α-Functionalization of ketones promoted by sunlight and heterogeneous catalysis in the aqueous phase

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Supporting Information

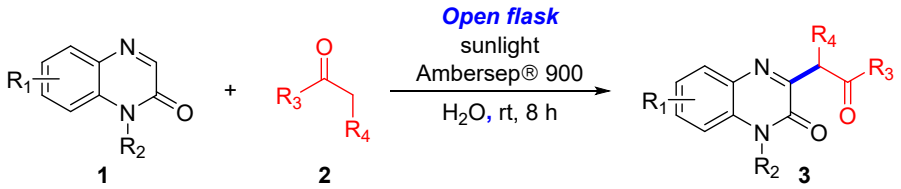
Table of contents

1. General Information

All reagents and deuterated solvents are commercially available and used without further purification. All products were separated by silica gel (200-300 mesh) column chrmomatography with petroleum ether (PE) (60°C-90°C) and ethyl acetate. (EA). ^{1}H and ^{13}C spectra were recorded on a Bruker Advance 500 spectrometer at ambient temperature with $CDCl_3$ as solvent on tetramethylsilane (TMS) as the internal standard. Melting points were determined on an X-5 Data microscopic melting point apparatus. Analytic 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.

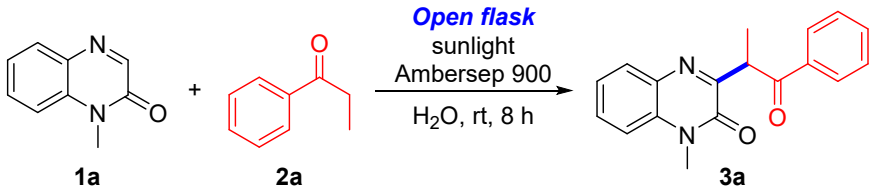
2. Experimental Section

2.1 General Procedure for the Synthesis of Product 3



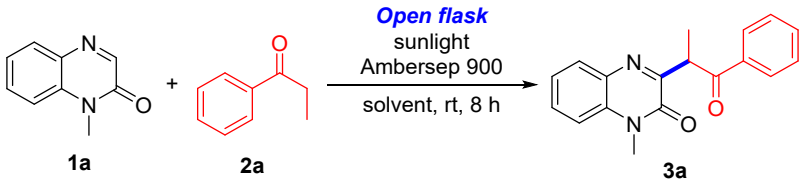
A mixture of quinoxalinones (**1**) (0.2 mmol), ketones (**2**) (0.4 mmol), Ambersep 900 (100 mg), and H_2O in a 10 mL tube was stirred under sunlight for 8 h. After the completion (as indicated by TLC), the resulting aqueous phase was extracted with EtOAc (5 mL x 3). The collected organic layer was washed with brine, dried with $MgSO_4$. Finally, the organic solvent was removed under reduced pressure, and the crude product was purified by silica gel column chromatography (200-300 mesh silica gel, PE/EA = 3:1) to afford product **3**.

2.2 General Procedure for the Gram-Scale Synthesis of Product 3a



A mixture of 1-methylquinoxalin-2(1*H*)-ones (1a) (8.0 mmol), propiophenone (2a) (16.0 mmol), Ambersep 900 (3.0 g), and H_2O (15 mL) in a 50 mL tube was vigorous stirred under sunlight. After the completion (as indicated by TLC), the resulting aqueous phase was extracted with EtOAc (25 mL x 3). The collected organic layer was washed with brine, dried with $MgSO_4$. Finally, the organic solvent was removed under reduced pressure, and the crude product was purified by silica gel column chromatography (200-300 mesh silica gel, PE/EA = 3:1) to afford product **3a** in 69% yield (1.6g).

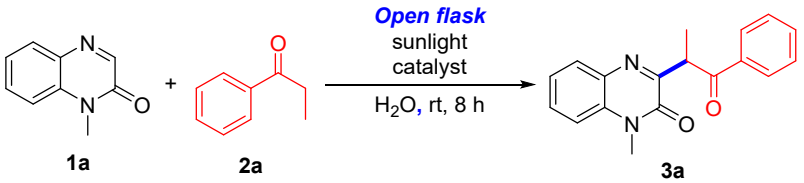
2.3 Optimization of Solvents[a]



entry	solvent	yield (%)[b]
1	H_2O	78
2	Toluene	60
3	DMSO	63
4	DMF	51
5	DMC	10
6	CH_3CN	82

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (2.0 equiv.), Ambersep 900 (100 mg), solvent (3.0 mL), sunlight, open flask, air, room temperature, 8 h. [b] Isolated yields.

2.4 Optimization of Homogeneous catalysts[a]



entry	catalyst	yield (%)[b]

1	K_2CO_3	23
2	NaOH	80
3	KOH	82

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (2.0 equiv.), catalyst (100 mg), H_2O (3.0 mL), sunlight, open flask, air, room temperature, 8 h. [b] Isolated yields.

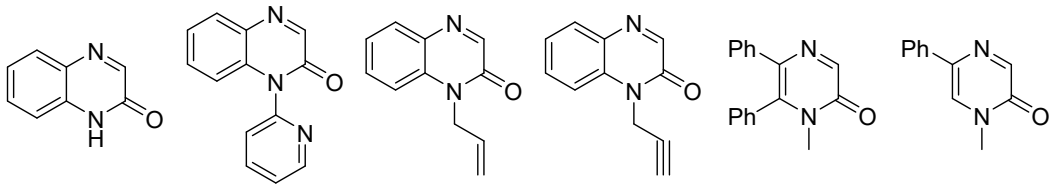
2.5 Testing of the Recycability of Catalytic System

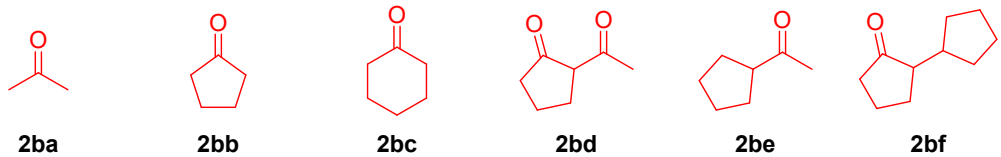
To a 15 mL tube was added quinoxalinone (1a) (0.2 mmol), propiophenone (2a) (0.6 mmol), Ambersep 900 (100 mg) and H_2O (3 mL). And the mixture was under vigorous stirring with the irradiation of sunlight for 8 hours. After the completion (as indicated by TLC), the resulting aqueous phase was extracted with ethyl acetate (3 mL x 5) and the collected organic layer was washed with brine and dried with $MgSO_4$. The solvent was removed under reduced pressure, and the crude product was further purified by silica gel column chromatography (200-300 mesh silica gel, PE/EA = 4:1) to afford the target product.

2.6 The Regeneration of Ambersep 900 Catalyst

After it was recycled for four times, Ambersep 900 catalyst was first washed with ethanol, ethyl acetate and 1, 2-dichloromethane continuously to remove the organic impurities. Then, the catalyst was washed with HCl (2M), distilled water and NaOH (2M) for three times to remove the water-soluble impurities. After that, the catalyst was immersed into saturated NaOH solution for 12 h, and the resulting catalyst was washed with distilled water repeatedly until the pH value is about 7. Finally, it was dried under vacuum condition to give the regenerated Ambersep 900 catalyst.

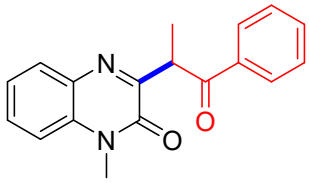
2.7 Ineffective substrates for the α-functionalization of asymmetric ketones





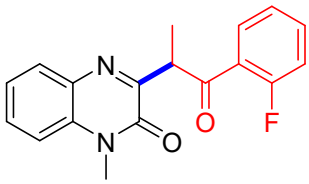
3. Characterization Data of Products

1-Methyl-3-(1-oxo-1-phenylpropan-2-yl)quinoxalin-2(1H)-one (3a)



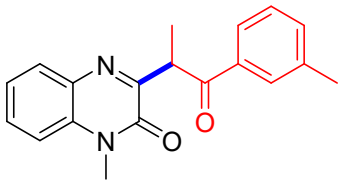
Obtained as white solid (46 mg, 78% yield); m.p. 132-133 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 – 8.06 (m, 2H), 7.88 (dd, J = 8.0, 1.5 Hz, 1H), 7.54 (td, J = 7.1, 1.4 Hz, 2H), 7.46 (t, J = 7.5 Hz, 2H), 7.36 – 7.31 (m, 1H), 7.29 (d, J = 8.4 Hz, 1H), 5.32 (q, J = 7.0 Hz, 1H), 3.68 (s, 3H), 1.64 (d, J = 7.0 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.67, 159.24, 154.39, 136.40, 133.07, 132.96, 132.81, 130.32, 130.17, 128.68, 128.62, 123.70, 113.62, 45.17, 29.24, 14.70; HRMS (ESI+): $[M + Na]^+$ Calculated for $C_{18}H_{16}N_2O_2Na$: 315.1104, Found 315.1100.

3-(1-(2-Fluorophenyl)-1-oxopropan-2-yl)-1-methylquinoxalin-2(1H)-one (3b)



Obtained as white solid 1:1 dr (46 mg, 75% yield); m.p. 148-149 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.99 (td, J = 7.6, 1.9 Hz, 1H), 7.83 (dd, J = 8.0, 1.6 Hz, 1H), 7.55 – 7.51 (m, 1H), 7.51 – 7.46 (m, 1H), 7.33 (d, J = 7.5 Hz, 1H), 7.29 (d, J = 8.7 Hz, 1H), 7.23 (t, J = 7.6 Hz, 1H), 7.09 (dd, J = 11.1, 8.6 Hz, 1H), 5.13 (q, J = 7.0 Hz, 1H), 3.68 (s, 3H), 1.64 (d, J = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) Mixture of diastereomers is observed. Ratio: 5/5. Major diastereomer: δ 197.57 (d, J = 4.4 Hz), 162.40, 160.38, 159.40, 154.38, 134.31 (d, J = 9.1 Hz), 133.15, 132.65, 131.33 (d, J = 2.6 Hz), 130.17 (d, J = 21.4 Hz), 125.42 (d, J = 12.5 Hz), 124.48 (d, J = 3.4 Hz), 123.60, 116.64 (d, J = 24.0 Hz), 113.58, 49.69, 29.18, 13.88; Minor diastereomer: δ 197.57 (d, J = 4.4 Hz), 162.40, 160.38, 159.40, 154.38, 134.31 (d, J = 9.1 Hz), 133.15, 132.65, 131.33 (d, J = 2.6 Hz), 130.17 (d, J = 21.4 Hz), 125.42 (d, J = 12.5 Hz), 124.48 (d, J = 3.4 Hz), 123.60, 116.64 (d, J = 24.0 Hz), 113.58, 49.64, 29.18, 13.88; ^{19}F NMR (471 MHz, $CDCl_3$) δ -110.42; HRMS (ESI+): $[M + Na]^+$ Calculated for $C_{18}H_{15}FN_2O_2Na$: 333.1010, Found 333.1007.

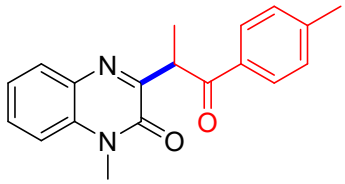
1-methyl-3-(1-oxo-1-(m-tolyl)propan-2-yl)quinoxalin-2(1H)-one (3c)



Obtained as white solid (46 mg, 76% yield); m.p. 131-132 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.91 – 7.86 (m, 3H), 7.54 – 7.50 (m, 1H), 7.35 – 7.30 (m, 3H), 7.28 (d, J = 8.3 Hz, 1H), 5.29 (q, J = 7.0 Hz, 1H), 3.66 (s, 3H), 2.40 (s, 3H), 1.63 (d, J = 7.0 Hz,

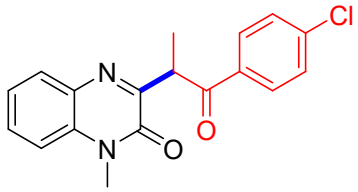
3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 199.92, 159.29, 154.40, 138.44, 136.43, 133.76, 133.08, 132.82, 130.29, 130.10, 129.12, 128.54, 125.85, 123.65, 113.60, 45.23, 29.19, 21.41, 14.69; HRMS (ESI+): $[M+Na]^+$ Calculated for $C_{19}H_{18}N_2O_2Na$: 329.1260, Found 329.1257.

1-Methyl-3-(1-oxo-1-(p-tolyl)propan-2-yl)quinoxalin-2(1H)-one (3d)



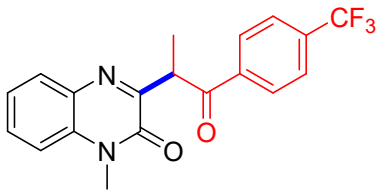
Obtained as white solid (48 mg, 79% yield); m.p. 163-164 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.98 (d, J = 8.2 Hz, 2H), 7.87 (dd, J = 8.0, 1.6 Hz, 1H), 7.53 (m, J = 8.6, 7.3, 1.6 Hz, 1H), 7.33 (m, J = 8.3, 7.3, 1.2 Hz, 1H), 7.28 (dd, J = 8.4, 1.2 Hz, 1H), 7.25 (d, J = 7.9 Hz, 2H), 5.30 (q, J = 7.0 Hz, 1H), 3.67 (s, 3H), 2.38 (s, 3H), 1.62 (d, J = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 199.22, 159.39, 154.39, 143.69, 133.89, 133.09, 132.83, 130.33, 130.09, 129.36, 128.75, 123.64, 113.57, 45.03, 29.21, 21.63, 14.76; HRMS (ESI+): $[M + Na]^+$ Calculated for $C_{19}H_{18}N_2O_2Na$: 329.1260, Found 329.1263.

3-(1-(4-Chlorophenyl)-1-oxopropan-2-yl)-1-methylquinoxalin-2(1H)-one (3e)



Obtained as white solid (47 mg, 72% yield); m.p. 68-69 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.01 (d, J = 8.5 Hz, 2H), 7.87 (dd, J = 8.1, 1.5 Hz, 1H), 7.57 – 7.53 (m, 1H), 7.42 (d, J = 8.6 Hz, 2H), 7.36 – 7.32 (m, 1H), 7.31 – 7.29 (m, 1H), 5.24 (q, J = 7.0 Hz, 1H), 3.68 (s, 3H), 1.62 (d, J = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 198.42, 158.93, 154.34, 139.31, 134.85, 133.06, 132.79, 130.34, 130.30, 130.01, 128.98, 123.78, 113.64, 45.21, 29.26, 14.61; HRMS (ESI+): $[M + Na]^+$ Calculated for $C_{18}H_{15}ClN_2O_2Na$: 349.0714, Found 349.0715.

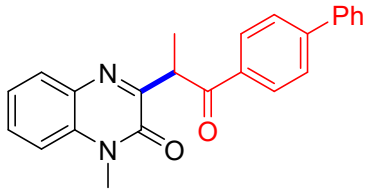
1-Methyl-3-(1-oxo-1-(4-(trifluoromethyl)phenyl)propan-2-yl)quinoxalin-2(1H)-one (3f)



Obtained as white solid (45 mg, 62% yield), m.p. 158-159 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.17 (d, J = 8.0 Hz, 2H), 7.87 (dd, J = 8.1, 1.5 Hz, 1H), 7.72 (d, J = 8.2 Hz, 2H), 7.56 (m, J = 8.6, 7.3, 1.5 Hz, 1H), 7.35 (m, J = 8.4, 7.4, 1.2 Hz, 1H), 7.31 (dd, J = 8.5, 1.3 Hz, 1H), 5.27 (q, J = 6.9 Hz, 1H), 3.69 (s, 3H), 1.64 (d, J = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 198.70, 158.73, 154.33, 139.38, 134.27, 134.01, 133.06, 132.78, 130.40, 130.36, 128.86, 125.74 (q, J = 3.6 Hz), 123.85, 113.68, 45.57, 29.28,

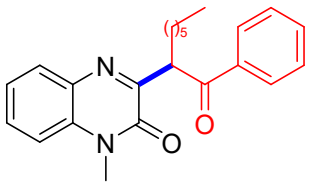
14.48; ^{19}F NMR (471 MHz, $CDCl_3$) δ -63.11; HRMS (ESI+): $[M + Na]^+$ Calculated for $C_{19}H_{15}F_3N_2O_2Na$ 383.0978, Found 383.0980.

3-(1-([1,1'-Biphenyl]-4-yl)-1-oxopropan-2-yl)-1-methylquinoxalin-2(1H)-one (3g)



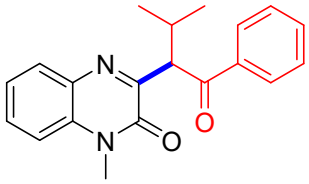
Obtained as white solid (57 mg, 77% yield); m.p. 139-140 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.15 (d, J = 8.4 Hz, 2H), 7.87 (dd, J = 8.0, 1.5 Hz, 1H), 7.66 (d, J = 8.4 Hz, 2H), 7.59 (dd, J = 8.4, 1.2 Hz, 2H), 7.52 – 7.48 (m, 1H), 7.43 (t, J = 7.6 Hz, 2H), 7.38 – 7.34 (m, 1H), 7.32 – 7.29 (m, 1H), 7.25 (dd, J = 8.4, 1.2 Hz, 1H), 5.33 (q, J = 7.0 Hz, 1H), 3.64 (s, 3H), 1.66 (d, J = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 199.26, 159.25, 154.41, 145.61, 139.96, 135.16, 133.08, 132.83, 130.30, 130.18, 129.24, 128.93, 128.15, 127.37, 127.26, 123.70, 113.65, 45.24, 29.24, 14.77; HRMS (ESI+): $[M + Na]^+$ Calculated for $C_{24}H_{20}N_2O_2Na$: 391.1417, Found 391.1440.

1-Methyl-3-(1-oxo-1-phenyloctan-2-yl)quinoxalin-2(1H)-one (3h)



Obtained as white solid (46 mg, 64% yield); m.p. 83-84 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.11 – 8.07 (m, 2H), 7.87 (dd, J = 8.1, 1.4 Hz, 1H), 7.54 – 7.52 (m, 1H), 7.51 – 7.49 (m, 1H), 7.44 (t, J = 7.6 Hz, 2H), 7.33 – 7.30 (m, 1H), 7.27 (d, J = 8.1 Hz, 1H), 5.32 (t, J = 6.8 Hz, 1H), 3.67 (s, 3H), 2.19 (td, J = 15.4, 14.4, 7.4 Hz, 1H), 2.10 (td, J = 14.1, 13.5, 6.3 Hz, 1H), 1.43 (tt, J = 6.3, 3.8 Hz, 2H), 1.39 – 1.34 (m, 2H), 1.26 (dq, J = 7.1, 3.7 Hz, 4H), 0.85 (t, J = 6.8 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 198.81, 158.24, 154.60, 137.04, 132.97, 132.90, 132.82, 130.38, 130.15, 128.65, 128.62, 123.67, 113.58, 50.16, 31.59, 29.95, 29.39, 29.30, 27.88, 22.58, 14.08; HRMS (ESI+): $[M + Na]^+$ Calculated for $C_{23}H_{26}N_2O_2Na$: 385.1886, Found 385.1888.

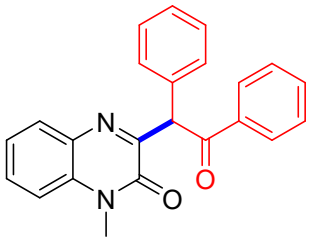
1-Methyl-3-(3-methyl-1-oxo-1-phenylbutan-2-yl)quinoxalin-2(1H)-one (3i)



Obtained as white solid (45 mg, 71% yield); m.p. 118-119 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.10 – 8.04 (m, 2H), 7.83 (dd, J = 8.1, 1.5 Hz, 1H), 7.47 – 7.41 (m, 2H), 7.36 (t, J = 7.5 Hz, 2H), 7.27 – 7.23 (m, 1H), 7.19 (d, J = 7.1 Hz, 1H), 5.25 (d, J = 9.2 Hz, 1H), 3.61 (s, 3H), 2.82 (dp, J = 9.2, 6.6 Hz, 1H), 0.99 (d, J = 6.7 Hz, 3H), 0.90 (d, J = 6.7 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 196.99, 156.50, 153.80, 136.89,

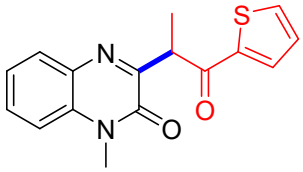
131.88, 131.82, 131.80, 129.49, 129.22, 127.69, 127.59, 122.68, 112.49, 54.64, 29.51, 28.42, 20.49, 19.70; HRMS (ESI+): $[M + Na]^+$ Calculated for $C_{20}H_{20}N_2O_2Na$: 343.1417, Found 343.1418.

1-Methyl-3-(2-oxo-1,2-diphenylethyl)quinoxalin-2(1H)-one (3j)



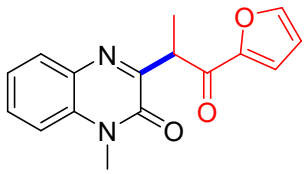
Obtained as white solid (50 mg, 70% yield); m.p. 144-145 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.08 – 8.04 (m, 2H), 7.75 (dd, J = 8.0, 1.5 Hz, 1H), 7.51 – 7.49 (m, 2H), 7.49 – 7.45 (m, 2H), 7.42 – 7.38 (m, 2H), 7.38 – 7.34 (m, 2H), 7.31 – 7.28 (m, 1H), 7.27 – 7.22 (m, 2H), 6.62 (s, 1H), 3.65 (d, J = 1.3 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 196.00, 157.63, 154.44, 136.55, 134.45, 133.08, 132.96, 132.67, 130.64, 130.32, 128.88, 128.64, 128.49, 127.61, 123.64, 113.56, 57.07, 29.33; HRMS (ESI+): $[M + Na]^+$ Calculated for $C_{23}H_{18}N_2O_2Na$: 377.1260, Found 377.1283.

1-Methyl-3-(1-oxo-1-(thiophen-2-yl)propan-2-yl)quinoxalin-2(1H)-one (3k)



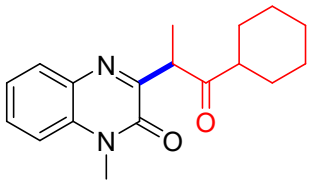
Obtained as white solid (31 mg, 52% yield); m.p. 139-140 °C. ^{1}H NMR (500 MHz, $CDCl_3$) ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.92 – 7.90 (m, 1H), 7.89 (d, J = 4.1 Hz, 1H), 7.62 (d, J = 4.7 Hz, 1H), 7.57 – 7.53 (m, 1H), 7.35 (t, J = 7.6 Hz, 1H), 7.30 (d, J = 8.4 Hz, 1H), 7.14 – 7.11 (m, 1H), 5.16 (q, J = 7.0 Hz, 1H), 3.68 (s, 3H), 1.67 (d, J = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 192.10, 158.52, 154.40, 143.60, 133.66, 133.11, 132.80, 132.41, 130.44, 130.27, 128.17, 123.73, 113.61, 46.61, 29.25, 15.04; HRMS (ESI+): $[M + Na]^+$ Calculated for $C_{16}H_{14}N_2O_2SNa$: 321.0668, Found 321.0667.

3-(1-(Furan-2-yl)-1-oxopropan-2-yl)-1-methylquinoxalin-2(1H)-one (3l)



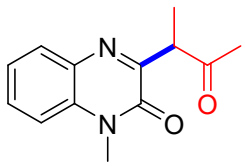
Obtained as white solid (31 mg, 55% yield); m.p. 136-137 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.90 (dd, J = 8.0, 1.6 Hz, 1H), 7.58 – 7.53 (m, 2H), 7.37 – 7.33 (m, 1H), 7.33 – 7.29 (m, 2H), 6.53 (dd, J = 3.5, 1.7 Hz, 1H), 5.09 (q, J = 7.0 Hz, 1H), 3.69 (s, 3H), 1.64 (d, J = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 188.25, 158.61, 154.39, 152.15, 146.38, 133.12, 132.79, 130.39, 130.19, 123.70, 117.65, 113.59, 112.32, 45.74, 29.21, 14.27; HRMS (ESI+): $[M+Na]^+$ Calculated for $C_{16}H_{14}N_2O_3Na$: 305.0897, Found 305.0899.

3-(1-Cyclohexyl-1-oxopropan-2-yl)-1-methylquinoxalin-2(1H)-one (3m)



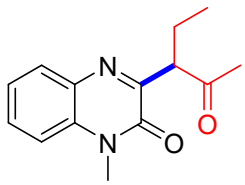
Obtained as white solid (38 mg, 63% yield); m.p. 96-97 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.87 (d, J = 7.9 Hz, 1H), 7.54 (t, J = 7.7 Hz, 1H), 7.34 (t, J = 7.7 Hz, 1H), 7.30 (d, J = 8.4 Hz, 1H), 4.57 (q, J = 7.0 Hz, 1H), 3.68 (s, 3H), 2.68 (tt, J = 11.5, 3.5 Hz, 1H), 2.03 (d, J = 13.0 Hz, 1H), 1.95 (d, J = 12.4 Hz, 1H), 1.82 – 1.77 (m, 2H), 1.66 (d, J = 10.9 Hz, 1H), 1.50 (d, J = 7.0 Hz, 3H), 1.46 – 1.30 (m, 2H), 1.29 – 1.16 (m, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 212.67, 159.14, 154.48, 133.08, 132.67, 130.24, 130.10, 123.65, 113.58, 50.36, 48.38, 29.17, 28.68, 25.88, 25.67, 14.00; HRMS (ESI+): $[M+Na]^+$ Calculated for $C_{18}H_{22}N_2O_2Na$: 321.1573, Found 321.1577.

1-Methyl-3-(3-oxobutan-2-yl)quinoxalin-2(1H)-one (3n)



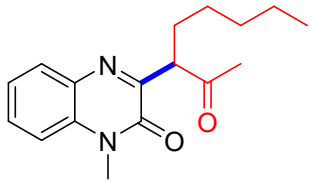
Obtained as white solid (24 mg, 52% yield); m.p. 78-79 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.88 (dd, J = 8.0, 1.5 Hz, 1H), 7.59 – 7.53 (m, 1H), 7.38 – 7.34 (m, 1H), 7.32 (d, J = 8.4 Hz, 1H), 4.39 (q, J = 7.1 Hz, 1H), 3.70 (s, 3H), 2.34 (s, 3H), 1.53 (d, J = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 207.52, 158.89, 154.53, 133.10, 132.70, 130.29, 130.28, 123.77, 113.64, 50.82, 29.20, 29.20, 13.65; HRMS (ESI): $[M+Na]^+$ Calculated for $C_{13}H_{14}N_2O_2Na$: 253.0947, Found 253.0964.

1-Methyl-3-(2-oxopentan-3-yl)quinoxalin-2(1H)-one (3o)



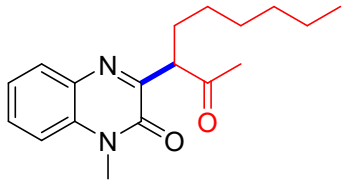
Obtained as white solid (29 mg, 59% yield); m.p. 80-81 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.89 (dd, J = 8.0, 1.5 Hz, 1H), 7.59 – 7.54 (m, 1H), 7.38 – 7.34 (m, 1H), 7.32 (d, J = 8.0 Hz, 1H), 4.31 (t, J = 7.0 Hz, 1H), 3.71 (s, 3H), 2.33 (s, 3H), 2.16 – 2.04 (m, 2H), 1.02 (t, J = 7.4 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 206.92, 157.80, 154.76, 133.01, 132.72, 130.37, 130.28, 123.75, 113.61, 57.74, 30.13, 29.23, 22.12, 12.42; HRMS (ESI): $[M+Na]^+$ Calculated for $C_{14}H_{16}N_2O_2Na$: 267.1104, Found 267.1115.

1-Methyl-3-(2-oxooctan-3-yl)quinoxalin-2(1H)-one (3p)



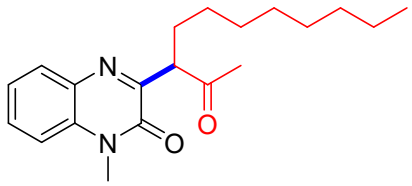
Obtained as white solid (31 mg, 54% yield); m.p. 110-111 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.89 (d, J = 7.8 Hz, 1H), 7.56 (t, J = 7.6 Hz, 1H), 7.36 (t, J = 7.5 Hz, 1H), 7.32 (d, J = 8.4 Hz, 1H), 4.37 (t, J = 7.0 Hz, 1H), 3.70 (s, 3H), 2.32 (s, 3H), 2.09 (dq, J = 15.1, 7.7, 6.8 Hz, 1H), 2.04 – 1.96 (m, 1H), 1.41 – 1.29 (m, 6H), 0.88 (t, J = 6.9 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 206.98, 157.91, 154.74, 133.00, 132.71, 130.37, 130.26, 123.74, 113.61, 56.23, 31.84, 30.05, 29.24, 28.74, 27.44, 22.43, 14.03; HRMS (ESI): $[M+Na]^+$ Calculated for $C_{17}H_{22}N_2O_2Na$: 309.1573, Found 309.1578.

1-Methyl-3-(2-oxononan-3-yl)quinoxalin-2(1H)-one (3q)



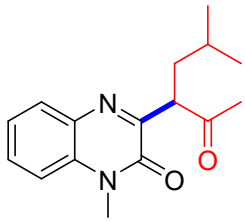
Obtained as white solid (34 mg, 56% yield); m.p. 121-122 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.89 (dd, J = 8.0, 1.5 Hz, 1H), 7.58–7.54 (m, 1H), 7.38–7.34 (m, 1H), 7.32 (d, J = 8.4 Hz, 1H), 4.39–4.35 (m, 1H), 3.71 (s, 3H), 2.32 (s, 3H), 2.13–2.05 (m, 1H), 2.04–1.96 (m, 1H), 1.37 (dd, J = 7.4, 4.3 Hz, 4H), 1.31–1.26 (m, 4H), 0.89–0.85 (m, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 209.96, 157.94, 154.74, 133.01, 132.72, 130.39, 130.25, 123.74, 113.60, 56.25, 31.60, 30.05, 29.33, 29.24, 28.80, 27.74, 22.56, 14.07. HRMS (ESI): $[M+Na]^+$ Calculated for $C_{18}H_{24}N_2O_2Na$: 323.1730, Found 323.173.

1-Methyl-3-(2-oxoundecan-3-yl)quinoxalin-2(1H)-one (3r)



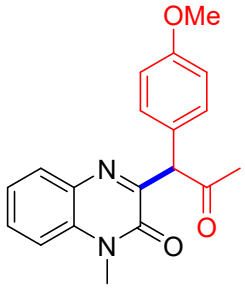
Obtained as white solid (33 mg, 51% yield); m.p. 147-148 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.89 (d, J = 7.9 Hz, 1H), 7.58–7.54 (m, 1H), 7.36 (t, J = 7.6 Hz, 1H), 7.32 (d, J = 8.4 Hz, 1H), 4.37 (t, J = 7.0 Hz, 1H), 3.70 (s, 3H), 2.32 (s, 3H), 2.09 (dq, J = 14.8, 7.3 Hz, 1H), 2.00 (dq, J = 14.0, 6.8 Hz, 1H), 1.43–1.30 (m, 6H), 1.30–1.26 (m, 6H), 0.87 (t, J = 6.7 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 206.96, 157.94, 154.74, 133.01, 132.73, 130.39, 130.25, 123.73, 113.59, 56.25, 31.86, 30.05, 29.71, 29.66, 29.36, 29.24, 28.80, 27.78, 22.66, 14.11; HRMS (ESI): $[M+Na]^+$ Calculated for $C_{20}H_{28}N_2O_2Na$: 351.2043, Found 351.2042.

1-Methyl-3-(5-methyl-2-oxohexan-3-yl)quinoxalin-2(1H)-one (3s)



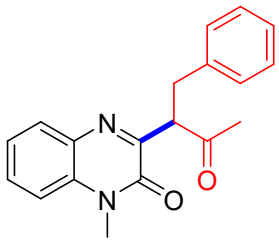
Obtained as white solid (33 mg, 60% yield); m.p. 103-104 °C. ^{1}H NMR (500 MHz, $CDCl_3$) 7.89 (dd, J = 8.0, 1.5 Hz, 1H), 7.58 – 7.54 (m, 1H), 7.38 – 7.34 (m, 1H), 7.32 (d, J = 8.4 Hz, 1H), 4.49 (dd, J = 8.1, 5.9 Hz, 1H), 3.71 (s, 3H), 2.31 (s, 3H), 2.06 (ddd, J = 14.2, 8.1, 6.4 Hz, 1H), 1.83 (ddd, J = 13.6, 7.7, 6.0 Hz, 1H), 1.66 (dd, J = 13.4, 6.7 Hz, 1H), 0.97 (d, J = 6.6 Hz, 3H), 0.95 (d, J = 6.5 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 206.86, 158.97, 154.74, 133.00, 132.71, 130.39, 130.26, 123.74, 113.60, 54.26, 37.67, 29.81, 29.25, 26.24, 22.90, 22.37; HRMS (ESI): $[M+Na]^+$ Calculated for $C_{16}H_{20}N_2O_2Na$: 295.1417, Found 295.1414.

3-(1-(4-Methoxyphenyl)-2-oxopropyl)-1-methylquinoxalin-2(1H)-one (3t)



Obtained as white solid (34 mg, 53% yield); m.p. 138-139 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84 (d, J = 7.8 Hz, 1H), 7.48 – 7.45 (m, 1H), 7.34 (d, J = 8.5 Hz, 2H), 7.29 – 7.26 (m, 1H), 7.21 (d, J = 8.7 Hz, 1H), 6.76 (d, J = 8.5 Hz, 2H), 4.17 (s, 1H), 3.69 (s, 3H), 3.60 (s, 3H), 1.18 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 204.76, 159.21, 157.50, 154.58, 133.13, 132.58, 131.53, 130.56, 130.33, 126.17, 123.67, 114.01, 113.56, 61.67, 55.24, 29.65, 29.28; HRMS (ESI): $[M+Na]^+$ Calculated for $C_{19}H_{18}N_2O_3Na$: 345.1210, Found 345.1203.

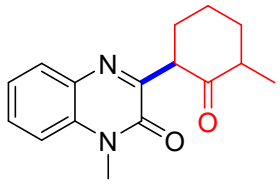
1-Methyl-3-(3-oxo-1-phenylbutan-2-yl)quinoxalin-2(1H)-one (3u)



Obtained as white solid (42 mg, 69% yield); m.p. 141-142 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.92 (dd, J = 8.1, 1.5 Hz, 1H), 7.56 (ddd, J = 8.5, 7.2, 1.5 Hz, 1H), 7.39 – 7.35 (m, 1H), 7.30 (d, J = 8.9 Hz, 2H), 7.29 – 7.27 (m, 2H), 7.26 – 7.24 (m, 1H), 7.20 – 7.16 (m, 1H), 4.76 (dd, J = 8.1, 6.7 Hz, 1H), 3.68 (s, 3H), 3.44 (dd, J = 13.9, 6.7 Hz, 1H), 3.31 (dd, J = 13.9, 8.1 Hz, 1H), 2.16 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ

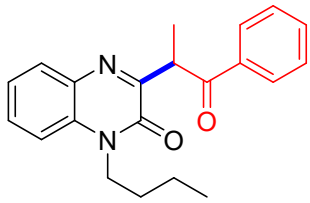
206.87, 157.11, 154.64, 139.38, 133.00, 132.65, 130.40, 130.39, 129.17, 128.45, 126.34, 123.82, 113.62, 57.67, 35.02, 31.07, 29.22; HRMS (ESI): $[M+Na]^+$ Calculated for $C_{19}H_{18}N_2O_3Na$: 329.1260, Found 329.1261.

1-Methyl-3-(3-methyl-2-oxocyclohexyl)quinoxalin-2(1H)-one (3v)



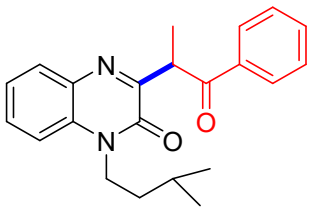
Obtained as white solid 1:1 dr (39 mg, 72% yield); m.p. 127-128 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.92 – 6.88 (m, 1H), 6.85 (dd, J = 8.0, 1.3 Hz, 1H), 6.79 – 6.74 (m, 1H), 6.66 (dd, J = 7.8, 1.4 Hz, 1H), 4.57 – 4.53 (m, 1H), 3.35 (s, 3H), 2.53 (tq, J = 11.9, 5.3 Hz, 1H), 2.13 (dq, J = 13.3, 3.0 Hz, 1H), 2.03 (dq, J = 9.7, 2.8 Hz, 1H), 1.87 – 1.79 (m, 3H), 1.38 (qd, J = 12.9, 5.0 Hz, 1H), 1.04 (d, J = 6.4 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) Mixture of diastereomers is observed. Ratio: 5/5. Major diastereomer: δ 214.64, 166.93, 135.27, 129.96, 127.37, 123.85, 118.60, 114.29, 113.63, 55.40, 53.28, 45.76, 37.18, 28.95, 24.87, 14.38; Major diastereomer: 214.64, 166.93, 135.27, 129.96, 127.37, 123.85, 118.60, 114.29, 113.63, 55.40, 53.28, 45.76, 37.18, 28.70, 24.87, 14.38; HRMS (ESI): Calculated for $C_{16}H_{18}N_2O_2$ $[M+Na]^+$ 293.1260, Found 293.1255.

1-Butyl-3-(1-oxo-1-phenylpropan-2-yl)quinoxalin-2(1H)-one (3w)



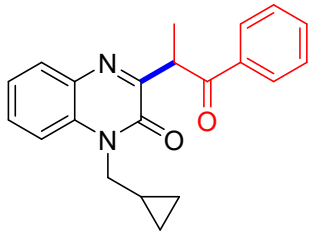
Obtained as white solid (53 mg, 79% yield); m.p. 97-98 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.07 (dd, J = 8.2, 1.4 Hz, 2H), 7.88 (dd, J = 8.0, 1.6 Hz, 1H), 7.54 – 7.50 (m, 2H), 7.44 (t, J = 7.6 Hz, 2H), 7.33 – 7.28 (m, 2H), 5.31 (q, J = 7.0 Hz, 1H), 4.30 – 4.23 (m, 1H), 4.17 (dt, J = 13.6, 8.0 Hz, 1H), 1.73 –1.67 (m, J = 9.6, 5.3, 1.8 Hz, 2H), 1.63 (d, J = 7.0 Hz, 3H), 1.42 (q, J = 7.5 Hz, 2H), 0.96 (t, J = 7.4 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 199.62, 159.26, 154.09, 136.49, 133.11, 132.87, 132.25, 130.55, 130.03, 128.64, 128.60, 123.44, 113.61, 45.17, 42.30, 29.30, 20.21, 14.72, 13.7; HRMS (ESI+): $[M+Na]^+$ Calculated for $C_{21}H_{22}N_2O_2Na$: 357.1573, Found 357.1570.

1-Isopentyl-3-(1-oxo-1-phenylpropan-2-yl)quinoxalin-2(1H)-one (3x)



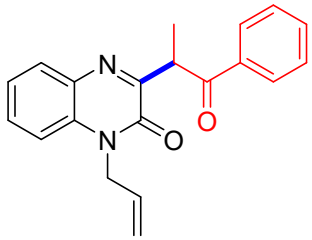
Obtained as white solid 1:1 dr (54 mg, 78% yield); m.p. 102-103 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.05 – 7.97 (m, 2H), 7.62 – 7.55 (m, 1H), 7.49 (t, J = 7.8 Hz, 2H), 6.91 (ddd, J = 18.0, 7.8, 1.3 Hz, 2H), 6.79 (td, J = 8.4, 1.4 Hz, 1H), 6.76 (dd, J = 7.8, 1.4 Hz, 1H), 4.48 (qd, J = 7.2, 2.4 Hz, 1H), 3.96 (dddd, J = 22.6, 15.7, 13.9, 6.7 Hz, 2H), 1.70 (dp, J = 13.3, 6.7 Hz, 1H), 1.57 (dtd, J = 8.9, 6.8, 1.9 Hz, 2H), 1.31 (d, J = 7.2 Hz, 3H), 1.00 (t, J = 6.5 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) Mixture of diastereomers is observed. Ratio: 5/5. δ 199.59, 159.23, 154.01, 136.45, 133.14, 132.89, 132.23, 130.58, 130.06, 128.64, 128.62, 123.44, 113.50, 45.14, 41.17, 35.77, 26.53, 22.48, 22.46, 14.74; Minor diastereomer: δ 199.6, 159.2, 154.0, 136.5, 133.1, 132.9, 132.2, 130.6, 130.1, 128.6, 128.6, 123.4, 113.5, 45.1, 41.2, 35.8, 26.5, 22.5, 22.5, 14.7; HRMS (ESI+): $[M+Na]^+$ Calculated for $C_{22}H_{24}N_2O_2Na$: 371.1730, Found 371.1731.

1-(Cyclopropylmethyl)-3-(1-oxo-1-phenylpropan-2-yl)quinoxalin-2(1H)-one (3y)



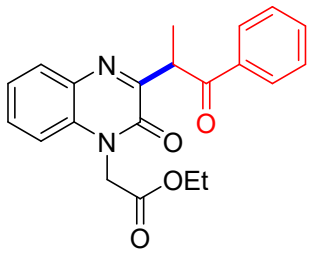
Obtained as white solid (45 mg, 68% yield); m.p. 113-114 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.06 (dd, J = 8.2, 1.3 Hz, 2H), 7.88 (d, J = 8.0 Hz, 1H), 7.52 (dt, J = 7.6, 4.6 Hz, 2H), 7.46 – 7.39 (m, 3H), 7.32 (t, J = 7.5 Hz, 1H), 5.31 (q, J = 6.9 Hz, 1H), 4.18 (h, J = 7.4 Hz, 2H), 1.64 (d, J = 7.0 Hz, 3H), 1.28 – 1.23 (m, 1H), 0.53 – 0.46 (m, 4H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 199.56, 159.49, 154.37, 136.52, 133.04, 132.86, 132.50, 130.52, 130.00, 128.64, 128.59, 123.45, 113.90, 46.19, 45.30, 14.74, 9.68, 4.19, 3.97; HRMS (ESI+): $[M+Na]^+$ Calculated for $C_{21}H_{20}N_2O_2Na$: 355.1417, Found 355.1419.

1-Allyl-3-(1-oxo-1-phenylpropan-2-yl)quinoxalin-2(1H)-one (3z)



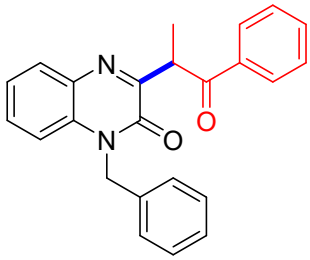
Obtained as white solid (34 mg, 54% yield); m.p. 131-132 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.09 – 8.05 (m, 2H), 7.88 (dd, J = 8.0, 1.5 Hz, 1H), 7.54 – 7.47 (m, 2H), 7.44 (t, J = 7.6 Hz, 2H), 7.33 – 7.29 (m, 1H), 7.27 – 7.24 (m, 1H), 5.89 (ddd, J = 22.2, 10.3, 5.0 Hz, 1H), 5.33 (q, J = 7.0 Hz, 1H), 5.22 (d, J = 10.4 Hz, 1H), 5.11 – 5.05 (m, 1H), 4.93 (dd, J = 16.4, 5.0 Hz, 1H), 4.81 (dd, J = 16.3, 5.0 Hz, 1H), 1.64 (d, J = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 199.65, 159.28, 153.99, 136.45, 132.99, 132.92, 132.28, 130.47, 130.40, 130.06, 128.65, 128.61, 123.66, 117.94, 114.17, 45.18, 44.59, 14.70; HRMS (ESI+): $[M+Na]^+$ Calculated for $C_{20}H_{18}N_2O_2Na$: 341.1260, Found 341.1262.

Ethyl-2-(2-oxo-3-(1-oxo-1-phenylpropan-2-yl)quinoxalin-1(2H)-yl)acetate (3aa)



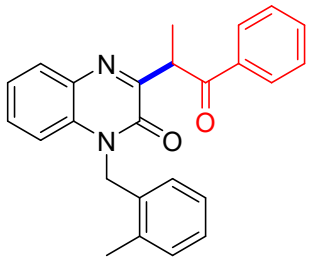
Obtained as white solid (49 mg, 67% yield), m.p. 133-134 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.98 (d, J = 7.2 Hz, 2H), 7.81 (d, J = 7.8 Hz, 1H), 7.45 (t, J = 7.4 Hz, 1H), 7.39 (dt, J = 20.3, 7.4 Hz, 3H), 7.25 (t, J = 7.5 Hz, 1H), 7.00 – 6.96 (m, 1H), 5.23 (q, J = 7.0 Hz, 1H), 5.07 (d, J = 17.2, 1.3 Hz, 1H), 4.75 (d, J = 17.3 Hz, 1H), 4.13 (qd, J = 7.1, 2.1 Hz, 2H), 1.56 (d, J = 7.0 Hz, 3H), 1.15 (t, J = 7.1 Hz, 3H); ^{13}C NMR (126 MHz,$CDCl_3$) δ 199.53, 166.93, 159.01, 154.04, 136.35, 132.99, 132.87, 132.22, 130.64, 130.31, 128.67, 128.61, 123.97, 113.04, 62.06, 45.18, 43.66, 14.65, 14.07; HRMS (ESI+): $[M+Na]^+$ Calculated for $C_{21}H_{20}N_2O_4Na$: 387.1315, Found 387.1317.

1-Benzyl-3-(1-oxo-1-phenylpropan-2-yl)quinoxalin-2(1H)-one (3ab)



Obtained as white solid (53 mg, 72% yield); m.p. 155-151 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.11 – 8.05 (m, 2H), 7.88 (dd, J = 8.0, 1.6 Hz, 1H), 7.55 – 7.51 (m, 1H), 7.44 (dd, J = 8.4, 7.1 Hz, 2H), 7.39 (ddd, J = 8.5, 7.3, 1.6 Hz, 1H), 7.30 – 7.25 (m, 3H), 7.24 – 7.19 (m, 2H), 7.12 (d, J = 7.3 Hz, 2H), 5.53 – 5.40 (m, 2H), 5.35 (q, J = 7.0 Hz, 1H), 1.68 (d, J = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 199.62, 159.44, 154.51, 136.57, 135.05, 133.10, 132.90, 132.36, 130.40, 130.14, 128.93, 128.66, 128.62, 127.66, 126.69, 123.74, 114.43, 45.95, 45.53, 14.73; HRMS (ESI+): $[M+Na]^+$ Calculated for $C_{24}H_{20}N_2O_2Na$: 391.1417, Found 391.1410.

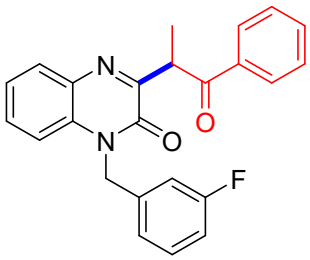
1-(2-Methylbenzyl)-3-(1-oxo-1-phenylpropan-2-yl)quinoxalin-2(1H)-one (3ac)



Obtained as white solid (53 mg, 69% yield); m.p. 187-188 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.08 – 8.04 (m, 2H), 7.91 (dd, J = 8.0, 1.6 Hz, 1H), 7.54 – 7.50 (m, 1H), 7.43 (t, J = 8.4, 7.0 Hz, 2H), 7.39 – 7.34 (m, 1H), 7.31 – 7.27 (m, 1H), 7.20 (d, J = 7.5 Hz, 1H), 7.15 – 7.11 (m, 1H), 7.00 – 6.96 (m, 2H), 6.46 (d, J = 7.7 Hz, 1H), 5.47 – 5.38 (m, 2H), 5.35 (dd, J = 8.0, 6.1 Hz, 1H), 2.42 (s, 3H), 1.68 (d, J = 7.0 Hz, 3H);

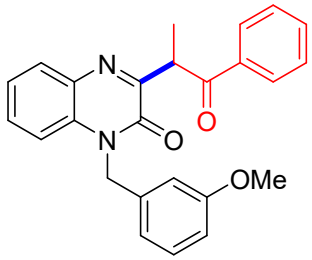
^{13}C NMR (126 MHz, $CDCl_3$) δ 199.59, 159.42, 154.47, 136.56, 134.90, 133.11, 132.88, 132.46, 132.22, 130.55, 130.39, 130.21, 128.64, 128.61, 127.33, 126.47, 124.41, 123.80, 114.51, 45.41, 44.06, 19.20, 14.70; HRMS (ESI+): $[M+Na]^+$ Calculated for $C_{25}H_{22}N_2O_2Na$: 405.1573, Found 405.1586.

1-(3-Fluorobenzyl)-3-(1-oxo-1-phenylpropan-2-yl)quinoxalin-2(1H)-one (3ad)



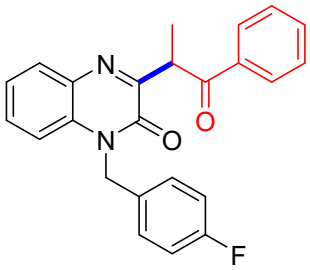
Obtained as white solid (46 mg, 60% yield); m.p. 132-133 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.10 – 8.04 (m, 2H), 7.90 (dd, J = 7.9, 1.5 Hz, 1H), 7.55 – 7.51 (m, 1H), 7.45 (t, J = 7.7 Hz, 2H), 7.43 – 7.39 (m, 1H), 7.33 – 7.28 (m, 1H), 7.27 – 7.22 (m, 1H), 7.16 (d, J = 8.3 Hz, 1H), 6.93 (td, J = 8.3, 2.3 Hz, 2H), 6.82 (d, J = 9.5 Hz, 1H), 5.52 – 5.38 (m, 2H), 5.35 (q, J = 7.0 Hz, 1H), 1.68 (d, J = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 199.57, 164.08, 162.12, 159.41, 154.42, 137.59 (d, J = 7.0 Hz), 136.51, 133.10, 132.96, 132.18, 130.60, 130.54 (d, J = 2.8 Hz), 130.22, 128.84 – 128.47 (m), 123.91, 122.29 (d, J = 3.1 Hz), 114.74 (d, J = 21.1 Hz), 114.14, 113.78 (d, J = 22.3 Hz), 45.52, 45.48, 14.68; ^{19}F NMR (471 MHz, $CDCl_3$) δ -111.96; HRMS (ESI+): $[M+Na]^+$ Calculated for $C_{24}H_{19}FN_2O_2Na$: 409.1323, Found 409.1334.

1-(3-Methoxybenzyl)-3-(1-oxo-1-phenylpropan-2-yl)quinoxalin-2(1H)-one (3ae)



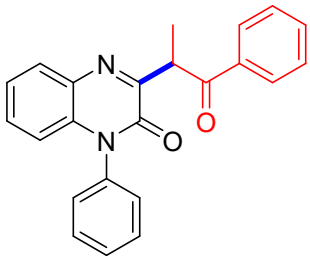
Obtained as white solid (49 mg, 62% yield); m.p. 147-148 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.08 (d, J = 7.5Hz, 2H), 7.87 (dd, J = 8.0, 1.6 Hz, 1H), 7.54 – 7.50 (m, 1H), 7.44 (t, J = 7.6 Hz, 2H), 7.40 – 7.36 (m, 1H), 7.28 – 7.24 (m, 1H), 7.21 (d, J = 8.4 Hz, 1H), 7.17 (t, J = 8.0 Hz, 1H), 6.76 (dd, J = 8.2, 3.0 Hz, 1H), 6.70 (d, J = 7.6 Hz, 2H), 5.47 – 5.38 (m, 2H), 5.36 (q, J = 7.0 Hz, 1H), 3.71 (s, 3H), 1.68 (d, J = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 199.67, 160.05, 159.40, 154.51, 136.66, 136.50, 133.07, 132.94, 132.37, 130.38, 130.16, 129.99, 128.69, 128.62, 123.76, 118.89, 114.44, 112.91, 112.53, 55.20, 45.88, 45.45, 14.71; HRMS (ESI+): $[M+Na]^+$ Calculated for $C_{25}H_{22}N_2O_3Na$: 421.1523; Found 421.1519.

1-(4-Fluorobenzyl)-3-(1-oxo-1-phenylpropan-2-yl)quinoxalin-2(1H)-one (3af)



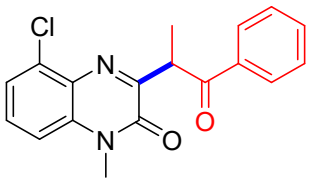
Obtained as white solid (49 mg, 63% yield); m.p. 177-178 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.11 – 8.05 (m, 2H), 7.89 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.56 – 7.52 (m, 1H), 7.45 (t, *J* = 7.7 Hz, 2H), 7.43 – 7.39 (m, 1H), 7.32 – 7.28 (m, 1H), 7.19 (d, *J* = 8.4 Hz, 1H), 7.14 – 7.09 (m, 2H), 6.95 (t, *J* = 8.6 Hz, 2H), 5.41 (q, *J* = 15.7 Hz, 2H), 5.33 (q, *J* = 7.0 Hz, 1H), 1.68 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 199.68, 163.15, 161.19, 159.41, 154.46, 136.51, 133.11, 132.95, 132.20, 130.80 (d, *J* = 3.2 Hz), 130.53, 130.18, 128.65 (d, *J* = 7.5 Hz), 128.54 (d, *J* = 8.2 Hz), 123.86, 115.88 (d, *J* = 21.6 Hz), 114.19, 45.58, 45.27, 14.68; ^{19}F NMR (471 MHz, $CDCl_3$) δ -114.40; HRMS (ESI+): $[M+Na]^+$ Calculated for $C_{24}H_{19}FN_2O_2Na$: 409.1323, Found 409.1327.

3-(1-Oxo-1-phenylpropan-2-yl)-1-phenylquinoxalin-2(1H)-one (3ag)



Obtained as white solid (50 mg, 71% yield); m.p. 190-191 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.11 – 8.04 (m, 2H), 7.96 – 7.89 (m, 1H), 7.59 – 7.55 (m, 2H), 7.51 (td, *J* = 7.3, 1.5 Hz, 2H), 7.43 (t, *J* = 7.6 Hz, 2H), 7.34 – 7.29 (m, 2H), 7.26 (ddt, *J* = 9.6, 7.2, 2.2 Hz, 2H), 6.71 – 6.64 (m, 1H), 5.36 (q, *J* = 7.0 Hz, 1H), 1.67 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 199.75, 159.83, 135.66, 133.91, 132.95, 132.71, 130.34, 130.22, 129.96, 129.80, 129.47, 128.71, 128.62, 128.39, 128.08, 123.88, 115.42, 44.92, 14.81; HRMS (ESI+): $[M+Na]^+$ Calculated for $C_{23}H_{18}N_2O_2Na$: 377.1260, Found 377.1266.

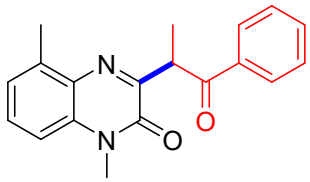
5-Chloro-1-methyl-3-(1-oxo-1-phenylpropan-2-yl)quinoxalin-2(1H)-one (3ah)



Obtained as white solid (47 mg, 72% yield); m.p. 147-148 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.11 – 8.07 (m, 2H), 7.58 – 7.54 (m, 1H), 7.50 – 7.46 (m, 2H), 7.45 – 7.40 (m, 2H), 7.20 (dd, *J* = 6.4, 3.2 Hz, 1H), 5.25 (q, *J* = 7.0 Hz, 1H), 3.65 (s, 3H), 1.69 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 199.88, 159.54, 154.11, 136.37, 135.28, 134.59, 133.02, 130.07, 129.43, 128.71, 128.65, 124.64, 112.48, 45.87, 29.57,

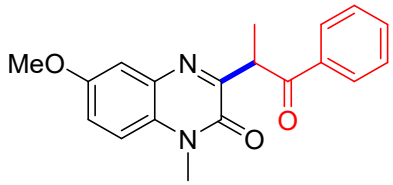
14.46; HRMS (ESI+): $[M+Na]^+$ Calculated for $C_{18}H_{15}ClN_2O_2Na$: 349.0714, Found 349.0711.

1,5-Dimethyl-3-(1-oxo-1-phenylpropan-2-yl)quinoxalin-2(1H)-one (3ai)



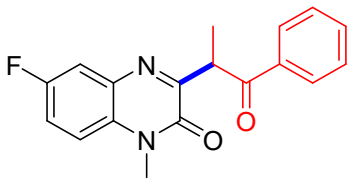
Obtained as white solid (43 mg, 70% yield); m.p. 128-129 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.07 (d, J = 7.6 Hz, 2H), 7.52 (t, J = 7.2 Hz, 1H), 7.45 (t, J = 7.6 Hz, 2H), 7.39 (t, J = 7.9 Hz, 1H), 7.17 (d, J = 7.4 Hz, 1H), 7.11 (d, J = 8.4 Hz, 1H), 5.28 (q, J = 7.0 Hz, 1H), 3.65 (d, J = 0.7 Hz, 3H), 2.63 (s, 3H), 1.64 (d, J = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 200.06, 157.32, 154.28, 139.16, 136.63, 133.18, 132.83, 131.24, 129.88, 128.64, 128.56, 124.98, 111.47, 45.38, 29.33, 17.39, 14.64; HRMS (ESI+): $[M+Na]^+$ Calculated for $C_{19}H_{18}N_2O_2Na$: 329.1260; Found 329.1273.

6-Methoxy-1-methyl-3-(1-oxo-1-phenylpropan-2-yl)quinoxalin-2(1H)-one (3aj)



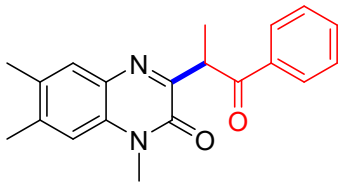
Obtained as white solid (48 mg, 75% yield); m.p. 13-138 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.09 – 8.06 (m, 2H), 7.55 – 7.51 (m, 1H), 7.45 (t, J = 7.7 Hz, 2H), 7.35 (d, J = 2.9 Hz, 1H), 7.21 (d, J = 9.1 Hz, 1H), 7.15 (dd, J = 9.1, 2.8 Hz, 1H), 5.35 (q, J = 7.0 Hz, 1H), 3.87 (s, 3H), 3.67 (s, 3H), 1.62 (d, J = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 199.57, 159.80, 156.02, 154.00, 136.41, 133.59, 132.93, 128.67, 128.63, 127.31, 119.48, 114.50, 111.66, 55.80, 45.07, 29.39, 14.78; HRMS (ESI+): $[M+Na]^+$ Calculated for $C_{19}H_{18}N_2O_3Na$: 342.1210, Found 345.1212.

6-Fluoro-1-methyl-3-(1-oxo-1-phenylpropan-2-yl)quinoxalin-2(1H)-one (3ak)



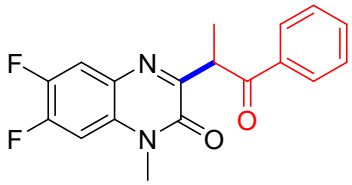
Obtained as white solid (36 mg, 58% yield); m.p. 136-137 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.09 – 8.05 (m, 2H), 7.59 (dd, J = 8.7, 2.8 Hz, 1H), 7.55 (t, J = 7.4 Hz, 1H), 7.47 (t, J = 7.6 Hz, 2H), 7.31 – 7.27 (m, 1H), 7.26 – 7.24 (m, 1H), 5.30 (q, J = 7.0 Hz, 1H), 3.67 (s, 3H), 1.62 (d, J = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 199.54, 160.80, 159.68, 157.75, 154.06, 136.28, 133.37 (d, J = 11.3 Hz), 133.05, 129.76, 128.67 (d, J = 11.0 Hz), 117.86 (d, J = 23.9 Hz), 115.74 (d, J = 22.5 Hz), 114.70 (d, J = 8.6 Hz), 45.29, 29.48, 14.60; ^{19}F NMR (471 MHz, $CDCl_3$) δ -118.89; HRMS (ESI+): $[M+Na]^+$ Calculated for $C_{18}H_{15}FN_2O_2Na$: 333.1010, Found 333.1010.

1,6,7-trimethyl-3-(1-oxo-1-phenylpropan-2-yl)quinoxalin-2(1H)-one (3al)



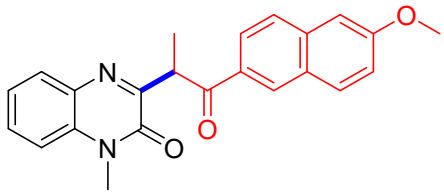
Obtained as white solid (46 mg, 72% yield); m.p. 128-129 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.07 – 8.05 (m, 2H), 7.63 (s, 1H), 7.51 (t, *J* = 7.3 Hz, 1H), 7.43 (t, *J* = 7.6 Hz, 2H), 7.05 (s, 1H), 5.29 (q, *J* = 7.0 Hz, 1H), 3.65 (s, 3H), 2.40 (s, 3H), 2.32 (s, 3H), 1.61 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 199.73, 157.99, 154.42, 139.98, 136.53, 132.81, 132.62, 131.27, 131.06, 130.36, 128.61, 128.59, 114.15, 45.07, 29.16, 20.54, 19.09, 14.72; HRMS (ESI+): $[M+Na]^+$ Calculated for $C_{20}H_{20}N_2O_2Na$: 343.1417, Found 343.1419.

6,7-Difluoro-1-methyl-3-(1-oxo-1-phenylpropan-2-yl)quinoxalin-2(1H)-one (3am)



Obtained as white solid (43 mg, 65% yield); m.p. 134-135 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.07 – 8.05 (m, 2H), 7.70 (dd, *J* = 10.2, 8.1 Hz, 1H), 7.58 – 7.54 (m, 1H), 7.47 (t, *J* = 7.7 Hz, 2H), 7.10 (dd, *J* = 11.3, 7.0 Hz, 1H), 5.27 (q, *J* = 7.0 Hz, 1H), 3.62 (s, 3H), 1.61 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 199.55, 159.79 (d, *J* = 3.6 Hz), 154.02, 152.37 (d, *J* = 14.4 Hz), 150.35 (d, *J* = 14.4 Hz), 147.67 (d, *J* = 13.9 Hz), 145.71 (d, *J* = 14.1 Hz), 136.17, 133.13, 130.32 (d, *J* = 7.5 Hz), 129.03 (dd, *J* = 9.4, 3.0 Hz), 128.68 (d, *J* = 15.9 Hz), 102.29 (d, *J* = 23.0 Hz), 45.16, 29.71, 14.56; ^{19}F NMR (471 MHz, $CDCl_3$) δ -130.73 (d, *J* = 22.3 Hz), -141.95 (d, *J* = 22.5 Hz); HRMS (ESI+): $[M+Na]^+$ Calculated for $C_{18}H_{14}F_2N_2O_2Na$: 351.0916, Found 351.0926.

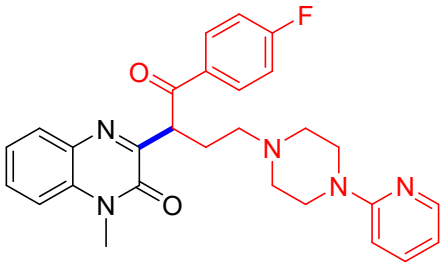
3-(1-(6-Methoxynaphthalen-2-yl)-1-oxopropan-2-yl)-1-methylquinoxalin-2(1H)-one (3an)



Obtained as white solid (46 mg, 62% yield); m.p. 110-111 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.57 (s, 1H), 8.09 (dd, *J* = 8.6, 1.8 Hz, 1H), 7.89 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.85 (d, *J* = 9.0 Hz, 1H), 7.76 (d, *J* = 8.6 Hz, 1H), 7.55 – 7.50 (m, 1H), 7.33 (t, *J* = 7.6 Hz, 1H), 7.28 (d, *J* = 8.5, 1H), 7.17 (dd, *J* = 8.9, 2.5 Hz, 1H), 7.13 (d, *J* = 2.5 Hz, 1H), 5.45 (q, *J* = 7.0 Hz, 1H), 3.93 (s, 3H), 3.67 (s, 3H), 1.69 (d, *J* = 7.0 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.34, 159.66, 159.39, 154.44, 137.27, 133.09, 132.85, 131.81, 131.28, 130.32, 130.10, 130.07, 127.99, 127.21, 125.25, 123.66, 119.54, 113.58, 105.66, 55.41, 45.11, 29.22, 14.90; HRMS (ESI+): $[M+H]^+$ Calculated for $C_{23}H_{20}N_2O_3Na$: 373.1547, Found 373.1556.

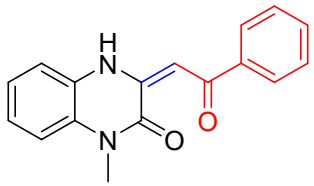
3-(1-(4-Fluorophenyl)-1-oxo-4-(4-(pyridin-2-yl)piperazin-1-yl)butan-2-yl)-1-

methylquinoxalin-2(1H)-one (3ao)



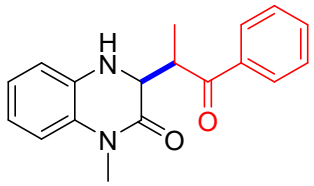
Obtained as white solid (34 mg, 35% yield). m.p. 133-134 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.21 – 8.11 (m, 3H), 7.85 (dd, J = 8.0, 1.5 Hz, 1H), 7.54 – 7.48 (m, 1H), 7.46 – 7.39 (m, 1H), 7.32 (t, J = 7.5 Hz, 1H), 7.25 (s, 1H), 7.10 (t, J = 8.6 Hz, 2H), 6.59 (dd, J = 7.1, 4.9 Hz, 1H), 6.53 (d, J = 8.6 Hz, 1H), 5.47 (t, J = 6.3 Hz, 1H), 3.67 (s, 3H), 3.25 (d, J = 24.1 Hz, 4H), 2.59 – 2.26 (m, 8H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 196.89, 166.65, 164.63, 159.32, 158.20, 154.76, 147.91, 137.40, 133.00, 132.78, 131.30 (d, J = 9.2 Hz), 130.18 (d, J = 4.1 Hz), 123.76, 115.77, 115.60, 113.56, 113.18, 106.92, 56.31, 52.57, 48.40, 44.91, 29.31, 27.31; HRMS (ESI+): $[M+Na]^+$ Calculated for $C_{28}H_{28}FN_5O_2Na$: 508.2119, Found 508.2123.

1-Methyl-3-(2-oxo-2-phenylethylidene)-3,4-dihydroquinoxalin-2(1H)-one (4)



Obtained as yellow solid (24 mg, 76% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ14.03 (s, 1H), 8.06 – 8.02 (m, 2H), 7.54 – 7.50 (m, 1H), 7.49 – 7.46 (m, 2H), 7.24 – 7.19 (m, 4H), 7.03 (s, 1H), 3.67 (s, 3H).

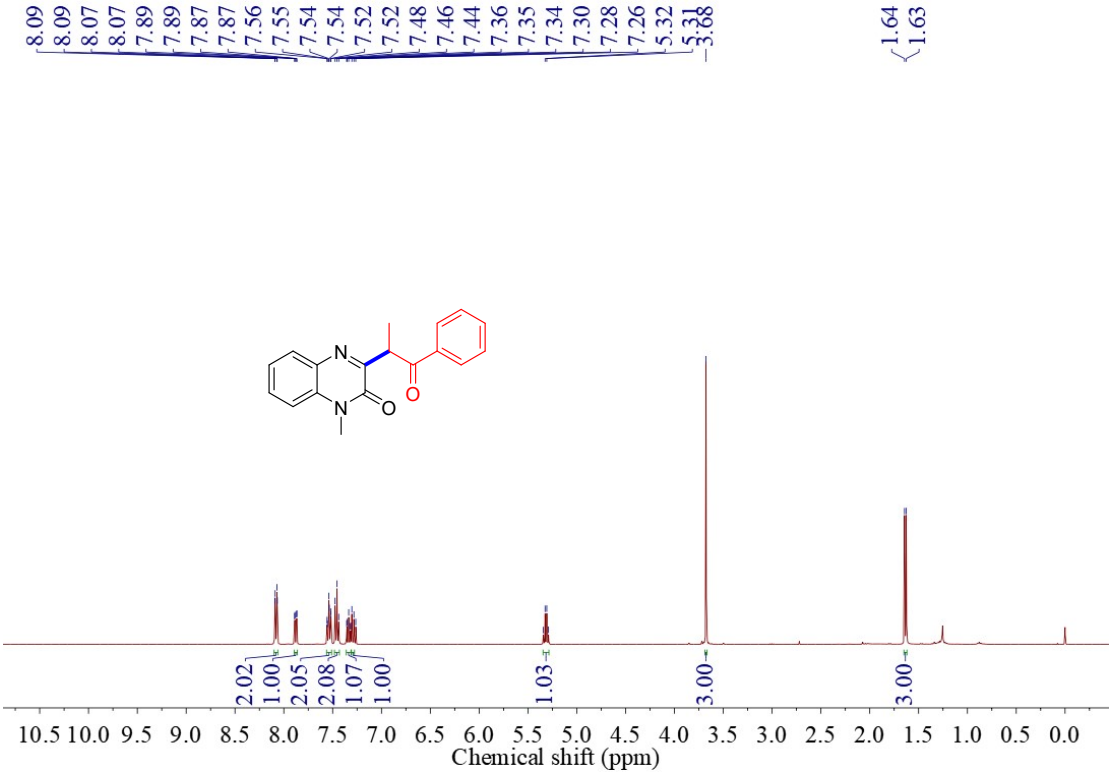
1-Methyl-3-(1-oxo-1-phenylpropan-2-yl)-3,4-dihydroquinoxalin-2(1H)-one (6)



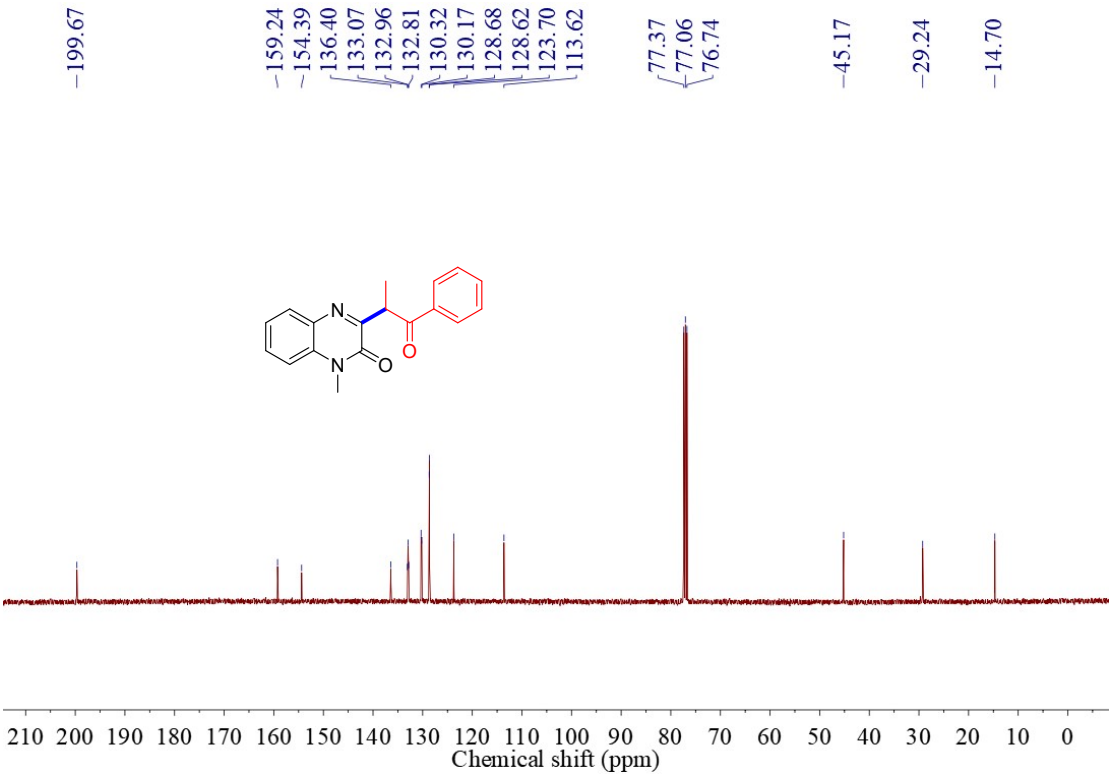
Obtained as white solid (41 mg, 70% yield); m.p. 102-103 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.02 (d, J = 7.4 Hz, 2H), 7.60 (t, J = 7.4 Hz, 1H), 7.50 (t, J = 7.7 Hz, 2H), 6.96 – 6.92 (m, 1H), 6.90 (d, J = 7.9 Hz, 1H), 6.81 (t, J = 7.6 Hz, 1H), 6.77 (d, J = 7.8 Hz, 1H), 4.99 (s, 1H), 4.49 (qd, J = 7.3, 2.4 Hz, 1H), 4.38 (d, J = 2.4 Hz, 1H), 3.39 (s, 3H), 1.32 (d, J = 7.3 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 204.07, 166.42, 135.45, 135.38, 133.59, 128.84, 128.70, 127.82, 123.89, 118.98, 114.44, 114.06, 57.21, 41.95, 29.18, 12.54; HRMS (ESI+): $[M+Na]^+$ Calculated for $C_{18}H_{18}N_2O_2Na$: 317.1260, Found 317.1261.

4.Copies of NMR Spectra

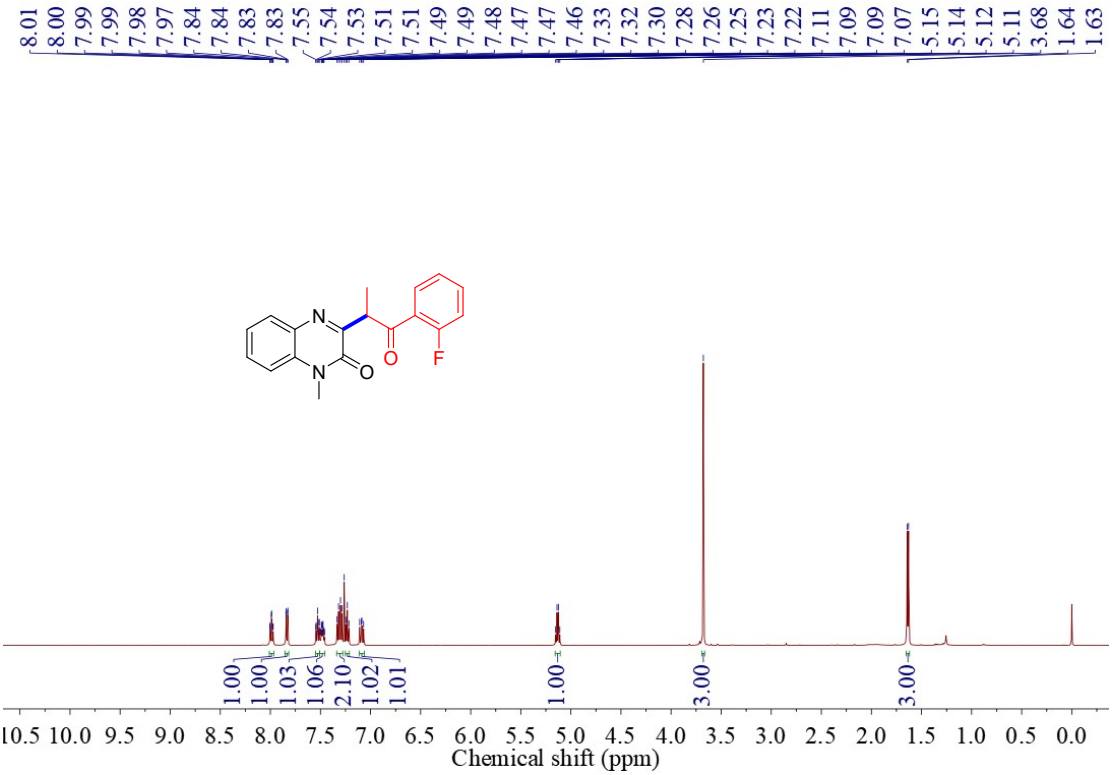
3a ^{1}H NMR



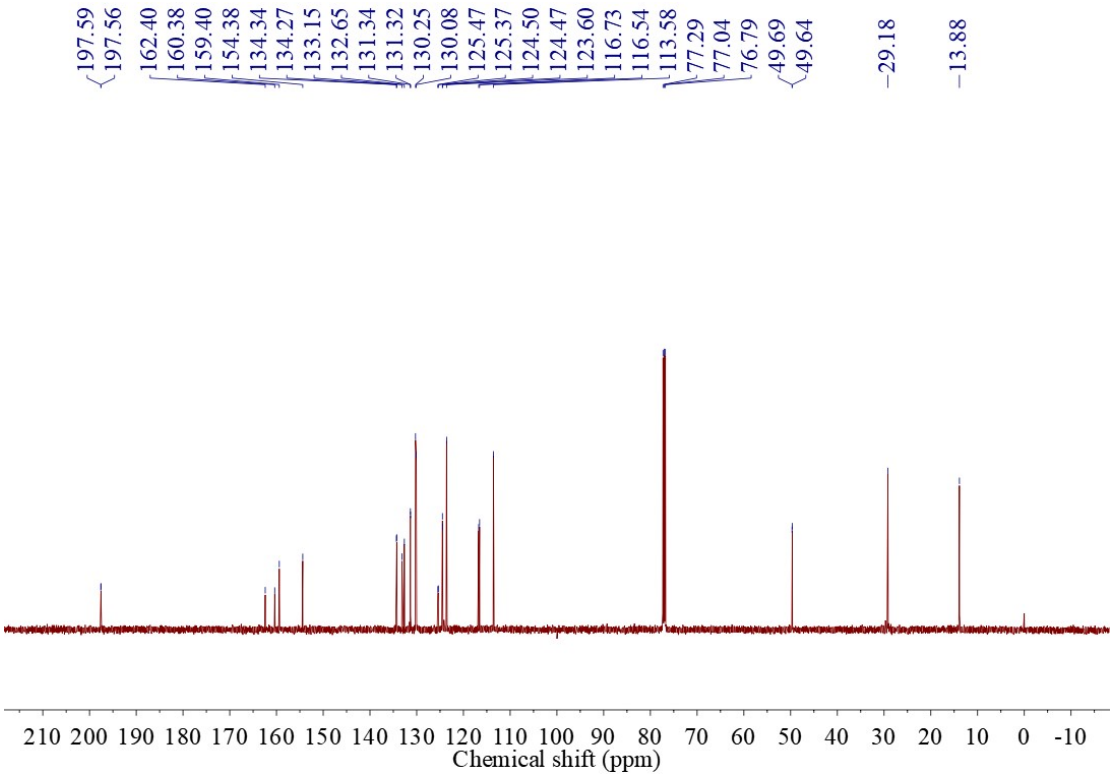
3a ^{13}C NMR



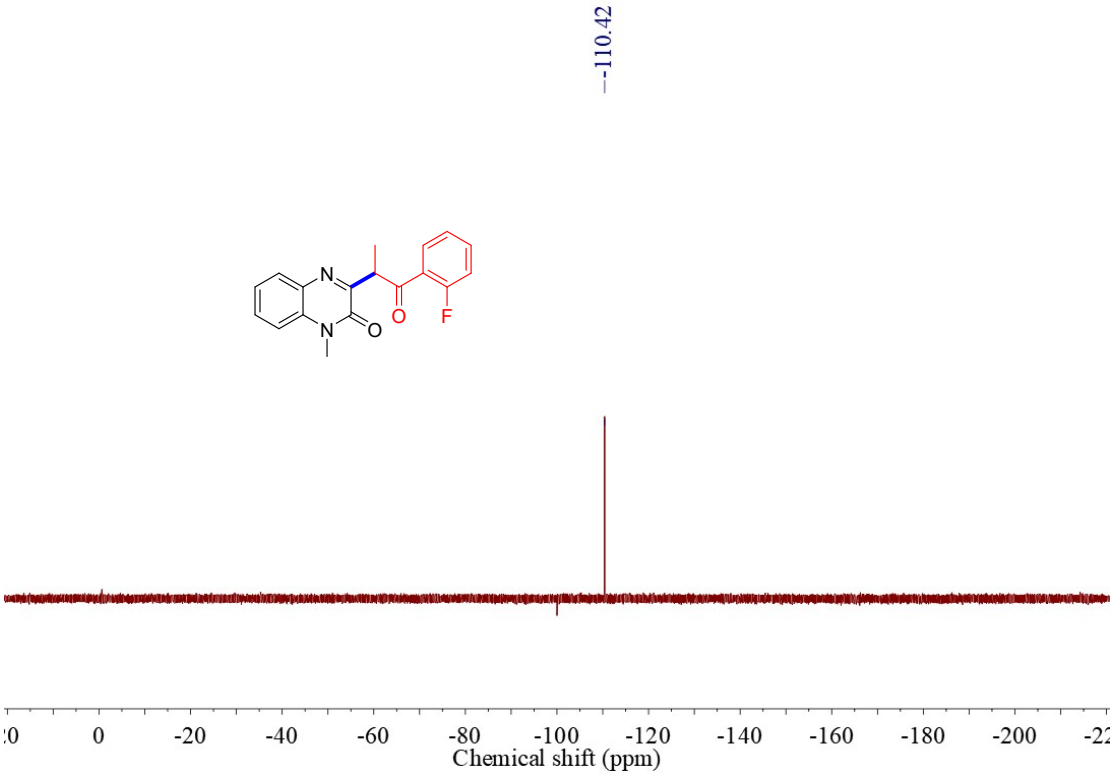
3b ^{1}H NMR



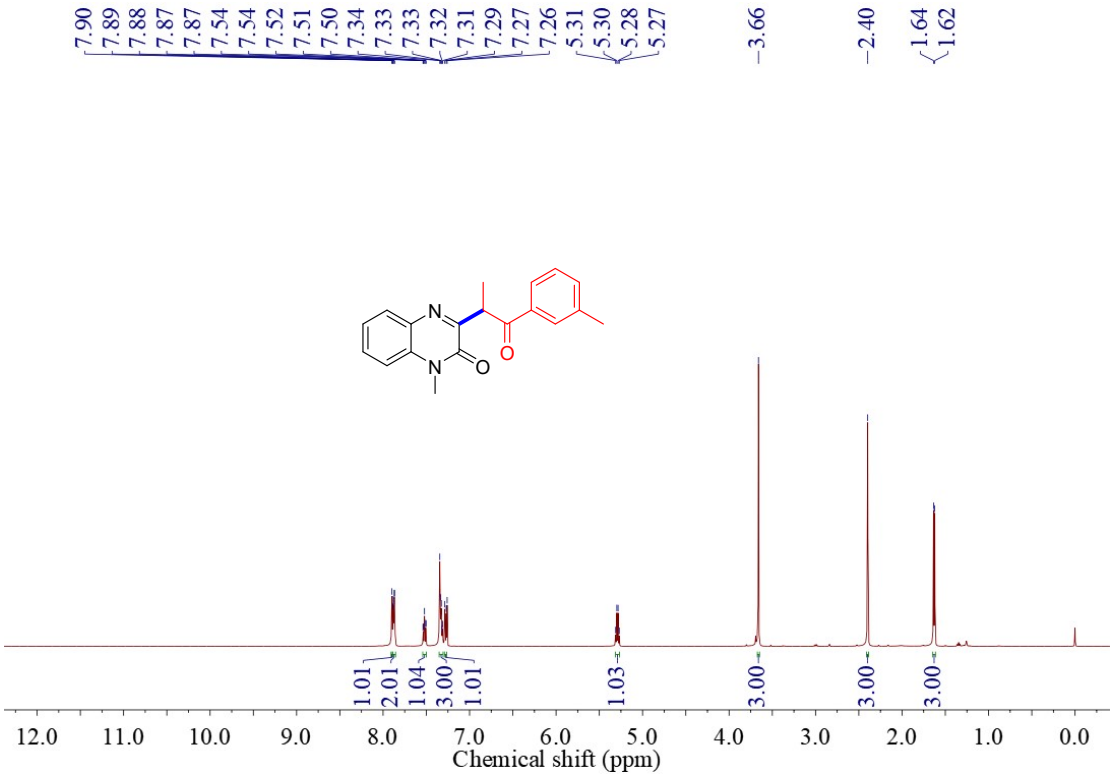
3b ^{13}C NMR



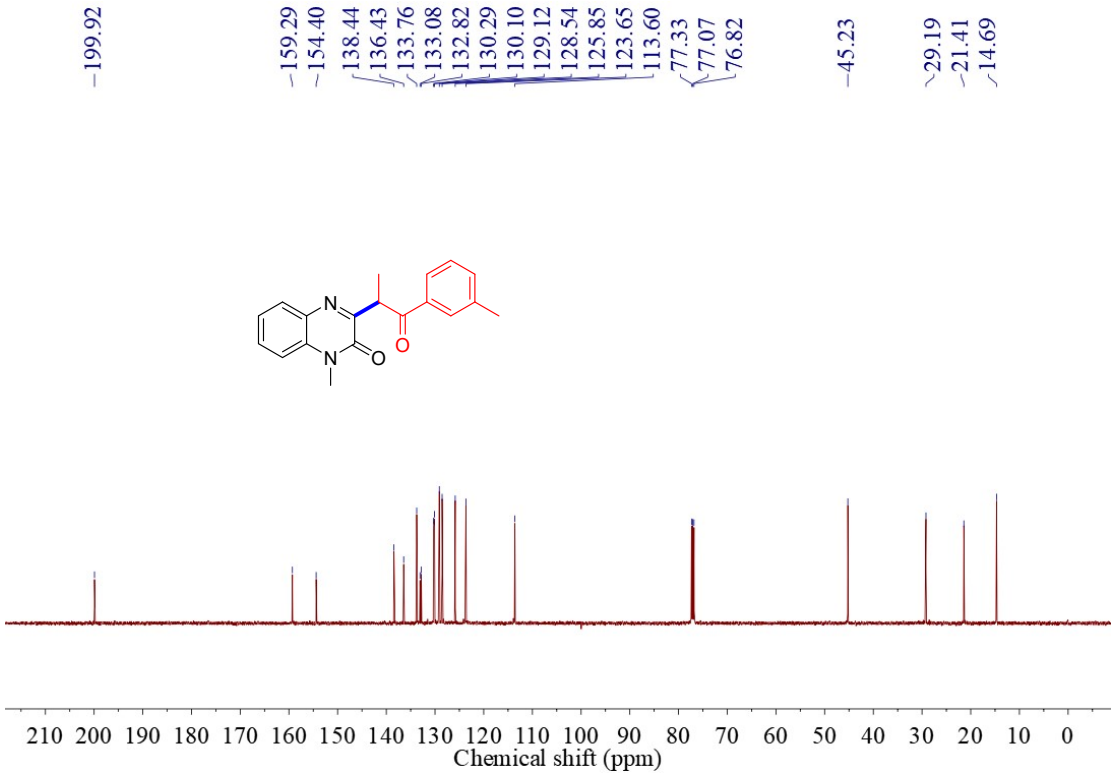
3b ^{19}F NMR



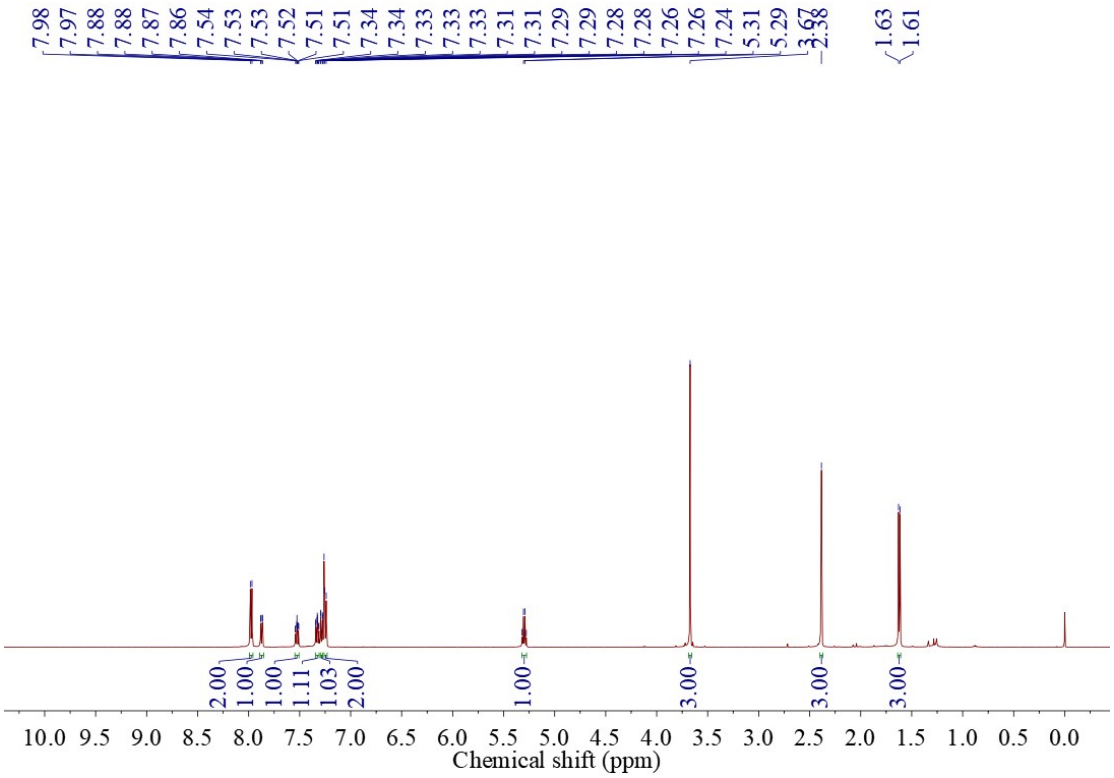
3c ^{1}H NMR



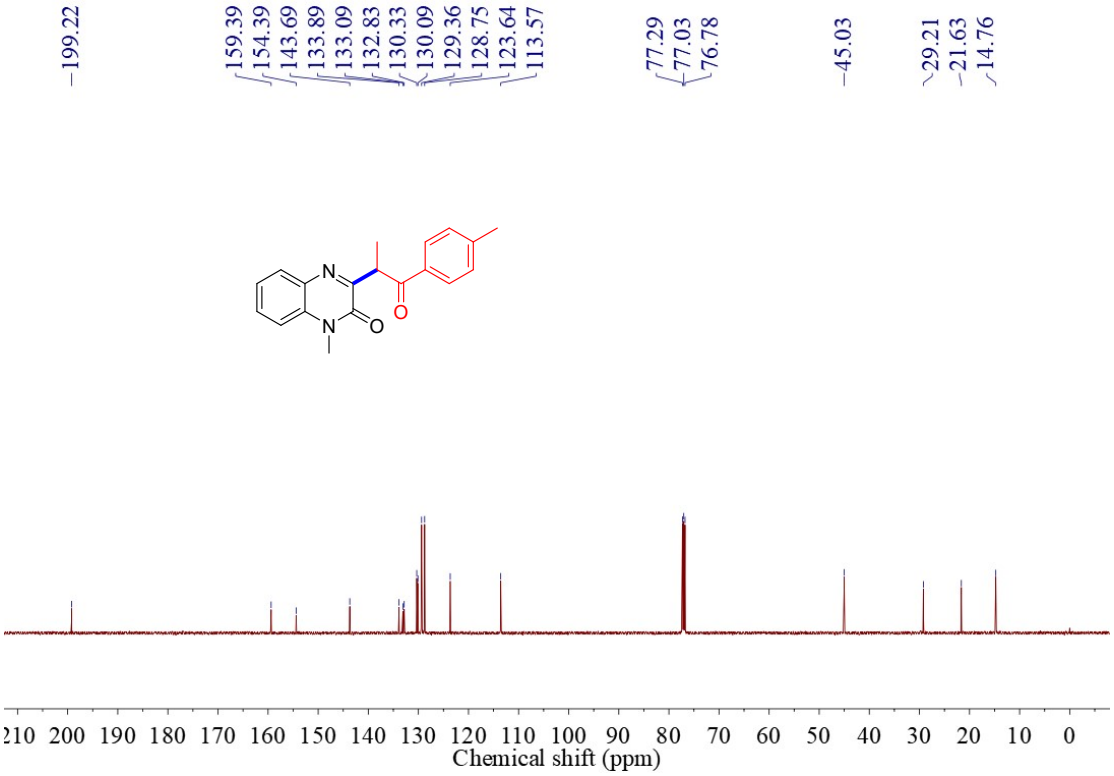
3c ^{13}C NMR



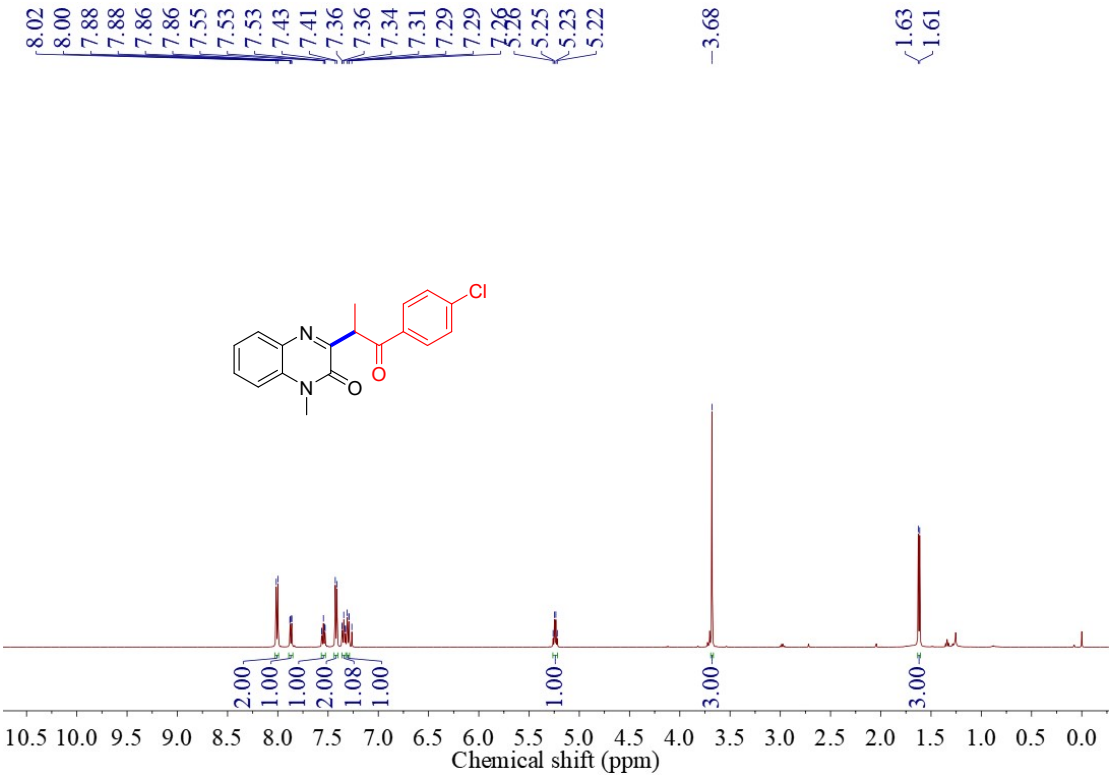
3d ^{13}C NMR



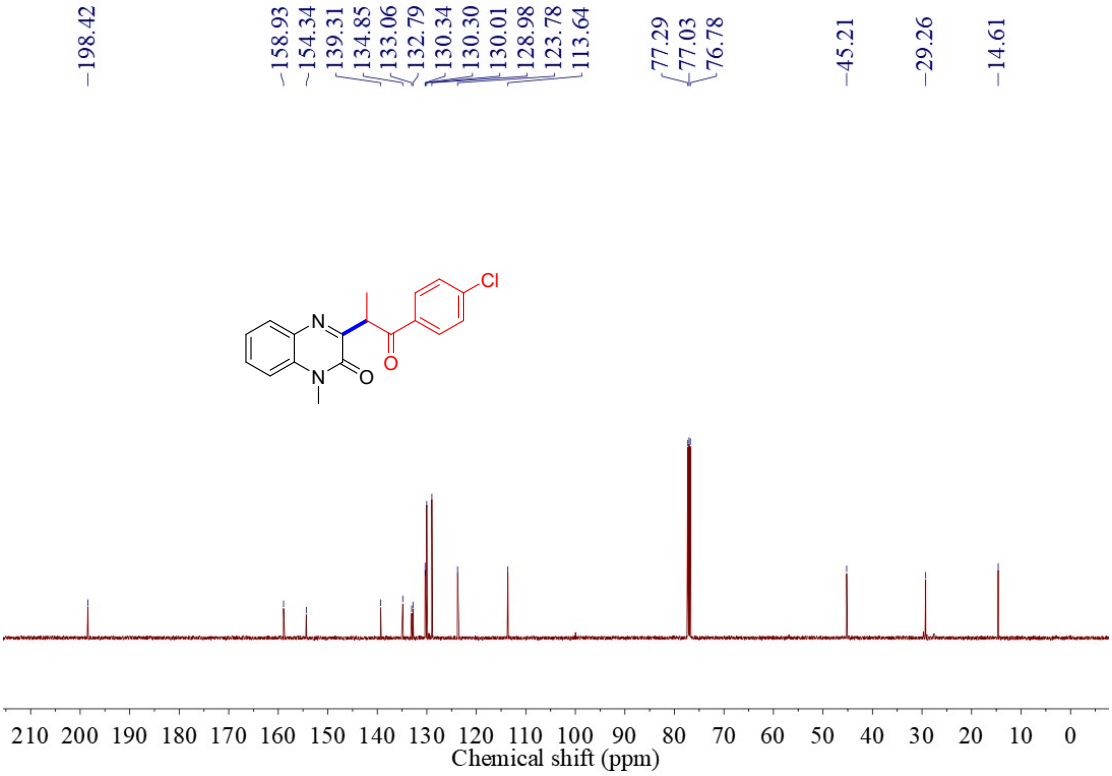
3d ^{13}C NMR



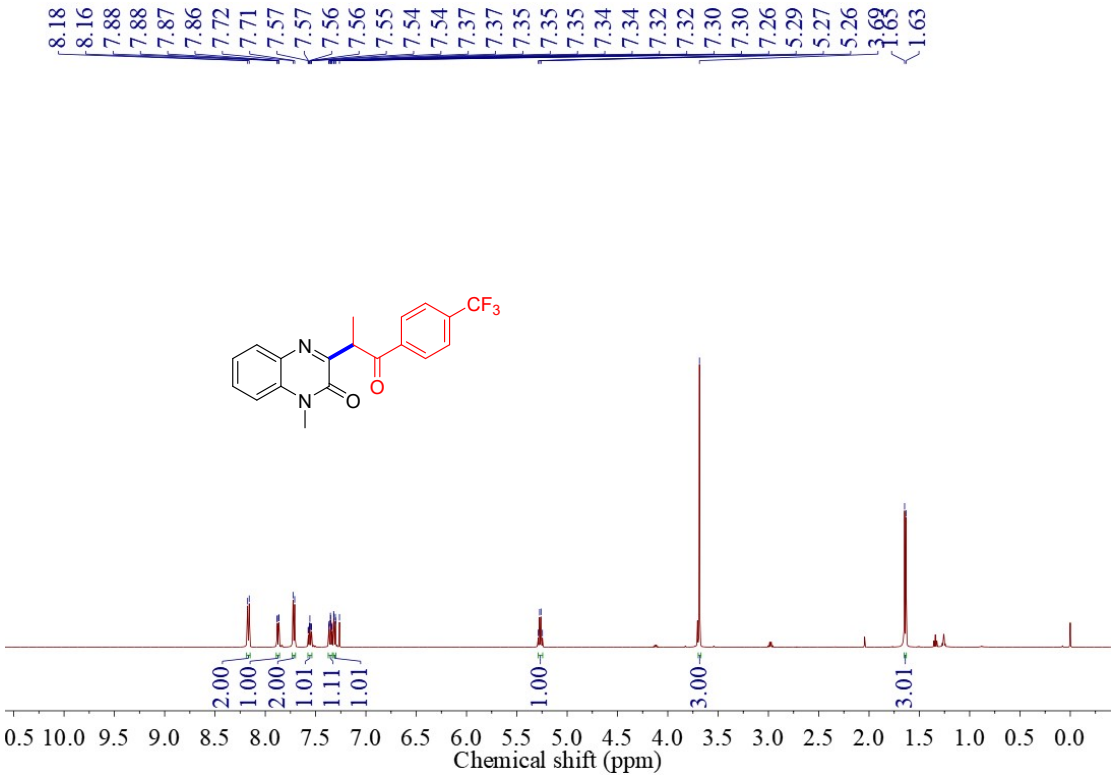
3e ^{1}H NMR



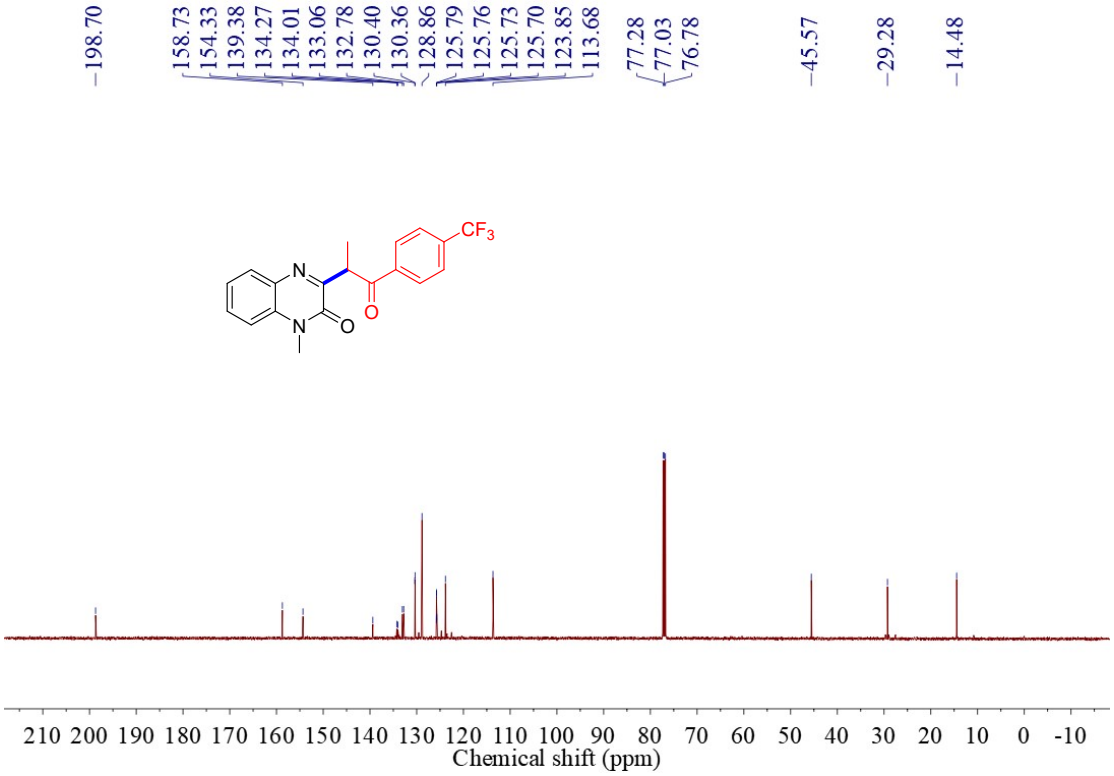
3e ^{13}C NMR



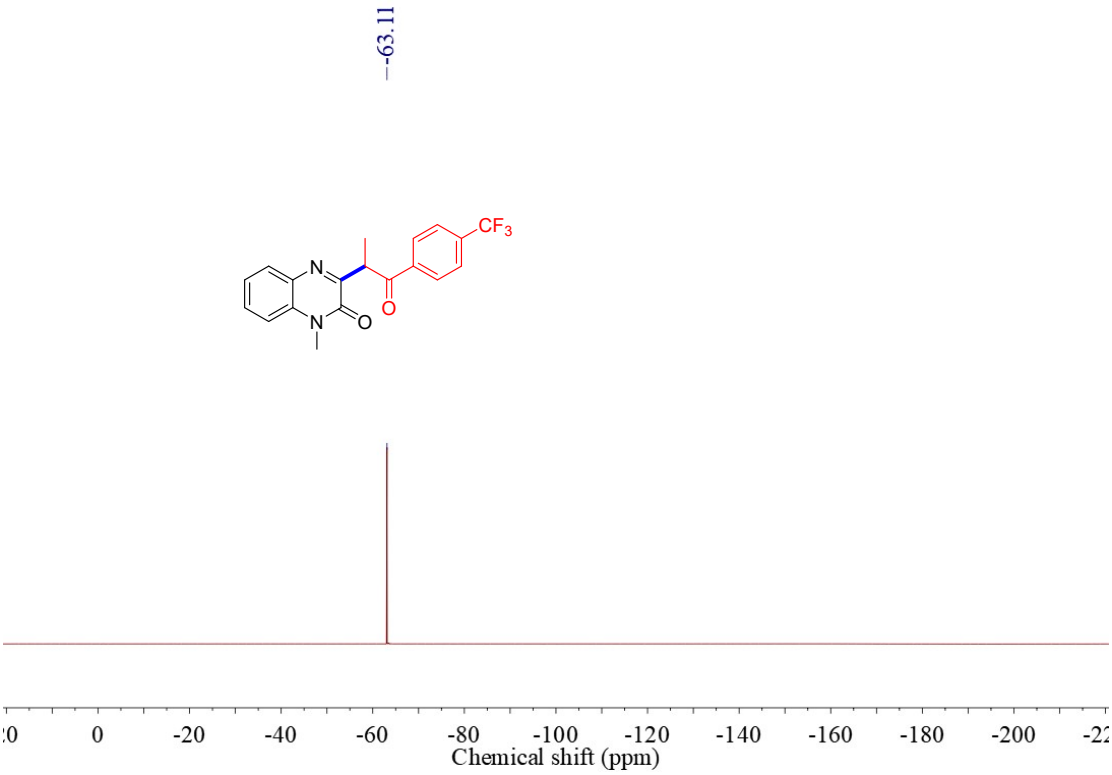
3f ^{1}H NMR



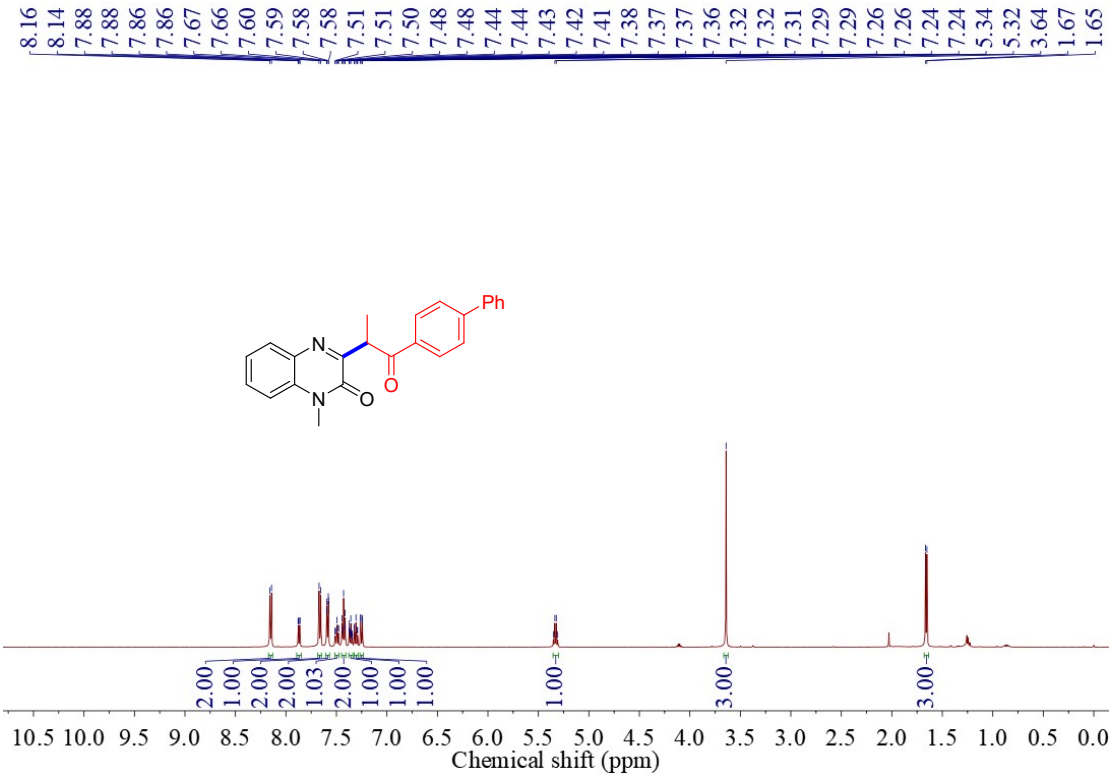
3f ^{13}C NMR



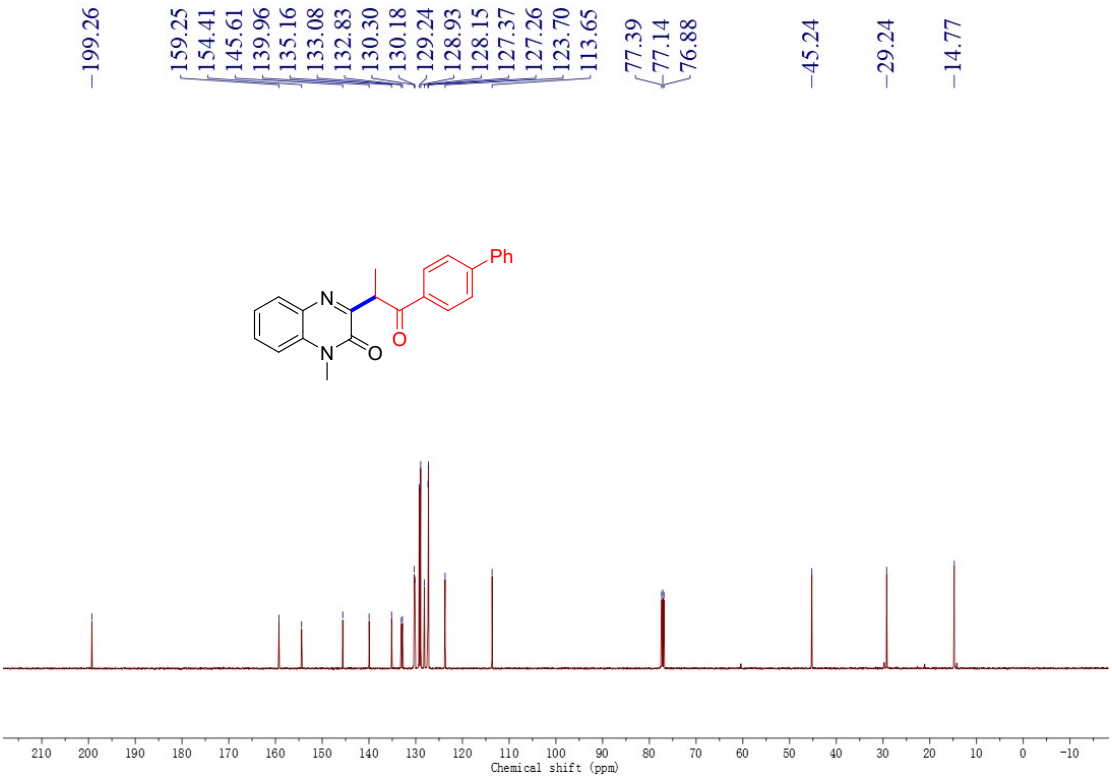
3f ^{19}F NMR


-63.11
CF3
N
N
O
O
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
Chemical shift (ppm)

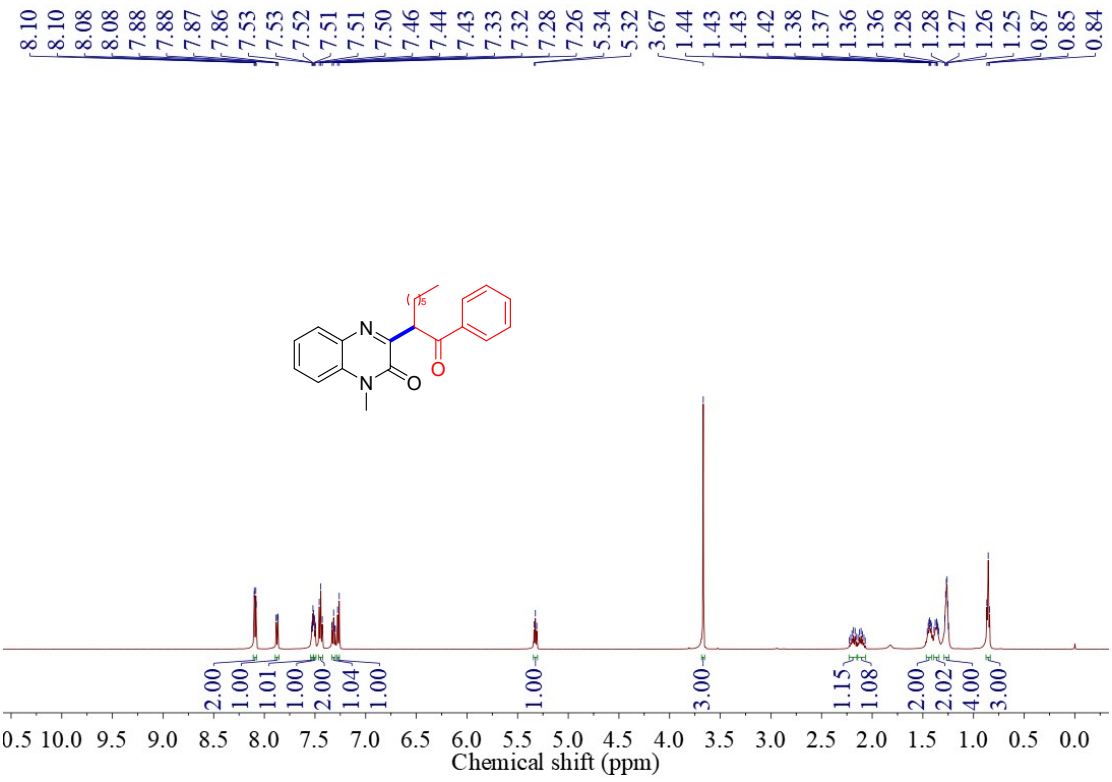
3g ^{1}H NMR


8.16
8.14
7.88
7.88
7.86
7.86
7.67
7.66
7.60
7.59
7.58
7.58
7.51
7.51
7.50
7.48
7.48
7.44
7.44
7.43
7.42
7.41
7.38
7.37
7.37
7.36
7.32
7.32
7.31
7.29
7.29
7.26
7.26
7.24
7.24
5.34
5.32
3.64
1.67
1.65
Ph
N
N
O
O
2.00
1.00
2.00
2.00
1.03
2.00
1.00
1.00
1.00
1.00
3.00
3.00
Chemical shift (ppm)

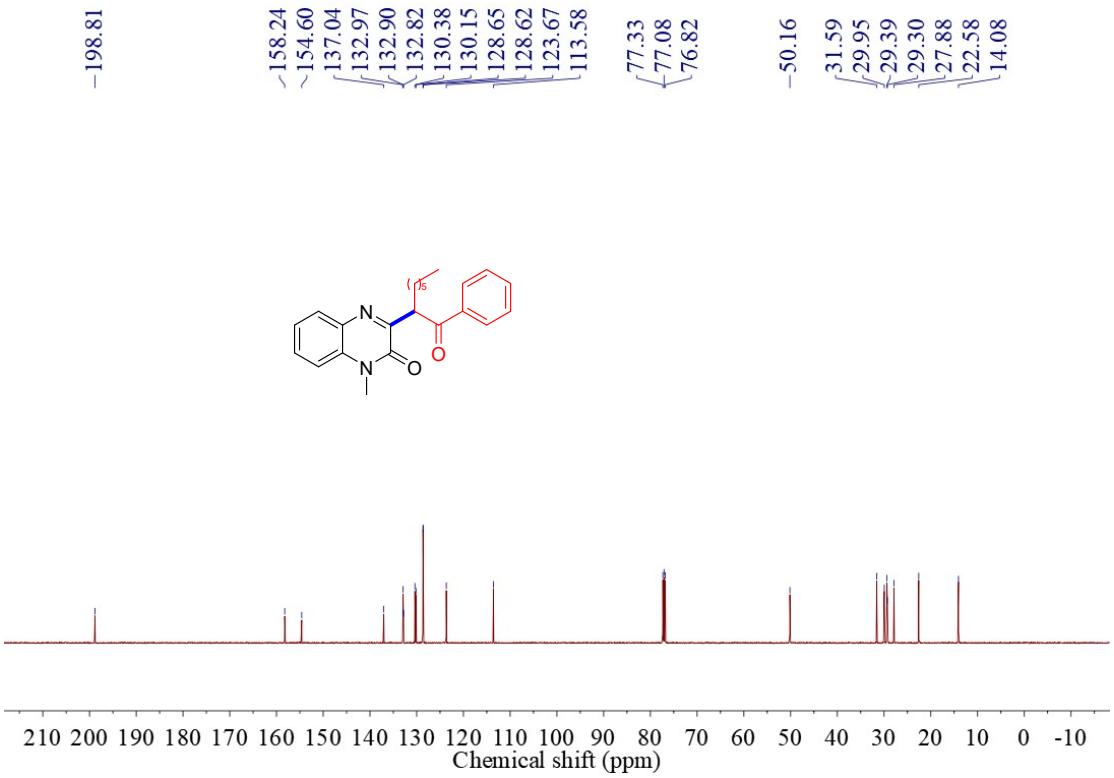
3g ^{13}C NMR



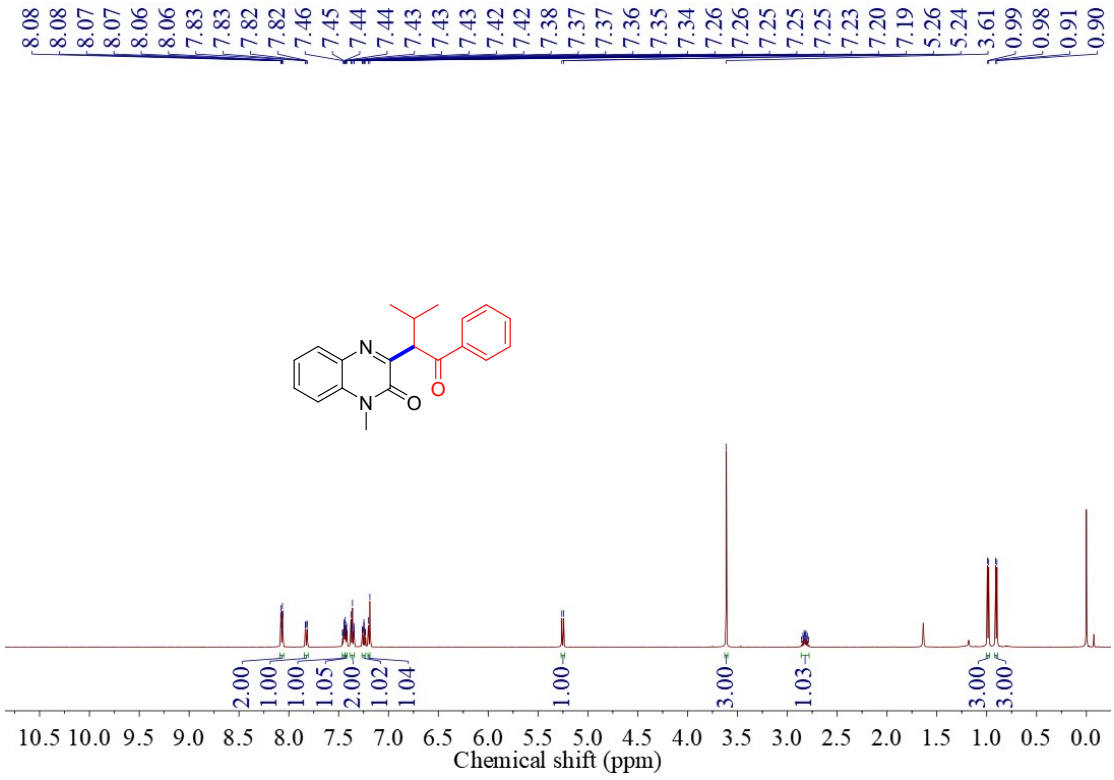
3h ^{1}H NMR



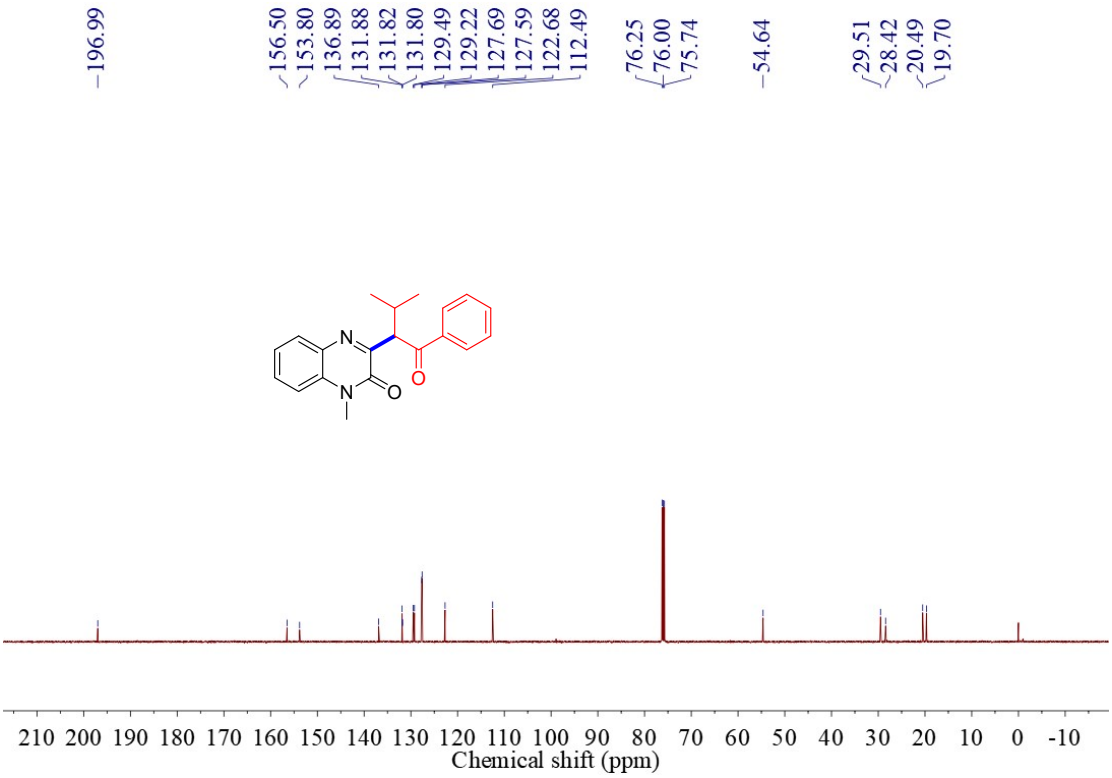
3h ^{13}C NMR



3i ^{1}H NMR



3i ^{13}C NMR



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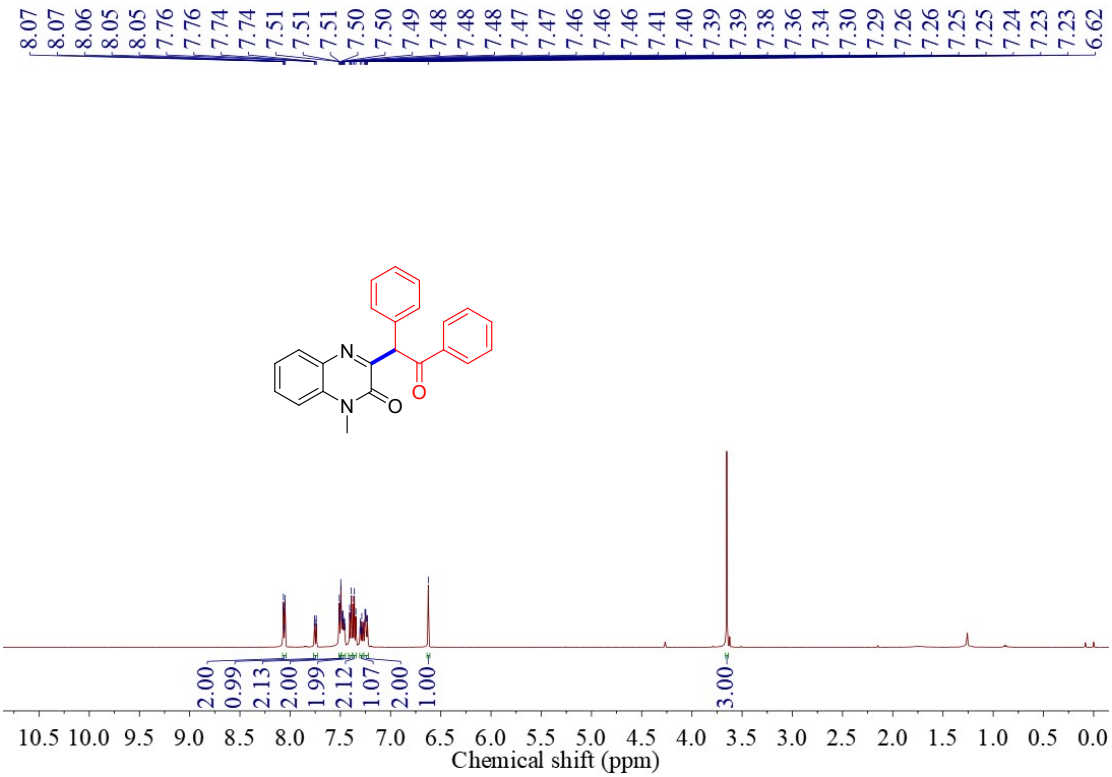
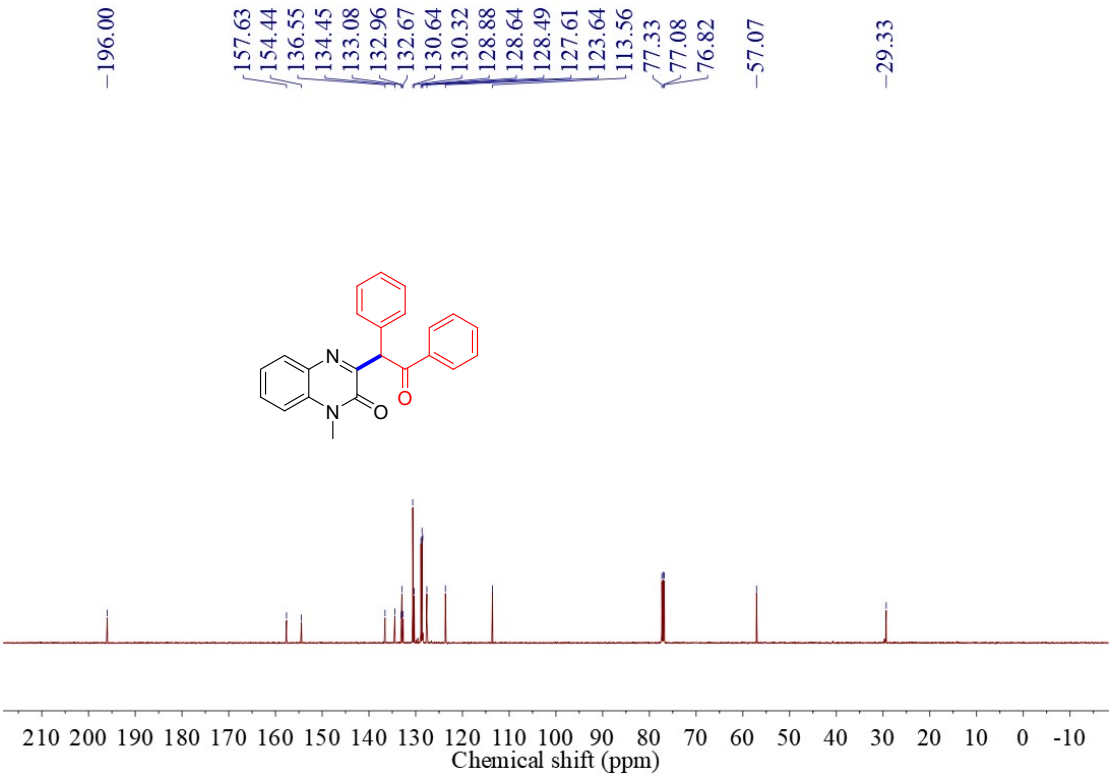


3j ^{13}C NMR



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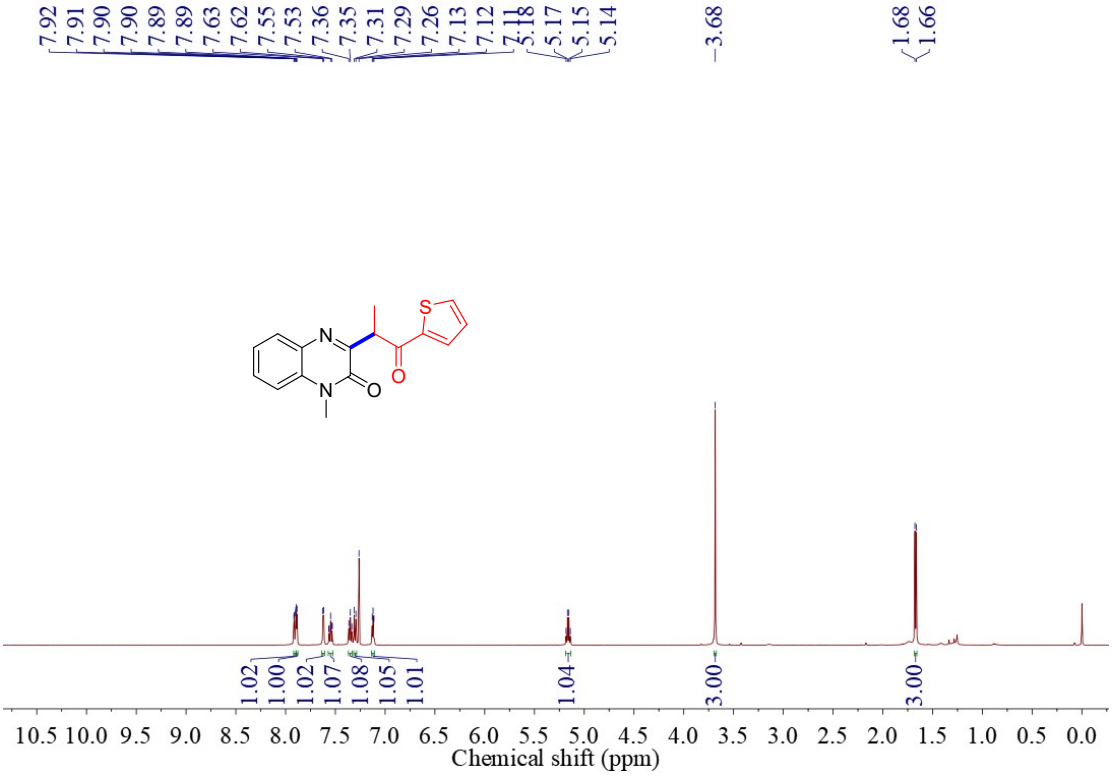

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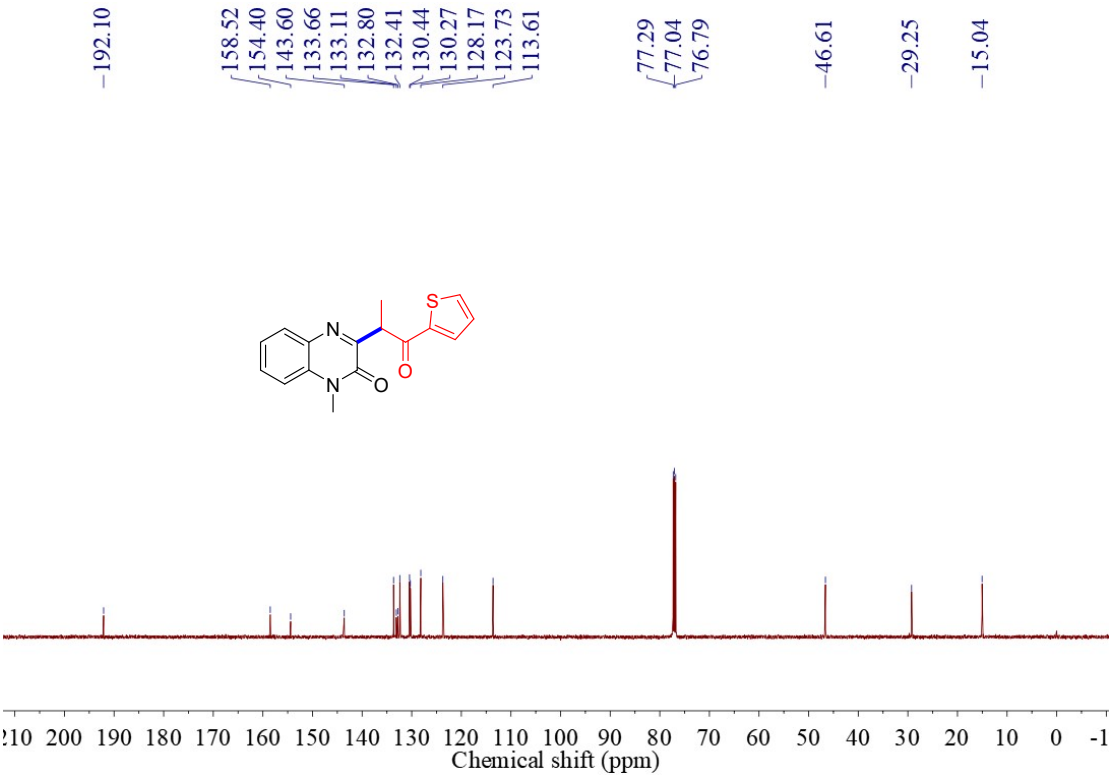
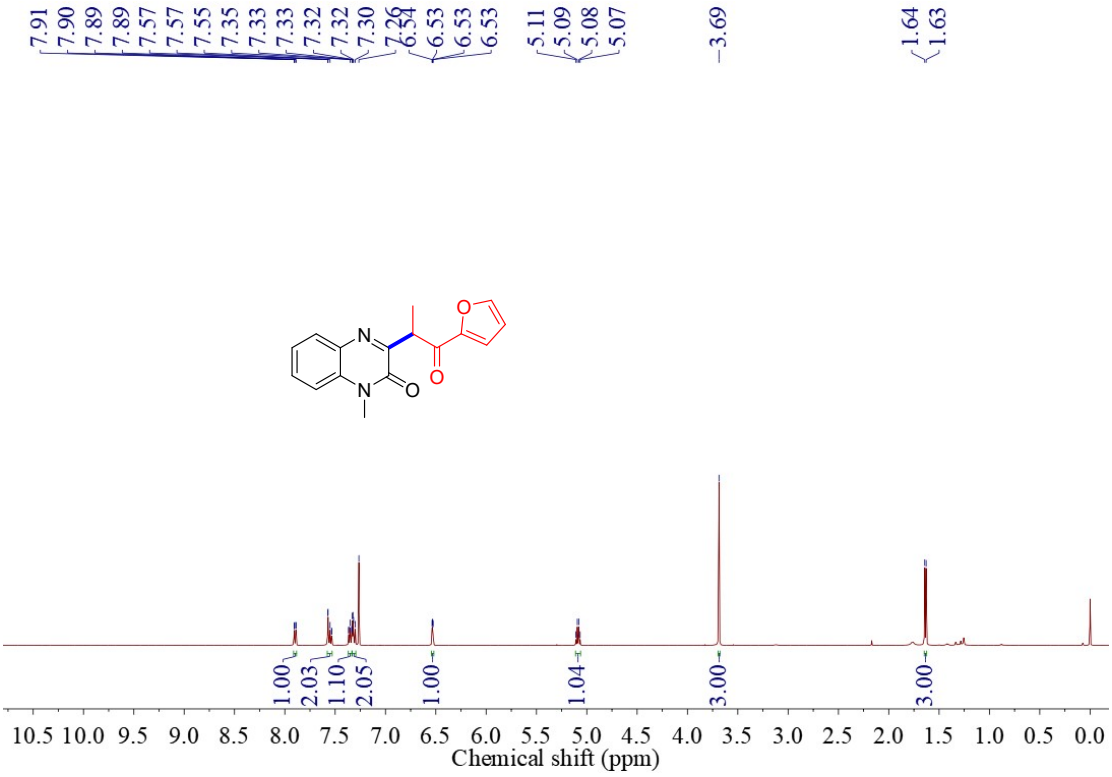


3l ^{1}H NMR



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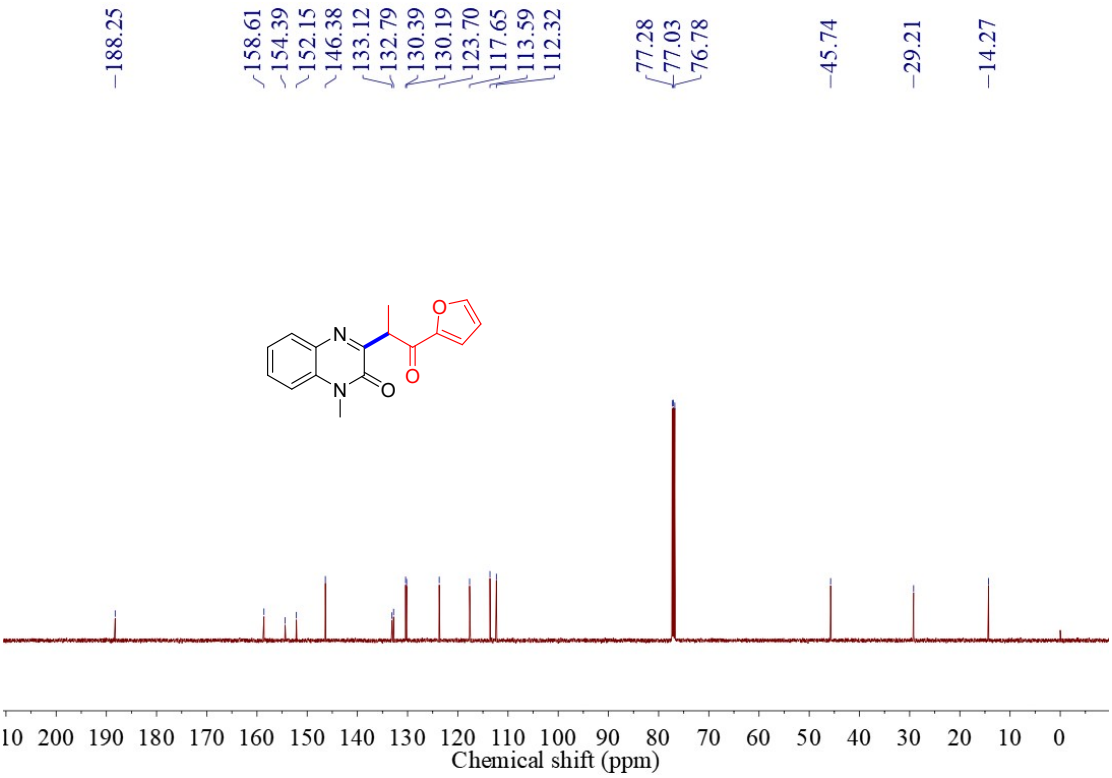
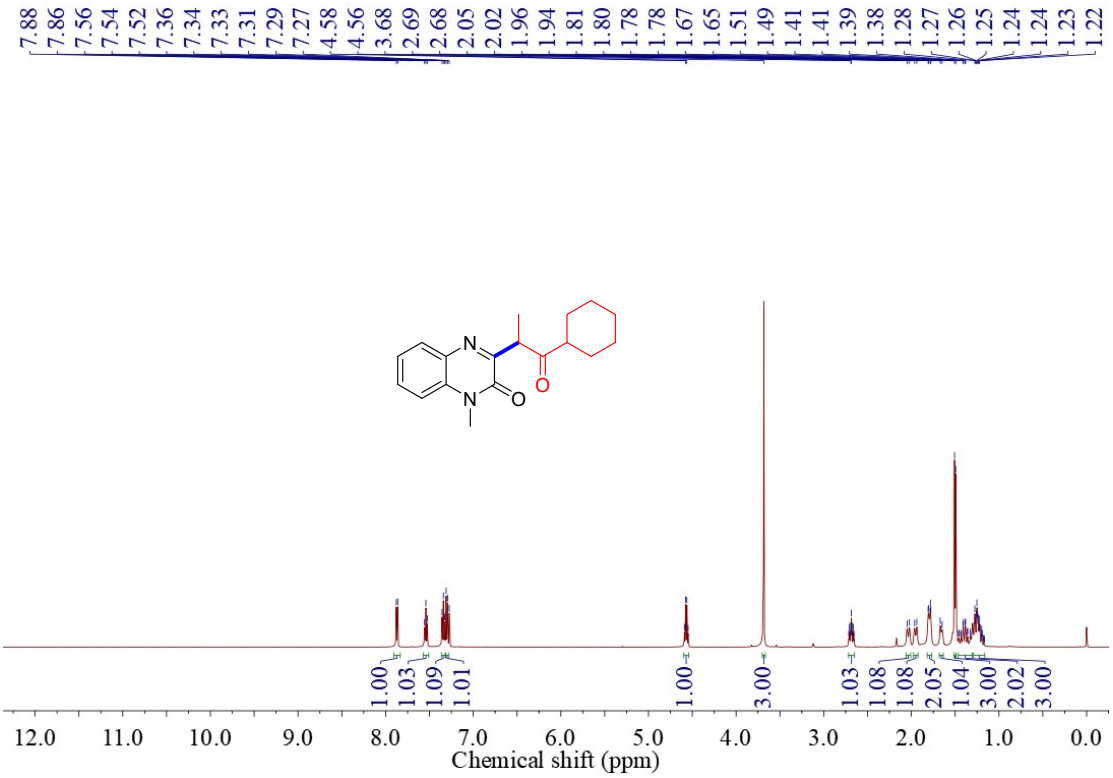
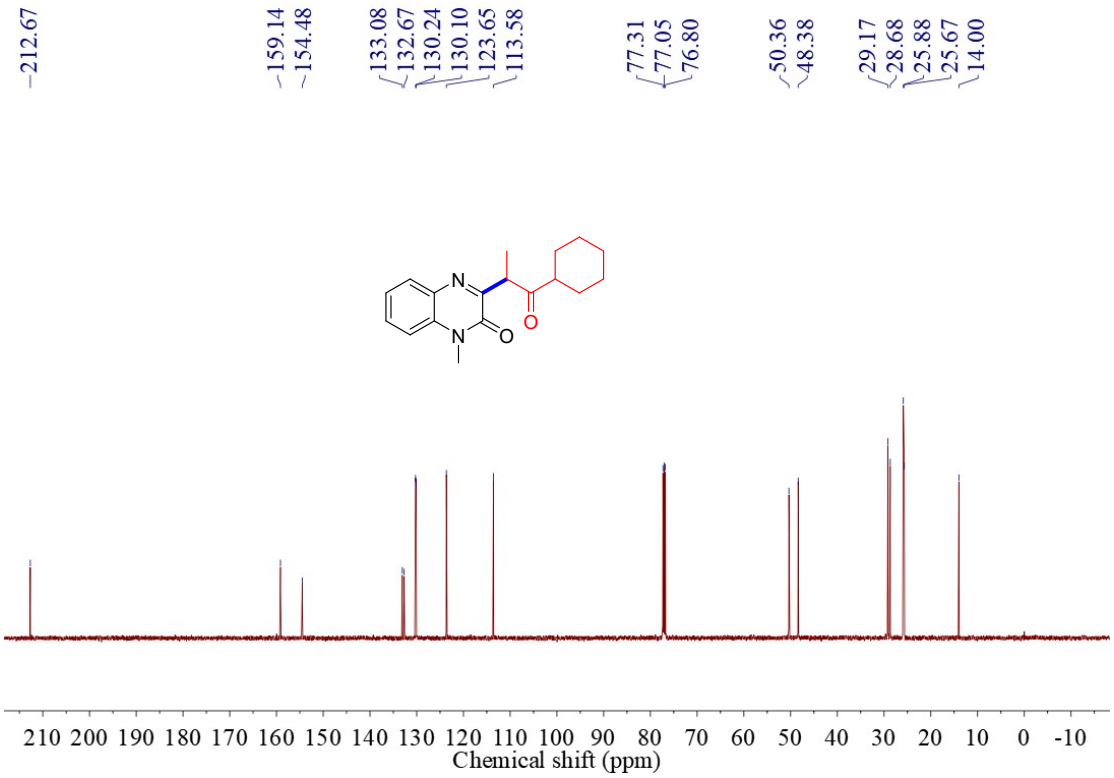


3m ^{1}H NMR



3m ^{13}C NMR



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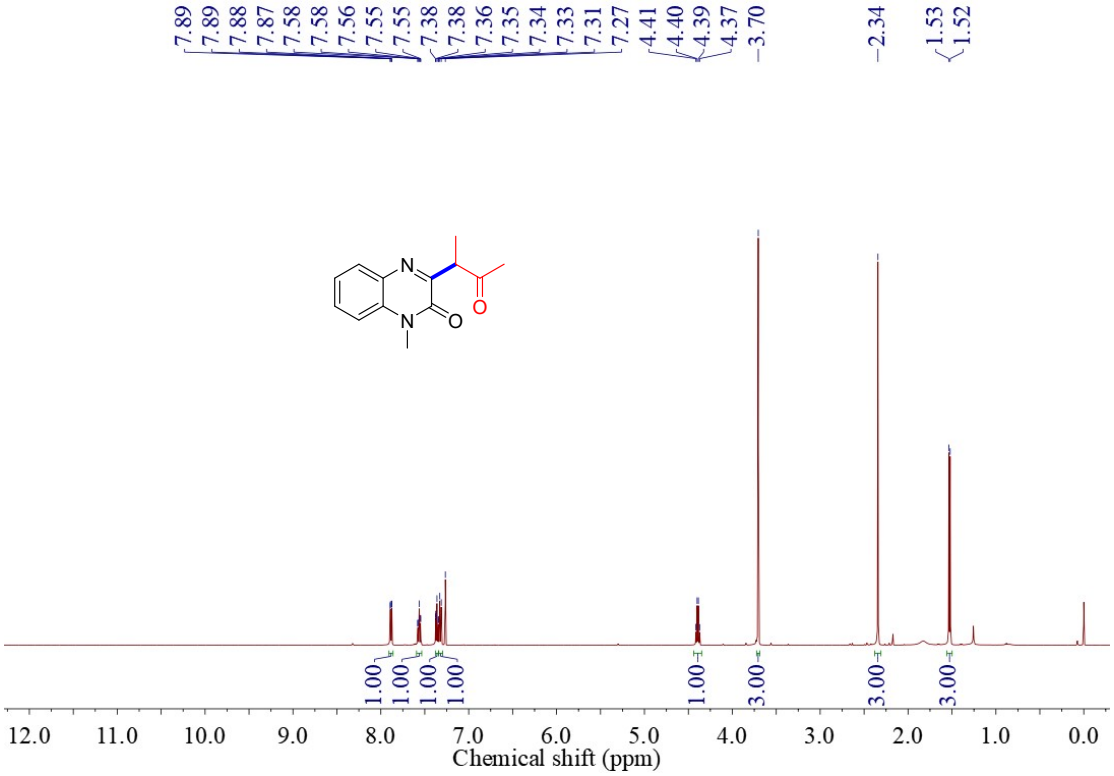
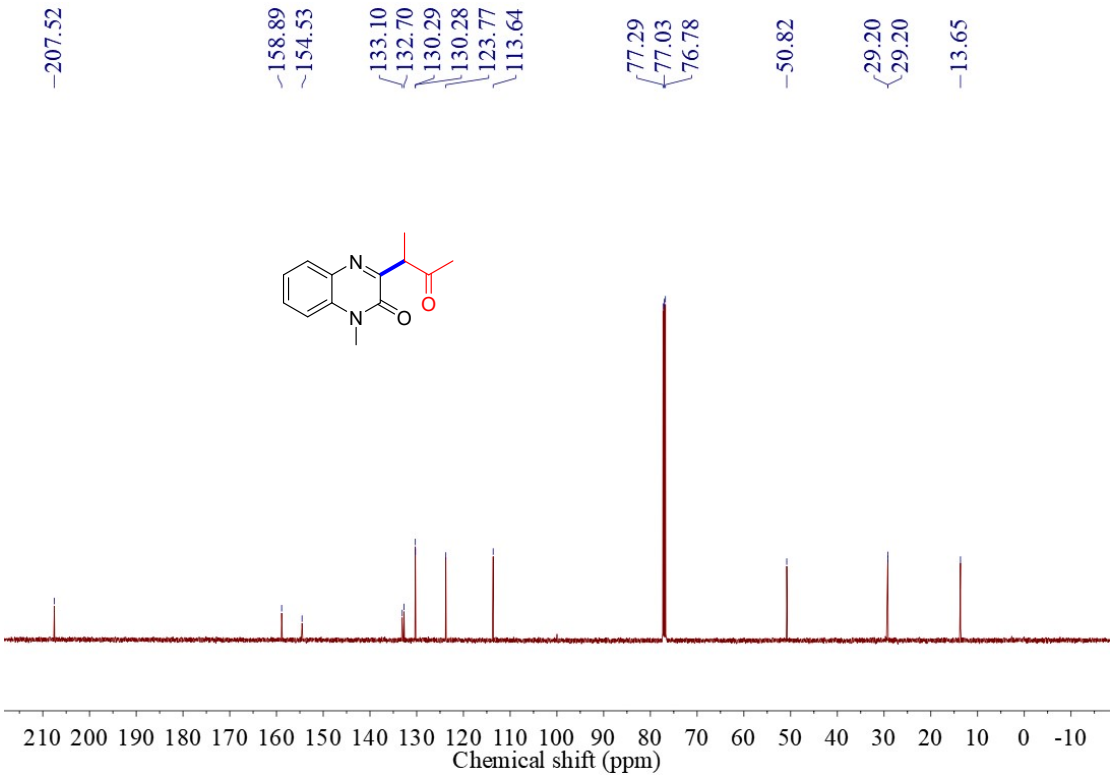
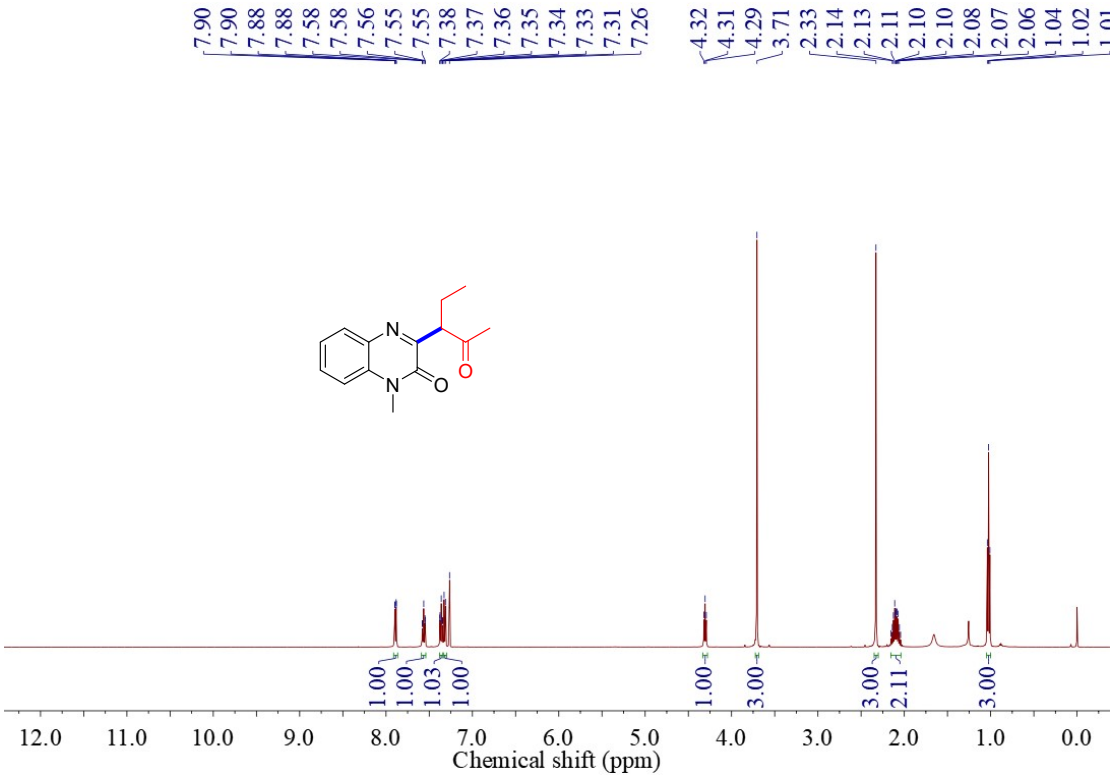


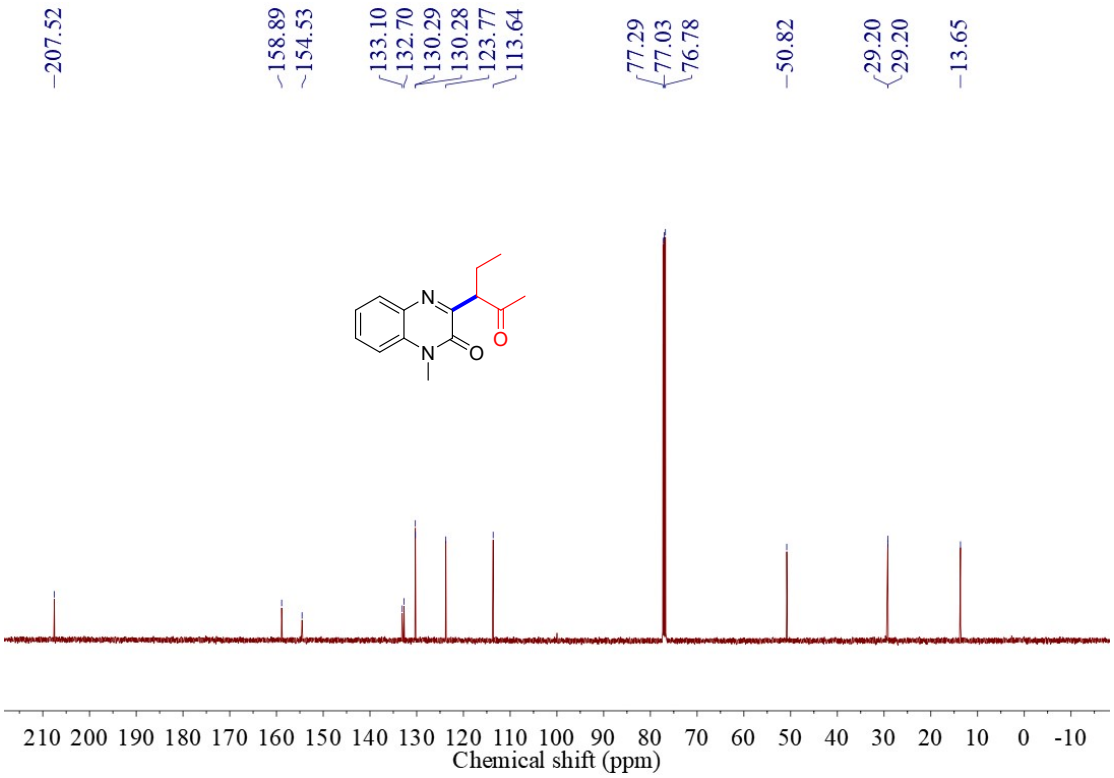
3n ^{13}C NMR



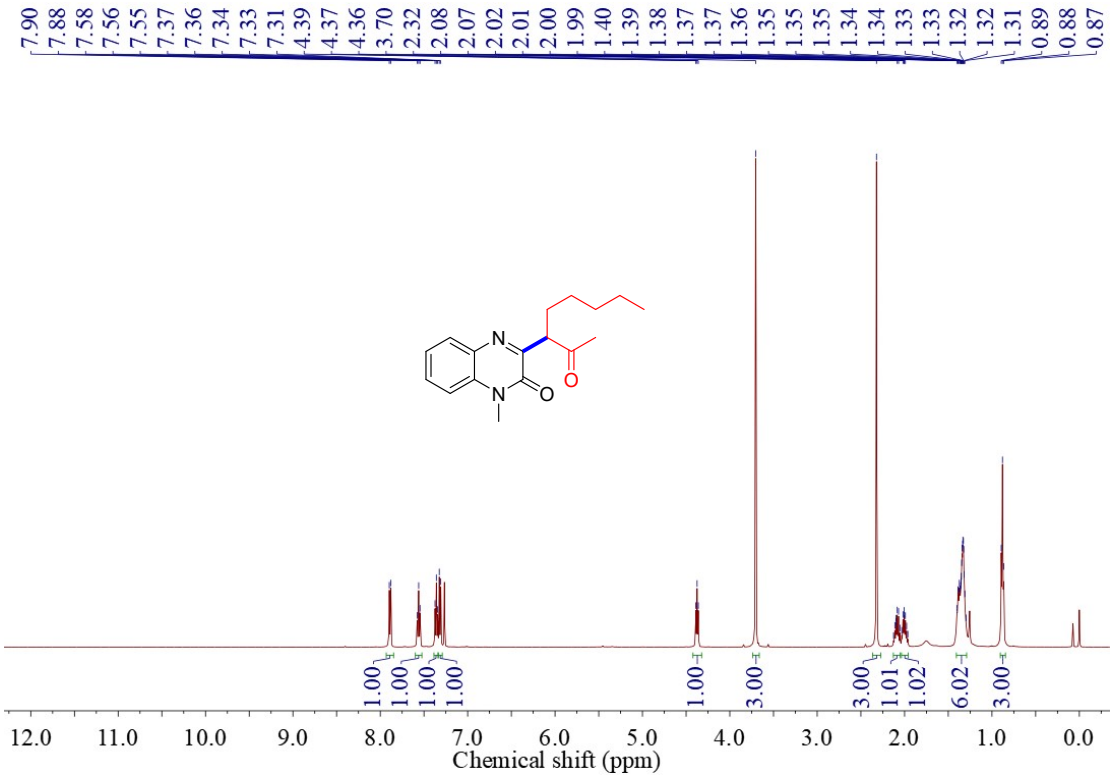
3o ^{1}H NMR



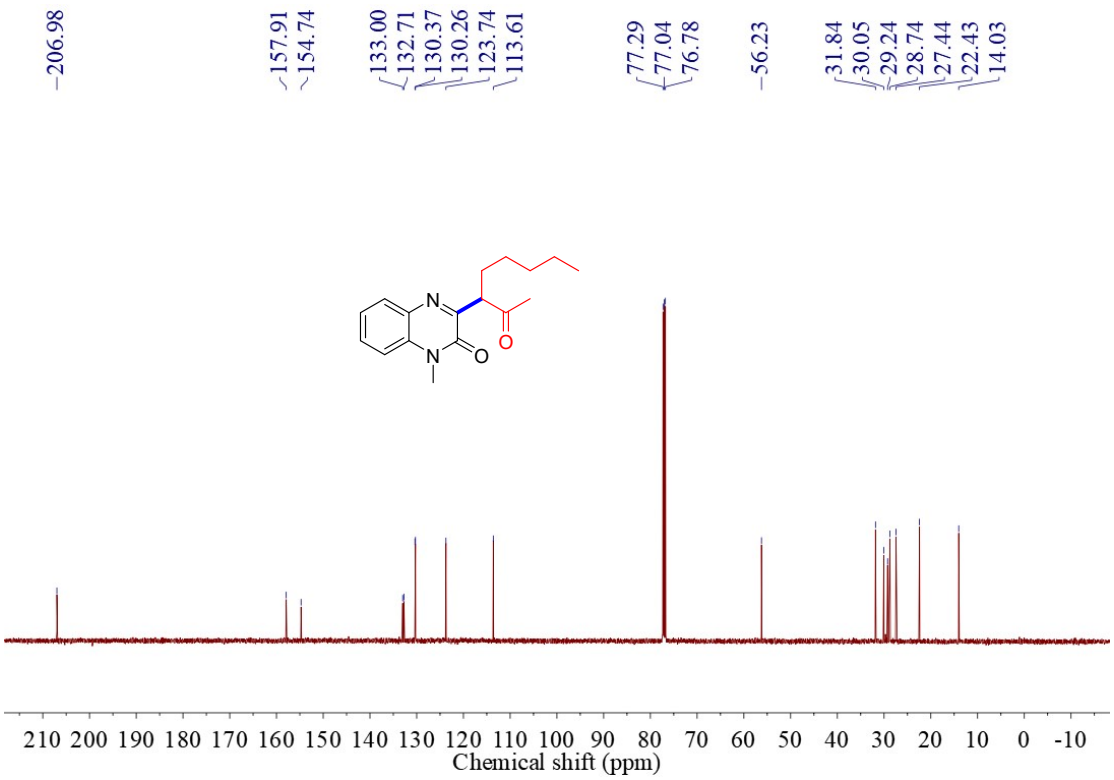
3o ^{13}C NMR



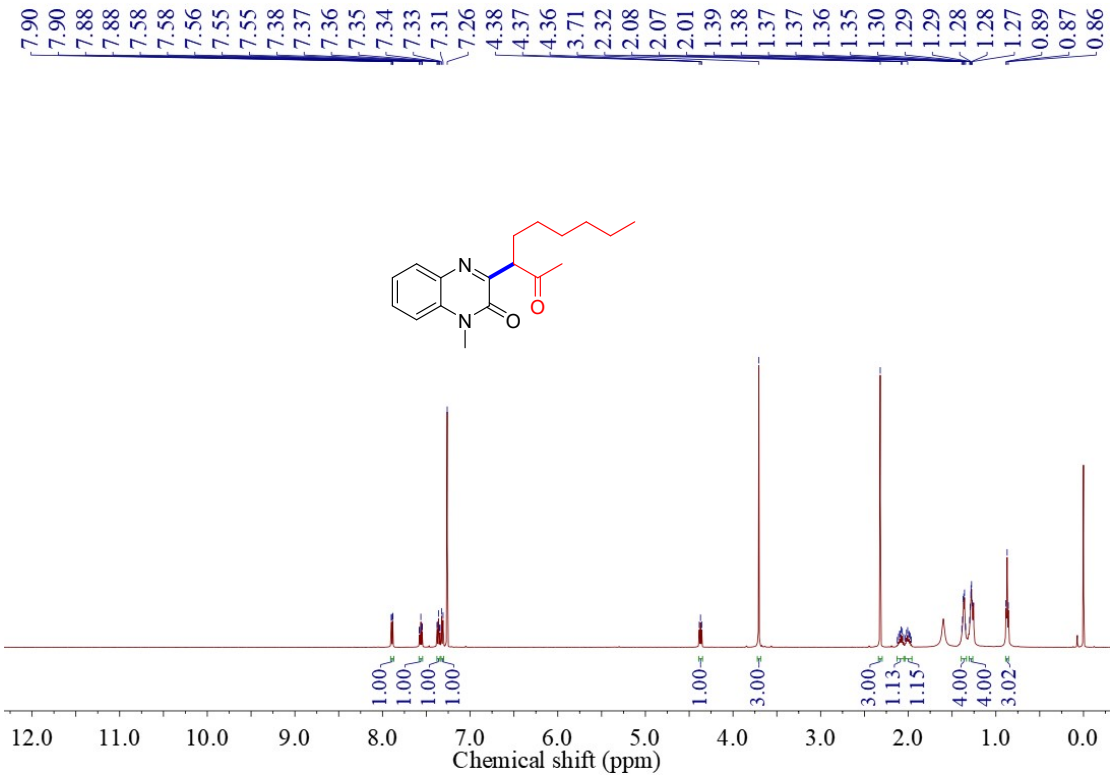
3p ^{1}H NMR



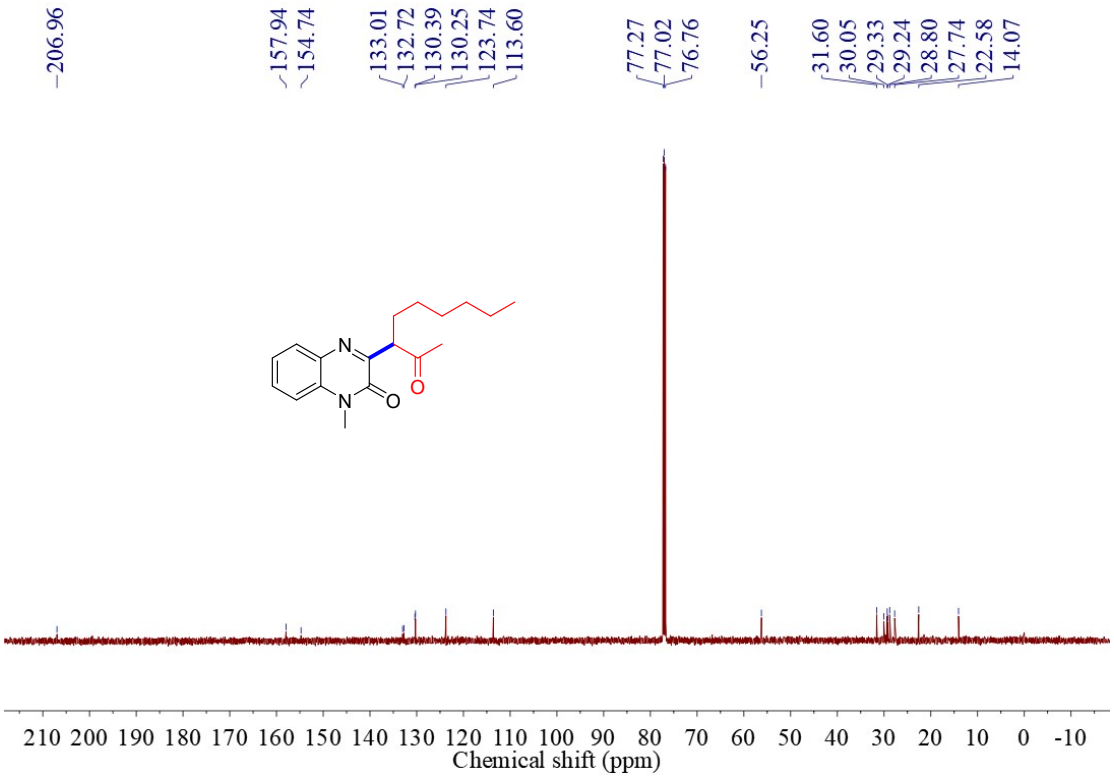
3p ^{13}C NMR



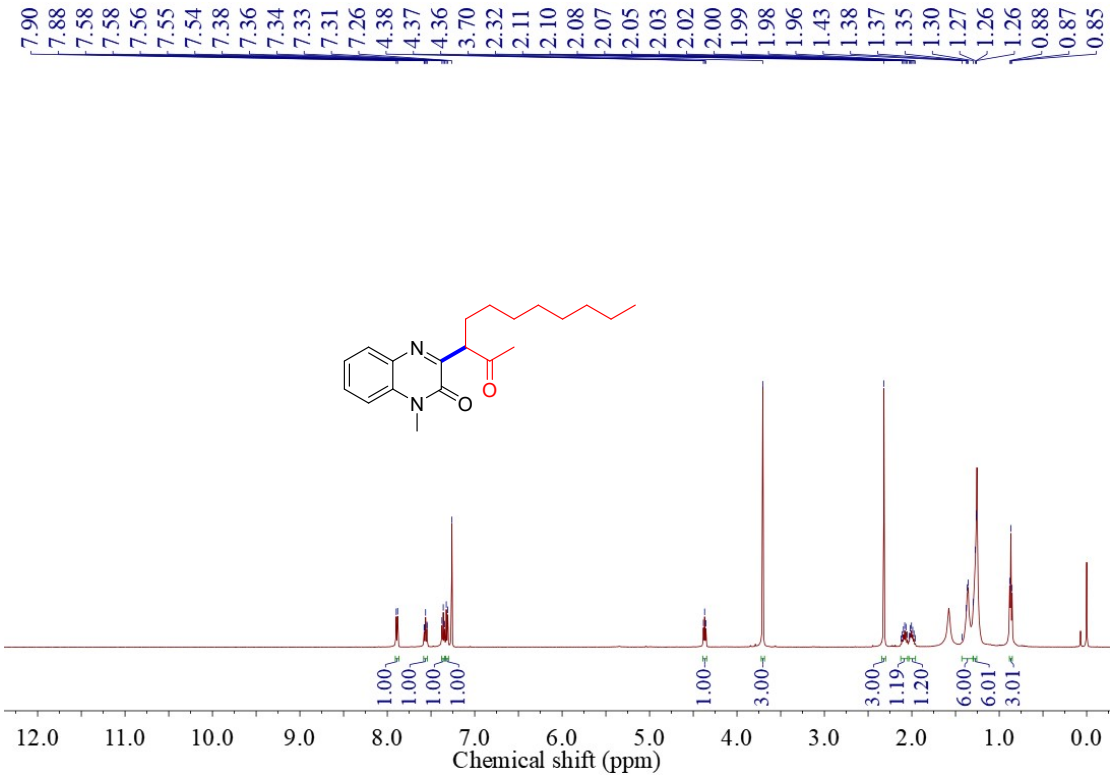
3q ^{1}H NMR



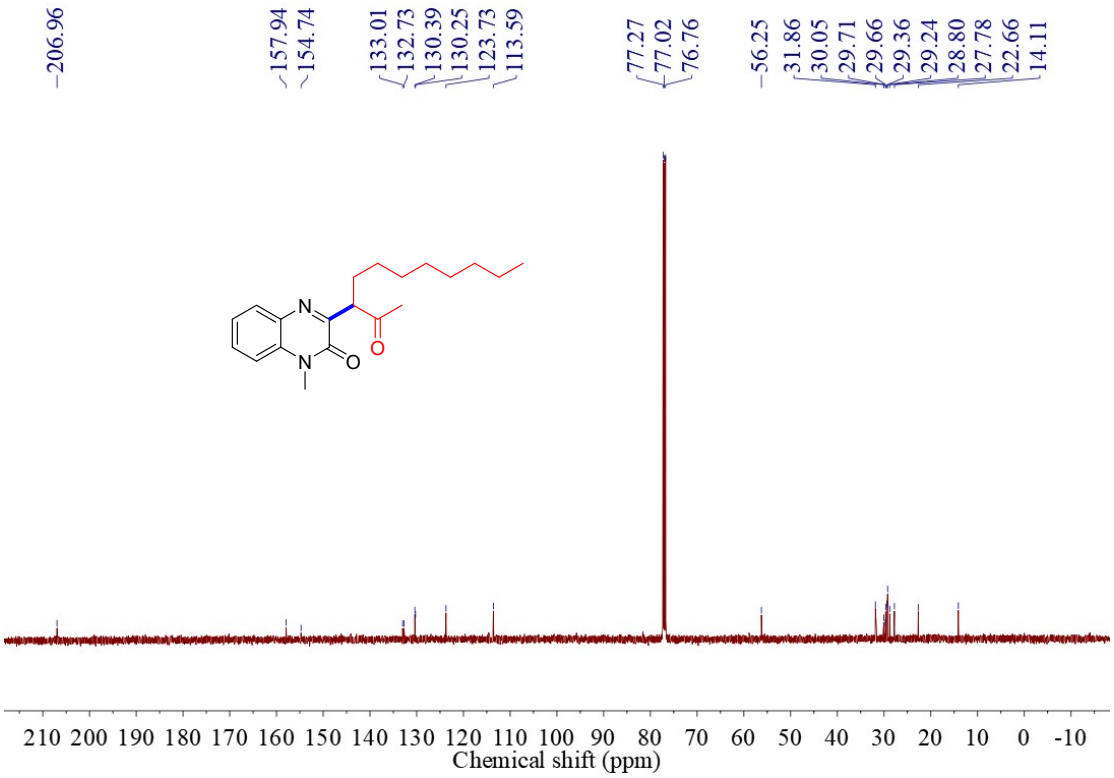
3q ^{13}C NMR



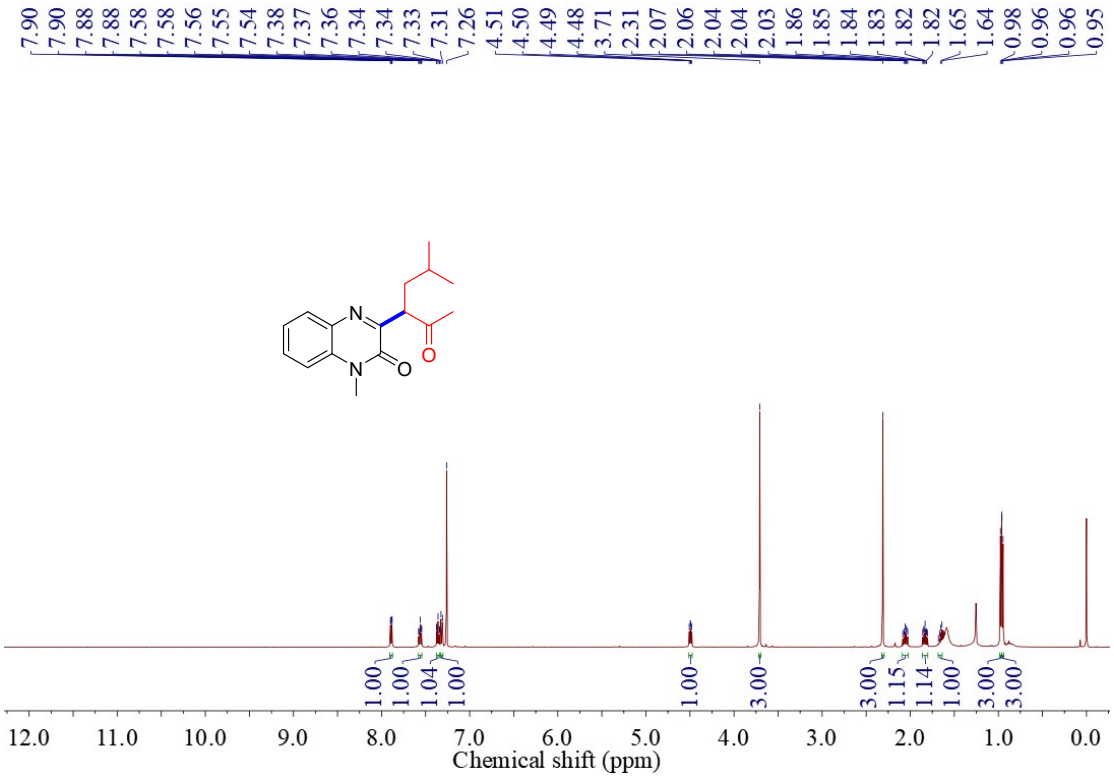
3r ^{1}H NMR



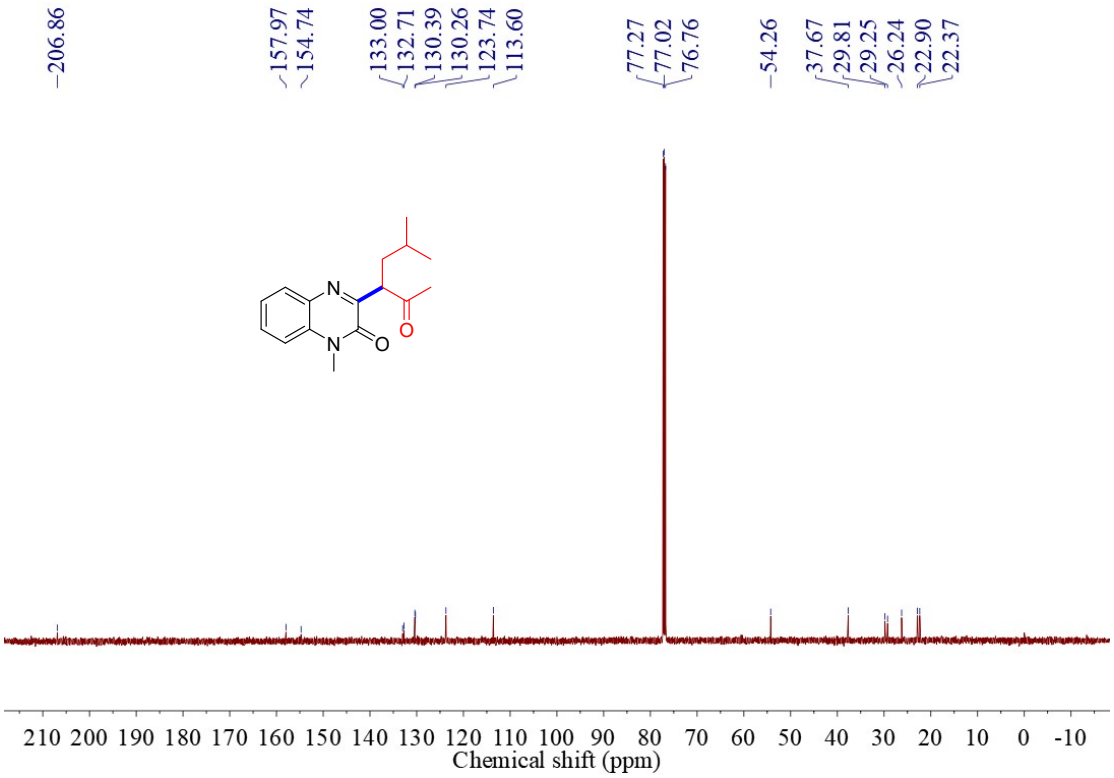
3r ^{13}C NMR



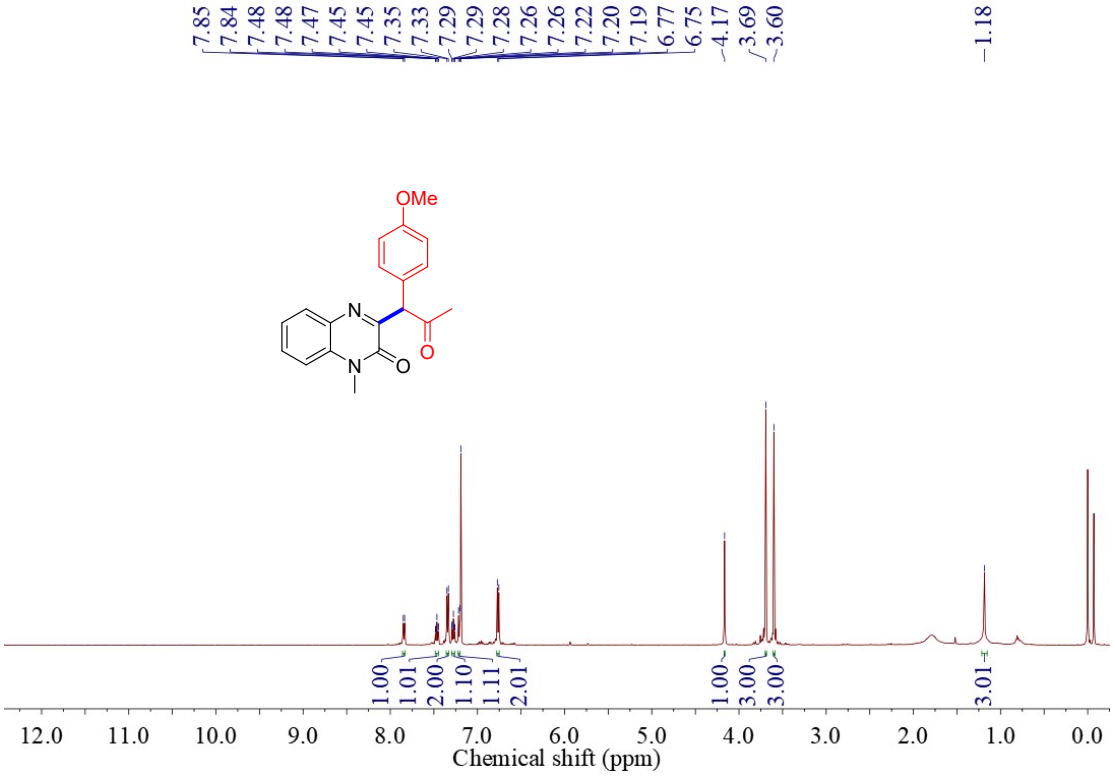
3s ^{1}H NMR



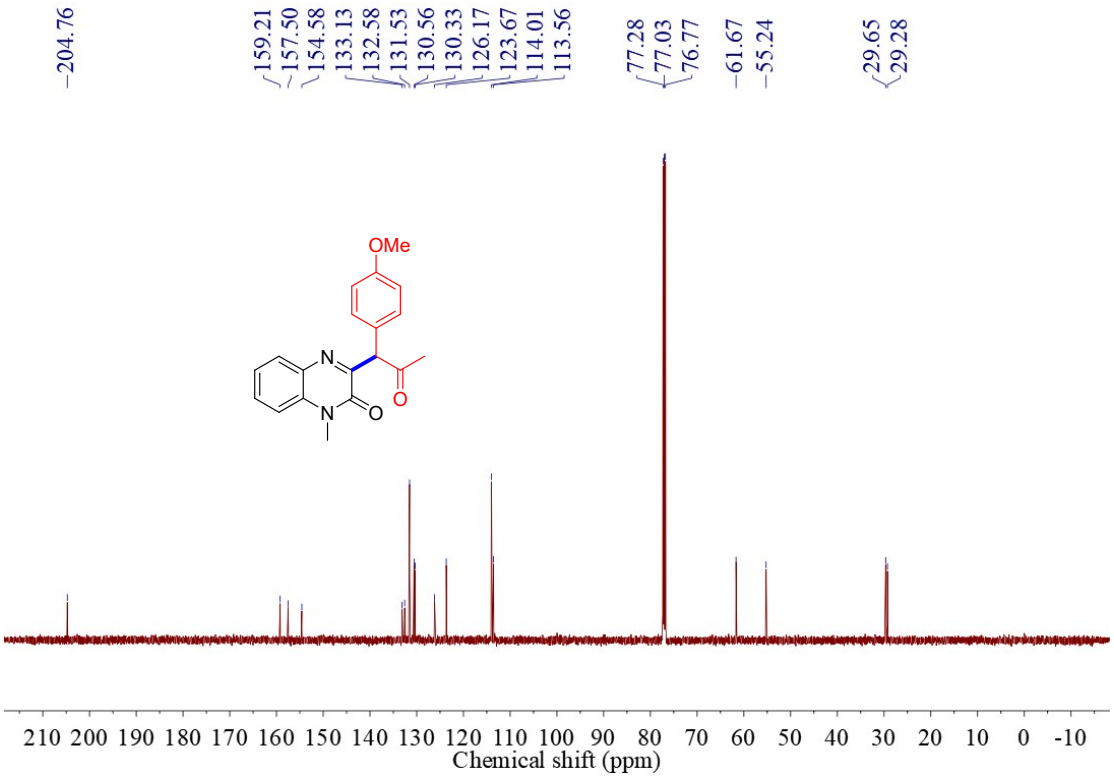
3s ^{13}C NMR



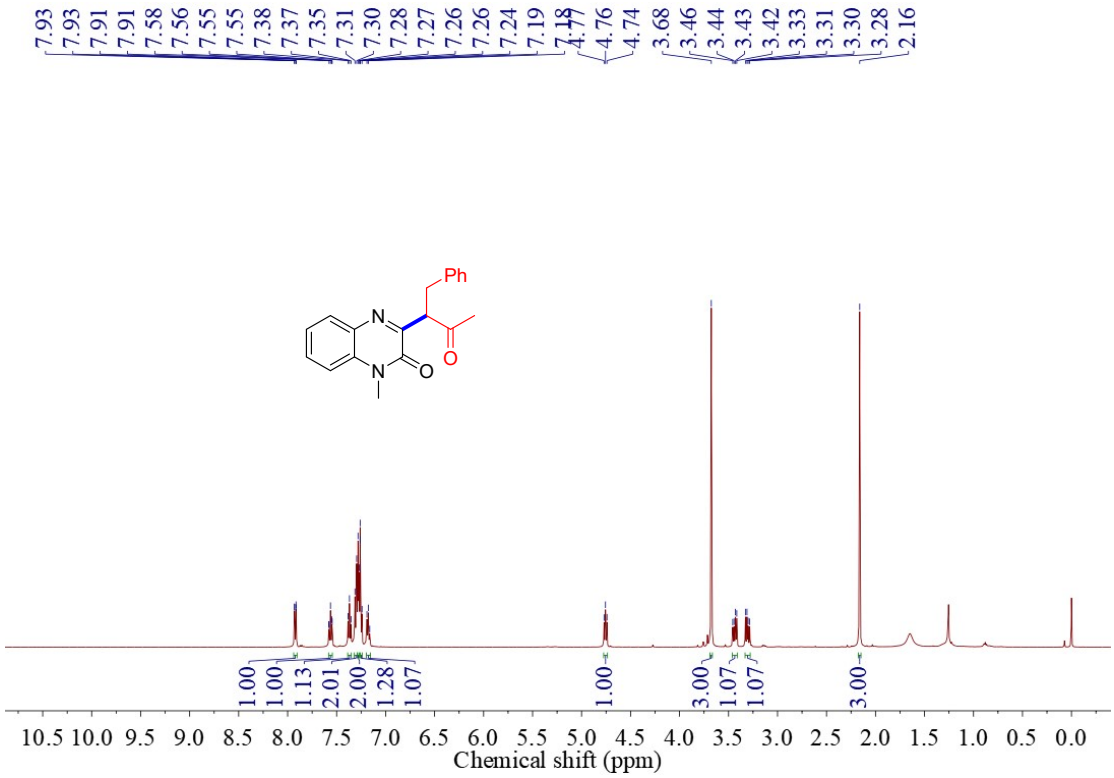
3t ^{1}H NMR



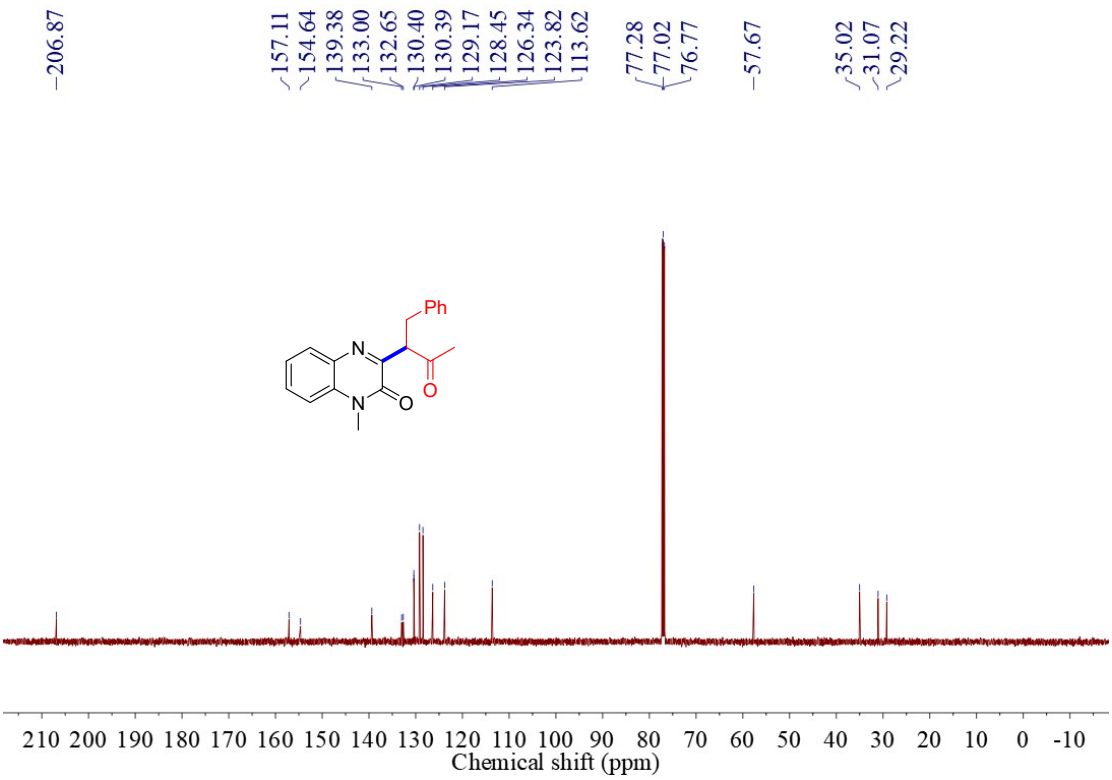
3t ^{13}C NMR



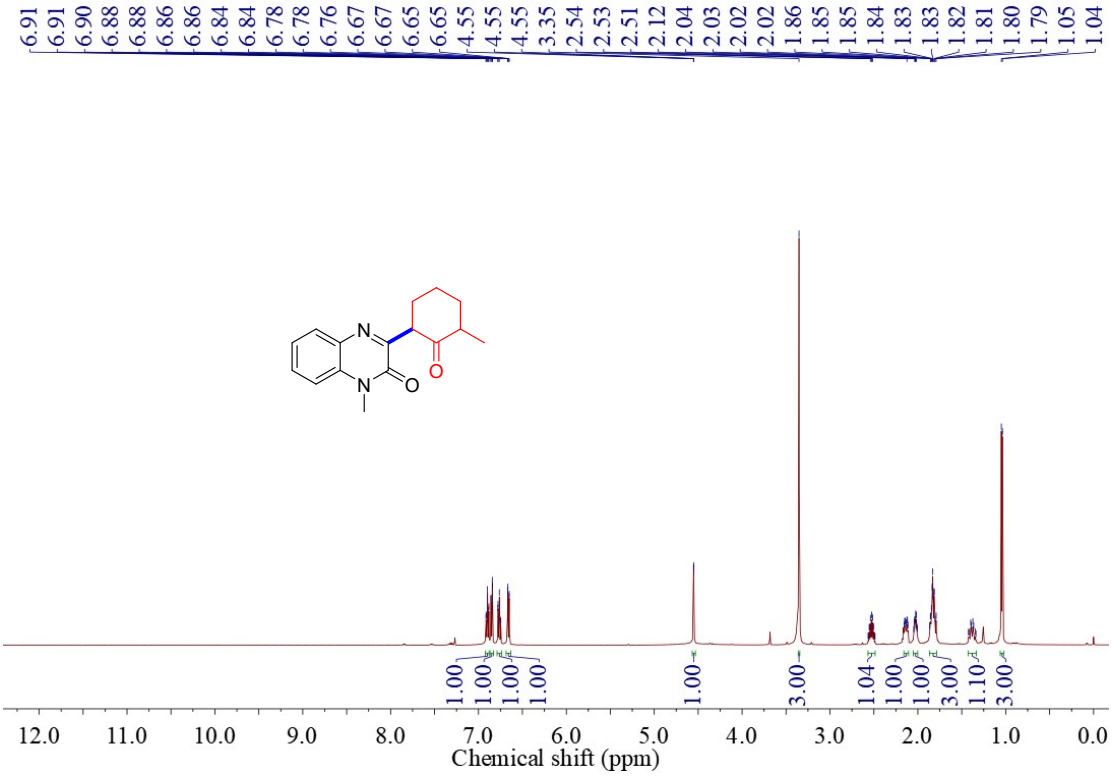
3u ^{1}H NMR



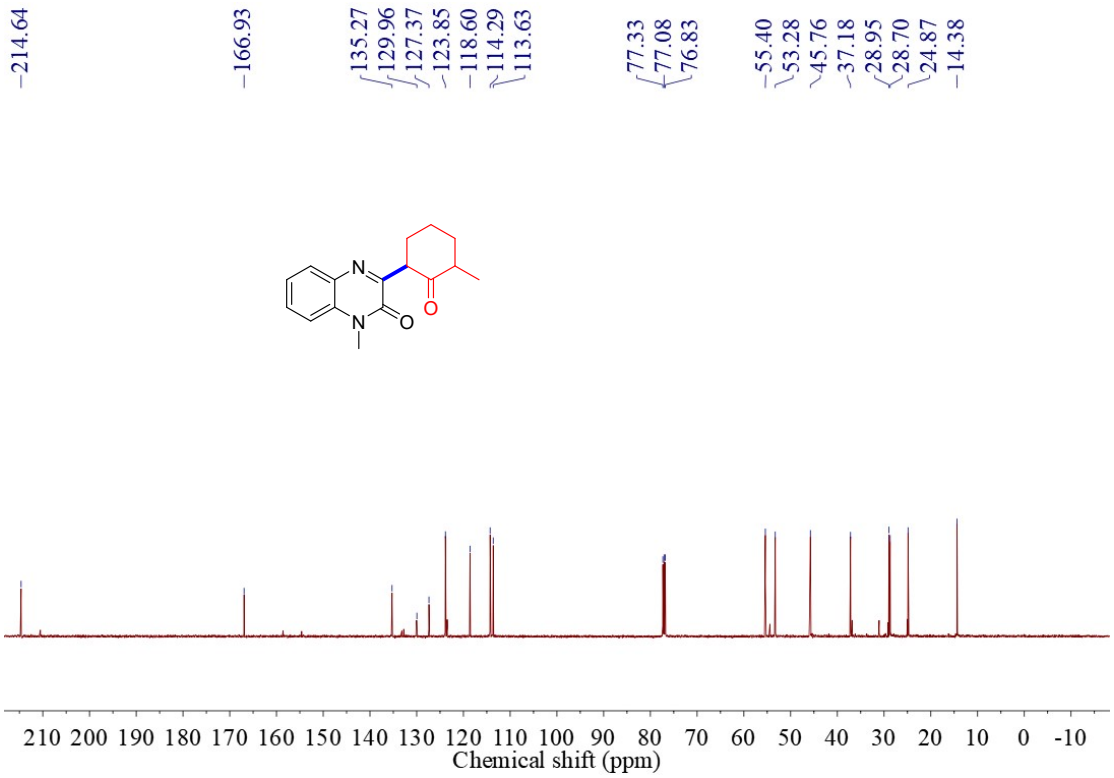
3u ^{13}C NMR



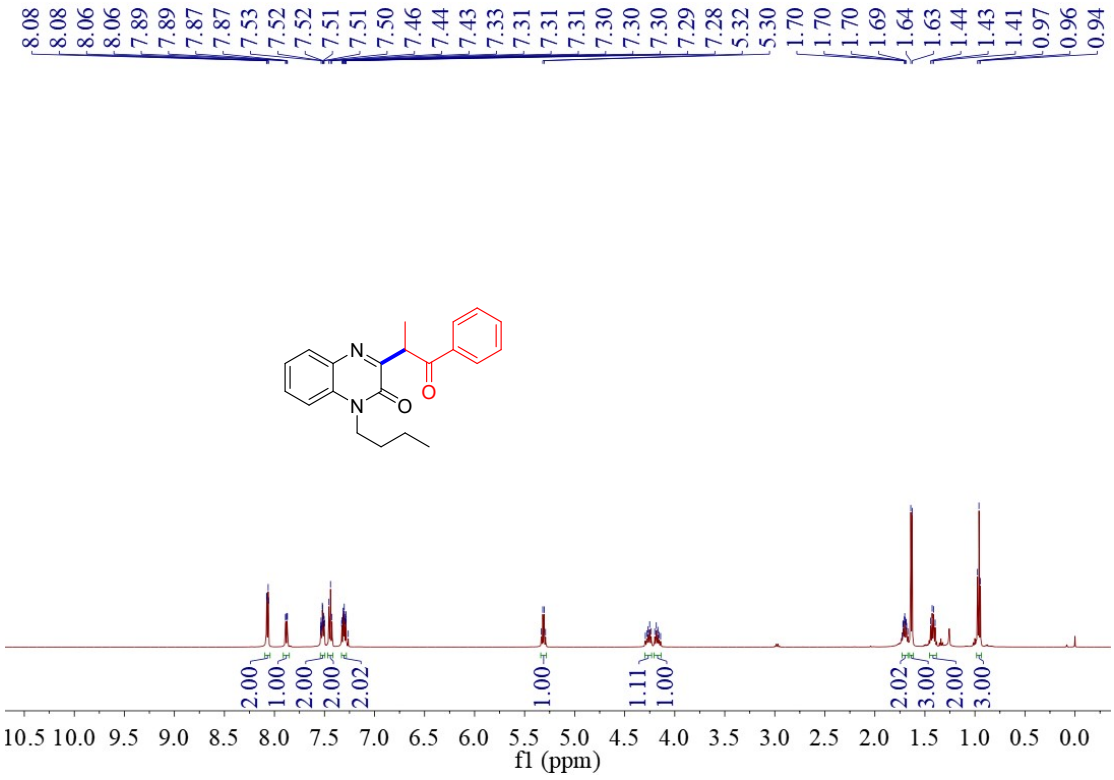
3v ^{1}H NMR



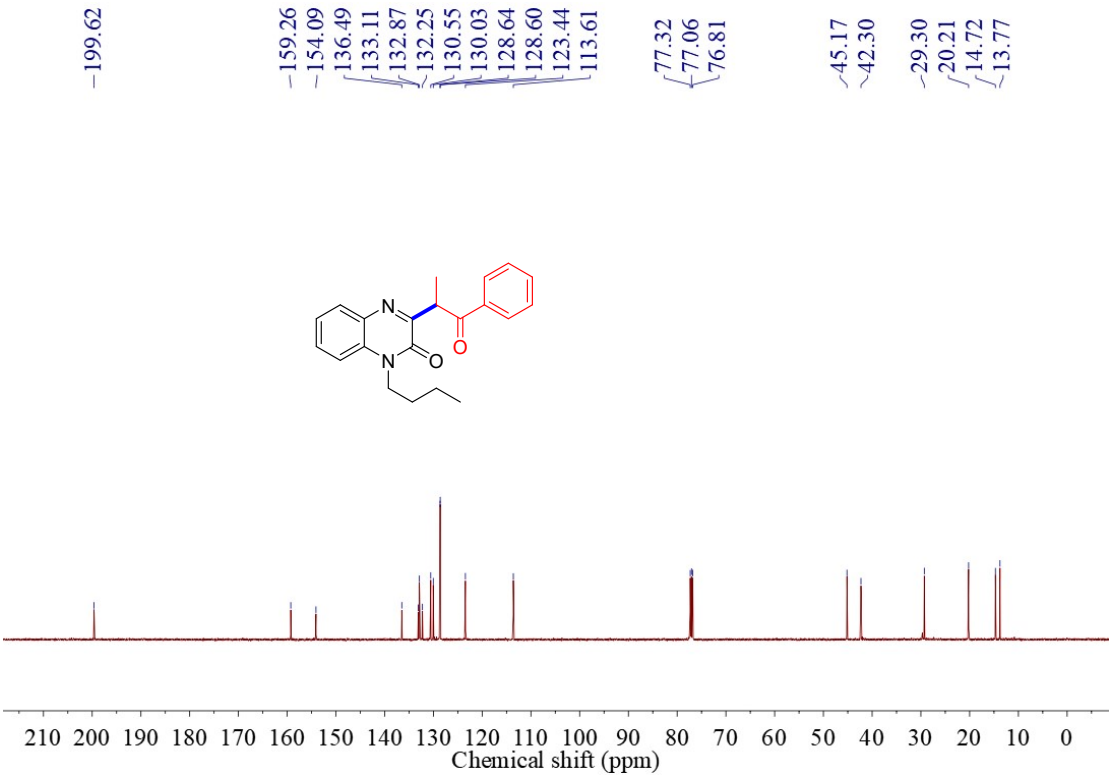
3v ^{13}C NMR



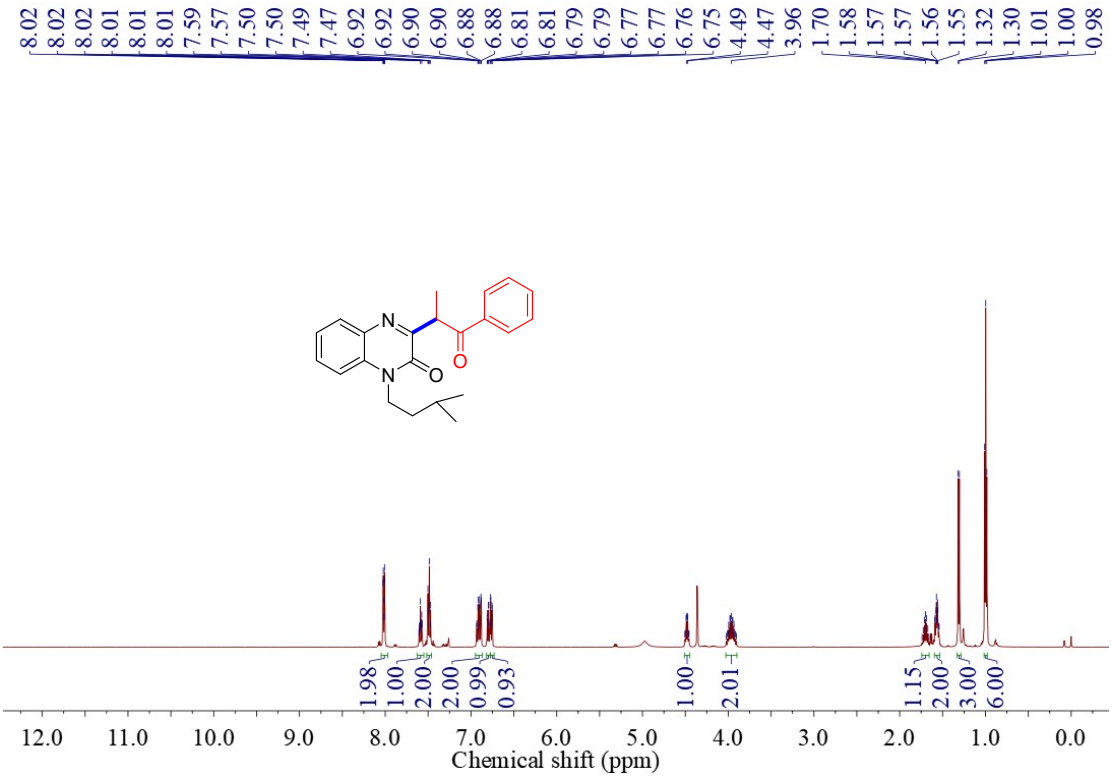
3w ^{1}H NMR



3w ^{13}C NMR



3x ^{1}H NMR



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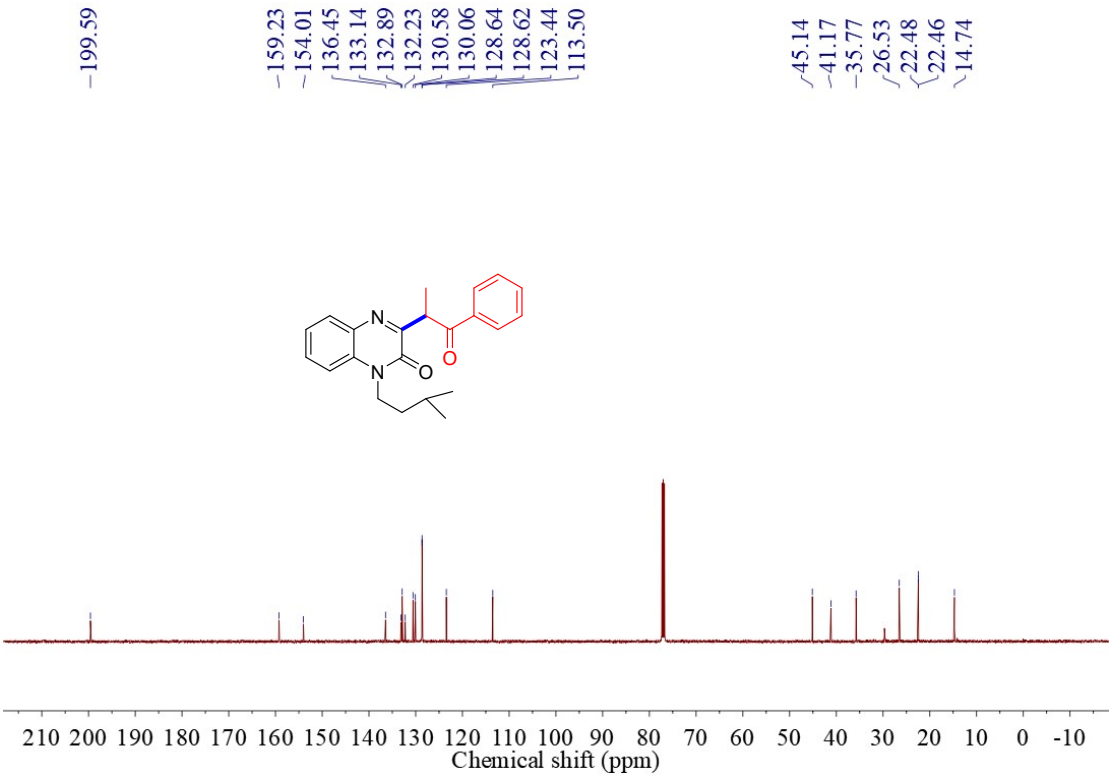

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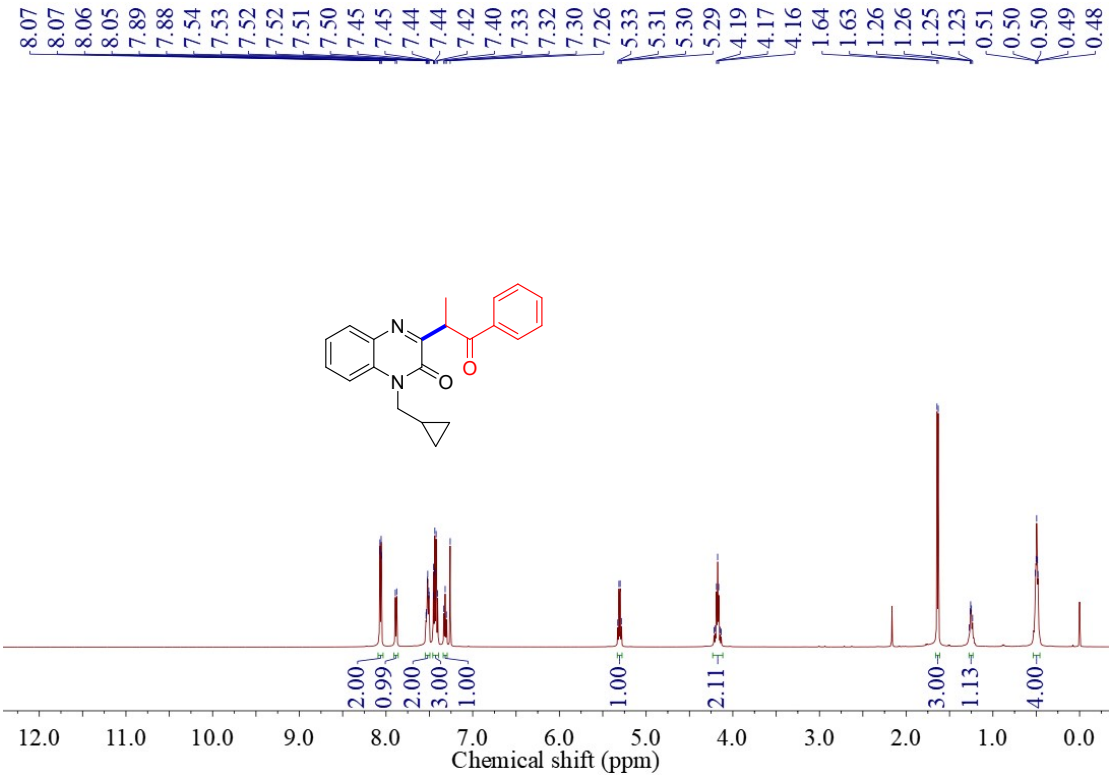

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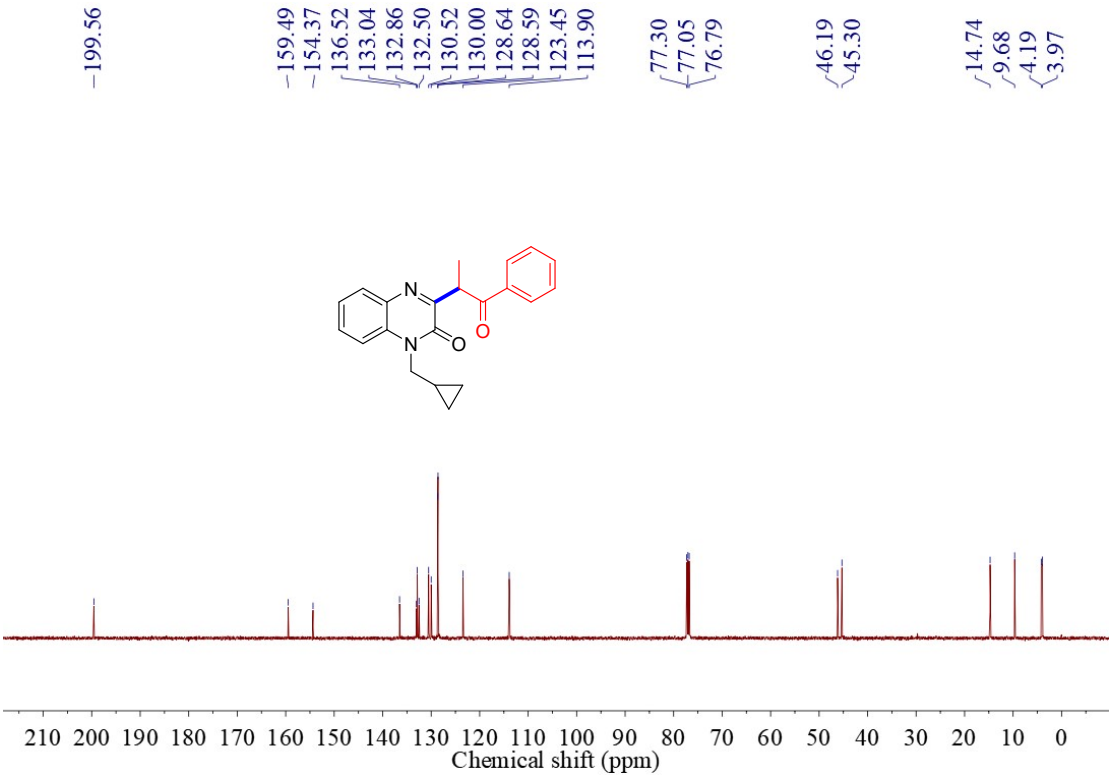

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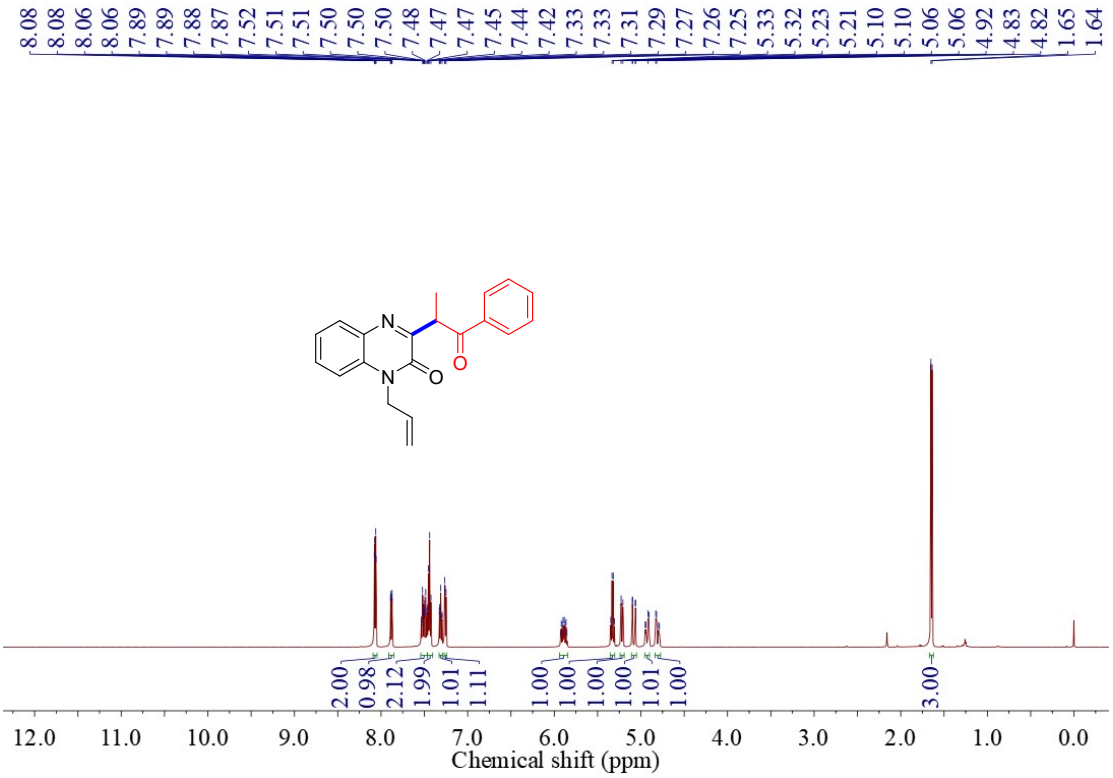

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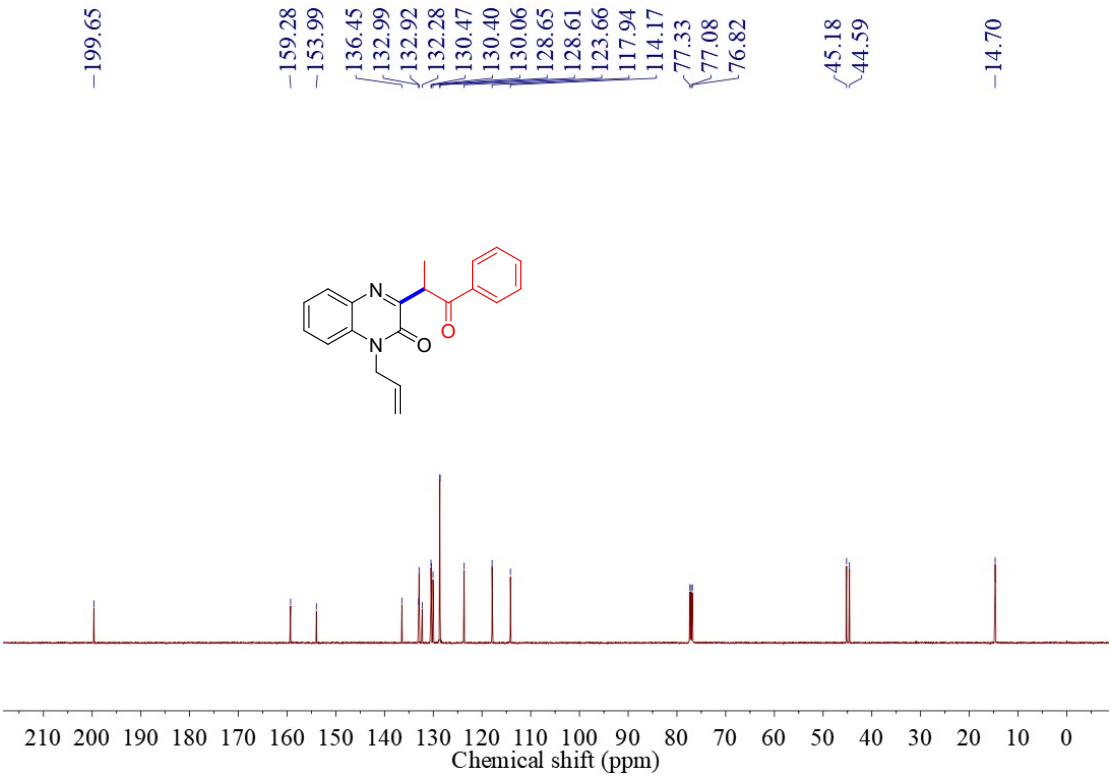
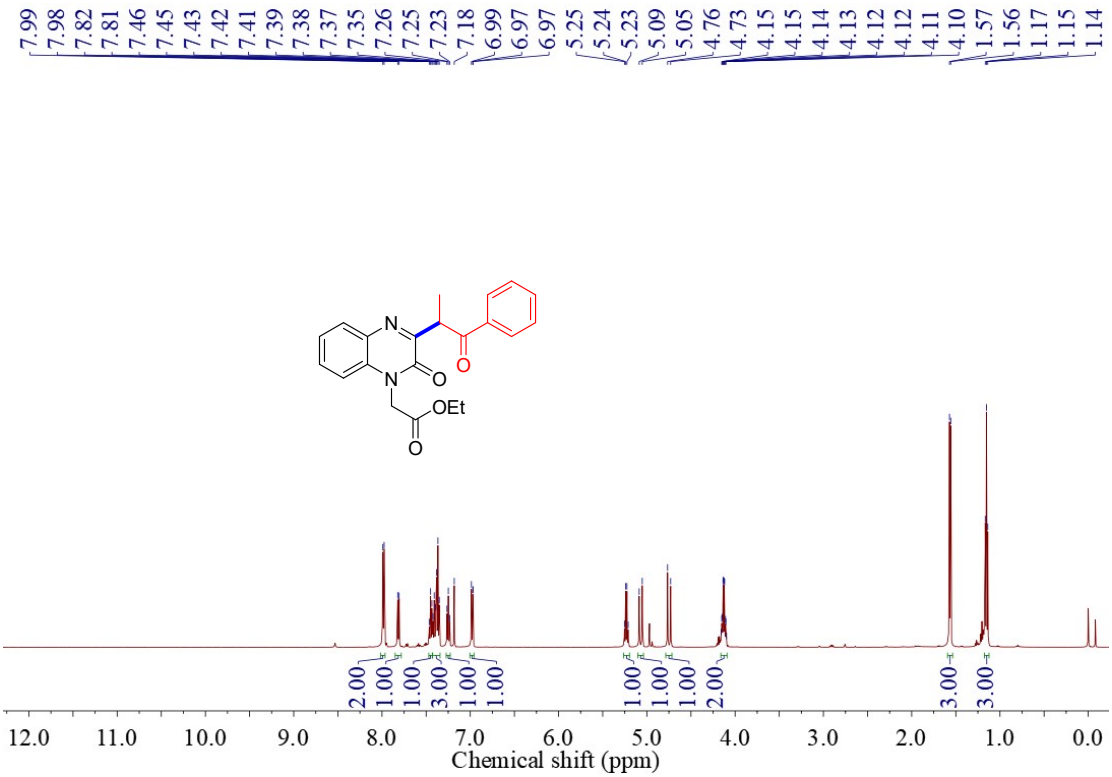


3aa ^{1}H NMR



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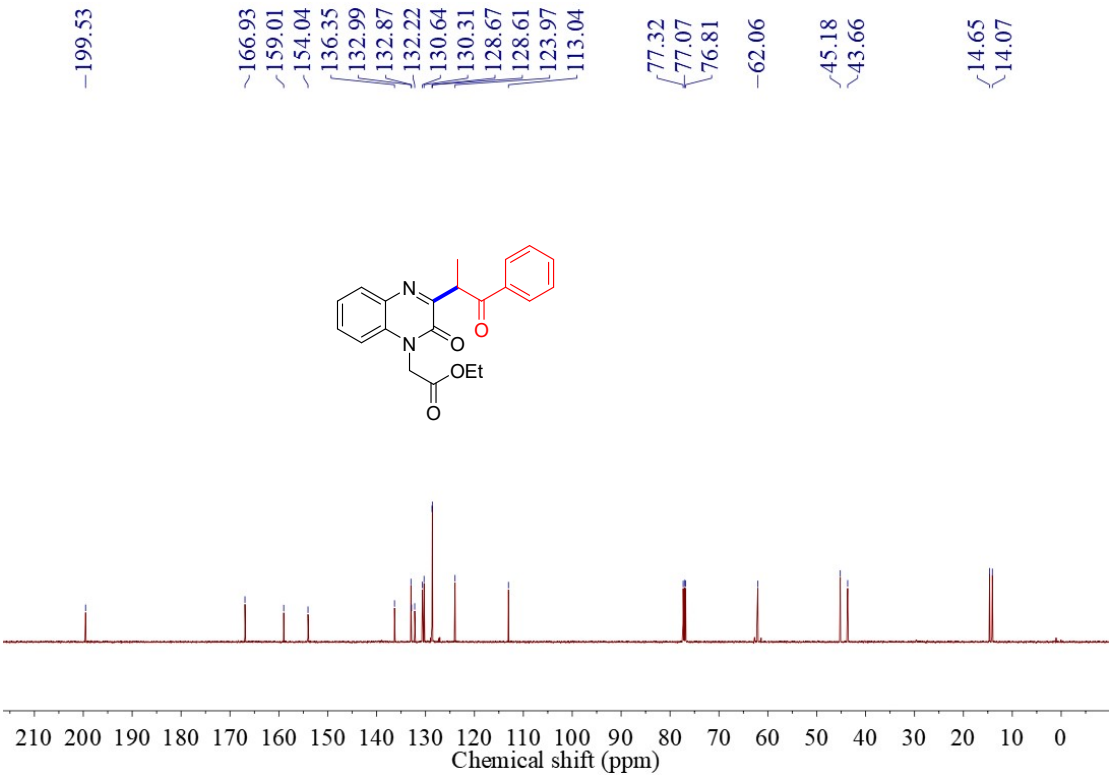

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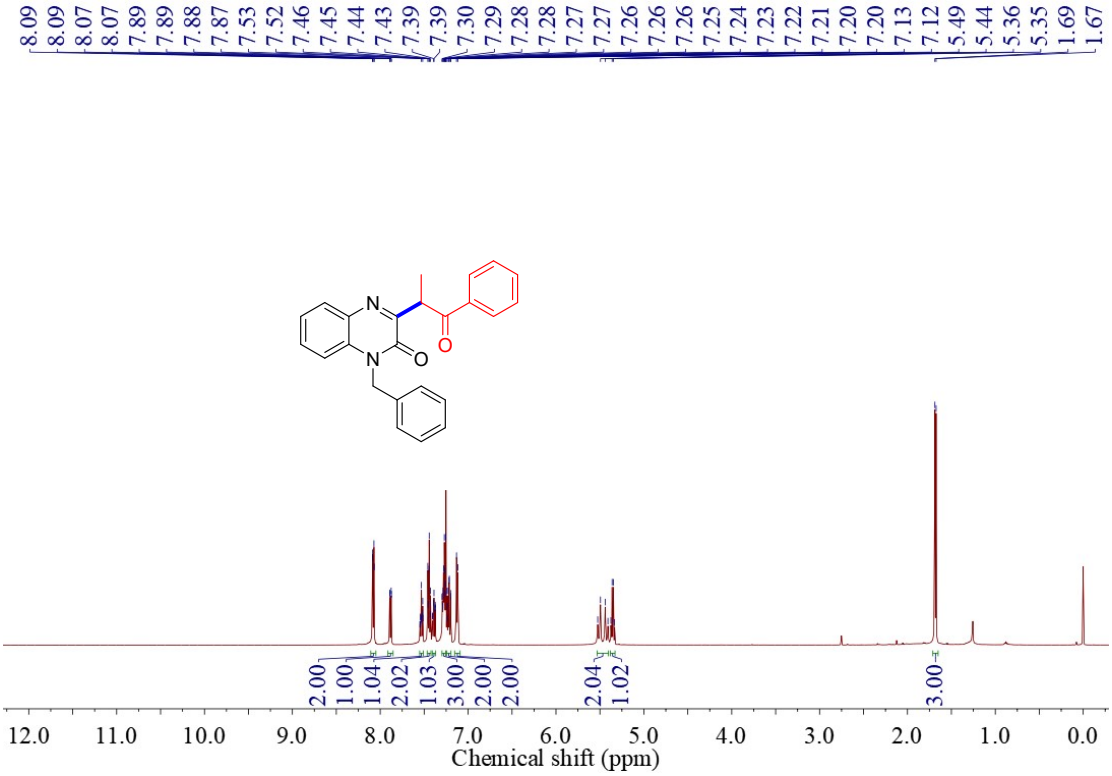

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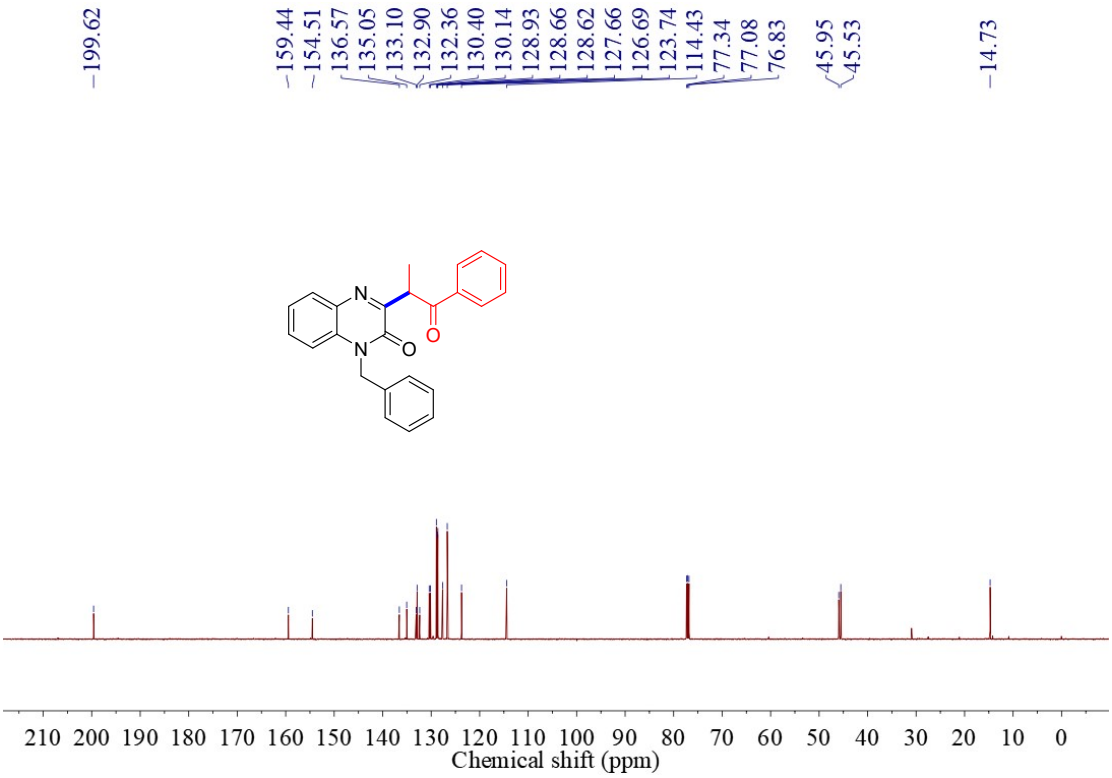

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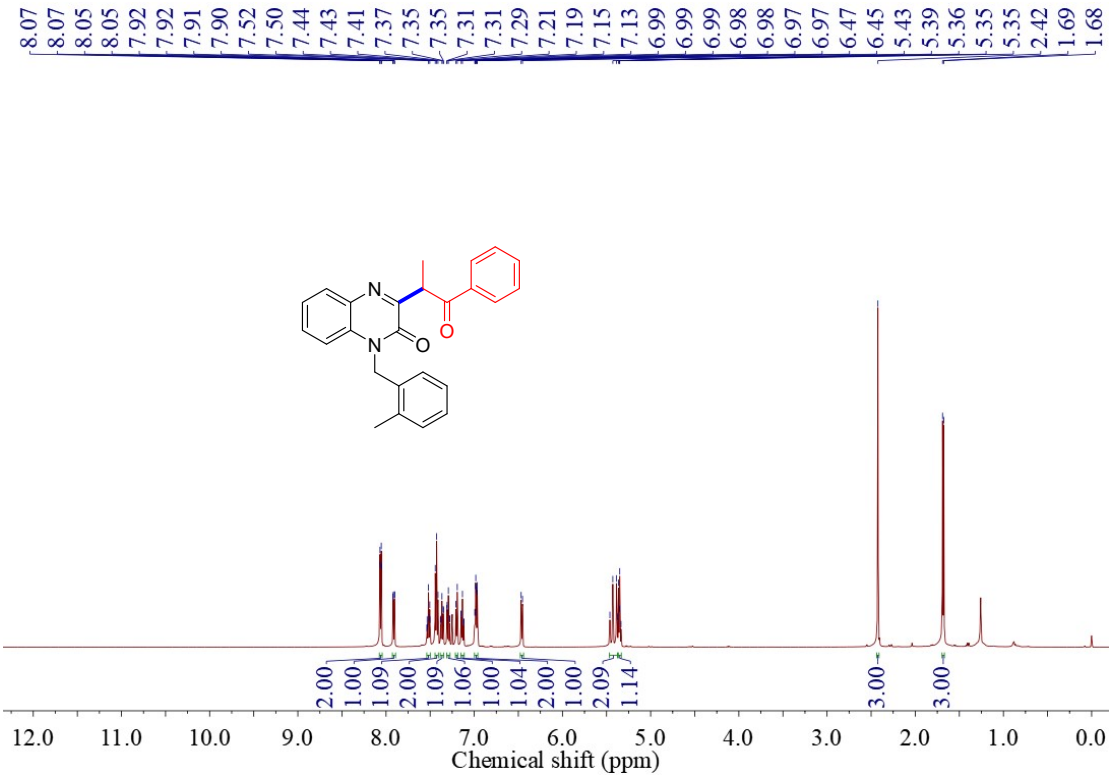

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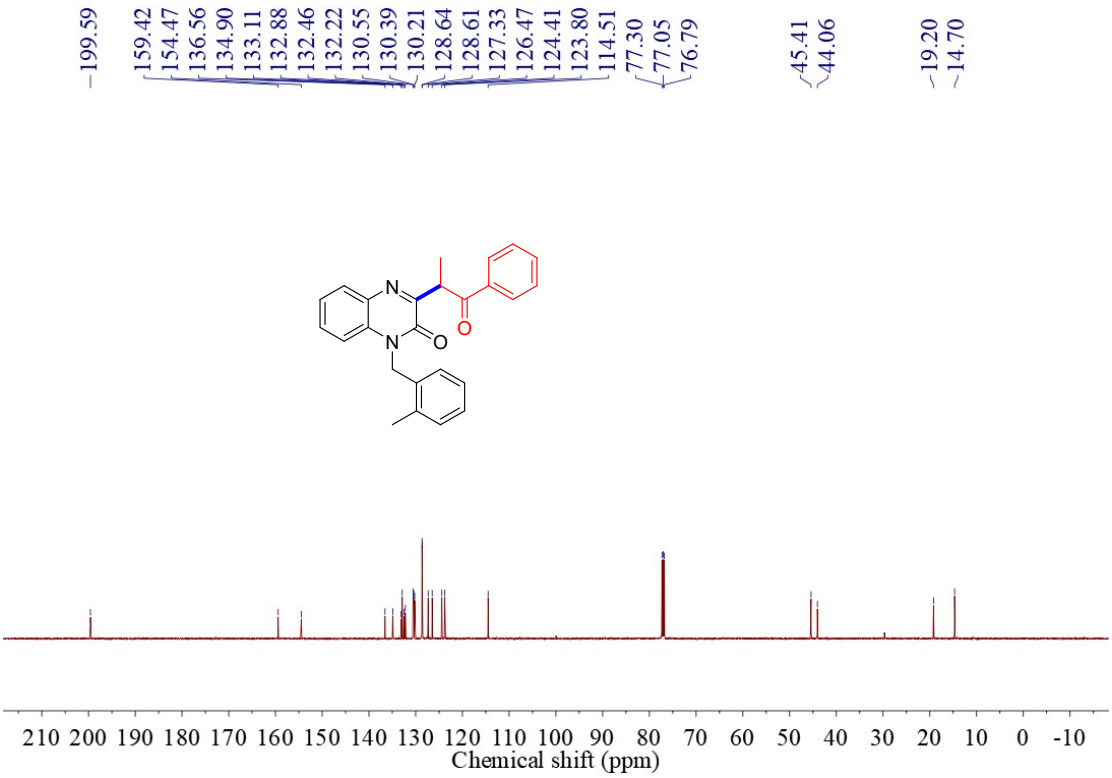
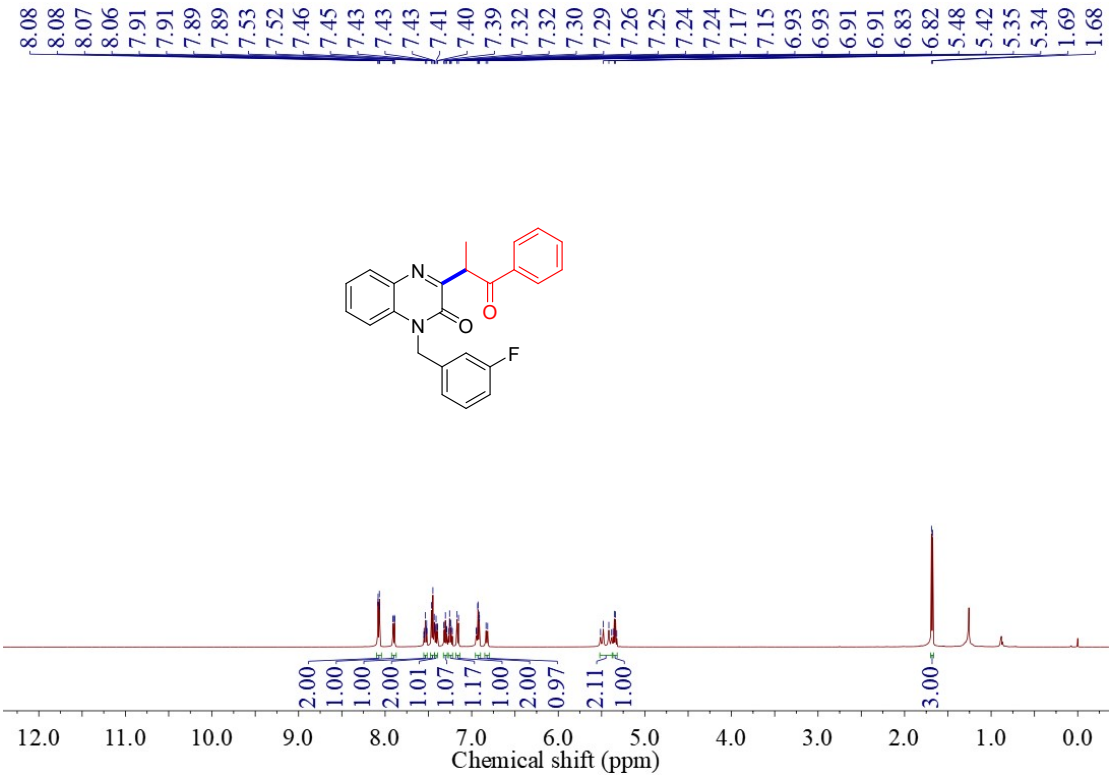


3ad ^{1}H NMR



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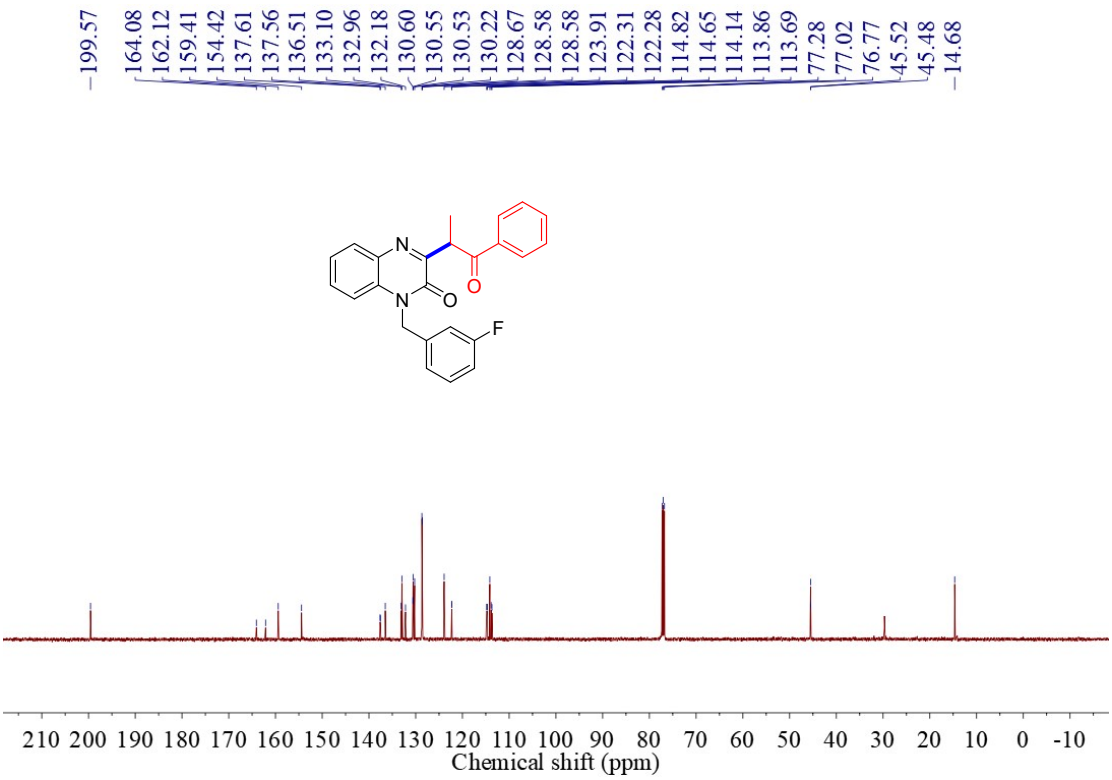
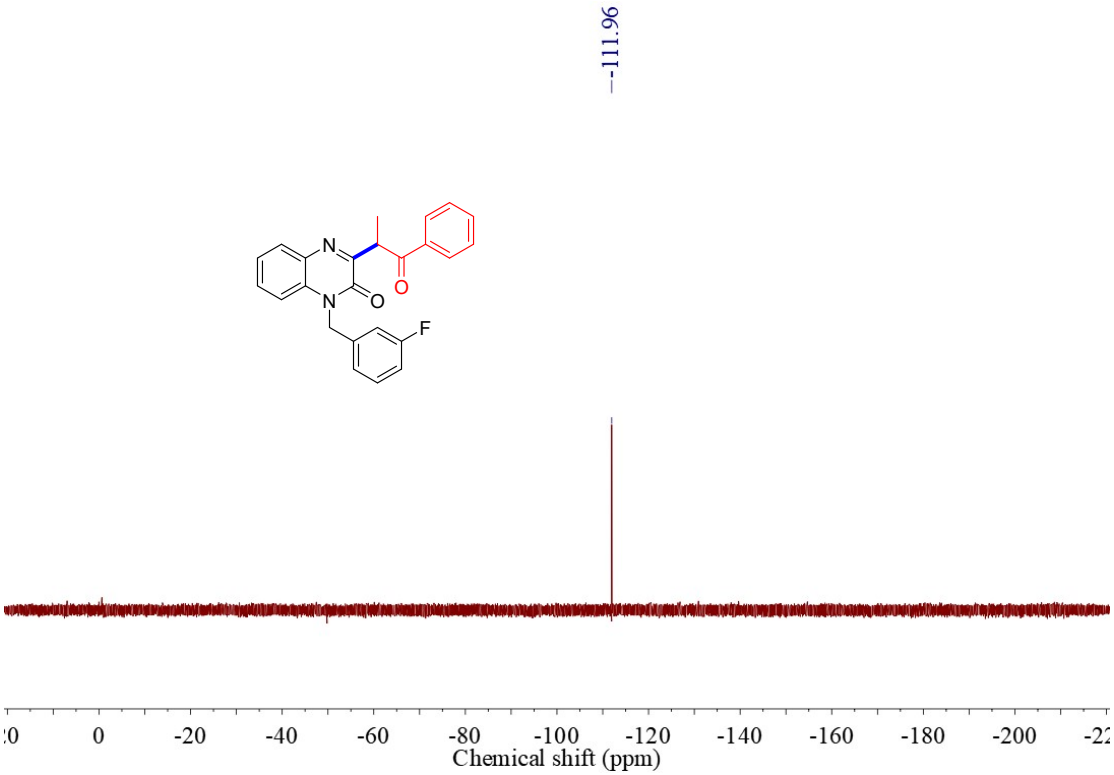
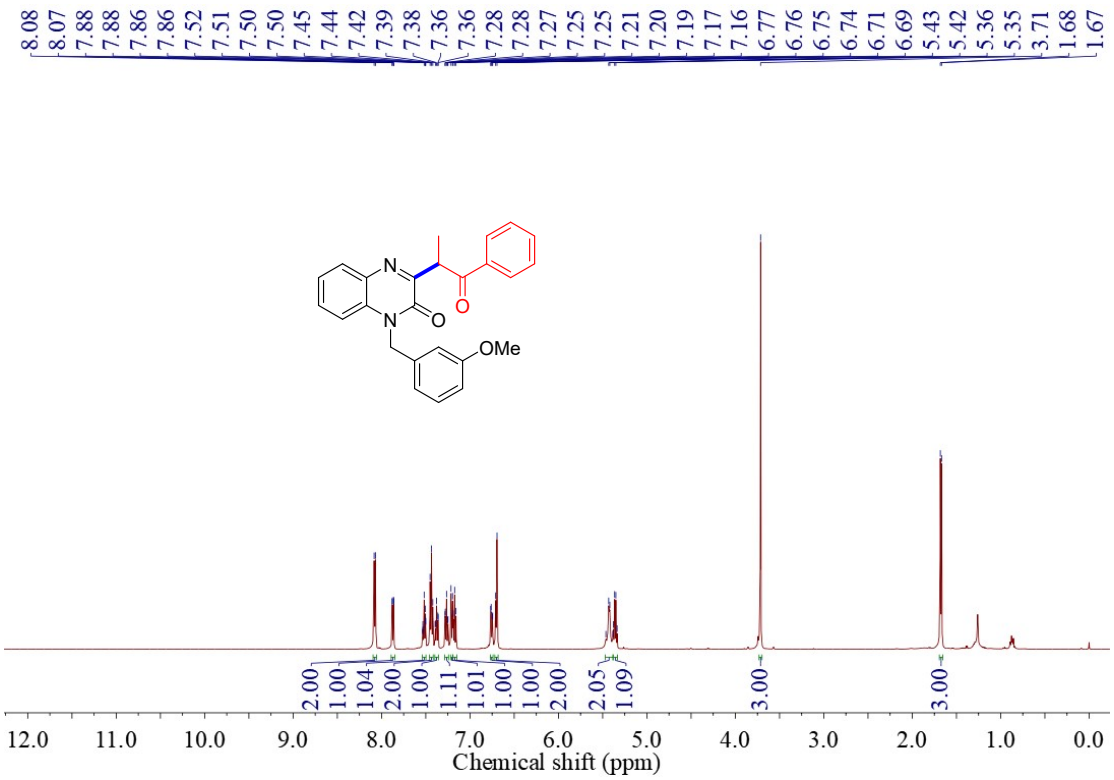


3ad ^{19}F NMR



3ae ^{1}H NMR



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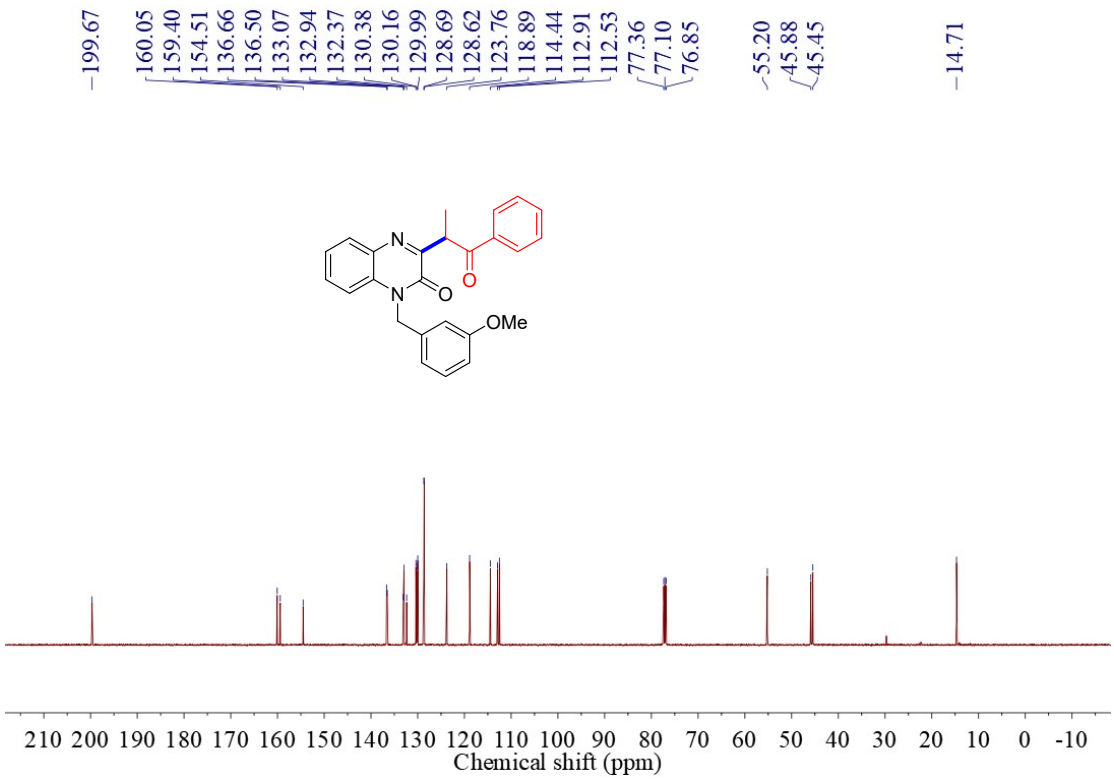

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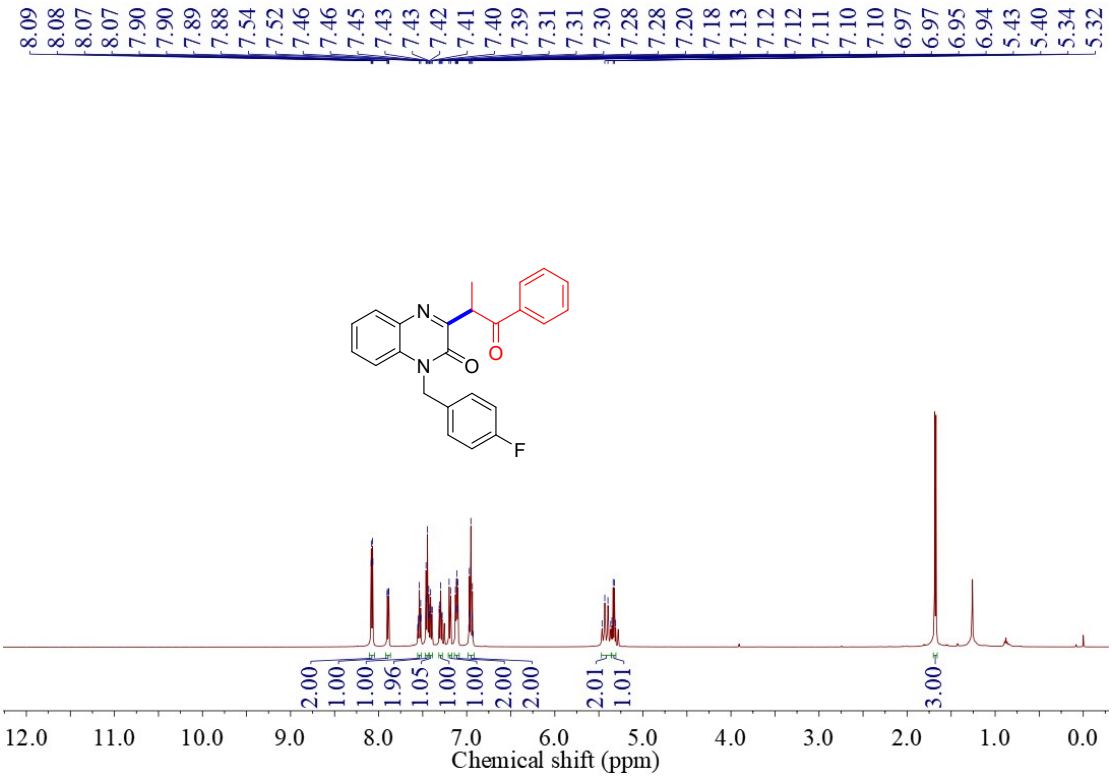

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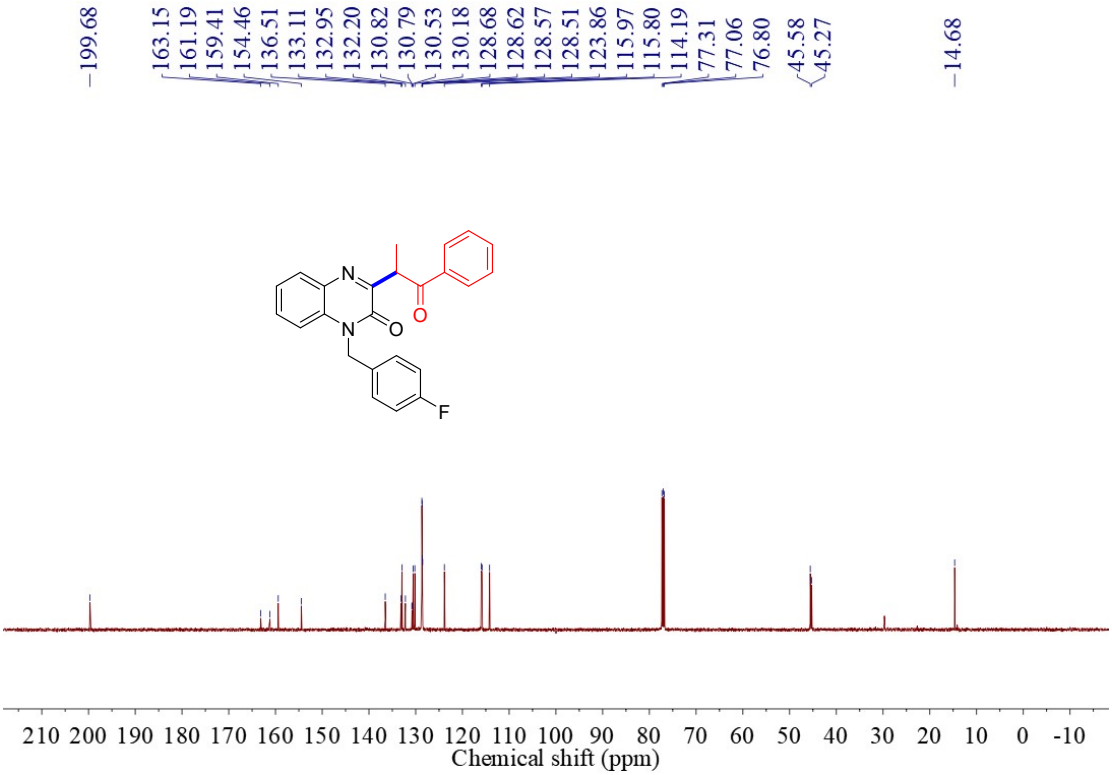

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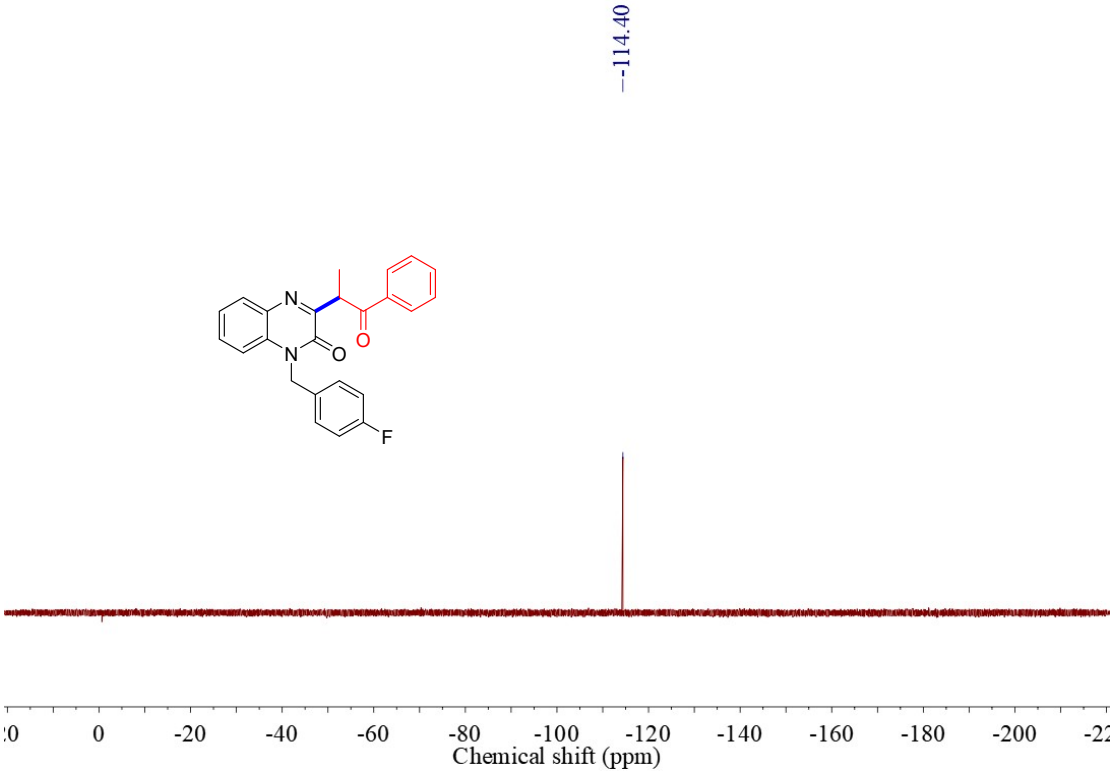

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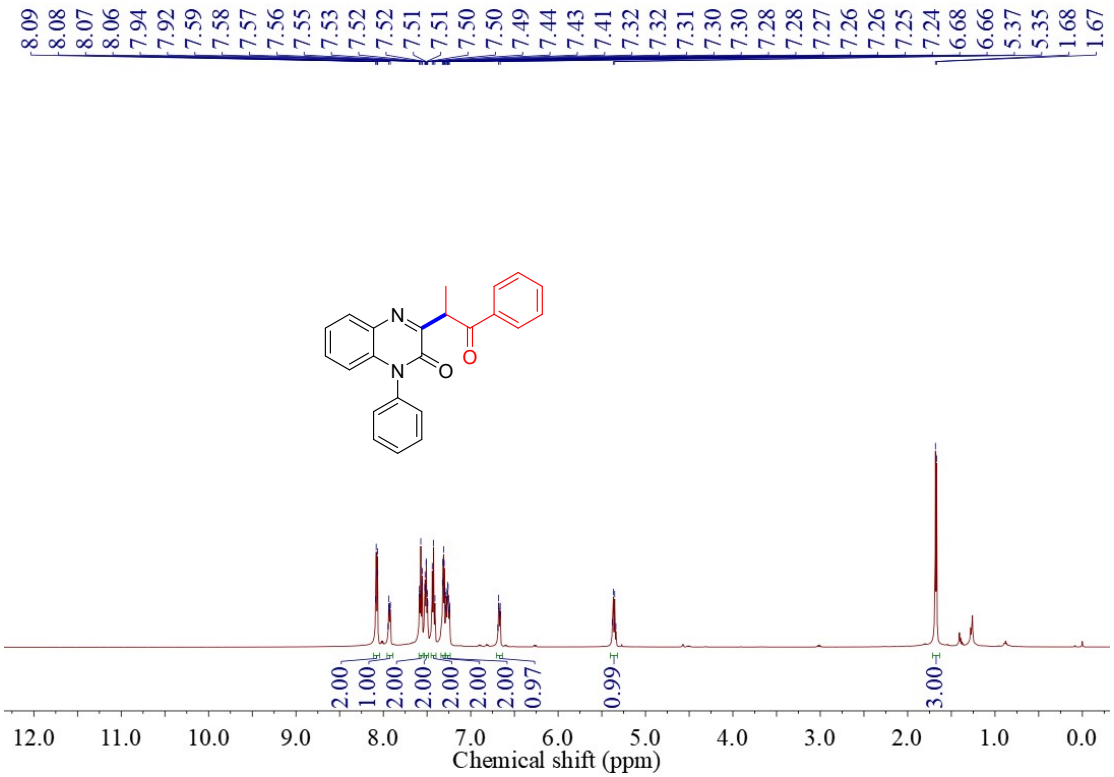

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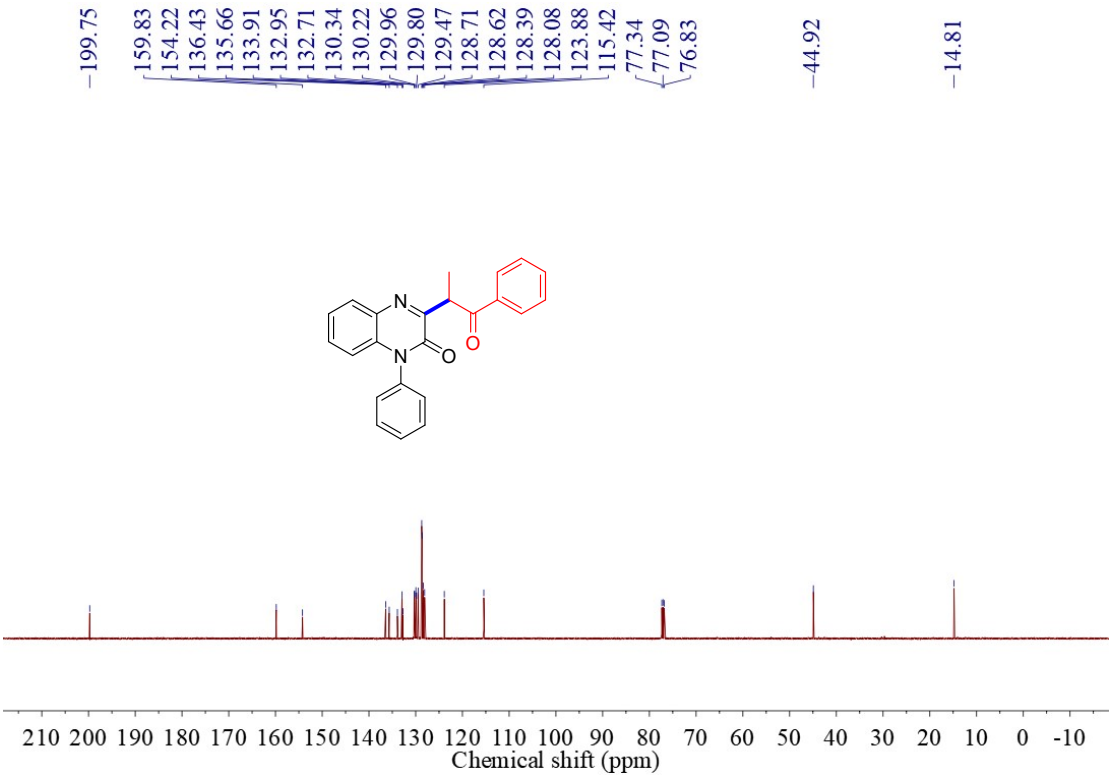

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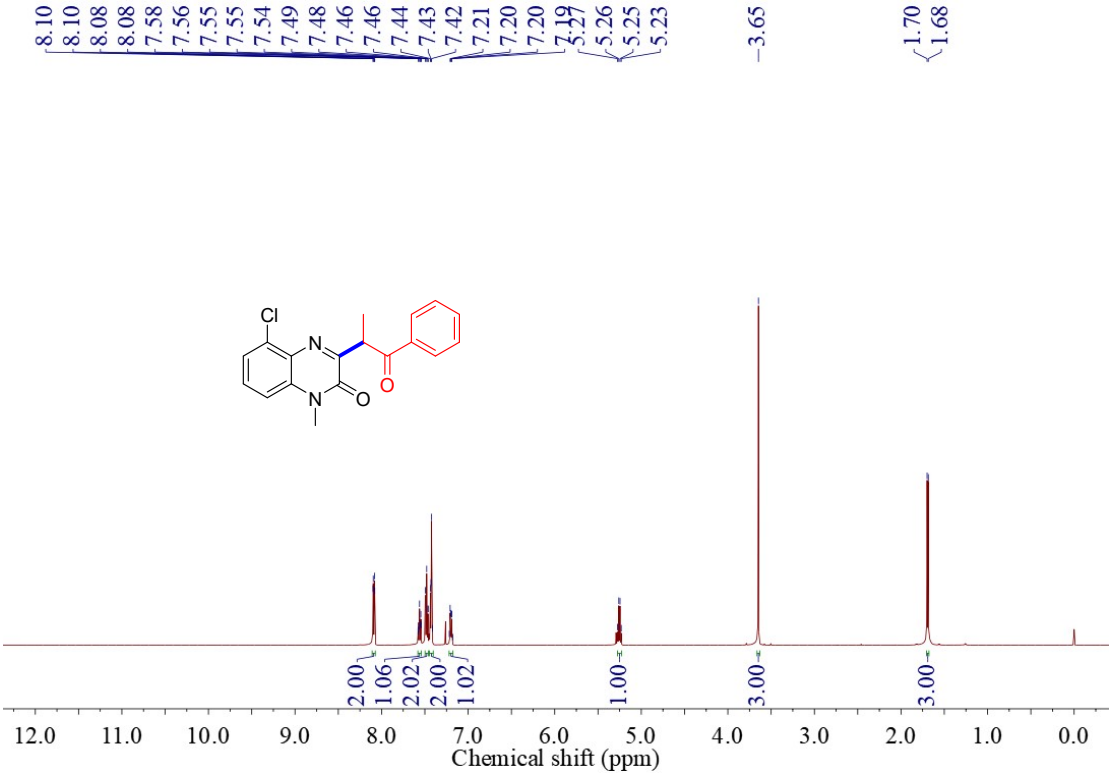

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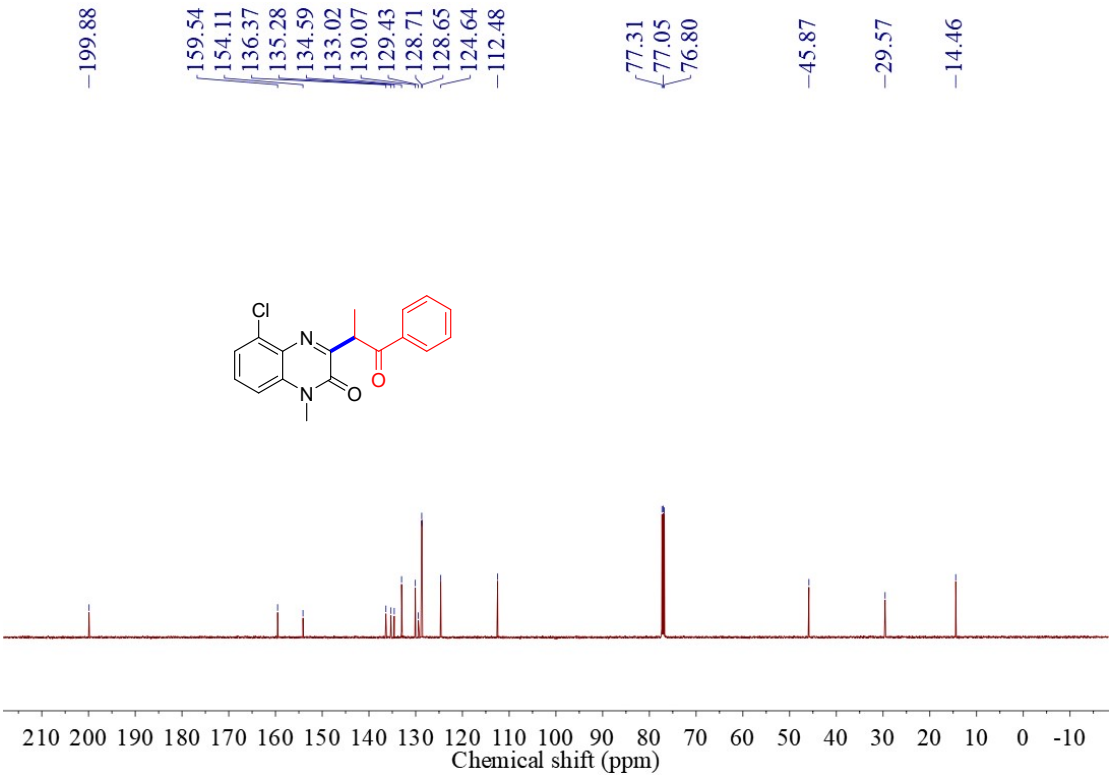

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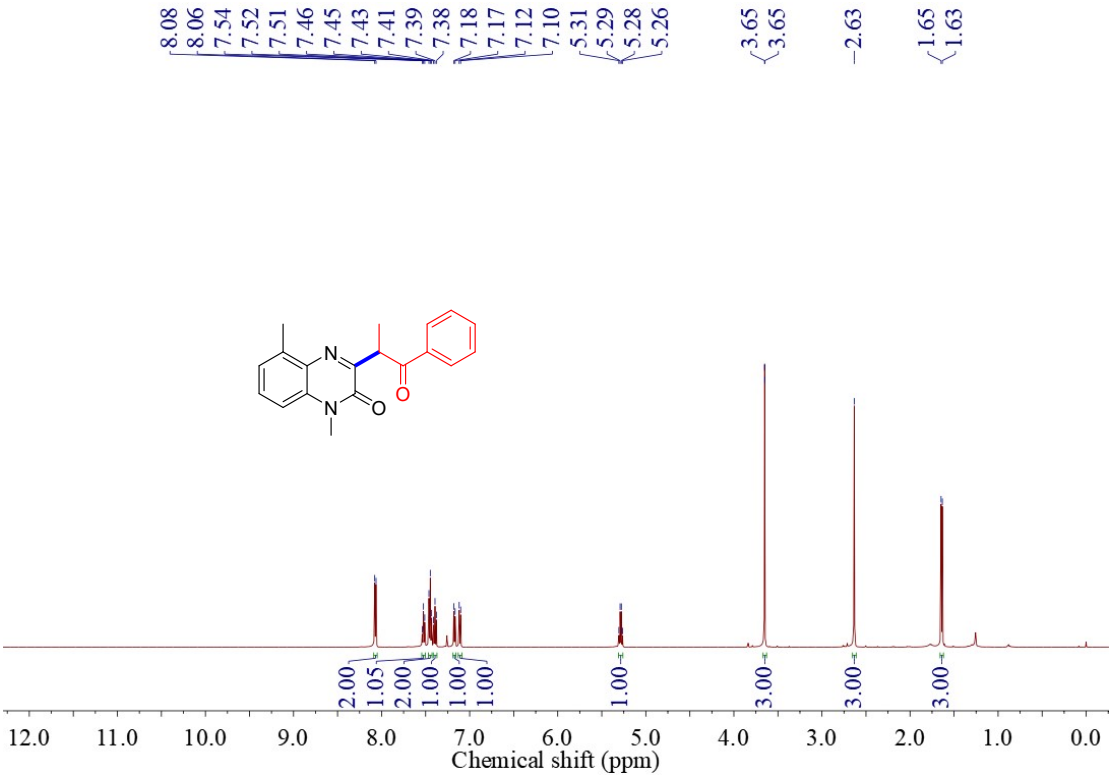

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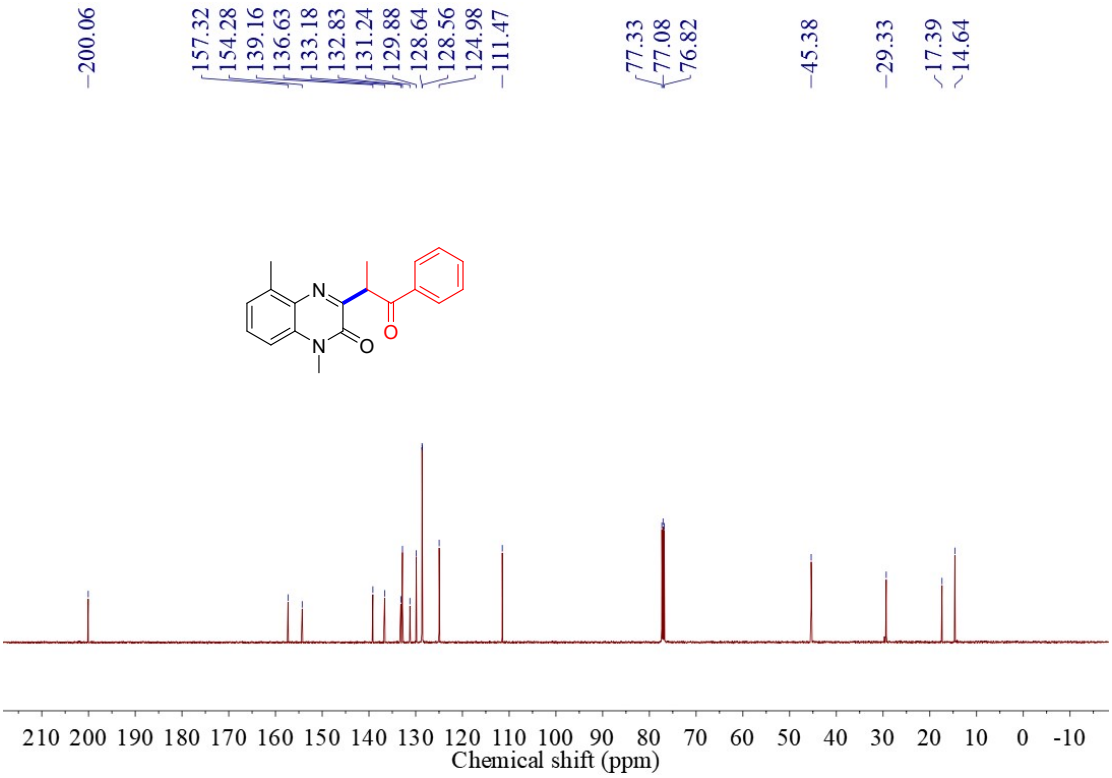

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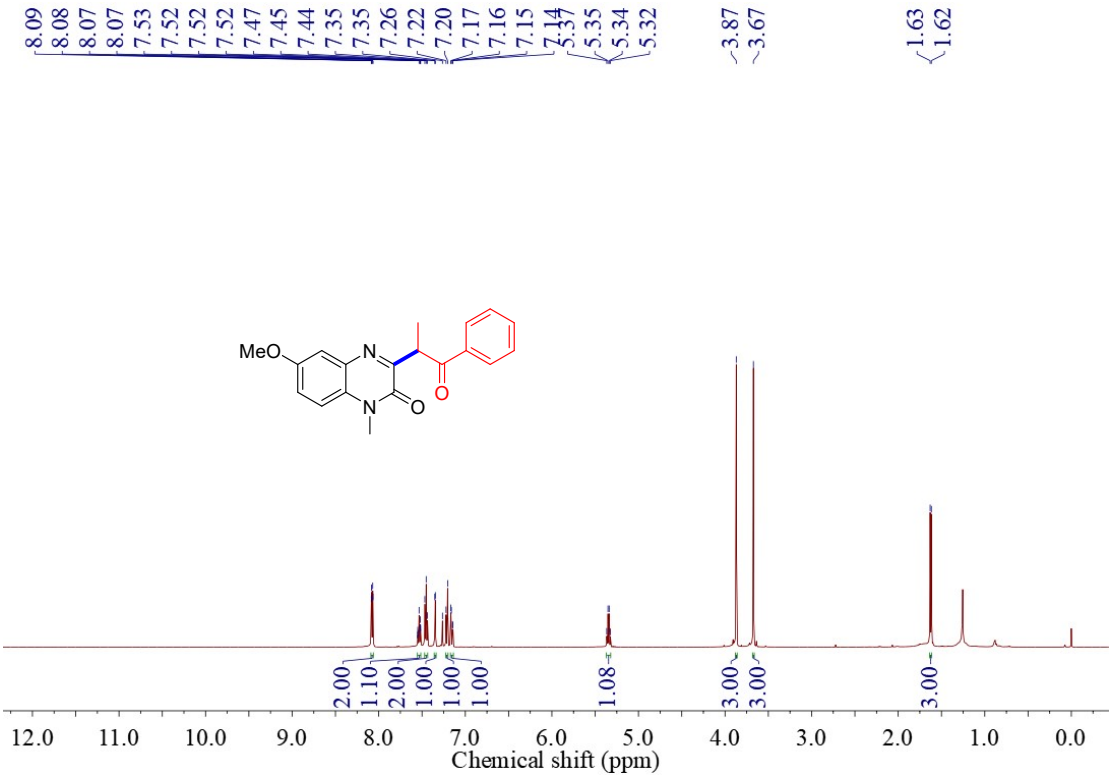

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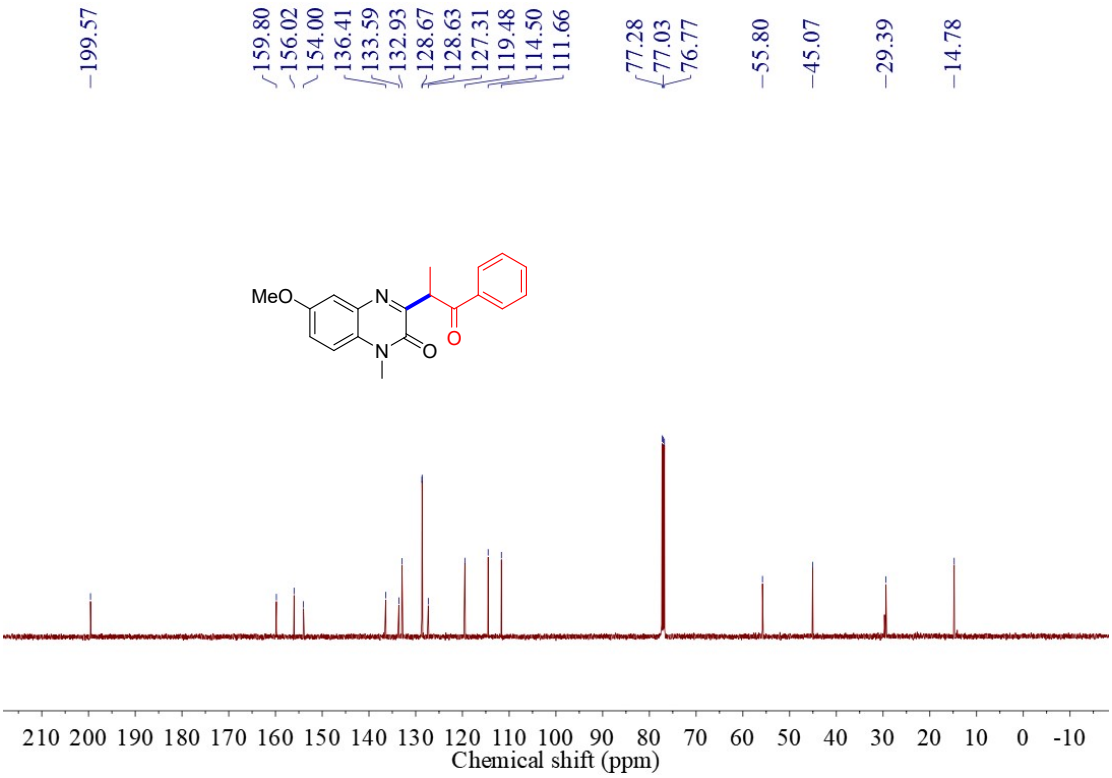

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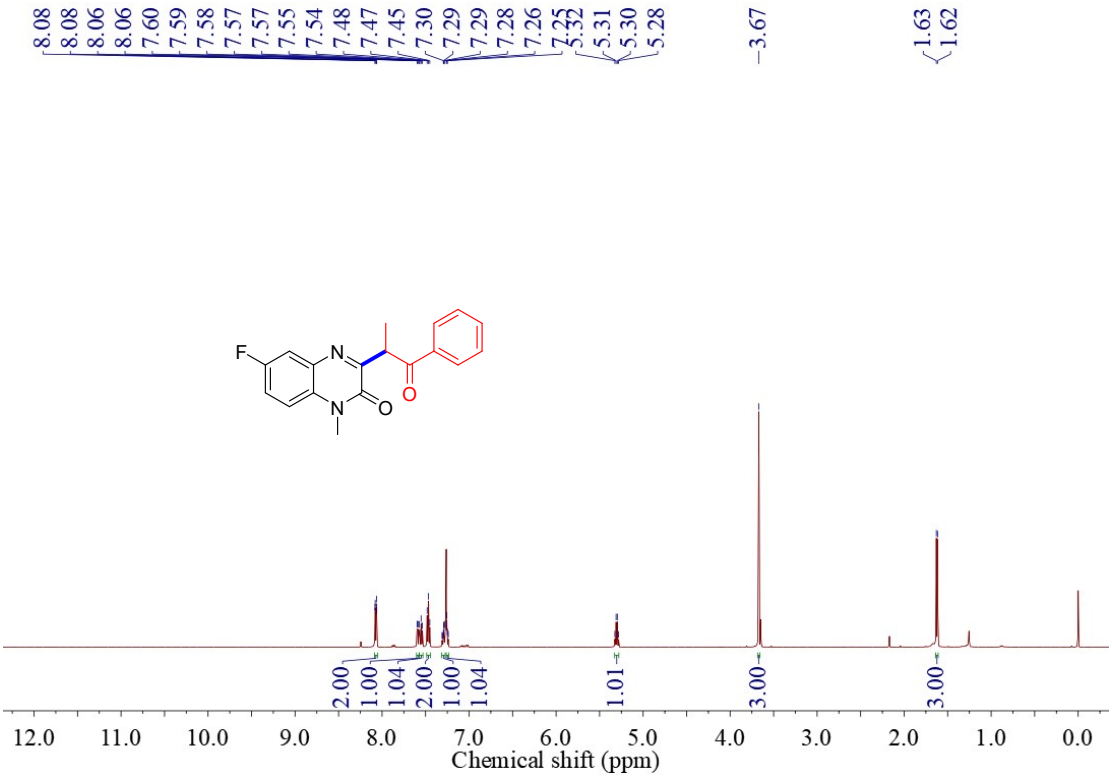

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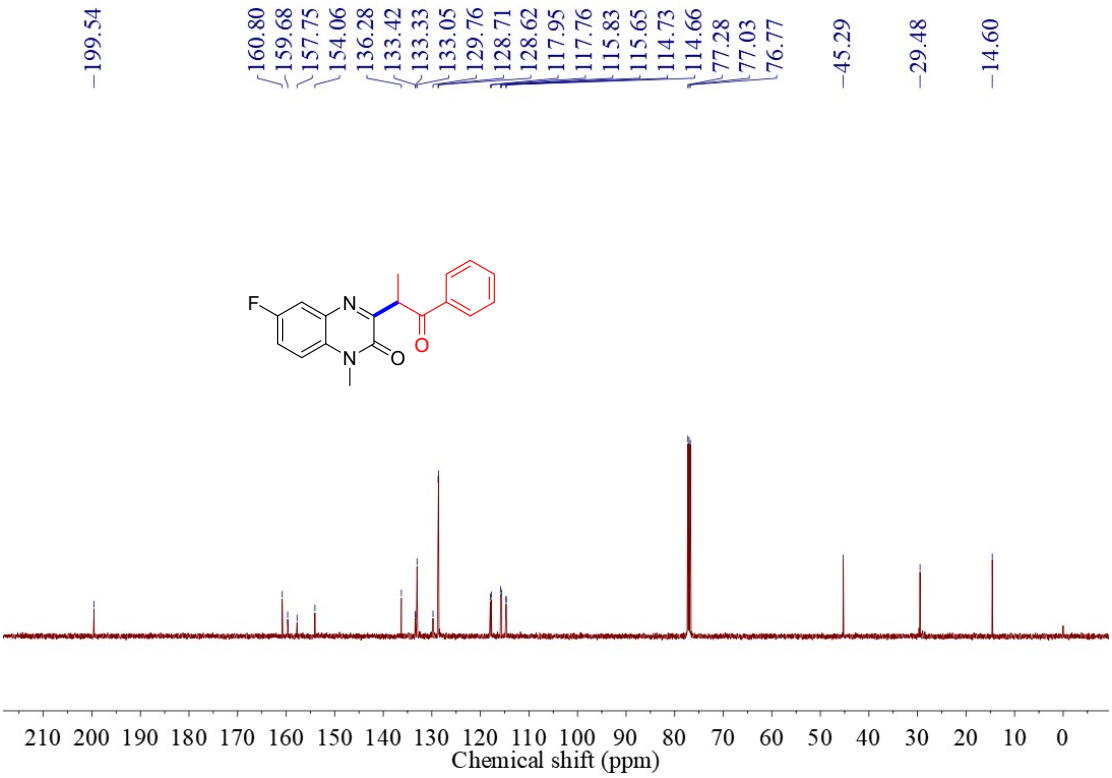
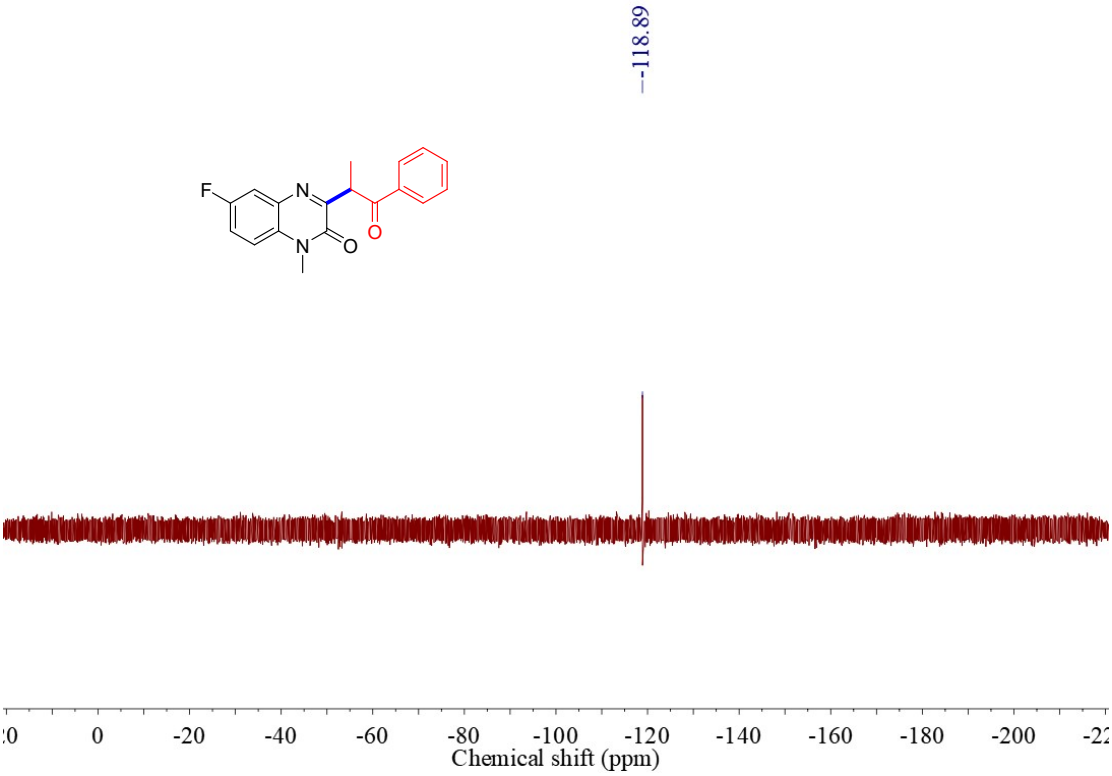


3ak ^{19}F NMR



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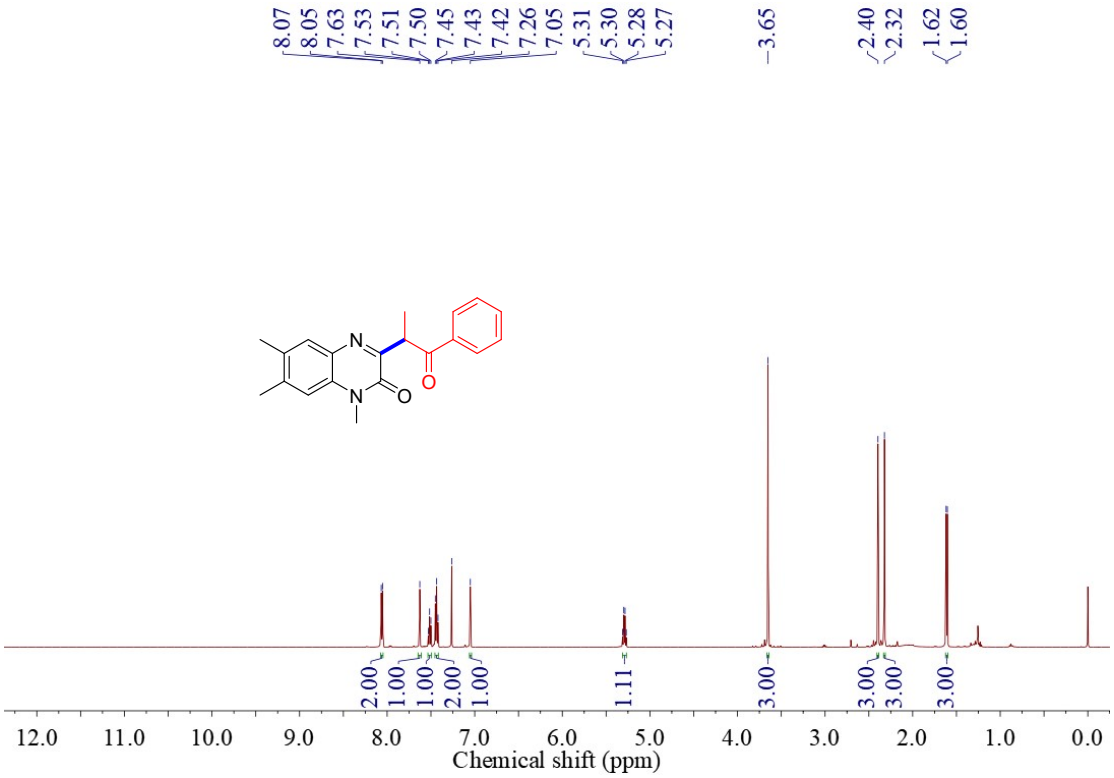

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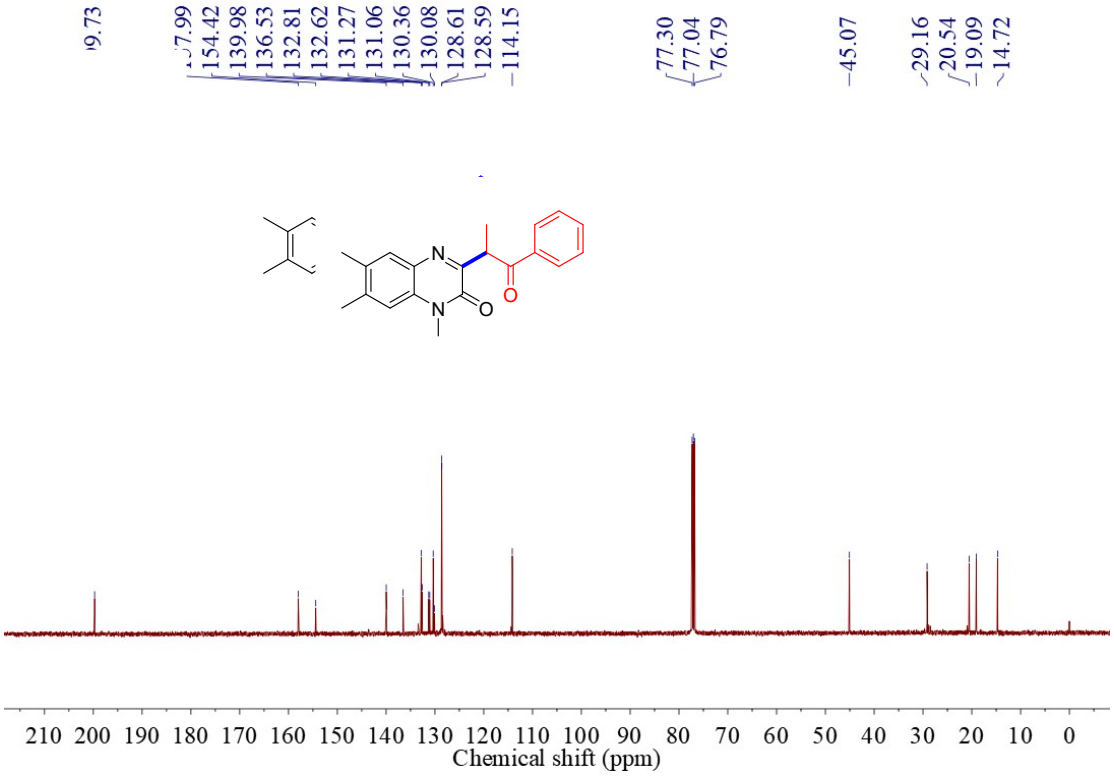

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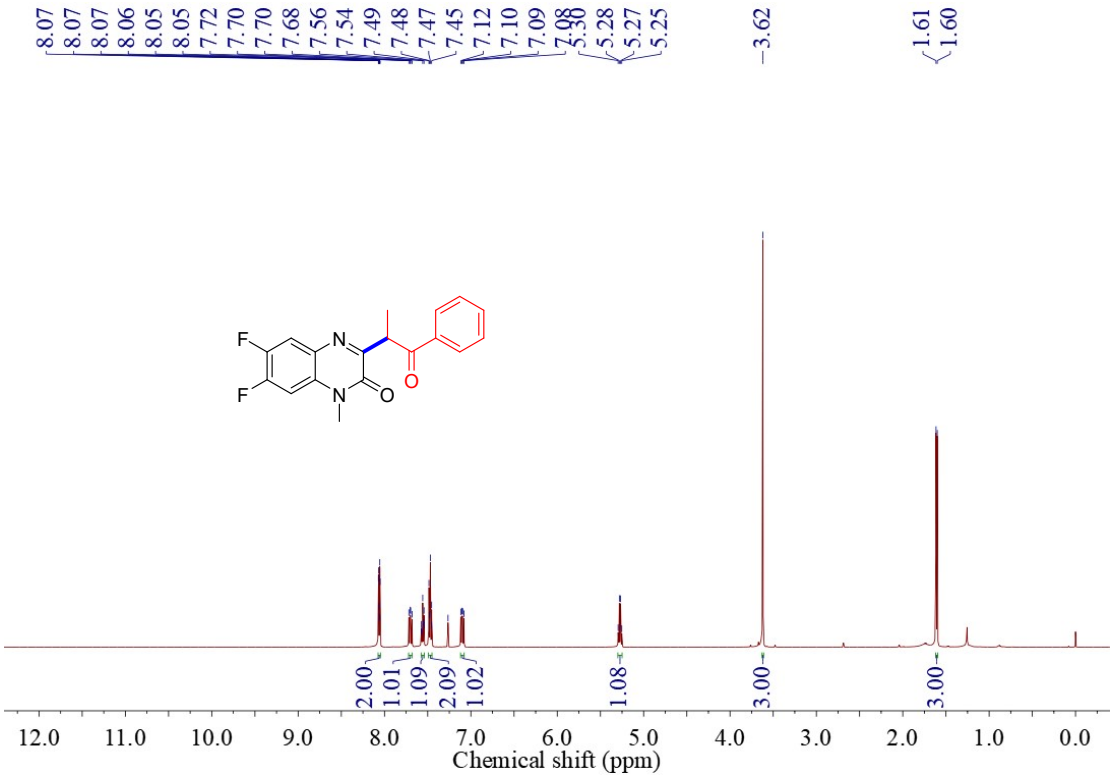

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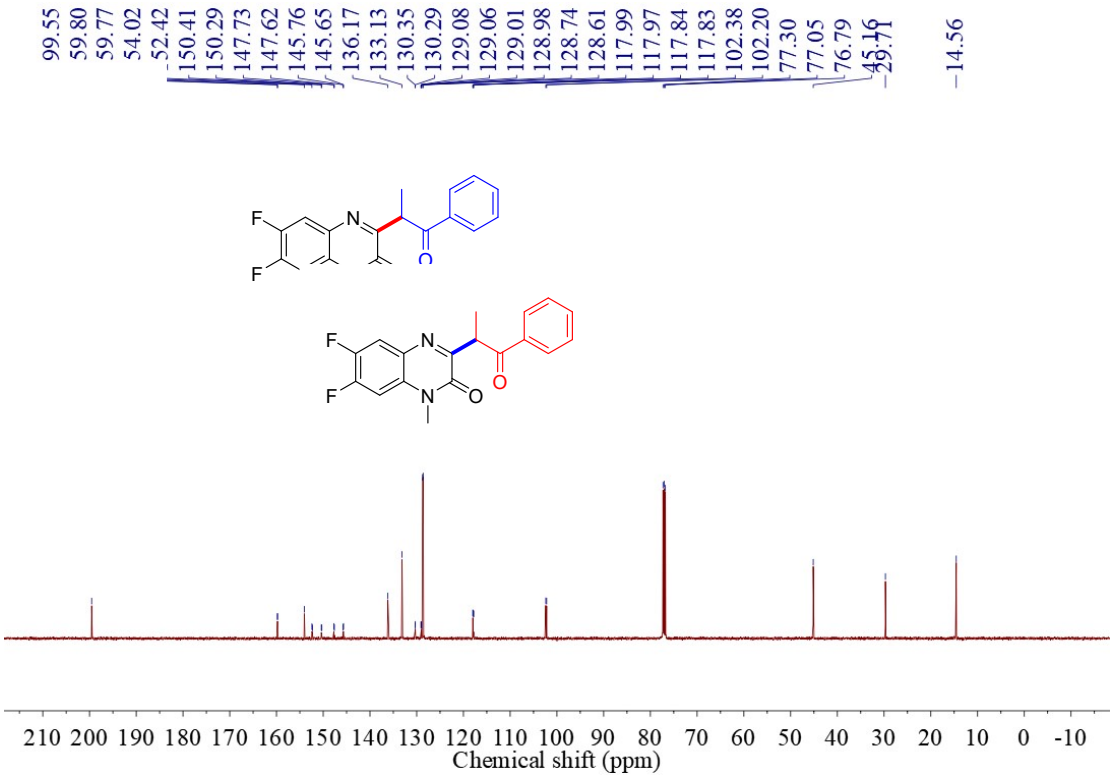

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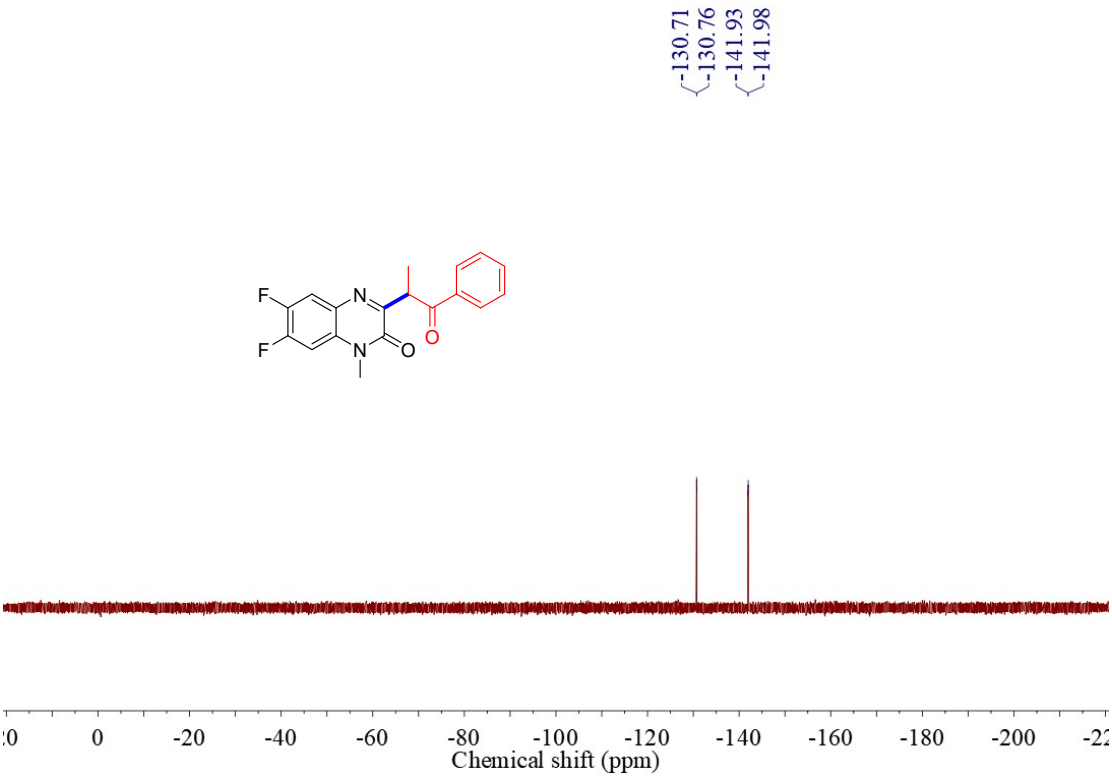

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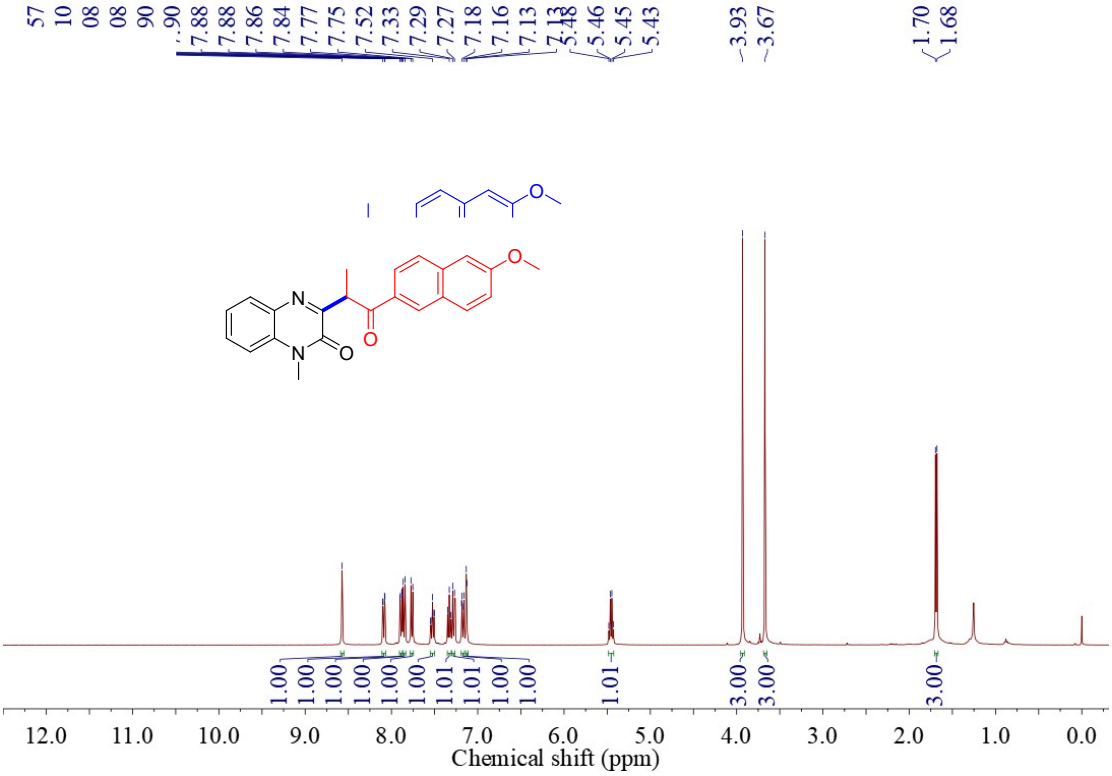

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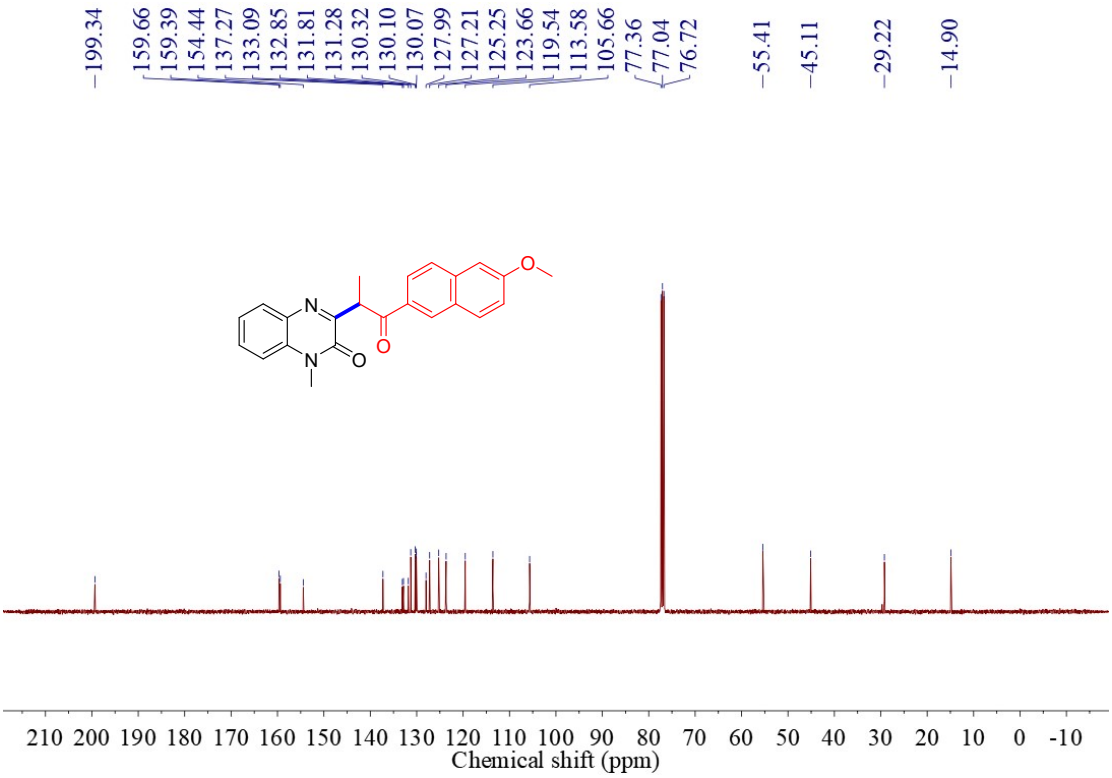

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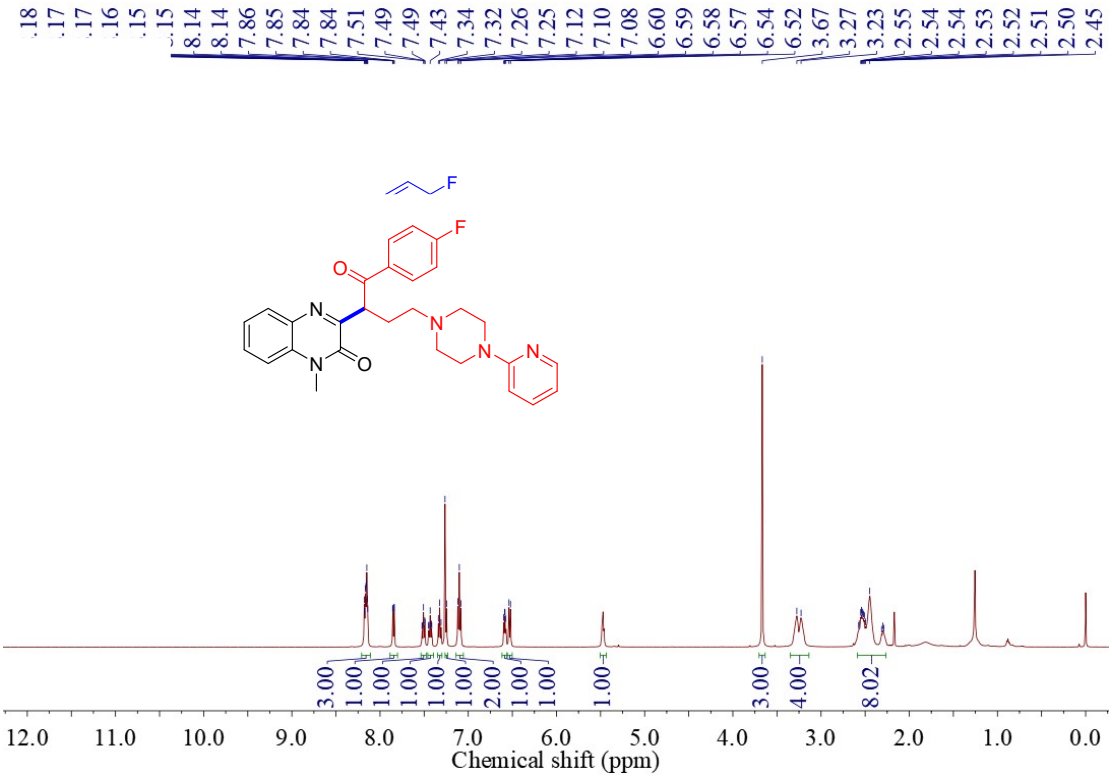
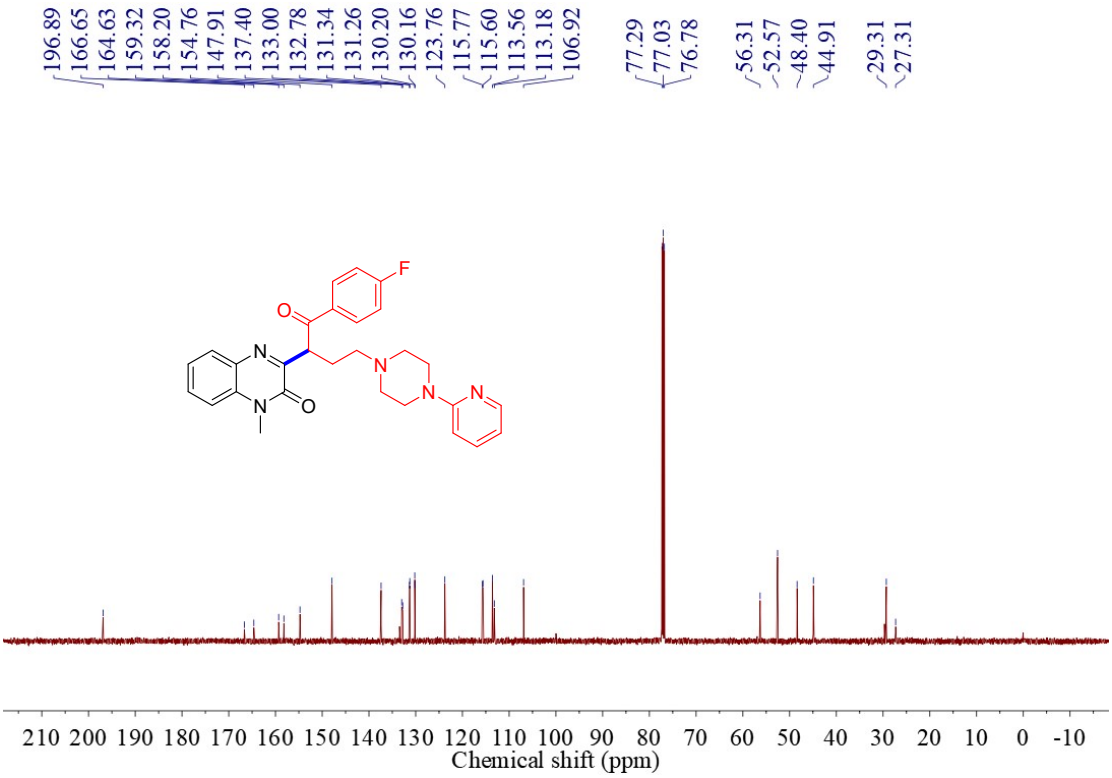
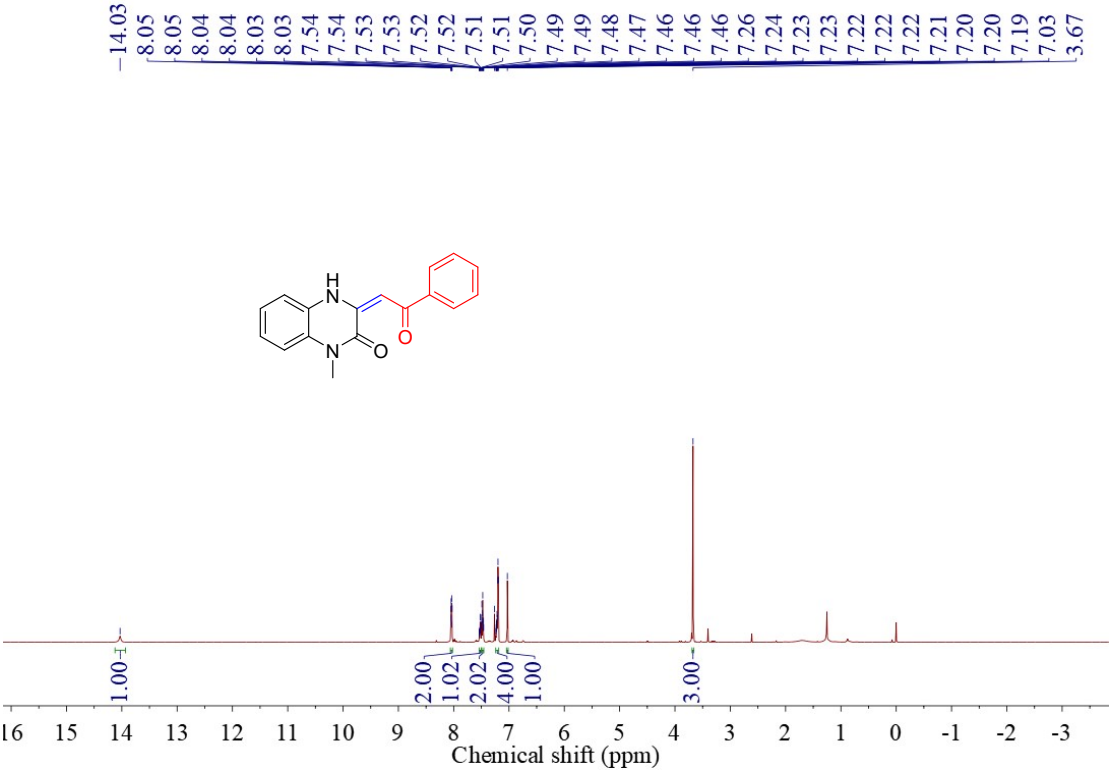


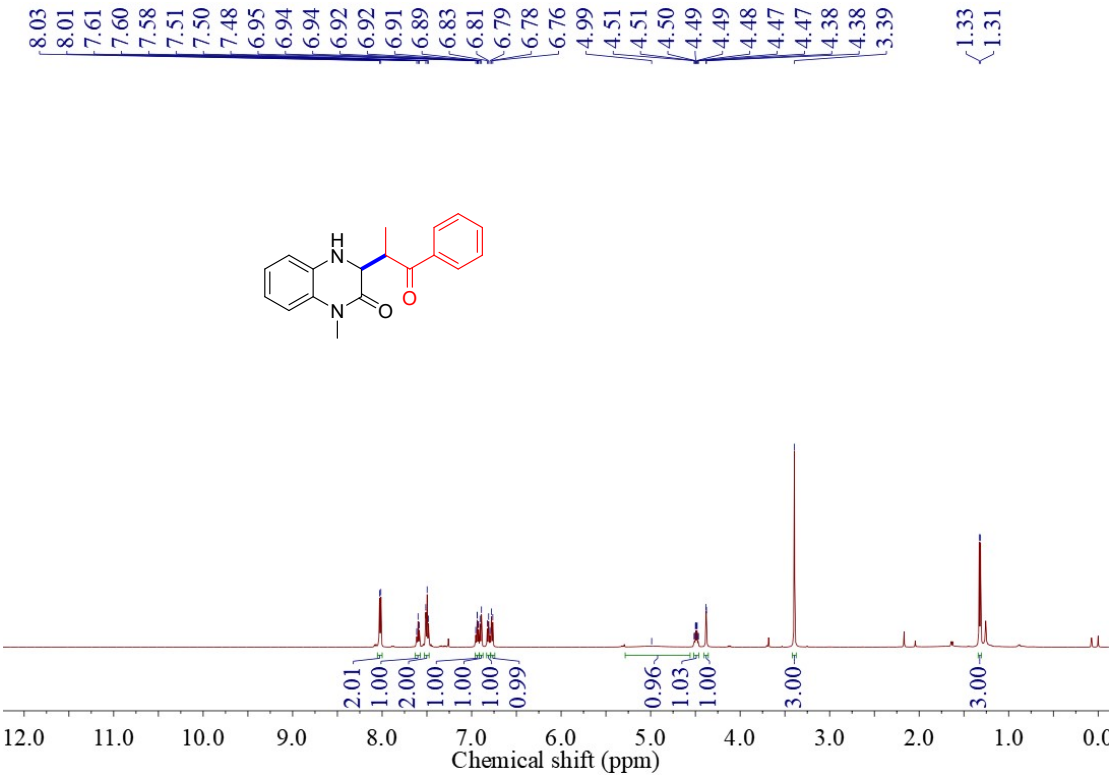
3ao ^{13}C NMR



4 ^{1}H NMR



6 ^{1}H NMR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4.49
4.48
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4.47
4.38
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3.39
1.33
1.31
H
N
O
N
O
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1.00
2.00
1.00
1.00
1.00
0.99
0.96
1.03
1.00
3.00
3.00
12.0
11.0
10.0
9.0
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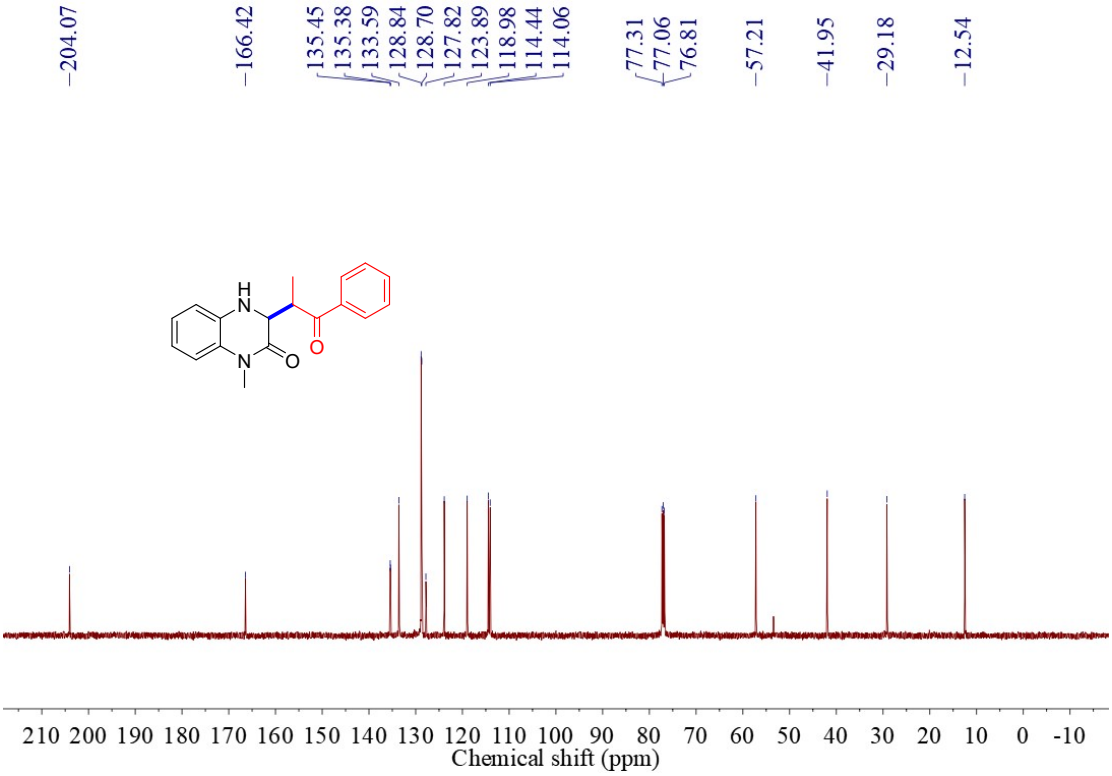
3.0
2.0
1.0
0.0
Chemical shift (ppm)

6 ^{13}C NMR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76.81
57.21
41.95
29.18
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H
N
O
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
Chemical shift (ppm)