

## Supporting Information

# Energy-transfer photocatalysis for Minisci C–H (amino)alkylation of heteroarenes using oxime esters as dual-role reagents

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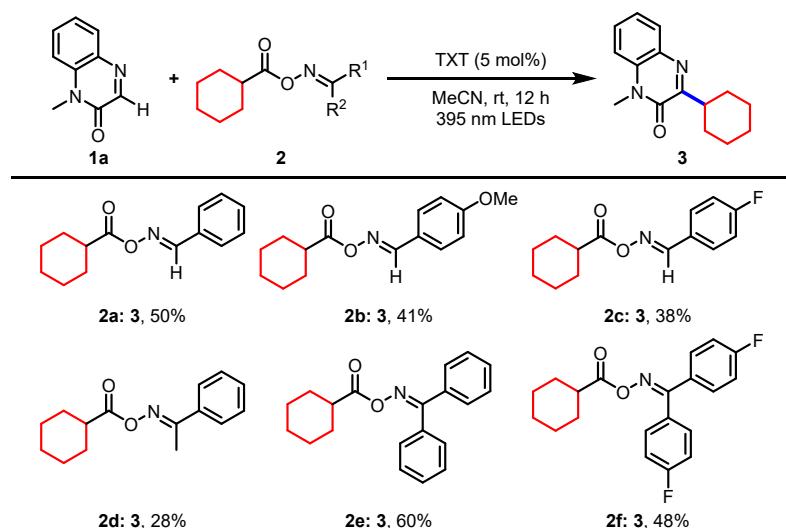
## **General Information**

All reagents and deuterated solvents were commercially available and used without further purification. The oxime esters were prepared according to previous references.<sup>1-3</sup> The quinoxalinones on the basis of our early reports.<sup>4-6</sup> All products were separated by silica gel (200-300 mesh) column chromatography with petroleum ether (PE) (60-90°C) and ethyl acetate (EA). <sup>1</sup>H, <sup>13</sup>C and <sup>19</sup>F NMR spectra were recorded on a Bruker Advance 500 spectrometer at ambient temperature with CDCl<sub>3</sub> as solvent and tetramethylsilane (TMS) as the internal standard. Analytical thin layer chromatography (TLC) was performed on Merk precoated TLC (silica gel 60 F254) plates. Compounds for HRMS were analyzed by positive mode electrospray ionization (ESI) using Agilent 6530 QTOF mass spectrometer.

## 1. Experimental Section

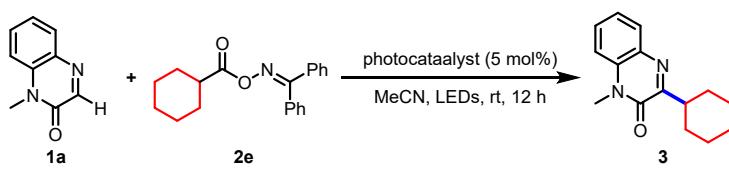
## 1.1 Details of Optimization

**Table S1.** Screening of oxime ester for the Minisci C–H (amino)alkylation.<sup>a,b</sup>



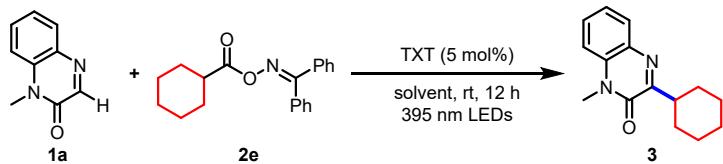
<sup>a</sup> Reaction conditions: **1a** (0.2 mmol), **2** (0.4 mmol), TXT (5 mol%), MeCN (1.0 mL), 395 nm LEDs, room temperature, N<sub>2</sub>, 12 h. <sup>b</sup> Isolated yields.

**Table S2.** Screening of catalyst for the Minisci C–H (amino)alkylation.<sup>a,b</sup>



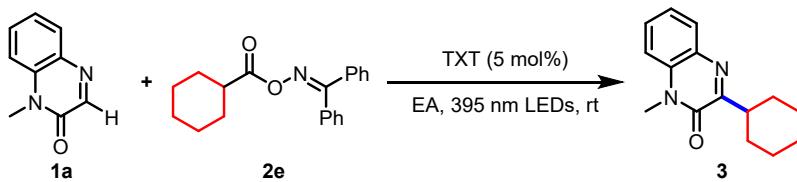
Entry	Photocatalyst	$E_T$ (kcal/mol)	Yield (%)
1	Thioxanthone (TXT)	65.5	59
2	[Ir(dF(CF <sub>3</sub> )ppy) <sub>2</sub> (dtbbpy)](PF <sub>6</sub> )	61.8	42
3	<i>fac</i> -Ir(ppy) <sub>3</sub>	58.1	n.d.
4	[Ru(bpy) <sub>3</sub> ](PF <sub>6</sub> ) <sub>2</sub>	46.5	n.d.
5	[Mes-Acr]ClO <sub>4</sub>	44.7	n.d.
6	None	-	n.d.

<sup>a</sup> Reaction conditions: **1a** (0.2 mmol), **2e** (0.4 mmol), photocatalyst (5 mol%), MeCN (1.0 mL), LEDs, room temperature, N<sub>2</sub>, 12 h. <sup>b</sup> Isolated yields are given.

**Table S3.** Screening of solvent for the Minisci C–H (amino)alkylation. <sup>a,b</sup>

Entry	Solvent	Yield (%)
1	MeCN	59
2	DCM	54
3	DMF	trace
4	Acetone	41
5	EA	68
6	MeOH	27
7	PEG	trace
8	H <sub>2</sub> O	trace
9	DCM/H <sub>2</sub> O (v/v = 1:1)	19
10	EA/H <sub>2</sub> O (v/v = 1:1)	24

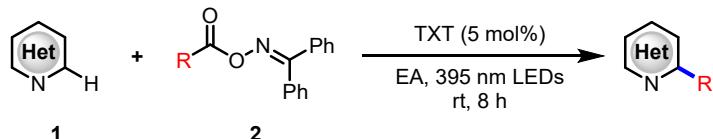
<sup>a</sup> Reaction conditions: **1a** (0.2 mmol), **2e** (0.4 mmol), TXT (5 mol%), solvent (1.0 mL), 395 nm LEDs, room temperature, N<sub>2</sub>, 12 h. <sup>b</sup> Isolated yields are given.

**Table S4.** Screening of reaction time for the Minisci C–H (amino)alkylation. <sup>a,b</sup>

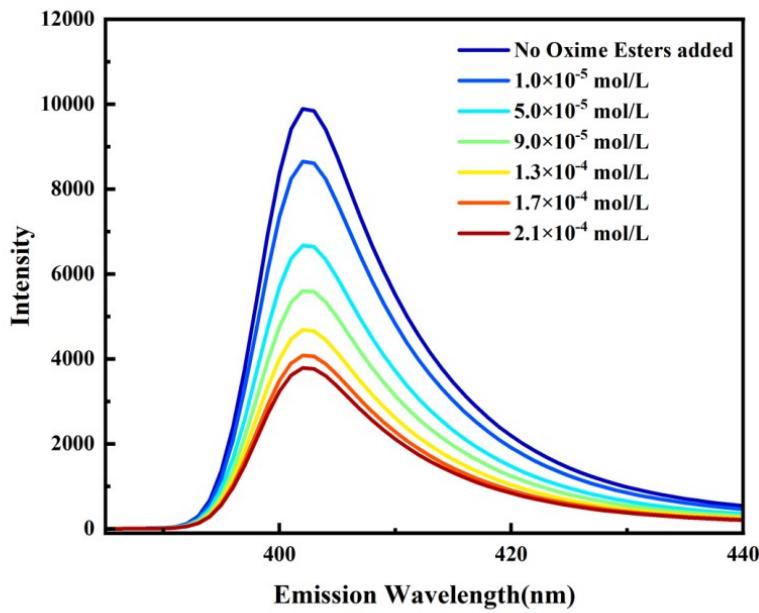
Entry	Reaction time (hour)	Yield (%)
1	2	26
2	4	43
3	6	59
4	8	71
5	10	73
6	12	68

<sup>a</sup> Reaction conditions: **1a** (0.2 mmol), **2e** (0.4 mmol), TXT (5 mol%), EA (1.0 mL), 395 nm LEDs, room temperature, N<sub>2</sub>. <sup>b</sup> Isolated yields are given.

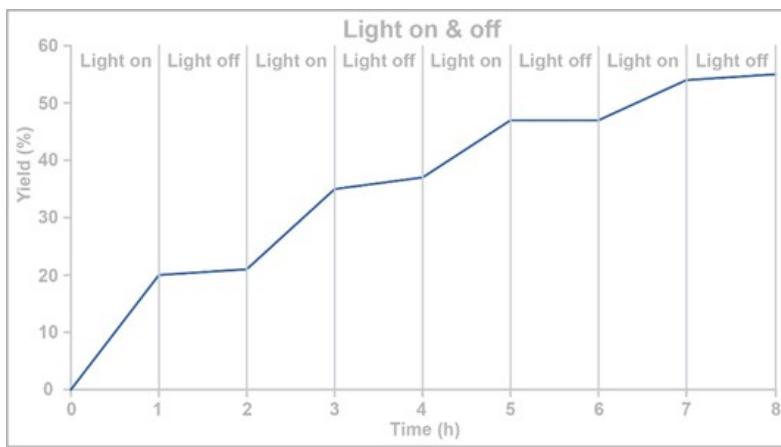
## 1.2 General Procedure for Photoinduced Minisci C–H (Amino)alkylation



A mixture of heteroarenes (**1**) (0.2 mmol), oxime ester (**2**) (0.4 mmol), thioxanthone (TXT) (5 mol%) and EA (2 mL) in a 25-mL tube was stirred under N<sub>2</sub> with the irradiation of 395 nm LEDs (10 W) for 8 h. After completing the reaction as indicated by TLC, a saturated NaHCO<sub>3</sub> solution was added to the mixture. The mixture was then extracted with EA, and the collected organic layer was washed with brine, and dried with MgSO<sub>4</sub>. The solvent was removed *in vacuo*, and the obtained residue was further purified by silica gel column chromatography (200-300 mesh silica gel).



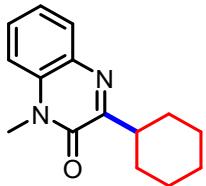
**Scheme S1.** Fluorescence quenching of thioxanthone by benzaldoxime ester



**Scheme S2** Visible light irradiation On/Off experiments.

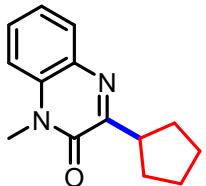
## 2. Characterization of Products

### 3-Cyclohexyl-1-methylquinoxalin-2(1*H*)-one (3)<sup>7</sup>



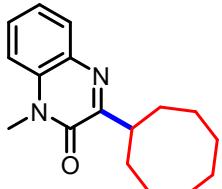
Obtained as a white solid (71% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.84 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.50 (ddd, *J* = 8.6, 7.3, 1.5 Hz, 1H), 7.36 – 7.28 (m, 1H), 7.28 (dd, *J* = 8.4, 1.2 Hz, 1H), 3.70 (s, 3H), 3.35 (tt, *J* = 11.6, 3.3 Hz, 1H), 1.99 – 1.92 (m, 2H), 1.87 (dt, *J* = 13.0, 3.4 Hz, 2H), 1.81 – 1.72 (m, 1H), 1.58 (qd, *J* = 12.5, 3.1 Hz, 2H), 1.47 (qt, *J* = 12.9, 3.3 Hz, 2H), 1.32 (dddd, *J* = 16.4, 12.7, 8.2, 4.3 Hz, 1H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 164.3, 154.5, 132.9, 132.8, 129.7, 129.4, 123.4, 113.5, 40.8, 30.5, 29.1, 26.3, 26.2.

### 3-Cyclopentyl-1-methylquinoxalin-2(1*H*)-one (4)<sup>7</sup>



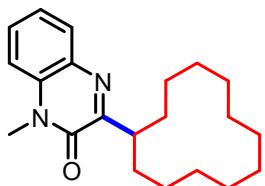
Obtained as a white solid (72% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.82 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.50 (ddd, *J* = 8.6, 7.3, 1.6 Hz, 1H), 7.34 – 7.27 (m, 2H), 3.72 (d, *J* = 8.2 Hz, 1H), 3.70 (s, 3H), 2.10 – 2.03 (m, 2H), 1.92 (dq, *J* = 12.3, 8.1 Hz, 2H), 1.82 (tdd, *J* = 12.2, 9.5, 5.2 Hz, 2H), 1.73 (ddd, *J* = 12.3, 8.0, 4.3 Hz, 2H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 163.7, 155.0, 133.0, 132.7, 129.8, 129.3, 123.4, 113.4, 42.7, 30.8, 29.0, 26.0.

### 3-Cyclooctyl-1-methylquinoxalin-2(1*H*)-one (5)<sup>7</sup>



Obtained as a white solid (69% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.85 (d, *J* = 8.8 Hz, 1H), 7.18 (ddd, *J* = 8.7, 2.5, 1.2 Hz, 1H), 7.10 (d, *J* = 2.4 Hz, 1H), 3.67 (s, 3H), 3.32 (tt, *J* = 11.5, 3.3 Hz, 1H), 1.98 – 1.90 (m, 2H), 1.87 (dt, *J* = 12.9, 3.2 Hz, 2H), 1.80 – 1.73 (m, 1H), 1.59 – 1.51 (m, 2H), 1.46 (td, *J* = 12.9, 9.3, 3.1 Hz, 2H), 1.31 (tt, *J* = 12.5, 3.7 Hz, 1H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 165.8, 154.5, 132.9, 132.7, 129.7, 129.3, 123.4, 113.4, 40.4, 30.6, 29.1, 26.7, 26.6, 25.9.

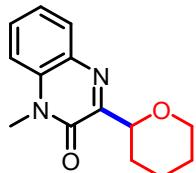
### 3-Cyclododecyl-1-methylquinoxalin-2(1*H*)-one (6)<sup>7</sup>



Obtained as a white solid (64% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.88 (d, *J* = 7.9 Hz, 1H), 7.51 (t, *J* = 7.8 Hz, 1H), 7.37 – 7.27 (m, 2H), 3.71 (s, 4H), 1.78 (q, *J* = 6.7 Hz, 3H), 1.61 (q, *J* = 6.2, 5.6

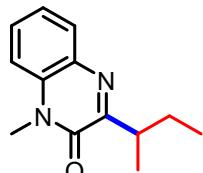
Hz, 2H), 1.50 – 1.42 (m, 6H), 1.39 – 1.28 (m, 9H), 0.84 (t,  $J$  = 6.3 Hz, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  164.5, 154.9, 132.9, 132.7, 129.7, 129.4, 123.4, 113.5, 36.2, 29.1, 28.1, 24.0, 23.9, 23.6, 23.3, 23.1.

### **1-Methyl-3-(tetrahydro-2*H*-pyran-2-yl)quinoxalin-2(*1H*)-one (7)<sup>8</sup>**



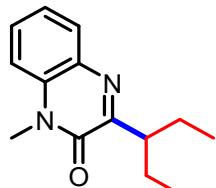
Obtained as a white solid (75% yield);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.98 (dd,  $J$  = 8.0, 1.5 Hz, 1H), 7.48 (ddd,  $J$  = 8.6, 7.3, 1.5 Hz, 1H), 7.29 – 7.23 (m, 2H), 4.93 (dd,  $J$  = 10.9, 2.1 Hz, 1H), 4.22 (dq,  $J$  = 9.9, 2.5 Hz, 1H), 3.63 (s, 4H), 2.08 (dt,  $J$  = 12.7, 2.1 Hz, 1H), 1.91 (dt,  $J$  = 11.6, 2.4 Hz, 1H), 1.79 – 1.70 (m, 2H), 1.59 – 1.49 (m, 2H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  158.8, 153.7, 133.0, 132.7, 130.6, 130.3, 123.7, 113.5, 76.5, 69.5, 30.2, 29.0, 25.6, 23.6.

### **3-(*sec*-Butyl)-1-methylquinoxalin-2(*1H*)-one (8)<sup>9</sup>**



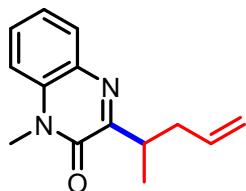
Obtained as a white solid (70% yield);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.84 (dd,  $J$  = 7.9, 1.6 Hz, 1H), 7.51 (ddd,  $J$  = 8.5, 7.3, 1.5 Hz, 1H), 7.36 – 7.27 (m, 2H), 3.70 (s, 3H), 3.46 (h,  $J$  = 6.9 Hz, 1H), 1.93 (dp,  $J$  = 14.4, 7.3 Hz, 1H), 1.61 (dt,  $J$  = 13.4, 7.2 Hz, 1H), 1.29 (d,  $J$  = 6.9 Hz, 3H), 0.94 (t,  $J$  = 7.4 Hz, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  164.5, 154.7, 132.9, 132.8, 129.8, 129.4, 123.4, 113.5, 37.8, 29.1, 27.5, 17.9, 12.1.

### **1-Methyl-3-(pentan-3-yl)quinoxalin-2(*1H*)-one (9)<sup>9</sup>**



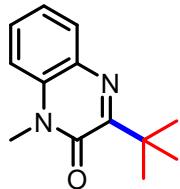
Obtained as a white solid (74% yield);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.85 (dd,  $J$  = 8.0, 1.3 Hz, 1H), 7.53 – 7.48 (m, 1H), 7.34 – 7.30 (m, 1H), 7.29 (d,  $J$  = 8.4 Hz, 1H), 3.70 (s, 3H), 3.38 – 3.31 (m, 1H), 1.90 – 1.83 (m, 2H), 1.70 (ddd,  $J$  = 13.4, 7.4, 5.9 Hz, 2H), 0.88 (t,  $J$  = 7.4 Hz, 6H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  163.8, 155.1, 132.8, 132.8, 129.8, 129.4, 123.3, 113.4, 44.6, 29.1, 25.7, 11.9.

### **1-Methyl-3-(pent-4-en-2-yl)quinoxalin-2(*1H*)-one (10)<sup>9</sup>**



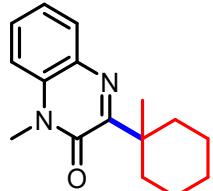
Obtained as a white solid (57% yield);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.85 (dd,  $J = 8.0, 1.6$  Hz, 1H), 7.52 (ddd,  $J = 8.5, 7.2, 1.5$  Hz, 1H), 7.36 – 7.28 (m, 2H), 5.90 – 5.80 (m, 1H), 5.05 (dq,  $J = 17.0, 1.7$  Hz, 1H), 4.97 (ddt,  $J = 10.2, 2.1, 1.1$  Hz, 1H), 3.70 (s, 3H), 3.63 (h,  $J = 6.9$  Hz, 1H), 2.66 (dtt,  $J = 14.2, 6.6, 1.4$  Hz, 1H), 2.34 (dtt,  $J = 13.9, 7.5, 1.2$  Hz, 1H), 1.30 (d,  $J = 6.9$  Hz, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  163.8, 154.6, 136.9, 132.9, 132.8, 129.8, 129.6, 123.4, 116.2, 113.5, 38.7, 36.0, 29.1, 17.9.

### **3-(*tert*-Butyl)-1-methylquinoxalin-2(1*H*)-one (11)<sup>10</sup>**



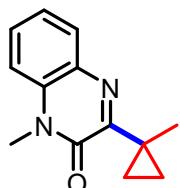
Obtained as a white solid (68% yield);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.83 (dd,  $J = 8.0, 1.5$  Hz, 1H), 7.50 (ddd,  $J = 8.6, 7.4, 1.5$  Hz, 1H), 7.33 – 7.25 (m, 2H), 3.67 (s, 3H), 1.49 (s, 9H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  165.3, 153.8, 133.3, 132.2, 130.1, 129.5, 123.2, 113.3, 39.5, 28.8, 27.9.

### **1-Methyl-3-(1-methylcyclohexyl)quinoxalin-2(1*H*)-one (12)<sup>10</sup>**



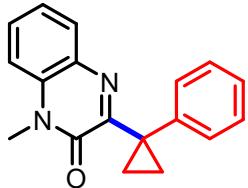
Obtained as a white solid (61% yield);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.84 (dd,  $J = 7.9, 1.5$  Hz, 1H), 7.50 (ddd,  $J = 8.5, 7.3, 1.5$  Hz, 1H), 7.31 (ddd,  $J = 8.3, 7.3, 1.2$  Hz, 1H), 7.29 – 7.25 (m, 1H), 3.67 (s, 3H), 2.46 (ddd,  $J = 12.3, 7.6, 3.3$  Hz, 2H), 1.66 (ddd,  $J = 13.0, 8.7, 3.7$  Hz, 2H), 1.58 (td,  $J = 7.4, 3.9$  Hz, 2H), 1.51 (ddd,  $J = 8.7, 4.4, 2.6$  Hz, 2H), 1.48 – 1.43 (m, 2H), 1.43 (s, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  164.8, 153.8, 133.1, 132.3, 130.1, 129.5, 123.1, 113.2, 43.0, 35.8, 28.8, 26.6, 24.5, 22.9.

### **1-Methyl-3-(1-methylcyclopropyl)quinoxalin-2(1*H*)-one (13)**



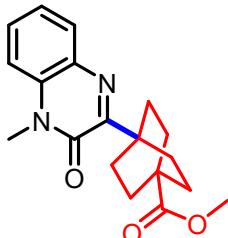
Obtained as a white solid (59% yield); M. P. = 108-109 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.82 (dd,  $J = 7.9, 1.5$  Hz, 1H), 7.51 (ddd,  $J = 8.6, 7.3, 1.5$  Hz, 1H), 7.35 – 7.30 (m, 1H), 7.28 (dd,  $J = 8.4, 1.2$  Hz, 1H), 3.69 (s, 3H), 1.57 (s, 3H), 1.28 (q,  $J = 4.2$  Hz, 2H), 0.86 – 0.79 (m, 2H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  162.0, 154.4, 133.3, 132.5, 129.8, 129.6, 123.4, 113.4, 28.9, 22.4, 22.3, 13.9; HRMS (ESI+): Calculated for  $\text{C}_{13}\text{H}_{14}\text{N}_2\text{O}$ :  $[\text{M}+\text{H}]^+$  215.1179, Found 215.1164.

### **1-Methyl-3-(1-phenylcyclopropyl)quinoxalin-2(1*H*)-one (14)<sup>9</sup>**



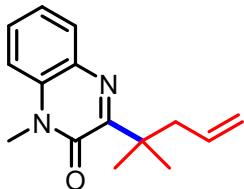
Obtained as a white solid (65% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.90 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.55 – 7.49 (m, 1H), 7.49 – 7.41 (m, 2H), 7.35 – 7.31 (m, 1H), 7.29 – 7.22 (m, 3H), 7.20 – 7.12 (m, 1H), 3.60 (s, 3H), 1.54 – 1.45 (m, 2H), 1.42 – 1.34 (m, 2H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 160.4, 154.4, 141.9, 133.6, 132.5, 130.1, 130.0, 128.6, 128.2, 126.5, 123.4, 113.5, 30.7, 29.0, 13.7.

### **Methyl 4-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)bicyclo[2.2.2]octane-1-carboxylate (15)<sup>9</sup>**



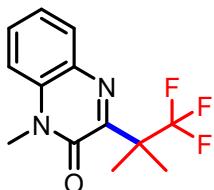
Obtained as a white solid (69% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.81 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.51 (ddd, *J* = 8.5, 7.3, 1.6 Hz, 1H), 7.34 – 7.29 (m, 1H), 7.27 (dd, *J* = 8.3, 1.2 Hz, 1H), 3.68 (s, 3H), 3.66 (s, 3H), 2.22 – 2.12 (m, 6H), 1.96 – 1.89 (m, 6H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 178.6, 163.7, 153.8, 133.1, 132.3, 130.1, 129.7, 123.3, 113.3, 51.7, 40.1, 39.1, 28.8, 28.2, 27.6.

### **1-Methyl-3-(2-methylpent-4-en-2-yl)quinoxalin-2(1*H*)-one (16)<sup>9</sup>**



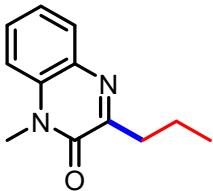
Obtained as a white solid (43% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.84 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.51 (ddd, *J* = 8.6, 7.3, 1.6 Hz, 1H), 7.31 (ddd, *J* = 8.2, 7.3, 1.2 Hz, 1H), 7.28 (d, *J* = 1.2 Hz, 1H), 5.71 (ddt, *J* = 17.5, 10.1, 7.4 Hz, 1H), 5.01 (ddt, *J* = 17.0, 2.6, 1.4 Hz, 1H), 4.91 (ddt, *J* = 10.2, 2.3, 1.1 Hz, 1H), 3.67 (s, 3H), 2.78 (d, *J* = 7.3 Hz, 2H), 1.46 (s, 6H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 164.2, 153.8, 135.6, 133.3, 132.2, 130.2, 129.6, 123.2, 116.9, 113.3, 44.1, 42.8, 28.8, 25.9.

### **1-Methyl-3-(1,1,1-trifluoro-2-methylpropan-2-yl)quinoxalin-2(1*H*)-one (17)<sup>9</sup>**



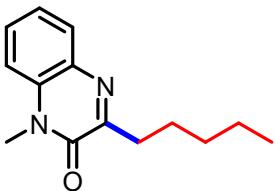
Obtained as a white solid (72% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.88 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.58 (ddd, *J* = 8.5, 7.3, 1.5 Hz, 1H), 7.35 (ddd, *J* = 8.3, 7.3, 1.2 Hz, 1H), 7.30 (dd, *J* = 8.4, 1.2 Hz, 1H), 3.69 (s, 3H), 1.80 – 1.74 (m, 6H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 156.0, 153.3, 133.4, 131.6, 130.9, 130.9, 127.9 (q, *J* = 284.8 Hz), 123.6, 113.4, 49.1 (d, *J* = 25.2 Hz), 29.1, 20.2 (d, *J* = 2.5 Hz); <sup>19</sup>F NMR (471 MHz, CDCl<sub>3</sub>) δ -73.59.

### **1-Methyl-3-propylquinoxalin-2(1*H*)-one (18)<sup>9</sup>**



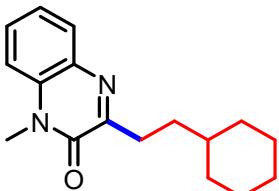
Obtained as a white solid (63% yield); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.83 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.52 (ddd, *J* = 8.5, 7.4, 1.5 Hz, 1H), 7.36 – 7.28 (m, 2H), 3.71 (s, 3H), 2.99 – 2.87 (m, 2H), 1.83 (h, *J* = 7.4 Hz, 2H), 1.05 (t, *J* = 7.4 Hz, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 161.2, 155.0, 133.1, 132.7, 129.6, 129.5, 123.5, 113.6, 36.3, 29.1, 20.3, 14.1.

### **1-Methyl-3-pentylquinoxalin-2(1*H*)-one (19)<sup>9</sup>**



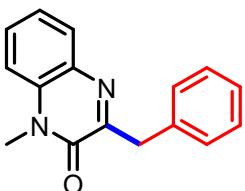
Obtained as a white solid (61% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.82 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.51 (ddd, *J* = 8.6, 7.2, 1.5 Hz, 1H), 7.36 – 7.17 (m, 2H), 3.69 (s, 3H), 2.98 – 2.88 (m, 2H), 1.89 – 1.68 (m, 2H), 1.50 – 1.34 (m, 4H), 0.92 (t, *J* = 7.1 Hz, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 161.4, 154.9, 133.1, 132.7, 129.6, 129.4, 123.5, 113.5, 34.3, 31.8, 29.0, 26.5, 22.5, 14.0.

### **3-(2-Cyclohexylethyl)-1-methylquinoxalin-2(1*H*)-one (20)<sup>9</sup>**



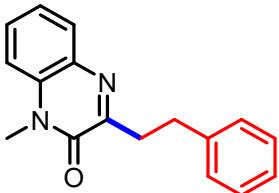
Obtained as a white solid (59% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.82 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.51 (ddd, *J* = 8.5, 7.3, 1.6 Hz, 1H), 7.32 (ddd, *J* = 8.3, 7.3, 1.3 Hz, 1H), 7.28 (dd, *J* = 8.4, 1.2 Hz, 1H), 3.69 (s, 3H), 3.07 – 2.87 (m, 2H), 1.87 – 1.80 (m, 2H), 1.77 – 1.60 (m, 5H), 1.38 (ddd, *J* = 11.0, 7.5, 4.1 Hz, 1H), 1.29 – 1.14 (m, 3H), 1.06 – 0.93 (m, 2H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 161.7, 154.9, 133.1, 132.7, 129.5, 129.4, 123.5, 113.5, 37.8, 34.2, 33.2, 31.9, 29.0, 26.7, 26.4.

### **3-Benzyl-1-methylquinoxalin-2(1*H*)-one (21)<sup>8</sup>**



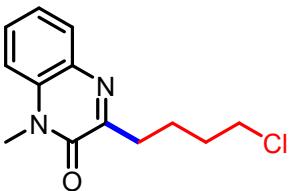
Obtained as a white solid (49% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.87 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.53 (ddd, *J* = 8.5, 7.3, 1.5 Hz, 1H), 7.51 – 7.41 (m, 2H), 7.34 (td, *J* = 7.8, 7.3, 1.2 Hz, 1H), 7.32 – 7.26 (m, 3H), 4.28 (s, 2H), 3.67 (s, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 159.3, 154.7, 137.0, 133.4, 132.6, 129.9, 129.9, 129.6, 128.4, 126.6, 123.6, 113.6, 40.7, 29.2.

### **1-Methyl-3-phenethylquinoxalin-2(1*H*)-one (22)<sup>10</sup>**



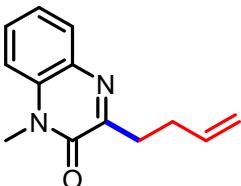
Obtained as a white solid (57% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.86 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.53 (ddd, *J* = 8.5, 7.2, 1.5 Hz, 1H), 7.38 – 7.26 (m, 6H), 7.24 – 7.15 (m, 1H), 3.71 (s, 3H), 3.32 – 3.25 (m, 2H), 3.18 – 3.10 (m, 2H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 160.1, 154.9, 141.6, 133.2, 132.6, 129.7, 129.7, 128.6, 128.4, 126.0, 123.6, 113.6, 36.0, 32.6, 29.1.

### **3-(4-Chlorobutyl)-1-methylquinoxalin-2(1*H*)-one (23)<sup>9</sup>**



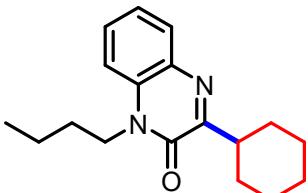
Obtained as a white solid (45% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.84 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.54 (ddd, *J* = 8.7, 7.3, 1.5 Hz, 1H), 7.38 – 7.28 (m, 2H), 3.71 (s, 3H), 3.61 (t, *J* = 6.2 Hz, 2H), 2.99 (t, *J* = 7.1 Hz, 2H), 2.00 – 1.92 (m, 4H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 160.3, 154.9, 133.1, 132.6, 129.8, 129.7, 123.6, 113.6, 44.8, 33.2, 32.3, 29.1, 23.9.

### **3-(But-3-en-1-yl)-1-methylquinoxalin-2(1*H*)-one (24)<sup>10</sup>**



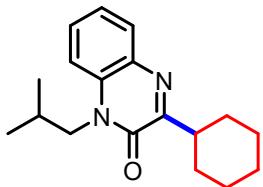
Obtained as a white solid (38% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.83 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.52 (ddd, *J* = 8.5, 7.3, 1.5 Hz, 1H), 7.33 (ddd, *J* = 8.2, 7.3, 1.3 Hz, 1H), 7.29 (dd, *J* = 8.4, 1.2 Hz, 1H), 5.96 (ddt, *J* = 16.8, 10.2, 6.6 Hz, 1H), 5.11 (dq, *J* = 17.2, 1.7 Hz, 1H), 5.00 (dq, *J* = 10.2, 1.4 Hz, 1H), 3.69 (s, 3H), 3.09 – 3.02 (m, 2H), 2.62 – 2.53 (m, 2H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 160.3, 154.8, 137.7, 133.1, 132.7, 129.7, 129.6, 123.5, 115.1, 113.6, 33.5, 30.6, 29.0.

### **1-Butyl-3-cyclohexylquinoxalin-2(1*H*)-one (25)<sup>7</sup>**



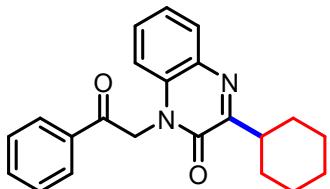
Obtained as a white solid (77% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.85 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.54 – 7.43 (m, 1H), 7.33 – 7.27 (m, 2H), 4.24 (dd, *J* = 9.0, 6.6 Hz, 2H), 3.46 – 3.26 (m, 1H), 1.96 (dd, *J* = 13.2, 3.3 Hz, 2H), 1.87 (dt, *J* = 13.1, 3.4 Hz, 2H), 1.74 (dq, *J* = 12.6, 8.0, 7.6 Hz, 3H), 1.58 (qd, *J* = 12.5, 3.1 Hz, 2H), 1.53 – 1.42 (m, 4H), 1.32 (tt, *J* = 12.6, 3.6 Hz, 1H), 1.00 (t, *J* = 7.3 Hz, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 164.3, 154.2, 133.2, 132.0, 130.0, 129.3, 123.1, 113.5, 42.1, 40.8, 30.5, 29.4, 26.4, 26.2, 20.3, 13.8.

### **3-Cyclohexyl-1-isobutylquinoxalin-2(1*H*)-one (26)<sup>8</sup>**



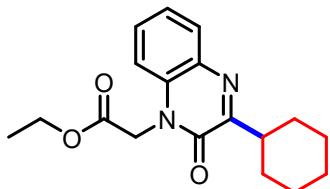
Obtained as a white solid (72% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.85 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.47 (ddd, *J* = 8.6, 7.2, 1.5 Hz, 1H), 7.32 – 7.26 (m, 2H), 4.13 (d, *J* = 7.5 Hz, 2H), 3.45 – 3.25 (m, 1H), 2.25 (dt, *J* = 13.8, 6.9 Hz, 1H), 2.01 – 1.92 (m, 2H), 1.87 (dt, *J* = 13.0, 3.4 Hz, 2H), 1.76 (dtd, *J* = 13.2, 3.3, 1.6 Hz, 1H), 1.58 (qd, *J* = 12.6, 3.1 Hz, 2H), 1.46 (qt, *J* = 12.9, 3.3 Hz, 2H), 1.32 (tt, *J* = 12.6, 3.6 Hz, 1H), 1.00 (d, *J* = 6.7 Hz, 6H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 164.3, 154.7, 133.0, 132.4, 130.0, 129.2, 123.2, 113.9, 49.0, 40.8, 30.5, 27.3, 26.3, 26.2, 20.3.

### **3-Cyclohexyl-1-(2-oxo-2-phenylethyl)quinoxalin-2(1*H*)-one (27)<sup>8</sup>**



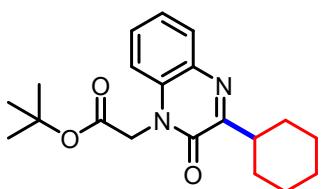
Obtained as a white solid (58% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.14 – 7.99 (m, 2H), 7.87 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.67 (t, *J* = 7.4 Hz, 1H), 7.55 (t, *J* = 7.7 Hz, 2H), 7.43 – 7.36 (m, 1H), 7.30 (t, *J* = 7.5 Hz, 1H), 6.93 (d, *J* = 8.3 Hz, 1H), 5.72 (s, 2H), 3.41 – 3.26 (m, 1H), 2.03 – 1.96 (m, 2H), 1.87 (dt, *J* = 13.2, 3.3 Hz, 2H), 1.79 – 1.73 (m, 1H), 1.61 (qd, *J* = 12.6, 3.3 Hz, 2H), 1.46 (qt, *J* = 12.9, 3.4 Hz, 2H), 1.32 (dddd, *J* = 16.4, 12.7, 8.0, 3.4 Hz, 1H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 191.4, 163.9, 154.3, 134.7, 134.3, 133.0, 132.3, 130.0, 129.5, 129.0, 128.2, 123.6, 113.3, 48.5, 40.9, 30.5, 26.3, 26.2.

### **Ethyl 2-(3-cyclohexyl-2-oxoquinoxalin-1(2*H*)-yl)acetate (28)<sup>8</sup>**



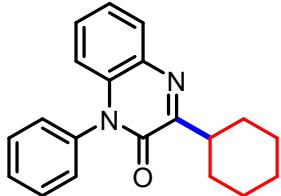
Obtained as a white solid (64% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.87 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.47 (ddd, *J* = 8.6, 7.3, 1.5 Hz, 1H), 7.38 – 7.28 (m, 1H), 7.05 (dd, *J* = 8.4, 1.2 Hz, 1H), 5.01 (s, 2H), 4.25 (q, *J* = 7.1 Hz, 2H), 3.40 – 3.27 (m, 1H), 1.97 (dt, *J* = 12.8, 2.7 Hz, 2H), 1.87 (dt, *J* = 13.1, 3.4 Hz, 2H), 1.80 – 1.73 (m, 1H), 1.59 (qd, *J* = 12.6, 3.2 Hz, 2H), 1.46 (qt, *J* = 12.8, 3.3 Hz, 2H), 1.36 – 1.30 (m, 1H), 1.27 (t, *J* = 7.2 Hz, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 167.3, 164.1, 154.1, 132.9, 132.0, 130.1, 129.6, 123.7, 112.9, 62.0, 43.6, 40.8, 30.5, 26.3, 26.1, 14.1.

### **tert-Butyl 2-(3-cyclohexyl-2-oxoquinoxalin-1(2*H*)-yl)acetate (29)<sup>7</sup>**



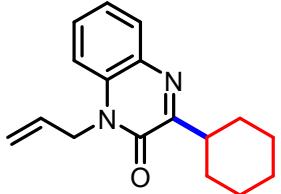
Obtained as a white solid (62% yield);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.85 (d,  $J = 7.9$  Hz, 1H), 7.46 (t,  $J = 7.8$  Hz, 1H), 7.31 (t,  $J = 7.6$  Hz, 1H), 7.04 (d,  $J = 8.3$  Hz, 1H), 4.93 (s, 2H), 3.33 (ddd,  $J = 11.7, 8.4, 3.3$  Hz, 1H), 2.02 – 1.93 (m, 2H), 1.86 (dt,  $J = 13.3, 3.5$  Hz, 2H), 1.76 (d,  $J = 13.1$  Hz, 1H), 1.58 (qd,  $J = 12.6, 3.1$  Hz, 2H), 1.49 (d,  $J = 9.1$  Hz, 1H), 1.45 (s, 9H), 1.35 – 1.29 (m, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  166.3, 164.1, 154.1, 132.9, 132.1, 130.0, 129.4, 123.6, 112.9, 83.0, 44.3, 40.8, 30.5, 28.0, 26.3, 26.2.

### 3-Cyclohexyl-1-phenylquinoxalin-2(1*H*)-one (30)<sup>8</sup>



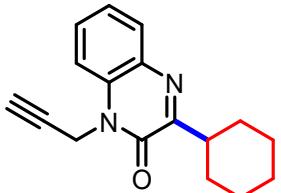
Obtained as a white solid (56% yield);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.80 (dd,  $J = 6.3, 3.2$  Hz, 1H), 7.53 (t,  $J = 7.6$  Hz, 2H), 7.47 (d,  $J = 7.4$  Hz, 1H), 7.30 – 7.19 (m, 4H), 6.66 – 6.50 (m, 1H), 3.27 (tt,  $J = 11.7, 3.3$  Hz, 1H), 1.98 – 1.90 (m, 2H), 1.80 (dt,  $J = 13.0, 3.4$  Hz, 2H), 1.72 – 1.66 (m, 1H), 1.56 (qd,  $J = 12.6, 3.4$  Hz, 2H), 1.43 – 1.33 (m, 2H), 1.30 – 1.23 (m, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  165.1, 154.3, 136.1, 133.7, 132.7, 130.2, 129.4, 129.3, 129.0, 128.3, 123.6, 115.3, 40.9, 30.6, 26.3, 26.2.

### 1-Allyl-3-cyclohexylquinoxalin-2(1*H*)-one (31)<sup>7</sup>



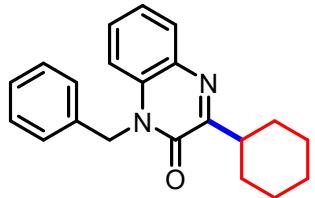
Obtained as a white solid (54% yield);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.85 (dd,  $J = 7.9, 1.6$  Hz, 1H), 7.46 (ddd,  $J = 8.5, 7.2, 1.5$  Hz, 1H), 7.34 – 7.24 (m, 2H), 5.94 (ddt,  $J = 17.2, 10.4, 5.2$  Hz, 1H), 5.26 (dq,  $J = 10.3, 1.4$  Hz, 1H), 5.17 (dq,  $J = 17.2, 1.6$  Hz, 1H), 4.90 (dt,  $J = 5.3, 1.8$  Hz, 2H), 3.35 (tt,  $J = 11.6, 3.3$  Hz, 1H), 2.02 – 1.93 (m, 2H), 1.87 (dt,  $J = 13.0, 3.4$  Hz, 2H), 1.80 – 1.73 (m, 1H), 1.58 (qd,  $J = 12.6, 3.1$  Hz, 2H), 1.46 (qt,  $J = 12.9, 3.3$  Hz, 2H), 1.31 (qt,  $J = 12.9, 3.7$  Hz, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  164.3, 154.1, 133.0, 132.1, 130.8, 129.9, 129.3, 123.4, 118.0, 114.0, 44.6, 40.8, 30.6, 26.3, 26.2.

### 3-Cyclohexyl-1-(prop-2-yn-1-yl)quinoxalin-2(1*H*)-one (32)<sup>8</sup>



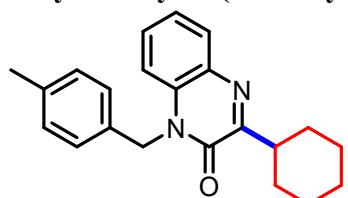
Obtained as a white solid (47% yield);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.86 (dd,  $J = 8.0, 1.4$  Hz, 1H), 7.60 – 7.48 (m, 1H), 7.44 (d,  $J = 8.3$  Hz, 1H), 7.35 (t,  $J = 7.6$  Hz, 1H), 5.05 (d,  $J = 2.6$  Hz, 2H), 3.40 – 3.28 (m, 1H), 2.28 (t,  $J = 2.6$  Hz, 1H), 2.01 – 1.93 (m, 2H), 1.87 (dt,  $J = 13.2, 3.3$  Hz, 2H), 1.80 – 1.73 (m, 1H), 1.58 (qd,  $J = 12.5, 3.2$  Hz, 2H), 1.47 (dddd,  $J = 16.3, 12.9, 8.0, 3.4$  Hz, 2H), 1.32 (tt,  $J = 12.5, 3.6$  Hz, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  164.2, 153.5, 133.1, 131.4, 129.9, 129.5, 123.8, 113.9, 77.2, 73.0, 40.8, 31.5, 30.5, 26.3, 26.2.

**1-Benzyl-3-cyclohexylquinoxalin-2(1*H*)-one (33)<sup>7</sup>**



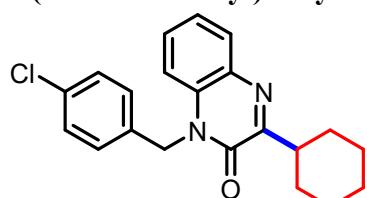
Obtained as a white solid (60% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.84 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.39 – 7.34 (m, 1H), 7.32 – 7.28 (m, 2H), 7.25 (dd, *J* = 12.3, 6.0 Hz, 4H), 5.48 (s, 2H), 3.40 (ddd, *J* = 11.6, 8.3, 3.3 Hz, 1H), 2.06 – 1.97 (m, 2H), 1.88 (dt, *J* = 13.0, 3.4 Hz, 2H), 1.77 (dt, *J* = 12.5, 3.6 Hz, 1H), 1.61 (qd, *J* = 12.6, 3.3 Hz, 2H), 1.48 (qt, *J* = 12.9, 3.4 Hz, 2H), 1.32 (qt, *J* = 12.8, 3.6 Hz, 1H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 164.4, 154.6, 135.5, 133.2, 132.2, 129.9, 129.4, 128.9, 127.6, 126.9, 123.5, 114.3, 46.0, 40.9, 30.6, 26.4, 26.2.

**3-Cyclohexyl-1-(4-methylbenzyl)quinoxalin-2(1*H*)-one (34)<sup>7</sup>**



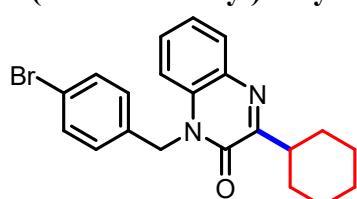
Obtained as a white solid (61% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.85 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.38 (td, *J* = 8.4, 7.8, 1.5 Hz, 1H), 7.28 – 7.24 (m, 2H), 7.19 – 7.06 (m, 4H), 5.45 (s, 2H), 3.41 (tt, *J* = 11.6, 3.3 Hz, 1H), 2.30 (s, 3H), 2.04 – 1.97 (m, 2H), 1.88 (dp, *J* = 9.9, 3.3 Hz, 2H), 1.81 – 1.74 (m, 1H), 1.61 (qd, *J* = 12.6, 3.2 Hz, 2H), 1.48 (qt, *J* = 12.9, 3.4 Hz, 2H), 1.33 (qt, *J* = 12.8, 3.5 Hz, 1H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 164.4, 154.6, 137.4, 133.1, 132.5, 132.3, 129.8, 129.6, 129.4, 127.0, 123.4, 114.3, 45.8, 40.8, 30.6, 26.4, 26.2, 21.1.

**1-(4-Chlorobenzyl)-3-cyclohexylquinoxalin-2(1*H*)-one (35)<sup>7</sup>**



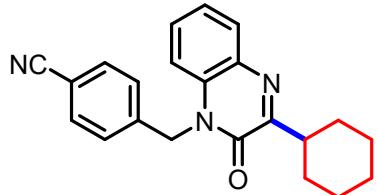
Obtained as a white solid (56% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.86 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.39 (ddd, *J* = 8.5, 7.2, 1.6 Hz, 1H), 7.34 – 7.26 (m, 3H), 7.24 – 7.12 (m, 3H), 5.44 (s, 2H), 3.39 (tt, *J* = 11.7, 3.3 Hz, 1H), 2.05 – 1.96 (m, 2H), 1.88 (dp, *J* = 10.1, 3.3 Hz, 2H), 1.81 – 1.75 (m, 1H), 1.61 (qd, *J* = 12.6, 3.2 Hz, 2H), 1.48 (qt, *J* = 12.8, 3.3 Hz, 2H), 1.32 (qt, *J* = 12.8, 3.5 Hz, 1H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 164.4, 154.5, 134.0, 133.5, 133.2, 132.0, 130.0, 129.5, 129.1, 128.4, 123.6, 114.0, 45.4, 40.9, 30.6, 26.3, 26.2.

**1-(4-Bromobenzyl)-3-cyclohexylquinoxalin-2(1*H*)-one (36)<sup>7</sup>**



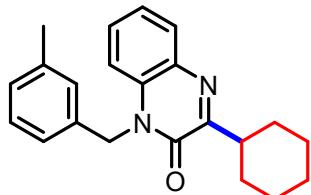
Obtained as a white solid (58% yield);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.86 (dd,  $J = 7.9, 1.5$  Hz, 1H), 7.51 – 7.42 (m, 2H), 7.39 (ddd,  $J = 8.6, 7.2, 1.6$  Hz, 1H), 7.29 (td,  $J = 7.7, 1.3$  Hz, 1H), 7.17 (dd,  $J = 8.4, 1.2$  Hz, 1H), 7.15 – 7.05 (m, 2H), 5.43 (s, 2H), 3.48 – 3.28 (m, 1H), 2.05 – 1.96 (m, 2H), 1.88 (dt,  $J = 12.9, 3.3$  Hz, 2H), 1.78 (dtd,  $J = 11.4, 3.3, 1.6$  Hz, 1H), 1.61 (qd,  $J = 12.6, 3.2$  Hz, 2H), 1.48 (qt,  $J = 12.9, 3.3$  Hz, 2H), 1.37 – 1.28 (m, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  164.4, 154.5, 134.6, 133.1, 132.0, 132.0, 130.0, 129.5, 128.7, 123.6, 121.6, 114.0, 45.4, 40.9, 30.6, 26.3, 26.2.

#### 4-((3-Cyclohexyl-2-oxoquinoxalin-1(2*H*)-yl)methyl)benzonitrile (37)<sup>7</sup>



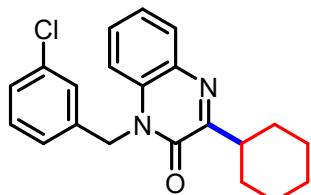
Obtained as a white solid (46% yield);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.80 (dd,  $J = 7.9, 1.5$  Hz, 1H), 7.61 – 7.47 (m, 2H), 7.32 (ddd,  $J = 8.5, 7.3, 1.6$  Hz, 1H), 7.30 – 7.19 (m, 3H), 7.01 (dd,  $J = 8.3, 1.2$  Hz, 1H), 5.45 (s, 2H), 3.29 (tt,  $J = 11.7, 3.3$  Hz, 1H), 1.97 – 1.88 (m, 2H), 1.81 (dt,  $J = 13.1, 3.3$  Hz, 2H), 1.74 – 1.68 (m, 1H), 1.53 (qd,  $J = 12.6, 3.2$  Hz, 2H), 1.40 (qt,  $J = 12.9, 3.4$  Hz, 2H), 1.25 (qt,  $J = 12.8, 3.6$  Hz, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  164.4, 154.4, 140.9, 133.2, 132.8, 131.8, 130.2, 129.6, 127.6, 123.9, 118.4, 113.7, 111.8, 45.6, 40.9, 30.6, 26.3, 26.1.

#### 3-Cyclohexyl-1-(3-methylbenzyl)quinoxalin-2(1*H*)-one (38)<sup>7</sup>



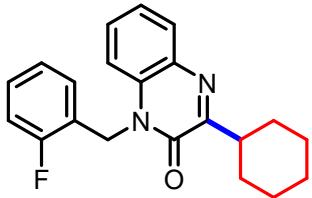
Obtained as a white solid (61% yield);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.84 (dd,  $J = 8.0, 1.5$  Hz, 1H), 7.37 (ddd,  $J = 8.5, 7.2, 1.6$  Hz, 1H), 7.29 – 7.22 (m, 2H), 7.18 (t,  $J = 7.7$  Hz, 1H), 7.04 (q,  $J = 7.6$  Hz, 3H), 5.45 (s, 2H), 3.41 (ddd,  $J = 11.6, 8.3, 3.2$  Hz, 1H), 2.29 (s, 3H), 2.05 – 1.98 (m, 2H), 1.88 (dp,  $J = 10.2, 3.3$  Hz, 2H), 1.81 – 1.74 (m, 1H), 1.61 (qd,  $J = 12.6, 3.2$  Hz, 2H), 1.48 (qt,  $J = 12.9, 3.4$  Hz, 2H), 1.38 – 1.28 (m, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  164.4, 154.6, 138.7, 135.4, 133.1, 132.3, 129.8, 129.4, 128.8, 128.4, 127.6, 124.0, 123.4, 114.3, 46.0, 40.8, 30.6, 26.4, 26.2, 21.5.

#### 1-(3-Chlorobenzyl)-3-cyclohexylquinoxalin-2(1*H*)-one (39)<sup>7</sup>



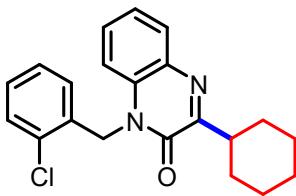
Obtained as a white solid (53% yield);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.86 (dd,  $J = 8.0, 1.5$  Hz, 1H), 7.40 (ddd,  $J = 8.5, 7.2, 1.4$  Hz, 1H), 7.30 (td,  $J = 7.7, 1.2$  Hz, 1H), 7.26 – 7.21 (m, 3H), 7.16 (dd,  $J = 8.4, 1.2$  Hz, 1H), 7.11 (td,  $J = 4.6, 2.2$  Hz, 1H), 5.45 (s, 2H), 3.39 (ddd,  $J = 11.7, 8.4, 3.3$  Hz, 1H), 2.05 – 1.98 (m, 2H), 1.89 (dt,  $J = 13.2, 3.3$  Hz, 2H), 1.80 – 1.75 (m, 1H), 1.61 (qd,  $J = 12.6, 3.2$  Hz, 2H), 1.48 (tdd,  $J = 13.0, 11.1, 3.4$  Hz, 2H), 1.37 – 1.28 (m, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  164.4, 154.5, 137.6, 134.9, 133.1, 132.0, 130.2, 130.0, 129.5, 128.0, 127.1, 125.1, 123.7, 114.0, 45.5, 40.9, 30.6, 26.3, 26.2.

### **3-Cyclohexyl-1-(2-fluorobenzyl)quinoxalin-2(1*H*)-one (40)<sup>7</sup>**



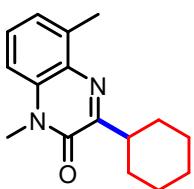
Obtained as a white solid (43% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.85 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.40 (ddd, *J* = 8.5, 7.2, 1.6 Hz, 1H), 7.29 (td, *J* = 7.7, 1.2 Hz, 1H), 7.24 (dd, *J* = 5.3, 3.3 Hz, 1H), 7.22 – 7.18 (m, 1H), 7.11 (dd, *J* = 10.3, 8.3 Hz, 1H), 7.07 – 6.92 (m, 2H), 5.55 (s, 2H), 3.40 (tt, *J* = 11.6, 3.2 Hz, 1H), 2.07 – 1.96 (m, 2H), 1.89 (dt, *J* = 13.1, 3.4 Hz, 2H), 1.82 – 1.74 (m, 1H), 1.62 (qd, *J* = 12.6, 3.3 Hz, 2H), 1.48 (qt, *J* = 13.0, 3.4 Hz, 2H), 1.38 – 1.30 (m, 1H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 164.3, 160.3 (d, *J* = 245.7 Hz), 154.7, 133.1, 131.9, 129.9, 129.6, 129.4 (d, *J* = 7.6 Hz), 128.5 (d, *J* = 3.8 Hz), 124.7 (d, *J* = 245.7 Hz), 123.6, 122.5 (d, *J* = 13.9 Hz), 115.5 (d, *J* = 21.4 Hz), 113.9 (d, *J* = 2.5 Hz), 40.9, 39.4, 39.3, 30.6, 26.3, 26.2; <sup>19</sup>F NMR (471 MHz, CDCl<sub>3</sub>) δ -118.38.

### **1-(2-Chlorobenzyl)-3-cyclohexylquinoxalin-2(1*H*)-one (41)<sup>7</sup>**



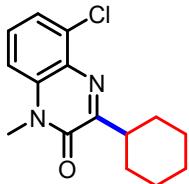
Obtained as a white solid (44% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.88 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.45 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.38 (ddd, *J* = 8.5, 7.3, 1.5 Hz, 1H), 7.30 (td, *J* = 7.7, 1.3 Hz, 1H), 7.21 (td, *J* = 7.7, 1.6 Hz, 1H), 7.09 (td, *J* = 7.7, 1.3 Hz, 1H), 7.02 (dd, *J* = 8.4, 1.2 Hz, 1H), 6.74 (dd, *J* = 7.8, 1.5 Hz, 1H), 5.58 (s, 2H), 3.40 (ddd, *J* = 11.6, 8.4, 3.2 Hz, 1H), 2.05 – 1.98 (m, 2H), 1.89 (dp, *J* = 9.9, 3.2 Hz, 2H), 1.82 – 1.75 (m, 1H), 1.63 (qd, *J* = 12.6, 3.3 Hz, 2H), 1.48 (qt, *J* = 13.0, 3.4 Hz, 2H), 1.39 – 1.31 (m, 1H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 164.4, 154.6, 133.1, 132.7, 132.5, 131.9, 129.9, 129.7, 129.7, 128.8, 127.3, 126.9, 123.7, 114.2, 43.6, 40.9, 30.6, 26.3, 26.2.

### **3-Cyclohexyl-1,5-dimethylquinoxalin-2(1*H*)-one (42)<sup>8</sup>**



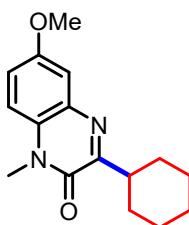
Obtained as a white solid (63% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.38 (dd, *J* = 8.4, 7.4 Hz, 1H), 7.18 (d, *J* = 7.4 Hz, 1H), 7.12 (d, *J* = 8.1 Hz, 1H), 3.68 (s, 3H), 3.33 (tt, *J* = 11.4, 3.4 Hz, 1H), 2.68 (s, 3H), 2.02 – 1.94 (m, 2H), 1.86 (dt, *J* = 12.8, 3.4 Hz, 2H), 1.76 (dddd, *J* = 12.8, 4.8, 3.2, 1.5 Hz, 1H), 1.56 (qd, *J* = 12.4, 2.8 Hz, 2H), 1.48 (qt, *J* = 12.9, 3.0 Hz, 2H), 1.32 (tt, *J* = 12.4, 3.7 Hz, 1H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 162.2, 154.5, 138.6, 132.9, 131.3, 129.0, 124.7, 111.3, 40.8, 30.7, 29.2, 26.3, 26.3, 17.4.

**5-Chloro-3-cyclohexyl-1-methylquinoxalin-2(1*H*)-one (43)<sup>8</sup>**



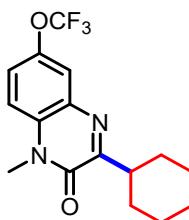
Obtained as a white solid (60% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.55 – 7.36 (m, 2H), 7.19 (dd, J = 6.7, 3.2 Hz, 1H), 3.69 (s, 3H), 3.34 (td, J = 11.2, 5.6 Hz, 1H), 1.99 (d, J = 12.9 Hz, 2H), 1.93 – 1.84 (m, 2H), 1.76 (d, J = 13.0 Hz, 1H), 1.62 (qd, J = 12.6, 3.4 Hz, 2H), 1.52 – 1.42 (m, 2H), 1.37 – 1.31 (m, 1H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 164.7, 154.2, 134.8, 134.3, 129.5, 129.3, 124.3, 112.3, 41.3, 30.5, 29.5, 26.2, 26.1.

**3-Cyclohexyl-6-methoxy-1-methylquinoxalin-2(1*H*)-one (44)<sup>7</sup>**



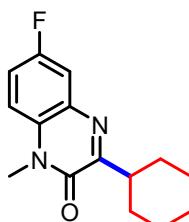
Obtained as a white solid (61% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.39 (d, J = 2.9 Hz, 1H), 7.21 (d, J = 9.2 Hz, 1H), 7.14 (dd, J = 9.1, 2.8 Hz, 1H), 3.89 (s, 3H), 3.69 (s, 3H), 3.41 – 3.34 (m, 1H), 2.05 – 1.91 (m, 2H), 1.87 (dt, J = 13.0, 3.4 Hz, 2H), 1.80 – 1.74 (m, 1H), 1.60 (qd, J = 12.6, 3.2 Hz, 2H), 1.47 (qt, J = 10.9, 2.4 Hz, 2H), 1.33 (tt, J = 13.3, 3.8 Hz, 1H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 164.9, 155.9, 154.2, 133.4, 127.1, 118.7, 114.4, 111.1, 55.8, 40.9, 30.6, 29.3, 26.3, 26.1.

**3-Cyclohexyl-1-methyl-6-(trifluoromethoxy)quinoxalin-2(1*H*)-one (45)<sup>8</sup>**



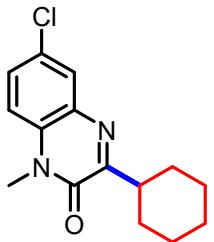
Obtained as a white solid (60% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.85 (d, J = 8.8 Hz, 1H), 7.18 (ddd, J = 8.7, 2.5, 1.2 Hz, 1H), 7.10 (d, J = 2.4 Hz, 1H), 3.67 (s, 3H), 3.32 (tt, J = 11.5, 3.3 Hz, 1H), 1.98 – 1.90 (m, 2H), 1.87 (dt, J = 12.9, 3.2 Hz, 2H), 1.80 – 1.73 (m, 1H), 1.59 – 1.51 (m, 2H), 1.46 (td, J = 12.9, 9.3, 3.1 Hz, 2H), 1.31 (tt, J = 12.5, 3.7 Hz, 1H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 164.7, 154.3, 149.4, 149.3, 133.9, 131.2, 118.3 (q, J = 258.3 Hz), 115.8, 106.1, 40.8, 30.5, 29.3, 26.3, 26.1; <sup>19</sup>F NMR (471 MHz, CDCl<sub>3</sub>) δ -57.68.

**3-Cyclohexyl-6-fluoro-1-methylquinoxalin-2(1*H*)-one (46)<sup>8</sup>**



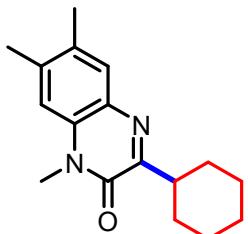
Obtained as a white solid (56% yield);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.63 – 7.46 (m, 1H), 7.28 – 7.20 (m, 2H), 3.69 (s, 3H), 3.40 – 3.27 (m, 1H), 1.98 – 1.91 (m, 2H), 1.87 (dt,  $J = 13.0, 3.3$  Hz, 2H), 1.77 (dd,  $J = 13.2, 4.8, 3.2, 1.6$  Hz, 1H), 1.59 – 1.51 (m, 2H), 1.50 – 1.40 (m, 2H), 1.35 – 1.26 (m, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  165.9, 158.6 (d,  $J = 243.2$  Hz), 154.2, 133.5 (d,  $J = 11.3$  Hz), 129.5 (d,  $J = 1.3$  Hz), 117.0 (d,  $J = 23.9$  Hz), 115.2 (d,  $J = 22.7$  Hz), 114.5 (d,  $J = 10.1$  Hz), 40.87, 30.49, 29.31, 26.26, 26.13;  $^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ )  $\delta$  -119.55.

### **6-Chloro-3-cyclohexyl-1-methylquinoxalin-2(1*H*)-one (47)<sup>8</sup>**



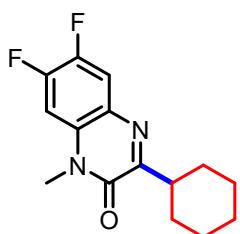
Obtained as a white solid (45% yield);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.84 (d,  $J = 2.4$  Hz, 1H), 7.45 (dd,  $J = 8.9, 2.4$  Hz, 1H), 7.20 (d,  $J = 8.9$  Hz, 1H), 3.67 (s, 3H), 3.38 – 3.26 (m, 1H), 1.94 (dd,  $J = 12.4, 3.4$  Hz, 2H), 1.86 (dt,  $J = 12.9, 3.2$  Hz, 2H), 1.80 – 1.74 (m, 1H), 1.58 – 1.50 (m, 2H), 1.50 – 1.41 (m, 2H), 1.31 (tt,  $J = 12.2, 3.5$  Hz, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  165.7, 154.2, 133.4, 131.6, 129.3, 129.2, 128.7, 114.6, 40.8, 30.5, 29.3, 26.3, 26.1.

### **3-Cyclohexyl-1,6,7-trimethylquinoxalin-2(1*H*)-one (48)<sup>8</sup>**



Obtained as a white solid (69% yield);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.62 (s, 1H), 7.04 (s, 1H), 3.67 (s, 3H), 3.32 (tt,  $J = 11.7, 3.2$  Hz, 1H), 2.40 (s, 3H), 2.34 (s, 3H), 1.99 – 1.91 (m, 2H), 1.86 (dt,  $J = 13.1, 3.5$  Hz, 2H), 1.76 (d,  $J = 12.9$  Hz, 1H), 1.57 (qd,  $J = 12.5, 3.1$  Hz, 2H), 1.46 (qt,  $J = 12.9, 3.2$  Hz, 2H), 1.32 (tt,  $J = 12.8, 3.7$  Hz, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  163.0, 154.6, 139.1, 132.3, 131.1, 130.9, 129.8, 114.1, 40.7, 30.6, 29.0, 26.4, 26.2, 20.5, 19.1.

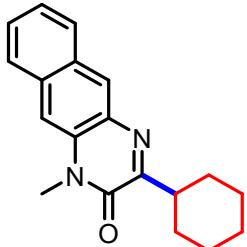
### **3-Cyclohexyl-6,7-difluoro-1-methylquinoxalin-2(1*H*)-one (49)<sup>7</sup>**



Obtained as a white solid (63% yield);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.65 (dd,  $J = 10.4, 8.2$  Hz, 1H), 7.07 (dd,  $J = 11.4, 7.1$  Hz, 1H), 3.64 (s, 3H), 3.30 (ddd,  $J = 11.4, 8.1, 3.2$  Hz, 1H), 1.93 (d,  $J = 12.4$  Hz, 2H), 1.89 – 1.81 (m, 2H), 1.80 – 1.73 (m, 1H), 1.49 (dd,  $J = 25.7, 16.0, 9.6, 3.2$  Hz, 4H), 1.31 (tt,  $J = 14.1, 4.0$  Hz, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  164.9 (d,  $J = 3.5$  Hz), 154.1, 150.9

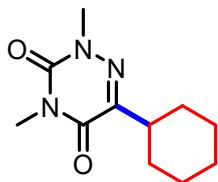
(dd,  $J = 252.2, 14.5$  Hz), 146.5 (dd,  $J = 246.2, 13.9$  Hz), 130.0 (dd,  $J = 8.9, 1.5$  Hz), 129.1 (dd,  $J = 9.2, 2.9$  Hz), 117.4 (dd,  $J = 18.0, 2.1$  Hz), 102.0 (d,  $J = 23.0$  Hz), 40.8, 30.5, 29.6, 26.2, 26.1;  $^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ )  $\delta$  -132.34 (d,  $J = 22.3$  Hz), -142.75 (d,  $J = 22.5$  Hz).

### 3-Cyclohexyl-1-methylbenzo[g]quinoxalin-2(1H)-one (50)<sup>8</sup>



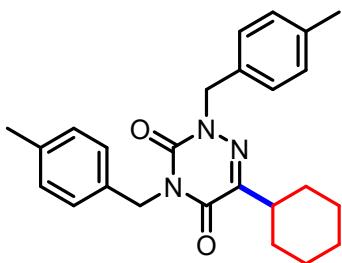
Obtained as a white solid (40% yield);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.37 (s, 1H), 7.96 (d,  $J = 8.2$  Hz, 1H), 7.90 (d,  $J = 8.3$  Hz, 1H), 7.55 (ddd,  $J = 8.2, 6.7, 1.3$  Hz, 1H), 7.47 (ddd,  $J = 8.1, 6.7, 1.2$  Hz, 1H), 3.76 (s, 3H), 3.44 – 3.35 (m, 1H), 2.04 – 1.96 (m, 2H), 1.89 (dt,  $J = 12.9, 3.4$  Hz, 2H), 1.81 – 1.76 (m, 1H), 1.63 (qd,  $J = 12.6, 3.2$  Hz, 2H), 1.49 (qt,  $J = 12.9, 3.4$  Hz, 2H), 1.35 (tt,  $J = 12.7, 3.6$  Hz, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  164.8, 154.4, 133.3, 132.3, 131.7, 129.7, 128.7, 128.4, 127.5, 127.1, 125.1, 109.7, 40.9, 30.7, 29.1, 26.3, 26.2.

### 6-Cyclohexyl-2,4-dimethyl-1,2,4-triazine-3,5(2H,4H)-dione (51)<sup>8</sup>



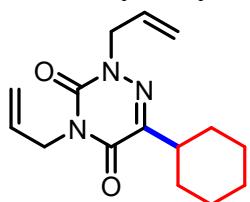
Obtained as a white solid (72% yield);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  3.61 (s, 3H), 3.34 (s, 3H), 2.96 – 2.80 (m, 1H), 1.90 – 1.78 (m, 4H), 1.76 – 1.71 (m, 1H), 1.38 (td,  $J = 9.8, 3.4$  Hz, 4H), 1.23 (d,  $J = 3.8$  Hz, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  156.1, 149.2, 148.3, 39.4, 38.3, 30.4, 27.1, 26.1, 26.0.

### 6-Cyclohexyl-2,4-bis(4-methylbenzyl)-1,2,4-triazine-3,5(2H,4H)-dione (52)



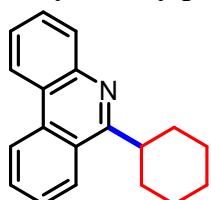
Obtained as a white solid (63% yield); M. P. = 112–113 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.38 (d,  $J = 7.9$  Hz, 2H), 7.30 (s, 2H), 7.14 (d,  $J = 7.8$  Hz, 2H), 7.10 (d,  $J = 7.8$  Hz, 2H), 5.02 (d,  $J = 2.4$  Hz, 4H), 2.85 (t,  $J = 7.6$  Hz, 1H), 2.33 (s, 3H), 2.31 (s, 3H), 1.85 (d,  $J = 8.1$  Hz, 2H), 1.80 (d,  $J = 5.6$  Hz, 2H), 1.71 (d,  $J = 12.7$  Hz, 1H), 1.35 (t,  $J = 10.4$  Hz, 4H), 1.28 – 1.18 (m, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  155.7, 148.9, 148.8, 137.9, 137.8, 133.0, 132.9, 129.6, 129.3, 129.2, 128.8, 55.0, 43.9, 38.4, 30.5, 26.5, 26.0, 21.2, 21.2; HRMS (ESI $^+$ ): Calculated for  $\text{C}_{25}\text{H}_{29}\text{N}_3\text{O}_2$ :  $[\text{M}+\text{Na}]^+$  426.2152, Found 426.2171.

**2,4-Diallyl-6-cyclohexyl-1,2,4-triazine-3,5(2*H*,4*H*)-dione (53)<sup>17</sup>**



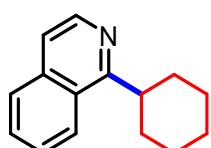
Obtained as a colourless liquid (36% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 6.04 – 5.78 (m, 2H), 5.36 – 5.15 (m, 4H), 4.54 (t, *J* = 5.3 Hz, 4H), 2.88 (ddd, *J* = 11.0, 8.0, 3.2 Hz, 1H), 1.87 (d, *J* = 7.2 Hz, 2H), 1.85 – 1.78 (m, 2H), 1.72 (d, *J* = 12.7 Hz, 1H), 1.38 (dd, *J* = 20.7, 11.1 Hz, 4H), 1.29 – 1.19 (m, 1H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 155.4, 148.9, 148.5, 131.7, 130.6, 119.1, 118.7, 53.9, 42.9, 38.4, 30.4, 26.1, 26.0; HRMS (ESI<sup>+</sup>): Calculated for C<sub>15</sub>H<sub>21</sub>N<sub>3</sub>O<sub>2</sub>: [M+Na]<sup>+</sup> 298.1526, Found 298.1538.

**6-Cyclohexylphenanthridine (54)<sup>11</sup>**



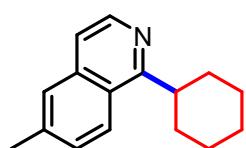
Obtained as a white solid (52% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.53 (d, *J* = 8.2 Hz, 1H), 8.47 – 8.38 (m, 1H), 8.21 (d, *J* = 8.2 Hz, 1H), 8.05 (d, *J* = 8.2 Hz, 1H), 7.69 (t, *J* = 7.6 Hz, 1H), 7.63 – 7.54 (m, 2H), 7.54 – 7.45 (m, 1H), 3.52 (tt, *J* = 11.3, 3.3 Hz, 1H), 2.02 – 1.96 (m, 2H), 1.87 (ddd, *J* = 15.2, 9.8, 3.4 Hz, 4H), 1.78 – 1.73 (m, 1H), 1.48 (dt, *J* = 13.2, 3.5 Hz, 2H), 1.36 (tt, *J* = 12.9, 3.4 Hz, 1H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 165.3, 143.9, 133.0, 130.1, 129.9, 128.4, 127.1, 126.2, 125.6, 124.7, 123.4, 122.6, 121.8, 42.0, 32.3, 26.9, 26.4.

**1-Cyclohexylisoquinoline (55)<sup>7</sup>**



Obtained as a colourless liquid (40% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.48 (d, *J* = 5.7 Hz, 1H), 8.23 (d, *J* = 8.5 Hz, 1H), 7.80 (d, *J* = 8.1 Hz, 1H), 7.65 (t, *J* = 7.5 Hz, 1H), 7.58 (ddd, *J* = 8.3, 6.7, 1.4 Hz, 1H), 7.48 (d, *J* = 5.7 Hz, 1H), 3.63 – 3.51 (m, 1H), 2.01 – 1.91 (m, 4H), 1.89 – 1.77 (m, 3H), 1.54 (qt, *J* = 12.9, 3.3 Hz, 2H), 1.41 (tt, *J* = 13.1, 3.7 Hz, 1H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 165.7, 141.8, 136.4, 129.6, 127.6, 126.9, 126.3, 124.8, 118.9, 41.5, 32.6, 26.9, 26.2.

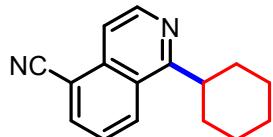
**1-Cyclohexyl-6-methylisoquinoline (56)<sup>18</sup>**



Obtained as a colourless liquid (36% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.43 (d, *J* = 5.7 Hz, 1H), 8.11 (d, *J* = 8.7 Hz, 1H), 7.58 (s, 1H), 7.41 (t, *J* = 6.4 Hz, 2H), 3.58 – 3.47 (m, 1H), 2.53 (s, 3H), 1.95 (t, *J* = 15.0 Hz, 4H), 1.84 (dd, *J* = 24.6, 12.8 Hz, 3H), 1.53 (td, *J* = 13.0, 3.4 Hz, 2H), 1.41 (t, *J*

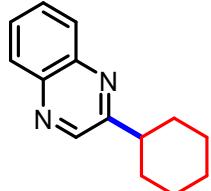
$= 12.8$  Hz, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  165.4, 141.8, 136.8, 130.5, 129.1, 126.5, 124.7, 124.6, 118.5, 41.5, 32.6, 26.9, 26.2, 21.8; HRMS (ESI $^+$ ): Calculated for  $\text{C}_{16}\text{H}_{19}\text{N}$ :  $[\text{M}+\text{H}]^+$  226.1590, Found 226.1592.

### 1-Cyclohexylisoquinoline-5-carbonitrile (57)<sup>14</sup>



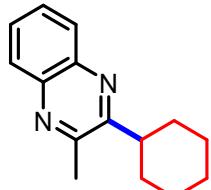
Obtained as a colourless liquid (23% yield);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.68 (d,  $J = 5.8$  Hz, 1H), 8.50 (d,  $J = 8.6$  Hz, 1H), 8.09 (d,  $J = 7.1$  Hz, 1H), 7.89 (d,  $J = 5.8$  Hz, 1H), 7.74 – 7.62 (m, 1H), 3.64 – 3.49 (m, 1H), 1.96 (d,  $J = 11.0$  Hz, 4H), 1.86 (dd,  $J = 22.8, 12.6$  Hz, 3H), 1.53 (dt,  $J = 16.0, 12.8$  Hz, 2H), 1.41 (t,  $J = 12.8$  Hz, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  166.7, 144.3, 136.0, 136.0, 130.1, 126.1, 125.7, 116.9, 115.9, 110.4, 41.8, 32.6, 26.7, 26.1; HRMS (ESI $^+$ ): Calculated for  $\text{C}_{16}\text{H}_{16}\text{N}_2$ :  $[\text{M}+\text{H}]^+$  237.1386, Found 237.1390.

### 2-Cyclohexylquinoxaline (58)<sup>16</sup>



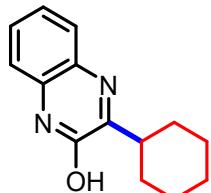
Obtained as a colourless liquid (35% yield);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.77 (s, 1H), 8.06 (t,  $J = 9.0$  Hz, 2H), 7.71 (ddd,  $J = 15.1, 14.0, 6.8$  Hz, 2H), 2.97 (t,  $J = 12.0$  Hz, 1H), 2.04 (d,  $J = 12.1$  Hz, 2H), 1.92 (d,  $J = 13.1$  Hz, 2H), 1.80 (d,  $J = 12.7$  Hz, 1H), 1.71 (dt,  $J = 15.5, 7.7$  Hz, 2H), 1.47 (ddd,  $J = 15.7, 12.8, 3.1$  Hz, 2H), 1.41 – 1.30 (m, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  161.1, 145.0, 142.2, 141.4, 129.8, 129.1, 129.0, 128.8, 45.0, 32.3, 26.4, 25.9.

### 2-Cyclohexyl-3-methylquinoxaline (59)<sup>12</sup>



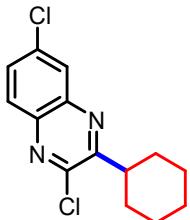
Obtained as a colourless liquid (38% yield);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.06 – 7.99 (m, 1H), 7.99 – 7.92 (m, 1H), 7.68 – 7.61 (m, 2H), 3.04 (tt,  $J = 11.5, 3.2$  Hz, 1H), 2.79 (s, 3H), 1.97 – 1.88 (m, 4H), 1.83 – 1.74 (m, 3H), 1.51 – 1.36 (m, 3H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  160.4, 152.6, 141.4, 140.5, 128.7, 128.7, 128.6, 128.1, 42.6, 31.6, 26.6, 26.0, 22.7.

### 3-Cyclohexylquinoxalin-2-ol (60)<sup>22</sup>



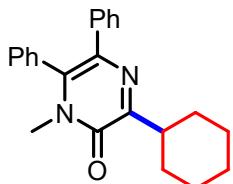
Obtained as a white solid (31% yield);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  11.68 (s, 1H), 7.83 (d,  $J = 7.2$  Hz, 1H), 7.66 (dd,  $J = 41.8, 9.2$  Hz, 1H), 7.52 – 7.43 (m, 1H), 7.32 (s, 1H), 3.35 (t,  $J = 11.0$  Hz, 1H), 1.99 (d,  $J = 11.0$  Hz, 2H), 1.89 (d,  $J = 11.1$  Hz, 2H), 1.79 (d,  $J = 9.8$  Hz, 1H), 1.66 – 1.57 (m, 2H), 1.49 (d,  $J = 12.5$  Hz, 2H), 1.33 (d,  $J = 12.2$  Hz, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  164.9, 132.9, 130.6, 129.5, 128.9, 126.3, 124.0, 115.4, 40.2, 30.5, 26.3, 26.1; HRMS (ESI $^+$ ): Calculated for  $\text{C}_{14}\text{H}_{16}\text{N}_2\text{O}$ :  $[\text{M}+\text{Na}]^+$  251.1155, Found 251.1162.

### 2,6-Dichloro-3-cyclohexylquinoxaline (61)



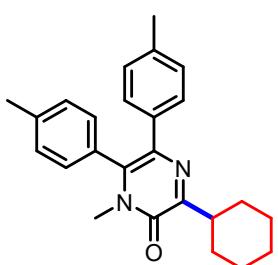
Obtained as a yellow solid (29% yield); M. P. = 66-67 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.05 (d,  $J = 2.2$  Hz, 1H), 7.90 (d,  $J = 8.9$  Hz, 1H), 7.64 (dd,  $J = 8.9, 2.3$  Hz, 1H), 3.33 (tt,  $J = 11.6, 3.2$  Hz, 1H), 2.01 (d,  $J = 12.1$  Hz, 2H), 1.93 (d,  $J = 13.2$  Hz, 2H), 1.84 – 1.77 (m, 1H), 1.67 (dd,  $J = 12.0, 3.1$  Hz, 2H), 1.49 (dd,  $J = 13.0, 3.3$  Hz, 2H), 1.39 – 1.30 (m, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  160.3, 147.7, 141.4, 139.1, 135.6, 130.8, 129.2, 127.9, 42.6, 31.2, 26.3, 25.9; HRMS (ESI $^+$ ): Calculated for  $\text{C}_{14}\text{H}_{14}\text{Cl}_2\text{N}_2$ :  $[\text{M}+\text{H}]^+$  281.0607, Found 281.0615.

### 3-Cyclohexyl-1-methyl-5,6-diphenylpyrazin-2(1*H*)-one (62)<sup>11</sup>



Obtained as a white solid (67% yield);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.39 (dd,  $J = 5.0, 2.1$  Hz, 3H), 7.26 – 7.19 (m, 2H), 7.19 – 7.14 (m, 2H), 7.14 – 7.07 (m, 3H), 3.30 (s, 4H), 2.04 – 1.96 (m, 2H), 1.86 (dt,  $J = 13.4, 3.4$  Hz, 2H), 1.77 – 1.73 (m, 1H), 1.61 (qd,  $J = 12.7, 3.4$  Hz, 2H), 1.52 – 1.43 (m, 2H), 1.31 – 1.27 (m, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  161.1, 155.3, 138.2, 135.8, 132.9, 132.1, 130.2, 130.1, 129.3, 129.0, 127.6, 126.7, 40.6, 34.0, 30.5, 26.4, 26.2.

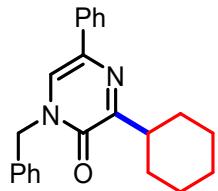
### 3-Cyclohexyl-1-methyl-5,6-di-p-tolylpyrazin-2(1*H*)-one (63)



Obtained as a white solid (62% yield); M. P. = 96-97 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.19 (d,  $J = 7.8$  Hz, 2H), 7.08 (dd,  $J = 11.6, 8.1$  Hz, 4H), 6.94 (d,  $J = 8.0$  Hz, 2H), 3.35 – 3.21 (m, 4H), 2.38 (s, 3H), 2.25 (s, 3H), 1.98 (d,  $J = 12.0$  Hz, 2H), 1.85 (d,  $J = 13.0$  Hz, 2H), 1.74 (d,  $J = 12.8$  Hz, 1H), 1.60 (dd,  $J = 27.7, 12.7$  Hz, 2H), 1.46 (dd,  $J = 28.8, 12.8$  Hz, 2H), 1.29 (t,  $J = 9.1$  Hz, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  160.8, 155.4, 139.2, 136.3, 135.5, 135.5, 132.0, 130.1, 130.0, 129.8,

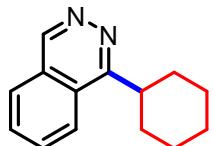
129.1, 128.4, 40.5, 33.9, 30.5, 26.4, 26.2, 21.4, 21.1; HRMS (ESI+): Calculated for C<sub>25</sub>H<sub>28</sub>N<sub>2</sub>O: [M+H]<sup>+</sup> 373.2274, Found 373.2275.

**1-Benzyl-3-cyclohexyl-5-phenylpyrazin-2(1*H*)-one (64)**



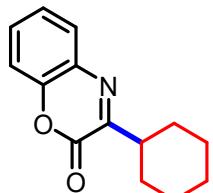
Obtained as a white solid (53% yield); M. P. = 82–83 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.74 (d, *J* = 7.4 Hz, 2H), 7.42 – 7.32 (m, 9H), 5.15 (s, 2H), 3.29 (tt, *J* = 11.5, 3.2 Hz, 1H), 1.98 (d, *J* = 12.0 Hz, 2H), 1.86 (d, *J* = 12.9 Hz, 2H), 1.76 (d, *J* = 12.9 Hz, 1H), 1.57 (dd, *J* = 12.0, 2.7 Hz, 2H), 1.49 – 1.43 (m, 2H), 1.30 (dd, *J* = 8.9, 3.6 Hz, 1H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 163.4, 154.8, 136.2, 135.3, 132.2, 129.1, 128.7, 128.5, 128.5, 127.7, 124.9, 121.8, 52.6, 40.6, 30.6, 26.4, 26.2; HRMS (ESI+): Calculated for C<sub>22</sub>H<sub>24</sub>N<sub>2</sub>O: [M+H]<sup>+</sup> 333.1961, Found 333.1966.

**1-Cyclohexylphthalazine (65)<sup>7</sup>**



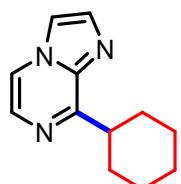
Obtained as a white solid (47% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.76 (s, 1H), 8.09 – 8.01 (m, 2H), 7.70 (dtd, *J* = 14.9, 6.9, 1.4 Hz, 2H), 2.96 (tt, *J* = 12.0, 3.4 Hz, 1H), 2.03 (d, *J* = 11.8 Hz, 2H), 1.92 (d, *J* = 13.3 Hz, 2H), 1.80 (d, *J* = 12.8 Hz, 1H), 1.75 – 1.66 (m, 2H), 1.47 (dd, *J* = 25.8, 12.8 Hz, 2H), 1.36 (t, *J* = 12.7 Hz, 1H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 161.1, 145.0, 142.2, 141.3, 129.8, 129.1, 129.0, 128.8, 45.0, 32.3, 26.4, 25.8.

**3-Cyclohexyl-2*H*-benzo[*b*][1,4]oxazin-2-one (66)<sup>19</sup>**



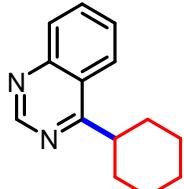
Obtained as a white solid (37% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.73 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.49 – 7.41 (m, 1H), 7.37 – 7.31 (m, 1H), 7.26 (d, *J* = 8.3 Hz, 1H), 3.23 – 3.09 (m, 1H), 1.99 (d, *J* = 12.0 Hz, 2H), 1.88 (d, *J* = 13.0 Hz, 2H), 1.77 (d, *J* = 12.8 Hz, 1H), 1.55 (ddd, *J* = 15.1, 12.6, 2.8 Hz, 2H), 1.49 – 1.37 (m, 2H), 1.37 – 1.22 (m, 1H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 161.3, 152.6, 146.2, 131.4, 130.3, 128.9, 125.3, 116.2, 41.4, 30.3, 26.1, 26.0; HRMS (ESI+): Calculated for C<sub>14</sub>H<sub>15</sub>NO<sub>2</sub>: [M+Na]<sup>+</sup> 252.0995, Found 252.1001.

**8-Cyclohexylimidazo[1,2-*a*]pyrazine (67)<sup>15</sup>**



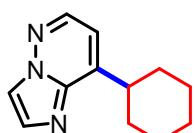
Obtained as a white solid (52% yield);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.94 (d,  $J = 4.5$  Hz, 1H), 7.82 (d,  $J = 4.5$  Hz, 1H), 7.76 (s, 1H), 7.66 (s, 1H), 3.67 (tt,  $J = 11.9, 3.3$  Hz, 1H), 2.04 (d,  $J = 11.9$  Hz, 2H), 1.89 (dd,  $J = 9.5, 6.6$  Hz, 2H), 1.82 – 1.72 (m, 3H), 1.53 (dt,  $J = 16.4, 6.4$  Hz, 2H), 1.41 – 1.35 (m, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  160.3, 139.7, 134.1, 129.0, 117.1, 113.8, 41.3, 31.1, 26.3, 26.1.

#### 4-Cyclohexylquinazoline (68)<sup>16</sup>



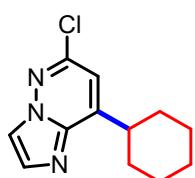
Obtained as a colourless liquid (50% yield);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  9.26 (s, 1H), 8.20 (d,  $J = 8.3$  Hz, 1H), 8.06 (d,  $J = 8.4$  Hz, 1H), 7.88 (t,  $J = 7.3$  Hz, 1H), 7.64 (t,  $J = 7.5$  Hz, 1H), 3.56 (dd,  $J = 15.9, 7.4$  Hz, 1H), 1.95 (d,  $J = 9.7$  Hz, 4H), 1.88 – 1.75 (m, 3H), 1.53 (dt,  $J = 16.0, 8.4$  Hz, 2H), 1.44 – 1.36 (m, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  175.3, 154.6, 149.9, 133.4, 129.2, 127.4, 124.2, 123.2, 41.3, 32.0, 26.5, 26.0.

#### 6-Chloro-2-cyclohexylimidazo[1,2-*b*]pyridazine (69)<sup>13</sup>



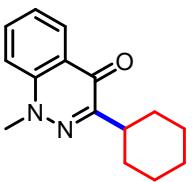
Obtained as a white solid (46% yield);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.89 (d,  $J = 1.3$  Hz, 1H), 7.72 (d,  $J = 1.2$  Hz, 1H), 6.86 (s, 1H), 3.36 (ddt,  $J = 11.6, 8.2, 3.4$  Hz, 1H), 2.09 (ddd,  $J = 8.4, 3.9, 2.0$  Hz, 2H), 1.90 (ddd,  $J = 10.1, 4.7, 2.4$  Hz, 2H), 1.82 (dtd,  $J = 12.8, 3.2, 1.6$  Hz, 1H), 1.52 (qd,  $J = 10.3, 8.5, 2.9$  Hz, 4H), 1.32 (tt,  $J = 12.5, 3.5$  Hz, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  148.1, 147.4, 137.9, 133.1, 117.2, 114.6, 38.8, 32.0, 26.2, 26.0.

#### 2-Cyclohexylimidazo[1,2-*b*]pyridazine (70)<sup>14</sup>



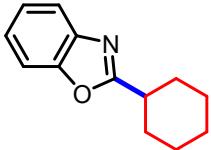
Obtained as a white solid (55% yield);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.24 (d,  $J = 4.7$  Hz, 1H), 7.95 (d,  $J = 1.2$  Hz, 1H), 7.74 (d,  $J = 1.2$  Hz, 1H), 6.84 (d,  $J = 4.7$  Hz, 1H), 3.39 (ddd,  $J = 11.6, 7.8, 3.0$  Hz, 1H), 2.13 – 2.06 (m, 2H), 1.93 – 1.86 (m, 2H), 1.85 – 1.79 (m, 1H), 1.54 (qd,  $J = 12.2, 11.7, 3.0$  Hz, 4H), 1.33 (td,  $J = 12.4, 3.7$  Hz, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  146.3, 143.5, 139.3, 132.4, 116.8, 112.5, 38.5, 32.2, 26.4, 26.1.

#### 3-Cyclohexyl-1-methylcinnolin-4(1*H*)-one (71)



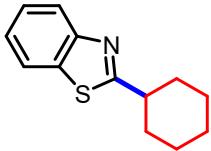
Obtained as a yellow liquid (68% yield); M. P. = 92–93 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.35 (dt,  $J$  = 3.4, 1.8 Hz, 1H), 7.78 – 7.57 (m, 1H), 7.47 – 7.33 (m, 1H), 4.07 (d,  $J$  = 2.6 Hz, 1H), 3.38 – 3.15 (m, 1H), 1.91 (dd,  $J$  = 13.8, 8.0 Hz, 1H), 1.87 – 1.79 (m, 1H), 1.78 – 1.73 (m, 1H), 1.53 – 1.41 (m, 1H), 1.32 – 1.27 (m, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  169.9, 154.5, 141.1, 133.3, 126.3, 123.9, 123.2, 114.4, 43.4, 37.2, 31.0, 26.5, 26.3; HRMS (ESI+): Calculated for  $\text{C}_{15}\text{H}_{18}\text{N}_2\text{O}$ : [M+H] $^+$  243.1492, Found 243.1491.

### 2-Cyclohexylbenzo[d]oxazole (72)<sup>20</sup>



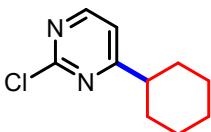
Obtained as a colourless liquid (20% yield);  $^1\text{H}$  NMR (500 MHz, DMSO)  $\delta$  7.74 – 7.62 (m, 2H), 7.38 – 7.29 (m, 2H), 3.00 (dd,  $J$  = 9.1, 5.5 Hz, 1H), 2.09 (dd,  $J$  = 12.8, 2.9 Hz, 2H), 1.77 (dd,  $J$  = 10.2, 6.4 Hz, 2H), 1.69 – 1.60 (m, 3H), 1.41 (dd,  $J$  = 24.6, 12.1 Hz, 2H), 1.29 (dd,  $J$  = 19.8, 7.8 Hz, 1H);  $^{13}\text{C}$  NMR (126 MHz, DMSO)  $\delta$  170.2, 150.5, 141.3, 125.1, 124.6, 119.8, 111.0, 37.3, 30.4, 25.8, 25.4; HRMS (ESI+): Calculated for  $\text{C}_{13}\text{H}_{15}\text{NO}$ : [M+H] $^+$  202.1226, Found 202.1232.

### 2-Cyclohexylbenzo[d]thiazole (73)<sup>15</sup>



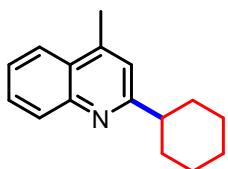
Obtained as a colourless liquid (26% yield);  $^1\text{H}$  NMR (500 MHz, DMSO)  $\delta$  8.03 (d,  $J$  = 8.0 Hz, 1H), 7.93 (d,  $J$  = 8.1 Hz, 1H), 7.47 (t,  $J$  = 7.5 Hz, 1H), 7.38 (dd,  $J$  = 10.9, 4.1 Hz, 1H), 3.09 (tt,  $J$  = 11.4, 3.6 Hz, 1H), 2.15 – 2.04 (m, 2H), 1.79 (d,  $J$  = 13.2 Hz, 2H), 1.68 (d,  $J$  = 12.8 Hz, 1H), 1.60 – 1.53 (m, 2H), 1.39 (dd,  $J$  = 12.5, 9.3 Hz, 2H), 1.30 – 1.23 (m, 1H);  $^{13}\text{C}$  NMR (126 MHz, DMSO)  $\delta$  177.1, 153.2, 134.5, 126.4, 125.2, 122.7, 122.5, 42.7, 33.2, 25.9, 25.8.

### 2-Chloro-4-cyclohexylpyrimidine (74)<sup>12</sup>



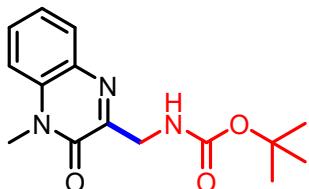
Obtained as a colourless liquid (18% yield);  $^1\text{H}$  NMR (500 MHz, DMSO)  $\delta$  8.58 (d,  $J$  = 5.0 Hz, 1H), 7.50 (d,  $J$  = 5.1 Hz, 1H), 2.66 (tt,  $J$  = 11.6, 3.2 Hz, 1H), 1.84 (d,  $J$  = 11.5 Hz, 2H), 1.78 (d,  $J$  = 12.7 Hz, 2H), 1.69 (d,  $J$  = 12.6 Hz, 1H), 1.44 (dd,  $J$  = 22.0, 12.5 Hz, 2H), 1.34 (dd,  $J$  = 19.4, 12.6 Hz, 2H), 1.22 (d,  $J$  = 8.9 Hz, 1H);  $^{13}\text{C}$  NMR (126 MHz, DMSO)  $\delta$  178.4, 160.7, 152.6, 119.1, 45.1, 31.6, 25.9, 25.7.

### 2-Cyclohexyl-4-methylquinoline (75)<sup>9</sup>



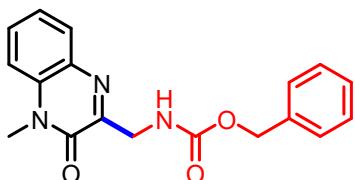
Obtained as a colourless liquid (15% yield);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.06 (d,  $J = 8.4$  Hz, 1H), 7.94 (d,  $J = 8.3$  Hz, 1H), 7.70 – 7.63 (m, 1H), 7.52 – 7.46 (m, 1H), 7.17 (s, 1H), 2.94 – 2.83 (m, 1H), 2.68 (s, 3H), 2.01 (d,  $J = 11.8$  Hz, 2H), 1.89 (d,  $J = 13.1$  Hz, 2H), 1.79 (d,  $J = 15.6$  Hz, 1H), 1.62 (dd,  $J = 23.6, 11.2$  Hz, 2H), 1.47 (q,  $J = 9.6$  Hz, 2H), 1.38 – 1.32 (m, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  166.5, 147.4, 144.4, 129.3, 129.0, 127.0, 125.4, 123.5, 120.2, 47.5, 32.8, 26.5, 26.1, 18.8.

#### *tert*-Butyl ((4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)methyl)carbamate (77)<sup>9</sup>



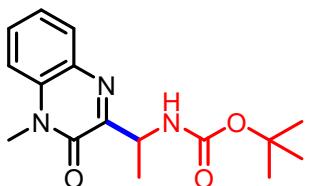
Obtained as a white solid (47% yield);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.82 (d,  $J = 7.9$  Hz, 1H), 7.51 (t,  $J = 7.4$  Hz, 1H), 7.30 (dd,  $J = 13.3, 5.7$  Hz, 2H), 5.72 (s, 1H), 4.52 (d,  $J = 3.8$  Hz, 2H), 3.65 (s, 3H), 1.43 (s, 9H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  155.8, 155.0, 154.0, 133.1, 132.1, 130.3, 129.9, 123.8, 113.7, 79.5, 43.0, 28.9, 28.4; HRMS (ESI $^+$ ): Calculated for  $\text{C}_{15}\text{H}_{19}\text{N}_3\text{O}_3$ :  $[\text{M}+\text{Na}]^+$  312.1319, Found 312.1328.

#### Benzyl ((4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)methyl)carbamate (78)<sup>9</sup>



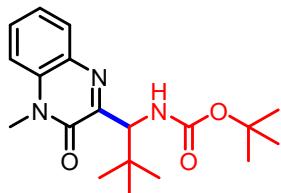
Obtained as a white solid (45% yield);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.75 (d,  $J = 7.9$  Hz, 1H), 7.49 (t,  $J = 7.7$  Hz, 1H), 7.35 – 7.23 (m, 7H), 6.04 (s, 1H), 5.09 (s, 2H), 4.57 (d,  $J = 4.8$  Hz, 2H), 3.62 (s, 3H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  156.3, 154.5, 153.9, 136.6, 133.1, 132.1, 130.4, 129.9, 128.6, 128.3, 128.2, 123.9, 113.8, 66.9, 43.3, 29.0; HRMS (ESI $^+$ ): Calculated for  $\text{C}_{18}\text{H}_{17}\text{N}_3\text{O}_3$ :  $[\text{M}+\text{Na}]^+$  346.1162, Found 346.1183.

#### *tert*-Butyl-(1-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)ethyl)carbamate (79)<sup>9</sup>



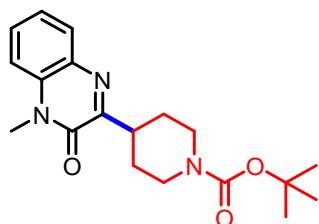
Obtained as a white solid (49% yield);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.86 (dd,  $J = 8.0, 1.1$  Hz, 1H), 7.57 (t,  $J = 7.8$  Hz, 1H), 7.36 (t,  $J = 7.6$  Hz, 1H), 7.32 (d,  $J = 8.4$  Hz, 1H), 5.94 (s, 1H), 5.26 (s, 1H), 3.71 (s, 3H), 1.51 (d,  $J = 6.7$  Hz, 3H), 1.47 (s, 9H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  161.1, 156.9, 155.4, 135.0, 133.9, 132.1, 131.7, 125.5, 115.5, 81.1, 50.5, 30.8, 30.2, 22.0; HRMS (ESI $^+$ ): Calculated for  $\text{C}_{16}\text{H}_{21}\text{N}_3\text{O}_3$ :  $[\text{M}+\text{Na}]^+$  326.1475, Found 326.1498.

**tert-Butyl-(2,2-dimethyl-1-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)propyl)carbamate (80)<sup>9</sup>**



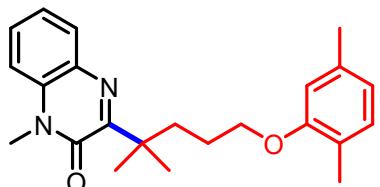
Obtained as a white solid (54% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.85 (d, *J* = 7.6 Hz, 1H), 7.56 (dd, *J* = 11.4, 4.2 Hz, 1H), 7.38 – 7.28 (m, 2H), 5.85 (d, *J* = 6.5 Hz, 1H), 5.33 (d, *J* = 9.6 Hz, 1H), 3.70 (s, 3H), 1.43 (s, 9H), 1.01 (s, 9H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 159.2, 155.5, 154.5, 133.2, 132.2, 130.3, 130.1, 123.5, 113.6, 79.0, 57.7, 37.1, 29.3, 28.4, 26.6; HRMS (ESI+): Calculated for C<sub>19</sub>H<sub>27</sub>N<sub>3</sub>O<sub>3</sub>: [M+Na]<sup>+</sup> 368.1945, Found 368.1936.

**tert-Butyl 4-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)piperidine-1-carboxylate (81)<sup>9</sup>**



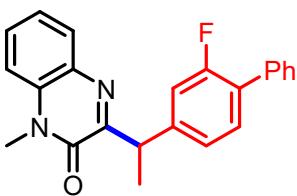
Obtained as a white solid (44% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.75 (d, *J* = 7.7 Hz, 1H), 7.46 (t, *J* = 7.4 Hz, 1H), 7.26 (t, *J* = 7.6 Hz, 1H), 7.22 (d, *J* = 8.4 Hz, 1H), 4.14 (d, *J* = 11.6 Hz, 1H), 4.04 (t, *J* = 10.6 Hz, 1H), 3.63 (s, 3H), 3.39 (d, *J* = 3.6 Hz, 1H), 3.17 (t, *J* = 11.8 Hz, 1H), 2.79 (t, *J* = 10.7 Hz, 1H), 2.11 (s, 1H), 1.75 (s, 1H), 1.58 (t, *J* = 9.4 Hz, 2H), 1.36 (s, 9H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 161.3, 154.8, 154.2, 133.0, 132.6, 129.9, 129.8, 123.5, 113.5, 79.3, 38.9, 29.2, 29.1, 28.4, 24.9; HRMS (ESI+): Calculated for C<sub>19</sub>H<sub>25</sub>N<sub>3</sub>O<sub>3</sub>: [M+Na]<sup>+</sup> 366.1788, Found 366.1798.

**3-(5-(2,5-Dimethylphenoxy)-2-methylpentan-2-yl)-1-methylquinoxalin-2(1*H*)-one (82)<sup>9</sup>**



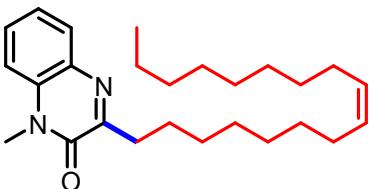
Obtained as a white solid (65% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.86 – 7.80 (m, 1H), 7.53 – 7.47 (m, 1H), 7.31 (t, *J* = 7.3 Hz, 1H), 7.24 (d, *J* = 9.8 Hz, 1H), 6.96 (d, *J* = 7.4 Hz, 1H), 6.61 (d, *J* = 7.4 Hz, 1H), 6.53 (s, 1H), 3.87 (t, *J* = 6.6 Hz, 2H), 3.63 (s, 3H), 2.24 (s, 3H), 2.21 – 2.16 (m, 2H), 2.15 (s, 3H), 1.67 (dd, *J* = 10.0, 6.4 Hz, 2H), 1.50 (s, 6H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 164.4, 157.0, 153.7, 136.3, 133.3, 132.2, 130.2, 129.6, 129.5, 123.6, 123.2, 120.4, 113.3, 111.9, 68.1, 42.6, 35.9, 28.7, 26.3, 25.4, 21.4, 15.8; HRMS (ESI+): Calculated for C<sub>23</sub>H<sub>28</sub>N<sub>2</sub>O<sub>2</sub>: [M+H]<sup>+</sup> 365.2224, Found 365.2235.

**3-(1-(2-Fluoro-[1,1'-biphenyl]-4-yl)ethyl)-1-methylquinoxalin-2(1*H*)-one (83)<sup>9</sup>**



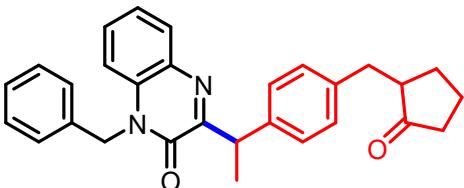
Obtained as a white solid (50% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.94 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.53 (dd, *J* = 10.4, 3.3 Hz, 1H), 7.49 (d, *J* = 7.9 Hz, 2H), 7.39 (t, *J* = 7.6 Hz, 2H), 7.37 – 7.33 (m, 2H), 7.32 (d, *J* = 4.4 Hz, 1H), 7.30 (s, 1H), 7.27 (d, *J* = 8.7 Hz, 1H), 7.22 (d, *J* = 12.9 Hz, 1H), 4.86 (q, *J* = 7.1 Hz, 1H), 3.65 (s, 3H), 1.71 (d, *J* = 7.1 Hz, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 161.2, 159.7 (d, *J* = 248.2 Hz), 154.5, 144.8 (d, *J* = 6.3 Hz), 135.8, 133.1, 132.7, 130.6 (d, *J* = 3.8 Hz), 130.2, 130.0, 129.0 (d, *J* = 3.8 Hz), 128.4, 127.4, 127.1 (d, *J* = 12.6 Hz), 124.2 (d, *J* = 2.5 Hz), 123.6, 115.5 (d, *J* = 22.7 Hz), 113.6, 41.4, 29.2, 19.6; <sup>19</sup>F NMR (471 MHz, CDCl<sub>3</sub>) δ -118.05; HRMS (ESI+): Calculated for C<sub>23</sub>H<sub>19</sub>FN<sub>2</sub>O: [M+H]<sup>+</sup> 359.1554, Found 359.1561.

#### (Z)-3-(Heptadec-8-en-1-yl)-1-methylquinoxalin-2(1H)-one (84)<sup>9</sup>



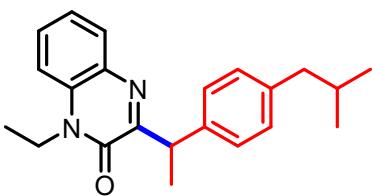
Obtained as a white solid (45% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.85 (d, *J* = 7.9 Hz, 1H), 7.55 – 7.49 (m, 1H), 7.37 – 7.31 (m, 1H), 7.30 (d, *J* = 8.3 Hz, 1H), 5.34 (t, *J* = 4.6 Hz, 2H), 3.70 (s, 3H), 3.02 – 2.89 (m, 2H), 2.01 (d, *J* = 5.1 Hz, 4H), 1.86 – 1.71 (m, 2H), 1.30 (dd, *J* = 35.9, 3.3 Hz, 20H), 0.87 (dd, *J* = 8.2, 5.5 Hz, 3H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 161.4, 154.9, 133.1, 132.8, 129.9, 129.9, 129.6, 129.5, 123.5, 113.5, 34.4, 31.9, 29.8, 29.8, 29.7, 29.7, 29.6, 29.5, 29.4, 29.3, 29.2, 29.0, 27.2, 26.9, 22.7, 14.1; HRMS (ESI+): Calculated for C<sub>26</sub>H<sub>40</sub>N<sub>2</sub>O: [M+Na]<sup>+</sup> 419.3033, Found 419.3045.

#### 1-Benzyl-3-(1-(4-((2-oxocyclopentyl)methyl)phenyl)ethyl)quinoxalin-2(1H)-one (85)



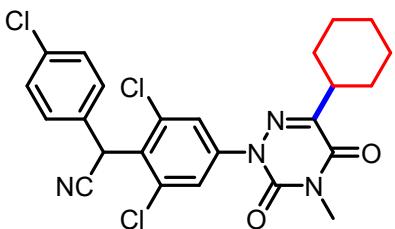
Obtained as a white solid (53% yield); M.P. = 119–120 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.83 (d, *J* = 8.0 Hz, 1H), 7.31 – 7.25 (m, 3H), 7.20 (d, *J* = 7.6 Hz, 1H), 7.18 – 7.14 (m, 3H), 7.10 (d, *J* = 8.3 Hz, 1H), 7.06 (d, *J* = 7.8 Hz, 2H), 7.00 (d, *J* = 8.0 Hz, 2H), 5.43 (d, *J* = 15.9 Hz, 1H), 5.20 (dd, *J* = 16.5, 8.2 Hz, 1H), 4.82 – 4.75 (m, 1H), 3.02 (dd, *J* = 13.9, 4.0 Hz, 1H), 2.37 (ddd, *J* = 13.8, 9.8, 1.5 Hz, 1H), 2.27 – 2.16 (m, 2H), 2.07 – 1.92 (m, 2H), 1.83 (dd, *J* = 6.4, 2.7 Hz, 1H), 1.64 – 1.57 (m, 4H), 1.44 (dd, *J* = 12.0, 6.5 Hz, 1H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 162.1, 154.5, 141.0, 138.2, 135.3, 133.0, 132.4, 130.2, 129.7, 128.9, 128.9, 128.9, 128.2, 127.6, 126.8, 123.5, 114.3, 51.1, 45.9, 41.4, 38.2, 35.3, 29.3, 20.6, 19.7; HRMS (ESI+): Calculated for C<sub>29</sub>H<sub>28</sub>N<sub>2</sub>O<sub>2</sub>: [M+H]<sup>+</sup> 437.2224, Found 437.2222.

#### 1-Ethyl-3-(1-(4-isobutylphenyl)ethyl)quinoxalin-2(1H)-one (86)



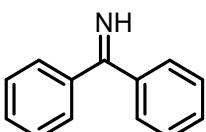
Obtained as a white solid (61% yield); M.P. = 115-116 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.91 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.50 – 7.44 (m, 1H), 7.35 (d, *J* = 8.1 Hz, 2H), 7.32 – 7.27 (m, 1H), 7.25 (d, *J* = 7.8 Hz, 1H), 7.05 (d, *J* = 8.0 Hz, 2H), 4.83 (q, *J* = 7.1 Hz, 1H), 4.29 (dq, *J* = 14.3, 7.2 Hz, 1H), 4.16 (dq, *J* = 14.2, 7.2 Hz, 1H), 2.40 (d, *J* = 7.2 Hz, 2H), 1.81 (dt, *J* = 13.5, 6.8 Hz, 1H), 1.67 (d, *J* = 7.1 Hz, 3H), 1.30 (t, *J* = 7.2 Hz, 3H), 0.86 (dd, *J* = 6.6, 2.2 Hz, 6H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 162.2, 153.9, 140.4, 139.8, 133.1, 132.0, 130.4, 129.6, 129.1, 127.8, 123.2, 113.3, 45.1, 41.2, 37.3, 30.2, 22.5, 22.5, 19.8, 12.4; HRMS (ESI+): Calculated for C<sub>22</sub>H<sub>26</sub>N<sub>2</sub>O: [M+H]<sup>+</sup> 335.2118, Found 335.2112.

### **2-(4-Chlorophenyl)-2-(2,6-dichloro-4-(6-cyclohexyl-4-methyl-3,5-dioxo-4,5-dihydro-1,2,4-triazin-2(3H)-yl)phenyl)acetonitrile (88)**



Obtained as a yellow solid (66% yield); M.P. = 98-99 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.78 (s, 2H), 7.30 (dt, *J* = 20.8, 10.4 Hz, 4H), 6.17 (s, 1H), 3.40 (s, 3H), 2.98 (d, *J* = 7.0 Hz, 1H), 1.93 (d, *J* = 7.3 Hz, 2H), 1.84 (d, *J* = 5.1 Hz, 2H), 1.74 (d, *J* = 12.1 Hz, 1H), 1.48 – 1.36 (m, 4H), 1.26 (d, *J* = 15.9 Hz, 1H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 155.1, 150.6, 148.1, 141.9, 135.6, 134.3, 130.9, 129.4, 129.1, 128.3, 124.7, 116.3, 38.8, 37.0, 30.4, 27.6, 26.1, 25.9; HRMS (ESI+): Calculated for C<sub>24</sub>H<sub>21</sub>Cl<sub>3</sub>N<sub>4</sub>O<sub>2</sub>: [M+Na]<sup>+</sup> 525.0622, Found 525.0615.

### **Diphenylmethanimine (90)<sup>21</sup>**

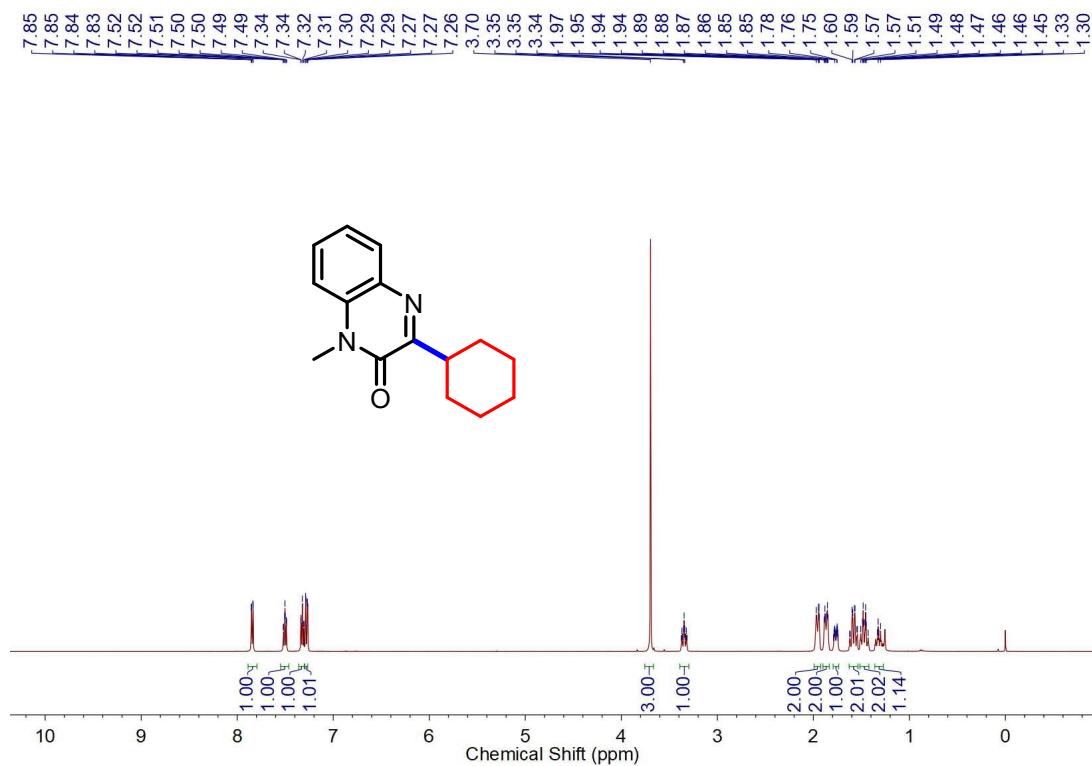


Obtained as a colourless liquid (64% yield); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.79 (s, 1H), 7.58 (d, *J* = 7.3 Hz, 4H), 7.45 (dt, *J* = 14.7, 5.6 Hz, 6H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 178.5, 139.1, 130.5, 128.6, 128.4; HRMS (ESI+): Calculated for C<sub>13</sub>H<sub>11</sub>N: [M+Na]<sup>+</sup> 204.0784, Found 204.0779.

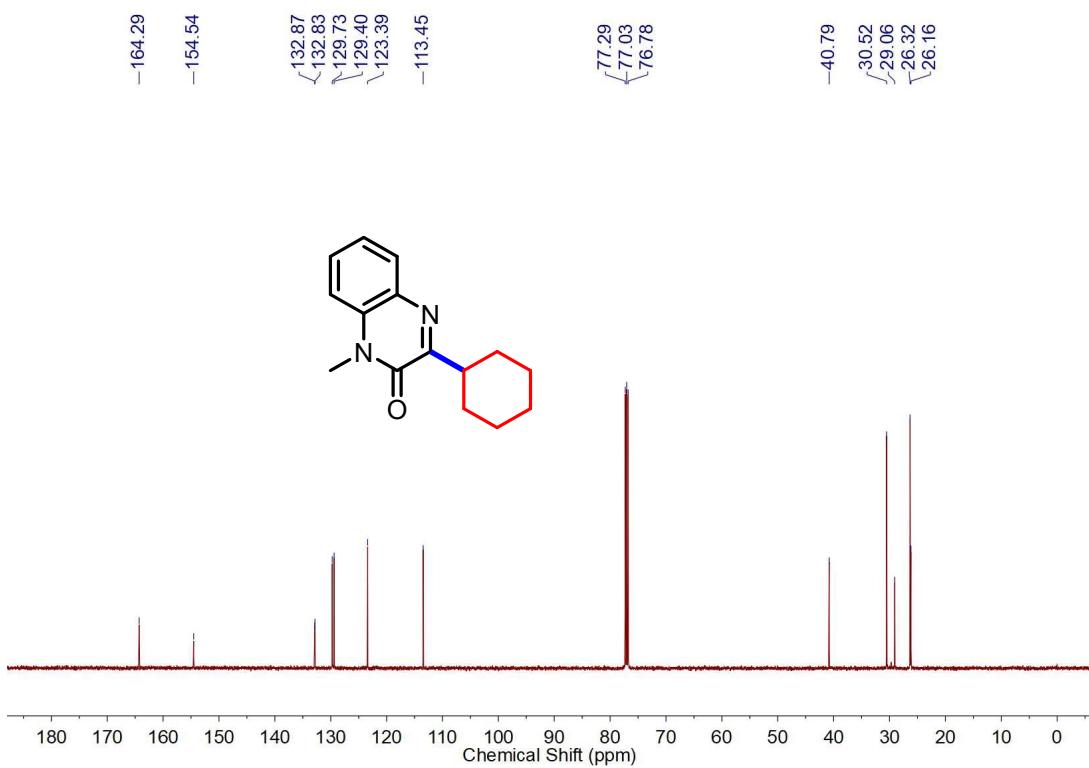
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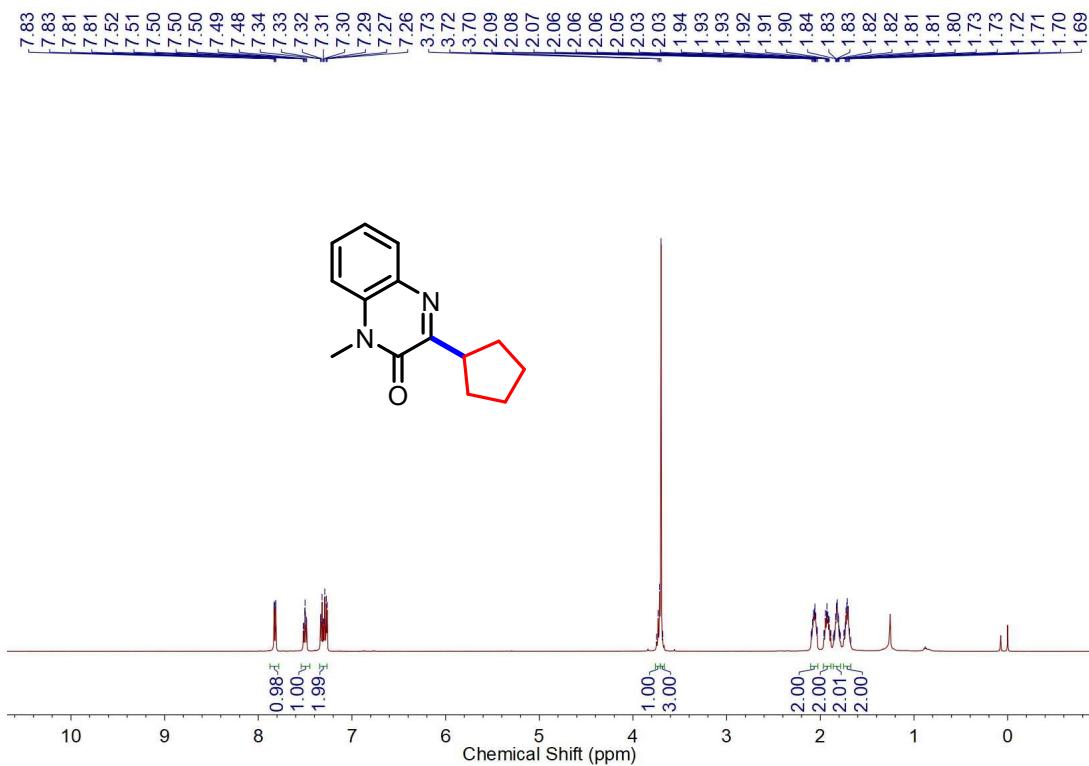
#### 4. Copies of $^1\text{H}$ , $^{13}\text{C}$ and $^{19}\text{F}$ NMR Spectra



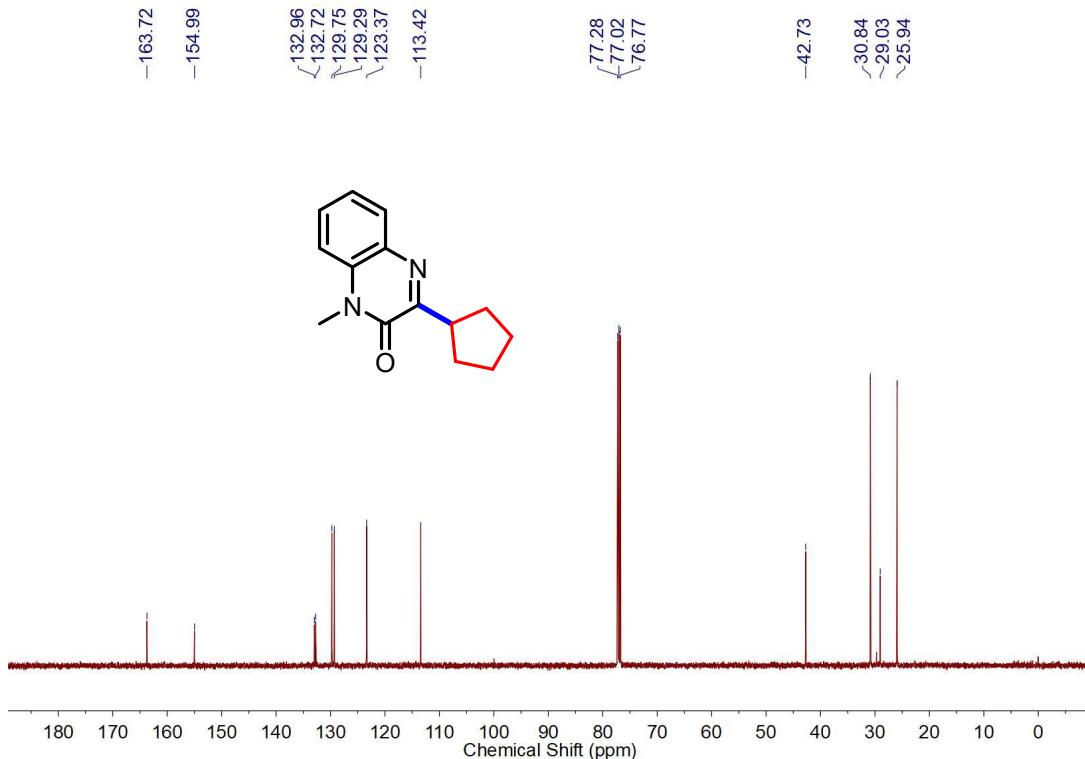
**Figure S1.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **3**



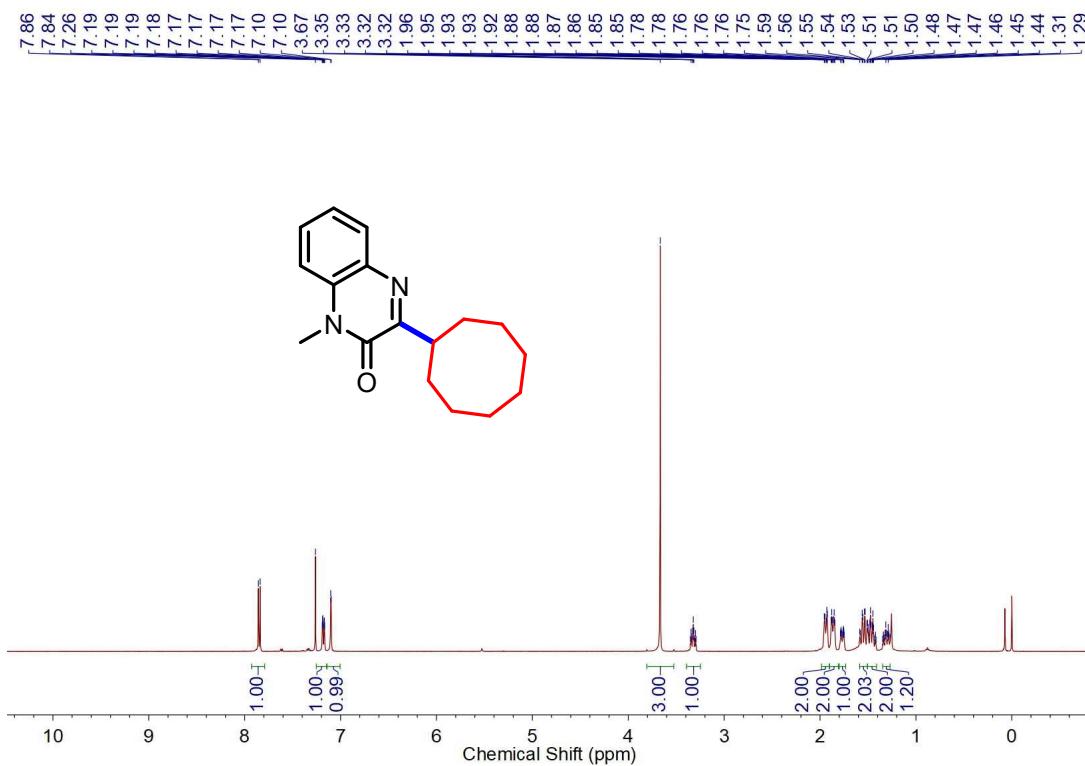
**Figure S2.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **3**



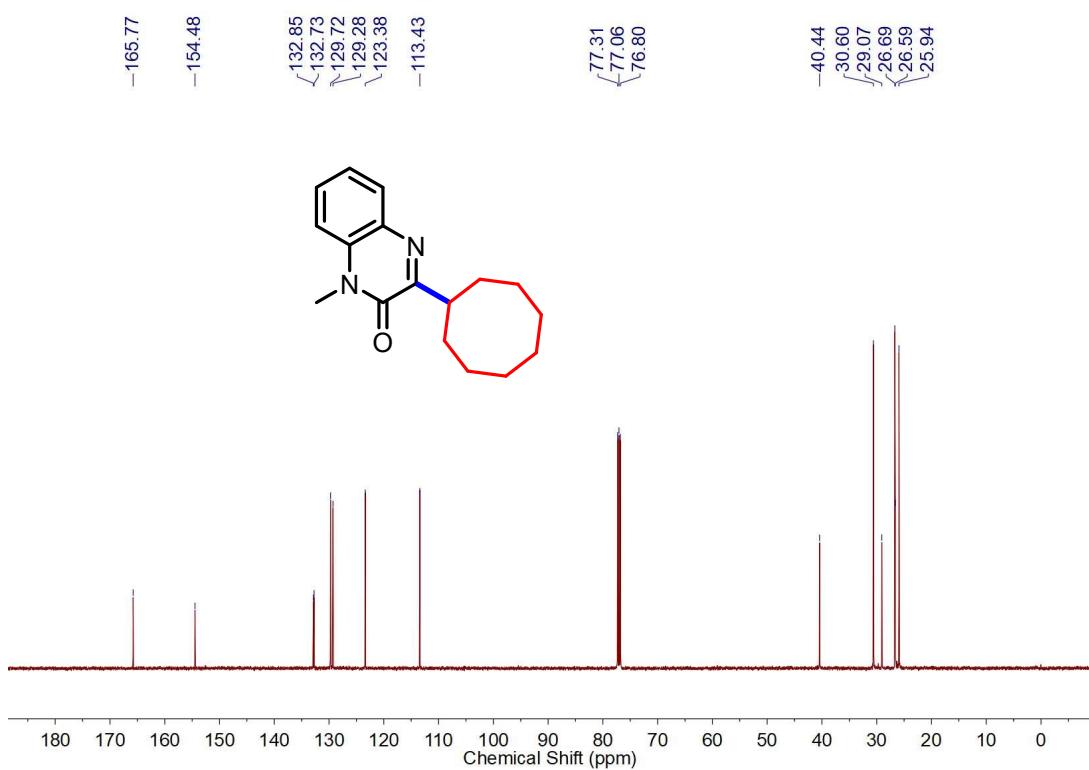
**Figure S3.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **4**



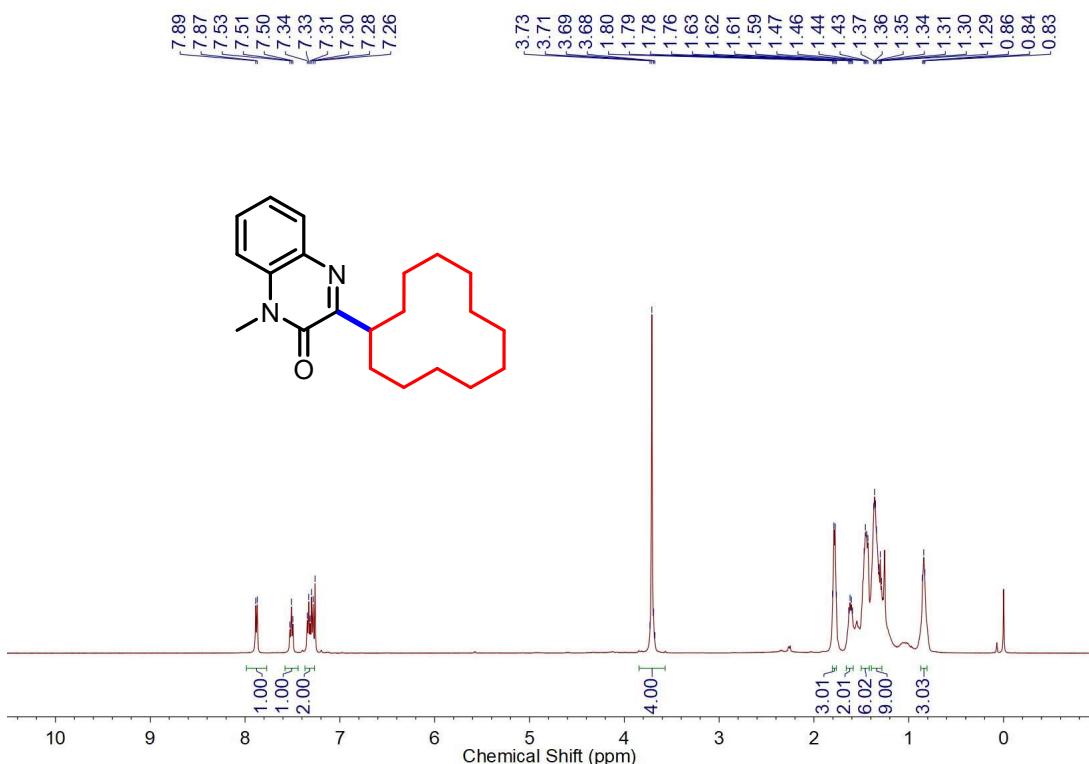
**Figure S4.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of 4



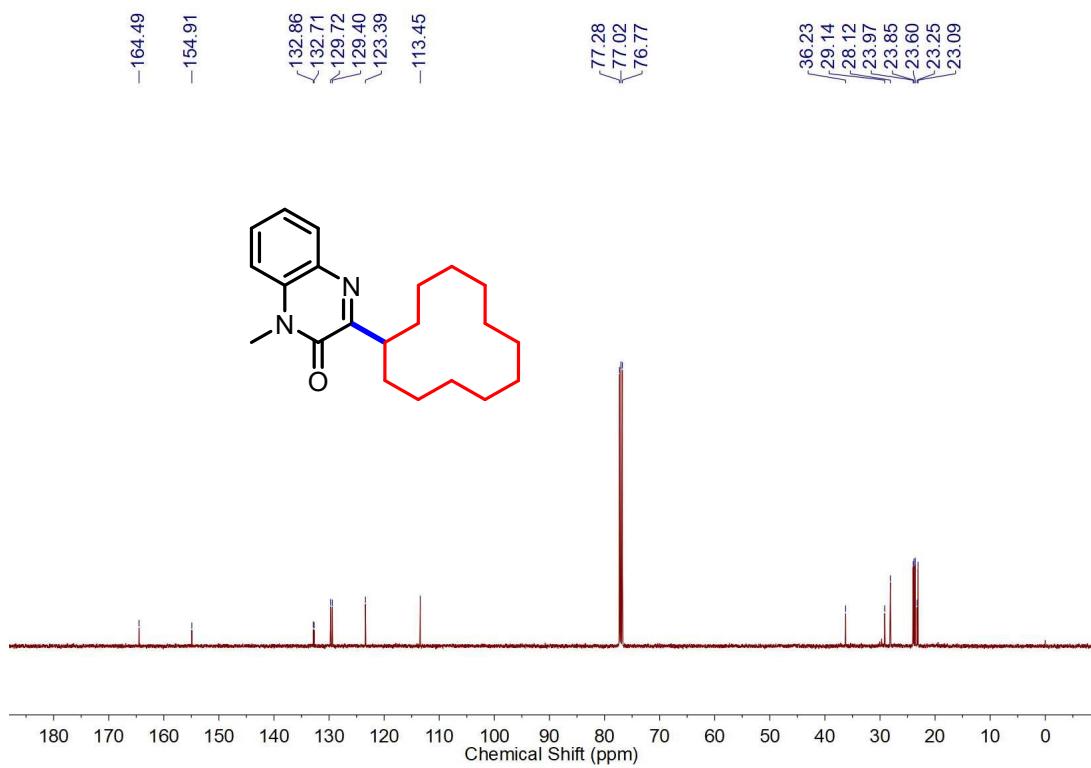
**Figure S5.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **5**



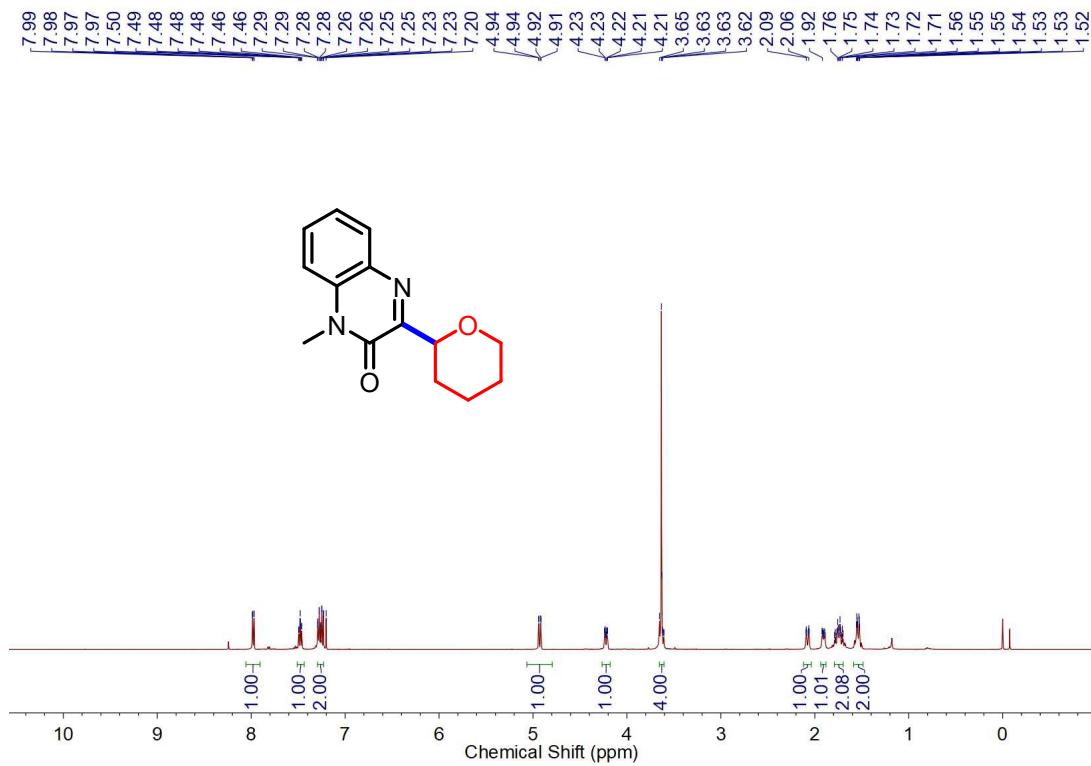
**Figure S6.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **5**



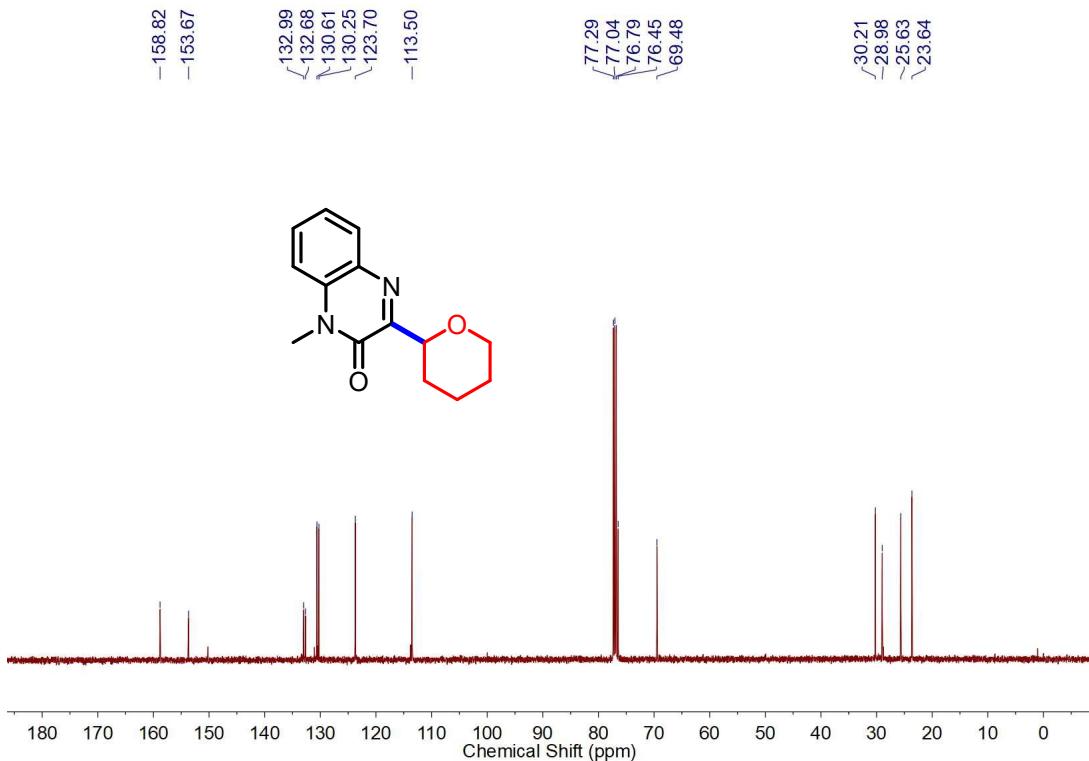
**Figure S7.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **6**



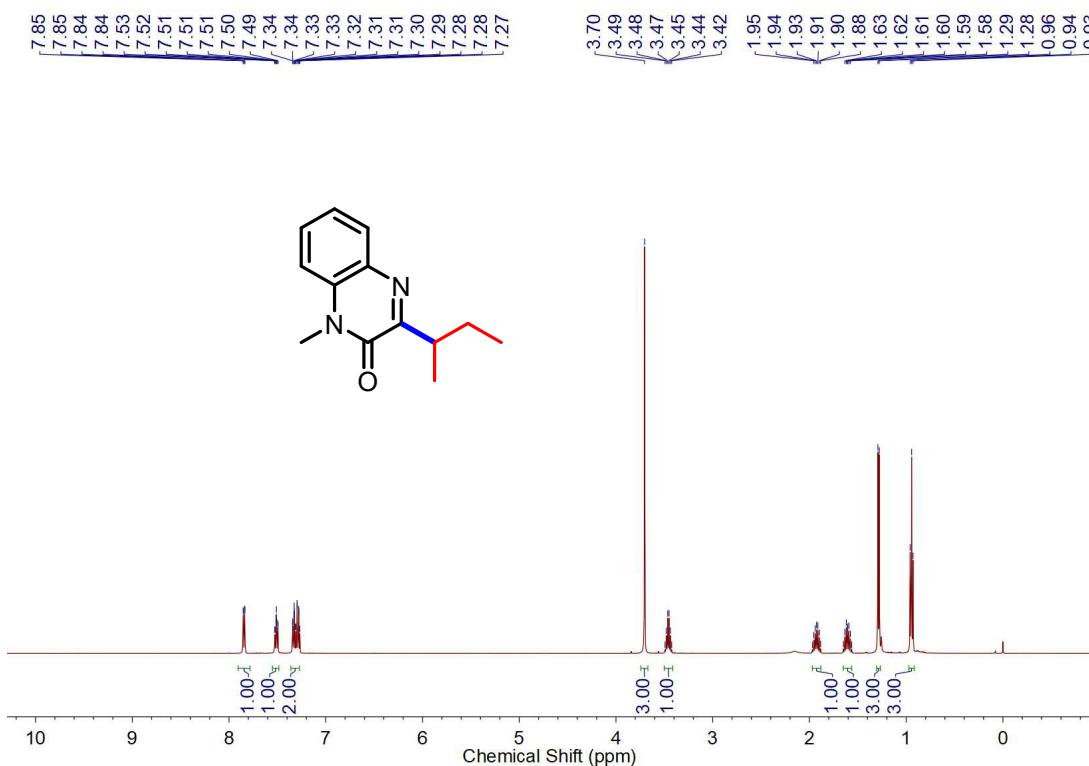
**Figure S8.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **6**



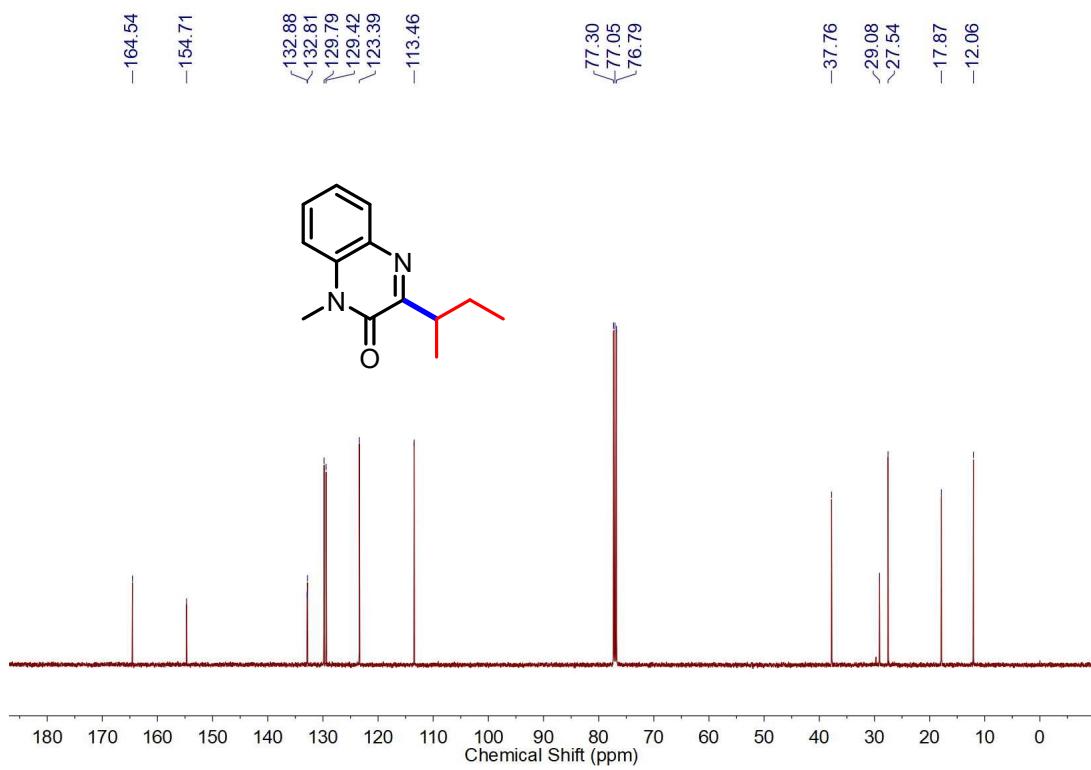
**Figure S9.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **7**



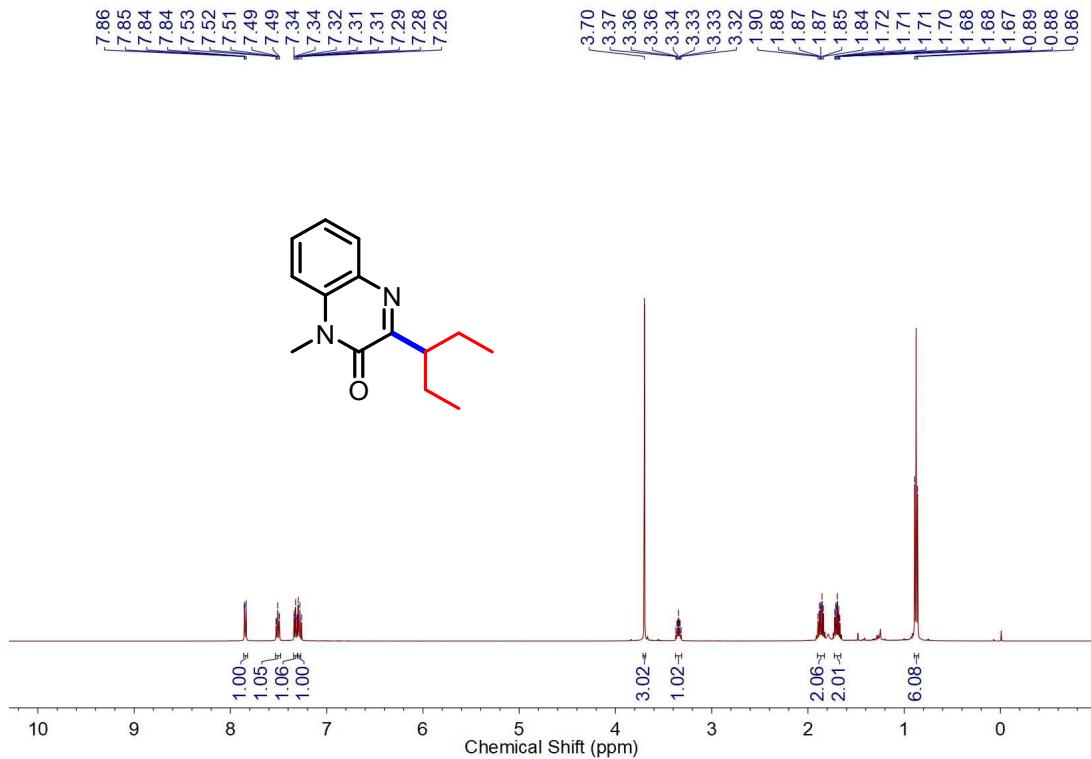
**Figure S10.** <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **7**



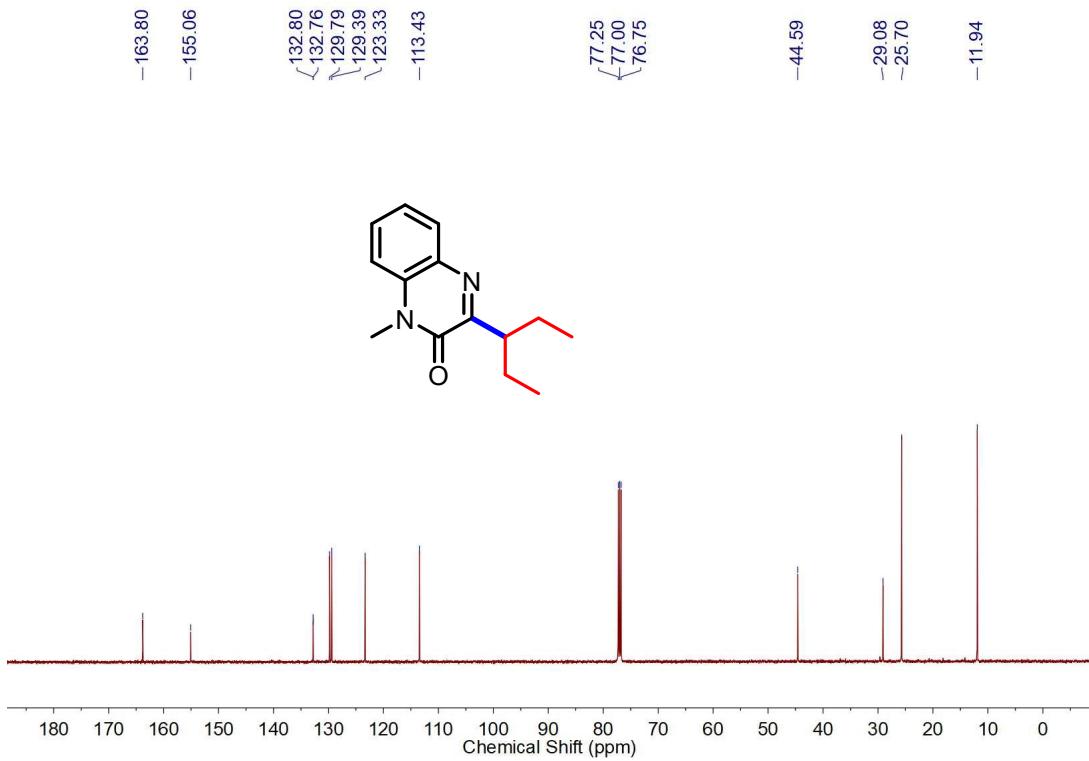
**Figure S11.** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **8**



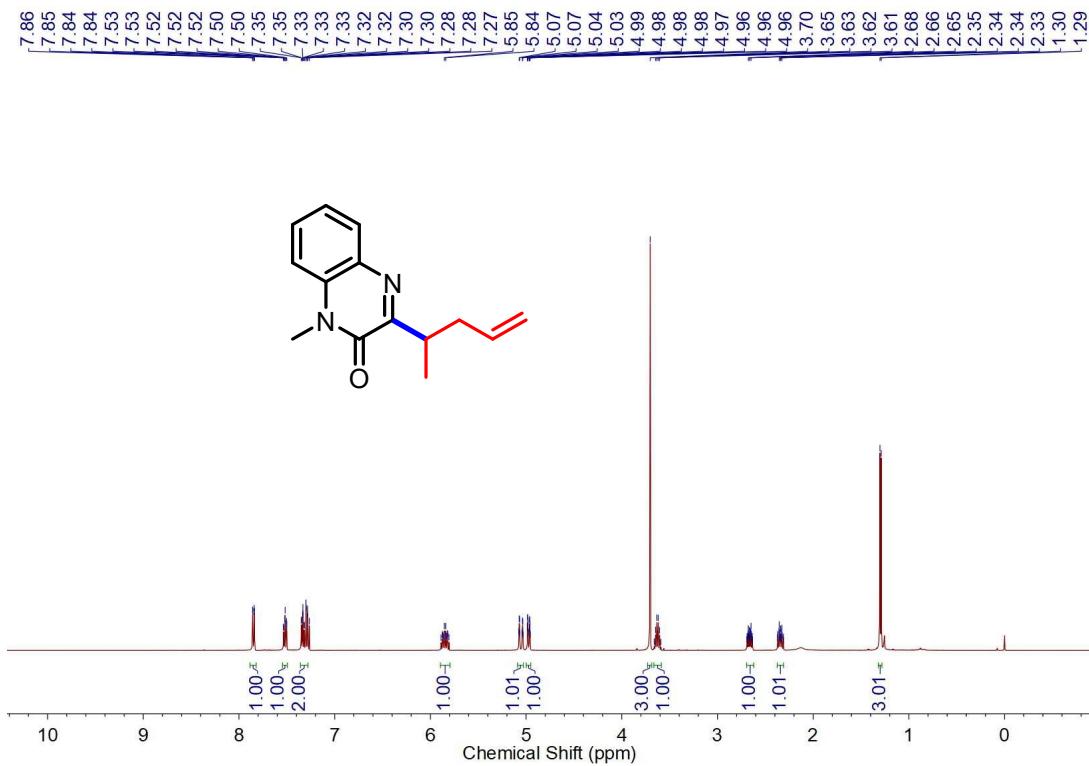
**Figure S12.** <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **8**



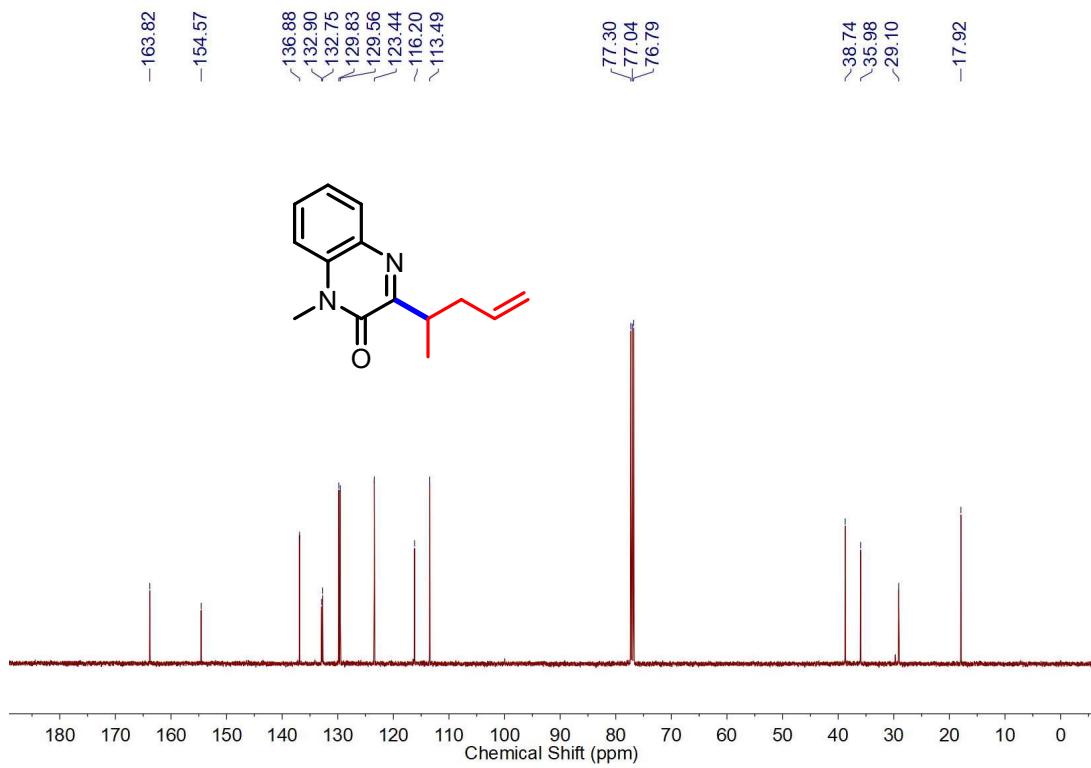
**Figure S13.** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **9**



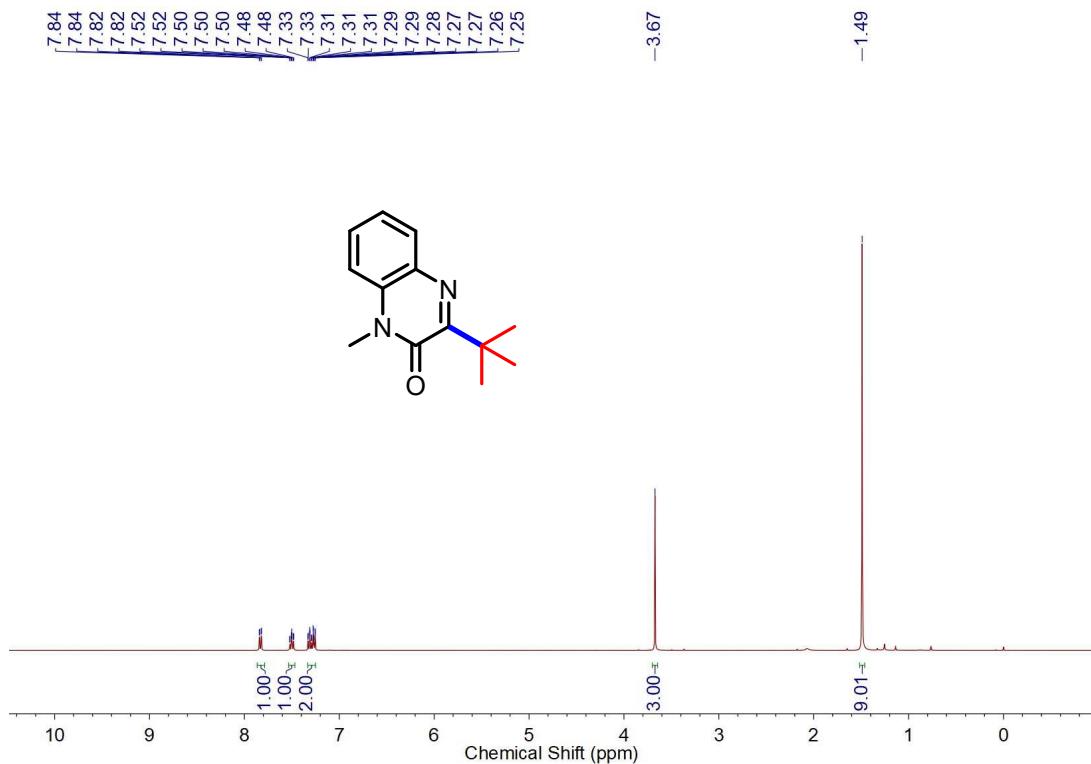
**Figure S14.** <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **9**



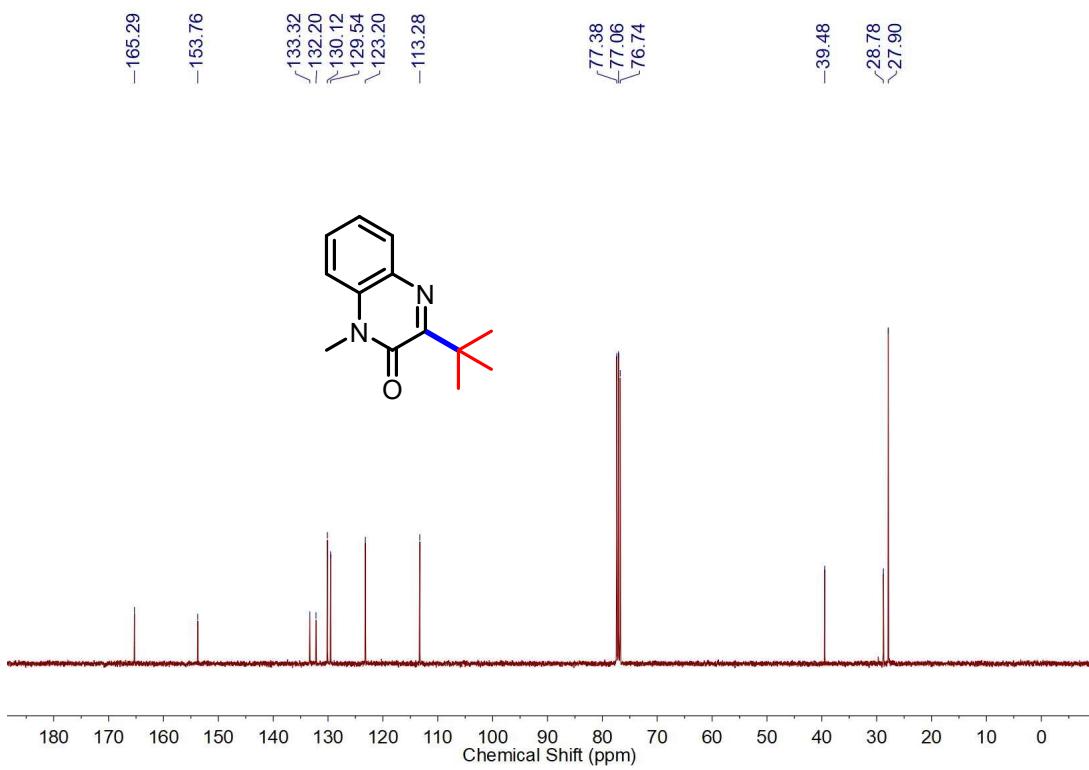
**Figure S15.** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **10**



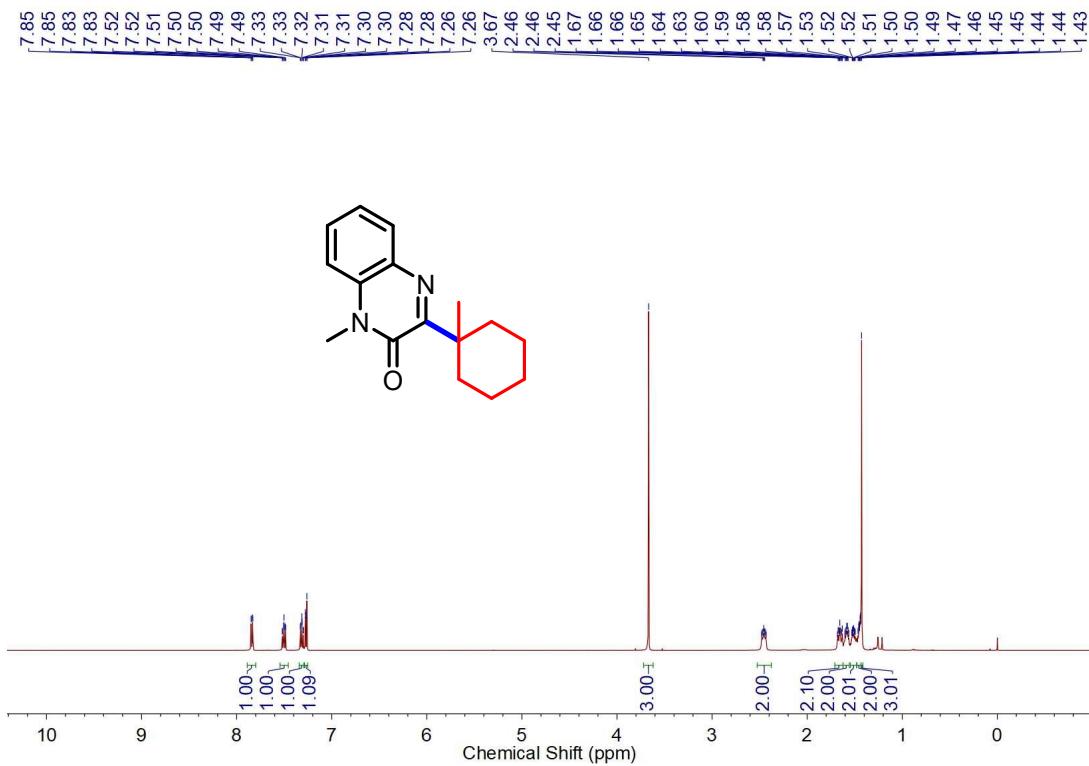
**Figure S16.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **10**



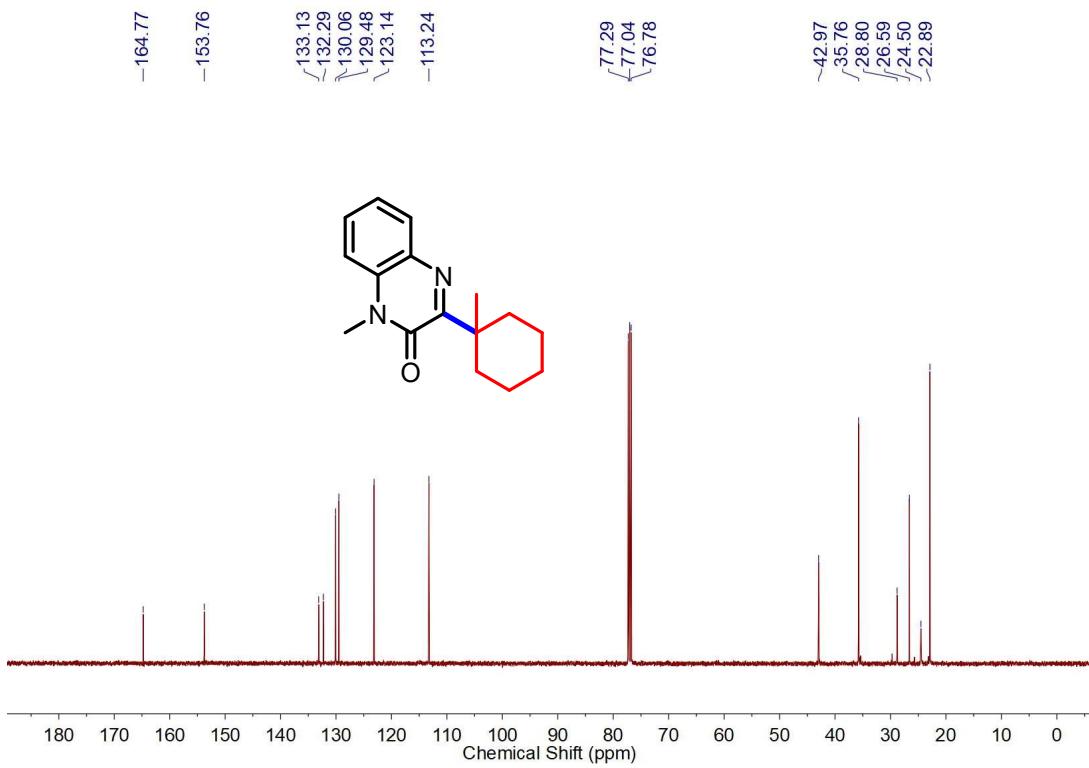
**Figure S17.**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of **11**



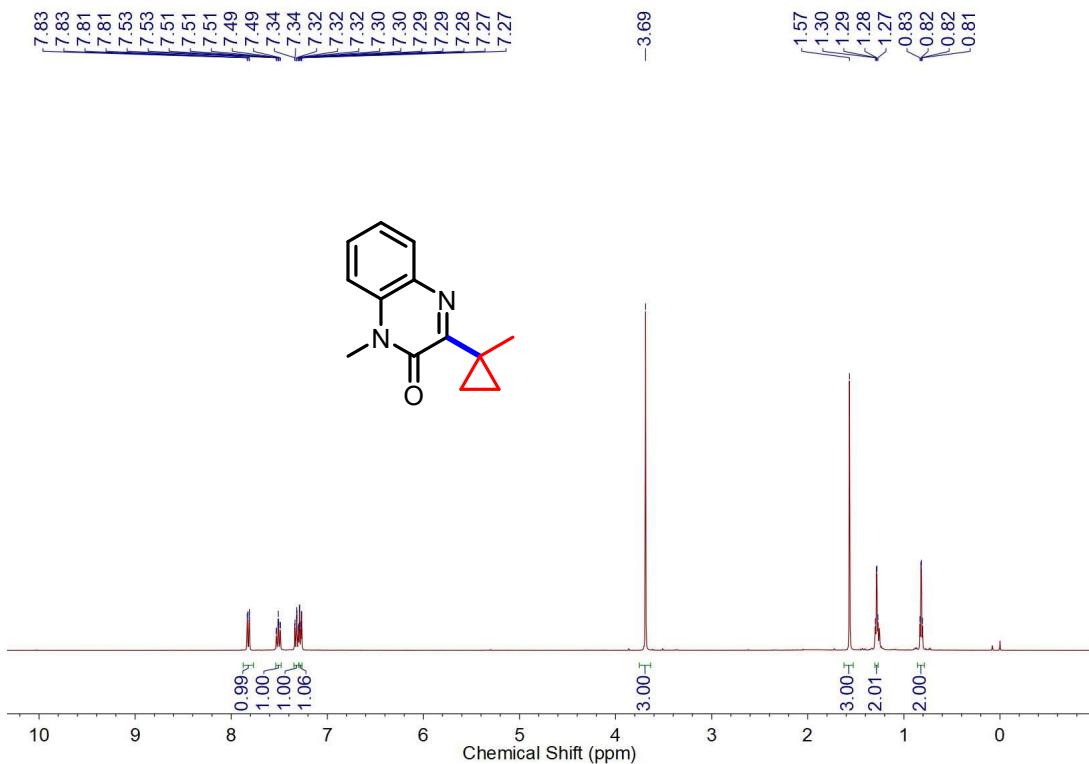
**Figure S18.**  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ) spectrum of **11**



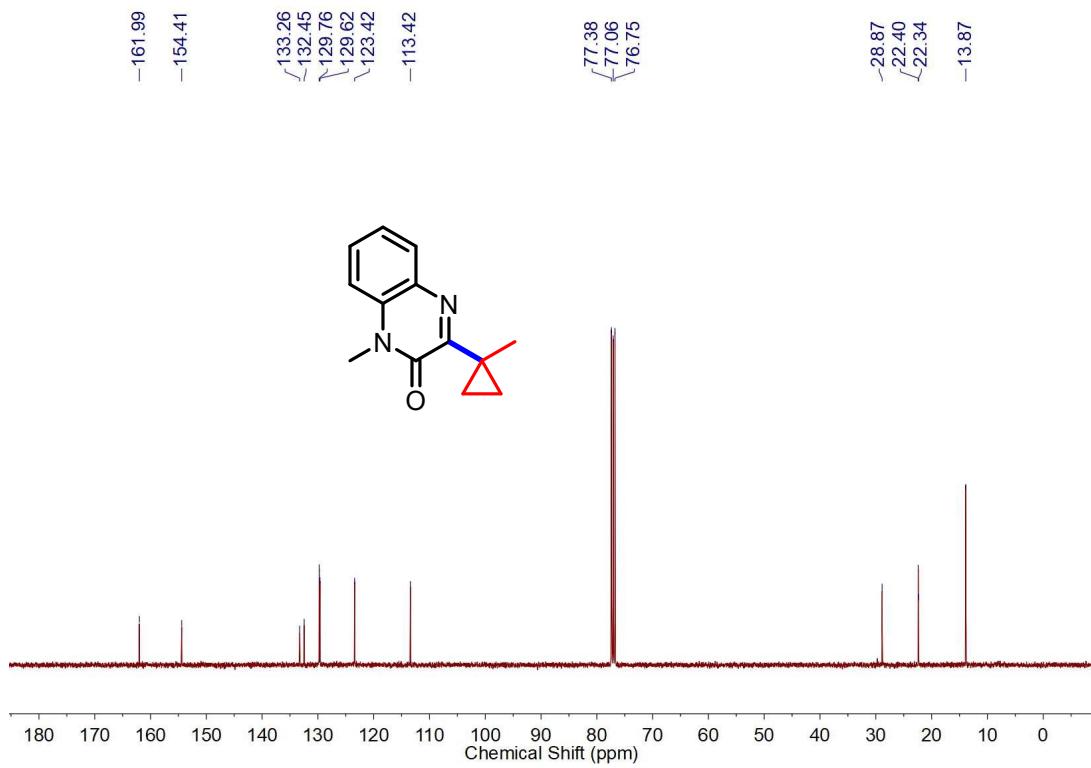
**Figure S19.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **12**



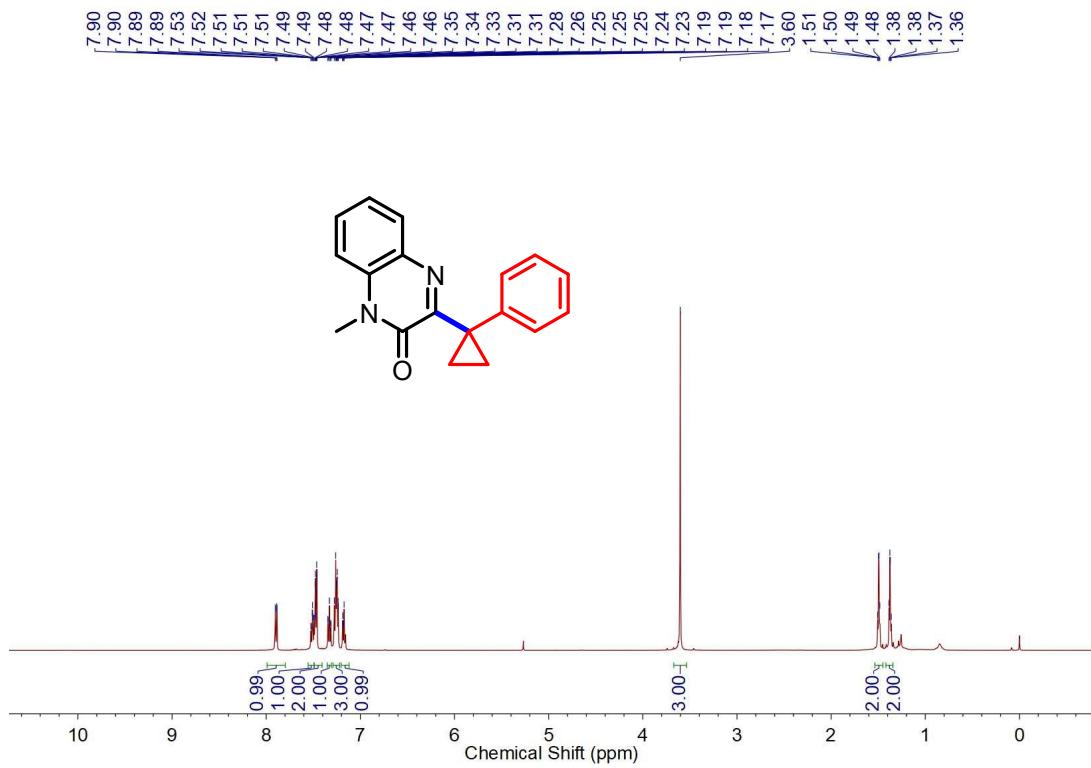
**Figure S20.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **12**



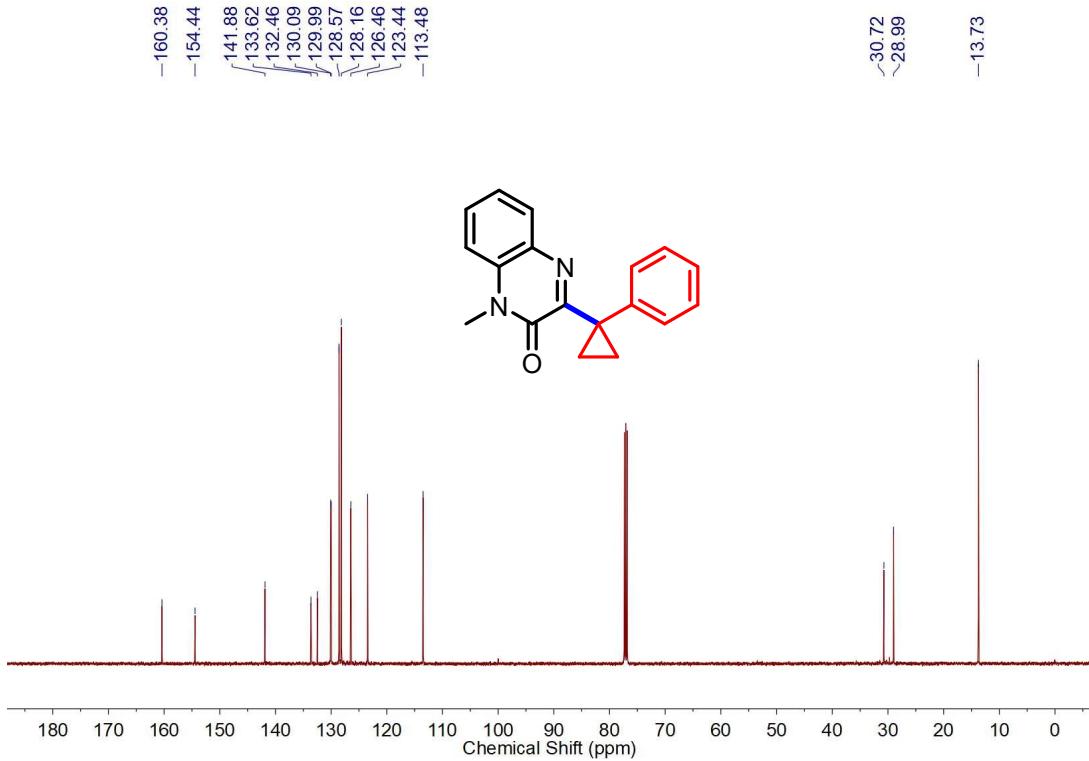
**Figure S21.**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of **13**



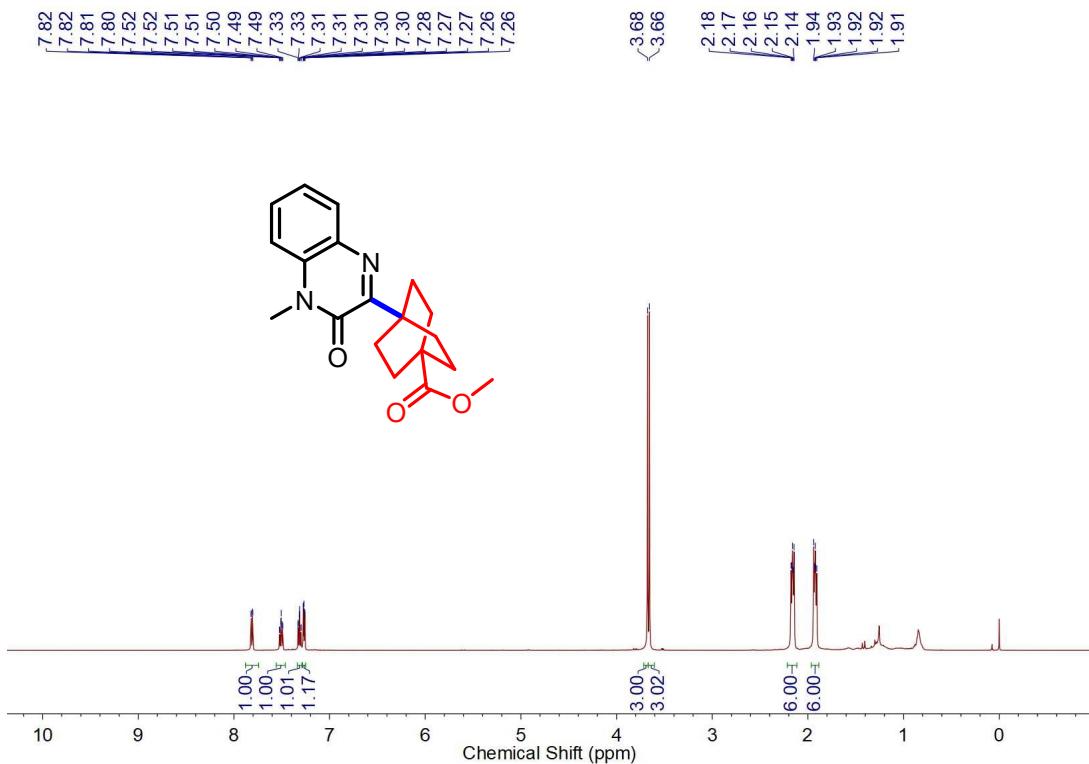
**Figure S22.**  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ) spectrum of **13**



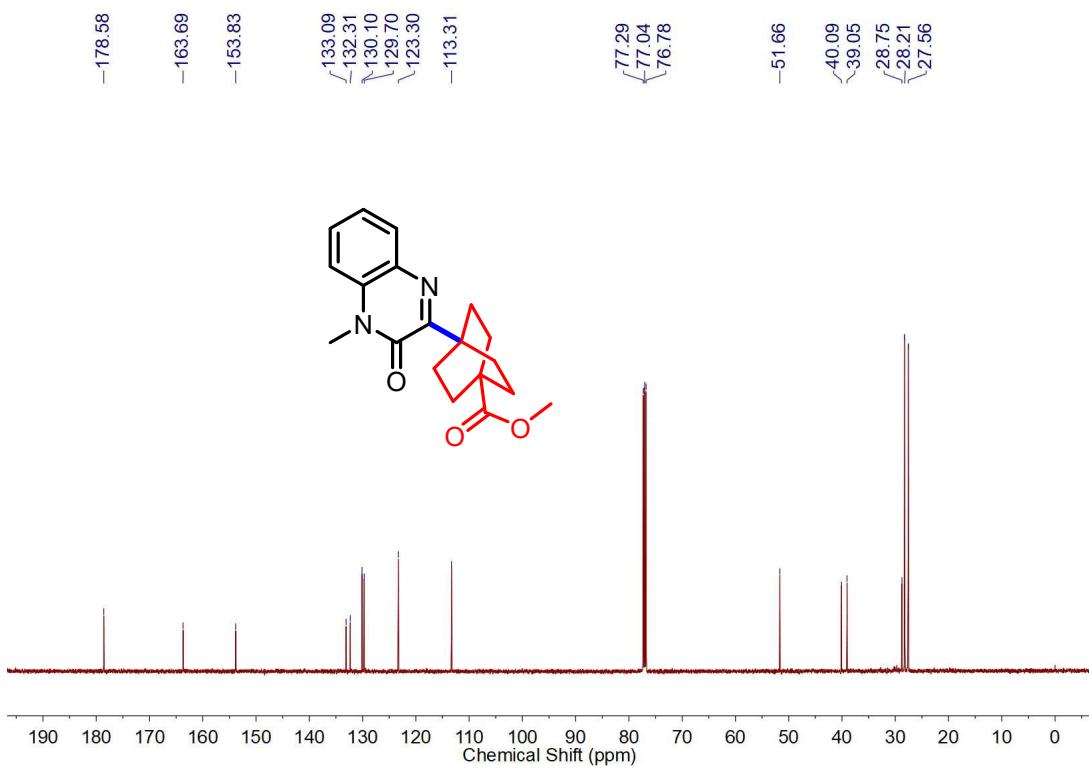
**Figure S23.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **14**



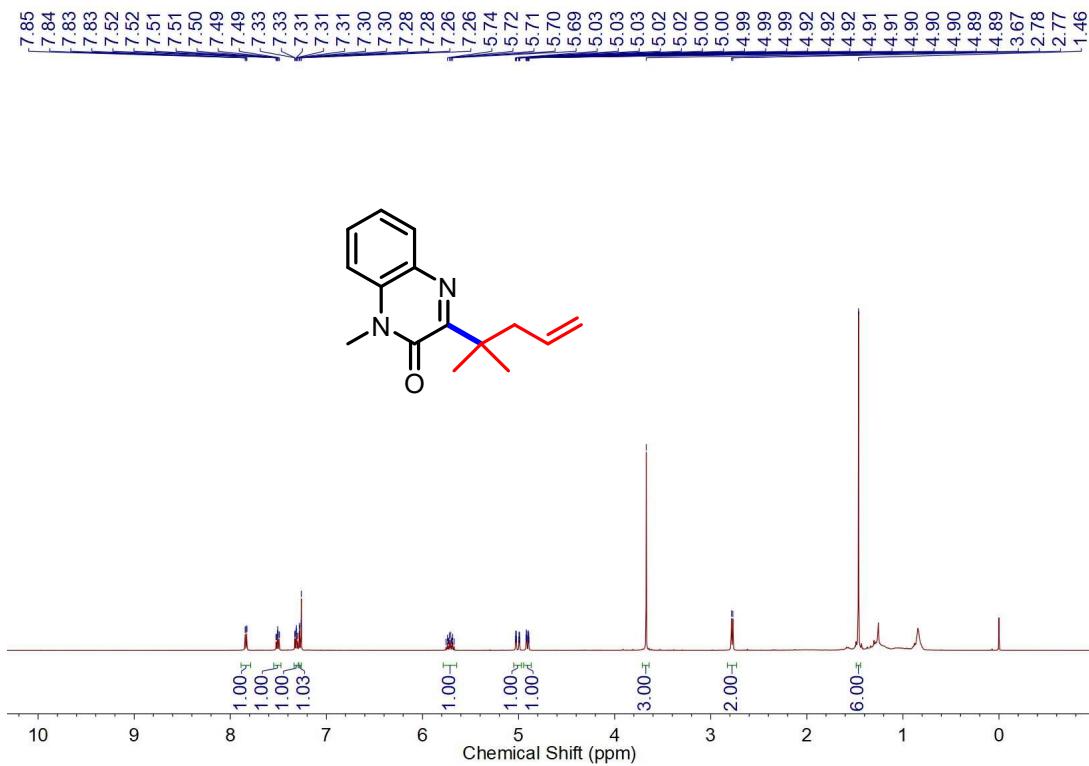
**Figure S24.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **14**



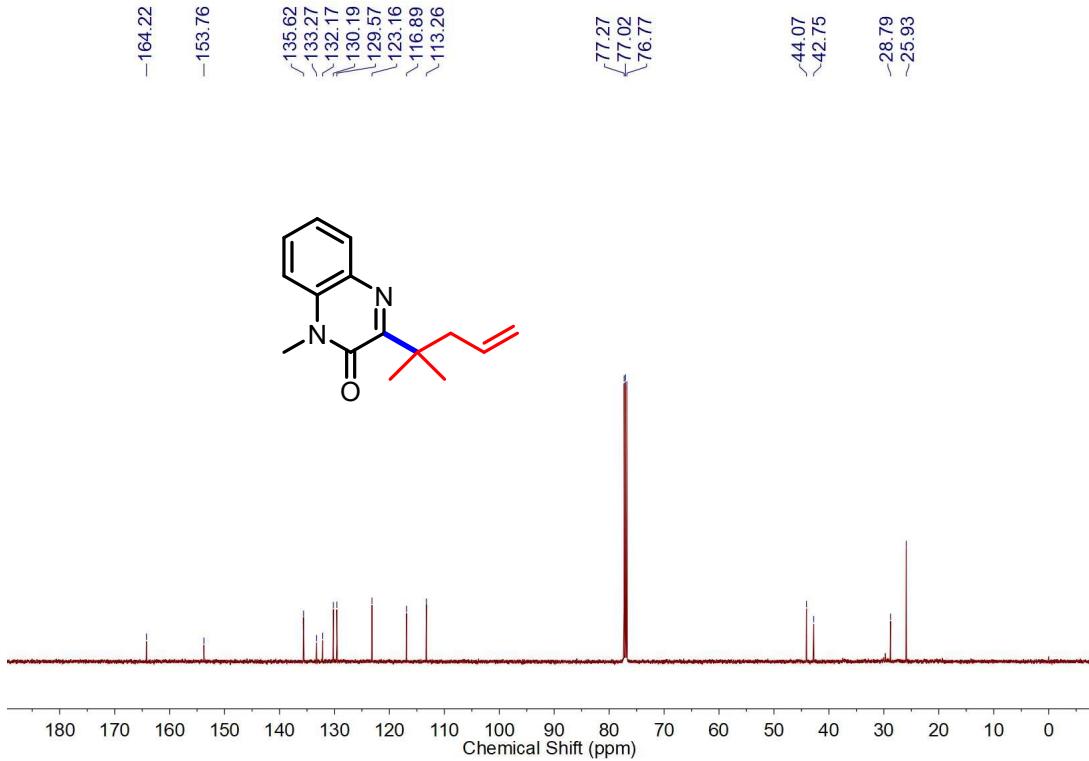
**Figure S25.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **15**



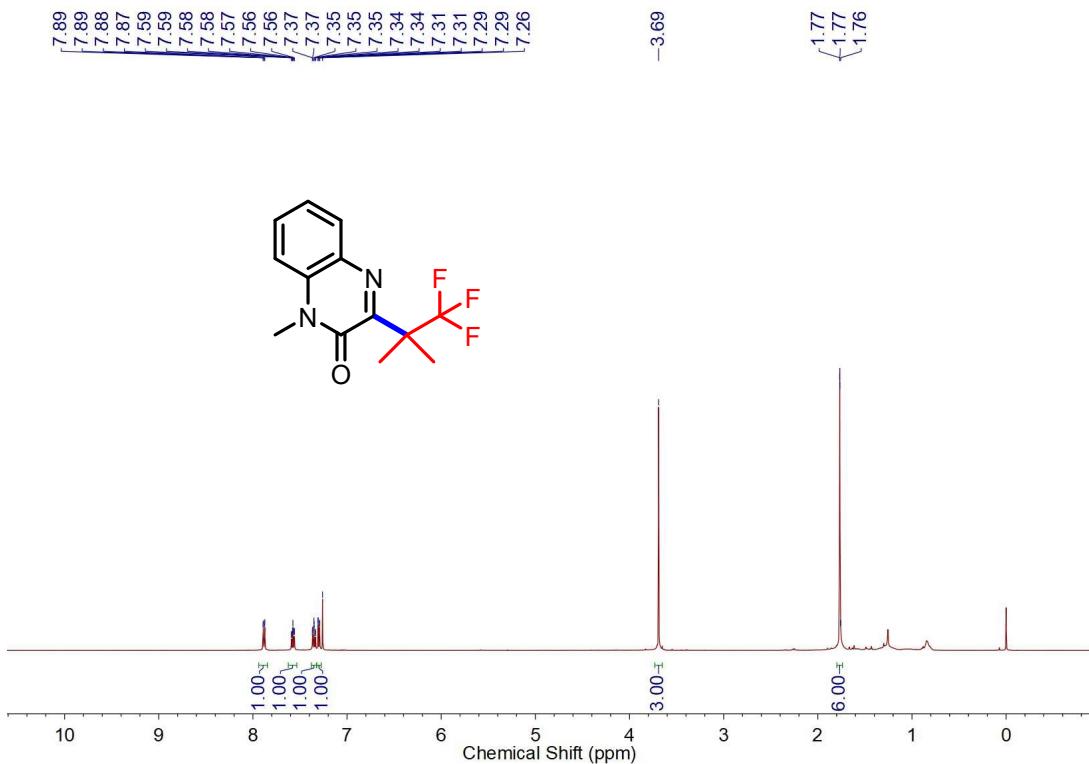
**Figure S26.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **15**



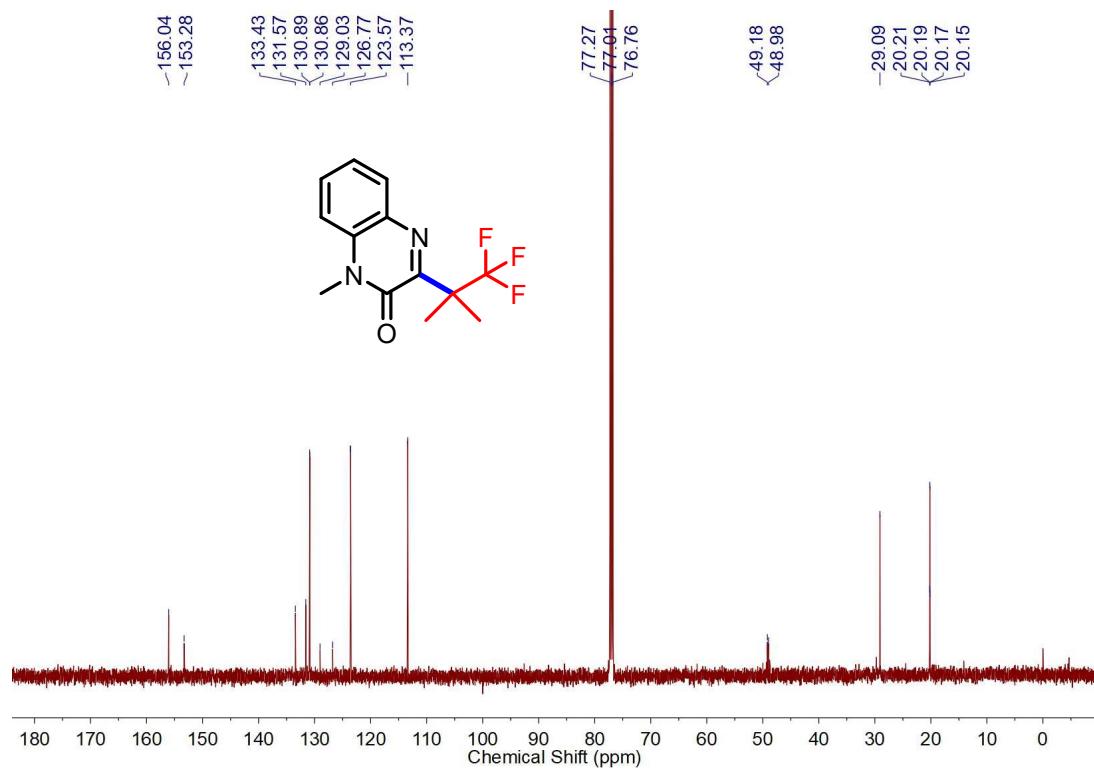
**Figure S27.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **16**



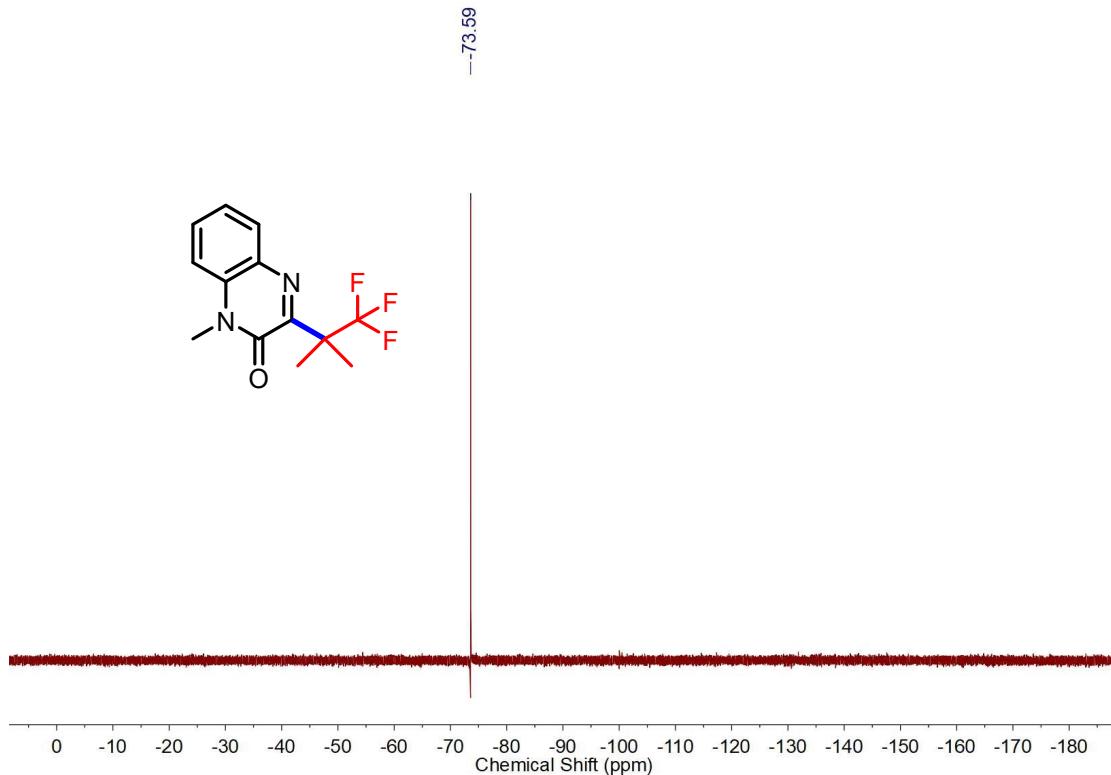
**Figure S28.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **16**



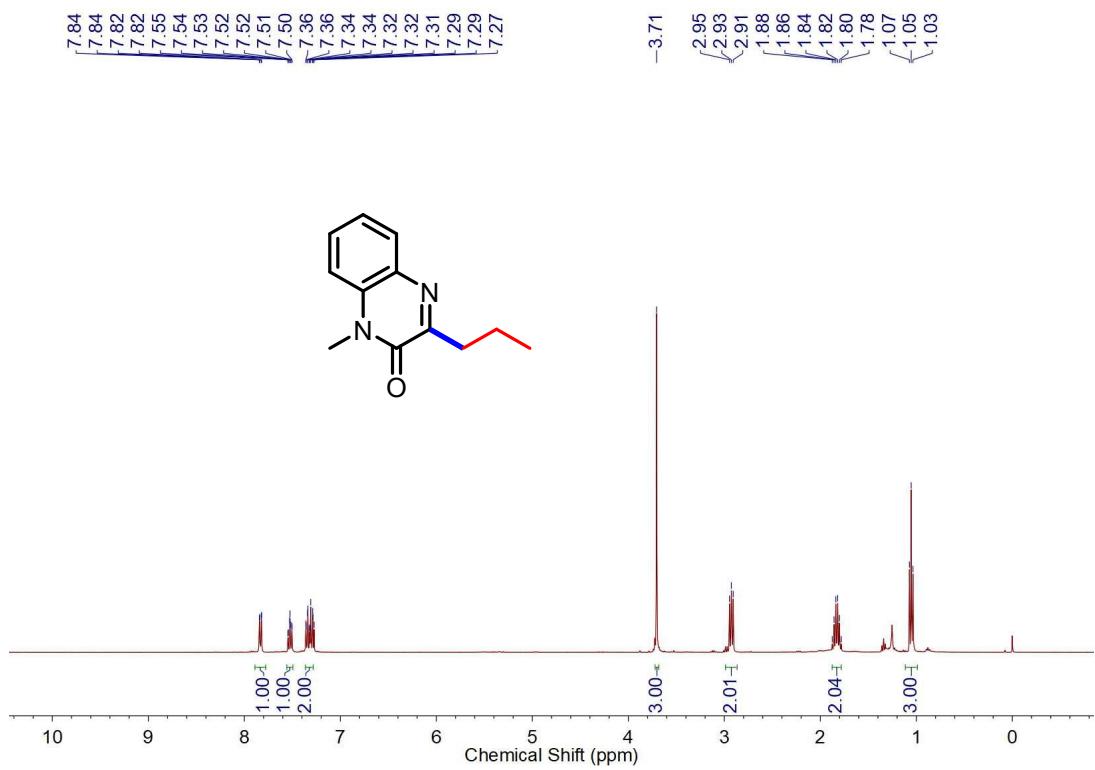
**Figure S29.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **17**



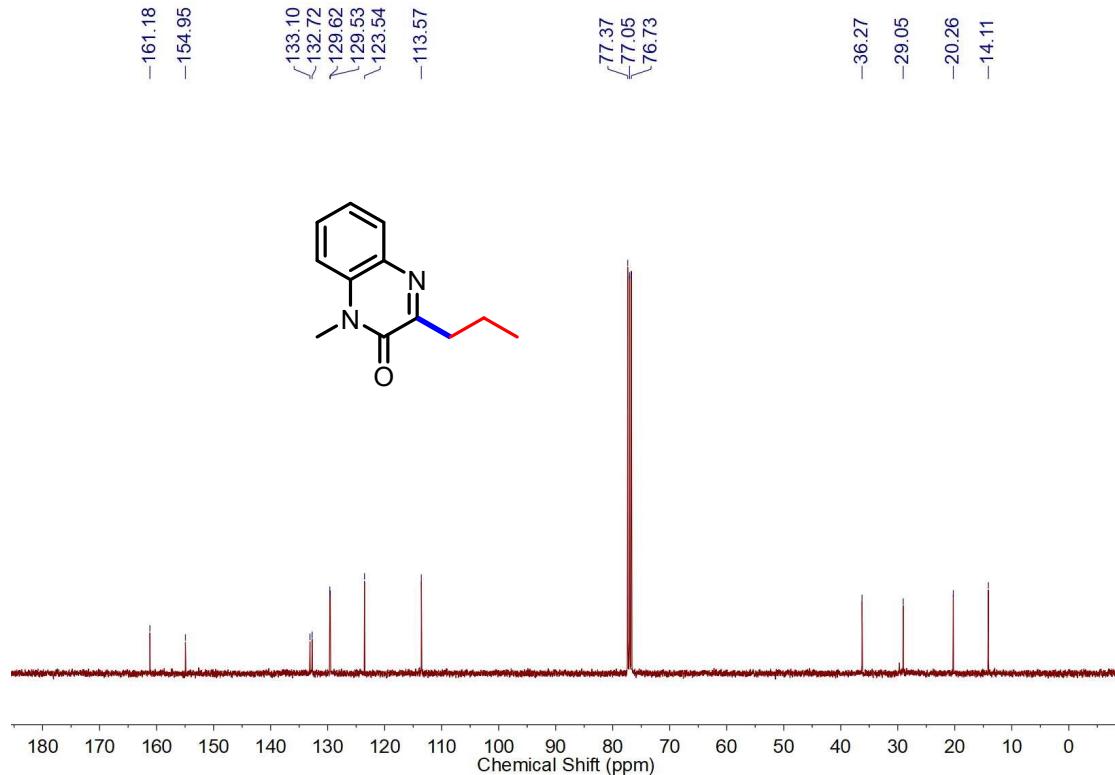
**Figure S30.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **17**



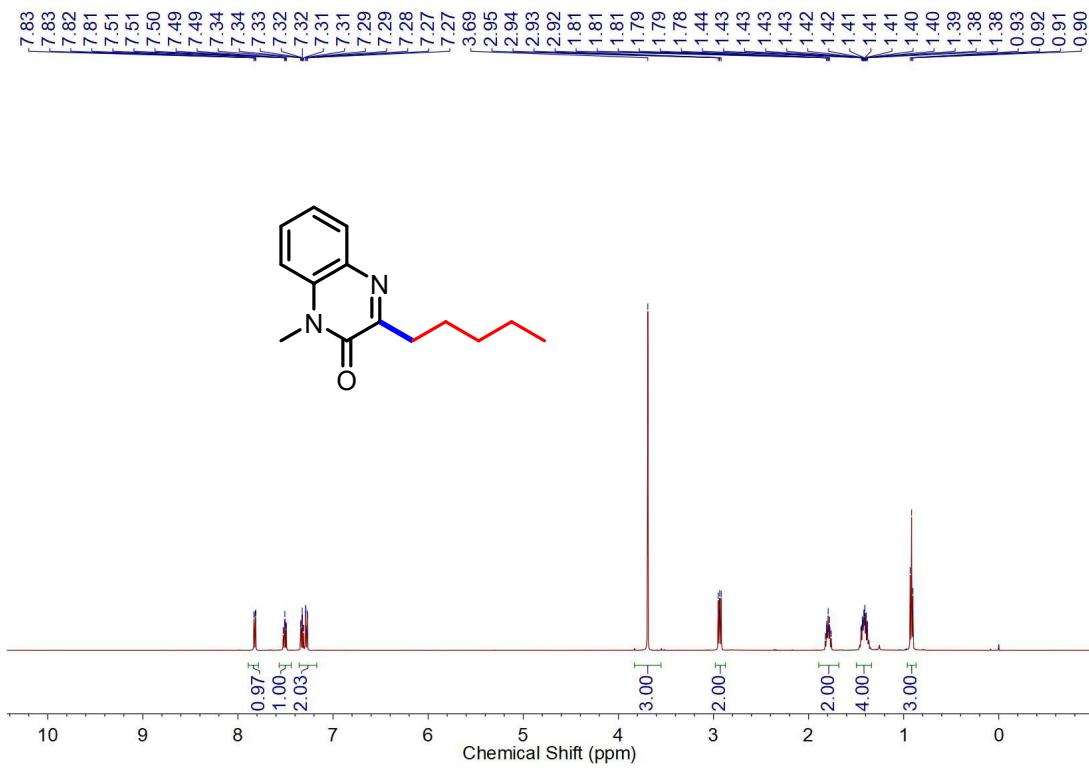
**Figure S31.**  $^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ ) spectrum of **17**



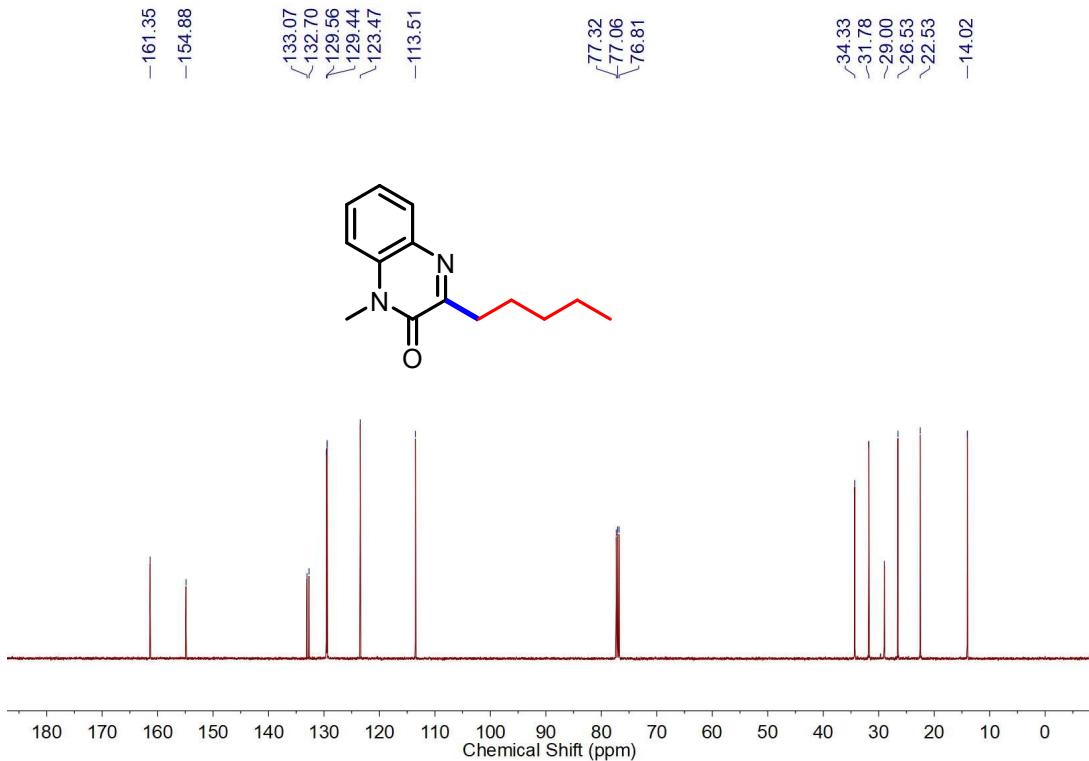
**Figure S32.**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of **18**



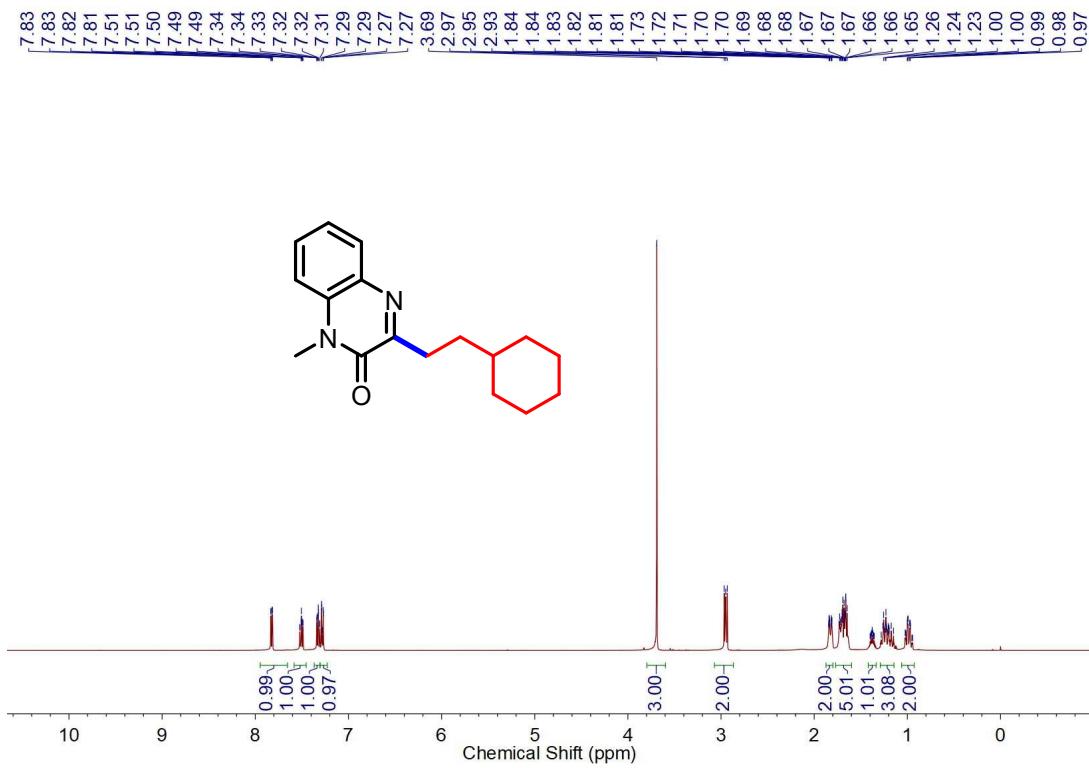
**Figure S33.**  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ) spectrum of **18**



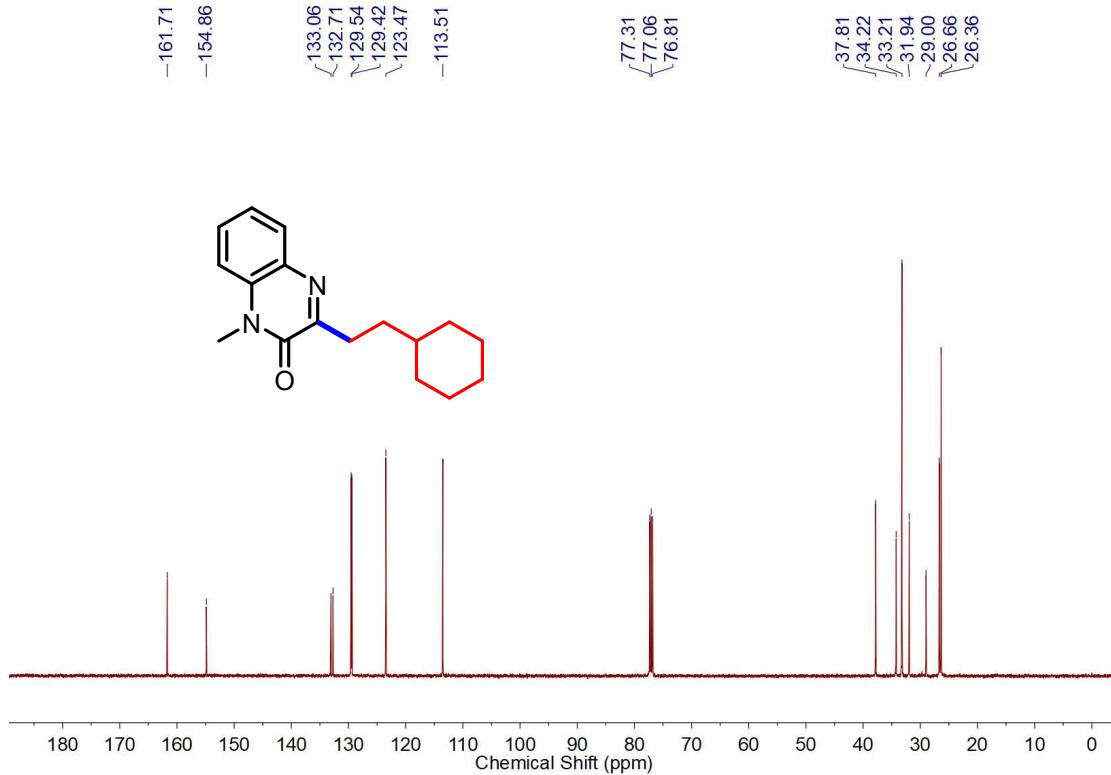
**Figure S34.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **19**



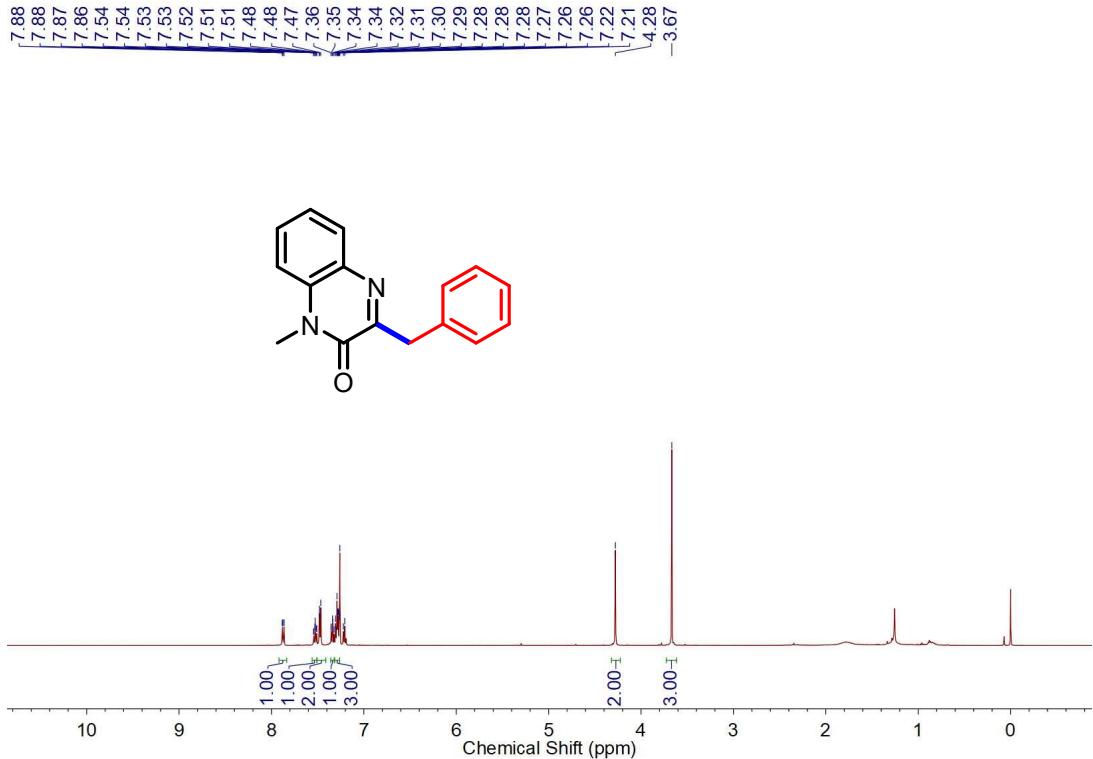
**Figure S35.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **19**



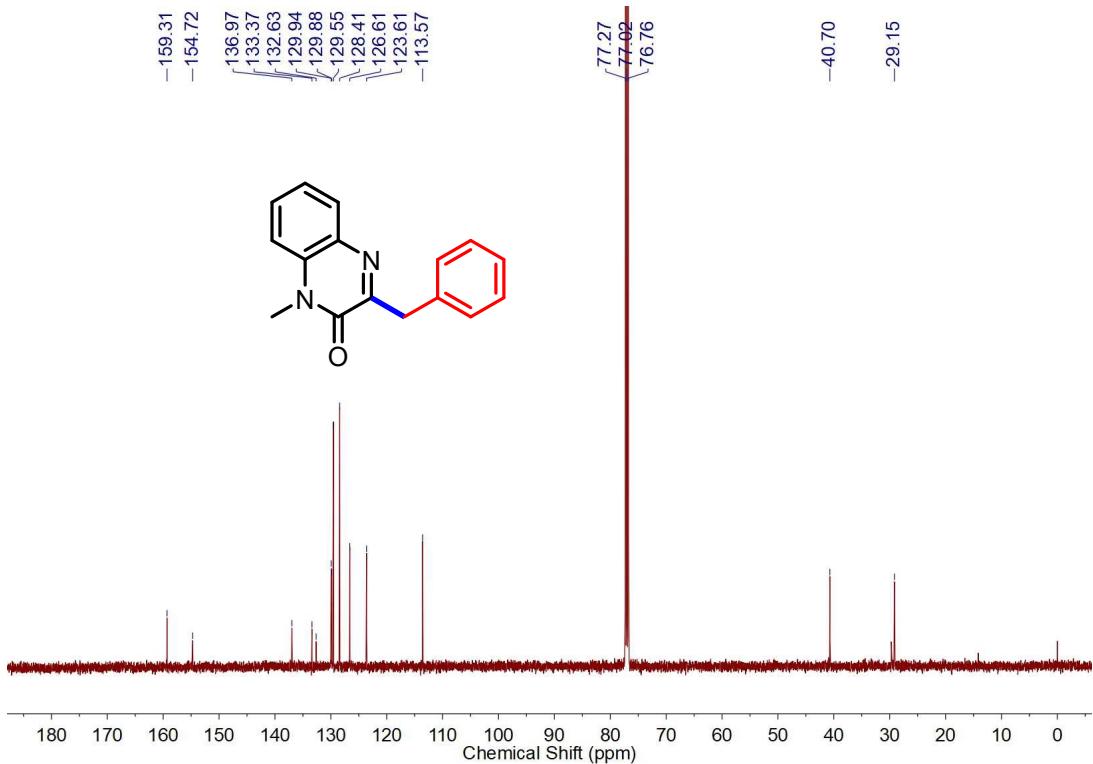
**Figure S36.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **20**



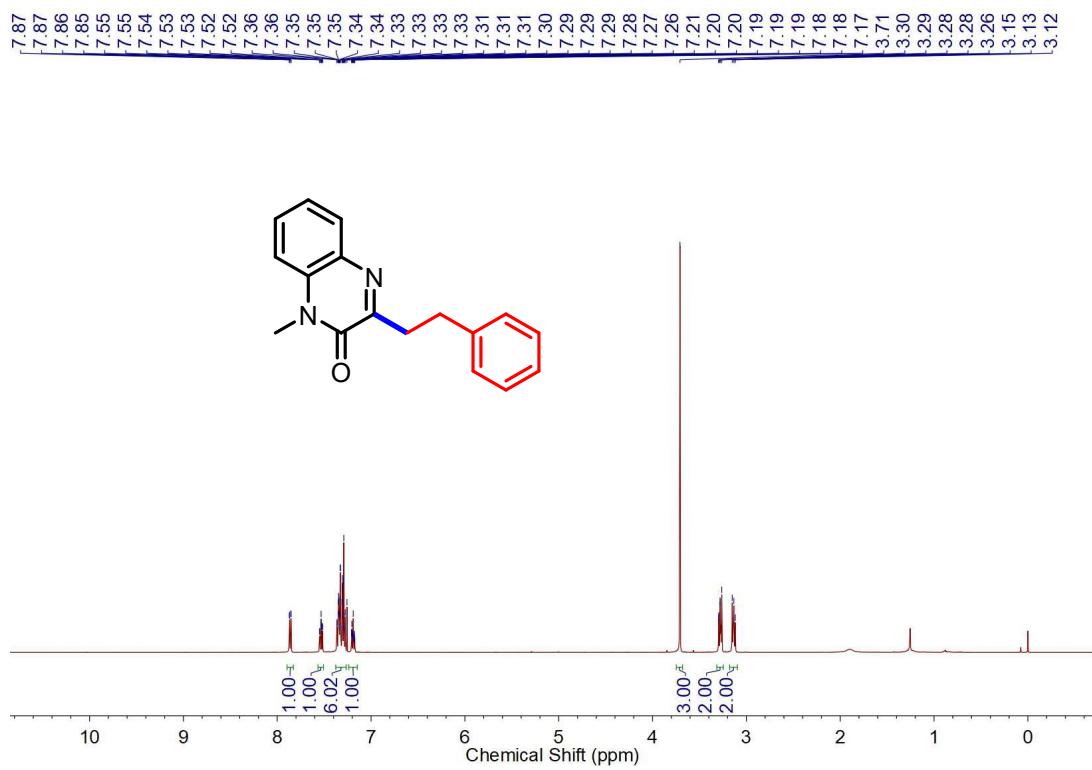
**Figure S37.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **20**



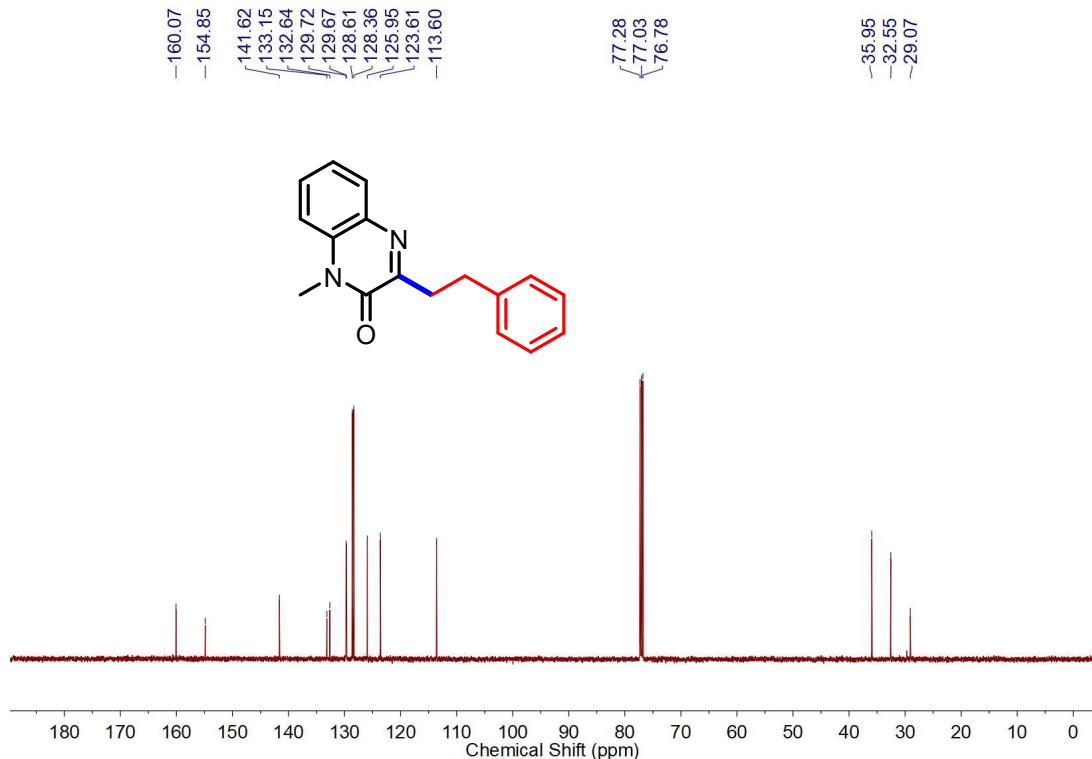
**Figure S38.** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **21**



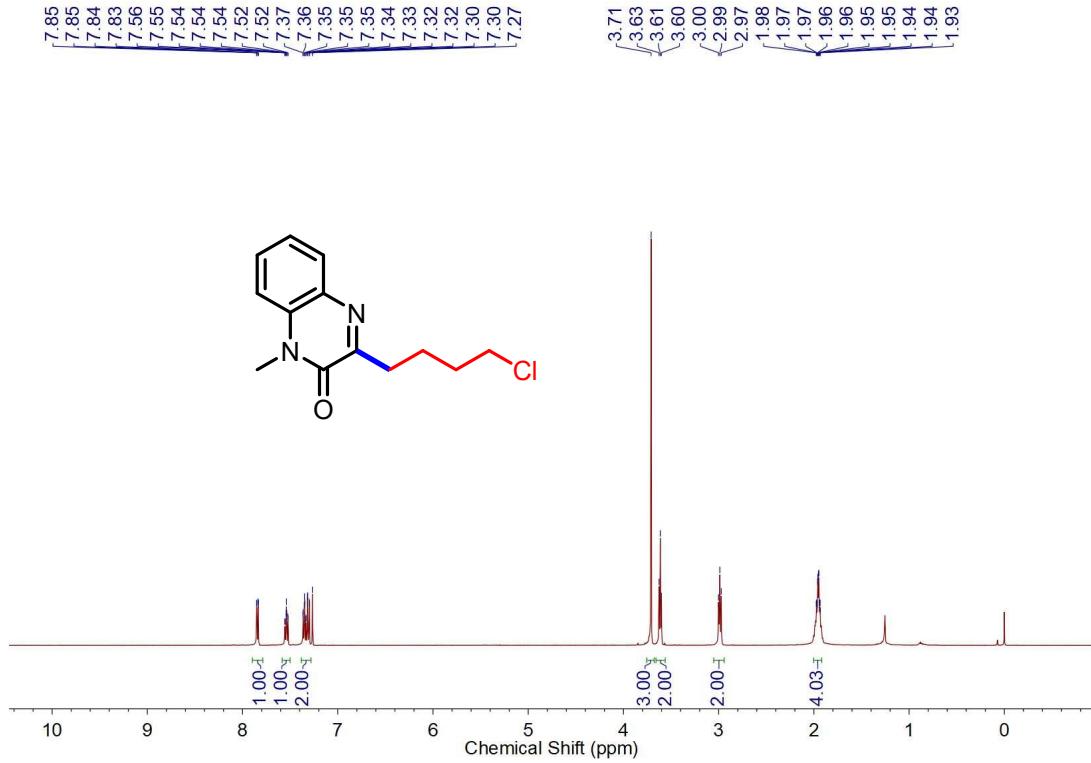
**Figure S39.** <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **21**



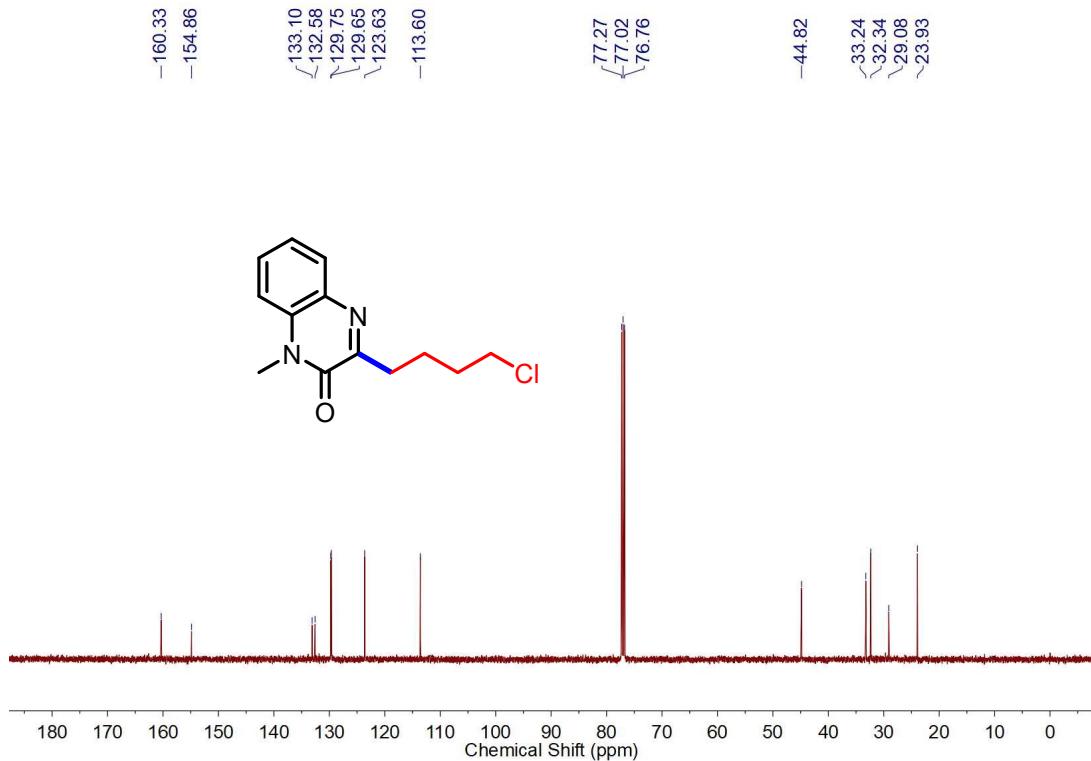
**Figure S40.** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **22**



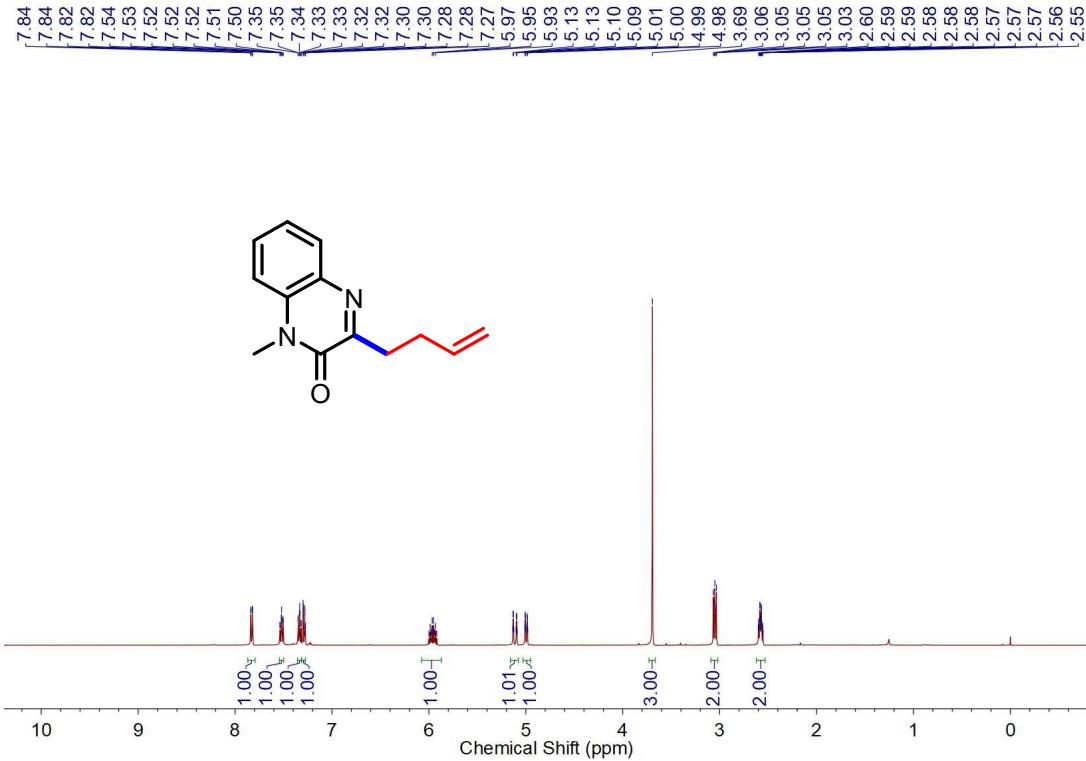
**Figure S41.** <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **22**



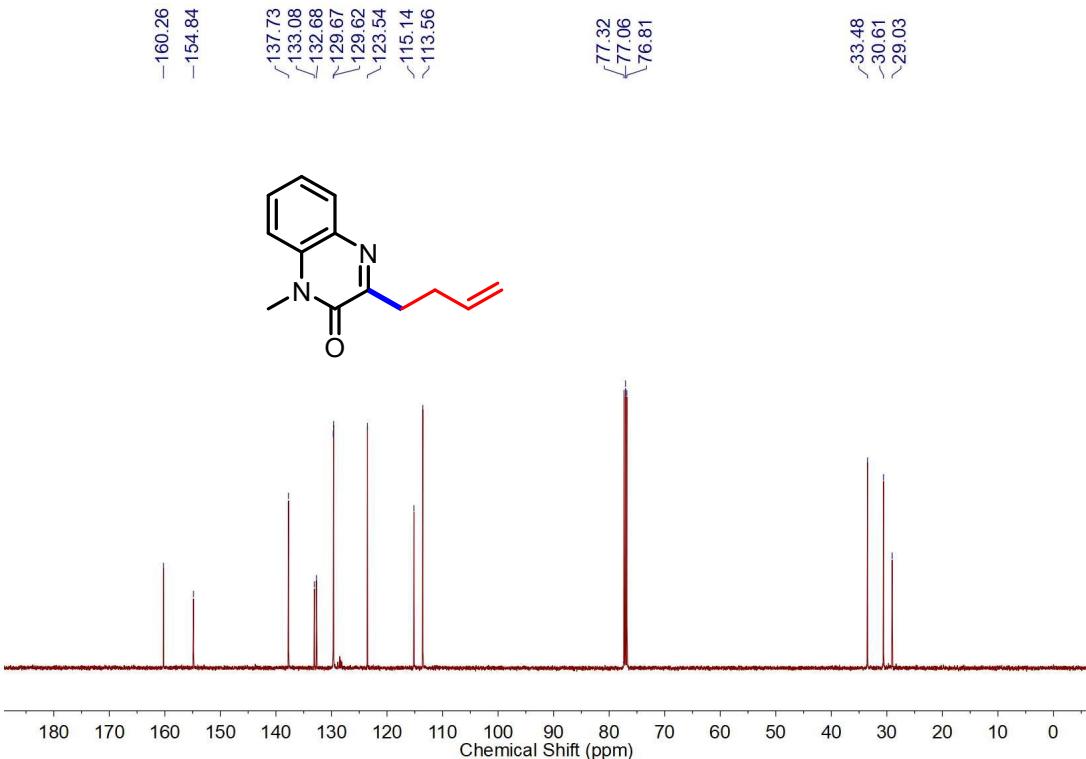
**Figure S42.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **23**

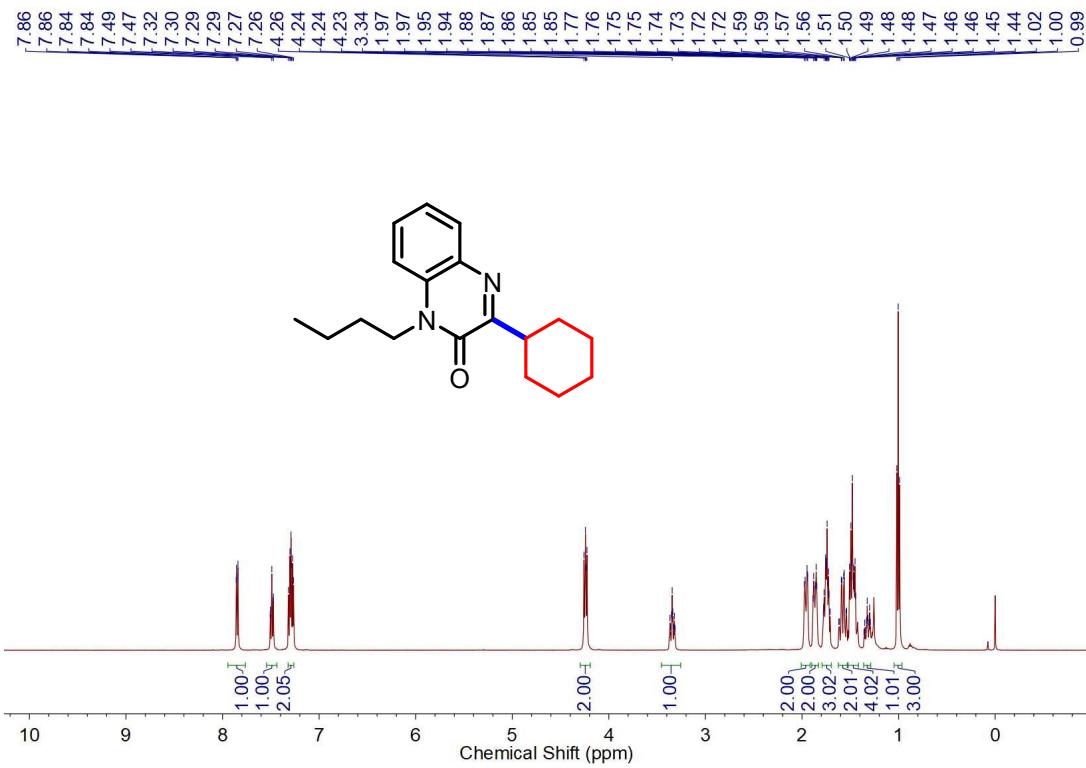


**Figure S43.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **23**

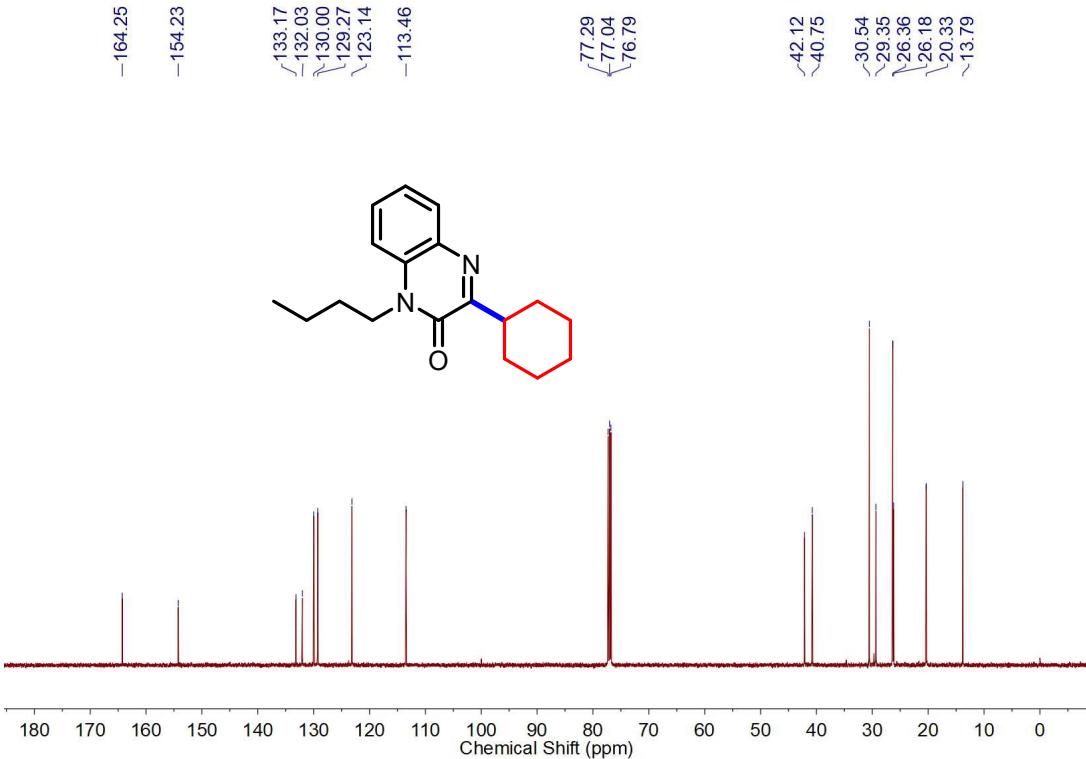


**Figure S44.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **24**

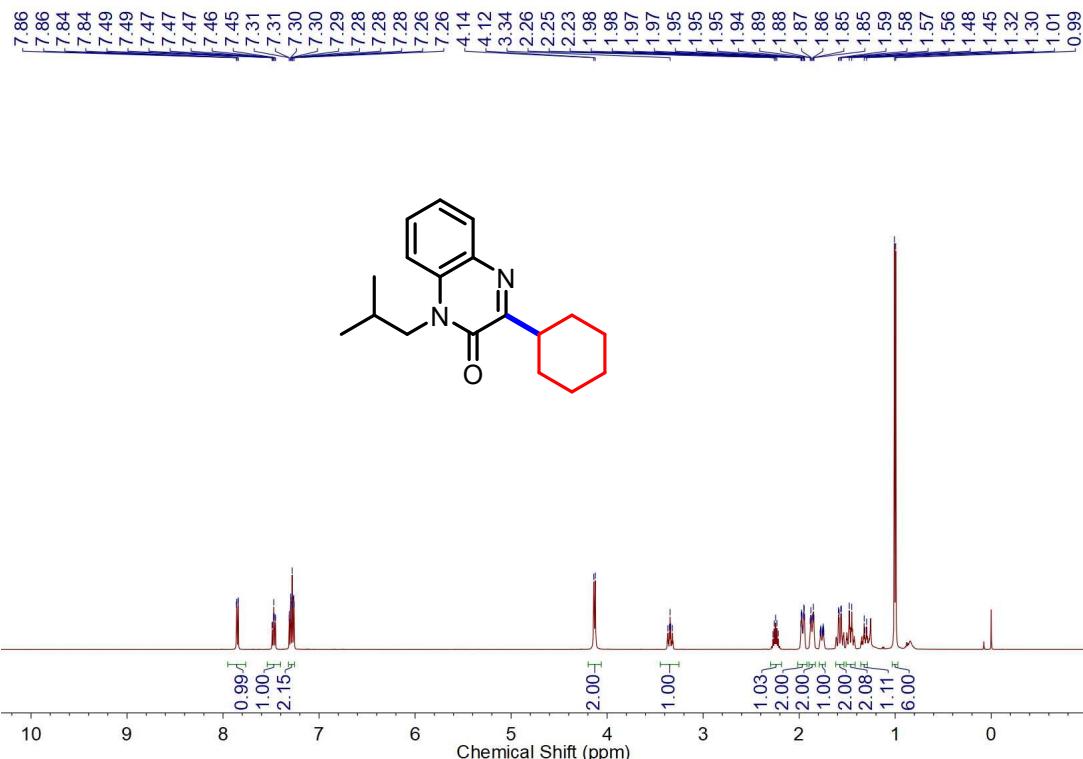




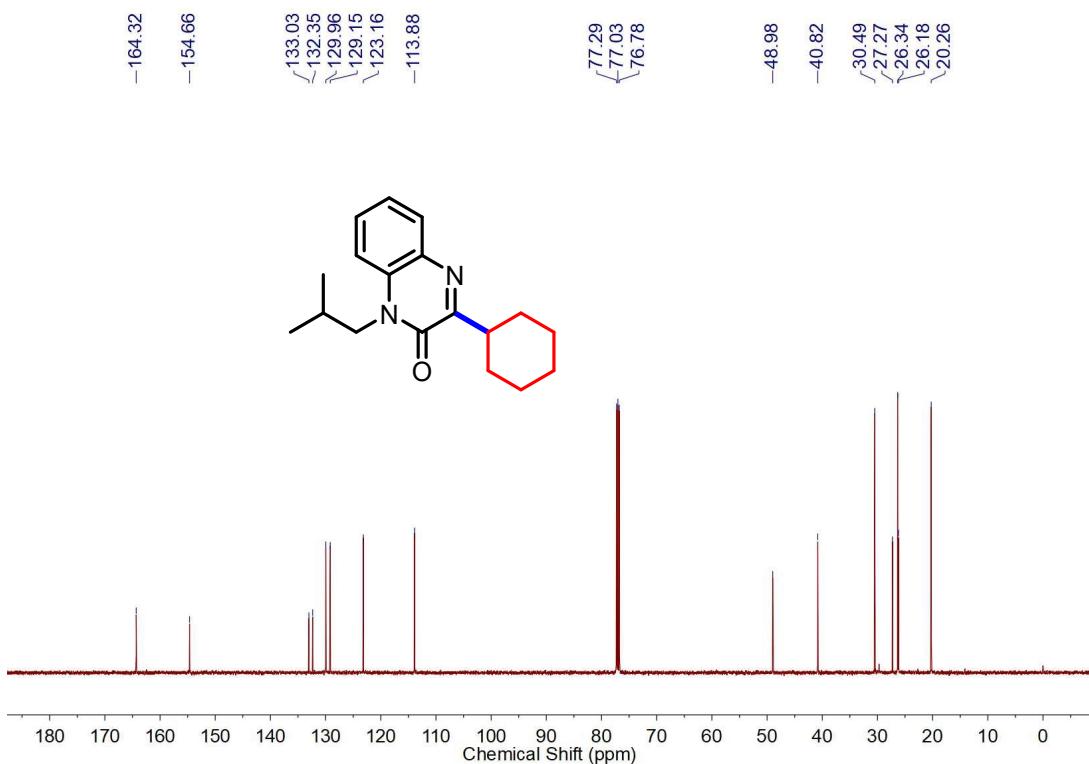
**Figure S46.** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **25**



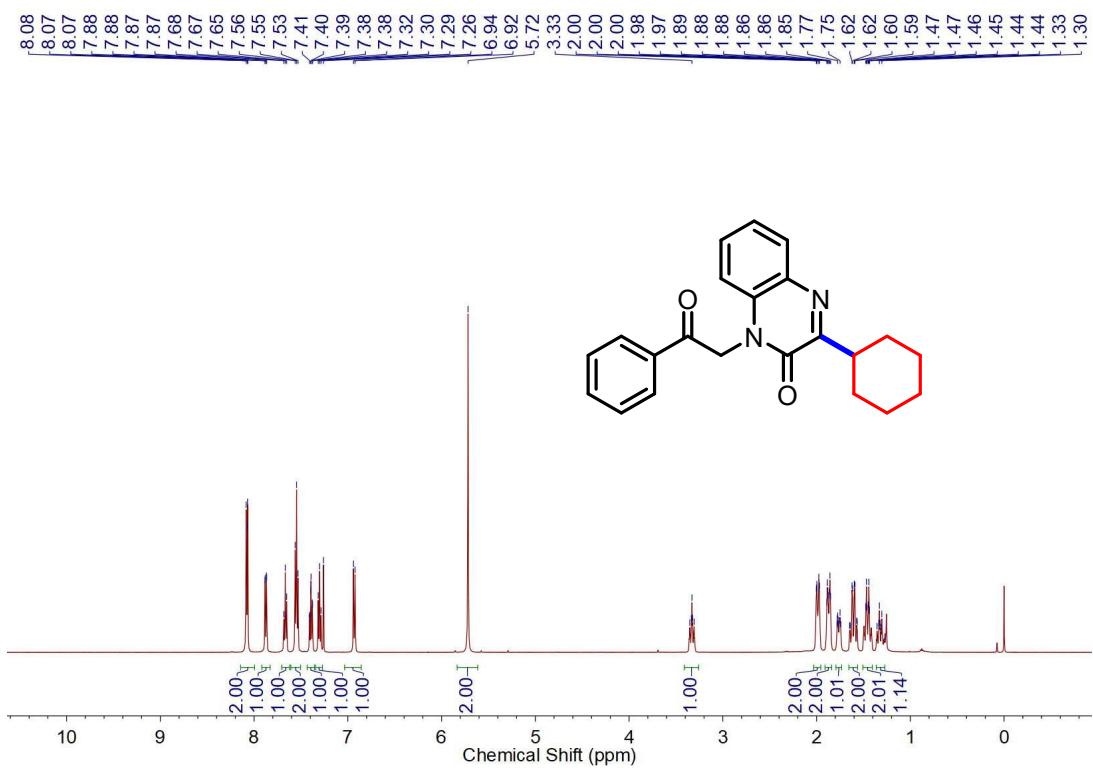
**Figure S47.** <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **25**



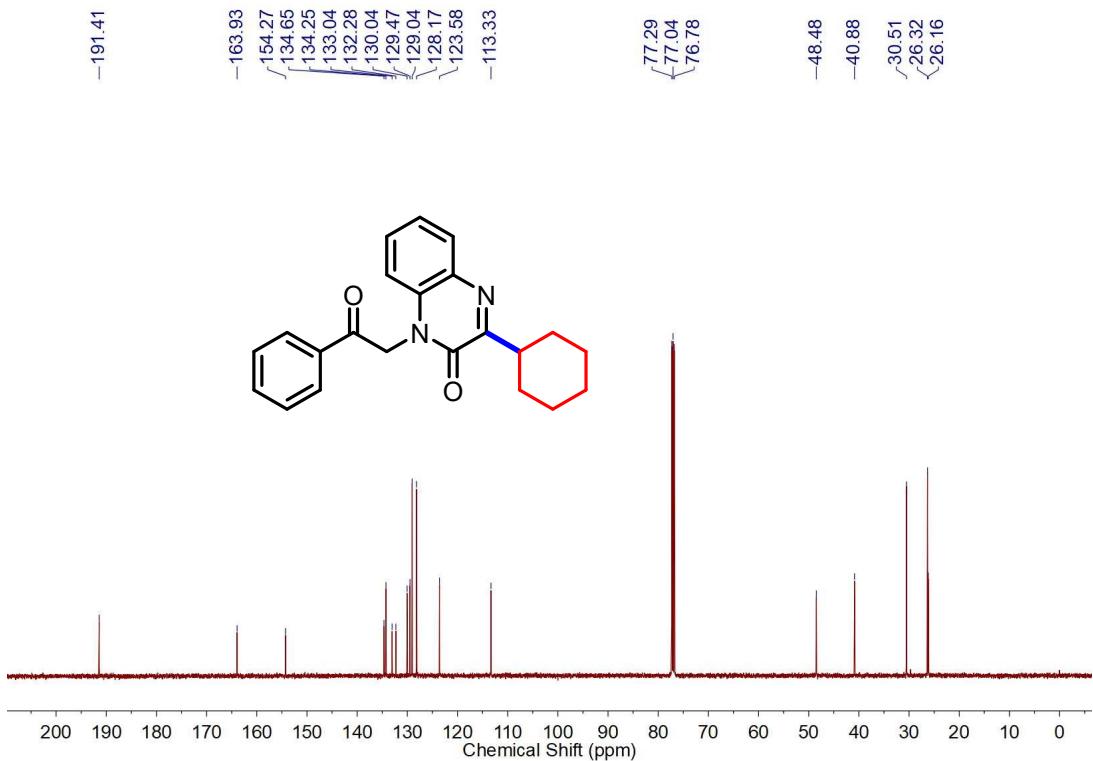
**Figure S48.** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **26**



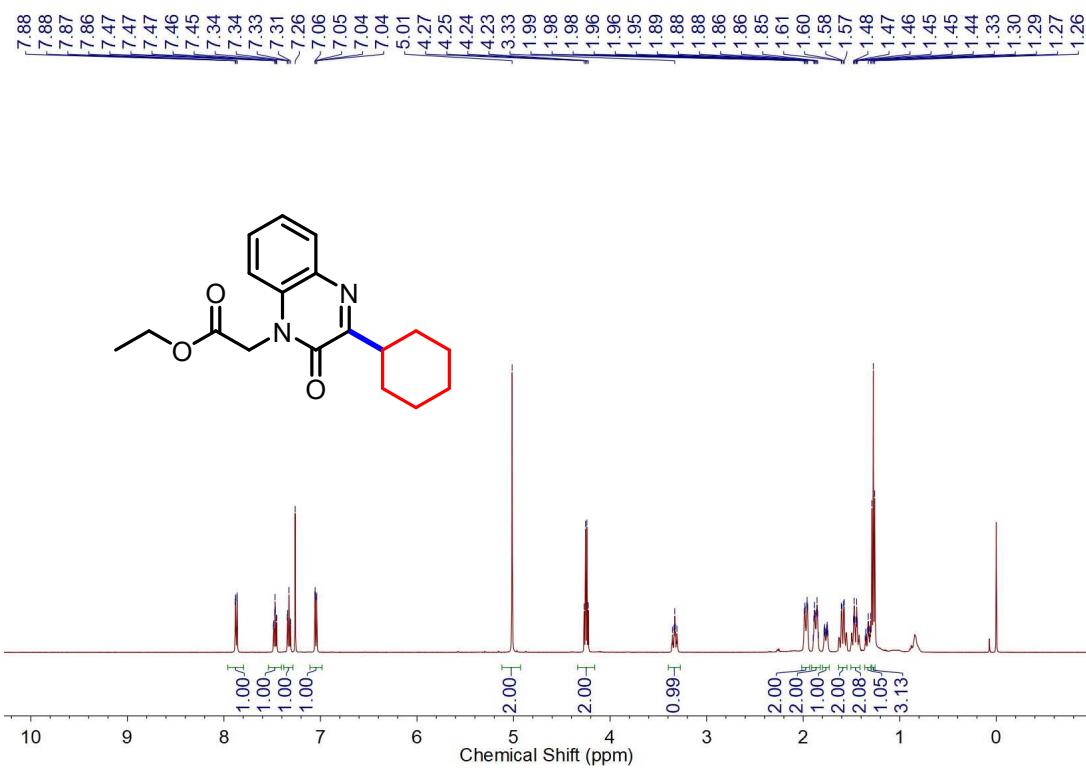
**Figure S49.** <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **26**



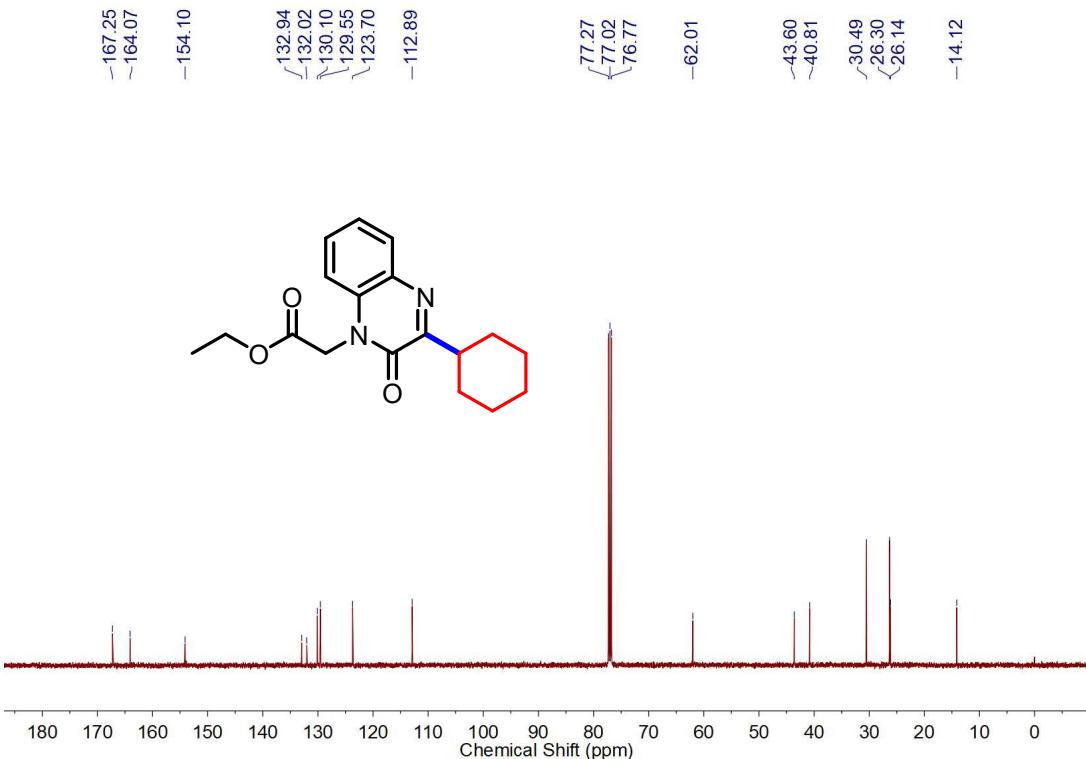
**Figure S50.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **27**



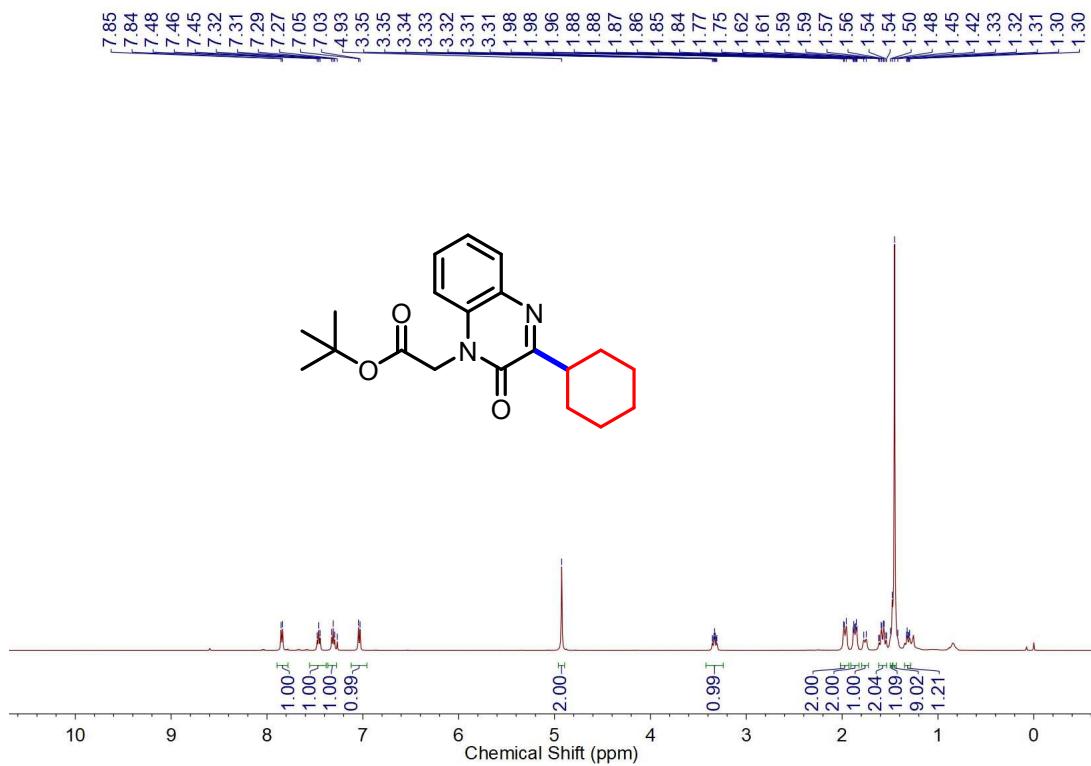
**Figure S51.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **27**



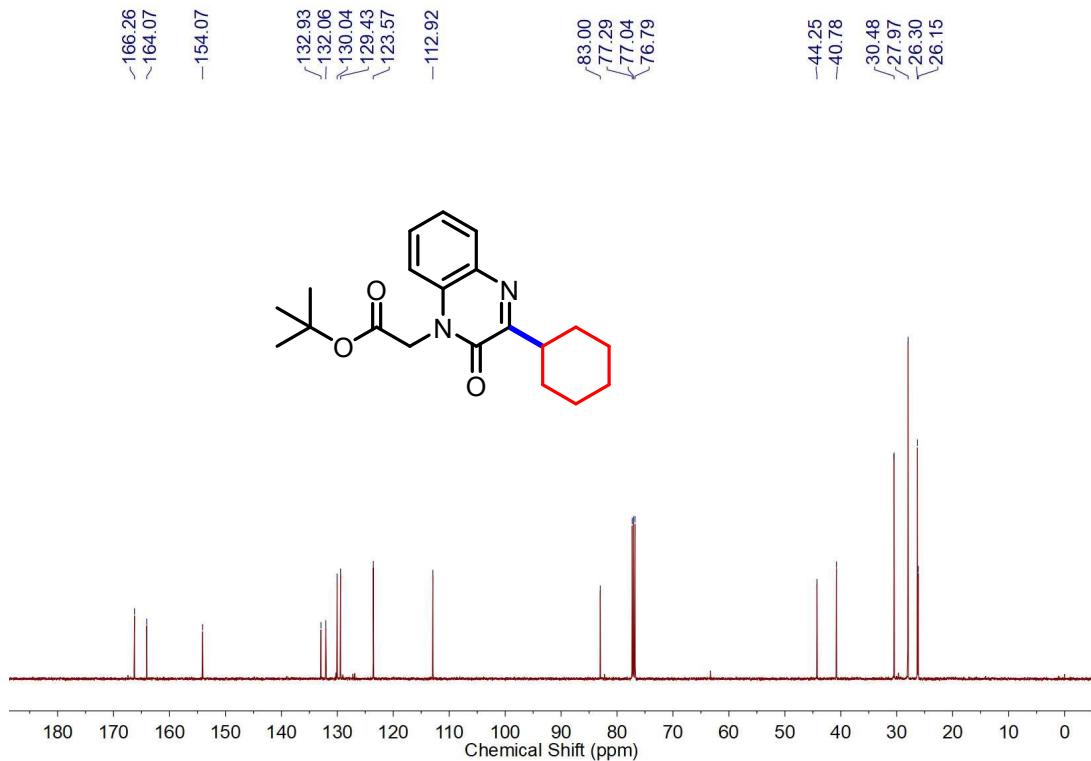
**Figure S52.** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **28**



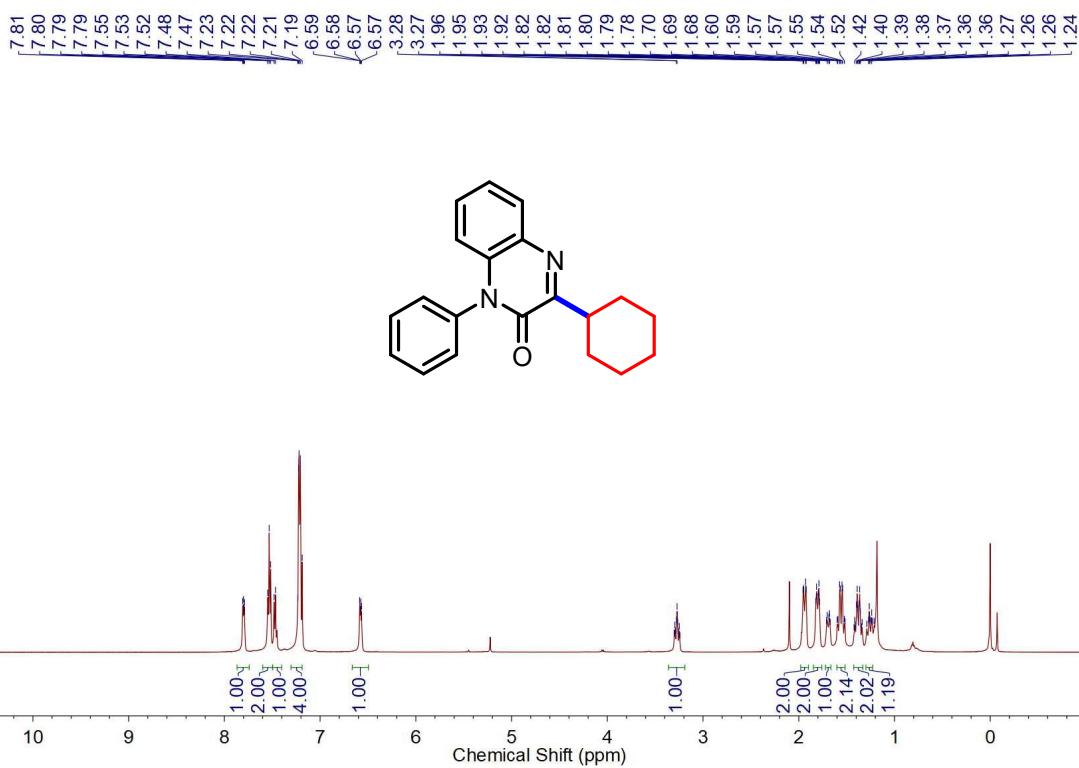
**Figure S53.** <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **28**



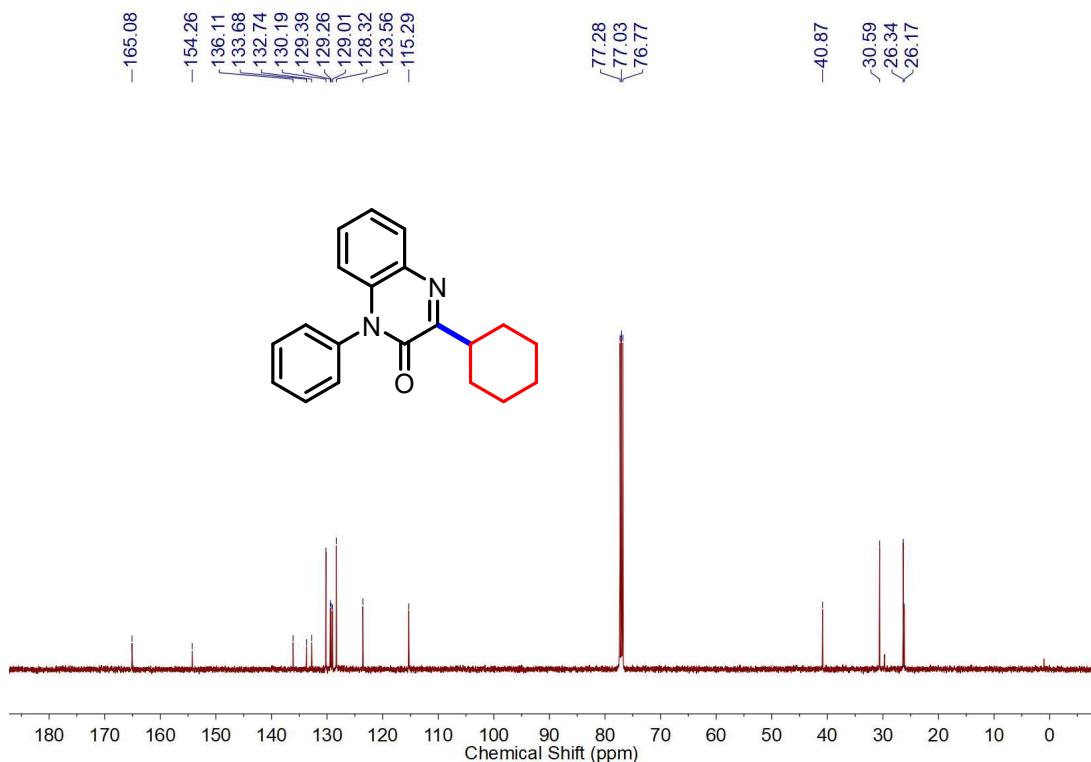
**Figure S54.** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **29**



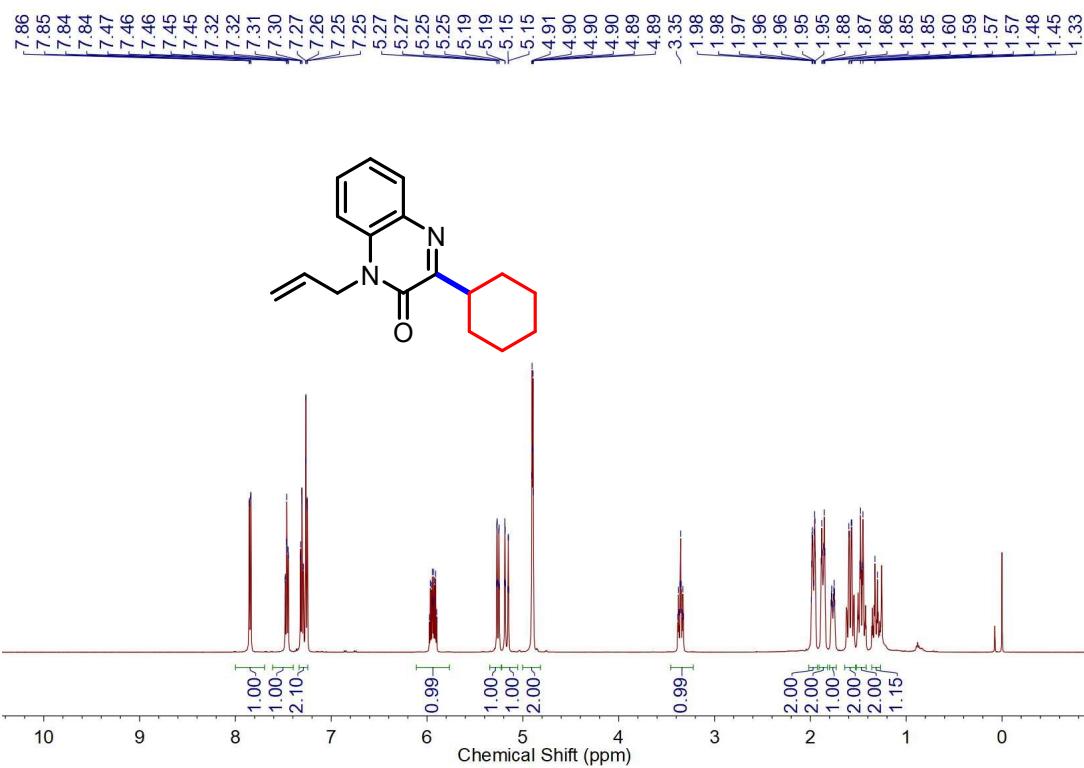
**Figure S55.** <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **29**



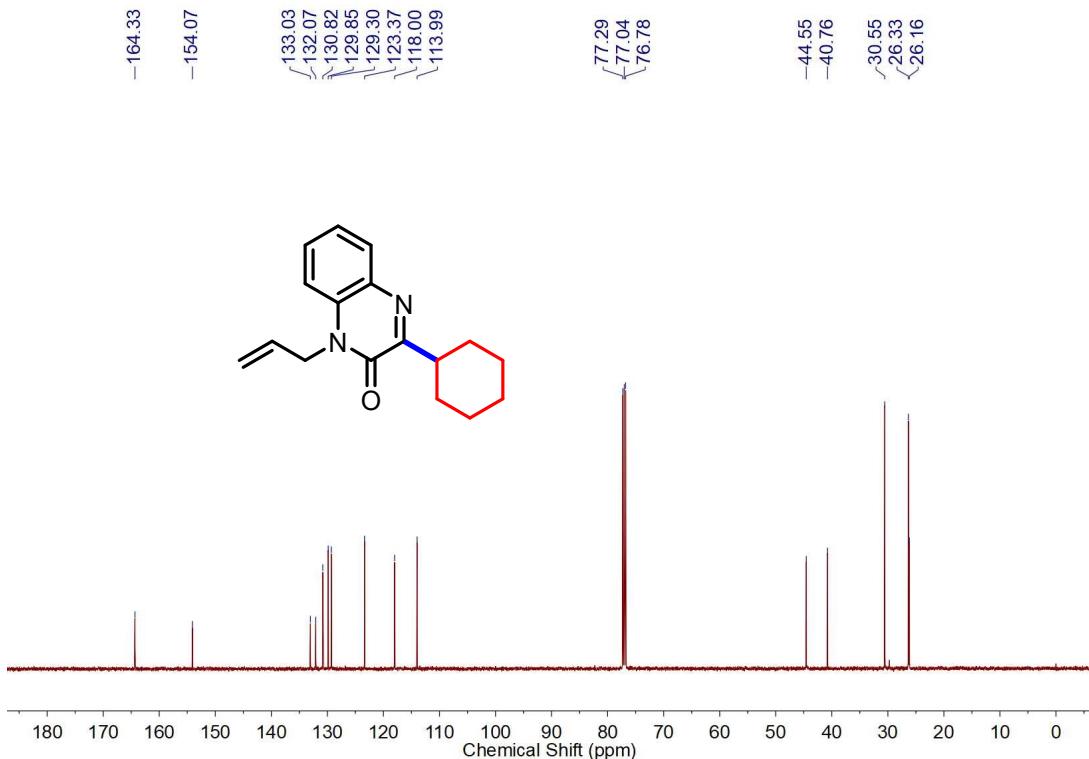
**Figure S56.** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **30**



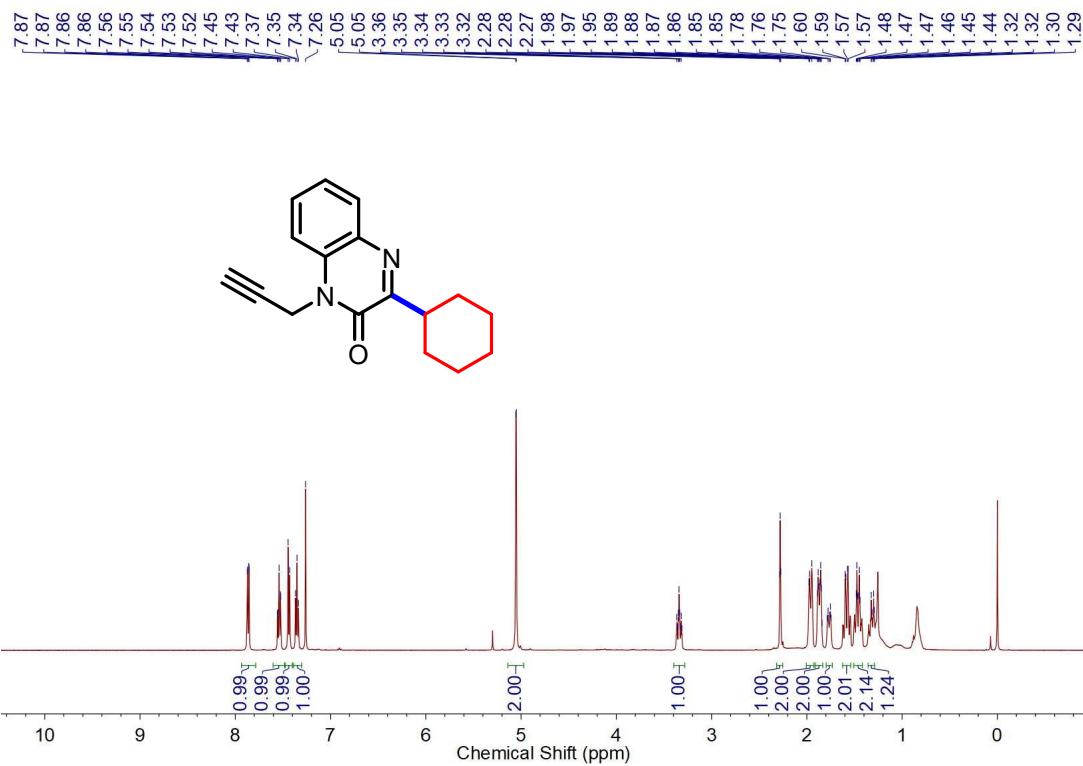
**Figure S57.** <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **30**



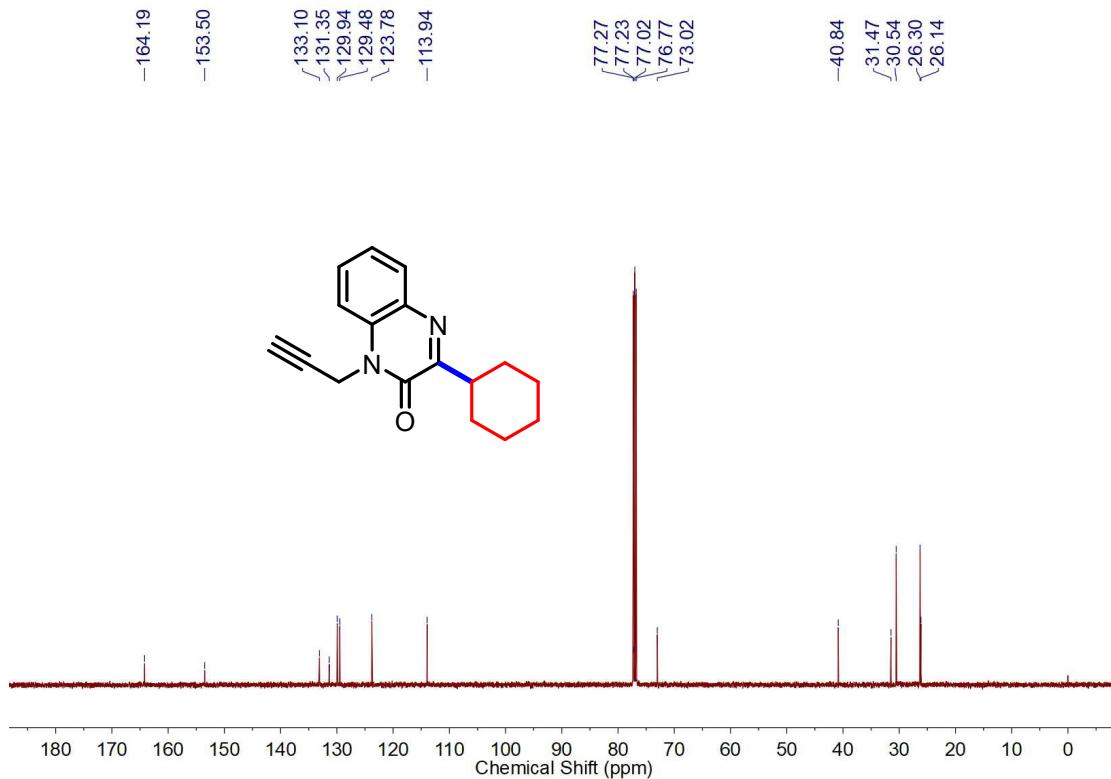
**Figure S58.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **31**



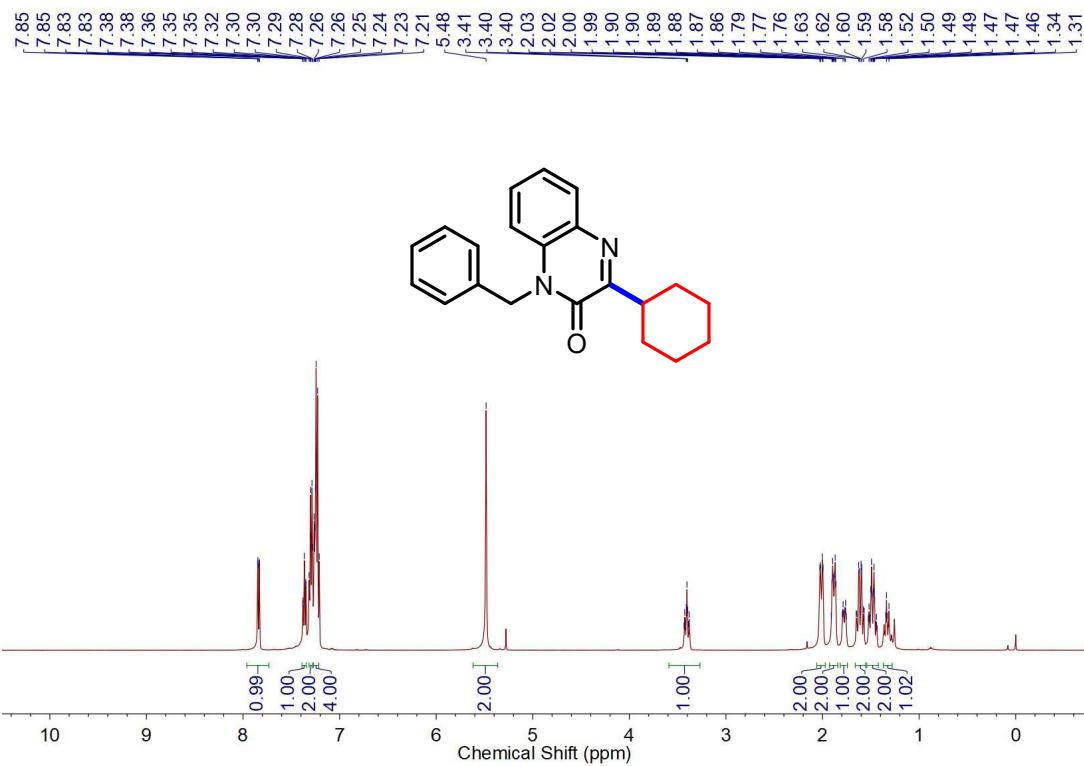
**Figure S59.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **31**



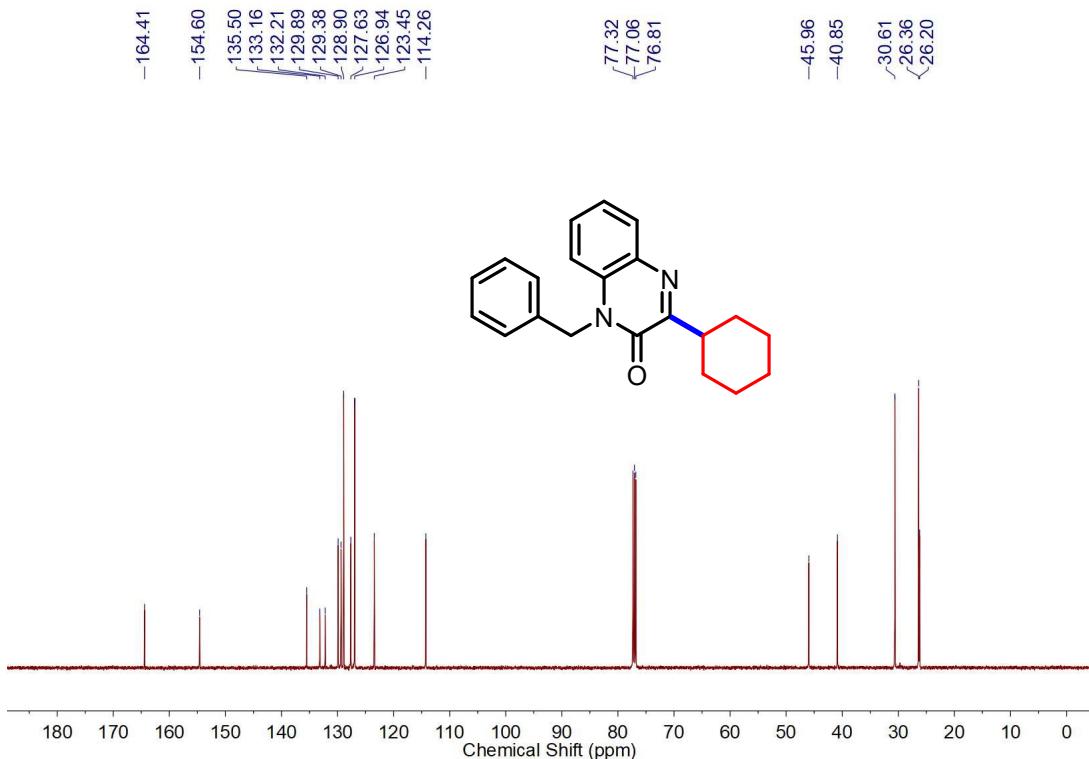
**Figure S60.** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **32**



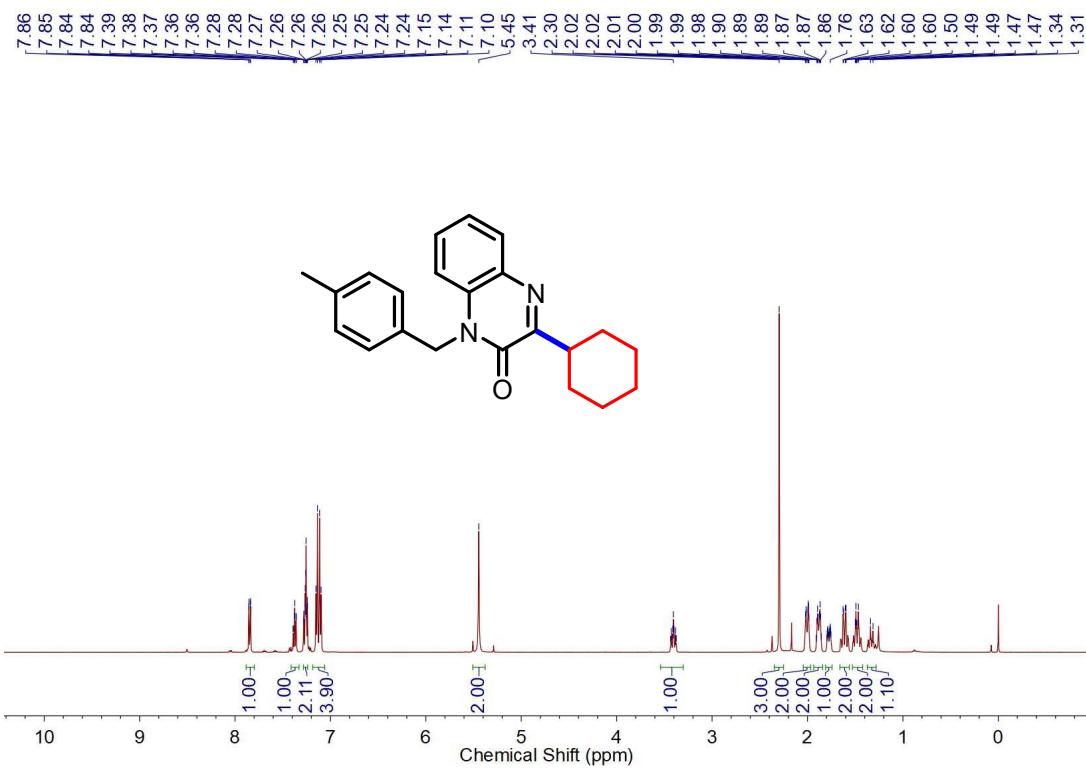
**Figure S61.** <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **32**



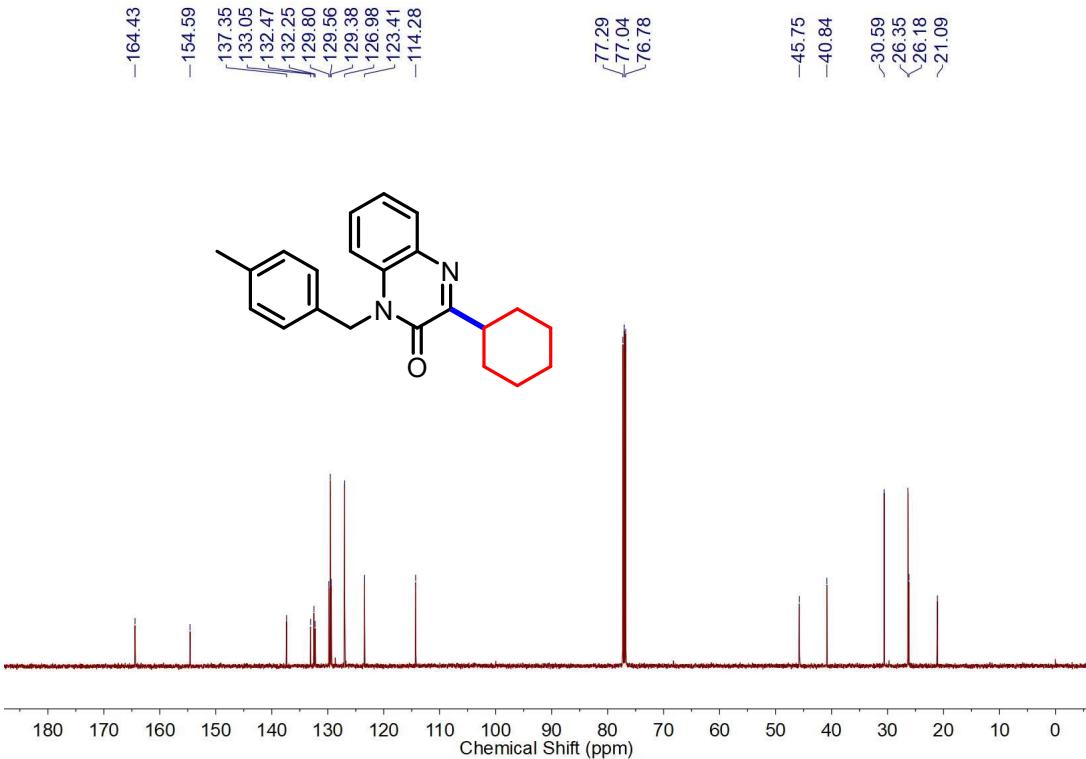
**Figure S62.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **33**



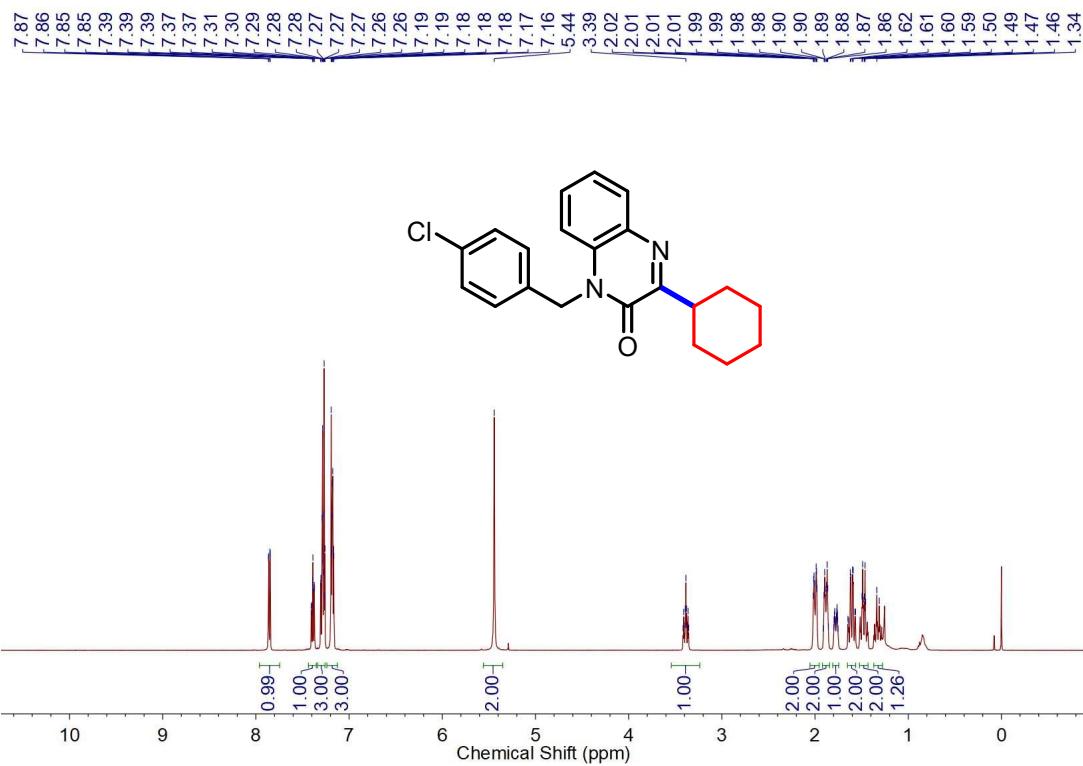
**Figure S63.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **33**



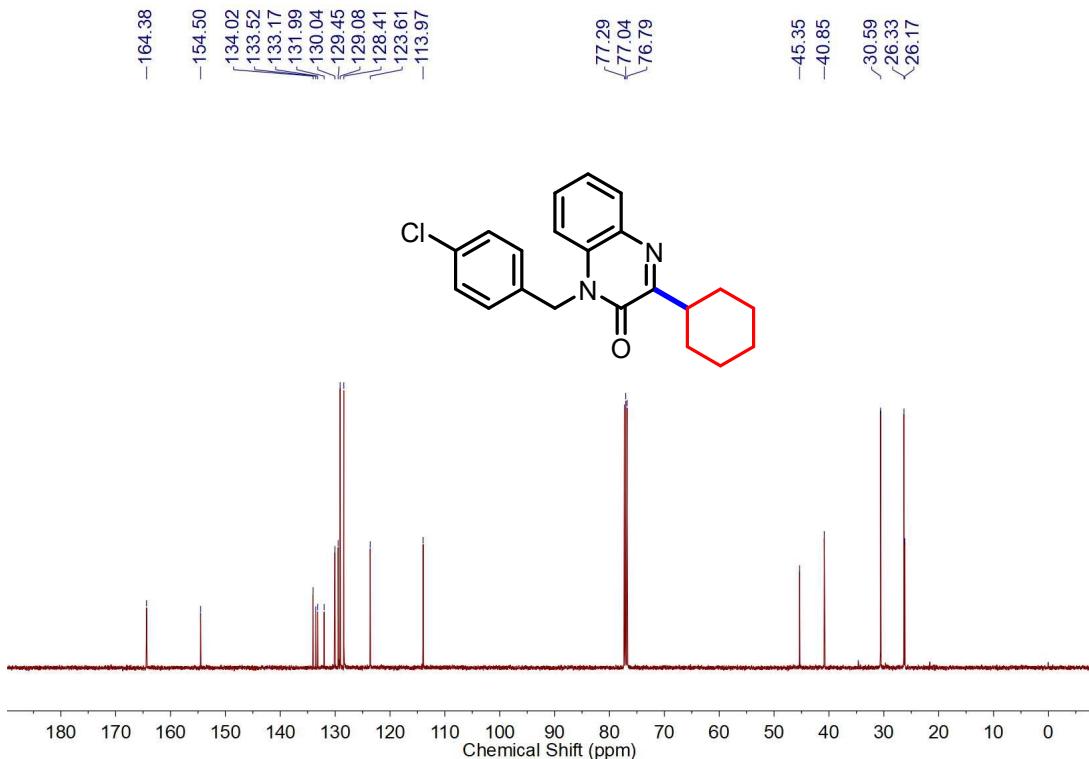
**Figure S64.** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **34**



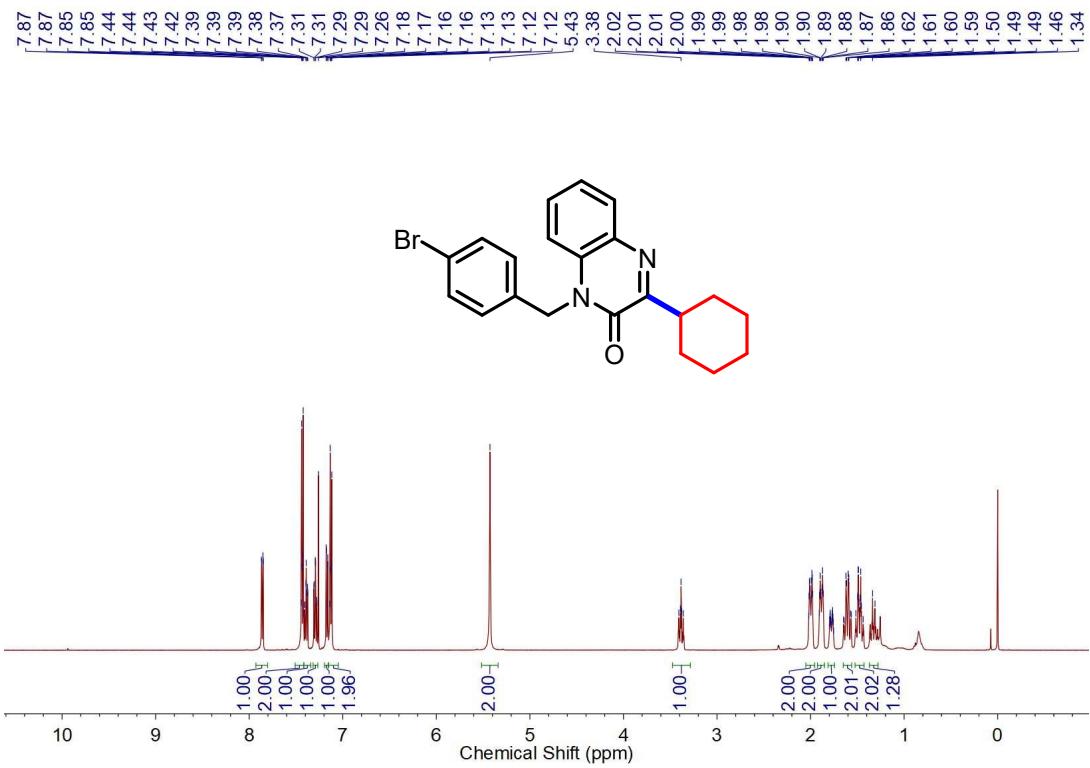
**Figure S65.** <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **34**



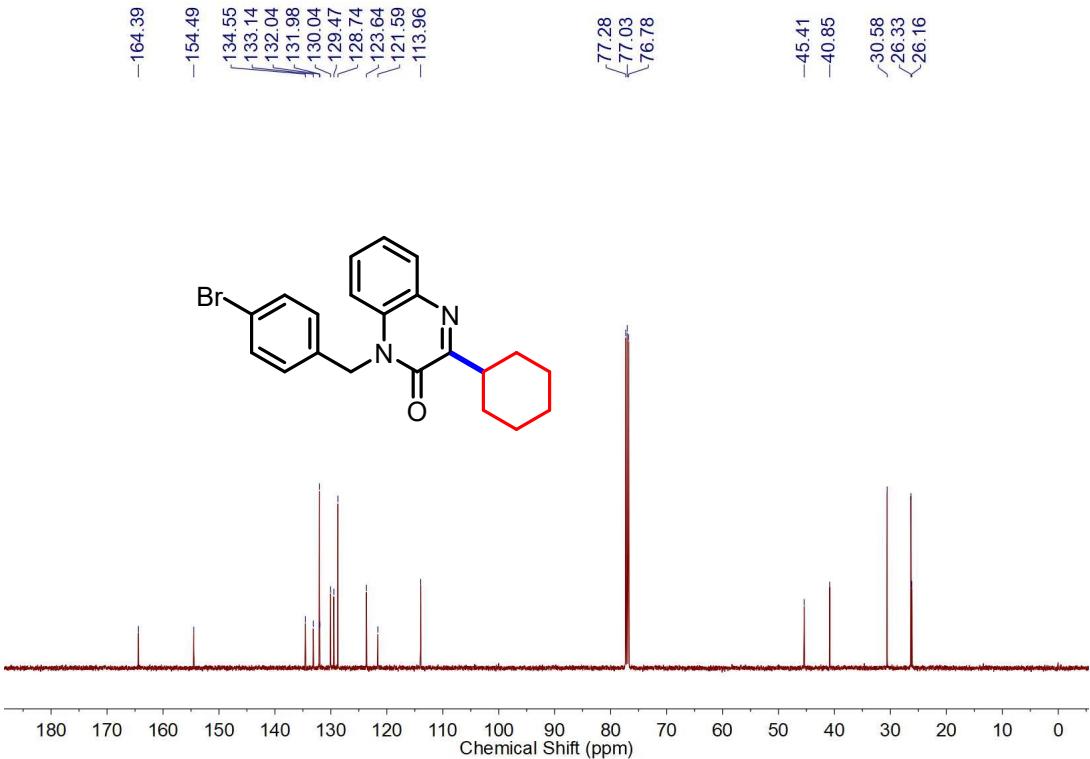
**Figure S66.** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **35**



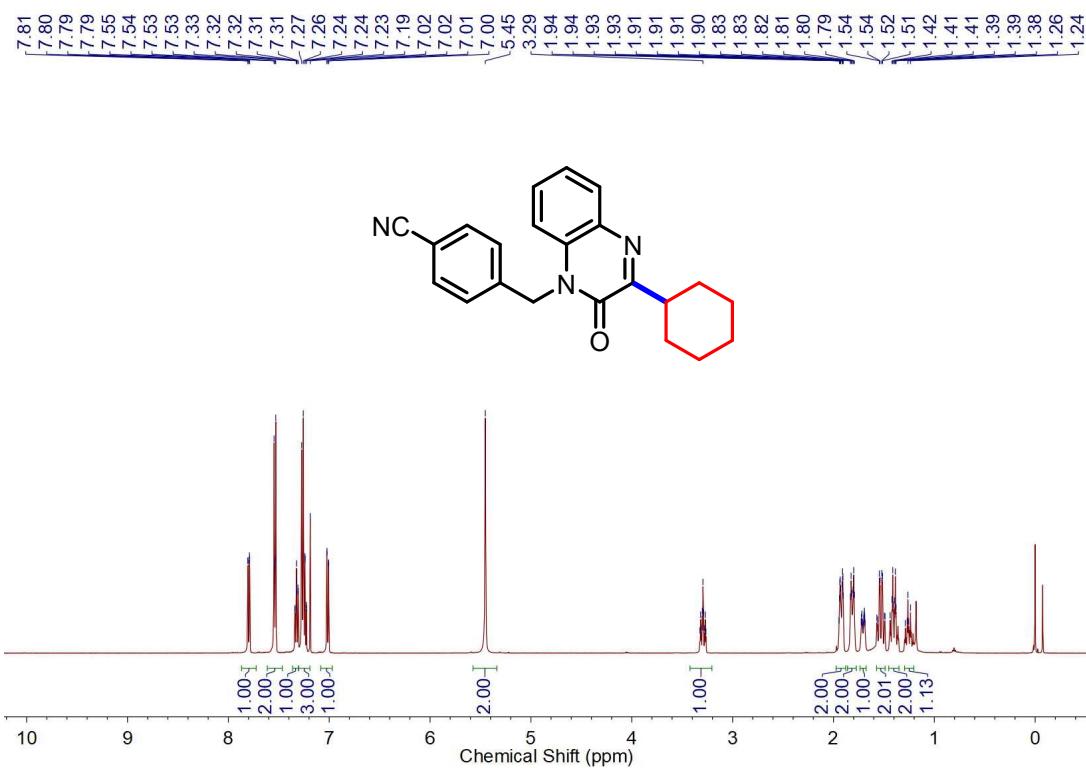
**Figure S67.** <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **35**



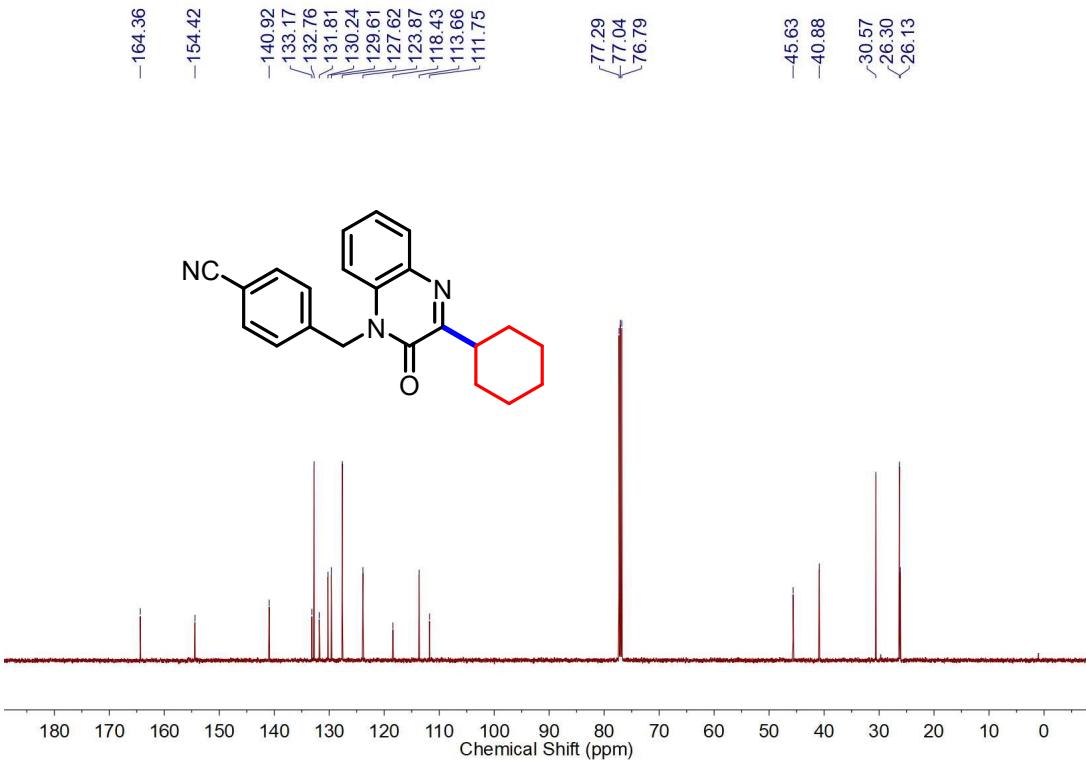
**Figure S68.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **36**



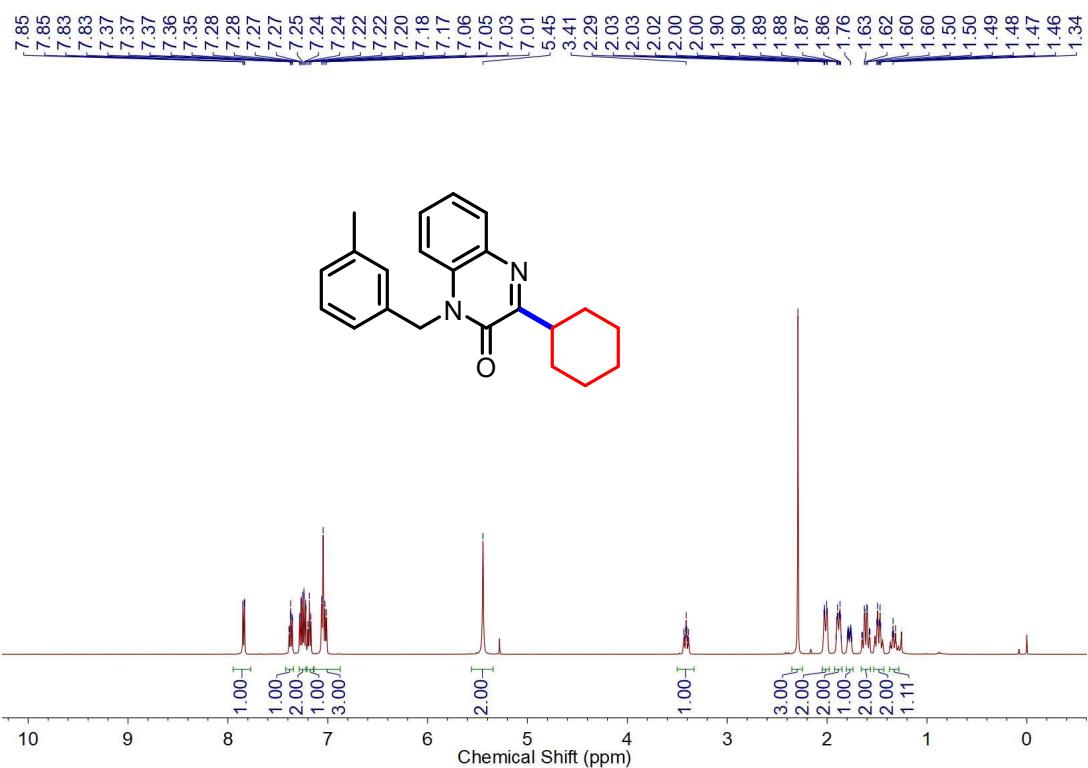
**Figure S69.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **36**



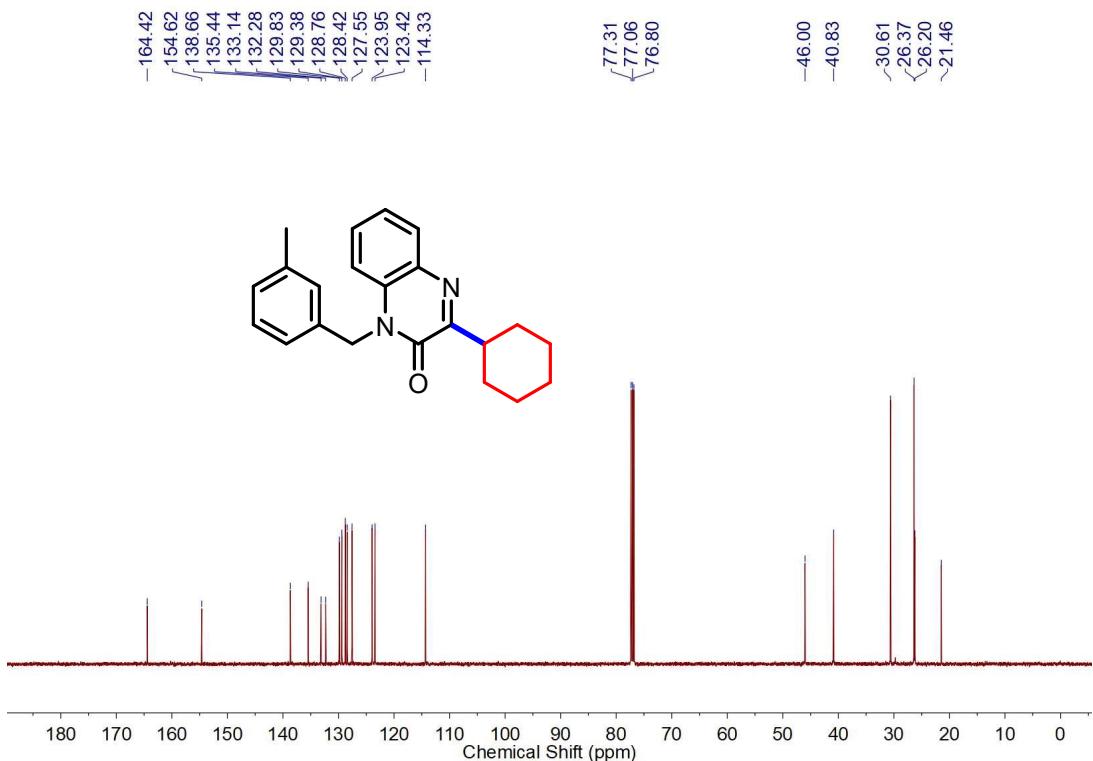
**Figure S70.** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **37**



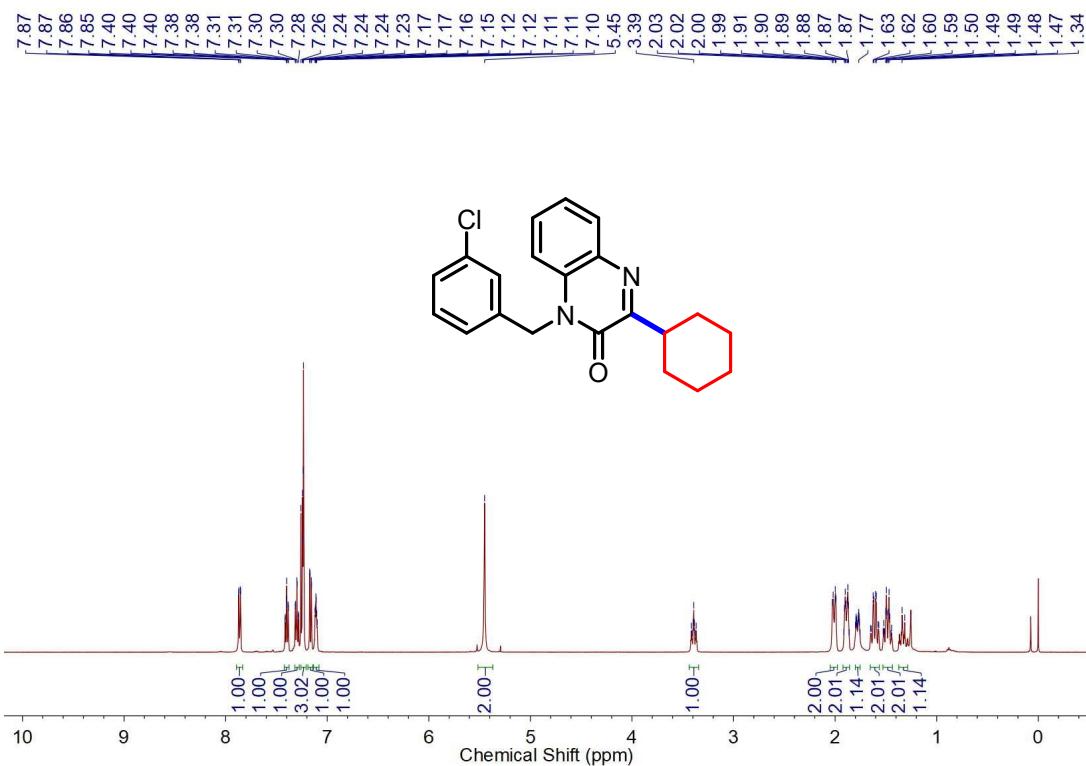
**Figure S71.** <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **37**



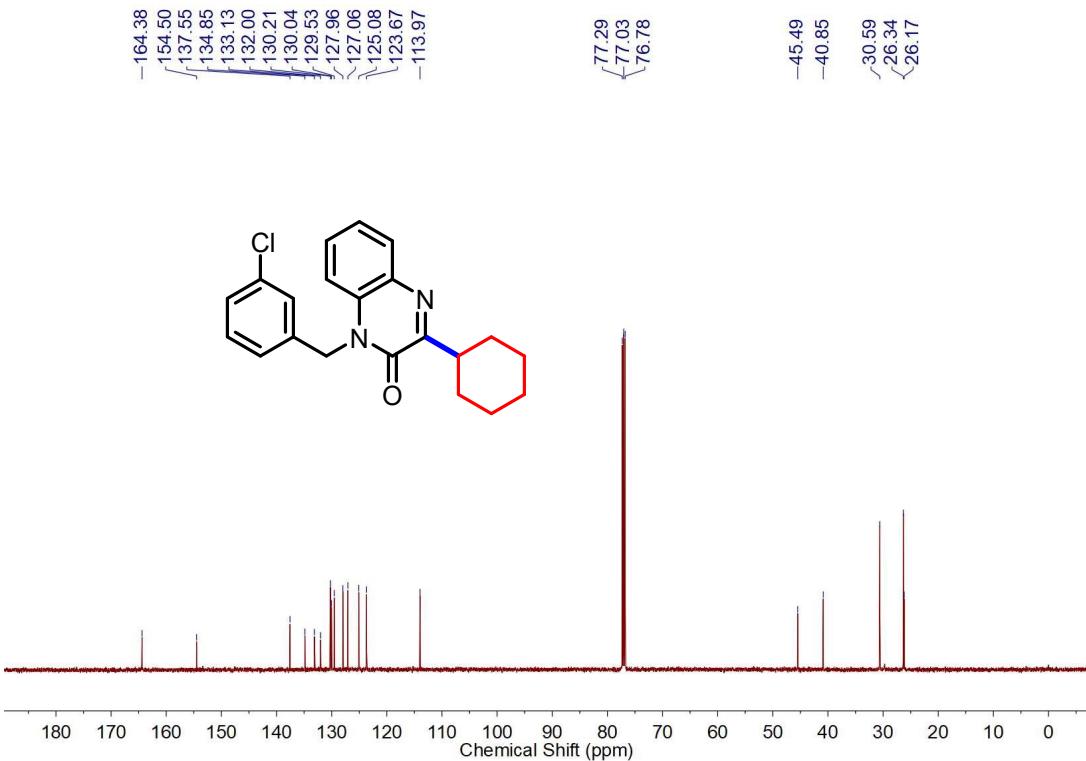
**Figure S72.** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **38**



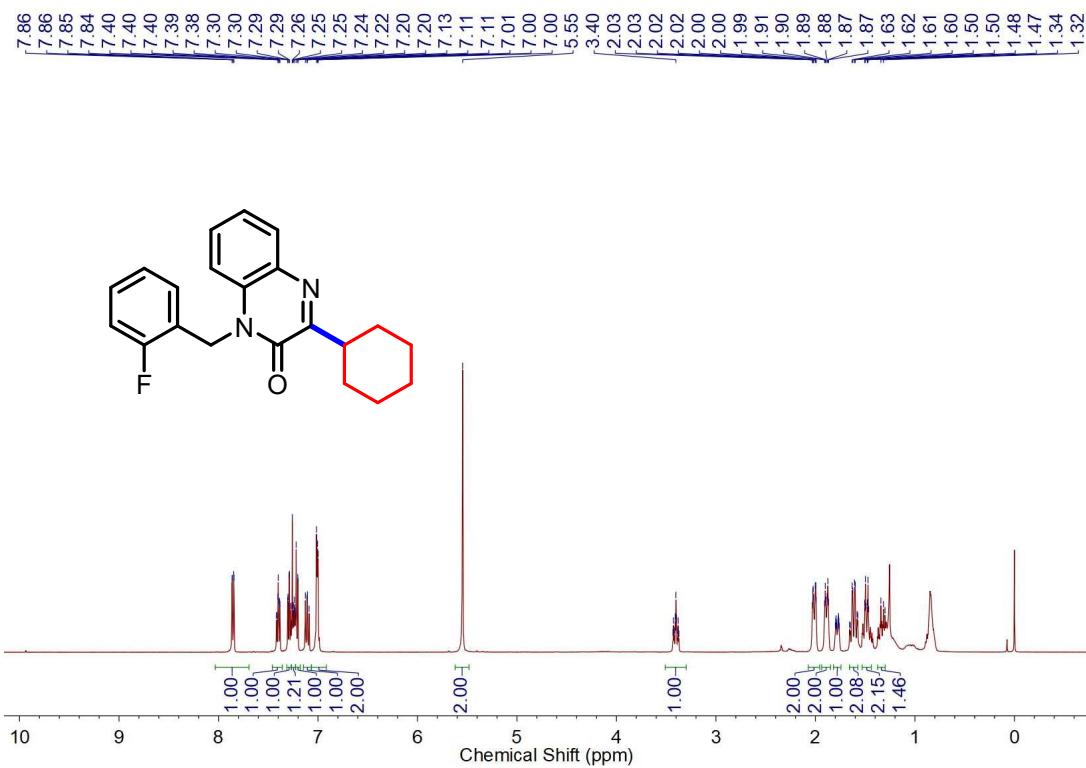
**Figure S73.** <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **38**



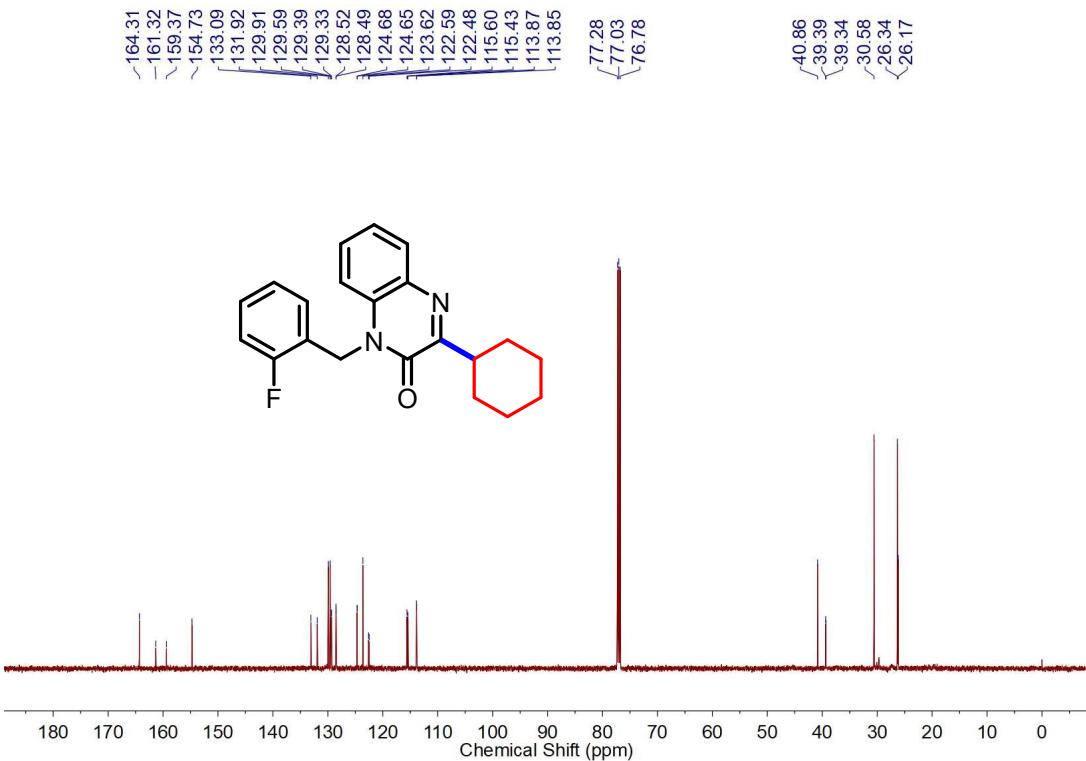
**Figure S74.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **39**



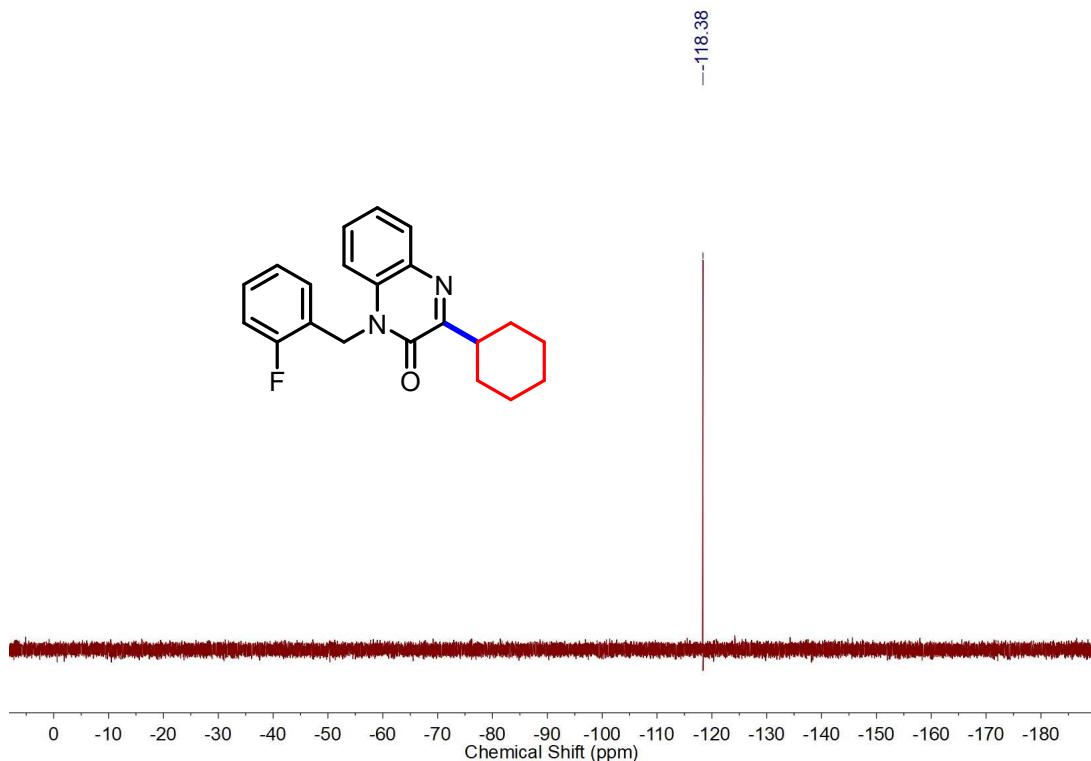
**Figure S75.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **39**



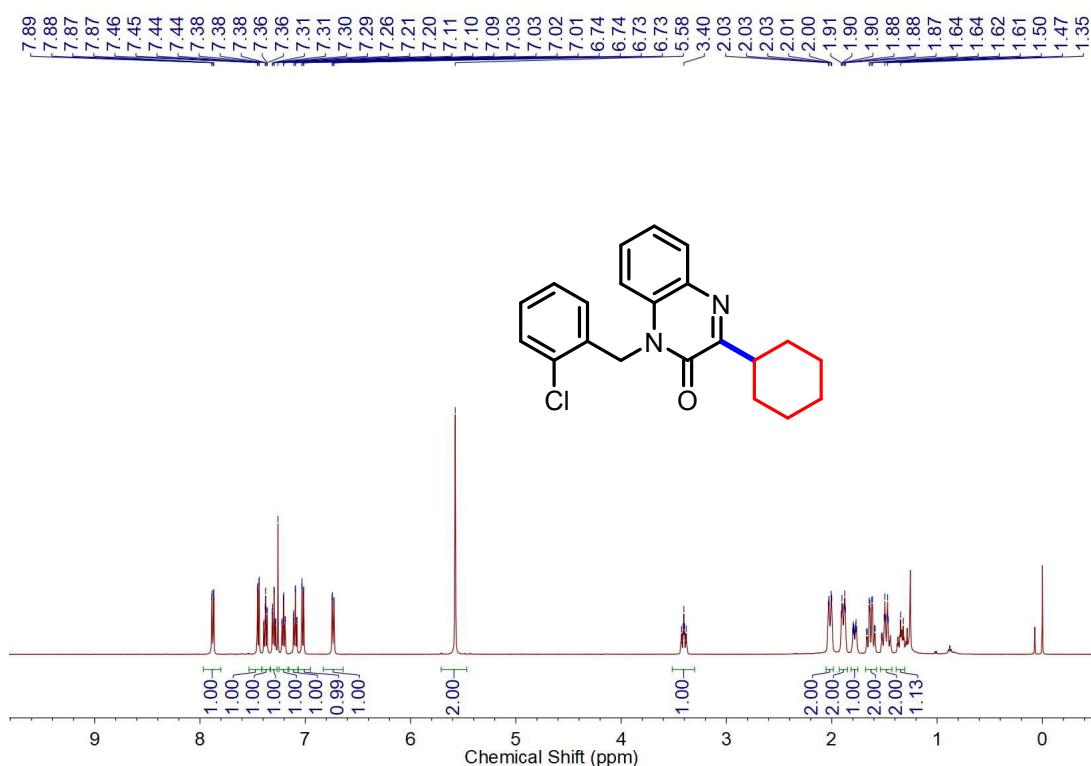
**Figure S76.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **40**



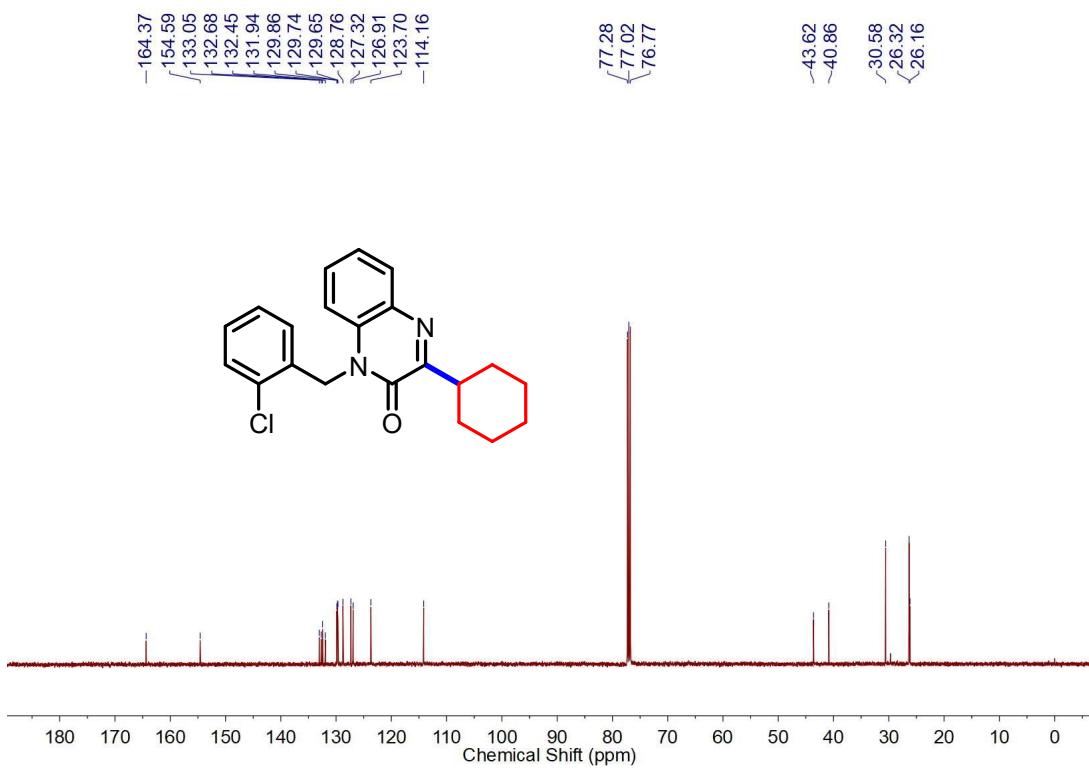
**Figure S77.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **40**



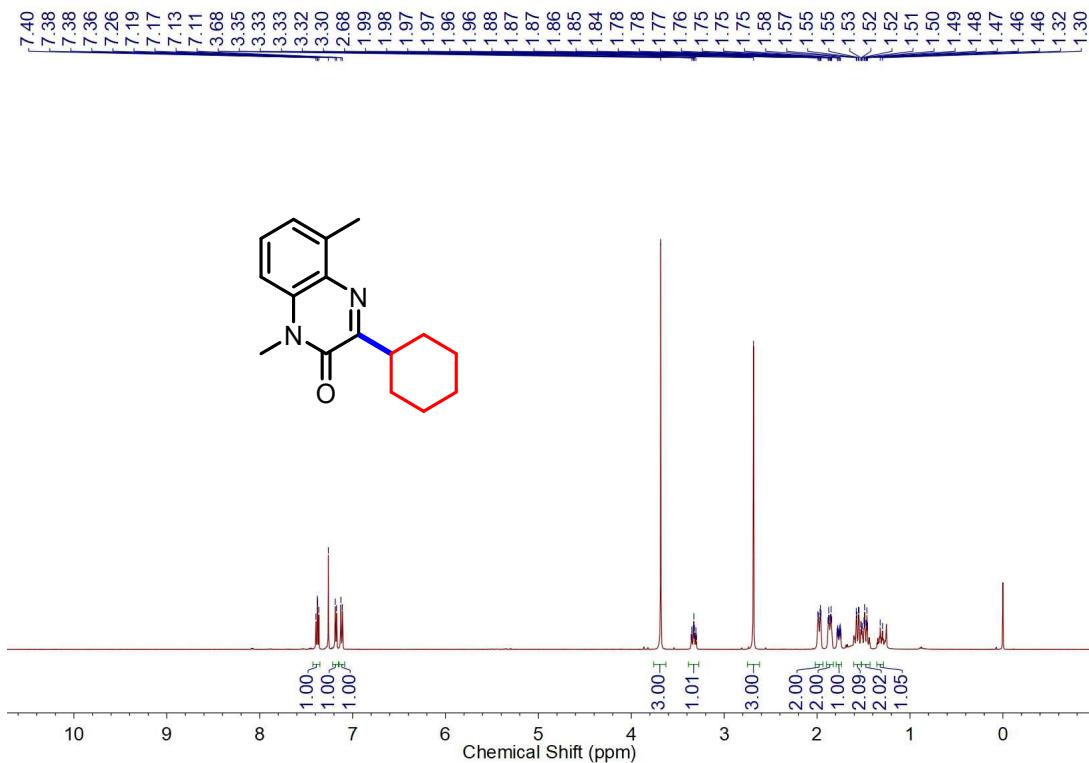
**Figure S78.**  $^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ ) spectrum of **40**



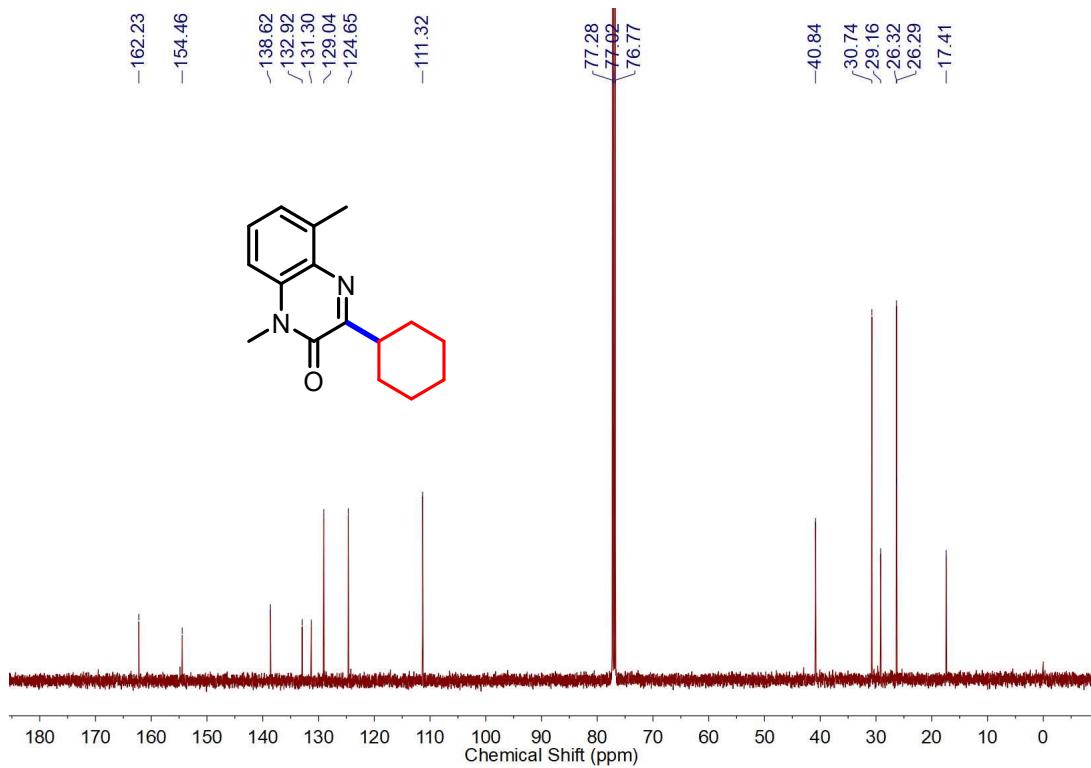
**Figure S79.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **41**



**Figure S80.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **41**

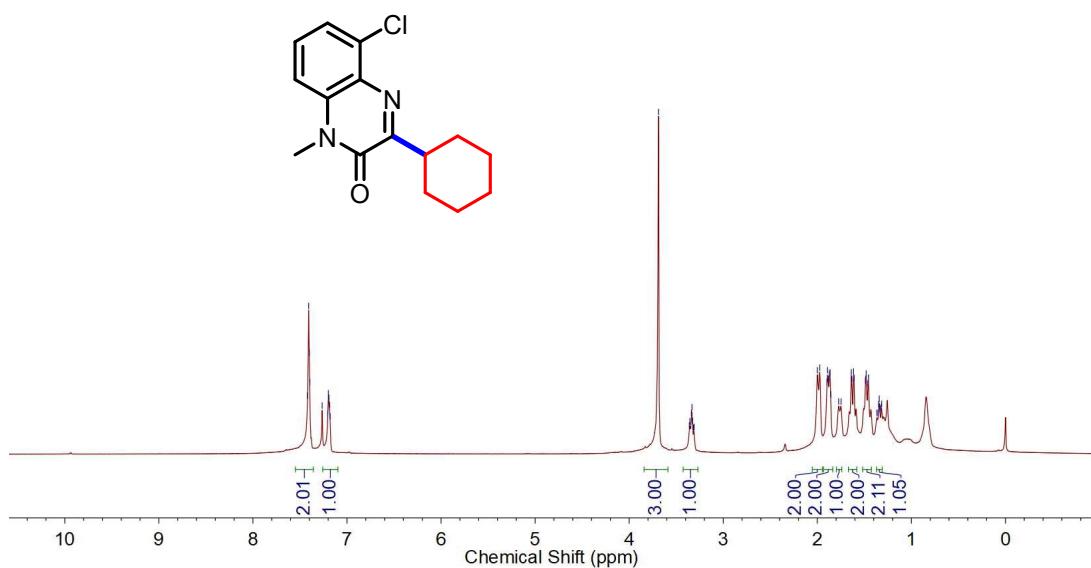


**Figure S81.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **42**

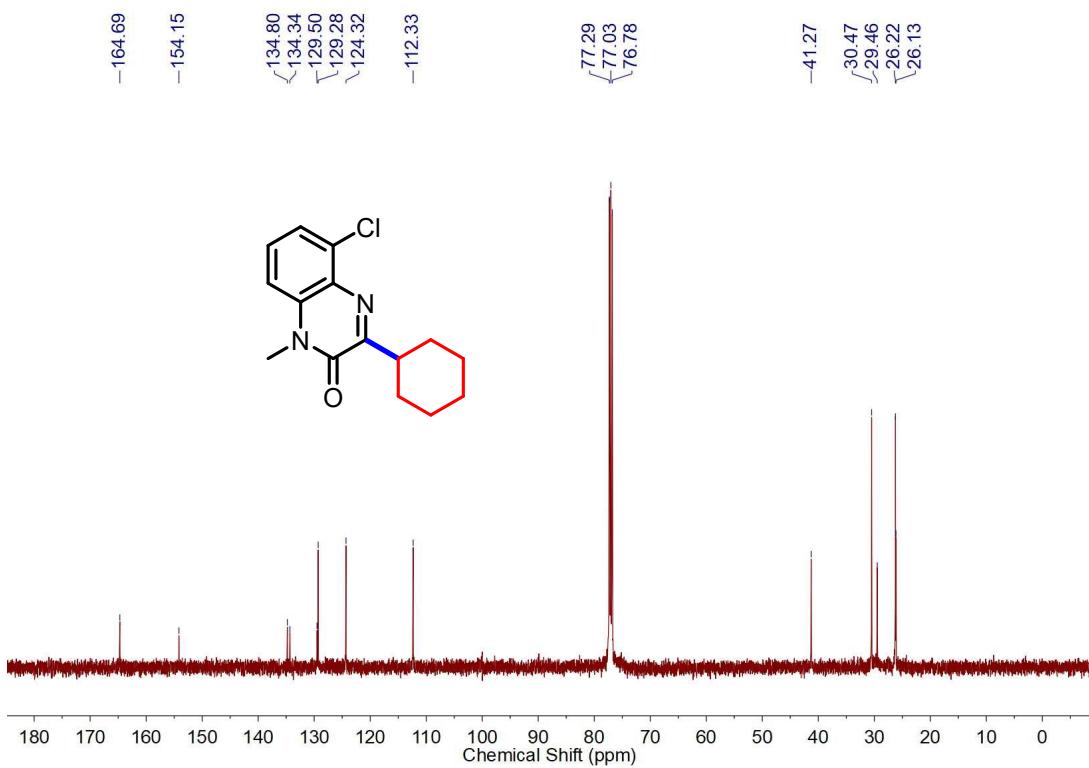


**Figure S82.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **42**

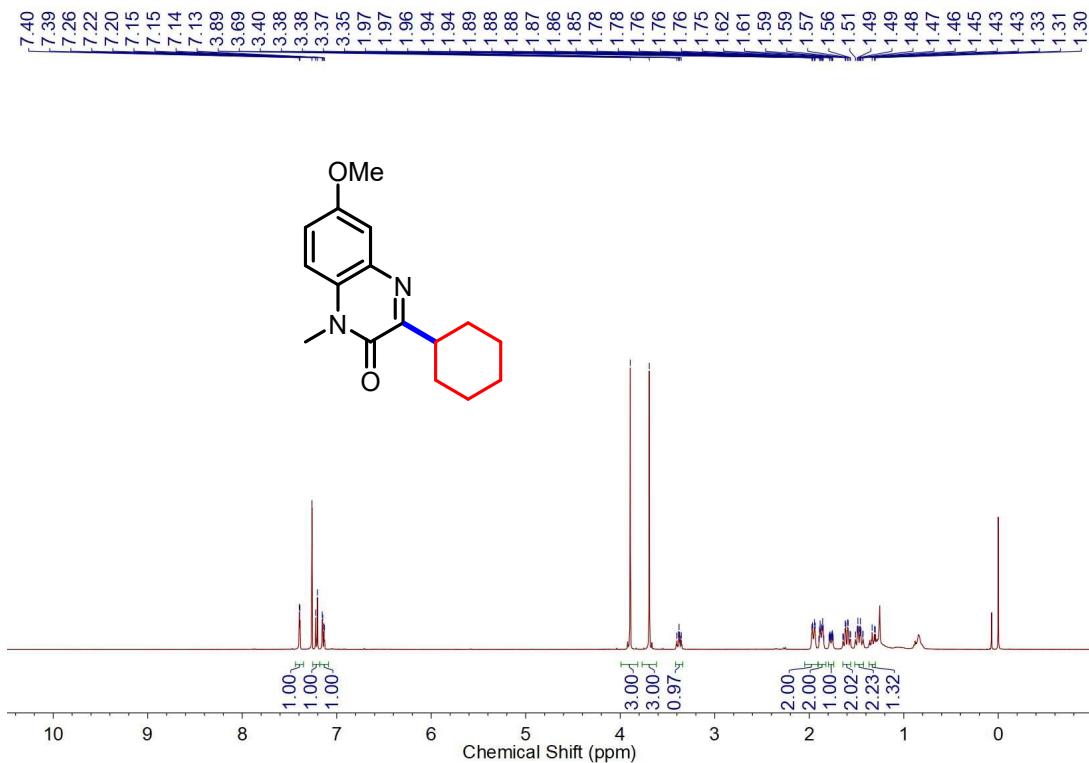
7.42  
7.41  
7.40  
7.39  
7.26  
7.20  
7.20  
7.19  
7.19  
7.18  
7.18  
3.69  
3.36  
3.35  
3.34  
3.33  
3.33  
3.32  
3.31  
2.00  
1.97  
1.90  
1.89  
1.88  
1.87  
1.86  
1.86  
1.77  
1.75  
1.63  
1.61  
1.61  
1.49  
1.48  
1.46  
1.46  
1.37  
1.35  
1.35  
1.34  
1.33  
1.32  
1.32



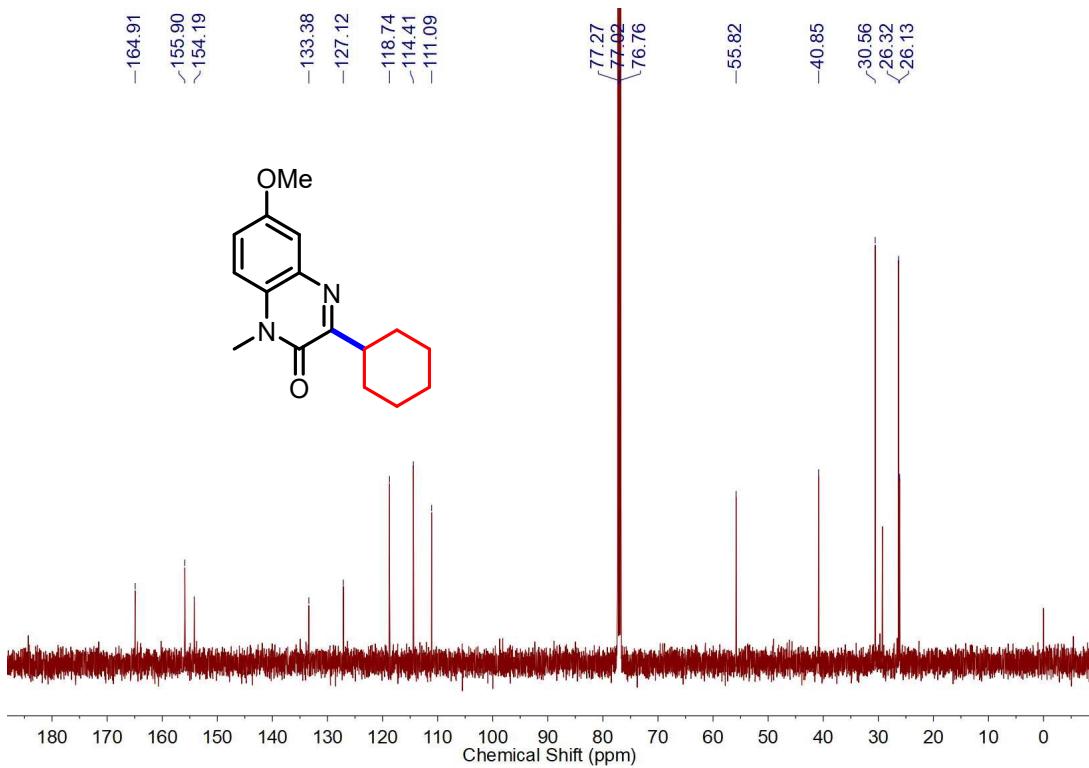
**Figure S83.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **43**



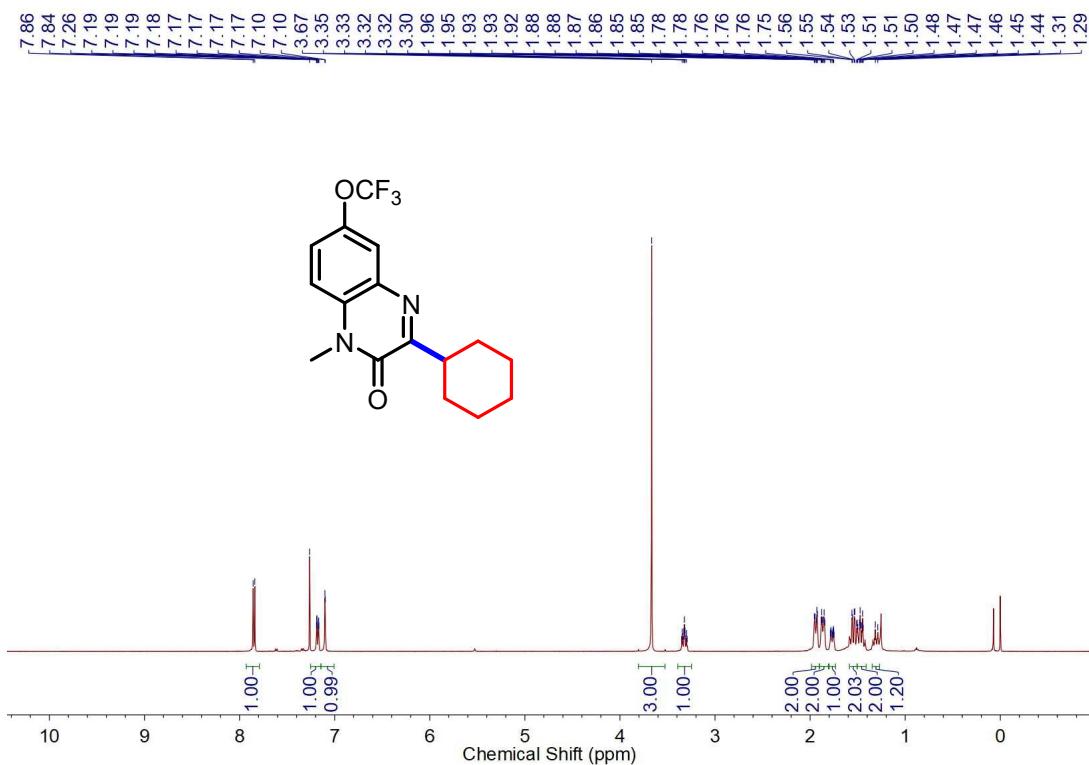
**Figure S84.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **43**



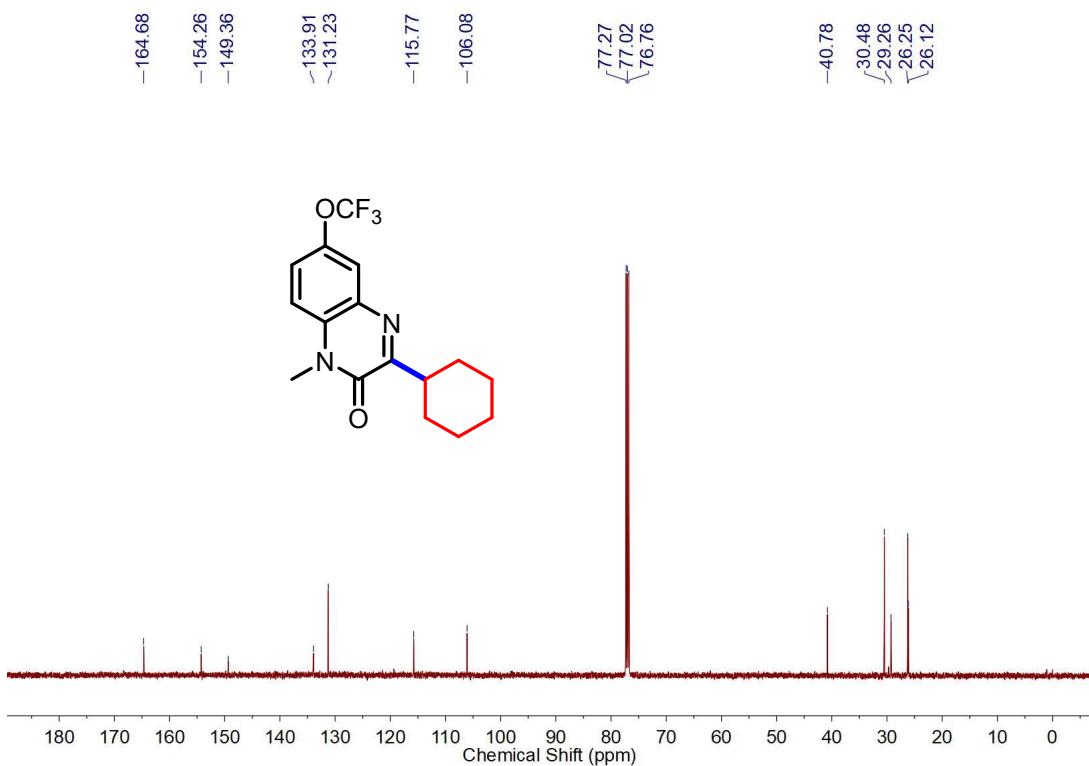
**Figure S85.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **44**



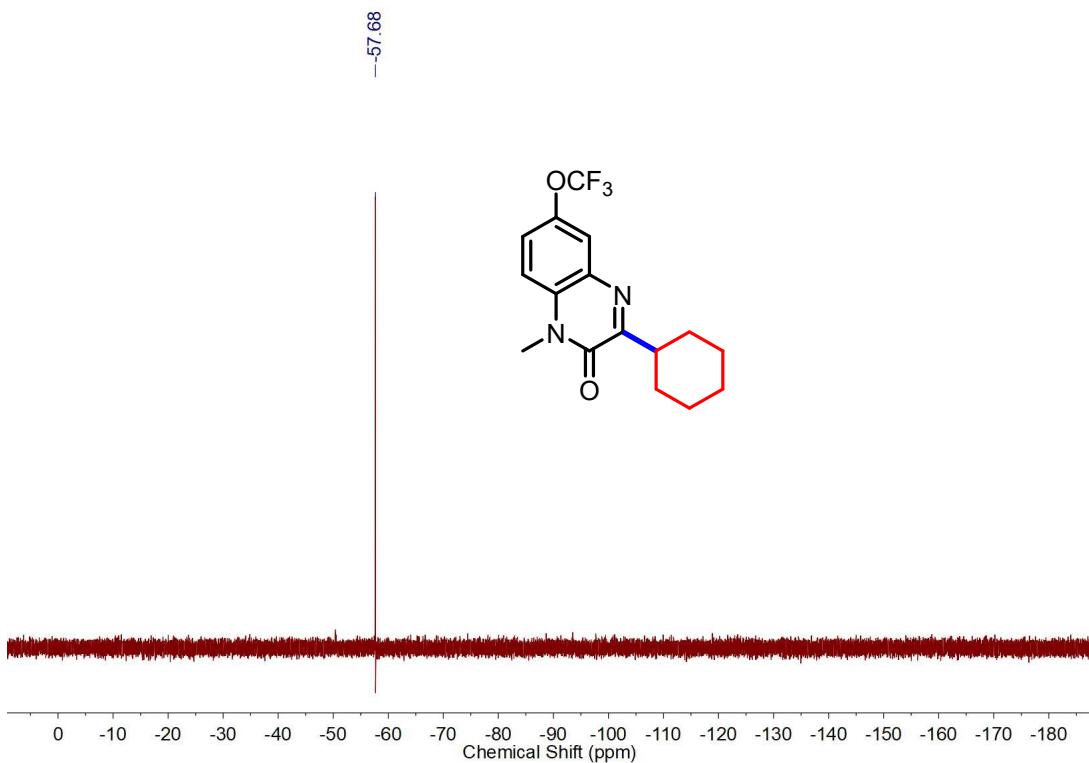
**Figure S86.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **44**



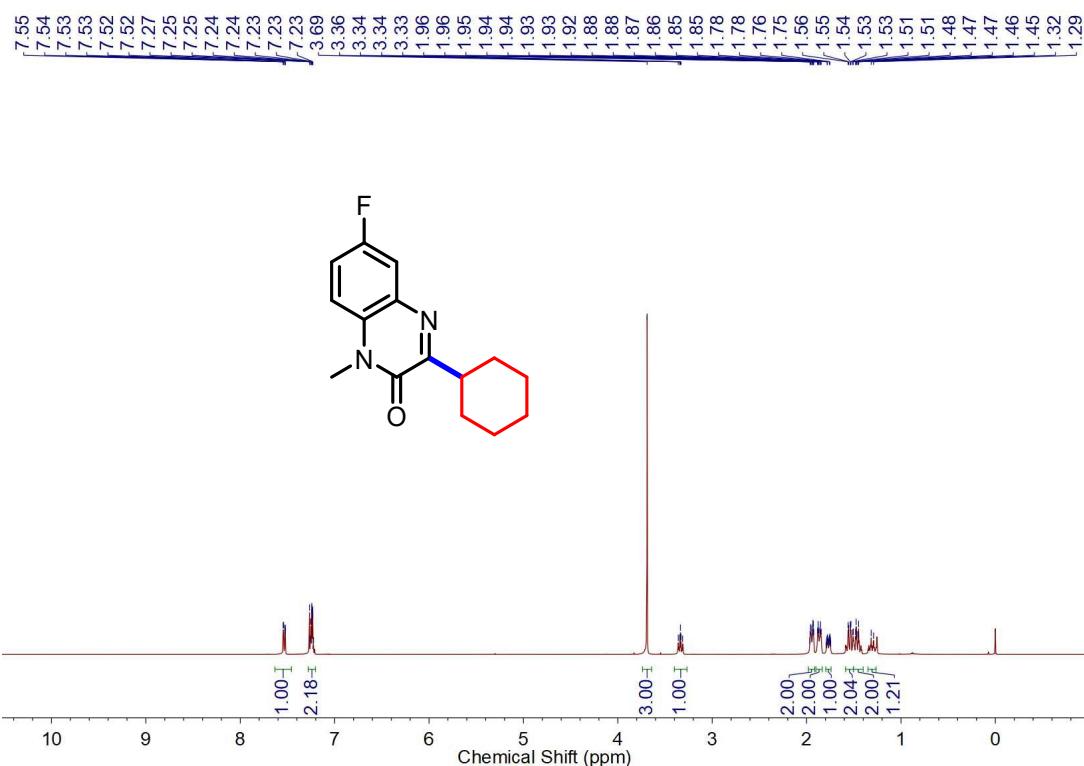
**Figure S87.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **45**



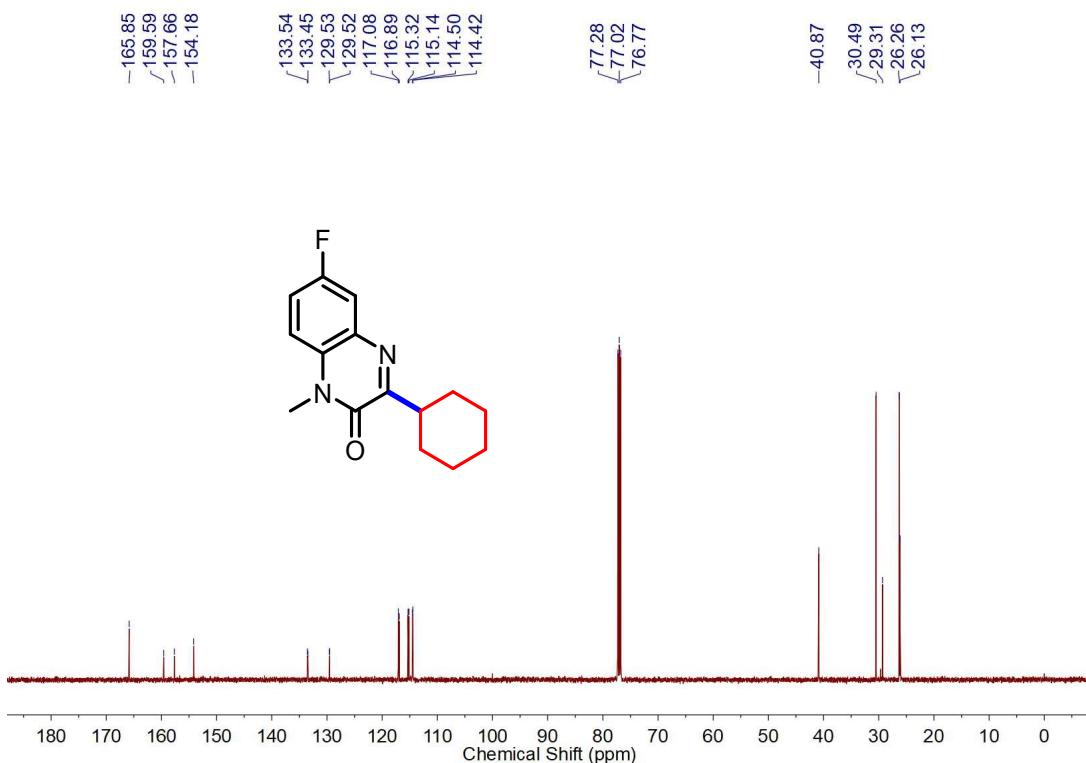
**Figure S88.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **45**



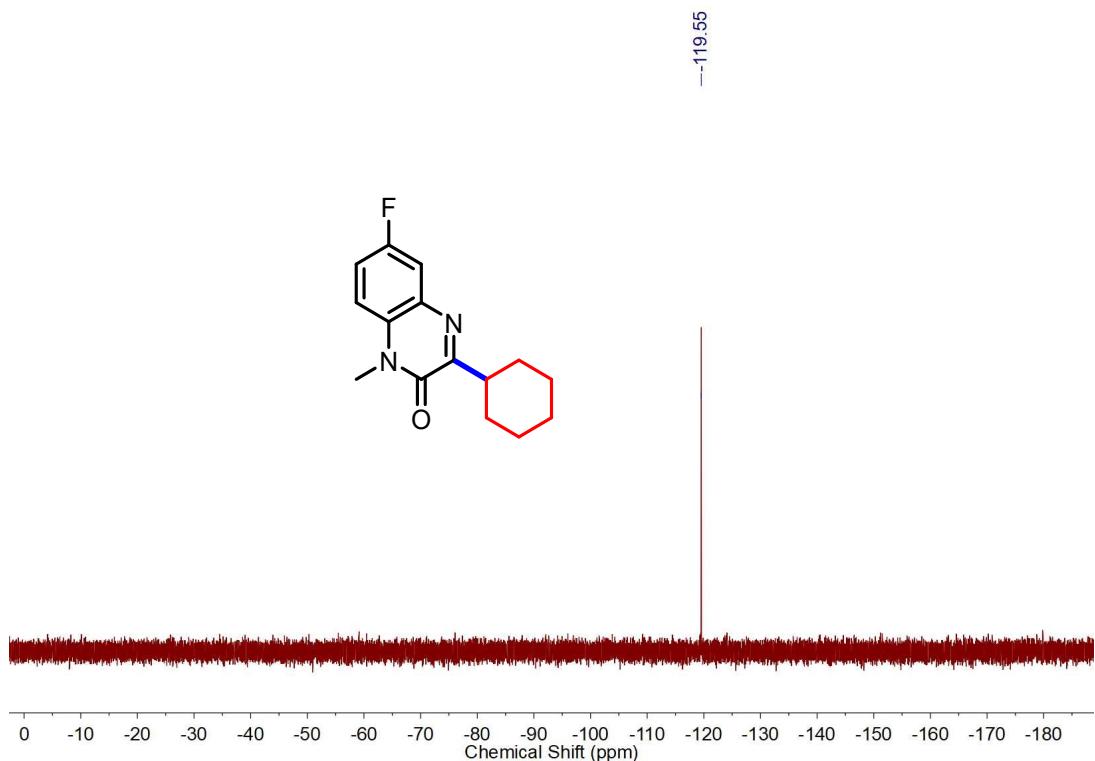
**Figure S89.**  $^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ ) spectrum of **45**



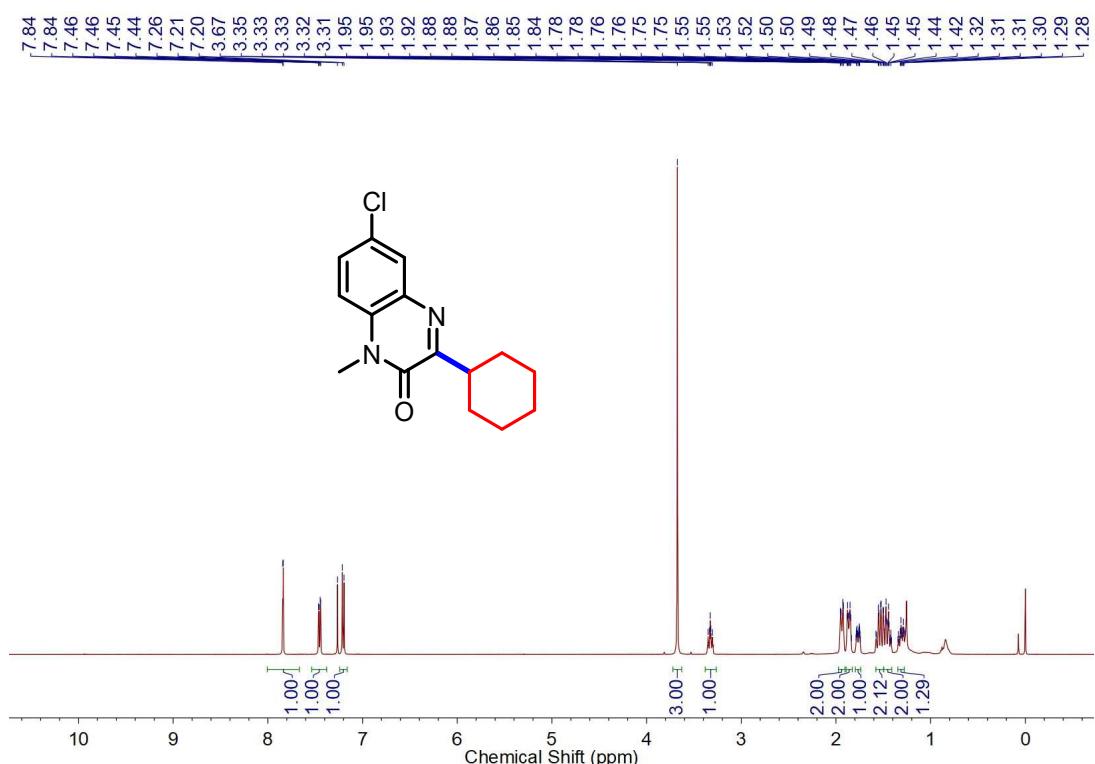
**Figure S90.** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **46**



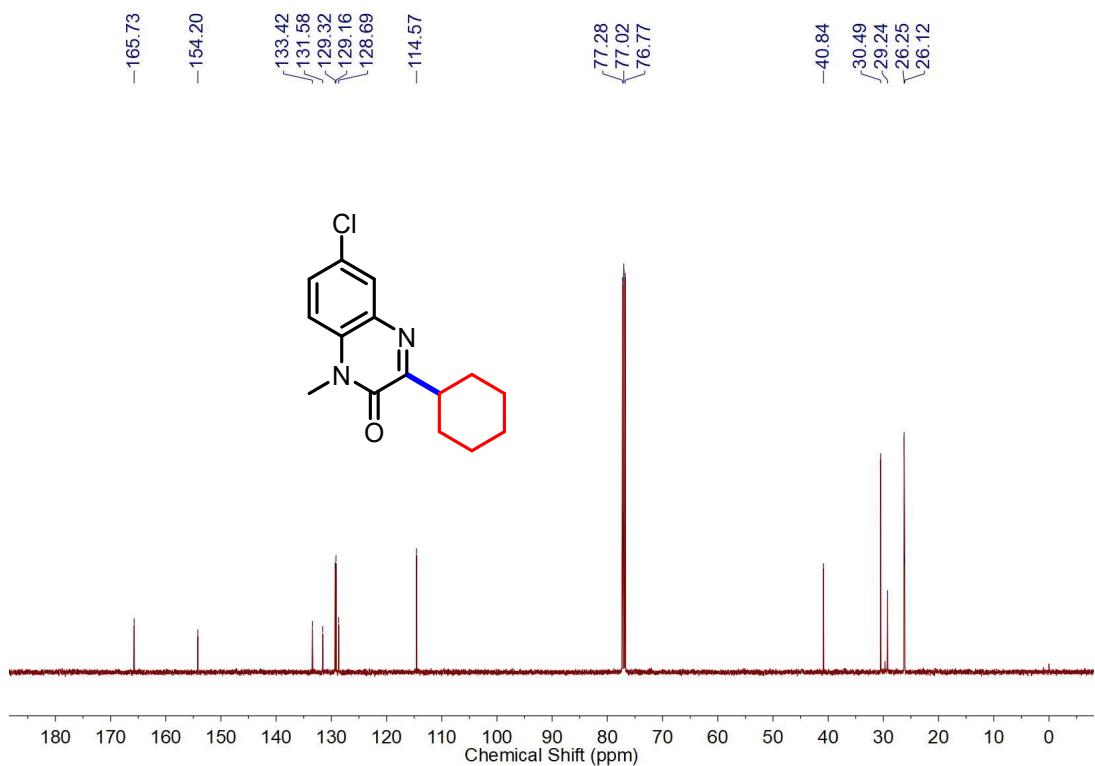
**Figure S91.** <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **46**



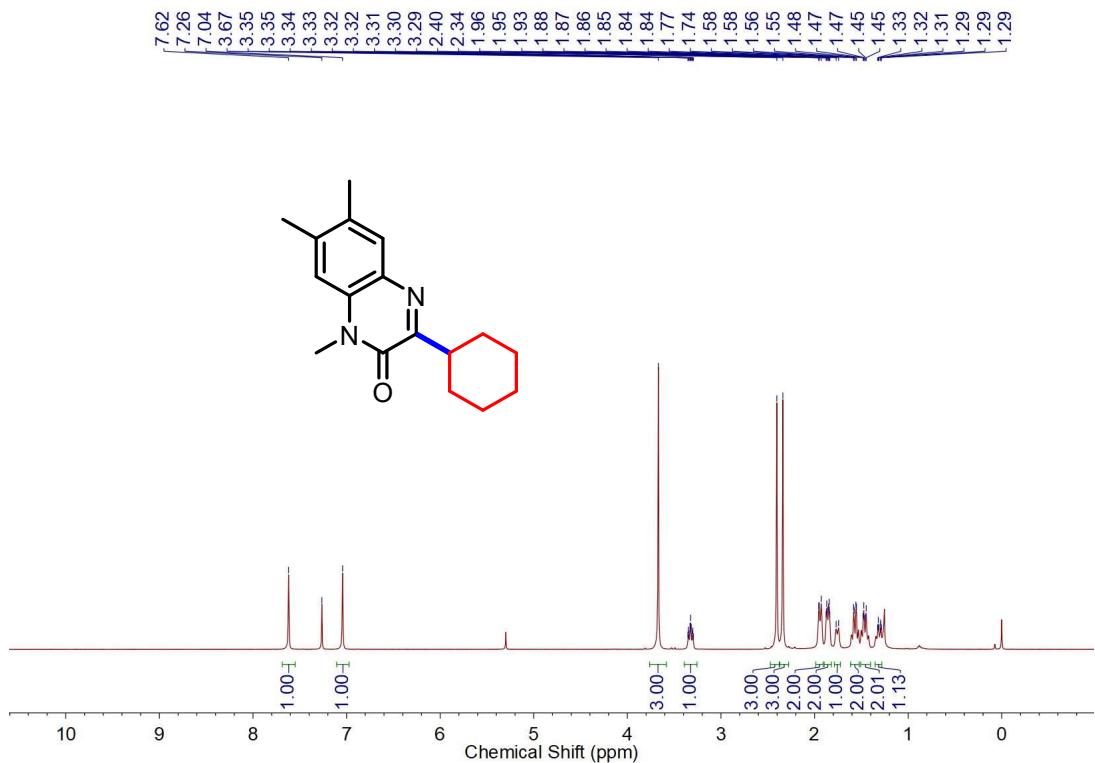
**Figure S92.**  $^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ ) spectrum of **46**



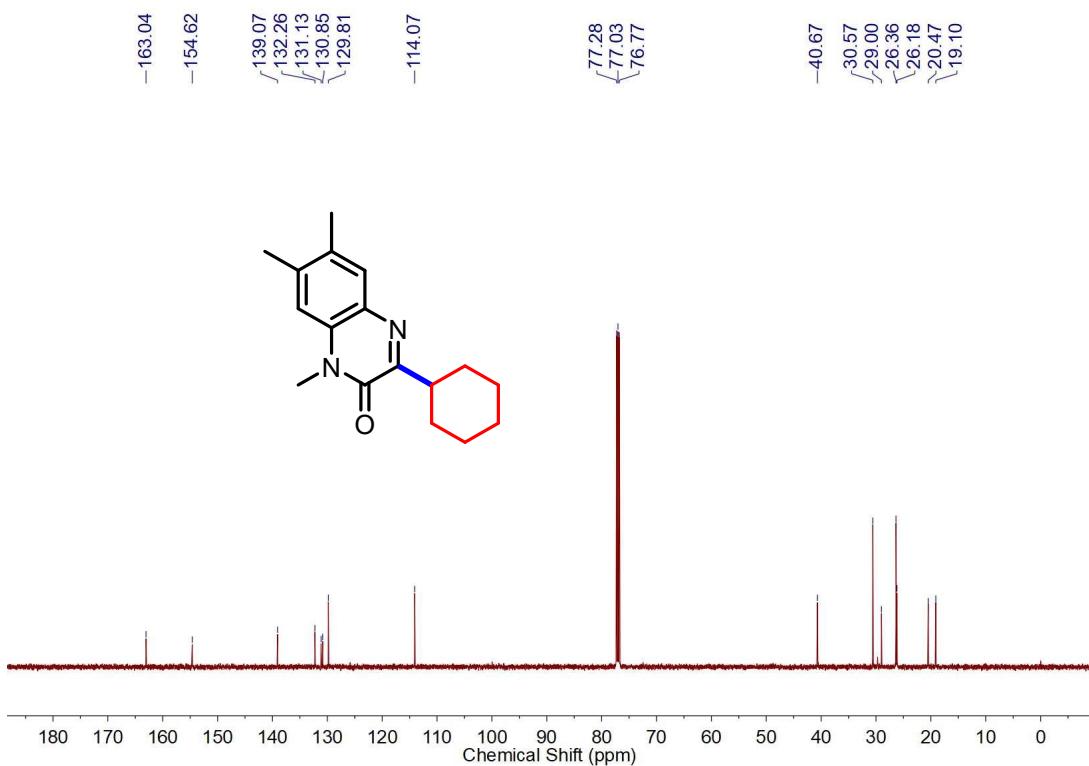
**Figure S93.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **47**



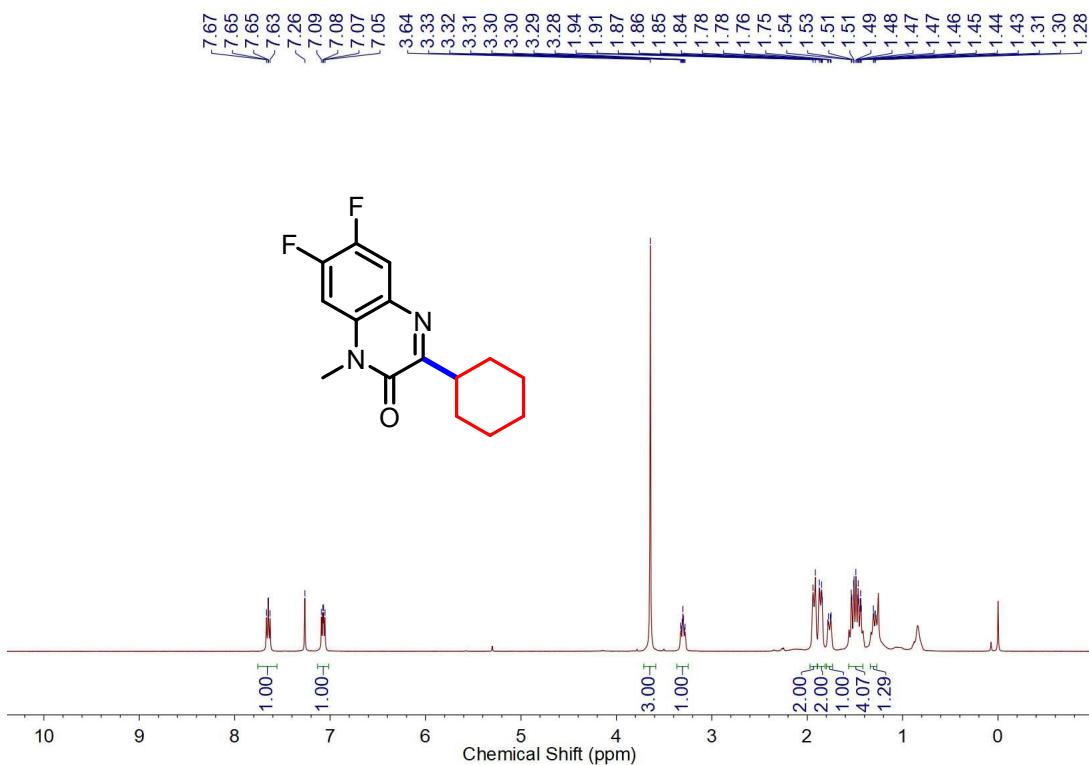
**Figure S94.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **47**



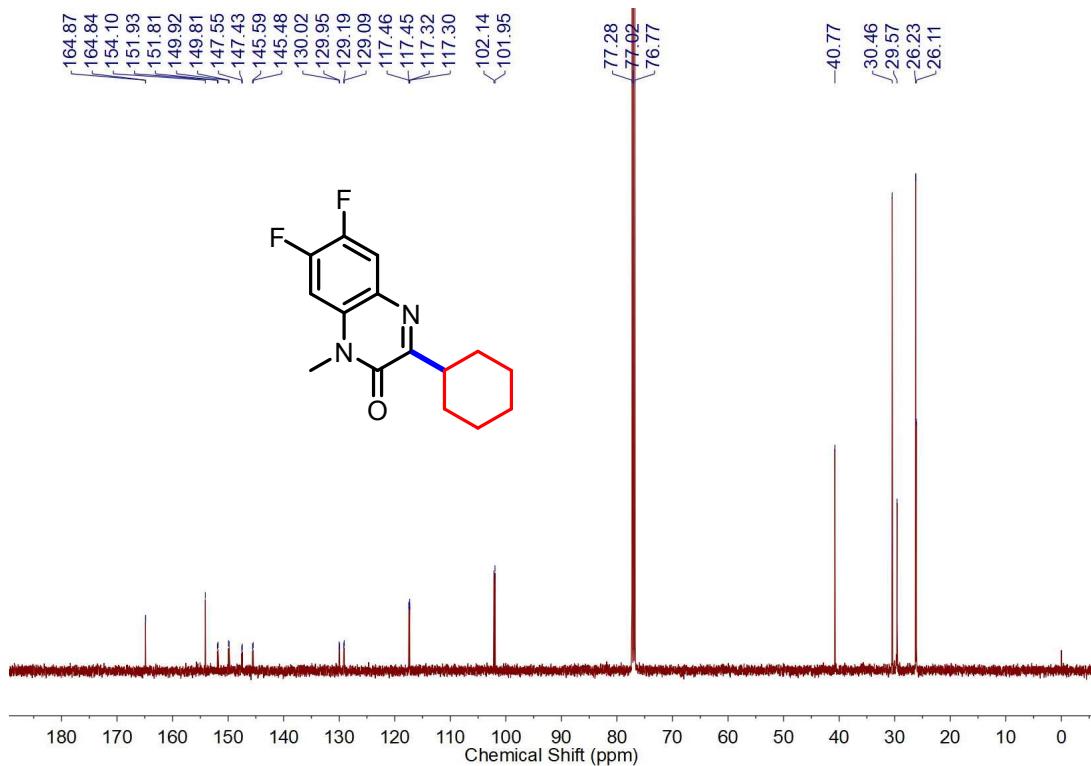
**Figure S95.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **48**



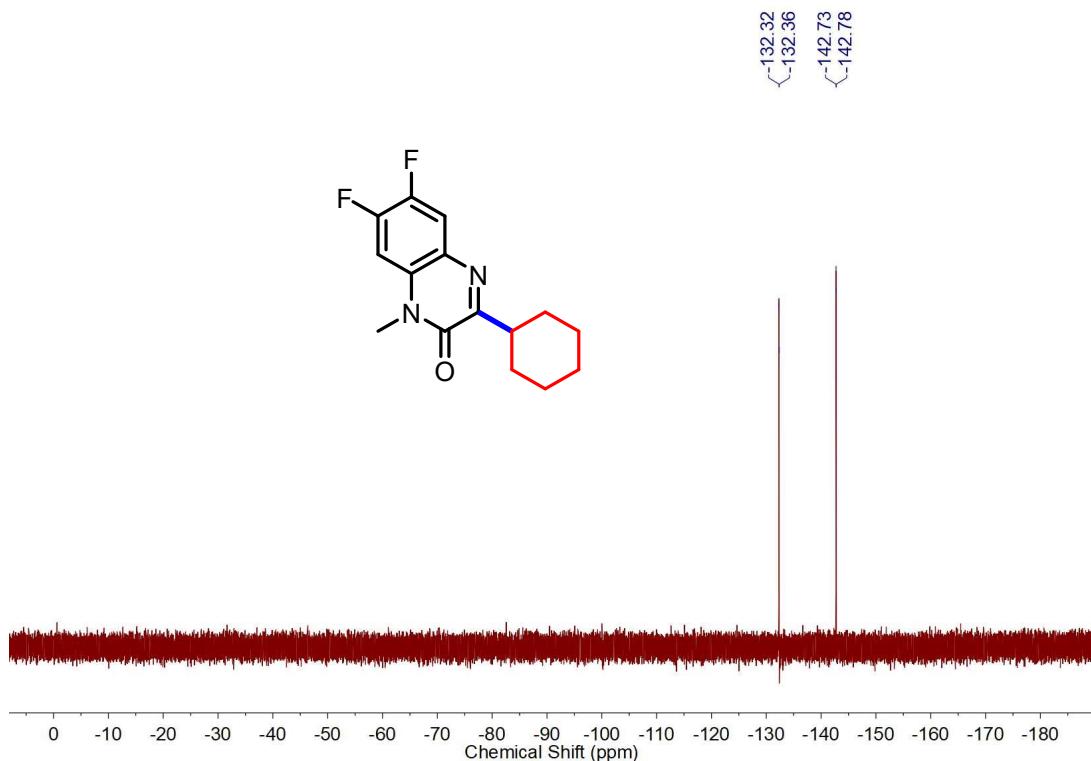
**Figure S96.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **48**



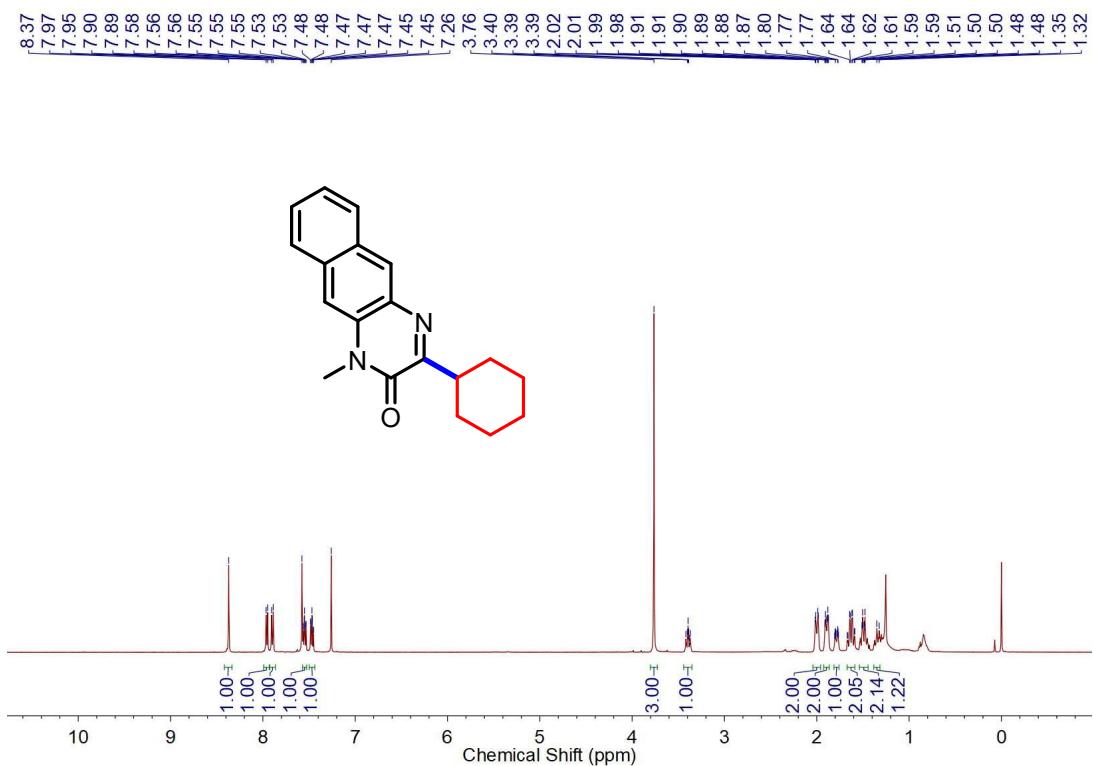
**Figure S97.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **49**



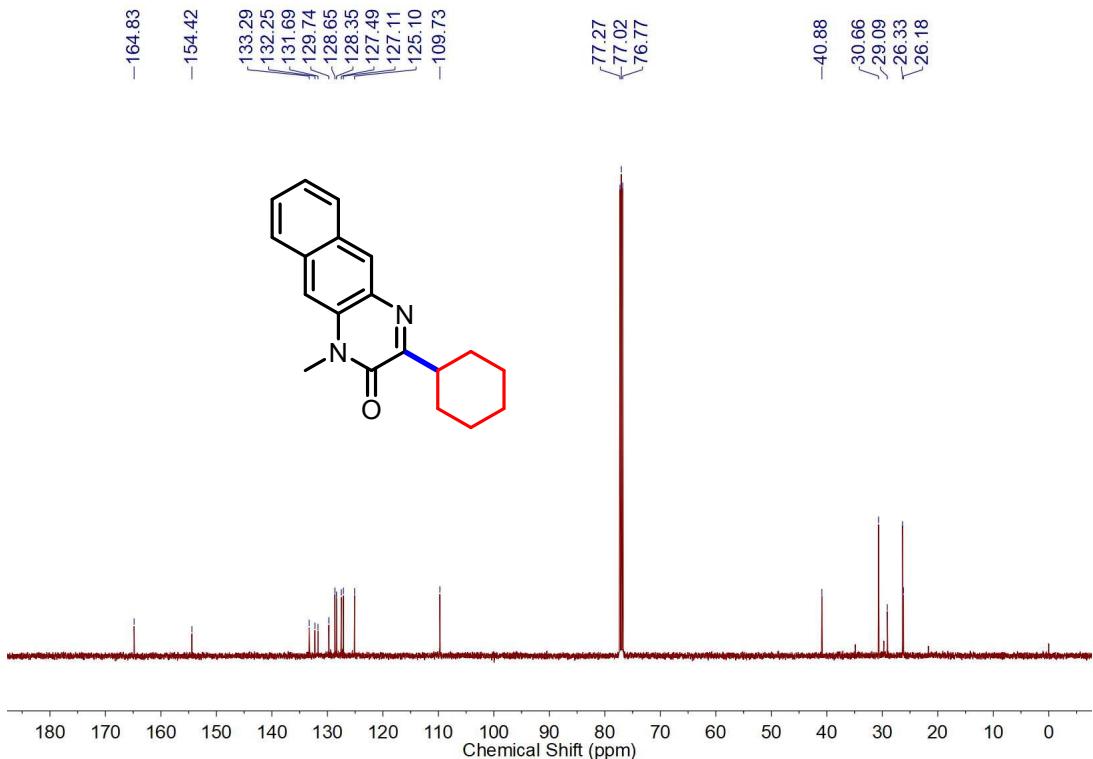
**Figure S98.** <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **49**



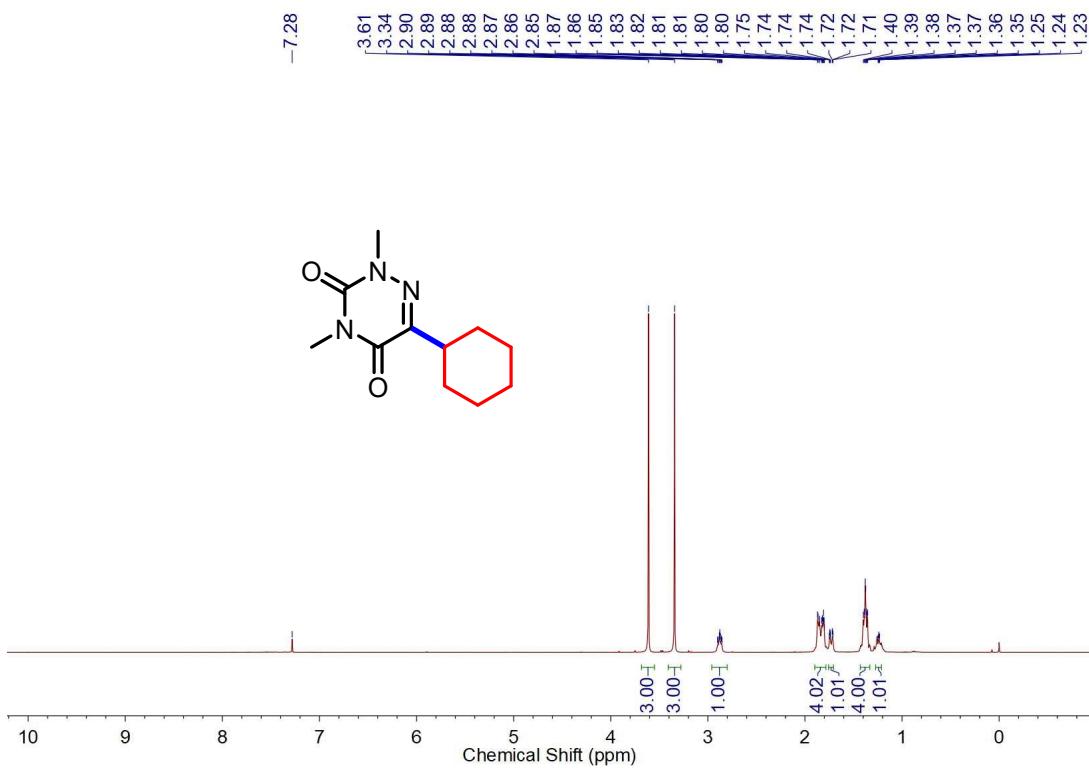
**Figure S99.** <sup>19</sup>F NMR (471 MHz, CDCl<sub>3</sub>) spectrum of **49**



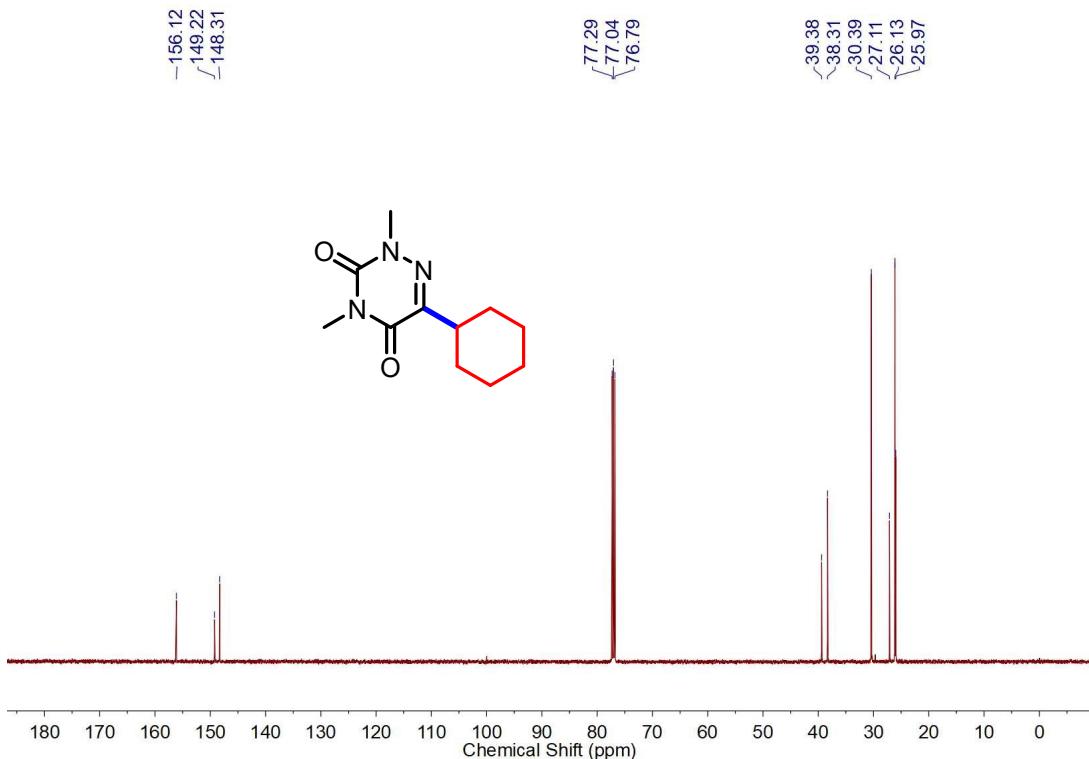
**Figure S100.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **50**



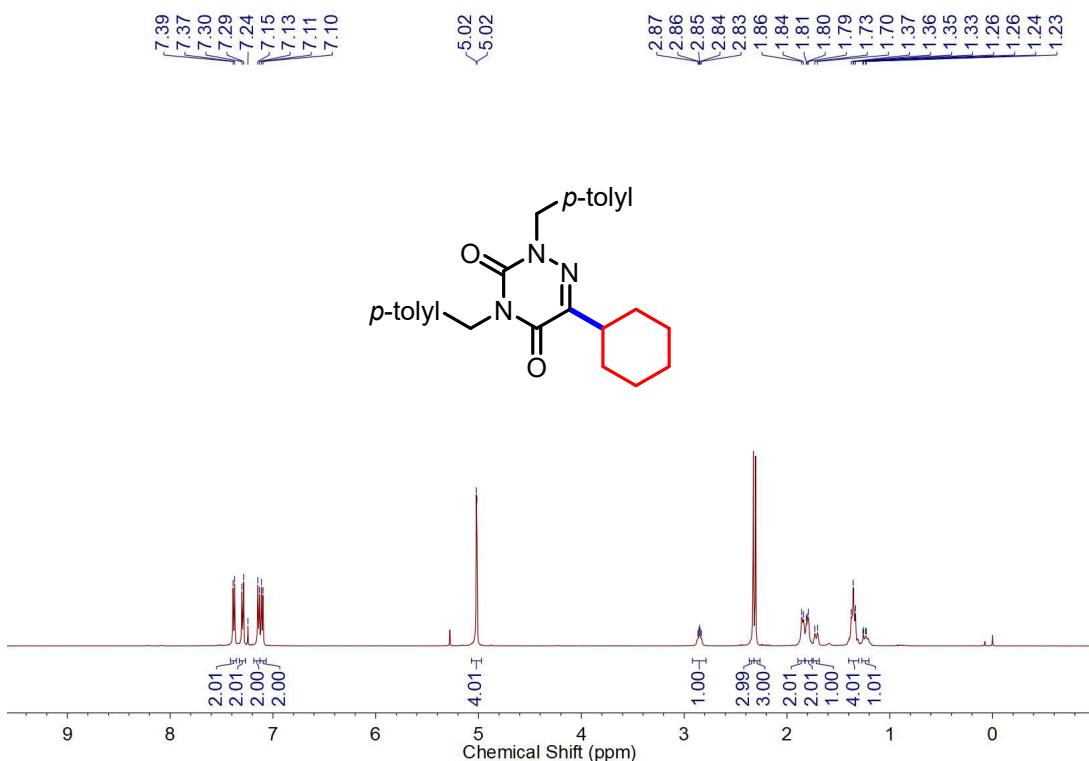
**Figure S101.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **50**



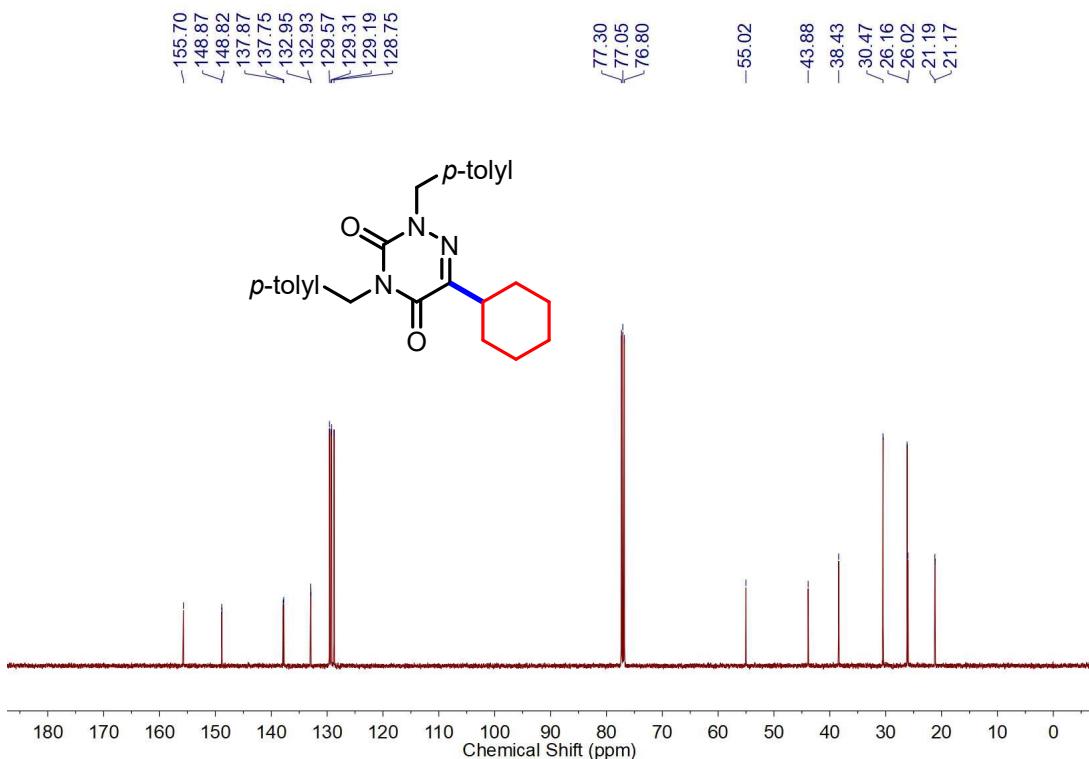
**Figure S102.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **51**



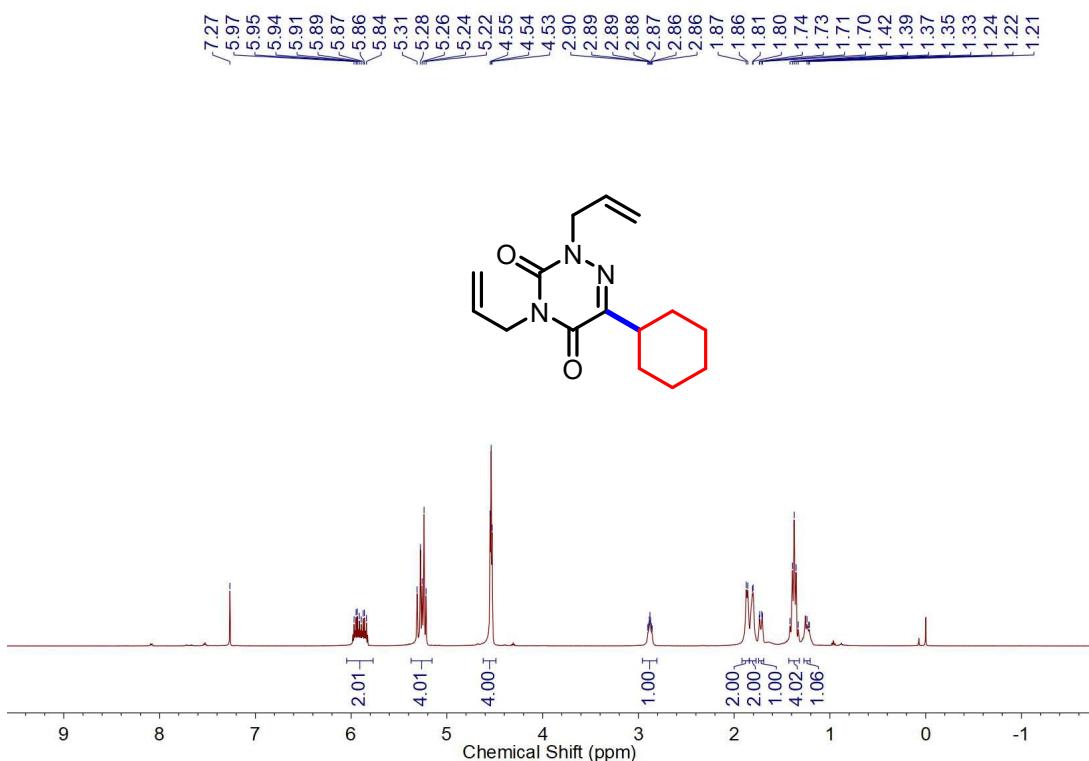
**Figure S103.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **51**



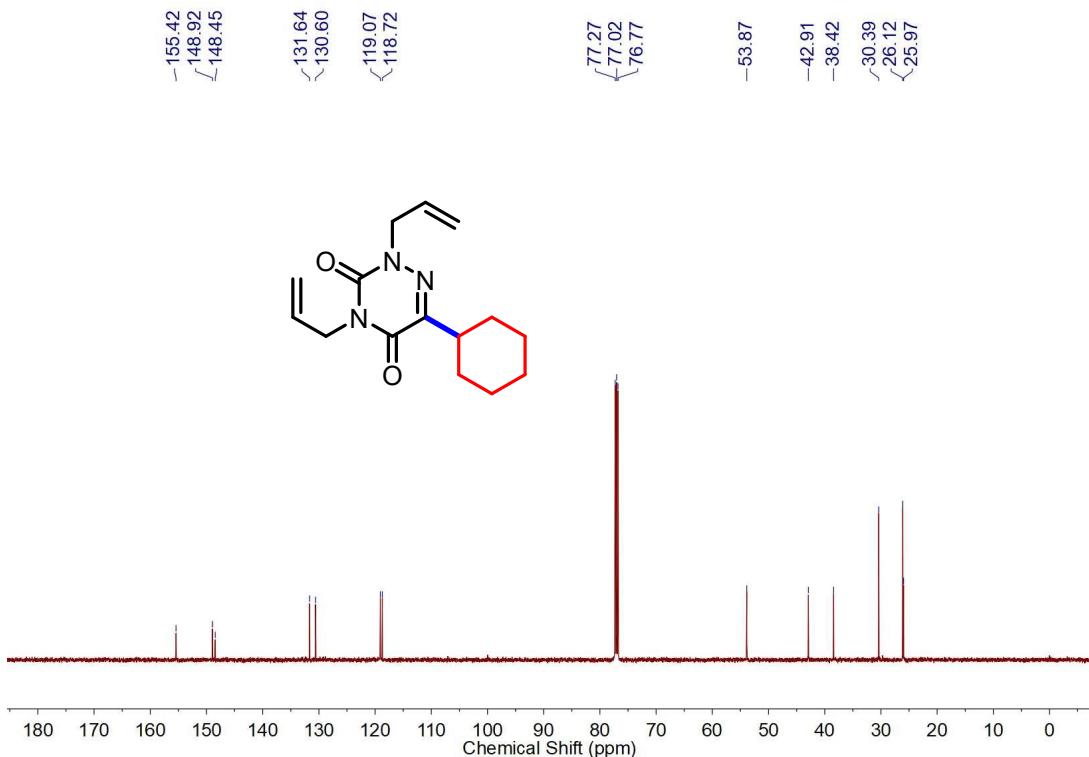
**Figure S104.** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **52**



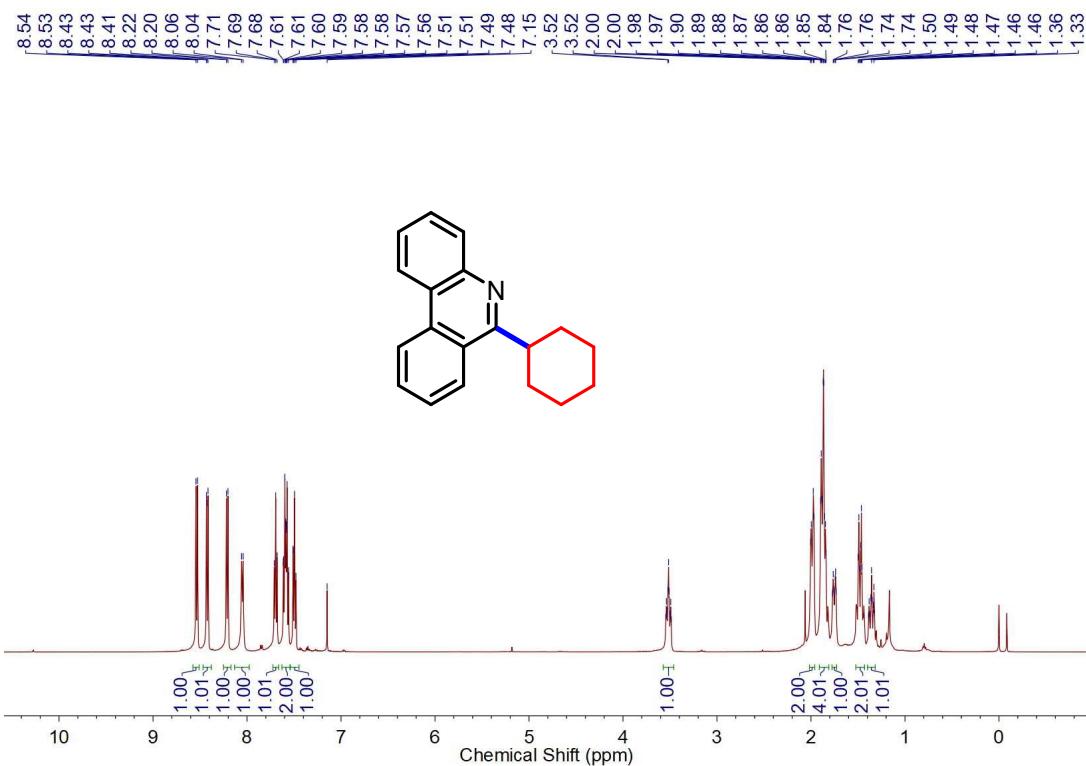
**Figure S105.** <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **52**



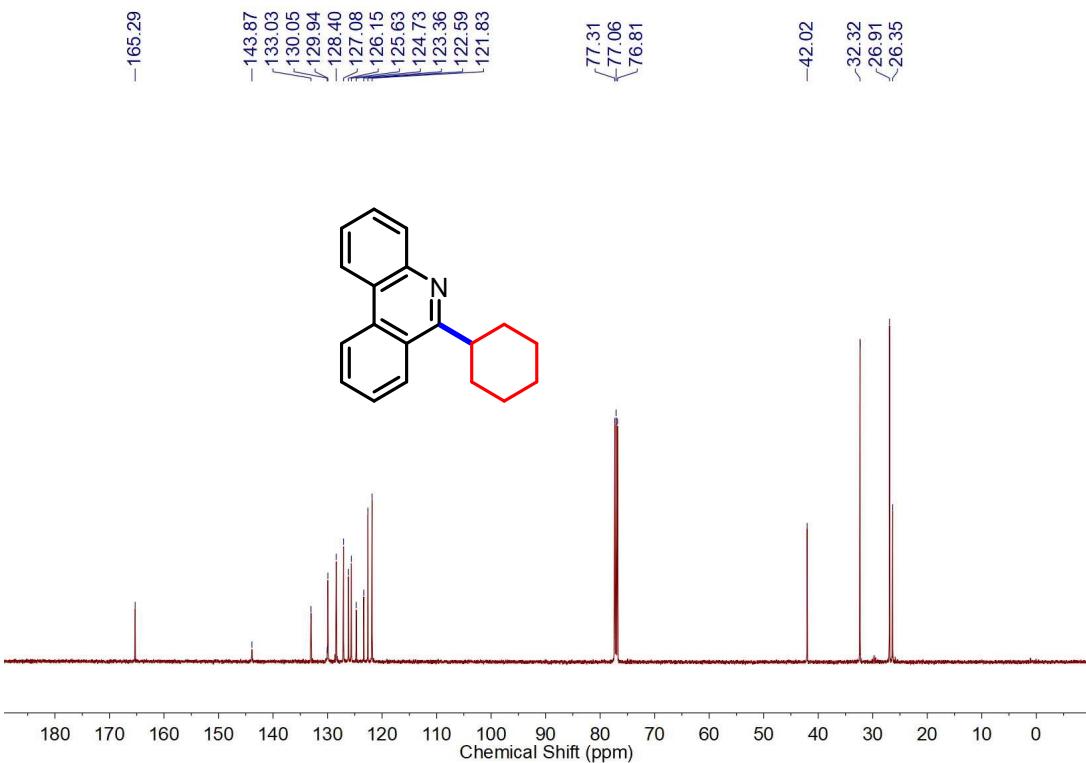
**Figure S106.** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **53**



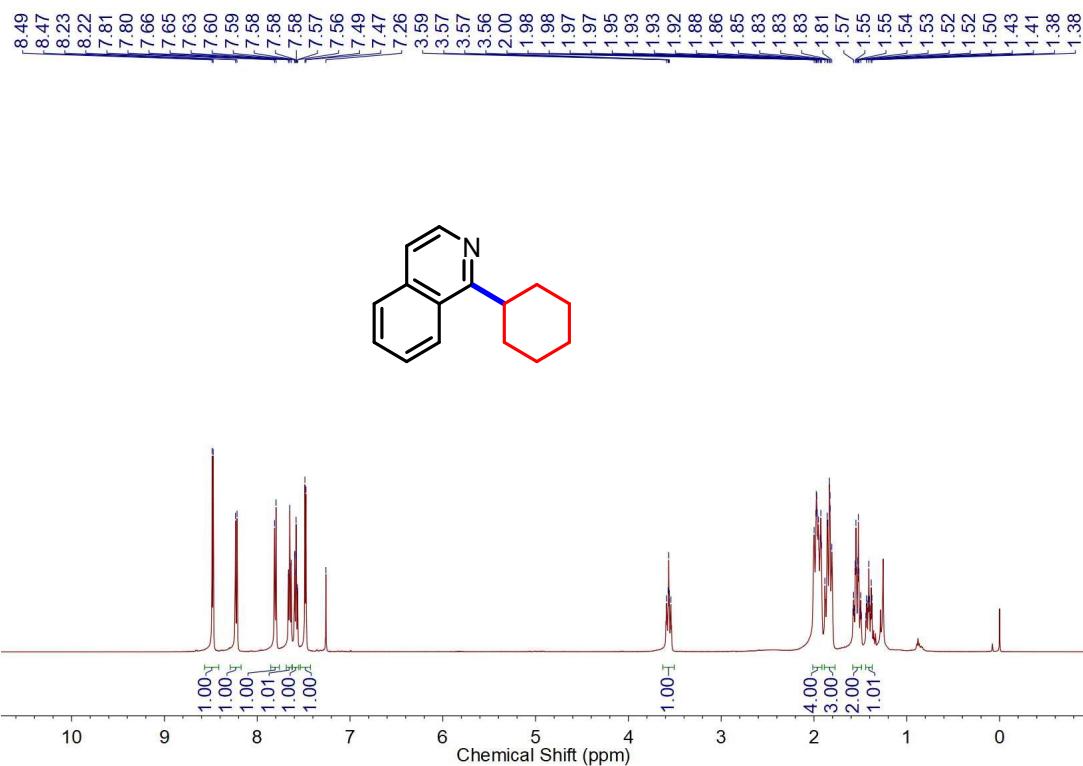
**Figure S107.** <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **53**



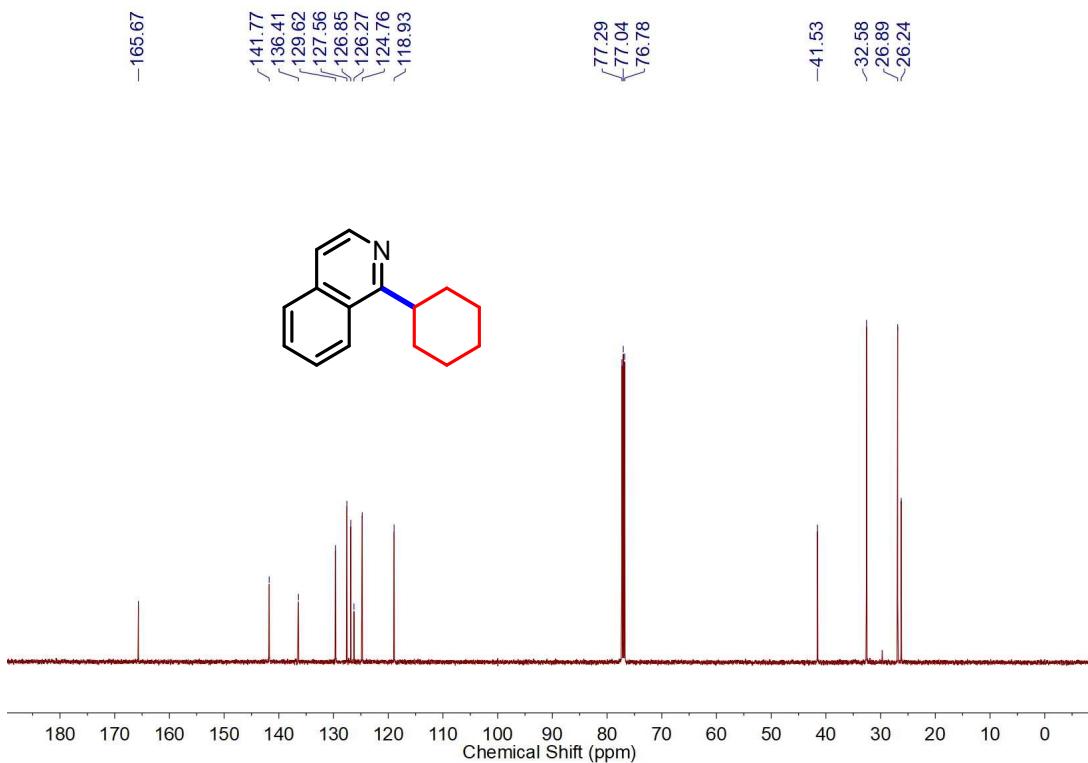
**Figure S108.** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **54**



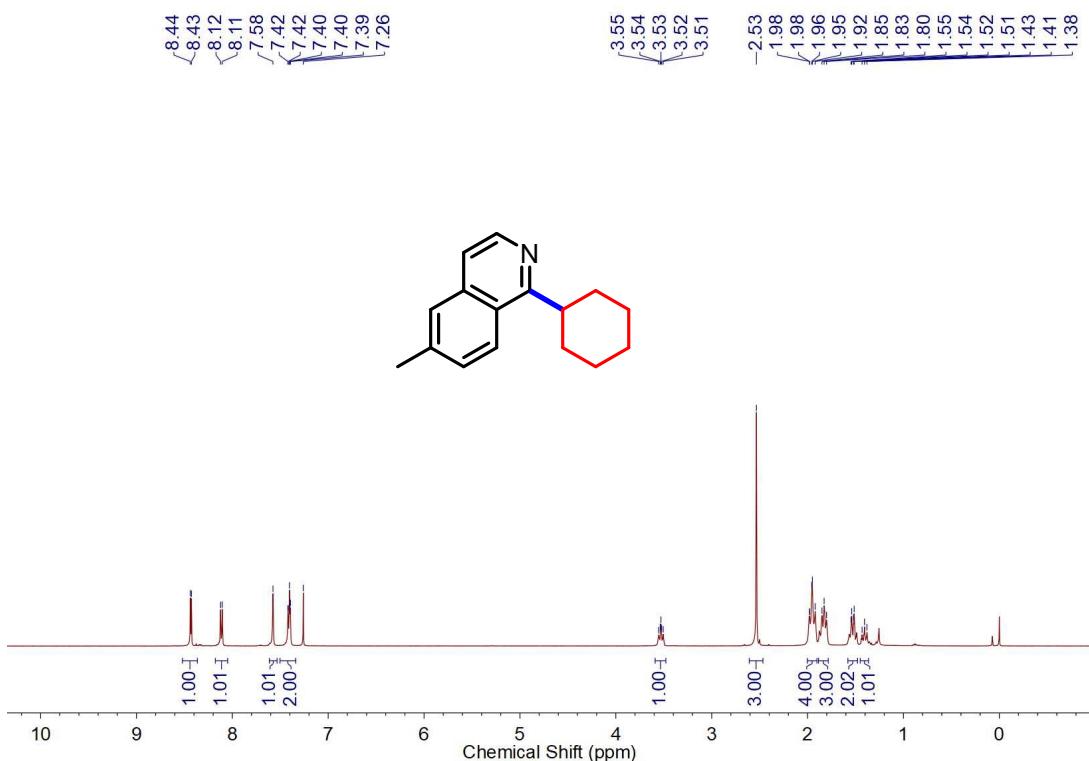
**Figure S109.** <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **54**



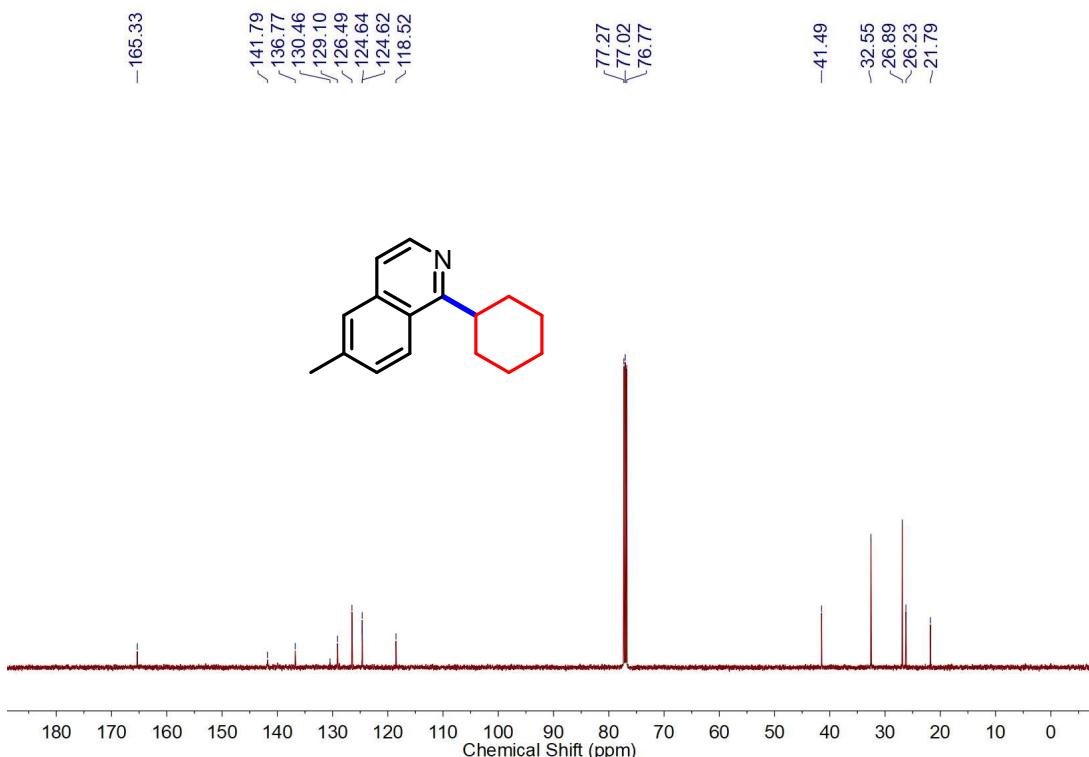
**Figure S110.** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **55**



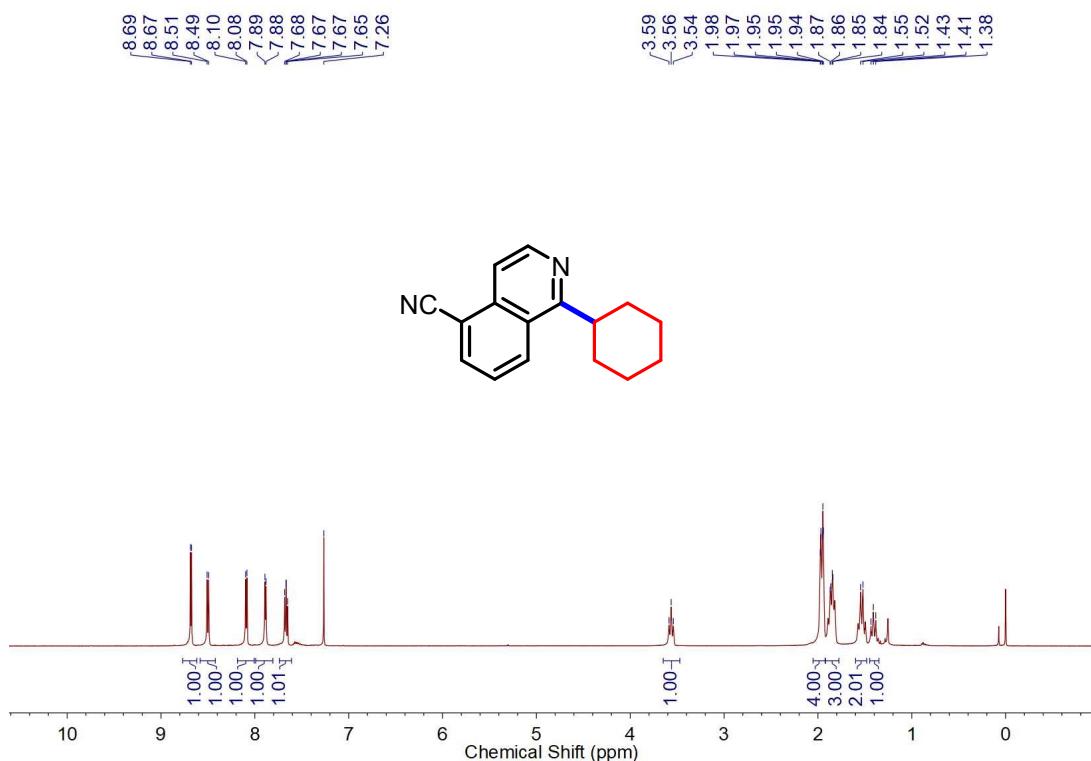
**Figure S111.** <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **55**



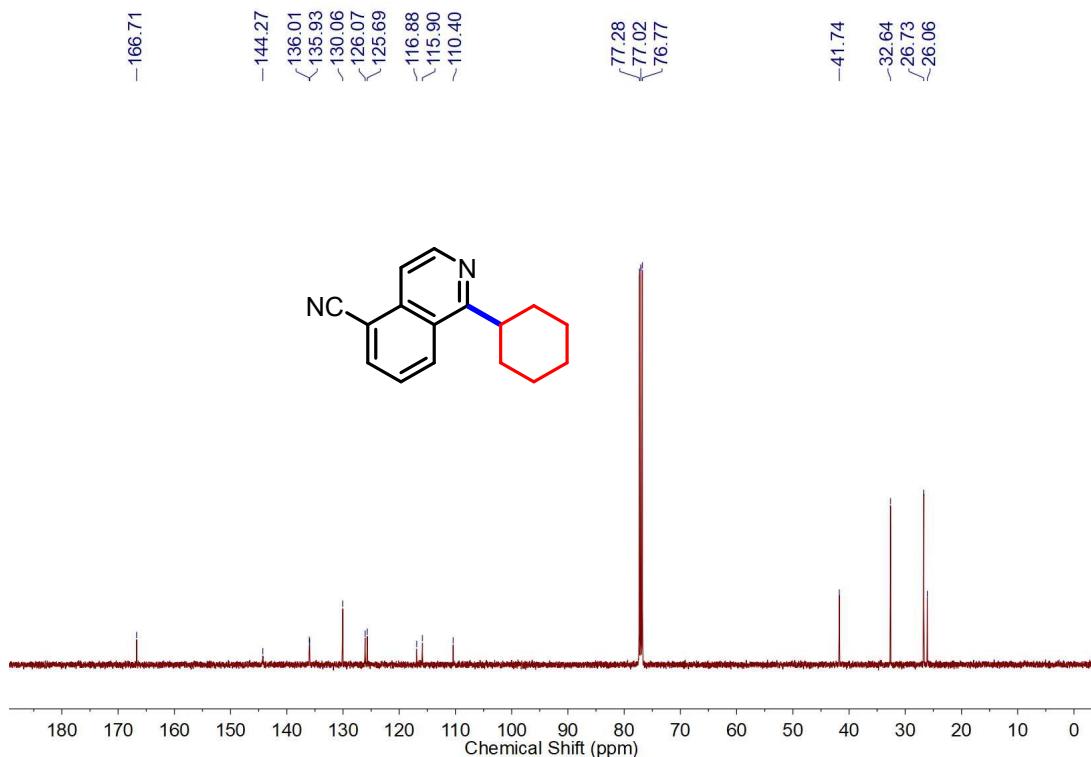
**Figure S112.** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **56**



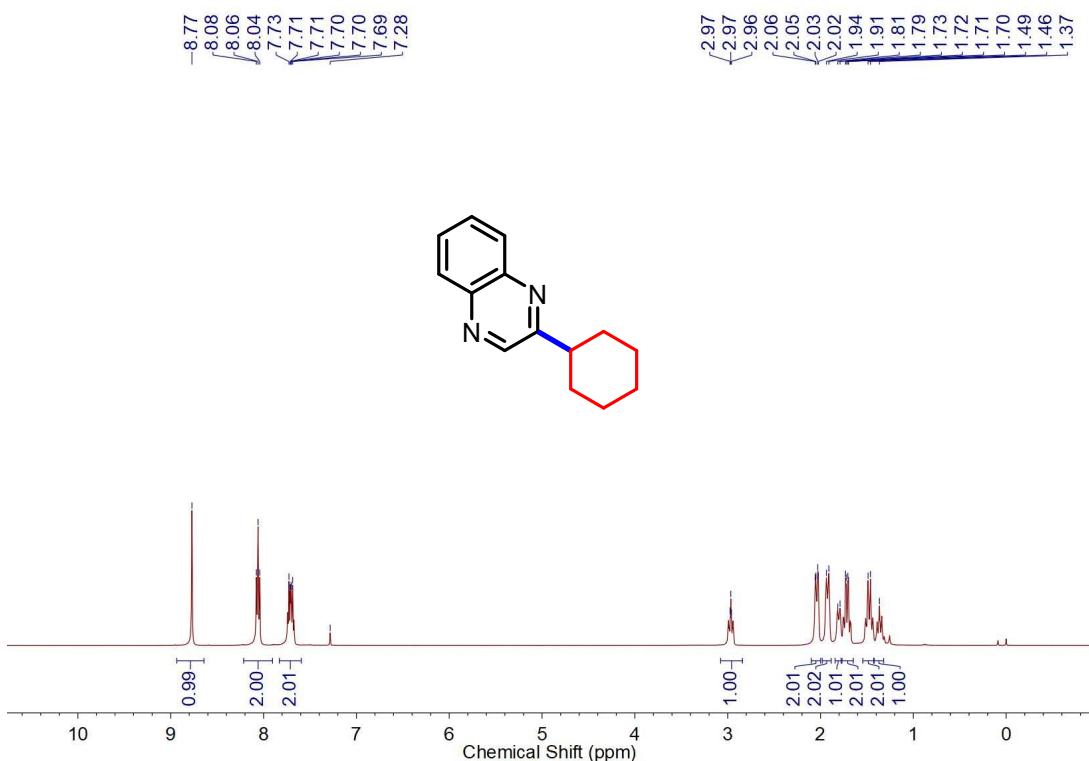
**Figure S113.** <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **56**



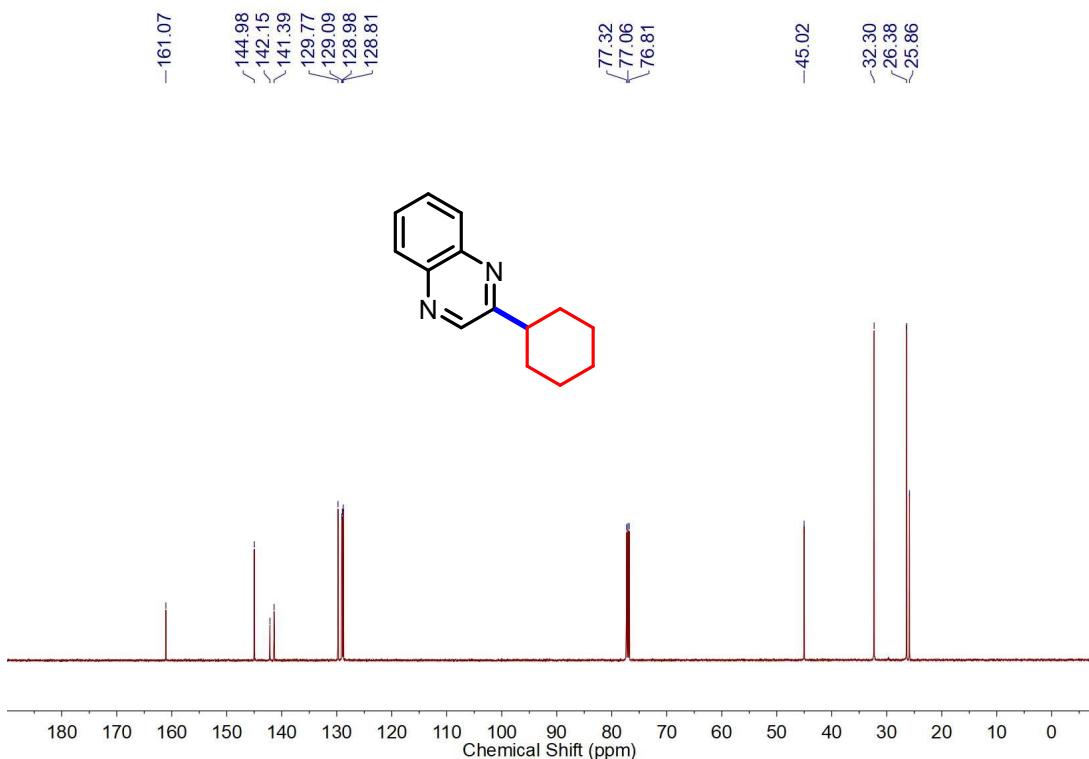
**Figure S114.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **57**



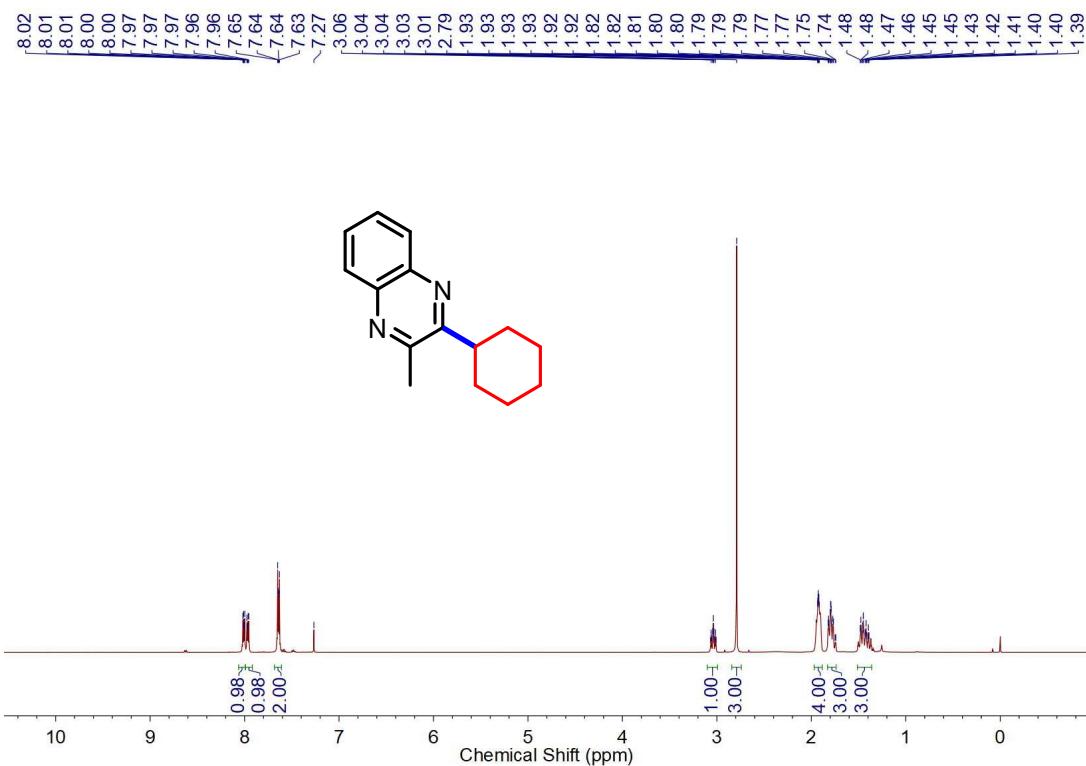
**Figure S115.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **57**



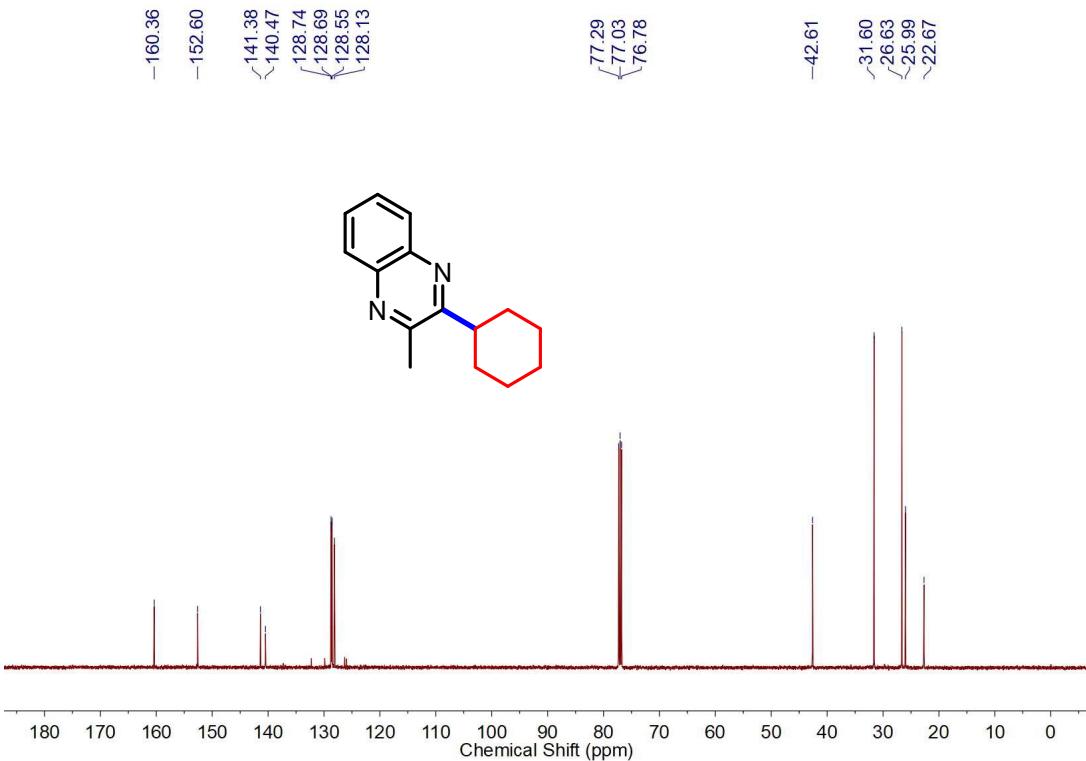
**Figure S116.** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **58**



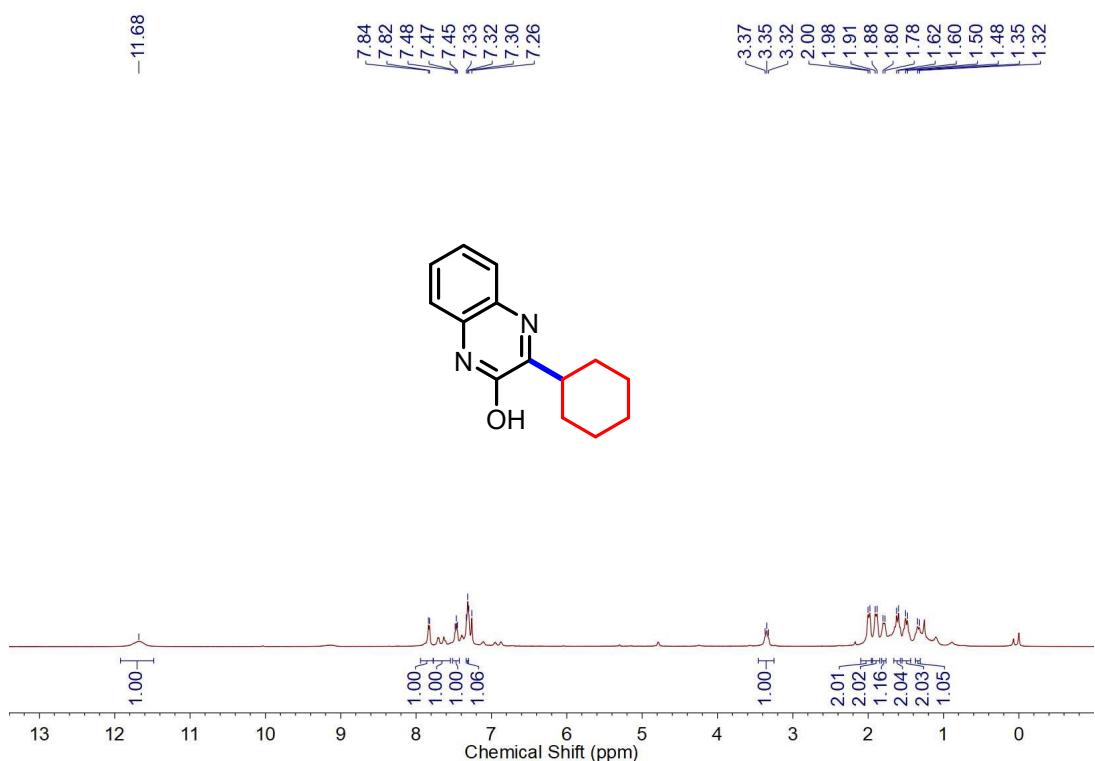
**Figure S117.** <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **58**



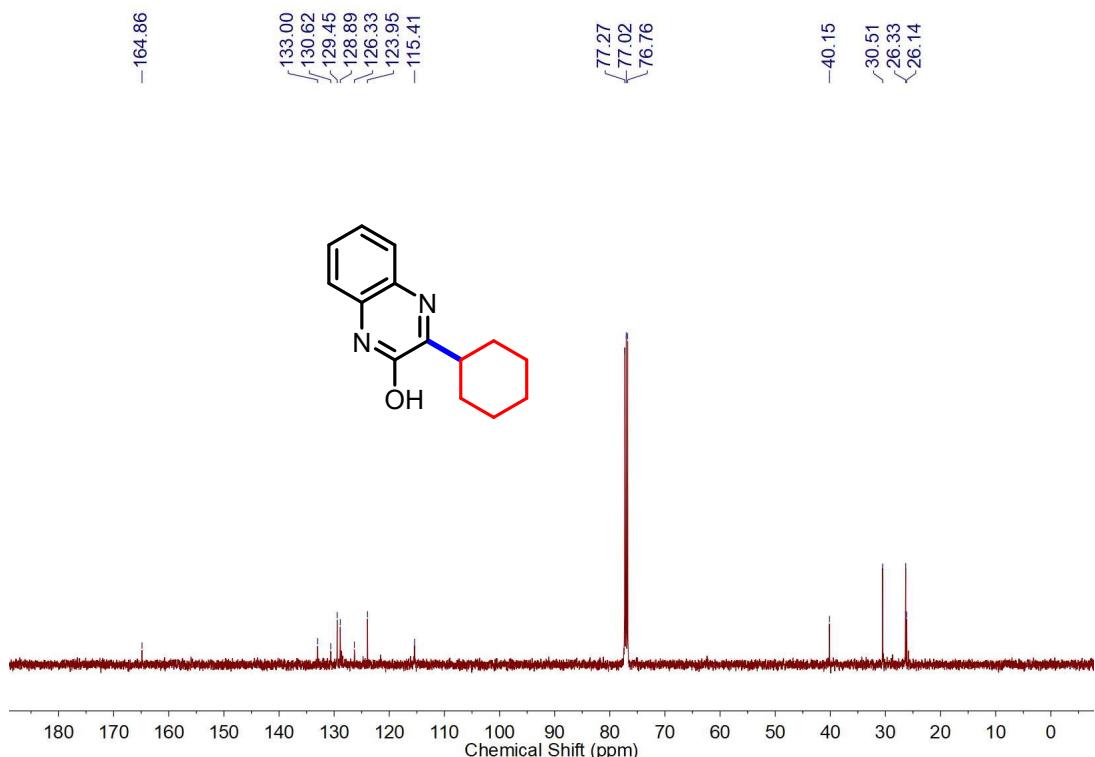
**Figure S118.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **59**



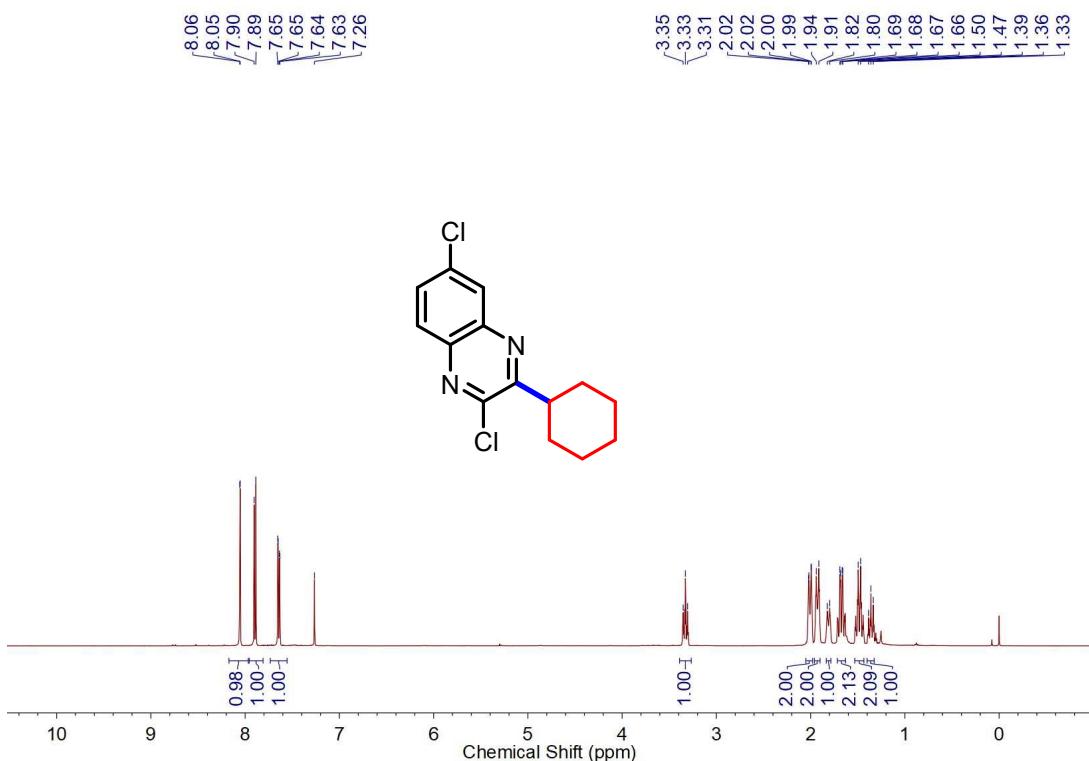
**Figure S119.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **59**



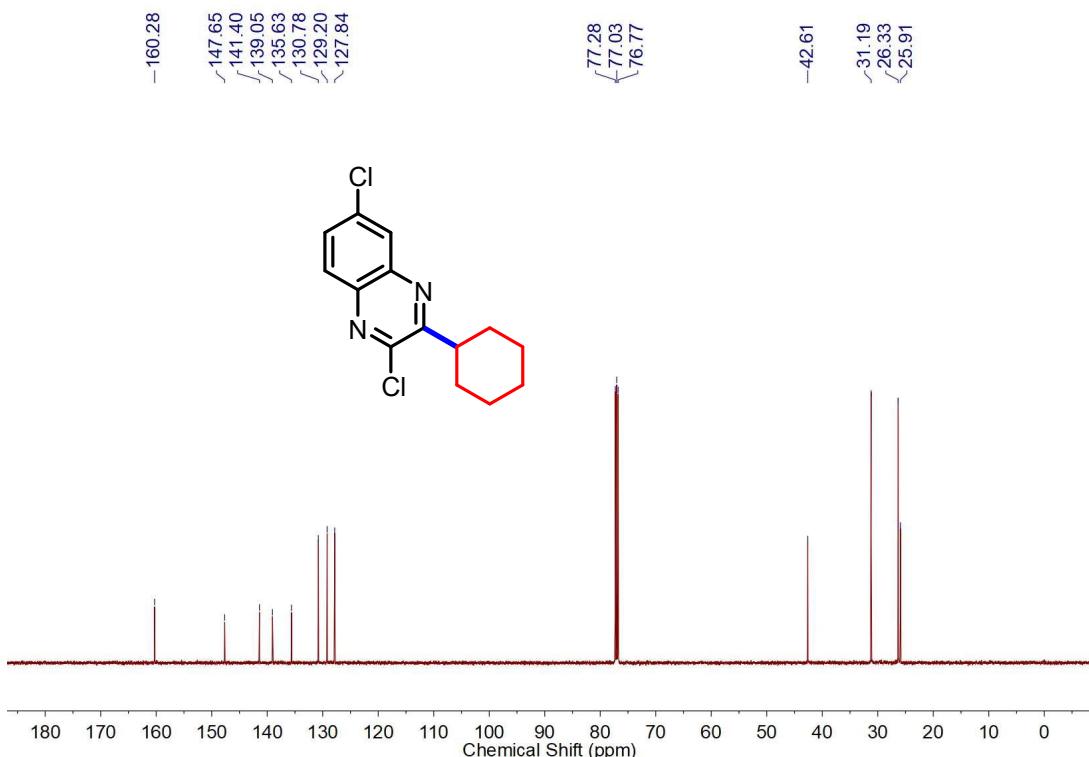
**Figure S120.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **60**



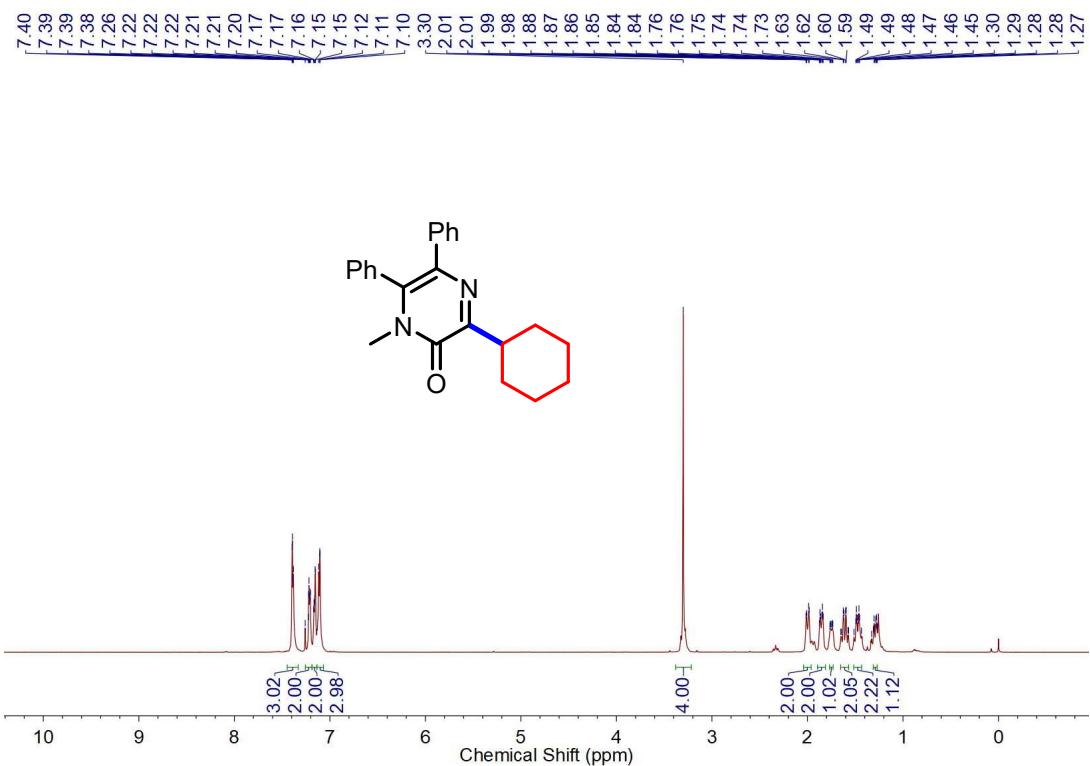
**Figure S121.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **60**



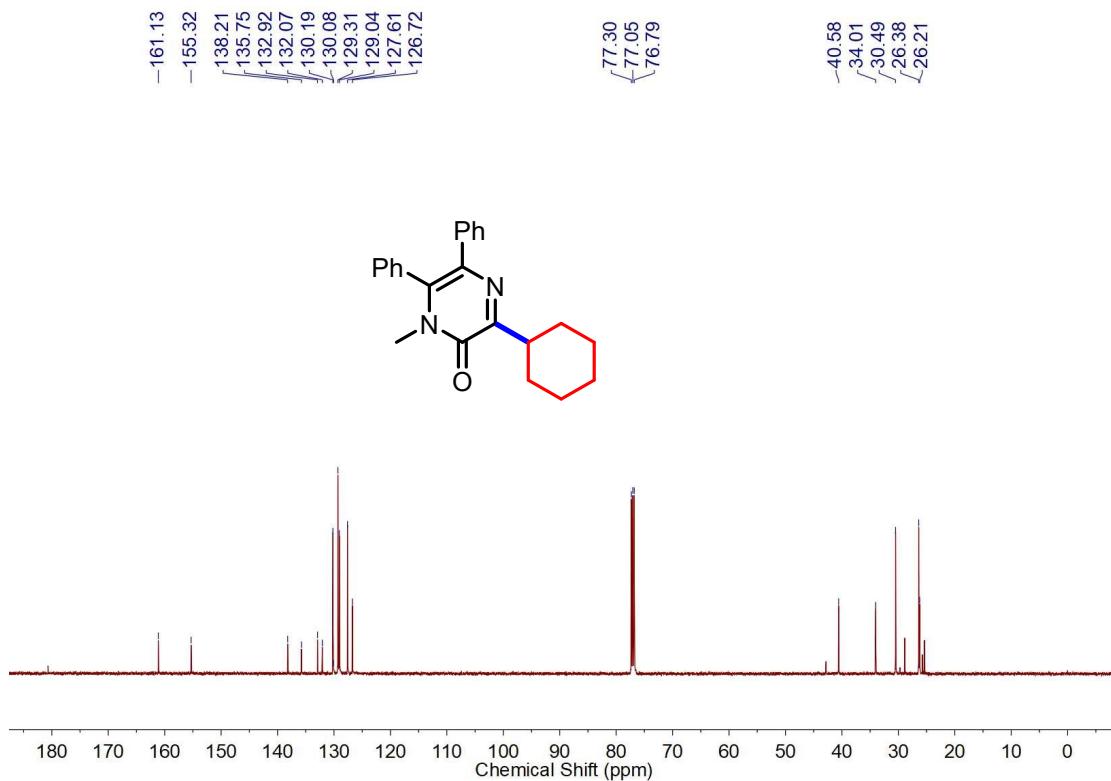
**Figure S122.** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **61**



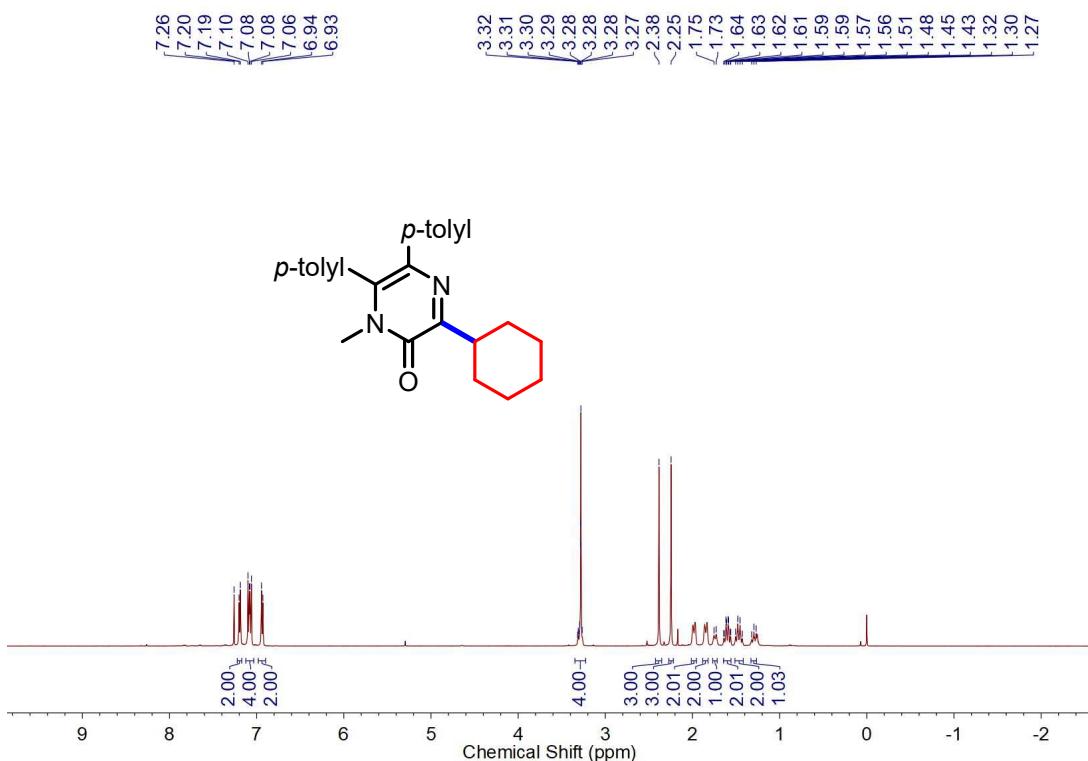
**Figure S123.** <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **61**



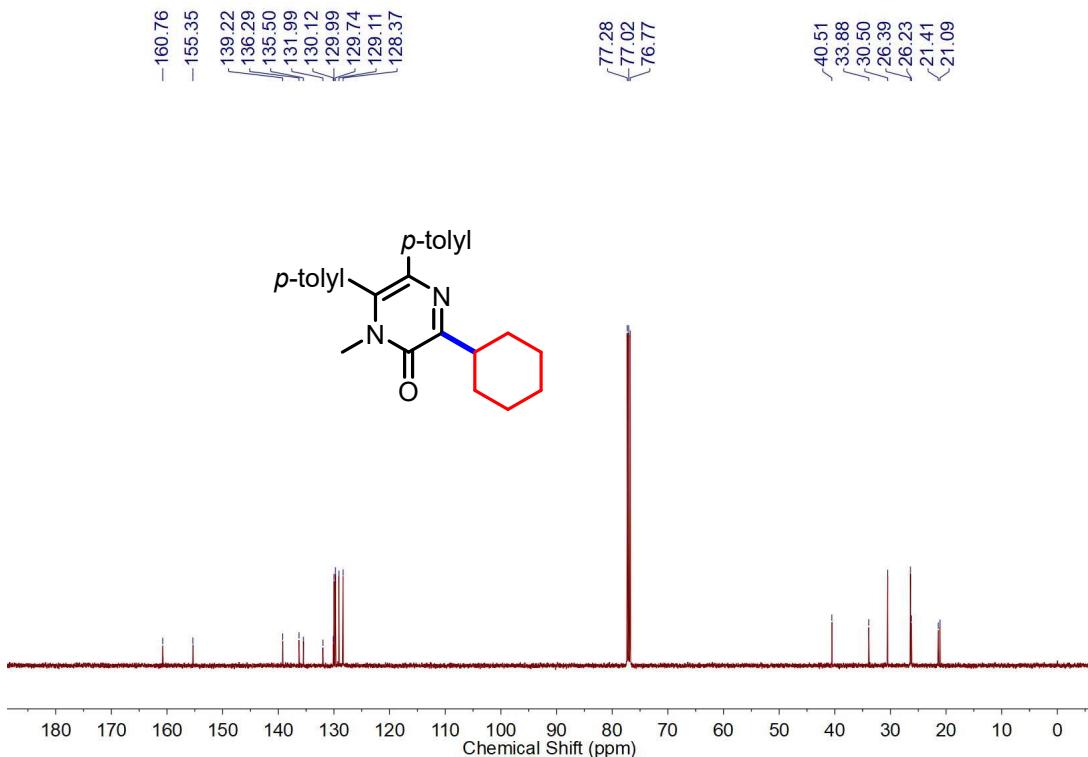
**Figure S124.** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **62**



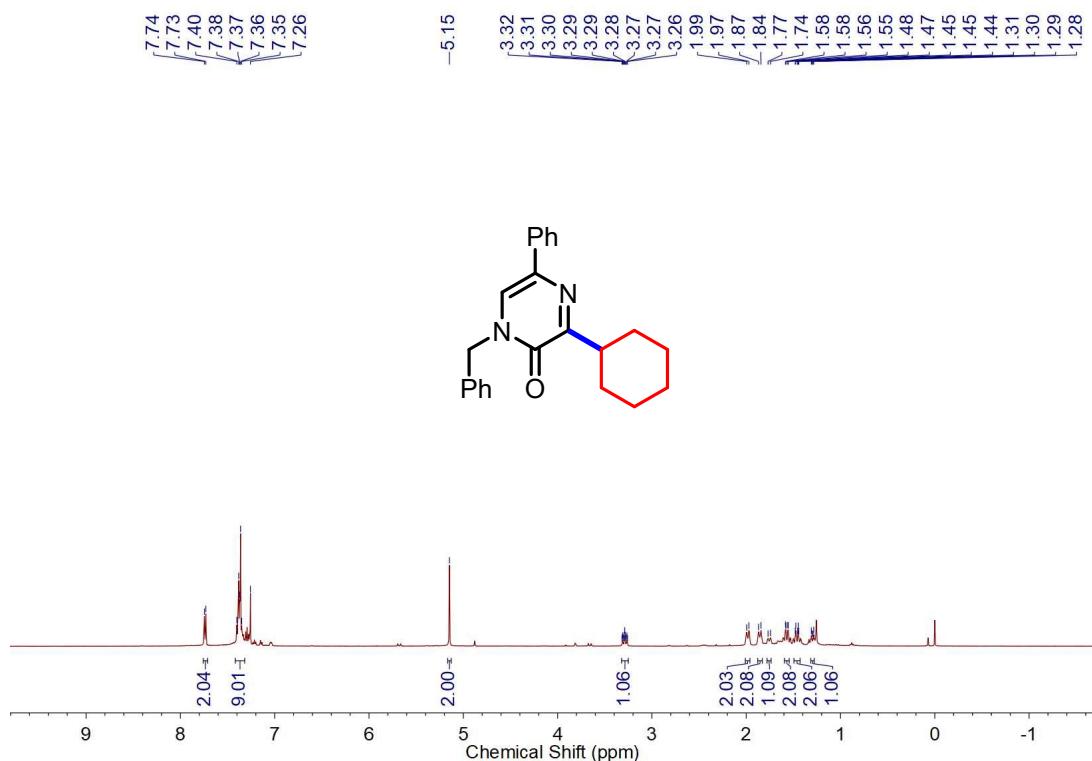
**Figure S125.** <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **62**



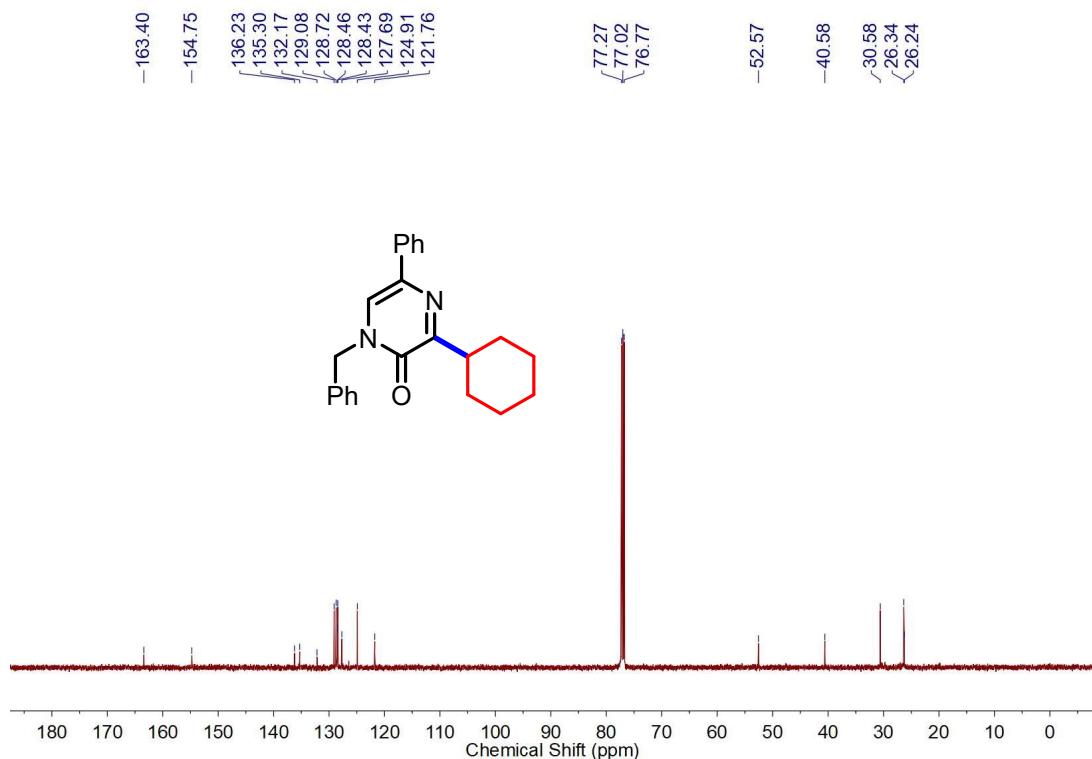
**Figure S126.** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **63**



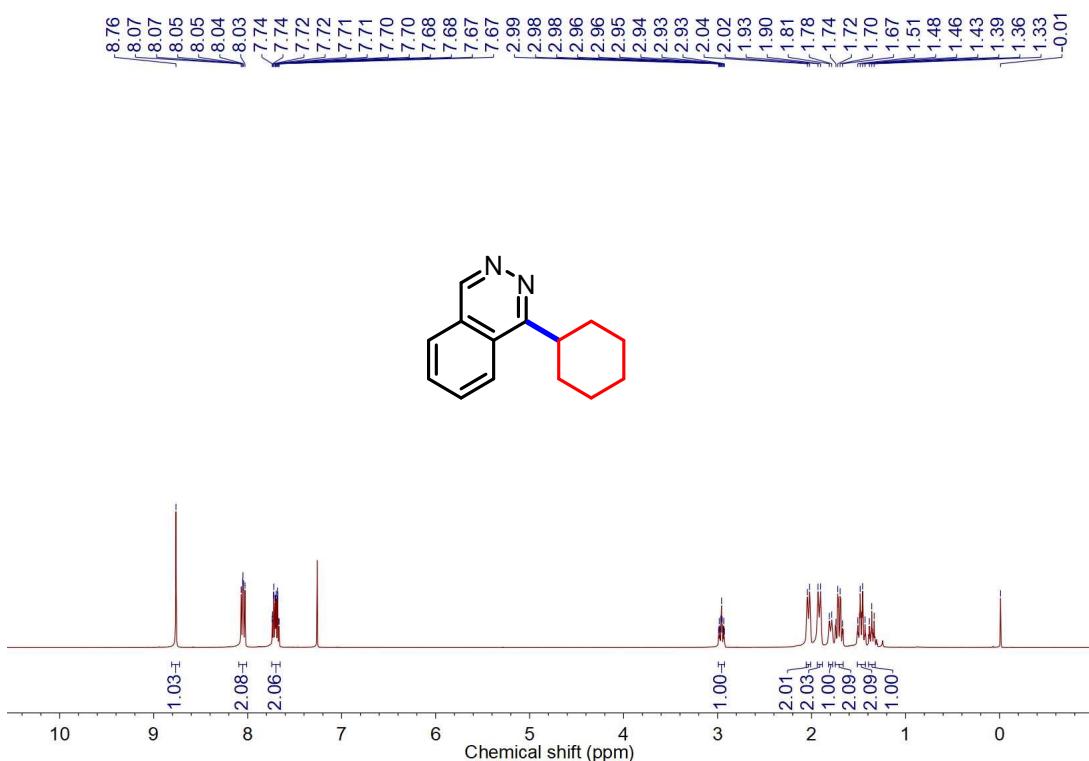
**Figure S127.** <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **63**



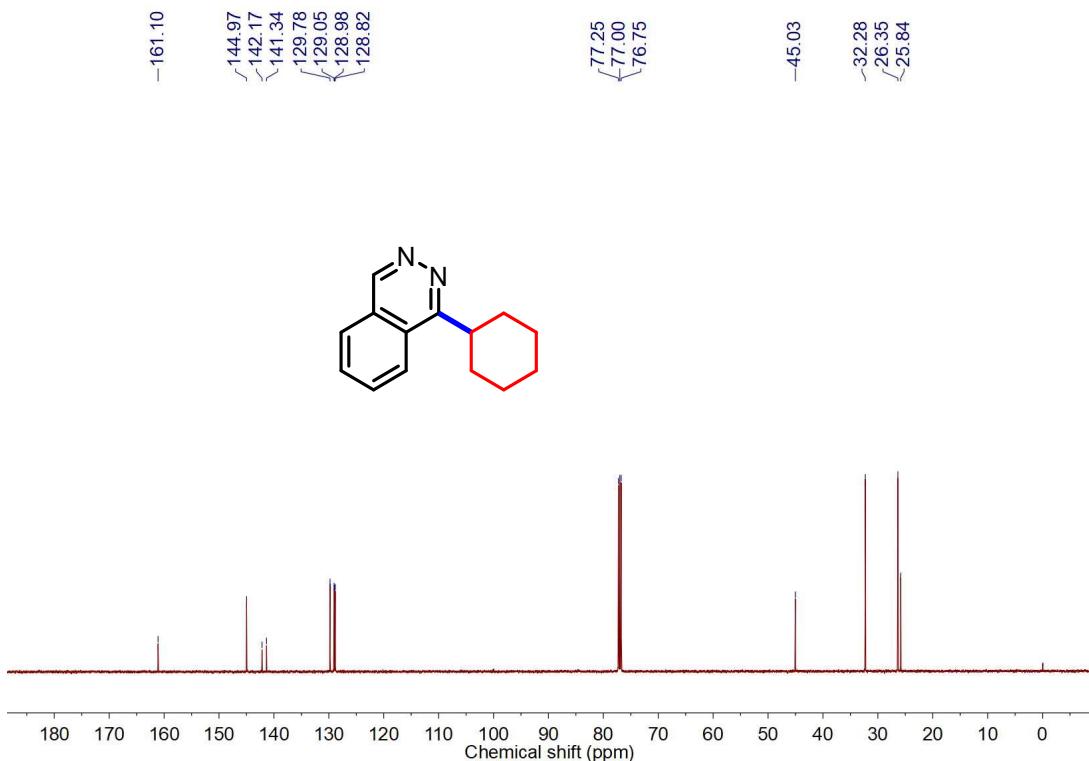
**Figure S128.** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **64**



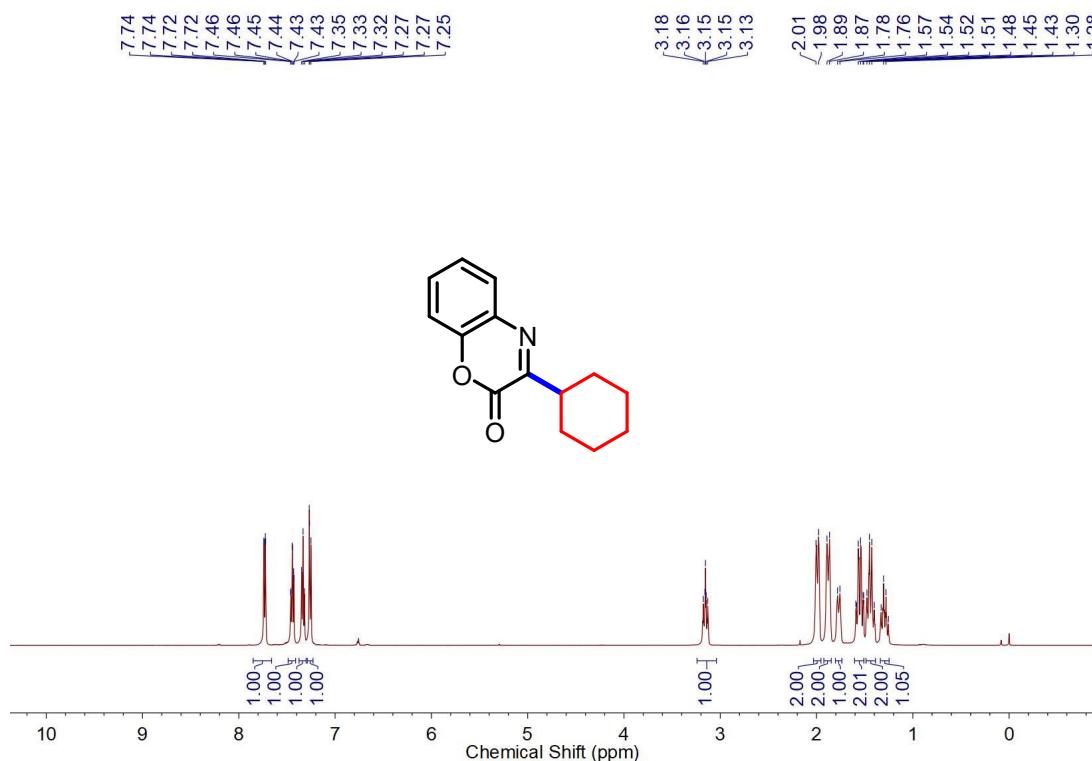
**Figure S129.** <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **64**



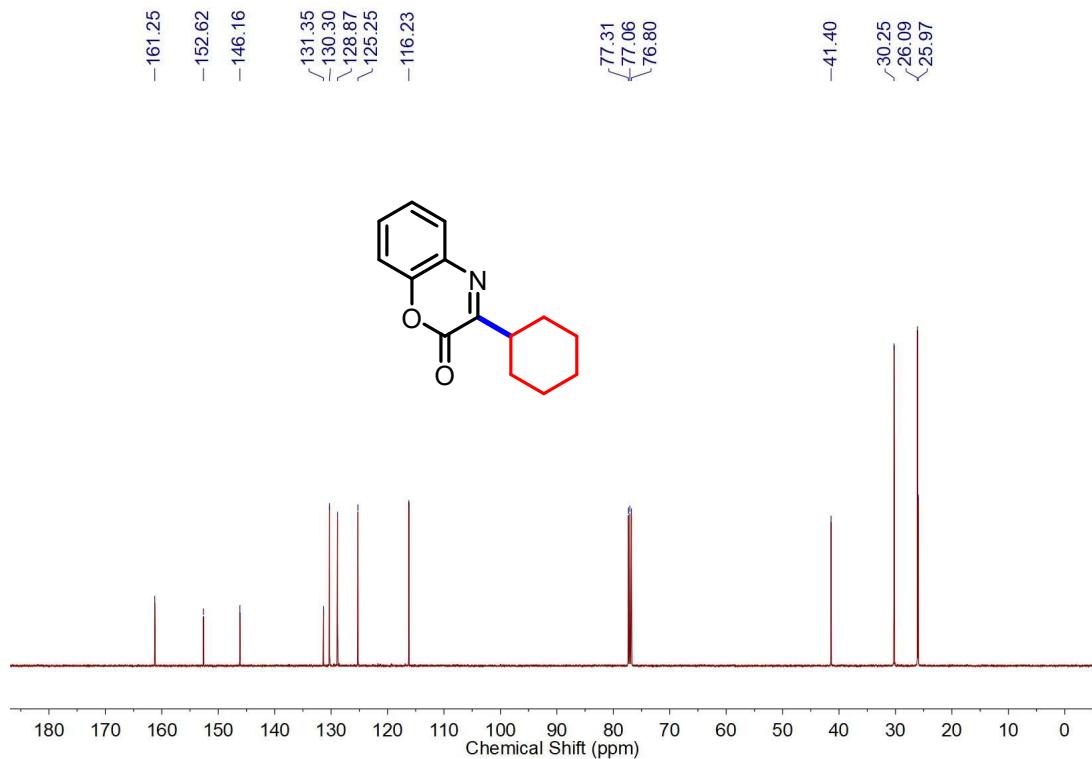
**Figure S130.** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **65**



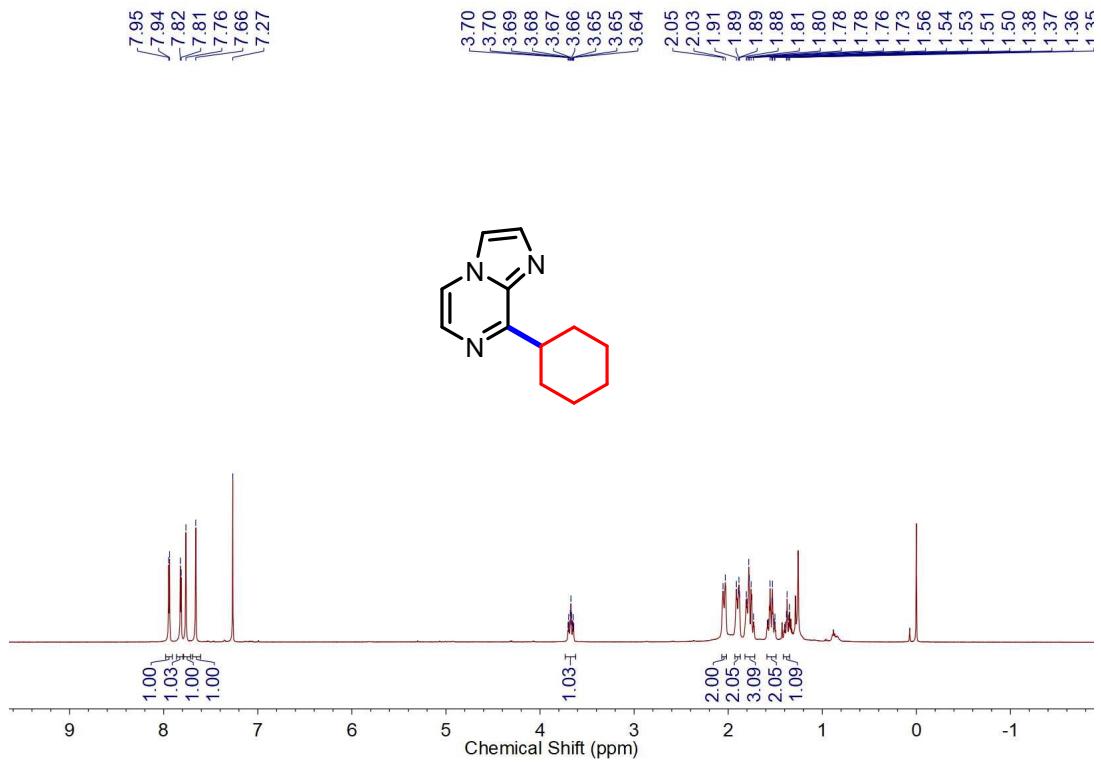
**Figure S131.** <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **65**



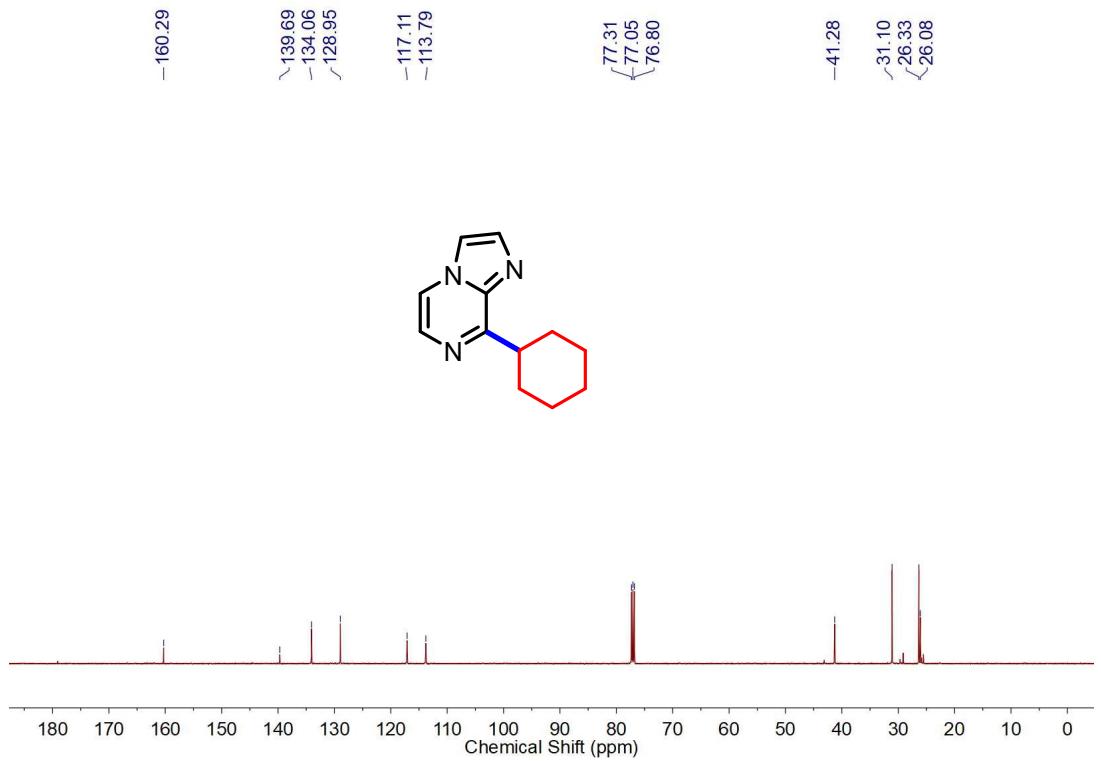
**Figure S132.** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **66**



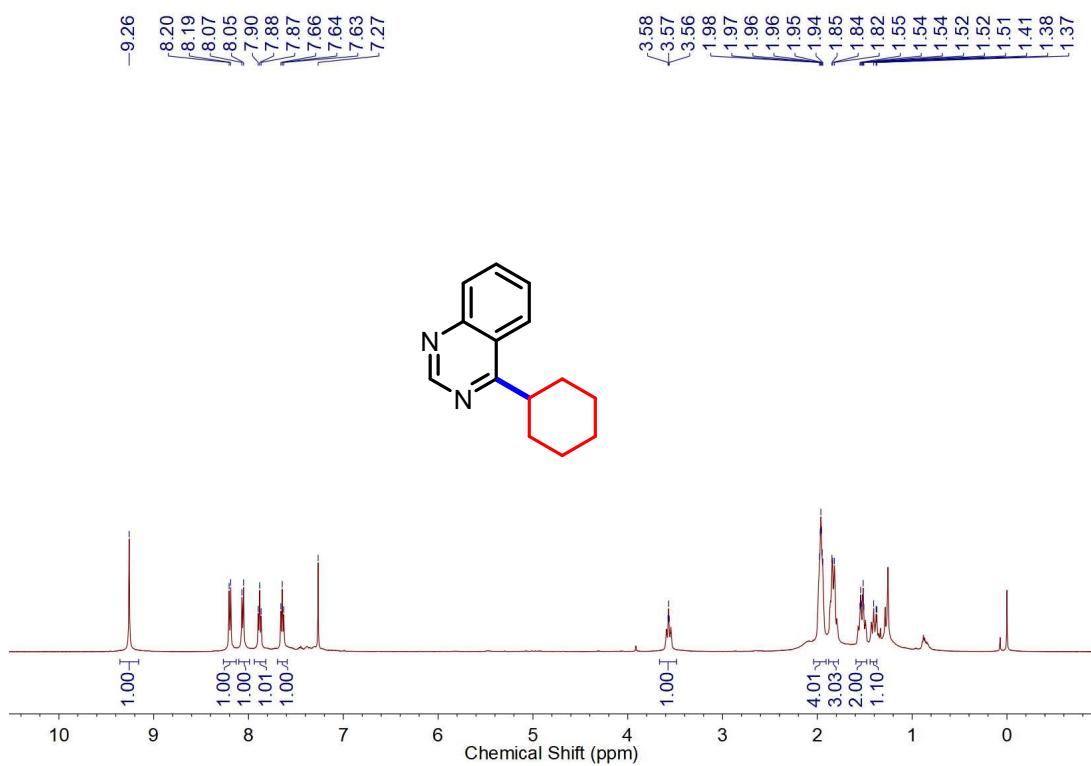
**Figure S133.** <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **66**



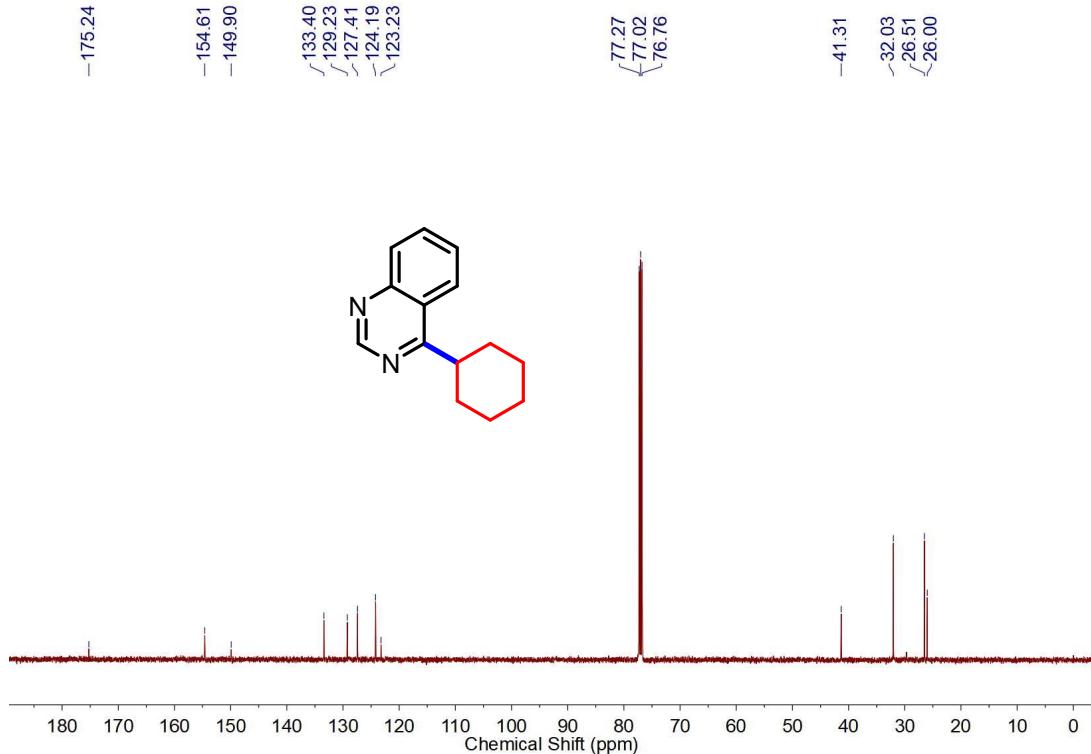
**Figure S134.** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **67**



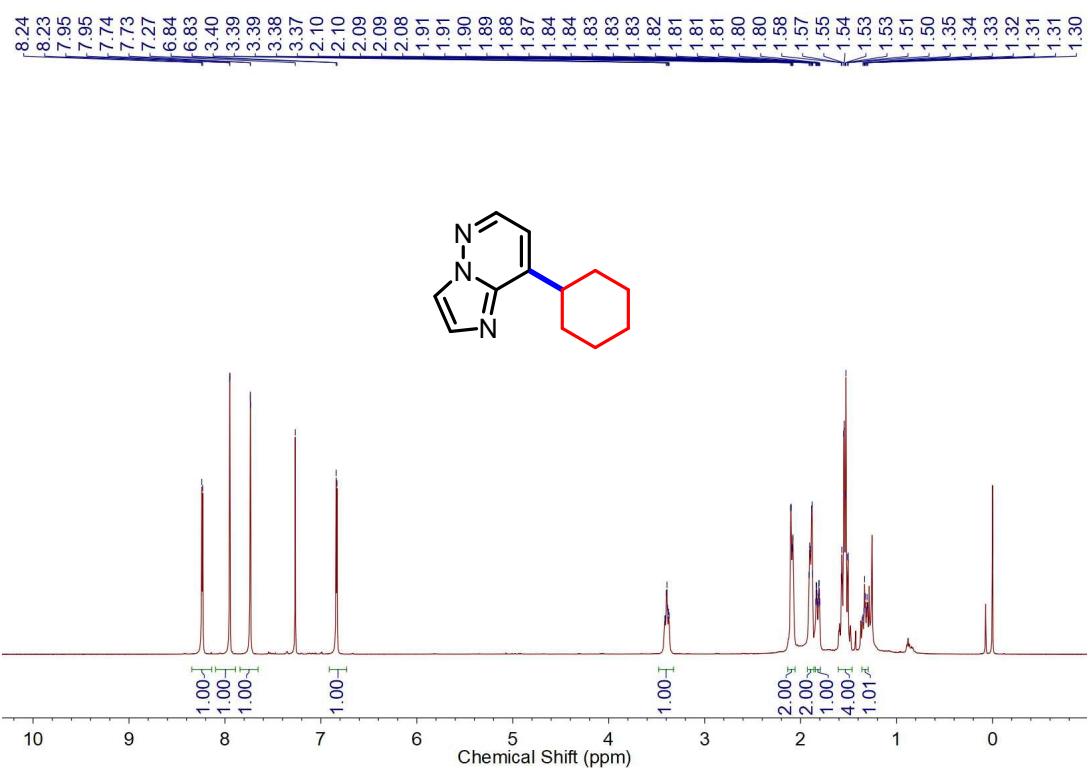
**Figure S135.** <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **67**



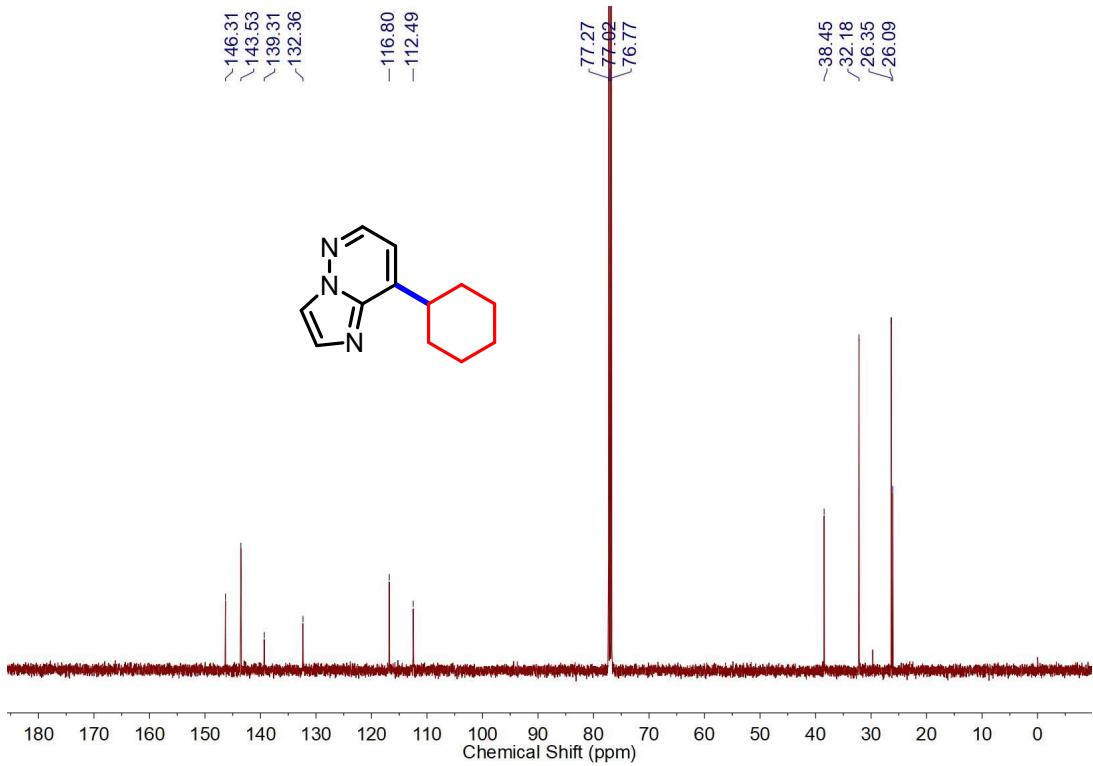
**Figure S136.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **68**



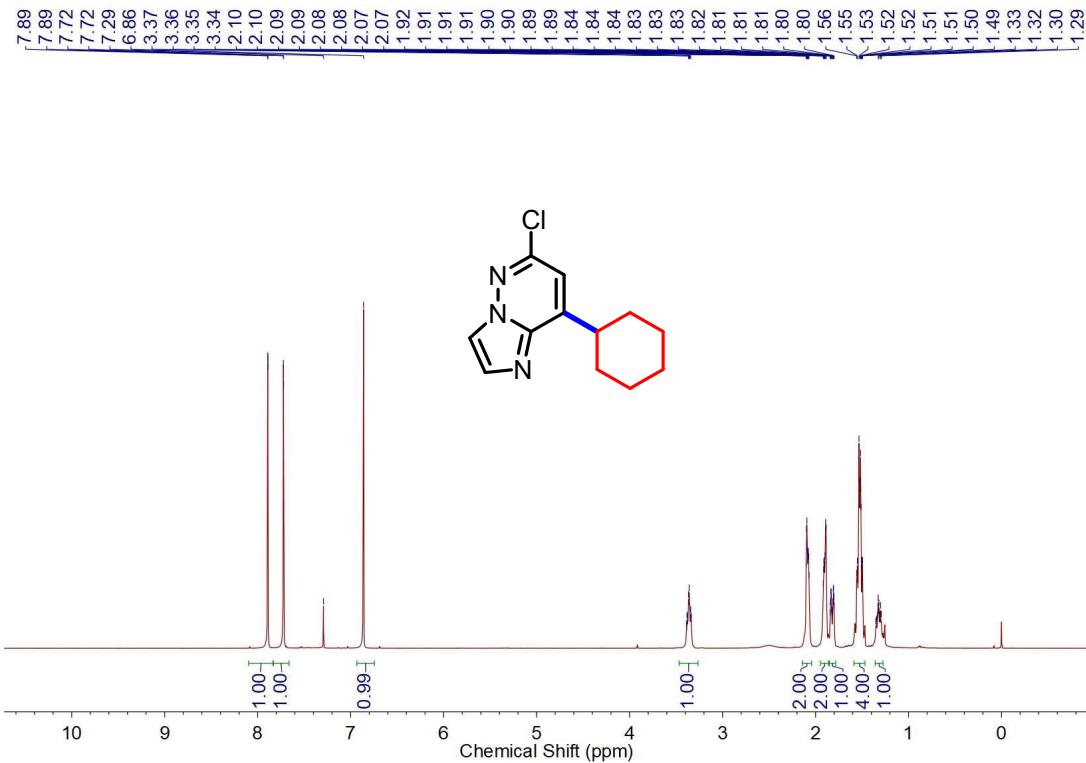
**Figure S137.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **68**



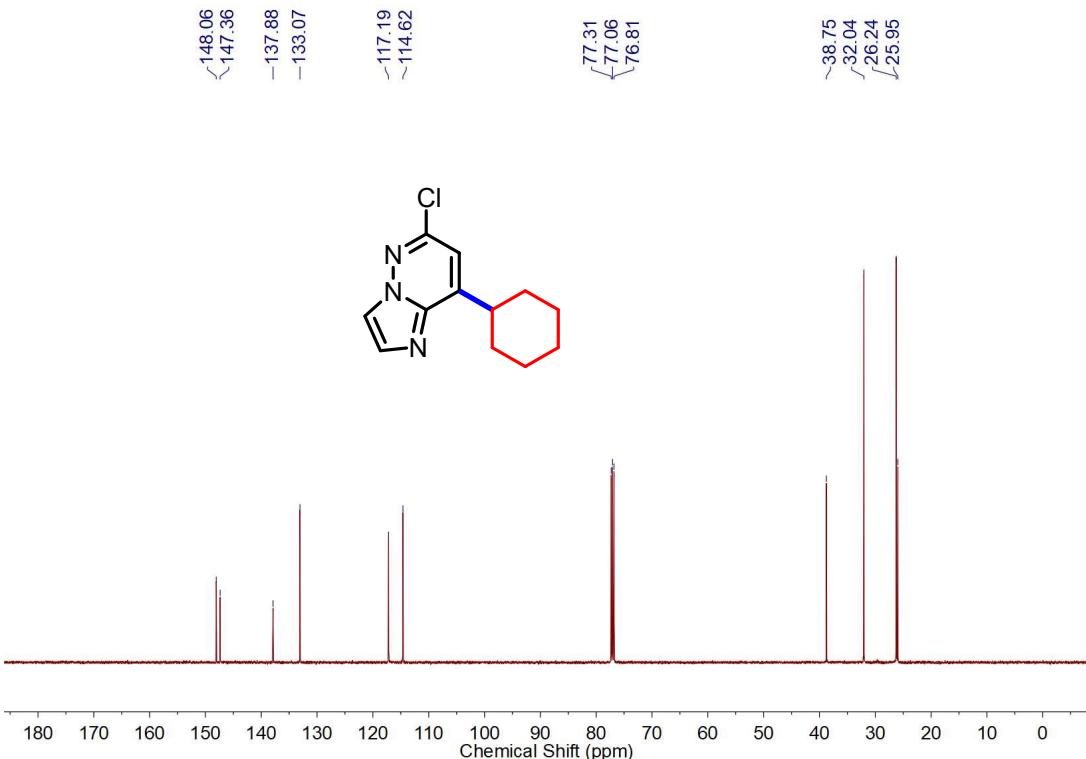
**Figure S138.** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of **69**



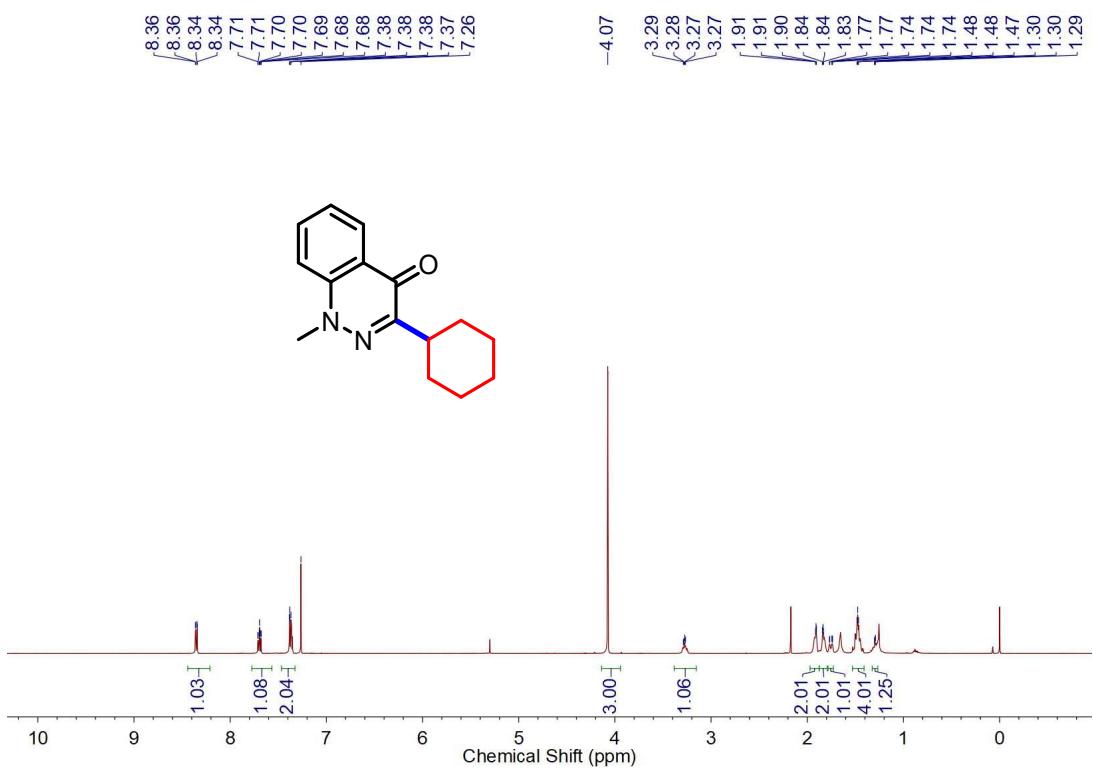
**Figure S139.** <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) spectrum of **69**



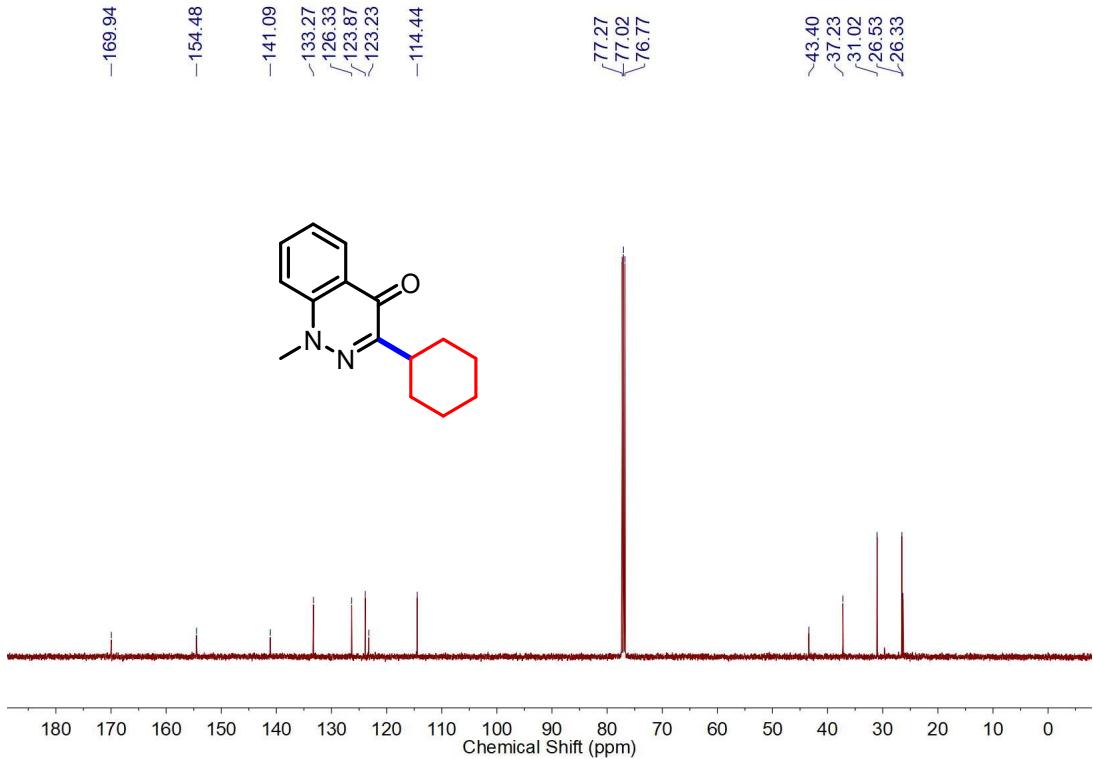
**Figure S140.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **70**



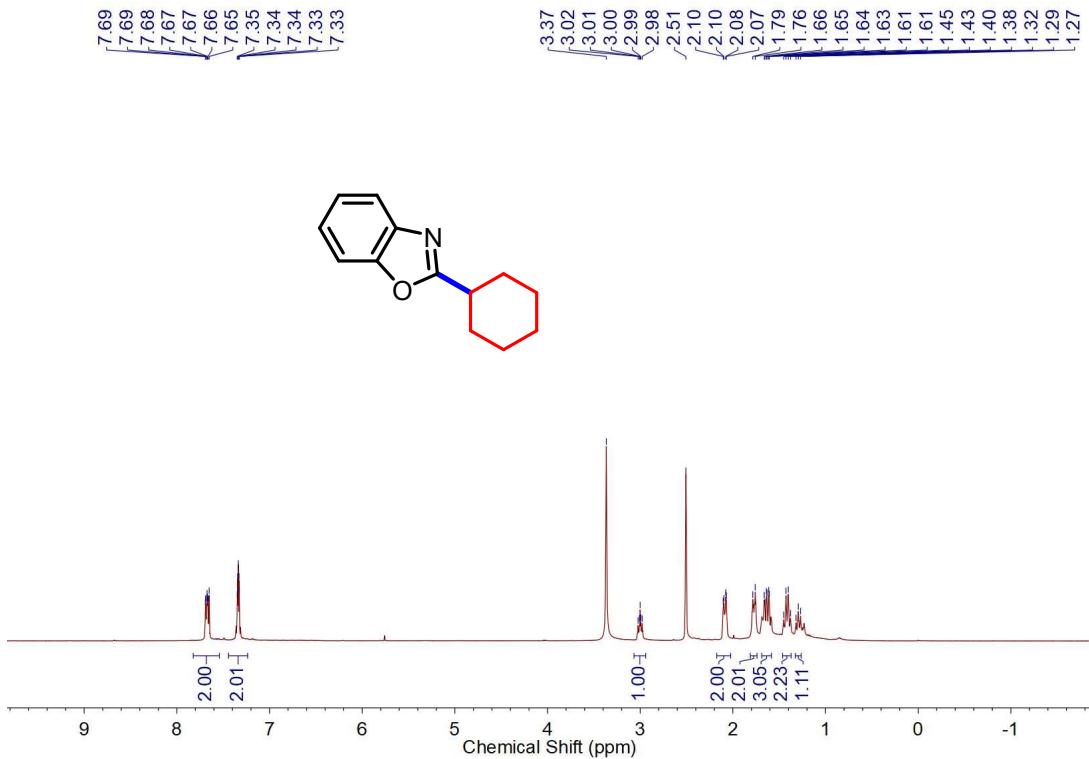
**Figure S141.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **70**



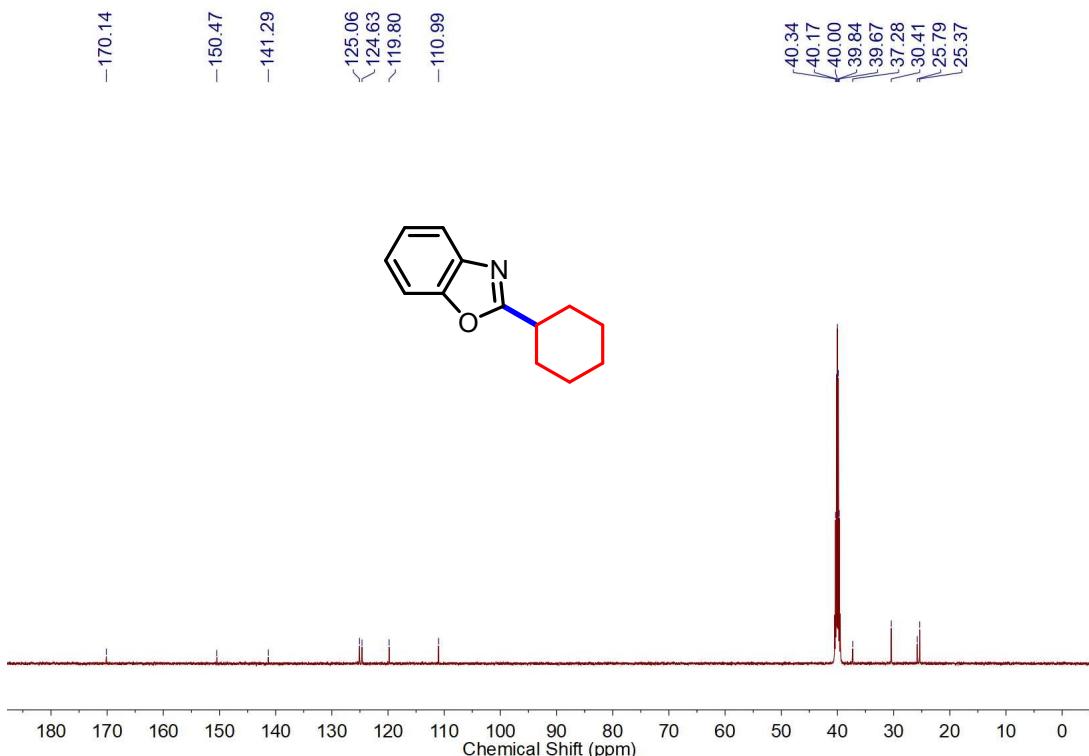
**Figure S142.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **71**



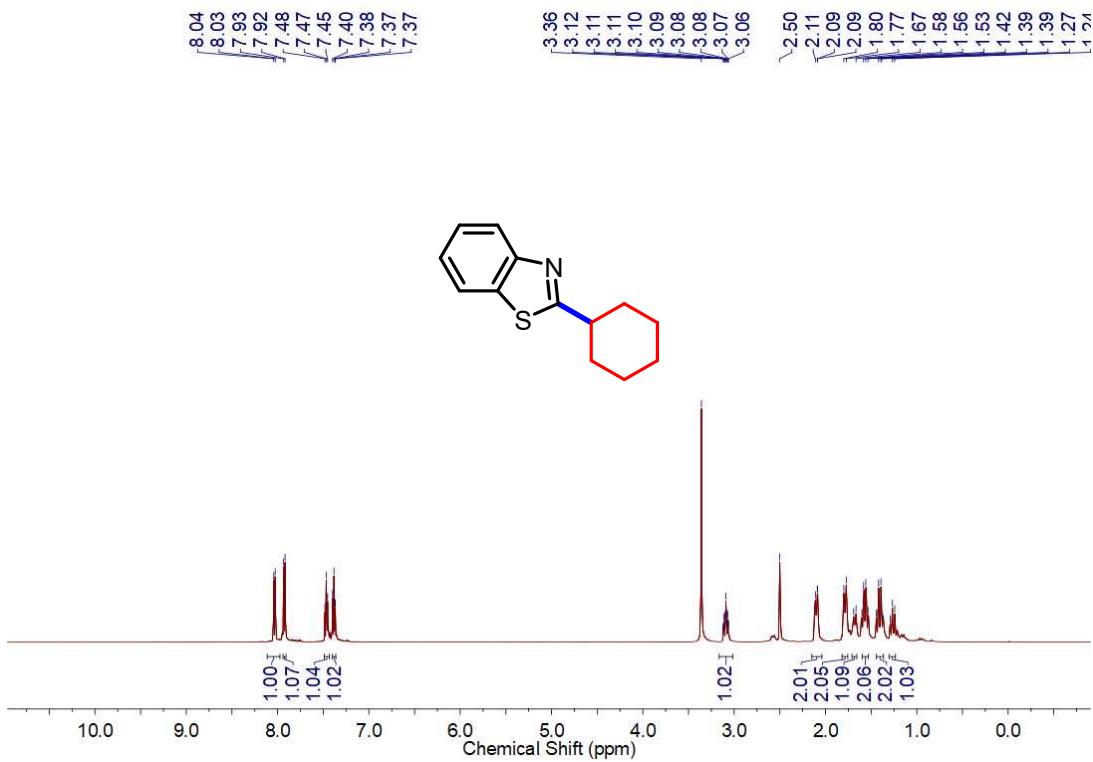
**Figure S143.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **71**



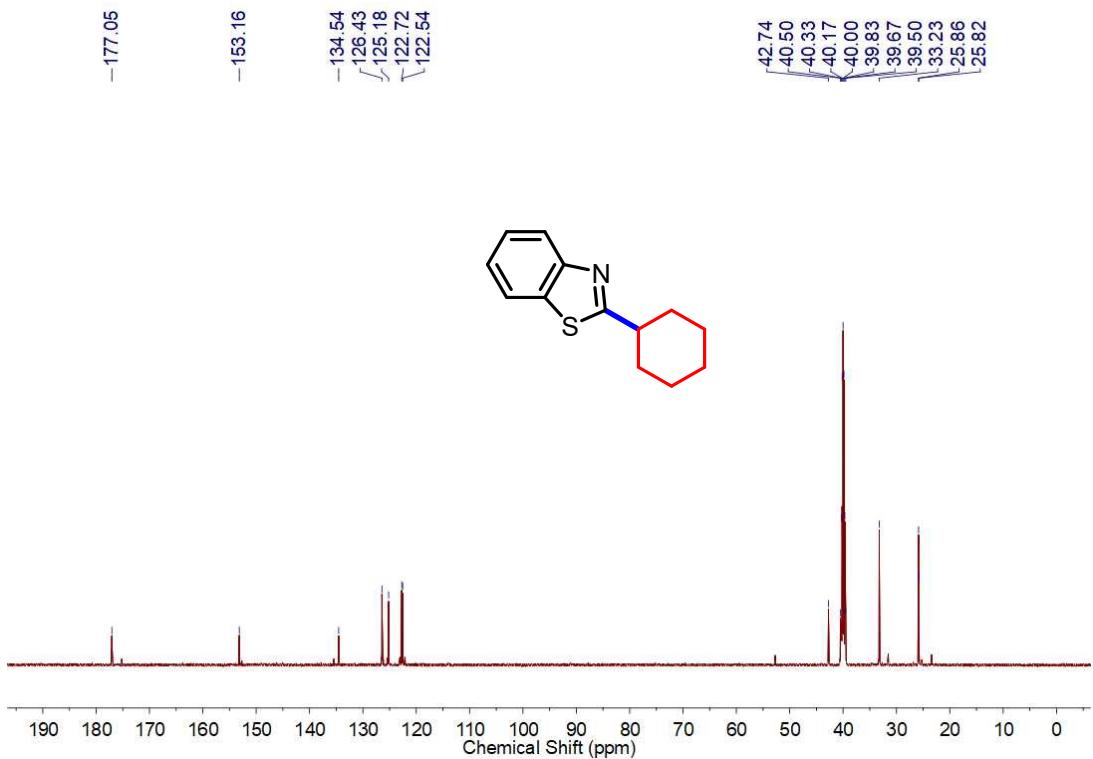
**Figure S144.**  $^1\text{H}$  NMR (500 MHz, DMSO) spectrum of **72**



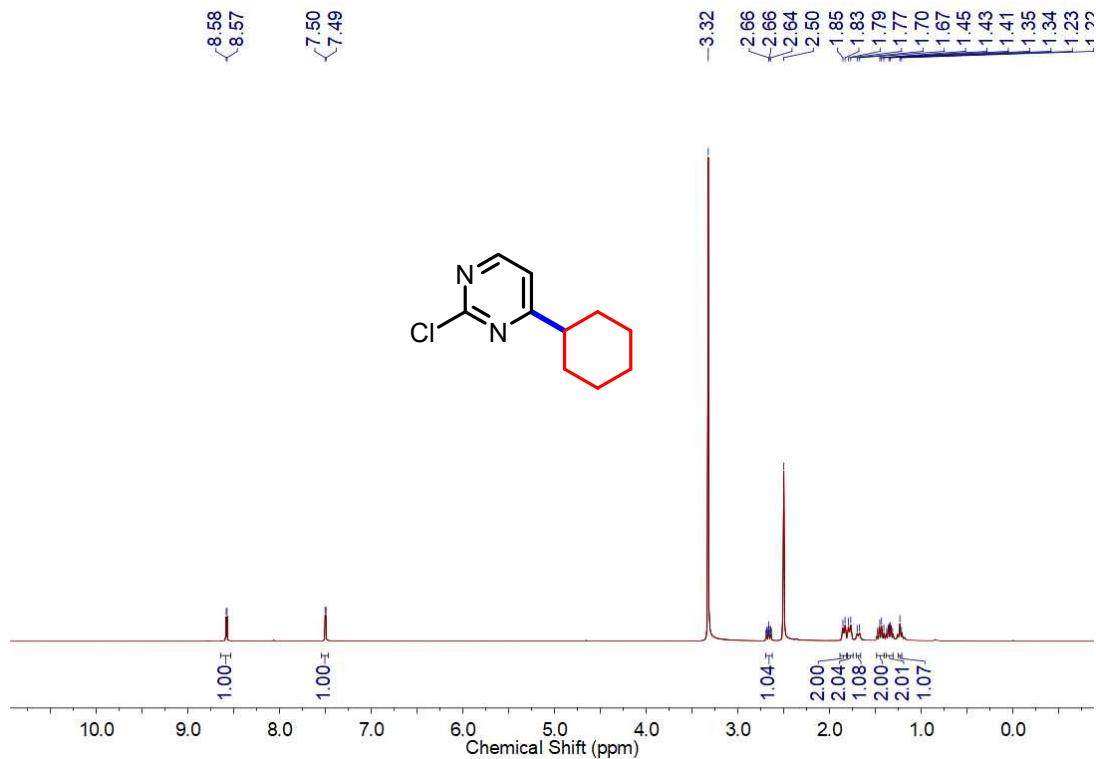
**Figure S145.**  $^{13}\text{C}$  NMR (471 MHz, DMSO) spectrum of **72**



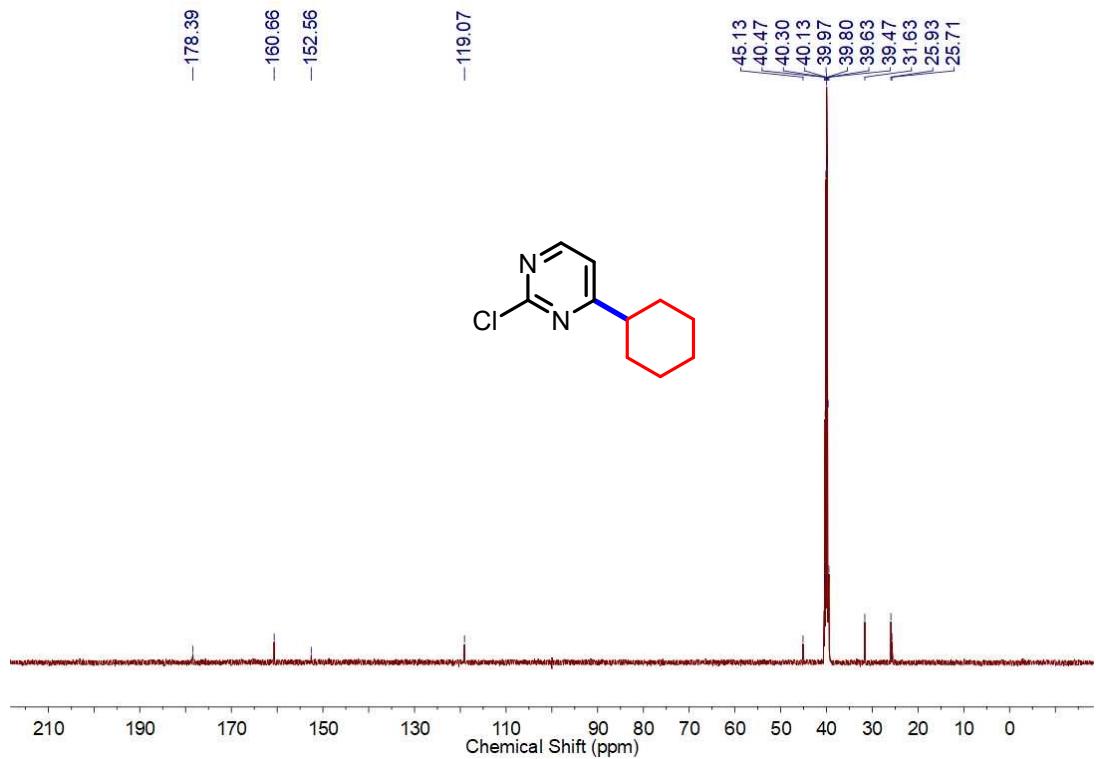
**Figure S146.** <sup>1</sup>H NMR (500 MHz, DMSO) spectrum of **73**



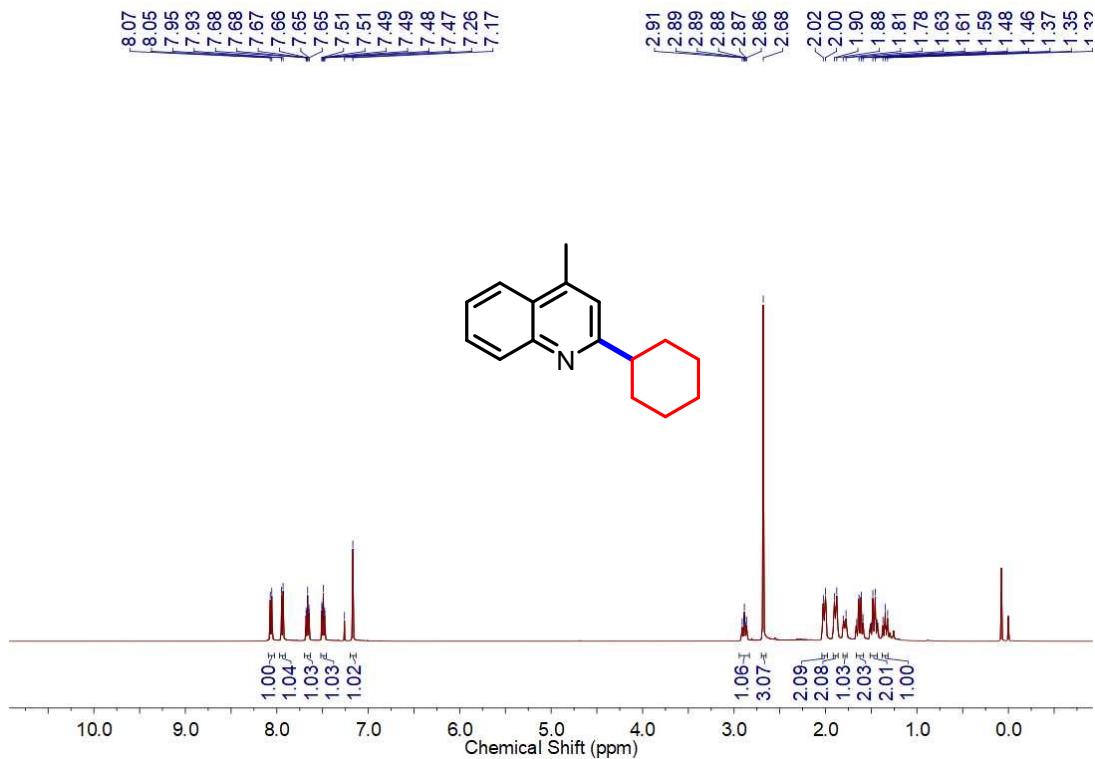
**Figure S147.** <sup>13</sup>C NMR (471 MHz, DMSO) spectrum of **73**



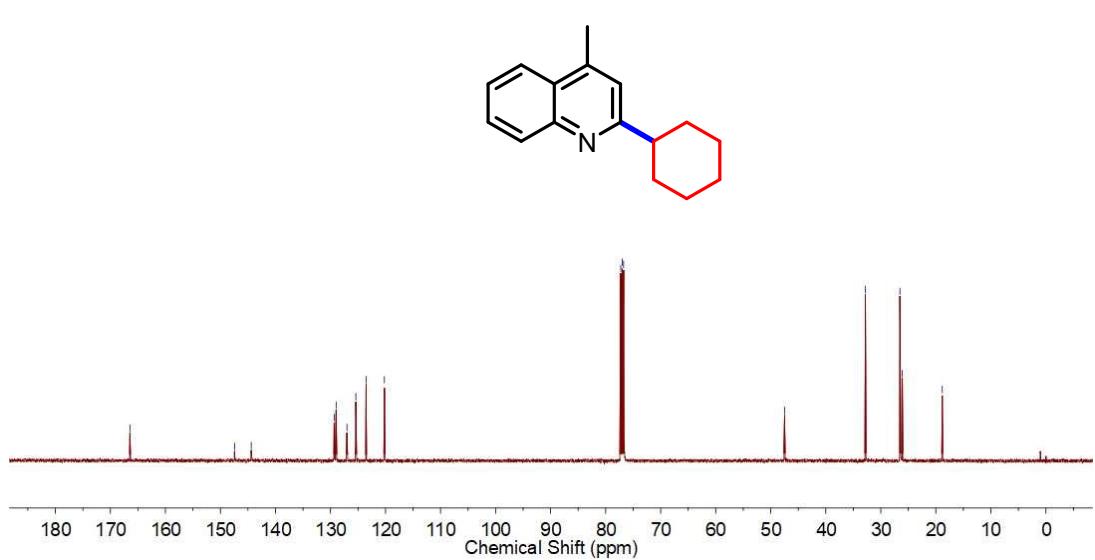
**Figure S148.**  $^1\text{H}$  NMR (500 MHz, DMSO) spectrum of **74**



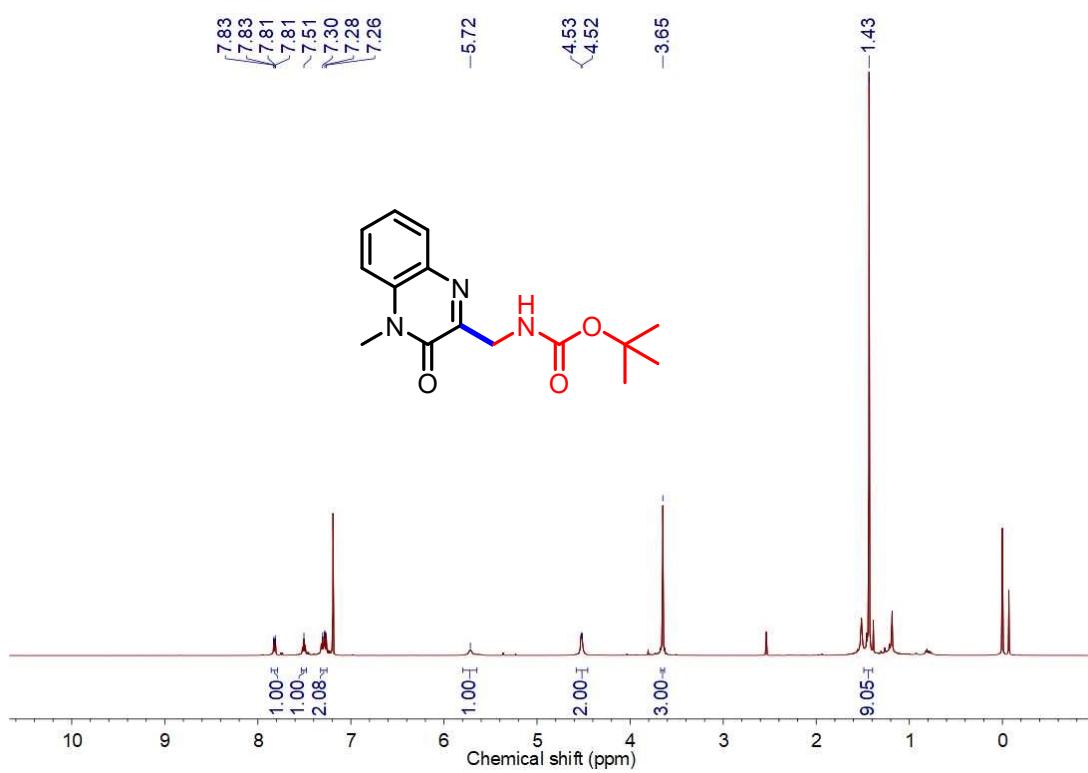
**Figure S149.**  $^{13}\text{C}$  NMR (471 MHz, DMSO) spectrum of **74**



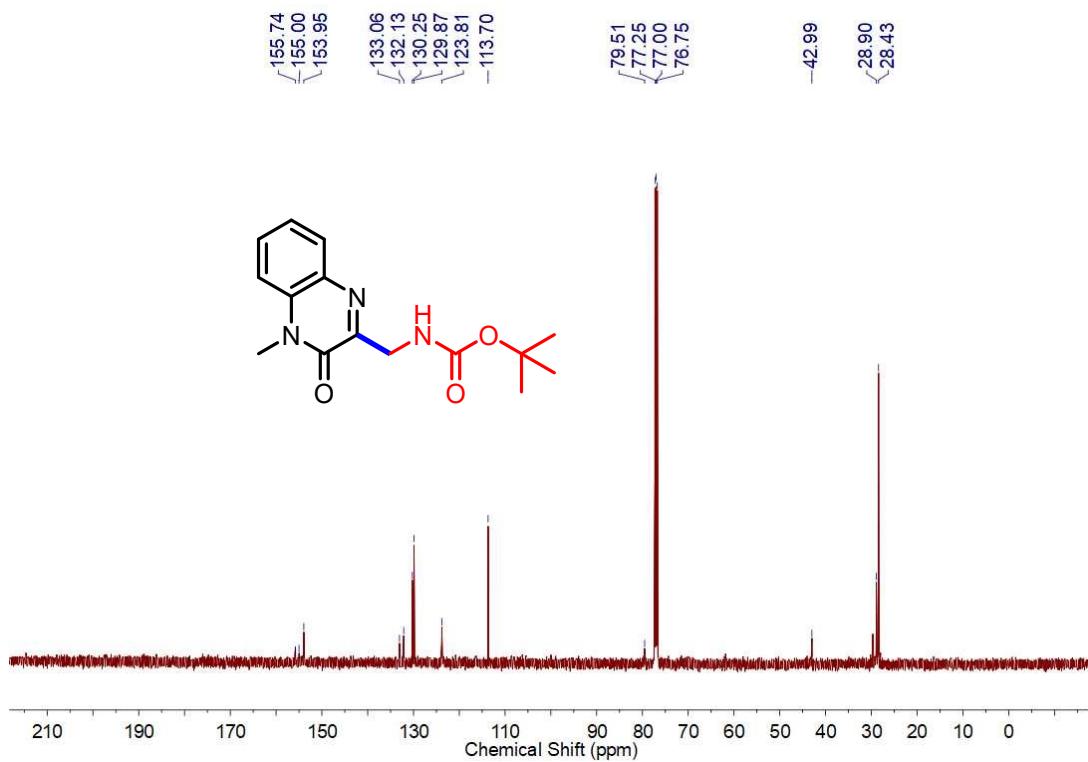
**Figure S150.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **75**



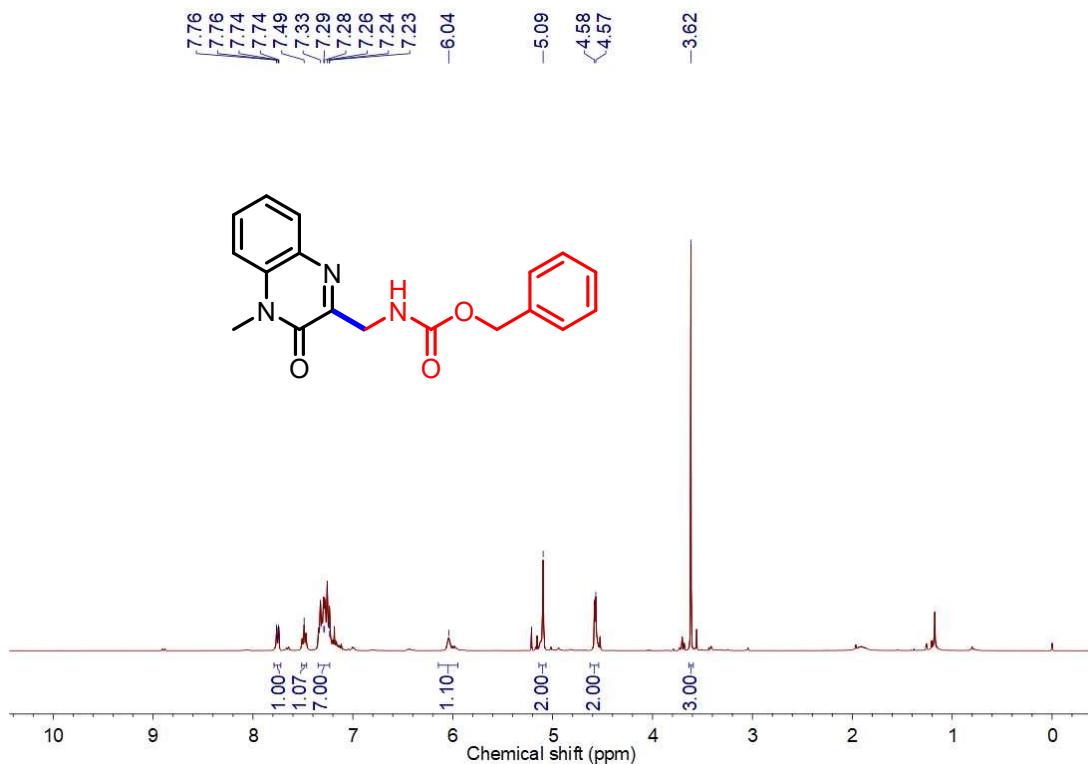
**Figure S151.**  $^{13}\text{C}$  NMR (471 MHz,  $\text{CDCl}_3$ ) spectrum of **75**



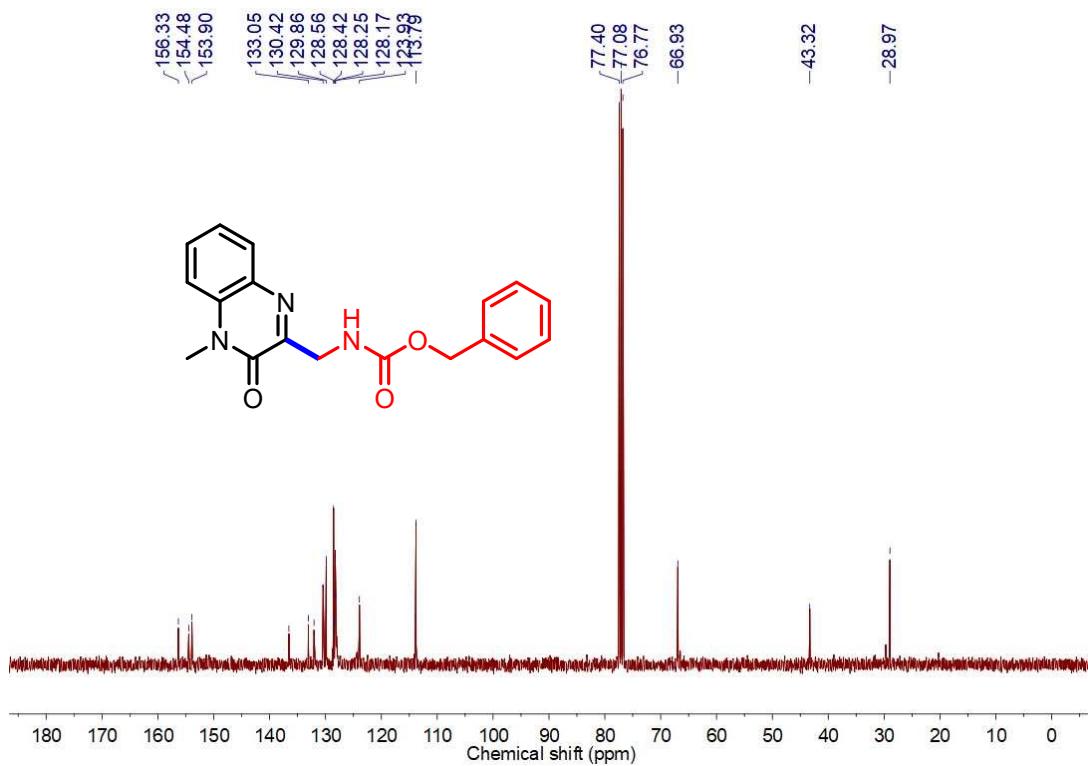
**Figure S152.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of 77



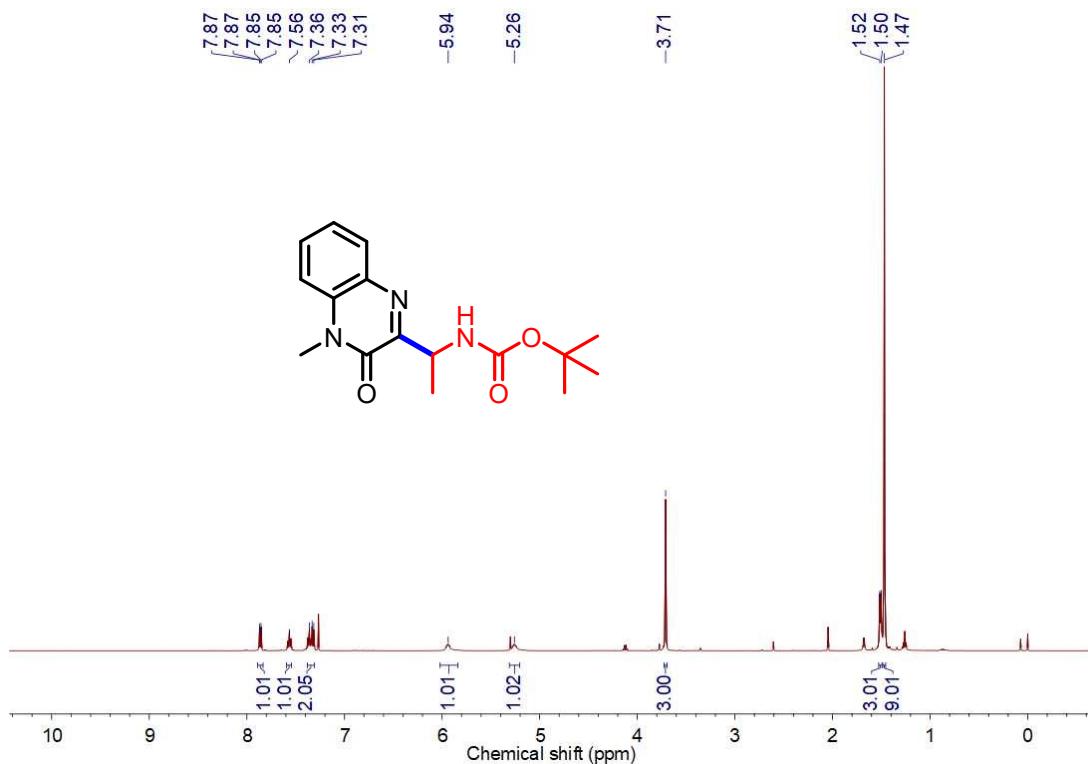
**Figure S153.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **77**



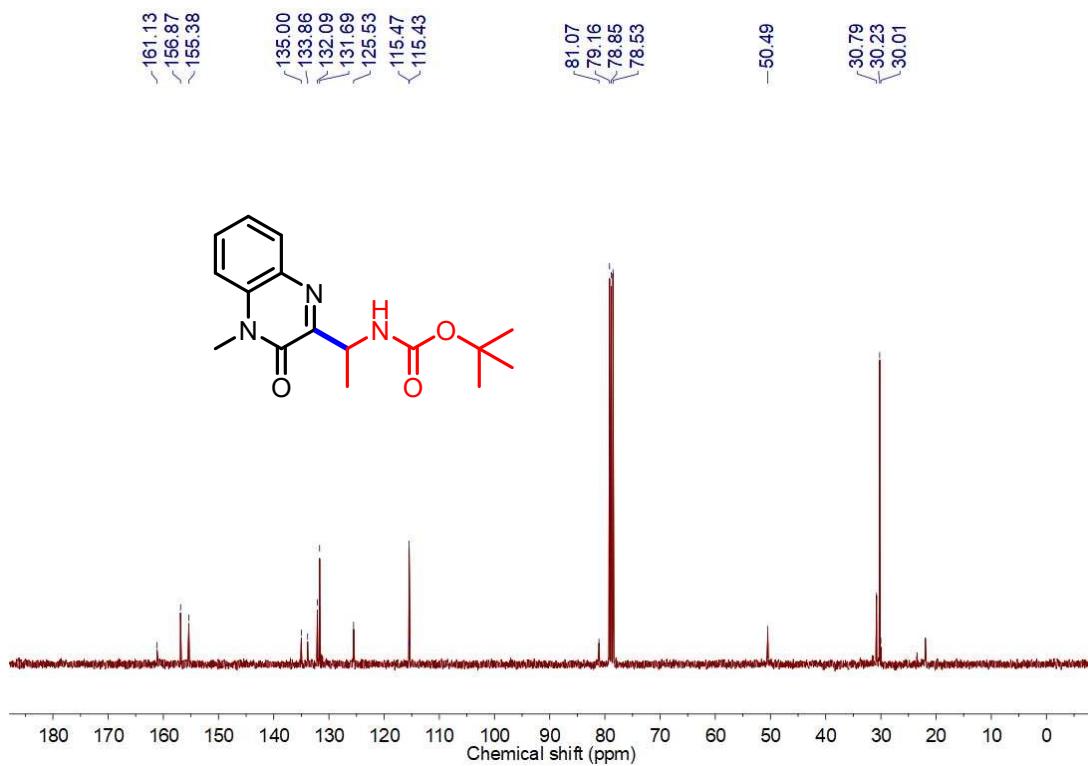
**Figure S154.**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of **78**



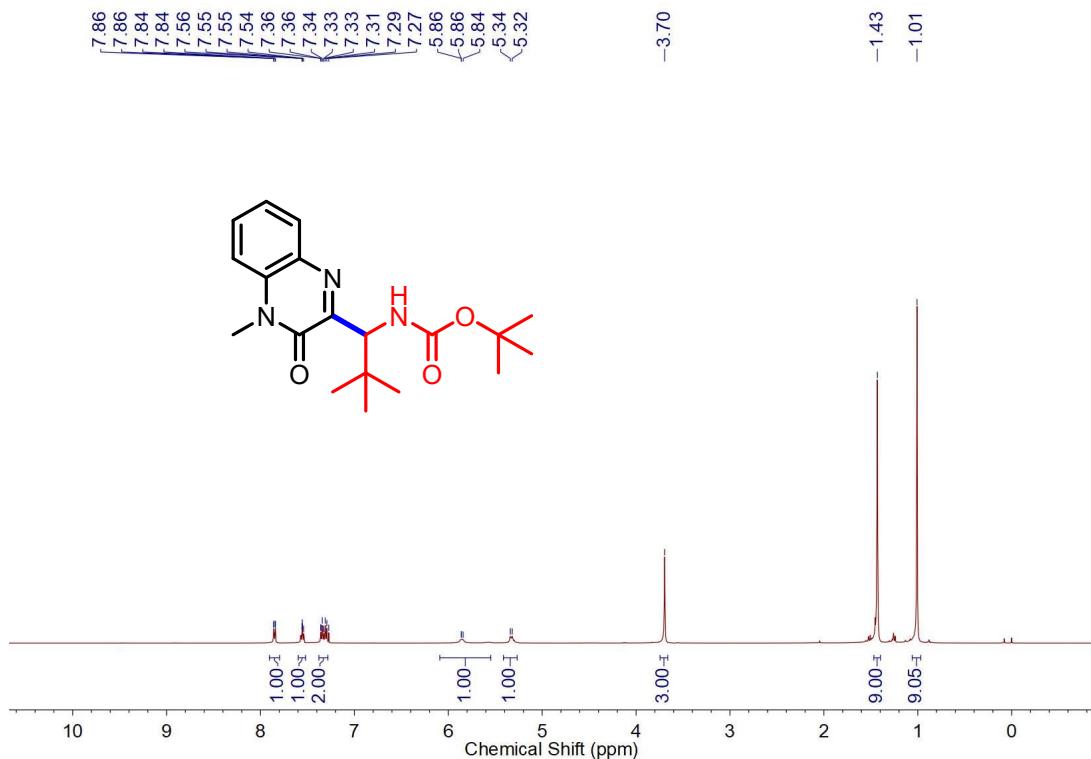
**Figure S155.**  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ) spectrum of **78**



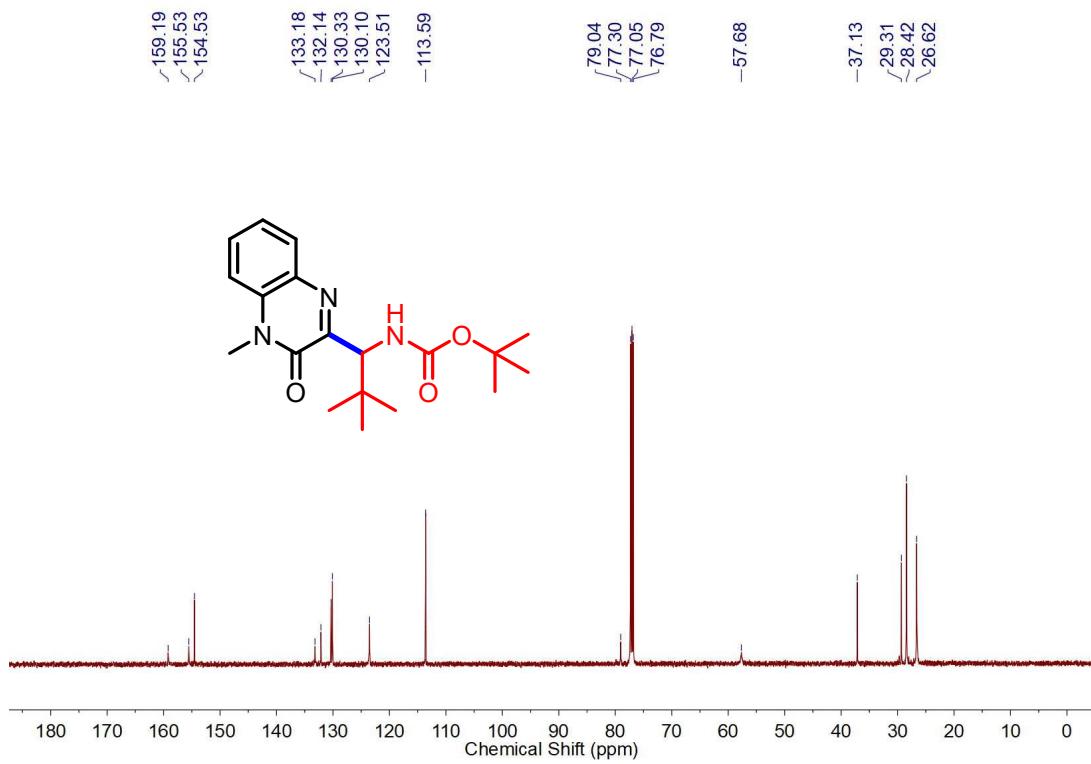
**Figure S156.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **79**



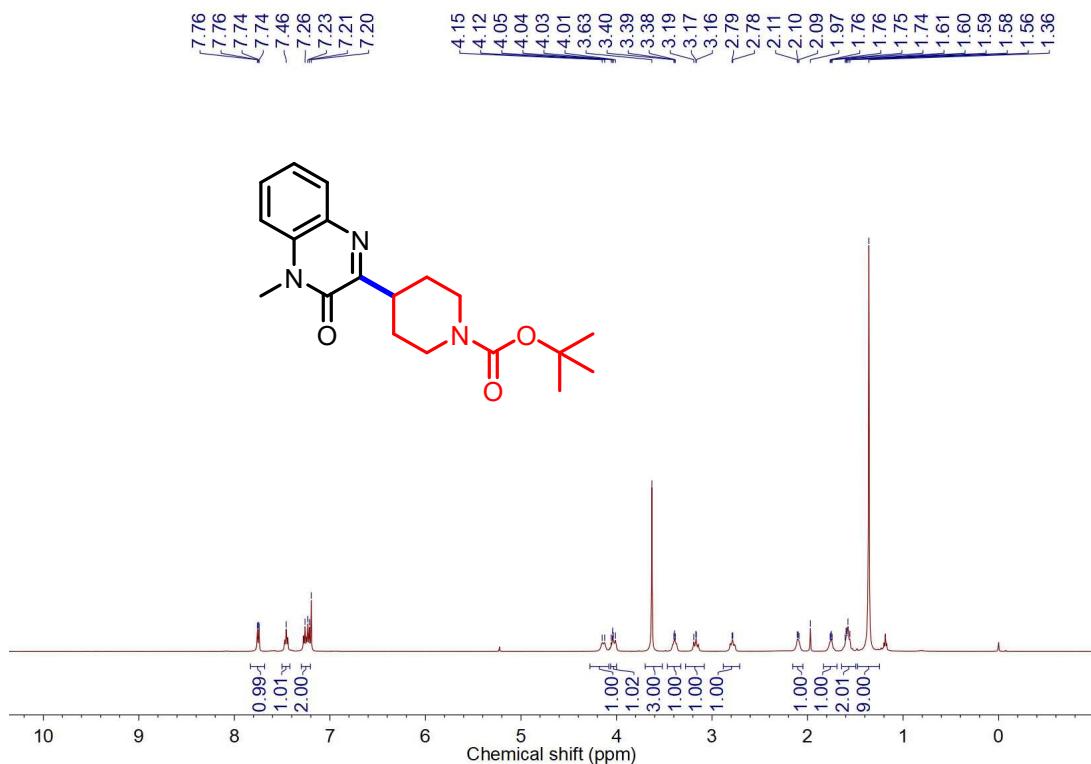
**Figure S157.**  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ) spectrum of **79**



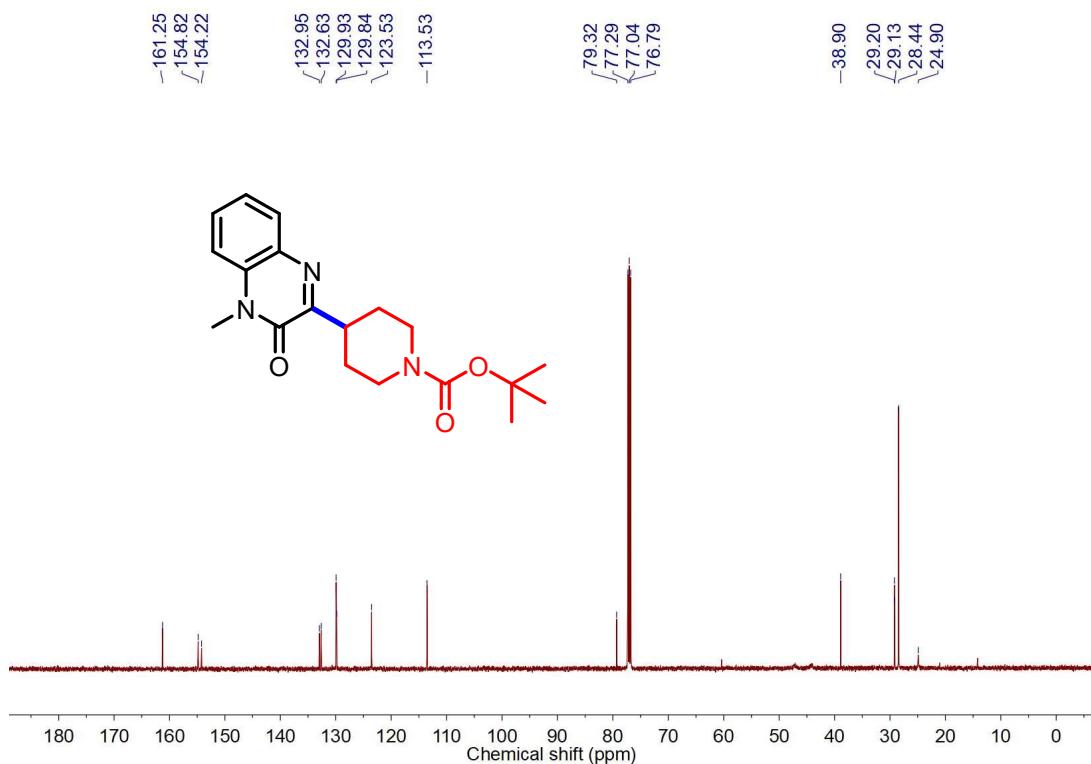
**Figure S158.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **80**



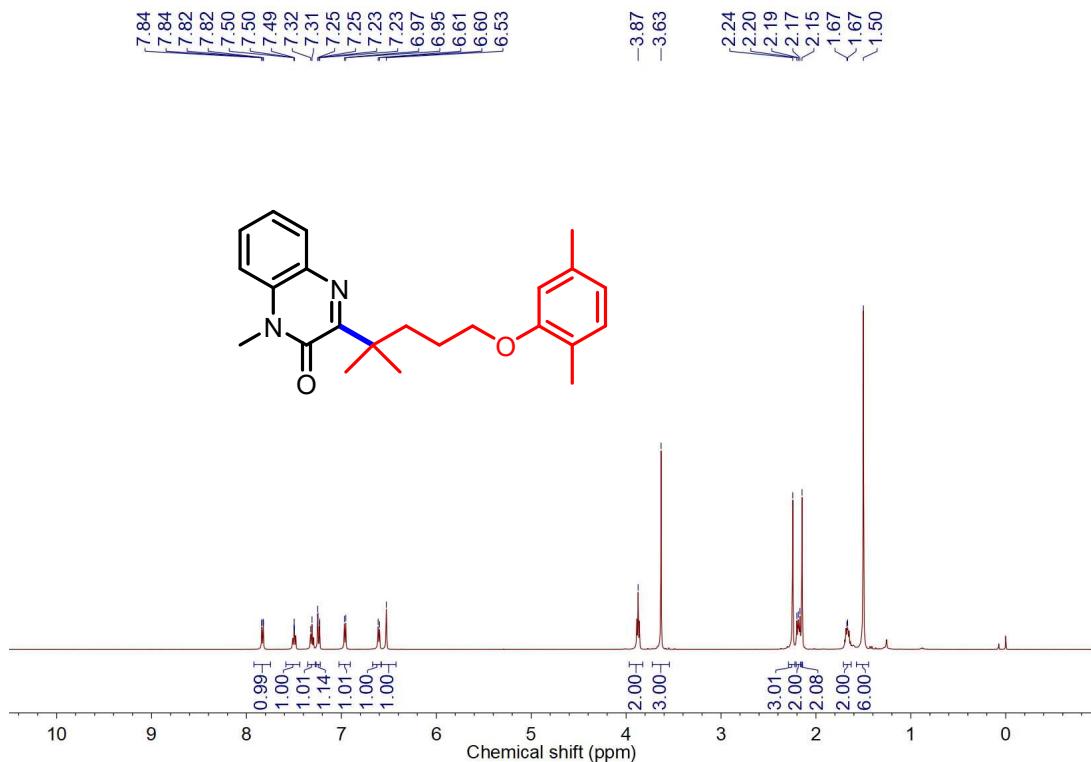
**Figure S159.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **80**



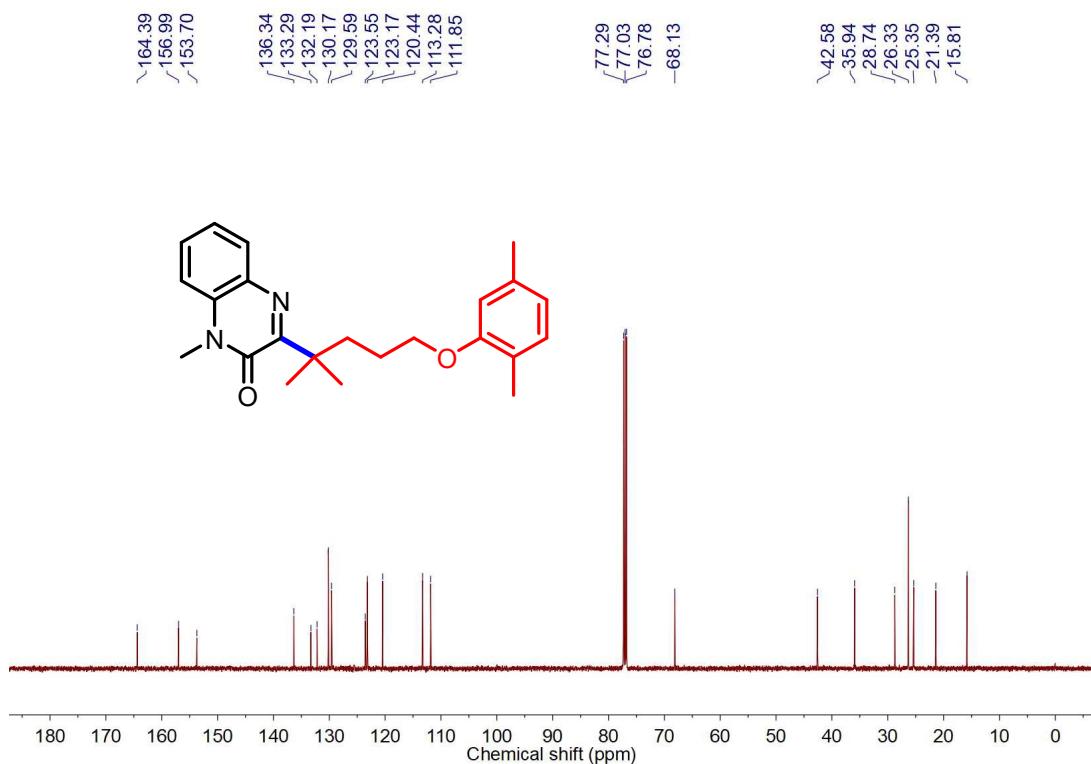
**Figure S160.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **81**



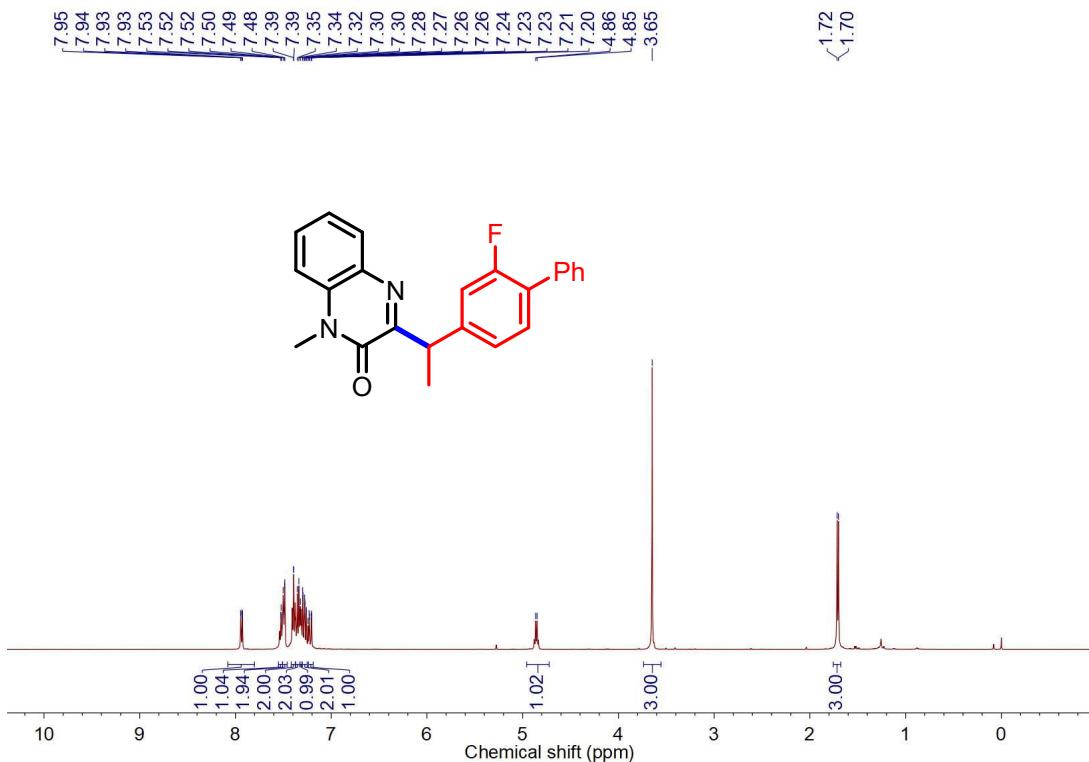
**Figure S161.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **81**



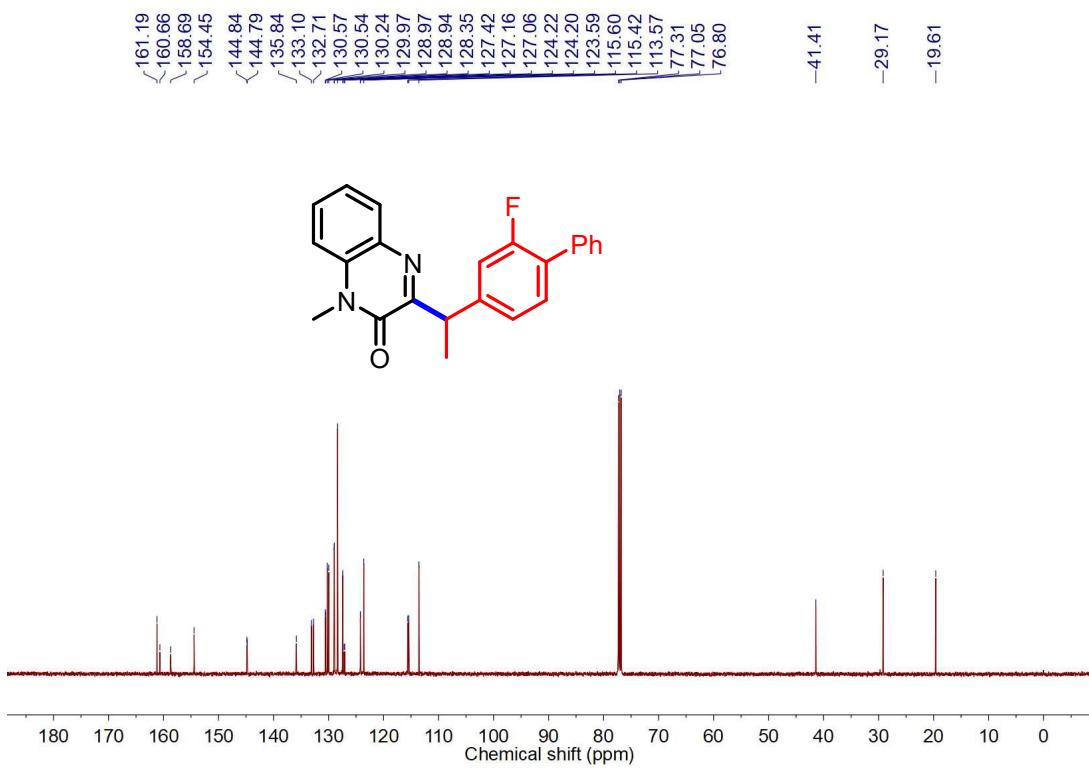
**Figure S162.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **82**



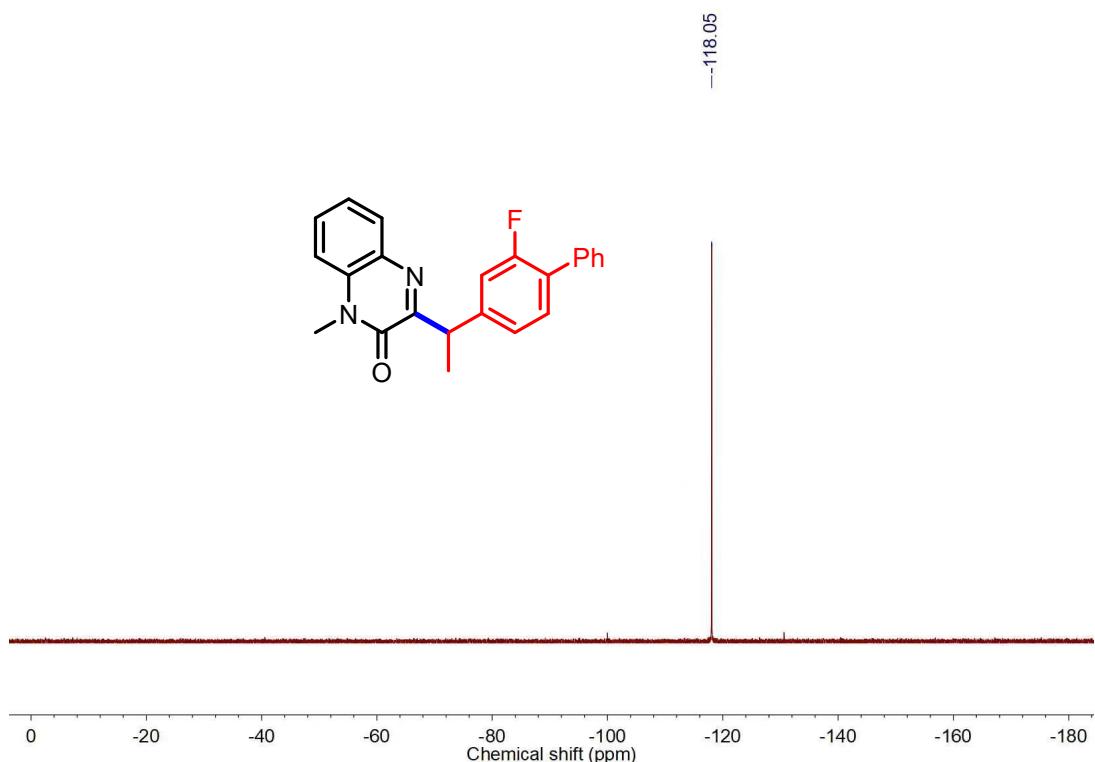
**Figure S163.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **82**



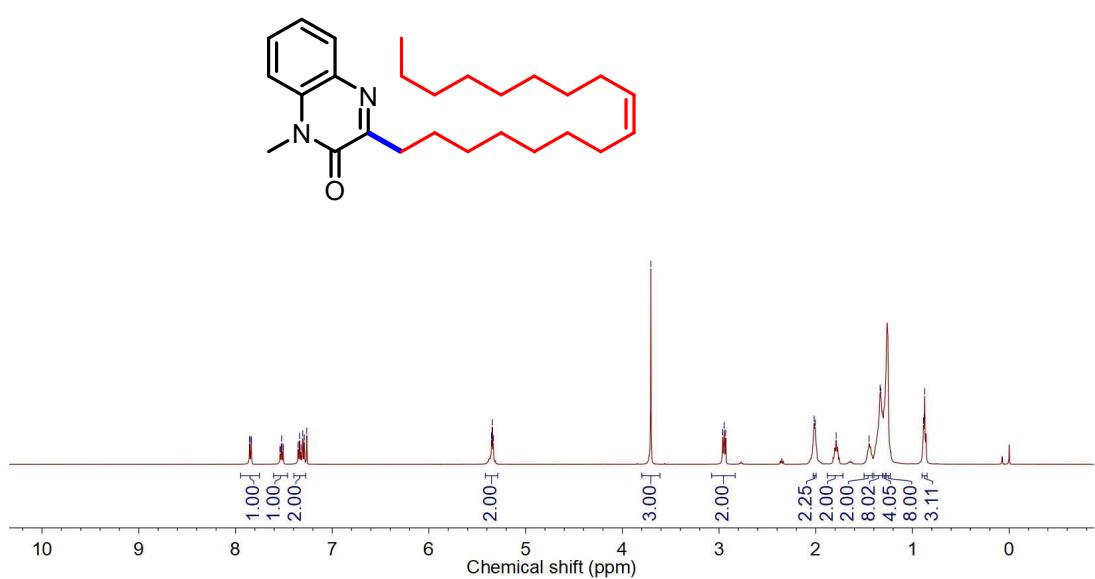
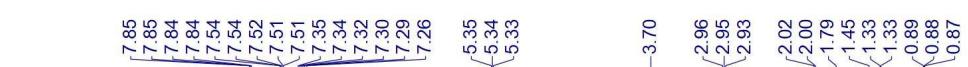
**Figure S164.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **83**



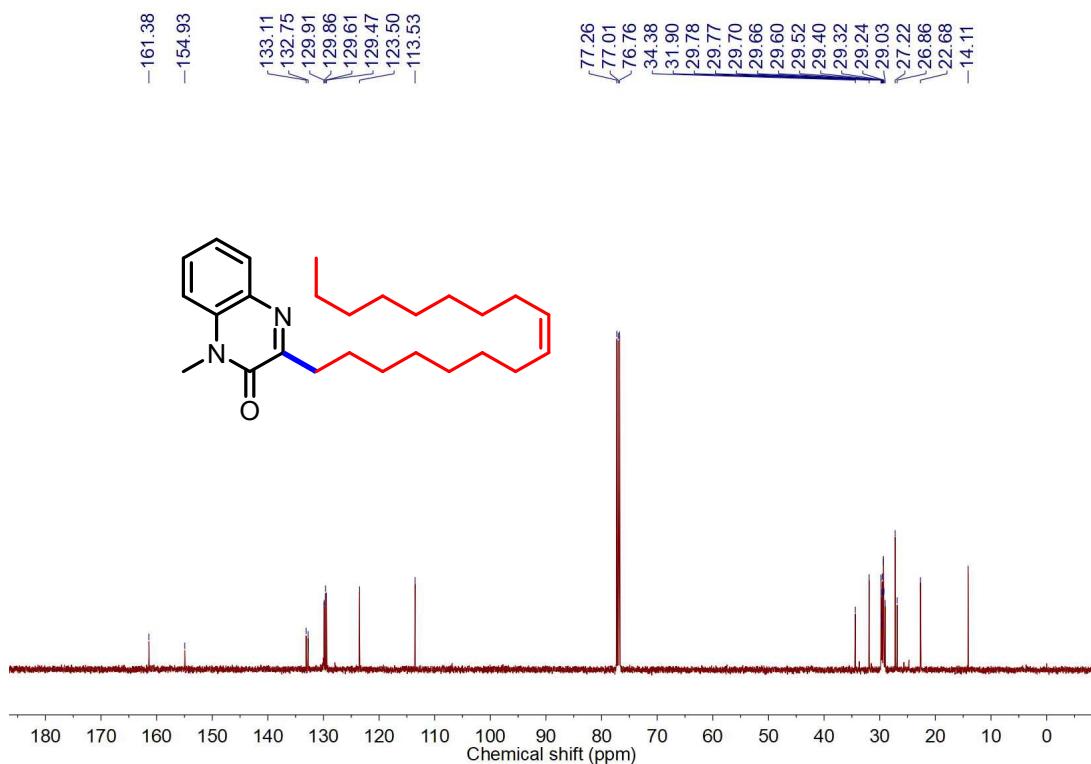
**Figure S165.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **83**



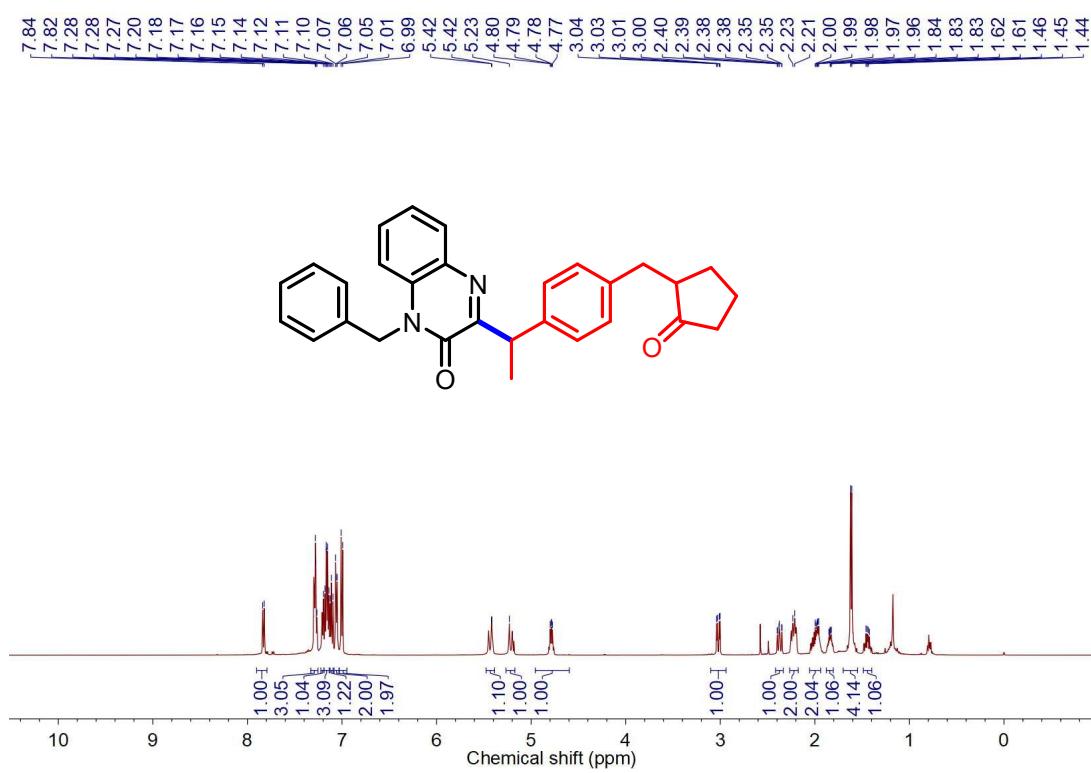
**Figure S166.**  $^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ ) spectrum of **83**



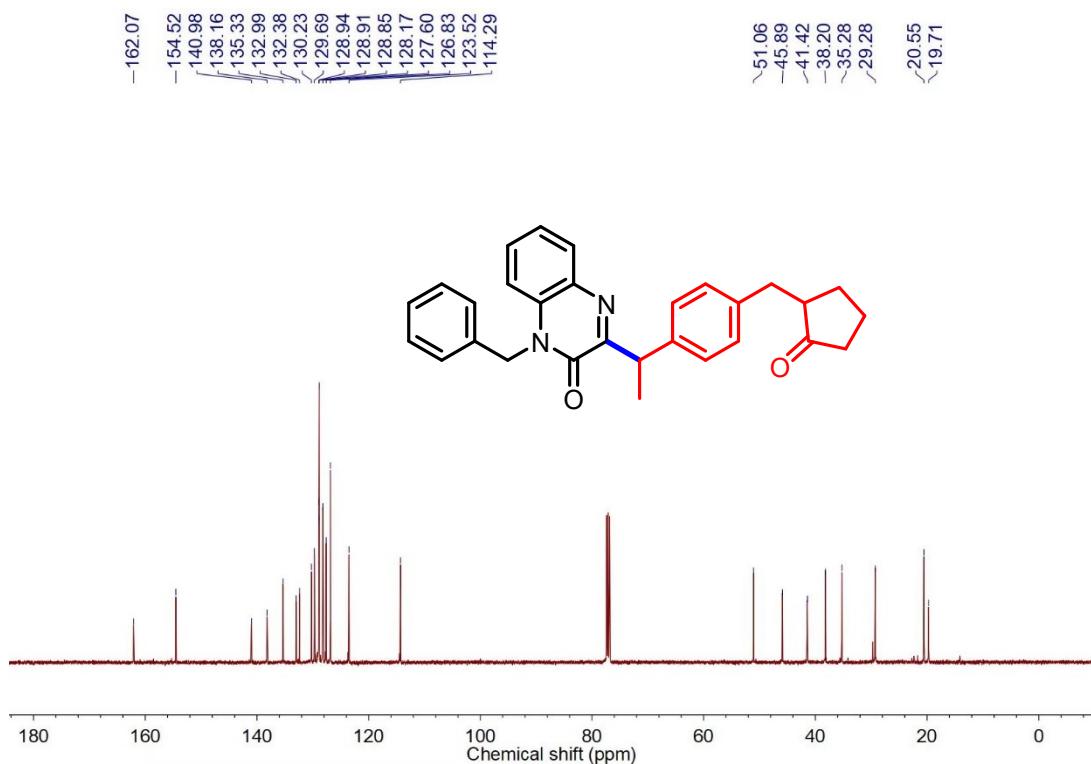
**Figure S167.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **84**



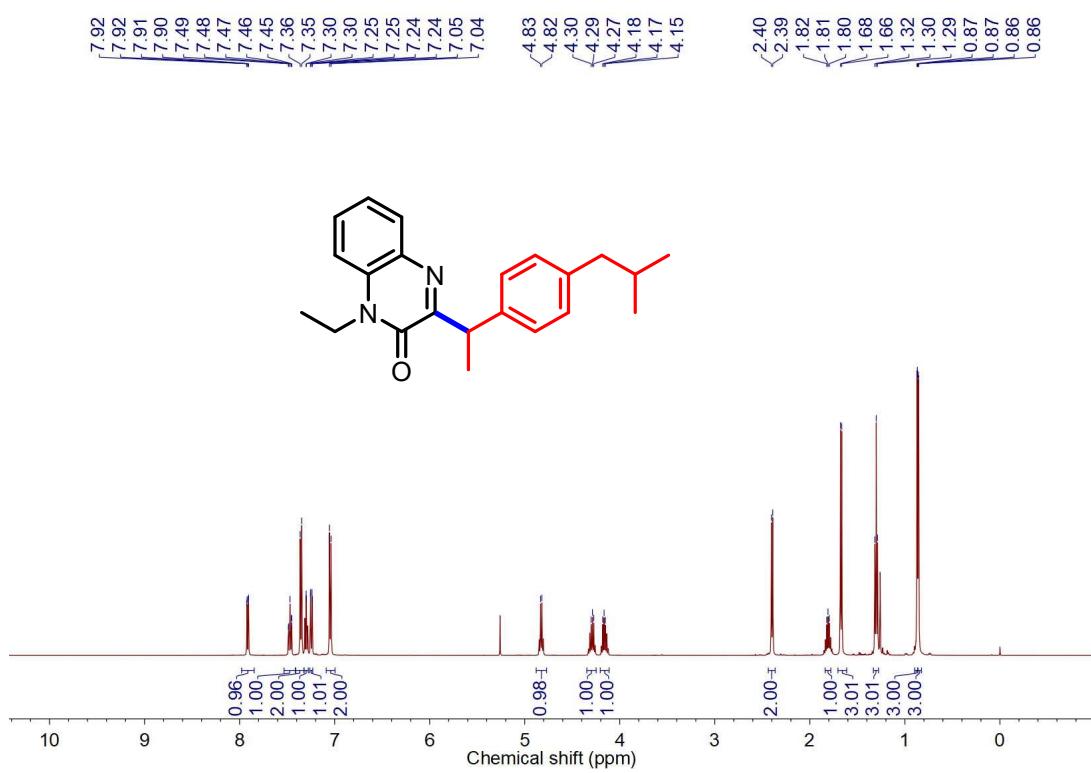
**Figure S168.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **84**



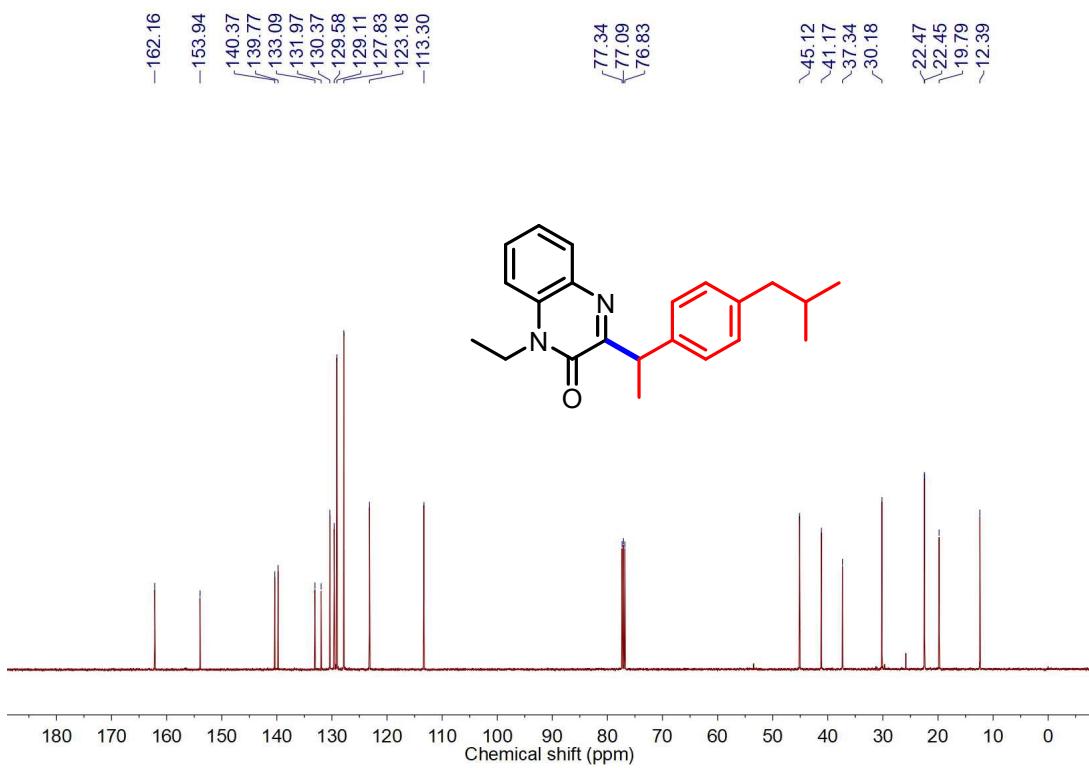
**Figure S169.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **85**



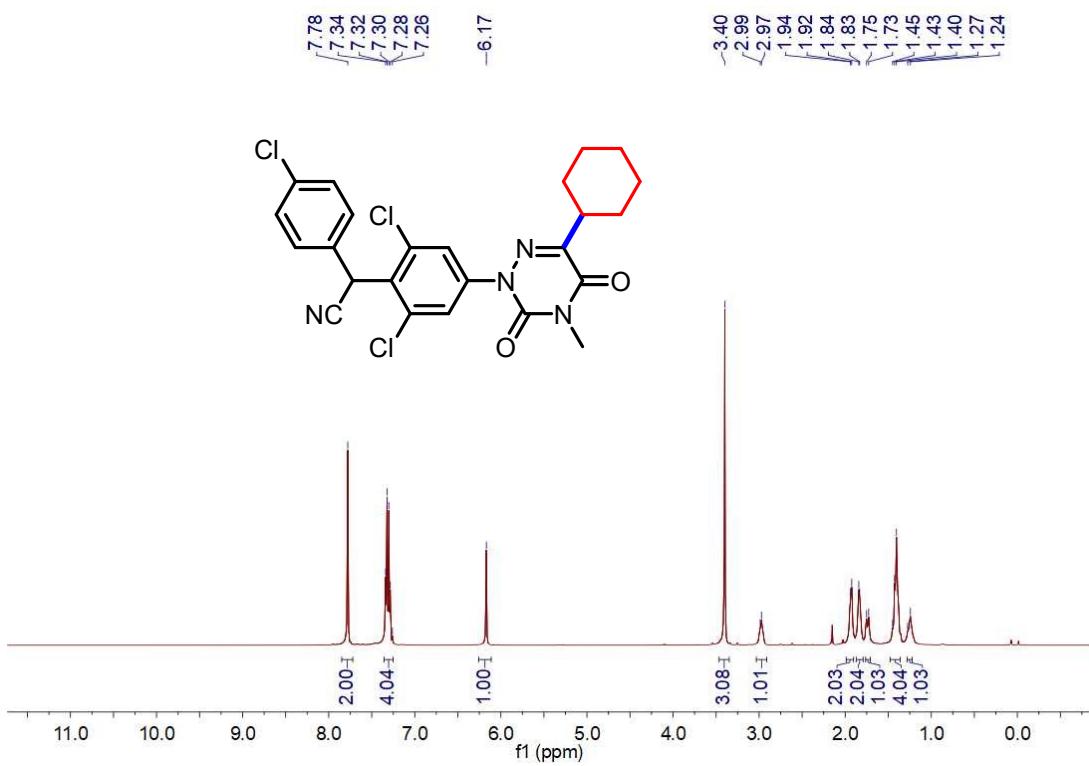
**Figure S170.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **85**



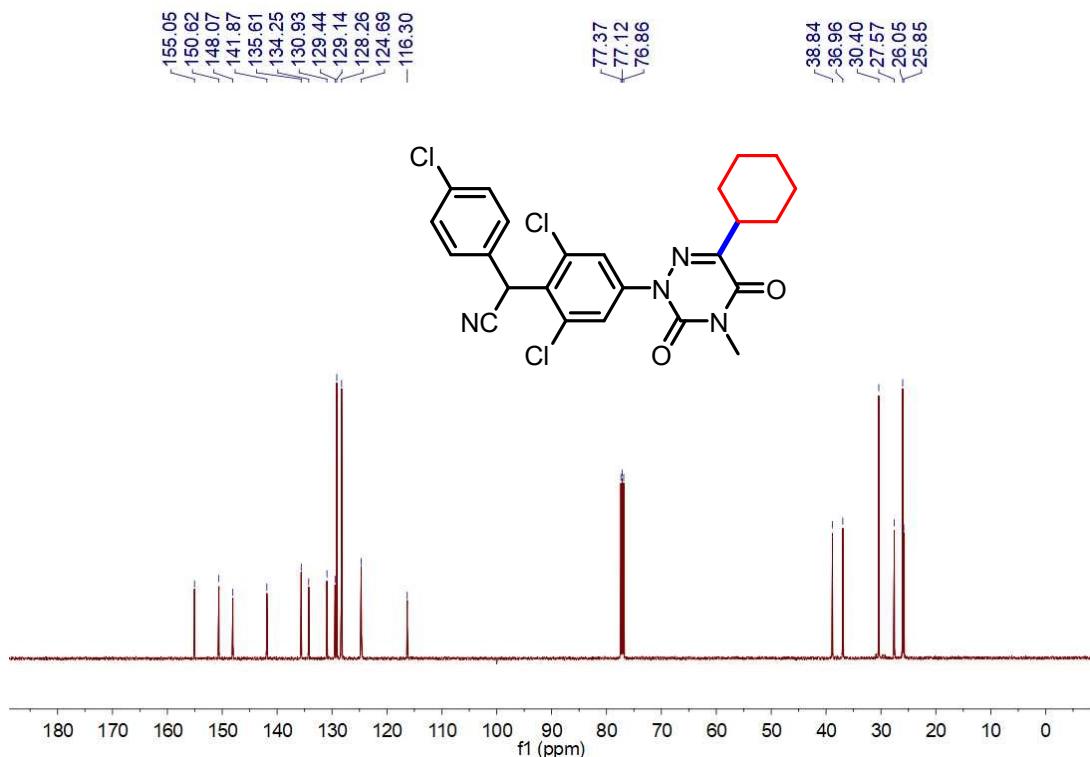
**Figure S171.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **86**



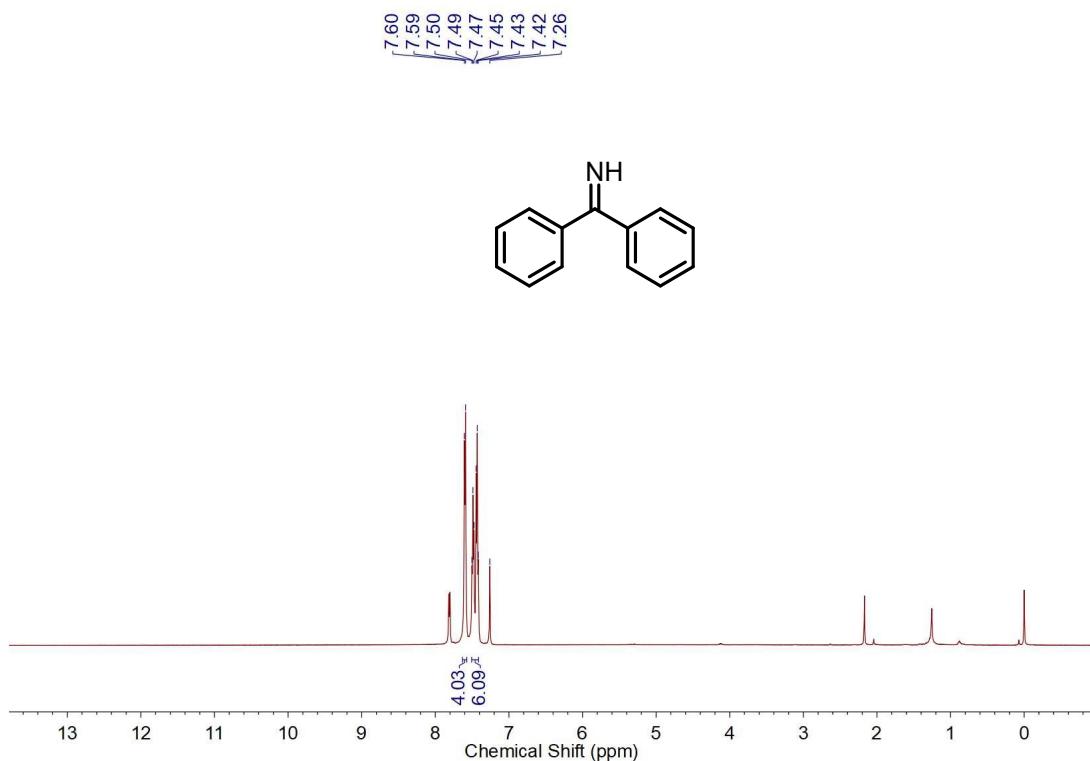
**Figure S172.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **86**



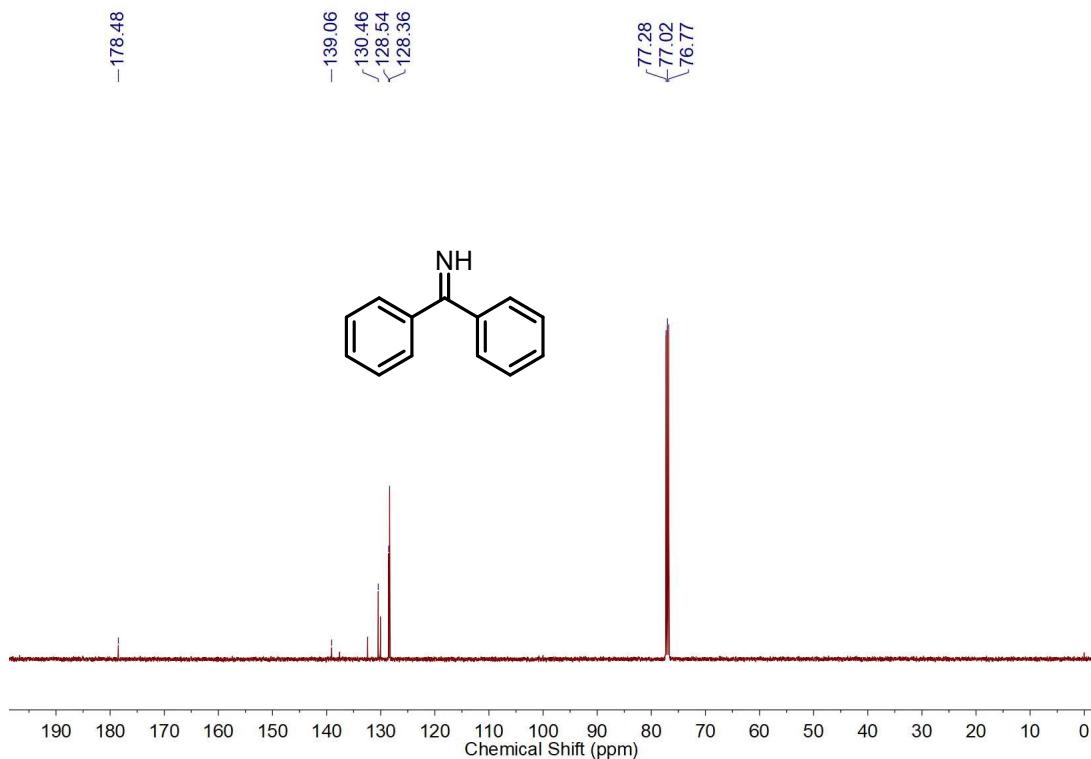
**Figure S173.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **88**



**Figure S174.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **88**



**Figure S175.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **90**



**Figure S176.**  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ ) spectrum of **90**