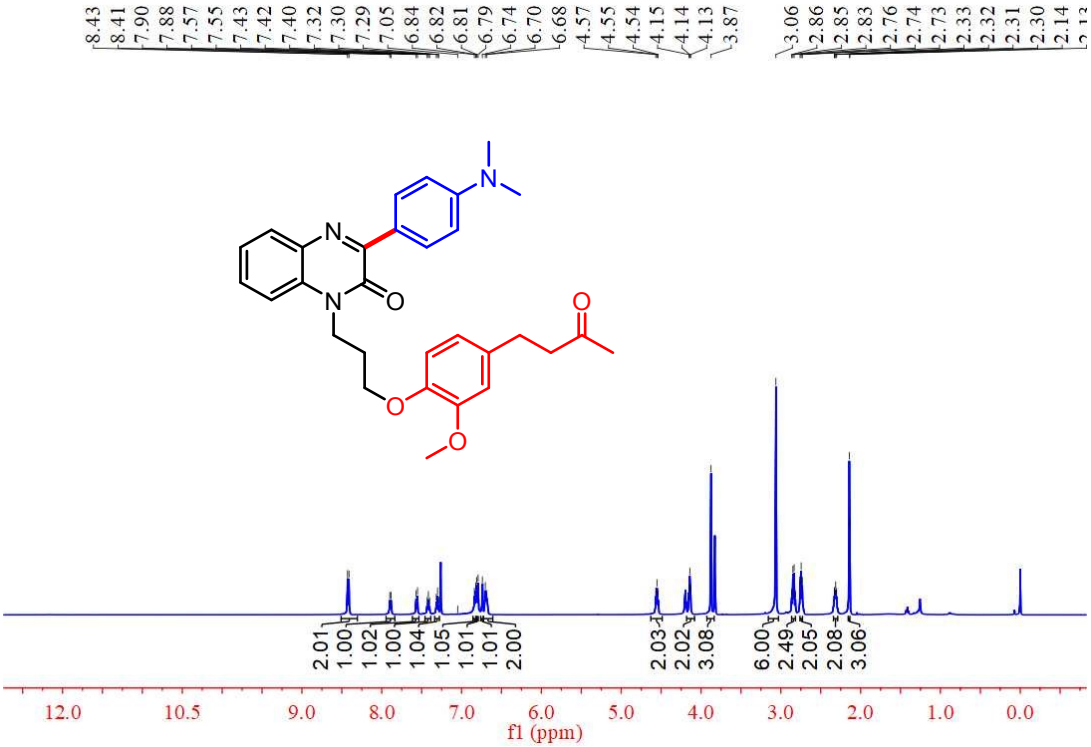
52 ^{1}H NMR (500 MHz, $CDCl_3$)



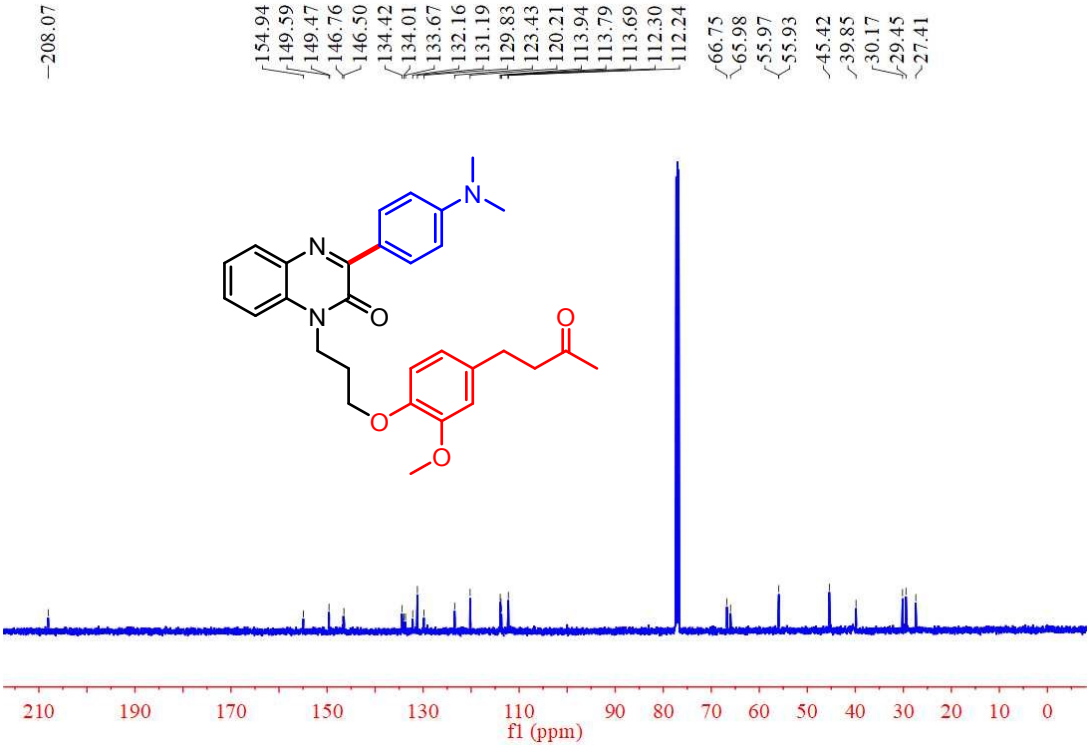
52 ^{13}C NMR (126 MHz, $CDCl_3$)



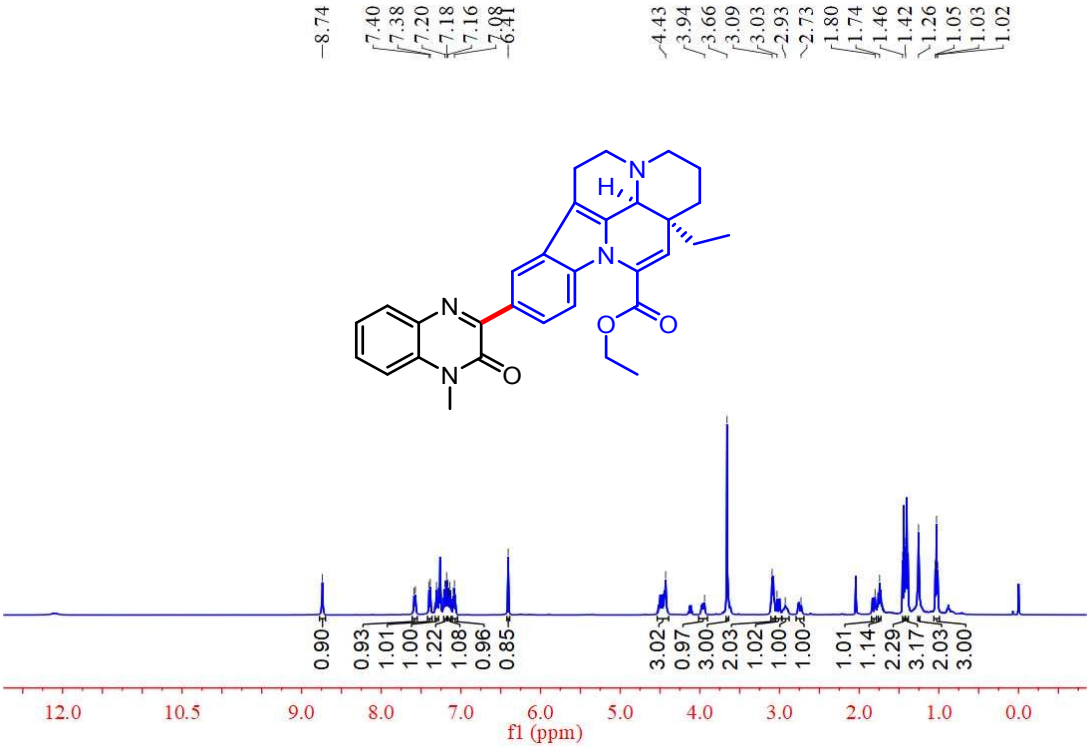
53 ^{1}H NMR (500 MHz, $CDCl_3$)



53 ^{13}C NMR (126 MHz, $CDCl_3$)



54 ^{1}H NMR (500 MHz, $CDCl_3$)



54 ^{13}C NMR (126 MHz, $CDCl_3$)