Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Visible-light-mediated ring opening and cyclization of aryl cyclopropanes: efficient synthesis of pyrrolo[*1,2-a*]quinoxalin-4(*5H*)-ones with antineoplastic activity

Jiabin Shen,[a,b]* Yong Yang,[a] Chao Chen,[a]* Hao Xu,[a] Chao Shen[a] and Pengfei Zhang[b]

[a] *Key Laboratory of Pollution Exposure and Health Intervention of Zhejiang Province, College of Biology and Environmental Engineering, Zhejiang Shuren University, Hangzhou 310015, P. R. China.*

[b] *College of Material Chemistry and Chemical Engineering, Hangzhou Normal University, Hangzhou 310036, China.*

Email: shenjiabinhznu@163.com (J. Shen); chenczju@163.com (C. Chen).

Supporting Information

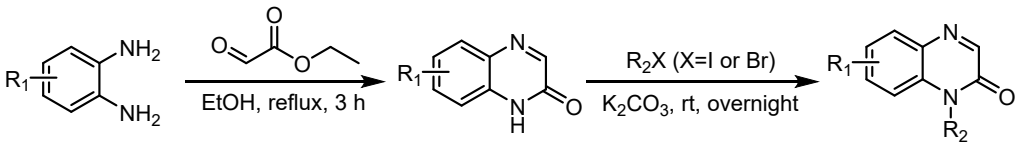
Table of contents

General Information

Commercial grade reagents, solvents, and starting materials were purchased of pure analytical grades and used as purchased without further purification unless otherwise stated. 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 and ^{13}C NMR spectra were recorded on a Bruker Advance 500 spectrometer at ambient temperature with $CDCl_3$ as solvent and tetramethylsilane (TMS) as the internal standard. Melting points were determined on an X-5 Datamicroscopic melting point apparatus. Analytical thin layer chromatography (TLC) was performed onMerk precoated TLC (silica gel 60 F254) plates. Compounds for HRMS were analyzed by positive mode electrospray ionization (ESI) using Agilent 6530 QTOF mass spectrometer.

1. Experimental Section

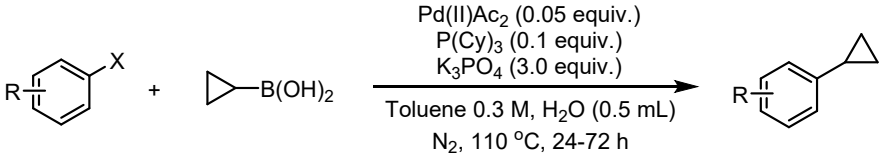
1.1 General procedure for the synthesis of quinoxalin-(*1H*)-ones 1a-1v.



1a-1v

Add corresponding 1,2-diaminobenzene derivatives (5 mmol), ethyl glyoxylate (6 mmol, 1.2 equiv), and ethanol (20 mL) into a 50 mL reaction flask and stir at 78 °C oil bath for 3 h. After the reaction is completed, the obtained reaction mixture is filtered and the filter residue is washed with ethanol, and the 2-hydroxyquinoxaline derivative is obtained after drying. Then, add 2-hydroxyquinoxaline (5 mmol, 1.0 equiv.), K_2CO_3 (6 mmol, 1.2 equiv.) and solvent *N, N*-dimethylformamide (20 mL) into a 50 mL reaction flask, and then drop halogenated alkanes (8 mmol, 1.6 equiv). Stir the reaction at room temperature for 12 h (TLC monitoring). After the reaction is complete, use ethyl acetate (30 mL × 3) And water extraction, the obtained organic phase is dried with anhydrous magnesium sulfate, filtered, and concentrated, and finally purified by silica gel column chromatography to obtain the required product.

1.2 General procedure for the synthesis of cyclopropanes 2a-2j.



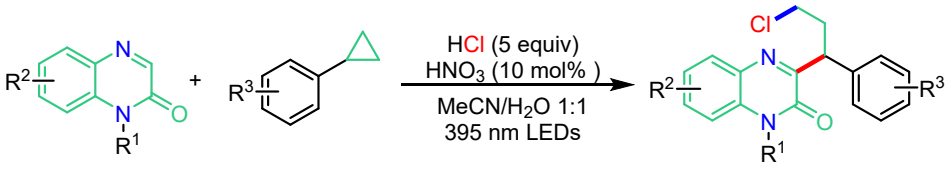
X = Br, I

2a-2j

Into a 20 mL microwave vial were weight the aryl halide (1.5-3 mmol, 1 equiv.), tricyclohexylphosphine (0.1 equiv.), palladium(II) acetate (0.05 equiv.), cesium carbonate (3 equiv.) and cyclopropylboronic acid (1.5 equiv.). A magnetic stirring bar, toluene (0.3M) and 0.5 mL of water were added, and the vial was closed. The reaction mixture was shaken briefly and set under inert atmosphere by bubbling nitrogen gas through the vial for 5 minutes. Afterwards, the vial was placed into an oil bath and stirred at 110 °C for 24-72 h. The reaction was monitored by LCMS or GC-FID. Upon completion, the reaction mixture was poured into a separatory funnel, diluted with ethyl acetate and washed with 15 mL water twice (sat. $NaHCO_3$ in case of pyridines). The organic layer was dried with Na_2SO_4, concentrated in vacuo and purified by column chromatography to give the title

compound.

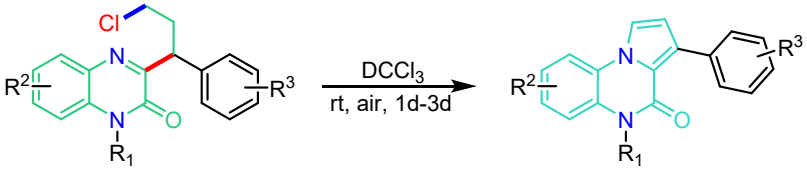
1.3 General procedure for ring opening of cyclopropanes.



1 2 3

To a 10 mL Shrek tube was added quinoxalinones (0.2 mmol), cyclopropanes (0.22 mmol), HCl (1 mL of 1.0 M, 1.0 mmol, 5.0 equiv), HNO_3 (10 mol%) and MeCN (1 mL). The above mixture was vigorous stirred under the irradiation of visible light (LEDs, 395 nm, 10 W) for 3 hours. After the completion, the reaction mixture was quenched and extracted with EtOAc. Then, the organic layer was dried over anhydrous $MgSO_4$, filtered, and concentrated in rotary evaporation. The resultant residue was purified by column chromatography using hexane/EtOAc to the chlorinated product **3a**-**3af**.

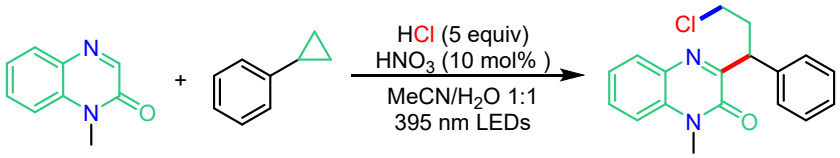
1.4 General procedure for cyclization of cyclopropanes.



3 4

The chlorinated products **3** could change into pyrrolo[1,2-a]quinoxalin-4(*5H*)-ones **4** in $DCCl_3$. Then, the organic layer was dried over anhydrous $MgSO_4$, filtered, and concentrated in rotary evaporation. The resultant residue was purified by column chromatography using hexane/EtOAc to the target product **4a**-**4s**.

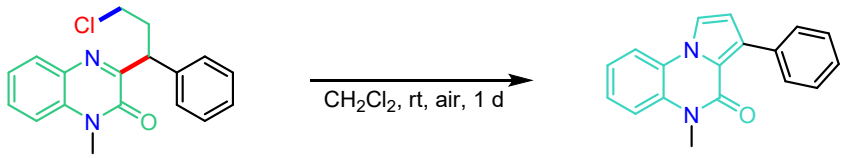
1.5 General procedure for the gram-scale synthesis of 3a.



1a (5.0 mmol) **2a** **3a** 82% (1.28 g)

To a 50 mL Shrek tube was added quinoxalinones (0.8 g, 5.0 mmol), cyclopropanes (0.65g, 5.5 mmol), HCl (2.5 mL of 1.0 M, 25.0 mmol, 5.0 equiv), HNO_3 (10 mol%) and MeCN (2.5 mL). The above mixture was vigorous stirred under the irradiation of visible light (LEDs, 395 nm, 10 W) for 3 hours. After the completion, the reaction mixture was quenched and extracted with EtOAc. Then, the organic layer was dried over anhydrous $MgSO_4$, filtered, and concentrated in rotary evaporation. The resultant residue was purified by column chromatography using hexane/EtOAc to the chlorinated product **3a** (82%, 1.28 g).

1.6 General procedure for the gram-scale synthesis of 4a.



3a (5.0 mmol) **4a** 84% (1.15 g)

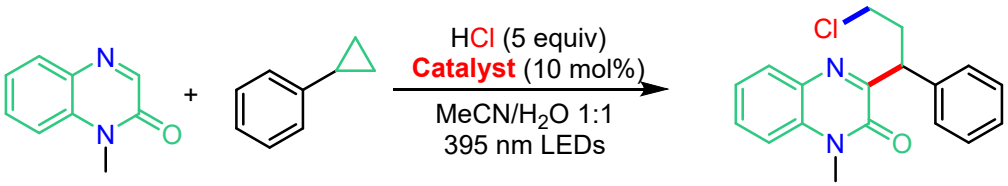
To a 50 mL Shrek tube was added the chlorinated product **3a** (1.56 g, 5.0 mmol) and CH_2Cl_2 (10 mL). The above mixture was vigorous stirred for 1 d. After the completion, the organic layer was dried over anhydrous $MgSO_4$, filtered, and concentrated in rotary evaporation. The resultant residue was purified by column chromatography using hexane/EtOAc to he target product **4a** (84%, 1.15 g).

1.7 Recyclable experiment.

A mixture of **1a** (80.0 mg, 0.5 mmol), cyclopropanes **2a** (0.65g, 5.5 mmol), HCl (2.5 mL of 1.0 M, 25.0 mmol, 5.0 equiv), HNO_3 (10 mol%) and MeCN (2.5 mL) in a 25 mL tube was stirred under the irradiation of visible light (LEDs, 395 nm, 10 W) for 3 hours. After cooling to room temperature, the mixture was extracted with EtOAc. According to the difference of the solubility to inorganic acids (HNO_3 and HCl) and organic compounds in H_2O and EtOAc, catalyst-in-water could be retrieved by an easy phase separation from the organic layer. And the retrieved catalyst-in-water was reutilized in the next round by the addition of starting materials(**1a**, **2a**) and HCl.

2. Optimization of reaction condition

2.1 Table S1: Catalyst screening.[a]

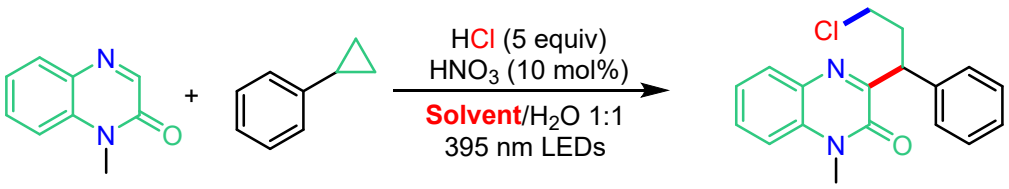


1a **2a** **3a**

Entry	Catalyst	Yield (%)[b]
1	SAS	45
2	HNO_3	87
3[c]	HNO_3	64
4[d]	HNO_3	85
5	-	trace
6	dark conditions	trace

[a]**1a** (0.2 mmol), **2a** (0.22 mmol, 1.1 equiv), HCl (1 mL of 1.0 M, 1.0 mmol), catalyst (10 mol%), MeCN (1 mL), rt, air, 3 h. [b] Isolated yields. [c] HNO_3 (5 mol%).[d] HNO_3 (20 mol%).

2.2 Table S2: Solvent screening.[a]

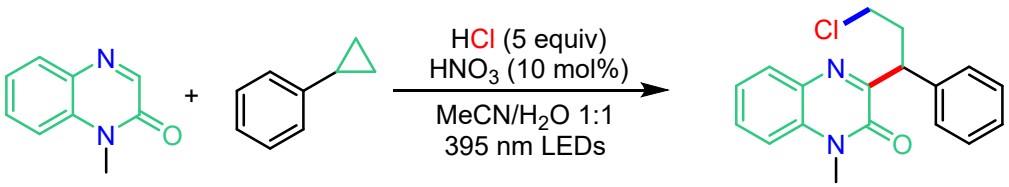


1a **2a** **3a**

Entry	Solvent	Yield (%)[b]
1	MeCN	87
2	DCE	26
3	THF	65
4	DMF	56
5	DMSO	63
6	NMP	53
7	Toluene	46
8	H_2O	15
9	CH_2Cl_2	61
10	EA	43

[a]**1a** (0.2 mmol), **2a** (0.22 mmol, 1.1 equiv), HCl (1 mL of 1.0 M, 1.0 mmol), HNO_3 (10 mol%), solvent (1 mL), rt, air, 3 h. [b] Isolated yields.

2.3 Table S3: Reaction temperature and time screening.[a]

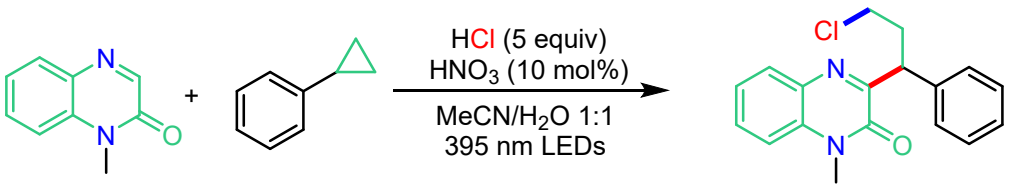


1a **2a** **3a**

Entry	Temperature	Yields[b] (%)
1	rt	87
2	40 °C	78
3	50 °C	67
4	60 °C	54
5	4 h	76
6	6 h	57
7	1 h	48
8[c]	rt	76

[a]**1a** (0.2 mmol), **2a** (0.22 mmol, 1.1 equiv), HCl (1 mL of 1.0 M, 1.0 mmol), HNO_3 (10 mol%), MeCN (1 mL), rt, air, 3 h. [b] Isolated yields. [c] under N_2.

2.4 Table S4: The dose of cyclopropyl benzene, HCl screening.[a]

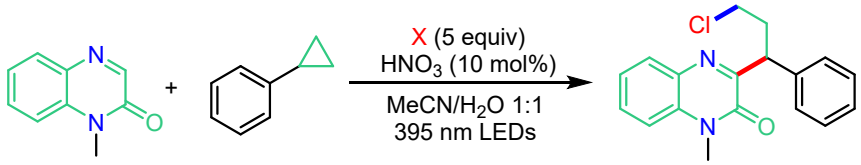


1a **2a** **3a**

Entry	**2a** (x equiv)	HCl (y equiv)	Yields[b] (%)
1	1.1	5	87
2	1.5	5	86
3	1	5	69
4	1.1	2	41
5	1.1	10	83

[a]**1a** (0.2 mmol), **2a** (x equiv), HCl (y equiv), HNO_3 (10 mol%), MeCN (1 mL), rt, air, 3 h. [b] Isolated yields.

2.5 Table S5: Chlorine source screening.

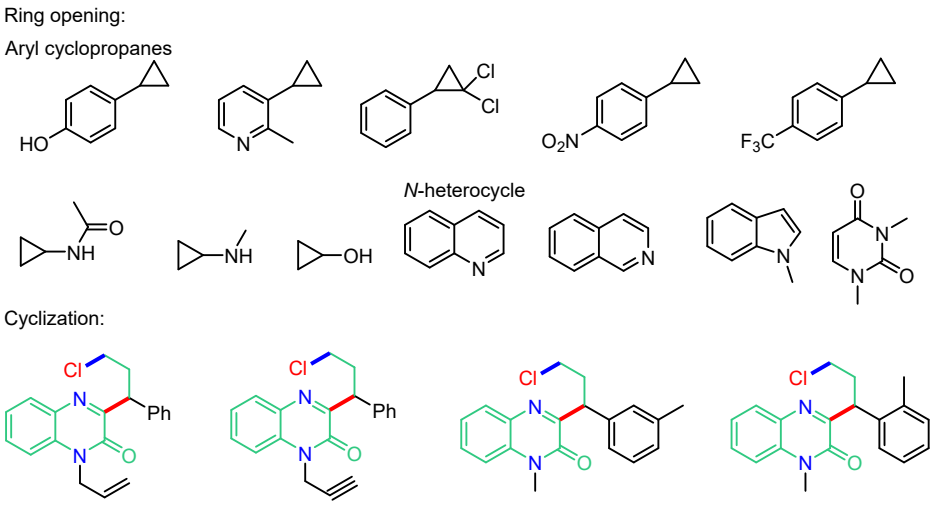


1a **2a** **3a**

Entry	**X**	Yields[b] (%)
1	HCl	87
2	KCl	71
3	NaCl	68
4	NCS	31

[a]**1a** (0.2 mmol), **2a** (0.22 mmol, 1.1 equiv), X (5.0 equiv), HNO_3 (10 mol%), MeCN (1 mL), rt, air, 3 h. [b] Isolated yields.

3. Unsuccessful substrate.

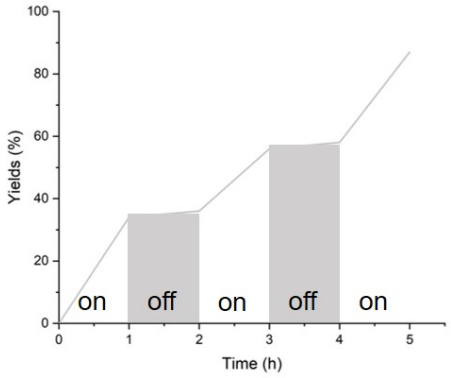


4. Crystallographic data of 4b

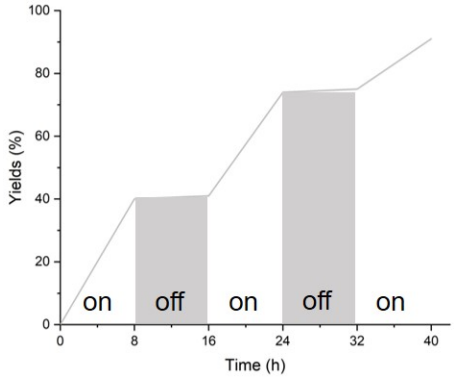
Deposition number	2281654

Empirical formula	C19H16N2O	
Formula weight	288.34	
Temperature	193 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a=8.8804(5) Å	a = 90°.
	b=7.0690(3) Å	b = 93.420(2)°.
	c=22.5844(13) Å	c = 90°.
Volume	1415.22(13) $Å^3$	
Z	4	
Density (calculated)	1.353 Mg/m^3	
Absorption coefficient	0.085 mm^{-1}	
F(000)	608	
h,k,lmax	11,9,29	
Nref	3253	
Completeness to theta = 27.494°	99.6 %	
Tmin,Tmax	0.989,0.992	
R (reflections)	0.0519 (2190)	
wR2 (reflections)	0.1364 (3240)	

5. Visible light irradiation On/Off experiment



The results of LEDs irradiation On/Off experiments demonstrate that the continuous irradiation of LEDs is indispensable for the ring opening reaction of aryl cyclopropanes.



The results of LEDs irradiation On/Off experiments demonstrate that the continuous irradiation of

LEDs is indispensable for the cyclization of aryl cyclopropanes.

6. Dipstick test experiment.

To a 10 mL Shrek tube was added the chlorinated product **3a** (0.156 g, 0.5 mmol) and CH_2Cl_2 (2 mL). The above mixture was vigorous stirred for 1 d. After the completion, the reaction mixture was quenched and extracted with EtOAc. Then, the aqueous phase was detected by a hydrogen peroxide dipstick.

7. The *in vitro* cytotoxicity assay of 4n,4l and 4p.

The in vitro cytotoxicity of the **4n**, 4l and 4p complexes were measured by an MTT (3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide) assay. The cells were plated in 96-well plates (4000-5000 cells per well) and incubated at 37 °C overnight. Then, cells were treated with a serial dilution of 4n,4l and 4p in various concentrations for an additional 48 h. Following exposure, 30 µL MTT solution (5 mg/mL in PBS) was added to each well. The MTT solution was removed from the wells after 4 h and the purple MTT-formazan crystals were then dissolved by the addition of DMSO (100 µL). The absorbance in each well was measured at 490 nm using a microplate reader (Multiskan FC, Thermo Scientific).

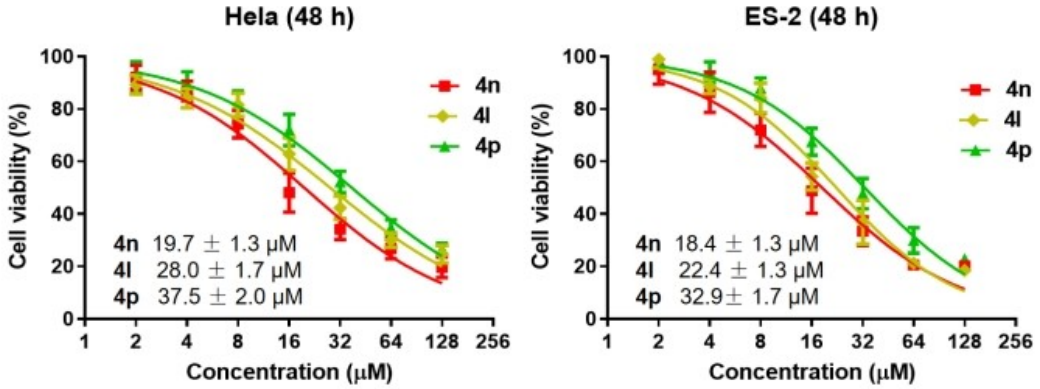


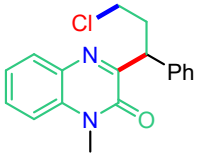
Fig.S5 MTT assay of **4n**, **4l**, and **4p** against human cancer cell lines HeLa and ES-2 after 48 h of drug exposure.

Reaction Set-up

All photochemical reactions were carried out using a PL-SX100A (http://www.bjplss.com/pl/) with wavelength of peak intensity of 395-525 nm.

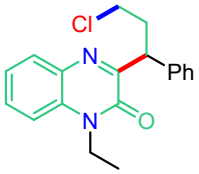
2. Characterization of Products

3-(3-Chloro-1-phenylpropyl)-1-methylquinoxalin-2(*1H*)-one (3a)



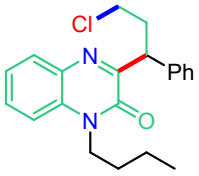
Obtained as yellow liquid (54 mg, 87% yield); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.92 (d, *J* = 7.9 Hz, 1H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.44 (d, *J* = 7.4 Hz, 2H), 7.36 (t, *J* = 7.5 Hz, 1H), 7.27 (dd, *J* = 11.8, 7.6 Hz, 3H), 7.20 (t, *J* = 7.2 Hz, 1H), 4.94 (t, *J* = 7.5 Hz, 1H), 3.67 – 3.53 (m, 4H), 3.51 – 3.43 (m, 1H), 2.73 (dd, *J* = 14.1, 7.0 Hz, 1H), 2.56 (dd, *J* = 14.1, 7.7 Hz, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 159.95, 154.35, 140.08, 133.14, 132.56, 130.17, 130.01, 128.68, 128.59, 127.05, 123.55, 113.58, 44.53, 43.20, 36.51, 29.15. **HRMS-ESI**: calcd for $C_{18}H_{17}ClN_2OH$ $[M+H]^+$ 313.1102, found 313.1095.

3-(3-Chloro-1-phenylpropyl)-1-ethylquinoxalin-2(*1H*)-one (3b)



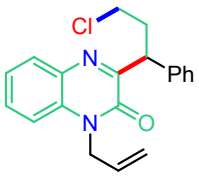
Obtained as yellow liquid (55 mg, 84% yield); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.93 (d, *J* = 7.8 Hz, 1H), 7.52 (t, *J* = 7.5 Hz, 1H), 7.44 (d, *J* = 7.3 Hz, 2H), 7.36 – 7.32 (m, 1H), 7.27 (dd, *J* = 13.8, 7.0 Hz, 3H), 7.19 (t, *J* = 7.0 Hz, 1H), 4.93 (t, *J* = 7.5 Hz, 1H), 4.28 (dt, *J* = 14.0, 7.0 Hz, 1H), 4.16 (dd, *J* = 13.8, 7.0 Hz, 1H), 3.62 – 3.52 (m, 1H), 3.52 – 3.40 (m, 1H), 2.72 (dd, *J* = 14.0, 7.0 Hz, 1H), 2.57 (dd, *J* = 14.0, 7.5 Hz, 1H), 1.30 (t, *J* = 7.0 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 160.02, 153.82, 140.13, 132.87, 132.07, 130.44, 129.97, 128.68, 128.58, 127.00, 123.34, 113.44, 44.45, 43.21, 37.44, 36.61, 12.38. **HRMS-ESI**: calcd for $C_{19}H_{19}ClN_2OH$ $[M+H]^+$ 327.1259, found 327.1249.

1-Butyl-3-(3-chloro-1-phenylpropyl)quinoxalin-2(*1H*)-one (3c)



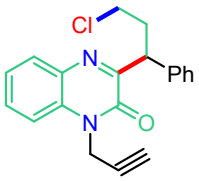
Obtained as yellow liquid (63 mg, 89% yield); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.93 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.56 – 7.49 (m, 1H), 7.43 (d, *J* = 7.3 Hz, 2H), 7.34 (t, *J* = 7.3 Hz, 1H), 7.28 (t, *J* = 7.6 Hz, 3H), 7.20 (t, *J* = 7.3 Hz, 1H), 4.98 – 4.88 (m, 1H), 4.28 – 4.20 (m, 1H), 4.12 – 4.02 (m, 1H), 3.62 – 3.54 (m, 1H), 3.51 – 3.43 (m, 1H), 2.72 (dd, *J* = 14.2, 7.2 Hz, 1H), 2.62 – 2.51 (m, 1H), 1.71 – 1.63 (m, 2H), 1.42 (dd, *J* = 15.0, 7.5 Hz, 2H), 0.95 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 159.98, 154.03, 140.13, 132.81, 132.33, 130.39, 129.90, 128.66, 128.57, 126.99, 123.32, 113.59, 44.50, 43.21, 42.31, 36.58, 29.22, 20.28, 13.74. **HRMS-ESI**: calcd for $C_{21}H_{23}ClN_2ONa$ $[M+Na]^+$ 377.1391, found 377.1396.

1-Allyl-3-(3-chloro-1-phenylpropyl)quinoxalin-2(*1H*)-one (3d)



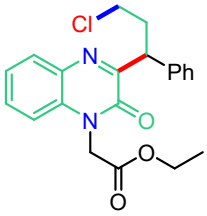
Obtained as yellow liquid (55 mg, 73% yield); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.92 (d, J = 7.9 Hz, 1H), 7.48 (t, J = 7.7 Hz, 1H), 7.44 (d, J = 7.4 Hz, 2H), 7.33 (t, J = 7.6 Hz, 1H), 7.29 – 7.23 (m, 3H), 7.19 (t, J = 7.3 Hz, 1H), 5.94 – 5.78 (m, 1H), 5.21 (d, J = 10.4 Hz, 1H), 5.11 (d, J = 17.2 Hz, 1H), 4.96 – 4.82 (m, 2H), 4.71 (dd, J = 16.1, 4.8 Hz, 1H), 3.57 (dt, J = 12.2, 6.3 Hz, 1H), 3.51 – 3.40 (m, 1H), 2.72 (dd, J = 14.1, 7.2 Hz, 1H), 2.63 – 2.49 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 160.06, 153.90, 140.05, 132.72, 132.37, 130.67, 130.28, 129.93, 128.67, 128.61, 127.05, 123.55, 118.16, 114.15, 44.66, 44.56, 43.19, 36.59. **HRMS-ESI**: calcd for $C_{20}H_{19}ClN_2OH$ $[M+H]^+$ 339.1259, found 339.1265.

3-(3-Chloro-1-phenylpropyl)-1-(prop-2-yn-1-yl)quinoxalin-2(*1H*)-one (3e)



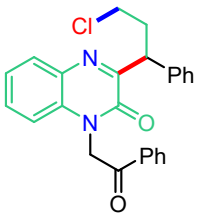
Obtained as yellow liquid (53 mg, 78% yield); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.93 (d, J = 7.7 Hz, 1H), 7.55 (t, J = 7.6 Hz, 1H), 7.42 (t, J = 7.9 Hz, 3H), 7.37 (t, J = 7.7 Hz, 1H), 7.27 (t, J = 7.5 Hz, 2H), 7.19 (t, J = 7.3 Hz, 1H), 5.06 (dd, J = 17.4, 2.1 Hz, 1H), 4.92 (t, J = 7.5 Hz, 1H), 4.82 (dd, J = 17.4, 2.0 Hz, 1H), 3.56 (dt, J = 12.1, 6.2 Hz, 1H), 3.45 (dt, J = 10.6, 7.4 Hz, 1H), 2.70 (dd, J = 14.1, 7.2 Hz, 1H), 2.56 (dd, J = 14.3, 8.1 Hz, 1H), 2.24 (s, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 159.92, 153.33, 139.82, 132.75, 131.63, 130.32, 130.13, 128.71, 128.64, 127.15, 123.96, 114.15, 73.31, 44.60, 43.13, 36.55, 31.59. **HRMS-ESI**: calcd for $C_{20}H_{17}ClN_2OH$ $[M+H]^+$ 337.1102, found 337.1108.

Ethyl -2-(3-(3-chloro-1-phenylpropyl)-2-oxoquinoxalin-1(*2H*)-yl)acetate (3f)



Obtained as yellow liquid (34 mg, 67% yield); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.94 (d, J = 7.8 Hz, 1H), 7.49 (t, J = 7.5 Hz, 1H), 7.42 (d, J = 7.4 Hz, 2H), 7.36 (t, J = 7.5 Hz, 1H), 7.27 (t, J = 7.4 Hz, 2H), 7.20 (d, J = 7.2 Hz, 1H), 7.03 (d, J = 8.3 Hz, 1H), 5.04 (d, J = 17.4 Hz, 1H), 4.91 (t, J = 7.5 Hz, 1H), 4.81 (d, J = 17.4 Hz, 1H), 4.18 (dt, J = 13.3, 6.6 Hz, 2H), 3.66 – 3.52 (m, 1H), 3.47 (dd, J = 12.2, 5.0 Hz, 1H), 2.72 (dd, J = 14.0, 7.1 Hz, 1H), 2.65 – 2.50 (m, 1H), 1.20 (t, J = 7.1 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 167.02, 159.83, 153.91, 139.83, 132.61, 132.29, 130.51, 130.17, 128.65, 128.62, 127.10, 123.87, 113.07, 62.02, 44.64, 43.61, 43.11, 36.49, 14.04. **HRMS-ESI**: calcd for $C_{21}H_{21}ClN_2O_3H$ $[M+H]^+$ 385.1313, found 385.1311.

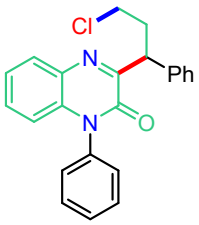
3-(3-Chloro-1-phenylpropyl)-1-(2-oxo-2-phenylethyl)quinoxalin-2(*1H*)-one (3g)



Obtained as yellow liquid (72 mg, 87% yield); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.01 – 7.93 (m, 3H), 7.62 (t, J = 7.5 Hz, 1H), 7.48 (t, J = 7.8 Hz, 2H), 7.41 (td, J = 8.9, 1.3 Hz, 3H), 7.36 – 7.31 (m, 1H), 7.27 (dd, J = 14.5, 6.7 Hz, 2H), 7.20 (t, J = 7.3 Hz, 1H), 6.91 (d, J = 8.1 Hz, 1H), 5.75 (d, J = 17.6 Hz, 1H), 5.50 (d, J = 17.5 Hz, 1H), 4.91 (dd, J = 8.4, 6.8 Hz, 1H), 3.59 (dt, J = 11.0, 6.2 Hz, 1H), 3.47 (ddd, J = 10.8, 7.7, 6.5 Hz, 1H), 2.74 (td, J = 14.3, 6.7 Hz, 1H), 2.58 (ddt, J = 14.4, 8.5,

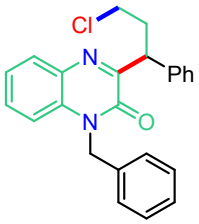
6.1 Hz, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 191.22, 159.69, 154.09, 139.94, 134.48, 134.27, 132.71, 132.58, 130.44, 130.09, 129.01, 128.67, 128.64, 128.12, 127.09, 123.75, 113.54, 48.60, 44.70, 43.16, 36.53. **HRMS-ESI**: calcd for $C_{25}H_{21}ClN_2O_2H$ $[M+H]^+$ 417.1365, found 417.1372.

3-(3-Chloro-1-phenylpropyl)-1-phenylquinoxalin-2(*1H*)-one (3h)



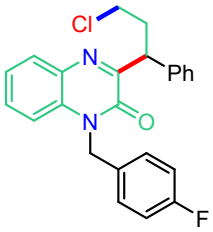
Obtained as yellow liquid (62 mg, 83% yield); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.95 (dd, *J* = 7.2, 2.1 Hz, 1H), 7.59 – 7.54 (m, 1H), 7.54 – 7.44 (m, 4H), 7.35 – 7.23 (m, 5H), 7.19 (dd, *J* = 15.3, 7.9 Hz, 1H), 7.12 (d, *J* = 7.2 Hz, 1H), 6.73 – 6.56 (m, 1H), 5.02 – 4.87 (m, 1H), 3.59 (dt, *J* = 12.3, 6.3 Hz, 1H), 3.47 (dt, *J* = 10.8, 7.2 Hz, 1H), 2.76 (dd, *J* = 14.2, 7.2 Hz, 1H), 2.63 (dt, *J* = 14.3, 7.1 Hz, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 160.82, 154.09, 139.91, 135.80, 133.96, 132.47, 130.23, 129.81, 129.70, 129.37, 128.85, 128.65, 128.37, 128.19, 127.09, 123.78, 115.45, 44.55, 43.21, 36.60. **HRMS-ESI**: calcd for $C_{23}H_{19}ClN_2OH$ $[M+H]^+$ 375.1259, found 375.1267.

1-Benzyl-3-(3-chloro-1-phenylpropyl)quinoxalin-2(*1H*)-one (3i)



Obtained as yellow liquid (71 mg, 91% yield); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.92 (d, *J* = 7.8 Hz, 1H), 7.46 (d, *J* = 7.3 Hz, 2H), 7.37 (d, *J* = 7.8 Hz, 1H), 7.29 (t, *J* = 7.3 Hz, 3H), 7.26 – 7.16 (m, 5H), 7.13 (d, *J* = 7.0 Hz, 2H), 5.50 (d, *J* = 15.6 Hz, 1H), 5.26 (d, *J* = 15.5 Hz, 1H), 4.99 (t, *J* = 7.3 Hz, 1H), 3.59 (dd, *J* = 10.7, 5.5 Hz, 1H), 3.49 (dd, *J* = 11.8, 4.9 Hz, 1H), 2.75 (dd, *J* = 13.9, 6.9 Hz, 1H), 2.60 (dd, *J* = 13.7, 7.2 Hz, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 160.20, 154.44, 140.08, 135.24, 132.83, 132.49, 130.30, 129.99, 128.91, 128.71, 128.65, 127.66, 127.10, 126.87, 123.62, 114.41, 45.99, 44.72, 43.22, 36.59. **HRMS-ESI**: calcd for $C_{24}H_{21}ClN_2OH$ $[M+H]^+$389.1415, found 389.1419.

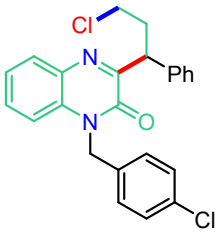
3-(3-Chloro-1-phenylpropyl)-1-(4-fluorobenzyl)quinoxalin-2(*1H*)-one (3j)



Obtained as yellow liquid (72 mg, 88% yield); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.84 (d, *J* = 7.8 Hz, 1H), 7.36 (d, *J* = 7.3 Hz, 2H), 7.32 (dd, *J* = 11.3, 4.1 Hz, 1H), 7.26 – 7.17 (m, 3H), 7.15 – 7.07 (m, 2H), 7.03 (dd, *J* = 8.2, 5.3 Hz, 2H), 6.84 (t, *J* = 8.6 Hz, 2H), 5.36 (d, *J* = 15.5 Hz, 1H), 5.15 (d, *J* = 15.6 Hz, 1H), 4.95 – 4.83 (m, 1H), 3.51 (dt, *J* = 12.1, 6.2 Hz, 1H), 3.39 (dt, *J* = 10.8, 7.2 Hz, 1H), 2.65 (dd, *J* = 14.2, 7.4 Hz, 1H), 2.57 – 2.44 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 162.18 (d, *J* = 246.4 Hz), 160.20, 154.37, 140.02, 132.84, 132.32, 131.01 (d, *J* = 3.2 Hz), 130.43, 130.05, 128.77, 128.70, 128.66,

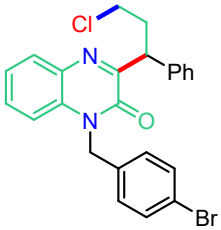
127.13, 123.75, 115.85 (d, *J* = 21.7 Hz), 114.17, 45.32, 44.69, 43.21, 36.55. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -114.37. **HRMS-ESI**: calcd for $C_{24}H_{20}ClFN_2ONa$ [M+Na] $^+$ 429.1140, found 429.1139.

3-(3-Chloro-1-phenylpropyl)-1-(4-chlorobenzyl)quinoxalin-2(*1H*)-one (3k)



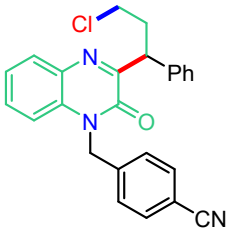
Obtained as yellow liquid (71 mg, 84% yield); **^{1}H NMR** (500 MHz, $CDCl_3$) *δ* 7.93 (d, *J* = 7.8 Hz, 1H), 7.44 (d, *J* = 7.4 Hz, 2H), 7.40 (t, *J* = 7.7 Hz, 1H), 7.34 – 7.27 (m, 3H), 7.25 – 7.18 (m, 3H), 7.15 (d, *J* = 8.3 Hz, 1H), 7.07 (d, *J* = 8.1 Hz, 2H), 5.45 (d, *J* = 15.7 Hz, 1H), 5.24 (d, *J* = 15.7 Hz, 1H), 4.98 (t, *J* = 7.5 Hz, 1H), 3.66 – 3.55 (m, 1H), 3.53 – 3.42 (m, 1H), 2.74 (dd, *J* = 14.1, 7.1 Hz, 1H), 2.60 (dt, *J* = 14.1, 7.0 Hz, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) *δ* 160.18, 154.34, 139.98, 133.76, 133.55, 132.82, 132.26, 130.44, 130.07, 129.09, 128.68, 128.66, 128.35, 127.14, 123.79, 114.12, 45.36, 44.70, 43.19, 36.52. **HRMS-ESI**: calcd for $C_{24}H_{20}Cl_2N_2OH$ [M+H] $^+$ 423.1025, found 423.1029.

1-(4-Bromobenzyl)-3-(3-chloro-1-phenylpropyl)quinoxalin-2(*1H*)-one (3l)



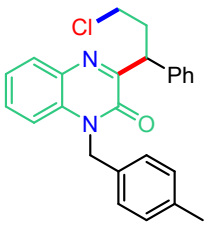
Obtained as yellow liquid (81 mg, 87% yield); **^{1}H NMR** (500 MHz, $CDCl_3$) *δ* 7.93 (d, *J* = 7.7 Hz, 1H), 7.44 (d, *J* = 7.4 Hz, 2H), 7.34 (ddt, *J* = 26.9, 19.0, 7.5 Hz, 6H), 7.21 (d, *J* = 7.2 Hz, 1H), 7.13 (d, *J* = 8.3 Hz, 1H), 7.00 (d, *J* = 8.0 Hz, 2H), 5.42 (d, *J* = 15.7 Hz, 1H), 5.21 (d, *J* = 15.7 Hz, 1H), 4.97 (t, *J* = 7.5 Hz, 1H), 3.59 (dd, *J* = 11.1, 5.6 Hz, 1H), 3.48 (dd, *J* = 12.1, 5.1 Hz, 1H), 2.74 (dd, *J* = 14.1, 7.1 Hz, 1H), 2.67 – 2.51 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) *δ* 160.18, 154.34, 139.98, 134.30, 132.82, 132.25, 132.04, 130.45, 130.09, 128.68, 127.15, 123.81, 121.63, 114.12, 45.42, 44.70, 43.21, 36.52. **HRMS-ESI**: calcd for $C_{24}H_20BrClN_2OH$ [M+H] $^+$ 467.0521, found 467.0527.

4-((3-(3-Chloro-1-phenylpropyl)-2-oxoquinoxalin-1(*2H*)-yl)methyl)benzonitrile (3m)



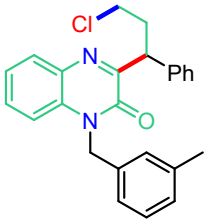
Obtained as yellow liquid (26 mg, 86% yield); **^{1}H NMR** (500 MHz, $CDCl_3$) *δ* 7.96 (d, *J* = 7.8 Hz, 1H), 7.54 (d, *J* = 8.0 Hz, 2H), 7.43 (dd, *J* = 11.6, 7.9 Hz, 3H), 7.35 (t, *J* = 7.5 Hz, 1H), 7.29 (t, *J* = 7.5 Hz, 2H), 7.22 (d, *J* = 8.1 Hz, 3H), 7.07 (d, *J* = 8.3 Hz, 1H), 5.51 (d, *J* = 16.2 Hz, 1H), 5.34 (d, *J* = 16.2 Hz, 1H), 4.97 (t, *J* = 7.5 Hz, 1H), 3.67 – 3.56 (m, 1H), 3.48 (dt, *J* = 10.8, 7.6 Hz, 1H), 2.74 (dd, *J* = 14.1, 7.2 Hz, 1H), 2.61 (dt, *J* = 14.3, 7.1 Hz, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) *δ* 160.16, 154.26, 140.63, 139.84, 132.81, 132.74, 132.07, 130.62, 130.24, 128.69, 128.67, 127.55, 127.21, 124.05, 118.41, 113.83, 111.73, 45.62, 44.69, 43.17, 36.45. **HRMS-ESI**: calcd for $C_{25}H_{20}ClN_3OH$ [M+H] $^+$ 414.1368, found 414.1365.

3-(3-Chloro-1-phenylpropyl)-1-(4-methylbenzyl)quinoxalin-2(*1H*)-one (3n)



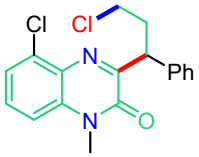
Obtained as yellow liquid (71 mg, 88% yield); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.92 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.49 – 7.42 (m, 2H), 7.42 – 7.37 (m, 1H), 7.29 (t, *J* = 7.7 Hz, 3H), 7.22 (dd, *J* = 8.0, 6.8 Hz, 2H), 7.08 – 7.01 (m, 4H), 5.47 (d, *J* = 15.5 Hz, 1H), 5.23 (d, *J* = 15.5 Hz, 1H), 4.99 (dd, *J* = 8.3, 6.9 Hz, 1H), 3.60 (dt, *J* = 10.9, 6.2 Hz, 1H), 3.49 (ddd, *J* = 10.8, 7.7, 6.6 Hz, 1H), 2.74 (dt, *J* = 14.3, 7.1 Hz, 1H), 2.61 (ddd, *J* = 16.4, 8.3, 6.2 Hz, 1H), 2.27 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 160.20, 154.45, 140.13, 137.39, 132.84, 132.52, 132.26, 130.28, 129.98, 129.58, 128.72, 128.65, 127.09, 126.94, 123.57, 114.44, 45.77, 44.71, 43.24, 36.61, 21.11. **HRMS-ESI**: calcd for $C_{25}H_{23}ClN_2OH$ $[M+H]^+$ 403.1572, found 403.1573.

3-(3-Chloro-1-phenylpropyl)-1-(3-methylbenzyl)quinoxalin-2(*1H*)-one (3o)



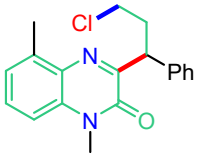
Obtained as yellow liquid (70 mg, 87% yield); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.93 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.46 (d, *J* = 7.2 Hz, 2H), 7.43 – 7.39 (m, 1H), 7.33 – 7.27 (m, 3H), 7.22 (t, *J* = 7.4 Hz, 2H), 7.14 (t, *J* = 7.6 Hz, 1H), 7.02 (d, *J* = 7.5 Hz, 1H), 6.97 – 6.89 (m, 2H), 5.47 (d, *J* = 15.6 Hz, 1H), 5.26 (d, *J* = 15.6 Hz, 1H), 5.00 (dd, *J* = 8.3, 6.9 Hz, 1H), 3.62 (dt, *J* = 10.9, 6.2 Hz, 1H), 3.50 (ddd, *J* = 10.8, 7.6, 6.6 Hz, 1H), 2.75 (dt, *J* = 14.3, 7.1 Hz, 1H), 2.65 – 2.56 (m, 1H), 2.24 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 160.17, 154.44, 140.06, 138.69, 135.14, 132.77, 132.52, 130.23, 129.99, 128.73, 128.68, 128.62, 128.44, 127.43, 127.07, 123.89, 123.58, 114.44, 45.98, 44.73, 43.21, 36.51, 21.40. **HRMS-ESI**: calcd for $C_{25}H_{23}ClN_2OH$ $[M+H]^+$ 403.1572, found 403.1573.

5-Chloro-3-(3-chloro-1-phenylpropyl)-1-methylquinoxalin-2(*1H*)-one (3p)



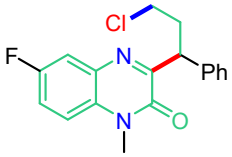
Obtained as yellow liquid (58 mg, 84% yield); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.45 (td, *J* = 8.2, 3.5 Hz, 4H), 7.29 (dd, *J* = 10.4, 4.7 Hz, 2H), 7.23 – 7.19 (m, 1H), 7.17 (dd, *J* = 7.3, 2.3 Hz, 1H), 4.97 (t, *J* = 7.6 Hz, 1H), 3.67 – 3.58 (m, 4H), 3.49 (ddd, *J* = 10.9, 7.6, 6.0 Hz, 1H), 2.76 (dd, *J* = 13.6, 7.1 Hz, 1H), 2.67 – 2.53 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 160.34, 153.97, 139.65, 135.19, 134.62, 129.97, 129.16, 128.84, 128.65, 127.16, 124.48, 112.44, 44.71, 43.17, 36.57, 29.57. **HRMS-ESI**: calcd for $C_{18}H_{16}Cl_2N_2OH$ $[M+H]^+$ 347.0712, found 347.0722.

3-(3-Chloro-1-phenylpropyl)-1,5-dimethylquinoxalin-2(*1H*)-one (3q)



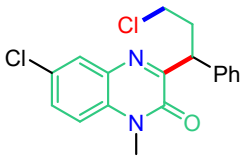
Obtained as yellow liquid (56 mg, 86% yield); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.47 – 7.35 (m, 3H), 7.28 (t, *J* = 7.6 Hz, 2H), 7.24 – 7.17 (m, 2H), 7.11 (d, *J* = 8.4 Hz, 1H), 4.93 (t, *J* = 7.6 Hz, 1H), 3.68 – 3.52 (m, 4H), 3.49 (dd, *J* = 12.4, 5.3 Hz, 1H), 2.82 – 2.67 (m, 4H), 2.57 (dt, *J* = 14.2, 7.1 Hz, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 158.01, 154.28, 140.22, 138.86, 133.24, 130.97, 129.80, 128.69, 128.57, 126.99, 124.88, 111.53, 44.69, 43.18, 36.83, 29.29, 17.59. **HRMS-ESI**: calcd for $C_{19}H_{19}ClN_2ONa$ [M+Na] $^+$ 349.1078, found 349.1061.

3-(3-Chloro-1-phenylpropyl)-6-fluoro-1-methylquinoxalin-2(*1H*)-one (3r)



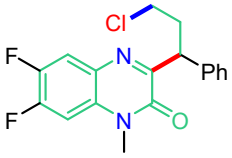
Obtained as yellow liquid (55 mg, 83% yield); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.98 – 7.80 (m, 1H), 7.45 – 7.40 (m, 2H), 7.28 (dd, *J* = 10.4, 4.7 Hz, 2H), 7.22 – 7.17 (m, 1H), 7.09 – 7.02 (m, 1H), 6.93 (dd, *J* = 10.0, 2.6 Hz, 1H), 4.99 – 4.84 (m, 1H), 3.59 – 3.53 (m, 4H), 3.46 (ddd, *J* = 10.8, 7.5, 6.4 Hz, 1H), 2.70 (td, *J* = 14.2, 6.8 Hz, 1H), 2.54 (ddt, *J* = 12.5, 8.3, 6.2 Hz, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 163.20 (d, *J* = 250.3 Hz), 158.84 (d, *J* = 3.4 Hz), 154.20, 139.94, 134.59 (d, *J* = 11.6 Hz), 132.03 (d, *J* = 10.4 Hz), 129.30 (d, *J* = 2.1 Hz), 128.65, 128.63, 127.12, 111.34 (d, *J* = 23.4 Hz), 100.55 (d, *J* = 27.8 Hz), 44.43, 43.14, 36.44, 29.39. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -107.52. **HRMS-ESI**: calcd for $C_{18}H_{16}ClFN_2ONa$ [M+Na] $^+$ 353.0827, found 353.0824.

6-Chloro-3-(3-chloro-1-phenylpropyl)-1-methylquinoxalin-2(*1H*)-one (3s)



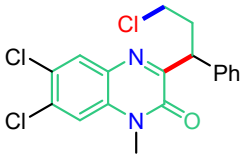
Obtained as yellow liquid (61 mg, 88% yield); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.93 (d, *J* = 2.3 Hz, 1H), 7.48 (dd, *J* = 8.9, 2.3 Hz, 1H), 7.42 (d, *J* = 7.4 Hz, 2H), 7.28 (t, *J* = 7.5 Hz, 2H), 7.20 (dd, *J* = 11.8, 6.5 Hz, 2H), 4.94 (t, *J* = 7.6 Hz, 1H), 3.64 – 3.52 (m, 4H), 3.51 – 3.40 (m, 1H), 2.69 (dd, *J* = 14.1, 7.2 Hz, 1H), 2.54 (dd, *J* = 14.3, 8.1 Hz, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 161.46, 154.00, 139.63, 133.05, 131.86, 129.98, 129.50, 128.89, 128.70, 128.66, 127.20, 114.74, 44.56, 43.06, 36.36, 29.34. **HRMS-ESI**: calcd for $C_{18}H_{16}Cl_2N_2ONa$ [M+Na] $^+$ 369.0532, found 369.0534.

3-(3-Chloro-1-phenylpropyl)-6,7-difluoro-1-methylquinoxalin-2(*1H*)-one (3t)



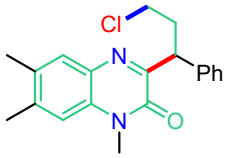
Obtained as yellow liquid (66 mg, 86% yield); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.81 – 7.66 (m, 1H), 7.41 (d, *J* = 7.4 Hz, 2H), 7.28 (t, *J* = 7.5 Hz, 2H), 7.20 (t, *J* = 7.3 Hz, 1H), 7.06 (dd, *J* = 11.2, 7.1 Hz, 1H), 4.91 (t, *J* = 7.6 Hz, 1H), 3.65 – 3.50 (m, 4H), 3.44 (dt, *J* = 10.8, 7.2 Hz, 1H), 2.67 (dd, *J* = 14.1, 7.2 Hz, 1H), 2.54 (dt, *J* = 14.3, 7.1 Hz, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 160.66, 153.89, 151.28 (dd, *J* = 253.2, 14.2 Hz), 146.63 (dd, *J* = 247.0, 14.0 Hz), 139.57, 130.38 (d, *J* = 8.9 Hz), 128.67, 127.23, 125.78, 117.75 (d, *J* = 18.0 Hz), 102.35, 102.17, 44.50, 43.02, 36.32, 29.66. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -131.04 (d, *J* = 22.4 Hz), -142.22 (d, *J* = 22.4 Hz). **HRMS-ESI**: calcd for $C_{18}H_{15}ClF_2N_2OH$ [M+H] $^+$ 349.0914, found 349.0906.

6,7-Dichloro-3-(3-chloro-1-phenylpropyl)-1-methylquinoxalin-2(*1H*)-one (3u)



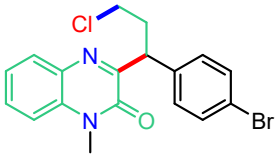
Obtained as yellow liquid (66 mg, 87% yield); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.40 (d, J = 7.2 Hz, 2H), 7.34 (s, 1H), 7.28 (t, J = 7.5 Hz, 2H), 7.22 (d, J = 7.3 Hz, 1H), 4.92 (dd, J = 8.0, 7.1 Hz, 1H), 3.59 – 3.53 (m, 4H), 3.47 – 3.41 (m, 1H), 2.66 (dt, J = 14.2, 7.1 Hz, 1H), 2.54 (ddd, J = 14.3, 8.3, 4.2 Hz, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 161.60, 153.73, 139.37, 134.07, 132.56, 131.58, 130.93, 128.71, 128.69, 127.36, 127.30, 115.12, 44.58, 42.98, 36.27, 29.42. **HRMS-ESI**: calcd for $C_{18}H_{15}Cl_3N_2OH$ $[M+H]^+$ 381.0323, found 381.0327.

3-(3-Chloro-1-phenylpropyl)-1,6,7-trimethylquinoxalin-2(*1H*)-one (3v)



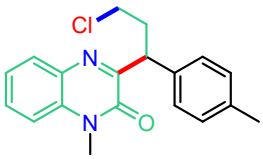
Obtained as yellow liquid (61 mg, 89% yield); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.69 (s, 1H), 7.43 (d, J = 7.3 Hz, 2H), 7.26 (dd, J = 10.4, 4.5 Hz, 2H), 7.18 (t, J = 7.3 Hz, 1H), 7.02 (s, 1H), 4.91 (t, J = 7.6 Hz, 1H), 3.63 – 3.52 (m, 4H), 3.47 (dt, J = 10.8, 7.0 Hz, 1H), 2.72 (dd, J = 14.1, 7.1 Hz, 1H), 2.53 (dd, J = 14.2, 7.9 Hz, 1H), 2.40 (s, 3H), 2.36 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 158.64, 154.43, 140.39, 139.79, 132.45, 131.13, 130.96, 130.23, 128.64, 128.54, 126.93, 114.17, 44.45, 43.27, 36.62, 29.06, 20.55, 19.15. **HRMS-ESI**: calcd for $C_{20}H_{21}ClN_2OH$ $[M+H]^+$ 341.1415, found 341.1407.

3-(1-(4-Bromophenyl)-3-chloropropyl)-1-methylquinoxalin-2(*1H*)-one (3w)



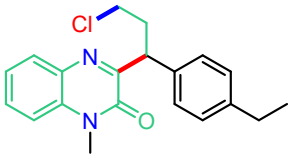
Obtained as yellow liquid (64 mg, 82% yield); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.91 (dd, J = 8.0, 1.1 Hz, 1H), 7.57 – 7.51 (m, 1H), 7.39 (d, J = 8.4 Hz, 2H), 7.36 (dd, J = 11.7, 4.4 Hz, 1H), 7.33 (t, J = 8.4 Hz, 2H), 7.27 (d, J = 8.3 Hz, 1H), 4.91 (t, J = 7.6 Hz, 1H), 3.69 – 3.51 (m, 4H), 3.51 – 3.37 (m, 1H), 2.71 (dd, J = 14.1, 7.2 Hz, 1H), 2.58 – 2.45 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 159.39, 154.28, 139.14, 133.13, 132.49, 131.71, 130.44, 130.23, 130.19, 123.68, 121.08, 113.67, 43.97, 42.97, 36.22, 29.19. **HRMS-ESI**: calcd for $C_{18}H_{16}BrClN_2OH$ $[M+H]^+$ 391.0208, found 391.0217.

3-(3-Chloro-1-(p-tolyl)propyl)-1-methylquinoxalin-2(*1H*)-one (3x)



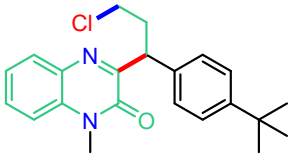
Obtained as yellow liquid (55 mg, 84% yield); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.91 (d, J = 7.8 Hz, 1H), 7.51 (t, J = 7.6 Hz, 1H), 7.34 (dd, J = 14.5, 7.6 Hz, 3H), 7.24 (d, J = 8.2 Hz, 1H), 7.08 (d, J = 7.6 Hz, 2H), 4.89 (t, J = 7.5 Hz, 1H), 3.65 – 3.54 (m, 4H), 3.48 (dd, J = 12.1, 5.2 Hz, 1H), 2.71 (dd, J = 14.0, 7.0 Hz, 1H), 2.55 (dt, J = 14.1, 7.0 Hz, 1H), 2.27 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 160.11, 154.34, 137.00, 136.65, 133.14, 132.56, 130.13, 129.94, 129.32, 128.56, 123.51, 113.56, 44.19, 43.26, 36.48, 29.13, 21.08. **HRMS-ESI**: calcd for $C_{19}H_{19}ClN_2OH$ $[M+H]^+$ 327.1259, found 327.1262.

3-(3-Chloro-1-(4-ethylphenyl)propyl)-1-methylquinoxalin-2(*1H*)-one (3y)



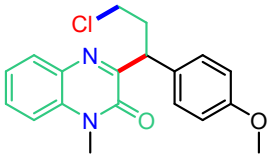
Obtained as yellow liquid (55 mg, 81% yield); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.91 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.56 – 7.48 (m, 1H), 7.34 (t, *J* = 7.7 Hz, 3H), 7.24 (d, *J* = 7.3 Hz, 1H), 7.11 (d, *J* = 8.0 Hz, 2H), 4.91 (t, *J* = 7.6 Hz, 1H), 3.65 – 3.52 (m, 4H), 3.48 (d, *J* = 7.1 Hz, 1H), 2.71 (dd, *J* = 14.1, 7.1 Hz, 1H), 2.57 (dt, *J* = 13.5, 6.8 Hz, 3H), 1.18 (t, *J* = 7.6 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 160.13, 154.36, 142.92, 137.19, 133.13, 132.58, 130.13, 129.93, 128.59, 128.10, 123.51, 113.56, 44.16, 43.30, 36.52, 29.14, 28.46, 15.41. **HRMS-ESI**: calcd for $C_{20}H_{21}ClN_2OH$ [M+H] $^+$ 341.1415, found 341.1407.

3-(1-(4-(*tert*-Butyl)phenyl)-3-chloropropyl)-1-methylquinoxalin-2(*1H*)-one (3z)



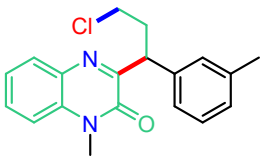
Obtained as yellow liquid (63 mg, 86% yield); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.91 (d, *J* = 7.8 Hz, 1H), 7.51 (t, *J* = 7.6 Hz, 1H), 7.35 (t, *J* = 9.9 Hz, 3H), 7.27 (dd, *J* = 19.5, 7.8 Hz, 3H), 4.92 (t, *J* = 7.5 Hz, 1H), 3.64 – 3.59 (m, 3H), 3.56 (dd, *J* = 11.5, 5.4 Hz, 1H), 3.49 (dd, *J* = 12.1, 5.2 Hz, 1H), 2.72 (dd, *J* = 14.0, 7.0 Hz, 1H), 2.56 (dd, *J* = 14.0, 7.4 Hz, 1H), 1.26 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 160.13, 154.40, 149.72, 136.88, 133.11, 132.61, 130.13, 129.90, 128.25, 125.50, 123.51, 113.55, 43.98, 43.33, 36.53, 34.42, 31.34, 29.15. **HRMS-ESI**: calcd for $C_{22}H_{25}ClN_2OH$ [M+H] $^+$ 369.1728, found 369.1736.

3-(3-Chloro-1-(4-methoxyphenyl)propyl)-1-methylquinoxalin-2(*1H*)-one (3aa)



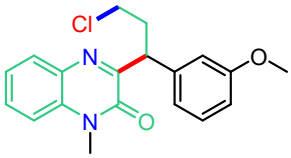
Obtained as yellow liquid (57 mg, 84% yield); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.91 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.58 – 7.46 (m, 1H), 7.39 – 7.33 (m, 1H), 7.28 – 7.23 (m, 1H), 7.20 (t, *J* = 7.9 Hz, 1H), 7.03 (d, *J* = 7.7 Hz, 1H), 7.00 – 6.96 (m, 1H), 6.74 (dd, *J* = 8.1, 2.2 Hz, 1H), 4.96 – 4.85 (m, 1H), 3.77 (s, 3H), 3.66 – 3.55 (m, 4H), 3.53 – 3.42 (m, 1H), 2.71 (dd, *J* = 14.1, 7.2 Hz, 1H), 2.61 – 2.49 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 159.74 (d, *J* = 15.4 Hz), 154.36, 141.74, 133.15, 132.54, 130.18, 130.03, 129.52, 123.54, 121.20, 114.39, 113.58, 112.24, 55.17, 44.48, 43.21, 36.56, 29.16. **HRMS-ESI**: calcd for $C_{19}H_{19}ClN_2O_2Na$ [M+Na] $^+$ 365.1027, found 365.1030.

3-(3-Chloro-1-(*m*-tolyl)propyl)-1-methylquinoxalin-2(*1H*)-one (3ab)



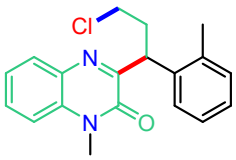
Obtained as yellow liquid (52 mg, 80% yield); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.92 (dd, *J* = 7.9, 1.0 Hz, 1H), 7.56 – 7.49 (m, 1H), 7.35 (t, *J* = 7.4 Hz, 1H), 7.24 (dd, *J* = 16.0, 4.6 Hz, 3H), 7.16 (t, *J* = 7.8 Hz, 1H), 7.01 (d, *J* = 7.4 Hz, 1H), 4.89 (t, *J* = 7.6 Hz, 1H), 3.60 (d, *J* = 11.8 Hz, 3H), 3.57 (dd, *J* = 10.8, 6.3 Hz, 1H), 3.52 – 3.44 (m, 1H), 2.72 (dd, *J* = 14.1, 7.1 Hz, 1H), 2.58 – 2.49 (m, 1H), 2.30 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 160.01, 154.36, 140.03, 138.16, 133.15, 132.58, 130.18, 129.96, 129.33, 128.45, 127.87, 125.68, 123.52, 113.58, 44.50, 43.27, 36.61, 29.15, 21.49. **HRMS-ESI**: calcd for $C_{19}H_{19}ClN_2OH$ [M+H] $^+$ 327.1259, found 327.1257.

3-(3-Chloro-1-(3-methoxyphenyl)propyl)-1-methylquinoxalin-2(*1H*)-one (3ac)



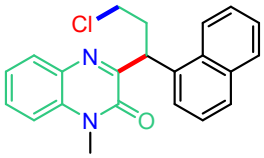
Obtained as yellow liquid (53 mg, 77% yield); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.91 (dd, *J* = 7.9, 0.9 Hz, 1H), 7.55 – 7.48 (m, 1H), 7.34 (t, *J* = 7.4 Hz, 1H), 7.27 – 7.22 (m, 1H), 7.20 (t, *J* = 7.9 Hz, 1H), 7.03 (d, *J* = 7.6 Hz, 1H), 6.98 (s, 1H), 6.74 (dd, *J* = 8.1, 2.1 Hz, 1H), 4.91 (t, *J* = 7.6 Hz, 1H), 3.76 (s, 3H), 3.60 (d, *J* = 5.3 Hz, 3H), 3.57 (dd, *J* = 11.6, 5.5 Hz, 1H), 3.52 – 3.45 (m, 1H), 2.71 (dd, *J* = 14.1, 7.1 Hz, 1H), 2.55 (dd, *J* = 14.2, 8.0 Hz, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 159.75 (d, *J* = 14.2 Hz), 154.35, 141.74, 133.14, 132.53, 130.17, 130.04, 129.52, 123.55, 121.20, 114.40, 113.58, 112.25, 55.17, 44.48, 43.21, 36.56, 29.16. **HRMS-ESI**: calcd for $C_{19}H_{19}ClN_2O_2H$ $[M+H]^+$ 343.1208, found 343.1202.

3-(3-Chloro-1-(o-tolyl)propyl)-1-methylquinoxalin-2(*1H*)-one (3ad)



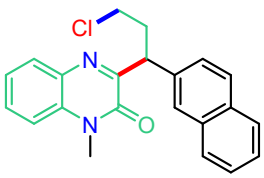
Obtained as yellow liquid (47 mg, 72% yield); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.94 (d, *J* = 7.8 Hz, 1H), 7.53 (t, *J* = 7.6 Hz, 1H), 7.36 (t, *J* = 7.5 Hz, 1H), 7.26 (d, *J* = 8.4 Hz, 1H), 7.19 (d, *J* = 7.2 Hz, 1H), 7.14 (d, *J* = 7.5 Hz, 1H), 7.08 (t, *J* = 7.1 Hz, 1H), 7.02 (t, *J* = 7.3 Hz, 1H), 5.16 (t, *J* = 7.3 Hz, 1H), 3.67 – 3.51 (m, 5H), 2.84 – 2.64 (m, 4H), 2.39 (dd, *J* = 14.0, 6.9 Hz, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 160.30, 154.46, 138.94, 137.44, 133.12, 132.53, 130.78, 130.14, 129.97, 126.89, 126.77, 125.95, 123.54, 113.60, 43.37, 39.97, 36.98, 29.14, 19.94. **HRMS-ESI**: calcd for $C_{19}H_{19}ClN_2OH$ $[M+H]^+$ 327.1259, found 327.1257.

3-(3-Chloro-1-(naphthalen-1-yl)propyl)-1-methylquinoxalin-2(*1H*)-one (3ae)



Obtained as yellow liquid (54 mg, 74% yield); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.63 (d, *J* = 8.6 Hz, 1H), 7.97 (d, *J* = 7.8 Hz, 1H), 7.84 (d, *J* = 8.1 Hz, 1H), 7.71 (d, *J* = 7.8 Hz, 1H), 7.62 (t, *J* = 7.5 Hz, 1H), 7.52 (dt, *J* = 23.2, 7.4 Hz, 2H), 7.41 – 7.29 (m, 3H), 7.26 (d, *J* = 8.4 Hz, 1H), 5.81 (t, *J* = 7.0 Hz, 1H), 3.69 – 3.52 (m, 5H), 2.94 (dt, *J* = 14.1, 7.0 Hz, 1H), 2.65 – 2.49 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 160.13, 154.53, 137.27, 134.18, 133.21, 132.55, 132.03, 130.17, 130.07, 128.82, 127.65, 126.50, 125.75, 125.23, 125.05, 123.85, 123.59, 113.65, 43.57, 39.38, 37.12, 29.15. **HRMS-ESI**: calcd for $C_{22}H_{19}ClN_2OH$ $[M+H]^+$ 363.1259, found 363.1256.

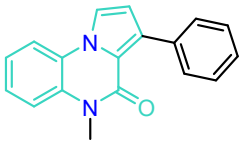
3-(3-chloro-1-(naphthalen-2-yl)propyl)-1-methylquinoxalin-2(*1H*)-one (3af)



Obtained as yellow liquid (57 mg, 79% yield); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.88 (d, *J* = 7.7 Hz, 1H), 7.79 (s, 1H), 7.73 – 7.63 (m, 3H), 7.52 (d, *J* = 8.2 Hz, 1H), 7.43 (t, *J* = 7.5 Hz, 1H), 7.29 (dd, *J* = 16.8, 9.3 Hz, 3H), 7.15 (d, *J* = 8.0 Hz, 1H), 5.02 (t, *J* = 7.3 Hz, 1H), 3.51 (d, *J* = 16.1 Hz, 4H), 3.45 – 3.38 (m, 1H), 2.72 (dd, *J* = 13.9, 7.0 Hz, 1H), 2.58 (dd, *J* = 13.9,

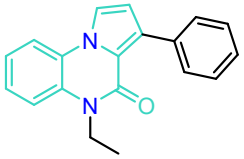
7.4 Hz, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 159.90, 154.37, 137.54, 133.50, 133.18, 132.64, 132.59, 130.22, 130.05, 128.29, 127.87, 127.60, 127.56, 126.74, 125.98, 125.71, 123.58, 113.61, 44.66, 43.22, 36.48, 29.14. **HRMS-ESI**: calcd for $C_{22}H_{19}ClN_2OH$ $[M+H]^+$ 363.1259, found 363.1248.

5-Methyl-3-phenylpyrrolo[1,2-*a*]quinoxalin-4(*5H*)-one (4a)



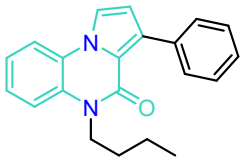
Obtained as yellow solid (50 mg, 91% yield); M. P. = 167-168 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.66 – 7.61 (m, 4H), 7.35 (t, *J* = 7.6 Hz, 2H), 7.28 – 7.23 (m, 3H), 7.18 – 7.15 (m, 1H), 6.68 (d, *J* = 2.8 Hz, 1H), 3.57 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 155.60, 134.79, 130.87, 130.34, 130.00, 127.70, 127.03, 125.66, 123.96, 122.79, 117.79, 115.53, 115.41, 115.07, 114.34, 28.36. **HRMS-ESI**: calcd for $C_{18}H_{14}N_2OH$ $[M+H]^+$ 275.1179, found 275.1184.

5-Ethyl-3-phenylpyrrolo[1,2-*a*]quinoxalin-4(*5H*)-one (4b)



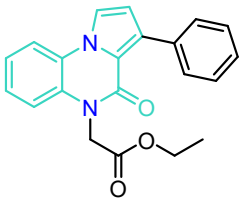
Obtained as yellow solid (50 mg, 87% yield); M. P. = 167-168 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.64 (dd, *J* = 15.7, 5.2 Hz, 4H), 7.35 (t, *J* = 7.6 Hz, 2H), 7.25 (dd, *J* = 9.7, 5.1 Hz, 3H), 7.18 – 7.13 (m, 1H), 6.68 (d, *J* = 2.8 Hz, 1H), 4.23 (q, *J* = 7.1 Hz, 2H), 1.28 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 155.18, 134.78, 130.61, 130.01, 129.13, 127.73, 126.99, 125.67, 124.12, 122.59, 117.74, 115.41, 115.23, 115.08, 114.65, 36.23, 12.78. **HRMS-ESI**: calcd for $C_{19}H_{16}N_2ONa$ $[M+Na]^+$ 311.1155, found 311.1158.

5-Butyl-3-phenylpyrrolo[1,2-*a*]quinoxalin-4(*5H*)-one (4c)



Obtained as yellow solid (50 mg, 88% yield); M. P. = 156-158 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.77 – 7.68 (m, 4H), 7.42 (t, *J* = 7.7 Hz, 2H), 7.35 – 7.28 (m, 3H), 7.25 – 7.20 (m, 1H), 6.75 (d, *J* = 2.9 Hz, 1H), 4.28 – 4.15 (m, 2H), 1.72 (dt, *J* = 21.8, 7.8 Hz, 2H), 1.47 (dd, *J* = 15.2, 7.5 Hz, 2H), 0.97 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 155.34, 134.84, 130.61, 130.00, 129.38, 127.74, 126.96, 125.61, 124.07, 122.56, 117.70, 115.55, 115.20, 115.11, 114.61, 41.22, 29.48, 20.33, 13.89. **HRMS-ESI**: calcd for $C_{21}H_{20}N_2OH$ $[M+H]^+$ 317.1648, found 317.1653.

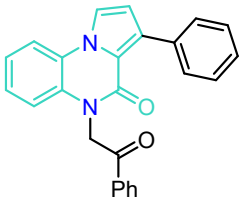
Ethyl 2-(4-oxo-3-phenylpyrrolo[1,2-*a*]quinoxalin-5(*4H*)-yl)acetate (4d)



Obtained as yellow solid (50 mg, 81% yield); M. P. = 141-144 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.66 – 7.61 (m, 4H), 7.36 – 7.32 (m, 2H), 7.26 – 7.23 (m, 1H), 7.23 – 7.19 (m, 1H), 7.17 (dd, *J* = 8.0, 1.3 Hz, 1H), 6.96 (dd, *J* = 8.2, 1.2 Hz, 1H), 6.69 (d, *J* = 2.9 Hz, 1H), 4.95 (s, 2H), 4.15 (q, *J* = 7.1 Hz, 2H), 1.17 (d, *J* = 7.1 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ

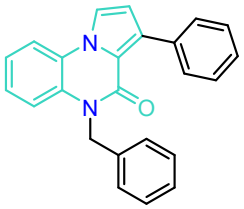
168.36, 155.29, 134.54, 131.68, 129.95, 129.38, 127.74, 127.16, 125.76, 123.98, 123.18, 117.25, 116.02, 115.16, 115.02, 114.72, 61.72, 42.72, 14.17. **HRMS-ESI**: calcd for $C_{21}H_{18}N_2O_3Na$ [M+Na] $^+$ 369.1210, found 369.1211.

5-(2-Oxo-2-phenylethyl)-3-phenylpyrrolo[1,2-*a*]quinoxalin-4(*5H*)-one (4e)



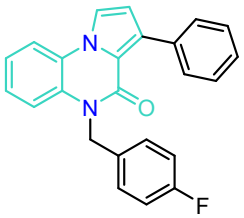
Obtained as yellow solid (64 mg, 84% yield); M. P. = 147-148 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.07 (d, J = 7.5 Hz, 2H), 7.73 (dd, J = 15.3, 5.1 Hz, 4H), 7.64 (t, J = 7.4 Hz, 1H), 7.52 (t, J = 7.7 Hz, 2H), 7.40 (t, J = 7.6 Hz, 2H), 7.31 (t, J = 7.4 Hz, 1H), 7.25 – 7.18 (m, 2H), 6.94 – 6.89 (m, 1H), 6.78 (d, J = 2.8 Hz, 1H), 5.74 (s, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 192.59, 155.52, 134.84, 134.64, 134.01, 131.49, 129.97, 129.56, 128.93, 128.13, 127.71, 127.10, 125.68, 124.03, 123.04, 119.74, 115.96, 115.46, 115.13, 114.70, 47.77. **HRMS-ESI**: calcd for $C_{25}H_{18}N_2O_2Na$ [M+Na] $^+$ 401.1260, found 401.1263.

5-Benzyl-3-phenylpyrrolo[1,2-*a*]quinoxalin-4(*5H*)-one (4f)



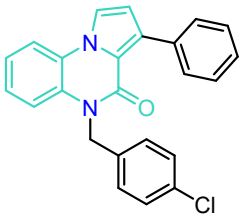
Obtained as yellow solid (60 mg, 86% yield); M. P. = 132-134 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.79 – 7.73 (m, 2H), 7.69 (d, J = 2.9 Hz, 1H), 7.65 (dd, J = 6.1, 3.2 Hz, 1H), 7.41 (t, J = 7.7 Hz, 2H), 7.31 (t, J = 7.4 Hz, 1H), 7.28 – 7.19 (m, 5H), 7.18 – 7.11 (m, 3H), 6.77 (d, J = 2.9 Hz, 1H), 5.46 (s, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 155.78, 136.58, 134.72, 131.33, 130.09, 129.49, 128.78, 127.80, 127.24, 127.12, 126.60, 125.64, 124.03, 122.89, 117.48, 116.49, 115.76, 115.24, 114.43, 44.96. **HRMS-ESI**: calcd for $C_{24}H_{18}N_2OH$ [M+H] $^+$ 351.1492, found 351.1501.

5-(4-Fluorobenzyl)-3-phenylpyrrolo[1,2-*a*]quinoxalin-4(*5H*)-one (4g)



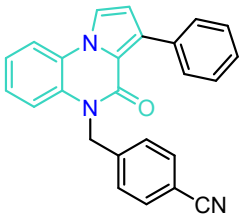
Obtained as yellow solid (61 mg, 83% yield); M. P. = 134-136 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.75 (d, J = 7.3 Hz, 2H), 7.67 (d, J = 2.9 Hz, 1H), 7.64 (dd, J = 6.1, 3.1 Hz, 1H), 7.41 (t, J = 7.7 Hz, 2H), 7.31 (t, J = 7.4 Hz, 1H), 7.21 (dd, J = 8.3, 5.5 Hz, 2H), 7.16 – 7.10 (m, 3H), 6.94 (t, J = 8.6 Hz, 2H), 6.76 (d, J = 2.8 Hz, 1H), 5.40 (s, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 162.02 (d, J = 245.3 Hz), 155.74, 134.66, 132.32 (d, J = 3.1 Hz), 131.44, 130.08, 129.30, 128.39, 128.32, 127.83, 127.18, 125.66, 124.03, 123.02, 117.37, 116.26, 115.88, 115.69 (d, J = 21.5 Hz), 115.29, 114.54, 44.31. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -115.25. **HRMS-ESI**: calcd for $C_{24}H_{17}FN_2OH$ [M+H] $^+$ 369.1398, found 369.1403.

5-(4-Chlorobenzyl)-3-phenylpyrrolo[1,2-*a*]quinoxalin-4(*5H*)-one (4h)



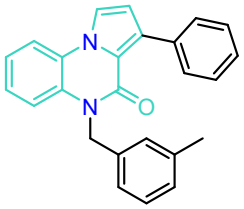
Obtained as yellow solid (67 mg, 87% yield); M. P. = 154-156 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.78 – 7.67 (m, 4H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.32 (t, *J* = 7.4 Hz, 1H), 7.26 – 7.15 (m, 6H), 7.10 (dd, *J* = 5.6, 4.0 Hz, 1H), 6.78 (d, *J* = 2.8 Hz, 1H), 5.43 (s, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 155.71, 135.15, 134.59, 133.03, 131.52, 130.04, 129.25, 128.95, 128.07, 127.81, 127.19, 125.69, 124.05, 123.07, 117.32, 116.24, 115.89, 115.31, 114.56, 44.38. **HRMS-ESI**: calcd for $C_{24}H_{17}ClN_2OH$ $[M+H]^+$ 385.1102, found 385.1100.

4-((4-Oxo-3-phenylpyrrolo[1,2-*a*]quinoxalin-5(*4H*)-yl)methyl)benzonitrile (4i)



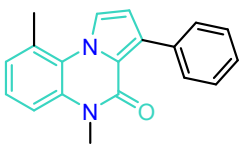
Obtained as yellow solid (63 mg, 84% yield); M. P. = 164-166 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.79 – 7.71 (m, 4H), 7.58 (d, *J* = 8.2 Hz, 2H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.38 – 7.31 (m, 3H), 7.25 – 7.16 (m, 2H), 7.04 (d, *J* = 7.9 Hz, 1H), 6.81 (d, *J* = 2.8 Hz, 1H), 5.53 (s, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 155.65, 142.23, 134.42, 132.66, 131.85, 129.99, 129.05, 128.41, 127.82, 127.29, 125.80, 124.10, 123.34, 118.65, 117.12, 116.14, 115.92, 115.42, 114.76, 111.28, 44.71. **HRMS-ESI**: calcd for $C_{25}H_{17}N_3OH$ $[M+H]^+$ 376.1444, found 376.1459.

5-(3-Methylbenzyl)-3-phenylpyrrolo[1,2-*a*]quinoxalin-4(*5H*)-one (4j)



Obtained as yellow solid (60 mg, 83% yield); M. P. = 167-168 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.85 – 7.63 (m, 4H), 7.42 (t, *J* = 7.5 Hz, 2H), 7.31 (t, *J* = 7.2 Hz, 1H), 7.16 (t, *J* = 8.2 Hz, 4H), 7.10 – 6.97 (m, 3H), 6.79 (d, *J* = 2.4 Hz, 1H), 5.44 (s, 2H), 2.27 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 155.79, 138.48, 136.51, 134.72, 131.27, 130.08, 129.57, 128.63, 128.03, 127.79, 127.15, 127.10, 125.66, 124.02, 123.65, 122.84, 117.51, 116.56, 115.69, 115.22, 114.39, 45.00, 21.48. **HRMS-ESI**: calcd for $C_{25}H_{20}N_2ONa$ $[M+Na]^+$ 387.1468, found 387.1478.

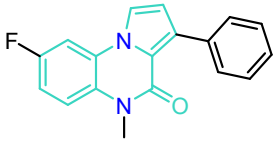
5,9-Dimethyl-3-phenylpyrrolo[1,2-a]quinoxalin-4(*5H*)-one (4k)



Obtained as yellow solid (50 mg, 86% yield); M. P. = 151-154 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.94 (d, *J* = 3.0 Hz, 1H), 7.60 (d, *J* = 7.2 Hz, 2H), 7.35 (t, *J* = 7.6 Hz, 2H), 7.26 (t, *J* = 7.4 Hz, 1H), 7.15 (dd, *J* = 9.4, 6.7 Hz, 2H), 7.03 – 6.98 (m, 1H), 6.66 (d, *J* = 2.9 Hz, 1H), 3.54 (s, 3H), 2.79 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 155.56, 135.05, 131.67, 130.38,

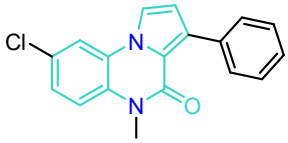
130.19, 127.63, 127.23, 127.03, 126.15, 124.99, 124.09, 121.34, 119.07, 114.23, 113.84, 29.06, 24.14. **HRMS-ESI**: calcd for $C_{19}H_{16}N_2OH$ $[M+H]^+$ 289.1335, found 289.1343.

8-Fluoro-5-methyl-3-phenylpyrrolo[1,2-*a*]quinoxalin-4(*5H*)-one (4l)



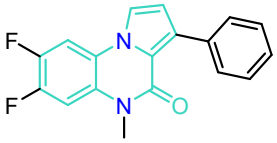
Obtained as yellow solid (48 mg, 83% yield); M. P. = 154-156 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.72 – 7.65 (m, 2H), 7.57 (d, *J* = 2.9 Hz, 1H), 7.40 (dt, *J* = 9.0, 5.1 Hz, 3H), 7.33 (t, *J* = 7.4 Hz, 1H), 7.24 (dd, *J* = 9.1, 4.9 Hz, 1H), 7.08 – 7.01 (m, 1H), 6.76 (d, *J* = 2.9 Hz, 1H), 3.61 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 158.35 (d, *J* = 242.9 Hz), 155.20, 134.46, 131.28, 129.98, 127.74, 127.19, 126.78, 124.55 (d, *J* = 10.2 Hz), 117.72, 116.68 (d, *J* = 9.0 Hz), 115.66, 115.57, 112.36 (d, *J* = 22.8 Hz), 101.86 (d, *J* = 27.4 Hz), 28.55. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -118.79. **HRMS-ESI**: calcd for $C_{18}H_{13}FN_2OH$ $[M+H]^+$ 293.1085, found 293.1078.

8-Chloro-5-methyl-3-phenylpyrrolo[1,2-*a*]quinoxalin-4(*5H*)-one (4m)



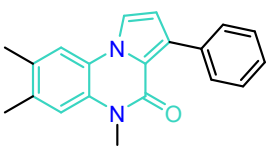
Obtained as yellow solid (54 mg, 87% yield); M. P. = 158-160 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.61 (d, *J* = 7.3 Hz, 2H), 7.57 (d, *J* = 1.8 Hz, 1H), 7.52 (d, *J* = 2.7 Hz, 1H), 7.34 (t, *J* = 7.5 Hz, 2H), 7.26 (d, *J* = 7.3 Hz, 1H), 7.21 – 7.18 (m, 1H), 7.12 (d, *J* = 8.8 Hz, 1H), 6.68 (d, *J* = 2.7 Hz, 1H), 3.51 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 155.20, 134.40, 131.42, 129.96, 129.03, 128.19, 127.75, 127.23, 125.45, 124.63, 117.64, 116.57, 115.63, 115.60, 114.48, 28.48. **HRMS-ESI**: calcd for $C_{18}H_{13}ClN_2OH$ $[M+H]^+$ 309.0789, found 309.0792.

7,8-Difluoro-5-methyl-3-phenylpyrrolo[1,2-*a*]quinoxalin-4(*5H*)-one (4n)



Obtained as yellow solid (52 mg, 84% yield); M. P. = 154-156 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.61 – 7.57 (m, 2H), 7.46 – 7.41 (m, 2H), 7.34 (t, *J* = 7.6 Hz, 2H), 7.29 – 7.26 (m, 1H), 7.05 (dd, *J* = 11.6, 7.2 Hz, 1H), 6.68 (d, *J* = 2.9 Hz, 1H), 3.50 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 155.17, 147.71 (d, *J* = 246.0 Hz), 145.63 (d, *J* = 252.1 Hz), 134.28, 131.56, 129.93, 128.66, 127.77, 127.30, 125.77, 117.42, 115.76, 115.59, 104.80 (d, *J* = 23.2 Hz), 103.74 (d, *J* = 22.7 Hz), 28.76. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -138.92 (d, *J* = 22.5 Hz), -142.78 (d, *J* = 22.5 Hz). **HRMS-ESI**: calcd for $C_{18}H_{12}F_2N_2OH$ $[M+H]^+$ 311.0990, found 311.0999.

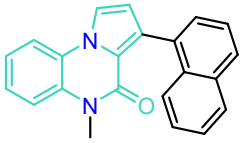
5,7,8-Trimethyl-3-phenylpyrrolo[1,2-*a*]quinoxalin-4(*5H*)-one (4o)



Obtained as yellow solid (50 mg, 83% yield); M. P. = 139-141 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.70 (d, *J* = 7.2 Hz, 2H), 7.62 (d, *J* = 2.8 Hz, 1H), 7.41 (dd, *J* = 13.7, 6.1 Hz, 3H), 7.31 (t, *J* = 7.4 Hz, 1H), 7.04 (s, 1H), 6.70 (d, *J* = 2.8 Hz, 1H), 3.59 (s, 3H), 2.35 (s, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 155.64, 135.01, 134.25, 131.33, 130.36, 130.01, 128.08,

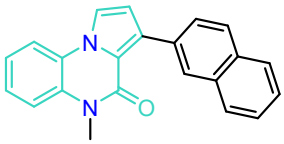
127.66, 126.87, 121.74, 117.77, 116.42, 115.18, 115.04, 114.64, 28.28, 19.95, 19.48. **HRMS-ESI**: calcd for $C_{20}H_{18}N_2OH$ $[M+H]^+$ 303.1492, found 303.1498.

5-Methyl-3-(naphthalen-1-yl)pyrrolo[1,2-*a*]quinoxalin-4(*5H*)-one (4p)



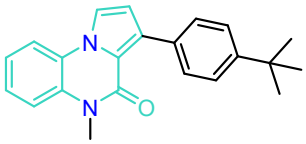
Obtained as yellow solid (40 mg, 61% yield); M. P. = 142-144 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.87 (dd, *J* = 12.2, 4.7 Hz, 2H), 7.83 (d, *J* = 8.5 Hz, 1H), 7.78 (dd, *J* = 5.8, 2.0 Hz, 2H), 7.58 – 7.52 (m, 2H), 7.47 – 7.41 (m, 1H), 7.40 – 7.34 (m, 2H), 7.33 – 7.26 (m, 2H), 6.76 (d, *J* = 2.8 Hz, 1H), 3.56 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 155.25, 133.55, 133.20, 132.61, 130.53, 128.21, 128.17, 128.03, 127.72, 126.33, 125.69, 125.46, 125.07, 124.02, 122.80, 119.57, 116.50, 115.61, 115.05, 114.36, 28.27. **HRMS-ESI**: calcd for $C_{22}H_{16}N_2ONa$ $[M+Na]^+$ 347.1155, found 347.1151.

5-Methyl-3-(naphthalen-2-yl)pyrrolo[1,2-*a*]quinoxalin-4(*5H*)-one (4q)



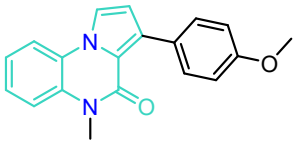
Obtained as yellow solid (37 mg, 57% yield); M. P. = 147-148 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) *δ* 8.12 (s, 1H), 7.91 – 7.82 (m, 4H), 7.72 – 7.66 (m, 2H), 7.48 – 7.41 (m, 2H), 7.31 (ddd, *J* = 14.8, 8.1, 4.0 Hz, 2H), 7.24 – 7.20 (m, 1H), 6.83 (d, *J* = 2.8 Hz, 1H), 3.62 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) *δ* 155.59, 133.28, 132.63, 132.49, 130.74, 130.33, 128.84, 128.33, 128.19, 127.62, 126.88, 125.77, 125.71, 125.68, 123.94, 122.81, 118.03, 115.53, 115.28, 114.36, 28.41. **HRMS-ESI**: calcd for $C_{22}H_{16}N_2ONa$ $[M+Na]^+$ 347.1155, found 347.1164.

3-(4-(*tert*-Butyl)phenyl)-5-methylpyrrolo[1,2-*a*]quinoxalin-4(*5H*)-one (4r)



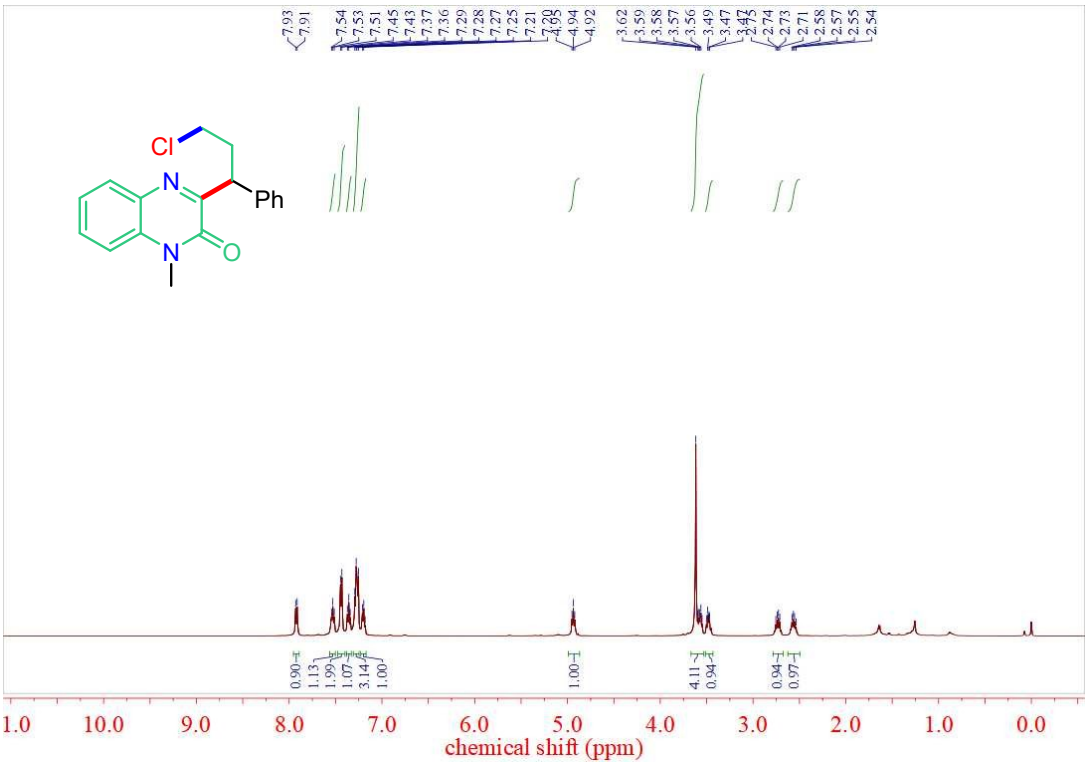
Obtained as yellow solid (41 mg, 62% yield); M. P. = 148-150 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) *δ* 7.62 – 7.56 (m, 4H), 7.40 – 7.35 (m, 2H), 7.26 – 7.20 (m, 2H), 7.17 – 7.12 (m, 1H), 6.66 (d, *J* = 2.9 Hz, 1H), 3.55 (s, 3H), 1.29 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) *δ* 154.60, 148.75, 130.74, 129.80, 129.26, 128.60, 124.51, 123.66, 122.95, 121.70, 116.64, 114.43, 114.34, 114.00, 113.23, 33.53, 30.37, 27.29. **HRMS-ESI**: calcd for $C_{22}H_{22}N_2OH$ $[M+H]^+$ 331.1805, found 331.1811.

3-(4-Methoxyphenyl)-5-methylpyrrolo[1,2-*a*]quinoxalin-4(*5H*)-one (4s)

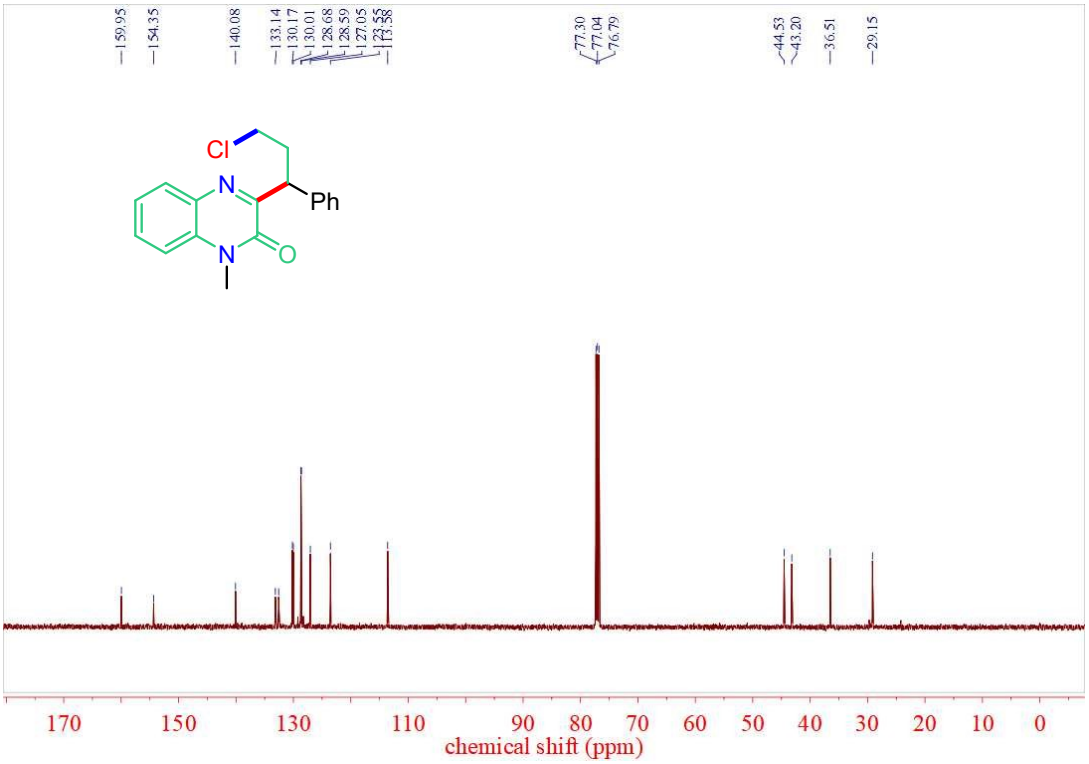


Obtained as yellow solid (36 mg, 60% yield); M. P. = 154-158 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) *δ* 7.59 (ddd, *J* = 9.5, 8.8, 5.0 Hz, 4H), 7.26 – 7.22 (m, 2H), 7.18 – 7.14 (m, 1H), 6.90 (d, *J* = 8.8 Hz, 2H), 6.64 (d, *J* = 2.8 Hz, 1H), 3.78 (s, 3H), 3.56 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) *δ* 158.83, 155.71, 131.12, 130.66, 130.33, 127.20, 125.54, 124.03, 122.75, 117.53, 115.49, 115.36, 114.81, 114.26, 113.25, 55.33, 28.33. **HRMS-ESI**: calcd for $C_{19}H_{16}N_2O_2H$ $[M+H]^+$ 305.1285, found 305.1280.

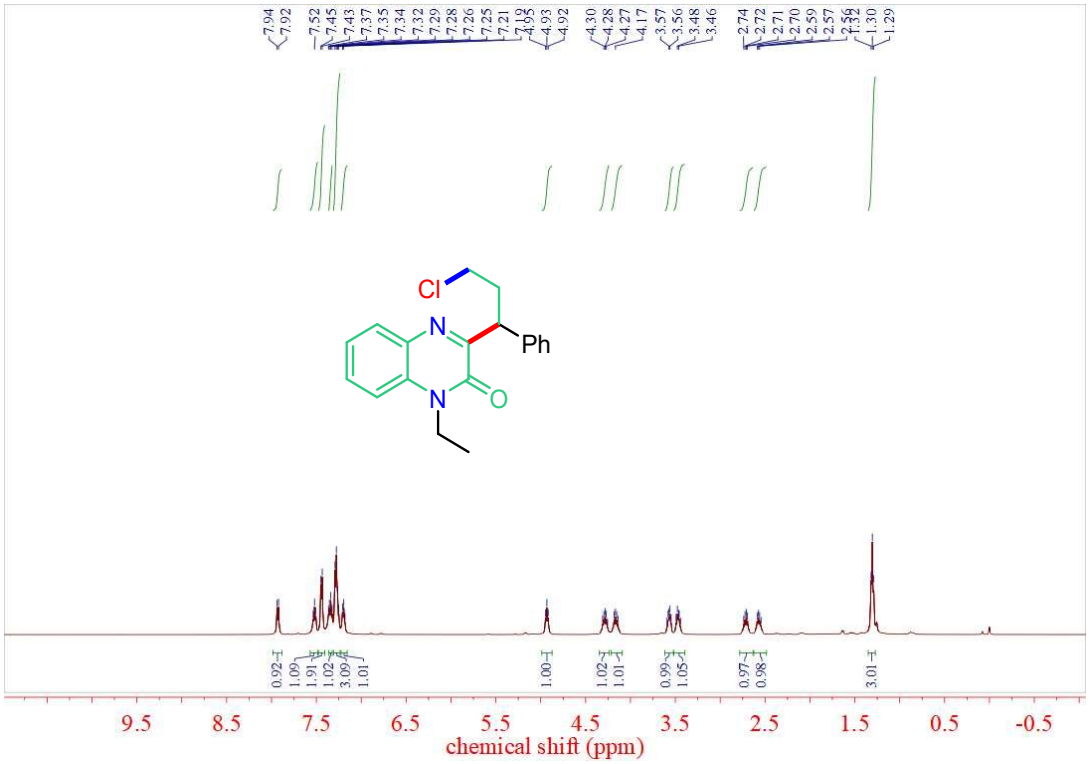
1. Copies of ^{1}H, ^{13}C and ^{19}F NMR Spectra



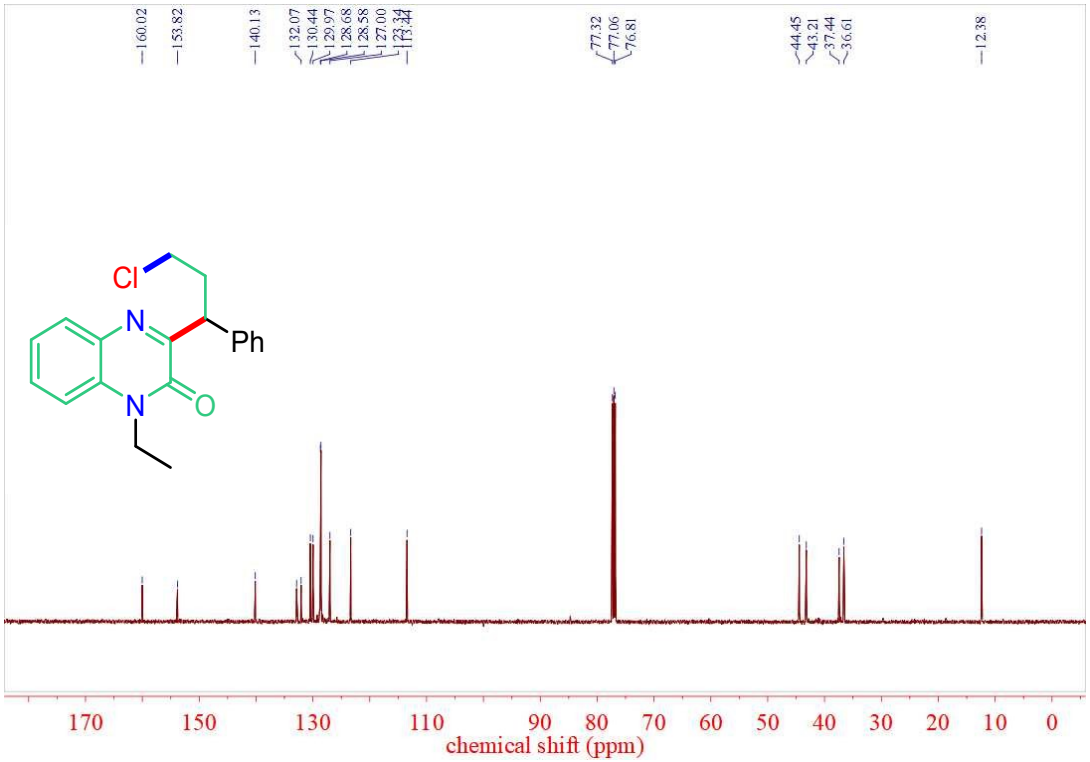
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3a**



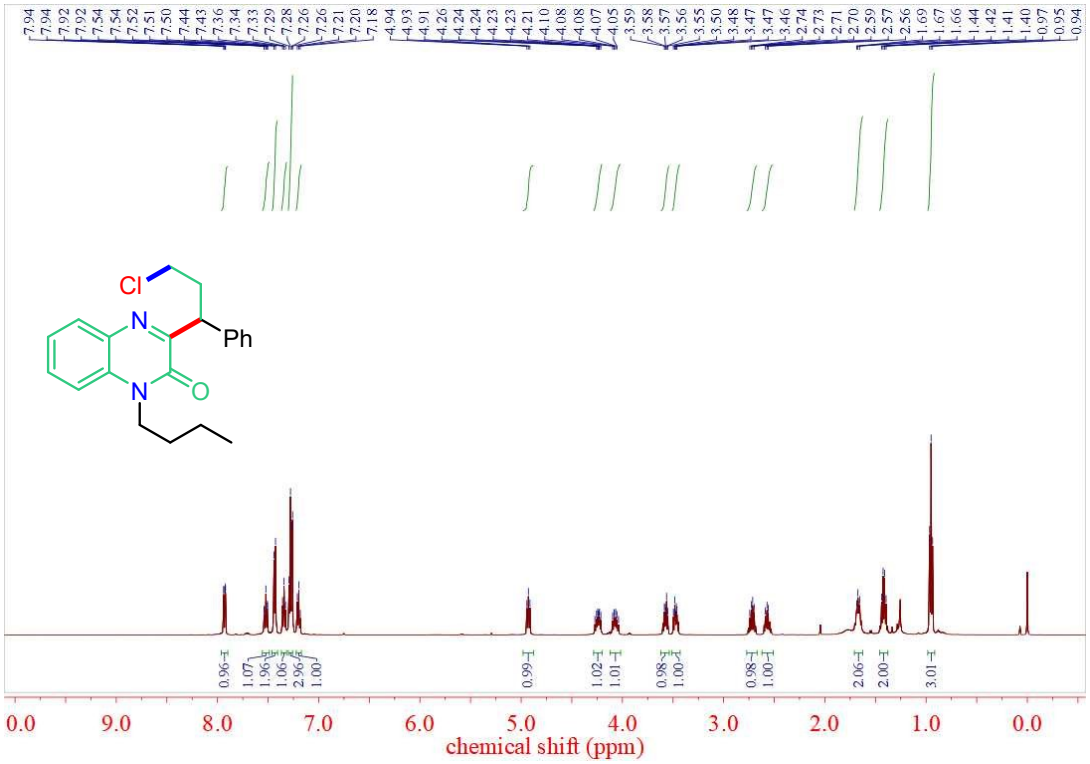
^{13}C NMR (126 MHz, $CDCl_3$) of compound **3a**



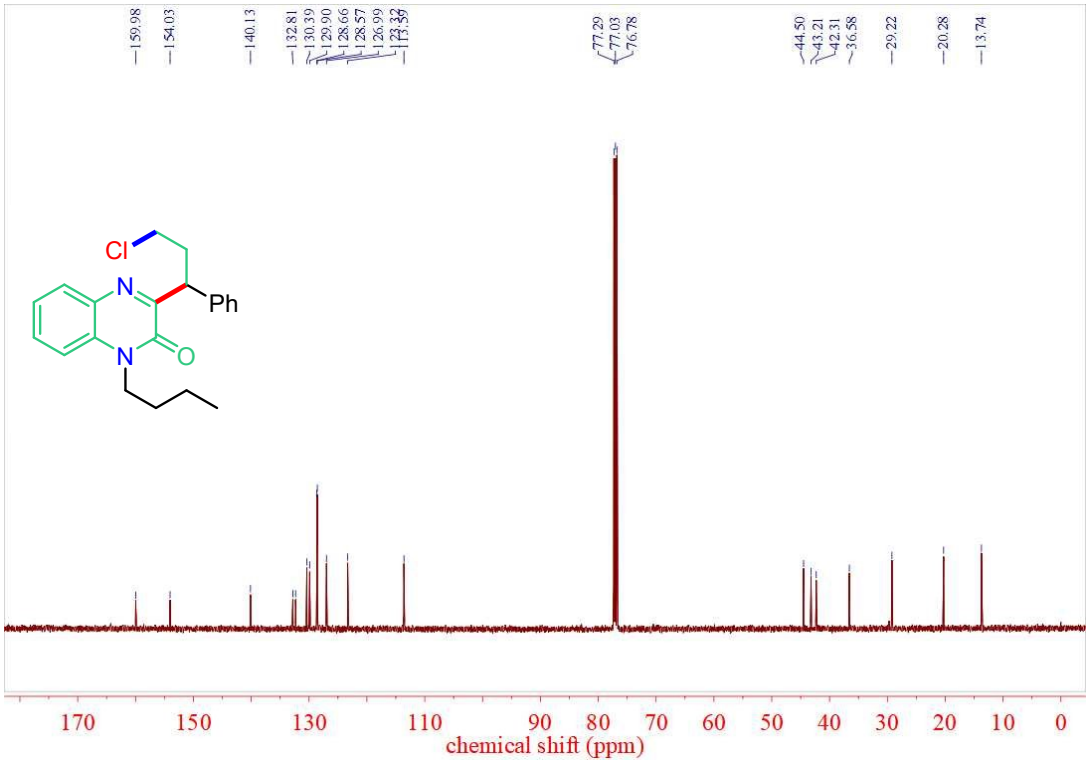
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3b**



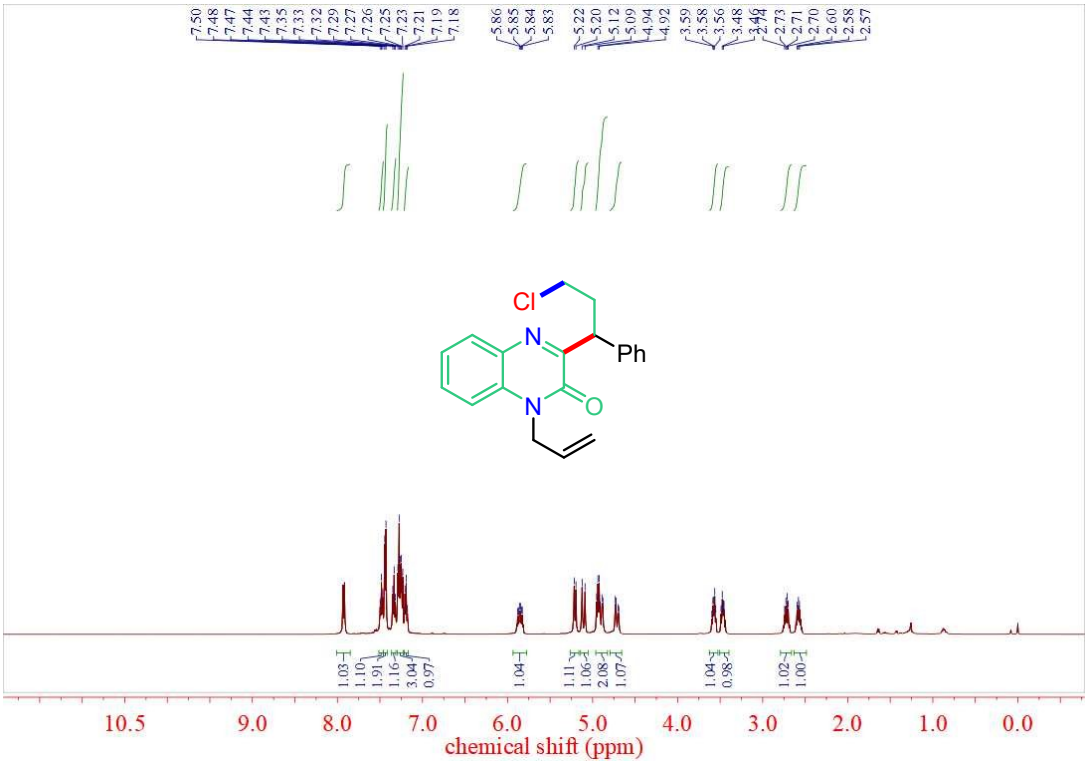
^{13}C NMR (126 MHz, $CDCl_3$) of compound **3b**



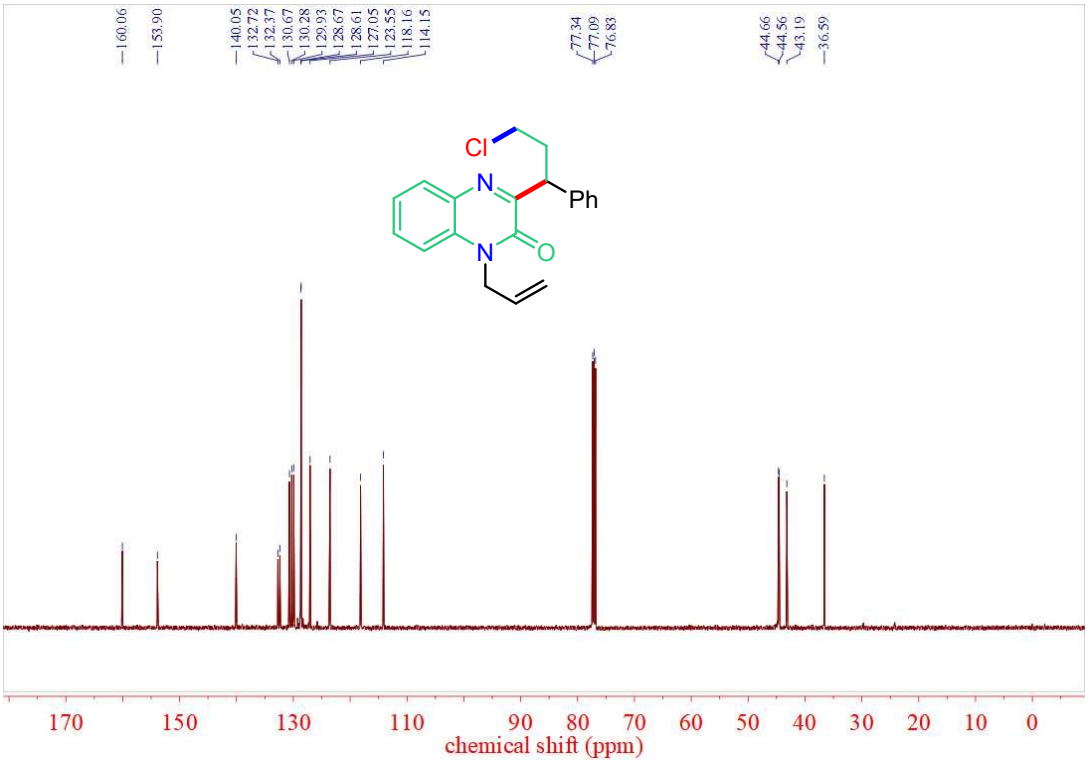
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3c**



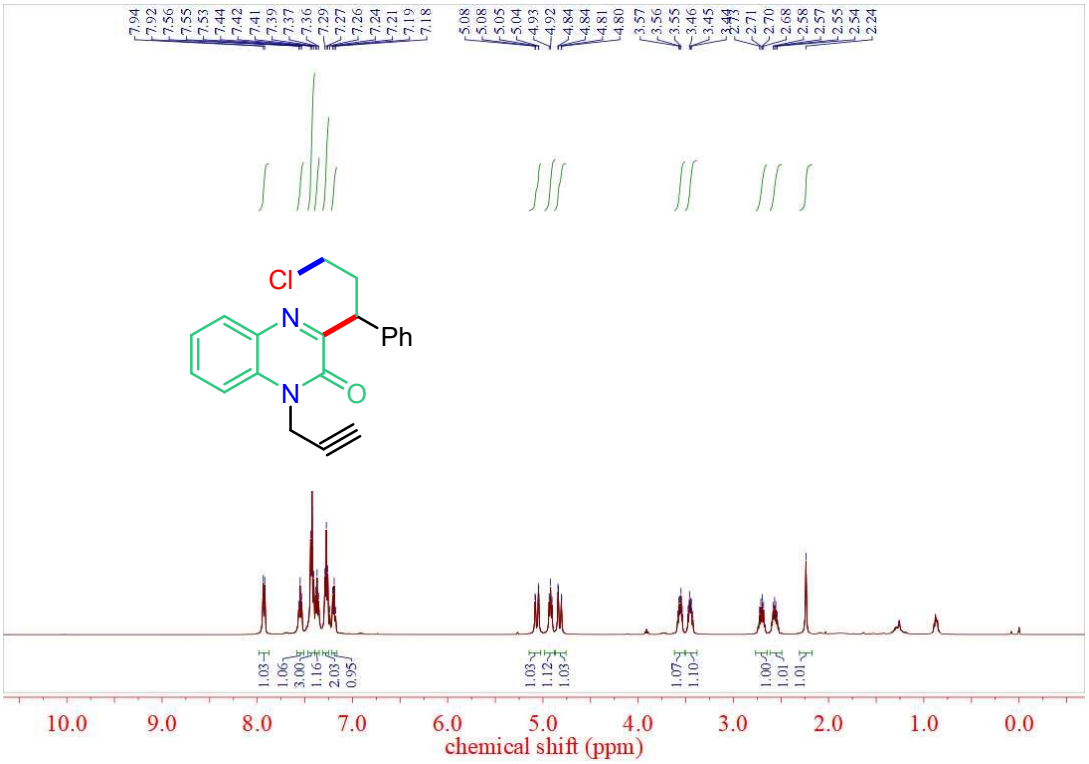
^{13}C NMR (126 MHz, $CDCl_3$) of compound **3c**



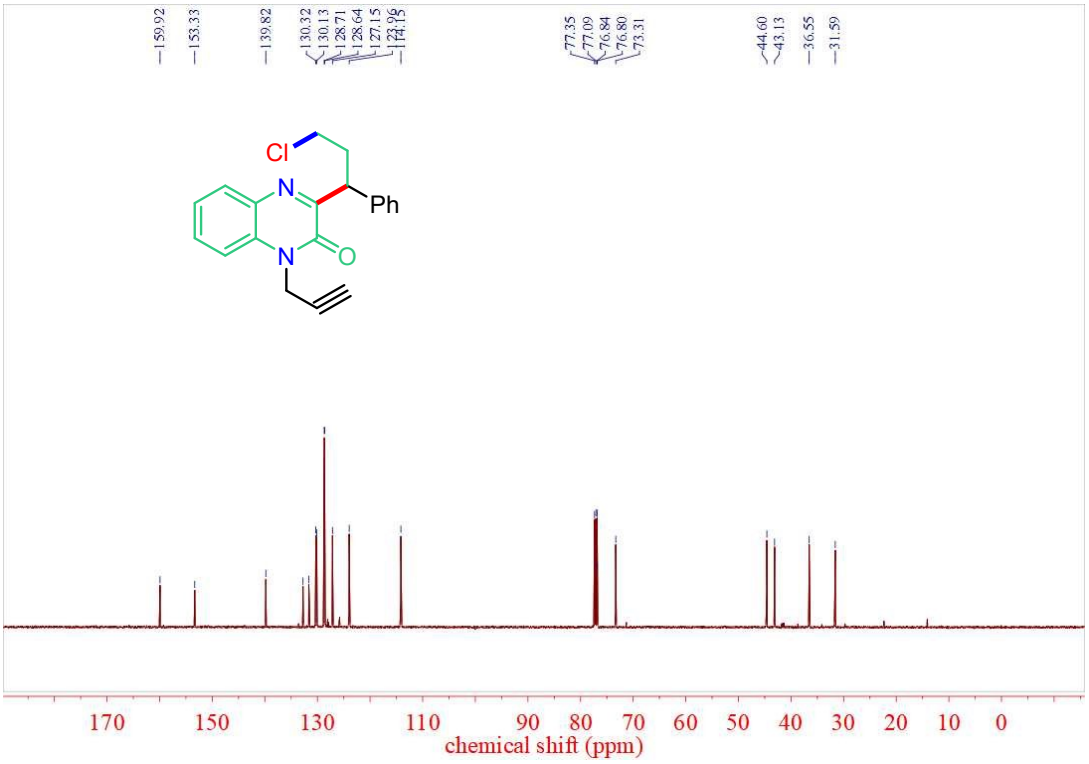
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3d**



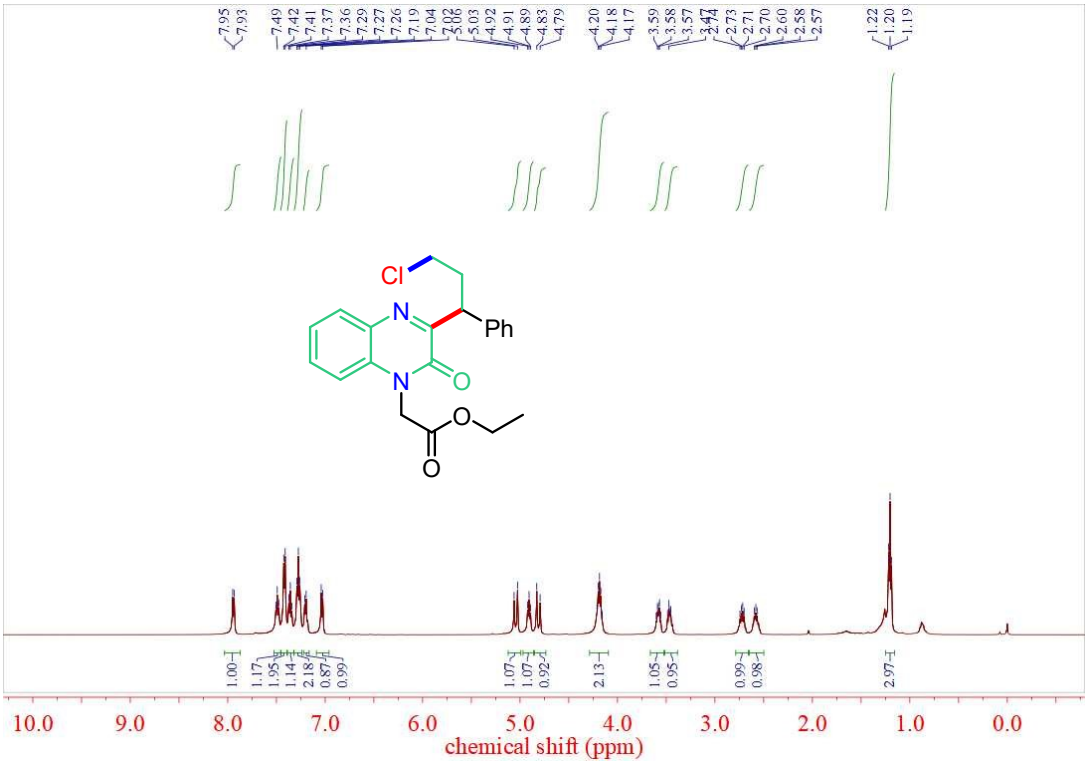
^{13}C NMR (126 MHz, $CDCl_3$) of compound **3d**



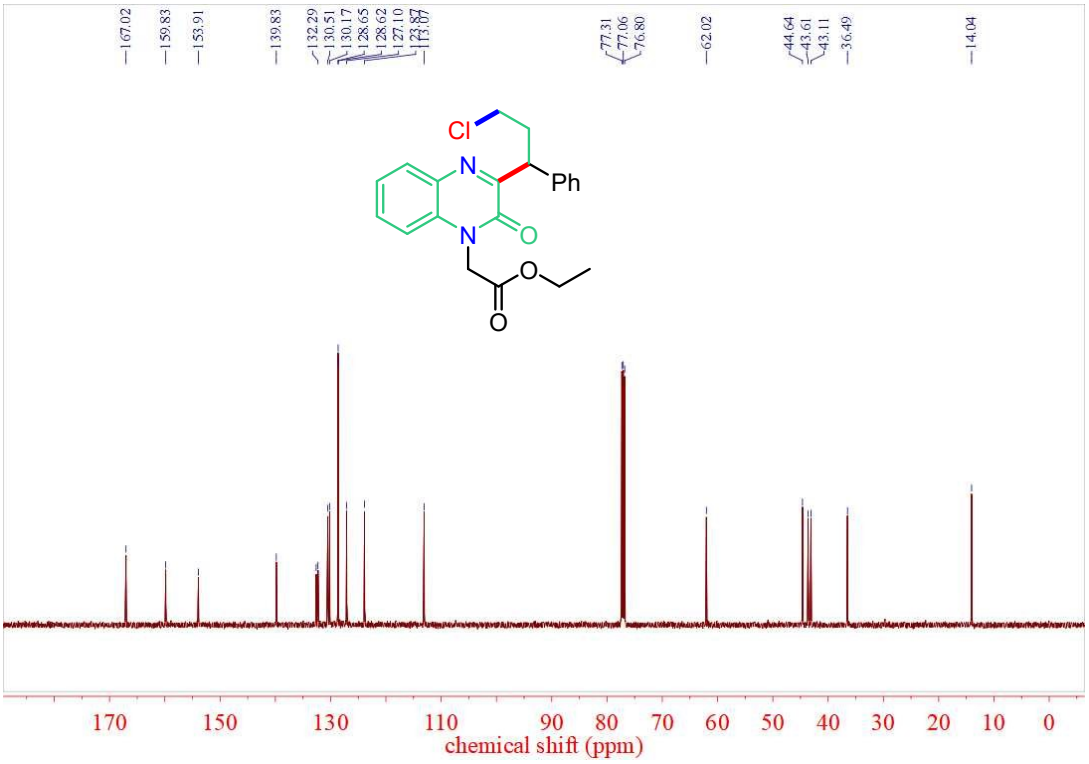
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3e**



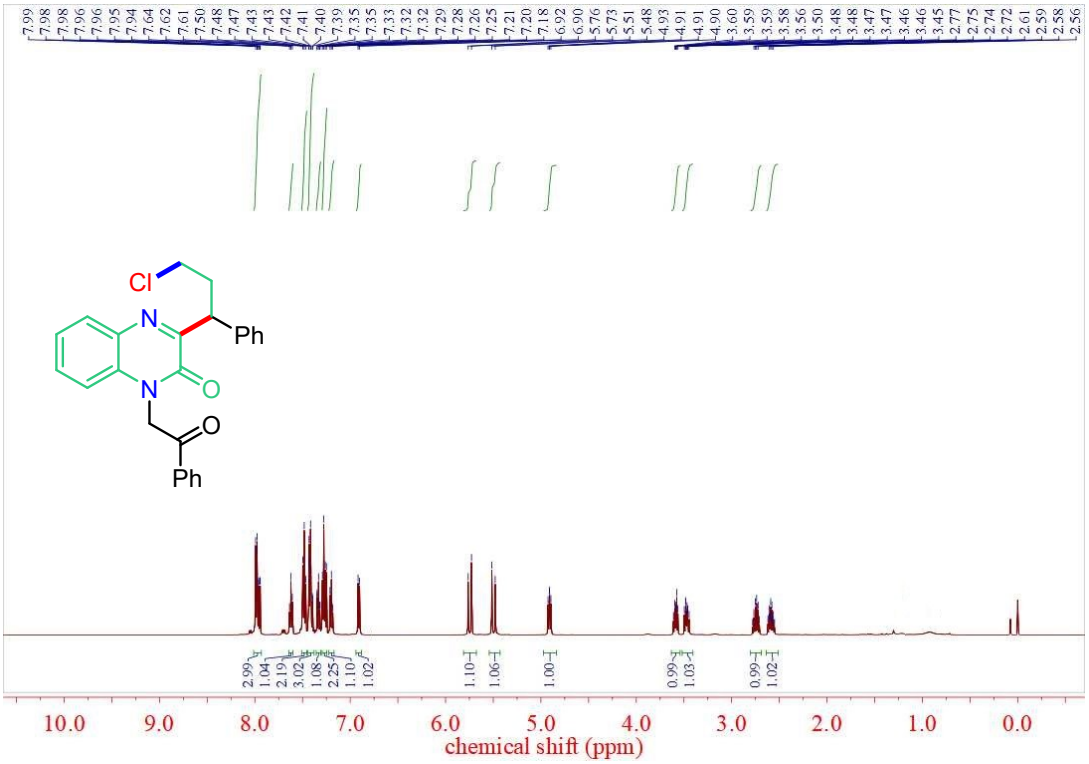
^{13}C NMR (126 MHz, $CDCl_3$) of compound **3e**



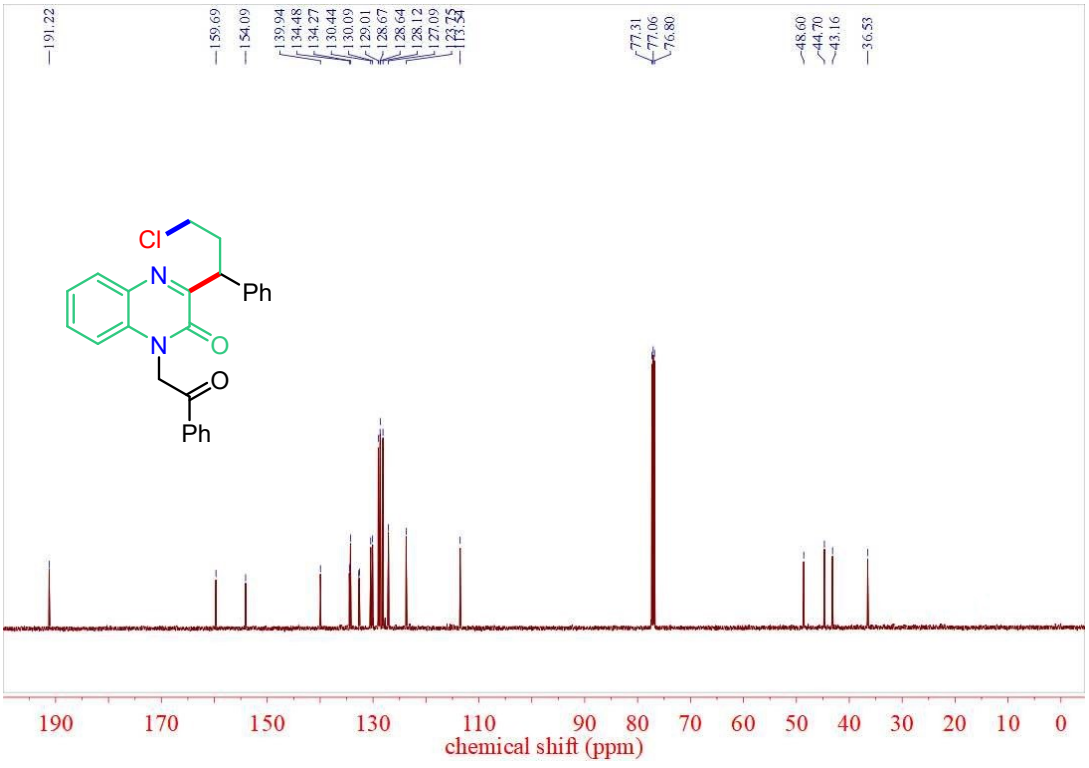
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3f**



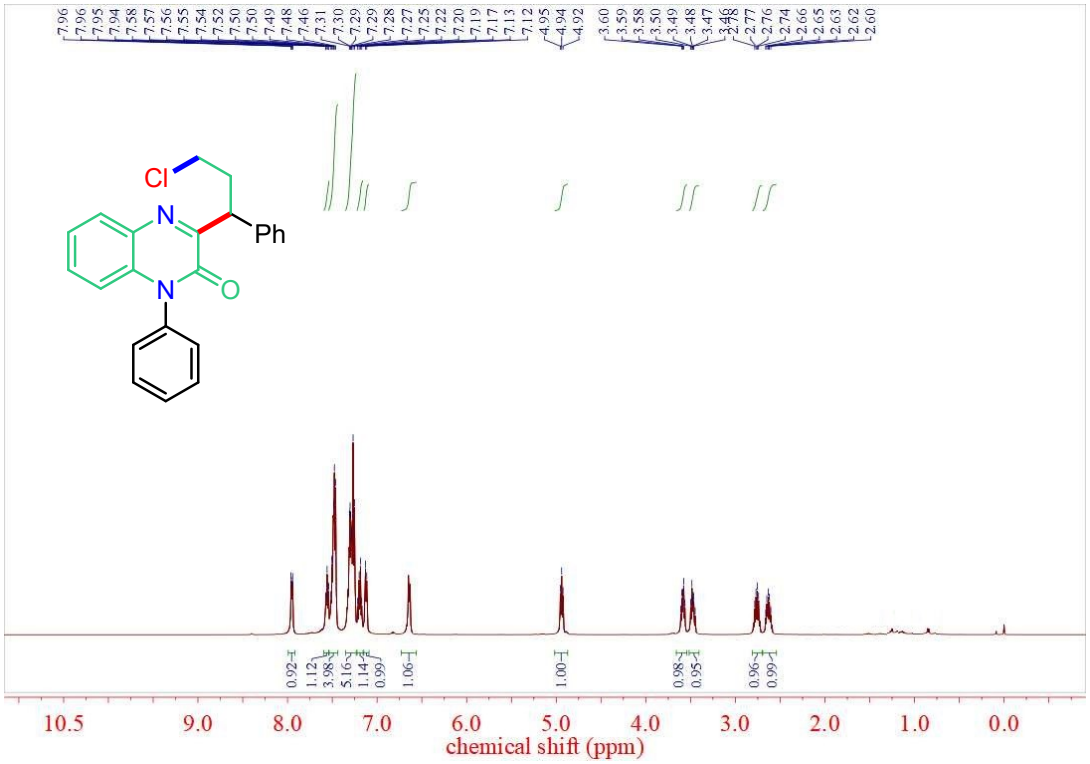
^{13}C NMR (126 MHz, $CDCl_3$) of compound **3f**



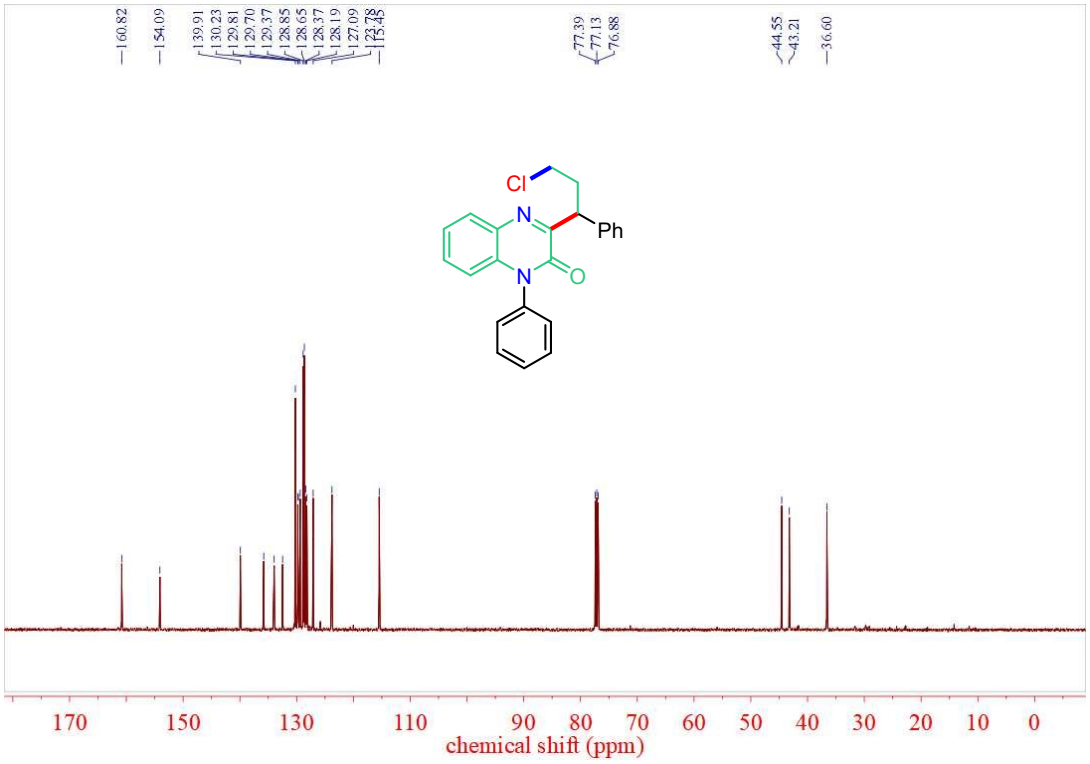
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3g**



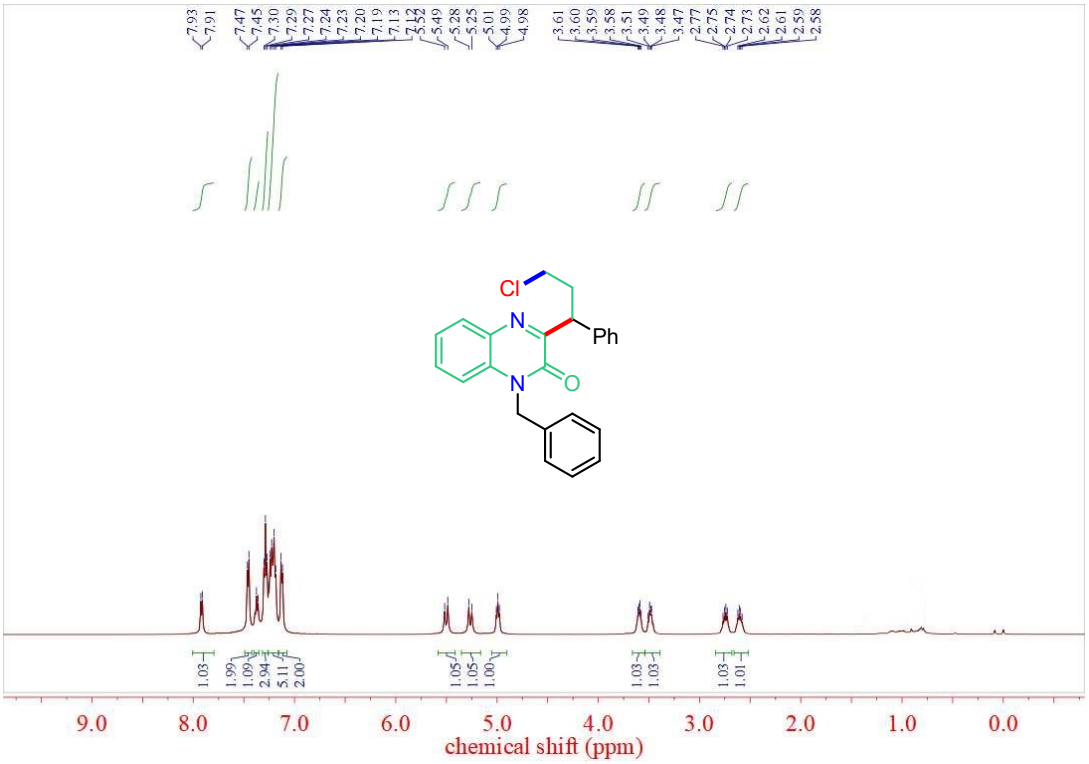
^{13}C NMR (126 MHz, $CDCl_3$) of compound **3g**



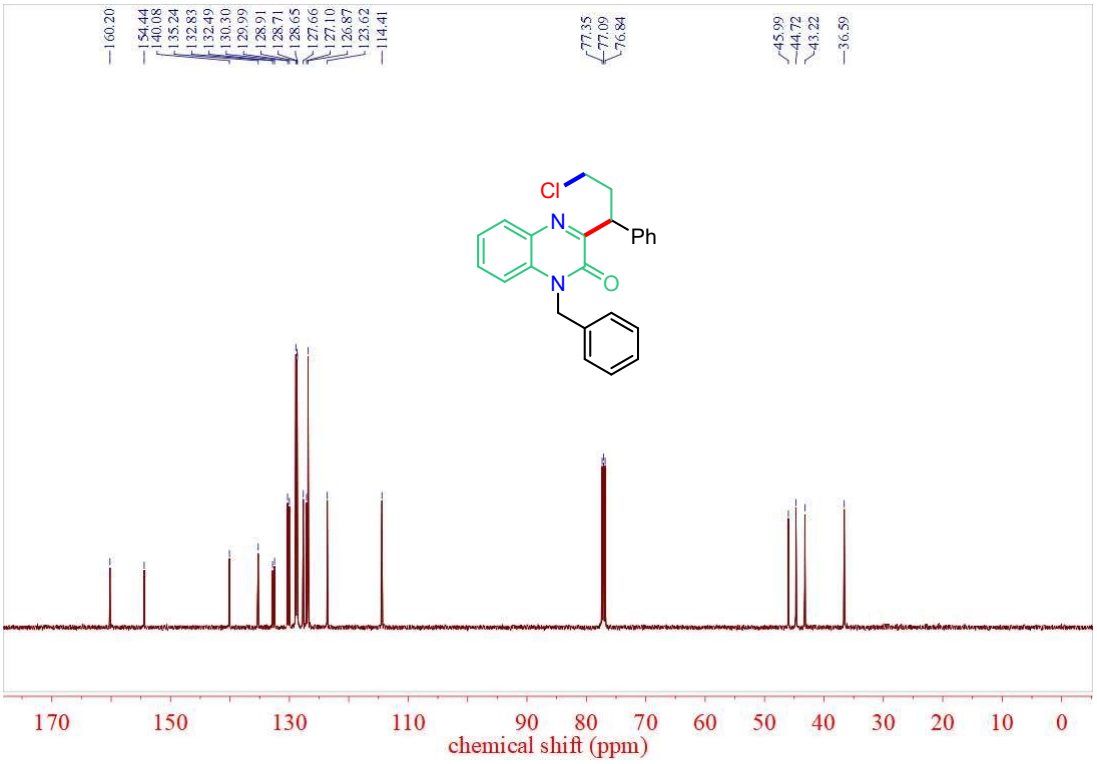
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3h**



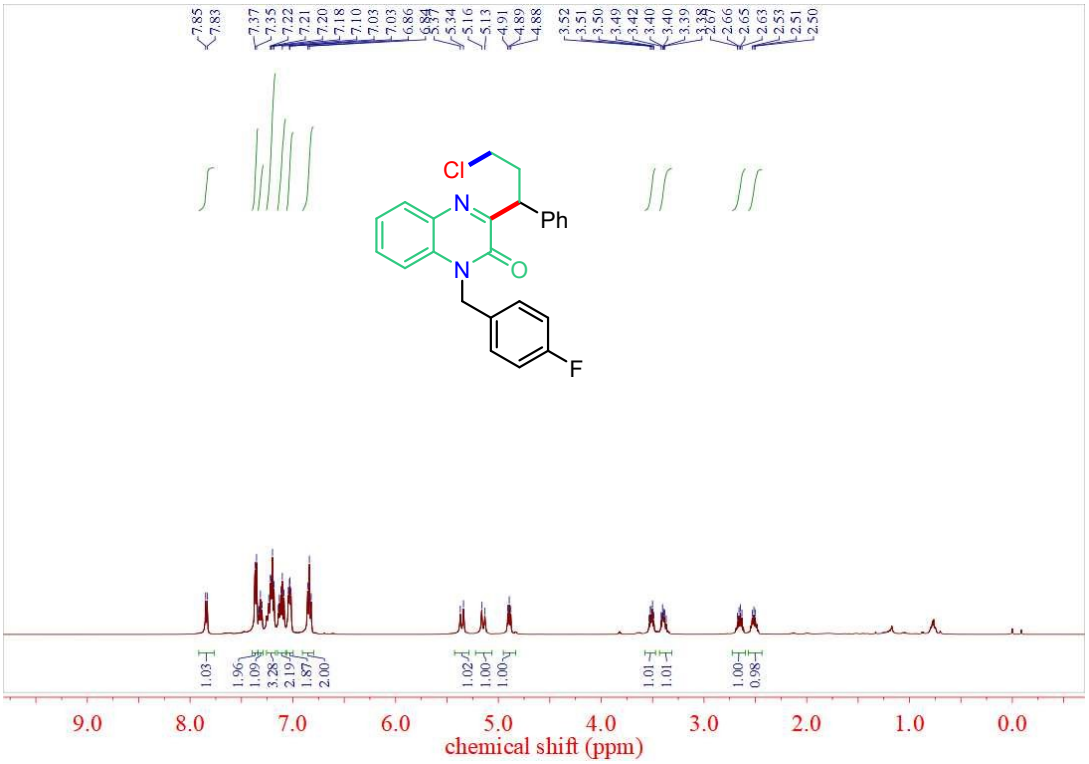
^{13}C NMR (126 MHz, $CDCl_3$) of compound **3h**



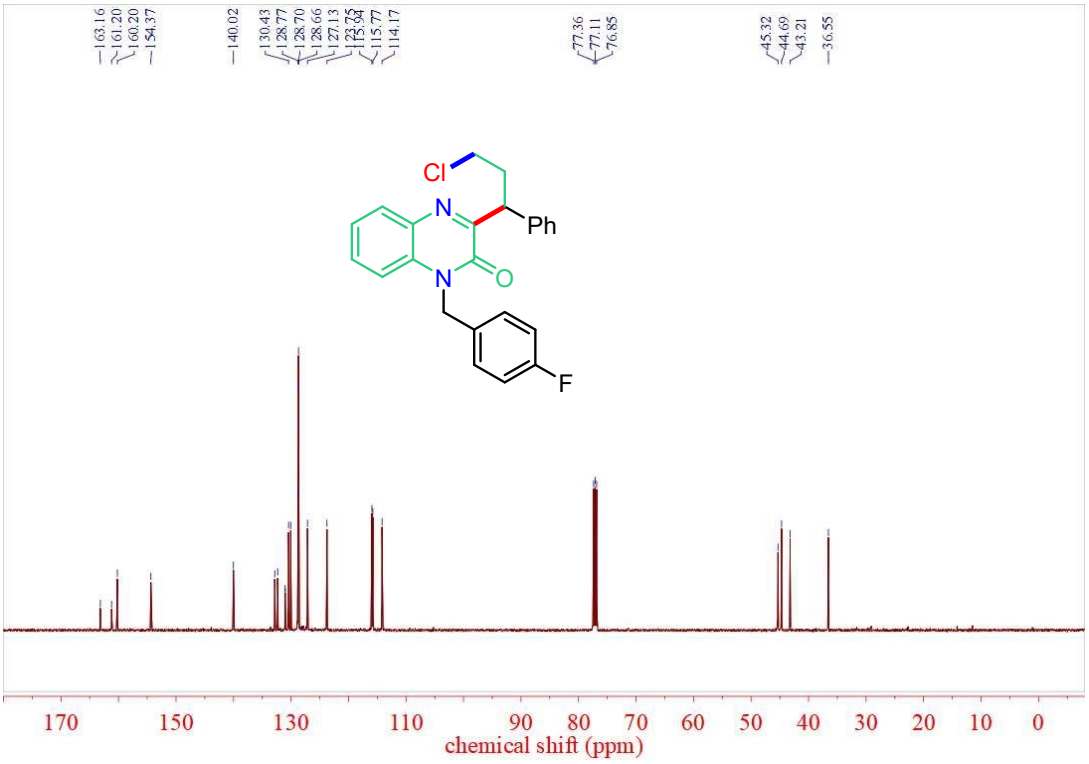
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3i**



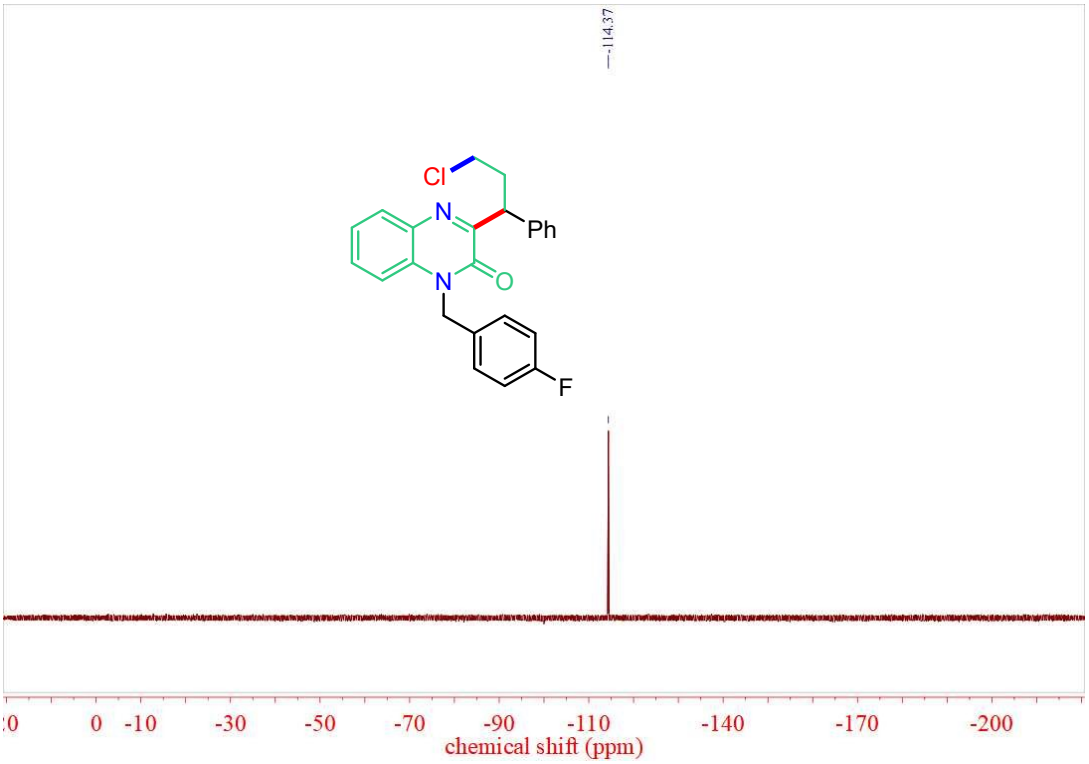
^{13}C NMR (126 MHz, $CDCl_3$) of compound **3i**



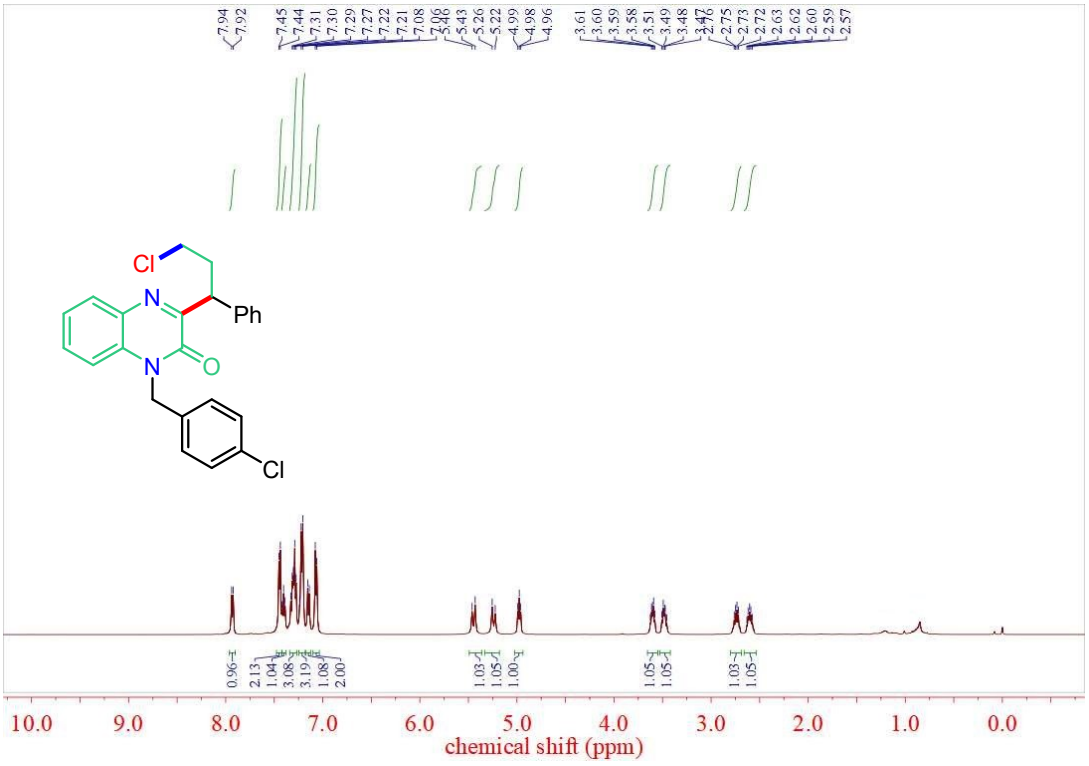
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3j**



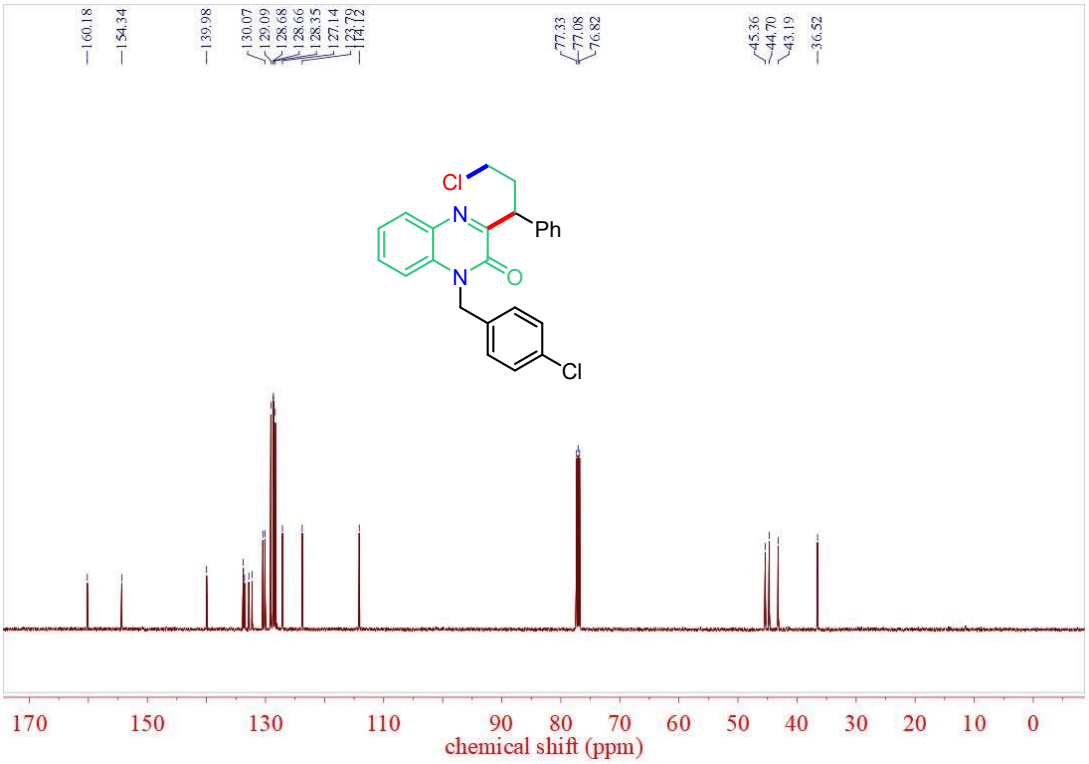
^{13}C NMR (126 MHz, $CDCl_3$) of compound **3j**



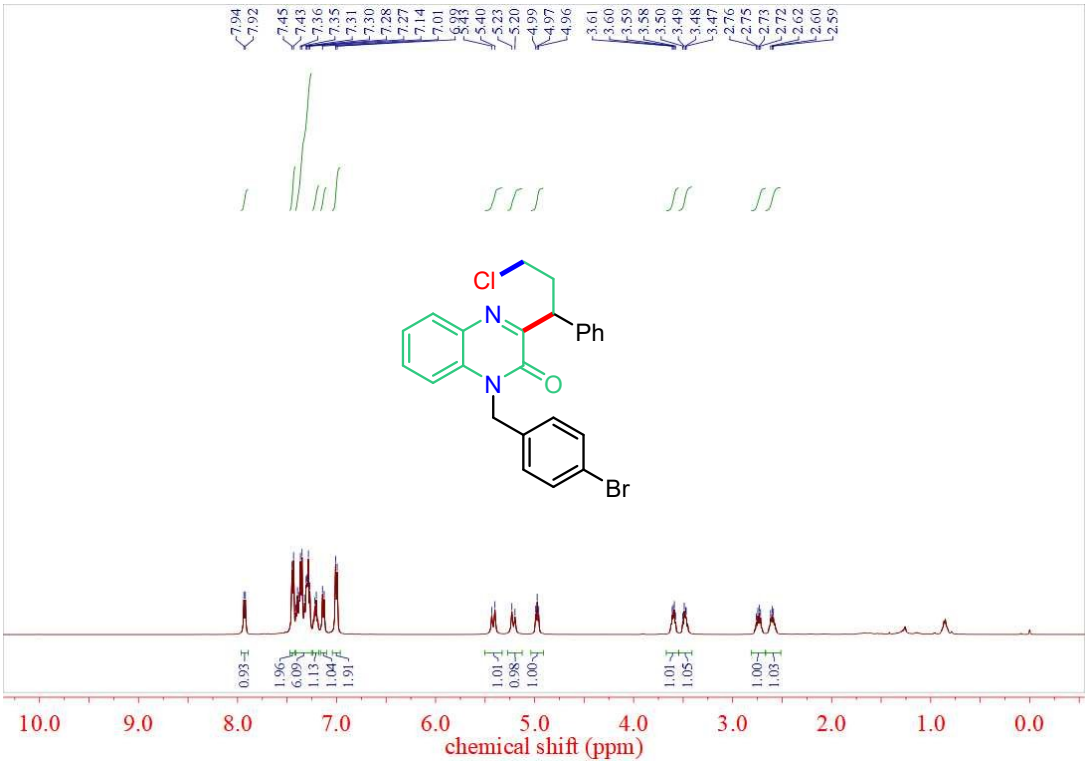
^{19}F NMR (471 MHz, $CDCl_3$) of compound **3j**



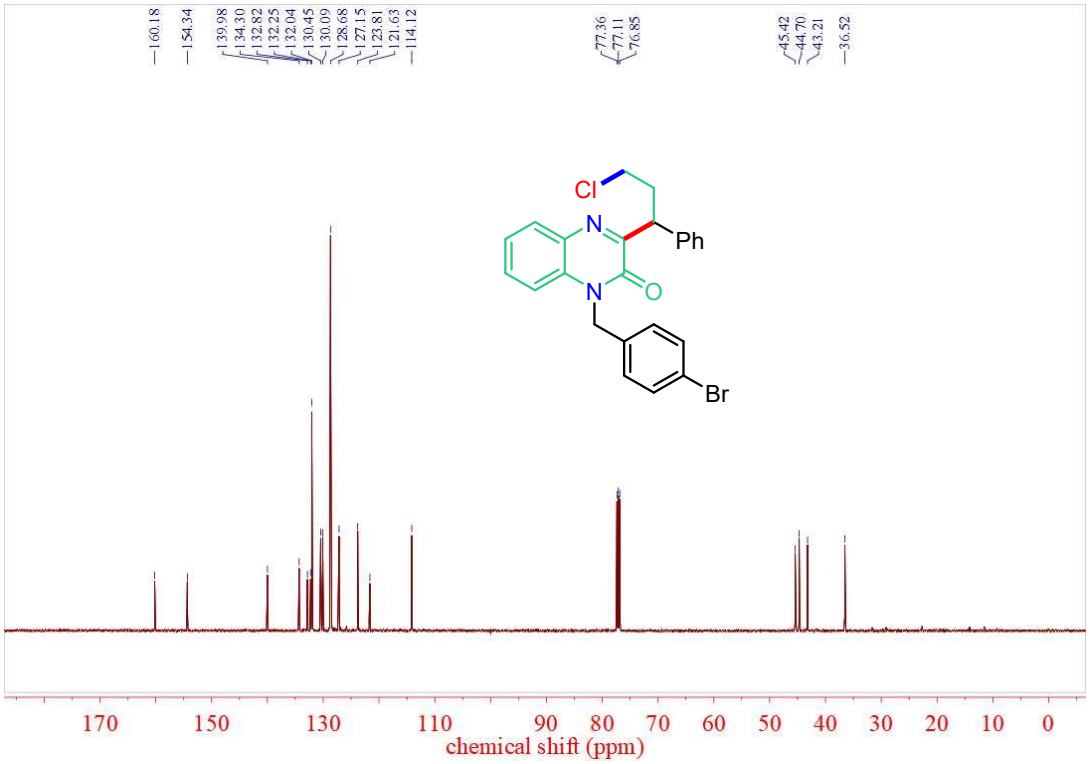
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3k**



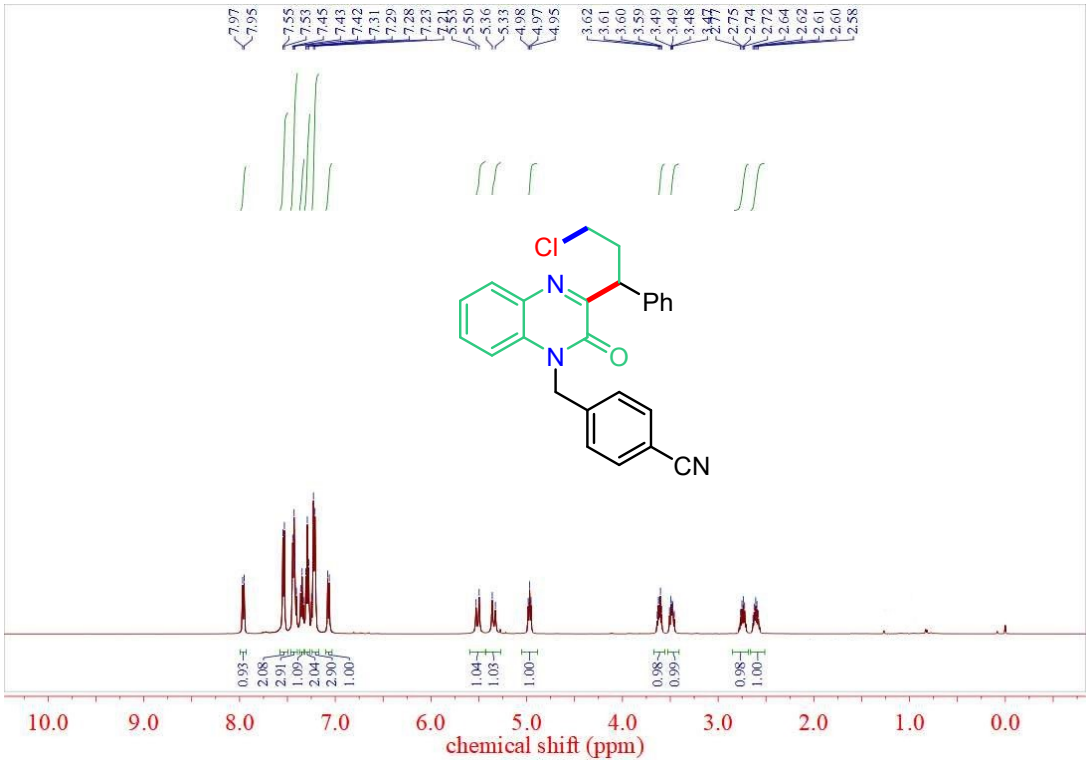
^{13}C NMR (126 MHz, $CDCl_3$) of compound **3k**



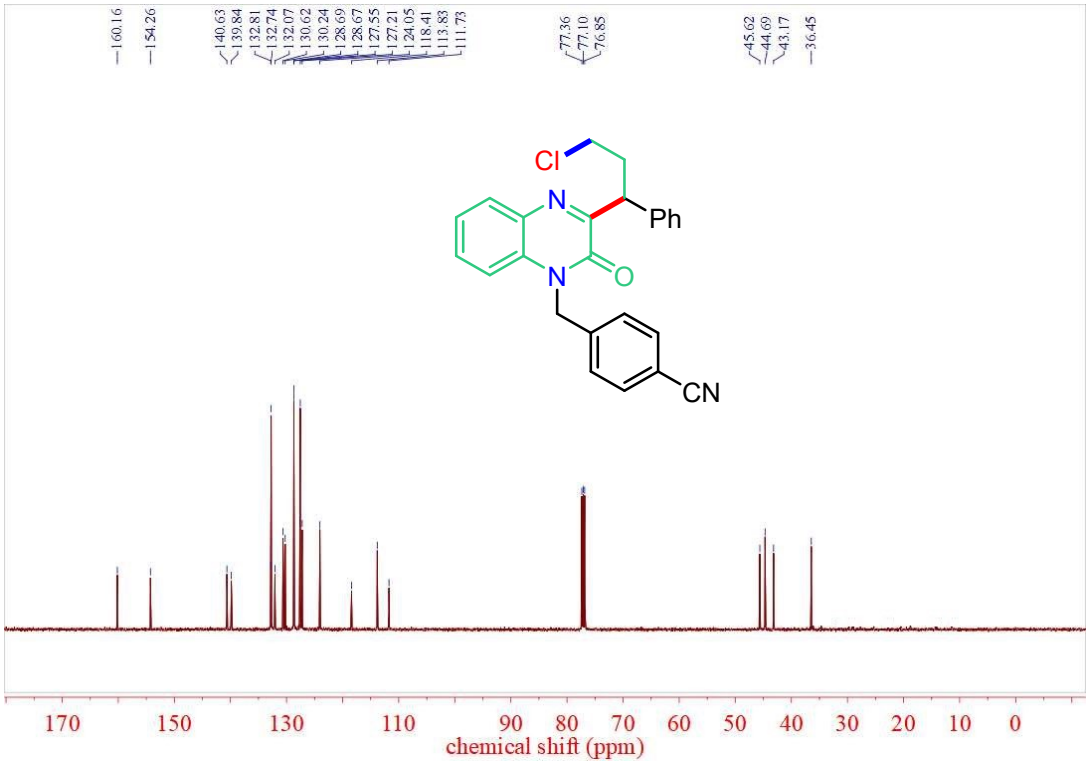
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3l**



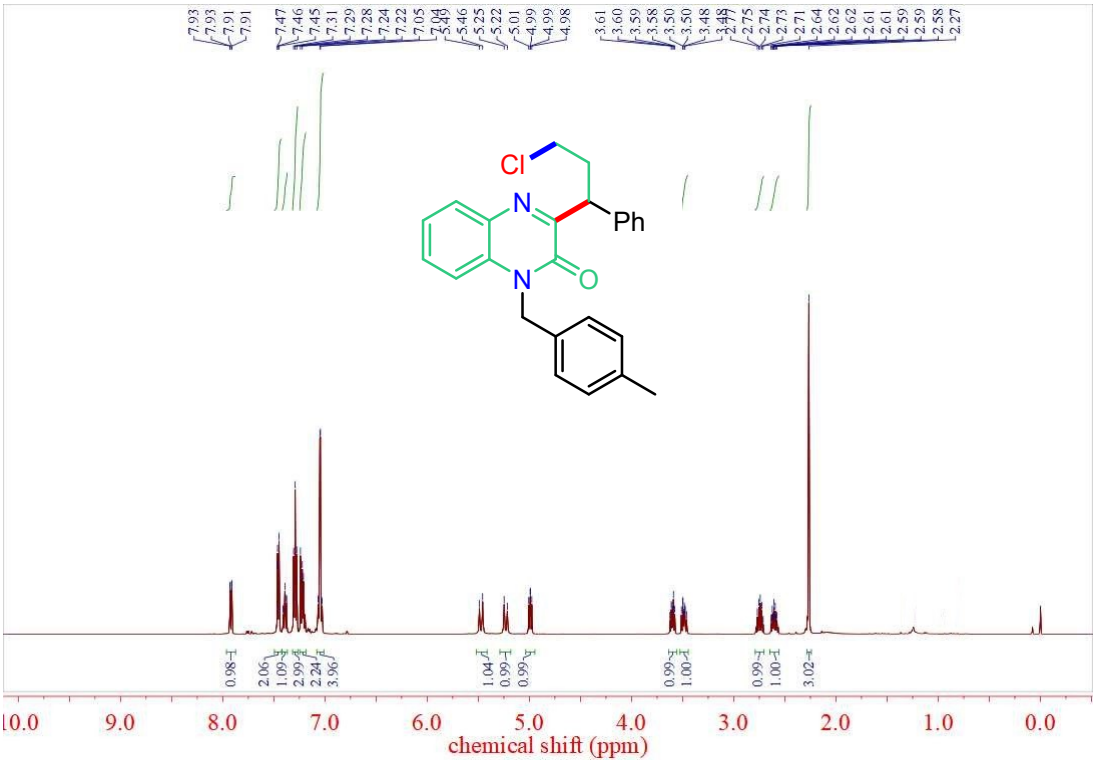
^{13}C NMR (126 MHz, $CDCl_3$) of compound **3l**



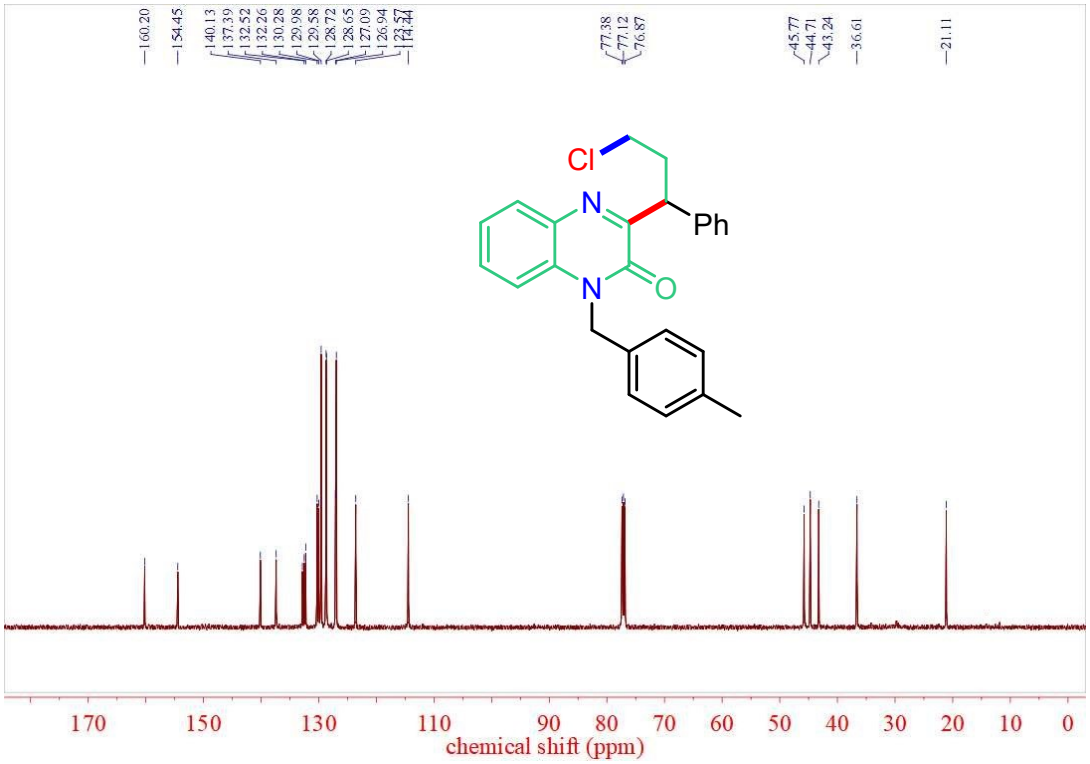
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3m**



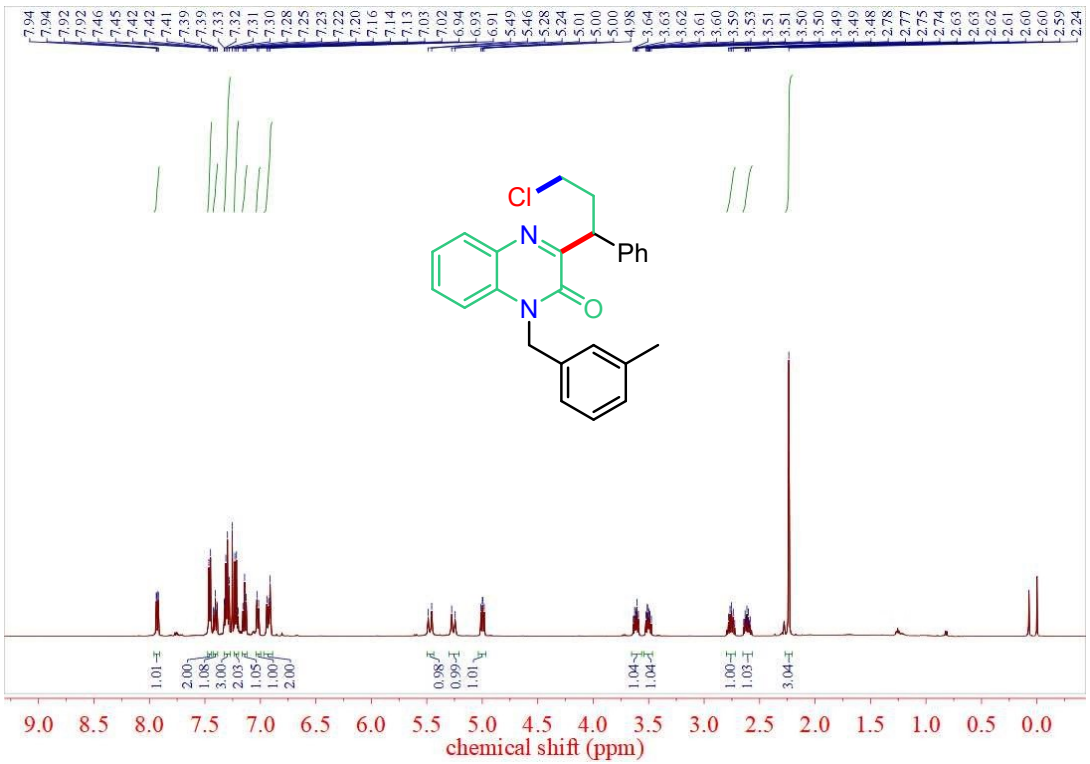
^{13}C NMR (126 MHz, $CDCl_3$) of compound **3m**



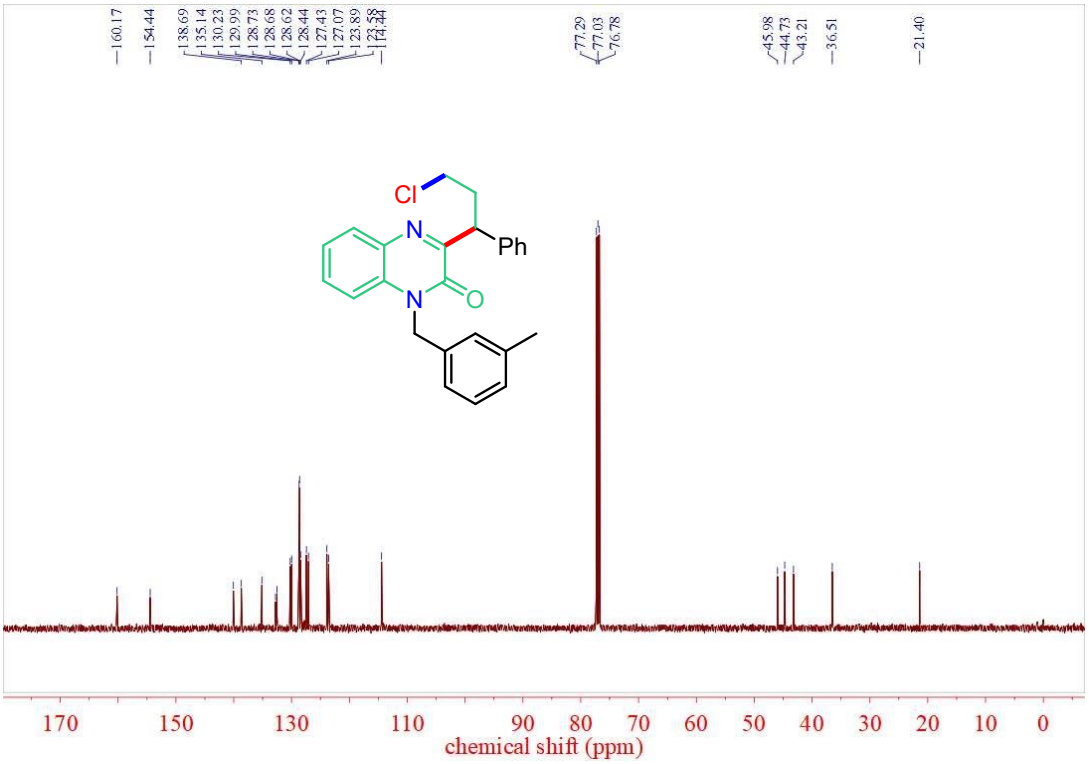
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3n**



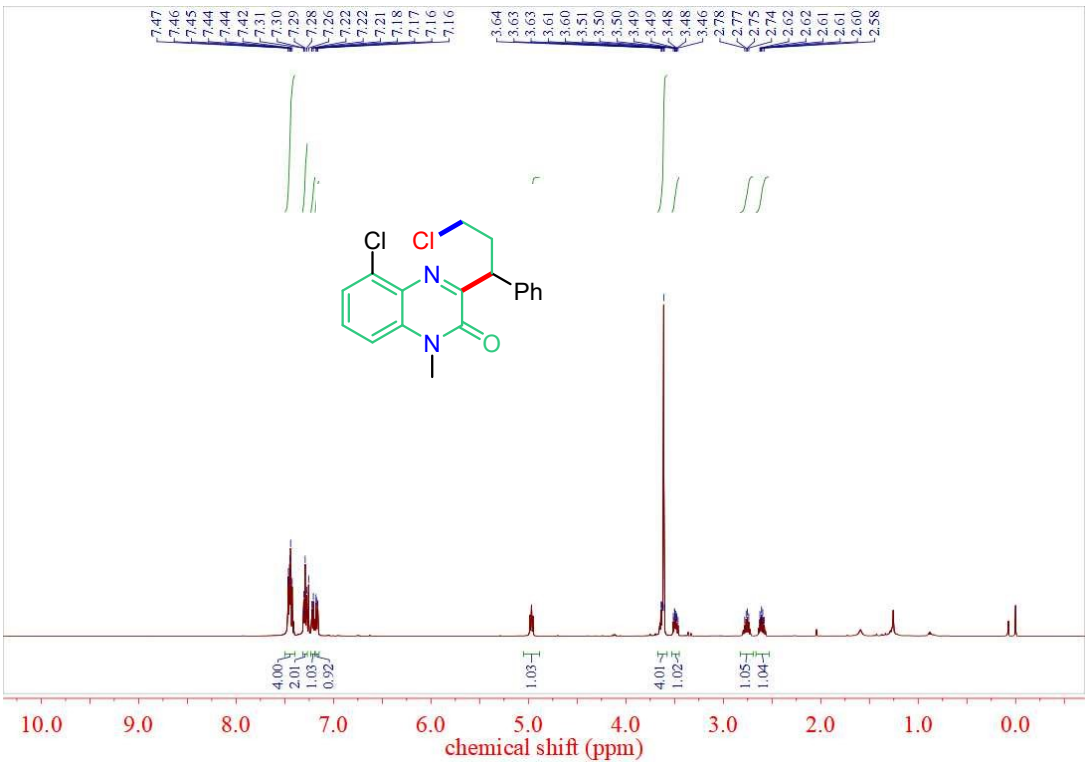
^{13}C NMR (126 MHz, $CDCl_3$) of compound **3n**



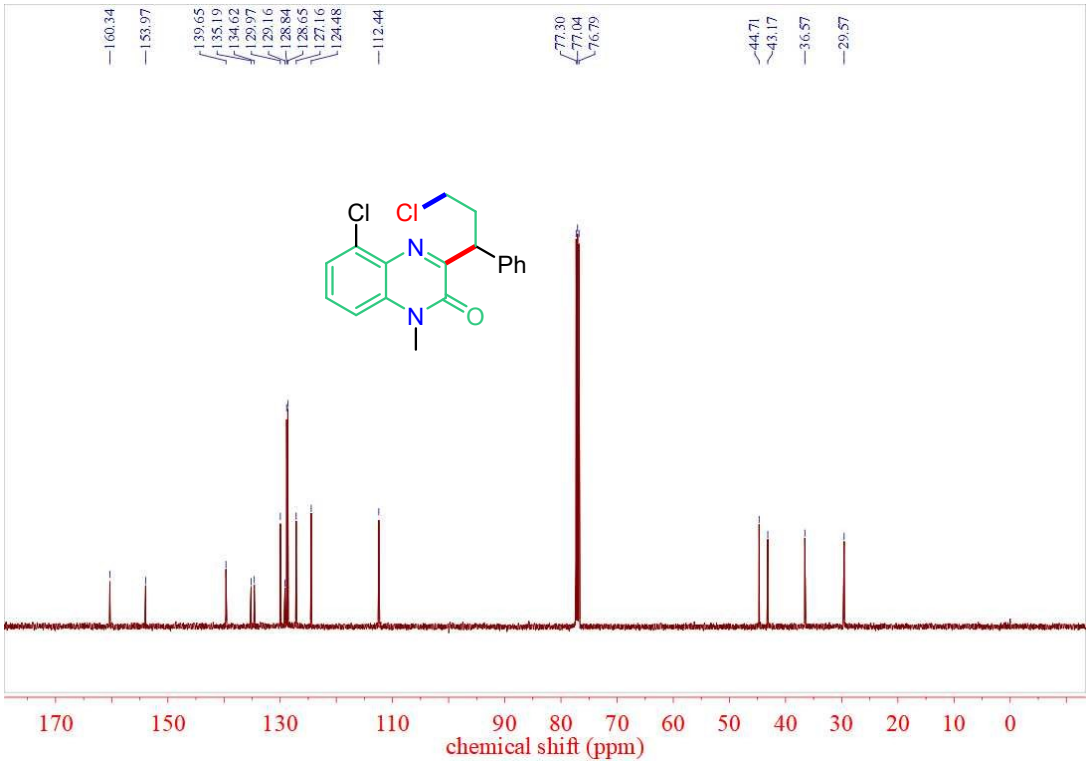
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3o**



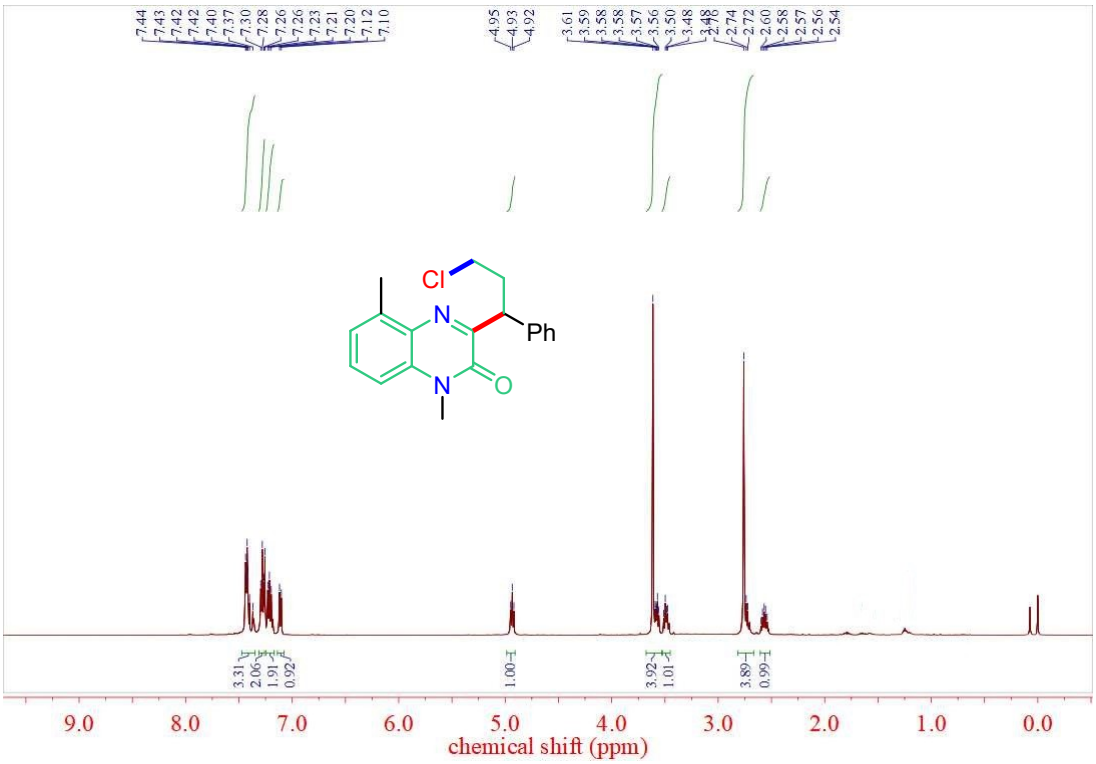
^{13}C NMR (126 MHz, $CDCl_3$) of compound **3o**



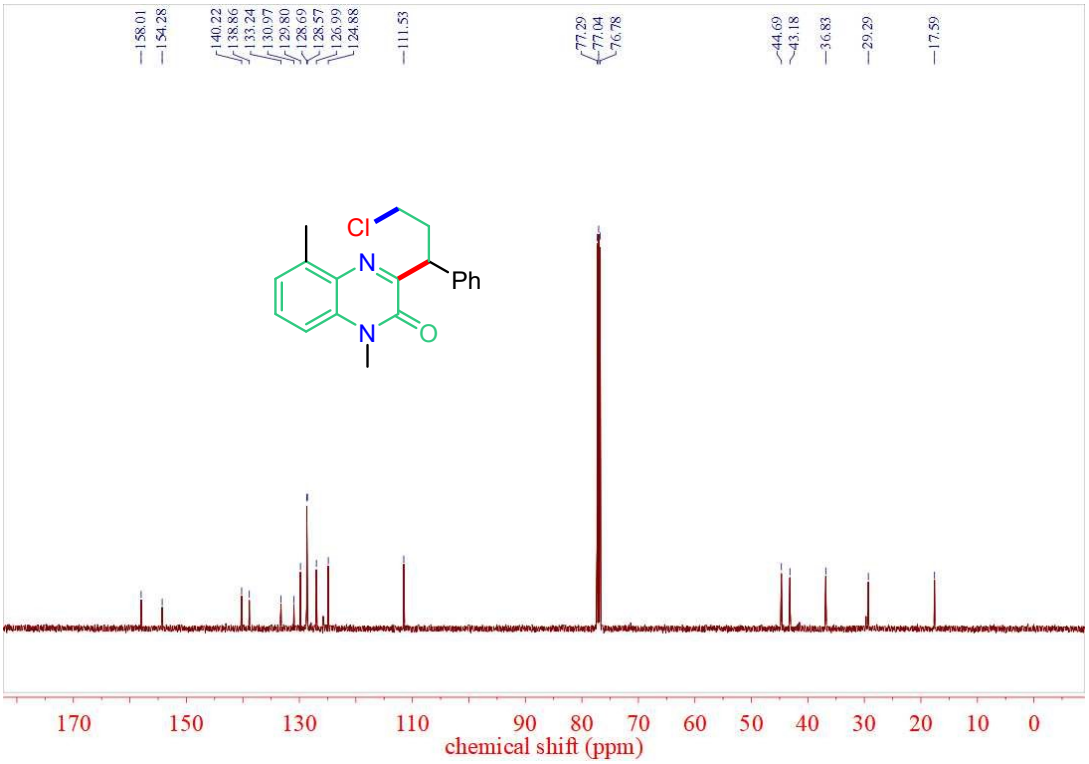
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3p**



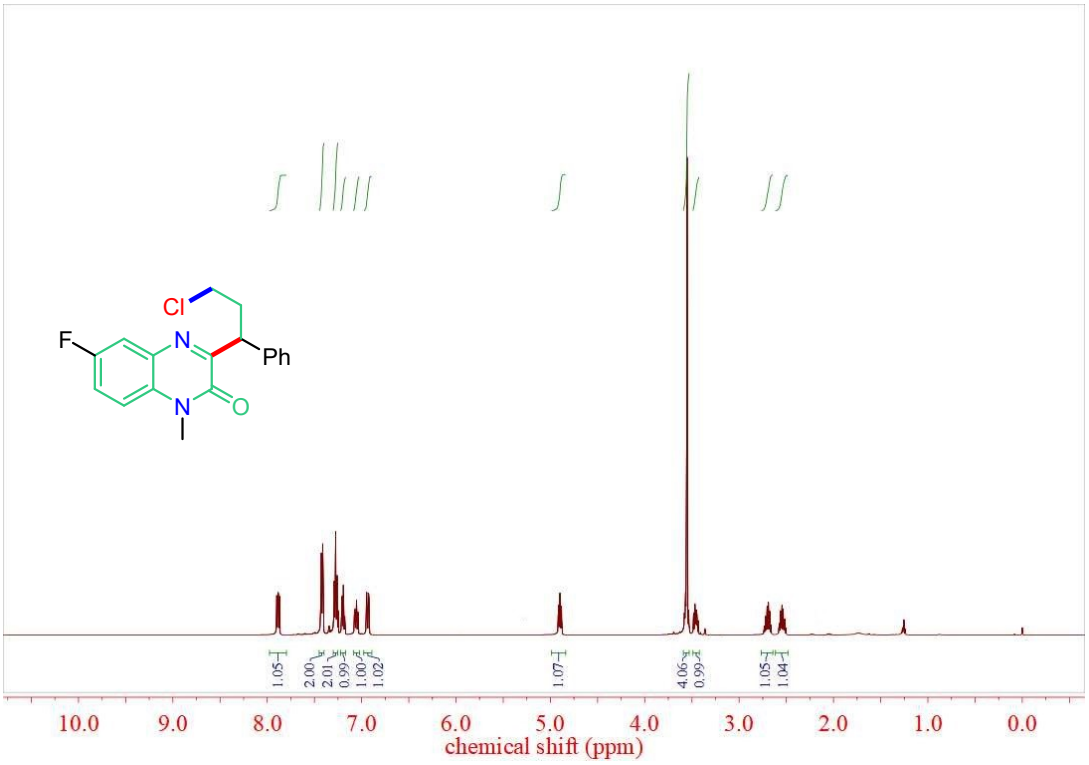
^{13}C NMR (126 MHz, $CDCl_3$) of compound **3p**



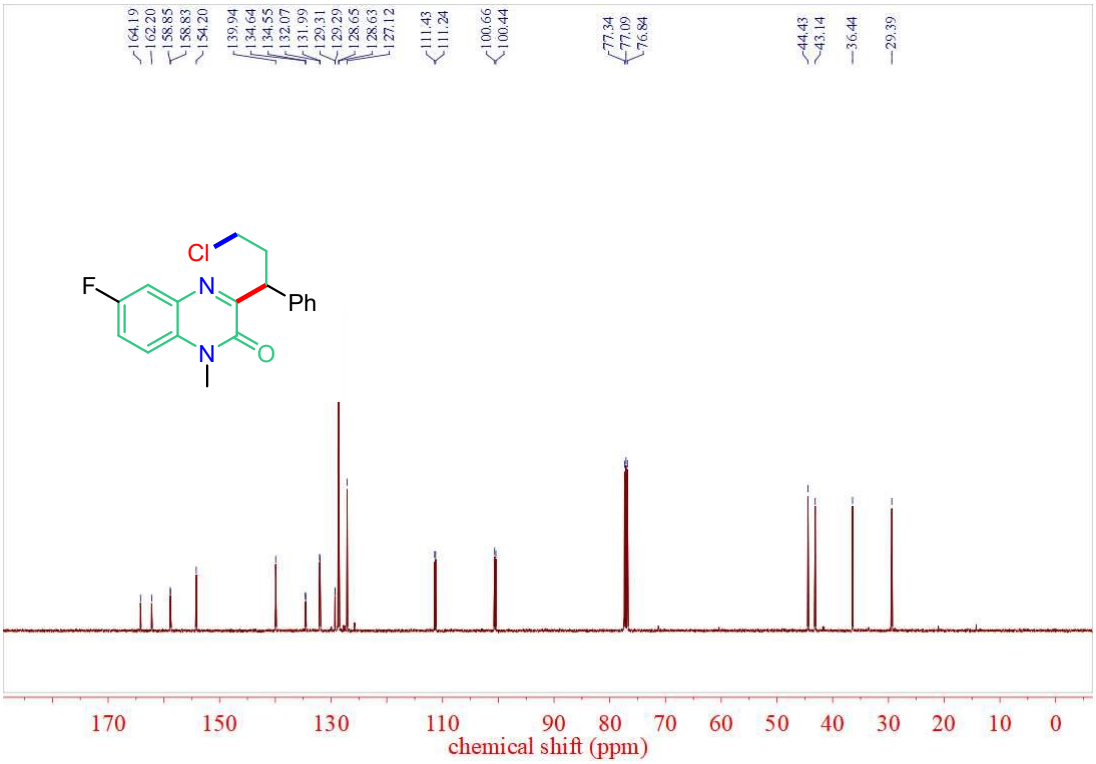
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3q**



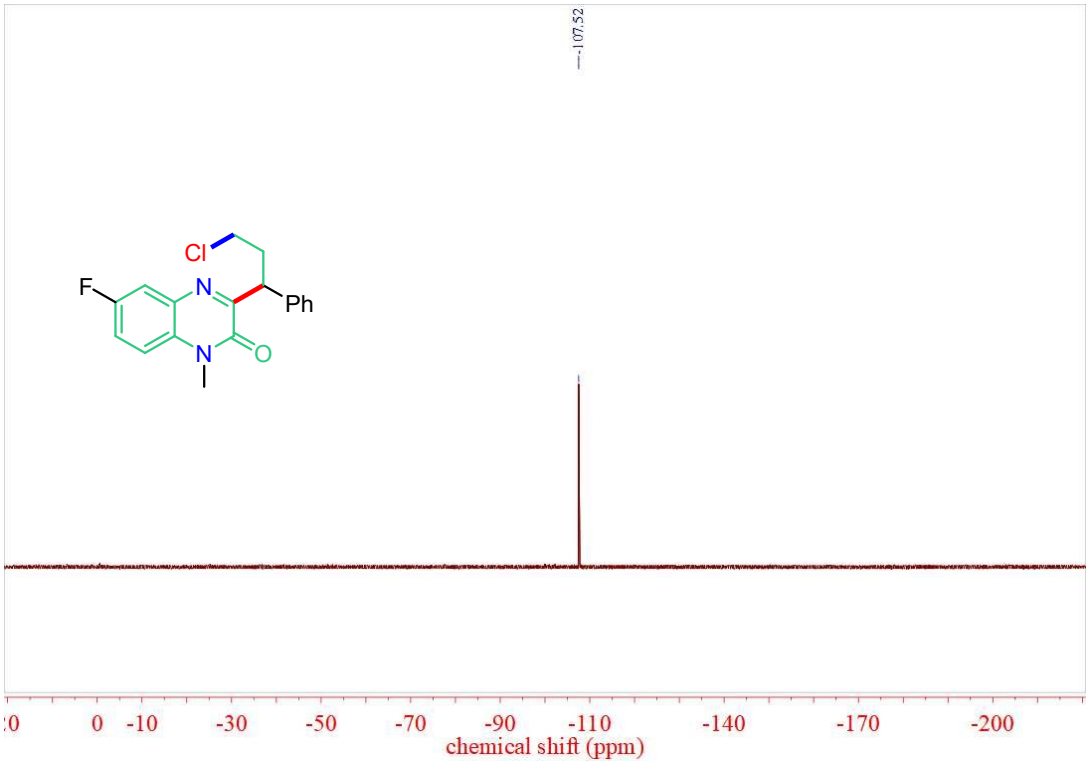
^{13}C NMR (126 MHz, $CDCl_3$) of compound **3p**



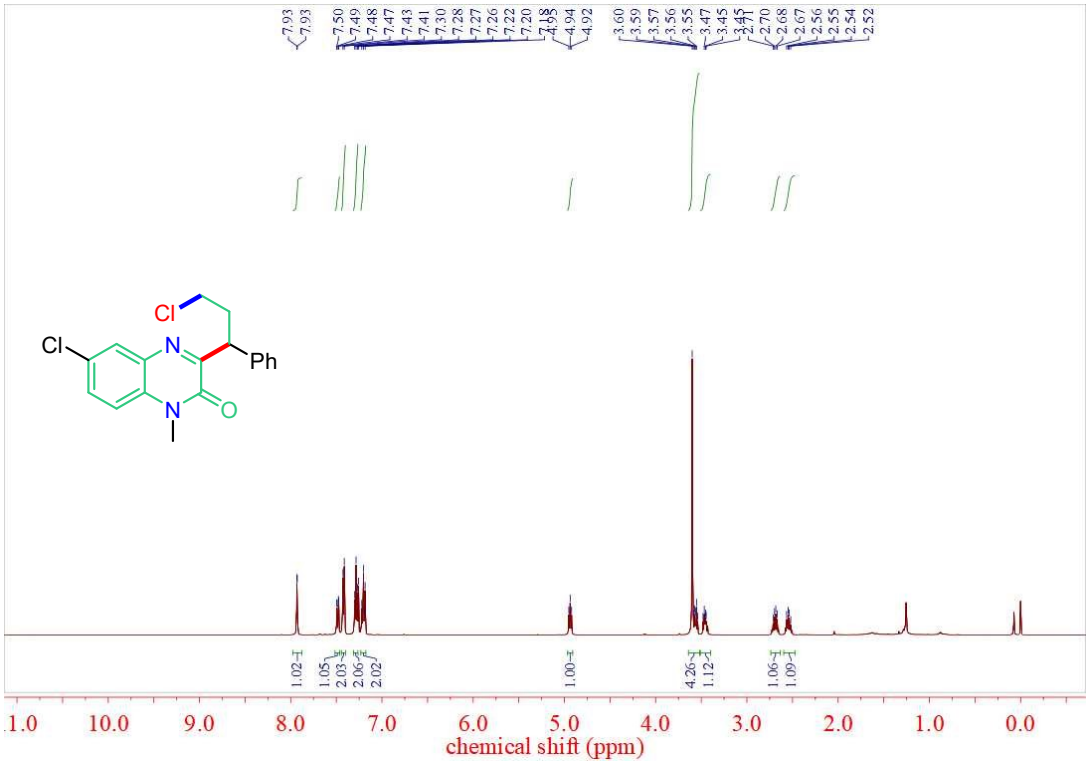
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3r**



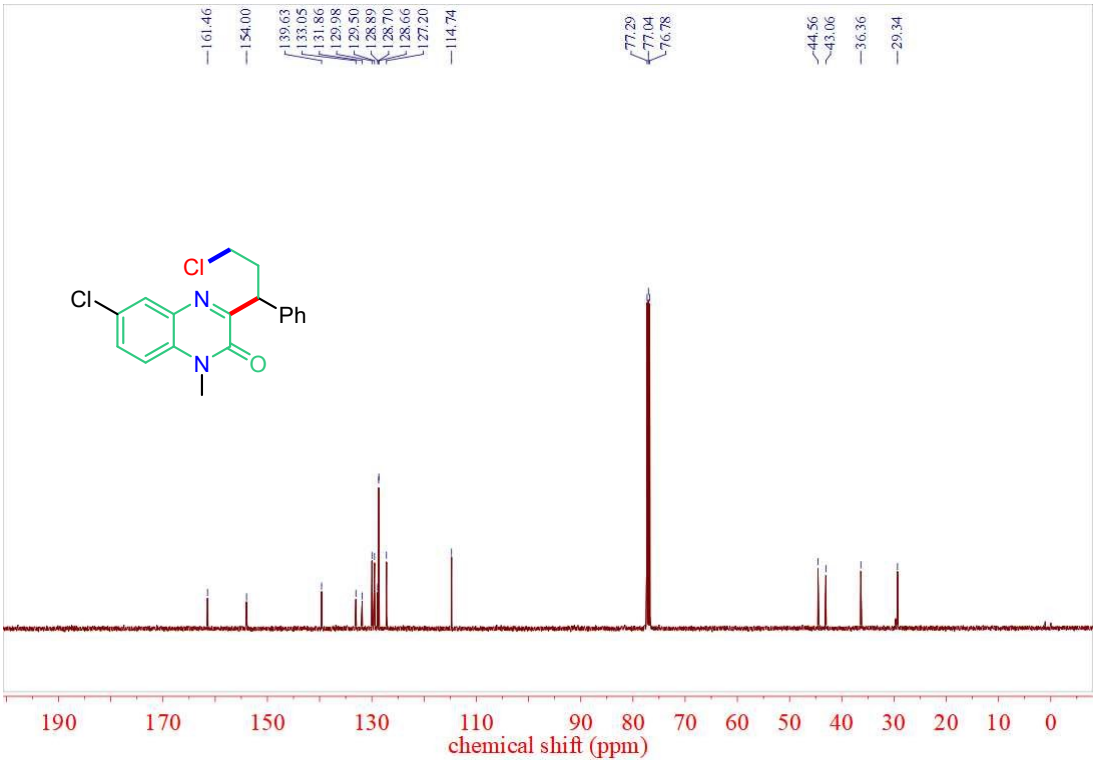
^{13}C NMR (126 MHz, $CDCl_3$) of compound **3r**



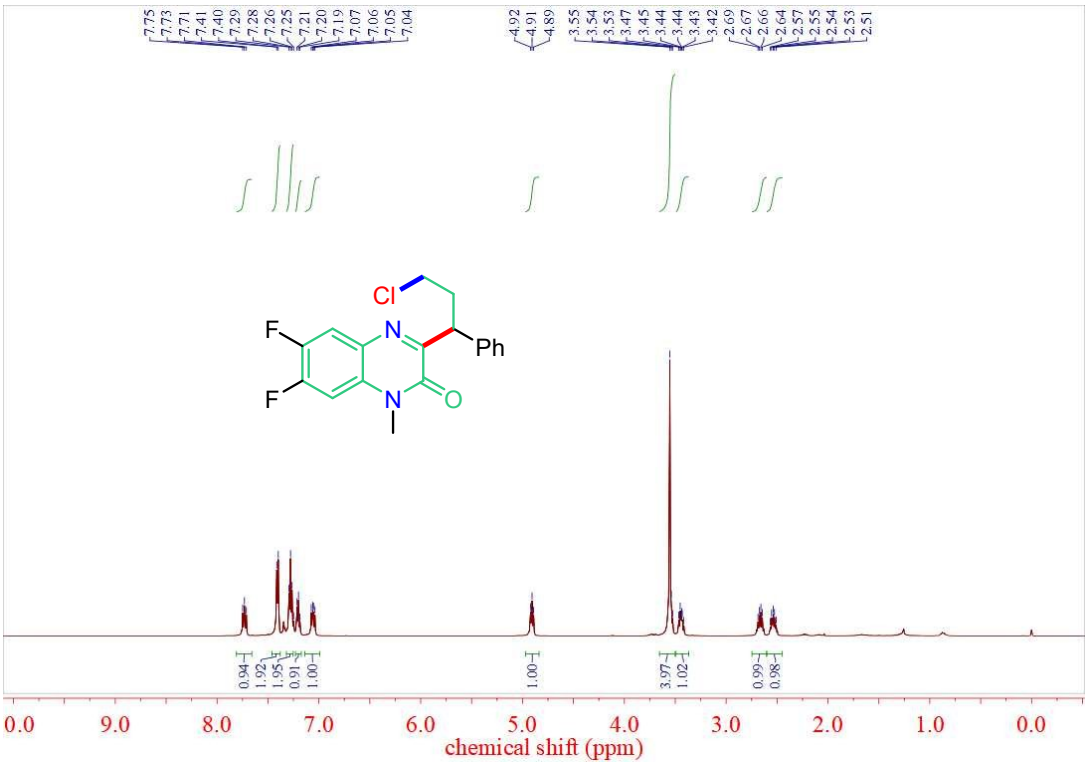
^{19}F NMR (471 MHz, $CDCl_3$) of compound **3r**



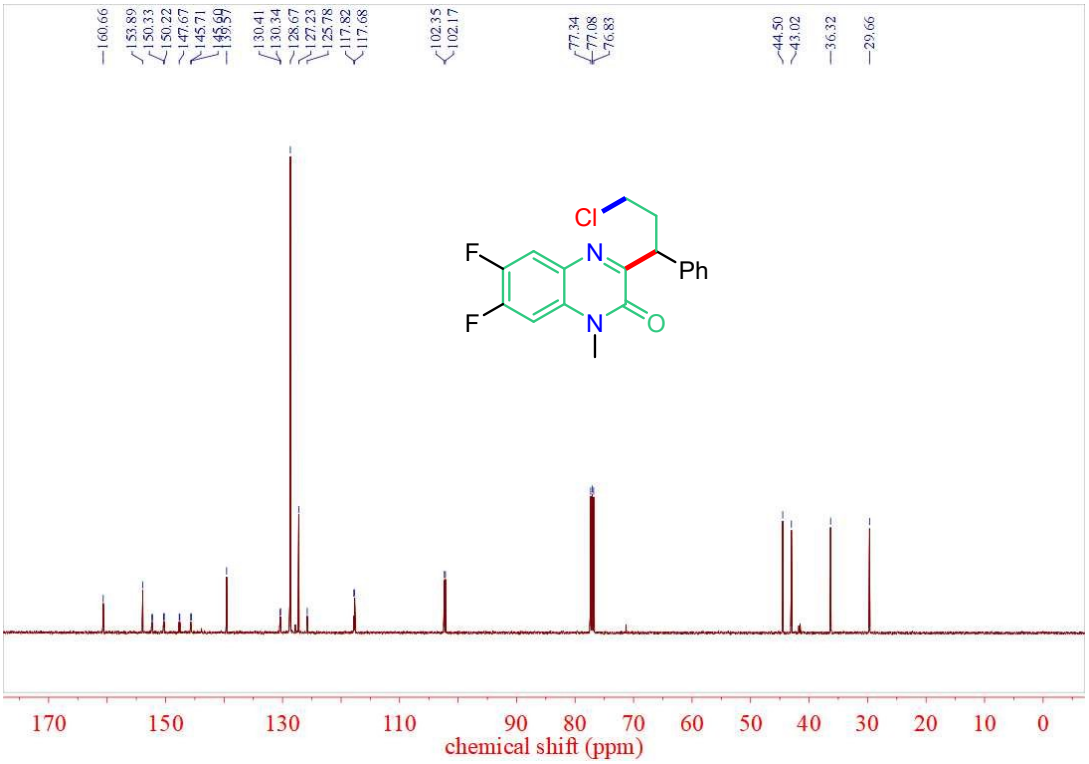
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3s**



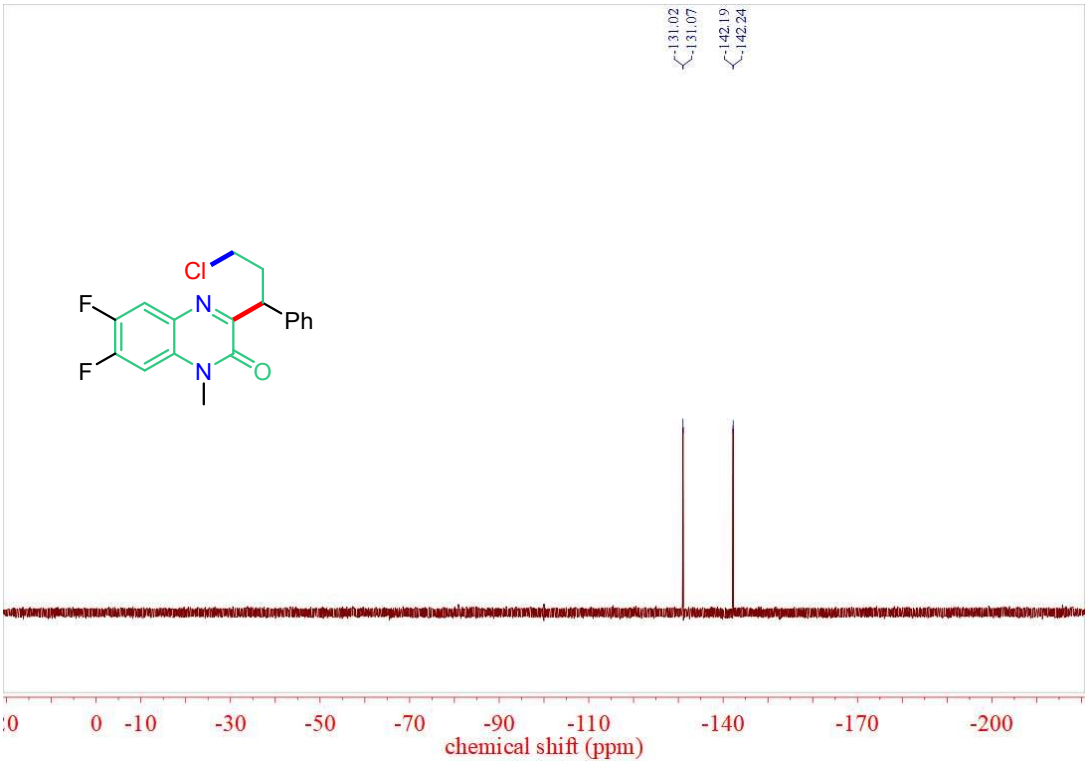
^{13}C NMR (126 MHz, $CDCl_3$) of compound **3s**



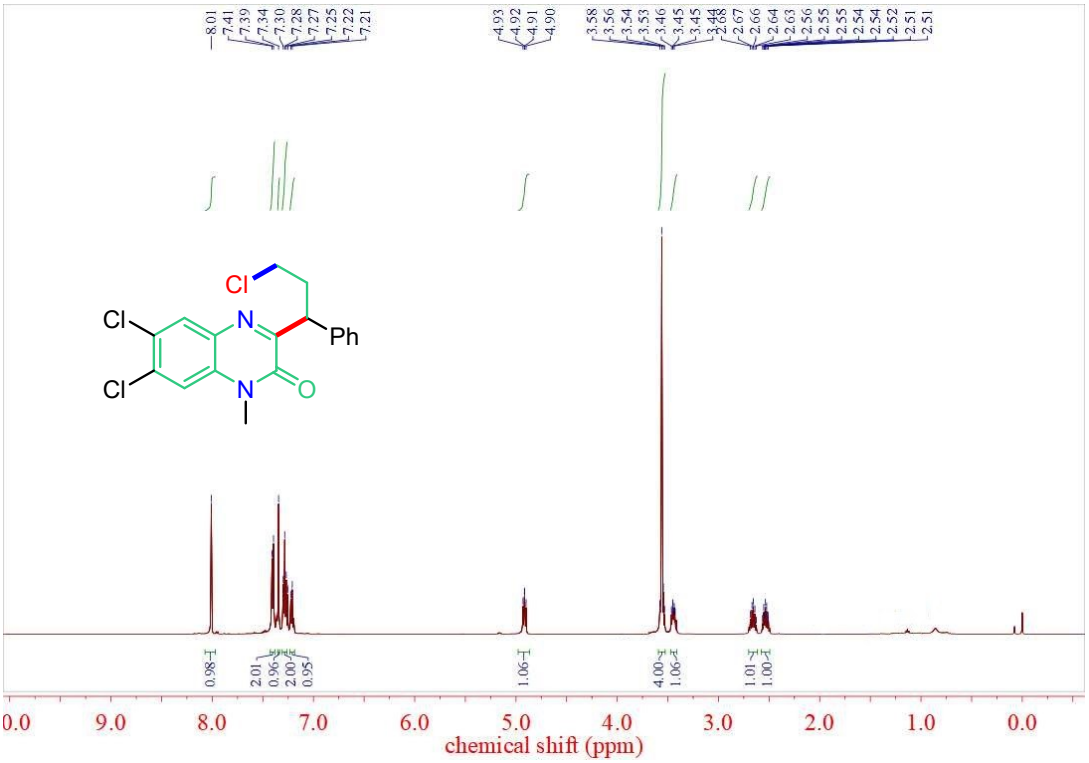
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3t**



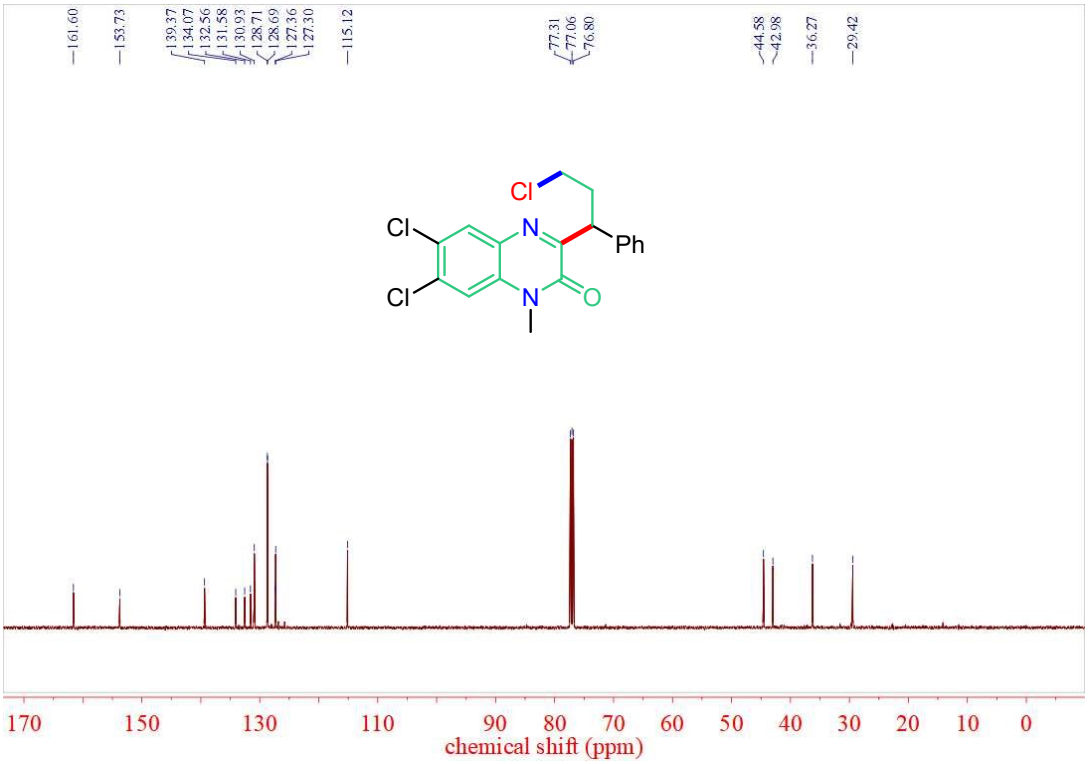
^{13}C NMR (126 MHz, $CDCl_3$) of compound **3t**



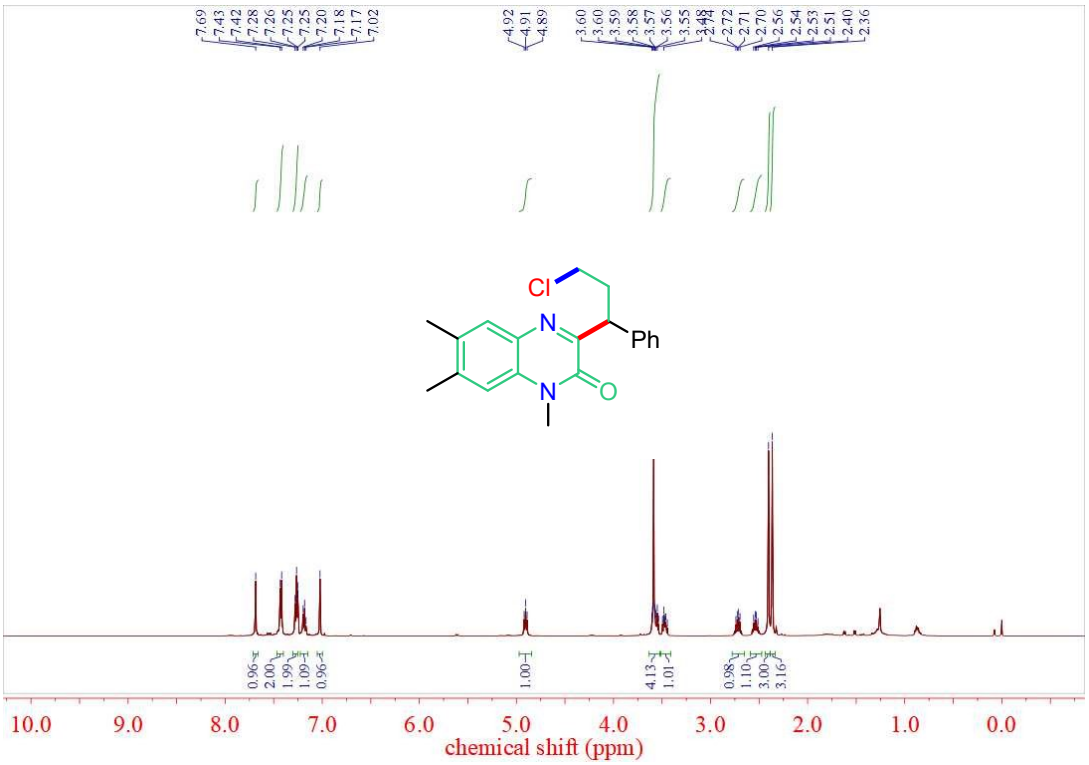
^{19}F NMR (471 MHz, $CDCl_3$) of compound **3r**



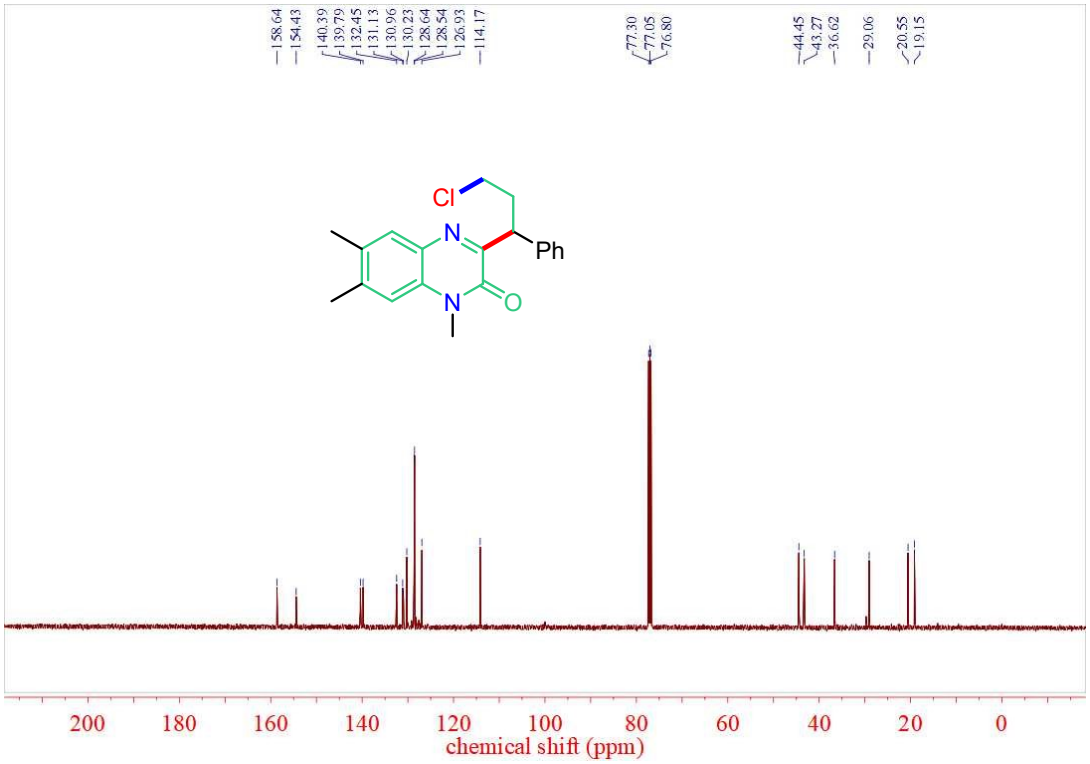
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3u**



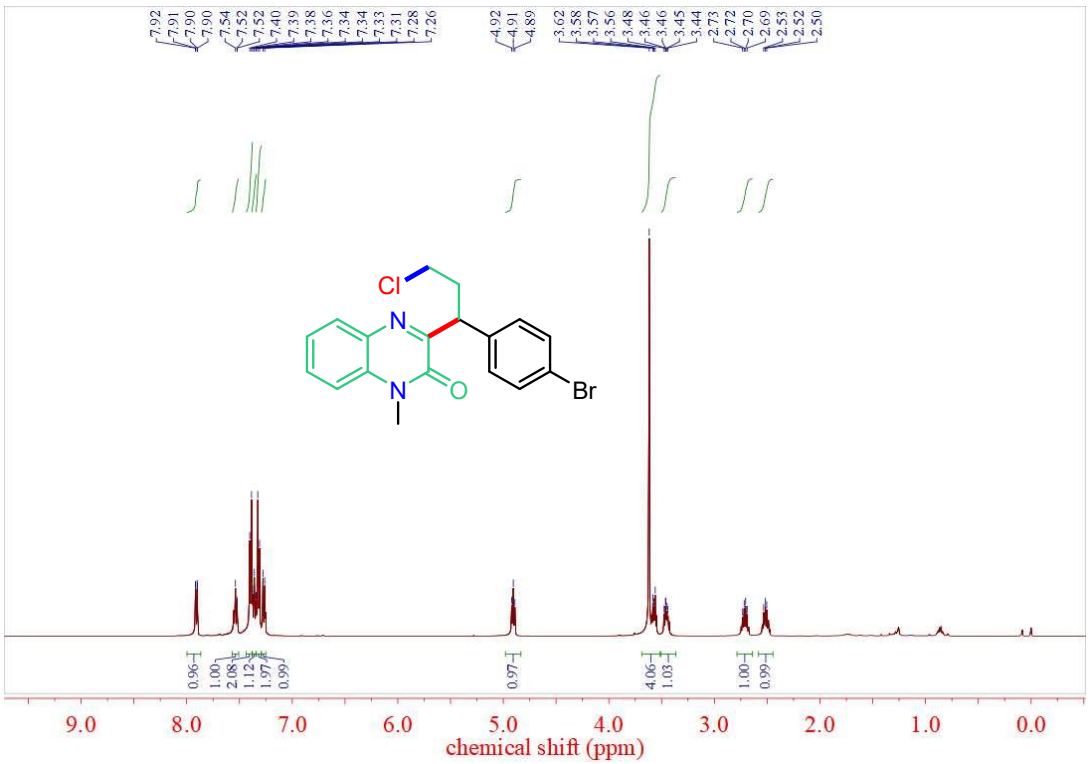
^{13}C NMR (126 MHz, $CDCl_3$) of compound **3u**



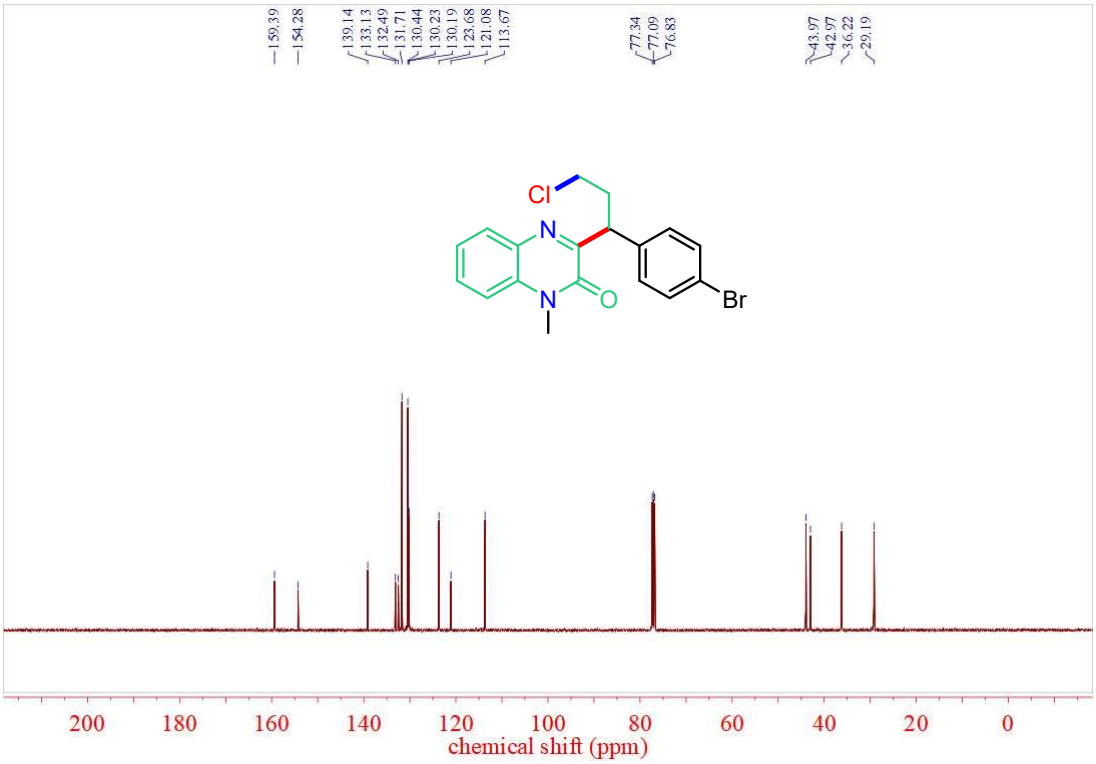
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3v**



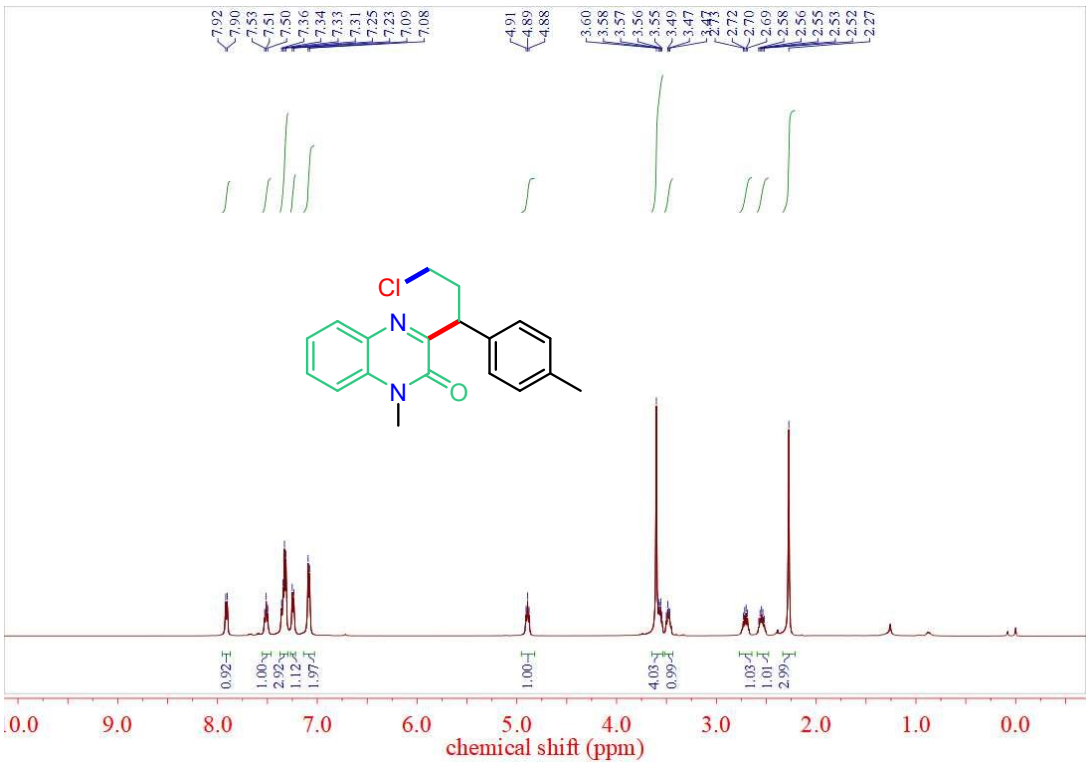
^{13}C NMR (126 MHz, $CDCl_3$) of compound **3v**



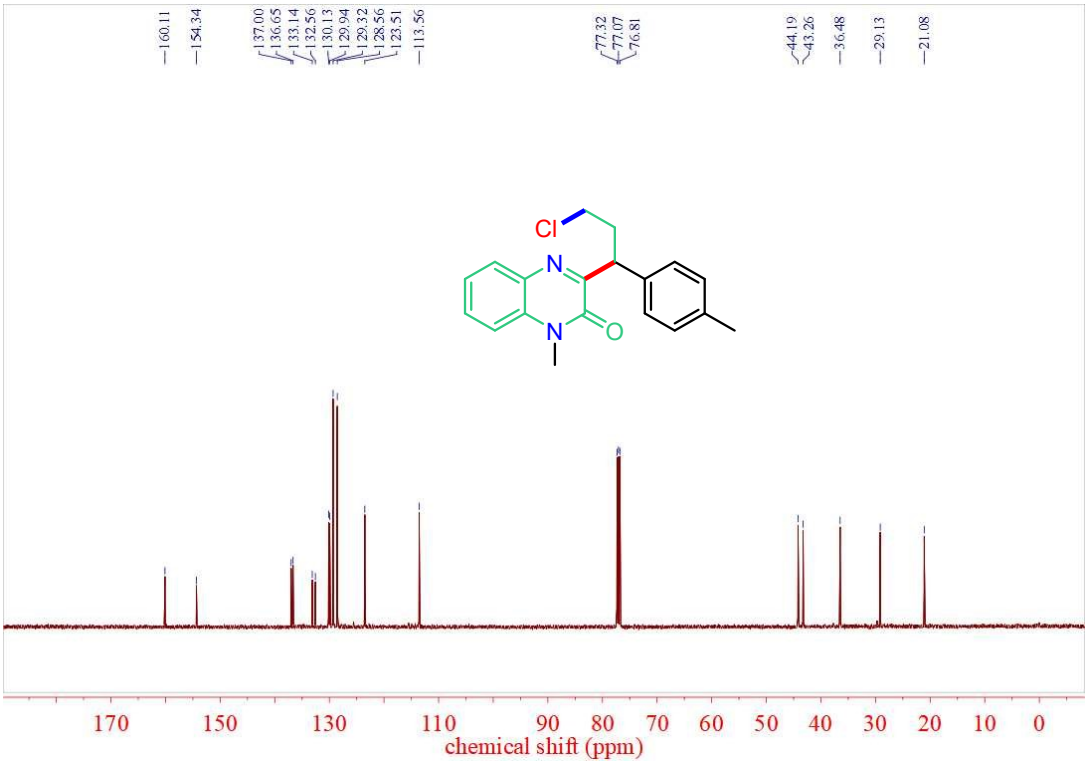
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3w**



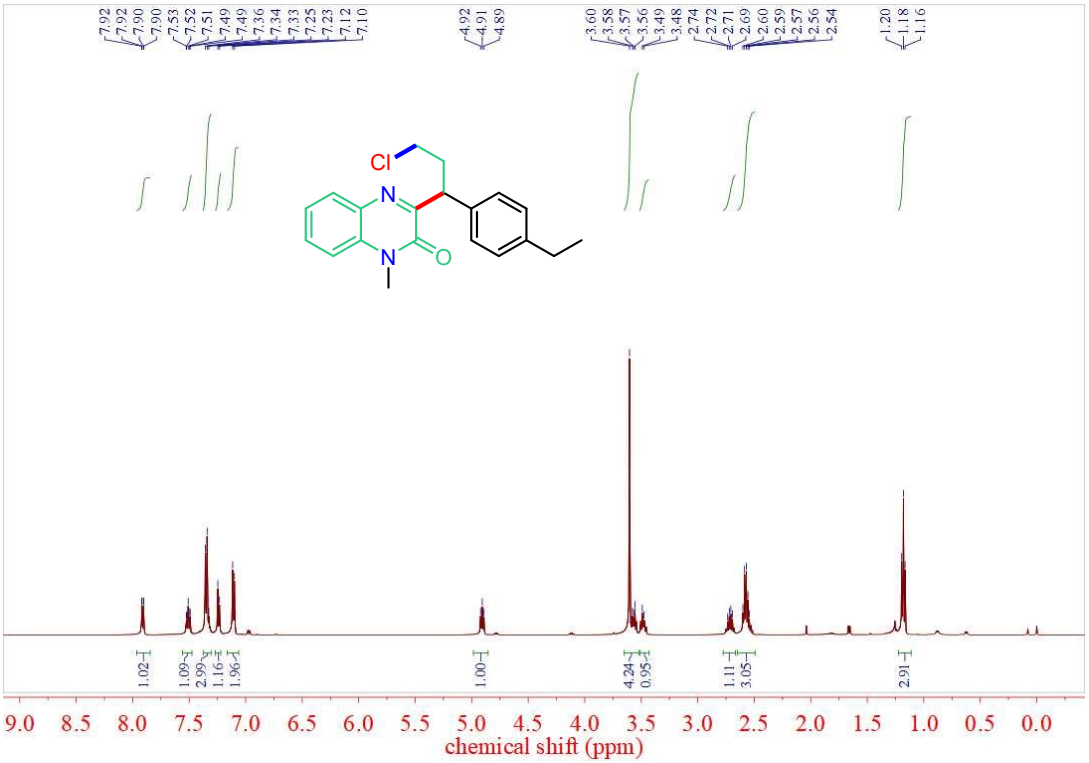
^{13}C NMR (126 MHz, $CDCl_3$) of compound **3w**



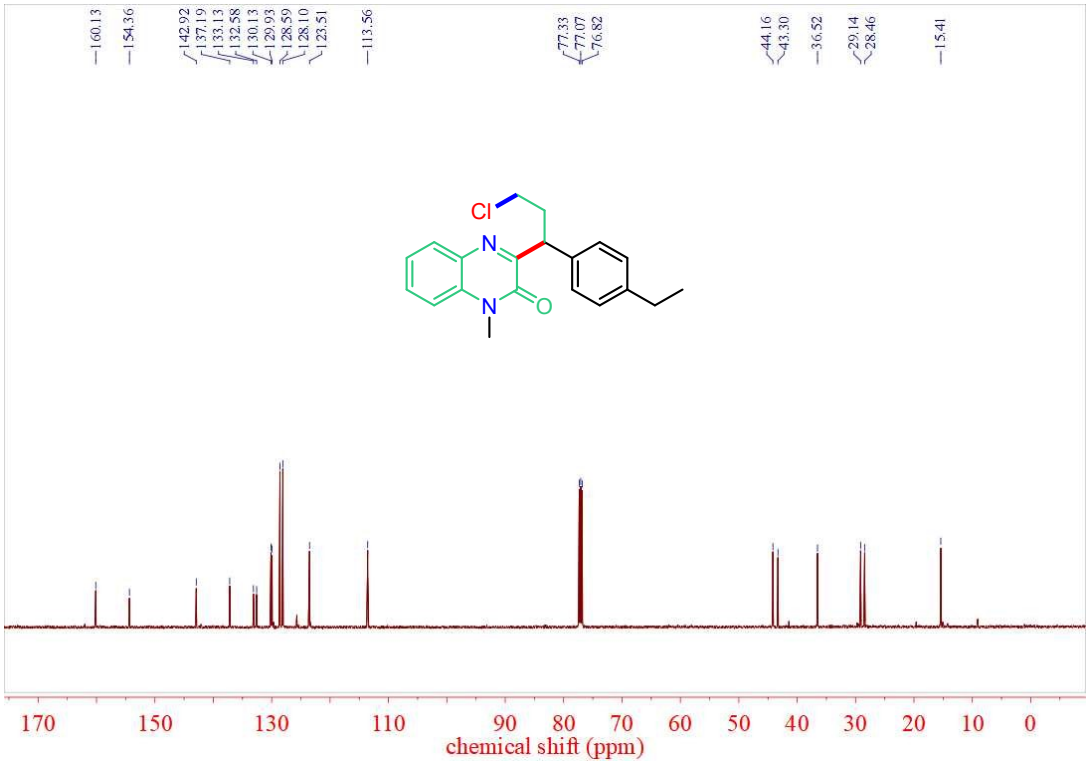
^{1}H NMR (500 MHz, CDCl3) of compound **3x**



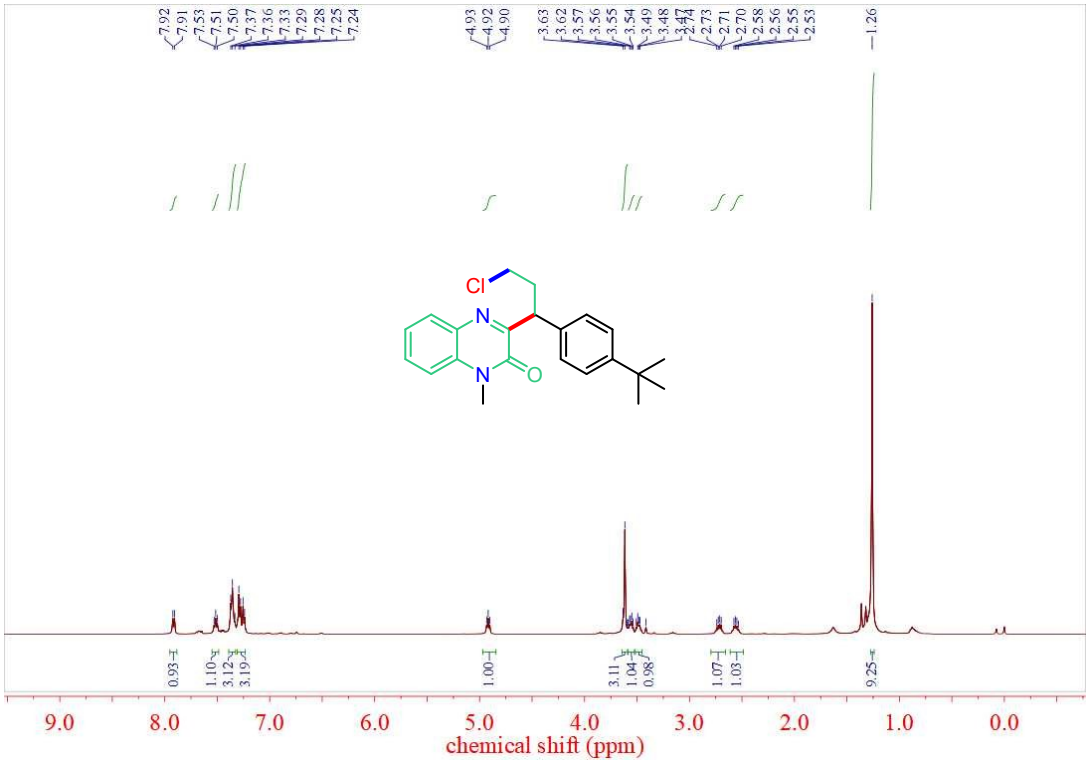
^{13}C NMR (126 MHz, $CDCl_3$) of compound **3x**



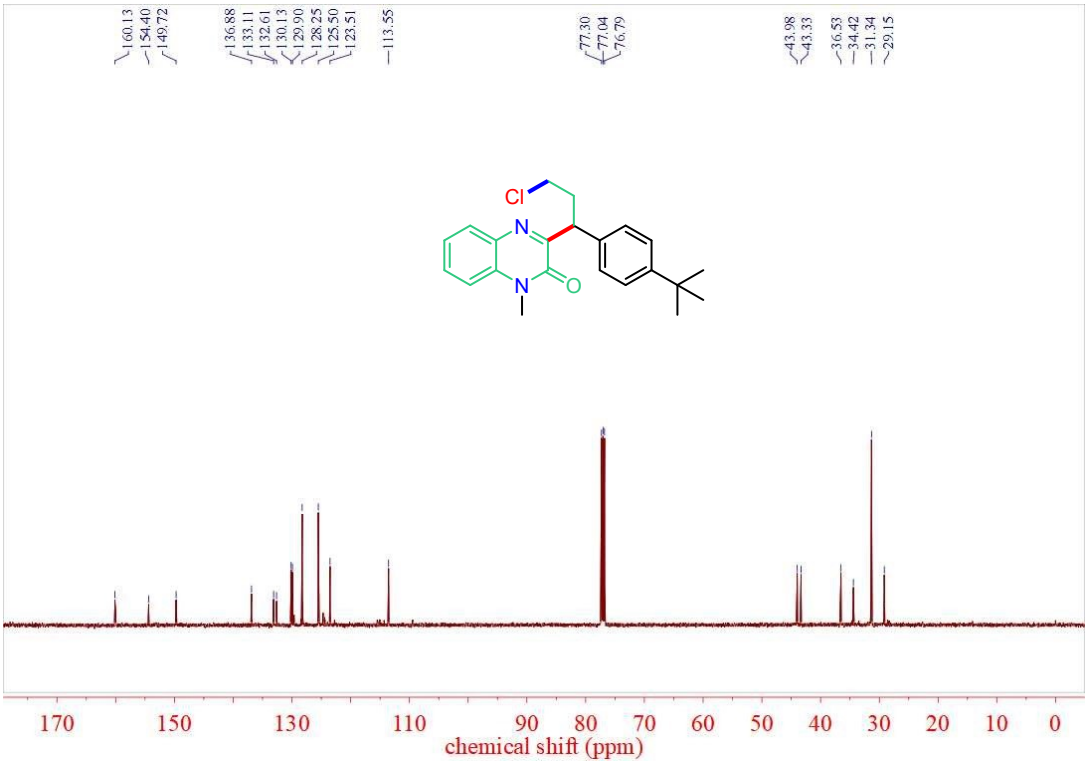
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3y**



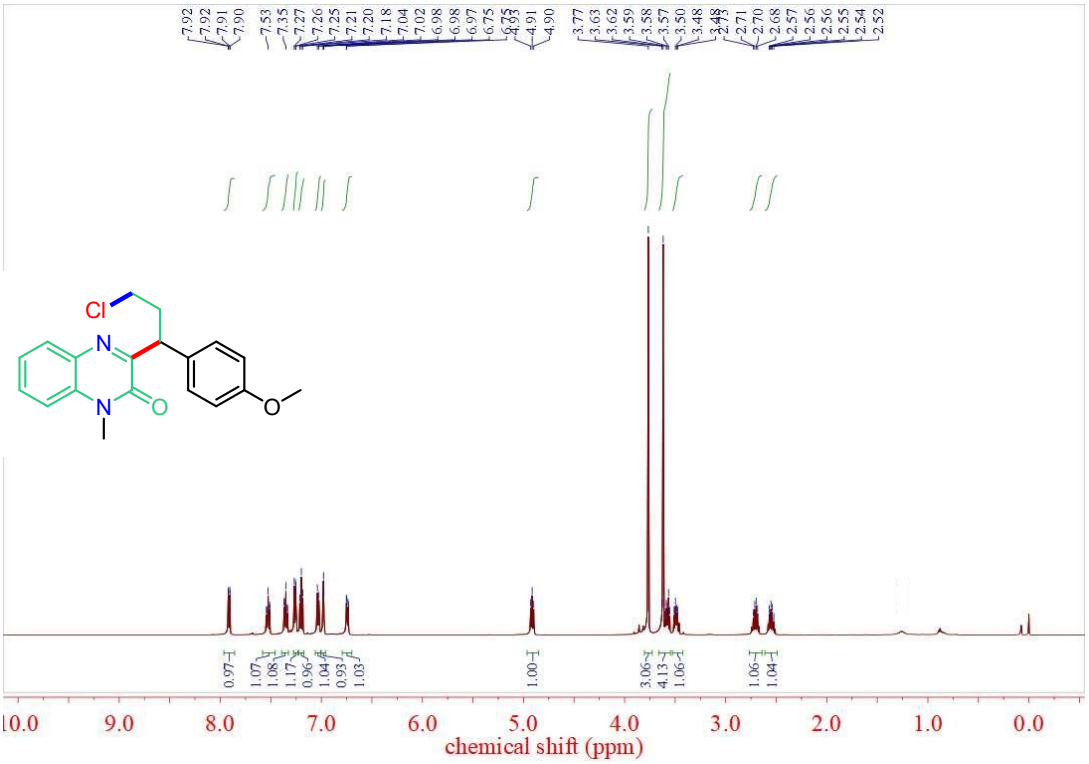
^{13}C NMR (126 MHz, $CDCl_3$) of compound **3y**



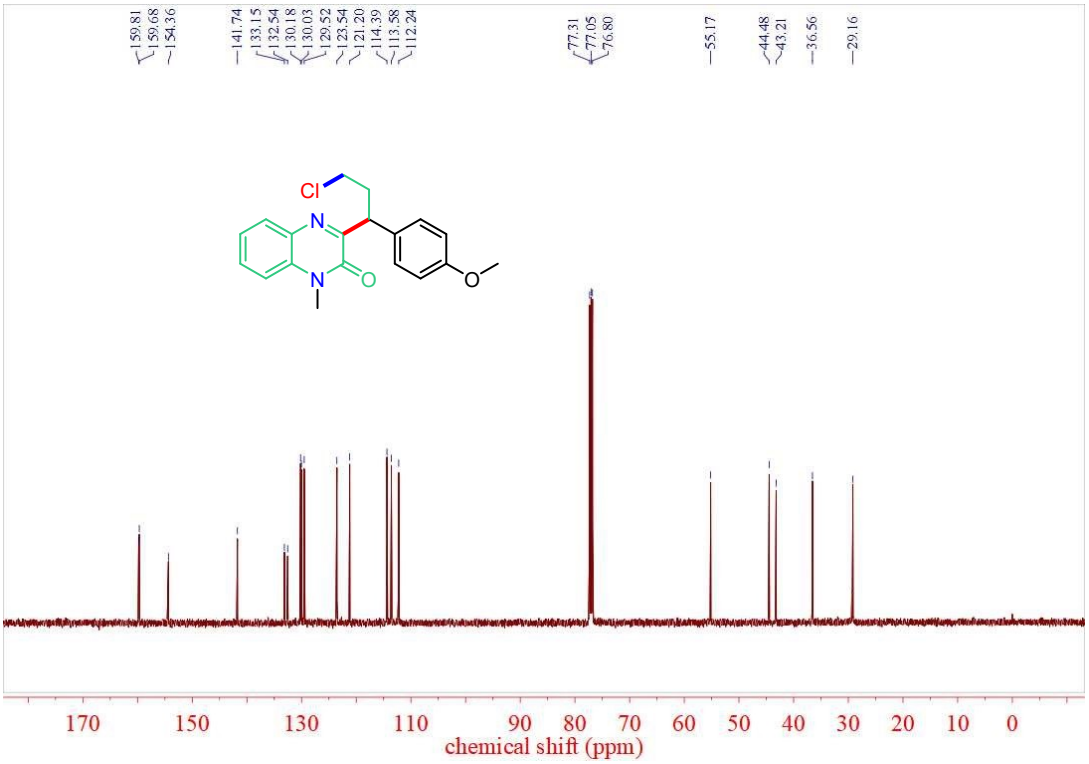
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3z**



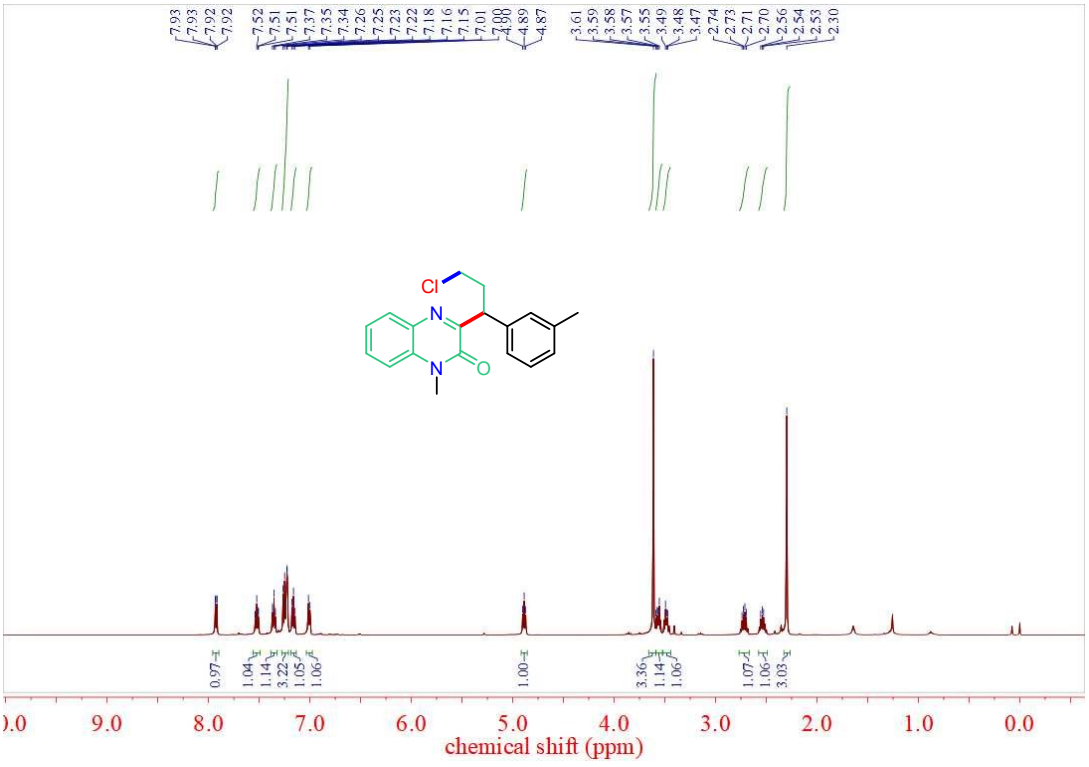
^{13}C NMR (126 MHz, $CDCl_3$) of compound **3z**



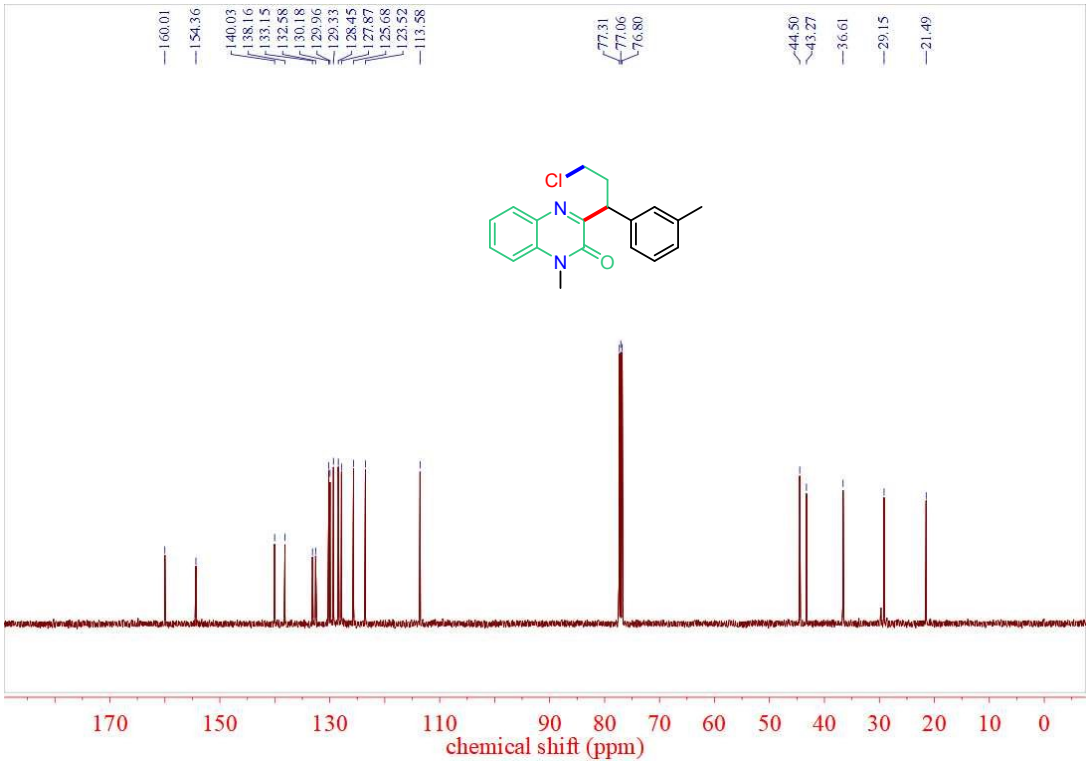
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3aa**



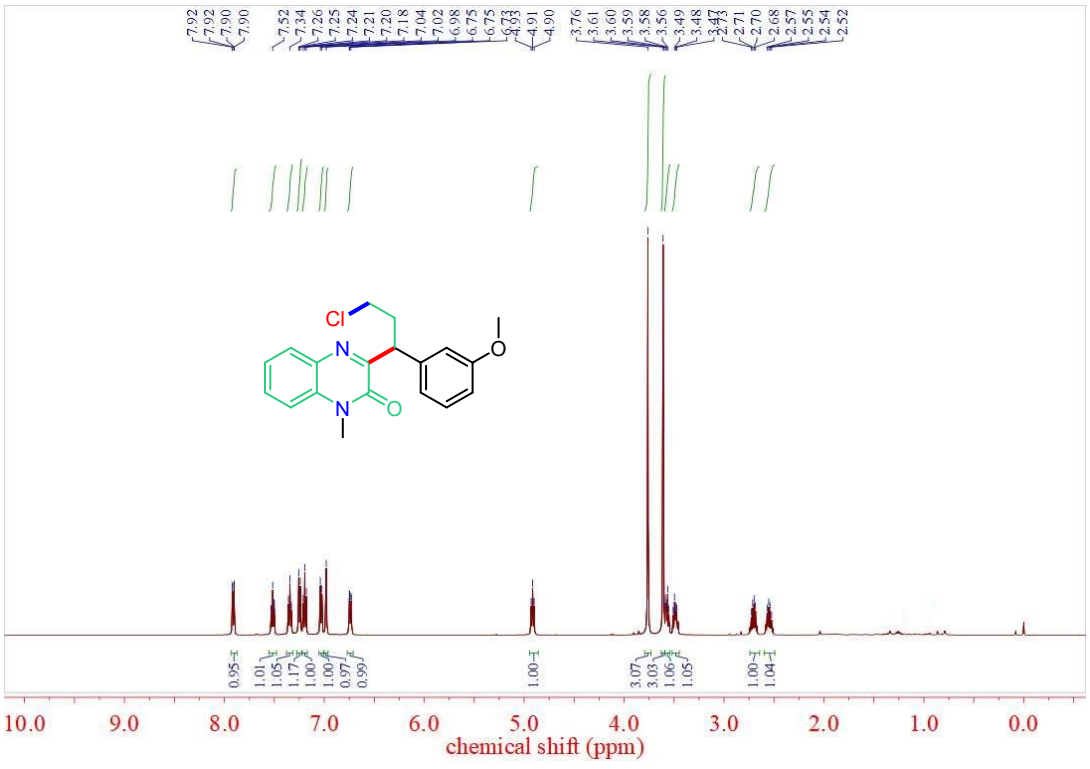
^{13}C NMR (126 MHz, $CDCl_3$) of compound **3aa**



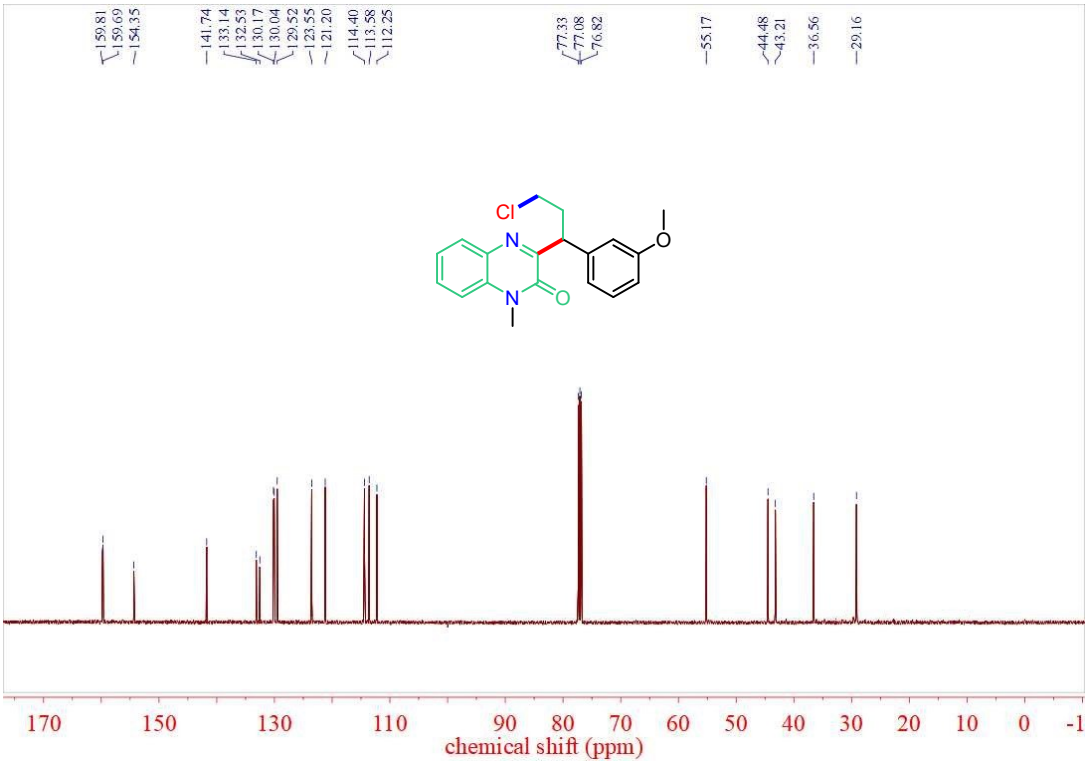
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3ab**



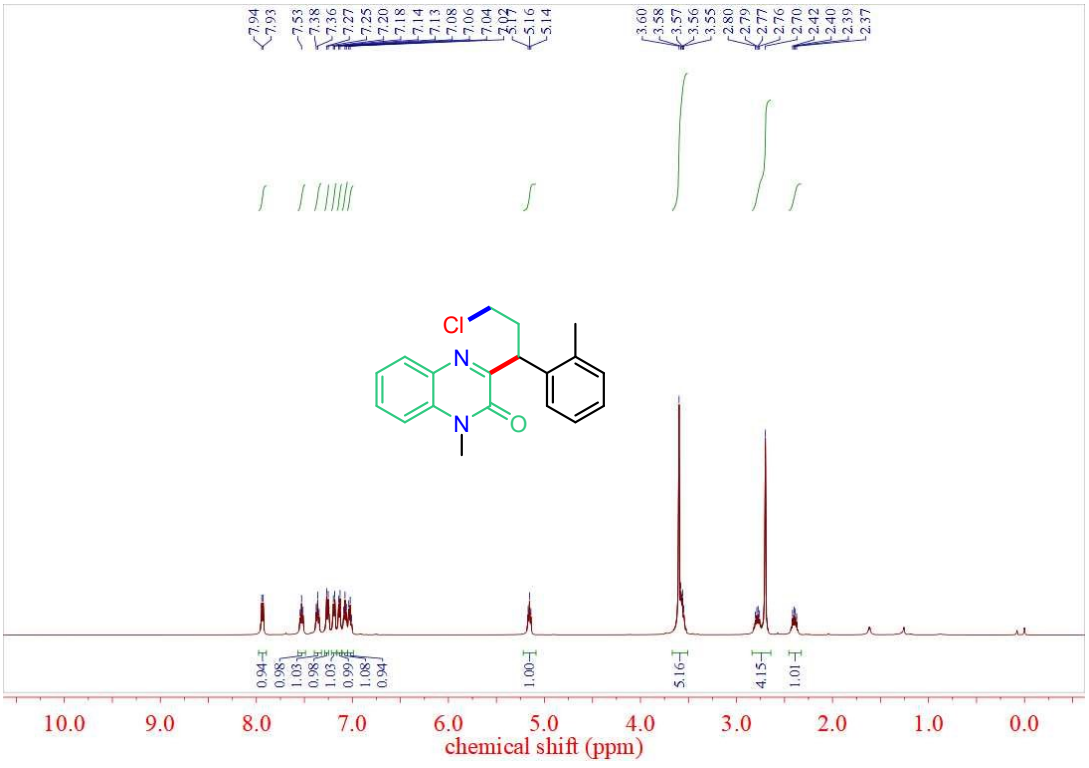
^{13}C NMR (126 MHz, $CDCl_3$) of compound **3ab**



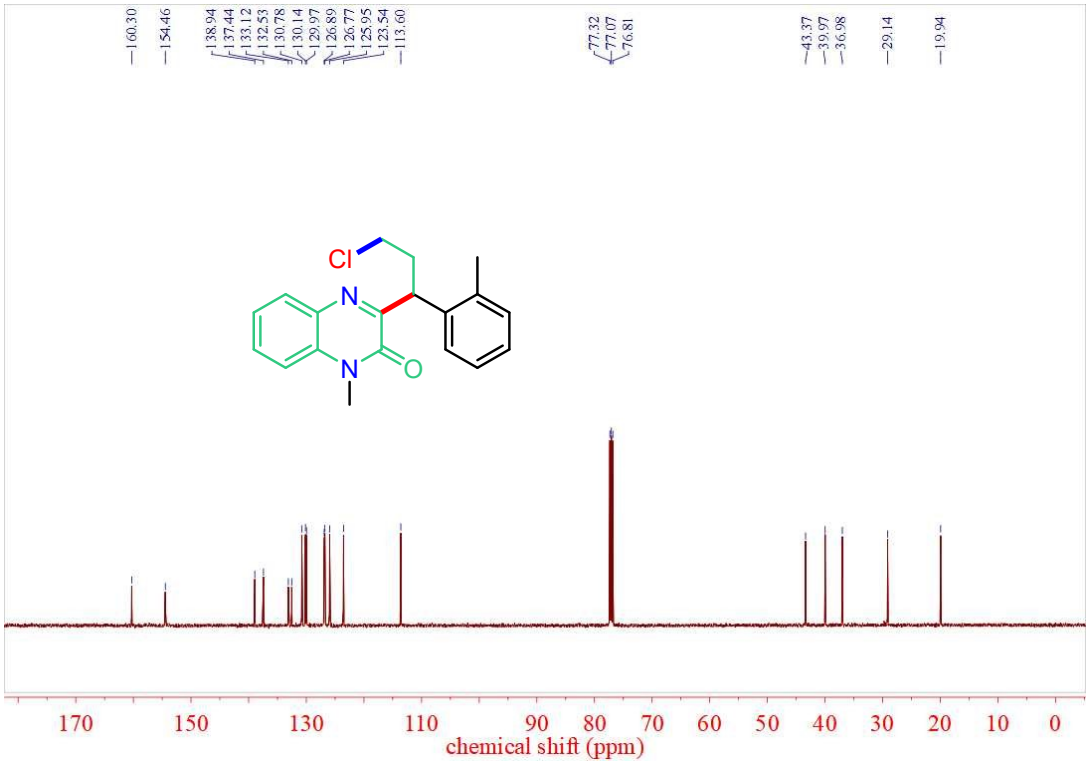
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3ac**



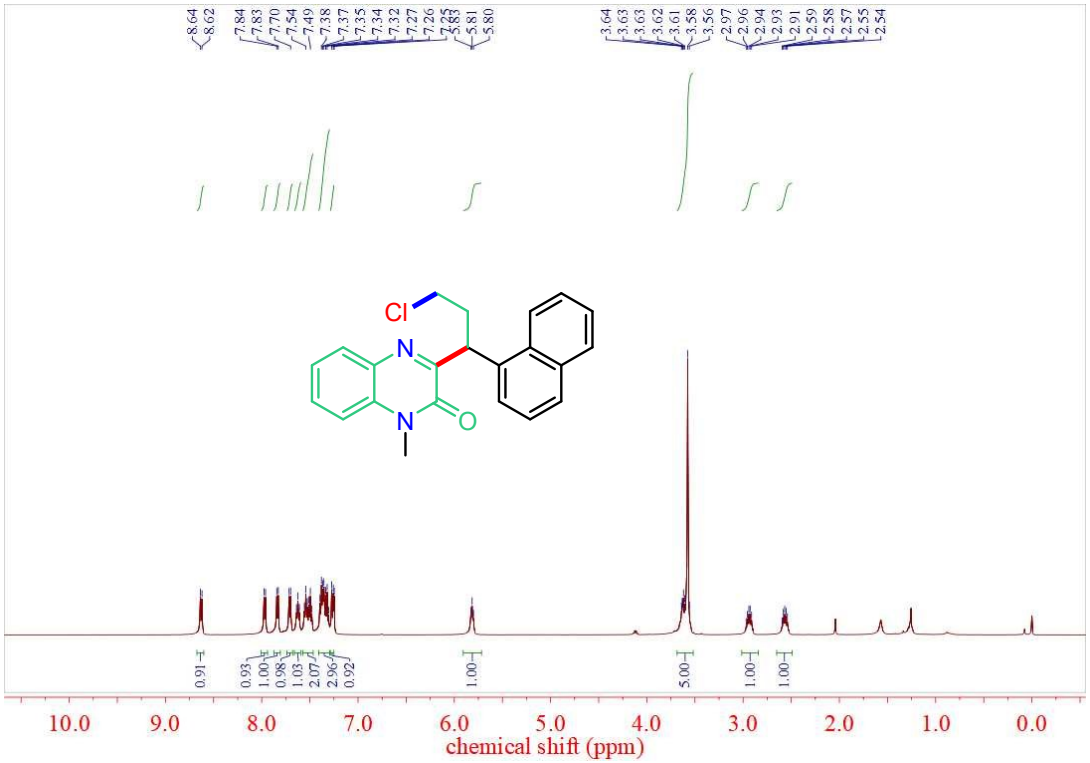
^{13}C NMR (126 MHz, $CDCl_3$) of compound **3ac**



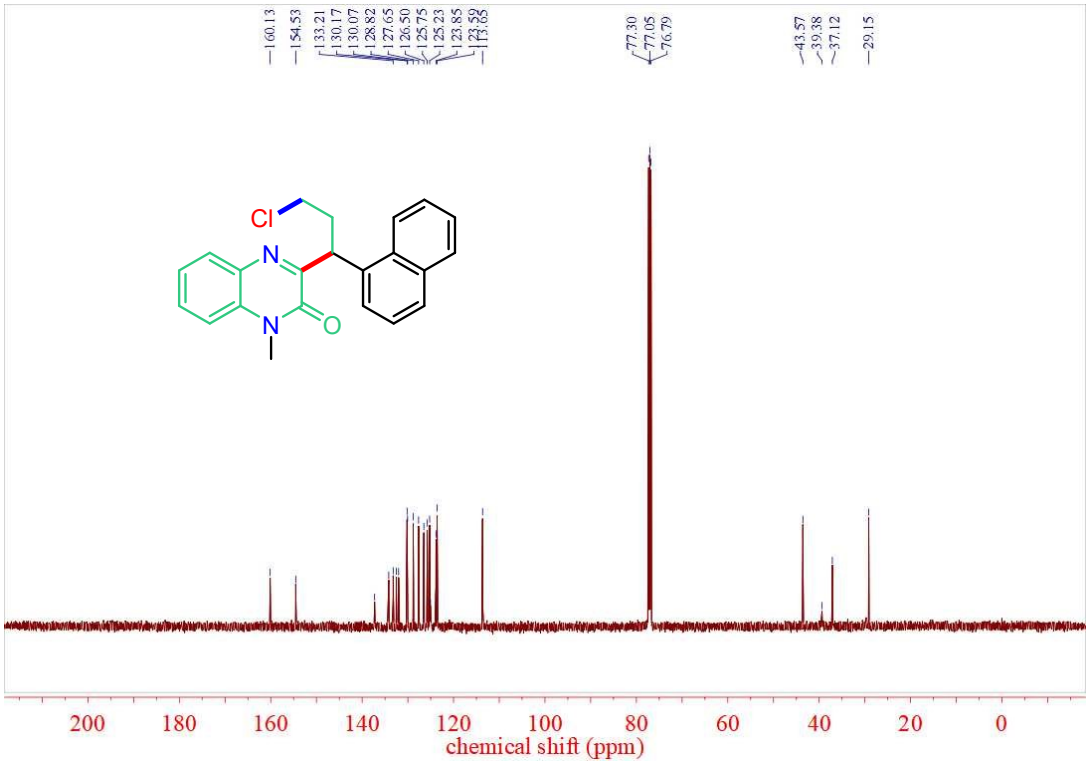
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3ad**



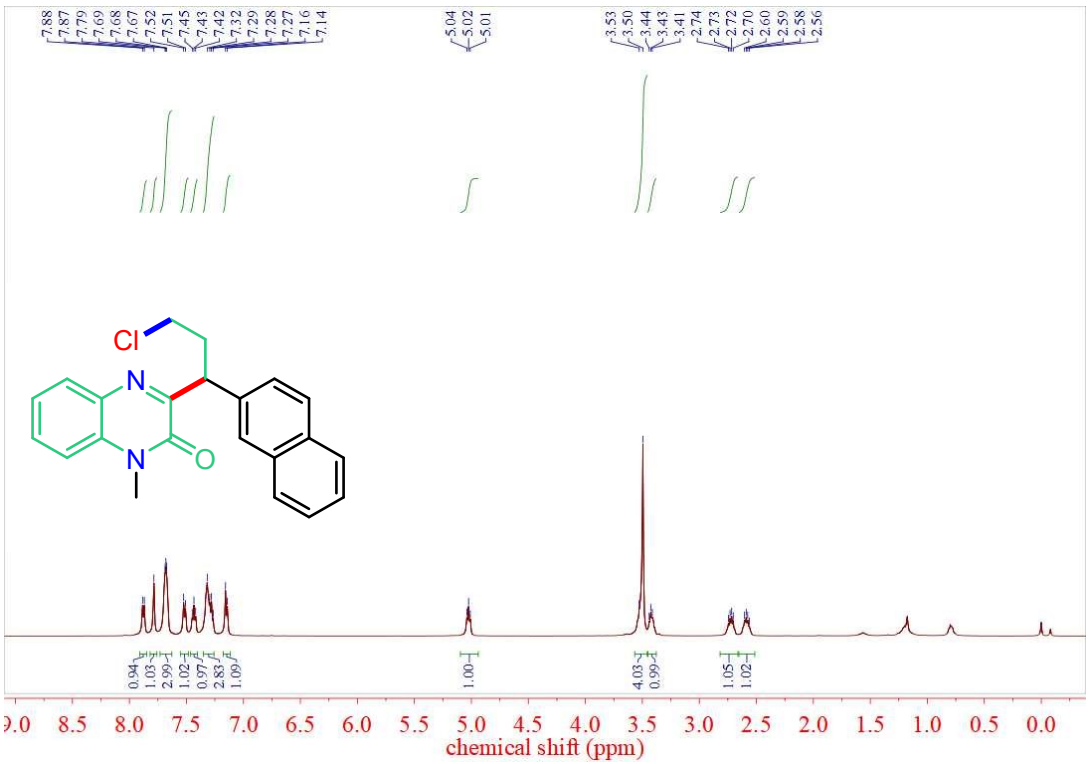
^{13}C NMR (126 MHz, $CDCl_3$) of compound **3ad**



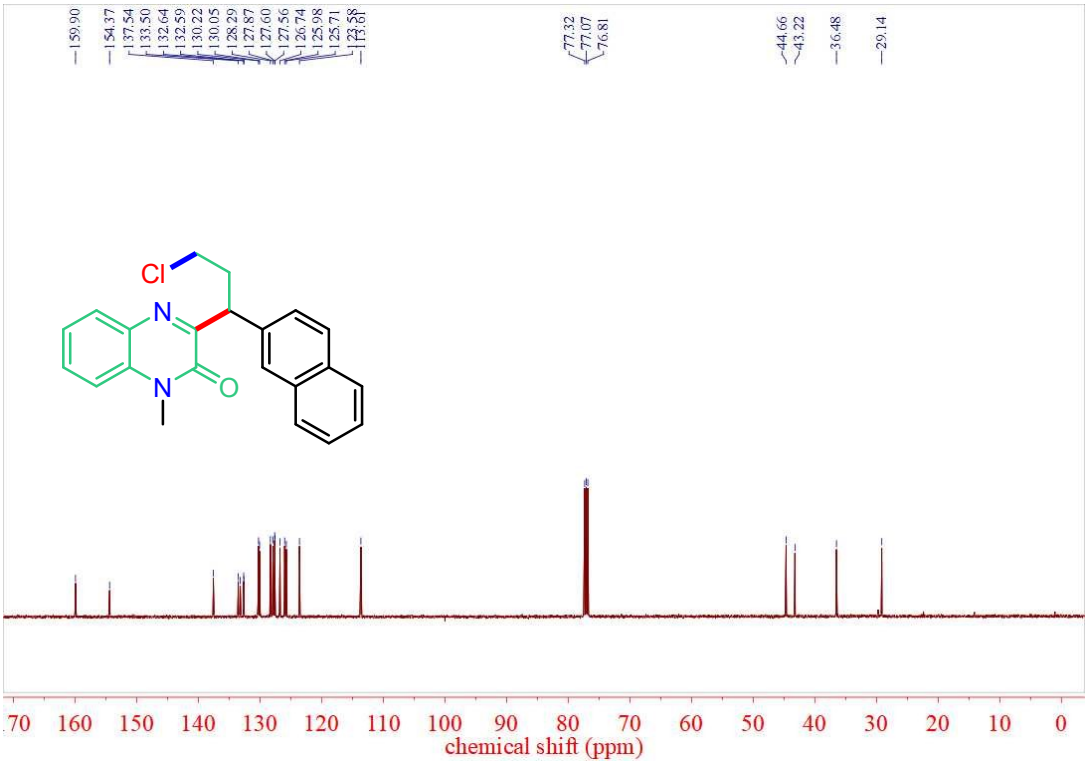
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3ae**



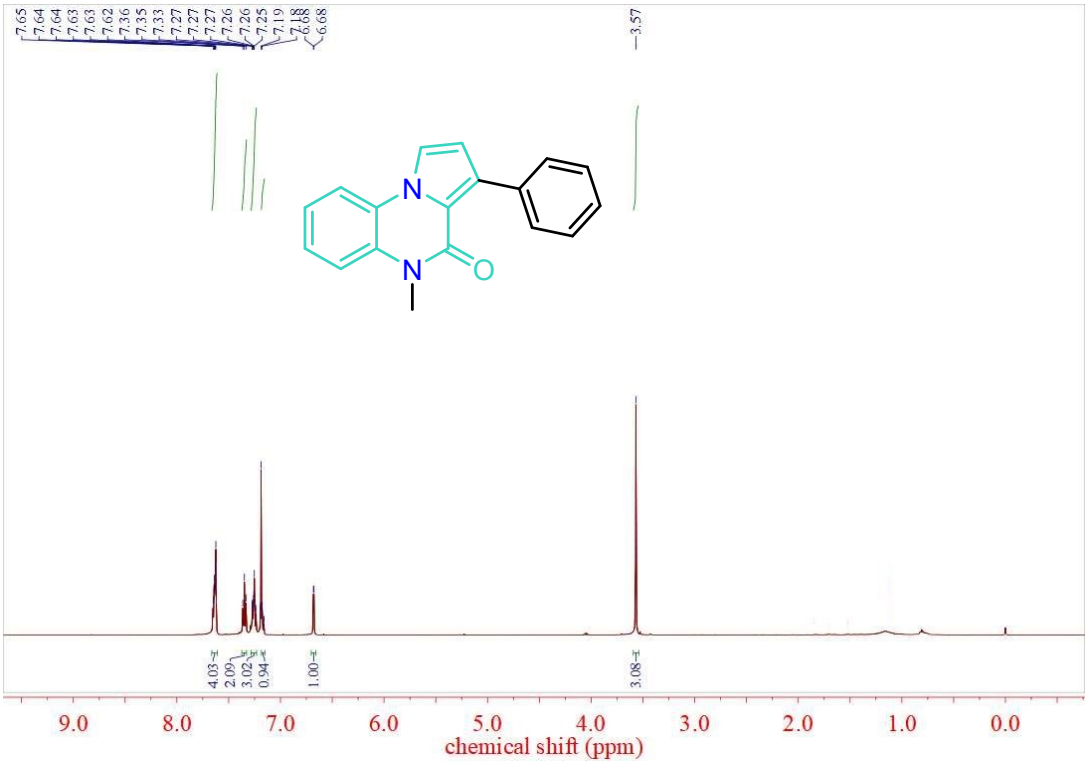
^{13}C NMR (126 MHz, $CDCl_3$) of compound **3ae**



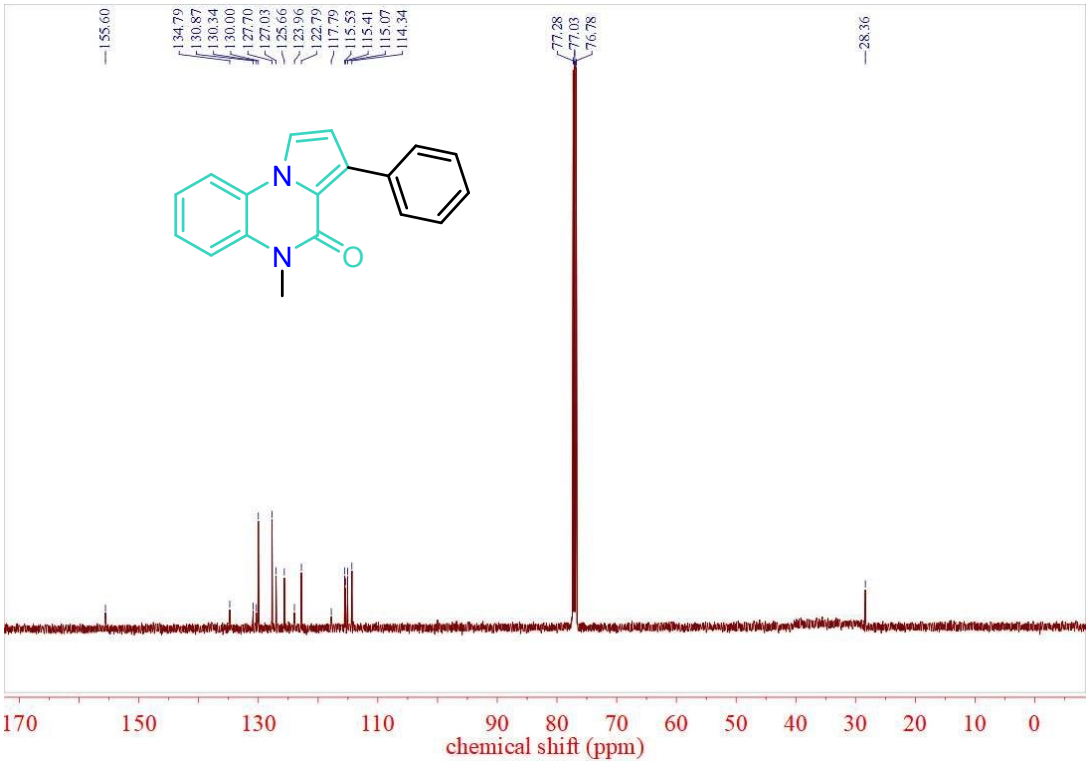
^{1}H NMR (500 MHz, $CDCl_3$) of compound **3af**



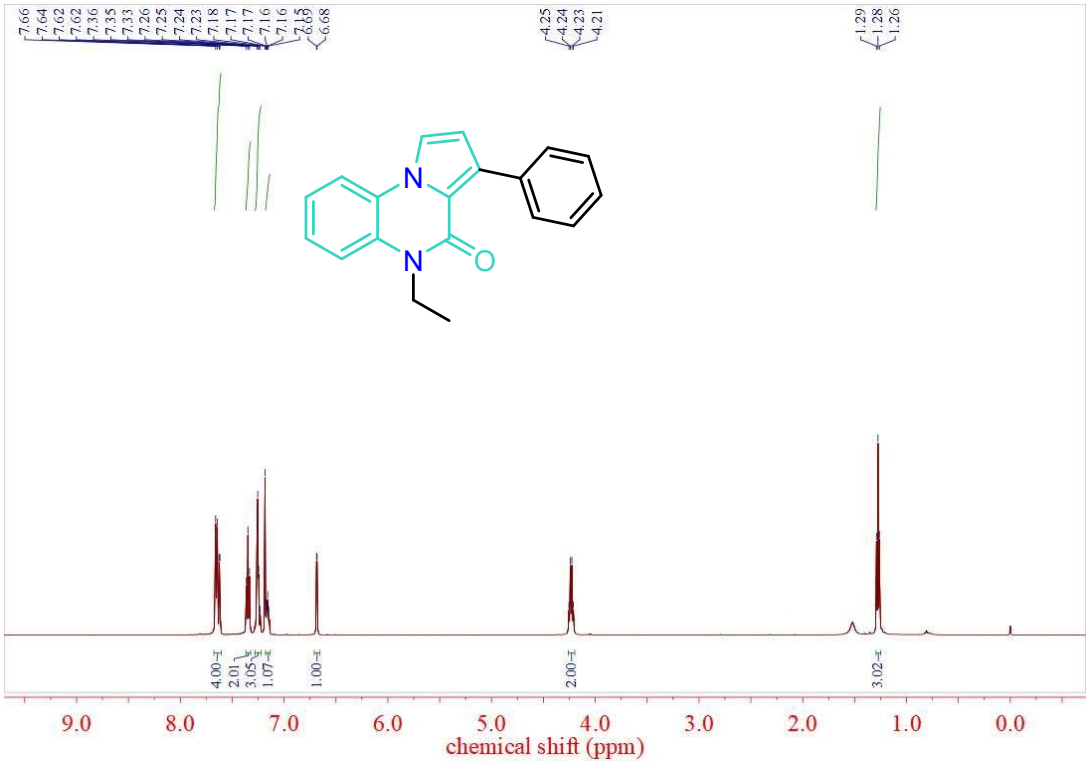
^{13}C NMR (126 MHz, $CDCl_3$) of compound **3af**



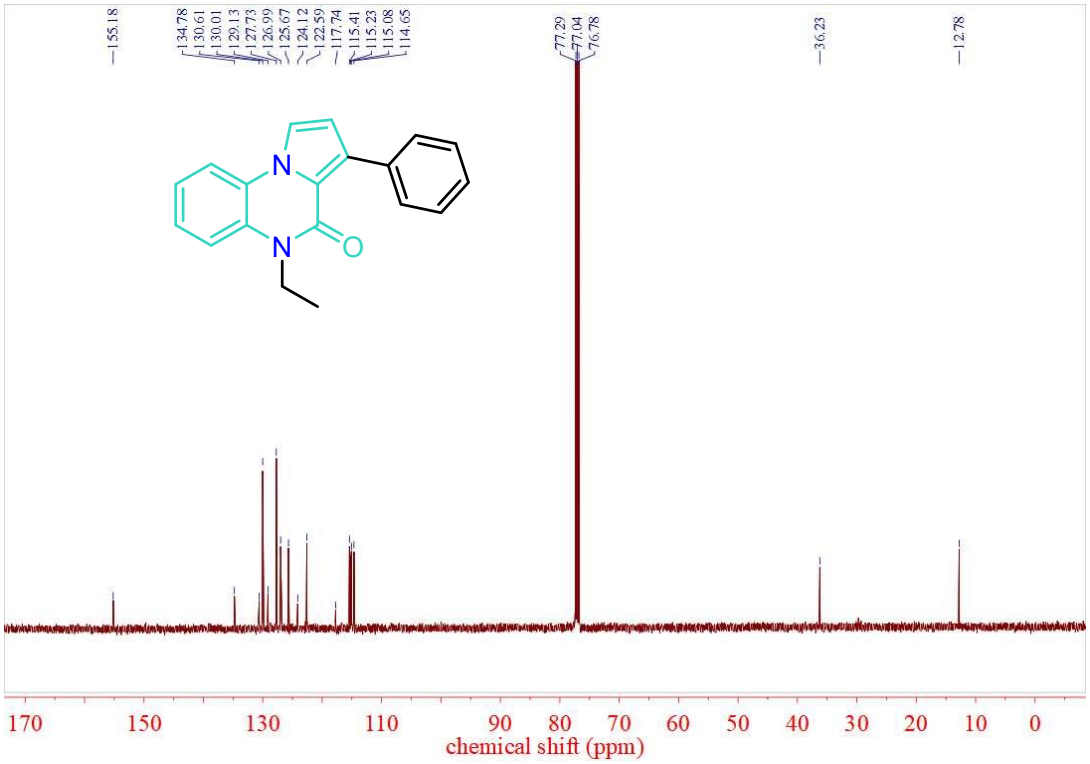
^{1}H NMR (500 MHz, $CDCl_3$) of compound **4a**



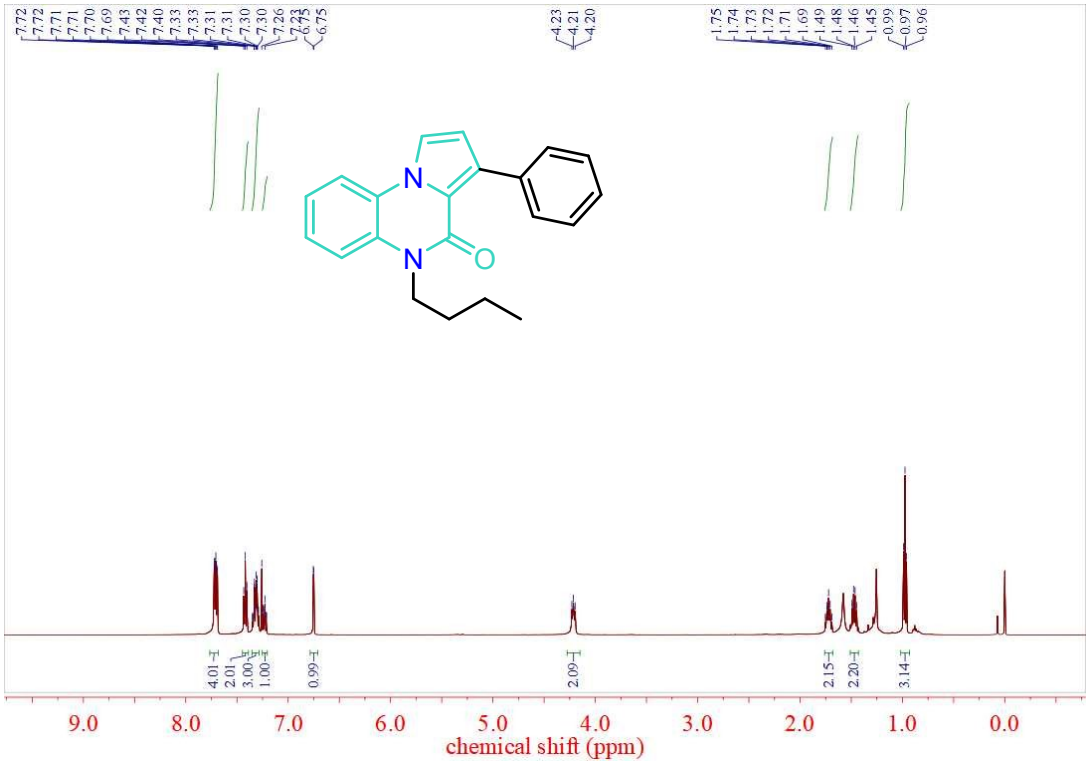
^{13}C NMR (126 MHz, $CDCl_3$) of compound **4a**



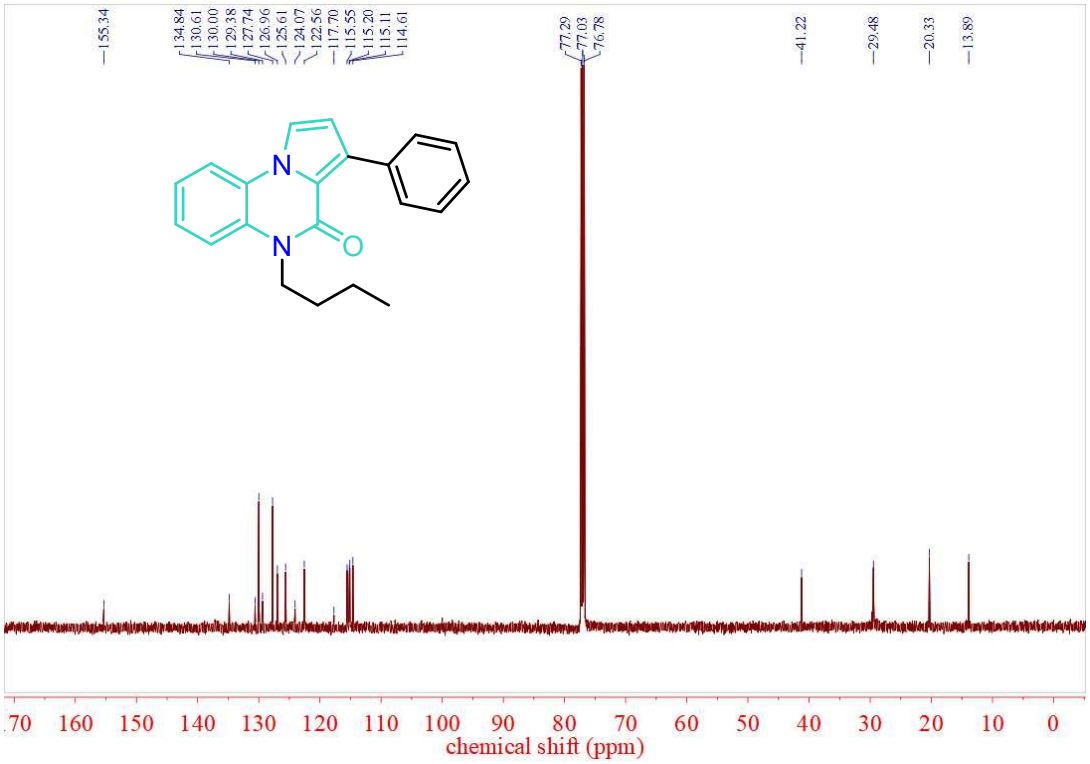
^{1}H NMR (500 MHz, $CDCl_3$) of compound **4b**



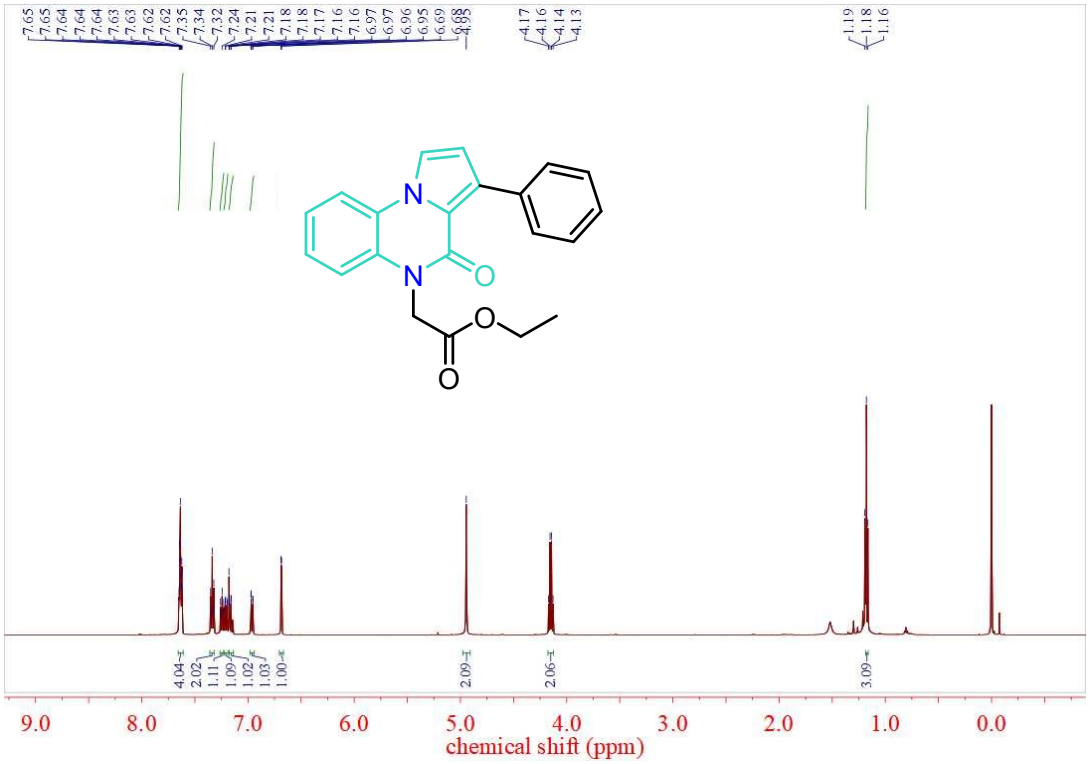
^{13}C NMR (126 MHz, $CDCl_3$) of compound **4b**



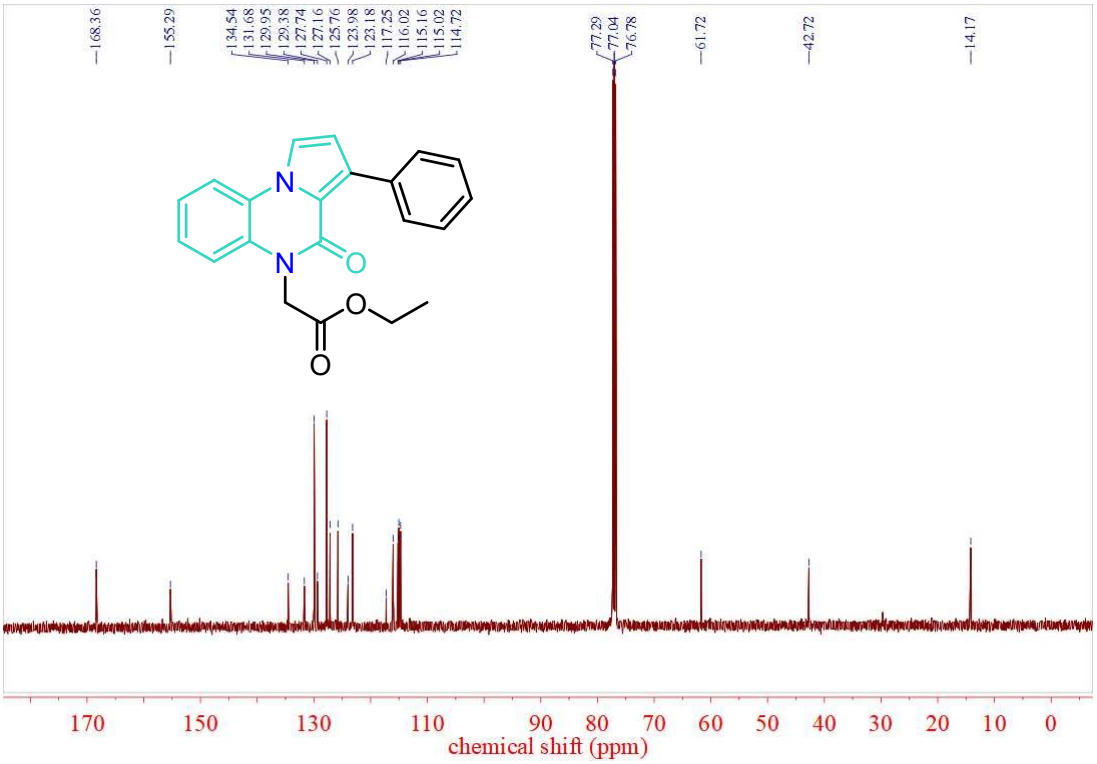
^{1}H NMR (500 MHz, $CDCl_3$) of compound **4c**



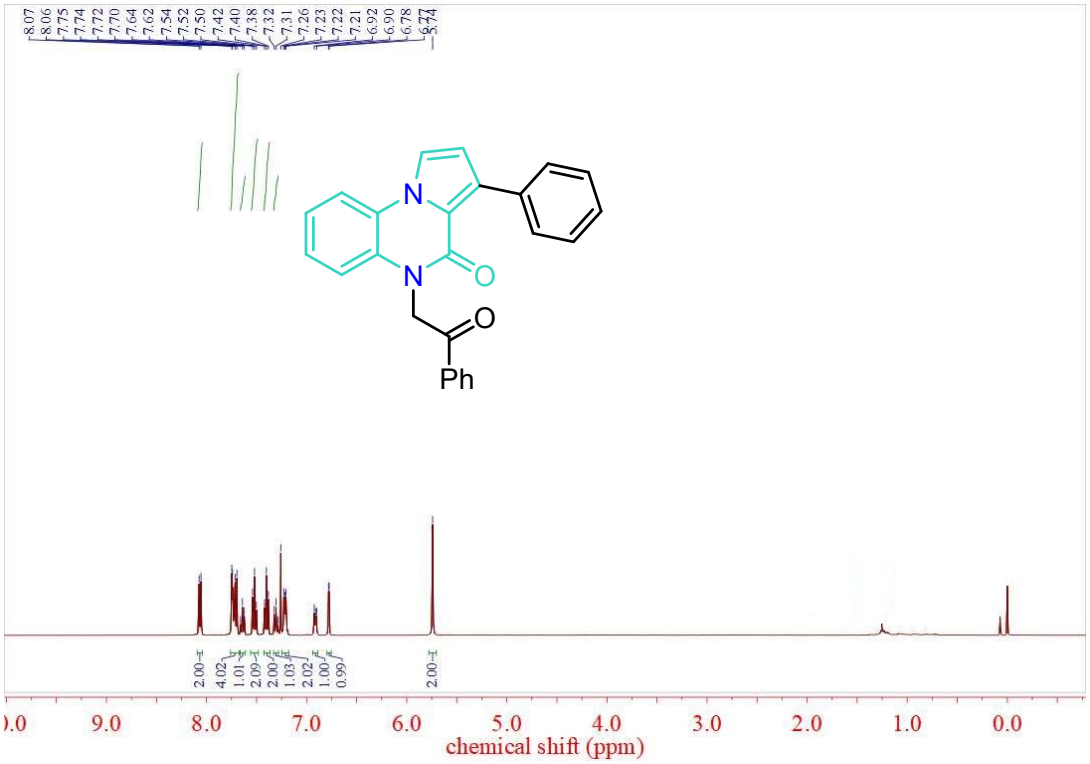
^{13}C NMR (126 MHz, $CDCl_3$) of compound **4c**



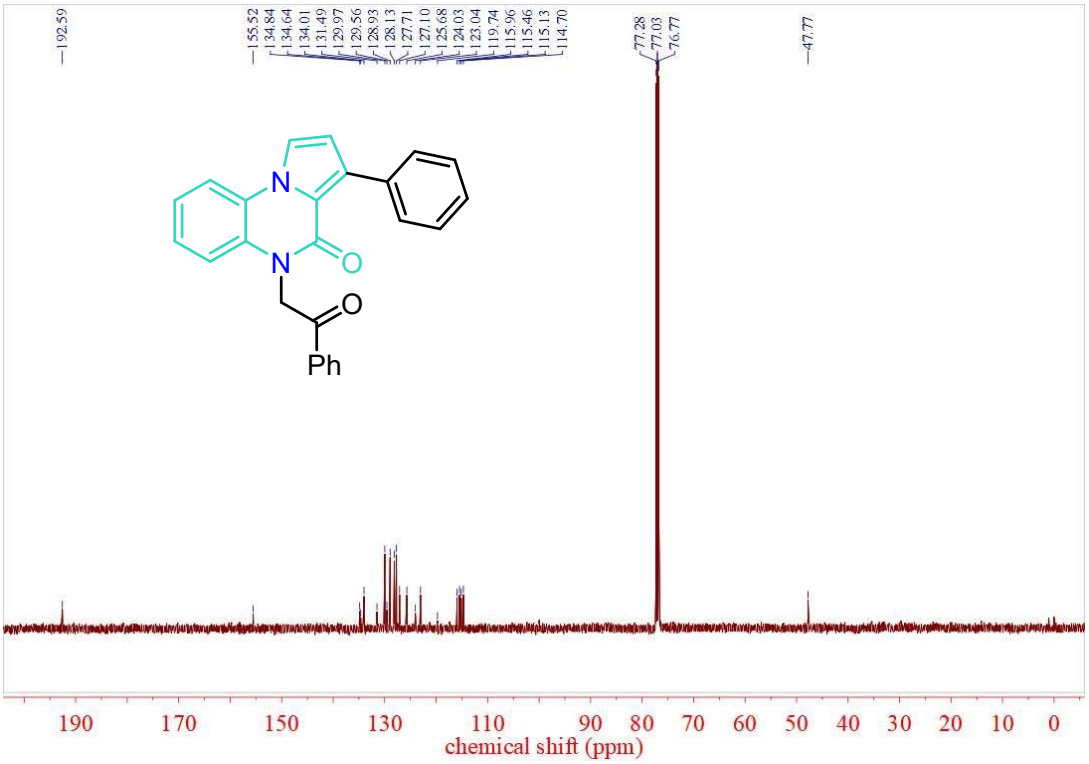
^{1}H NMR (500 MHz, $CDCl_3$) of compound **4d**



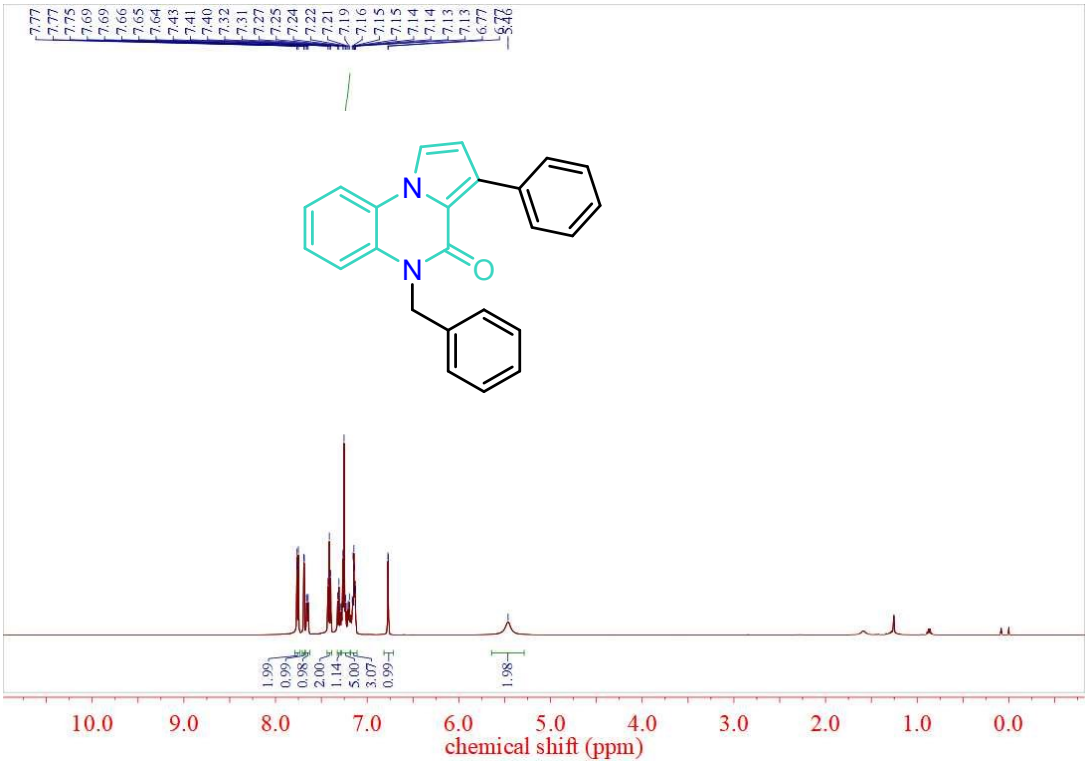
^{13}C NMR (126 MHz, $CDCl_3$) of compound **4d**



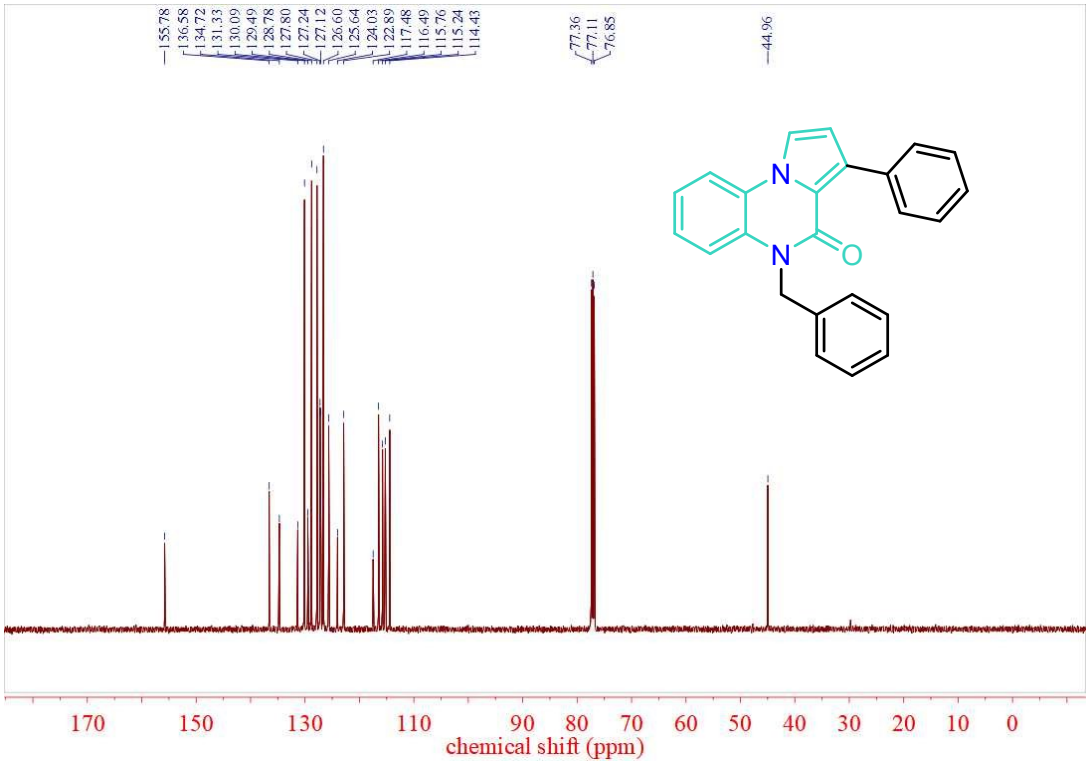
^{1}H NMR (500 MHz, $CDCl_3$) of compound **4e**



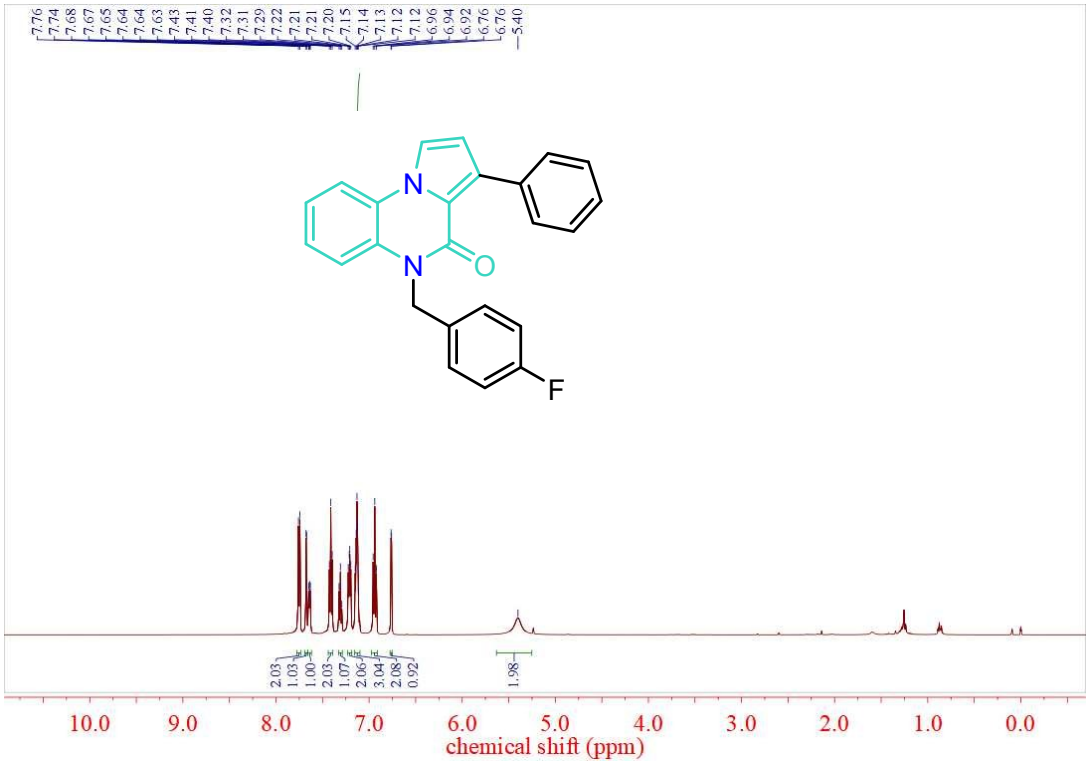
^{13}C NMR (126 MHz, $CDCl_3$) of compound **4e**



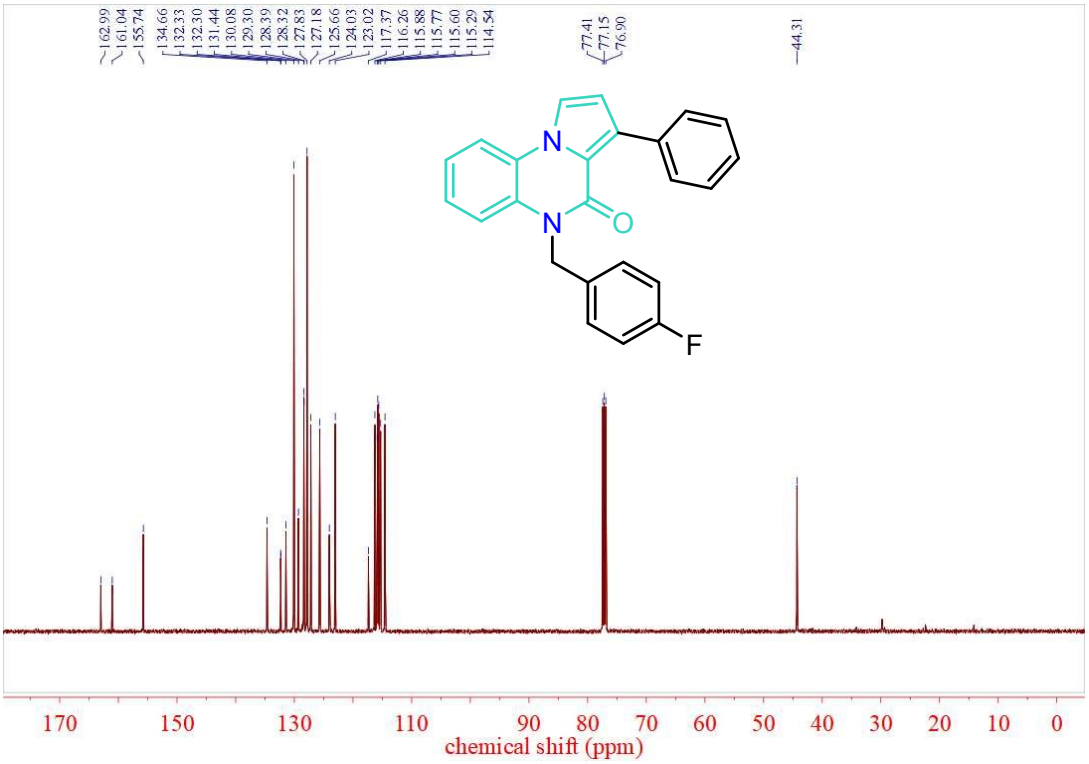
^{1}H NMR (500 MHz, $CDCl_3$) of compound **4f**



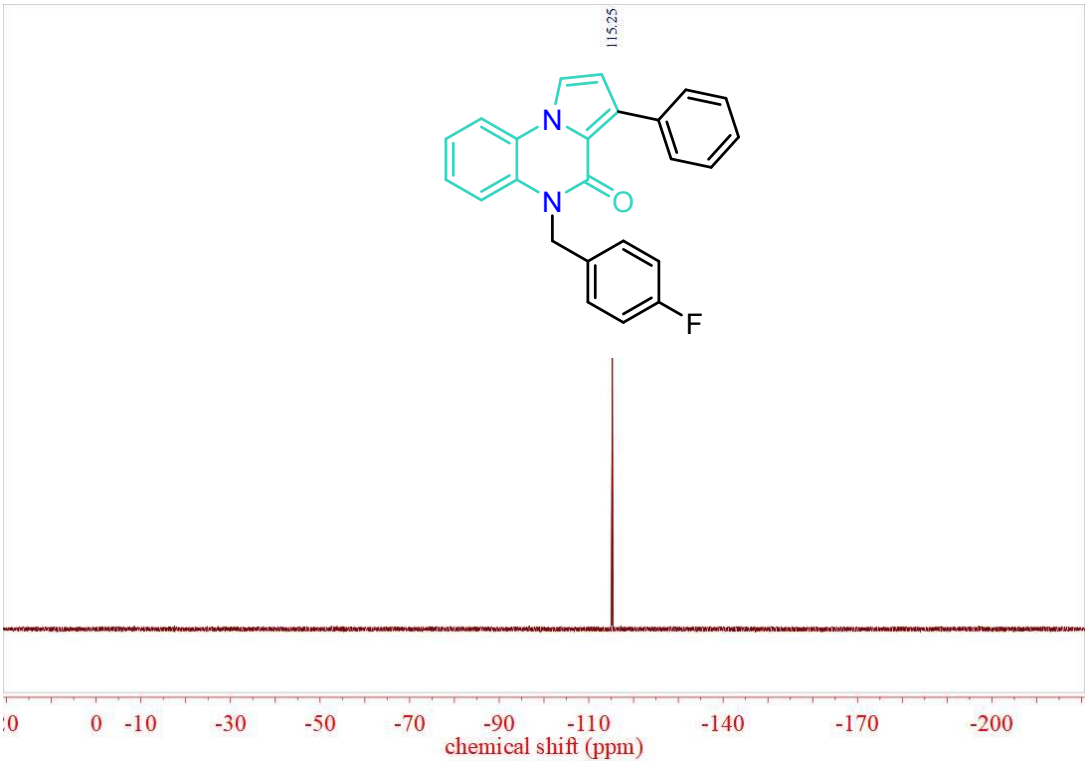
^{13}C NMR (126 MHz, $CDCl_3$) of compound **4f**



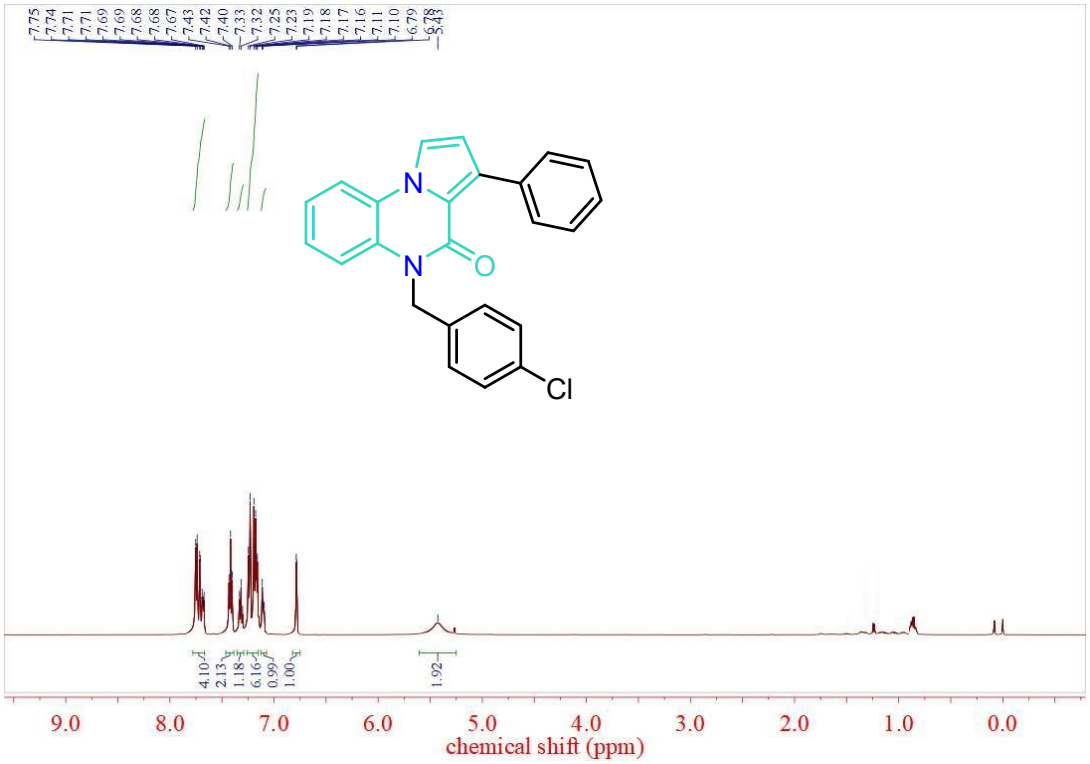
^{1}H NMR (500 MHz, $CDCl_3$) of compound **4g**



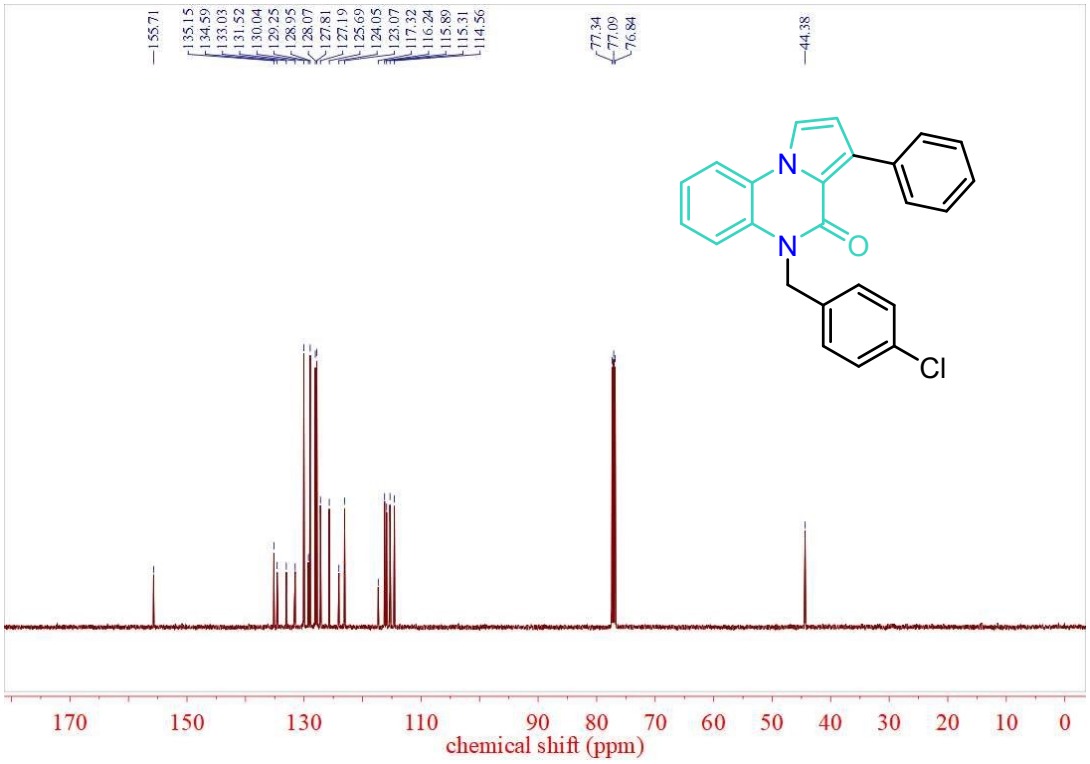
^{13}C NMR (126 MHz, $CDCl_3$) of compound **4g**



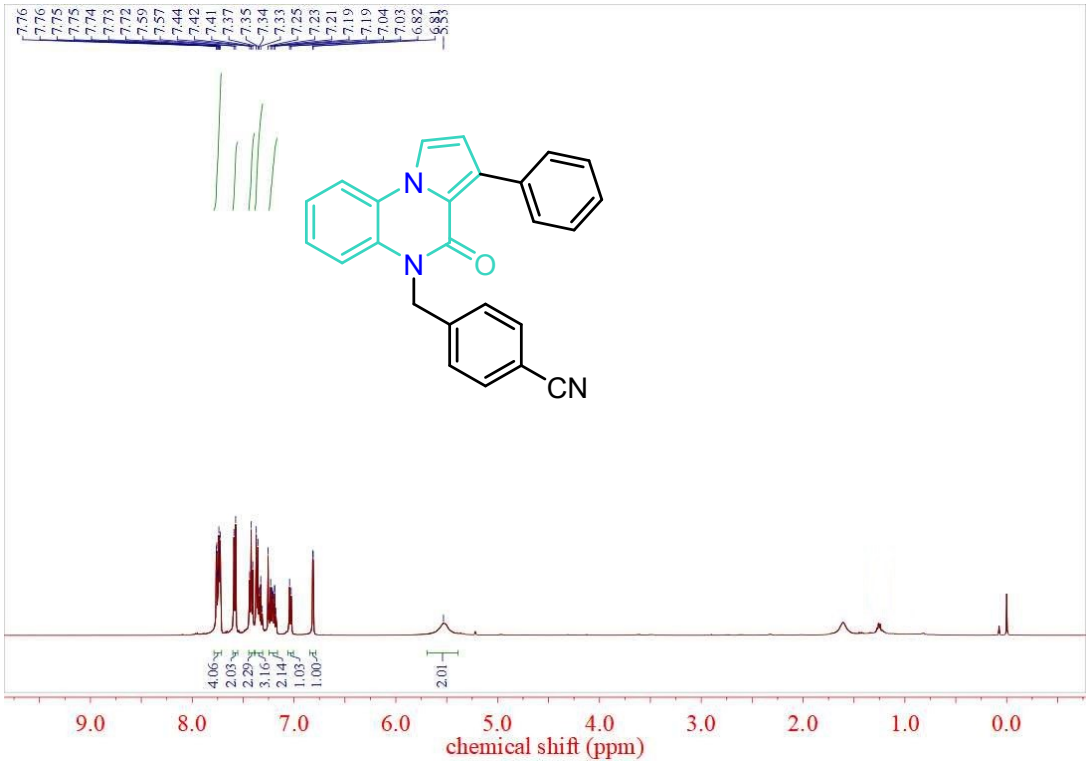
^{19}F NMR (471 MHz, $CDCl_3$) of compound **4g**



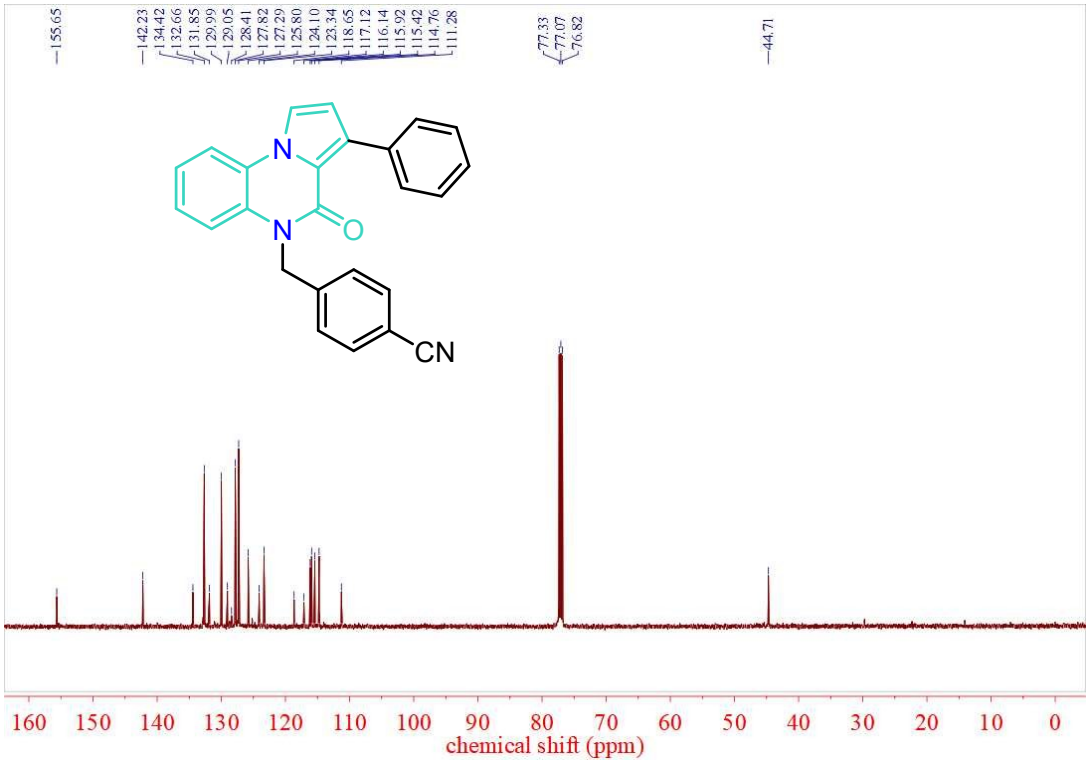
^{1}H NMR (500 MHz, $CDCl_3$) of compound **4h**



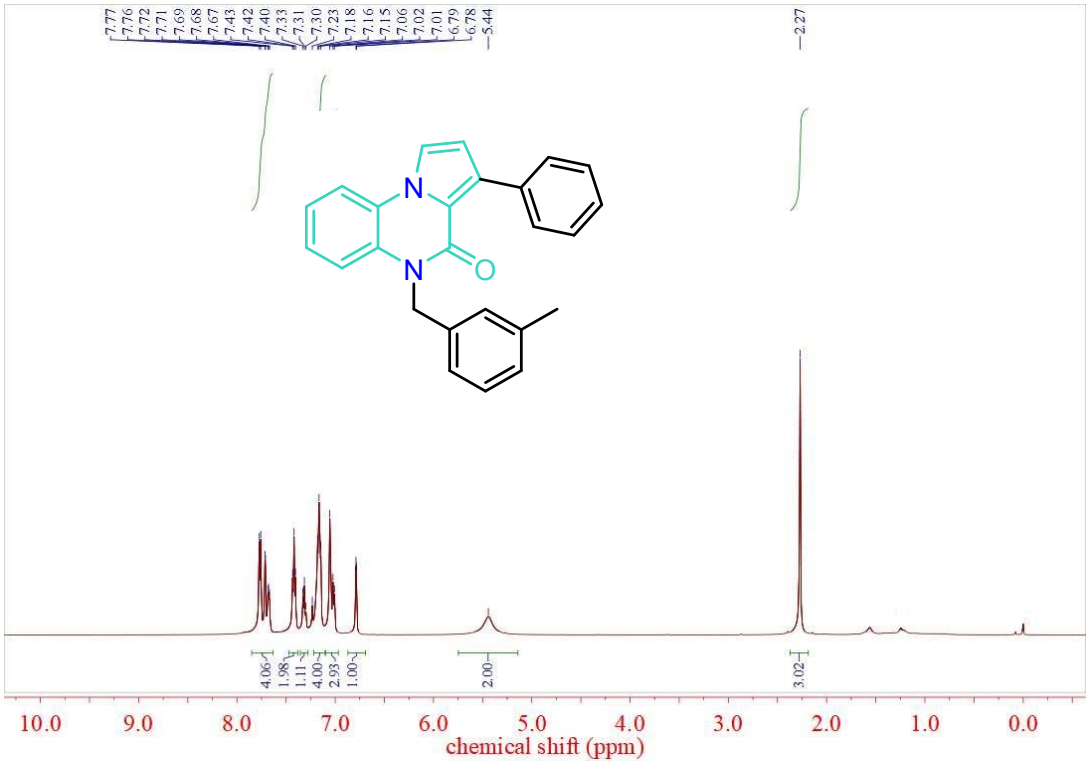
^{13}C NMR (126 MHz, $CDCl_3$) of compound **4h**



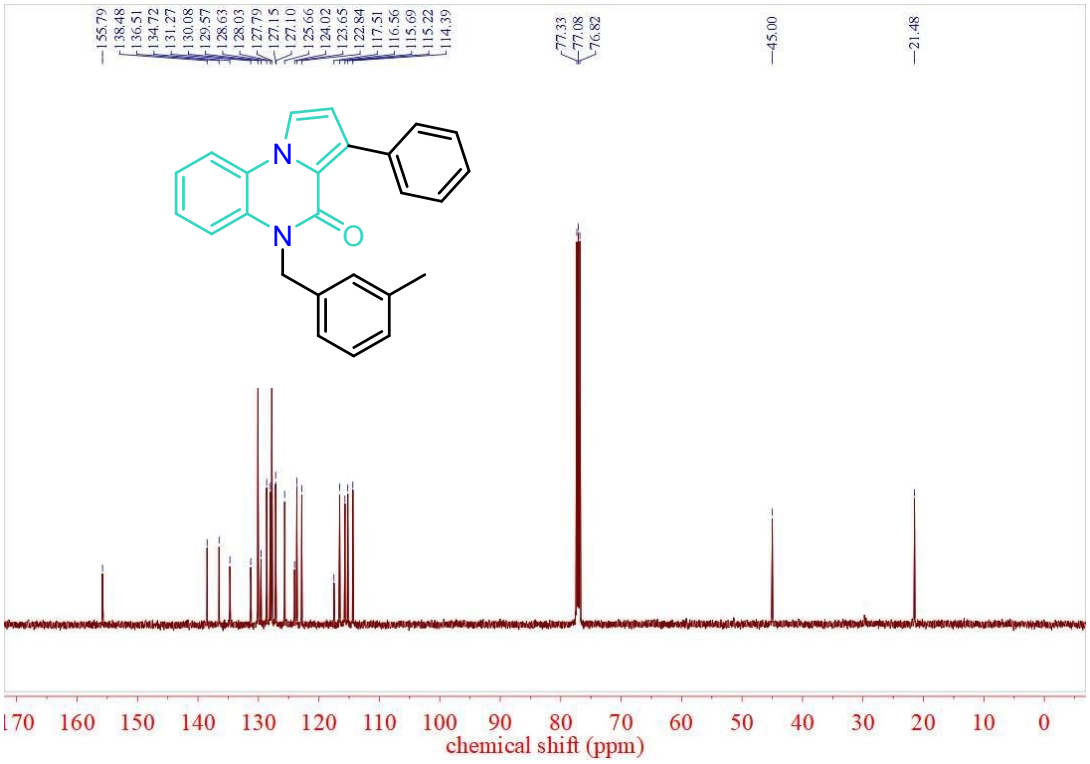
^{1}H NMR (500 MHz, $CDCl_3$) of compound **4i**



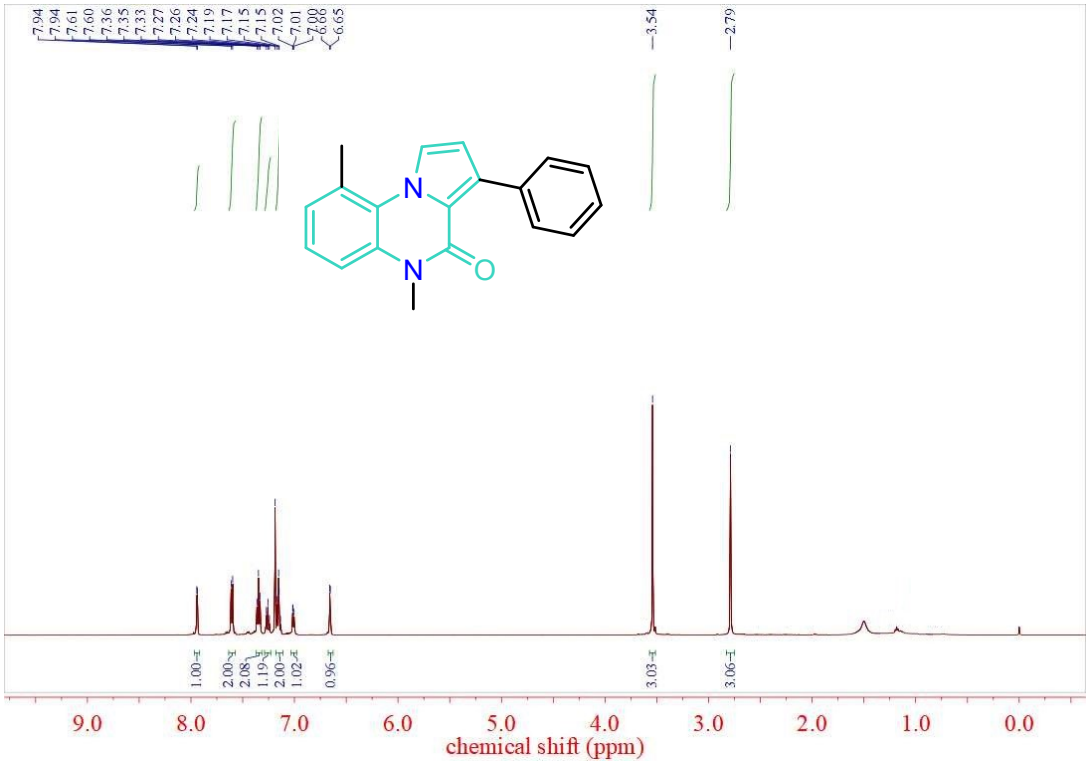
^{13}C NMR (126 MHz, $CDCl_3$) of compound **4i**



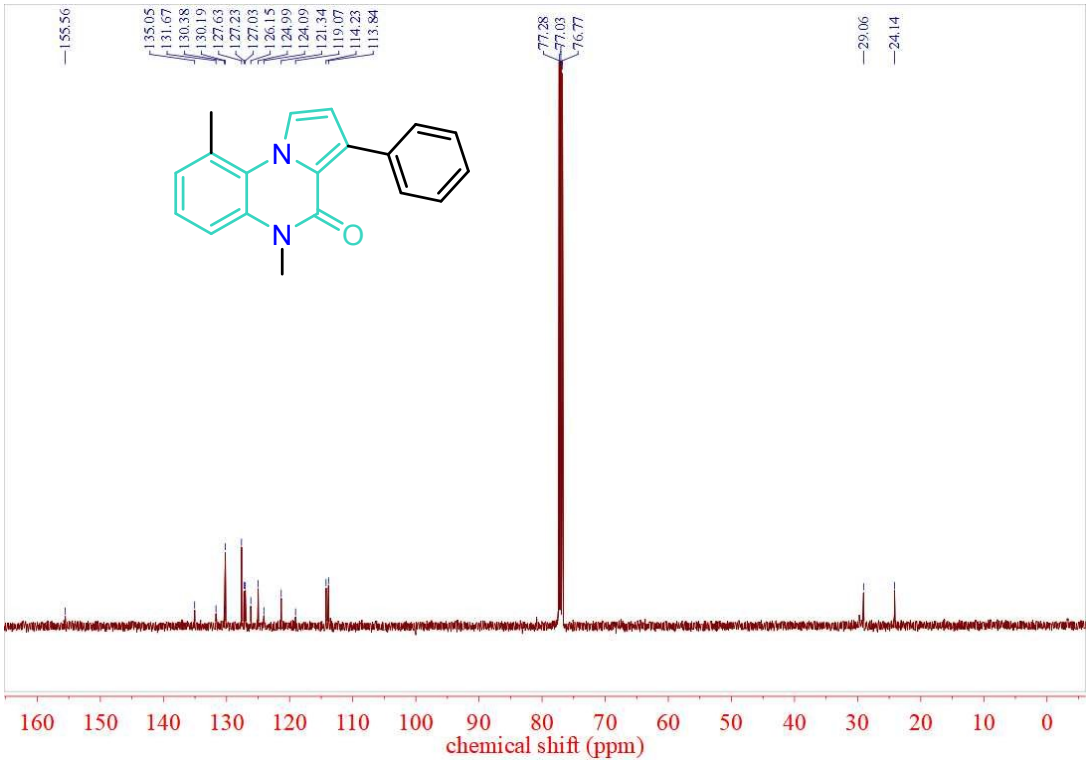
^{1}H NMR (500 MHz, $CDCl_3$) of compound **4j**



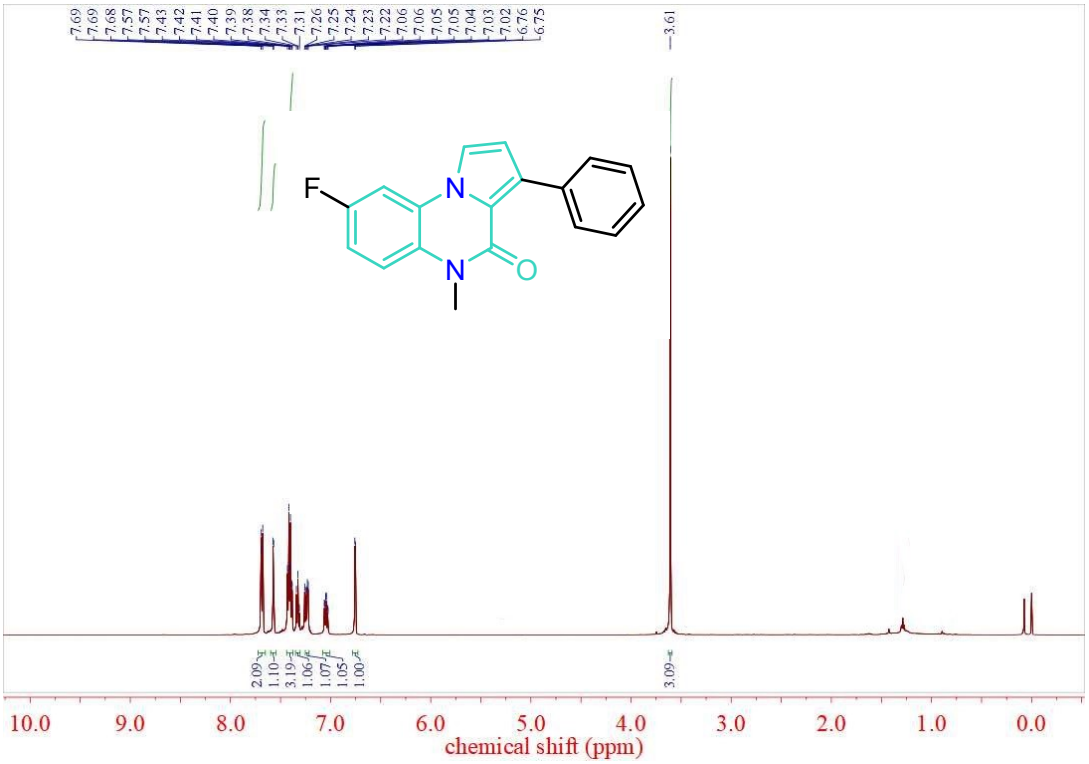
^{13}C NMR (126 MHz, $CDCl_3$) of compound **4j**



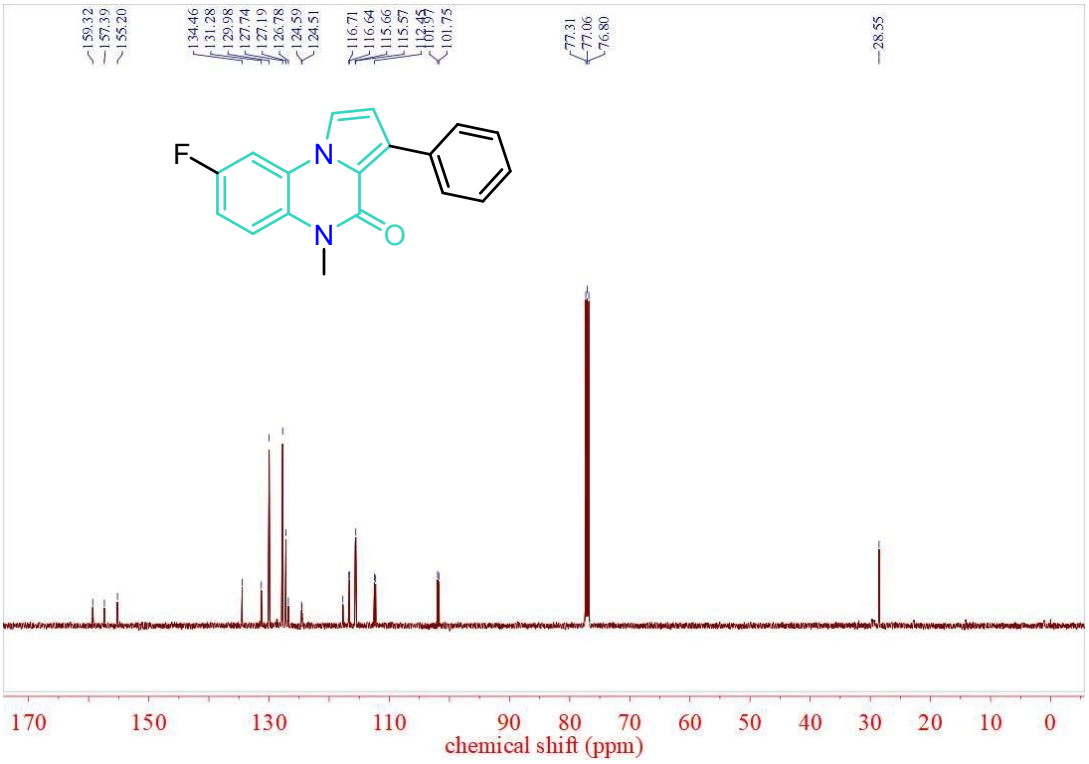
^{1}H NMR (500 MHz, $CDCl_3$) of compound **4k**



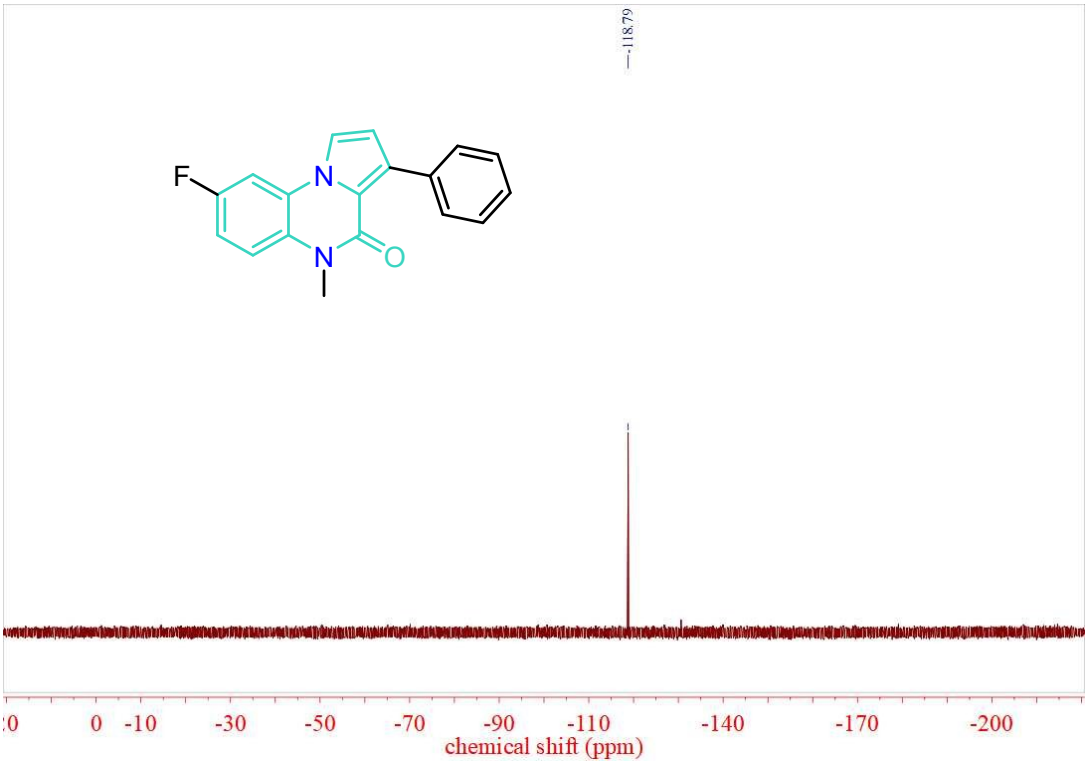
^{13}C NMR (126 MHz, $CDCl_3$) of compound **4k**



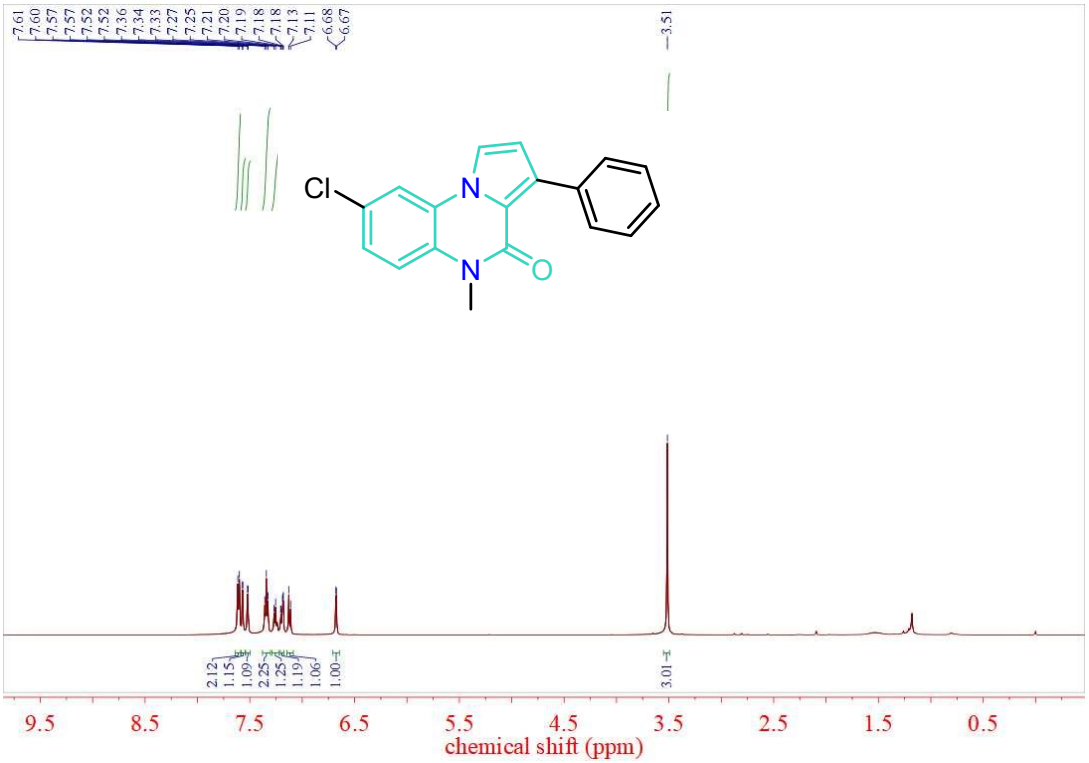
^{1}H NMR (500 MHz, $CDCl_3$) of compound **4l**



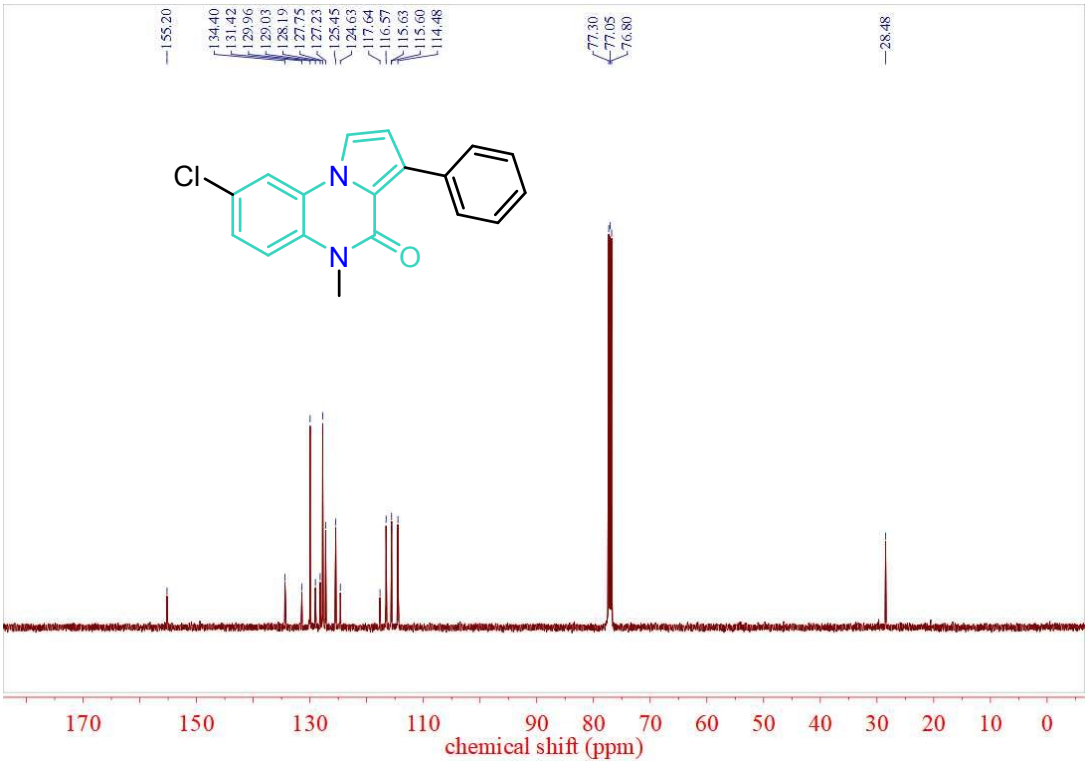
^{13}C NMR (126 MHz, $CDCl_3$) of compound **4l**



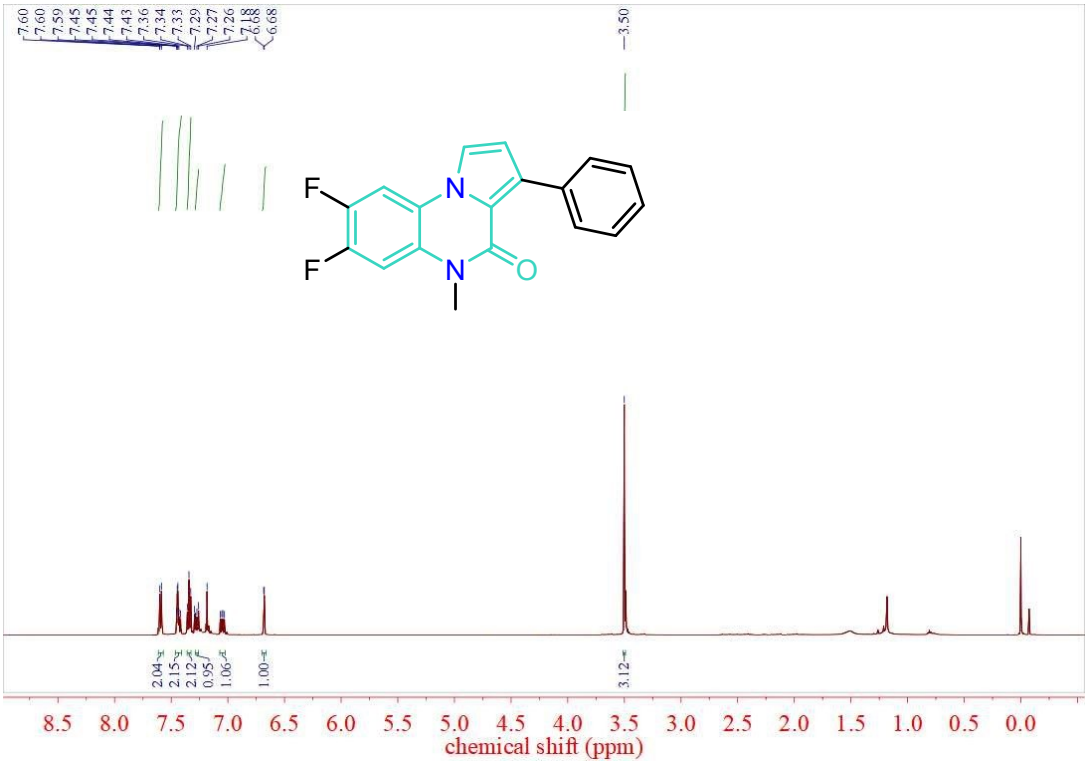
^{19}F NMR (471 MHz, $CDCl_3$) of compound **4l**



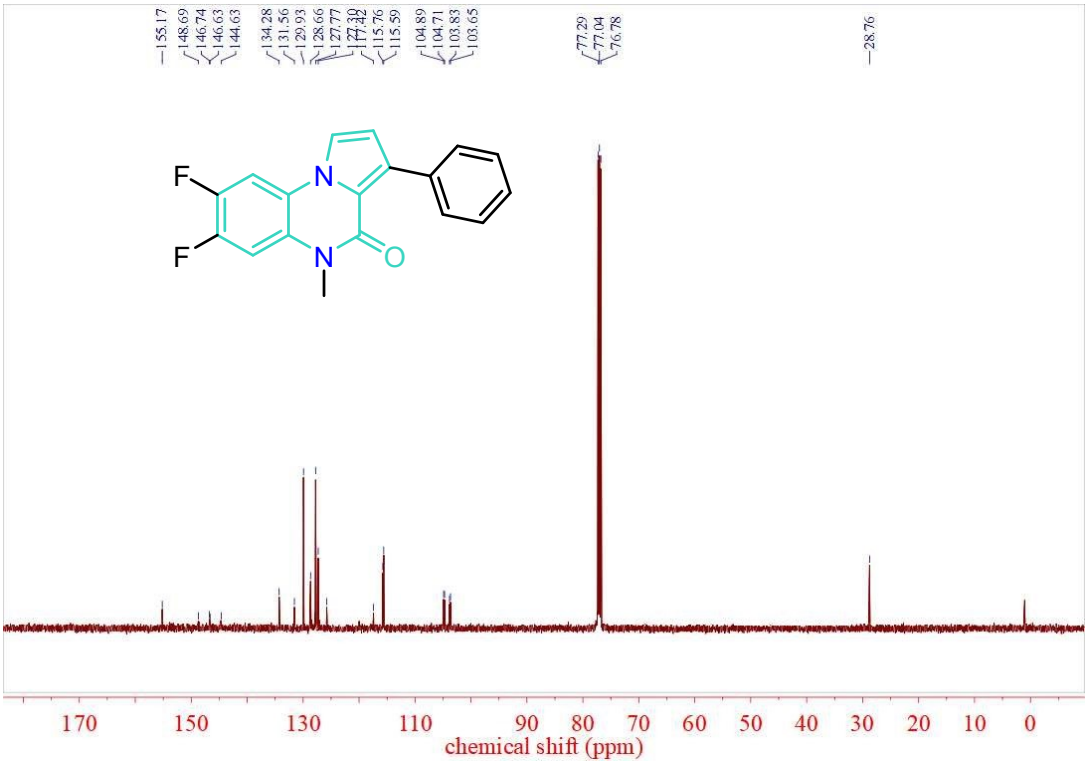
^{1}H NMR (500 MHz, $CDCl_3$) of compound **4m**



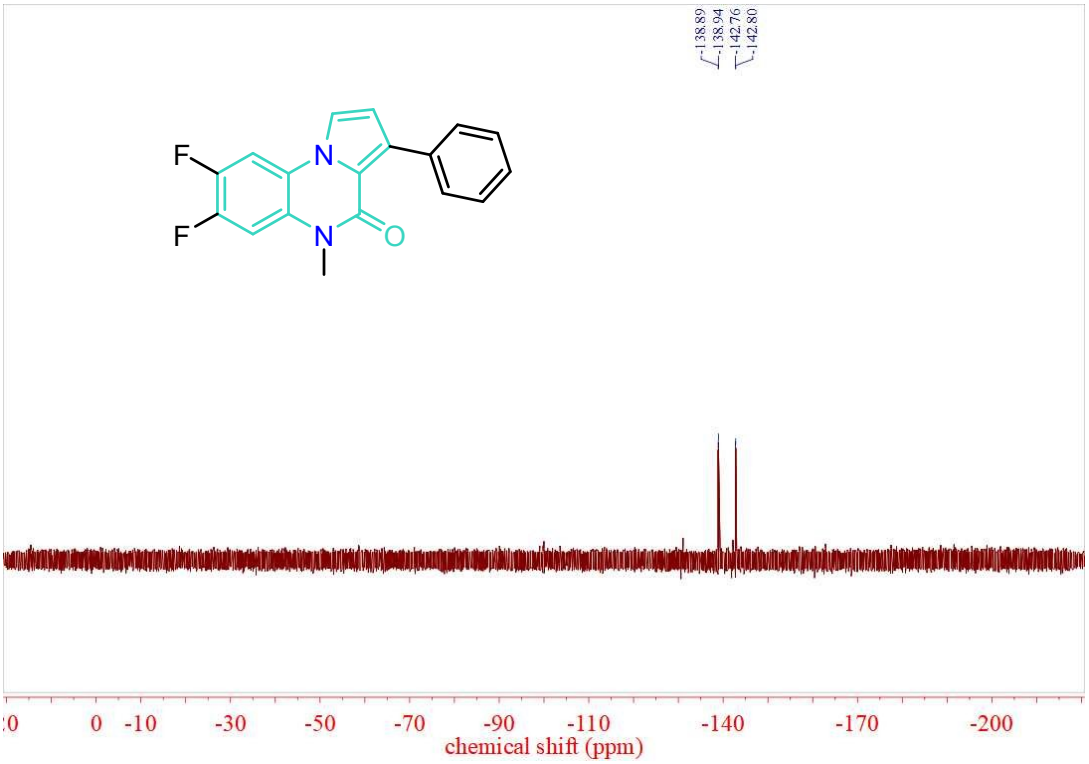
^{13}C NMR (126 MHz, $CDCl_3$) of compound **4m**



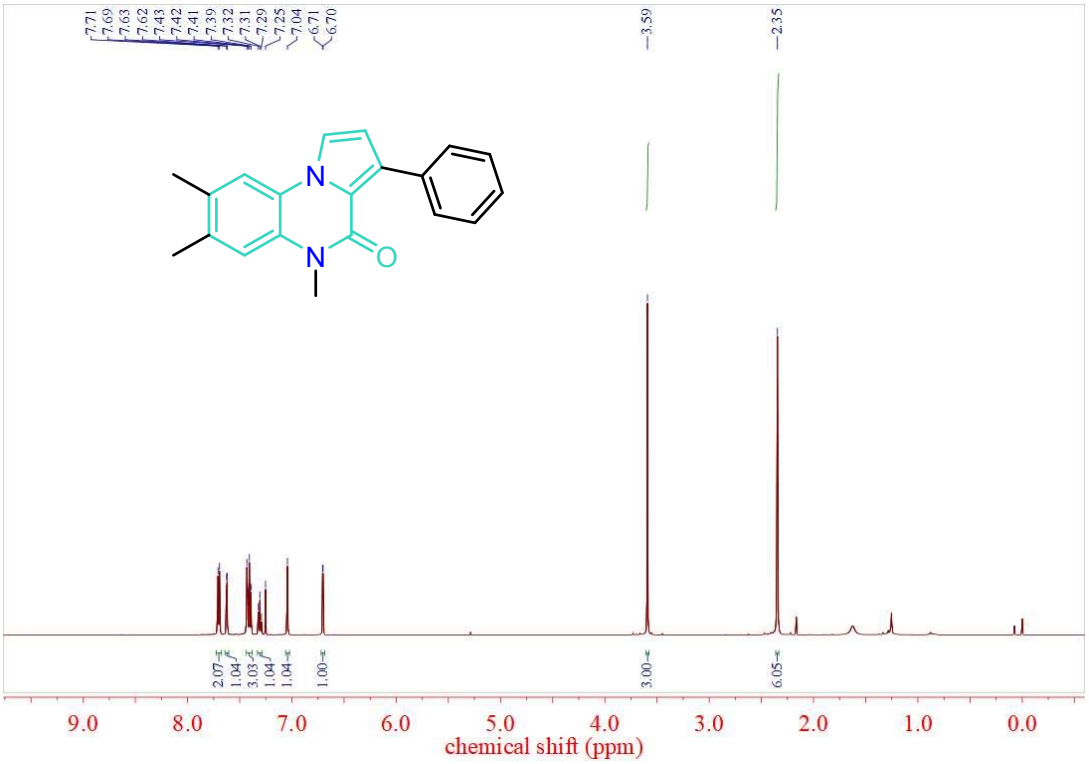
^{1}H NMR (500 MHz, $CDCl_3$) of compound **4n**



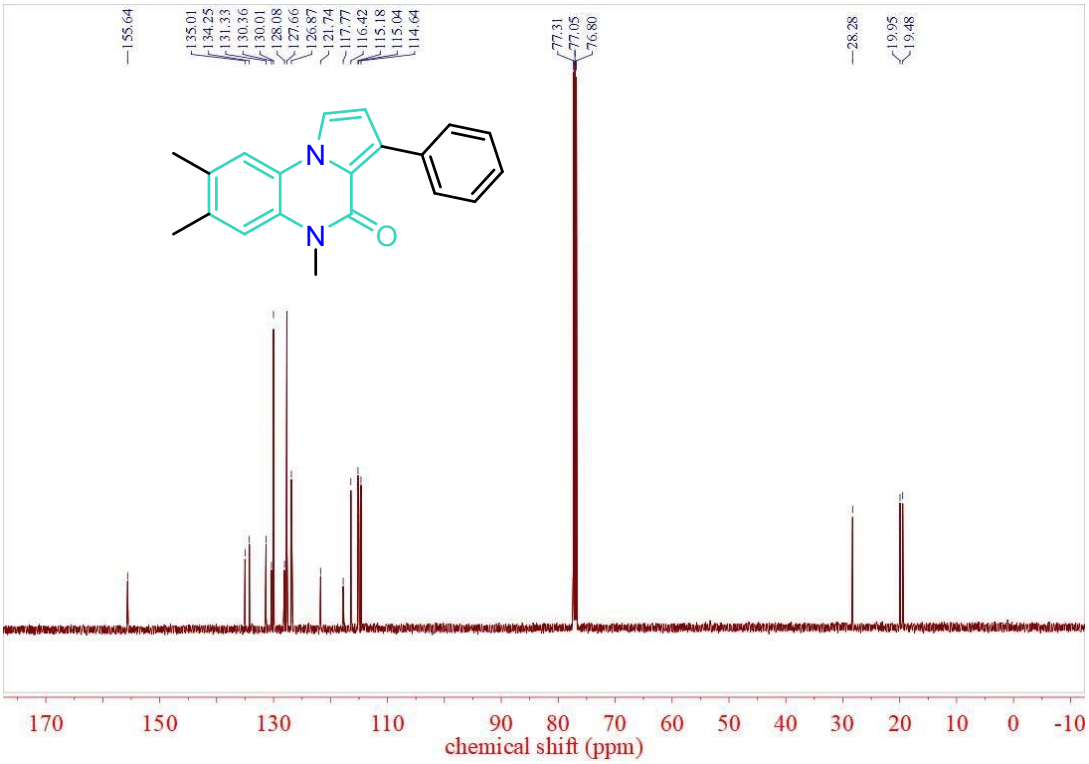
^{13}C NMR (126 MHz, $CDCl_3$) of compound **4n**



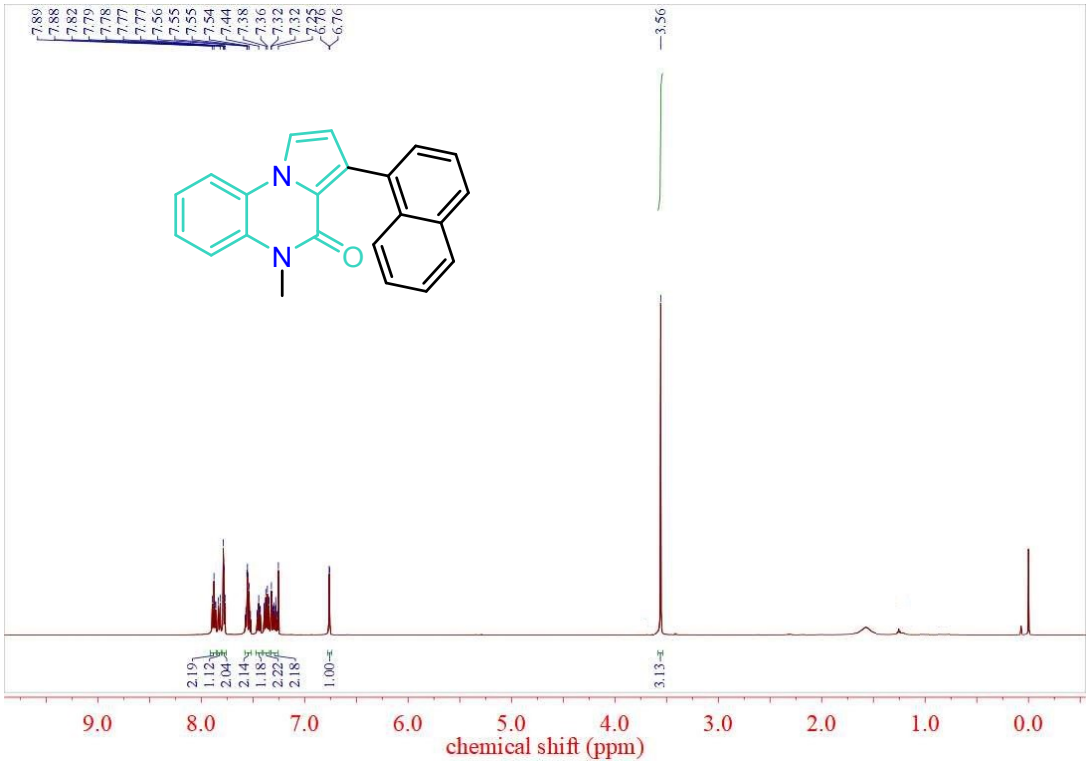
^{19}F NMR (471 MHz, $CDCl_3$) of compound **4n**



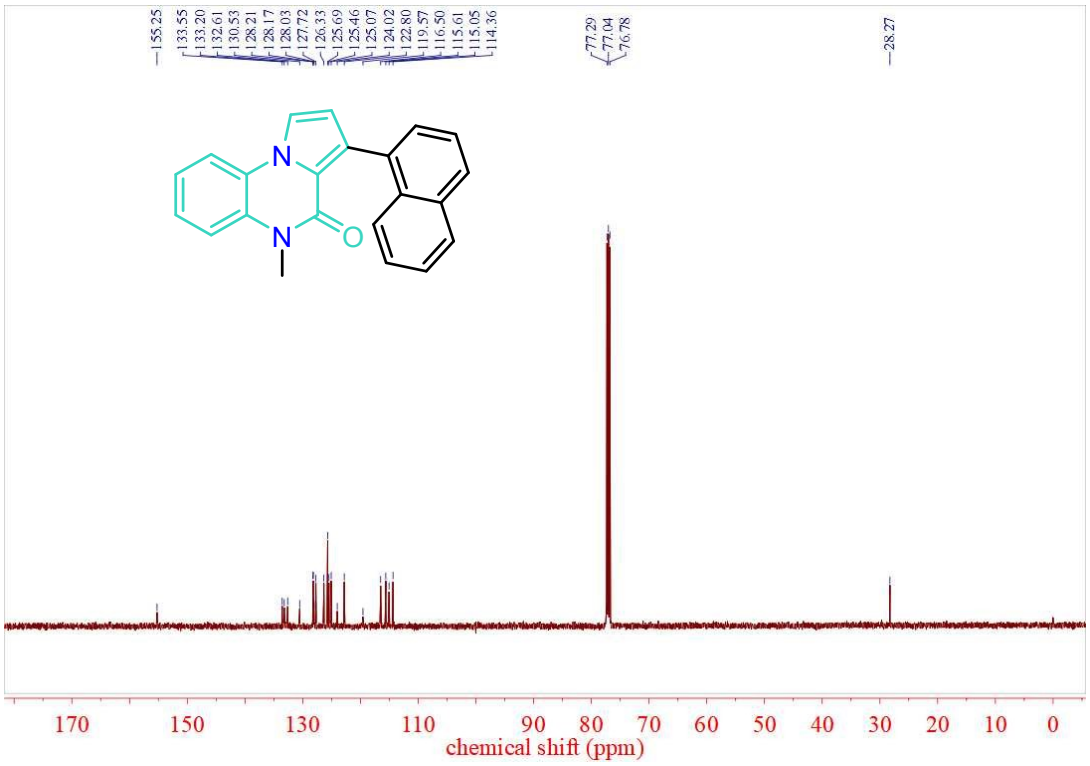
^{1}H NMR (500 MHz, $CDCl_3$) of compound **4o**



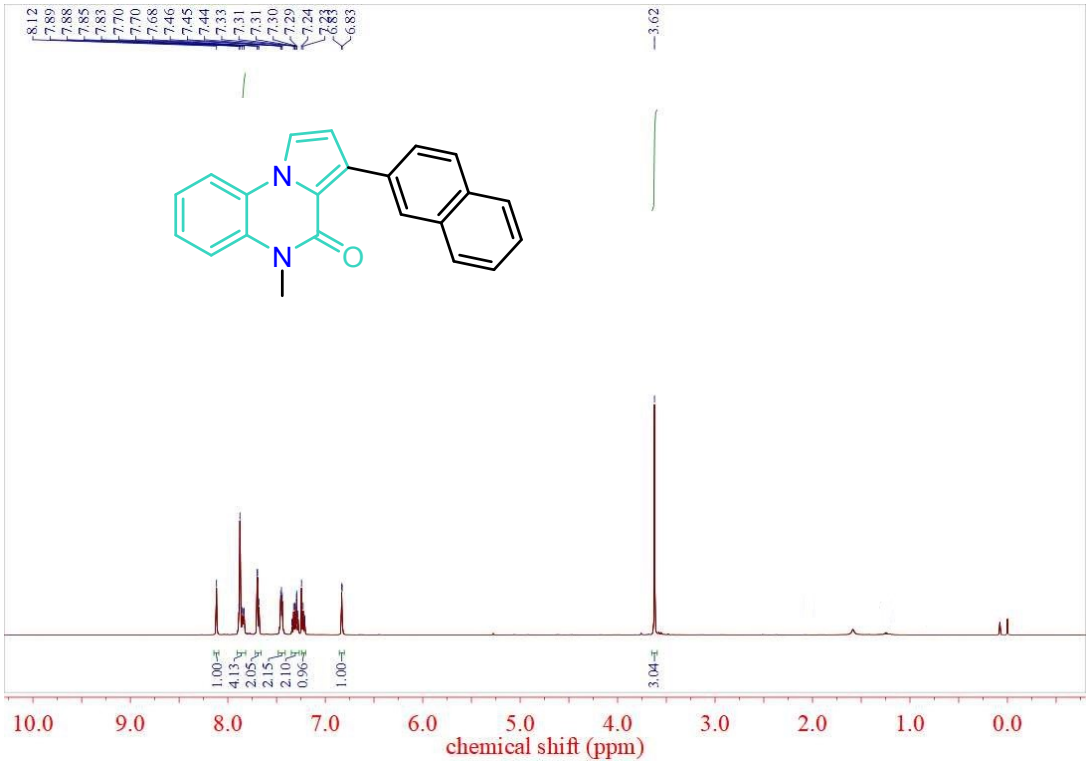
^{13}C NMR (126 MHz, $CDCl_3$) of compound **4o**



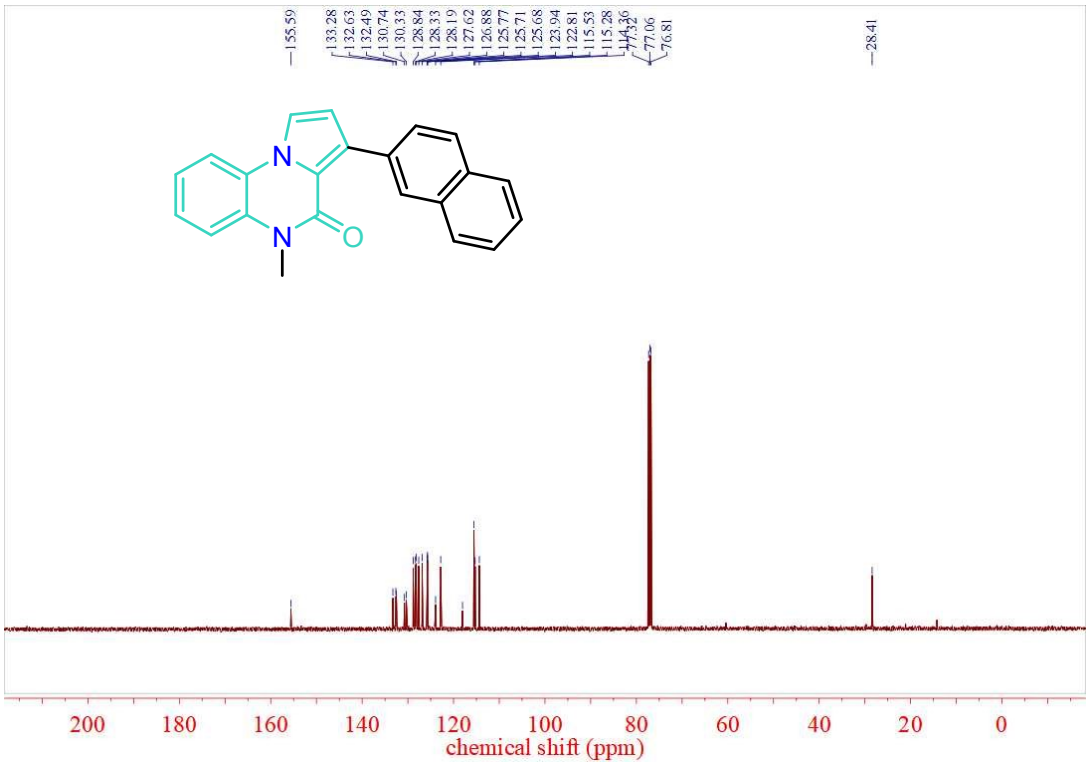
^{1}H NMR (500 MHz, $CDCl_3$) of compound **4p**



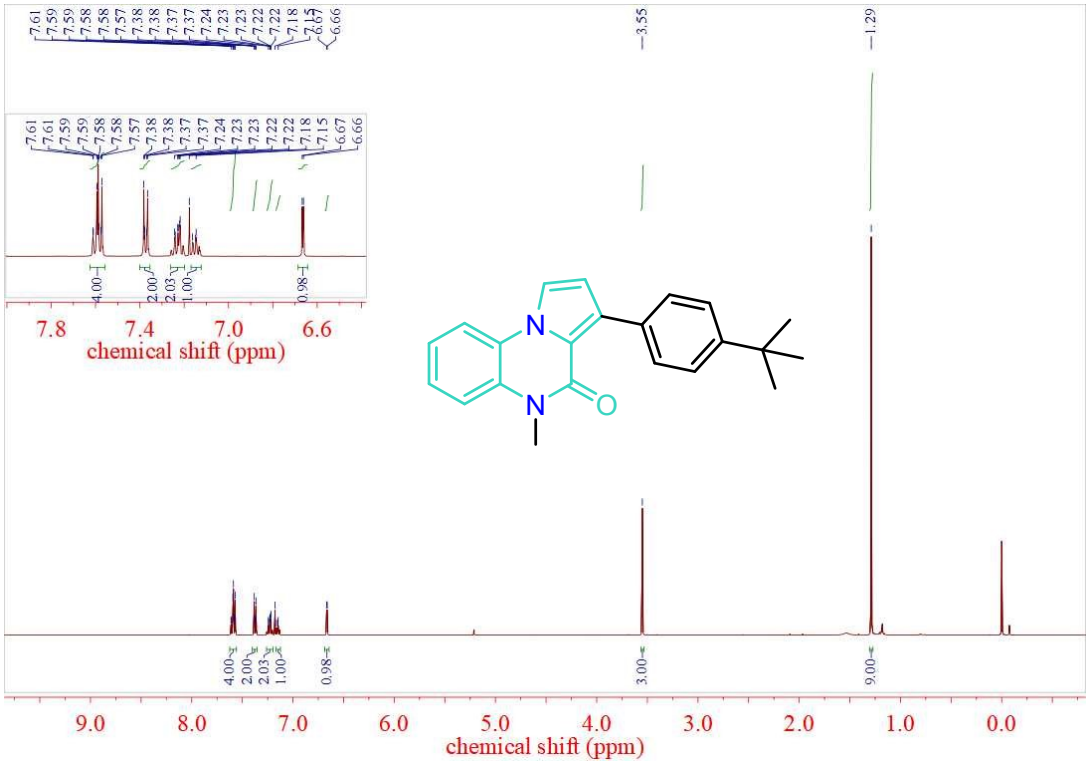
^{13}C NMR (126 MHz, $CDCl_3$) of compound **4p**



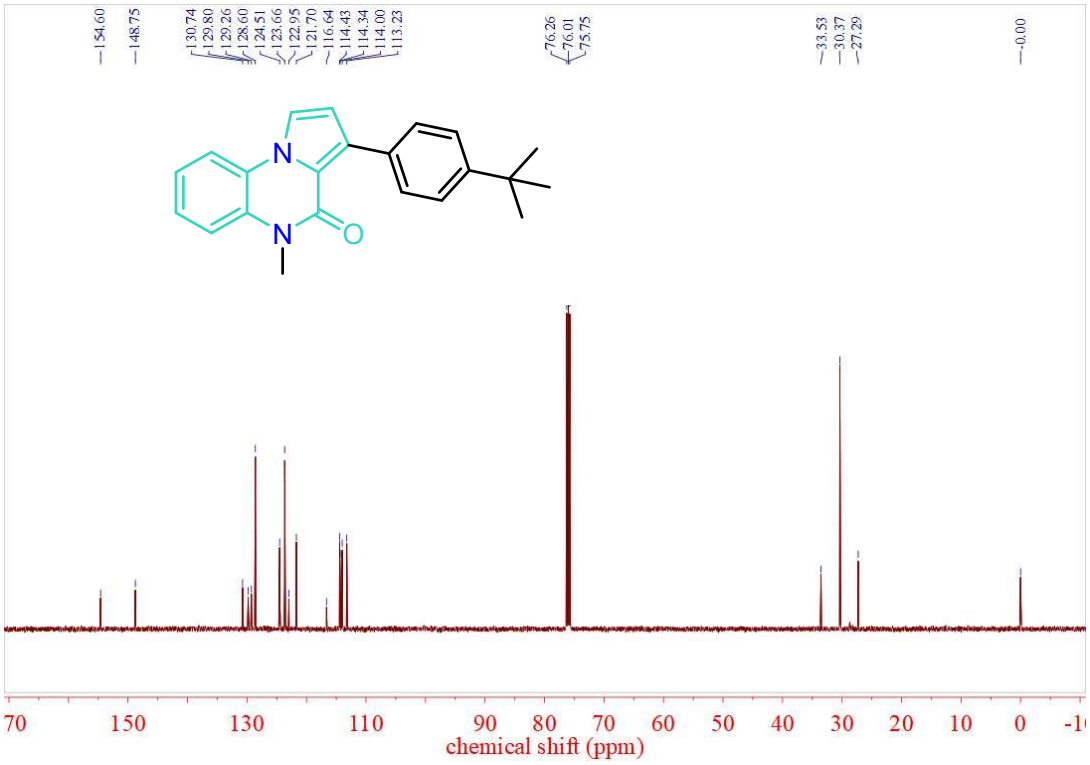
^{1}H NMR (500 MHz, $CDCl_3$) of compound **4q**



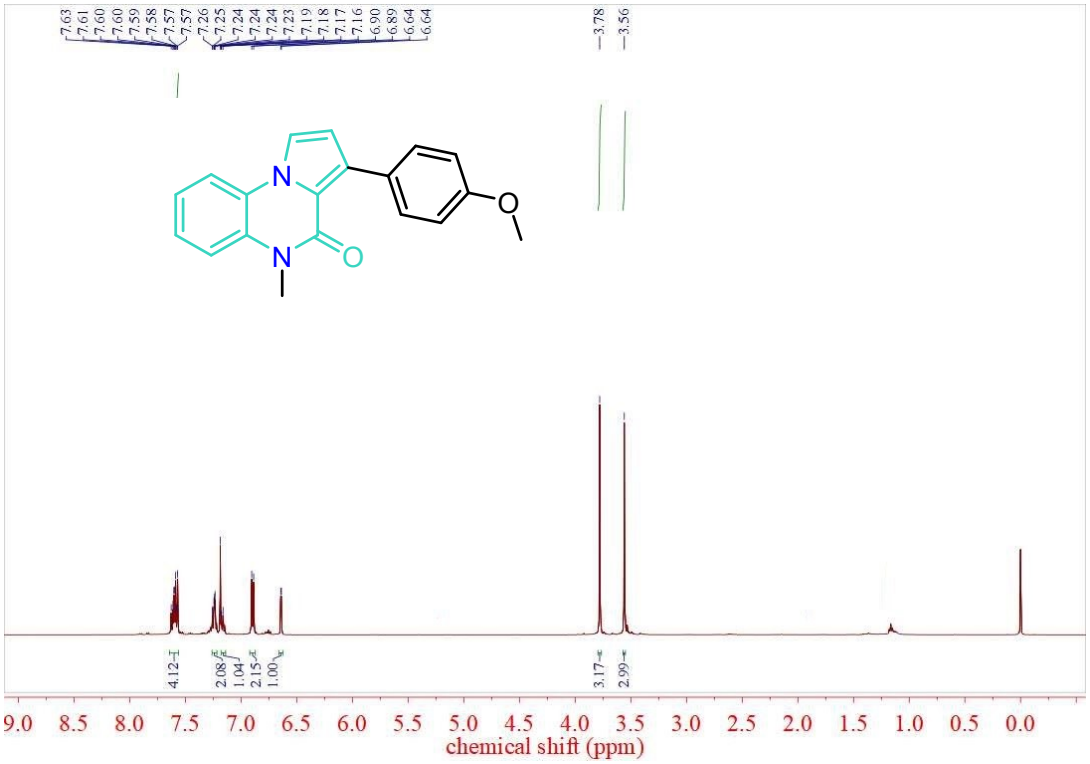
^{13}C NMR (126 MHz, $CDCl_3$) of compound **4q**



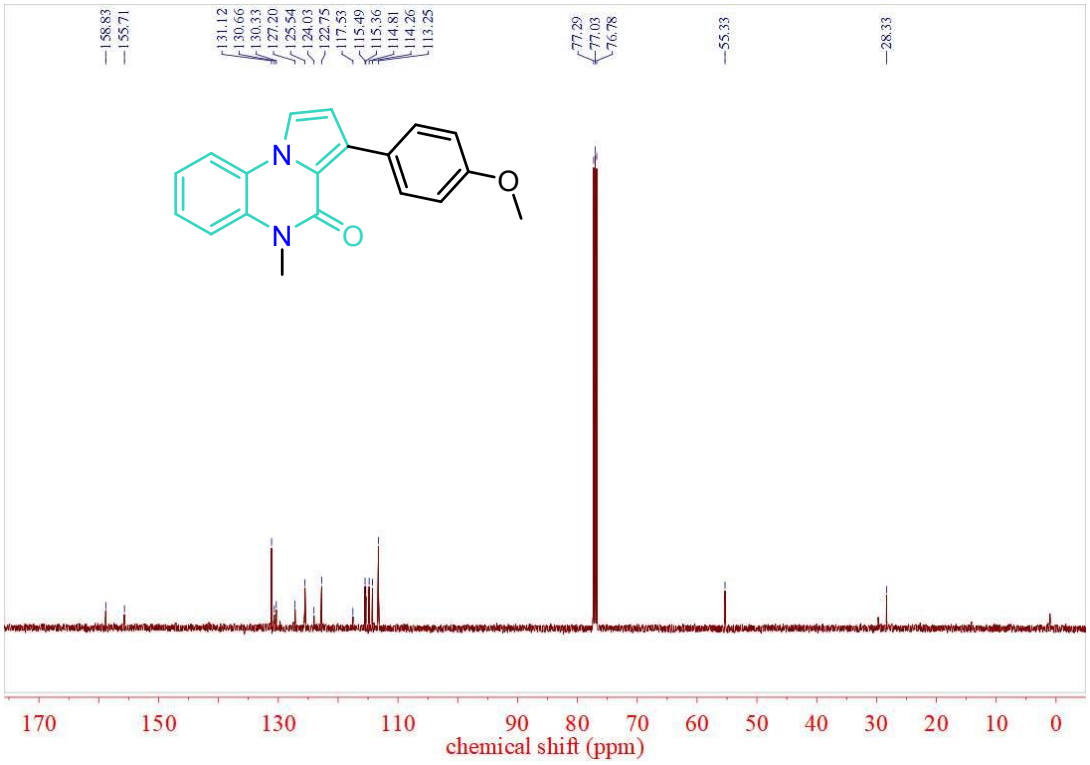
^{1}H NMR (500 MHz, $CDCl_3$) of compound **4r**



^{13}C NMR (126 MHz, $CDCl_3$) of compound **4r**



^{1}H NMR (500 MHz, $CDCl_3$) of compound **4s**



^{13}C NMR (126 MHz, $CDCl_3$) of compound **4s**