Photo-induced, metal- and photosensitizer-free decarboxylative C−H (amino)alkylation of heteroarenes in a sustainable solvent

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Supporting Information

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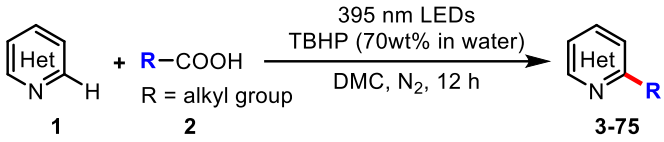
General Information

All reagents and deuterated solvents were commercially available and used without further purification. All products were separated by silica gel (200-300 mesh) column chromatography with petroleum ether (PE) (60-90°C) and ethyl acetate (EA). ^{1}H, ^{13}C and ^{19}F NMR spectra were recorded on a Bruker Advance 400 or 500 spectrometers at ambient temperature with $CDCl_3$ as solvent and tetramethylsilane (TMS) as the internal standard. Analytical thin layer chromatography (TLC) was performed on Merk precoated TLC (silica gel 60 F254) plates. Compounds for HRMS were analyzed by positive mode electrospray ionization (ESI) using Agilent 6530 QTOF mass spectrometer.

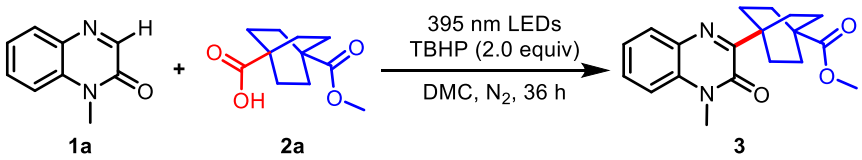
1. Experimental Section

1.1 General procedure for photoinduced decarboxylative C−H alkylation of heteroarenes



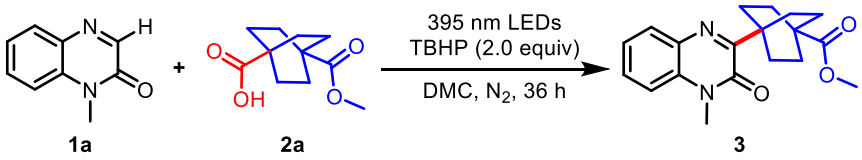
To a 15 mL tube was added heteroarenes (**1**) (0.2 mmol), carboxylic acids (**2**) (0.4 mmol), *tert*-butyl hydroperoxide (TBHP) (0.4 mmol, 70 wt% in water) and dimethyl carbonate (DMC) (1.0 mL). The above mixture was vigorously stirred under the irradiation of 395 nm LEDs in N_2 atmosphere for 12 hours. After completion, the reaction mixture was diluted with water. The resulting mixture was extracted with ethyl acetate and the collected organic layer was washed with brine, dried with $MgSO_4$. After the solvent was removed under reduced pressure, the crude product was further purified by silica gel column chromatography (200-300 mesh silica gel) to afford the target product.

1.2 General procedure for large-scale decarboxylative C−H alkylation of quinoxalinone with bicyclo[2.2.2]octane-1-carboxylic acid



To a 150 mL flask was added quinoxalinone (**1a**) (5.0 mmol), bicyclo[2.2.2]octane-1-carboxylic acid (**2a**) (10.0 mmol), tert-butyl hydroperoxide (TBHP) (10.0 mmol, 70 wt% in water) and dimethyl carbonate (DMC) (50.0 mL). The above mixture was vigorously stirred under the irradiation of 395 nm LEDs in N_2 atmosphere for 36 hours. After completion, the reaction mixture was diluted with water. The resulting mixture was extracted with ethyl acetate and the collected organic layer was washed with brine, dried with $MgSO_4$. After the solvent was removed under reduced pressure, the crude product was further purified by silica gel column chromatography (200-300 mesh silica gel) to afford the target product.

1.3 Testing of the recyclability of the solvent



To a 150 mL flask was added quinoxalinone (**1a**) (5.0 mmol), bicyclo[2.2.2]octane-1-carboxylic acid (**2a**) (10.0 mmol), *tert*-butyl hydroperoxide (TBHP) (10.0 mmol, 70 wt% in water) and dimethyl carbonate (DMC) (50.0 mL). The above mixture was vigorously stirred under the irradiation of 395

nm LEDs in N_2 atmosphere for 36 hours. After completion, the solvent was recycled through vacuum distillation and was reused for the next reaction. The crude product was further purified by silica gel column chromatography (200-300 mesh silica gel, PE(*v*)/EA(*v*) = 3:1, 800 mL) to afford the target product.

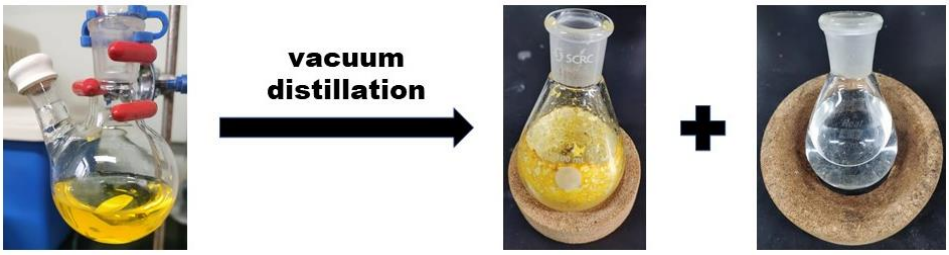


Figure S1 The schematic of recovering solvent

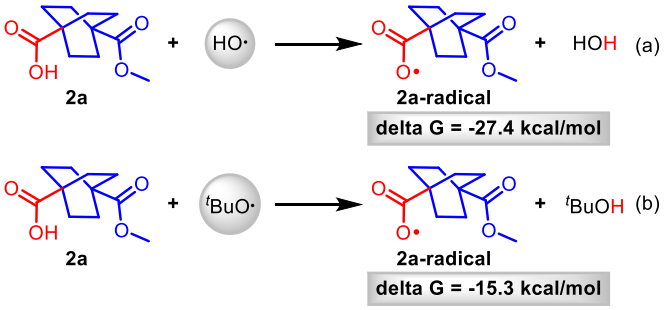
Table S1 Calculation of green chemistry metrics

Steps	Reagent 1	Reagent 2	Solvent	Oxidant	Yield	Product
1	Quinoxalinone (**1a**), 5 mmol, MW: 160.2, 801.0 mg	Carboxylic acid (**2a**), 10 mmol, MW: 212.2, 2122.0 mg	DMC, 593.7 mmol, MW: 90.1, 53492.4 mg	TBHP, 10 mmol, MW: 90.1, 901.0 mg	72%	**3**, 3.6 mmol, MW: 326.4, 1175.0 mg

$$Atom\ Economy = \frac{326.4}{160.2 + 212.2 + 90.1}\ \mathrm{X}\ 100\% = 70.6\%$$

With solvent recycling:

$$E - factor = \frac{\sum 801.0 + 2122.0 + 901.0 - 1175.0}{1175.0} = 2.3$$

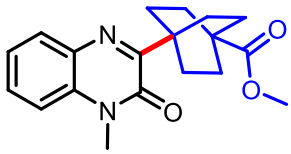


Scheme S1 Gibbs energy calculation for the HAT of **2a** with *tert*-butoxy and hydroxyl radicals

Based on the radical-relay strategy, we assumed that some simple oxygen radicals can initiate the carboxyl radicals, which can further transform into alkyl radicals. Then, we selected *tert*-butoxy and hydroxyl radicals to calculate the possibility. The Gibbs energy show that these two pathways are possible. Then, we further conducted experimental studies.

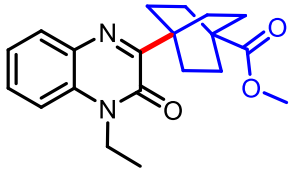
Characterization of Products

Methyl 4-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)bicyclo[2.2.2]octane-1-carboxylate (3)



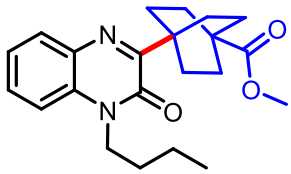
Obtained as a yellow solid (52 mg, 80% yield); M. P. = 122-123 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 7.9 Hz, 1H), 7.43 (t, *J* = 7.3 Hz, 1H), 7.23 (t, *J* = 7.6 Hz, 1H), 7.19 (d, *J* = 8.4 Hz, 1H), 3.60 (s, 3H), 3.58 (s, 3H), 2.08 (dd, *J* = 9.6, 6.1 Hz, 6H), 1.84 (dd, *J* = 9.6, 6.1 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) 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; HRMS (ESI+): Calculated for $C_{19}H_{22}N_2O_3$: $[M+H]^+$ 327.1703, Found 327.1734.

Methyl 4-(4-ethyl-3-oxo-3,4-dihydroquinoxalin-2-yl)bicyclo[2.2.2]octane-1-carboxylate (4)



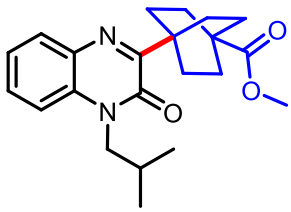
Obtained as a yellow liquid (53 mg, 78% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.82 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.52 – 7.47 (m, 1H), 7.29 (ddd, *J* = 8.4, 6.4, 2.1 Hz, 2H), 4.27 (q, *J* = 7.2 Hz, 2H), 3.67 (s, 3H), 2.15 (dd, *J* = 9.6, 6.2 Hz, 6H), 1.92 (dd, *J* = 9.6, 6.2 Hz, 6H), 1.35 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 178.6, 163.7, 153.3, 132.6, 132.0, 130.4, 129.7, 123.1, 113.2, 51.7, 40.0, 39.1, 37.1, 28.2, 27.6, 12.4; HRMS (ESI+): Calculated for $C_{20}H_{24}N_2O_3$: $[M+Na]^+$ 363.1679, Found 363.1695.

Methyl 4-(4-butyl-3-oxo-3,4-dihydroquinoxalin-2-yl)bicyclo[2.2.2]octane-1-carboxylate (5)



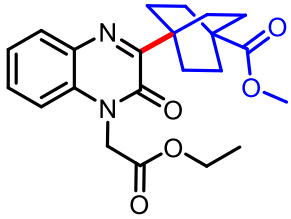
Obtained as a yellow liquid (53 mg, 72% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.73 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.41 (ddd, *J* = 8.5, 7.4, 1.5 Hz, 1H), 7.23 – 7.17 (m, 2H), 4.15 – 4.09 (m, 2H), 3.59 (s, 3H), 2.08 (dd, *J* = 9.7, 6.2 Hz, 6H), 1.84 (dd, *J* = 9.6, 6.2 Hz, 6H), 1.63 (t, *J* = 7.8 Hz, 2H), 1.40 (dd, *J* = 15.0, 7.5 Hz, 2H), 0.92 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 178.6, 163.7, 153.5, 132.6, 132.3, 130.3, 129.6, 123.1, 113.3, 51.7, 41.9, 40.0, 39.1, 29.3, 28.2, 27.6, 20.4, 13.8; HRMS (ESI+): Calculated for $C_{22}H_{28}N_2O_3$: $[M+H]^+$ 369.2173, Found 369.2188.

Methyl 4-(4-isobutyl-3-oxo-3,4-dihydroquinoxalin-2-yl)bicyclo[2.2.2]octane-1-carboxylate (6)



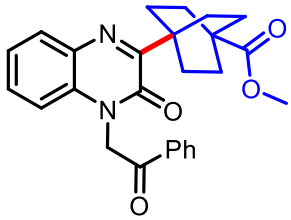
Obtained as a white solid (56 mg, 76% yield); M. P. = 125-126 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.73 (d, *J* = 7.9 Hz, 1H), 7.39 (t, *J* = 7.8 Hz, 1H), 7.19 (dd, *J* = 18.1, 8.1 Hz, 2H), 4.02 (d, *J* = 7.1 Hz, 2H), 3.59 (s, 3H), 2.15 – 2.06 (m, 7H), 1.87 – 1.80 (m, 6H), 0.90 (d, *J* = 6.7 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 178.6, 163.7, 153.9, 132.6, 132.5, 130.3, 129.5, 123.1, 113.7, 51.7, 48.5, 40.0, 39.1, 28.2, 27.6, 27.2, 20.2; HRMS (ESI+): Calculated for $C_{22}H_{28}N_2O_3$: $[M+H]^+$ 369.2173, Found 369.2175.

Methyl-4-(4-(2-ethoxy-2-oxoethyl)-3-oxo-3,4-dihydroquinoxalin-2-yl)bicyclo[2.2.2]octane-1-carboxylate (7)



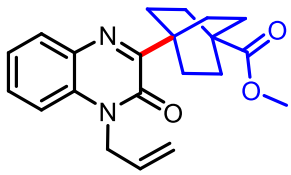
Obtained as a white solid (56 mg, 70% yield); M. P. = 110-111 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.49 – 7.43 (m, 1H), 7.34 – 7.28 (m, 1H), 7.03 (d, *J* = 7.8 Hz, 1H), 4.96 (s, 2H), 4.23 (q, *J* = 7.1 Hz, 2H), 3.67 (s, 3H), 2.15 (dd, *J* = 9.7, 6.2 Hz, 6H), 1.91 (dd, *J* = 9.6, 6.2 Hz, 6H), 1.26 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 178.6, 167.3, 163.6, 153.4, 132.4, 132.3, 130.4, 129.9, 123.6, 112.8, 62.0, 51.7, 43.4, 40.1, 39.1, 28.2, 27.6, 14.1; HRMS (ESI+): Calculated for $C_{22}H_{26}N_2O_5$: $[M+Na]^+$ 421.1734, Found 421.1740.

Methyl-4-(3-oxo-4-(2-oxo-2-phenylethyl)-3,4-dihydroquinoxalin-2-yl)bicyclo[2.2.2]octane-1-carboxylate (8)



Obtained as a yellow liquid (52 mg, 60% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.10 – 8.05 (m, 2H), 7.85 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.67 (t, *J* = 7.5 Hz, 1H), 7.54 (t, *J* = 7.8 Hz, 2H), 7.43 – 7.38 (m, 1H), 7.33 – 7.28 (m, 1H), 6.93 (d, *J* = 8.3 Hz, 1H), 5.69 (s, 2H), 3.67 (s, 3H), 2.17 (dd, *J* = 9.6, 6.2 Hz, 6H), 1.92 (dd, *J* = 9.5, 6.3 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 191.4, 178.6, 163.4, 153.5, 134.6, 134.3, 132.6, 132.5, 130.4, 129.8, 129.0, 128.2, 123.5, 113.2, 51.7, 48.3, 40.1, 39.1, 28.2, 27.6; HRMS (ESI+): Calculated for $C_{26}H_{26}N_2O_4$: $[M+H]^+$ 431.1965, Found 431.1995.

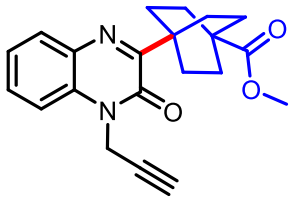
Methyl 4-(4-allyl-3-oxo-3,4-dihydroquinoxalin-2-yl)bicyclo[2.2.2]octane-1-carboxylate (9)



Obtained as a yellow solid (42 mg, 60% yield); M. P. = 95-96 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.81 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.49 – 7.43 (m, 1H), 7.31 – 7.26 (m, 1H), 7.23 (d, *J* = 8.3 Hz, 1H), 5.92 (ddt, *J* = 17.1, 10.3, 5.1 Hz, 1H), 5.24 (dd, *J* = 10.4, 0.7 Hz, 1H), 5.13 (dd, *J* = 17.3, 0.6 Hz, 1H), 4.88 – 4.81 (m, 2H), 3.66 (s, 3H), 2.15 (dd, *J* = 9.6, 6.2 Hz, 6H), 1.91 (dd, *J* = 9.6, 6.2 Hz, 6H); ^{13}C NMR

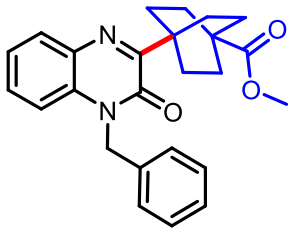
(126 MHz, $CDCl_3$) δ 178.6, 163.8, 153.3, 132.5, 132.3, 130.8, 130.2, 129.6, 123.3, 117.9, 113.8, 51.7, 44.3, 40.1, 39.1, 28.2, 27.6; HRMS (ESI+): Calculated for $C_{21}H_{24}N_2O_3$: $[M+Na]^+$ 375.1679, Found 375.1685.

Methyl-4-(3-oxo-4-(prop-2-yn-1-yl)-3,4-dihydroquinoxalin-2-yl)bicyclo[2.2.2]octane-1-carboxylate (10)



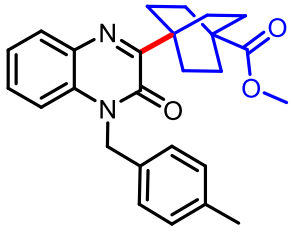
Obtained as a yellow solid (39 mg, 56% yield); M. P. = 140-141 °C; ^1H NMR (500 MHz, $CDCl_3$) δ 7.82 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.56 – 7.51 (m, 1H), 7.41 (d, *J* = 8.0 Hz, 1H), 7.37 – 7.31 (m, 1H), 5.01 (d, *J* = 2.4 Hz, 2H), 3.67 (s, 3H), 2.27 (t, *J* = 2.4 Hz, 1H), 2.15 (dd, *J* = 9.6, 6.2 Hz, 6H), 1.92 (dd, *J* = 9.6, 6.2 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 178.6, 163.7, 152.7, 132.5, 131.6, 130.3, 129.8, 123.7, 113.8, 77.1, 72.9, 51.7, 40.2, 39.0, 31.2, 28.2, 27.6; HRMS (ESI+): Calculated for $C_{21}H_{22}N_2O_3$: $[M+H]^+$ 351.1703, Found 351.1708.

Methyl 4-(4-benzyl-3-oxo-3,4-dihydroquinoxalin-2-yl)bicyclo[2.2.2]octane-1-carboxylate (11)



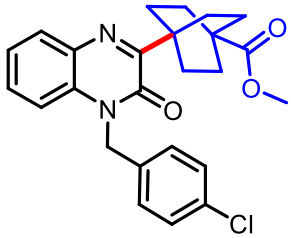
Obtained as a yellow liquid (55 mg, 68% yield); ^1H NMR (500 MHz, $CDCl_3$) δ 7.82 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.37 (dd, *J* = 12.1, 5.0 Hz, 1H), 7.30 (t, *J* = 7.3 Hz, 2H), 7.26 (t, *J* = 5.2 Hz, 2H), 7.21 (t, *J* = 8.9 Hz, 3H), 5.46 (s, 2H), 3.68 (s, 3H), 2.20 (dd, *J* = 9.6, 6.3 Hz, 6H), 1.94 (dd, *J* = 9.6, 6.3 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 178.6, 163.9, 153.8, 135.5, 132.6, 132.5, 130.2, 129.7, 128.9, 127.6, 126.8, 123.4, 114.1, 51.7, 45.6, 40.2, 39.1, 28.2, 27.7; HRMS (ESI+): Calculated for $C_{25}H_{26}N_2O_3$: $[M+H]^+$ 403.2016, Found 403.2022.

Methyl-4-(4-(4-methylbenzyl)-3-oxo-3,4-dihydroquinoxalin-2-yl)bicyclo[2.2.2]octane-1-carboxylate (12)



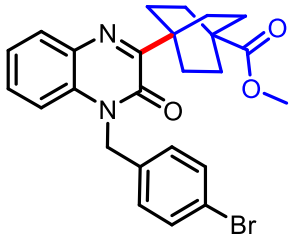
Obtained as a yellow liquid (57 mg, 68% yield); ^1H NMR (500 MHz, $CDCl_3$) δ 7.81 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.42 – 7.34 (m, 1H), 7.27 – 7.24 (m, 1H), 7.22 (d, *J* = 8.4 Hz, 1H), 7.09 (d, *J* = 5.6 Hz, 4H), 5.41 (s, 2H), 3.68 (s, 3H), 2.29 (s, 3H), 2.20 (dd, *J* = 9.6, 6.2 Hz, 6H), 1.94 (dd, *J* = 9.5, 6.3 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 178.6, 163.9, 153.8, 137.3, 132.6, 132.5, 132.5, 130.2, 129.7, 129.6, 126.8, 123.3, 114.1, 51.7, 45.4, 40.2, 39.1, 28.2, 27.6, 21.1; HRMS (ESI+): Calculated for $C_{26}H_{28}N_2O_3$: $[M+H]^+$ 417.2173, Found 417.2173.

Methyl-4-(4-(4-chlorobenzyl)-3-oxo-3,4-dihydroquinoxalin-2-yl)bicyclo[2.2.2]octane-1-carboxylate (13)



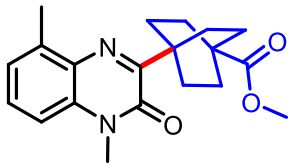
Obtained as a yellow solid (51 mg, 58% yield); M. P. = 145-146 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.42 – 7.37 (m, 1H), 7.30 – 7.26 (m, 3H), 7.18 – 7.13 (m, 3H), 5.41 (s, 2H), 3.68 (s, 3H), 2.19 (dd, *J* = 9.6, 6.2 Hz, 6H), 1.94 (dd, *J* = 9.6, 6.2 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 178.6, 163.9, 153.7, 134.1, 133.5, 132.6, 132.3, 130.4, 129.8, 129.1, 128.3, 123.6, 113.8, 51.7, 45.0, 40.2, 39.1, 28.2, 27.6; HRMS (ESI+): Calculated for $C_{25}H_{25}ClN_2O_3$: $[M+H]^+$ 437.1626, Found 437.1620.

Methyl-4-(4-(4-bromobenzyl)-3-oxo-3,4-dihydroquinoxalin-2-yl)bicyclo[2.2.2]octane-1-carboxylate (14)



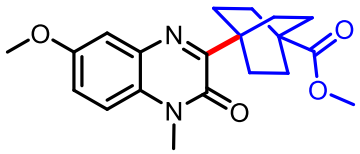
Obtained as a yellow solid (52 mg, 54% yield); M. P. = 154-155 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.42 (d, *J* = 8.4 Hz, 2H), 7.41 – 7.37 (m, 1H), 7.31 – 7.27 (m, 1H), 7.15 (d, *J* = 8.3 Hz, 1H), 7.09 (d, *J* = 8.4 Hz, 2H), 5.39 (s, 2H), 3.68 (s, 3H), 2.19 (dd, *J* = 9.6, 6.2 Hz, 6H), 1.94 (dd, *J* = 9.5, 6.3 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 178.5, 163.9, 153.70 134.6, 132.6, 132.3, 132.1, 130.4, 129.8, 128.6, 123.6, 121.5, 113.8, 51.7, 45.1, 40.2, 39.1, 28.2, 27.7; HRMS (ESI+): Calculated for $C_{25}H_{25}BrN_2O_3$: $[M+H]^+$ 481.1121, Found 481.1161.

Methyl-4-(4,8-dimethyl-3-oxo-3,4-dihydroquinoxalin-2-yl)bicyclo[2.2.2]octane-1-carboxylate (15)



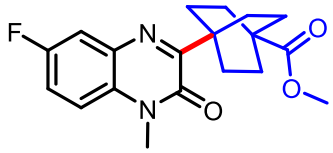
Obtained as a white solid (35 mg, 51% yield); M. P. = 110-111 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38 (t, *J* = 7.9 Hz, 1H), 7.17 (d, *J* = 7.4 Hz, 1H), 7.10 (d, *J* = 8.4 Hz, 1H), 3.67 (s, 3H), 3.64 (s, 3H), 2.66 (s, 3H), 2.16 (dd, *J* = 9.6, 6.2 Hz, 6H), 1.92 (dd, *J* = 9.6, 6.2 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 178.7, 161.7, 153.8, 139.0, 133.2, 130.7, 129.5, 124.6, 111.2, 51.7, 40.4, 39.1, 28.9, 28.3, 27.6, 17.4; HRMS (ESI+): Calculated for $C_{20}H_{24}N_2O_3$: $[M+H]^+$ 341.1860, Found 341.1874.

Methyl-4-(7-methoxy-4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)bicyclo[2.2.2]octane-1-carboxylate (16)



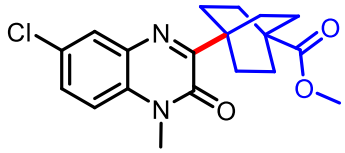
Obtained as a yellow solid (45 mg, 63% yield); M. P. = 133-134 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.8 Hz, 1H), 6.89 (dd, *J* = 8.9, 2.5 Hz, 1H), 6.67 (d, *J* = 2.5 Hz, 1H), 3.91 (s, 3H), 3.67 (s, 3H), 3.61 (s, 3H), 2.13 (dd, *J* = 9.6, 6.2 Hz, 6H), 1.91 (dd, *J* = 9.6, 6.2 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 178.7, 160.8, 160.1, 154.1, 134.5, 131.3, 127.3, 110.3, 97.6, 55.8, 51.7, 39.7, 39.1, 28.8, 28.3, 27.6; HRMS (ESI+): Calculated for $C_{20}H_{24}N_2O_4$: $[M+H]^+$ 357.1809, Found 357.1833.

Methyl-4-(7-fluoro-4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)bicyclo[2.2.2]octane-1-carboxylate (17)



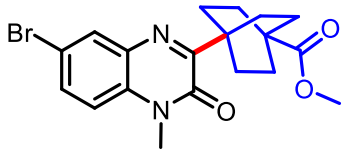
Obtained as a yellow solid (41 mg, 60% yield); M. P. = 172-173 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51 (dd, *J* = 8.8, 2.7 Hz, 1H), 7.24 (ddd, *J* = 11.0, 8.8, 5.0 Hz, 2H), 3.68 (s, 3H), 3.65 (s, 3H), 2.14 (dd, *J* = 9.6, 6.2 Hz, 6H), 1.92 (dd, *J* = 9.6, 6.2 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 178.5, 165.3, 158.6 (d, *J* = 243.2 Hz), 153.5, 132.9 (d, *J* = 11.3 Hz), 129.8 (d, *J* = 2.5 Hz), 117.4 (d, *J* = 23.9 Hz), 115.5 (d, *J* = 22.7 Hz), 114.4 (d, *J* = 8.8 Hz), 51.7, 40.3, 39.0, 29.0, 28.2, 27.5; ^{19}F NMR (471 MHz, $CDCl_3$) δ -119.62; HRMS (ESI+): Calculated for $C_{19}H_{21}FN_2O_3$: $[M+H]^+$ 345.1609, Found 345.1608.

Methyl-4-(7-chloro-4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)bicyclo[2.2.2]octane-1-carboxylate (18)



Obtained as a yellow solid (38 mg, 53% yield); M. P. = 177-178 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.82 (d, *J* = 2.4 Hz, 1H), 7.46 (dd, *J* = 8.9, 2.4 Hz, 1H), 7.20 (d, *J* = 8.9 Hz, 1H), 3.68 (s, 3H), 3.64 (s, 3H), 2.13 (dd, *J* = 9.7, 6.1 Hz, 6H), 1.92 (dd, *J* = 9.7, 6.2 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 178.5, 165.3, 153.5, 132.9, 131.8, 129.7, 129.5, 128.6, 114.5, 51.7, 40.4, 39.0, 29.0, 28.1, 27.5; HRMS (ESI+): Calculated for $C_{19}H_{21}ClN_2O_3$: $[M+H]^+$ 361.1314, Found 361.1316.

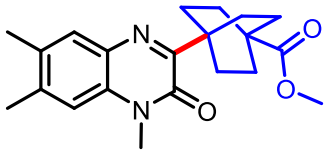
Methyl-4-(7-bromo-4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)bicyclo[2.2.2]octane-1-carboxylate (19)



Obtained as a yellow solid (40 mg, 49% yield); M. P. = 202-203 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.97 (d, *J* = 2.3 Hz, 1H), 7.58 (dd, *J* = 8.9, 2.3 Hz, 1H), 7.13 (d, *J* = 8.9 Hz, 1H), 3.67 (s, 3H), 3.63 (s, 3H), 2.12 (dd, *J* = 9.7, 6.1 Hz, 6H), 1.91 (dd, *J* = 9.7, 6.2 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ

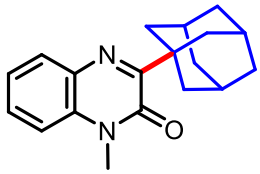
178.5, 165.2, 153.5, 133.2, 132.5, 132.4, 132.3, 115.8, 114.8, 51.7, 40.4, 39.0, 28.9, 28.1, 27.5; HRMS (ESI+): Calculated for $C_{19}H_{21}BrN_2O_3$: $[M+H]^+$ 405.0808, Found 405.0809.

Methyl-4-(4,6,7-trimethyl-3-oxo-3,4-dihydroquinoxalin-2-yl)bicyclo[2.2.2]octane-1-carboxylate (20)



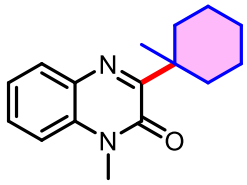
Obtained as a yellow solid (54 mg, 76% yield); M. P. = 174-175 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.55 (s, 1H), 7.01 (s, 1H), 3.66 (s, 3H), 3.61 (s, 3H), 2.38 (s, 3H), 2.32 (s, 3H), 2.17 – 2.11 (m, 6H), 1.92 – 1.87 (m, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 178.7, 162.4, 153.9, 139.4, 132.2, 131.1, 130.7, 130.2, 113.9, 51.6, 39.9, 39.1, 28.6, 28.2, 27.6, 20.5, 19.1; HRMS (ESI+): Calculated for $C_{21}H_{26}N_2O_3$: $[M+H]^+$ 355.2016, Found 355.2024.

3-(Adamantan-1-yl)-1-methylquinoxalin-2(1*H*)-one (21)



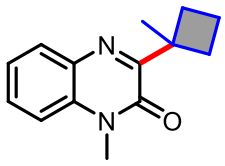
Obtained as a white solid (42 mg, 71% yield); M. P. = 155-156 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.53 – 7.47 (m, 1H), 7.34 – 7.29 (m, 1H), 7.27 (d, *J* = 5.5 Hz, 1H), 3.66 (s, 3H), 2.24 (d, *J* = 2.7 Hz, 6H), 2.11 (s, 3H), 1.85 – 1.77 (m, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.8, 153.7 133.0, 132.42, 130.1, 129.5, 123.2, 113.3, 42.0, 38.8, 37.0, 28.7, 28.6; HRMS (ESI+): Calculated for $C_{19}H_{22}N_2O$: $[M+H]^+$ 295.1805, Found 295.1819.

1-Methyl-3-(1-methylcyclohexyl)quinoxalin-2(1*H*)-one (22)



Obtained as a yellow solid (35 mg, 68% yield); M. P. = 105-106 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (dd, *J* = 7.9, 1.1 Hz, 1H), 7.48 – 7.40 (m, 1H), 7.25 (t, *J* = 7.6 Hz, 1H), 7.22 (s, 1H), 3.60 (s, 3H), 2.43 – 2.32 (m, 2H), 1.56 (dd, *J* = 25.4, 12.6 Hz, 5H), 1.44 (dd, *J* = 8.9, 5.0 Hz, 3H), 1.35 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.8, 153.8, 133.1, 132.3, 130.1, 129.5, 123.2, 113.3, 43.0, 35.8, 28.8, 26.6, 24.5, 22.9; HRMS (ESI+): Calculated for $C_{16}H_{20}N_2O$: $[M+H]^+$ 257.1648, Found 257.1653.

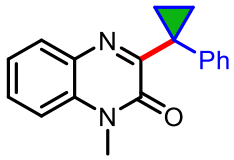
1-Methyl-3-(1-methylcyclobutyl)quinoxalin-2(1H)-one (23)



Obtained as a yellow liquid (29 mg, 64% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.52 – 7.46 (m, 1H), 7.33 – 7.28 (m, 1H), 7.28 – 7.24 (m, 1H), 3.65 (s, 3H), 2.71 – 2.57 (m,

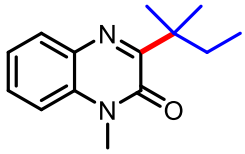
2H), 2.18 – 2.07 (m, 3H), 1.82 – 1.70 (m, 1H), 1.62 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.8, 153.4, 133.2, 132.5, 129.8, 129.4, 123.4, 113.4, 45.2, 32.6, 28.6, 24.7, 15.6; HRMS (ESI+): Calculated for $C_{14}H_{16}N_2O$: $[M+H]^+$ 229.1335, Found 229.1362.

1-Methyl-3-(1-phenylcyclopropyl)quinoxalin-2(1*H*)-one (24)



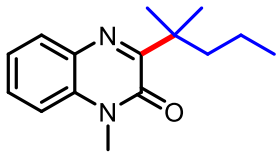
Obtained as a yellow solid (41 mg, 74% yield); M. P. = 120-121 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.0 Hz, 1H), 7.37 (d, *J* = 8.5 Hz, 3H), 7.21 (t, *J* = 7.6 Hz, 1H), 7.19 – 7.11 (m, 3H), 7.07 (t, *J* = 7.3 Hz, 1H), 3.49 (s, 3H), 1.42 – 1.37 (m, 2H), 1.30 – 1.25 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.4, 154.5, 141.9, 133.6, 132.5, 130.1, 130.0, 128.6, 128.2, 126.5, 123.4, 113.5, 30.7, 29.0, 13.8; HRMS (ESI+): Calculated for $C_{18}H_{16}N_2O$: $[M+Na]^+$ 299.1155, Found 299.1183.

1-Methyl-3-(tert-pentyl)quinoxalin-2(1*H*)-one (25)



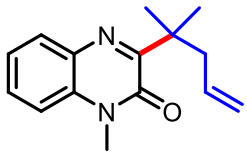
Obtained as a yellow liquid (34 mg, 74% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84 (d, *J* = 7.9 Hz, 1H), 7.53 – 7.47 (m, 1H), 7.31 (t, *J* = 7.6 Hz, 1H), 7.27 (d, *J* = 7.8 Hz, 1H), 3.67 (s, 3H), 2.05 (q, *J* = 7.5 Hz, 2H), 1.44 (s, 6H), 0.75 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.8, 153.8, 133.3, 132.3, 130.2, 129.5, 123.2, 113.3, 43.1, 32.4, 28.8, 25.9, 9.5; HRMS (ESI+): Calculated for $C_{14}H_{18}N_2O$: $[M+Na]^+$ 253.1311, Found 253.1329.

1-Methyl-3-(2-methylpentan-2-yl)quinoxalin-2(1*H*)-one (26)



Obtained as a yellow liquid (39 mg, 80% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.53 – 7.47 (m, 1H), 7.31 (t, *J* = 7.6 Hz, 1H), 7.27 – 7.25 (m, 1H), 3.67 (s, 3H), 2.01 – 1.95 (m, 2H), 1.45 (s, 6H), 1.14 (dd, *J* = 16.6, 7.5 Hz, 2H), 0.86 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.9, 153.8, 133.3, 132.2, 130.2, 129.5, 123.1, 113.3, 42.9, 42.3, 28.8, 26.4, 18.5, 14.8; HRMS (ESI+): Calculated for $C_{15}H_{20}N_2O$: $[M+Na]^+$ 267.1468, Found 267.1474.

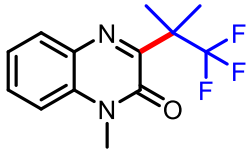
1-Methyl-3-(2-methylpent-4-en-2-yl)quinoxalin-2(1*H*)-one (27)



Obtained as a yellow liquid (26 mg, 54% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.50 (ddd, *J* = 8.6, 7.4, 1.5 Hz, 1H), 7.34 – 7.29 (m, 1H), 7.27 (d, *J* = 7.9 Hz, 1H), 5.71 (td, *J* = 17.4, 7.4 Hz, 1H), 5.06 – 4.97 (m, 1H), 4.94 – 4.87 (m, 1H), 3.67 (s, 3H), 2.78 (d, *J* = 7.4 Hz, 2H), 1.46 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.2, 153.8, 135.6, 133.3, 132.2, 130.2, 129.6, 123.2,

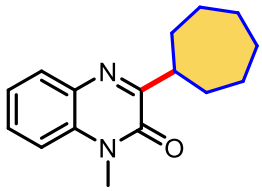
116.9, 113.3, 44.1, 42.8, 28.8, 25.9; HRMS (ESI+): Calculated for $C_{15}H_{18}N_2O$: $[M+H]^+$ 243.1492, Found 243.1515.

1-Methyl-3-(1,1,1-trifluoro-2-methylpropan-2-yl)quinoxalin-2(1*H*)-one (28)



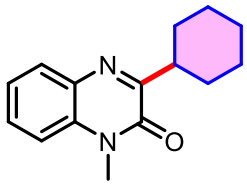
Obtained as a yellow solid (43 mg, 80% yield); M. P. = 116-117 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.88 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.60 – 7.55 (m, 1H), 7.37 – 7.33 (m, 1H), 7.30 (d, *J* = 8.4 Hz, 1H), 3.69 (s, 3H), 1.77 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.0, 153.3, 133.4, 131.6, 130.9, 130.9, 127.9 (q, *J* = 284.8 Hz), 123.6, 113.4, 49.1 (q, *J* = 25.2 Hz), 29.1, 20.2 (q, *J* = 1.3 Hz); ^{19}F NMR (471 MHz, $CDCl_3$) δ -73.57; HRMS (ESI+): Calculated for $C_{13}H_{13}F_3N_2O$: $[M+Na]^+$ 293.0872, Found 293.0872.

3-Cycloheptyl-1-methylquinoxalin-2(1*H*)-one (29)



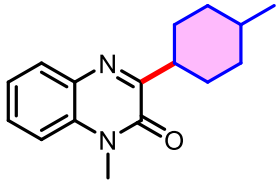
Obtained as a yellow solid (39 mg, 76% yield); M. P. = 86-87 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.53 – 7.46 (m, 1H), 7.34 – 7.29 (m, 1H), 7.29 – 7.26 (m, 1H), 3.69 (s, 3H), 3.52 – 3.45 (m, 1H), 2.01 – 1.95 (m, 2H), 1.82 (dd, *J* = 18.7, 10.1 Hz, 4H), 1.72 – 1.68 (m, 2H), 1.65 – 1.58 (m, 4H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.3, 154.5, 132.9, 132.8, 129.7, 129.3, 123.4, 113.5, 42.4, 32.3, 29.1, 28.2, 27.1; HRMS (ESI+): Calculated for $C_{16}H_{20}N_2O$: $[M+H]^+$ 257.1648, Found 257.1668.

3-Cyclohexyl-1-methylquinoxalin-2(1*H*)-one (30)



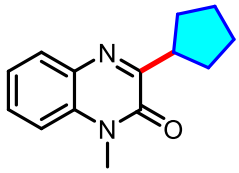
Obtained as a yellow solid (40 mg, 83% yield); M. P. = 98-99 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.47 – 7.40 (m, 1H), 7.28 – 7.22 (m, 1H), 7.20 (d, *J* = 9.6 Hz, 1H), 3.62 (s, 3H), 3.27 (tt, *J* = 11.5, 3.2 Hz, 1H), 1.88 (d, *J* = 11.3 Hz, 2H), 1.82 – 1.75 (m, 2H), 1.69 (d, *J* = 12.6 Hz, 1H), 1.50 (dd, *J* = 24.8, 9.9 Hz, 2H), 1.44 – 1.32 (m, 2H), 1.25 (t, *J* = 14.2 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.3, 154.6, 132.9, 132.9, 129.8, 129.4, 123.4, 113.5, 40.8, 30.5, 29.1, 26.3, 26.2; HRMS (ESI+): Calculated for $C_{15}H_{18}N_2O$: $[M+Na]^+$ 265.1311, Found 265.1318.

1-Methyl-3-(4-methylcyclohexyl)quinoxalin-2(1*H*)-one (31)



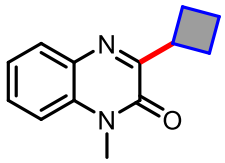
Obtained as a yellow solid (40 mg, 78% yield, 1.2:1 dr); M. P. = 118-119 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84 (t, *J* = 9.4 Hz, 1H), 7.50 (t, *J* = 7.8 Hz, 1H), 7.32 (t, *J* = 7.6 Hz, 1H), 7.28 (d, *J* = 8.2 Hz, 1H), 3.69 (d, *J* = 1.4 Hz, 3H), 3.32 (dt, *J* = 27.2, 12.3 Hz, 1H), 1.99 – 1.80 (m, 4H), 1.77 – 1.57 (m, 4H), 1.15 (dt, *J* = 13.1, 9.9 Hz, 1H), 0.99 (dd, *J* = 42.3, 6.8 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.3, 164.1, 154.6, 154.5, 132.9, 132.9, 132.8, 132.8, 129.9, 129.8, 129.4, 129.3, 123.4, 123.4, 113.5, 113.4, 40.5, 39.9, 35.0, 32.4, 31.5, 30.4, 29.1, 29.0, 28.4, 25.5, 22.8, 18.9; HRMS (ESI+): Calculated for $C_{16}H_{20}N_2O$: $[M+Na]^+$ 279.1468, Found 279.1459.

3-Cyclopentyl-1-methylquinoxalin-2(1*H*)-one (32)



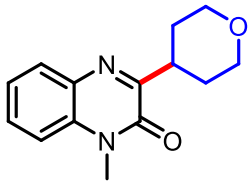
Obtained as a yellow liquid (34 mg, 75% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.44 – 7.38 (m, 1H), 7.25 – 7.21 (m, 1H), 7.20 – 7.18 (m, 1H), 3.65 – 3.60 (m, 4H), 1.98 (t, *J* = 7.9 Hz, 2H), 1.87 – 1.81 (m, 2H), 1.77 – 1.70 (m, 2H), 1.63 (dd, *J* = 11.2, 7.1 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.7, 155.0, 132.9, 132.7, 129.7, 129.3, 123.4, 113.4, 42.7, 30.8, 29.0, 25.9; HRMS (ESI+): Calculated for $C_{14}H_{16}N_2O$: $[M+H]^+$ 229.1335, Found 229.1337.

3-Cyclobutyl-1-methylquinoxalin-2(1*H*)-one (33)



Obtained as a yellow liquid (29 mg, 68% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.88 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.54 – 7.48 (m, 1H), 7.37 – 7.32 (m, 1H), 7.29 (d, *J* = 8.3 Hz, 1H), 4.07 (p, *J* = 8.4 Hz, 1H), 3.68 (s, 3H), 2.50 – 2.37 (m, 4H), 2.12 (dd, *J* = 19.1, 9.7 Hz, 1H), 1.95 – 1.86 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.3, 154.6, 133.0, 132.9, 129.8, 129.4, 123.5, 113.5, 38.4, 28.9, 26.3, 18.2; HRMS (ESI+): Calculated for $C_{13}H_{14}N_2O$: $[M+H]^+$ 215.1179, Found 215.1197.

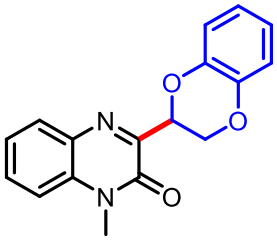
1-Methyl-3-(tetrahydro-2*H*-pyran-4-yl)quinoxalin-2(1*H*)-one (34)



Obtained as a yellow solid (39 mg, 80% yield); M. P. = 154-155 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.86 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.54 (ddd, *J* = 8.5, 7.4, 1.5 Hz, 1H), 7.37 – 7.33 (m, 1H), 7.32 – 7.29 (m, 1H), 4.14 – 4.06 (m, 2H), 3.71 (s, 3H), 3.62 (t, *J* = 11.7 Hz, 2H), 3.56 (ddd, *J* = 15.2, 7.6, 3.9 Hz,

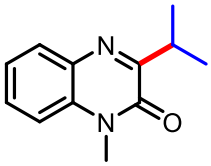
1H), 1.96 (dd, *J* = 24.1, 12.5 Hz, 2H), 1.91 – 1.86 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.0, 154.4, 132.9, 132.8, 130.0, 129.8, 123.6, 113.5, 67.9, 38.1, 30.1, 29.1; HRMS (ESI+): Calculated for $C_{14}H_{16}N_2O_2$: $[M+H]^+$ 245.1285, Found 245.1310.

3-(2,3-Dihydrobenzo[b][1,4]dioxin-2-yl)-1-methylquinoxalin-2(1*H*)-one (35)



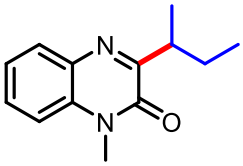
Obtained as a yellow solid (37 mg, 63% yield); M. P. = 139-140 ºC; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.90 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.63 – 7.57 (m, 1H), 7.38 – 7.32 (m, 2H), 7.09 – 7.04 (m, 1H), 6.89 (dd, *J* = 8.0, 1.5 Hz, 3H), 5.79 (dd, *J* = 6.7, 2.5 Hz, 1H), 4.61 (dd, *J* = 11.3, 2.5 Hz, 1H), 4.46 (dd, *J* = 11.3, 6.7 Hz, 1H), 3.74 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.8, 153.4, 143.7, 143.2, 133.3, 132.6, 131.3, 131.0, 124.0, 121.6, 121.5, 117.5, 117.1, 113.7, 71.4, 66.1, 29.1; HRMS (ESI+): Calculated for $C_{17}H_{14}N_2O_3$: $[M+Na]^+$ 317.0897, Found 317.0924.

3-Isopropyl-1-methylquinoxalin-2(1*H*)-one (36)



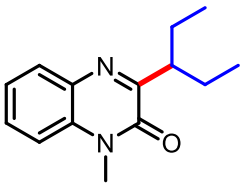
Obtained as a yellow solid (34 mg, 84% yield); M. P. = 90-91 ºC; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.54 – 7.48 (m, 1H), 7.35 – 7.31 (m, 1H), 7.29 (d, *J* = 8.4 Hz, 1H), 3.70 (s, 3H), 3.63 (dt, *J* = 13.7, 6.8 Hz, 1H), 1.32 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.0, 154.5, 133.0, 132.7, 129.8, 129.5, 123.4, 113.5, 31.2, 29.1, 20.2; HRMS (ESI+): Calculated for $C_{12}H_{14}N_2O$: $[M+Na]^+$ 225.0998, Found 225.1000.

3-(*Sec*-butyl)-1-methylquinoxalin-2(1*H*)-one (37)



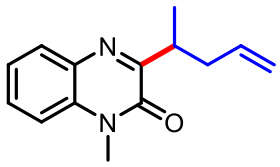
Obtained as a yellow liquid (35 mg, 81% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.55 – 7.46 (m, 1H), 7.36 – 7.27 (m, 2H), 3.71 (s, 3H), 3.46 (h, *J* = 6.9 Hz, 1H), 1.99 – 1.85 (m, 1H), 1.67 – 1.54 (m, 1H), 1.29 (d, *J* = 6.9 Hz, 3H), 0.94 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.6, 154.7, 132.9, 132.8, 129.8, 129.5, 123.4, 113.5, 37.8, 29.1, 27.6, 17.9, 12.1; HRMS (ESI+): Calculated for $C_{13}H_{16}N_2O$: $[M+H]^+$ 217.1335, Found 217.1347.

1-Methyl-3-(pentan-3-yl)quinoxalin-2(1*H*)-one (38)



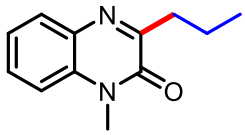
Obtained as a yellow liquid (36 mg, 78% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.0 Hz, 1H), 7.52 (t, *J* = 7.8 Hz, 1H), 7.33 (t, *J* = 8.2 Hz, 1H), 7.29 (d, *J* = 8.4 Hz, 1H), 3.71 (s, 3H), 3.39 – 3.32 (m, 1H), 1.91 – 1.84 (m, 2H), 1.74 – 1.67 (m, 2H), 0.88 (t, *J* = 7.4 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.9, 155.1, 132.9, 132.8, 129.8, 129.4, 123.4, 113.5, 44.6, 29.1, 25.8, 12.0; HRMS (ESI+): Calculated for $C_{14}H_{18}N_2O$: $[M+H]^+$ 231.1492, Found 231.1504.

1-Methyl-3-(pent-4-en-2-yl)quinoxalin-2(1*H*)-one (39)



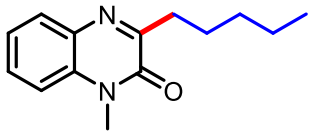
Obtained as a yellow liquid (28 mg, 61% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.52 (ddd, *J* = 8.6, 7.3, 1.5 Hz, 1H), 7.35 – 7.31 (m, 1H), 7.29 (dd, *J* = 8.4, 0.9 Hz, 1H), 5.85 (ddd, *J* = 17.0, 7.4, 6.7 Hz, 1H), 5.05 (dd, *J* = 17.1, 2.0 Hz, 1H), 5.00 – 4.94 (m, 1H), 3.70 (s, 3H), 3.63 (dd, *J* = 14.0, 6.9 Hz, 1H), 2.66 (dt, *J* = 12.9, 6.5 Hz, 1H), 2.34 (dt, *J* = 15.0, 7.5 Hz, 1H), 1.30 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 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; HRMS (ESI+): Calculated for $C_{14}H_{16}N_2O$: $[M+H]^+$ 229.1335, Found 229.1352.

1-Methyl-3-propylquinoxalin-2(1*H*)-one (40)



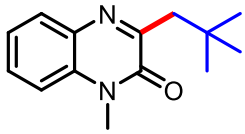
Obtained as a yellow solid (29 mg, 72% yield); M. P. = 105-106 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.55 – 7.49 (m, 1H), 7.36 – 7.31 (m, 1H), 7.30 (d, *J* = 8.4 Hz, 1H), 3.70 (s, 3H), 2.97 – 2.88 (m, 2H), 1.83 (dd, *J* = 15.1, 7.5 Hz, 2H), 1.05 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.2, 155.0, 133.1, 132.7, 129.6, 129.5, 123.5, 113.6, 36.2, 29.1, 20.3, 14.1; HRMS (ESI+): Calculated for $C_{12}H_{14}N_2O$: $[M+Na]^+$ 225.0998, Found 225.1000.

1-Methyl-3-pentylquinoxalin-2(1*H*)-one (41)



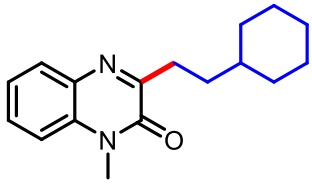
Obtained as a yellow solid (35 mg, 76% yield); M. P. = 110-111 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (dd, *J* = 7.9, 1.1 Hz, 1H), 7.54 – 7.47 (m, 1H), 7.32 (t, *J* = 7.6 Hz, 1H), 7.28 (d, *J* = 8.4 Hz, 1H), 3.69 (s, 3H), 2.96 – 2.88 (m, 2H), 1.77 (dd, *J* = 15.2, 7.5 Hz, 2H), 1.45 – 1.34 (m, 4H), 0.90 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.4, 154.9, 133.1, 132.7, 129.6, 129.5, 123.5, 113.6, 34.4, 31.8, 29.0, 26.6, 22.6, 14.1; HRMS (ESI+): Calculated for $C_{14}H_{18}N_2O$: $[M+H]^+$ 231.1492, Found 231.1513.

1-Methyl-3-neopentylquinoxalin-2(1*H*)-one (42)



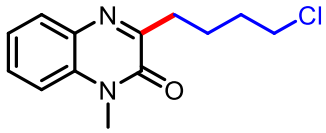
Obtained as a yellow liquid (32 mg, 70% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84 (d, *J* = 7.9 Hz, 1H), 7.53 (dd, *J* = 11.4, 4.2 Hz, 1H), 7.33 (t, *J* = 7.6 Hz, 1H), 7.30 – 7.25 (m, 1H), 3.70 (s, 3H), 2.92 (s, 2H), 1.06 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.2, 155.5, 133.2, 132.6, 129.8, 129.7, 123.5, 113.5, 45.2, 33.3, 29.9, 29.3; HRMS (ESI+): Calculated for $C_{14}H_{18}N_2O$: $[M+H]^+$ 231.1492, Found 231.1490.

3-(2-Cyclohexylethyl)-1-methylquinoxalin-2(1*H*)-one (43)



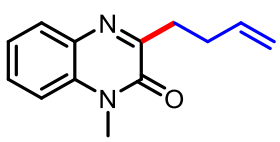
Obtained as a yellow solid (43 mg, 80% yield); M. P. = 134-135 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.55 – 7.49 (m, 1H), 7.36 – 7.28 (m, 2H), 3.70 (s, 3H), 3.00 – 2.91 (m, 2H), 1.83 (d, *J* = 13.0 Hz, 2H), 1.74 – 1.63 (m, 6H), 1.26 – 1.19 (m, 3H), 0.98 (dd, *J* = 21.1, 11.9 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.8, 154.9, 133.1, 132.8, 129.6, 129.5, 123.5, 113.6, 37.8, 34.3, 33.2, 32.0, 29.1, 26.7, 26.4; HRMS (ESI+): Calculated for $C_{17}H_{22}N_2O$: $[M+H]^+$ 271.1805, Found 271.1817.

3-(4-Chlorobutyl)-1-methylquinoxalin-2(1*H*)-one (44)



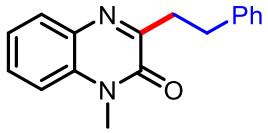
Obtained as a yellow liquid (21 mg, 42% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.0 Hz, 1H), 7.53 (t, *J* = 8.5 Hz, 1H), 7.34 (t, *J* = 7.1 Hz, 1H), 7.30 (d, *J* = 8.4 Hz, 1H), 3.70 (s, 3H), 3.61 (t, *J* = 6.4 Hz, 2H), 2.98 (t, *J* = 7.2 Hz, 2H), 1.96 – 1.93 (m, 2H), 1.26 (dd, *J* = 6.9, 3.8 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.3, 154.9, 133.1, 132.7, 129.7, 129.7, 123.6, 113.6, 44.8, 33.3, 32.4, 29.1, 23.9; HRMS (ESI+): Calculated for $C_{13}H_{15}ClN_2O$: $[M+H]^+$ 251.0946, Found 251.0953.

3-(But-3-en-1-yl)-1-methylquinoxalin-2(1*H*)-one (45)



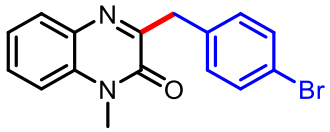
Obtained as a yellow liquid (22 mg, 51% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 7.9 Hz, 1H), 7.53 (t, *J* = 7.8 Hz, 1H), 7.34 (t, *J* = 7.6 Hz, 1H), 7.30 (d, *J* = 8.4 Hz, 1H), 5.96 (td, *J* = 16.9, 6.6 Hz, 1H), 5.11 (dd, *J* = 17.1, 1.6 Hz, 1H), 5.00 (d, *J* = 10.2 Hz, 1H), 3.71 (s, 3H), 3.09 – 3.02 (m, 2H), 2.58 (dd, *J* = 14.9, 7.1 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.3, 154.9, 137.7, 133.1, 132.7, 129.7, 123.6, 115.6, 115.2, 113.6, 33.5, 30.7, 29.1; HRMS (ESI+): Calculated for $C_{13}H_{14}N_2O$: $[M+Na]^+$ 237.0998, Found 237.1027.

1-Methyl-3-phenethylquinoxalin-2(1*H*)-one (46)



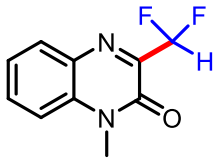
Obtained as a yellow solid (33 mg, 62% yield); M. P. = 105-106 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.54 (t, *J* = 7.1 Hz, 1H), 7.38 – 7.32 (m, 3H), 7.29 (t, *J* = 7.6 Hz, 3H), 7.19 (t, *J* = 7.1 Hz, 1H), 3.71 (s, 3H), 3.27 (dd, *J* = 9.5, 6.1 Hz, 2H), 3.13 (dd, *J* = 9.6, 6.4 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.1, 154.9, 141.7, 133.1, 132.7, 129.7, 129.7, 128.6, 128.4, 126.0, 123.6, 113.6, 36.0, 32.6, 29.1; HRMS (ESI+): Calculated for $C_{17}H_{16}N_2O$: $[M+Na]^+$ 287.1155, Found 287.1164.

3-(4-Bromobenzyl)-1-methylquinoxalin-2(1*H*)-one (47)



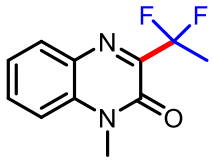
Obtained as a white solid (33 mg, 50% yield); M. P. = 124-125 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.56 – 7.51 (m, 1H), 7.40 (d, *J* = 8.4 Hz, 2H), 7.35 (dd, *J* = 11.5, 4.5 Hz, 3H), 7.28 (d, *J* = 8.4 Hz, 1H), 4.21 (s, 2H), 3.67 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 158.7, 154.7, 136.0, 133.3, 132.7, 131.5, 131.3, 130.1, 130.0, 123.7, 120.6, 113.6, 40.2, 29.2; HRMS (ESI+): Calculated for $C_{16}H_{13}BrN_2O$: $[M+H]^+$ 329.0284, Found 329.0308.

3-(Difluoromethyl)-1-methylquinoxalin-2(1*H*)-one (48)



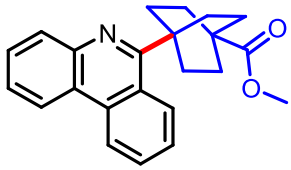
Obtained as a yellow solid (29 mg, 69% yield); M. P. = 67-68 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.00 (d, *J* = 7.9 Hz, 1H), 7.69 (t, *J* = 7.7 Hz, 1H), 7.43 (t, *J* = 7.6 Hz, 1H), 7.38 (d, *J* = 8.4 Hz, 1H), 6.96 (t, *J* = 53.7 Hz, 1H), 3.74 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.2, 148.7 (t, *J* = 21.4 Hz), 134.1, 132.7, 131.9, 131.5, 124.4, 114.0, 110.1 (t, *J* = 241.9 Hz), 29.0; ^{19}F NMR (471 MHz, $CDCl_3$) δ -124.36; HRMS (ESI+): Calculated for $C_{10}H_8F_2N_2O$: $[M+Na]^+$ 233.0497, Found 233.0500.

3-(1,1-Difluoroethyl)-1-methylquinoxalin-2(1*H*)-one (49)



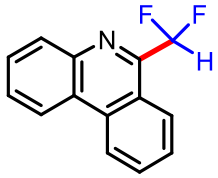
Obtained as a yellow solid (34 mg, 76% yield); M. P. = 104-105 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (dd, *J* = 8.0, 0.9 Hz, 1H), 7.68 – 7.62 (m, 1H), 7.42 – 7.32 (m, 2H), 3.72 (s, 3H), 2.13 (t, *J* = 18.9 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.4, 150.3 (t, *J* = 34.0 Hz), 134.2, 132.3, 131.3, 131.2, 124.1, 122.0, 119.6 (t, *J* = 303.7 Hz), 117.2, 113.8, 29.03, 22.45 (t, *J* = 32.8 Hz); HRMS (ESI+): Calculated for $C_{11}H_{10}F_2N_2O$: $[M+Na]^+$ 247.0653, Found 247.0682.

Methyl-4-(phenanthridin-6-yl)bicyclo[2.2.2]octane-1-carboxylate (50)



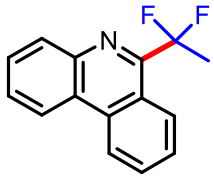
Obtained as a white solid (19 mg, 46% yield); M. P. = 132-133 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.68 (d, *J* = 8.2 Hz, 1H), 8.62 (d, *J* = 8.4 Hz, 1H), 8.52 (d, *J* = 8.0 Hz, 1H), 8.12 (s, 1H), 7.78 (t, *J* = 7.5 Hz, 1H), 7.73 – 7.68 (m, 1H), 7.66 – 7.59 (m, 2H), 3.72 (s, 3H), 2.42 – 2.37 (m, 6H), 2.08 – 2.04 (m, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 178.6, 164.9, 143.0, 134.0, 130.2, 129.4, 128.5, 127.9, 126.6, 125.9, 124.5, 123.3, 123.1, 121.7, 51.8, 41.1, 39.4, 30.6, 28.7; HRMS (ESI+): Calculated for $C_{23}H_{23}NO_2$: $[M+H]^+$ 346.1802, Found 346.1807.

6-(Difluoromethyl)phenanthridine (51)



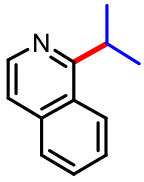
Obtained as a white solid (28 mg, 61% yield); M. P. = 97-98 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.68 (d, *J* = 8.3 Hz, 1H), 8.59 (t, *J* = 7.0 Hz, 2H), 8.27 – 8.17 (m, 1H), 7.91 (t, *J* = 7.7 Hz, 1H), 7.84 – 7.72 (m, 3H), 7.03 (t, *J* = 54.4 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 151.4 (t, *J* = 31.5 Hz), 142.5, 133.8, 131.2, 130.6, 129.1, 128.6, 128.0, 127.8, 126.5 (t, *J* = 3.8 Hz), 125.0, 122.4, 122.2, 118.37 (t, *J* = 243.2 Hz); ^{19}F NMR (471 MHz, $CDCl_3$) δ -110.56; HRMS (ESI+): Calculated for $C_{14}H_9F_2N$: $[M+H]^+$ 230.0776, Found 230.0777.

6-(1,1-Difluoroethyl)phenanthridine (52)



Obtained as a yellow liquid (32 mg, 66% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.67 (d, *J* = 8.6 Hz, 2H), 8.61 – 8.56 (m, 1H), 8.19 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.87 (ddd, *J* = 8.3, 7.1, 1.1 Hz, 1H), 7.78 – 7.71 (m, 3H), 2.35 (t, *J* = 19.5 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.0 (t, *J* = 31.5 Hz), 142.0, 133.9, 130.8, 130.7, 128.8, 128.3, 127.6 (t, *J* = 6.3 Hz), 127.5, 124.8, 124.1 (t, *J* = 239.4 Hz), 122.7, 122.3, 122.0, 23.1 (t, *J* = 26.5 Hz); ^{19}F NMR (471 MHz, $CDCl_3$) δ -83.42; HRMS (ESI+): Calculated for $C_{15}H_{11}F_2N$: $[M+H]^+$ 244.0932, Found 244.0933.

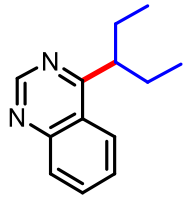
1-Isopropylisoquinoline (53)



Obtained as a colourless liquid (9 mg, 26% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.49 (d, *J* = 5.7 Hz, 1H), 8.23 (d, *J* = 8.5 Hz, 1H), 7.81 (d, *J* = 8.1 Hz, 1H), 7.68 – 7.62 (m, 1H), 7.58 (ddd, *J* = 8.2, 6.9, 1.2 Hz, 1H), 7.49 (d, *J* = 5.7 Hz, 1H), 3.96 (dt, *J* = 13.6, 6.8 Hz, 1H), 1.45 (d, *J* = 6.8 Hz, 6H); ^{13}C

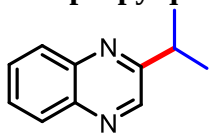
NMR (126 MHz, $CDCl_3$) δ 166.3, 141.9, 136.4, 129.6, 127.6, 126.9, 126.3, 124.8, 119.0, 31.0, 22.2; HRMS (ESI+): Calculated for $C_{12}H_{13}N$: $[M+H]^+$ 172.1121, Found 172.1122.

4-(Pentan-3-yl)quinazoline (54)



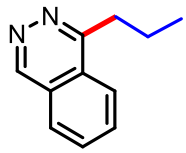
Obtained as a colourless liquid (9 mg, 22% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.30 (s, 1H), 8.21 (d, *J* = 8.4 Hz, 1H), 8.07 (d, *J* = 8.0 Hz, 1H), 7.89 (t, *J* = 7.4 Hz, 1H), 7.70 – 7.57 (m, 1H), 3.52 (ddd, *J* = 8.3, 5.4, 2.9 Hz, 1H), 2.01 – 1.94 (m, 2H), 1.89 – 1.80 (m, 2H), 0.80 (t, *J* = 7.4 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 175.2, 154.7, 149.9, 133.5, 129.2, 127.4, 125.1, 124.4, 44.9, 27.8, 12.2; HRMS (ESI+): Calculated for $C_{13}H_{16}N_2$: $[M+H]^+$ 201.1386, Found 201.1385.

2-Isopropylquinoxaline (55)



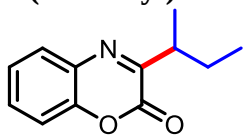
Obtained as a colourless liquid (7 mg, 20% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.79 (s, 1H), 8.11 – 8.03 (m, 2H), 7.79 – 7.66 (m, 2H), 3.33 (dt, *J* = 13.9, 6.9 Hz, 1H), 1.45 (d, *J* = 6.9 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.9, 144.8, 142.1, 141.4, 129.9, 129.1, 129.0, 128.9, 35.0, 22.0; HRMS (ESI+): Calculated for $C_{11}H_{12}N_2$: $[M+H]^+$ 173.1073, Found 173.1074.

1-Propylphthalazine (56)



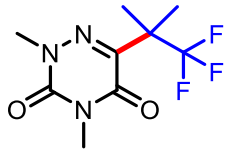
Obtained as a colourless liquid (6 mg, 17% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.42 (s, 1H), 8.14 (d, *J* = 7.8 Hz, 1H), 7.98 – 7.89 (m, 3H), 3.38 – 3.33 (m, 2H), 1.95 (dd, *J* = 15.2, 7.5 Hz, 2H), 1.09 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.5, 150.4, 132.4, 132.0, 127.0, 126.6, 125.7, 124.1, 35.2, 22.8, 14.3; HRMS (ESI+): Calculated for $C_{11}H_{12}N_2$: $[M+H]^+$ 173.1073, Found 173.1073.

3-(*sec*-Butyl)-2*H*-benzo[*b*][1,4]oxazin-2-one (57)



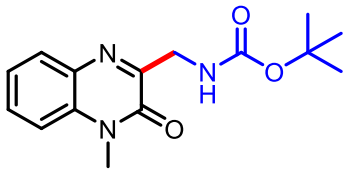
Obtained as a yellow liquid (17 mg, 42% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.42 (s, 1H), 8.14 (d, *J* = 7.8 Hz, 1H), 7.98 – 7.89 (m, 3H), 3.38 – 3.33 (m, 2H), 1.95 (dd, *J* = 15.2, 7.5 Hz, 2H), 1.09 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.6, 152.7, 146.2, 131.3, 130.4, 128.9, 125.3, 116.3, 38.5, 27.3, 17.5, 11.9; HRMS (ESI+): Calculated for $C_{12}H_{13}NO_2$: $[M+H]^+$ 204.1019, Found 204.1015.

2,4-Dimethyl-6-(1,1,1-trifluoro-2-methylpropan-2-yl)-1,2,4-triazine-3,5(2*H*,4*H*)-dione (58)



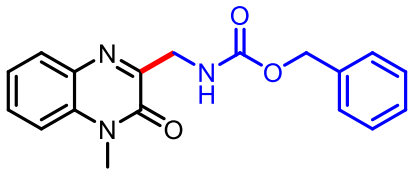
Obtained as a white solid (11 mg, 22% yield); M. P. = 107-108 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 3.64 (s, 3H), 3.33 (s, 3H), 1.59 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.8, 148.9, 140.6, 127.3 (q, *J* = 284.8 Hz), 46.4 (q, *J* = 26.5 Hz), 39.9, 27.3, 20.3; ^{19}F NMR (471 MHz, $CDCl_3$) δ -74.58; HRMS (ESI+): Calculated for $C_9H_{12}F_3N_3O_2$: $[M+H]^+$ 252.0954, Found 252.0955.

***Tert*-butyl ((4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)methyl)carbamate (59)**



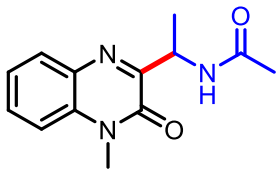
Obtained as a yellow solid (35 mg, 61% yield); M. P. = 152-153 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.88 (d, *J* = 7.9 Hz, 1H), 7.57 (dd, *J* = 11.4, 4.2 Hz, 1H), 7.36 (t, *J* = 7.9 Hz, 1H), 7.33 (d, *J* = 8.4 Hz, 1H), 5.79 (s, 1H), 4.58 (d, *J* = 3.3 Hz, 2H), 3.71 (s, 3H), 1.49 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.8, 155.0, 154.0, 133.1, 132.2, 130.3, 129.9, 123.8, 113.7, 76.8, 43.0, 28.9, 28.5; HRMS (ESI+): Calculated for $C_{15}H_{19}N_3O_3$: $[M+Na]^+$ 312.1319, Found 312.1325.

Benzyl-((4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)methyl)carbamate (60)



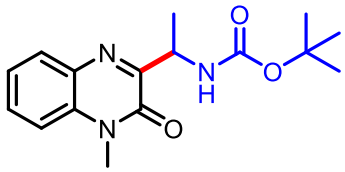
Obtained as a yellow liquid (35 mg, 54% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84 (d, *J* = 7.8 Hz, 1H), 7.57 (t, *J* = 7.7 Hz, 1H), 7.36 (dd, *J* = 29.0, 13.0 Hz, 7H), 6.09 (s, 1H), 5.18 (s, 2H), 4.66 (d, *J* = 4.5 Hz, 2H), 3.70 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.3, 154.5, 153.9, 136.6, 133.1, 132.1, 130.4, 129.9, 128.5, 128.2, 128.1, 123.9, 113.8, 66.9, 43.3, 29.0; HRMS (ESI+): Calculated for $C_{18}H_{17}N_3O_3$: $[M+Na]^+$ 346.1162, Found 346.1183.

***N*-(1-(4-Methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)ethyl)acetamide (61)**



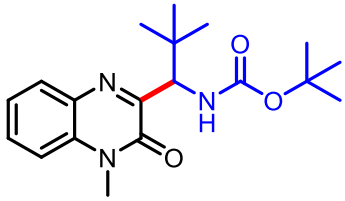
Obtained as a yellow solid (26 mg, 53% yield); M. P. = 129-130 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.86 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.62 – 7.55 (m, 1H), 7.40 – 7.36 (m, 1H), 7.34 (d, *J* = 8.4 Hz, 1H), 7.02 (d, *J* = 7.0 Hz, 1H), 5.57 – 5.49 (m, 1H), 3.72 (s, 3H), 2.08 (s, 3H), 1.53 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 169.2, 158.9, 153.6, 133.3, 132.0, 130.5, 129.9, 123.9, 113.8, 47.7, 29.1, 23.6, 20.0; HRMS (ESI+): Calculated for $C_{13}H_{15}N_3O_2$: $[M+Na]^+$ 268.1056, Found 268.1073.

***Tert*-butyl-(1-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)ethyl)carbamate (62)**



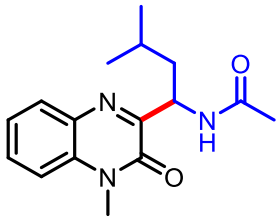
Obtained as a yellow solid (39 mg, 64% yield); M. P. = 75-76 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.55 (t, *J* = 7.4 Hz, 1H), 7.33 (dd, *J* = 18.0, 8.0 Hz, 2H), 5.94 (d, *J* = 6.6 Hz, 1H), 5.30 – 5.07 (m, 1H), 3.69 (s, 3H), 1.49 (d, *J* = 6.8 Hz, 3H), 1.45 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 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 $C_{16}H_{21}N_3O_3$: $[M+Na]^+$ 326.1475, Found 326.1488.

***Tert*-butyl-(2,2-dimethyl-1-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)propyl)carbamate (63)**



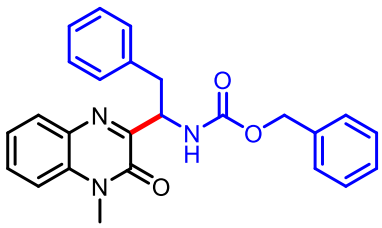
Obtained as a yellow liquid (41 mg, 59% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (d, *J* = 7.9 Hz, 1H), 7.55 (t, *J* = 7.8 Hz, 1H), 7.34 (t, *J* = 7.6 Hz, 1H), 7.30 (d, *J* = 8.4 Hz, 1H), 5.86 (d, *J* = 6.5 Hz, 1H), 5.33 (d, *J* = 9.7 Hz, 1H), 3.69 (s, 3H), 1.43 (s, 9H), 1.01 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.2, 155.6, 154.5, 133.2, 132.1, 130.4, 130.1, 123.5, 113.6, 79.1, 57.6, 37.1, 29.3, 28.4, 26.6; HRMS (ESI+): Calculated for $C_{19}H_{27}N_3O_3$: $[M+Na]^+$ 368.1945, Found 368.1966.

***N*-(3-Methyl-1-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)butyl)acetamide (64)**



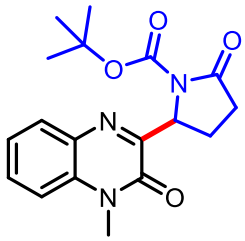
Obtained as a yellow solid (34 mg, 59% yield); M. P. = 105-106 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.59 – 7.52 (m, 1H), 7.36 (t, *J* = 7.6 Hz, 1H), 7.32 (d, *J* = 8.4 Hz, 1H), 6.72 (d, *J* = 9.1 Hz, 1H), 5.57 (td, *J* = 9.2, 4.6 Hz, 1H), 3.70 (s, 3H), 2.04 (s, 3H), 1.68 (dt, *J* = 17.0, 10.8 Hz, 3H), 1.04 (d, *J* = 5.9 Hz, 3H), 0.95 (d, *J* = 6.0 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.5, 158.9, 154.0, 133.2, 132.3, 130.4, 130.0, 123.9, 113.7, 50.9, 43.2, 29.0, 25.3, 23.6, 23.2, 22.0; HRMS (ESI+): Calculated for $C_{16}H_{21}N_3O_2$: $[M+H]^+$ 288.1707, Found 288.1740.

Benzyl-(1-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)-2-phenylethyl)carbamate (65)



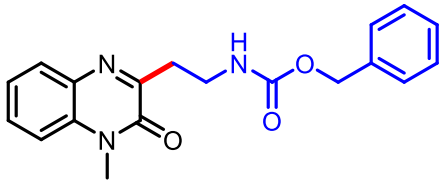
Obtained as a yellow solid (45 mg, 54% yield); M. P. = 128-129 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.62 (d, *J* = 7.8 Hz, 1H), 7.43 (t, *J* = 7.6 Hz, 1H), 7.19 (dd, *J* = 12.6, 8.1 Hz, 7H), 7.06 (t, *J* = 7.6 Hz, 4H), 6.99 (d, *J* = 6.7 Hz, 1H), 5.98 (d, *J* = 8.6 Hz, 1H), 5.49 (dd, *J* = 13.4, 7.3 Hz, 1H), 4.97 (dd, *J* = 27.3, 12.2 Hz, 2H), 3.58 (s, 3H), 3.29 (dd, *J* = 13.7, 5.0 Hz, 1H), 3.04 (dd, *J* = 13.7, 7.1 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.4, 155.7, 153.8, 136.9, 136.7, 133.2, 132.1, 130.5, 130.1, 129.7, 128.5, 128.2, 128.1, 128.1, 126.5, 123.8, 113.7, 66.6, 54.1, 39.2, 29.1; HRMS (ESI+): Calculated for $C_{25}H_{23}N_3O_3$: $[M+H]^+$ 414.1812, Found 414.1826.

***Tert*-butyl-2-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)-5-oxopyrrolidine-1-carboxylate (66)**



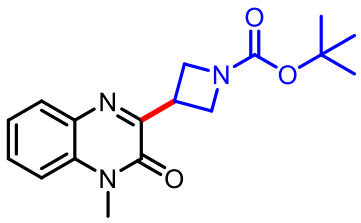
Obtained as a yellow liquid (43 mg, 63% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.86 – 7.80 (m, 1H), 7.60 – 7.54 (m, 1H), 7.35 (t, *J* = 8.1 Hz, 2H), 5.73 (dd, *J* = 8.7, 2.1 Hz, 1H), 3.73 (s, 3H), 2.62 (dt, *J* = 17.3, 8.5 Hz, 1H), 2.57 – 2.48 (m, 2H), 2.00 (dd, *J* = 11.7, 9.8 Hz, 1H), 1.33 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 174.7, 157.2, 153.7, 149.7, 133.2, 132.2, 130.6, 130.4, 124.1, 113.7, 82.7, 58.1, 31.2, 29.0, 27.9, 22.7; HRMS (ESI+): Calculated for $C_{18}H_{21}N_3O_4$: $[M+Na]^+$ 366.1424, Found 366.1444.

Benzyl-(2-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)ethyl)carbamate (67)



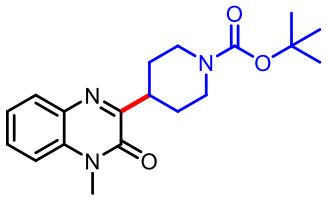
Obtained as a yellow solid (35 mg, 52% yield); M. P. = 72-73 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.82 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.58 – 7.52 (m, 1H), 7.38 – 7.27 (m, 7H), 5.57 (s, 1H), 5.06 (s, 2H), 3.74 (d, *J* = 5.7 Hz, 2H), 3.70 (s, 3H), 3.16 (t, *J* = 5.8 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 158.7, 156.4, 155.0, 136.7, 133.1, 132.4, 130.1, 129.8, 128.5, 128.2, 128.1, 123.7, 113.7, 66.6, 37.8, 33.9, 29.1; HRMS (ESI+): Calculated for $C_{19}H_{19}N_3O_3$: $[M+Na]^+$ 360.1319, Found 360.1303.

***Tert*-butyl 3-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)azetidine-1-carboxylate (68)**



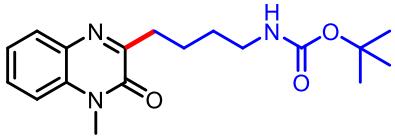
Obtained as a yellow solid (43 mg, 68% yield); M. P. = 84-85 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.60 – 7.54 (m, 1H), 7.41 – 7.35 (m, 1H), 7.33 (d, *J* = 8.4 Hz, 1H), 4.31 (d, *J* = 7.1 Hz, 4H), 4.23 – 4.13 (m, 1H), 3.70 (s, 3H), 1.45 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.4, 156.5, 154.4, 133.1, 132.5, 130.3, 130.2, 123.9, 113.7, 79.4, 52.4, 32.0, 29.0, 28.4; HRMS (ESI+): Calculated for $C_{17}H_{21}N_3O_3$: $[M+Na]^+$ 338.1475, Found 338.1479.

***Tert*-butyl 4-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)piperidine-1-carboxylate (69)**



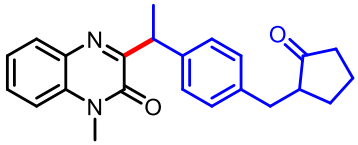
Obtained as a yellow solid (34 mg, 50% yield); M. P. = 99-100 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.57 – 7.50 (m, 1H), 7.38 – 7.32 (m, 1H), 7.30 (d, *J* = 8.3 Hz, 1H), 4.23 (s, 2H), 3.71 (s, 3H), 3.52 – 3.42 (m, 1H), 2.91 (t, *J* = 12.3 Hz, 2H), 1.93 (d, *J* = 12.7 Hz, 2H), 1.76 (ddd, *J* = 25.1, 12.6, 4.3 Hz, 2H), 1.47 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.2, 154.8, 154.4, 132.9, 132.7, 130.0, 129.8, 123.6, 113.6, 79.4, 48.0, 39.0, 29.4, 29.1, 28.5; HRMS (ESI+): Calculated for $C_{19}H_{25}N_3O_3$: $[M+Na]^+$ 366.1788, Found 366.1798.

***Tert*-butyl (4-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)butyl)carbamate (70)**



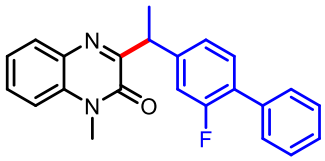
Obtained as a yellow liquid (38 mg, 57% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (d, *J* = 7.9 Hz, 1H), 7.53 (dd, *J* = 11.4, 4.1 Hz, 1H), 7.33 (t, *J* = 7.5 Hz, 1H), 7.30 (d, *J* = 8.3 Hz, 1H), 4.79 (s, 1H), 3.70 (s, 3H), 3.19 (d, *J* = 4.2 Hz, 2H), 2.96 (t, *J* = 7.5 Hz, 2H), 1.85 (dd, *J* = 15.1, 7.5 Hz, 2H), 1.63 (dd, *J* = 14.9, 7.2 Hz, 2H), 1.44 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.6, 156.0, 154.9, 133.1, 132.6, 129.7, 129.7, 123.6, 113.6, 76.8, 40.4, 33.6, 29.7, 29.1, 28.5, 23.6; HRMS (ESI+): Calculated for $C_{18}H_{25}N_3O_3$: $[M+H]^+$ 332.1969, Found 332.1983.

1-Methyl-3-(4-((2-oxocyclopentyl)methyl)phenyl)ethyl)quinoxalin-2(1*H*)-one (71)



Obtained as a yellow liquid (45 mg, 62% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.0 Hz, 1H), 7.51 (t, *J* = 7.8 Hz, 1H), 7.35 (dd, *J* = 8.3, 1.9 Hz, 3H), 7.25 (d, *J* = 7.2 Hz, 1H), 7.07 (d, *J* = 8.0 Hz, 2H), 4.81 (dd, *J* = 7.1, 3.2 Hz, 1H), 3.63 (s, 3H), 3.09 (dd, *J* = 13.9, 3.8 Hz, 1H), 2.44 (dd, *J* = 13.9, 9.8 Hz, 1H), 2.35 – 2.27 (m, 2H), 2.14 – 2.04 (m, 2H), 1.96 – 1.88 (m, 1H), 1.69 (dd, *J* = 23.7, 7.8 Hz, 4H), 1.53 (dd, *J* = 17.0, 6.0 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.9, 161.9, 154.4, 141.0, 138.2, 133.1, 132.7, 130.1, 129.7, 128.9, 128.2, 123.4, 113.5, 51.0, 41.4, 38.2, 35.3, 29.3, 29.1, 20.5, 19.7; HRMS (ESI+): Calculated for $C_{23}H_{24}N_2O_2$: $[M+Na]^+$ 383.1730, Found 383.1754.

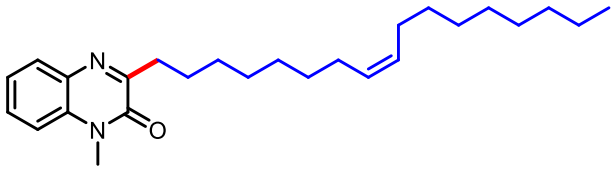
3-(1-(2-Fluoro-[1,1'-biphenyl]-4-yl)ethyl)-1-methylquinoxalin-2(1*H*)-one (72)



Obtained as a yellow liquid (39 mg, 54% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.41 (dd, *J* = 11.7, 7.6 Hz, 3H), 7.29 (t, *J* = 7.6 Hz, 2H), 7.23 (dt, *J* = 11.9, 8.8 Hz, 4H), 7.15 (dd, *J* = 13.9, 9.3 Hz, 2H), 4.77 (q, *J* = 7.1 Hz, 1H), 3.54 (s, 3H), 1.62 (d, *J* = 7.1 Hz, 3H); ^{13}C NMR

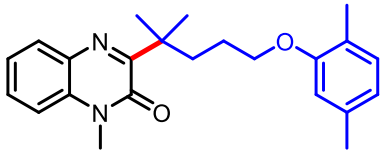
(126 MHz, $CDCl_3$) δ 161.2, 159.7 (d, *J* = 248.2 Hz), 154.5, 144.9 (d, *J* = 7.6 Hz), 135.9, 133.1, 132.7, 130.6 (d, *J* = 3.8 Hz), 130.2, 130.0, 129.0 (d, *J* = 2.5 Hz), 128.4, 127.5, 127.1 (d, *J* = 13.9 Hz), 124.2 (d, *J* = 3.8 Hz), 123.6, 115.5 (d, *J* = 23.9 Hz), 113.6, 41.4, 29.2, 19.6; ^{19}F NMR (471 MHz, $CDCl_3$) δ -118.04; HRMS (ESI+): Calculated for $C_{23}H_{19}FN_2O$: $[M+H]^+$ 359.1554, Found 359.1575.

3-(Heptadec-8-en-1-yl)-1-methylquinoxalin-2(1*H*)-one (73)



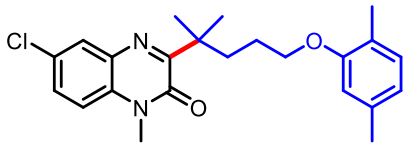
Obtained as a yellow liquid (60 mg, 76% yield); ^1H NMR (400 MHz, $CDCl_3$) δ 7.76 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.48 – 7.42 (m, 1H), 7.29 – 7.24 (m, 1H), 7.22 (d, *J* = 8.3 Hz, 1H), 5.32 – 5.22 (m, 2H), 3.63 (s, 3H), 2.90 – 2.82 (m, 2H), 1.94 (d, *J* = 5.4 Hz, 4H), 1.71 (dt, *J* = 15.4, 7.6 Hz, 2H), 1.34 – 1.07 (m, 20H), 0.80 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.4, 154.9, 133.1, 132.8, 129.9, 129.9, 129.6, 129.5, 123.5, 113.6, 34.4, 31.9, 29.8, 29.8, 29.7, 29.7, 29.6, 29.6, 29.4, 29.3, 29.3, 29.1, 27.2, 26.9, 22.7, 14.2; HRMS (ESI+): Calculated for $C_{26}H_{40}N_2O$: $[M+Na]^+$ 419.3033, Found 419.3059.

3-(5-(2,5-Dimethylphenoxy)-2-methylpentan-2-yl)-1-methylquinoxalin-2(1*H*)-one (74)



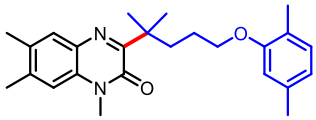
Obtained as a yellow liquid (55 mg, 76% yield); M. P. = 107-108 °C; ^1H NMR (500 MHz, $CDCl_3$) δ 7.83 (d, *J* = 7.9 Hz, 1H), 7.49 (t, *J* = 7.7 Hz, 1H), 7.30 (t, *J* = 7.6 Hz, 1H), 7.23 (d, *J* = 8.5 Hz, 1H), 6.96 (d, *J* = 7.4 Hz, 1H), 6.60 (d, *J* = 7.4 Hz, 1H), 6.52 (s, 1H), 3.87 (t, *J* = 6.6 Hz, 2H), 3.63 (s, 3H), 2.24 (s, 3H), 2.22 – 2.17 (m, 2H), 2.15 (s, 3H), 1.69 – 1.64 (m, 2H), 1.50 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.4, 157.0, 153.7, 136.4, 133.3, 132.2, 130.2, 129.6, 129.5, 123.6, 123.2, 120.5, 113.3, 111.9, 68.1, 42.6, 36.0, 28.8, 26.4, 25.4, 21.4, 15.8; HRMS (ESI+): Calculated for $C_{23}H_{28}N_2O_2$: $[M+Na]^+$ 387.2043, Found 387.2061.

6-Chloro-3-(5-(2,5-dimethylphenoxy)-2-methylpentan-2-yl)-1-methylquinoxalin-2(1*H*)-one (75)



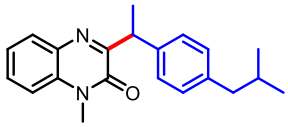
Obtained as a yellow solid (43 mg, 54% yield); M. P. = 121-122 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 2.4 Hz, 1H), 7.45 (dd, *J* = 8.9, 2.4 Hz, 1H), 7.15 (d, *J* = 8.9 Hz, 1H), 6.97 (d, *J* = 7.4 Hz, 1H), 6.61 (d, *J* = 7.4 Hz, 1H), 6.51 (s, 1H), 3.87 (t, *J* = 6.6 Hz, 2H), 3.60 (s, 3H), 2.25 (s, 3H), 2.20 – 2.14 (m, 5H), 1.70 – 1.64 (m, 2H), 1.48 (d, *J* = 4.8 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.9, 156.9, 153.3, 136.4, 132.7, 132.0, 130.2, 129.6, 129.5, 128.5, 123.5, 120.5, 114.5, 111.8, 67.9, 42.8, 35.8, 28.9, 26.3, 25.3, 21.4, 15.8; HRMS (ESI+): Calculated for $C_{23}H_{27}ClN_2O_2$: $[M+H]^+$ 399.1834, Found 399.1838.

3-(5-(2,5-Dimethylphenoxy)-2-methylpentan-2-yl)-1,6,7-trimethylquinoxalin-2(1*H*)-one (76)



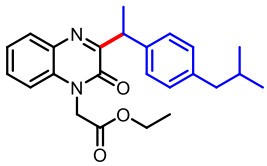
Obtained as a white solid (55 mg, 70% yield); M. P. = 99-100 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (s, 1H), 7.01 (s, 1H), 6.97 (d, *J* = 7.4 Hz, 1H), 6.61 (d, *J* = 7.4 Hz, 1H), 6.53 (s, 1H), 3.87 (t, *J* = 6.7 Hz, 2H), 3.62 (s, 3H), 2.41 (s, 3H), 2.35 (s, 3H), 2.25 (s, 3H), 2.18 (dd, *J* = 7.6, 4.4 Hz, 2H), 2.15 (s, 3H), 1.66 (dd, *J* = 10.4, 6.1 Hz, 2H), 1.50 (s, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.1, 157.0, 153.8, 139.3, 136.3, 132.0, 131.3, 130.6, 130.3, 130.2, 123.5, 120.4, 113.9, 111.8, 68.1, 42.4, 35.9, 28.7, 26.4, 25.4, 21.4, 20.5, 19.1, 15.8; HRMS (ESI+): Calculated for $C_{25}H_{32}N_2O_2$: $[M+Na]^+$ 415.2356, Found 415.2390.

3-(1-(4-Isobutylphenyl)ethyl)-1-methylquinoxalin-2(1*H*)-one (77)



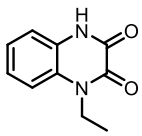
Obtained as a white solid (48 mg, 75% yield); M. P. = 113-114 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.91 (d, *J* = 7.9 Hz, 1H), 7.49 (t, *J* = 7.4 Hz, 1H), 7.33 (t, *J* = 8.1 Hz, 3H), 7.25 – 7.23 (m, 1H), 7.04 (d, *J* = 8.0 Hz, 2H), 4.81 (q, *J* = 7.1 Hz, 1H), 3.62 (s, 3H), 2.40 (d, *J* = 7.1 Hz, 2H), 1.81 (dt, *J* = 13.5, 6.7 Hz, 1H), 1.67 (d, *J* = 7.1 Hz, 3H), 0.87 (dd, *J* = 6.6, 2.1 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.1, 154.5, 140.3, 139.8, 133.1, 132.8, 130.1, 129.6, 129.1, 127.8, 123.4, 113.5, 45.1, 41.4, 30.2, 29.1, 22.5, 22.4, 19.7; HRMS (ESI+): Calculated for $C_{21}H_{24}N_2O$: $[M+H]^+$ 321.1961, Found 321.1954.

Ethyl-2-(3-(1-(4-isobutylphenyl)ethyl)-2-oxoquinoxalin-1(2H)-yl)acetate (78)



Obtained as a white solid (56 mg, 71% yield); M. P. = 124-125 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.94 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.51 – 7.44 (m, 1H), 7.37 – 7.31 (m, 3H), 7.04 (dd, *J* = 11.3, 8.3 Hz, 3H), 5.08 (d, *J* = 17.3 Hz, 1H), 4.86 – 4.76 (m, 2H), 4.24 – 4.16 (m, 2H), 2.40 (d, *J* = 7.2 Hz, 2H), 1.82 (dt, *J* = 13.5, 6.8 Hz, 1H), 1.68 (d, *J* = 7.1 Hz, 3H), 1.22 (t, *J* = 7.1 Hz, 3H), 0.87 (dd, *J* = 6.6, 2.4 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 167.2, 161.9, 154.1, 140.1, 139.9, 132.8, 132.2, 130.5, 129.8, 129.2, 127.8, 123.7, 112.9, 62.0, 45.1, 43.6, 41.4, 30.2, 22.5, 22.4, 19.7, 14.1; HRMS (ESI+): Calculated for $C_{24}H_{28}N_2O_3$: $[M+H]^+$ 393.2173, Found 393.2173.

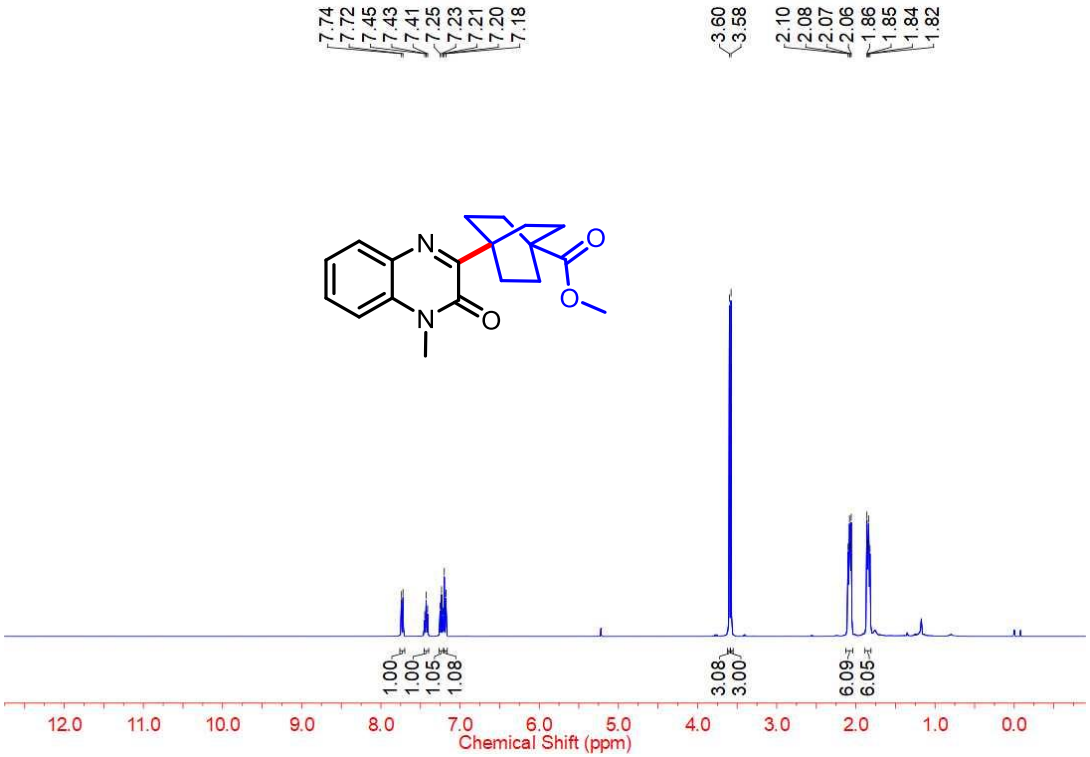
1-Ethyl-1,4-dihydroquinoxaline-2,3-dione (82)



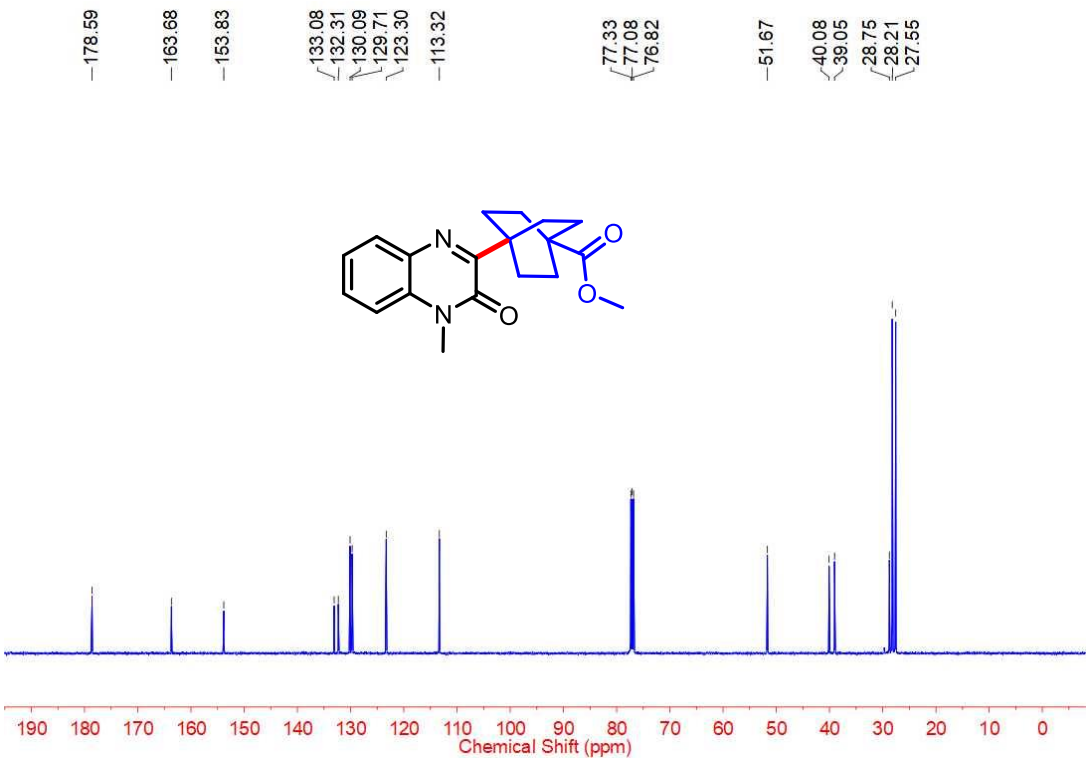
Obtained as a white solid (27 mg, 71% yield); ^{1}H NMR (500 MHz, DMSO) δ 12.03 (s, 1H), 7.41 (d, *J* = 7.8 Hz, 1H), 7.22 – 7.17 (m, 3H), 4.15 (q, *J* = 7.1 Hz, 2H), 1.22 (t, *J* = 7.1 Hz, 3H).

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

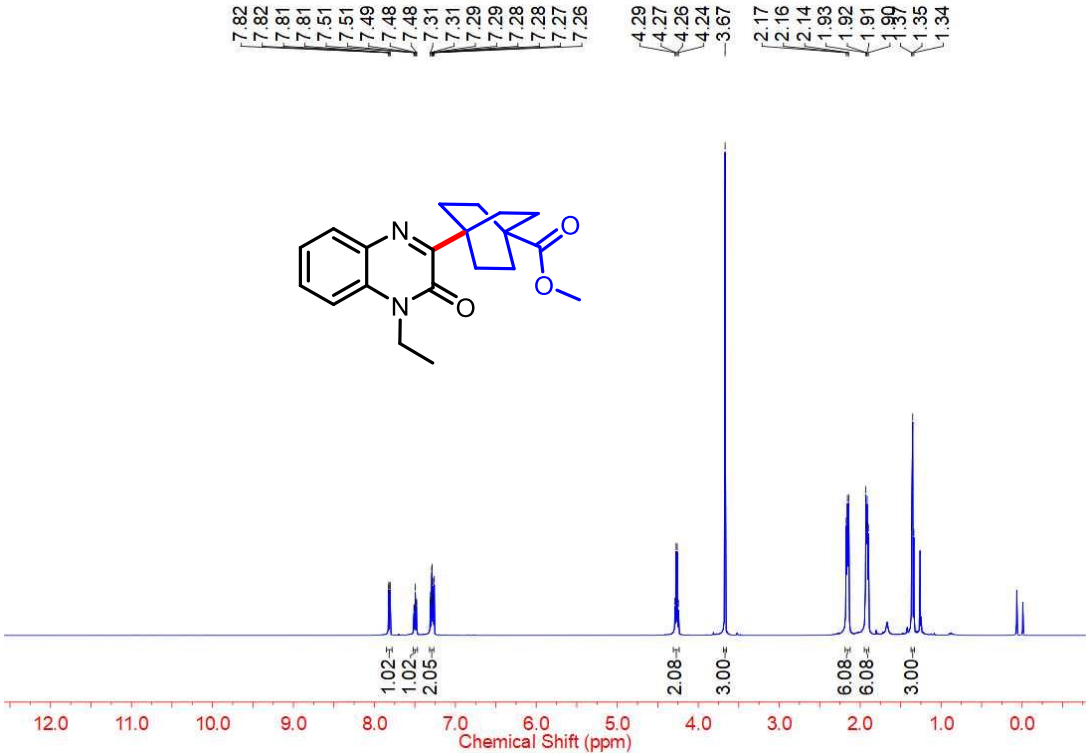
3 ^{1}H NMR (400 MHz, $CDCl_3$)



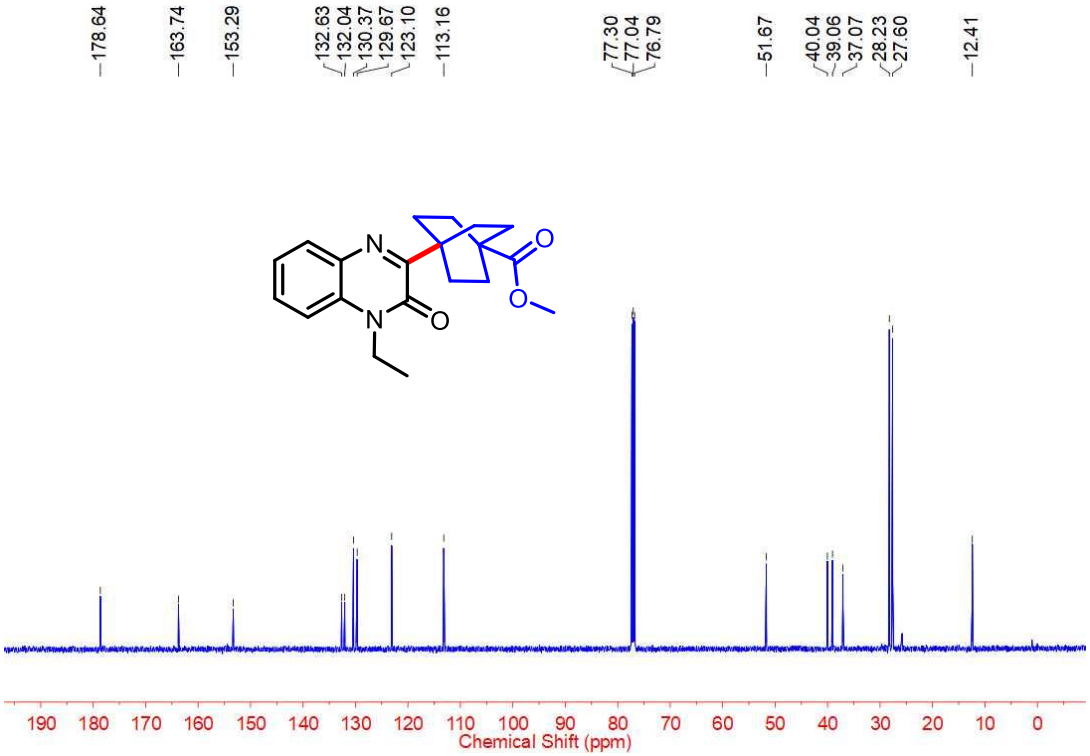
3 ^{13}C NMR (100 MHz, $CDCl_3$)



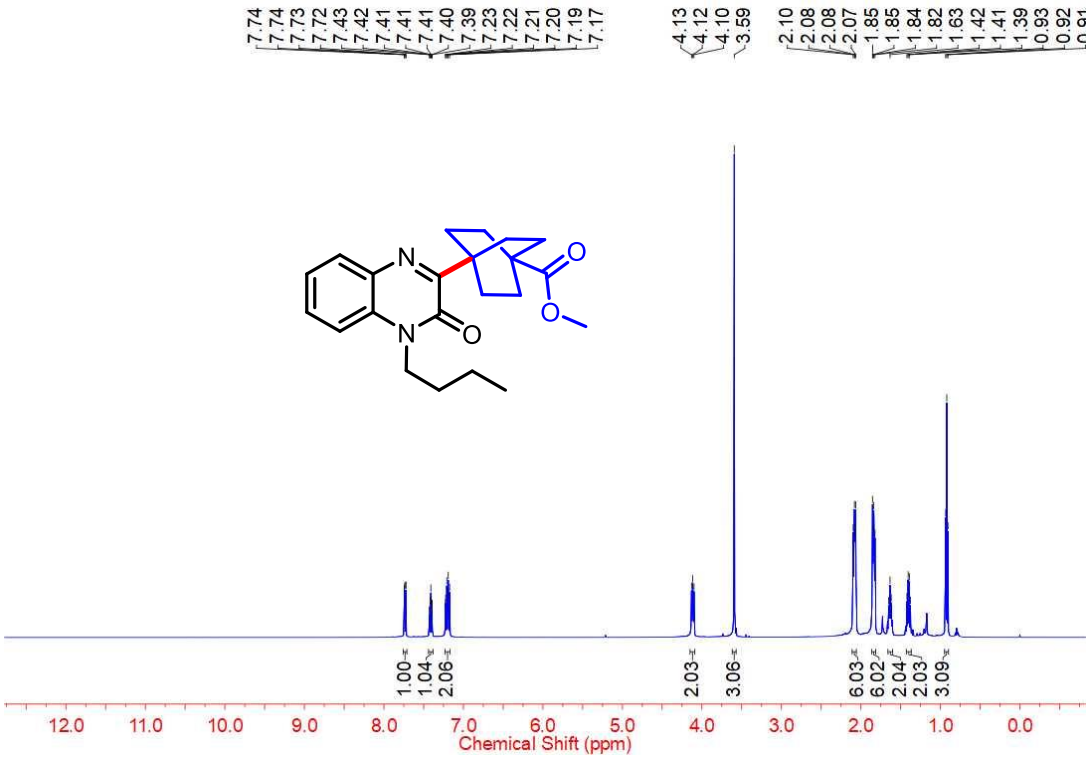
4 ^{1}H NMR (500 MHz, $CDCl_3$)



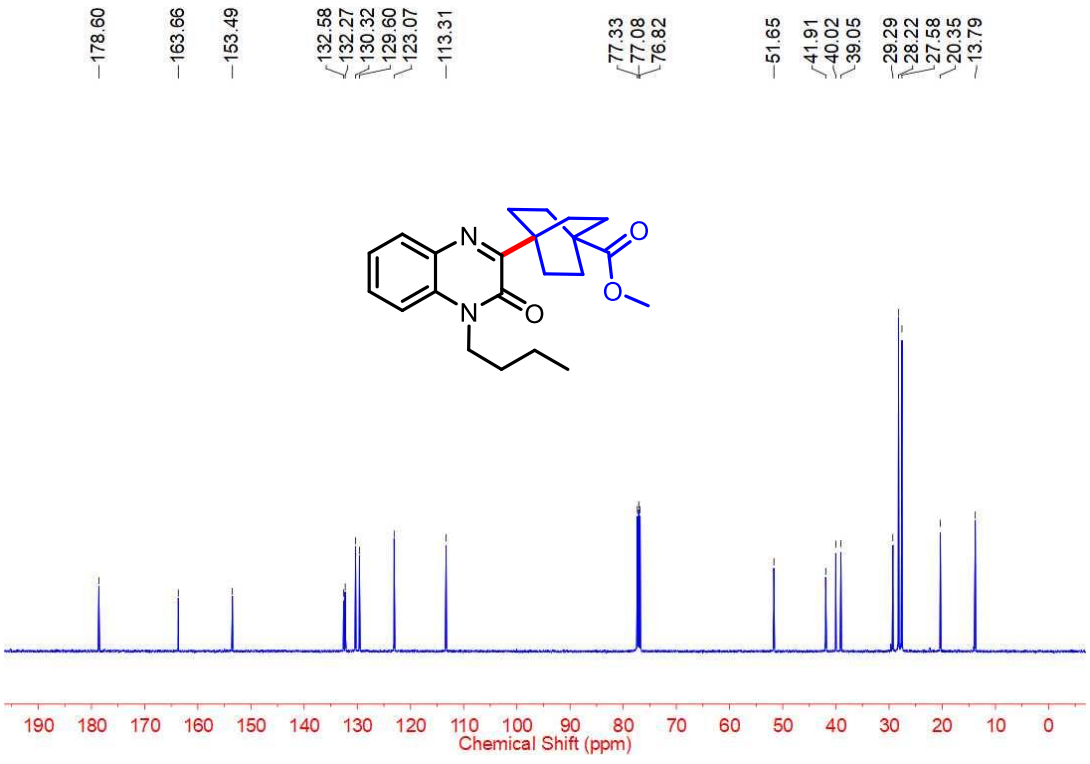
4 ^{13}C NMR (126 MHz, $CDCl_3$)



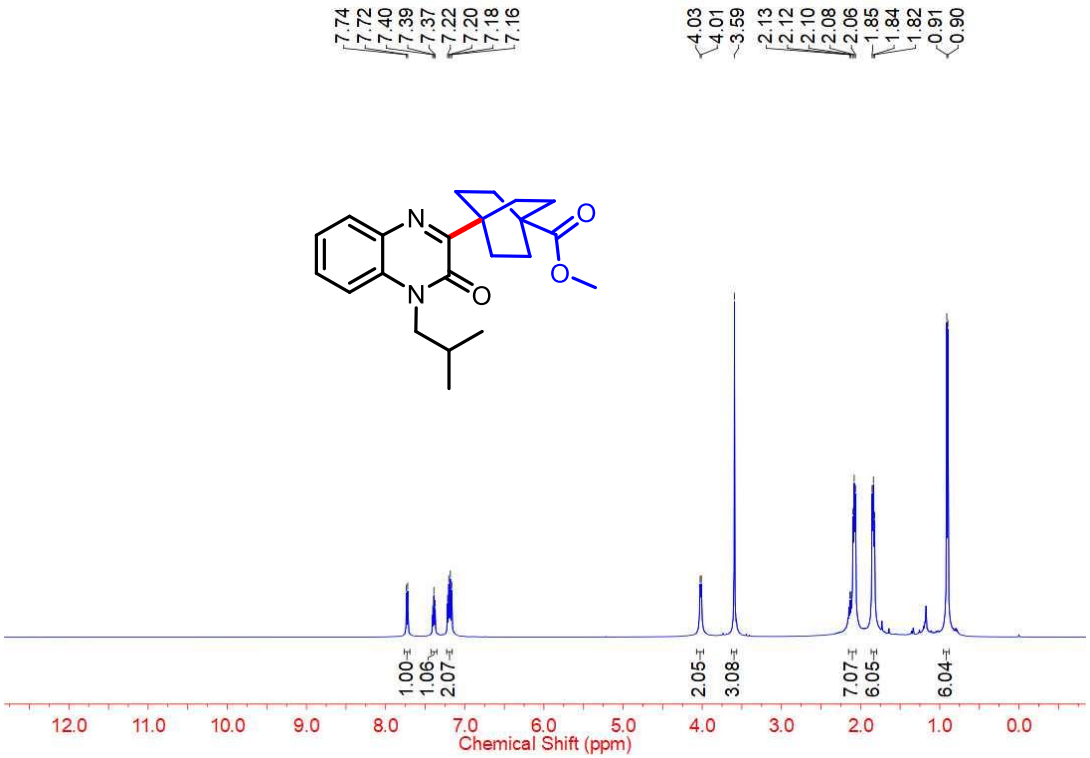
5 ^{1}H NMR (500 MHz, $CDCl_3$)



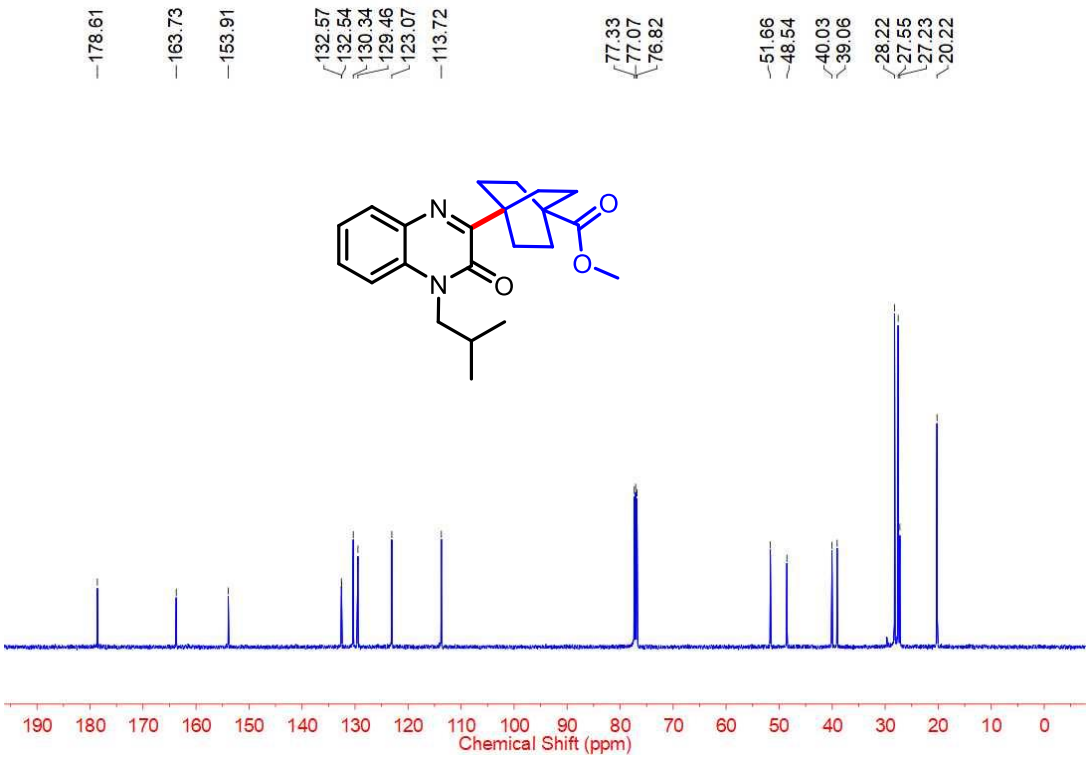
5 ^{13}C NMR (126 MHz, $CDCl_3$)



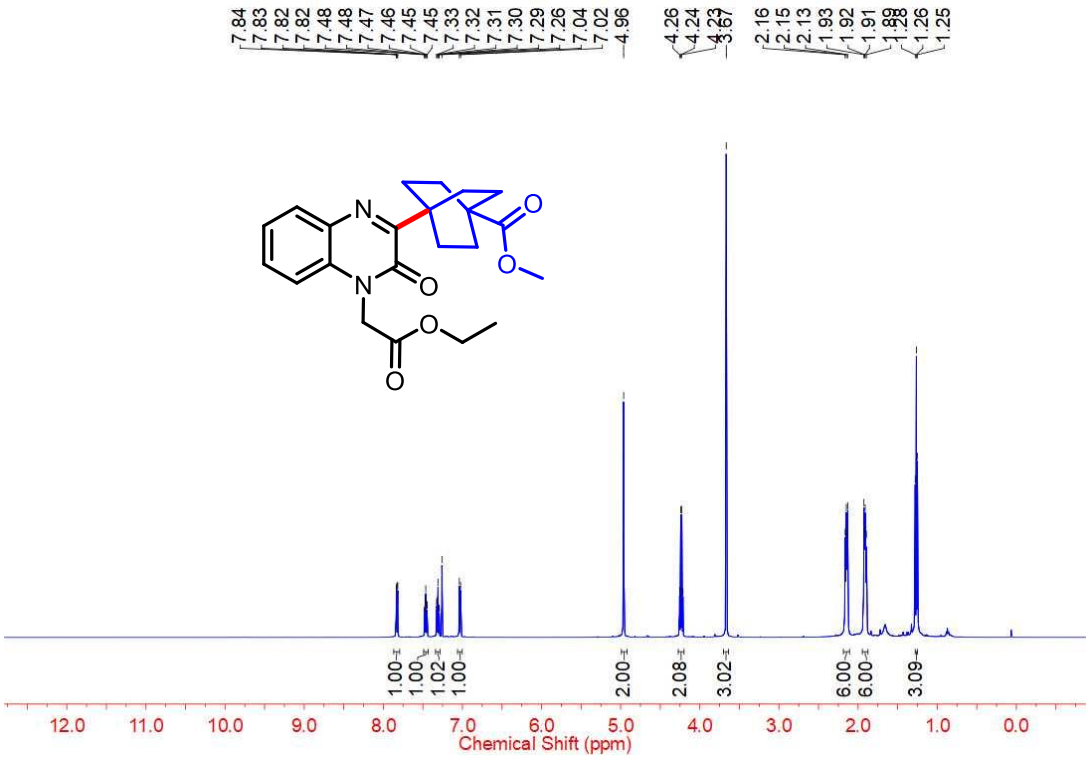
6 ^{1}H NMR (500 MHz, $CDCl_3$)



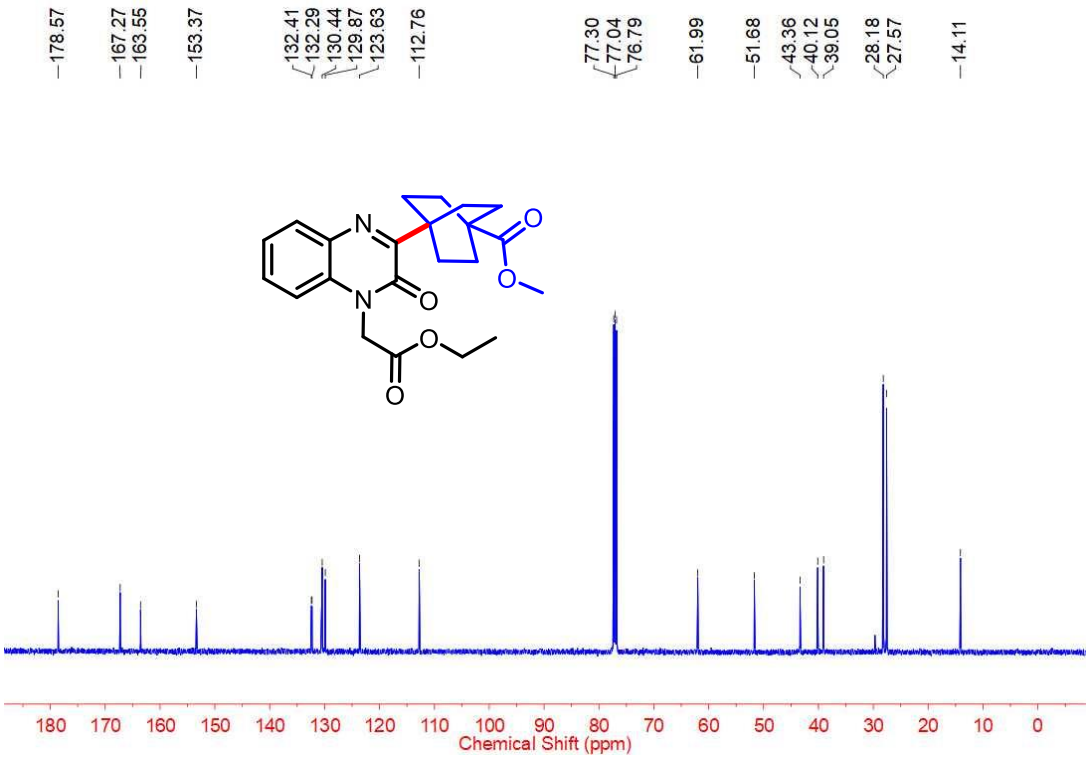
6 ^{13}C NMR (126 MHz, $CDCl_3$)



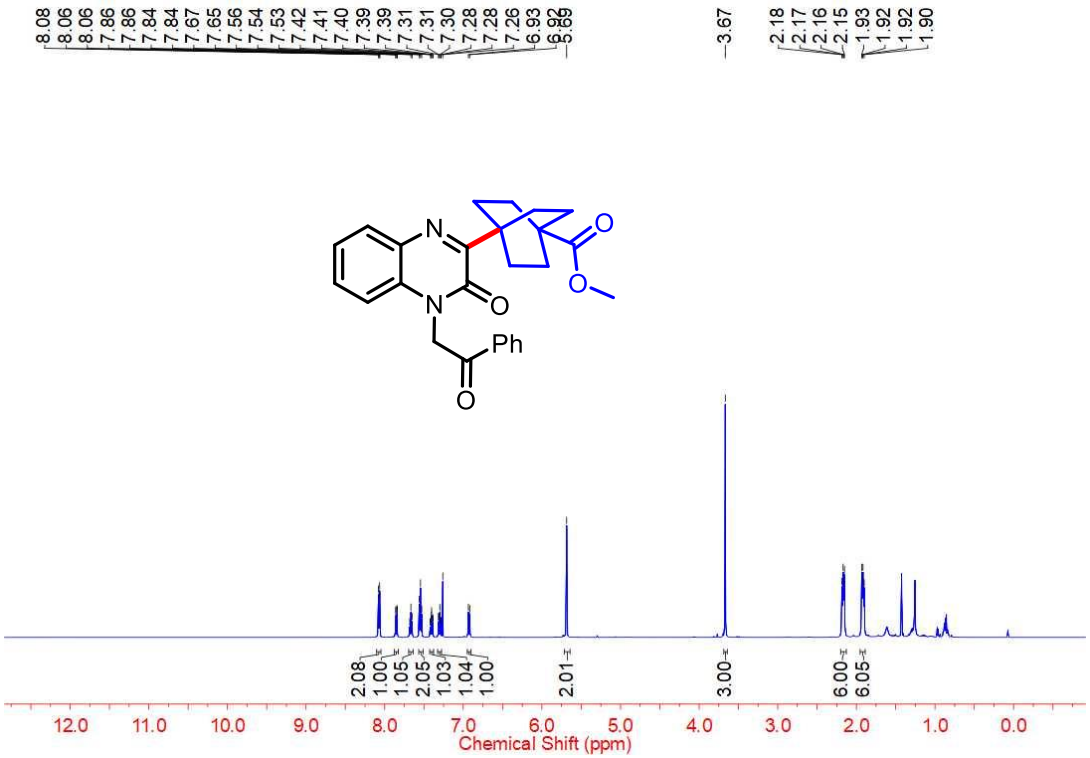
7 ^{1}H NMR (500 MHz, $CDCl_3$)



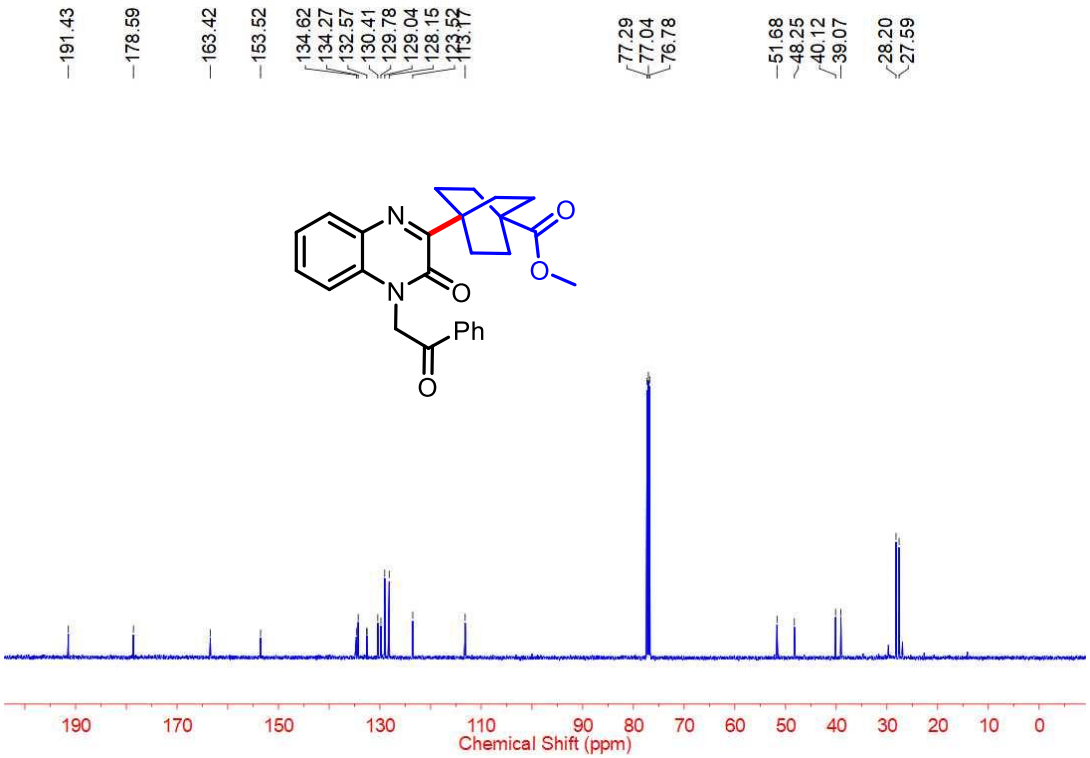
7 ^{13}C NMR (126 MHz, $CDCl_3$)



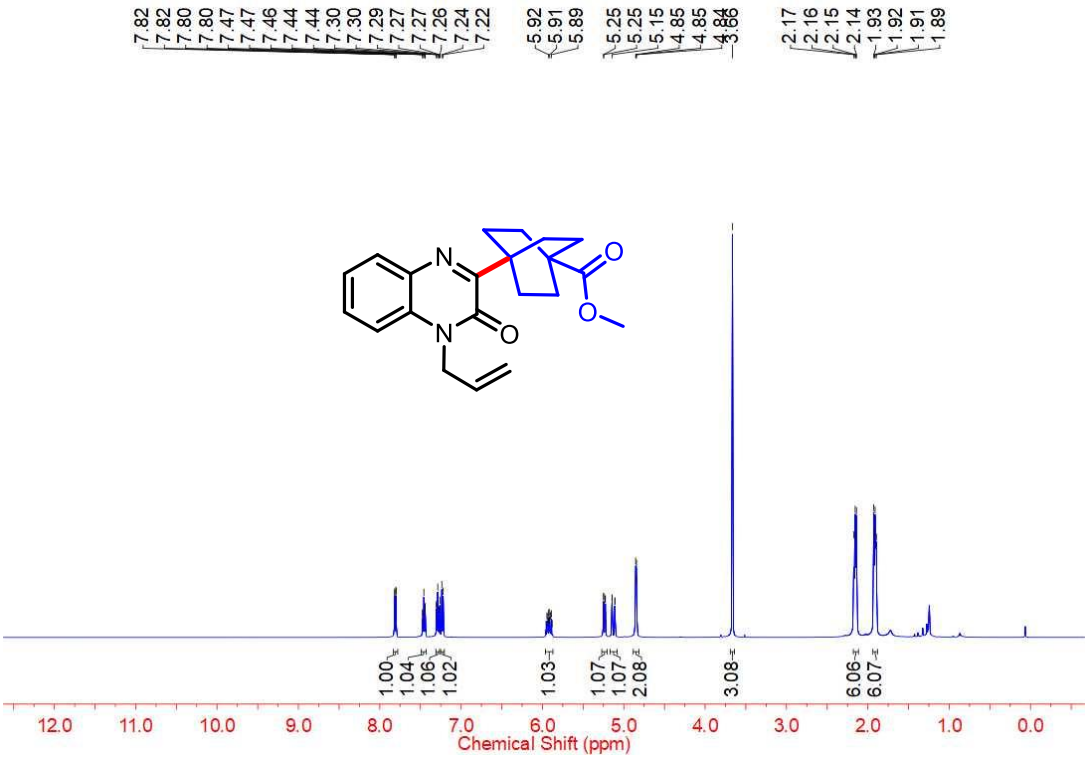
8 ^{1}H NMR (500 MHz, $CDCl_3$)



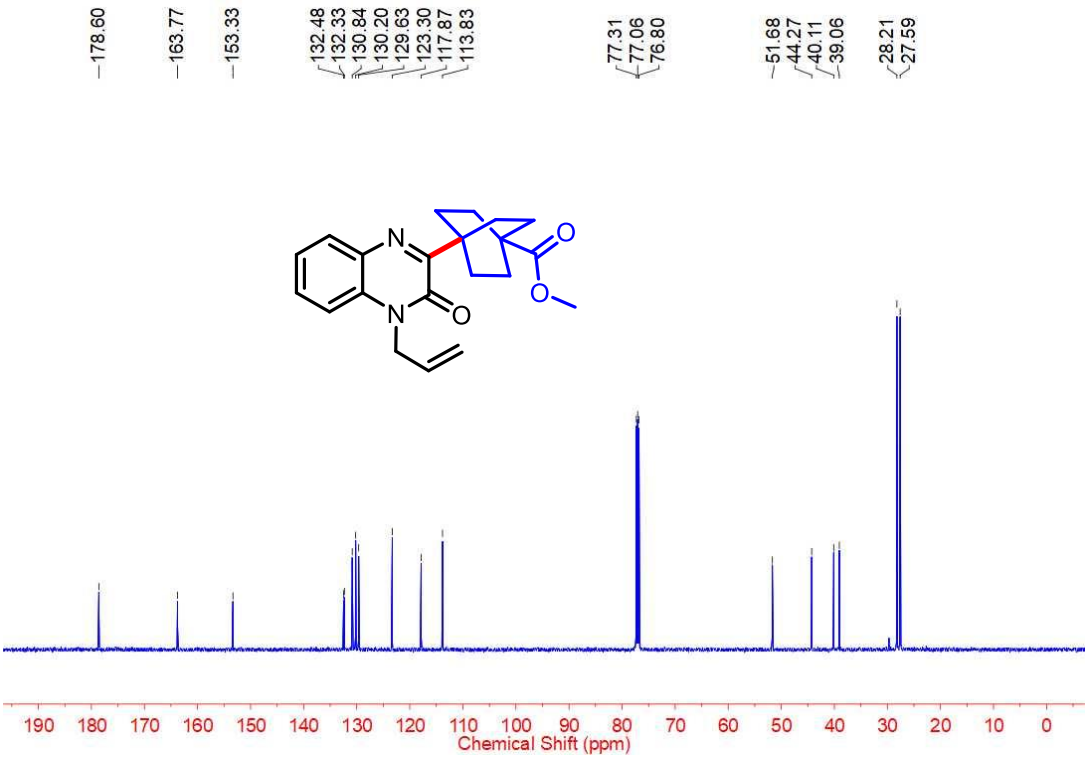
8 ^{13}C NMR (126 MHz, $CDCl_3$)



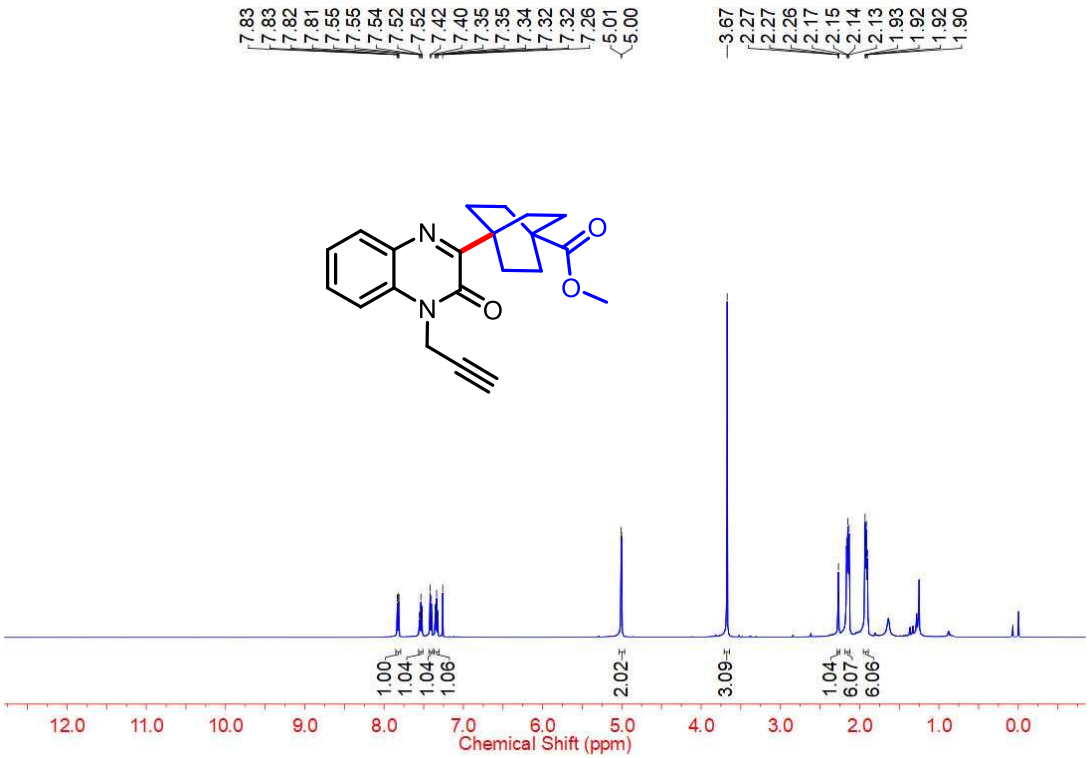
9 ^{1}H NMR (500 MHz, $CDCl_3$)



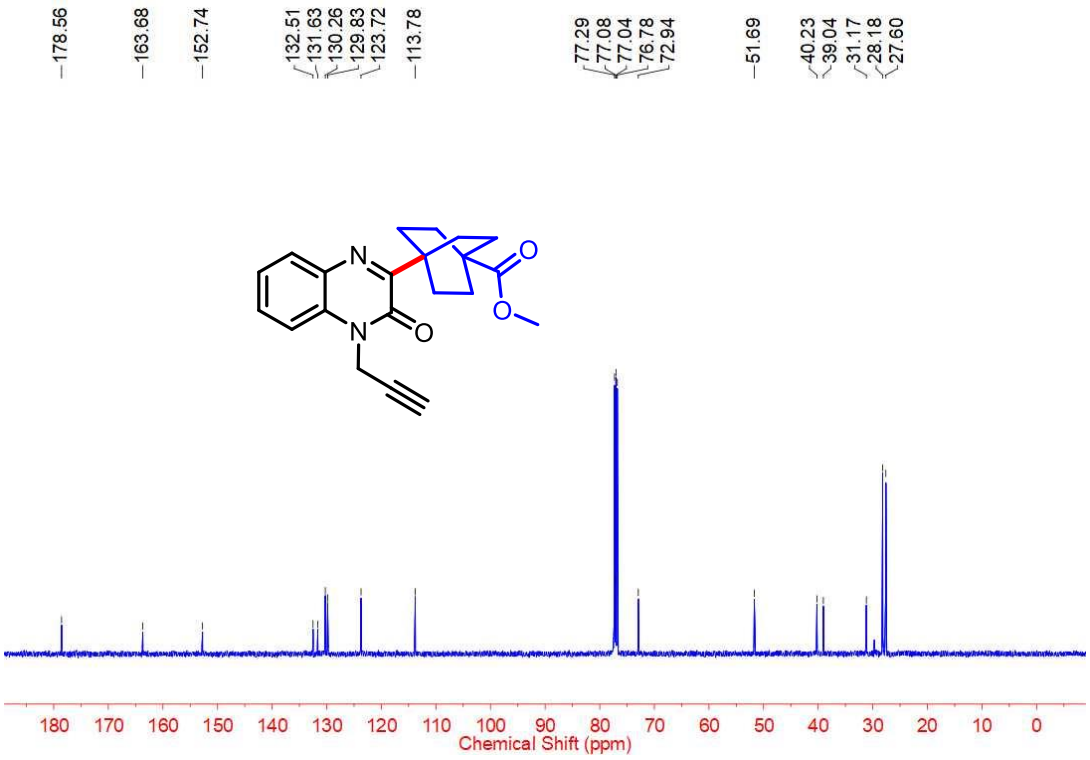
9 ^{13}C NMR (126 MHz, $CDCl_3$)



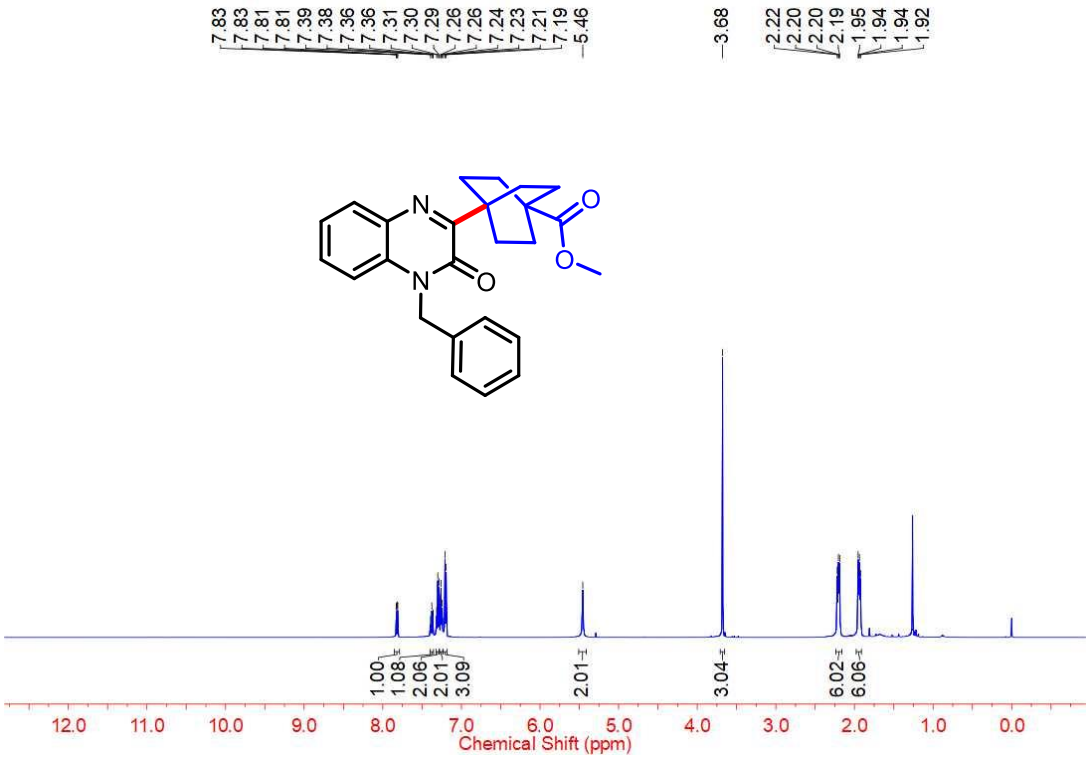
10 ^{1}H NMR (500 MHz, $CDCl_3$)



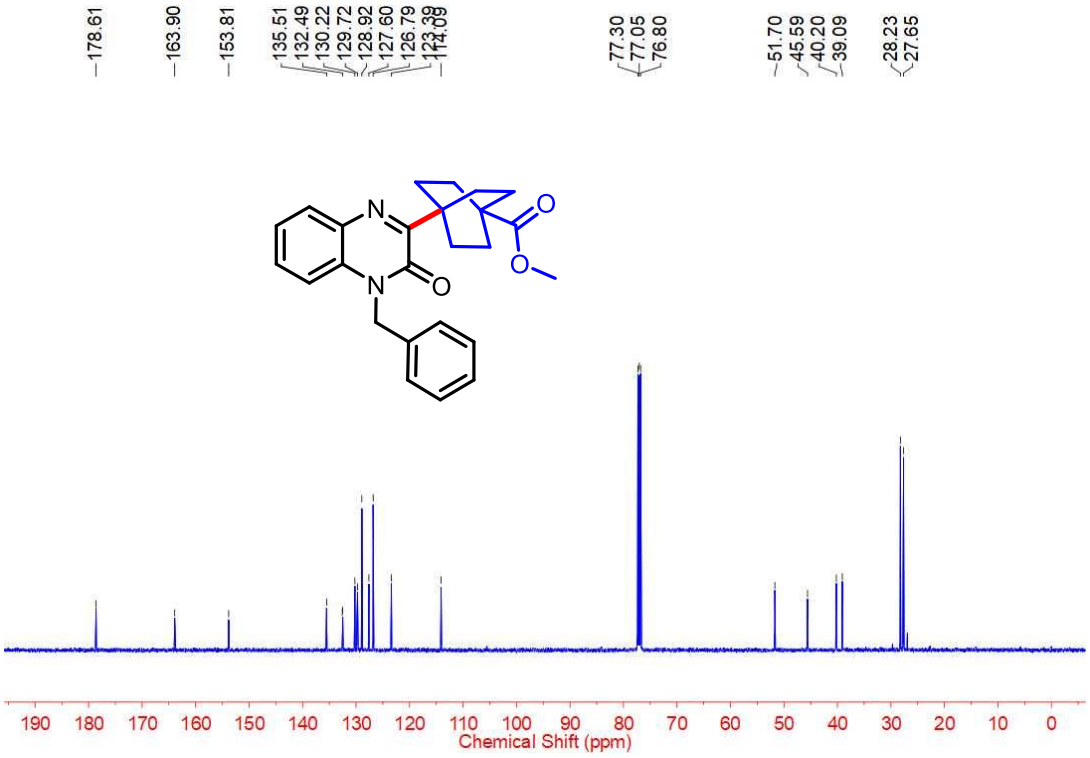
10 ^{13}C NMR (126 MHz, $CDCl_3$)



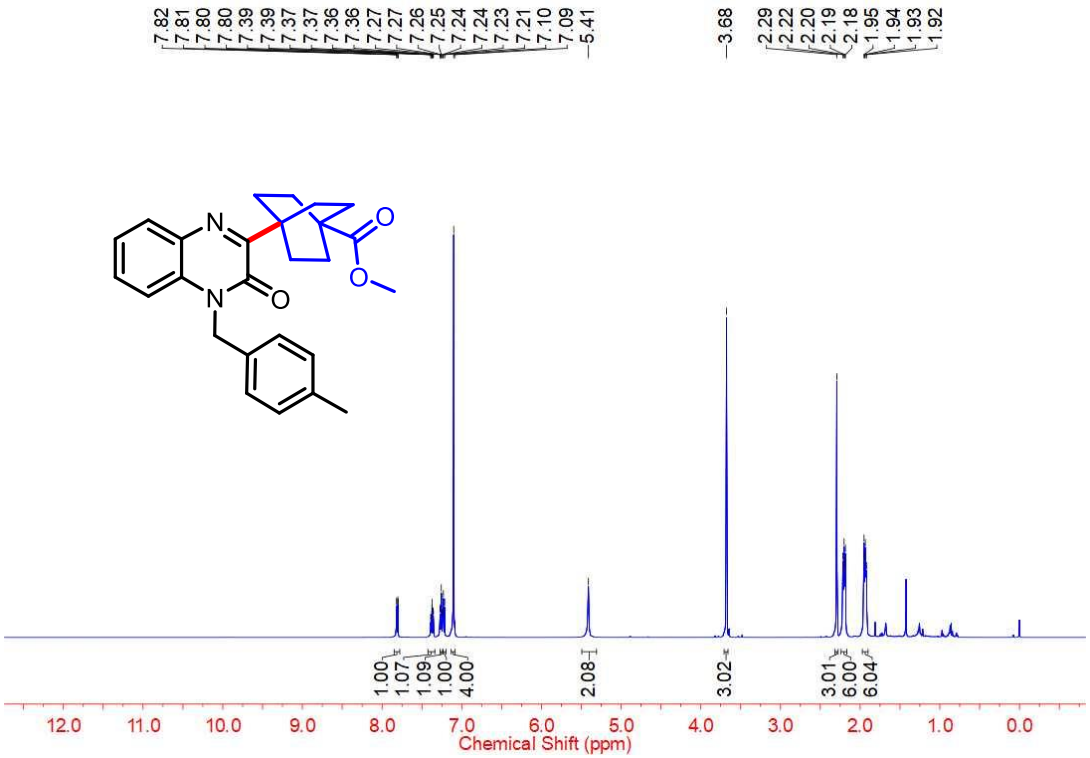
11 ^{1}H NMR (500 MHz, $CDCl_3$)



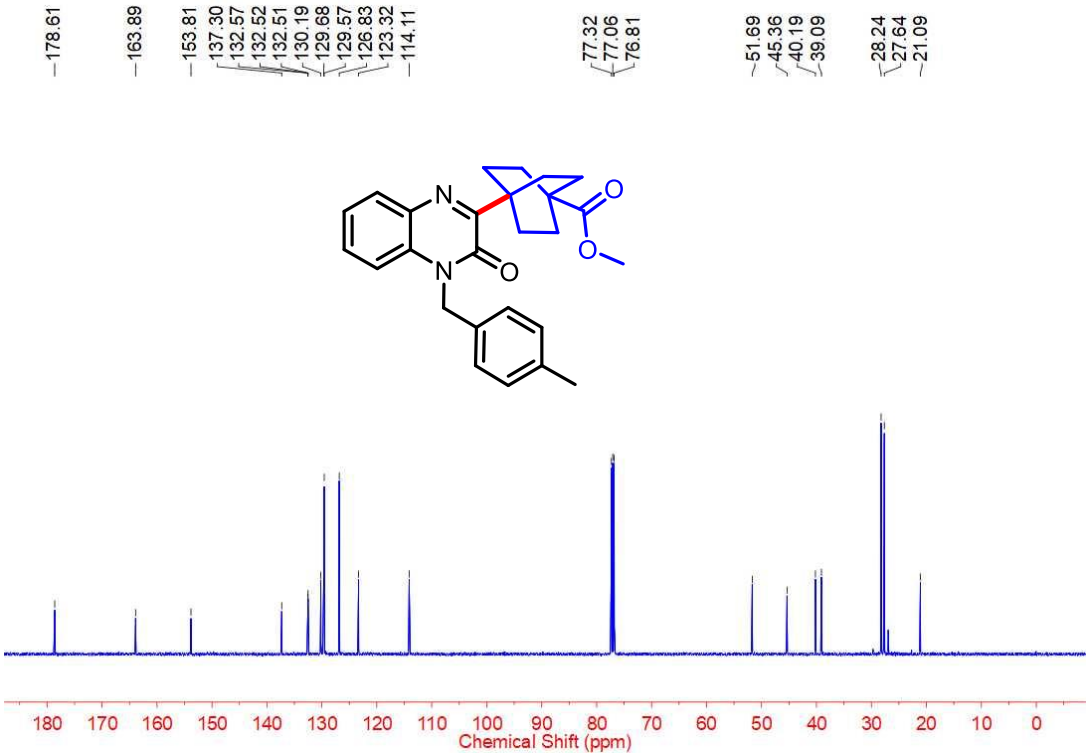
11 ^{13}C NMR (126 MHz, $CDCl_3$)



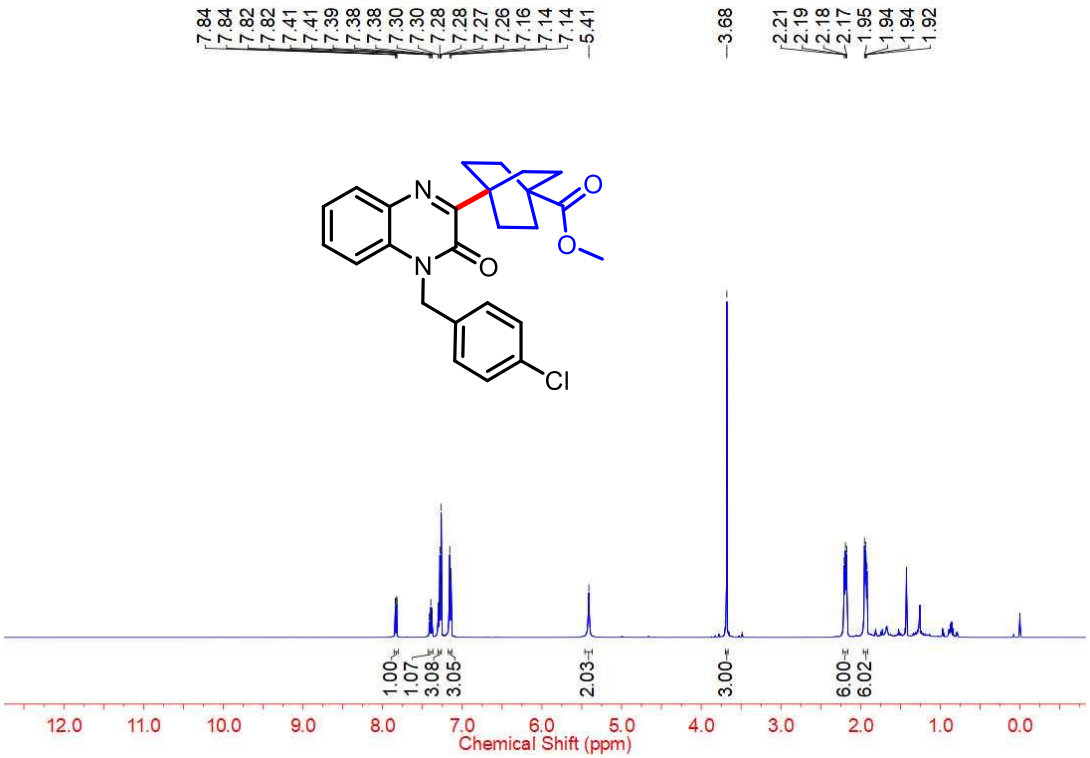
12 ^{1}H NMR (500 MHz, $CDCl_3$)



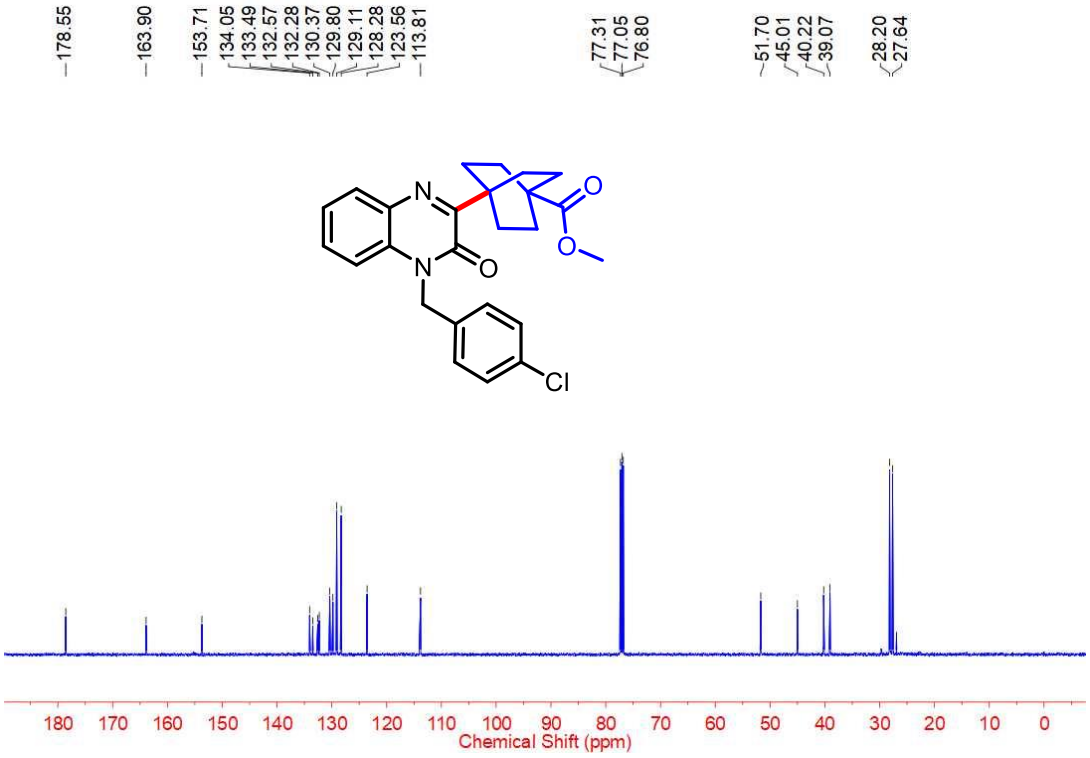
12 ^{13}C NMR (126 MHz, $CDCl_3$)



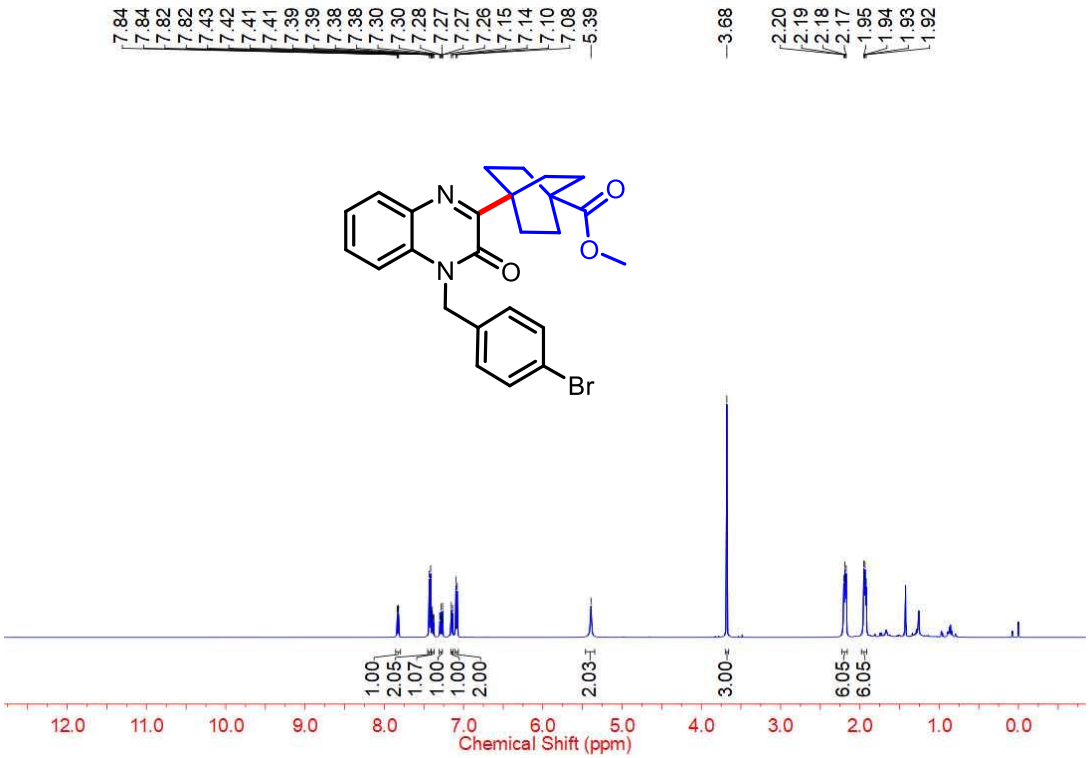
13 ^{1}H NMR (500 MHz, $CDCl_3$)



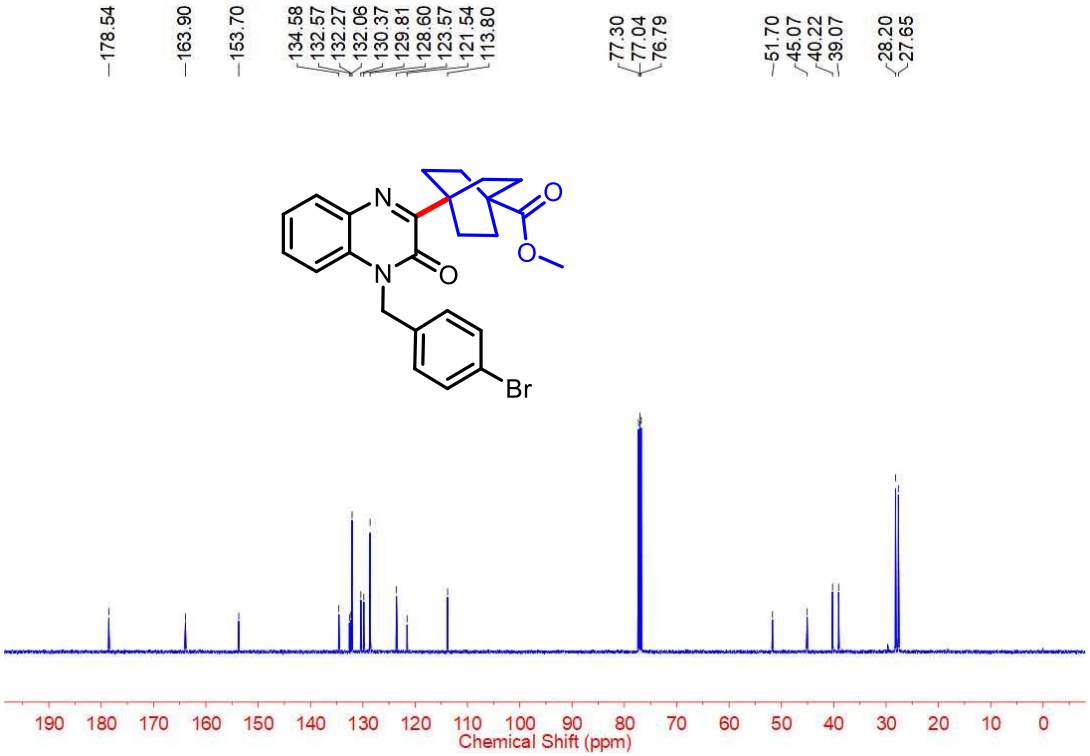
13 ^{13}C NMR (126 MHz, $CDCl_3$)



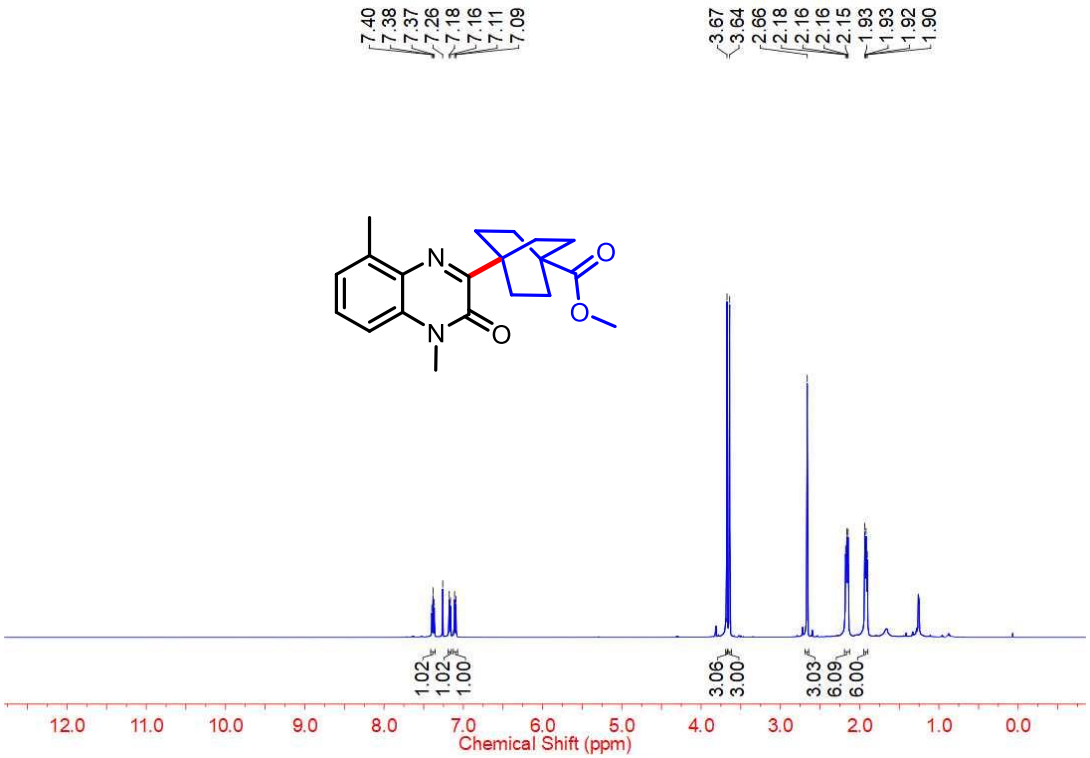
14 ^{1}H NMR (500 MHz, $CDCl_3$)



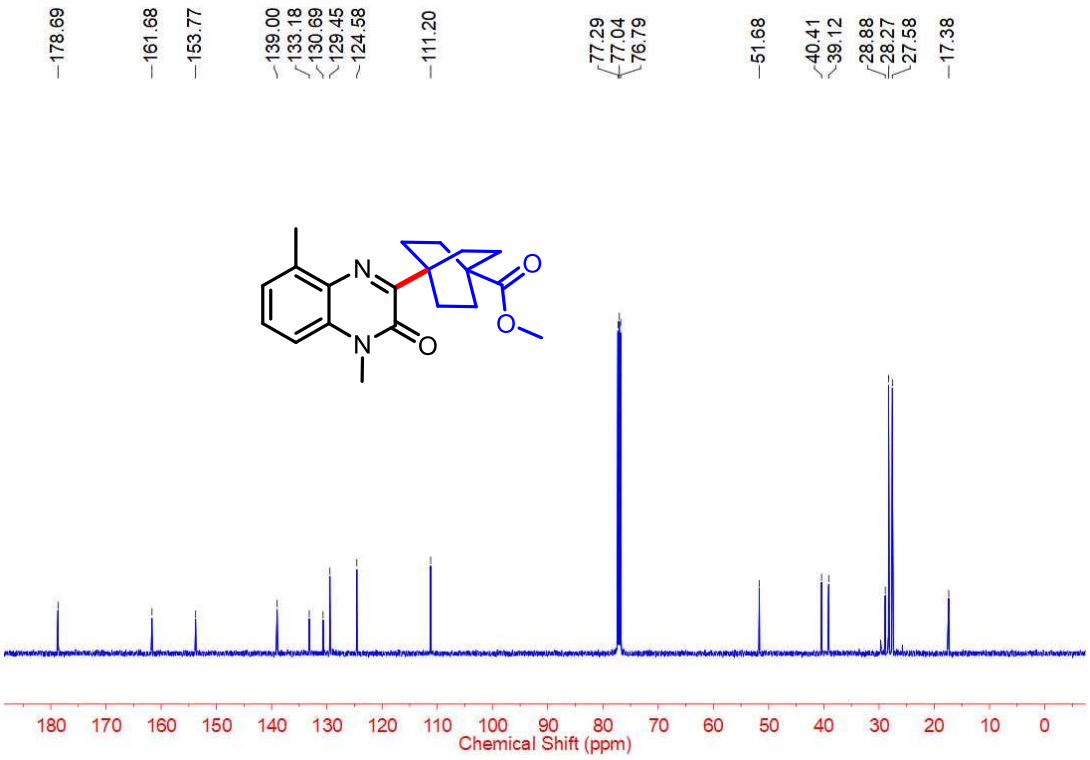
14 ^{13}C NMR (126 MHz, $CDCl_3$)



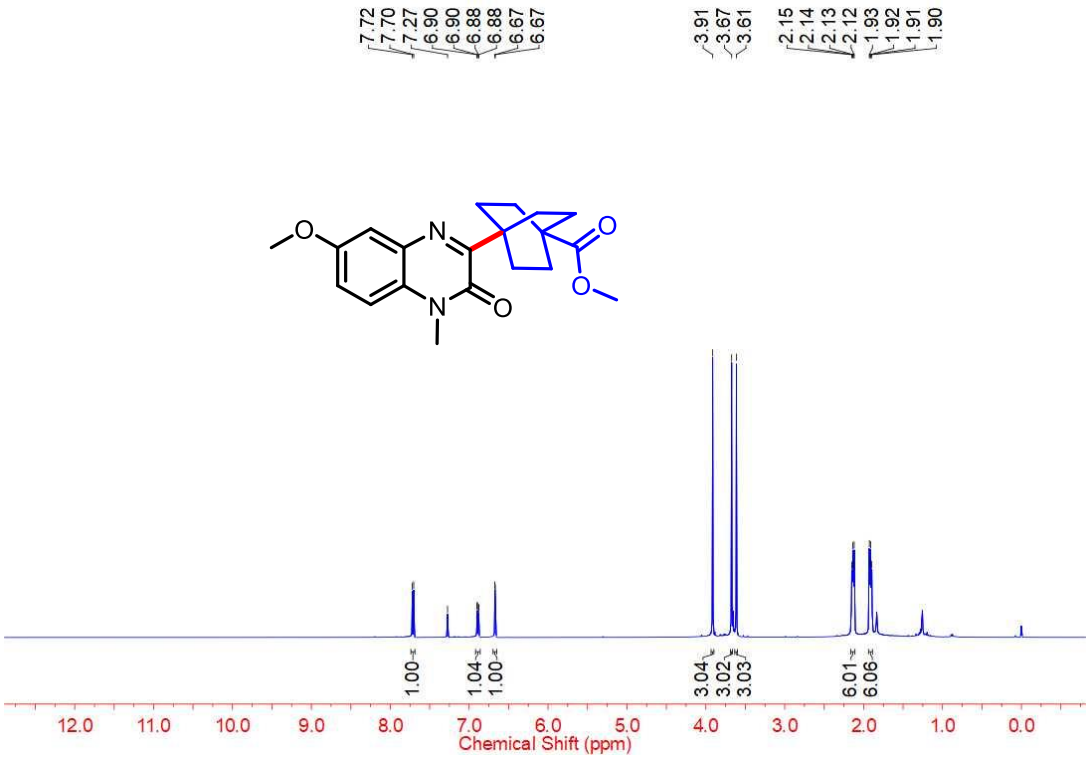
15 ^{1}H NMR (500 MHz, $CDCl_3$)



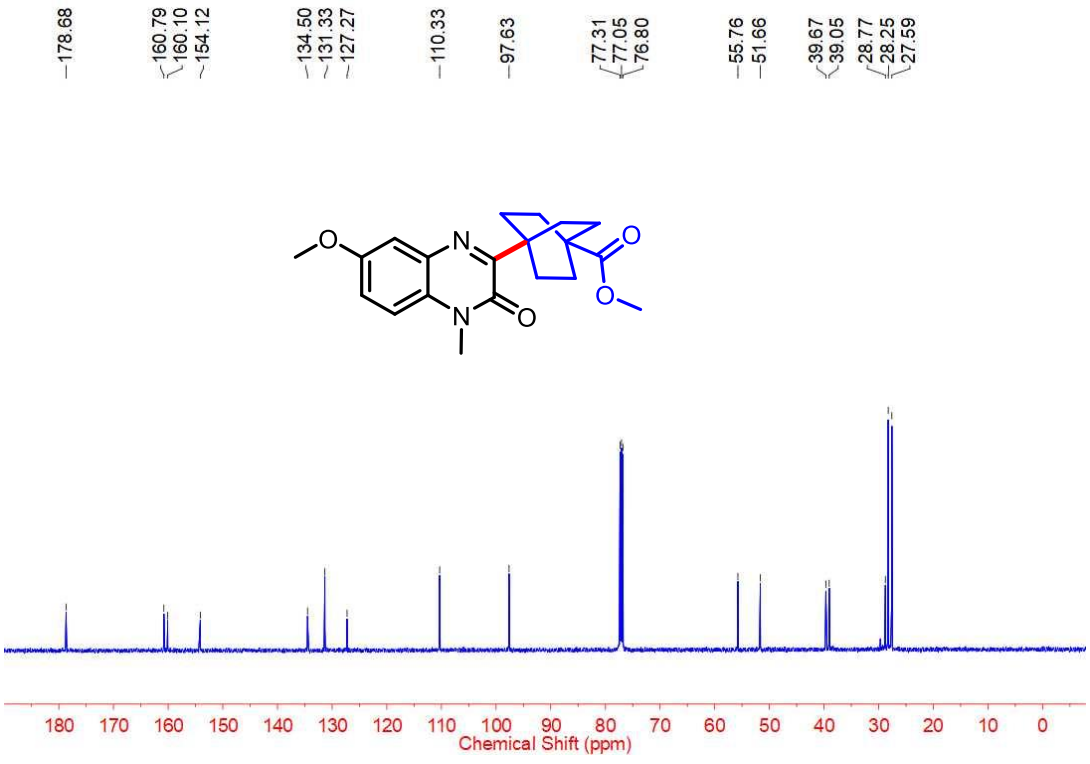
15 ^{13}C NMR (126 MHz, $CDCl_3$)



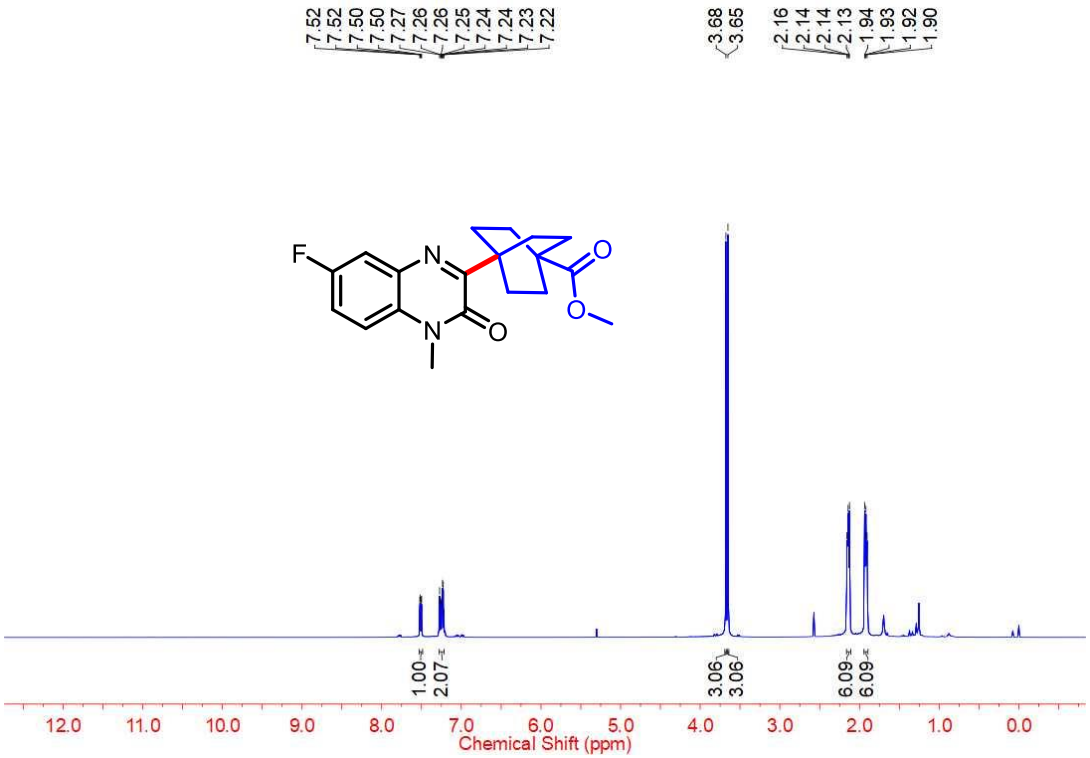
16 ^{1}H NMR (500 MHz, $CDCl_3$)



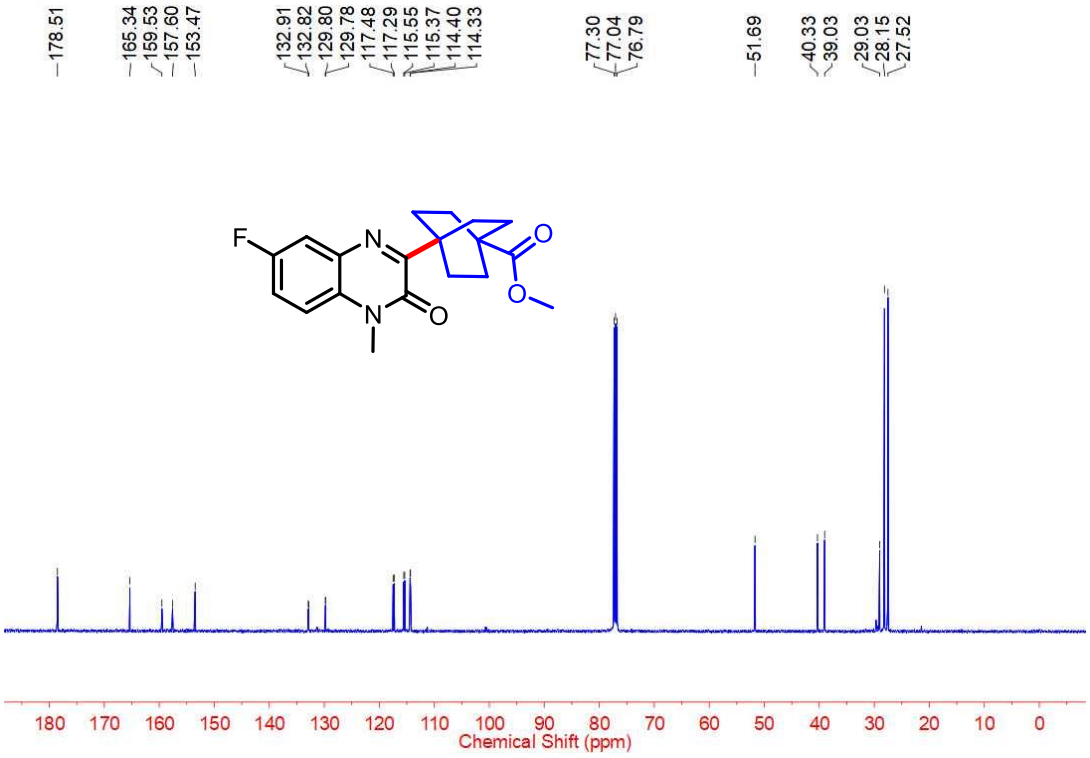
16 ^{13}C NMR (126 MHz, $CDCl_3$)



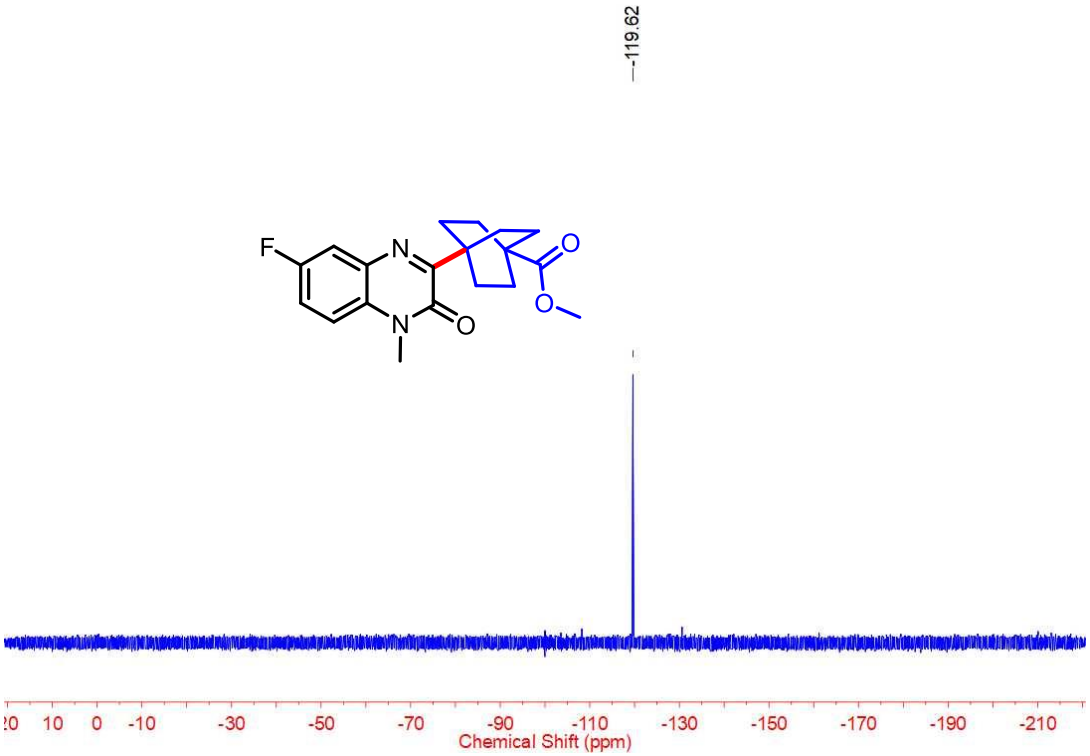
17 ^{1}H NMR (500 MHz, $CDCl_3$)



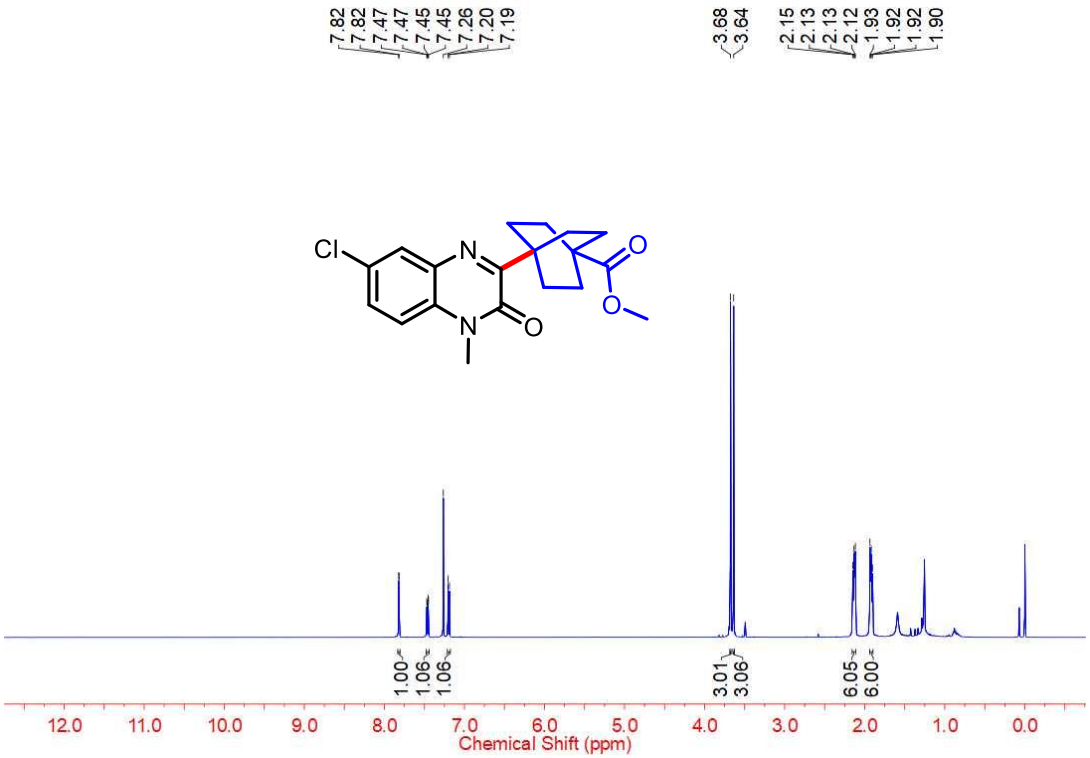
17 ^{13}C NMR (126 MHz, $CDCl_3$)



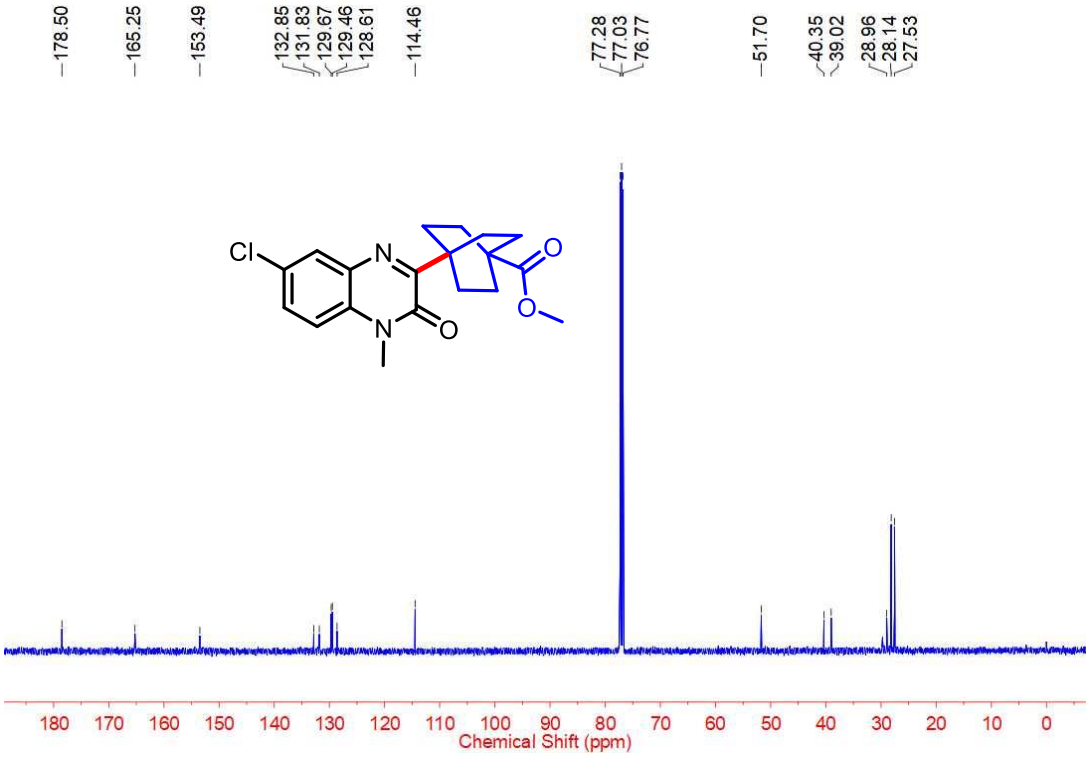
17 ^{19}F NMR (471 MHz, $CDCl_3$)



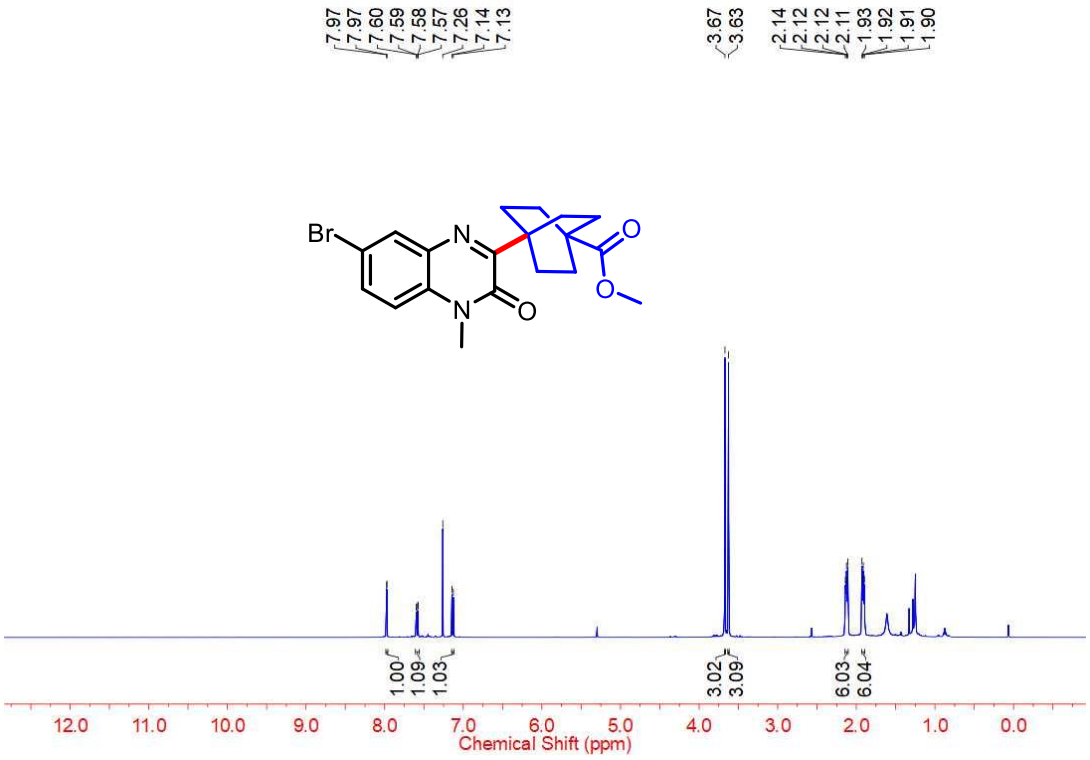
18 ^{1}H NMR (500 MHz, $CDCl_3$)



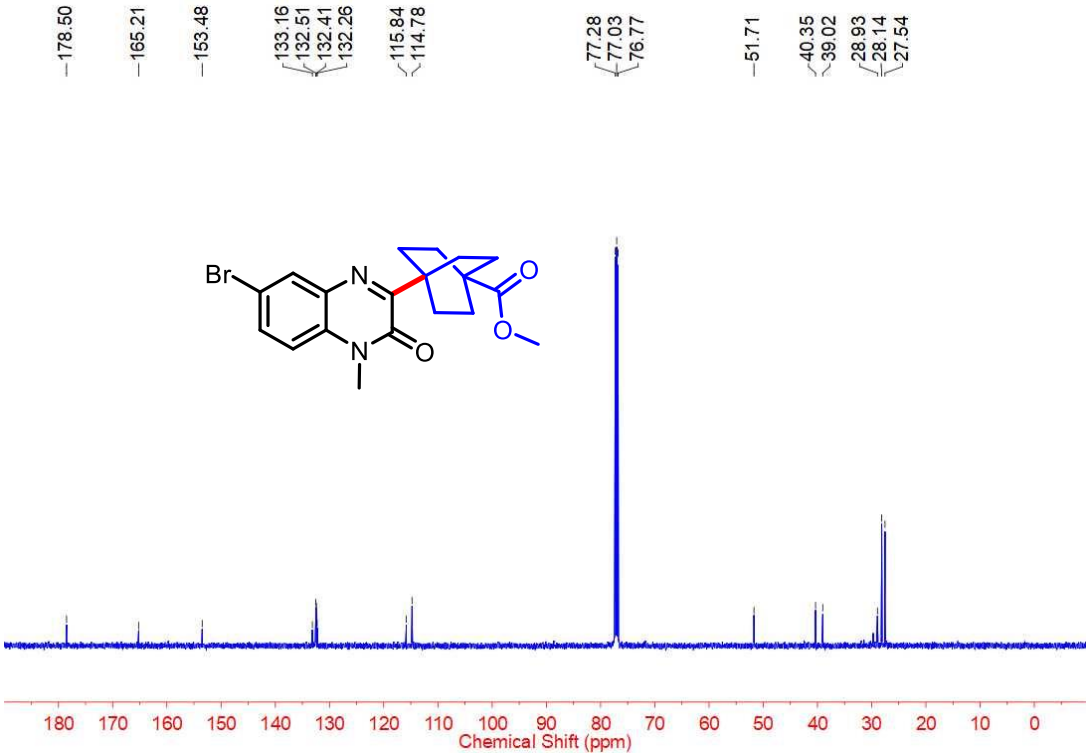
18 ^{13}C NMR (126 MHz, $CDCl_3$)



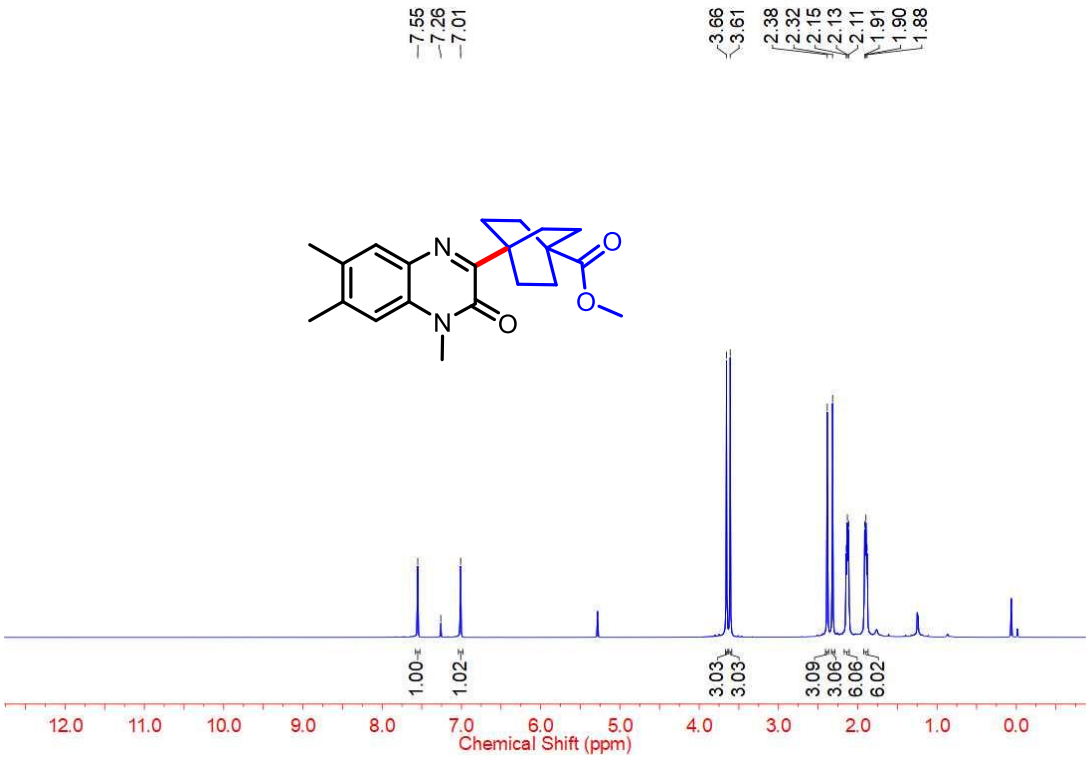
19 ^{1}H NMR (500 MHz, $CDCl_3$)



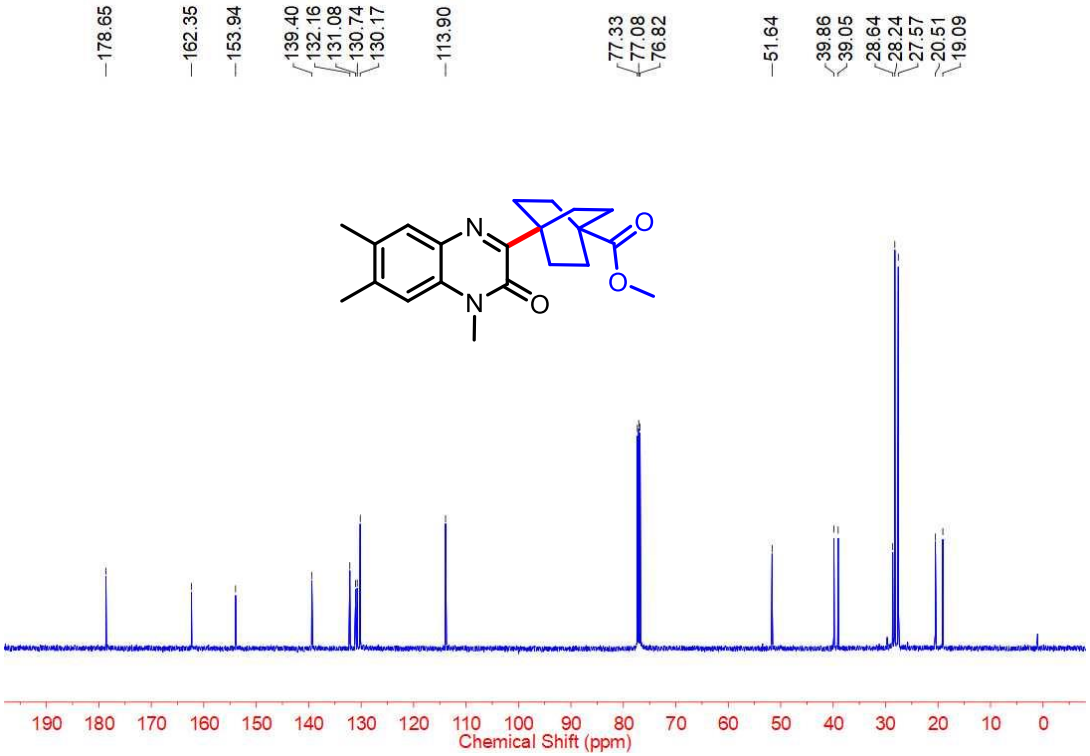
19 ^{13}C NMR (126 MHz, $CDCl_3$)



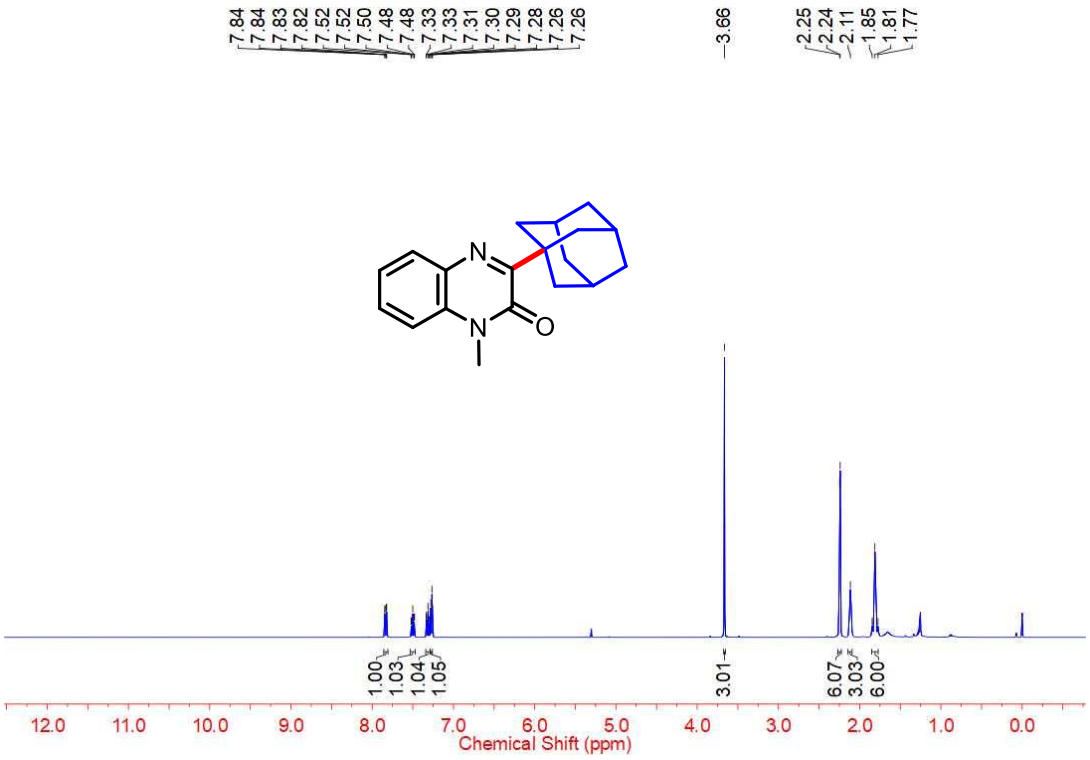
20 ^{1}H NMR (500 MHz, $CDCl_3$)



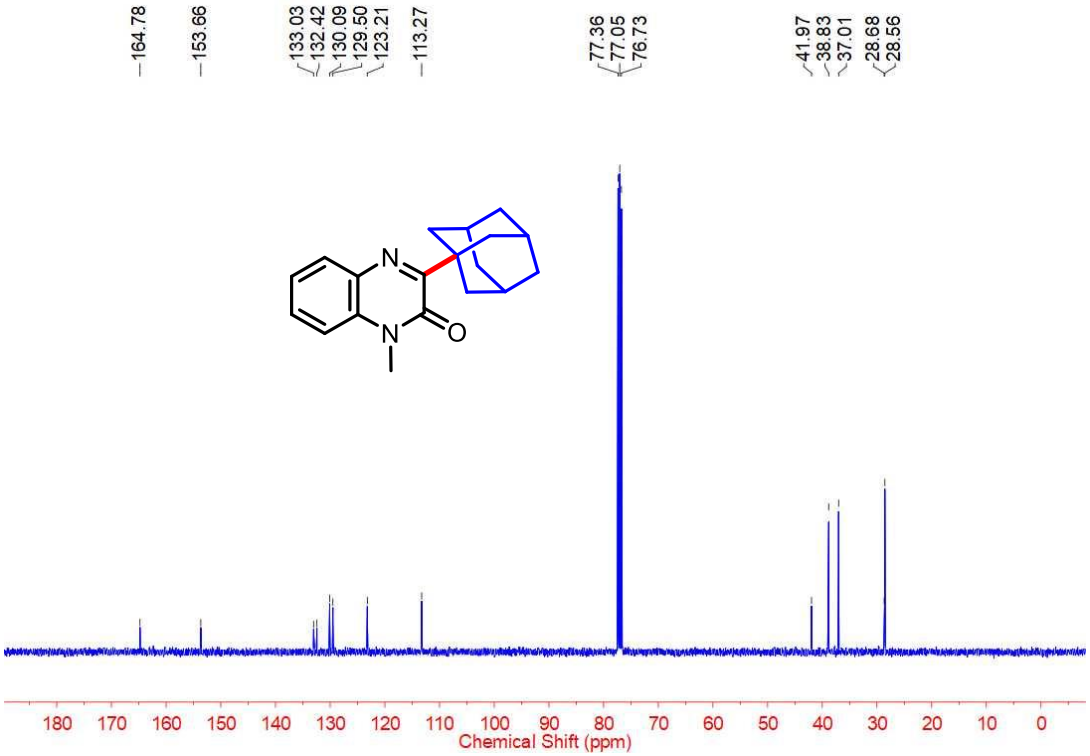
20 ^{13}C NMR (126 MHz, $CDCl_3$)



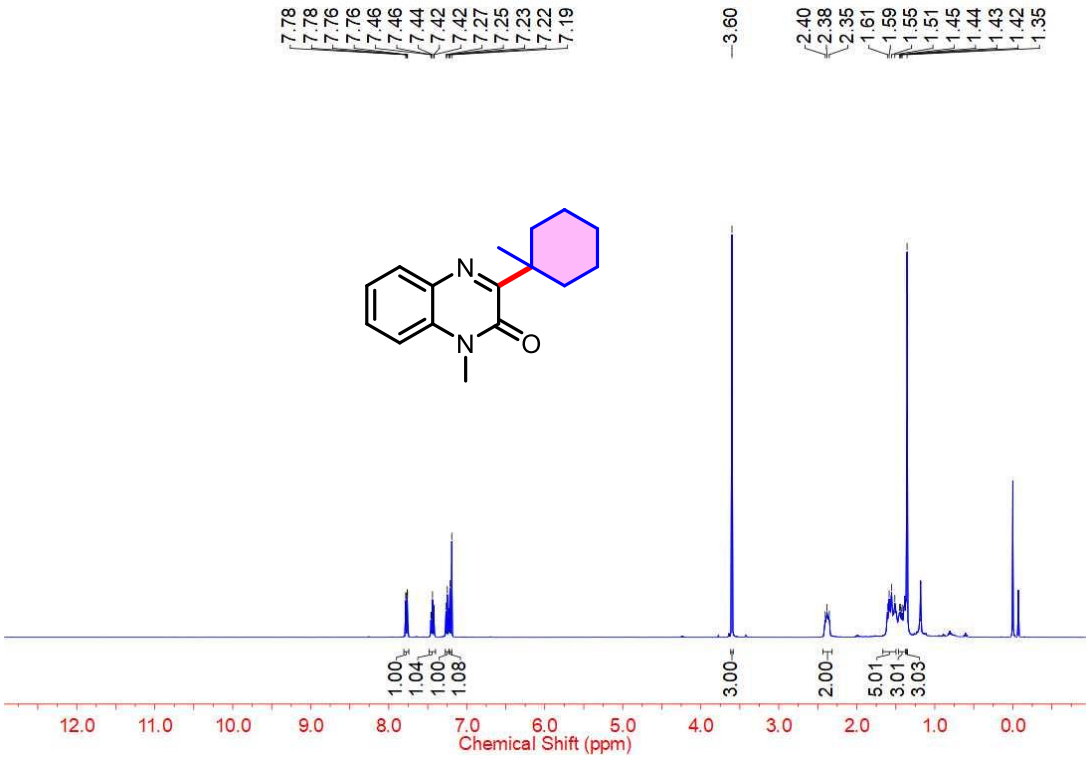
21 ^{1}H NMR (400 MHz, $CDCl_3$)



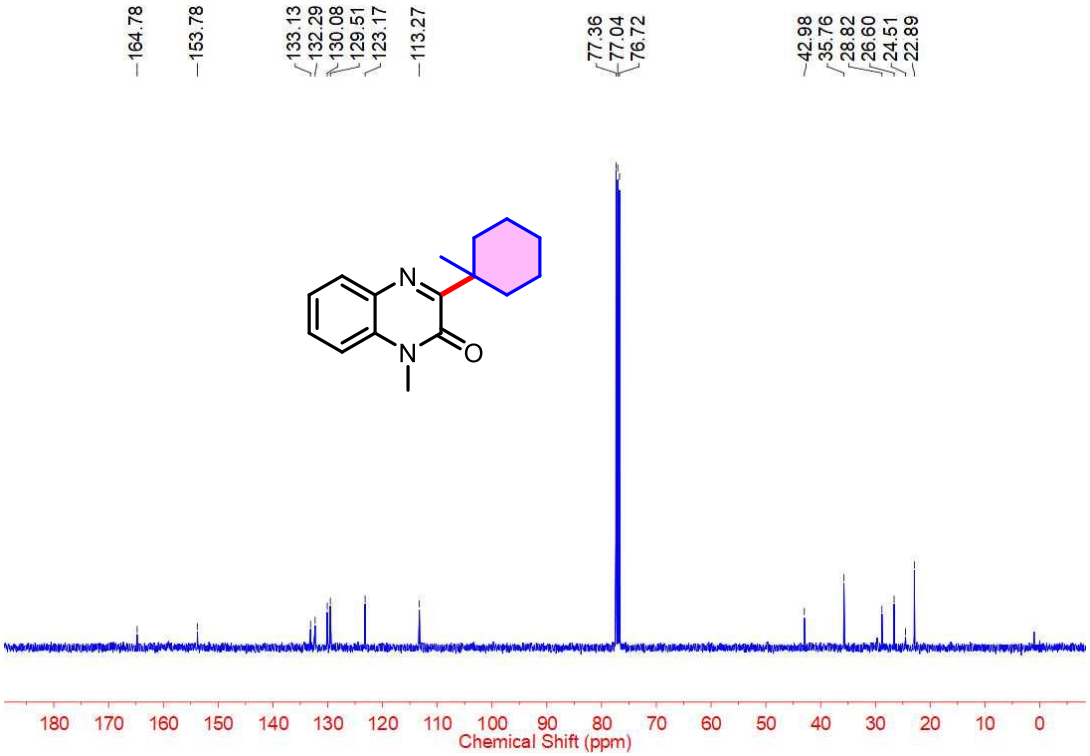
21 ^{13}C NMR (100 MHz, $CDCl_3$)



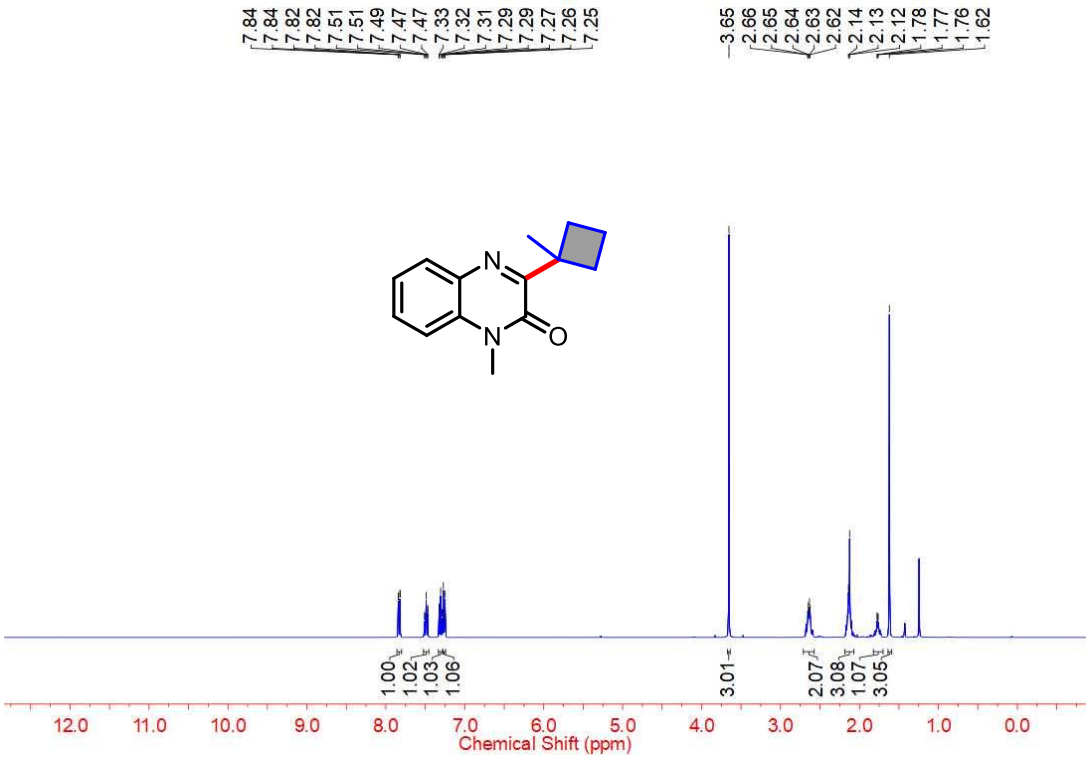
22 ^{1}H NMR (400 MHz, $CDCl_3$)



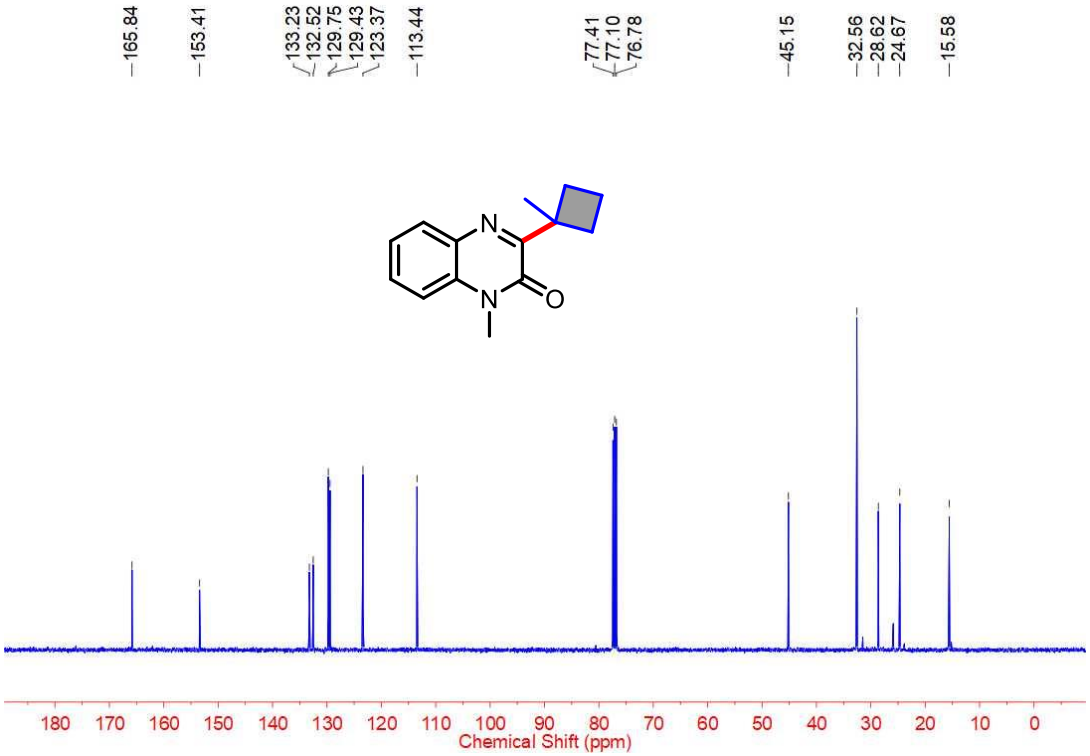
22 ^{13}C NMR (100 MHz, $CDCl_3$)



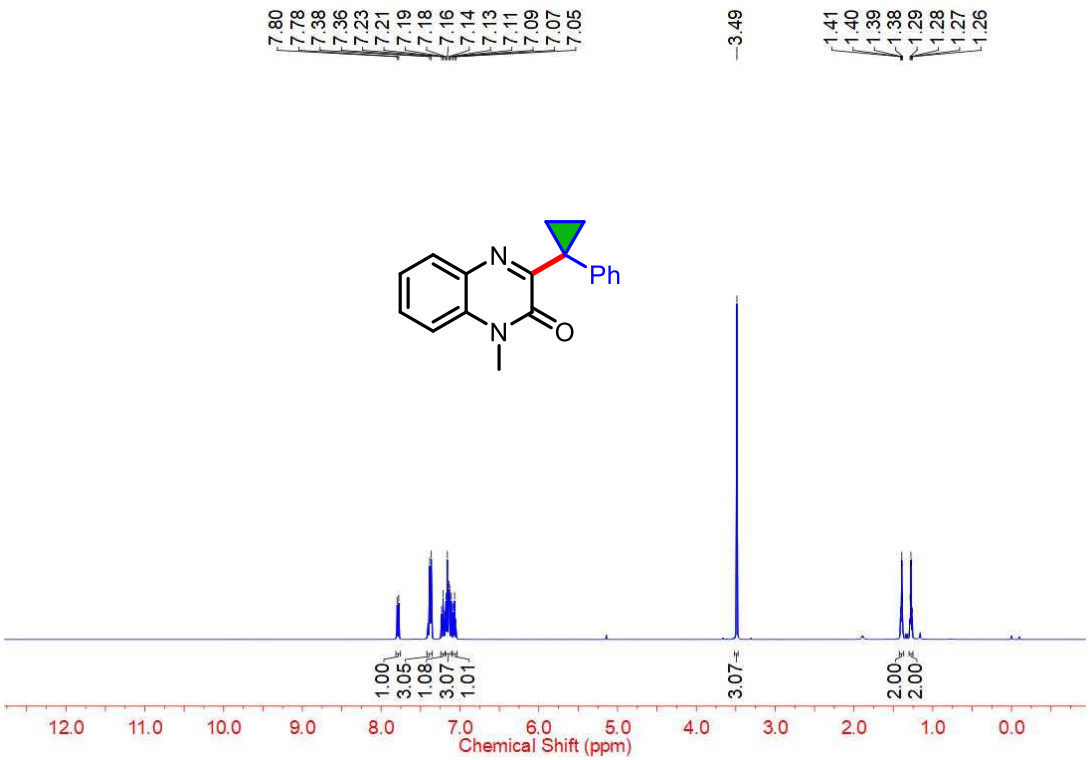
23 ^{1}H NMR (400 MHz, $CDCl_3$)



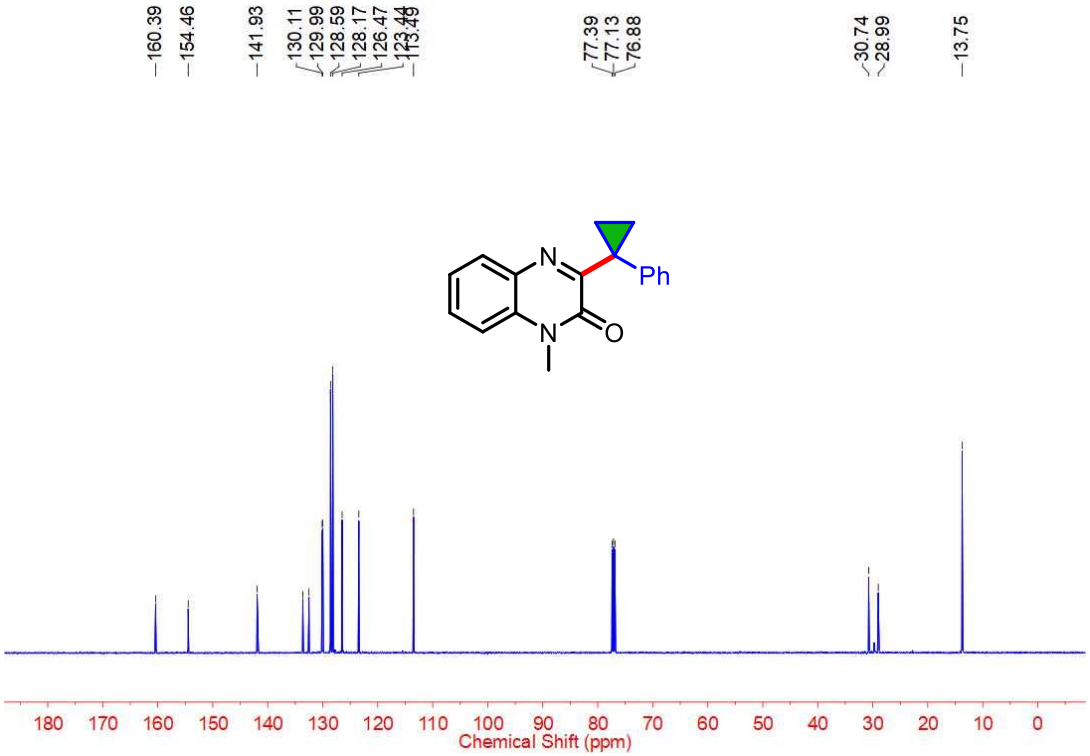
23 ^{13}C NMR (100 MHz, $CDCl_3$)



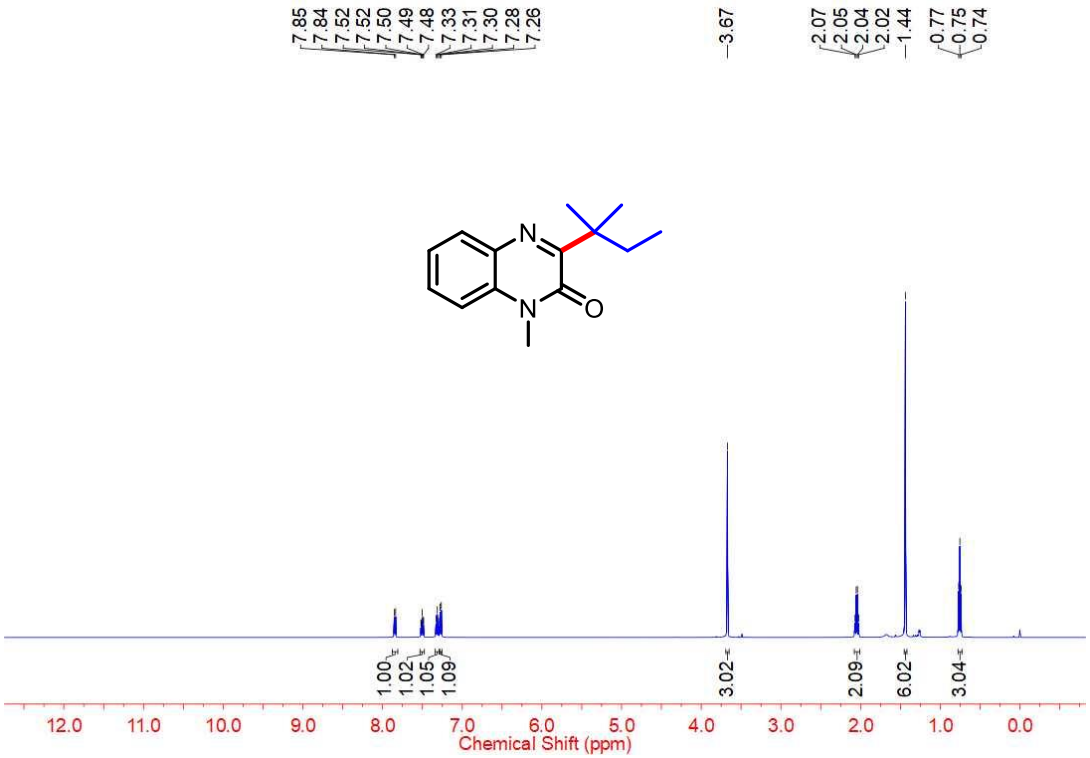
24 ^{1}H NMR (400 MHz, $CDCl_3$)



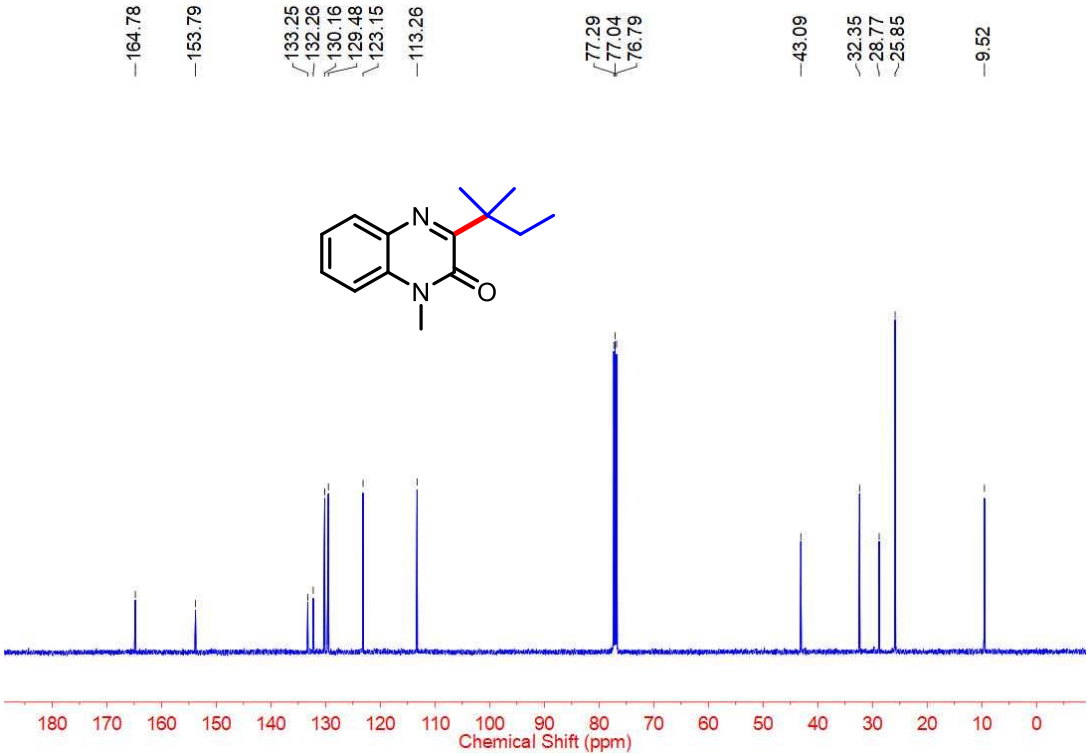
24 ^{13}C NMR (100 MHz, $CDCl_3$)



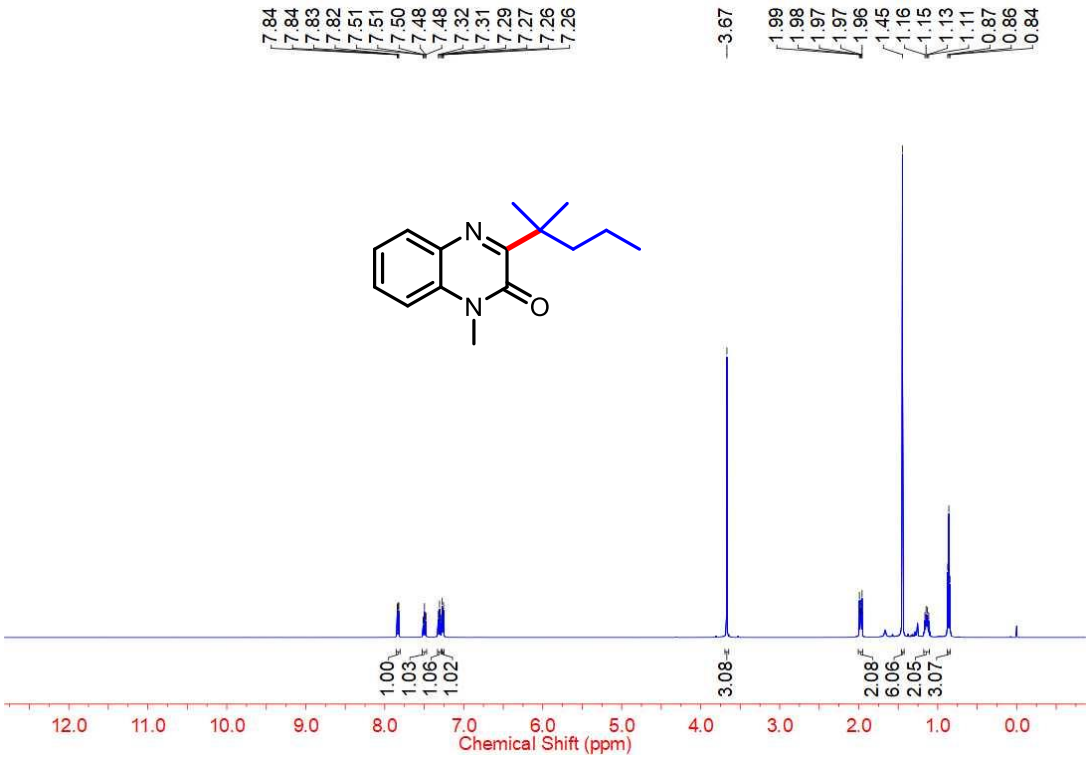
25 ^{1}H NMR (500 MHz, $CDCl_3$)



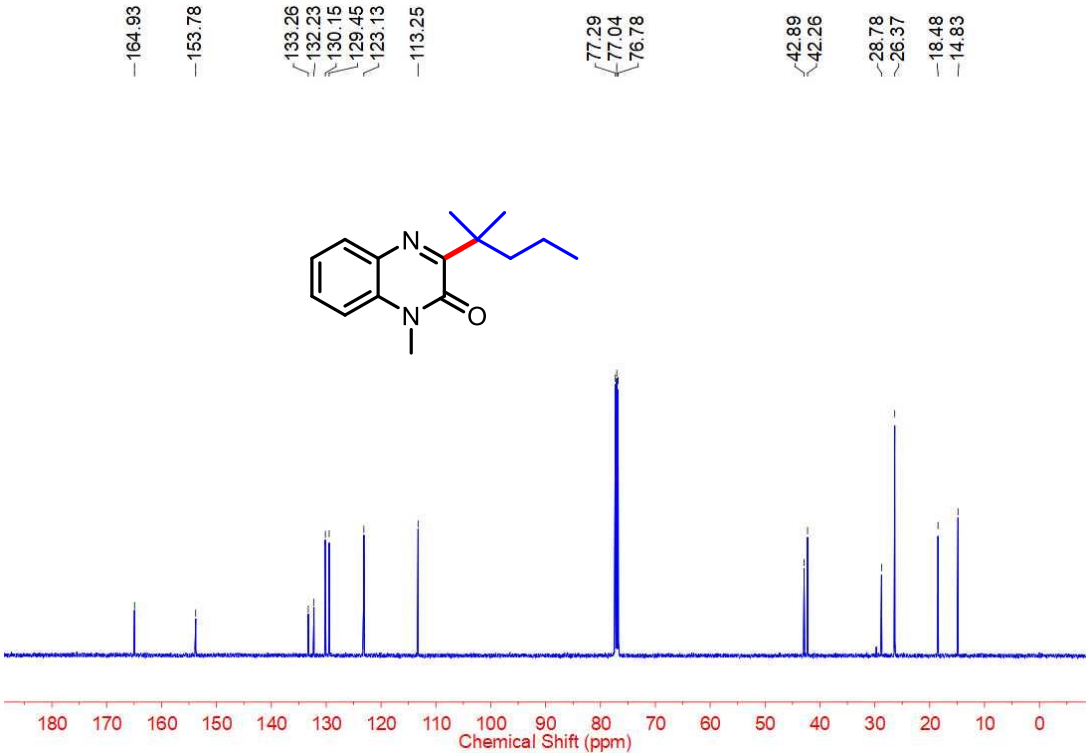
25 ^{13}C NMR (126 MHz, $CDCl_3$)



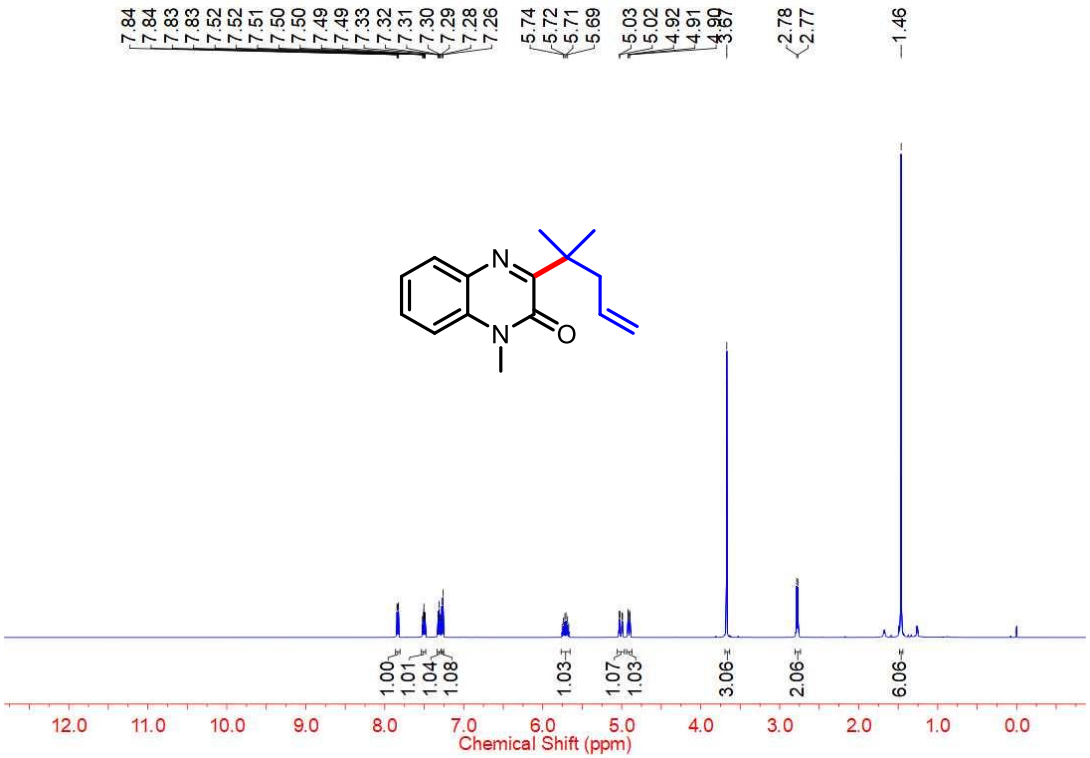
26 ^{1}H NMR (500 MHz, $CDCl_3$)



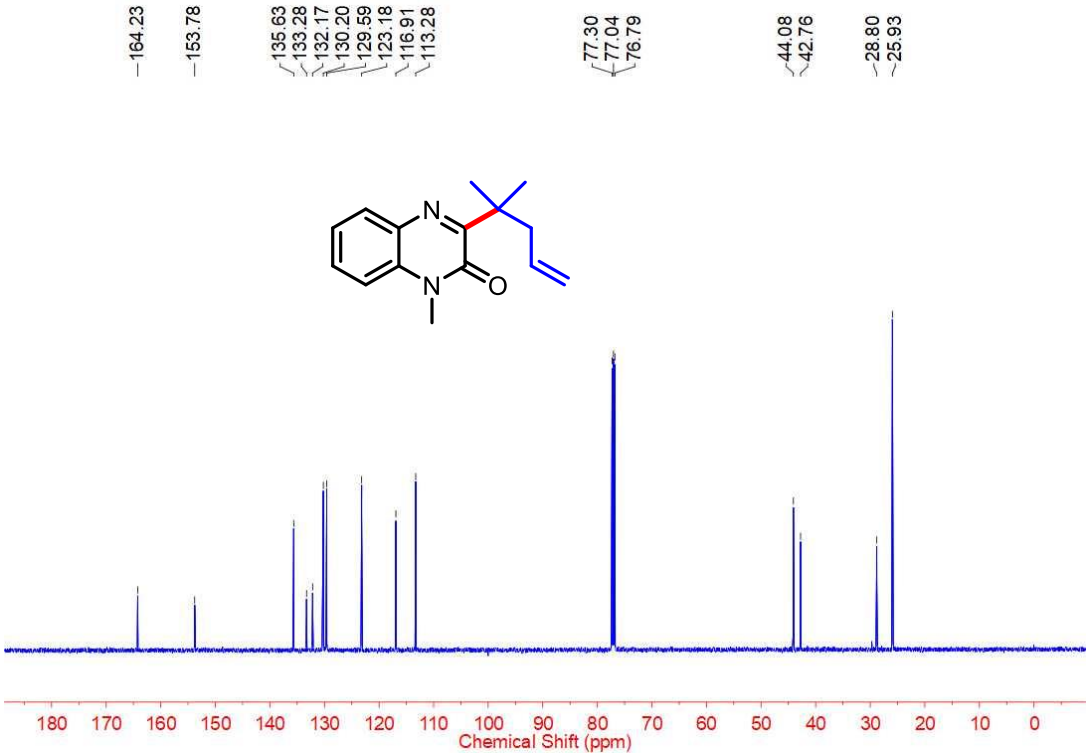
26 ^{13}C NMR (126 MHz, $CDCl_3$)



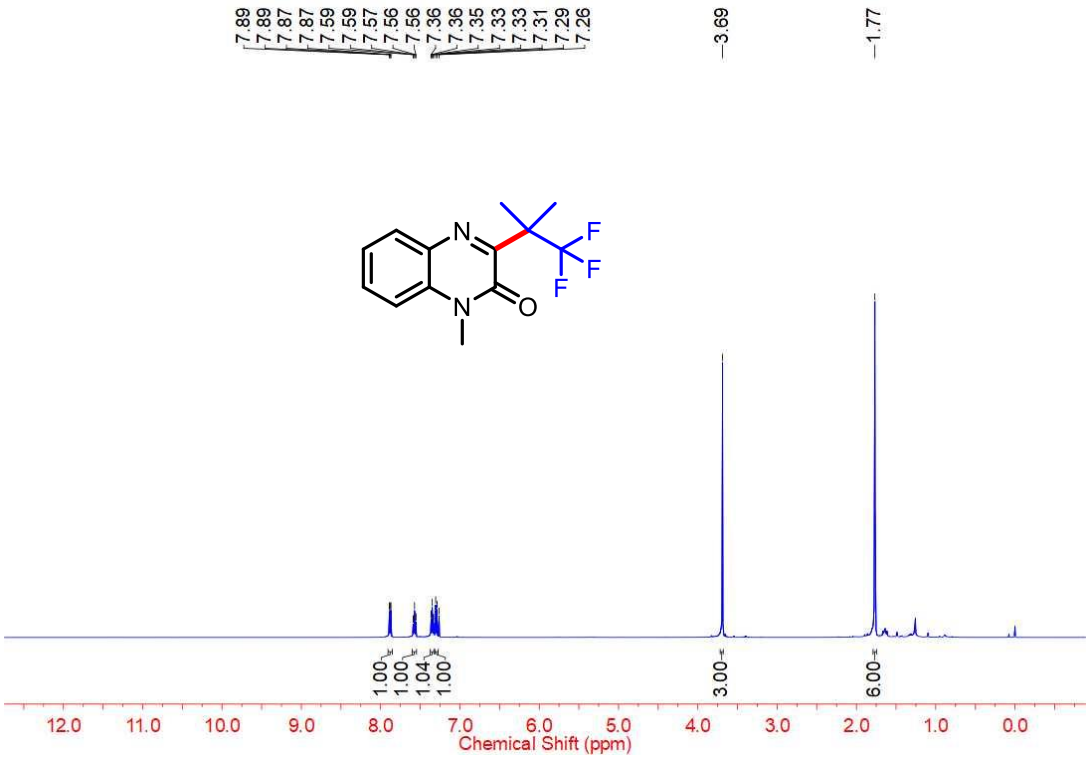
27 ^{1}H NMR (500 MHz, $CDCl_3$)



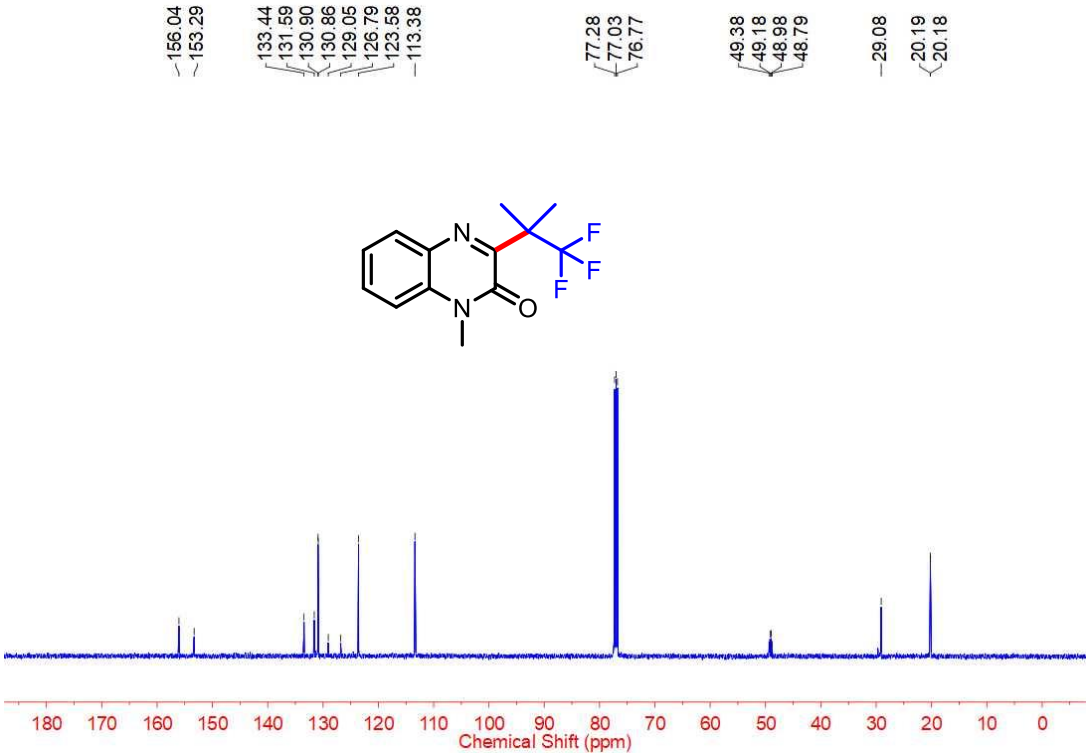
27 ^{13}C NMR (126 MHz, $CDCl_3$)



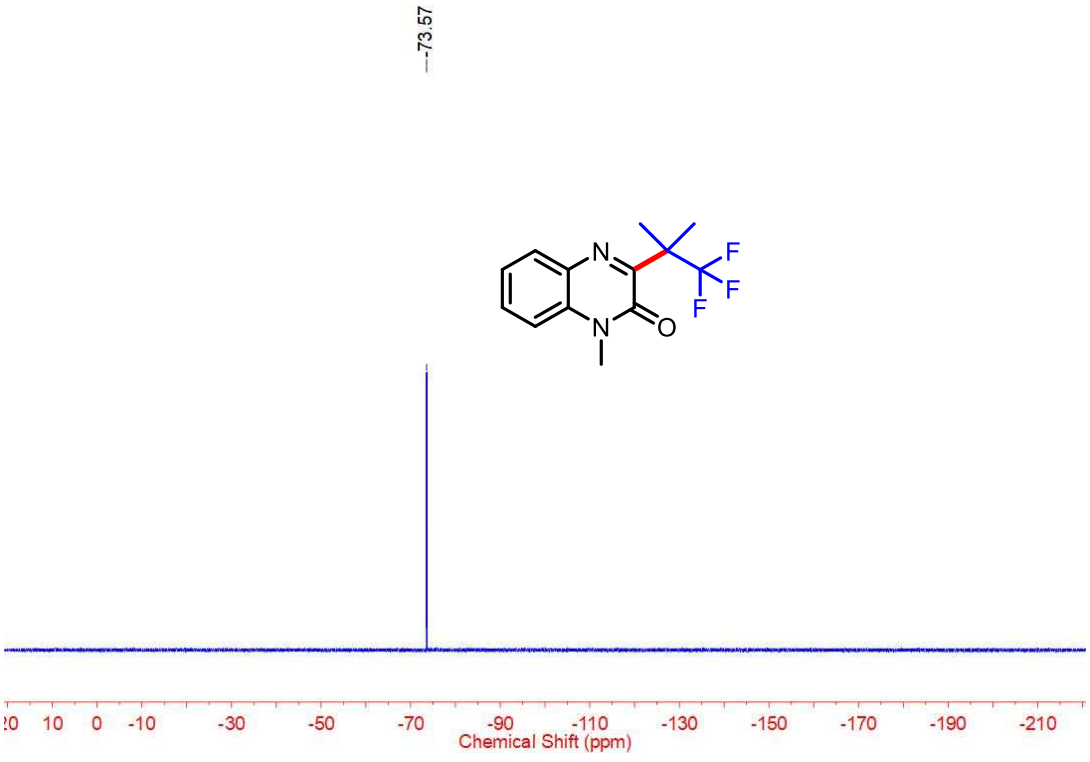
28 ^{1}H NMR (500 MHz, $CDCl_3$)



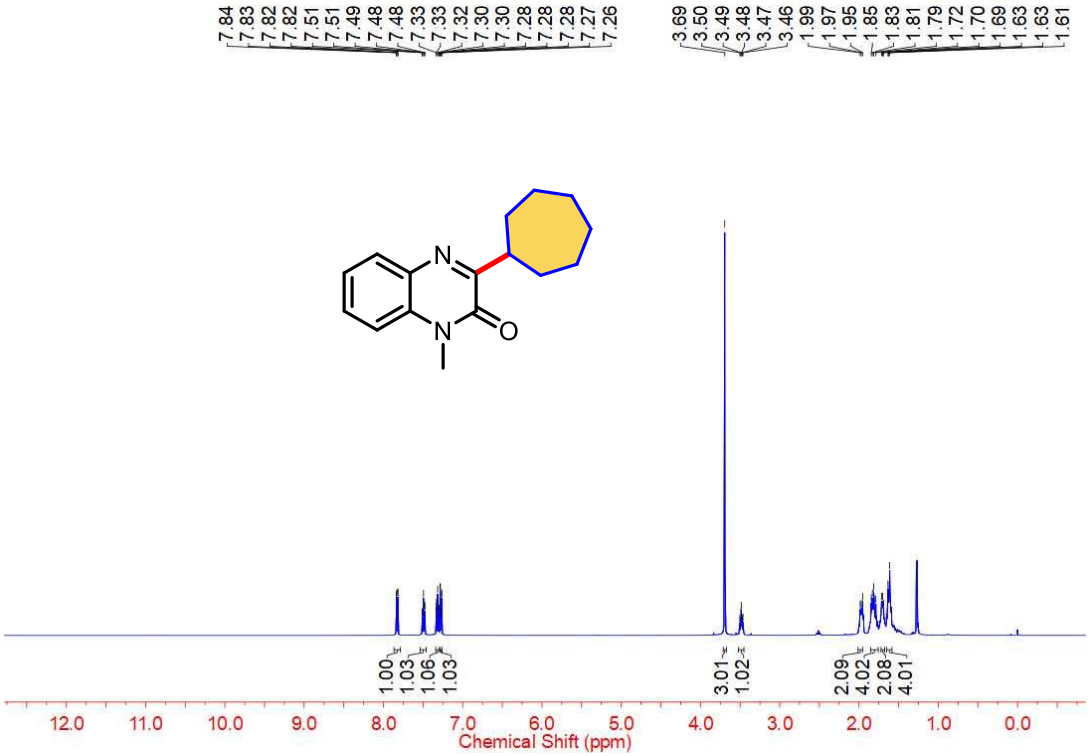
28 ^{13}C NMR (126 MHz, $CDCl_3$)



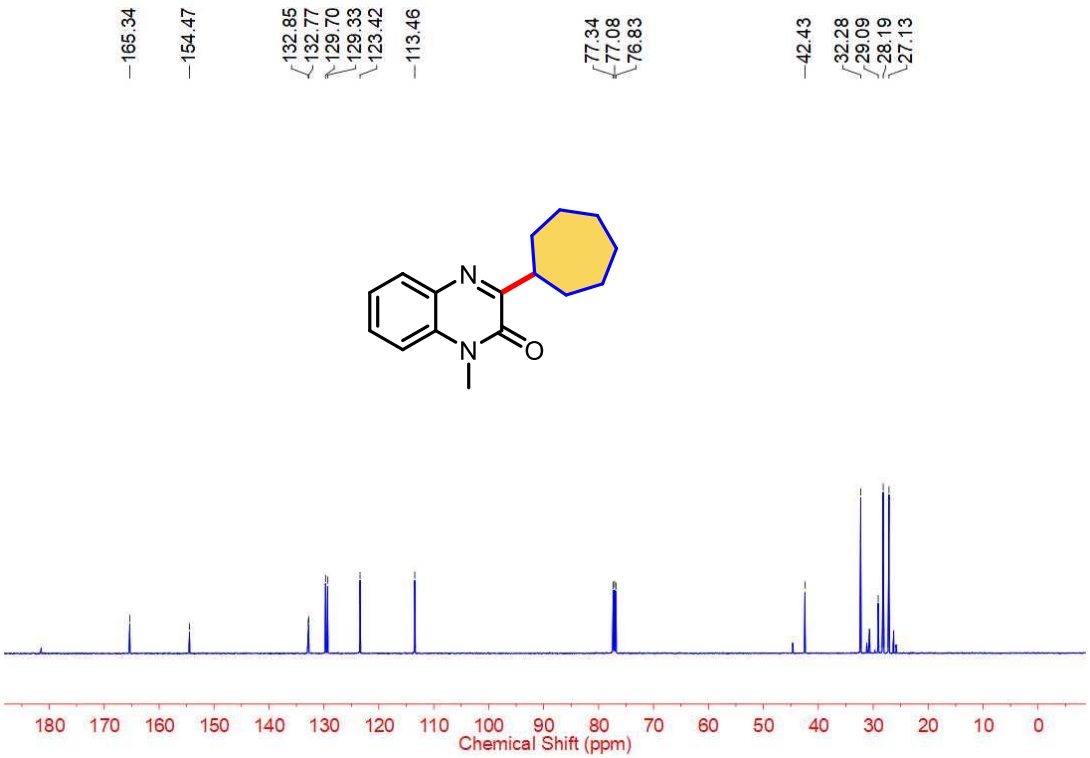
28 ^{19}F NMR (471 MHz, $CDCl_3$)



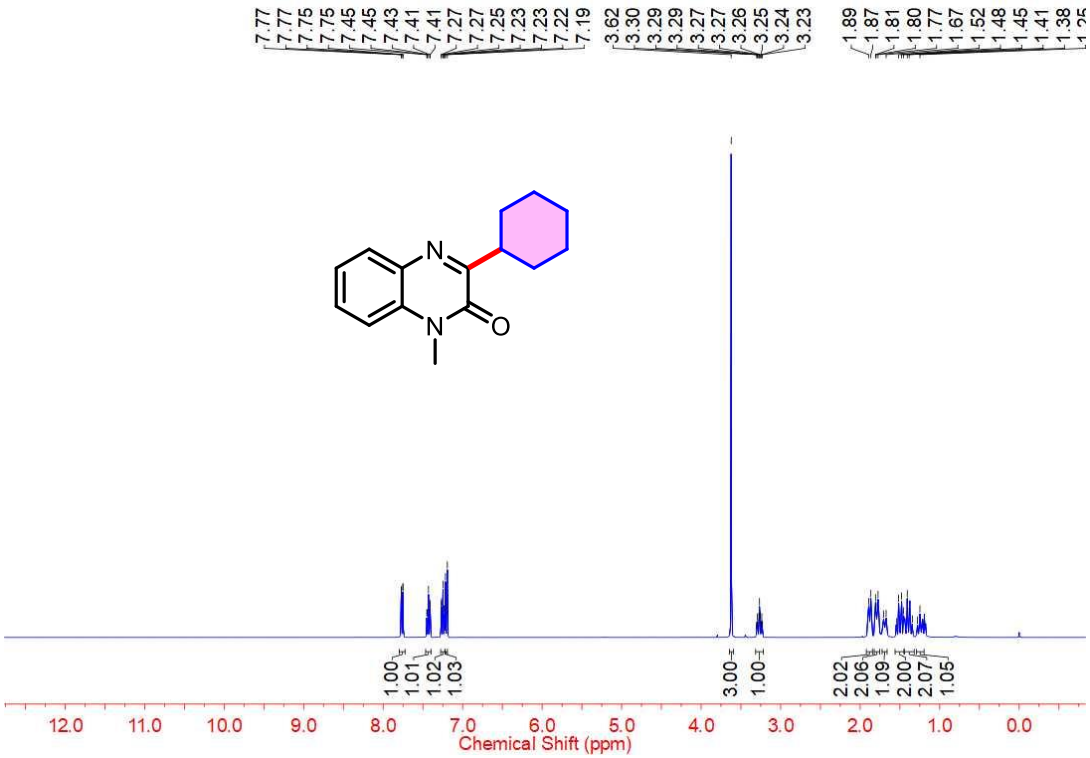
29 ^{1}H NMR (500 MHz, $CDCl_3$)



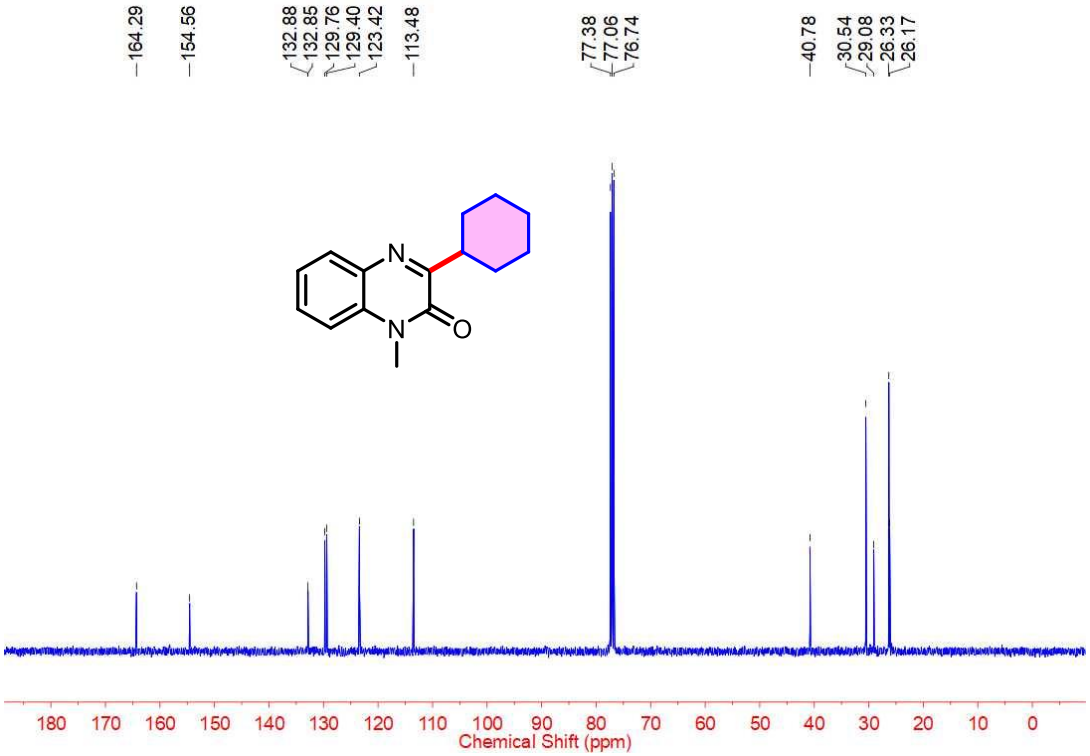
29 ^{13}C NMR (126 MHz, $CDCl_3$)



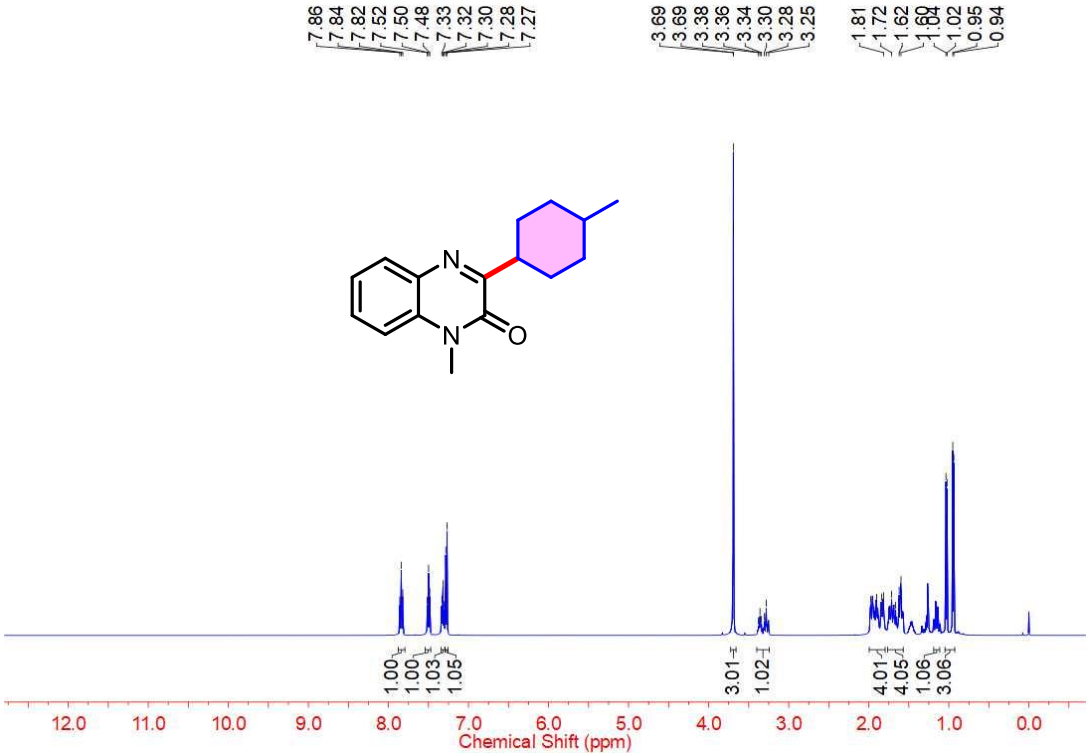
30 ^{1}H NMR (400 MHz, $CDCl_3$)



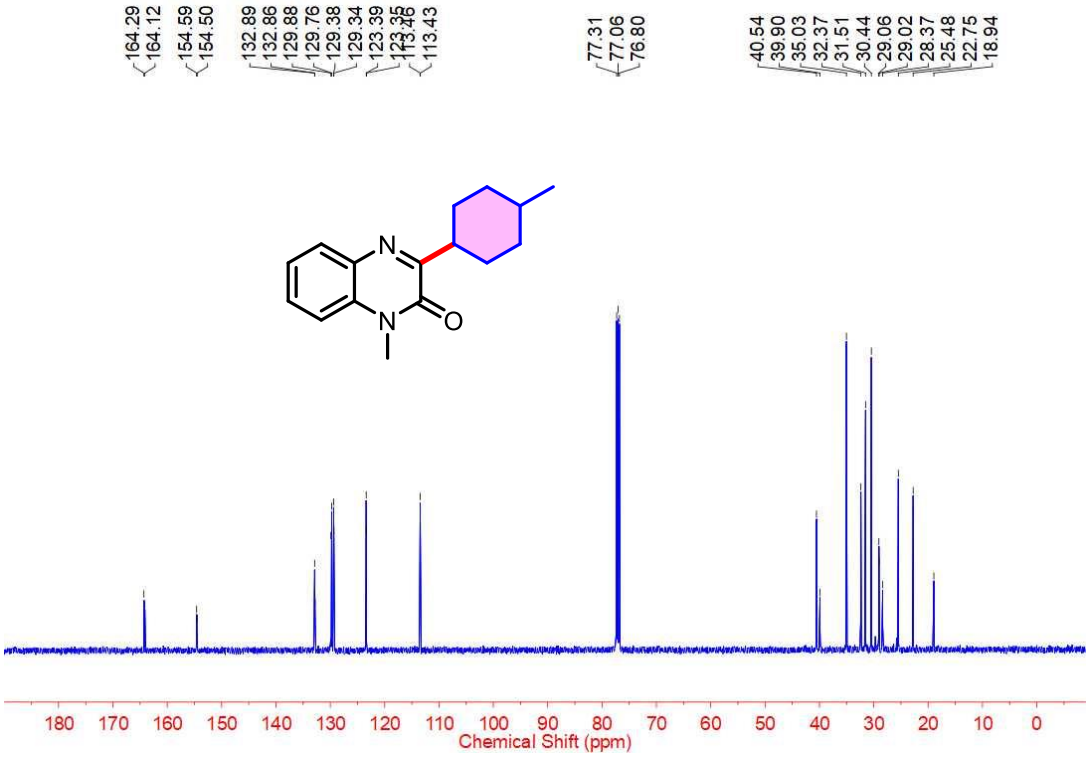
30 ^{13}C NMR (100 MHz, $CDCl_3$)



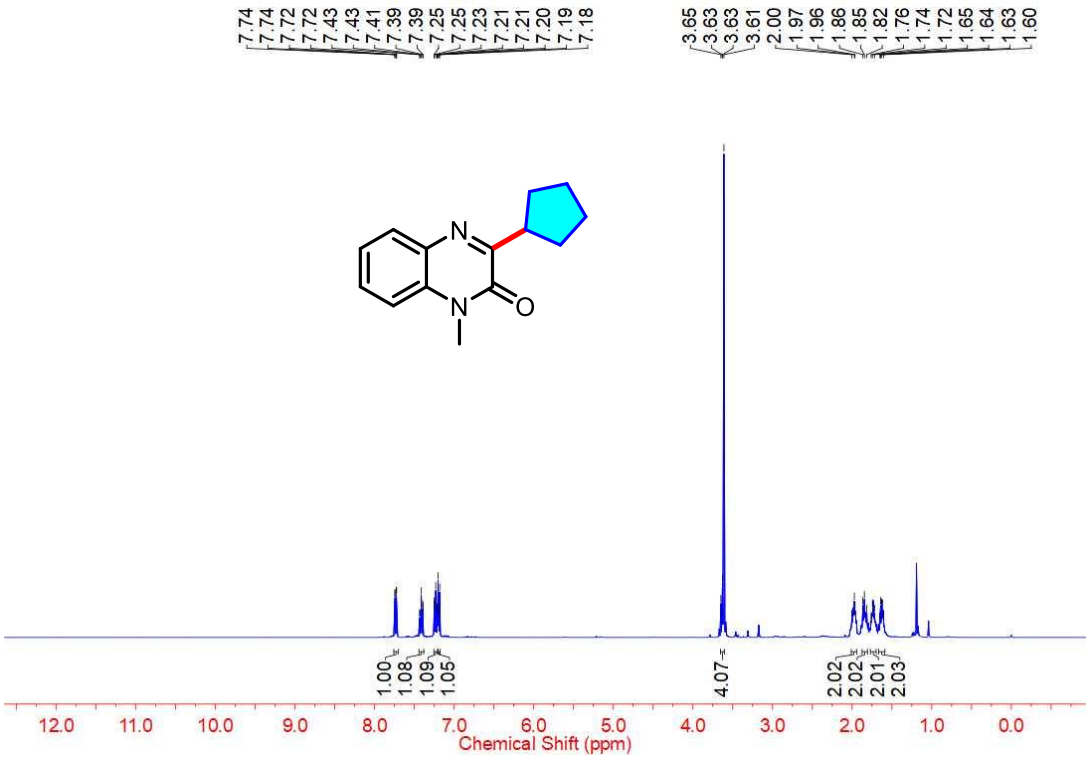
31 ^{1}H NMR (500 MHz, $CDCl_3$)



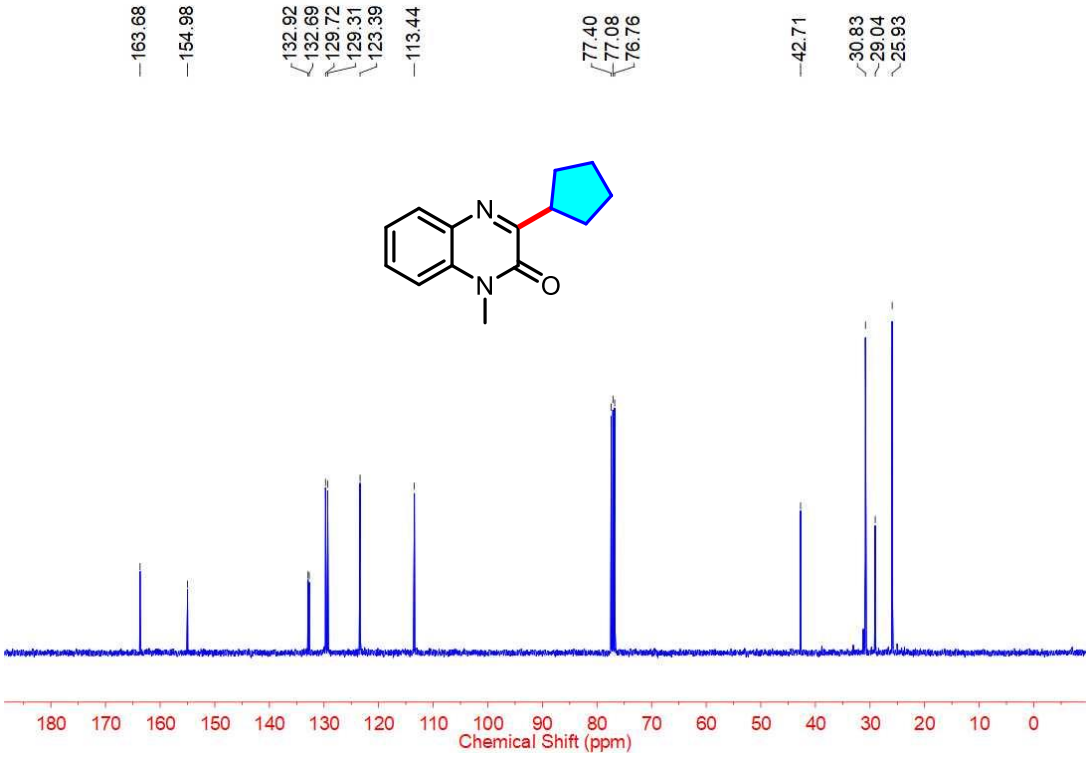
31 ^{13}C NMR (126 MHz, $CDCl_3$)



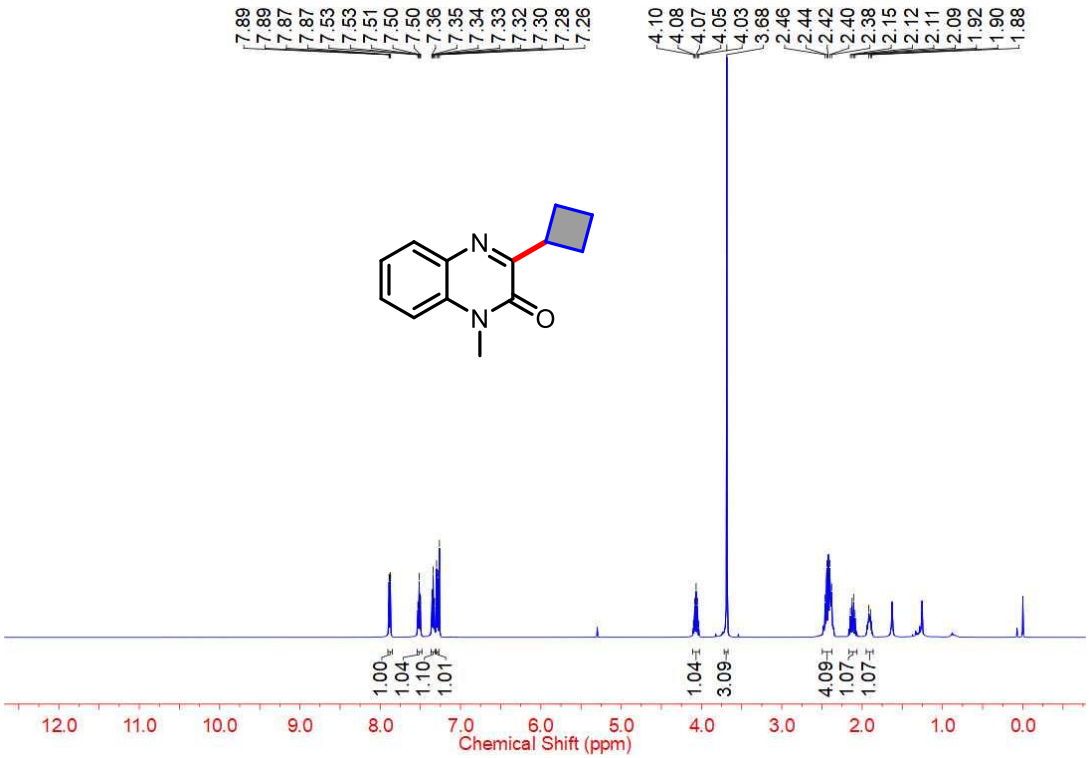
32 ^{1}H NMR (400 MHz, $CDCl_3$)



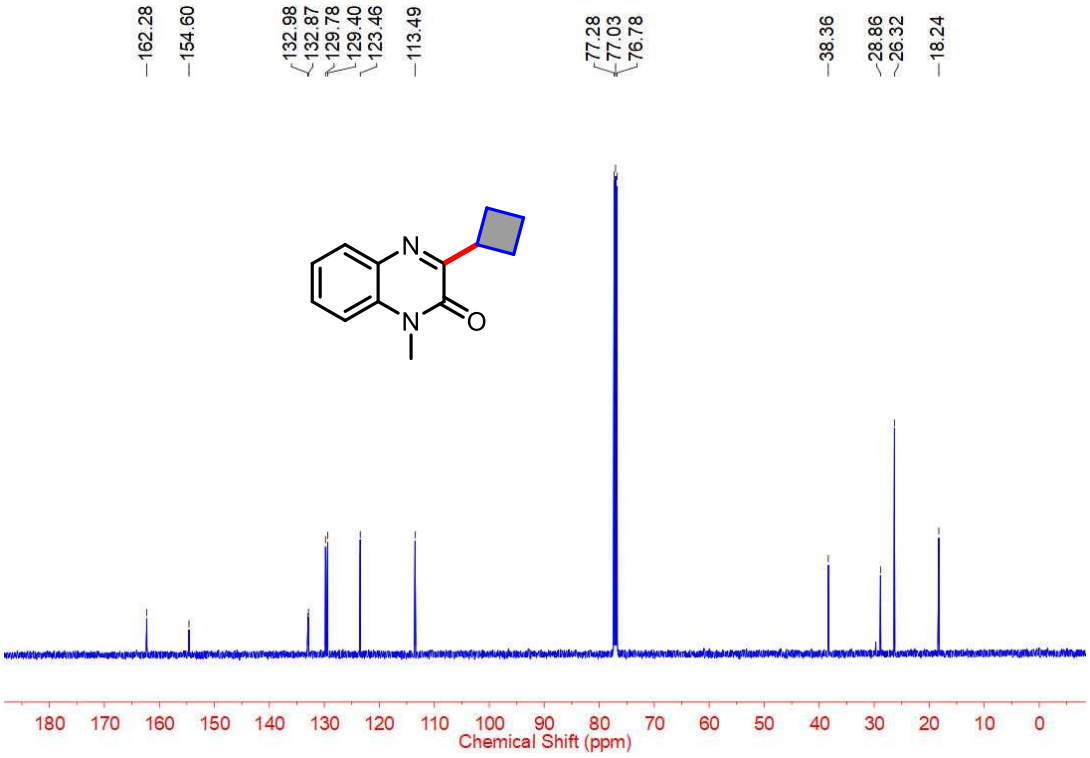
32 ^{13}C NMR (100 MHz, $CDCl_3$)



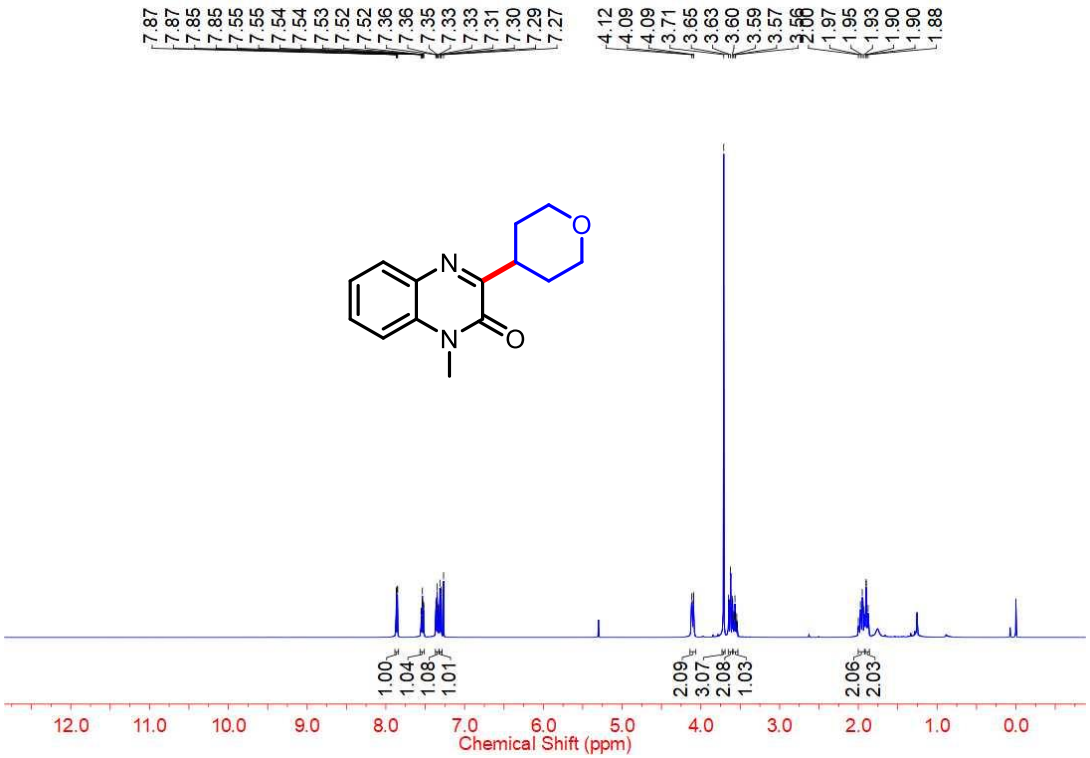
33 ^{1}H NMR (500 MHz, $CDCl_3$)



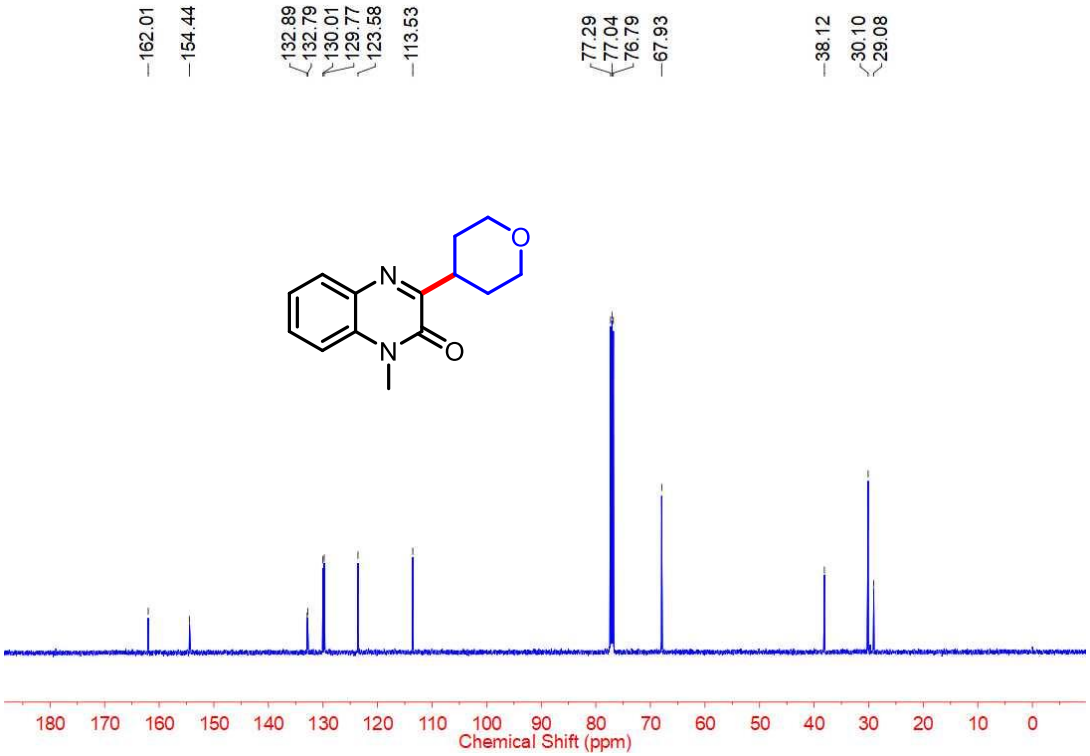
33 ^{13}C NMR (126 MHz, $CDCl_3$)



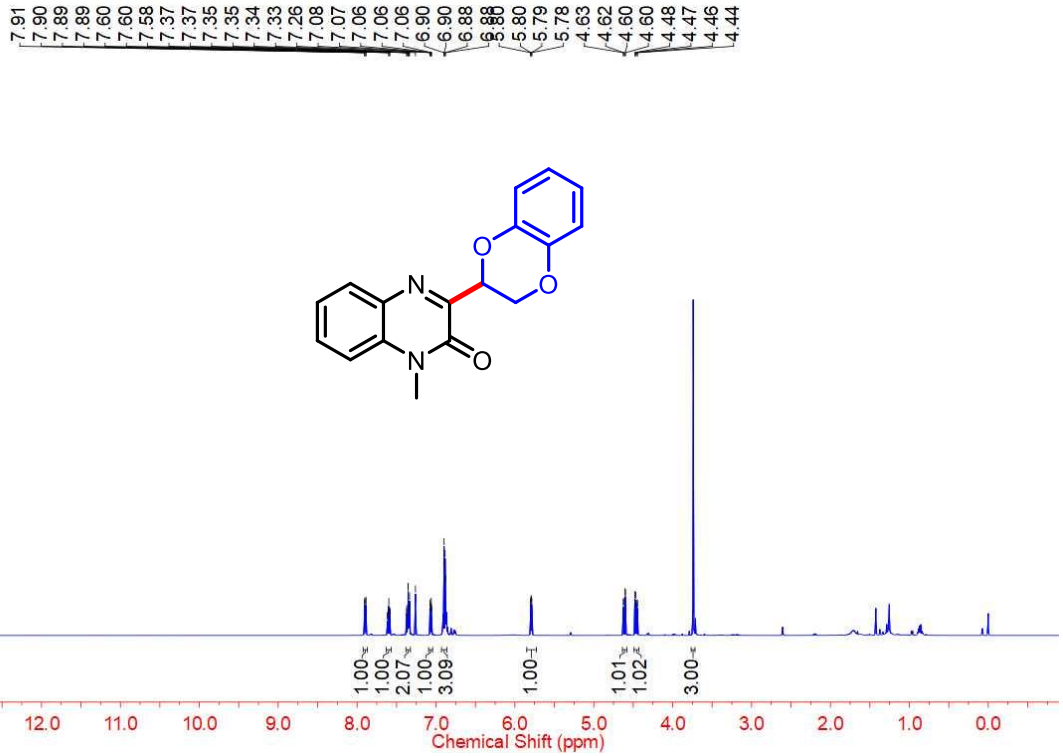
34 ^{1}H NMR (500 MHz, $CDCl_3$)



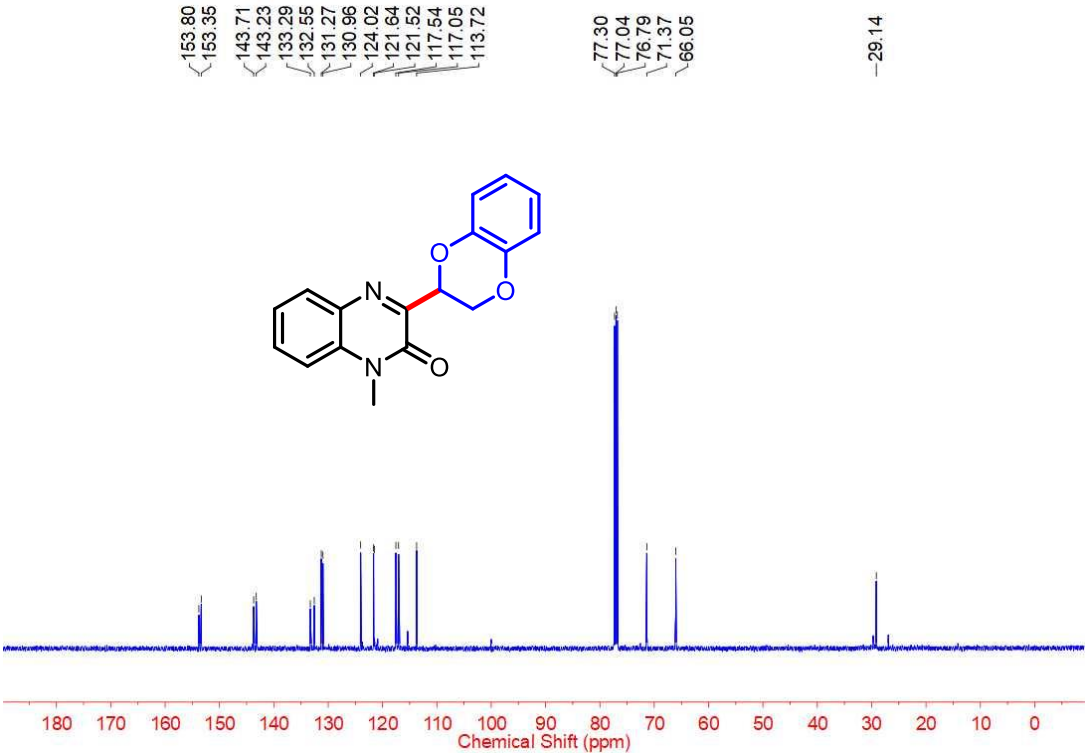
34 ^{13}C NMR (126 MHz, $CDCl_3$)



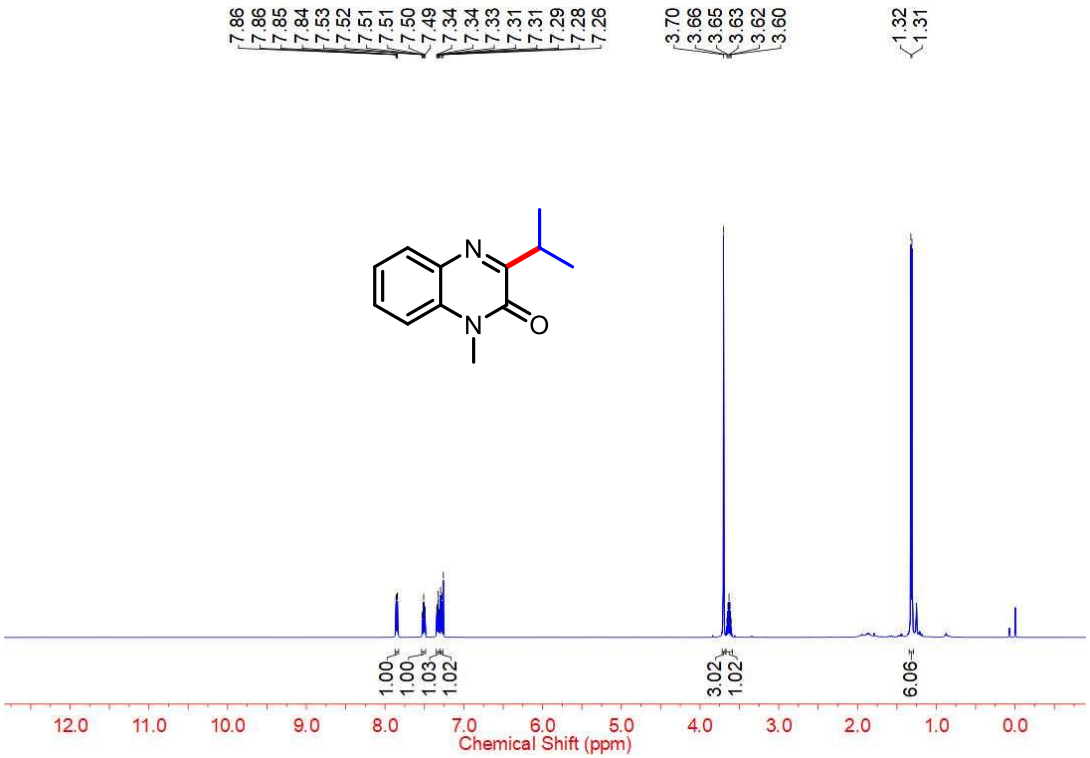
35 ^{1}H NMR (500 MHz, $CDCl_3$)



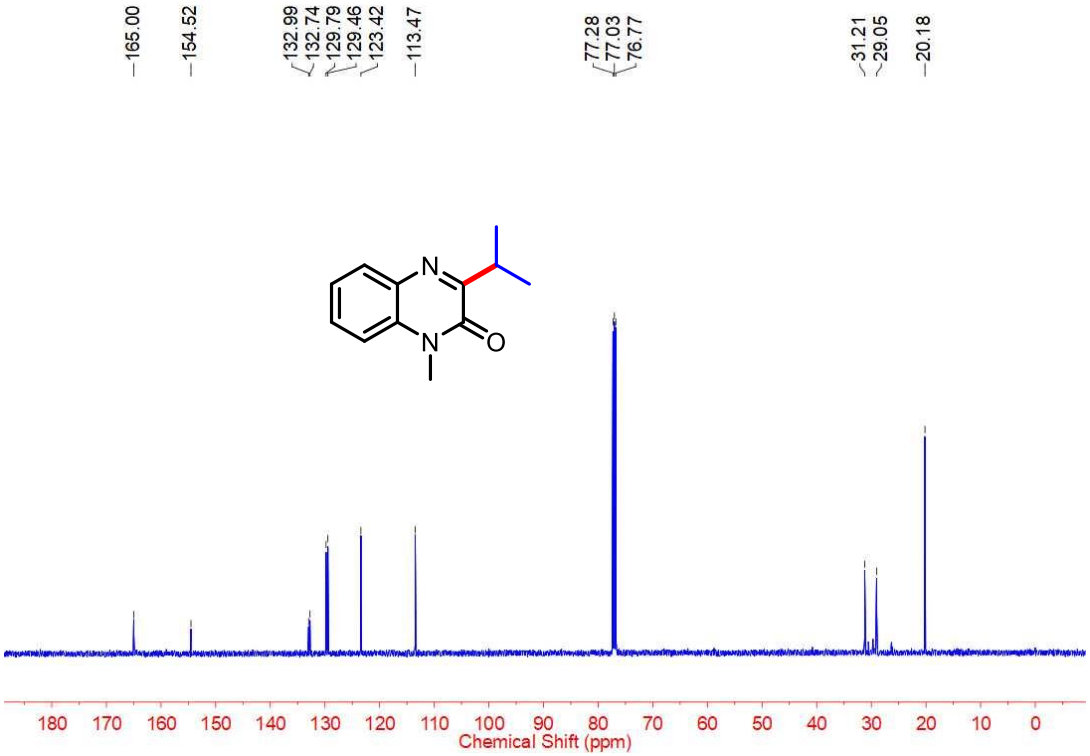
35 ^{13}C NMR (126 MHz, $CDCl_3$)



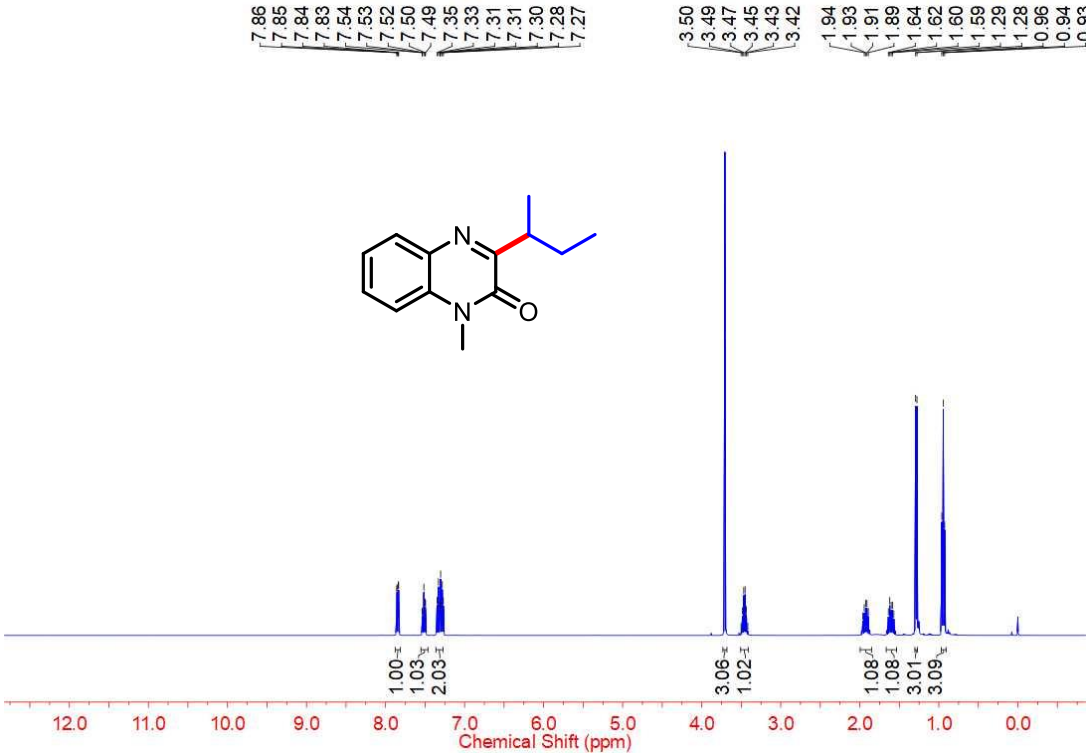
36 ^{1}H NMR (500 MHz, $CDCl_3$)



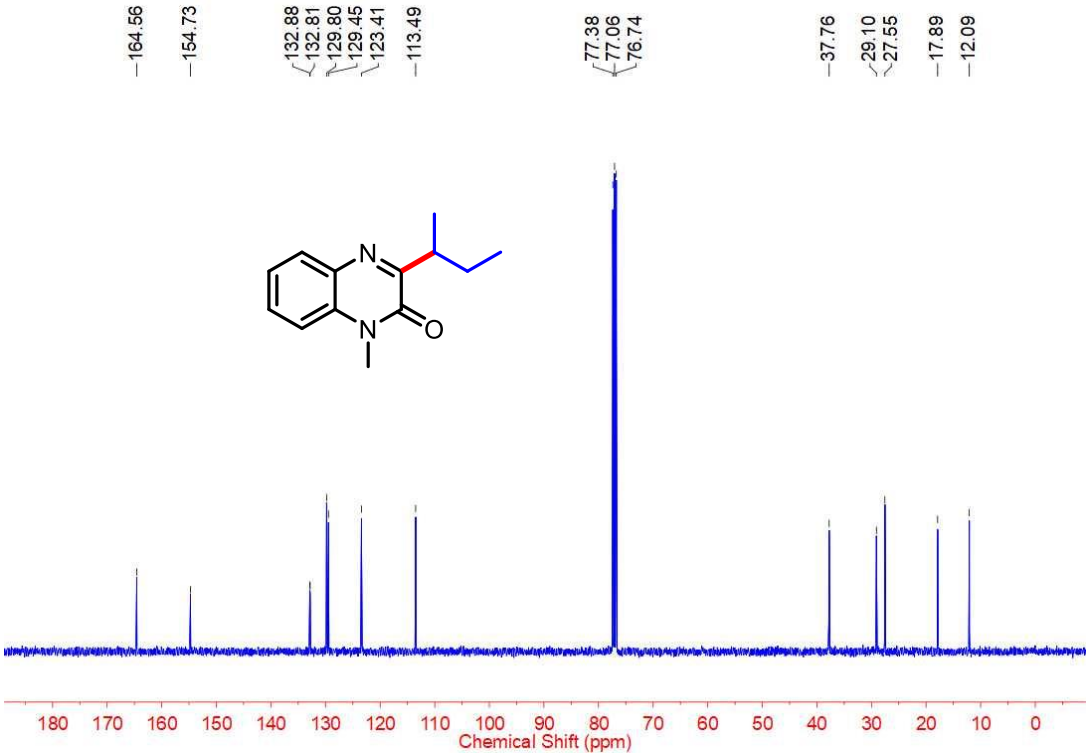
36 ^{13}C NMR (126 MHz, $CDCl_3$)



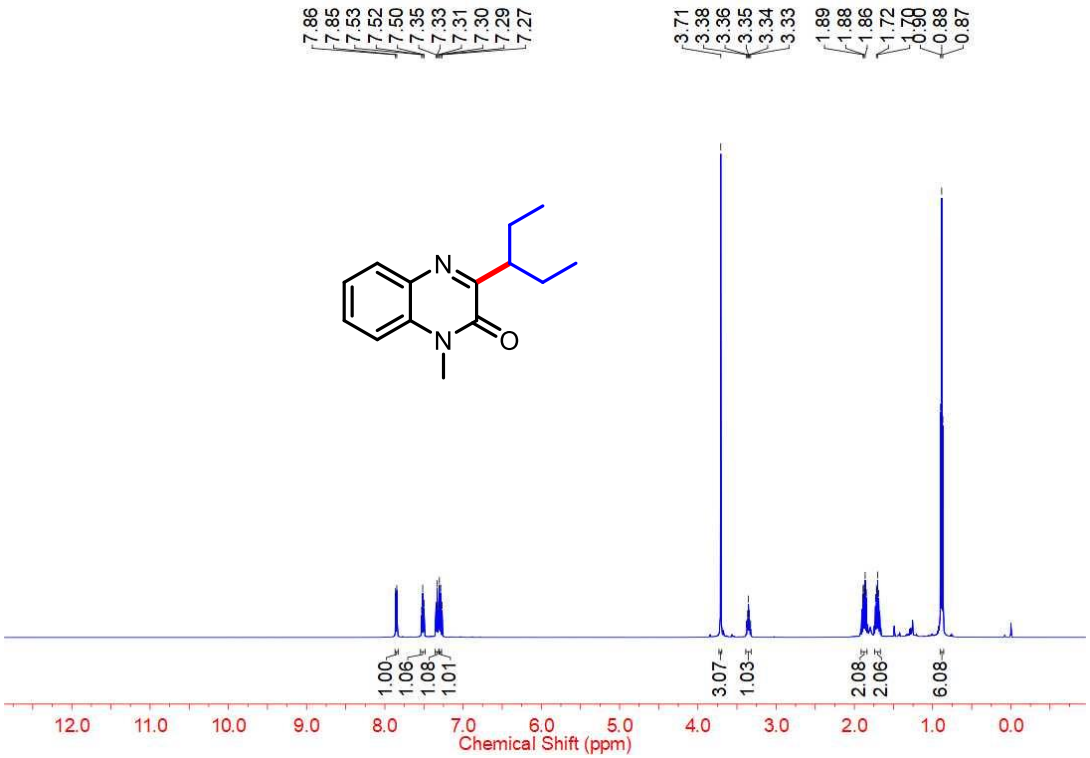
37 ^{1}H NMR (400 MHz, $CDCl_3$)



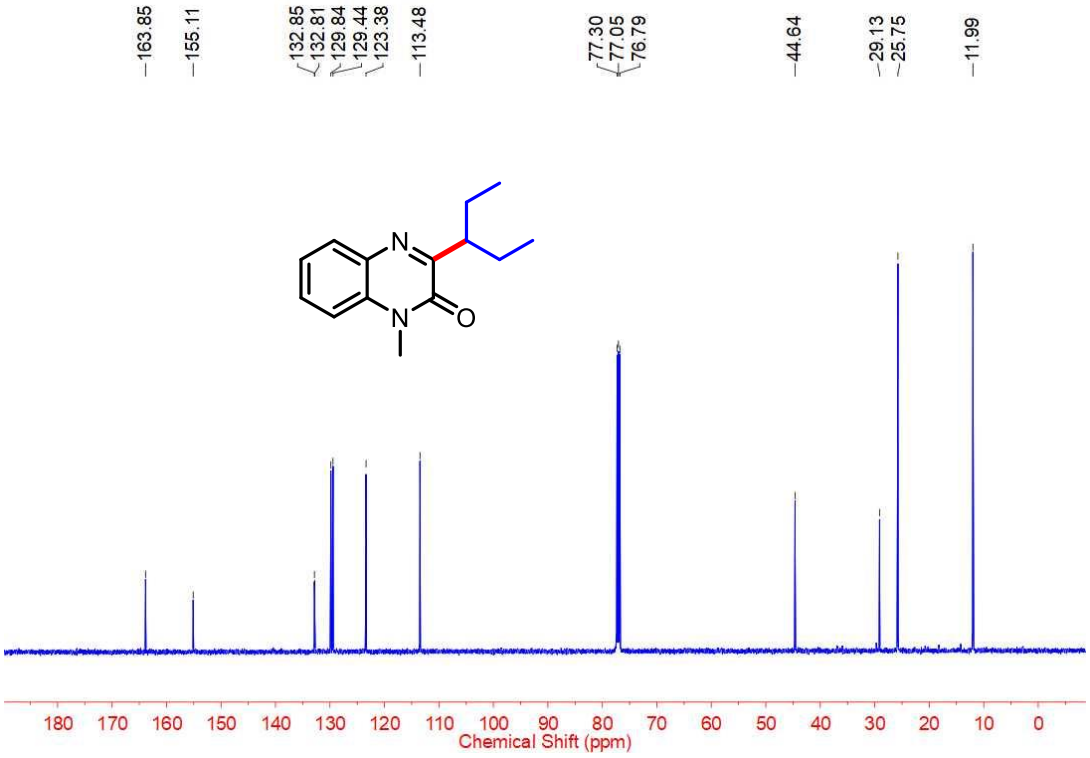
37 ^{13}C NMR (100 MHz, $CDCl_3$)



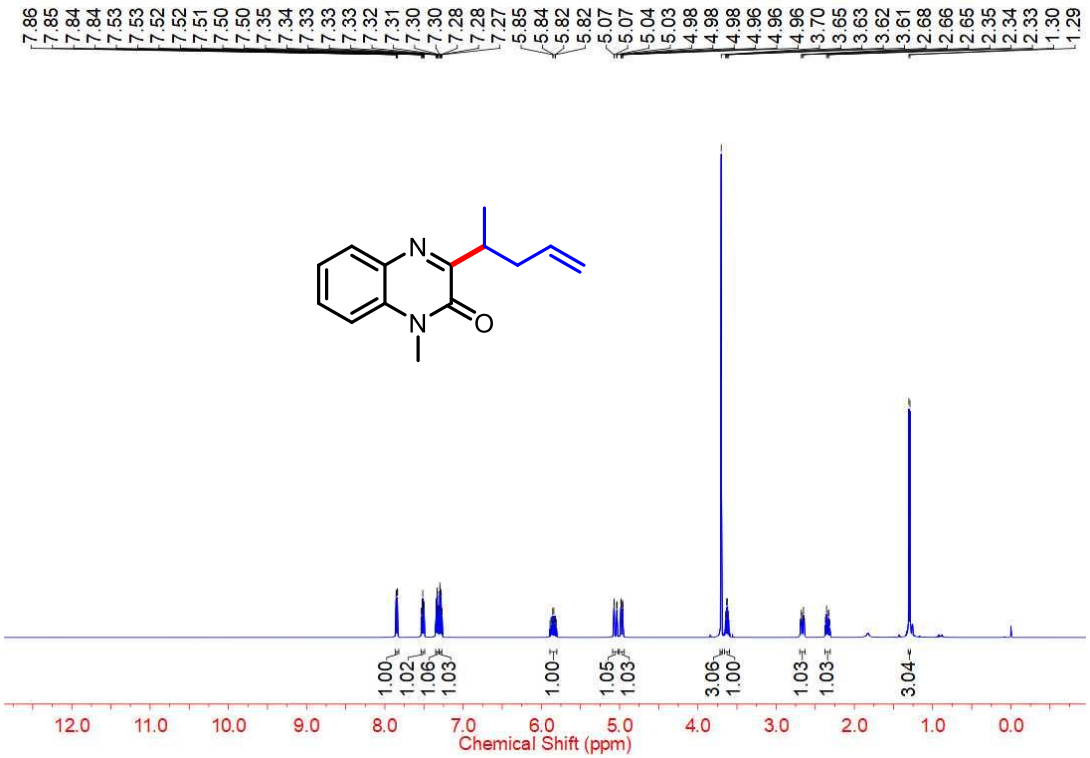
38 ^{1}H NMR (500 MHz, $CDCl_3$)



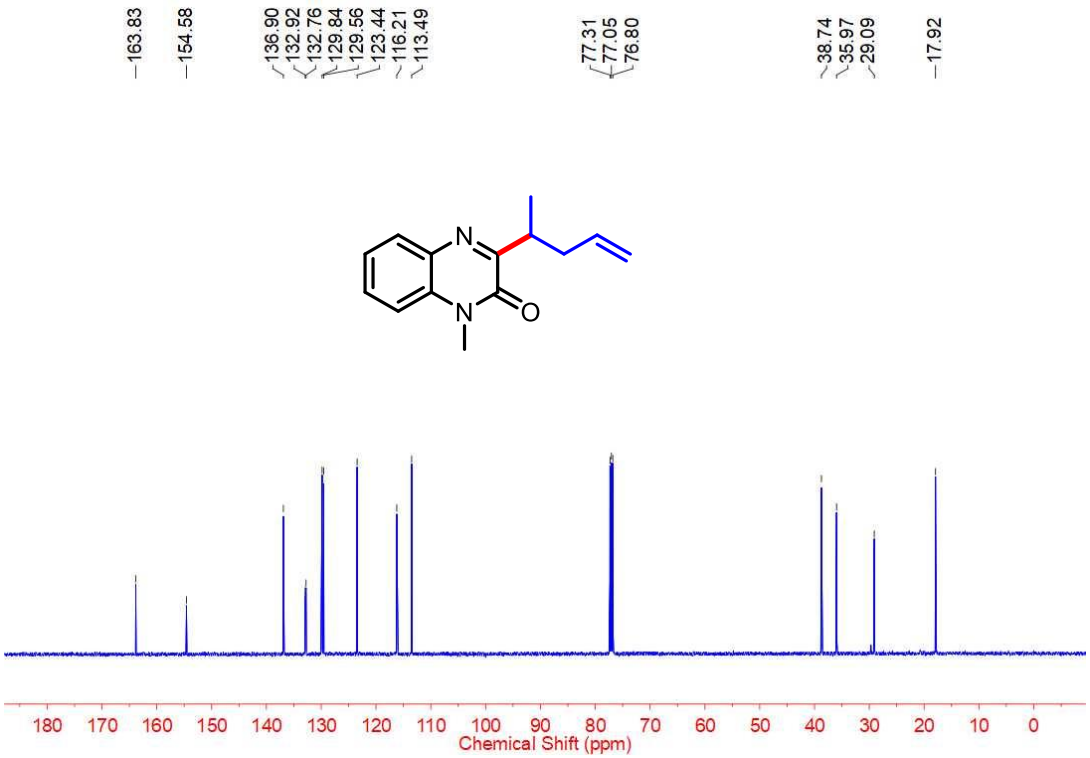
38 ^{13}C NMR (126 MHz, $CDCl_3$)



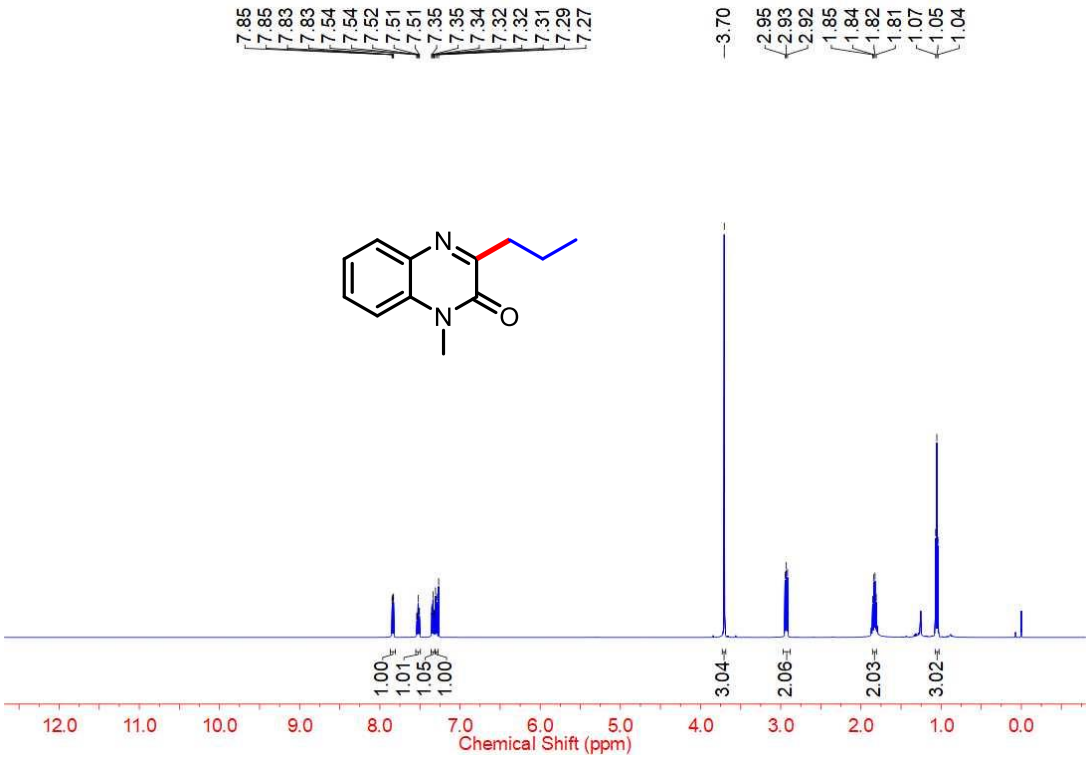
39 ^{1}H NMR (500 MHz, $CDCl_3$)



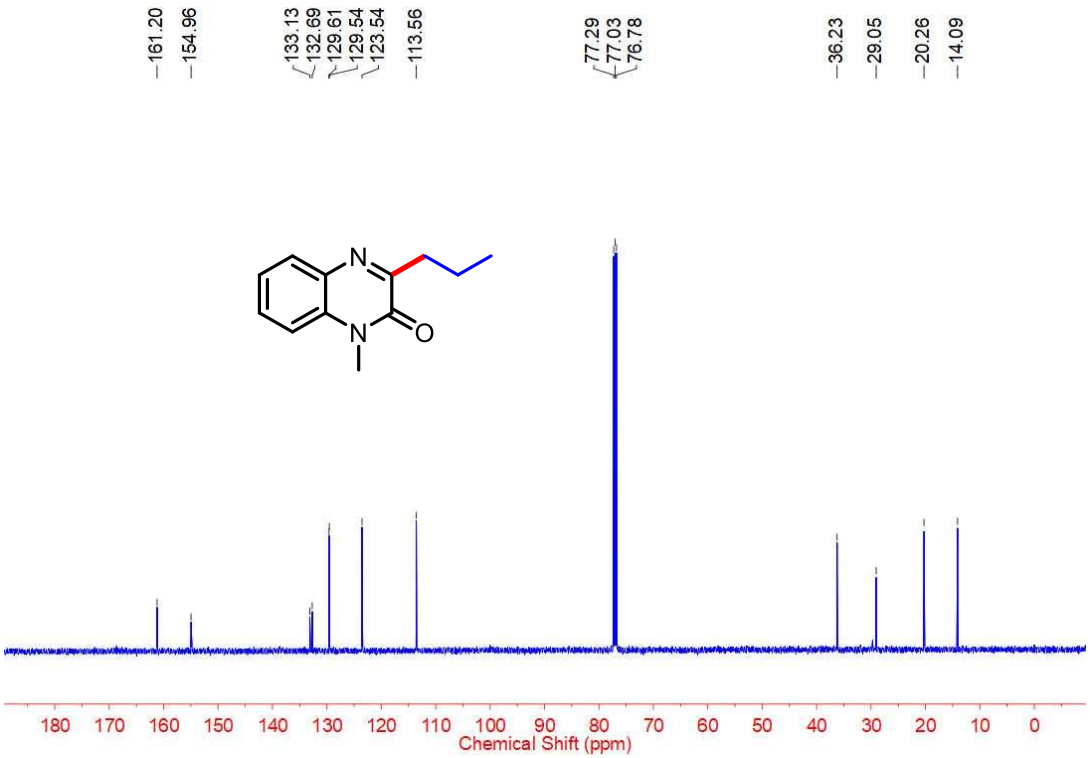
39 ^{13}C NMR (126 MHz, $CDCl_3$)



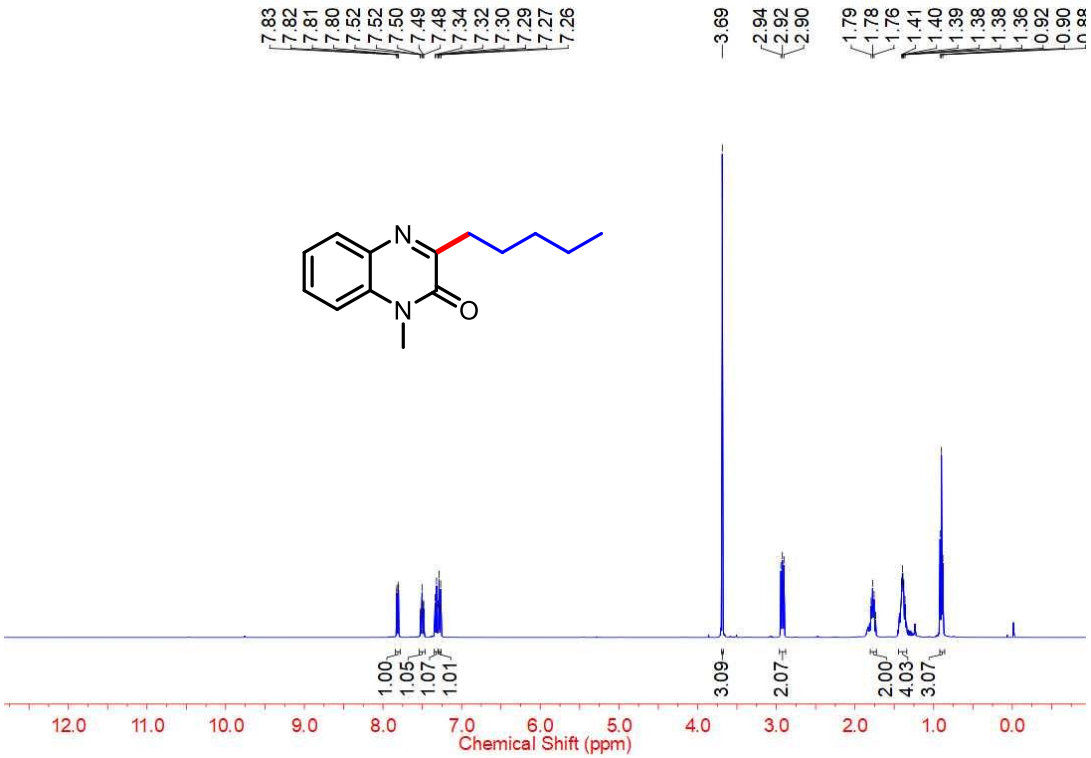
40 ^{1}H NMR (500 MHz, $CDCl_3$)



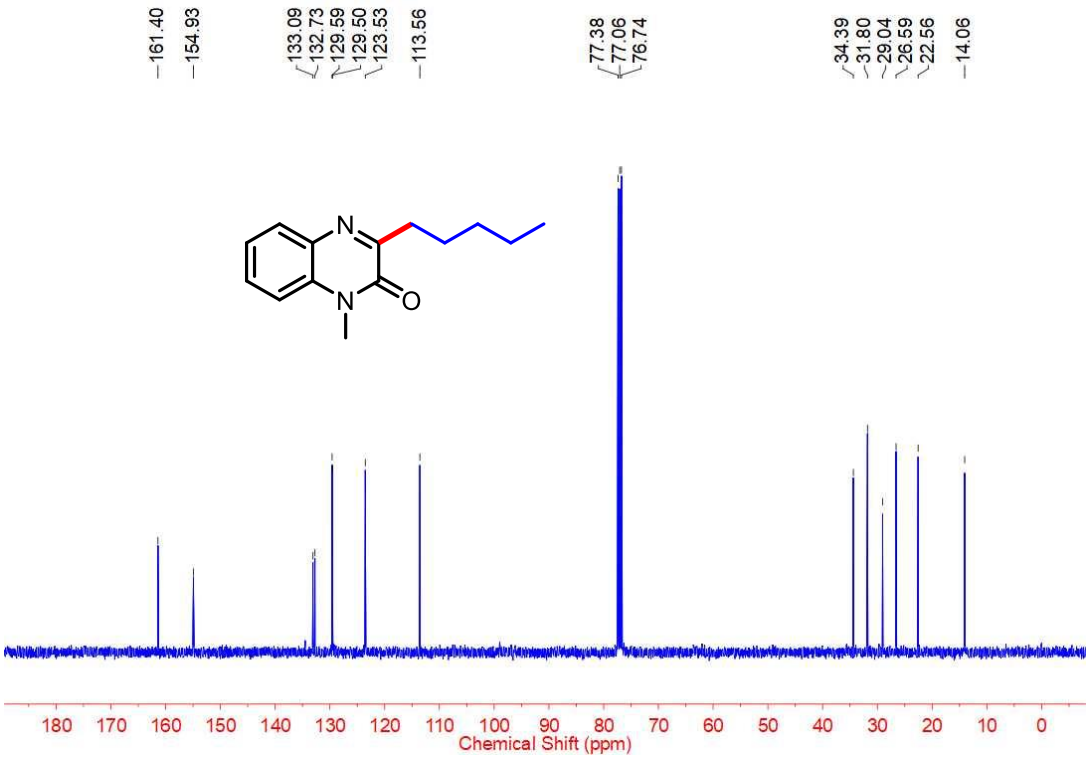
40 ^{13}C NMR (126 MHz, $CDCl_3$)



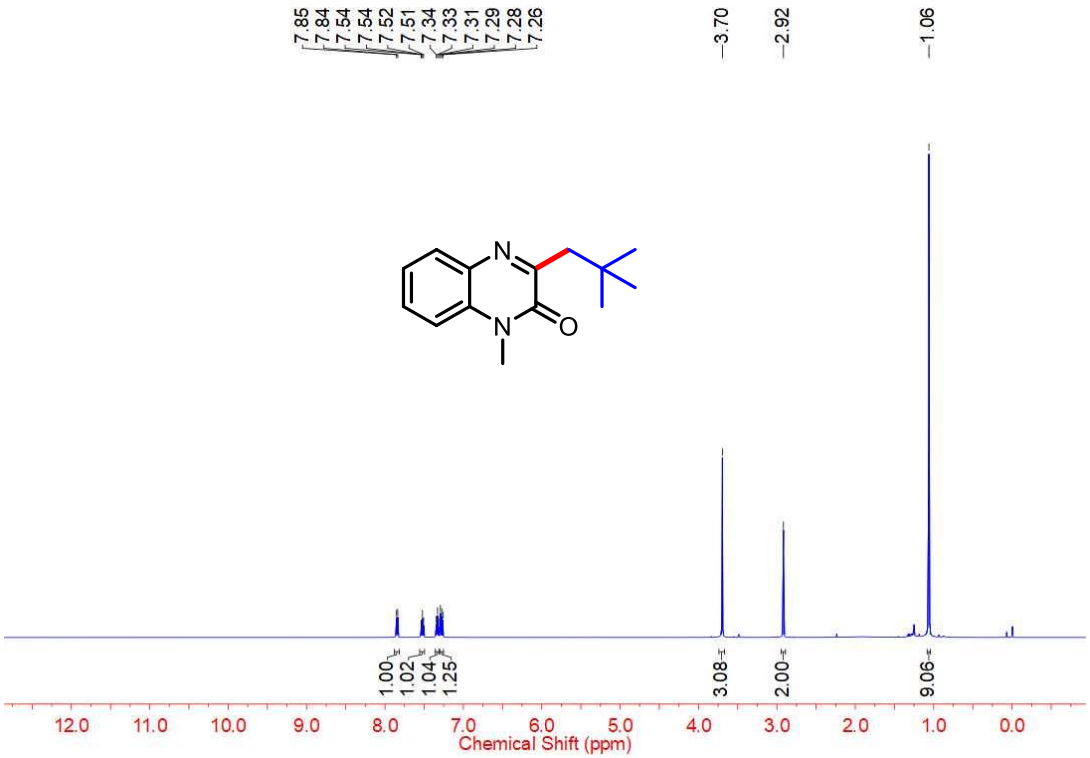
41 ^{1}H NMR (400 MHz, $CDCl_3$)



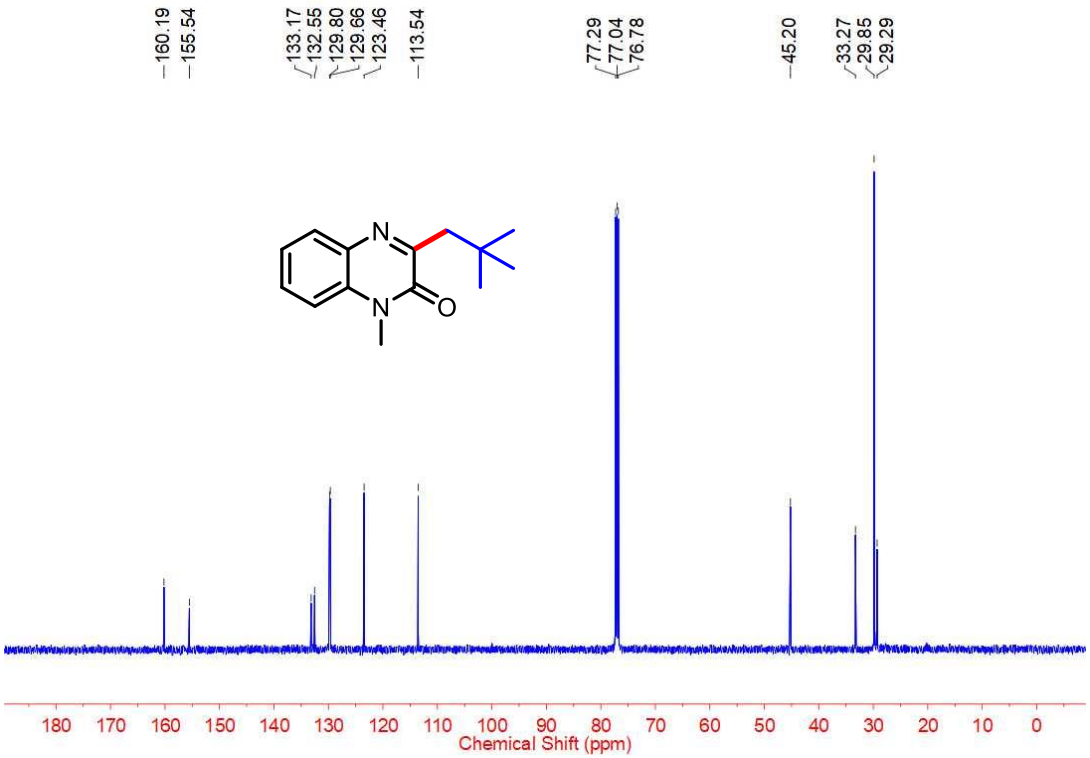
41 ^{13}C NMR (100 MHz, $CDCl_3$)



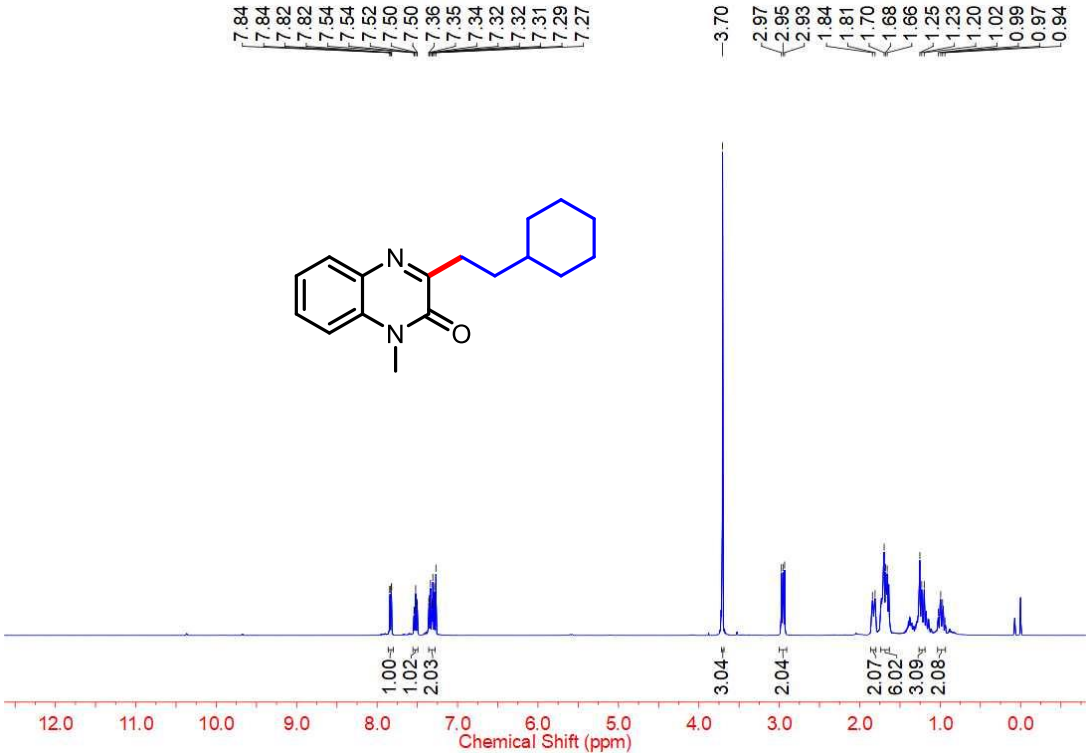
42 ^{1}H NMR (500 MHz, $CDCl_3$)



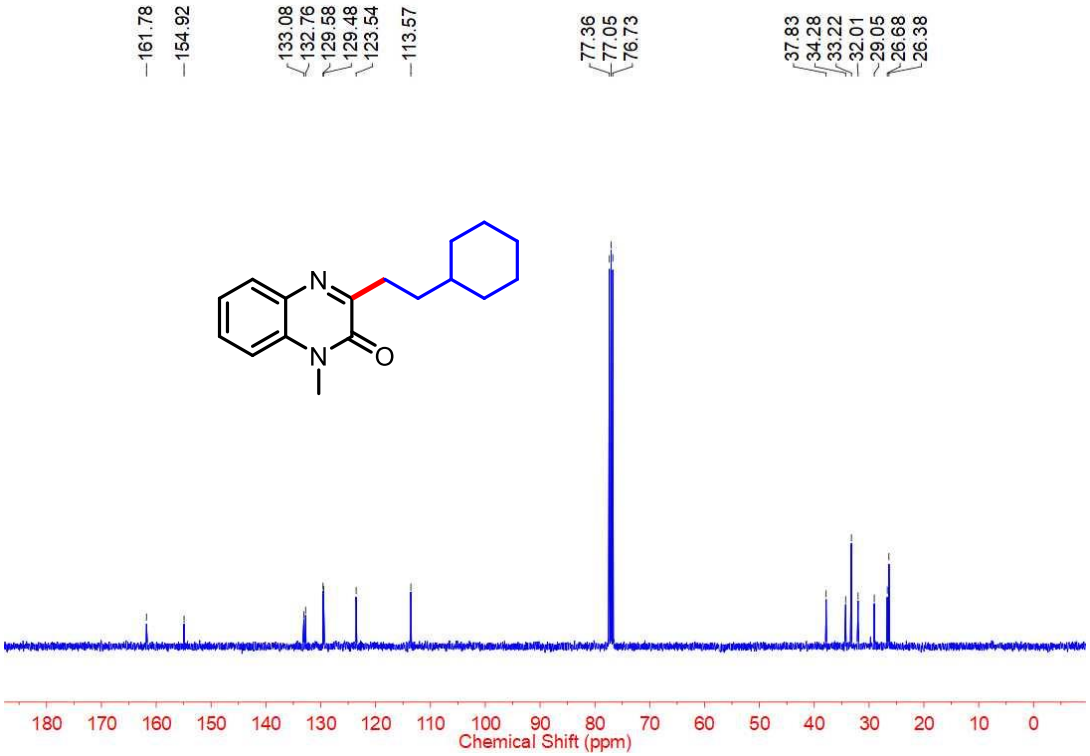
42 ^{13}C NMR (126 MHz, $CDCl_3$)



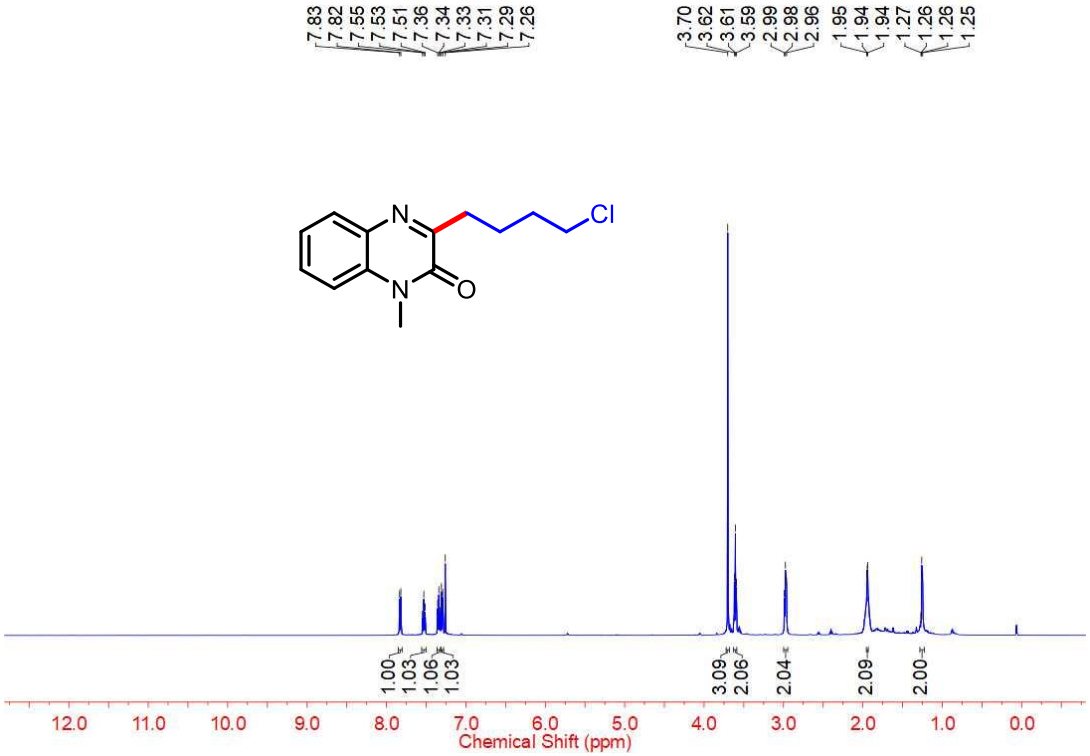
43 ^{1}H NMR (400 MHz, $CDCl_3$)



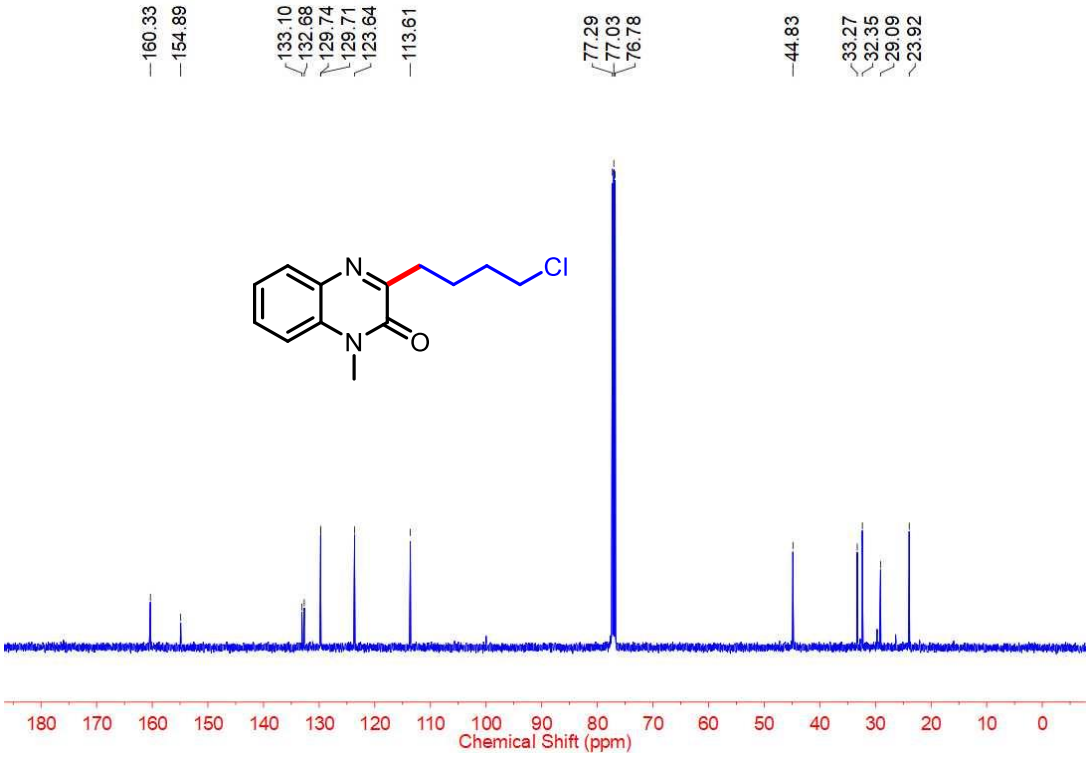
43 ^{13}C NMR (100 MHz, $CDCl_3$)



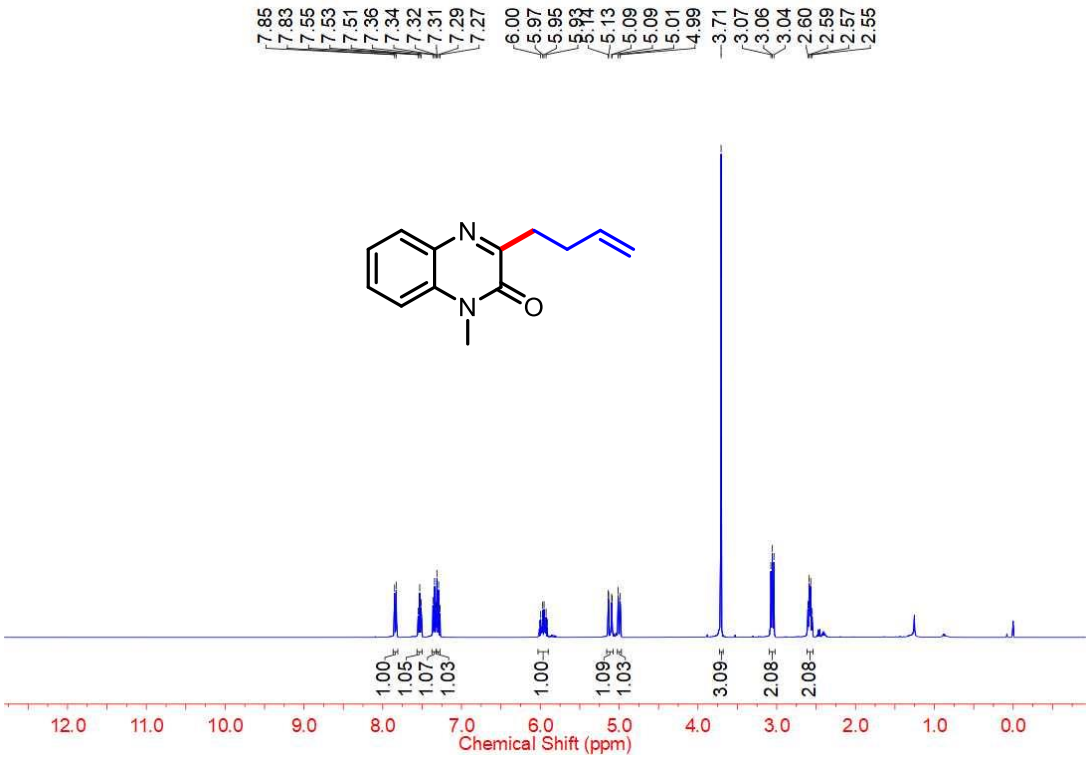
44 ^{1}H NMR (500 MHz, $CDCl_3$)



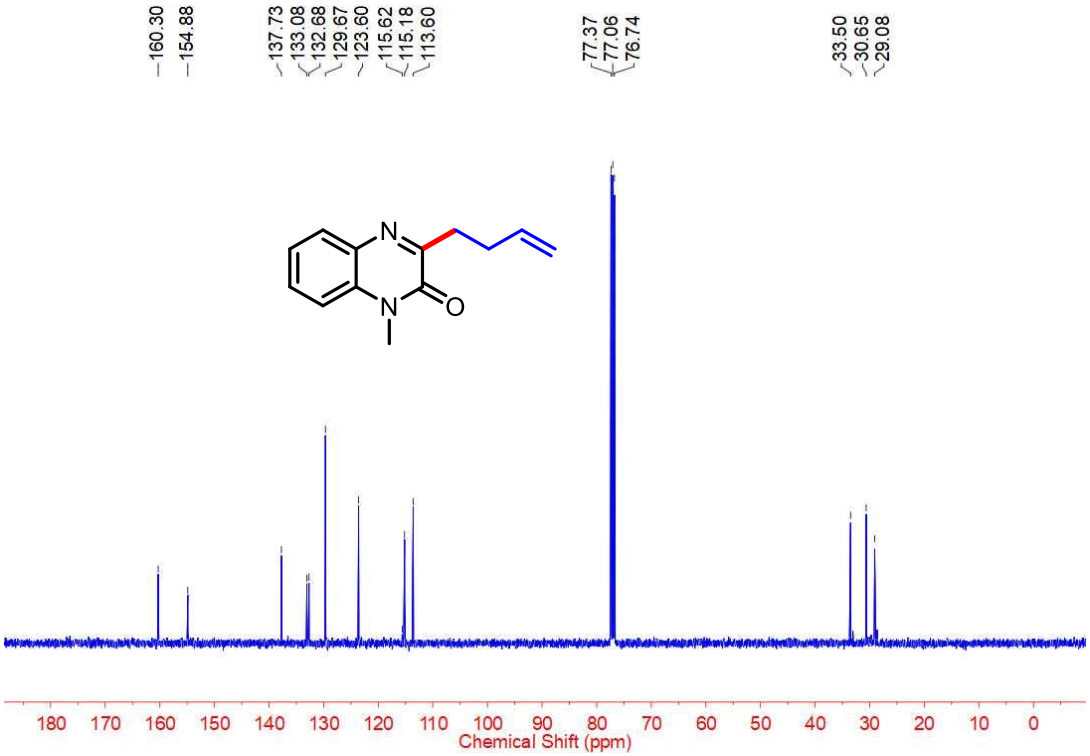
44 ^{13}C NMR (126 MHz, $CDCl_3$)



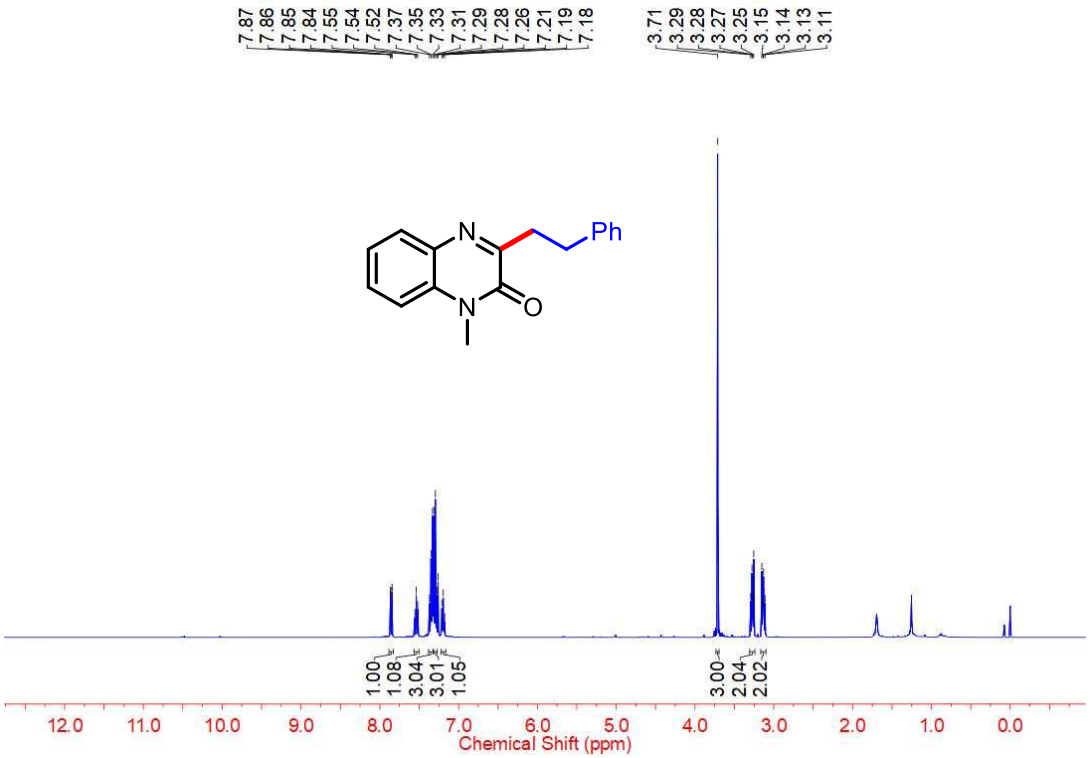
45 ^{1}H NMR (400 MHz, $CDCl_3$)



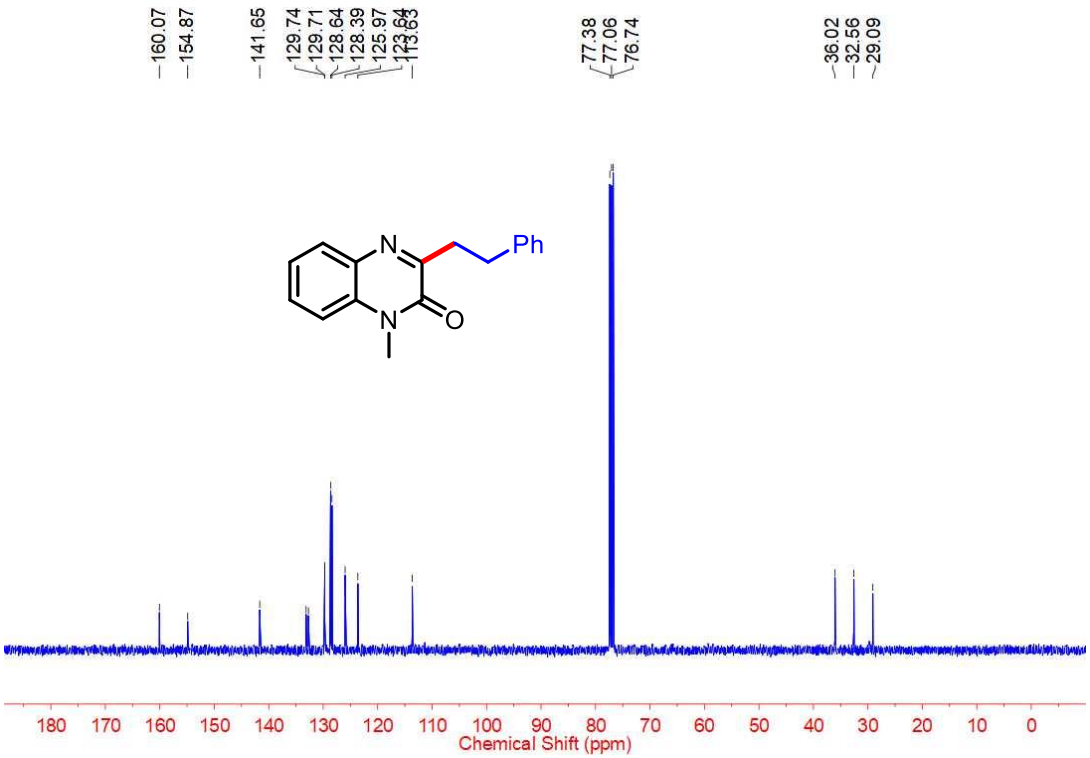
45 ^{13}C NMR (100 MHz, $CDCl_3$)



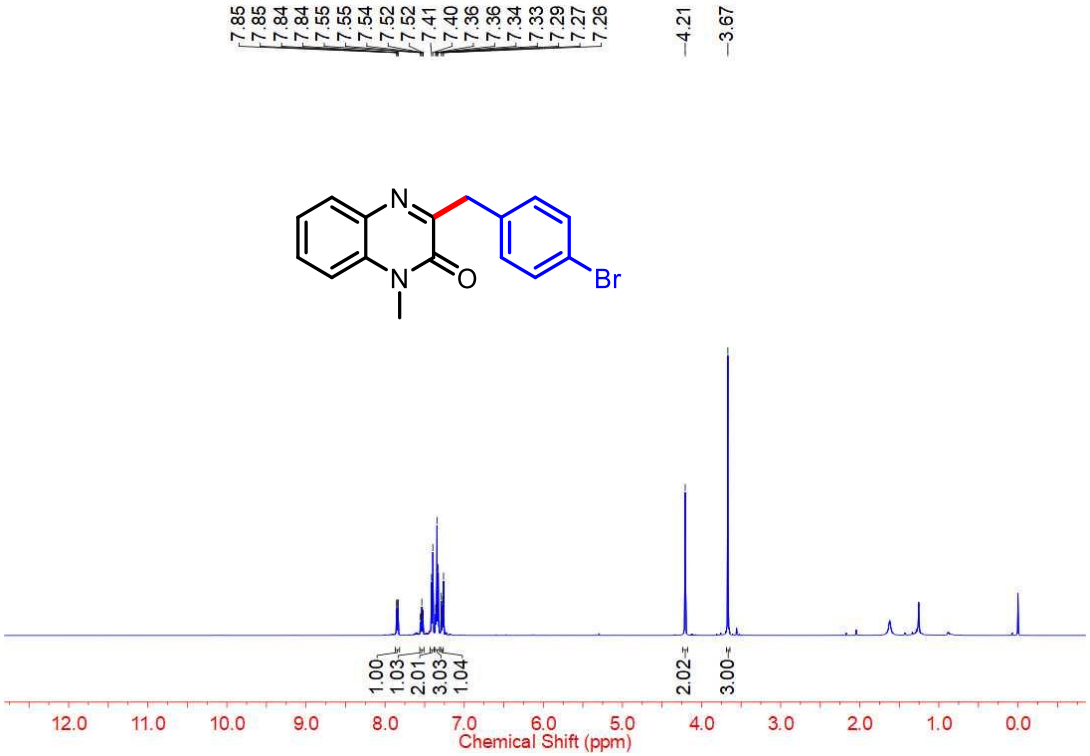
46 ^{1}H NMR (400 MHz, $CDCl_3$)



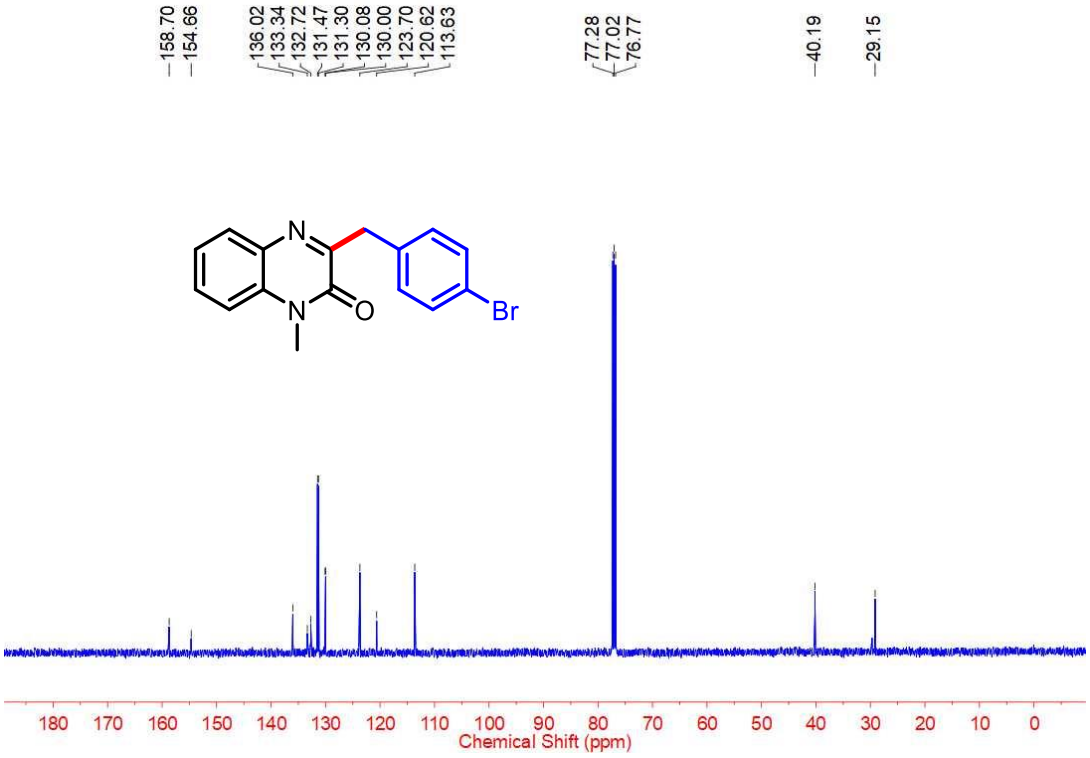
46 ^{13}C NMR (100 MHz, $CDCl_3$)



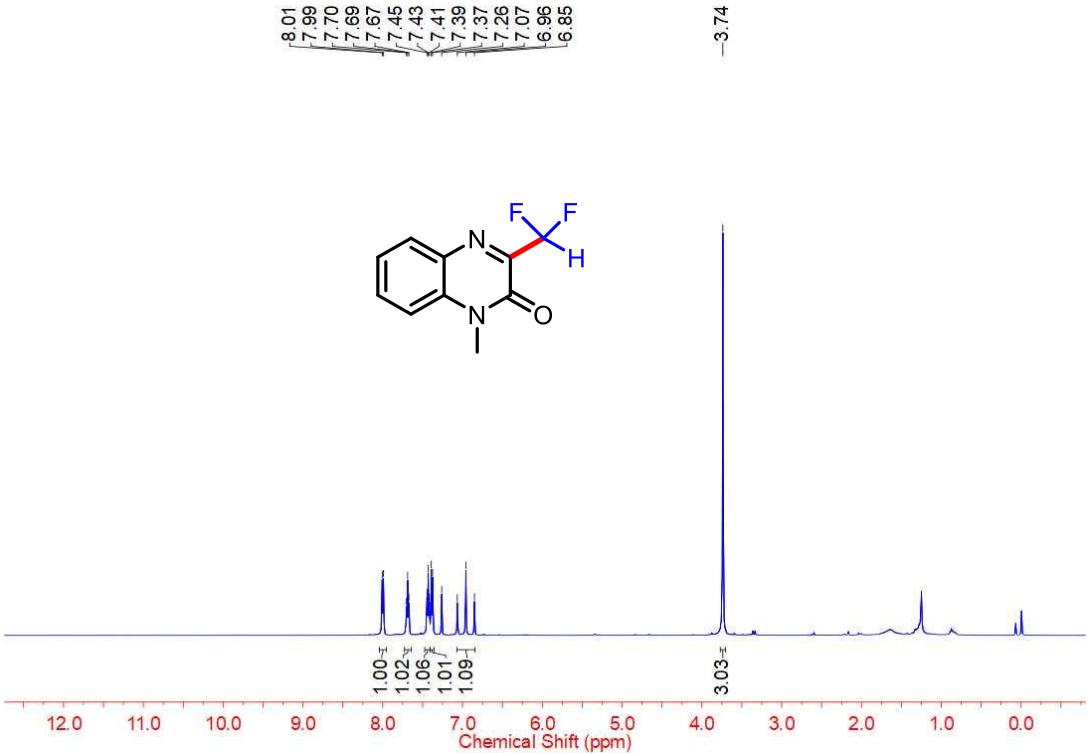
47 ^{1}H NMR (500 MHz, $CDCl_3$)



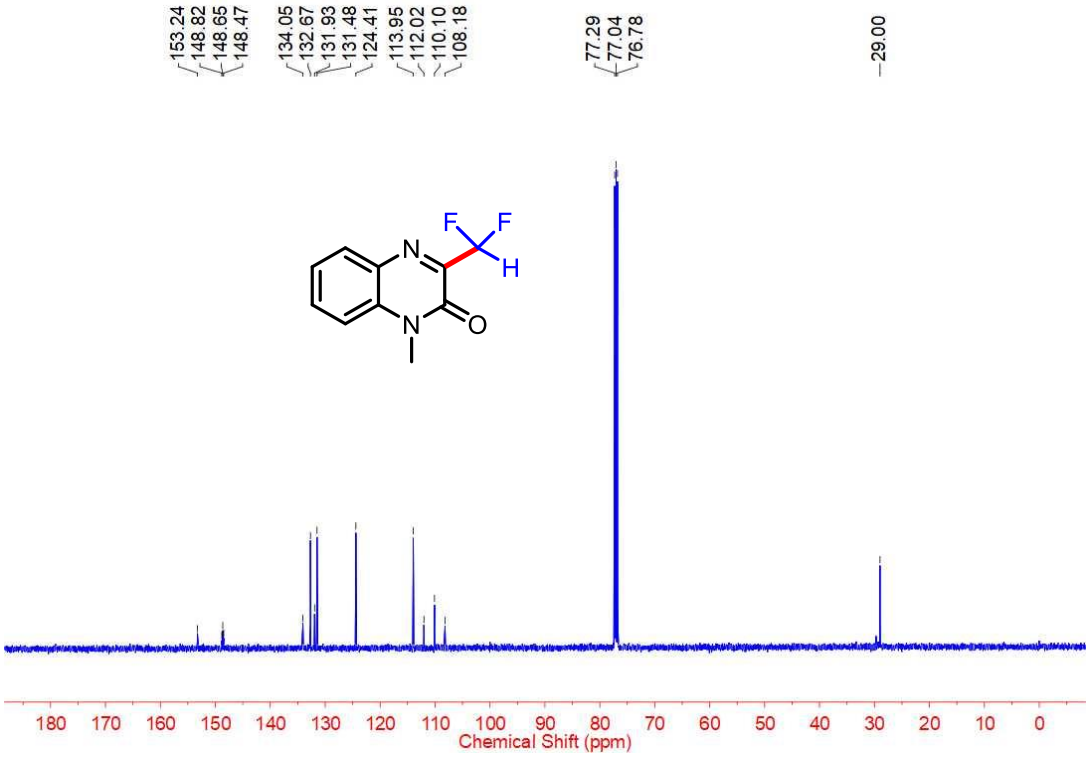
47 ^{13}C NMR (126 MHz, $CDCl_3$)



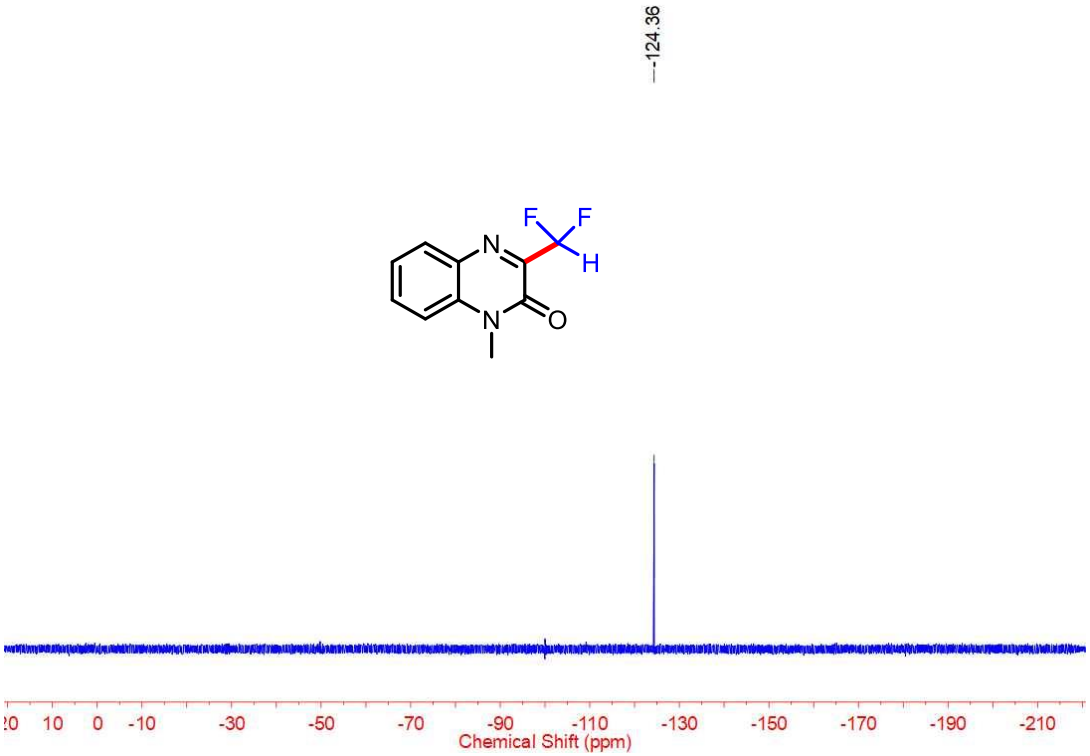
48 ^{1}H NMR (500 MHz, $CDCl_3$)



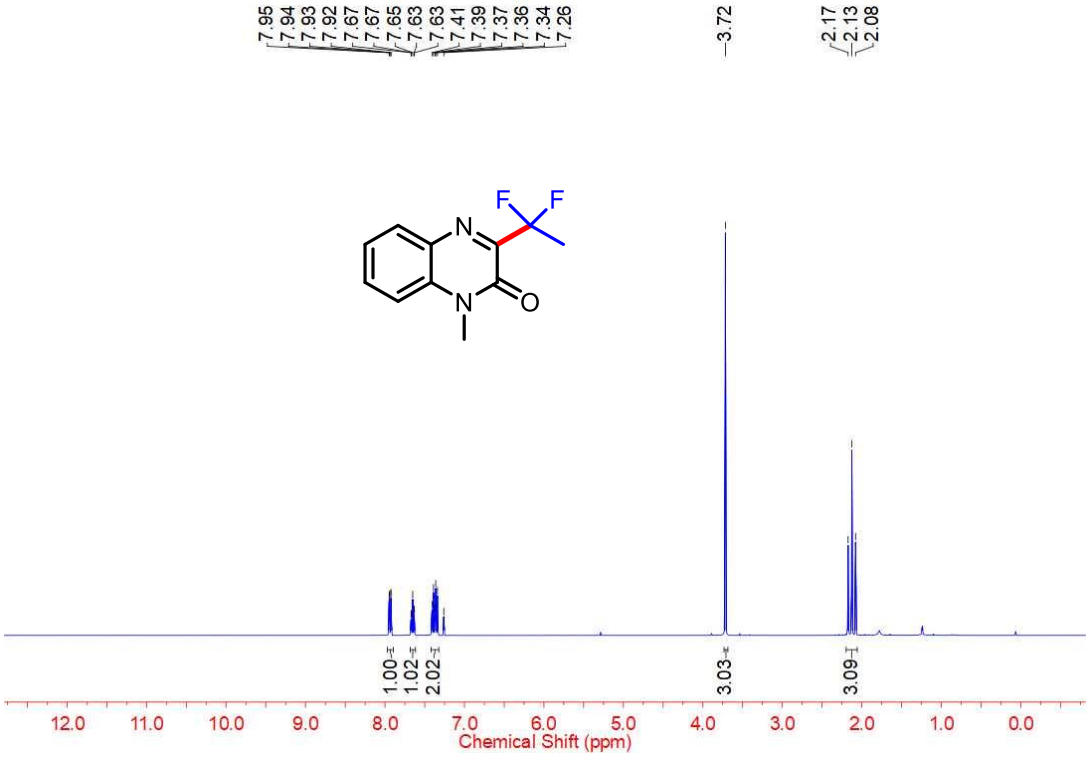
48 ^{13}C NMR (126 MHz, $CDCl_3$)



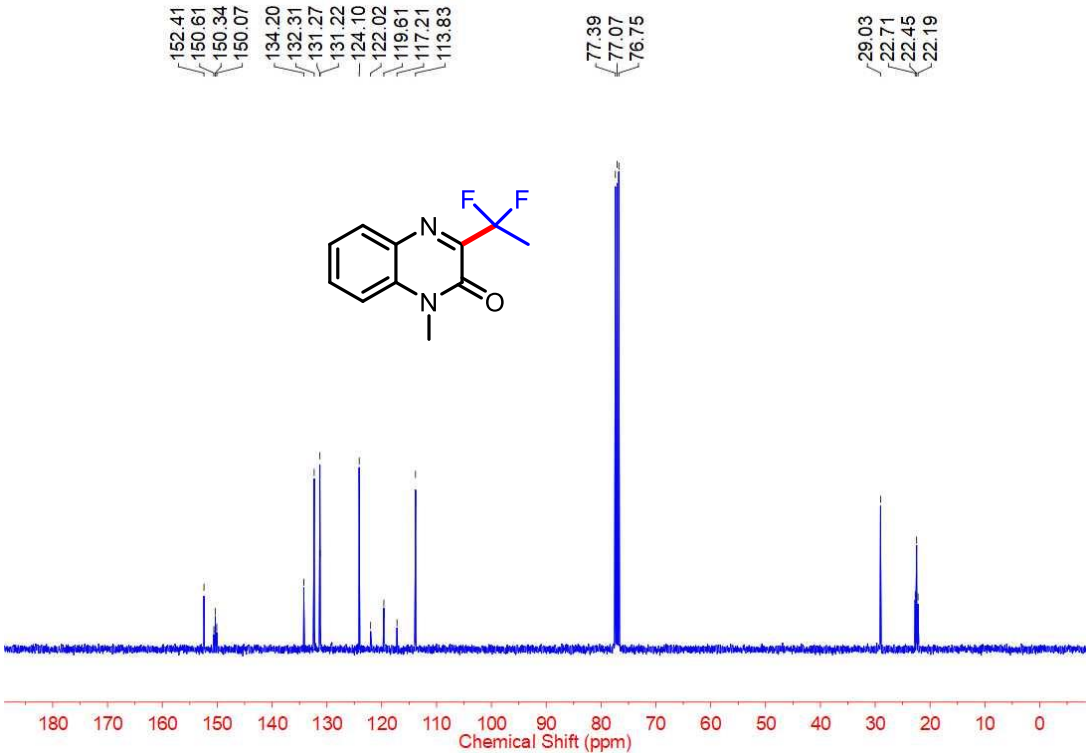
48 ^{19}F NMR (471 MHz, $CDCl_3$)



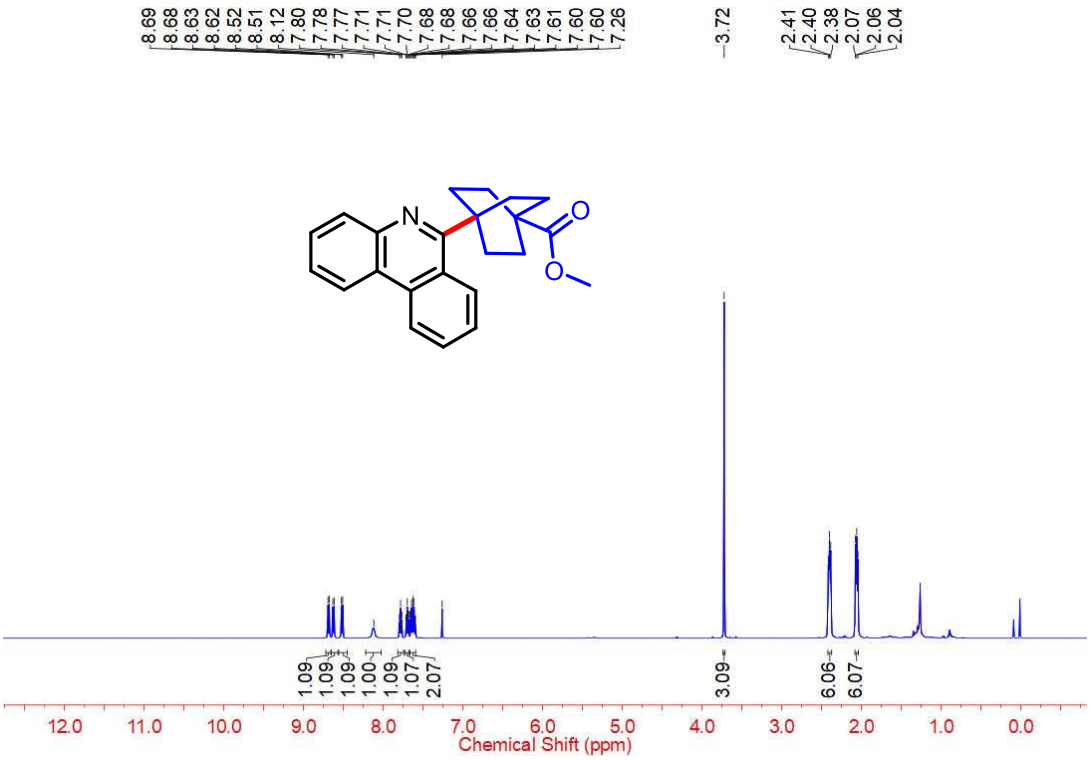
49 ^{1}H NMR (400 MHz, $CDCl_3$)



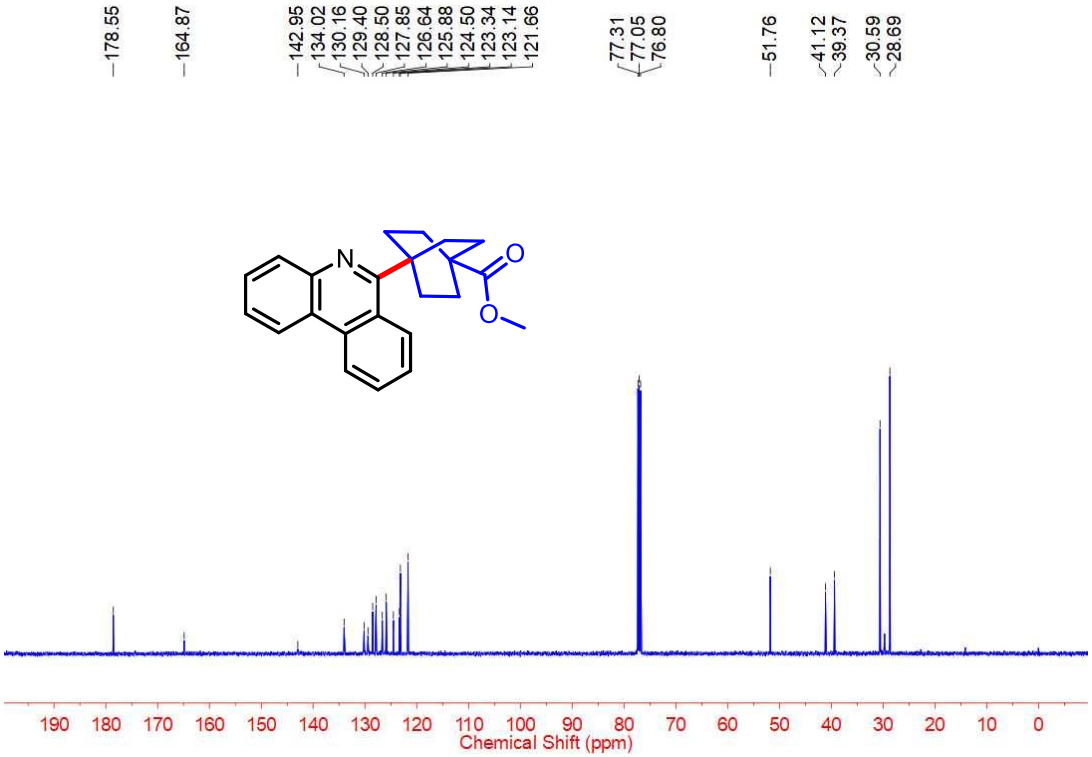
49 ^{13}C NMR (100 MHz, $CDCl_3$)



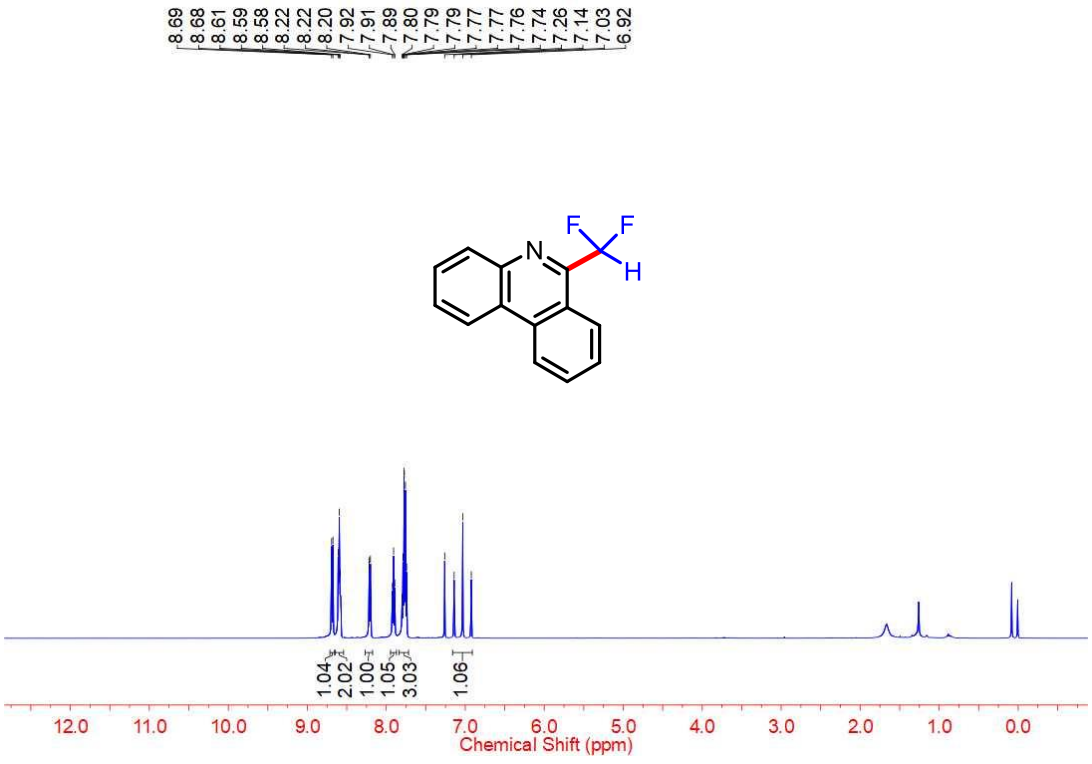
50 ^{1}H NMR (500 MHz, $CDCl_3$)



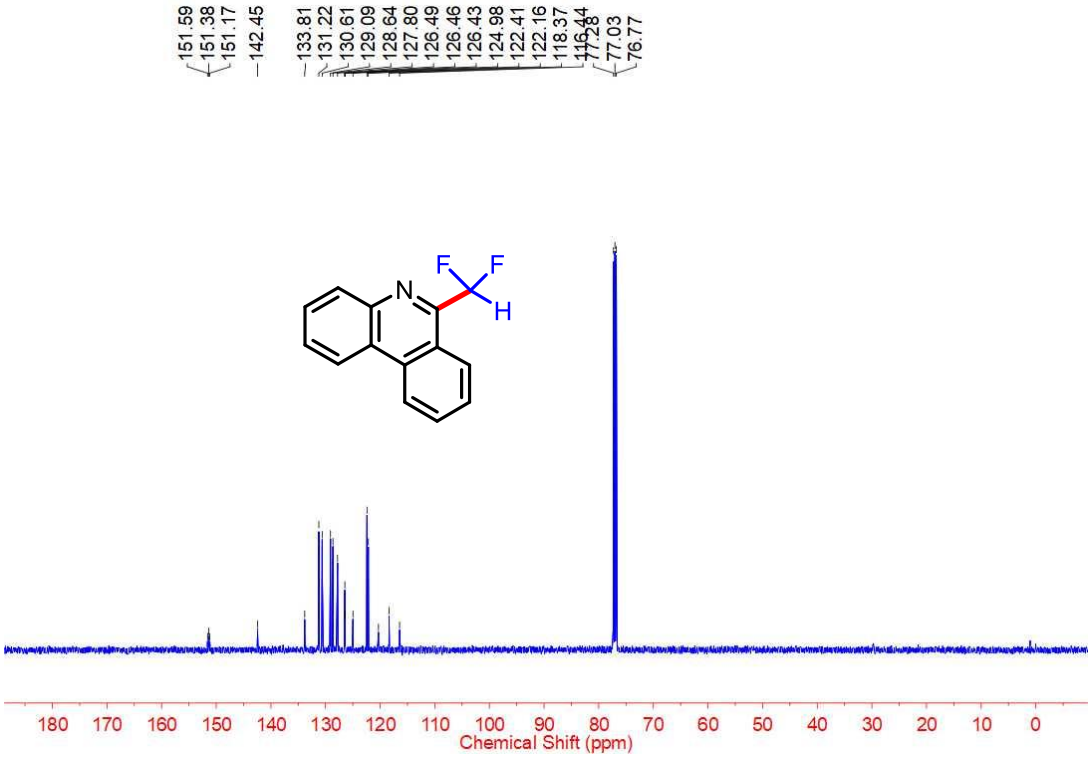
50 ^{13}C NMR (126 MHz, $CDCl_3$)



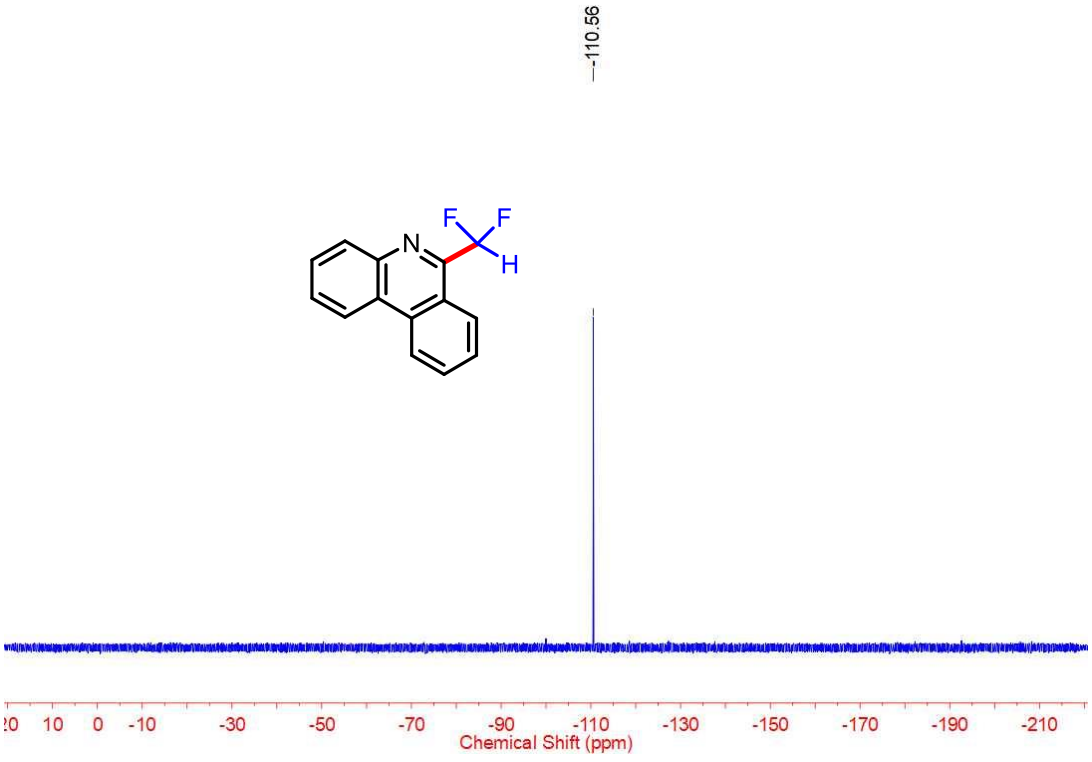
51 ^{1}H NMR (500 MHz, $CDCl_3$)



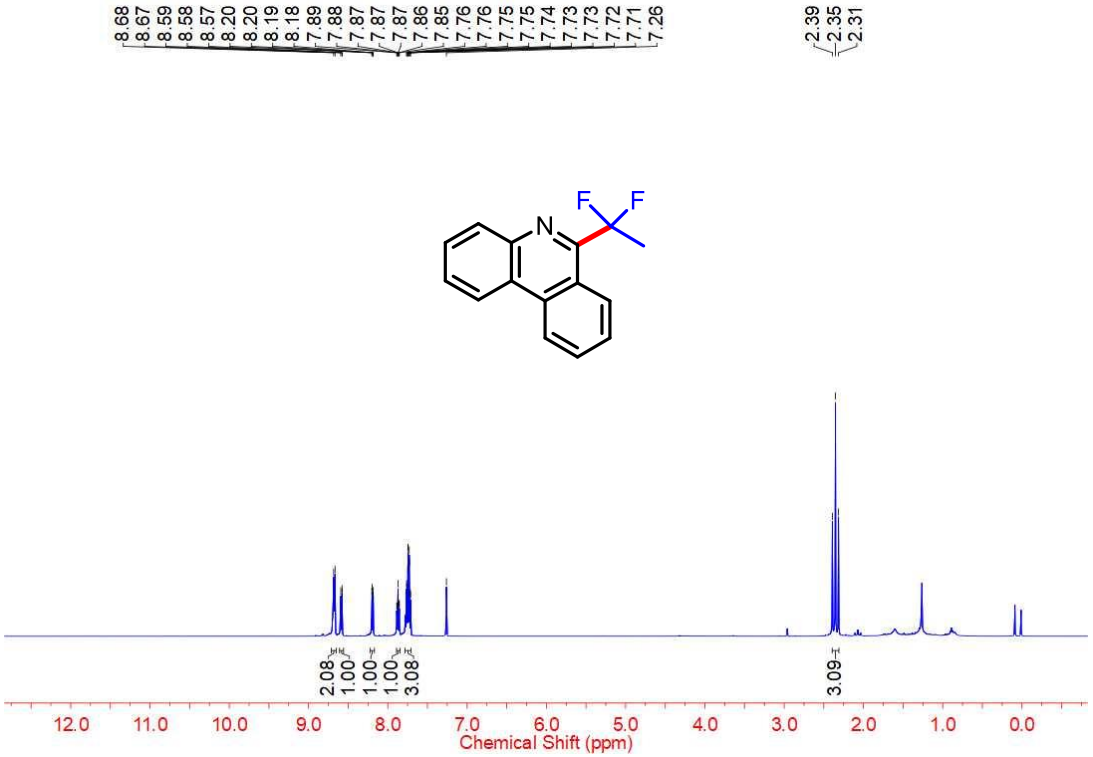
51 ^{13}C NMR (126 MHz, $CDCl_3$)



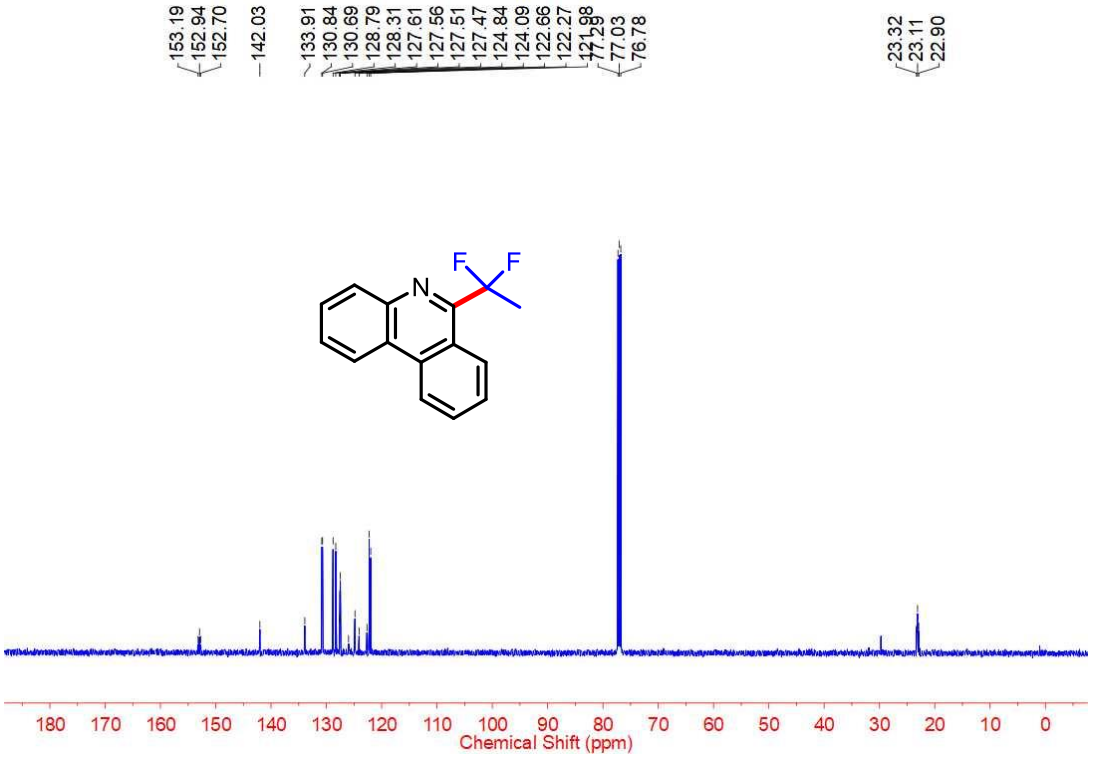
51 ^{19}F NMR (471 MHz, $CDCl_3$)



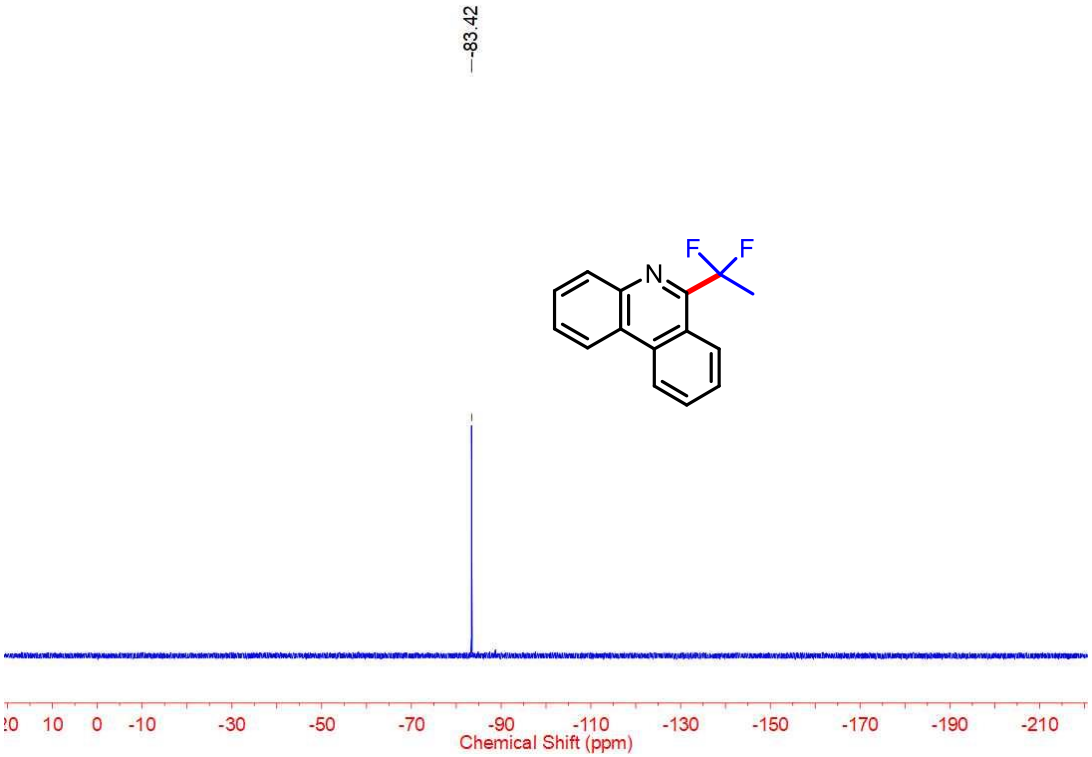
52 ^{1}H NMR (500 MHz, $CDCl_3$)



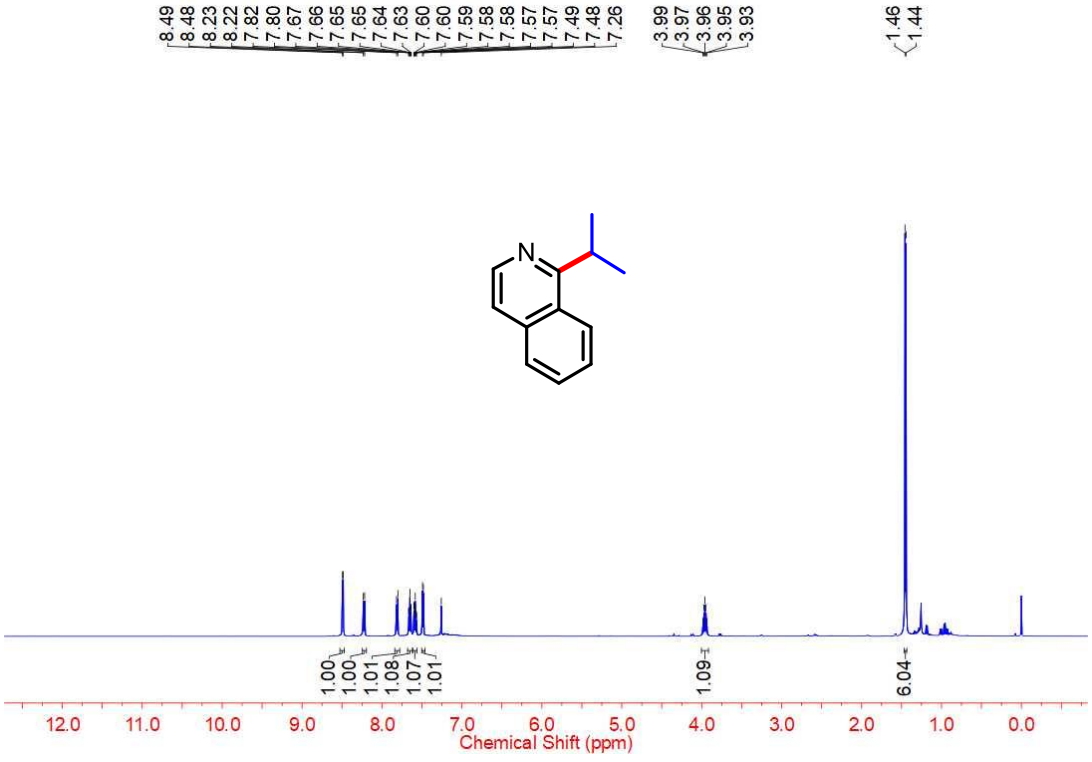
52 ^{13}C NMR (126 MHz, $CDCl_3$)



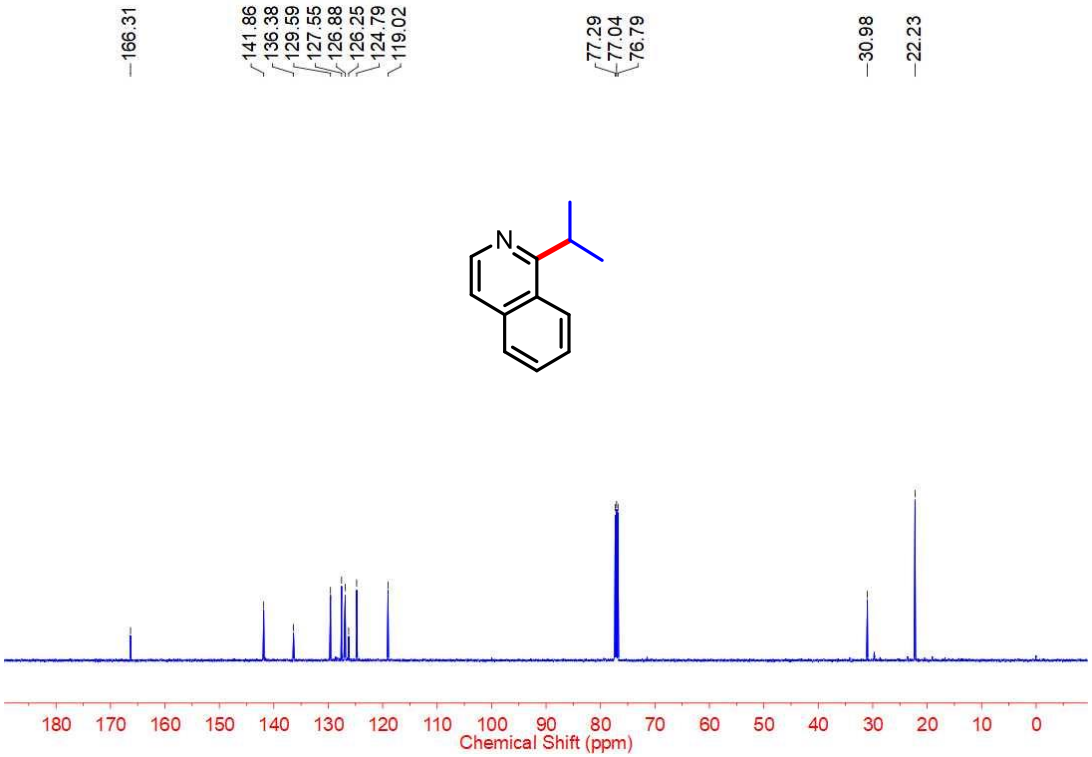
52 ^{19}F NMR (471 MHz, $CDCl_3$)



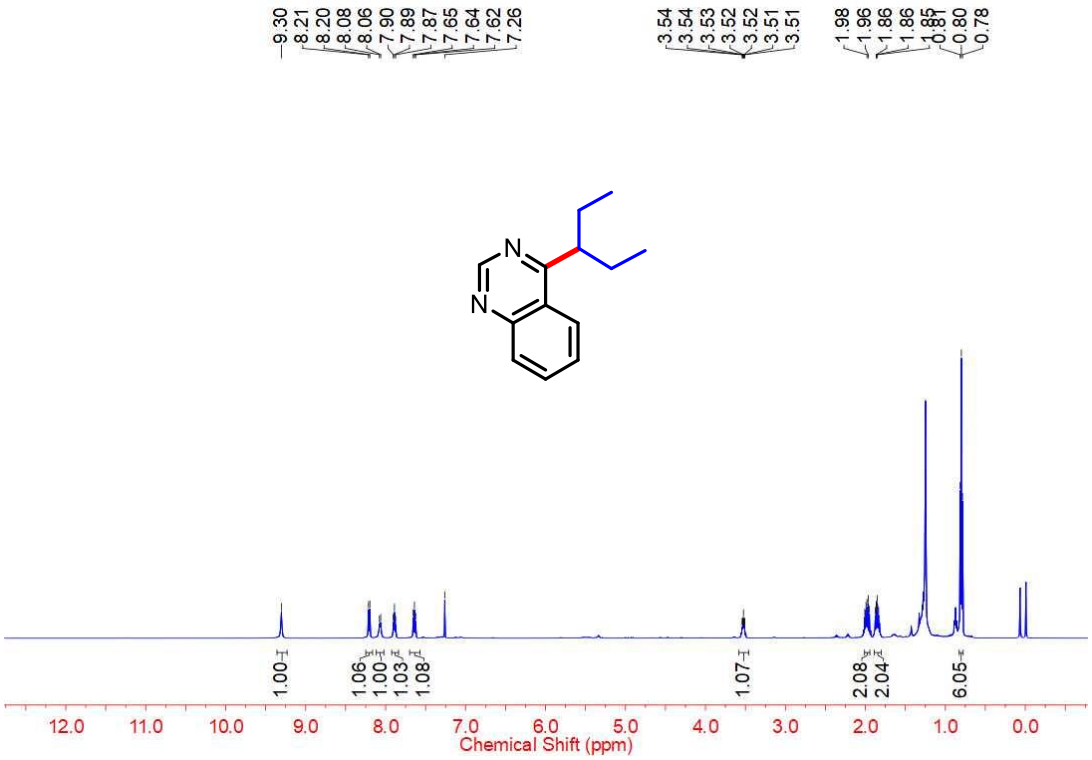
53 ^{1}H NMR (500 MHz, $CDCl_3$)



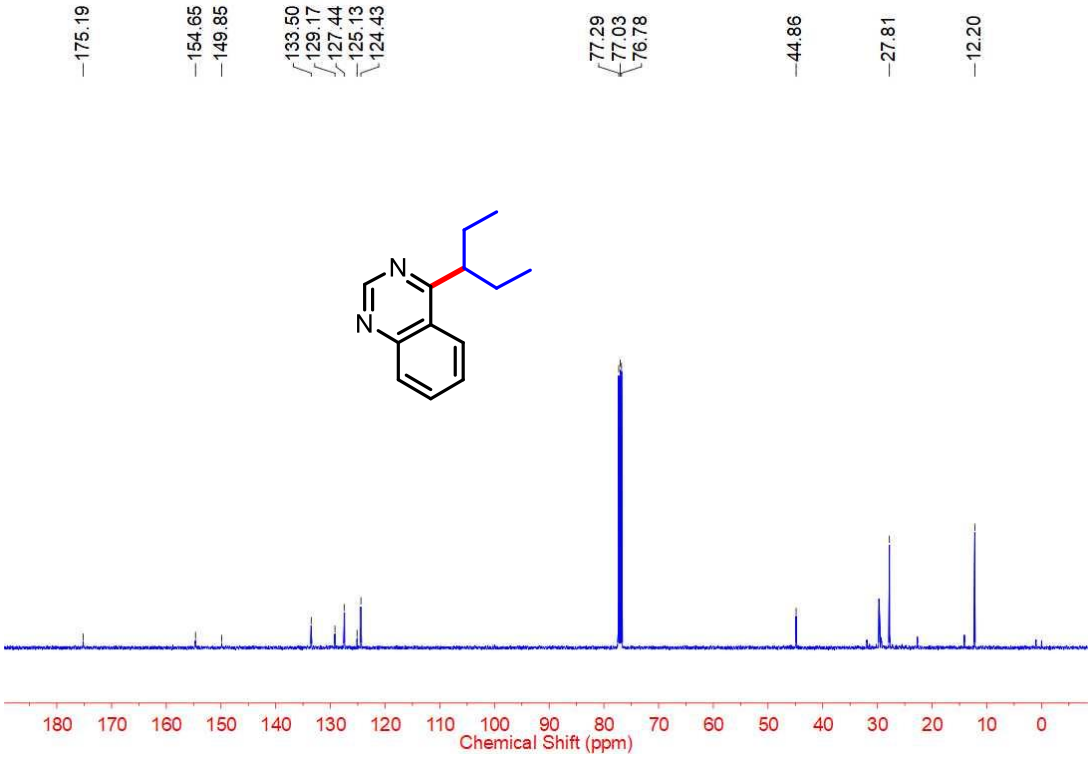
53 ^{13}C NMR (126 MHz, $CDCl_3$)



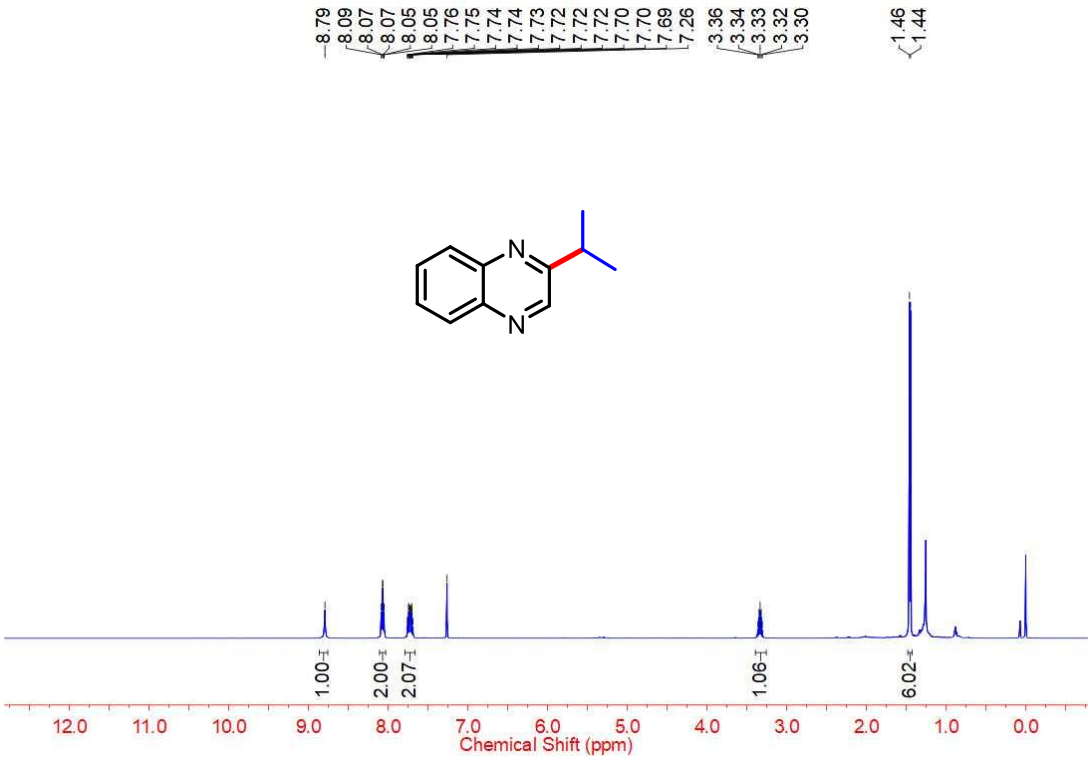
54 ^{1}H NMR (500 MHz, $CDCl_3$)



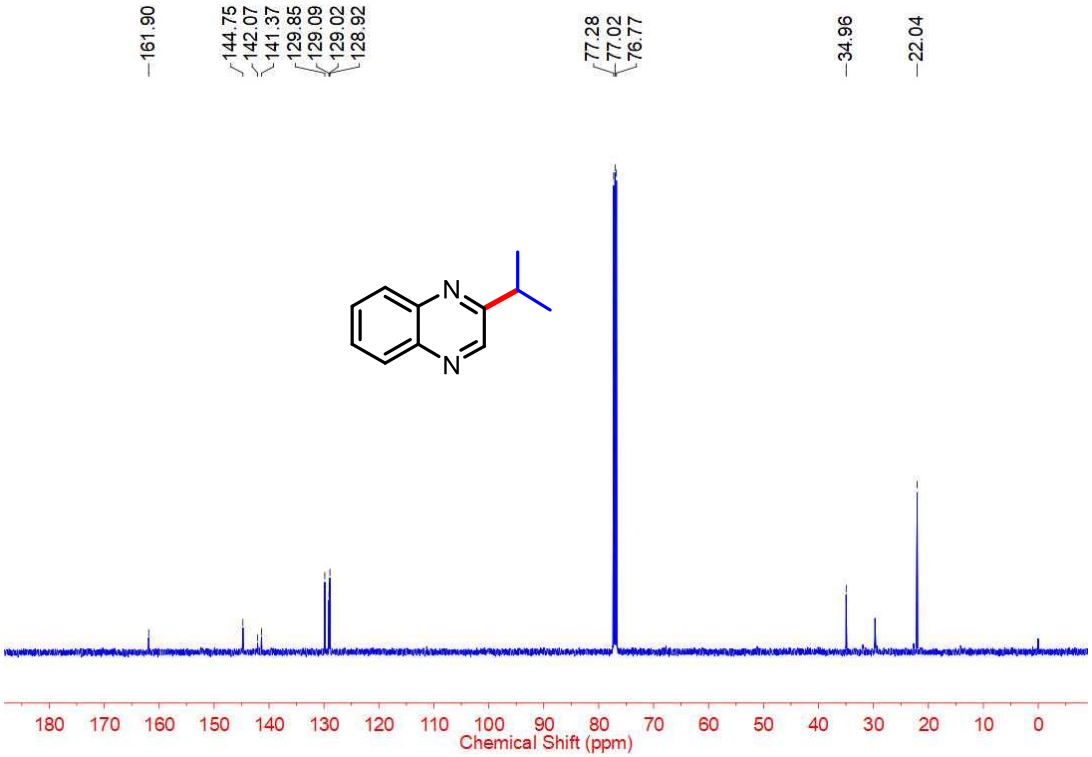
54 ^{13}C NMR (126 MHz, $CDCl_3$)



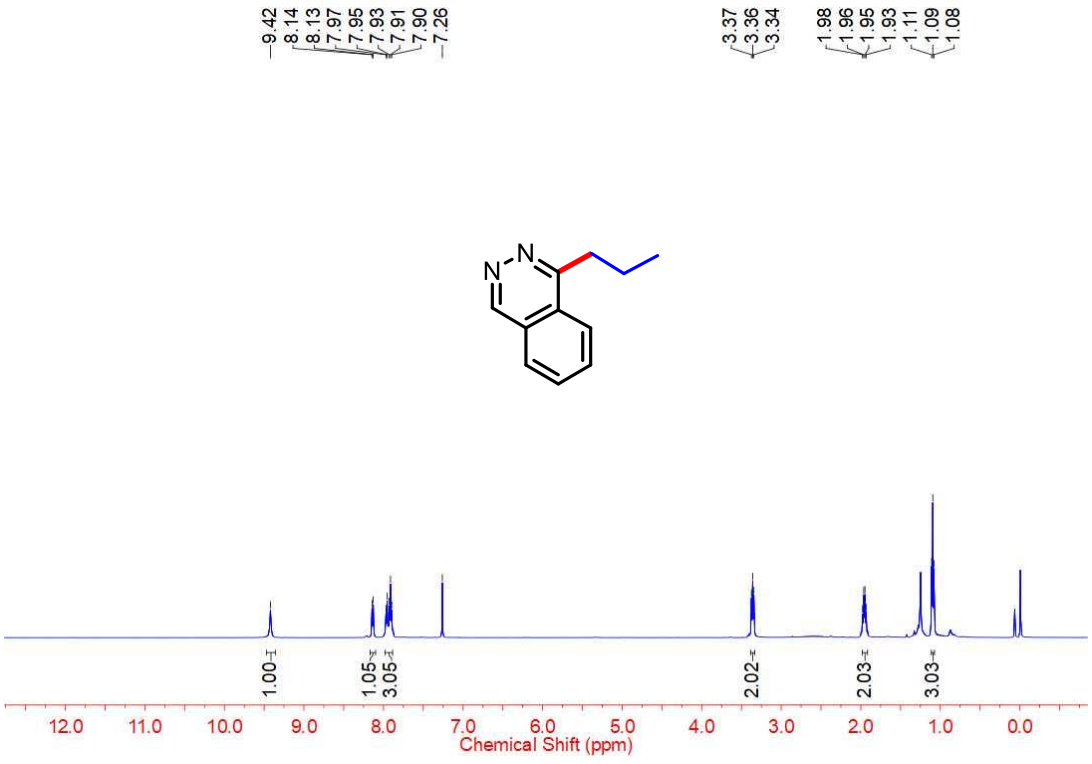
55 ^{1}H NMR (500 MHz, $CDCl_3$)



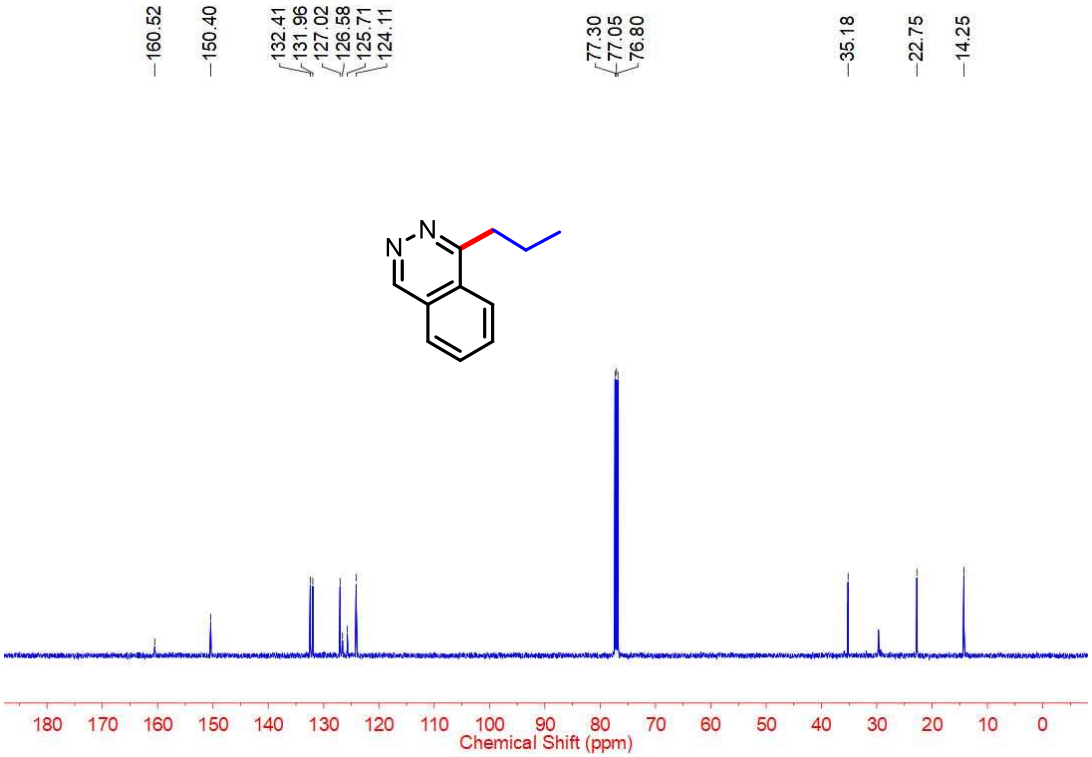
55 ^{13}C NMR (126 MHz, $CDCl_3$)



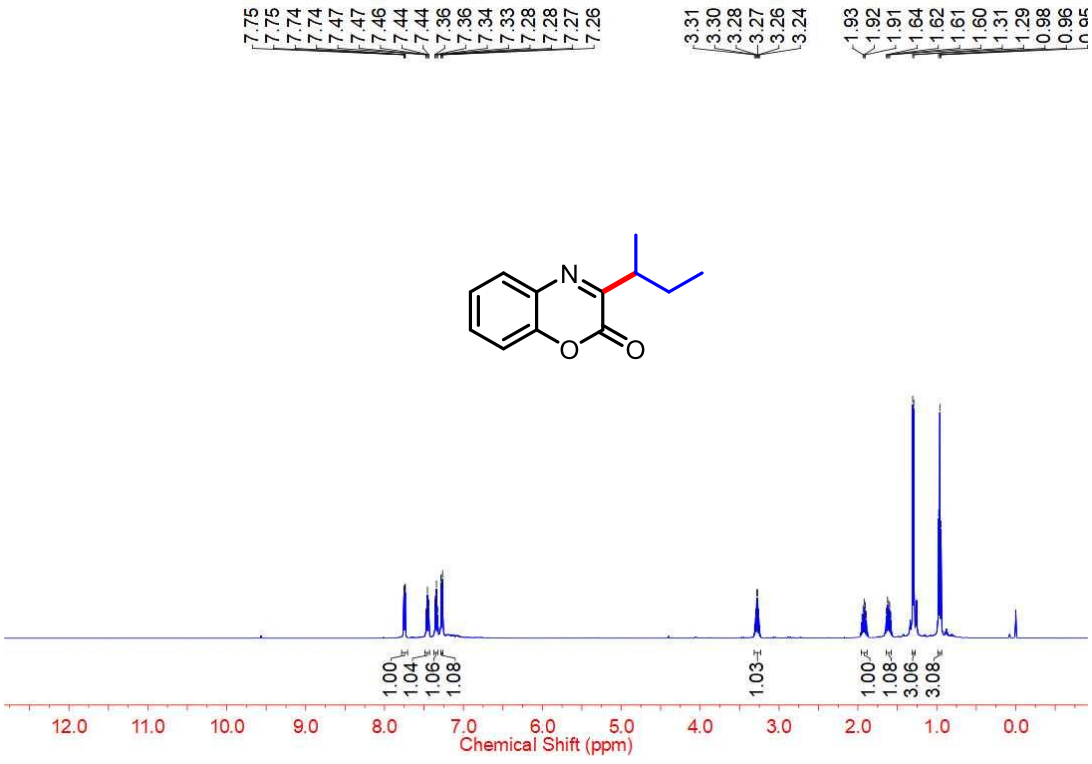
56 ^{1}H NMR (500 MHz, $CDCl_3$)



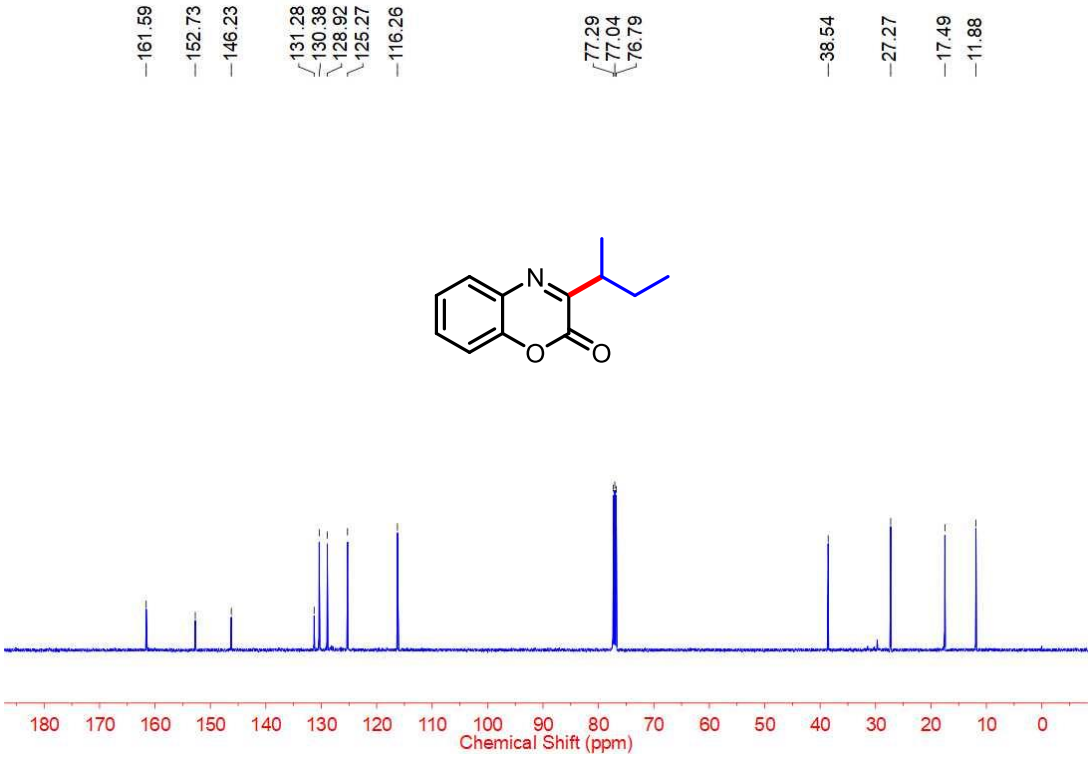
56 ^{13}C NMR (126 MHz, $CDCl_3$)



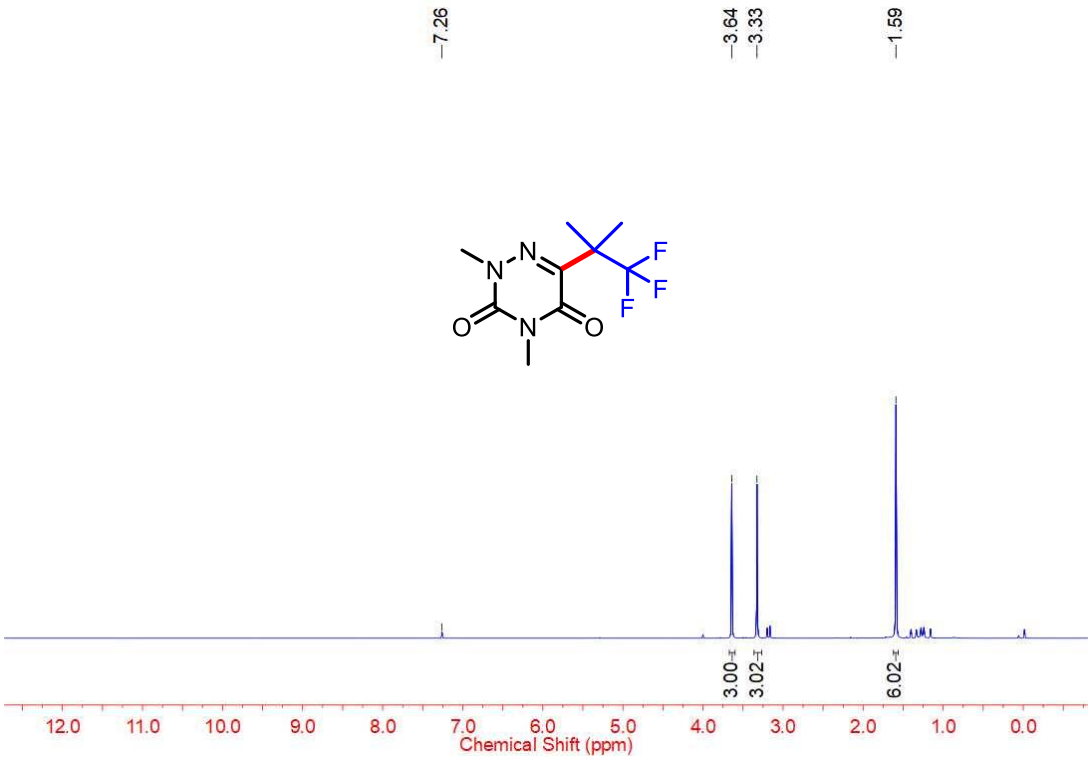
57 ^{1}H NMR (500 MHz, $CDCl_3$)



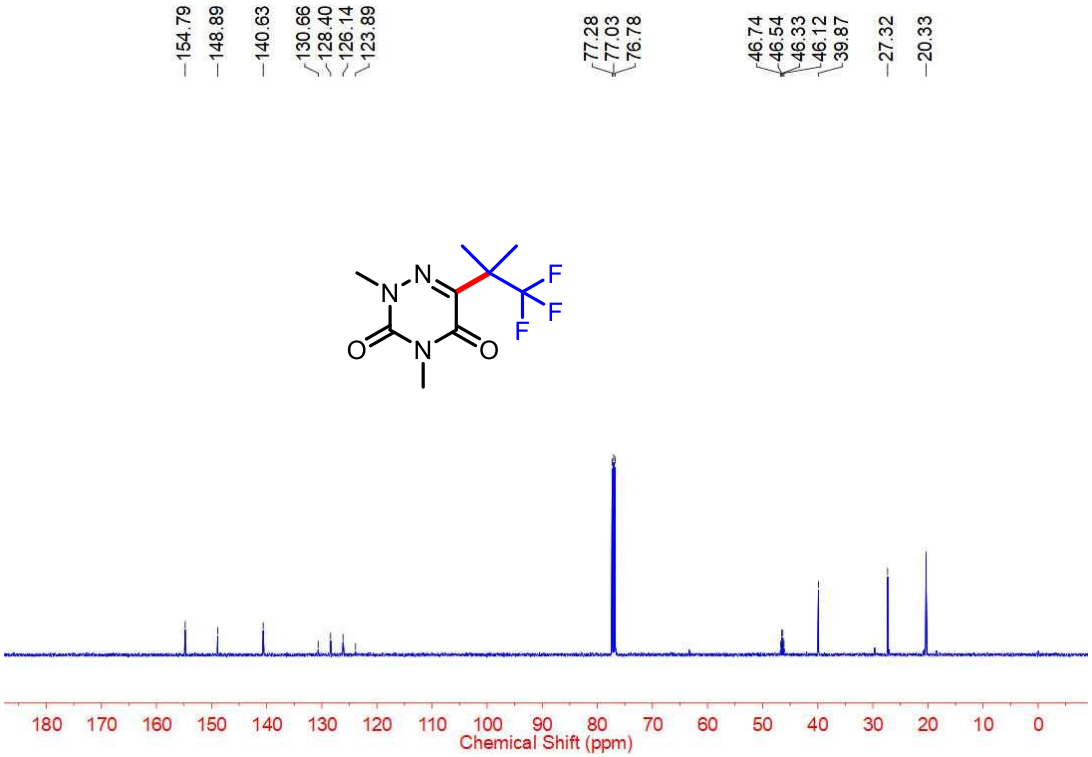
57 ^{13}C NMR (126 MHz, $CDCl_3$)



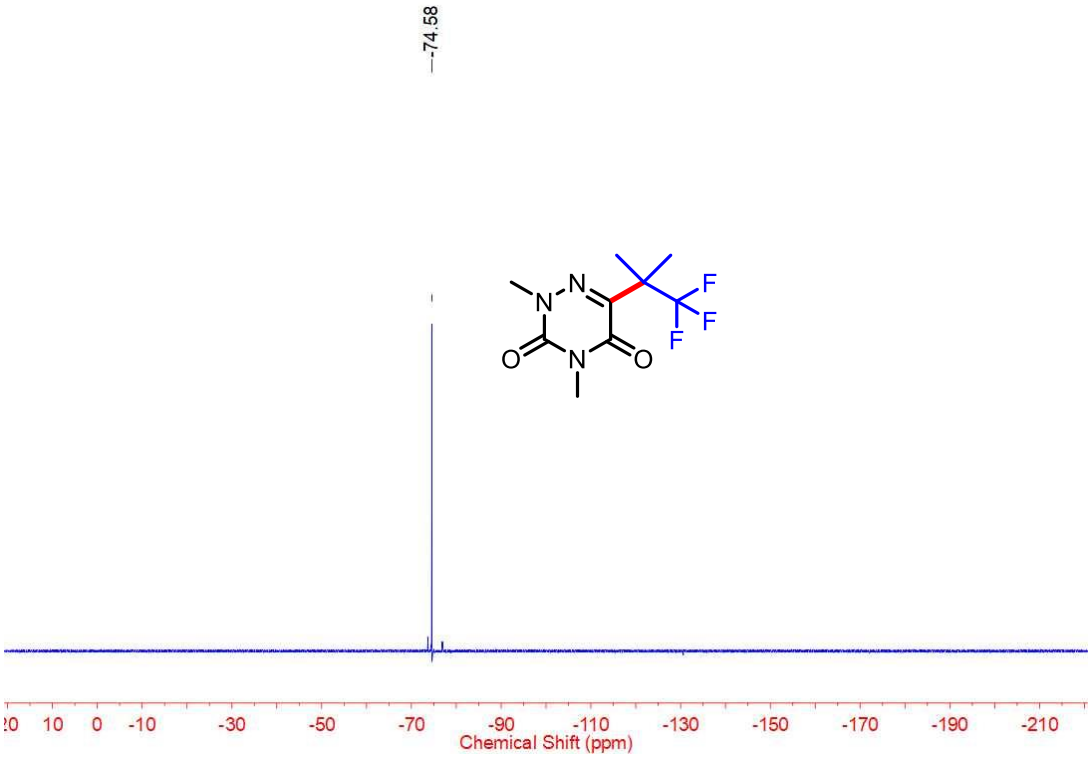
58 ^{1}H NMR (500 MHz, $CDCl_3$)



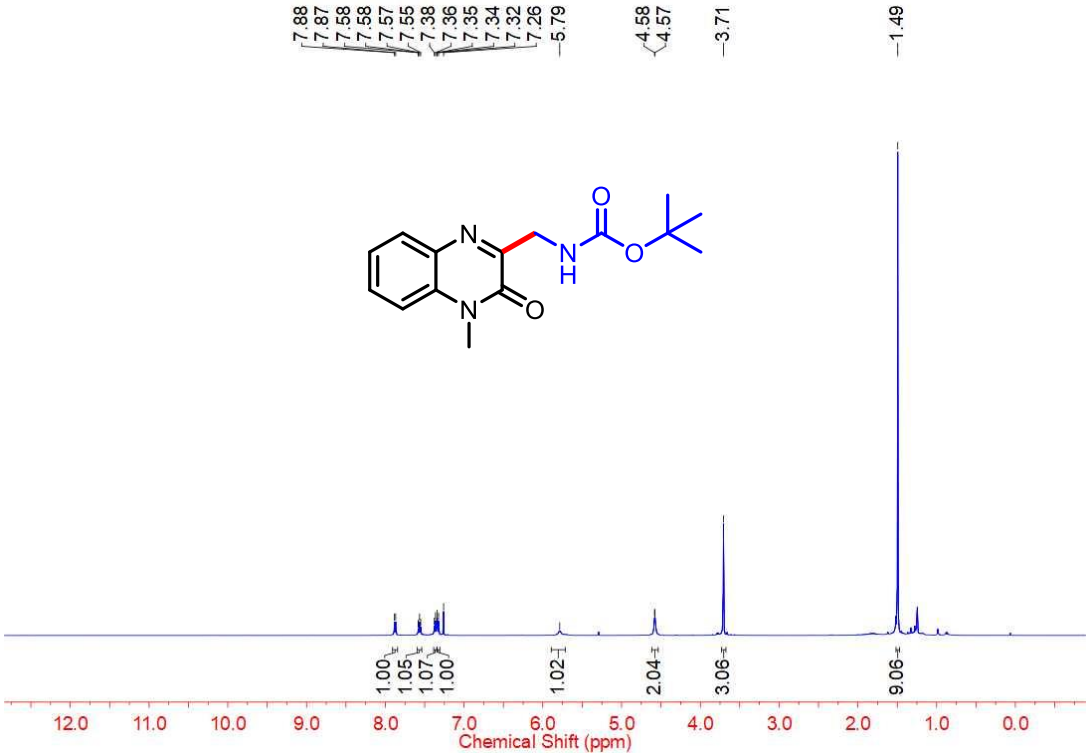
58 ^{13}C NMR (126 MHz, $CDCl_3$)



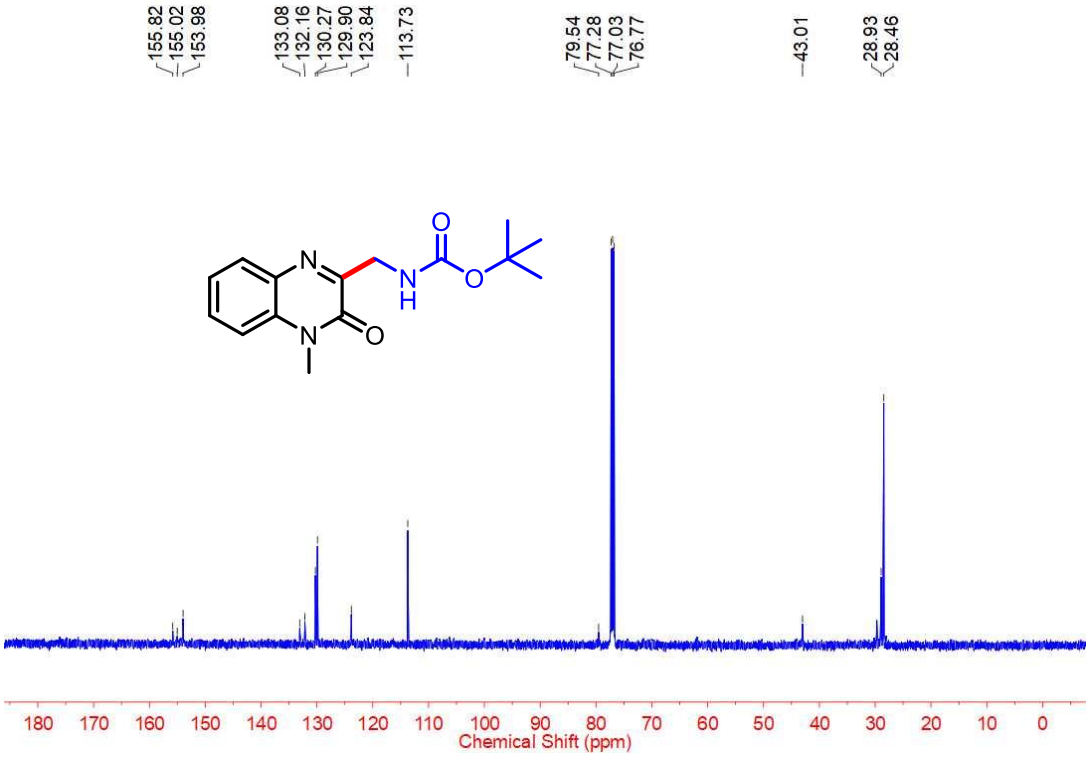
58 ^{19}F NMR (471 MHz, $CDCl_3$)



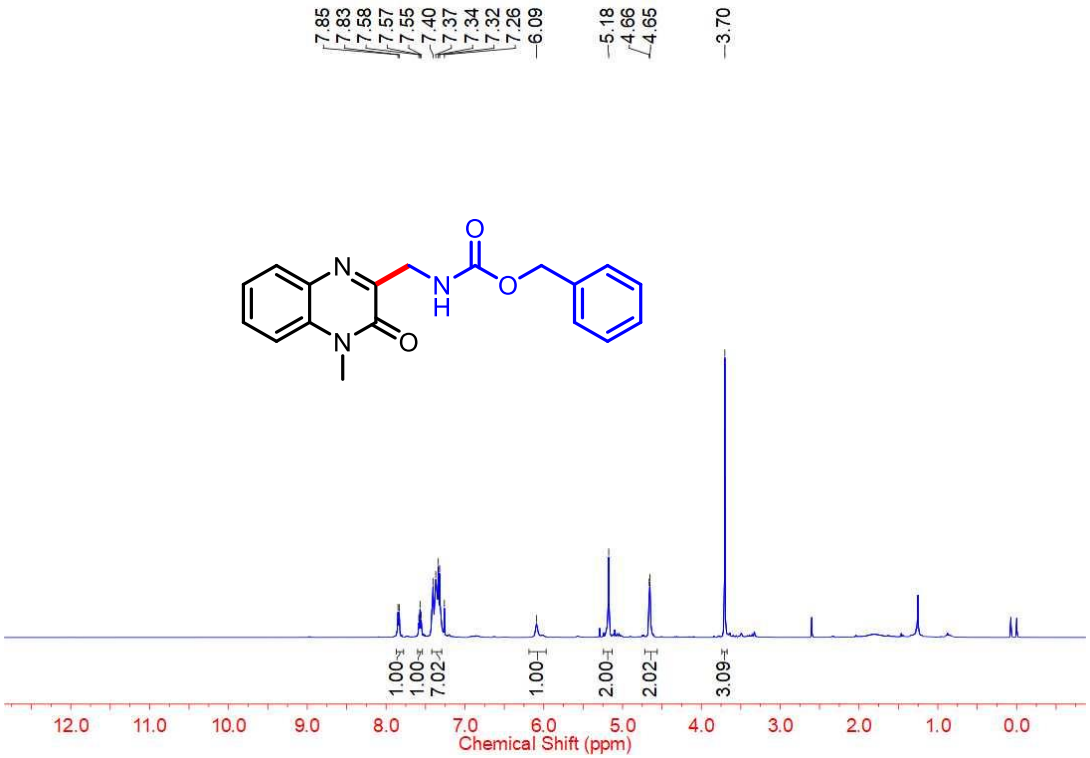
59 ^{1}H NMR (500 MHz, $CDCl_3$)



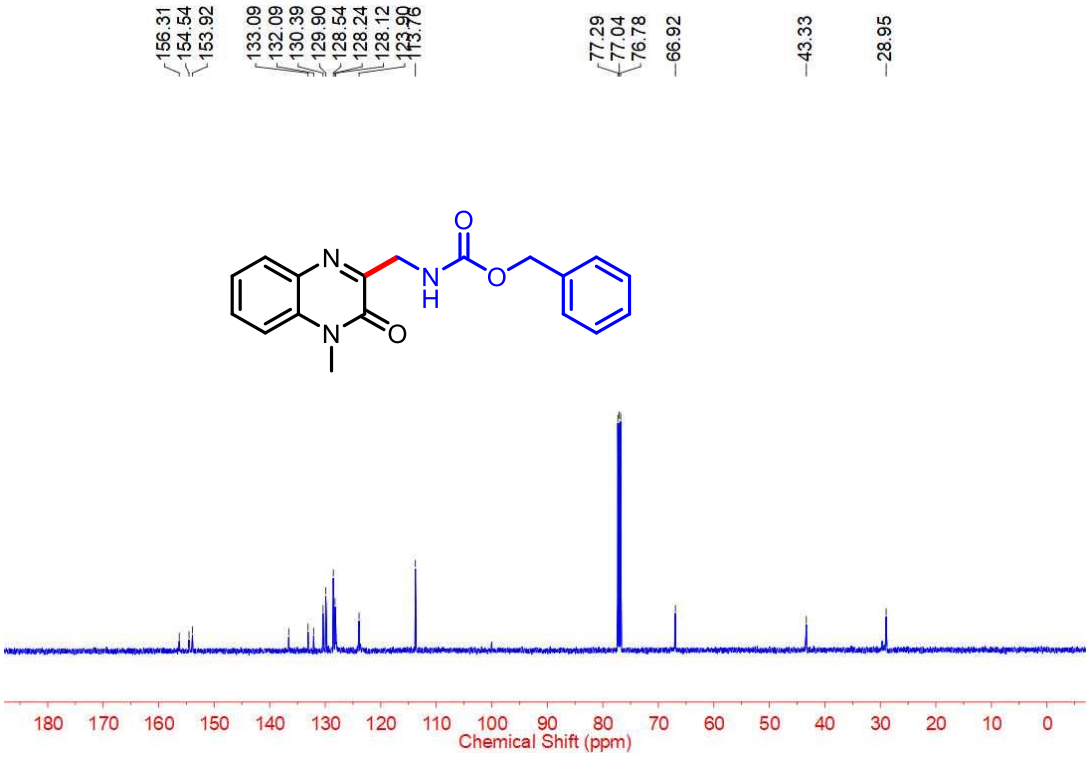
59 ^{13}C NMR (126 MHz, $CDCl_3$)



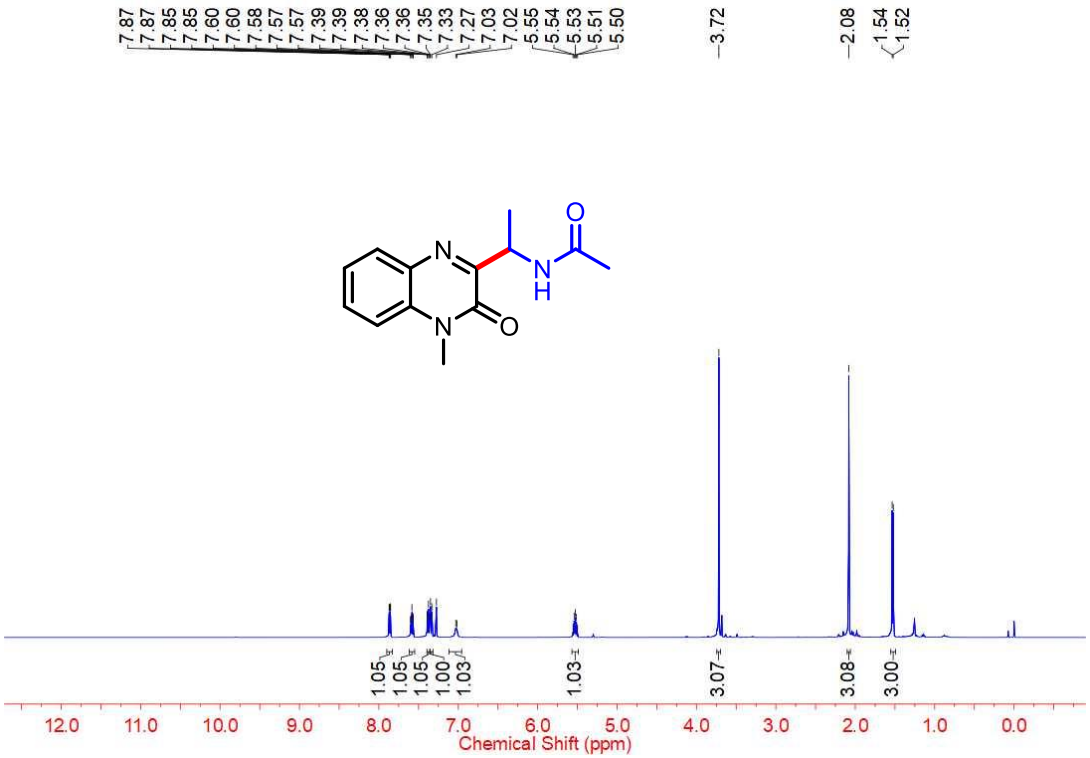
60 ^{1}H NMR (500 MHz, $CDCl_3$)



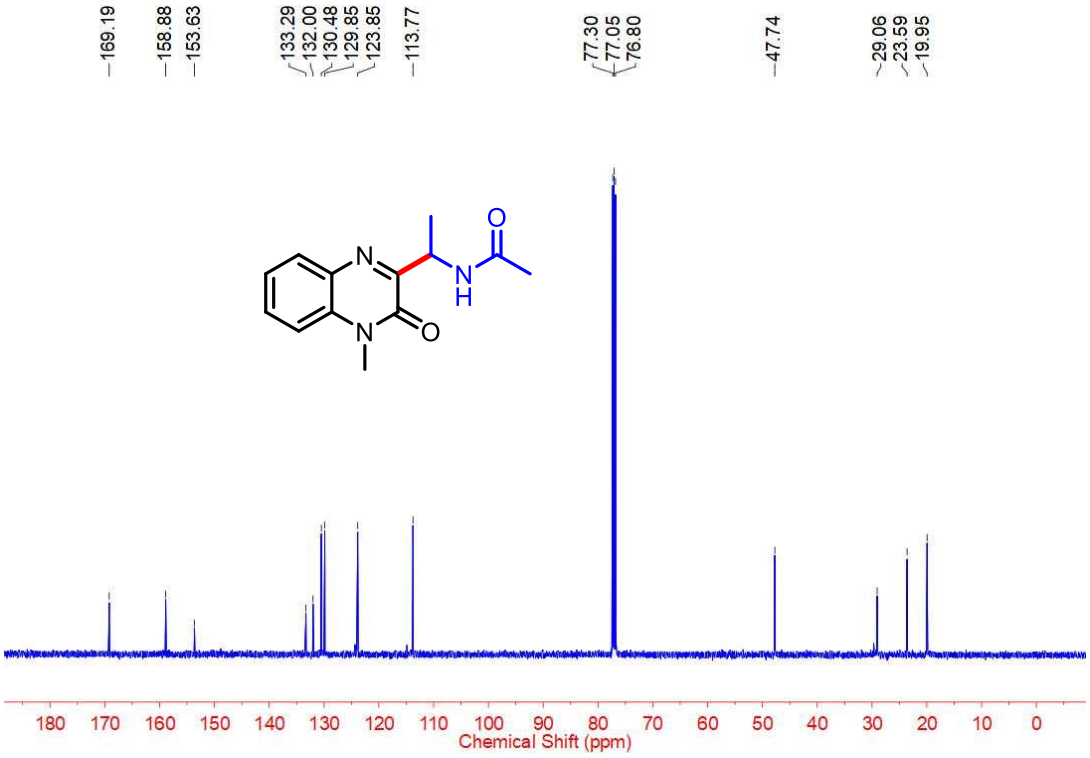
60 ^{13}C NMR (126 MHz, $CDCl_3$)



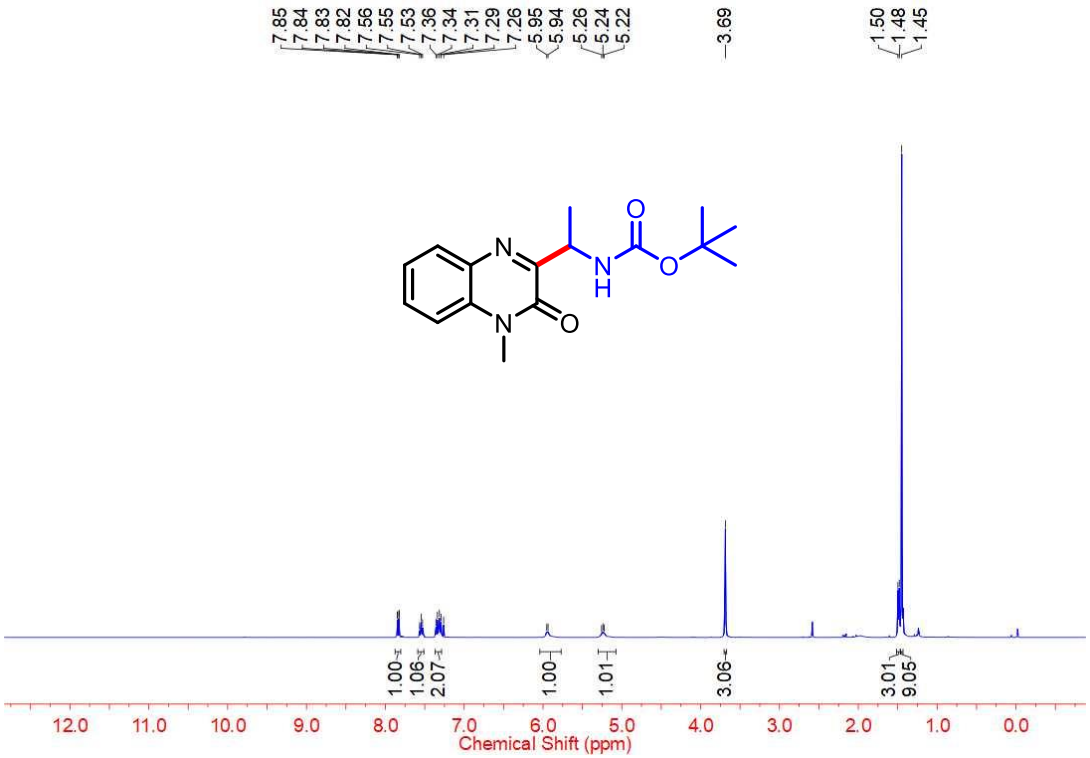
61 ^{1}H NMR (500 MHz, $CDCl_3$)



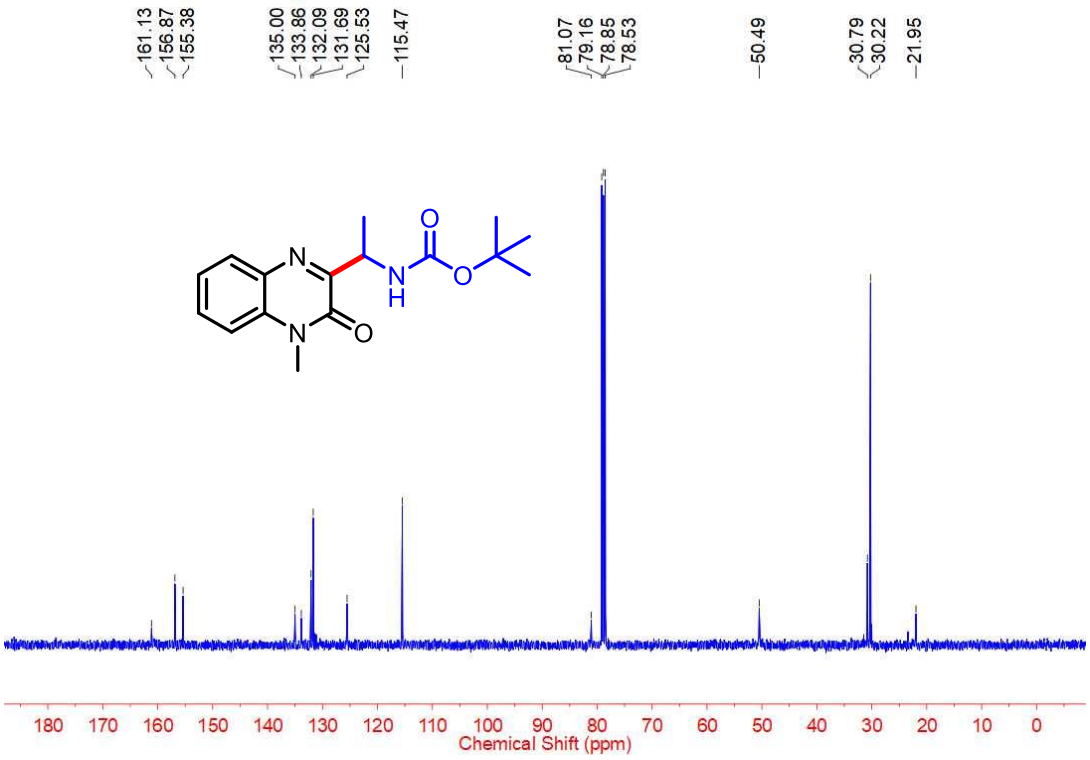
61 ^{13}C NMR (126 MHz, $CDCl_3$)



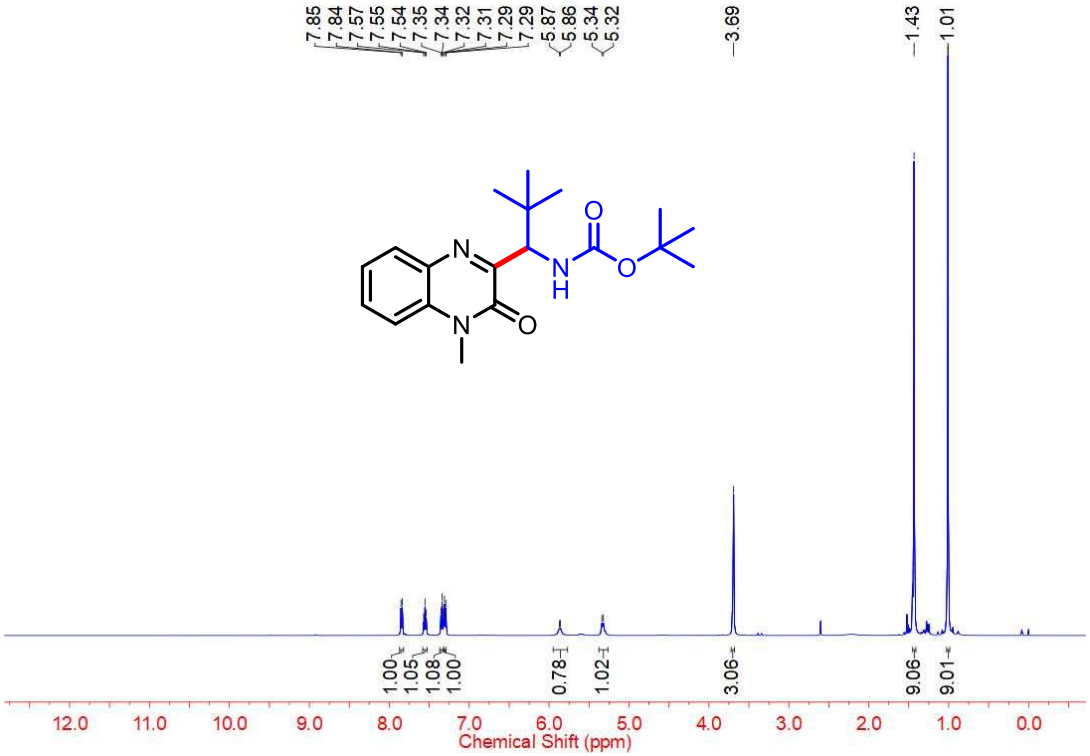
62 ^{1}H NMR (400 MHz, $CDCl_3$)



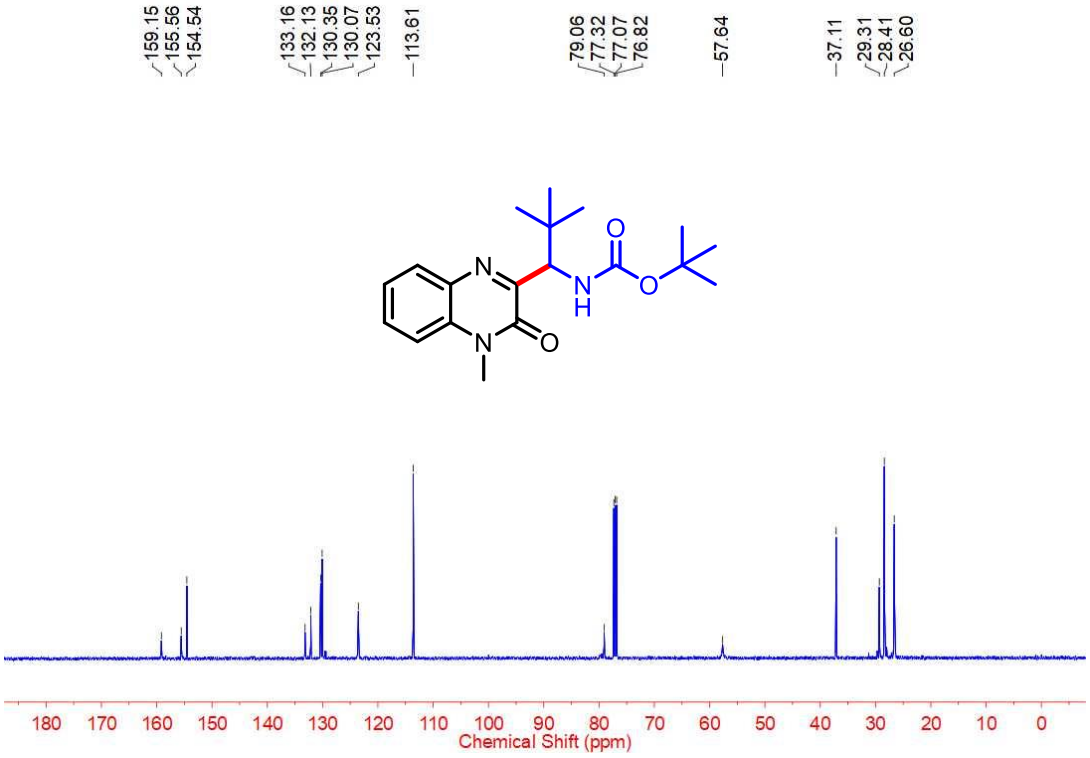
62 ^{13}C NMR (100 MHz, $CDCl_3$)



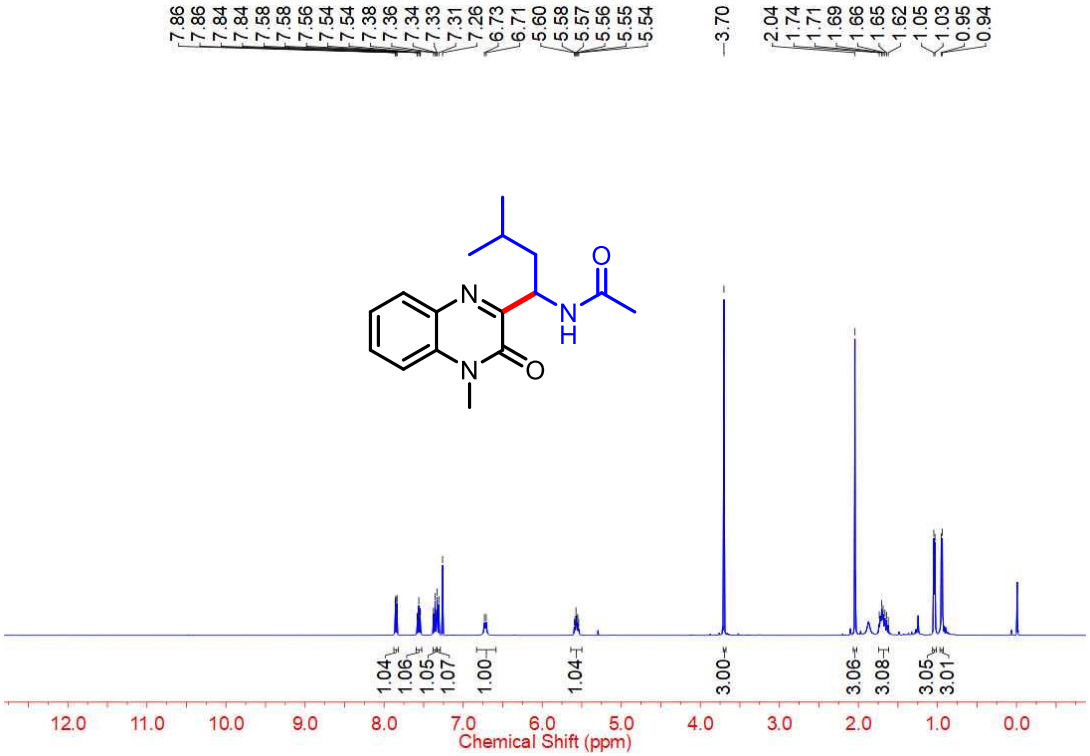
63 ^{1}H NMR (500 MHz, $CDCl_3$)



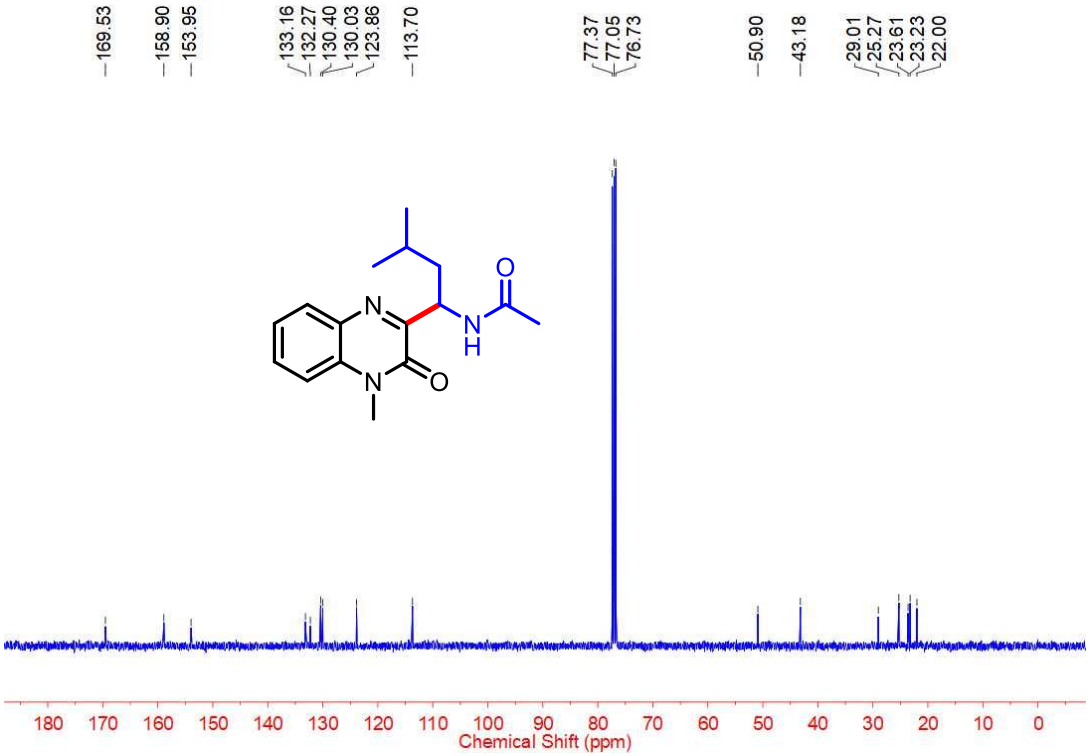
63 ^{13}C NMR (126 MHz, $CDCl_3$)



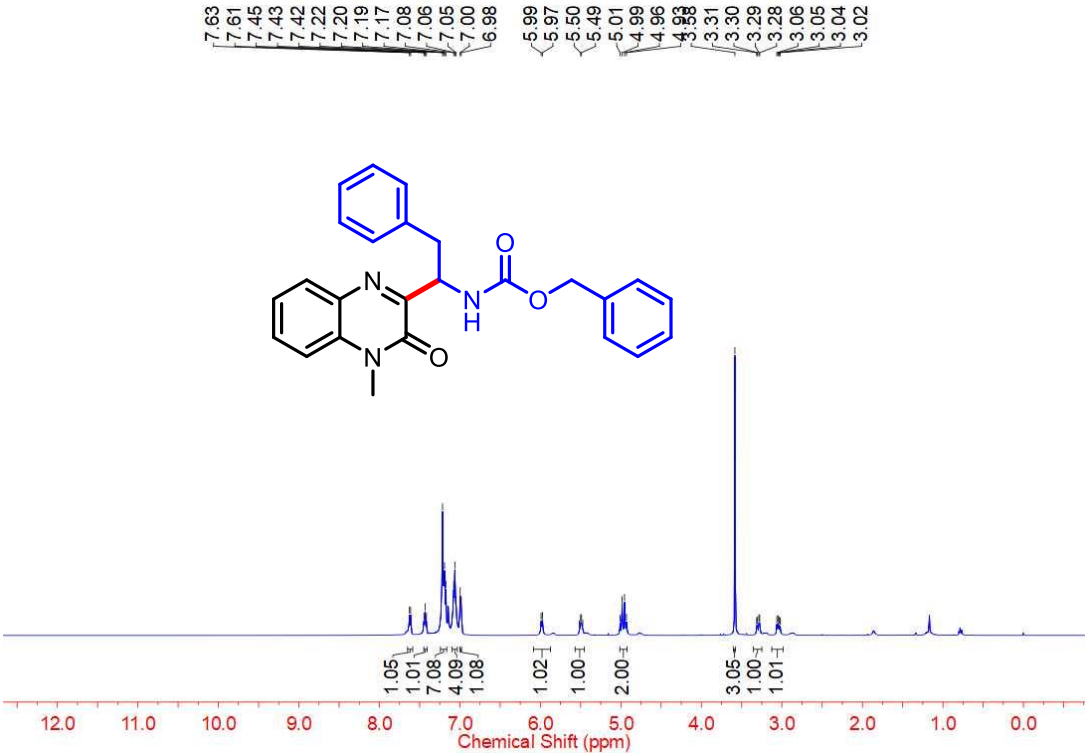
64 ^{1}H NMR (400 MHz, $CDCl_3$)



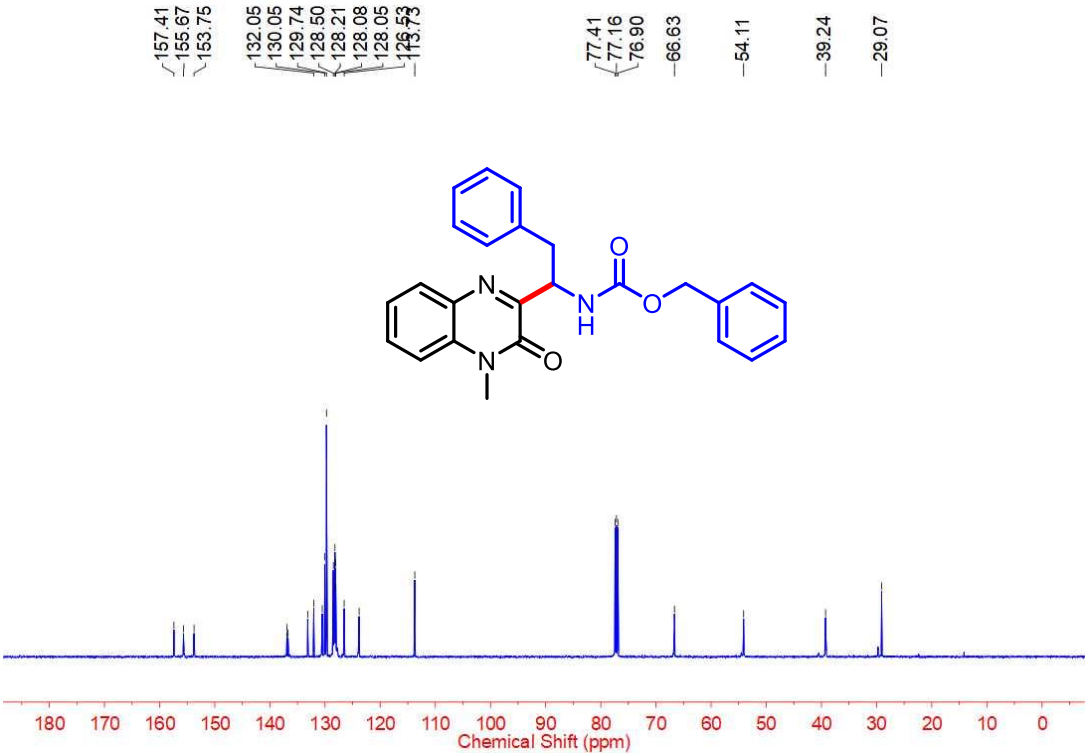
64 ^{13}C NMR (100 MHz, $CDCl_3$)



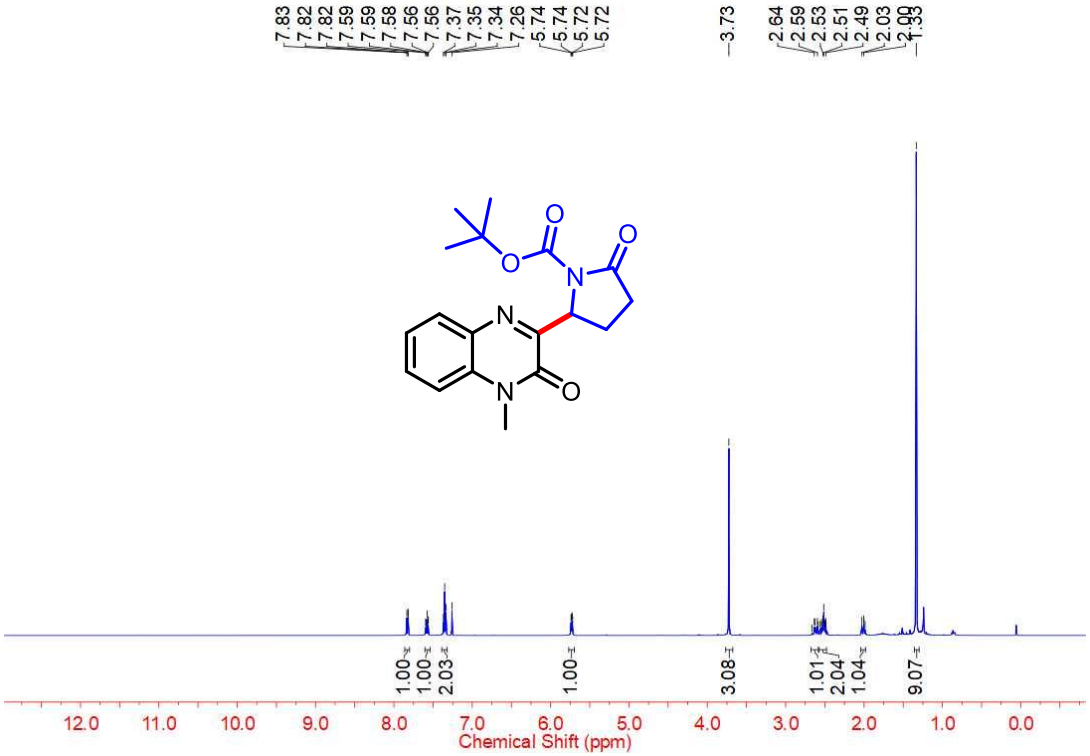
65 ^{1}H NMR (500 MHz, $CDCl_3$)



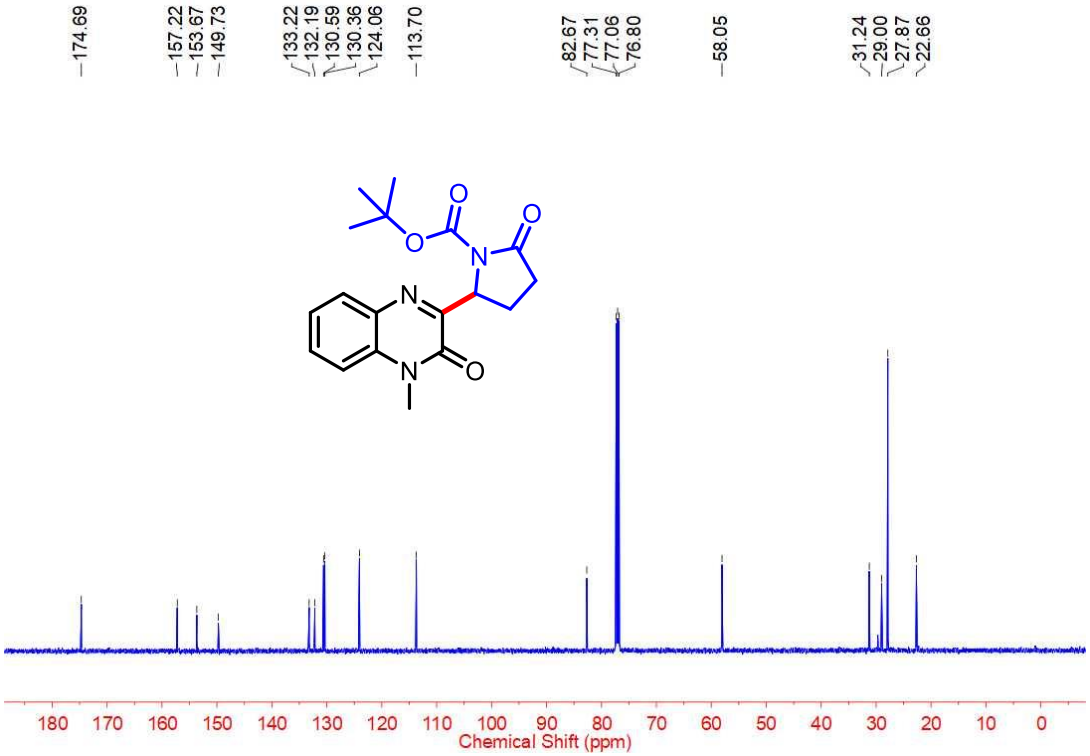
65 ^{13}C NMR (126 MHz, $CDCl_3$)



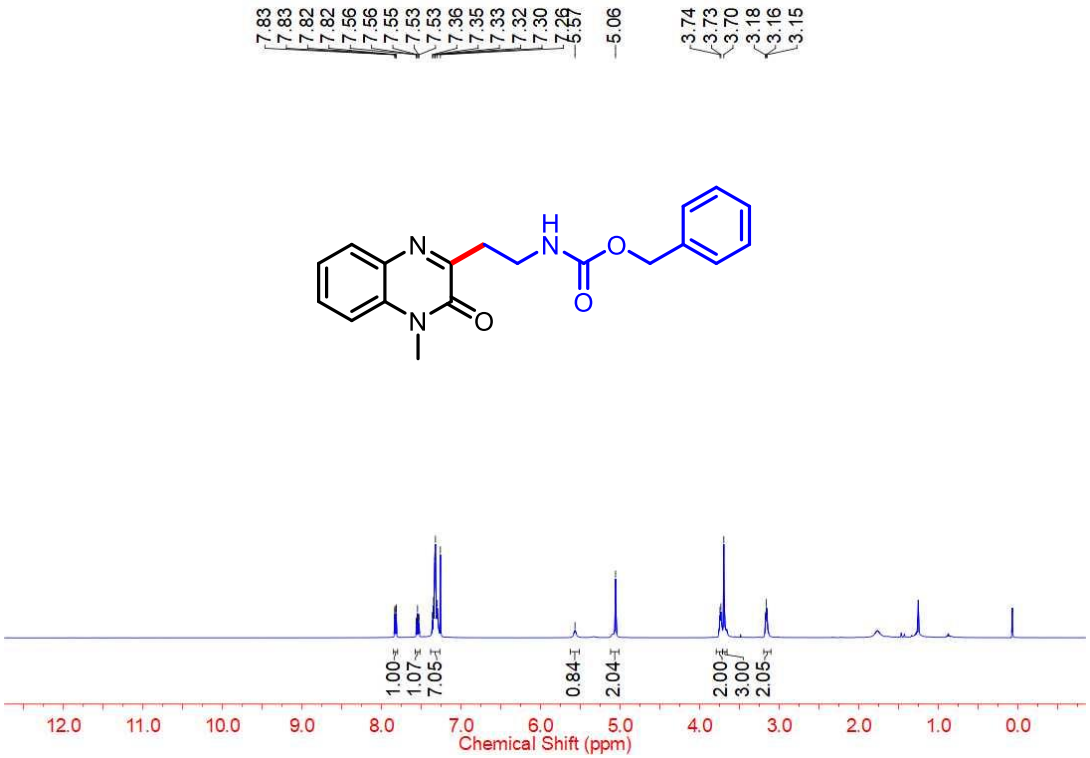
66 ^{1}H NMR (500 MHz, $CDCl_3$)



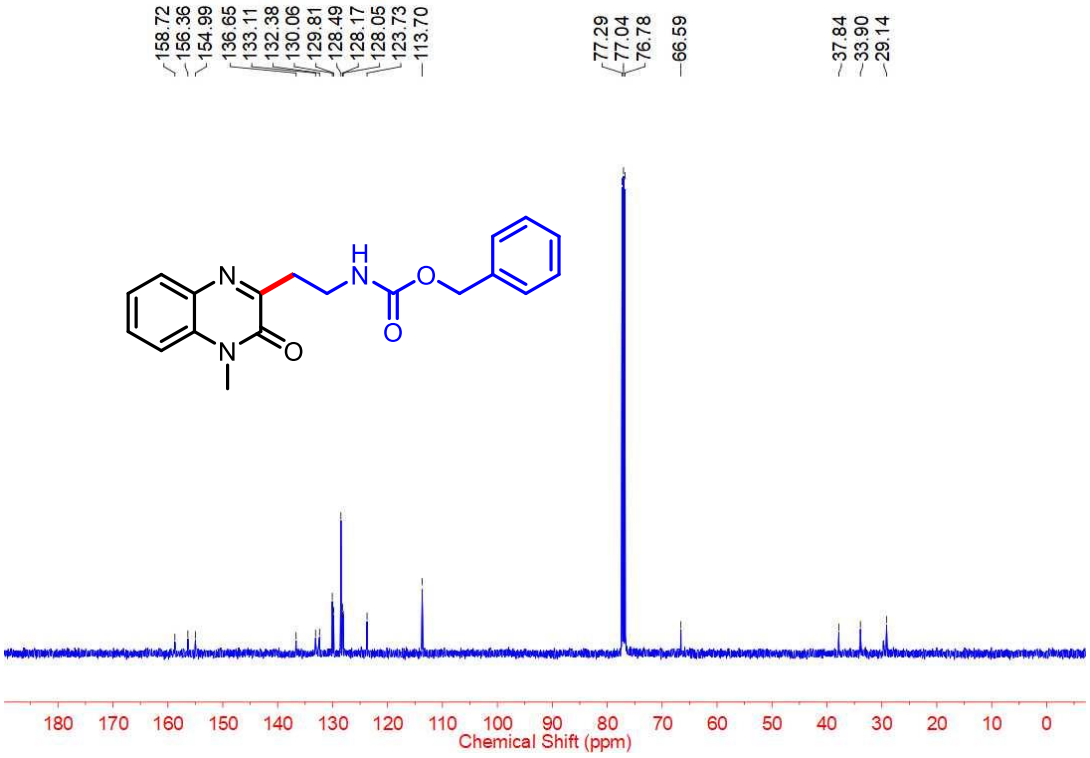
66 ^{13}C NMR (126 MHz, $CDCl_3$)



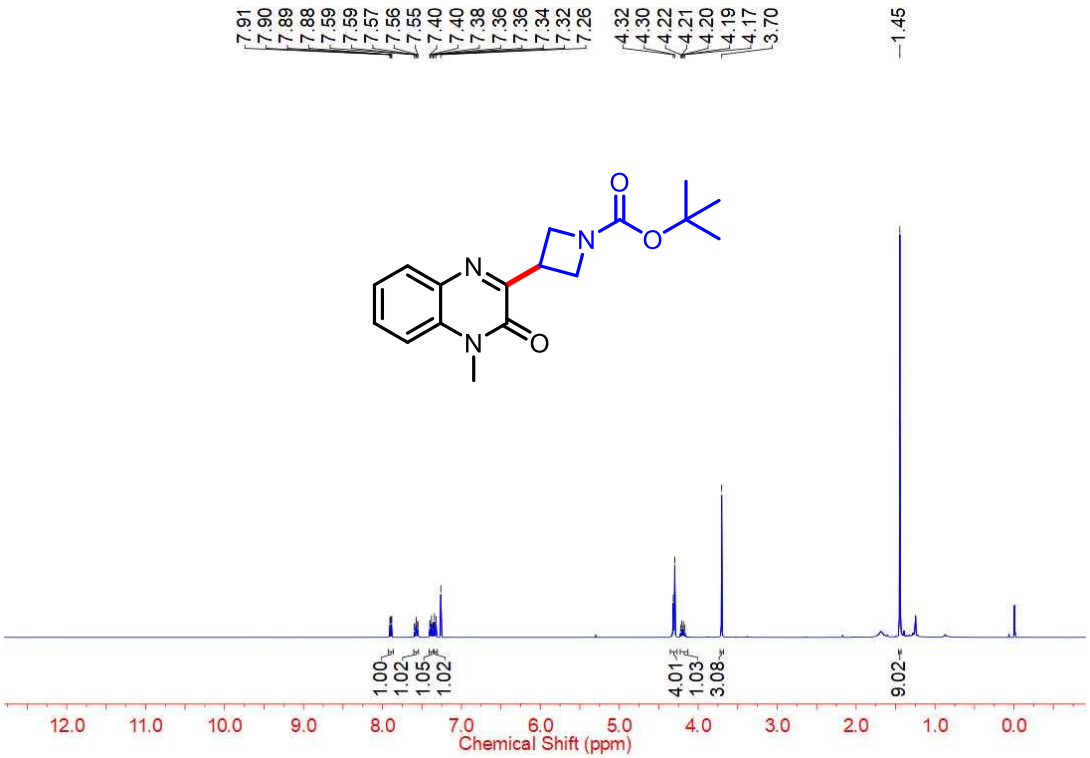
67 ^{1}H NMR (500 MHz, $CDCl_3$)



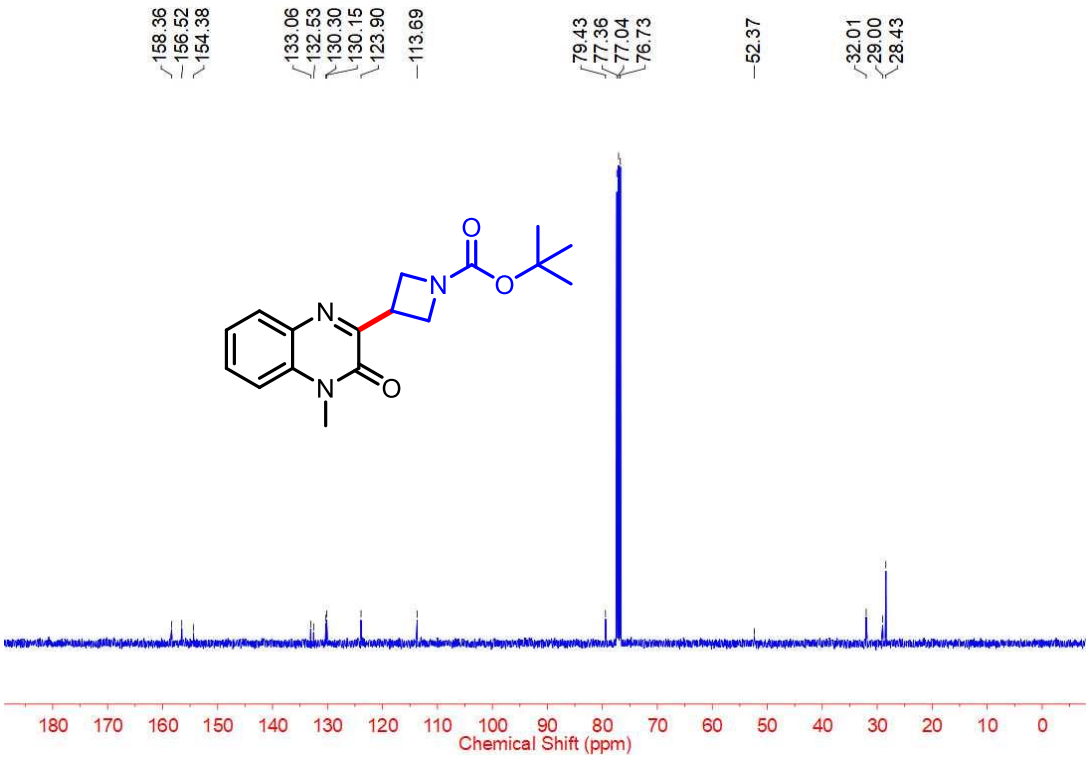
67 ^{13}C NMR (126 MHz, $CDCl_3$)



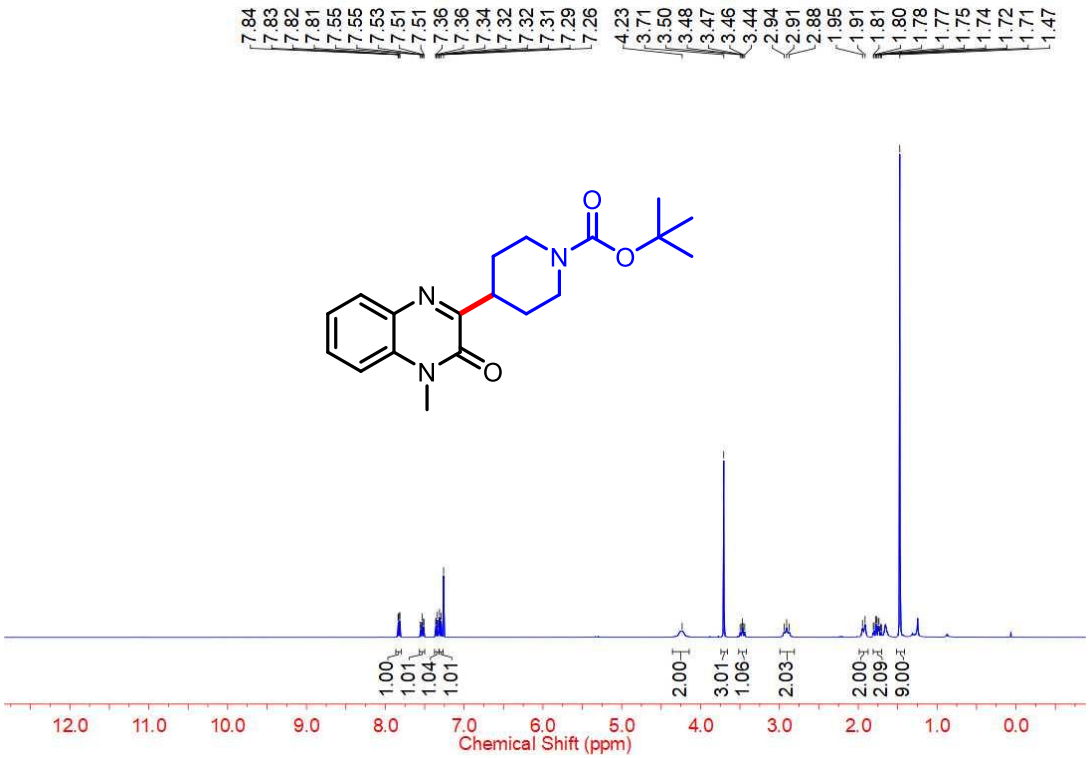
68 ^{1}H NMR (400 MHz, $CDCl_3$)



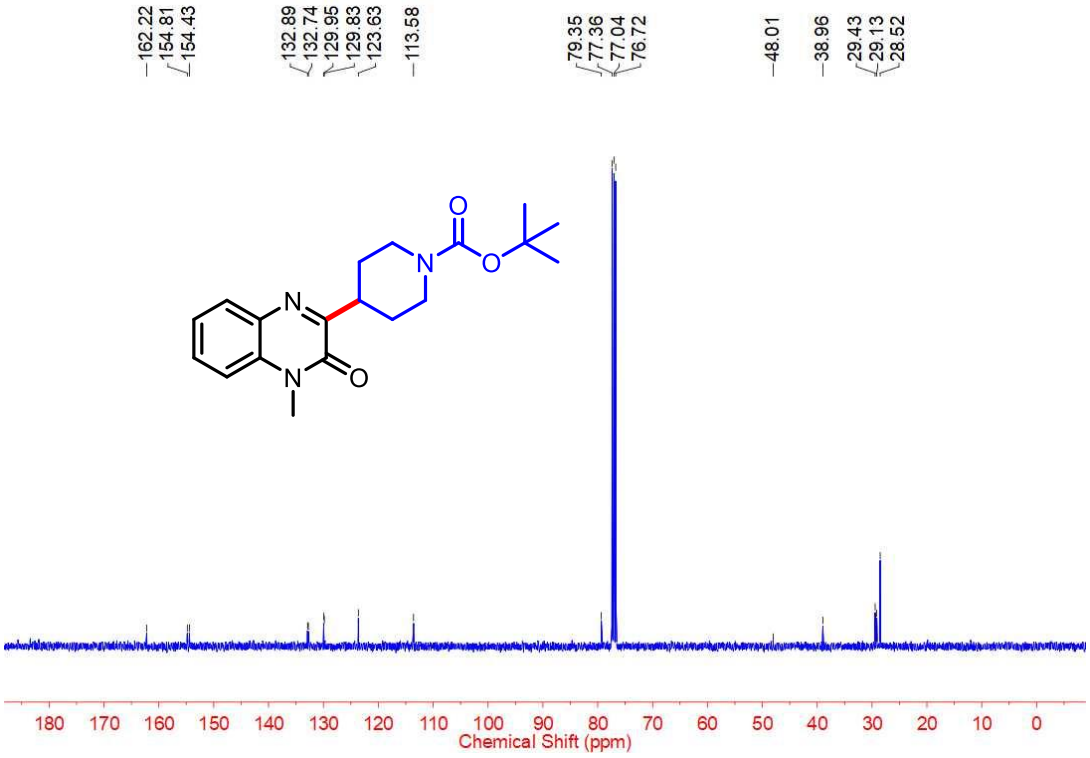
68 ^{13}C NMR (100 MHz, $CDCl_3$)



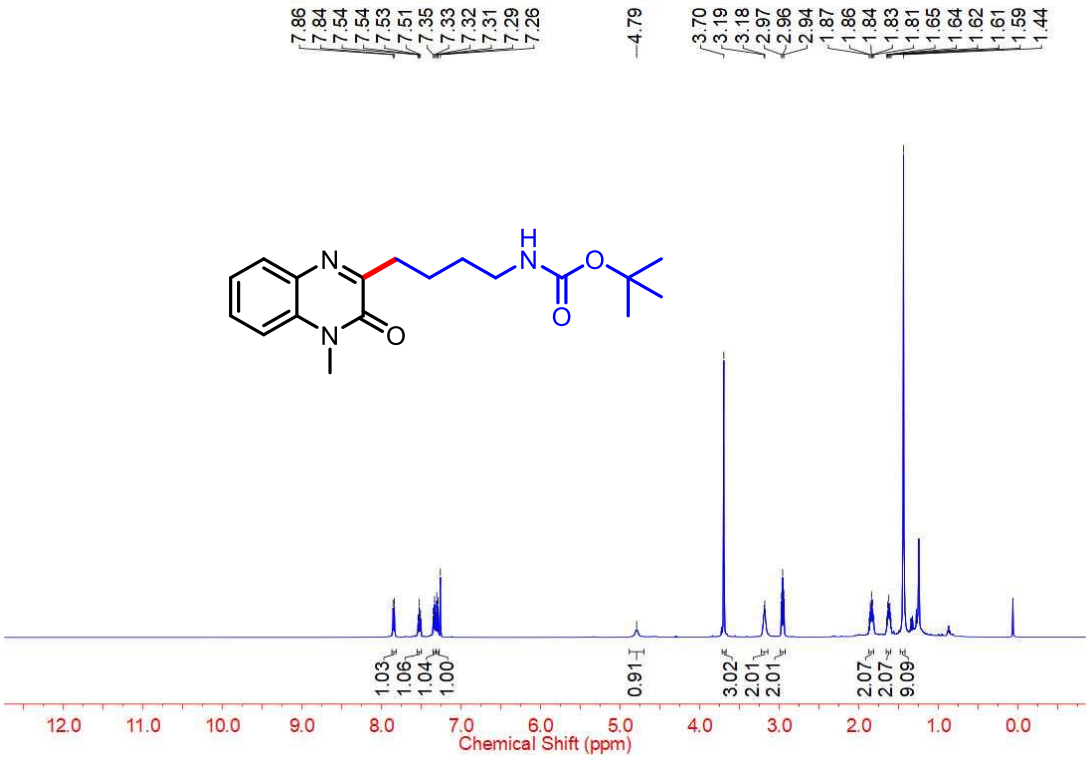
69 ^{1}H NMR (400 MHz, $CDCl_3$)



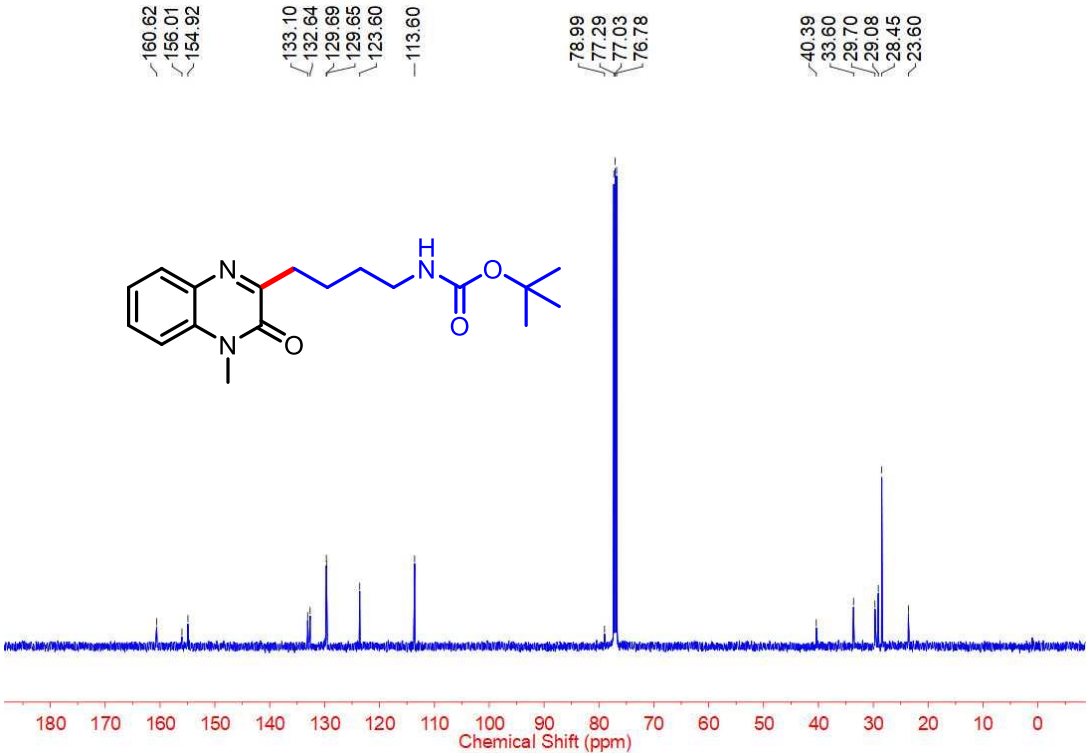
69 ^{13}C NMR (100 MHz, $CDCl_3$)



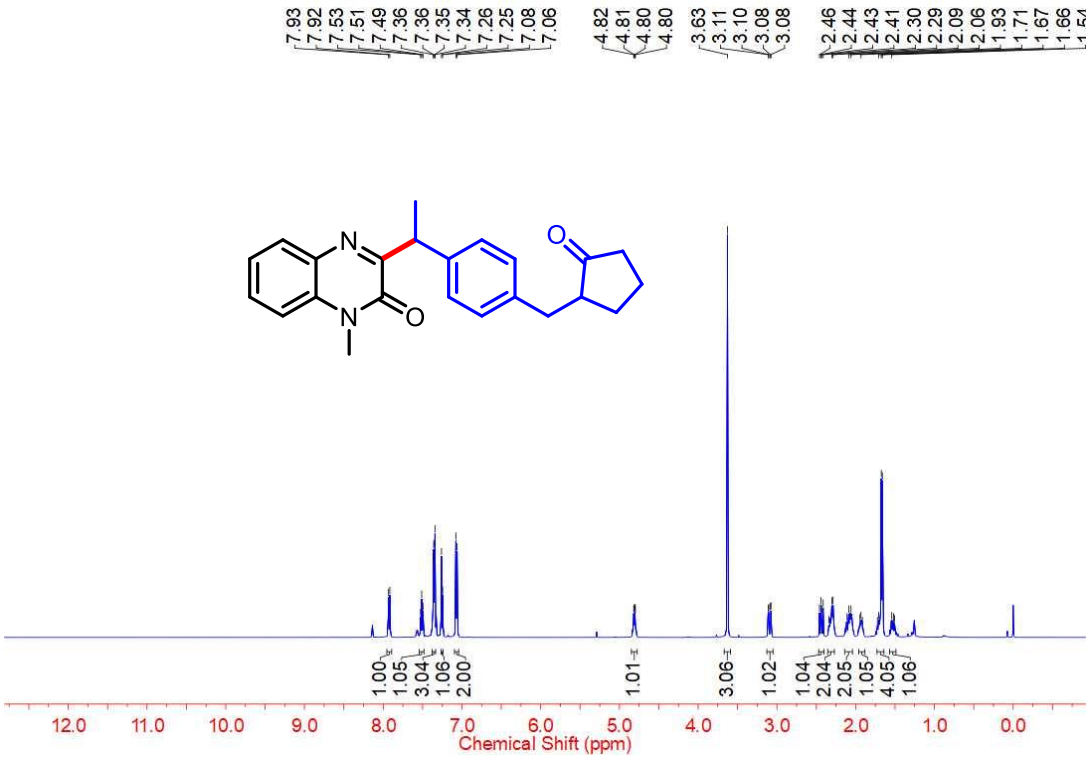
70 ^{1}H NMR (500 MHz, $CDCl_3$)



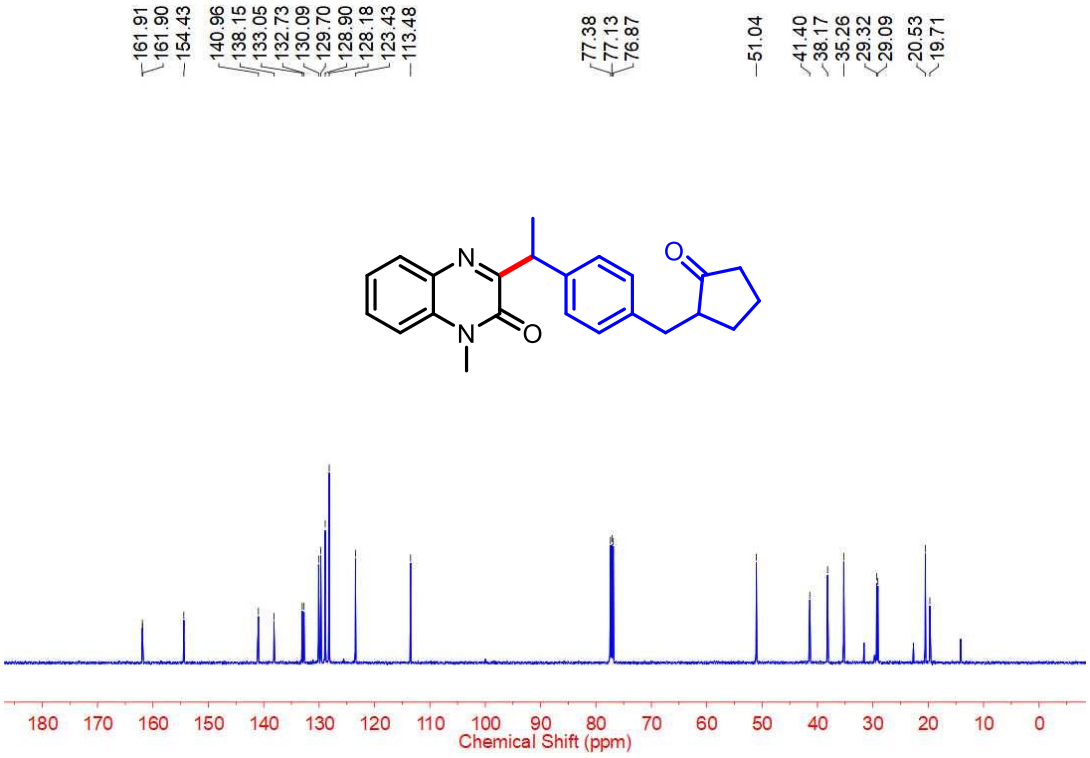
70 ^{13}C NMR (126 MHz, $CDCl_3$)



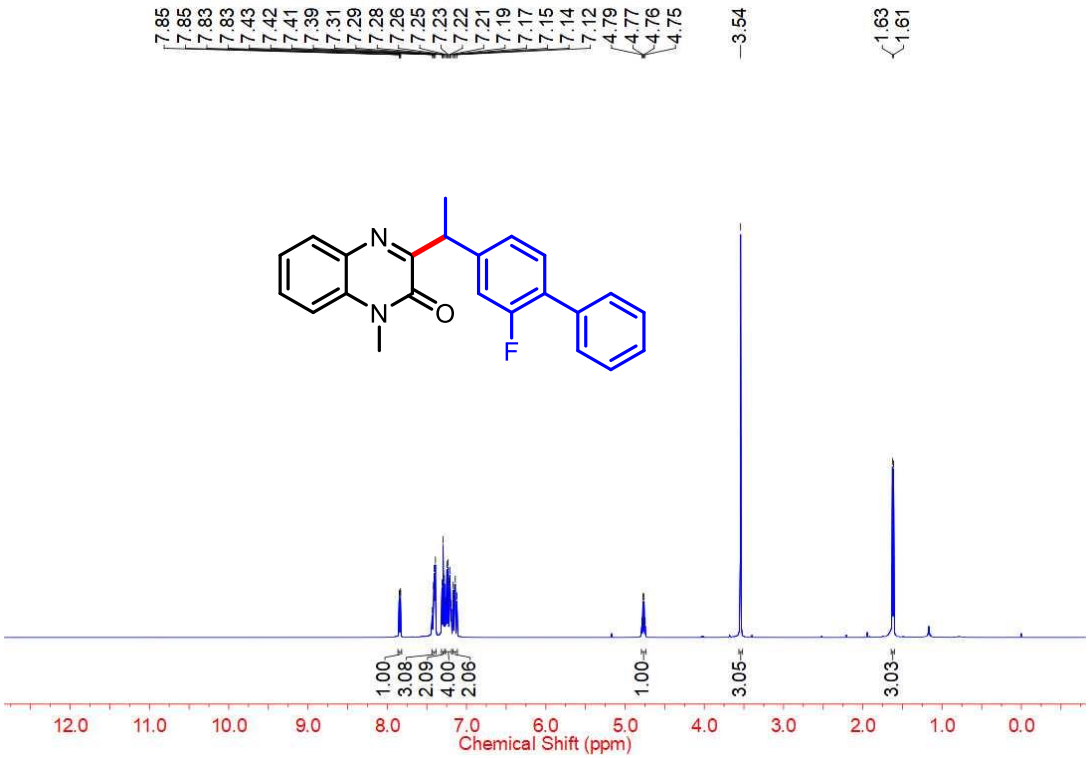
71 ^{1}H NMR (500 MHz, $CDCl_3$)



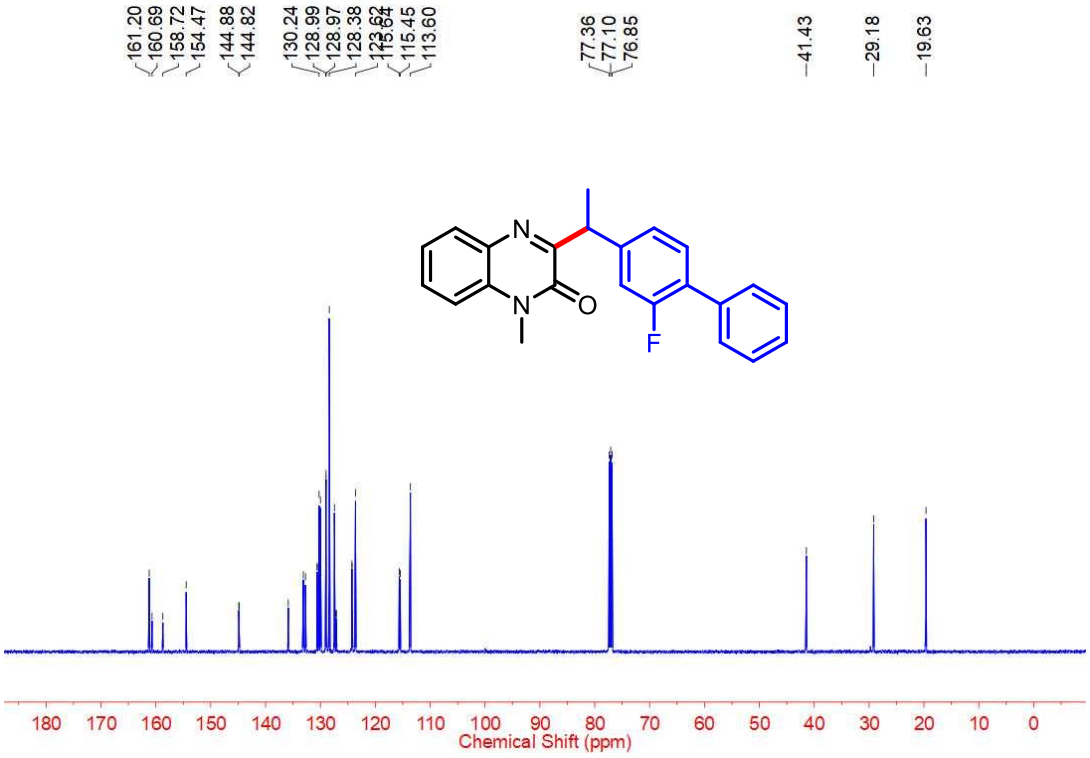
71 ^{13}C NMR (126 MHz, $CDCl_3$)



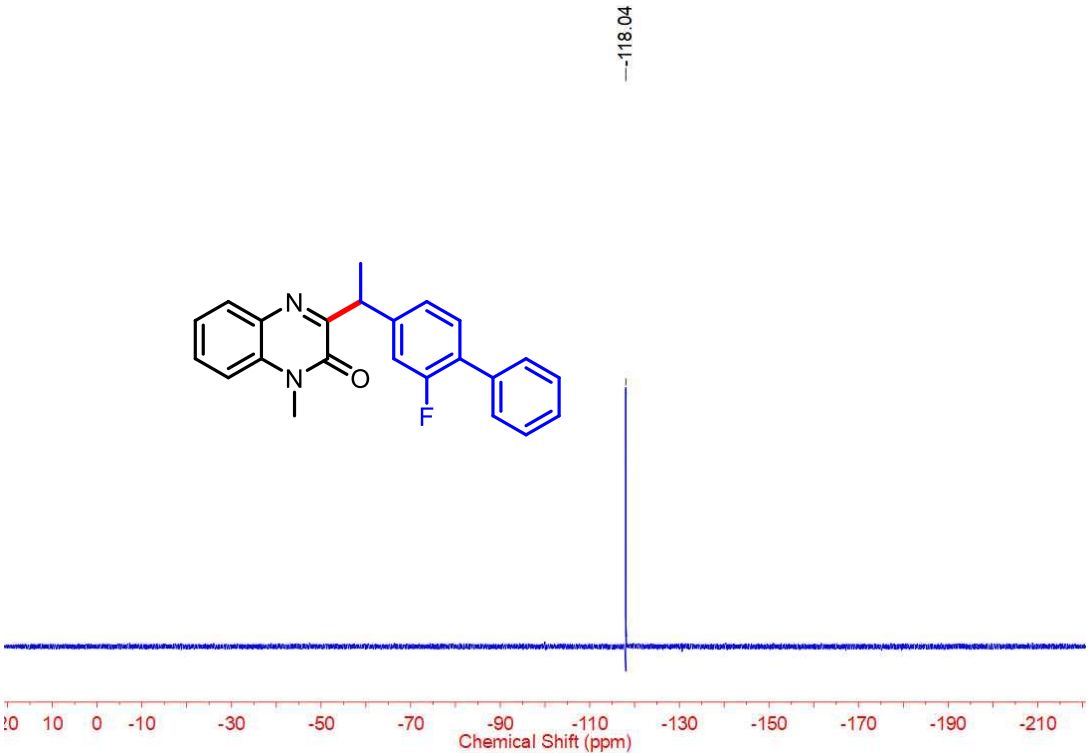
72 ^{1}H NMR (500 MHz, $CDCl_3$)



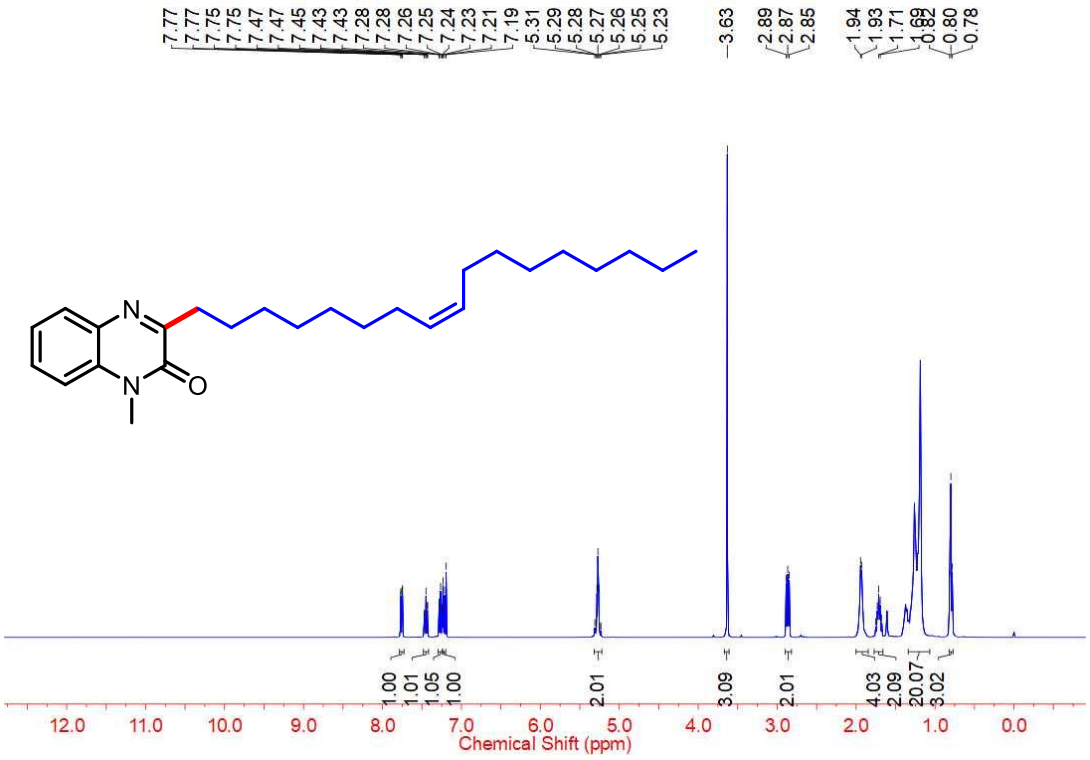
72 ^{13}C NMR (126 MHz, $CDCl_3$)



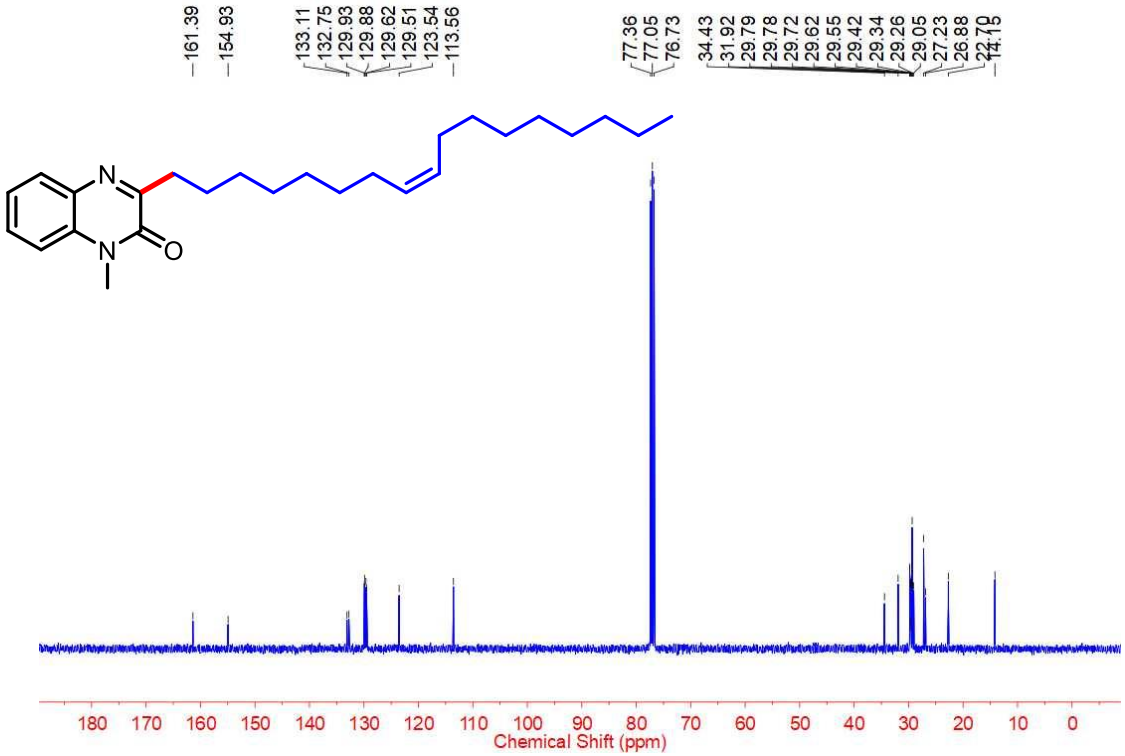
72 ^{19}F NMR (471 MHz, $CDCl_3$)



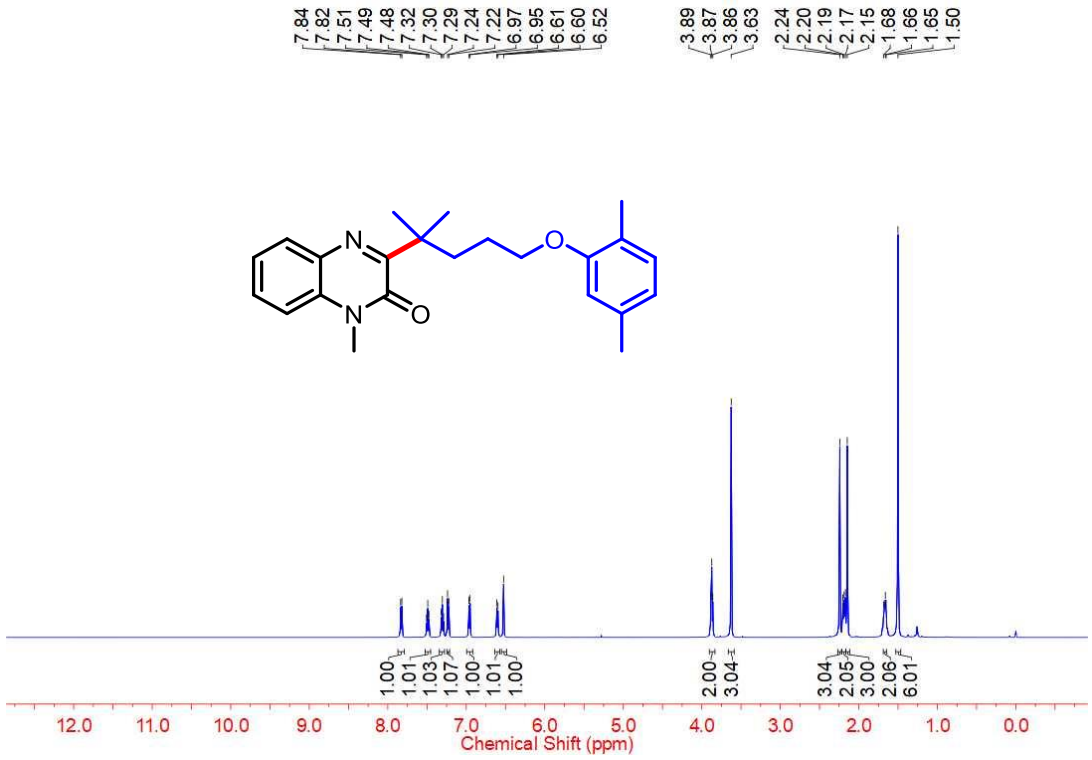
73 ^{1}H NMR (400 MHz, $CDCl_3$)



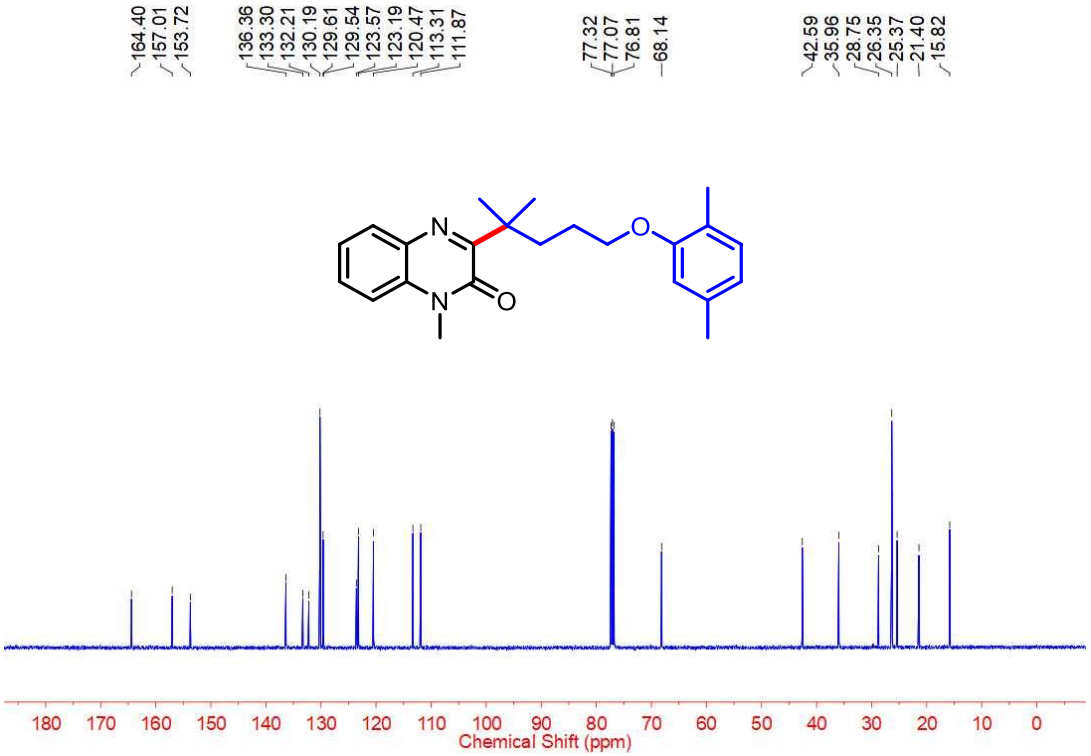
73 ^{13}C NMR (100 MHz, $CDCl_3$)



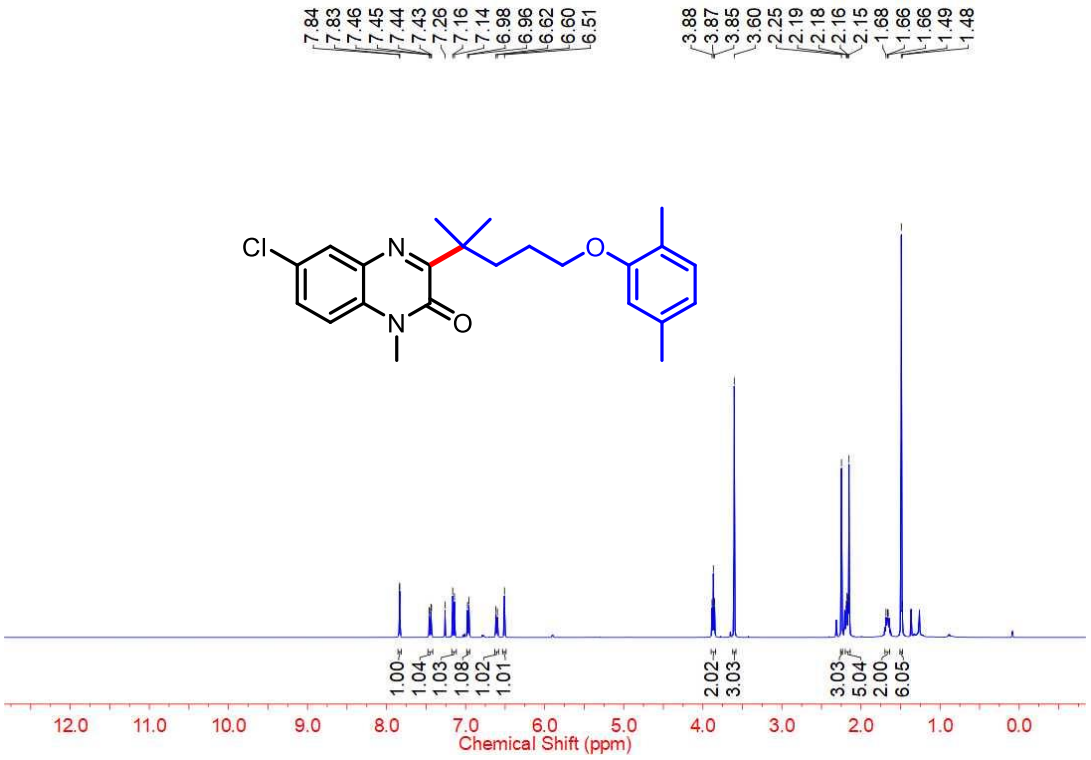
74 ^{1}H NMR (500 MHz, $CDCl_3$)



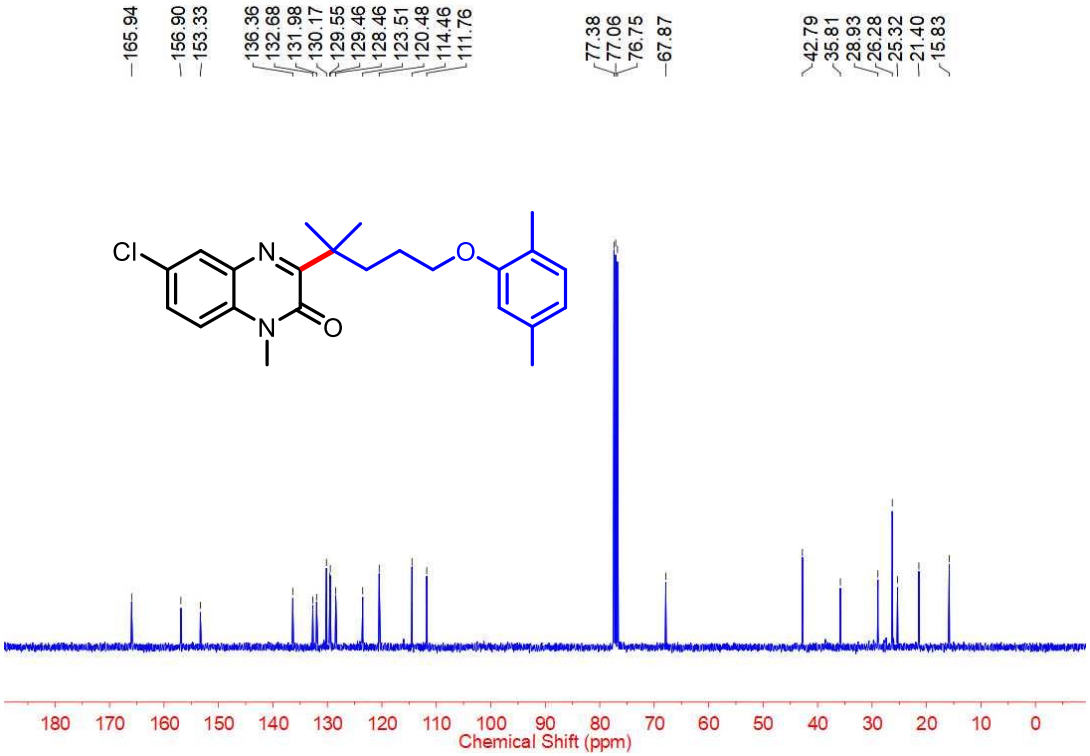
74 ^{13}C NMR (126 MHz, $CDCl_3$)



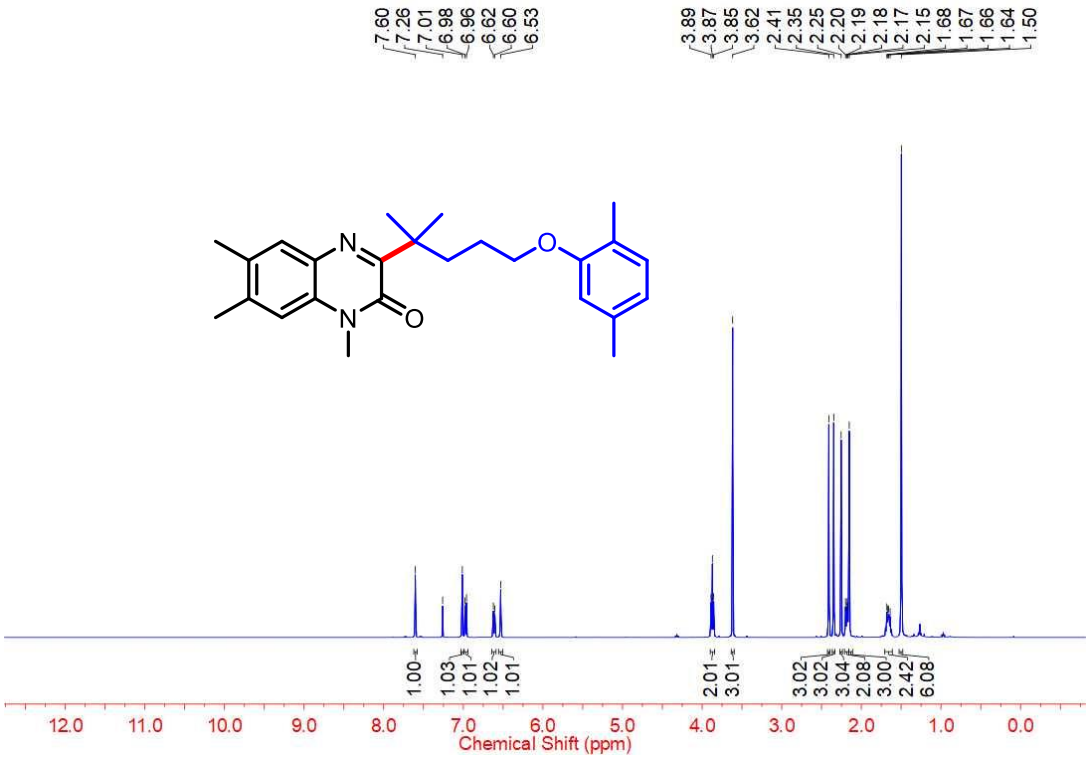
75 ^{1}H NMR (400 MHz, $CDCl_3$)



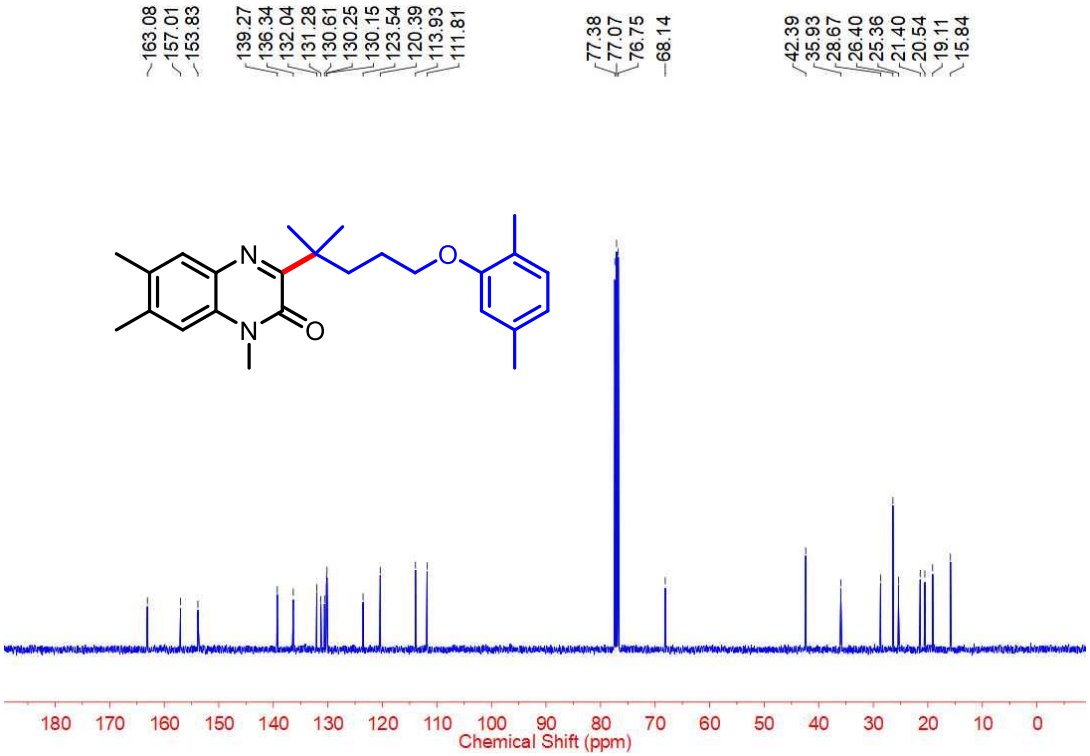
75 ^{13}C NMR (100 MHz, $CDCl_3$)



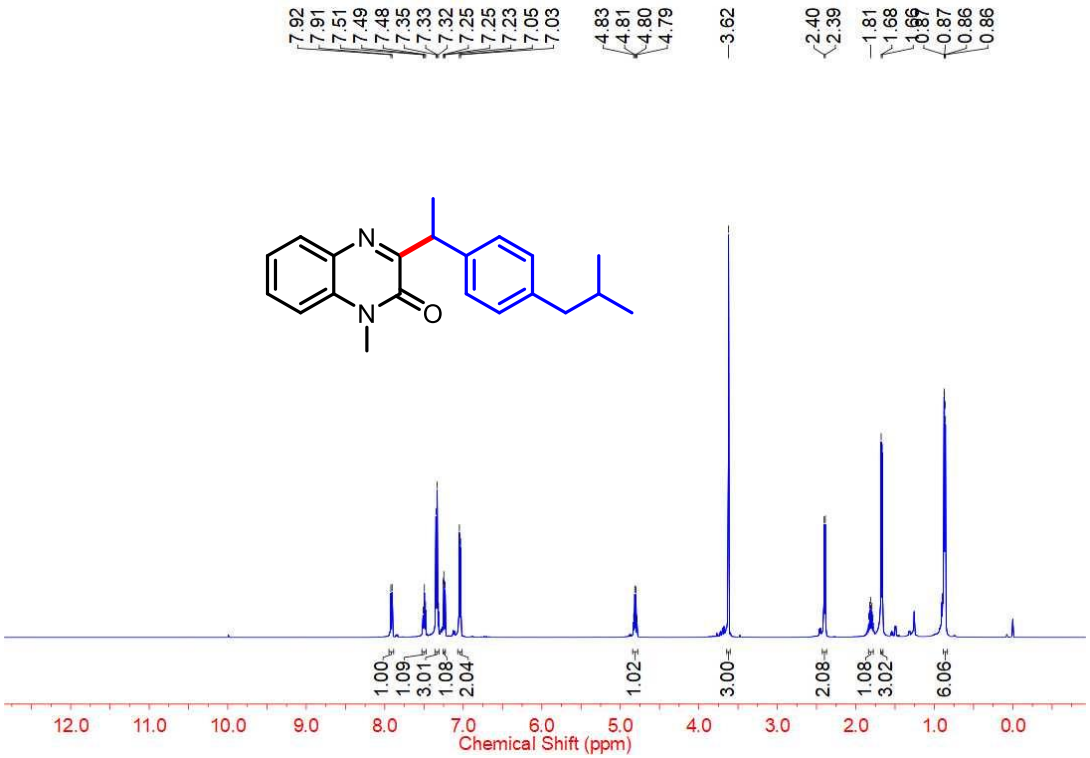
76 ^{1}H NMR (400 MHz, $CDCl_3$)



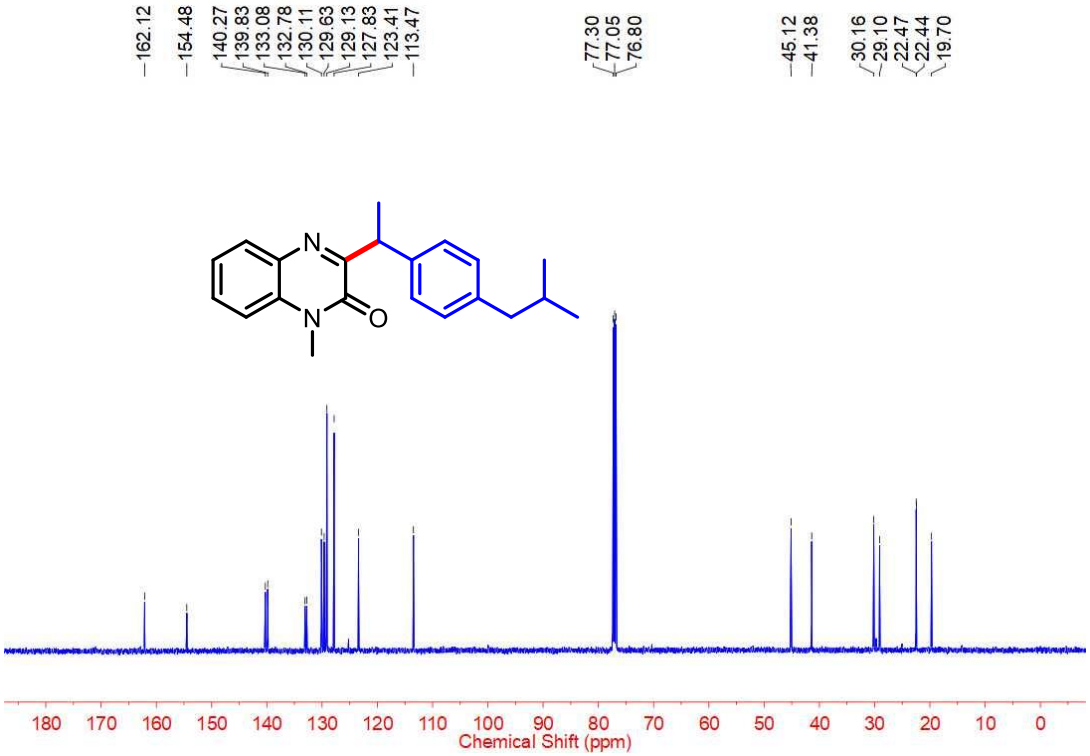
76 ^{13}C NMR (100 MHz, $CDCl_3$)



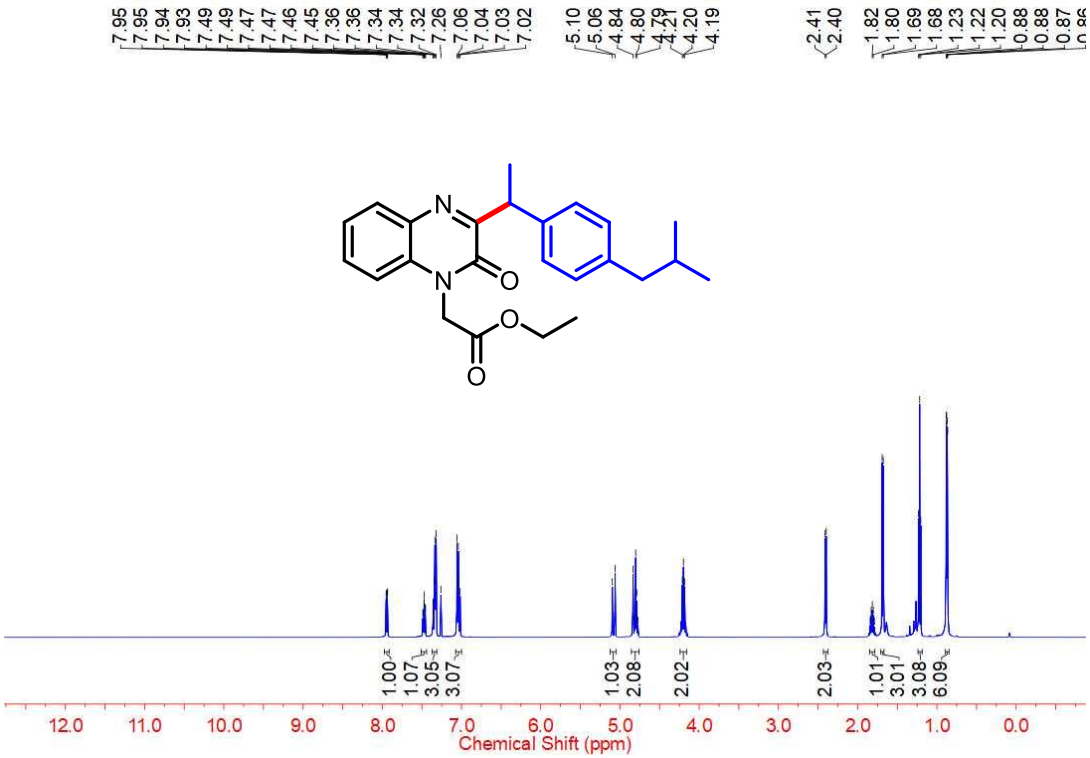
77 ^{1}H NMR (500 MHz, $CDCl_3$)



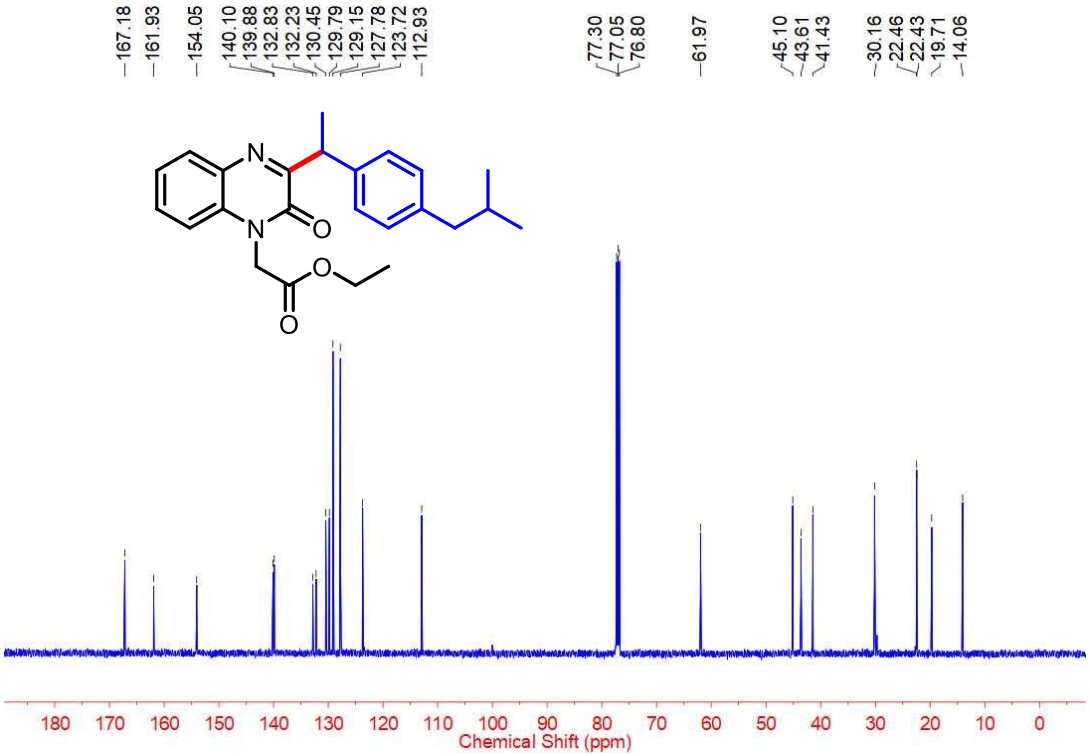
77 ^{13}C NMR (126 MHz, $CDCl_3$)



78 ^{1}H NMR (500 MHz, $CDCl_3$)



78 ^{13}C NMR (126 MHz, $CDCl_3$)



82 ^{1}H NMR (500 MHz, DMSO)