Supporting Information

For

Ru(II)-Catalyzed Site-Selective *N*-Directed C(sp²)–H Alkylation of Quinoxalinones with Maleimide

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Content

General Information

All chemicals and solvents were purchased from Alfa-Aesar by Thermo Fischer Scientific, India Pvt. Limited, Sigma-Aldrich Chemicals Pvt. Limited India and from local commercial sources, and were used without any further purification unless otherwise specified. Solvents for column chromatography were dried and distilled prior to use. Solvents were removed under reduced pressure using rotary evaporator, followed by further removal of the residual solvent under high vacuum. Column chromatography was performed on silica gel (100-200 mesh). Melting points were determined on Buchi M-560 instrument and are uncorrected. HRMS analysis was carried out using Agilent G6530AA LC Q-TOF mass spectrometer using ESI method. All experiments were performed in a screw capped reaction vial under conventional heating. Reactions were monitored by thin layer chromatography (TLC) on Merck gel 60 F_{254} plates. The ^{1}H- and the ^{13}C-NMR spectra were recorded on Bruker-Avance Neo 400 FT-NMR spectrometers by using tetramethylsilane (TMS) as internal standard. The chemical shift values are on δ scale and the coupling constant (J) are in Hz. TBHP 70% aqueous and 5-6 M in decane solution were used. 1-Methyl-3-phenylquinoxalin-2(1*H*)-one derivatives were prepared according to the literature procedures. [1-4]

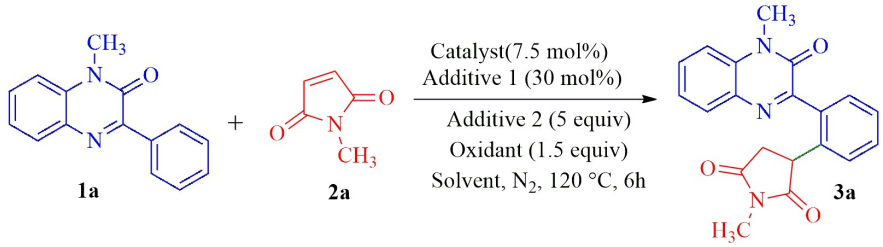
General procedure for the synthesis of compounds (3aa-5de)

An oven dried 10 mL screw capped reaction vial with a small stirring bar was charged with a mixture of *N*-methyl-3-phenylquinoxalin-2(1*H*)-one **1** (0.4 mmol), *N*-methylmaleimide **2** (0.8 mmol), $[Ru(p\text{-cymene})Cl_2]_2$ (7.5 mol%), $AgSbF_6$ (30 mol %), $Cu(OAc)_2.H_2O$ (1.5 equiv.) and 1,2-dichloroethane (DCE) (2mL) under nitrogen atmosphere. The resulting mixture was stirred at 120 ^{o}C for 6 hours. The progress of the reaction was monitored by TLC. After Completion of the reaction, the reaction mixture was cooled up to ambient temperature, diluted with DCM and passed through celite. The organic layer was concentrated on a rotary evaporator to obtained the crude product. The crude product thus obtained was further purified on a silica gel column using hexane/ethyl acetate (70:30) as eluent to afford the pure targeted products.

References

1. Xue, Z.-Y.; Jiang, Y.; Peng, X.-Z.; Yuan, W.-C.; Zhang, X.-M., *Adv. Synth. Catal.* **2010**, *352*, 2132-2136.
2. Núñez-Rico, J. L.; Vidal-Ferran, A., *Org. Lett.* **2013**, *15*, 2066-2069.
3. Carrër, A.; Brion, J.-D.; Messaoudi, S.; Alami, M., *Org. Lett.* **2013**, *15*, 5606-5609.
4. Zhang, Y.; Huang, T.; Li, X.; Zhang, M.; Song, Y.; Huang, K.; Su, W. *RSC Advances* **2020**, *10*, 22216-22221.

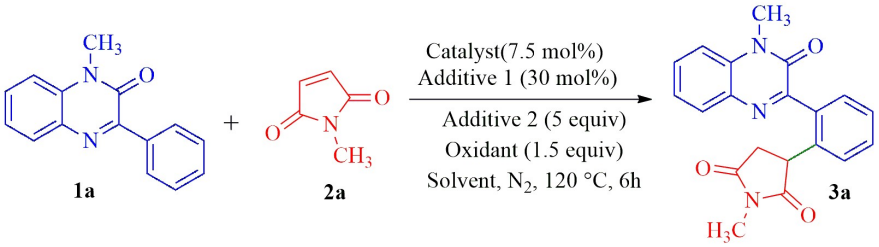
Table S1: Optimization of Solvents.[a]



S. No.	Catalyst (7.5 mol%)	Solvent (2 ml)	Yield (%)[b]
1	$[Ru(p\text{-cymene})Cl_2]_2$	H_2O	30
2	$[Ru(p\text{-cymene})Cl_2]_2$	MeOH	50
3	$[Ru(p\text{-cymene})Cl_2]_2$	HFIP	75
4	$[Ru(p\text{-cymene})Cl_2]_2$	THF	72
5	$[Ru(p\text{-cymene})Cl_2]_2$	1,4-dioxane	0
6	$[Ru(p\text{-cymene})Cl_2]_2$	ACN	0
7	$[Ru(p\text{-cymene})Cl_2]_2$	Toluene	Trace
8	$[Ru(p\text{-cymene})Cl_2]_2$	Acetone	70

[a] Reagents and conditions: a mixture of *N*-methyl-3-phenylquinoxalin-2(1*H*)-one (1a, 0.4 mmol), *N*-methylmaleimide (2a, 0.8 mmol), catalyst (7.5 mol %), $AgSbF_6$ (30 mol %), AcOH (5 equivalent) and $Cu(OAc)_2.H_2O$ (1.5 equivalent) in the indicated solvent (2 mL) were stirred at 120 °C for 6 h under N_2 atmosphere. [b] Isolated yields are reported.

Table S2: Optimization of catalysts.[a]

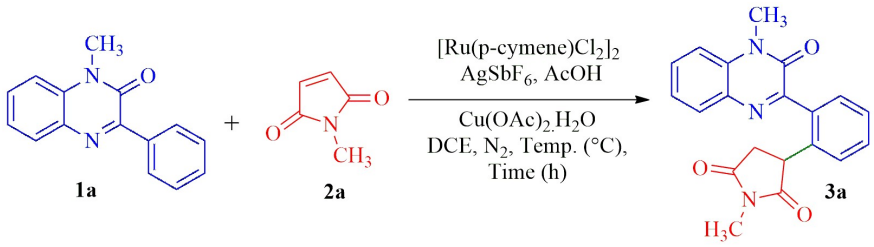


S. No.	Catalyst (7.5 mol%)	Yield (%)[b]
1	$RuCl_3.xH_2O$	Trace
2	$Pd(OAc)_2$	0
3	$PdCl_2$	0
4	$Pd(PPh_3)_2Cl_2$	0
5	$Pd_2(dba)_3$	0

6	$Pd(PPh_3)_4$	0
7	Rh(II)acetate dimer	0
8	$[Cp^*RhCl_2]_2$	70
9	$[Ru(p\text{-cymene})Cl_2]_2$	30[c]
10	$[Ru(p\text{-cymene})Cl_2]_2$	54[d]
11	$[Ru(p\text{-cymene})Cl_2]_2$	62[e]
12	$[Ru(p\text{-cymene})Cl_2]_2$	85[f]
13	$Cp^*Co(CO)I_2$	0

[a] Reagents and conditions: a mixture of *N*-methyl-3-phenylquinoxalin-2(1*H*)-one (1a, 0.4 mmol), *N*-methylmaleimide (2a, 0.8 mmol), catalyst (7.5 mol %), $AgSbF_6$ (30 mol %), AcOH (5 equivalent) and $Cu(OAc)_2.H_2O$ (1.5 equivalent) in DCE (2 mL) were stirred at 120 °C for 6 h under N_2 atmosphere. [b] Isolated yields are reported. [c] reaction was carried out in absence of N_2. [d-f] 0.4 mmol, 0.6 mmol and 1 mmol of *N*-methylmaleimide was used.

Table S3: Effect of concentration of catalyst, additives, oxidant, time and temprature on reaction yield.[a]



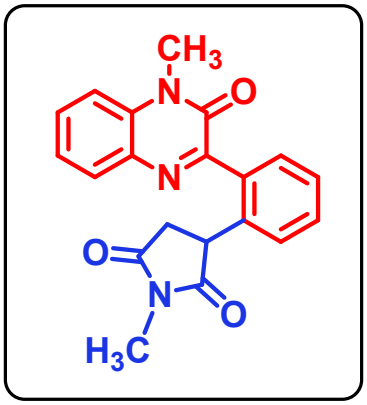
S. No.	$[Ru(p\text{-cymene})Cl_2]_2$ (mol %)	$AgSbF_6$ (mol %)	AcOH (5 equiv.)	$Cu(OAc)_2.H_2O$ (1.5 equiv.)	Time (h)	Temperature (°C)	Yield (%)[b]
1	5	30	5	1.5	6	120	70
2	10	30	5	1.5	6	120	87
3	7.5	25	5	1.5	6	120	75
4	7.5	35	5	1.5	6	120	70
5	7.5	30	3	1.5	6	120	47
6	7.5	30	7	1.5	6	120	85
7	7.5	30	10	1.5	6	120	63
8	7.5	30	5	1	6	120	70
9	7.5	30	5	2	6	120	84
10	7.5	30	5	2.5	6	120	79
12	7.5	30	5	1.5	4	120	70

13	7.5	30	5	1.5	7	120	86
14	7.5	30	5	1.5	8	120	80
15	7.5	30	5	1.5	12	120	71
16	7.5	30	5	1.5	6	100	42
17	7.5	30	5	1.5	6	110	60
18	7.5	30	5	1.5	6	130	80

[a] Reagents and conditions: a mixture of *N*-methyl-3-phenylquinoxalin-2(1*H*)-one (1a, 0.4 mmol), *N*-methylmaleimide (2a, 0.8 mmol), $[Ru(p\text{-cymene})Cl_2]_2$ catalyst, $AgSbF_6$ (additive), AcOH (co-additive) and $Cu(OAc)_2.H_2O$ (oxidant) in the DCE (2 mL) was stirred as indicated temprature for given time under N_2 atmosphere. [b] Isolated yields are reported.

Analytical Data

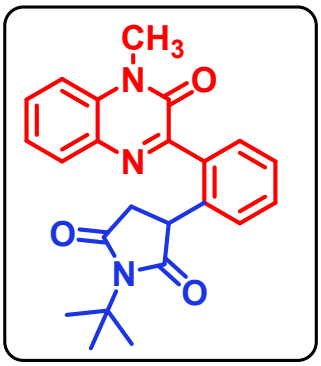
1-methyl-3-(2-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)phenyl)pyrrolidine-2,5-dione (3aa)



It was obtained as white solid having melting point 150-152°C with 85% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.78-7.74 (m, 2H), 7.62-7.58 (m, 1H), 7.48-7.40 (m, 2H), 7.39-7.35 (m, 2H), 7.27 (d, *J* = 1.8 Hz, 1H), 4.27 (dd, *J* = 9.4, 6.0 Hz, 1H), 3.77 (s, 3H), 3.25 (dd, *J* = 18.3, 9.4 Hz, 1H), 3.14 (dd, *J* = 18.3, 6.0 Hz, 1H), 2.68 (s, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 178.42, 176.61, 156.64, 154.57, 136.36, 135.37, 133.66, 132.33, 131.25,131.10, 130.29, 129.57, 127.46, 124.03, 113.94, 45.16, 38.80, 29.65, 24.92.
HRMS (ESI$^+$): m/z [M+H]$^+$ calculated for C:348.1343; found: 348.1357.

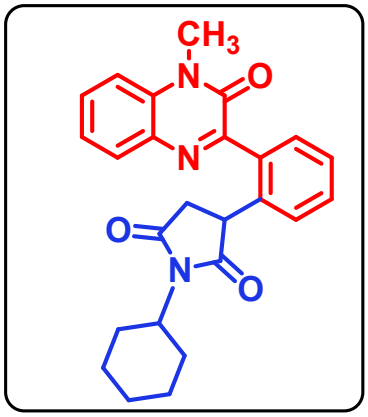
1-(tert-butyl)-3-(2-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)phenyl)pyrrolidine-2,5-dione (3ab)



It was obtained as white solid having melting point 154-156°C with 78% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.87 (dd, *J* = 8.1, 1.5 Hz, 1H), 7.67 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.61 (td, *J* = 8.0, 1.5 Hz, 1H), 7.48 - 7.44 (m, 1H), 7.42 - 7.39 (m, 1H), 7.38 - 7.35 (m, 2H), 7.23 - 7.19 (m, 1H), 4.16 - 4.10 (m, 1H), 3.77 (s, 3H), 3.13 (dd, *J* = 18.2, 9.8 Hz, 1H), 3.00 (dd, *J* = 18.2, 6.1 Hz, 1H), 1.44 (s, 9H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 179.11, 177.55, 156.87, 154.64, 137.54, 136.07, 133.74, 132.75, 131.05, 130.86,130.64, 130.28, 128.09, 127.28, 124.00, 113.85, 58.58, 44.58, 39.39, 29.62, 28.33.
HRMS (ESI$^+$): m/z [M+H]$^+$ calculated for C:390.1812; found:390.1830.

1-cyclohexyl-3-(2-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)phenyl)pyrrolidine-2,5-dione (3ac)

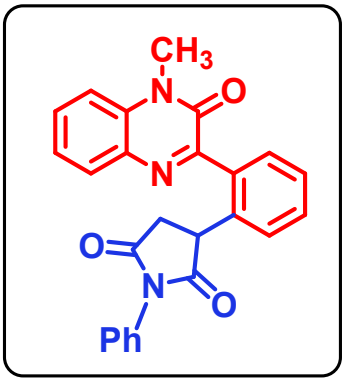


It was obtained as pale-yellow solid having melting point 220-222°C with 75% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.86 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.69 (dd, *J* = 7.4, 1.8 Hz, 1H), 7.63-7.58 (m, 1H), 7.47 - 7.40 (m, 2H), 7.40 - 7.35 (m, 2H), 7.19 (dd, *J* = 7.5, 1.5 Hz, 1H), 4.22 (dd, *J* = 9.5, 5.6 Hz, 1H), 3.96-3.88 (m, 1H), 3.77 (s, 3H), 3.19 (dd, *J* = 18.4, 9.6 Hz, 1H), 3.00 (dd, *J* = 18.4, 5.6 Hz, 1H), 2.05 (m, 2H), 1.74 (d, *J* = 11.3 Hz, 2H), 1.61 (s, 2H), 1.38 (t, *J* = 14.0 Hz, 2H), 1.26 - 1.19 (m, 2H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 178.19, 176.73, 156.68, 154.64, 137.27, 136.09, 133.72, 132.72, 131.07, 130.86,

130.59, 130.34, 127.88, 127.37, 124.04, 113.86, 51.96, 44.07, 38.90, 29.64, 28.81, 28.62, 25.90, 25.05.
HRMS (ESI$^+$): m/z $[M+H]^+$ calculated for C:416.1969; found:416.1973.

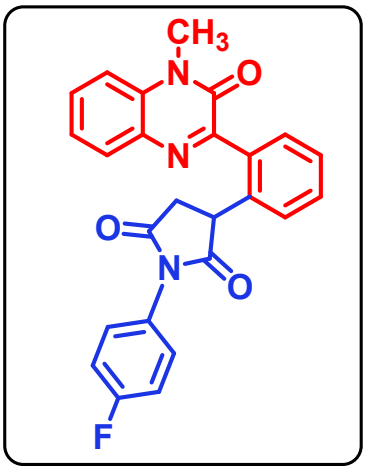
3-(2-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)phenyl)-1-phenylpyrrolidine-2,5-dione (3ad)



It was obtained as white solid having melting point 220-222^{o}C with 91% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.84 (dd, *J* = 8.3, 1.5 Hz, 1H), 7.77 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.63-7.59 (m, 1H), 7.53-7.43 (m, 2H), 7.38-7.34 (m, 4H), 7.32-7.30 (m, 2H), 7.00 (dd, *J* = 8.1, 1.7 Hz, 2H), 4.49 (dd, *J* = 9.4, 6.4 Hz, 1H), 3.76 (s, 3H), 3.44 (dd, *J* = 18.4, 9.4 Hz, 1H), 3.35 (dd, *J* = 18.5, 6.5 Hz, 1H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 177.03, 175.42, 156.72, 154.59, 136.43, 135.82, 133.80, 132.63, 132.05, 131.27, 131.14, 130.56, 130.38, 129.09, 129.03, 128.45, 127.61, 126.26, 124.10, 113.95, 45.17, 38.99, 29.67.
HRMS (ESI$^+$): m/z $[M+H]^+$ calculated for C:410.1499; found:410.1513.

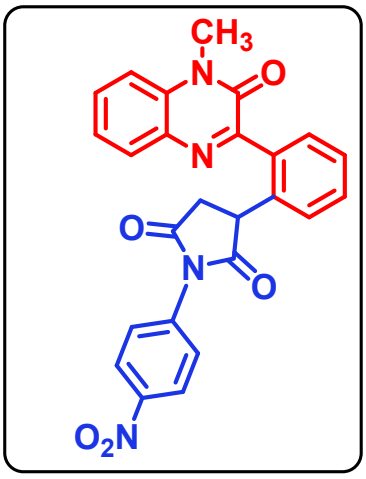
1-(4-fluorophenyl)-3-(2-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)phenyl)pyrrolidine-2,5-dione (3ae)



It was obtained as pink solid having melting point 198-200^{o}C with 72% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.82 (d, *J* = 8.1 Hz, 1H), 7.77 (d, *J* = 7.6 Hz, 1H), 7.61 (t, *J* = 7.9 Hz, 1H), 7.48 (m, 2H), 7.35 (d, *J* = 8.0 Hz, 3H), 7.03-6.94 (m, 4H), 4.48 (t, *J* = 7.8 Hz, 1H), 3.75 (s, 3H), 3.40 (q, *J* = 8.0 Hz, 2H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 177.00, 175.34, 163.29, 156.74, 154.56, 136.15, 135.72, 133.79, 132.57, 131.34, 131.19, 130.51, 130.39, 129.27, 128.07, 127.98, 127.68, 124.13, 116.12, 115.89, 113.98, 45.23, 38.89, 31.04.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -112.69.
HRMS (ESI$^+$): m/z $[M+H]^+$ calculated for C:428.1405; found:428.1399.

3-(2-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)phenyl)-1-(4-nitrophenyl)pyrrolidine-2,5-dione (3af)

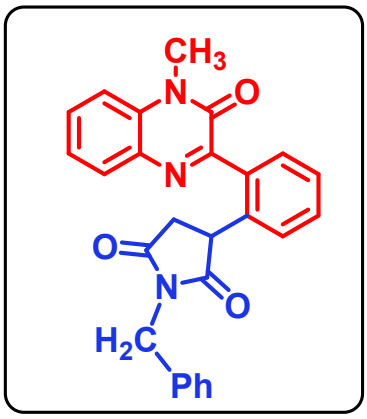


It was obtained as yellow solid having melting point 204-206 ^{o}C with 73% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.18 (d, *J* = 8.8 Hz, 2H), 7.82 (dd, *J* = 11.9, 8.0 Hz, 2H), 7.65-7.62 (m, 1H), 7.56 -7.49 (m, 2H), 7.41-7.34 (m, 3H), 7.29 (d, *J* = 4.1 Hz, 2H), 4.54 (t, *J* = 8.1 Hz, 1H), 3.78 (s, 3H), 3.50 (d, *J* = 8.1 Hz, 2H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 176.40, 174.54, 156.72, 154.48, 146.70, 137.47, 135.58, 135.47, 133.76, 132.41,

131.51, 131.30, 130.41, 130.35, 129.81, 127.82, 126.44, 124.12, 124.09, 114.03, 45.56, 38.81, 29.69.
HRMS (ESI$^+$): m/z $[M+H]^+$ calculated for C:455.1350; found:455.1372.

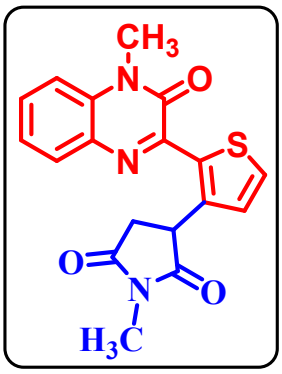
1-benzyl-3-(2-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)phenyl)pyrrolidine-2,5-dione (3ag)



It was obtained as white solid having melting point 190-192^{o}C with 93% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.82 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.73-7.71 (m, 1H), 7.63-7.59 (m, 1H), 7.43-7.40 (m, 2H), 7.38-7.35 (m, 2H), 7.34-7.31 (m, 3H), 7.24 (d, *J* = 1.7 Hz, 2H), 7.17- 7.15 (m, 1H), 4.47 (d, *J* = 13.9 Hz, 1H), 4.36 (d, *J* = 14.0 Hz, 1H), 4.26 (dd, *J* = 9.5, 5.7 Hz, 1H), 3.77 (s, 3H), 3.25 (dd, *J* = 18.4, 9.6 Hz, 1H), 3.05 (dd, *J* = 18.5, 5.7 Hz, 1H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 177.87, 176.17, 156.52, 154.58, 136.71, 135.87, 135.66, 133.64, 132.45, 131.11, 131.04, 130.38, 130.33, 128.95, 128.72, 128.68, 128.00, 127.43, 124.03, 113.94, 44.71, 42.42, 38.89, 29.62.
HRMS (ESI$^+$): m/z $[M+H]^+$ calculated for C:424.1656; found:424.1665.

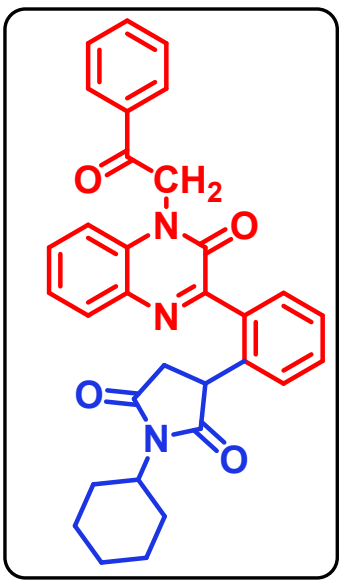
1-methyl-3-(5-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)thiophen-2-yl)pyrrolidine-2,5-dione (3da)



It was obtained as white solid having melting point 205-207^{o}C with 55% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.61 (d, *J* = 5.2 Hz, 1H), 7.58-7.53 (m, 2H), 7.38-7.33 (m, 2H), 7.06 (d, *J* = 5.2 Hz, 1H), 4.92 (dd, *J* = 9.2, 6.4 Hz, 1H), 3.79 (s, 3H), 3.33 (dd, *J* = 17.9, 9.2 Hz, 1H), 3.10 (d, *J* = 6.5 Hz, 1H), 3.04 (s, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 178.10, 177.00, 154.05, 148.98, 139.09, 132.55, 132.39, 131.89,131.78, 130.40, 130.03, 129.20, 124.39, 113.99, 43.24, 37.28, 29.76, 25.53.
HRMS (ESI$^+$): m/z $[M+H]^+$ calculated for C:354.0907; found:354.0913.

1-cyclohexyl-3-(2-(3-oxo-4-(2-oxo-2-phenylethyl)-3,4-dihydroquinoxalin-2-yl)phenyl)pyrrolidine-2,5-dione (3fc)

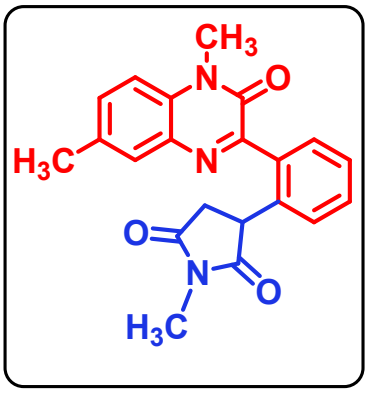


It was obtained as white solid having melting point 270-272^{o}C with 74% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.10-8.08 (m, 2H), 7.90 (d, *J* = 6.8 Hz, 1H), 7.71-7.67 (m, 2H), 7.56 (t, *J* = 7.7 Hz, 2H), 7.52-7.43 (m, 2H), 7.42-7.34 (m, 2H), 7.18 (d, *J* = 7.5 Hz, 1H), 7.01 (d, *J* = 8.4 Hz, 1H), 5.79 (q, *J* = 17.5 Hz, 2H), 4.22 (dd, *J* = 9.6, 5.5 Hz, 1H), 3.97-3.91 (m, 1H), 3.19 (dd, *J* = 18.4, 9.6 Hz, 1H), 2.97 (dd, *J* = 18.4, 5.6 Hz, 1H), 2.092.04 (m, 2H), 1.74 (d, *J* =

12.0 Hz, 2H), 1.60 (d, *J* = 10.4 Hz, 1H), 1.40 (d, *J* = 11.1 Hz, 2H), 1.28-1.20 (m, 3H).
^{13}C NMR (100 MHz Chloroform-*d*) δ 191.26, 178.27, 176.80, 156.49, 154.44, 137.57, 135.98, 134.71, 134.52, 133.18, 133.02, 131.12, 130.95, 130.91, 130.45, 129.25, 128.36, 127.77, 127.43, 124.23, 113.74, 52.05, 48.97, 44.11, 38.95, 28.87, 28.71, 25.97, 25.11.
HRMS (ESI$^+$): m/z [M+H]$^+$ calculated for C:520.2231; found:520.2237.

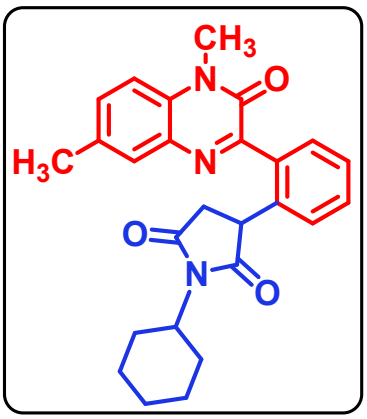
3-(2-(4,7-dimethyl-3-oxo-3,4-dihydroquinoxalin-2-yl)phenyl)-1-methylpyrrolidine-2,5-dione (4aa)



It was obtained as yellow solid having melting point 160-162^{o}C with 90% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.11 (d, *J* = 8.1 Hz, 1H), 7.63 (t, *J* = 7.8 Hz, 1H), 7.30 (d, *J* = 7.9 Hz, 2H), 7.26-7.24 (m, 2H), 7.09 (s, 1H), 4.67 (d, *J* = 8.9 Hz, 1H), 3.33 (dd, *J* = 17.9, 9.4 Hz, 1H), 3.14 (dd, *J* = 18.1, 6.4 Hz, 1H), 2.96 (s, 3H), 2.82 (s, 3H), 2.43 (s, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 178.38, 176.56, 157.89, 154.17, 141.17, 136.44, 135.06, 133.00, 132.06, 131.52,131.27, 130.90, 129.76, 128.33, 127.85, 115.43, 44.69, 38.71, 29.95, 25.13, 21.57.
HRMS (ESI$^+$): m/z [M+H]$^+$ calculated for C:362.1499; found:362.1516.

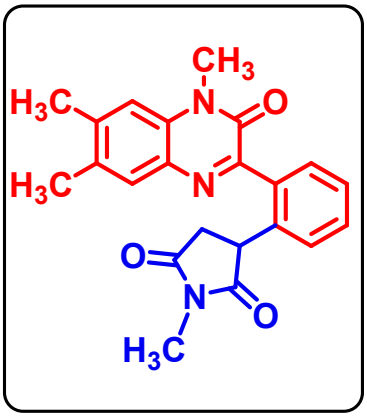
1-cyclohexyl-3-(2-(4,7-dimethyl-3-oxo-3,4-dihydroquinoxalin-2-KKyl)phenyl)pyrrolidine-2,5-dione (4ab)



It was obtained as pale-yellow solid having melting point 235-237^{o}C with 71% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.77 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.52 (m, 2H), 7.31-7.27 (m, 2H), 7.14 (dd, *J* = 8.0, 1.7 Hz, 1H), 6.90 (s, 1H), 4.14 (dd, *J* = 9.6, 5.6 Hz, 1H), 3.85 (m, 1H), 3.69 (s, 3H), 3.12 (dd, *J* = 18.4, 9.6 Hz, 1H), 2.93 (dd, *J* = 18.4, 5.6 Hz, 1H), 2.31 (s, 3H), 2.02-1.95 (m, 2H), 1.69 – 1.65 (m, 2H), 1.53 (d, *J* = 13.3 Hz, 1H), 1.32 (t, *J* = 14.8 Hz, 2H), 1.19-1.10 (m, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 178.40, 176.92, 156.78, 154.81, 140.55, 137.28, 133.77, 133.34, 132.84, 130.95, 130.60, 128.64, 128.24, 124.03, 113.89, 52.06, 44.14, 39.07, 29.71, 28.94, 28.73, 26.02, 25.16, 21.67.
HRMS (ESI$^+$): m/z [M+H]$^+$ calculated for C: 430.2125; found:430.2144.

1-methyl-3-(2-(4,6,7-trimethyl-3-oxo-3,4-dihydroquinoxalin-2-yl)phenyl)pyrrolidine-2,5-dione (4ba)

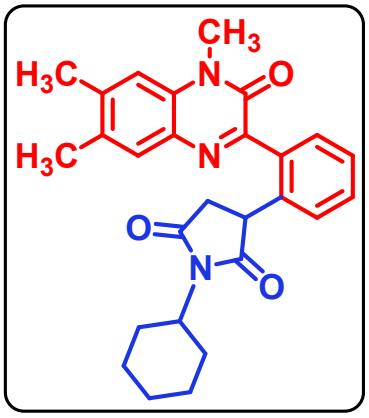


It was obtained as yellow solid having melting point 170-172^{o}C with 87% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.74-7.72 (m, 1H), 7.52 (s, 1H), 7.46-7.38 (m, 2H), 7.25-7.23 (m, 1H), 7.11 (s, 1H), 4.27 (dd, *J* = 9.4, 5.9 Hz, 1H), 3.73 (s, 3H), 3.24 (dd, *J* = 18.3, 9.4 Hz, 1H), 3.07 (dd, *J* = 18.3, 5.8 Hz, 1H), 2.74 (s, 3H), 2.44 (s, 3H), 2.35 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 178.37, 176.66, 155.22, 154.67, 141.15, 136.50, 135.85, 133.02, 131.74, 131.24,130.94, 130.38, 130.04, 129.19, 127.40, 114.45, 45.06, 38.88, 29.53, 24.95, 20.78, 19.24.
HRMS (ESI$^+$): m/z [M+H]$^+$ calculated for C:376.1656; found:376.1664.

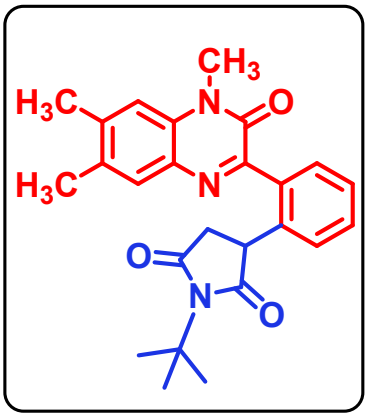
1-cyclohexyl-3-(2-(4,6,7-trimethyl-3-oxo-3,4-dihydroquinoxalin-2-yl)phenyl)pyrrolidine-2,5-dione (4bb)



It was obtained as yellow solid having melting point 152-154^{o}C with 60% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.68 (d, *J* = 7.5 Hz, 1H), 7.61 (s, 1H), 7.40 (q, *J* = 8.2 Hz, 2H), 7.17 (d, *J* = 7.7 Hz, 1H), 7.12 (s, 1H), 4.23-4.20 (m, 1H), 3.94 (t, *J* = 12.5 Hz, 1H), 3.74 (s, 3H), 3.20 (dd, *J* = 18.5, 9.6 Hz, 1H), 2.93 (dd, *J* = 18.6, 5.5 Hz, 1H), 2.44 (s, 3H), 2.36 (s, 3H), 2.09 (d, *J* = 12.8 Hz, 2H), 1.76 (d, *J* = 11.6 Hz, 2H), 1.61 (s, 2H), 1.44 (d, *J* = 12.2 Hz, 2H), 1.24 (s, 2H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 178.26, 176.85, 155.24, 154.76, 141.15,137.43, 136.44, 133.04, 131.79, 131.24, 130.88, 130.62, 130.14, 127.57, 127.31, 114.40, 52.00, 43.95, 39.02, 29.81, 29.53, 28.87, 28.76, 25.95, 25.10, 20.78, 19.26.
HRMS (ESI$^+$): m/z [M+H]$^+$ calculated for C:444.2282; found:444.2294.

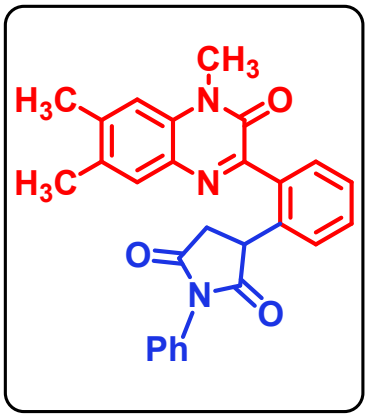
1-(tert-butyl)-3-(2-(4,6,7-trimethyl-3-oxo-3,4-dihydroquinoxalin-2-yl)phenyl)pyrrolidine-2,5-dione (4bc)



It was obtained as white solid having melting point 168-170^{o}C with 80% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.66 (d, *J* = 7.4 Hz, 1H), 7.60 (s, 1H), 7.45-7.36 (m, 2H), 7.19 (d, *J* = 7.4 Hz, 1H), 7.11 (s, 1H), 4.12 (dd, *J* = 9.8, 5.9 Hz, 1H), 3.73 (s, 3H), 3.13 (dd, *J* = 18.2, 9.9 Hz, 1H), 2.94 (dd, *J* = 18.2, 6.0 Hz, 1H), 2.44 (s, 3H), 2.36 (s, 3H), 1.47 (s, 9H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 179.15, 177.67, 155.35, 154.69, 141.07, 137.67, 136.37, 132.96, 131.74, 131.20, 130.83, 130.59, 130.04, 127.75, 127.18, 114.38, 58.55, 44.41, 39.49, 29.49, 28.37, 20.78, 19.25.
HRMS (ESI$^+$): m/z [M+H]$^+$ calculated for C:418.2125; found:418.2149.

1-phenyl-3-(2-(4,6,7-trimethyl-3-oxo-3,4-dihydroquinoxalin-2-yl)phenyl)pyrrolidine-2,5-dione (4bd)

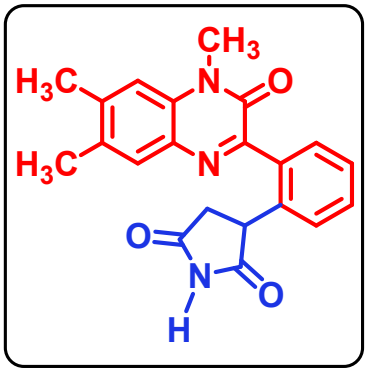


It was obtained as pale-yellow solid having melting point 218-220^{o}C with 85% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.76 (d, *J* = 6.6 Hz, 1H), 7.57 (s, 1H), 7.50-7.41 (m, 2H), 7.36-7.31 (m, 4H), 7.11 (s, 1H), 7.07 (d, *J* = 7.0 Hz, 2H), 4.48 (dd, *J* = 9.6, 6.1 Hz, 1H), 3.72 (s, 3H), 3.43 (dd, *J* = 18.5, 9.6 Hz, 1H), 3.26 (dd, *J* = 18.5, 6.2 Hz, 1H), 2.44 (s, 3H), 2.32 (s, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 177.07, 175.56, 155.11, 154.64, 141.24, 136.43, 136.06, 133.09, 132.04, 131.76, 131.20, 131.06, 130.52, 130.14, 128.98, 128.86, 128.42, 127.53, 126.29, 114.46, 45.02, 39.00, 29.54, 20.78, 19.23.
HRMS (ESI$^+$): m/z [M+Na]$^+$ calculated for C:460.1632; found:460.1623.

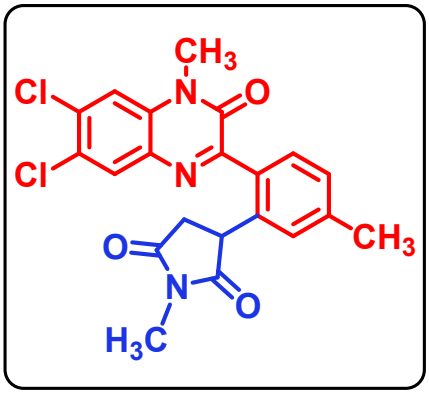
3-(2-(4,6,7-trimethyl-3-oxo-3,4-dihydroquinoxalin-2-yl)phenyl)pyrrolidine-2,5-dione (4bf)



It was obtained as white solid having melting point 178-180^{o}C with 82% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.73 (s, 1H), 7.72 (d, *J* = 7.4 Hz, 1H), 7.58 (s, 1H), 7.46-7.39 (m, 2H), 7.28 (d, *J* = 8.1 Hz, 1H), 7.12 (s, 1H), 4.33 (t, *J* = 8.0 Hz, 1H), 3.73 (s, 3H), 3.25 (dd, *J* = 18.6, 9.6 Hz, 1H), 3.02 (dd, *J* = 18.7, 6.0 Hz, 1H), 2.43 (s, 3H), 2.34 (s, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 178.85, 177.01, 155.04, 154.70, 141.25, 136.17, 135.89, 133.19, 131.69, 131.18, 130.97, 130.32, 130.16, 128.88, 127.54, 114.51, 46.10, 39.90, 29.58, 20.79, 19.28.
HRMS (ESI$^+$): m/z [M+H]$^+$ calculated for C:362.1499; found:362.1514.

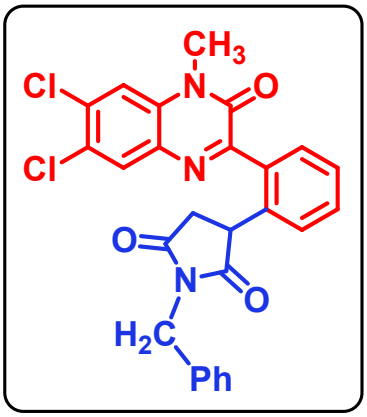
3-(2-(6,7-dichloro-4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)-5-methylphenyl)-1-methylpyrrolidine-2,5-dione (4ca)



It was obtained as yellow solid having melting point 120-130^{o}C with 60% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.84 (s, 1H), 7.63 (d, *J* = 8.0 Hz, 1H), 7.43 (s, 1H), 7.23 (s, 1H), 7.04 (s, 1H), 4.28 (s, 1H), 3.71 (s, 3H), 3.24 (dd, *J* = 18.4, 9.7 Hz, 1H), 3.03 (d, *J* = 18.3 Hz, 1H), 2.82 (s, 3H), 2.40 (s, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 178.37, 176.54, 157.88, 154.16, 141.17, 136.45, 135.04, 133.01, 132.07, 131.52, 131.26, 130.89, 129.75, 128.31, 127.84, 115.42, 44.69, 38.69, 29.93, 25.12, 21.56.
HRMS (ESI$^+$): m/z [M+H]$^+$ calculated for C:430.0720; found:430.0723.

1-benzyl-3-(2-(6,7-dichloro-4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)phenyl)pyrrolidine-2,5-dione (4de)



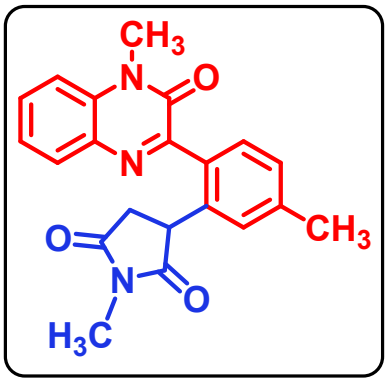
It was obtained as yellow solid having melting point 200-202^{o}C with 62% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.86 (s, 1H), 7.69 (dd, *J* = 7.2, 2.0 Hz, 1H), 7.50-7.39 (m, 4H), 7.33 (dd, *J* = 6.6, 3.0 Hz, 2H), 7.25 (d, *J* = 2.6 Hz, 2H), 7.15 (dd, *J* = 7.1, 1.8 Hz, 1H), 4.56 (d, *J* = 13.9 Hz, 1H), 4.46 (d, *J* = 13.9 Hz, 1H), 4.27 (dd, *J* = 9.5, 5.7 Hz, 1H), 3.71 (s, 3H), 3.25 (dd, *J* = 18.5, 9.5 Hz, 1H), 3.03 (dd, *J* = 18.4, 5.7 Hz, 1H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 177.72, 175.98, 157.81, 154.09, 136.71, 135.79, 135.27, 135.16, 133.00, 131.55,131.12,

131.06, 130.81, 129.09, 128.91, 128.72, 128.58, 128.08, 127.92, 127.52, 115.48, 44.58, 42.70, 38.77, 29.92.

HRMS (ESI$^+$): m/z [M+H]$^+$ calculated for C:492.0876; found:492.0879.

1-methyl-3-(2-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)phenyl)pyrrolidine-2,5-dione (5aa)

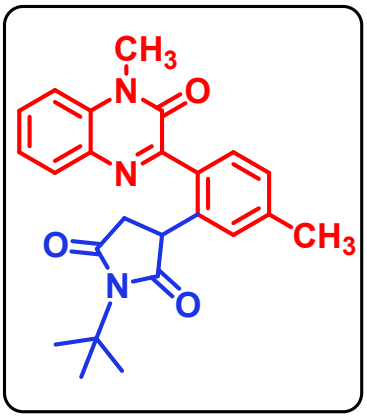


It was obtained as yellow solid having melting point 161-163^{o}C with 89% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.73 (d, *J* = 8.0 Hz, 1H), 7.65 (d, *J* = 7.9 Hz, 1H), 7.57 (t, *J* = 7.9 Hz, 1H), 7.34 (t, *J* = 7.5 Hz, 2H), 7.22 (d, *J* = 7.9 Hz, 1H), 7.05 (s, 1H), 4.25-4.21 (m, 1H), 3.74 (s, 3H), 3.24 (dd, *J* = 18.4, 9.5 Hz, 1H), 3.12 (dd, *J* = 18.2, 6.0 Hz, 1H), 2.68 (s, 3H), 2.39 (s, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ178.51, 176.72, 156.61, 154.61, 140.46, 136.30, 133.58, 132.50, 132.33, 131.19, 130.87, 130.21, 130.17, 128.19, 123.91, 113.87, 45.10, 38.88, 29.60, 24.90, 21.47.

HRMS (ESI$^+$): m/z [M+H]$^+$ calculated for C:362.1499; found:362.1507.

1-(tert-butyl)-3-(5-methyl-2-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)phenyl)pyrrolidine-2,5-dione (5ab)

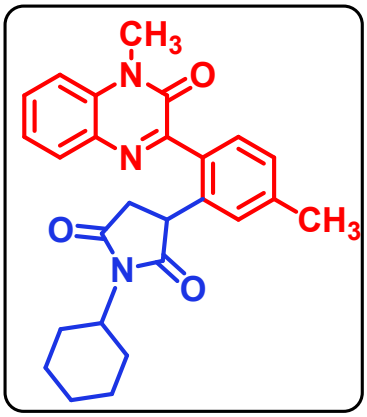


It was obtained as white solid having melting point 158-160^{o}C with 81% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.85 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.61-7.57 (m, 2H), 7.38-7.33 (m, 2H), 7.21 (dd, *J* = 8.0, 1.7 Hz, 1H), 6.99 (s, 1H), 4.11 (dd, *J* = 9.8, 6.2 Hz, 1H), 3.76 (s, 3H), 3.12 (dd, *J* = 18.1, 9.8 Hz, 1H), 3.00 (dd, *J* = 18.2, 6.1 Hz, 1H), 2.39 (s, 3H), 1.44 (s, 9H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 179.21, 177.64, 156.84, 154.68, 140.32, 137.39, 133.65, 133.18, 132.72, 130.82, 130.50,128.79, 128.03, 123.88, 113.79, 58.50, 44.52, 39.42, 29.58, 28.30, 21.58.

HRMS (ESI$^+$): m/z [M+H]$^+$ calculated for C:404.1969; found:404.2000.

1-cyclohexyl-3-(5-methyl-2-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)phenyl)pyrrolidine-2,5-dione (5ac)

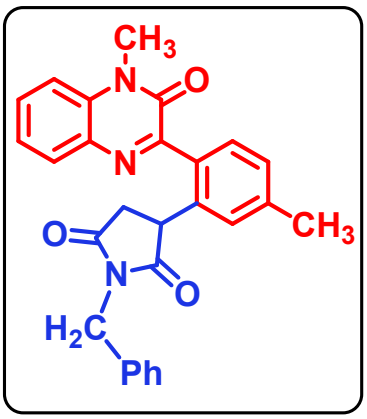


It was obtained as pale-yellow solid having melting point 236-238^{o}C with 85% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.84 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.59 (t, *J* = 8.2 Hz, 2H), 7.38-7.33 (m, 2H), 7.21 (dd, *J* = 8.0, 1.7 Hz, 1H), 6.97 (s, 1H), 4.20 (dd, *J* = 9.6, 5.7 Hz, 1H), 3.96-3.88 (m, 1H), 3.76 (s, 3H), 3.19 (dd, *J* = 18.4, 9.6 Hz, 1H), 2.99 (dd, *J* = 18.5, 5.7 Hz, 1H), 2.38 (s, 3H), 2.08-2.02 (m, 2H), 1.75-1.72 (m, 2H), 1.59 (d, *J* = 13.3 Hz, 1H), 1.44-1.34 (m, 2H), 1.26-1.17 (m, 3H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 178.30, 176.82, 156.68, 154.71, 140.45, 137.18, 133.67, 133.24, 132.74, 130.85, 130.50, 128.54, 128.14, 123.93, 113.79, 51.96, 44.04, 38.97, 29.61, 28.84, 28.63, 25.92, 25.06, 21.57.
HRMS (ESI$^+$): m/z [M+H]$^+$ calculated for C:430.2125; found:430.2134.

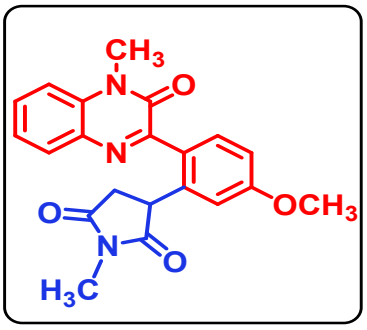
1-benzyl-3-(5-methyl-2-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)phenyl)pyrrolidine-2,5-dione (5ae)



It was obtained as pale-yellow solid having melting point 194-196°C with 92% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.81-7.79 (m, 1H), 7.64-7.57 (m, 2H), 7.49 (t, *J* = 7.8 Hz, 1H), 7.39-7.33 (m, 4H), 7.26-7.20 (m, 3H), 6.90 (s, 1H), 4.50 (d, *J* = 14.0 Hz, 1H), 4.39 (d, *J* = 14.0 Hz, 1H), 4.25-4.21 (m, 1H), 3.76 (s, 3H), 3.25 (dd, *J* = 18.5, 9.5 Hz, 1H), 3.03 (dd, *J* = 18.5, 5.5 Hz, 1H), 2.33 (s, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 178.04, 176.34, 156.56, 154.73, 140.57, 136.86, 136.02, 133.65, 132.85, 132.58,131.06, 130.93, 130.39, 129.18, 129.03, 128.71, 128.23, 128.04, 123.98, 113.89, 44.62, 42.51, 39.06, 29.64, 21.48.
HRMS (ESI$^+$): m/z [M+H]$^+$ calculated for C:438.1812; found:438.1827.

3-(5-methoxy-2-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)phenyl)-1-methylpyrrolidine-2,5-dione (5ba)

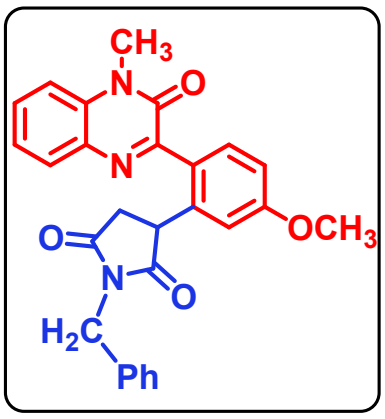


It was obtained as white solid having melting point 150-152°C with 54% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.79 (d, *J* = 8.7 Hz, 1H), 7.72 (d, *J* = 7.9 Hz, 1H), 7.57 (t, *J* = 7.5 Hz, 1H), 7.34 (t, *J* = 8.1 Hz, 2H), 6.95 (dd, *J* = 8.7, 2.6 Hz, 1H), 6.77 (d, *J* = 2.6 Hz, 1H), 4.28 (dd, *J* = 9.3, 6.1 Hz, 1H), 3.86 (s, 3H), 3.76 (s, 3H), 3.26 (dd, *J* = 18.2, 9.3 Hz, 1H), 3.16 (dd, *J* = 18.2, 6.1 Hz, 1H), 2.68 (s, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ178.22, 176.59, 160.93, 156.23, 154.75, 138.27, 133.60, 133.11, 132.41, 130.72, 130.10, 127.82, 123.92, 115.94, 113.86, 112.20, 55.59, 45.37, 38.85, 29.64, 24.94.

HRMS (ESI$^+$): m/z [M+H]$^+$ calculated for C:378.1448; found:378.1464.

1-benzyl-3-(5-methoxy-2-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)phenyl)pyrrolidine-2,5-dione (5be)

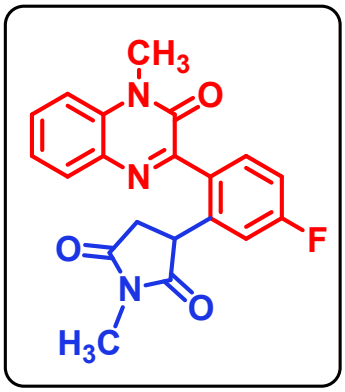


It was obtained as yellow solid having melting point 148-150°C with 52% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.70 (t, *J* = 9.3 Hz, 2H), 7.51 (t, *J* = 7.9 Hz, 1H), 7.27 (d, *J* = 7.5 Hz, 4H), 7.18 (d, *J* = 6.1 Hz, 3H), 6.85 (d, *J* = 7.1 Hz, 1H), 6.55 (s, 1H), 4.44 - 4.29 (m, 2H), 4.23 (dd, *J* = 9.4, 5.5 Hz, 1H), 3.69 (s, 3H), 3.68 (s, 3H), 3.20 (dd, *J* = 18.4, 9.5 Hz, 1H), 2.98 (dd, *J* = 18.5, 5.5 Hz, 1H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 177.78, 176.21, 160.97, 156.03, 154.78, 138.75, 136.00, 133.55, 132.87, 132.53, 130.74,130.20, 128.99, 128.71, 128.05, 128.01, 123.95, 114.37, 113.87, 112.69, 55.45, 44.82, 42.49, 39.02, 29.64.
HRMS (ESI$^+$): m/z [M+H]$^+$ calculated for C:454.1761; found:454.1771.

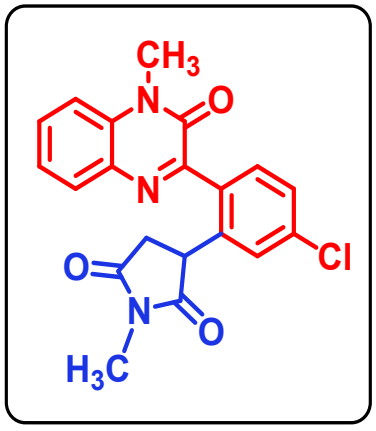
3-(5-fluoro-2-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)phenyl)-1-methylpyrrolidine-2,5-dione (5ca)



It was obtained as white solid having melting point 152-154^{o}C with 58% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.80-7.74 (m, 2H), 7.61 (t, *J* = 7.9 Hz, 1H), 7.36 (t, *J* = 8.2 Hz, 2H), 7.13 (t, *J* = 7.9 Hz, 1H), 6.99 (dd, *J* = 9.7, 2.5 Hz, 1H), 4.28 (dd, *J* = 9.5, 6.1 Hz, 1H), 3.77 (s, 3H), 3.25 (dd, *J* = 18.2, 9.4 Hz, 1H), 3.12 (dd, *J* = 18.3, 6.1 Hz, 1H), 2.68 (s, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 177.71, 176.14, 164.63, 162.14, 155.66, 154.53, 139.07, 133.55, 132.27, 131.21, 130.26, 124.10, 116.67, 116.45, 114.69, 113.97, 45.03, 38.55, 29.67, 24.97.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -110.03.
HRMS (ESI$^+$): m/z [M+H]$^+$ calculated for C: 366.1248; found:366.1239.

3-(5-chloro-2-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)phenyl)-1-methylpyrrolidine-2,5-dione (5da)

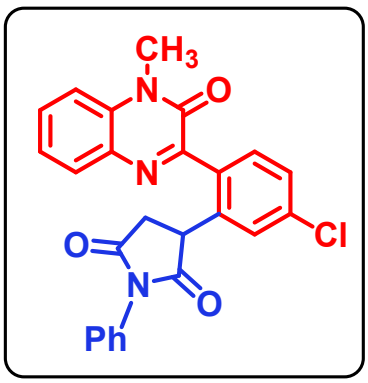


It was obtained as yellow solid having melting point 92-95^{o}C with 67% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.76-7.72 (m, 2H), 7.63-7.59 (m, 1H), 7.42-7.35 (m, 3H), 7.26 (s, 1H), 4.25 (dd, *J* = 9.4, 6.1 Hz, 1H), 3.76 (s, 3H), 3.25 (dd, *J* = 18.2, 9.4 Hz, 1H), 3.13 (dd, *J* = 18.3, 6.1 Hz, 1H), 2.67 (s, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 177.69, 176.12, 155.62, 154.45, 138.33, 136.10, 133.87, 133.72, 132.78, 132.31, 131.35, 130.36, 129.74, 127.69, 124.16, 114.00, 44.99, 38.60, 29.70, 25.01.

HRMS (ESI$^+$): m/z [M+H]$^+$ calculated for C:382.0953; found:382.0960.

3-(5-chloro-2-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)phenyl)-1-phenylpyrrolidine-2,5-dione (5dd)

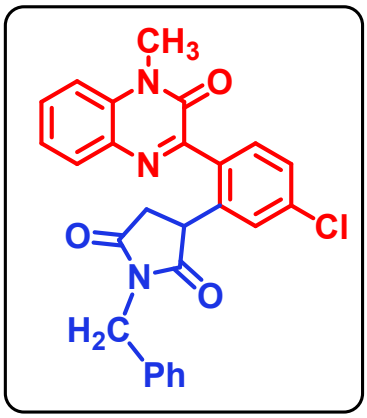


It was obtained as yellow solid having melting point 194-196^{o}C with 63% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.82 (d, *J* = 7.3 Hz, 1H), 7.75 (d, *J* = 8.4 Hz, 1H), 7.62 (t, *J* = 7.8 Hz, 1H), 7.43 (dd, *J* = 8.4, 2.1 Hz, 1H), 7.38 - 7.33 (m, 4H), 7.31 (s, 2H), 6.99 (d, *J* = 6.4 Hz, 2H), 4.48 (dd, *J* = 9.5, 6.6 Hz, 1H), 3.75 (s, 3H), 3.42 (dd, *J* = 18.4, 9.5 Hz, 1H), 3.34 (dd, *J* = 18.4, 6.6 Hz, 1H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 176.41, 174.99, 155.65, 154.44, 138.21, 136.18, 134.21, 133.80, 132.78, 132.54, 131.88, 131.40, 130.59, 129.46, 129.07, 128.55, 127.85, 126.19, 124.25, 114.02, 45.04, 38.72, 29.73.
HRMS (ESI$^+$): m/z [M+H]$^+$ calculated for C:444.1109; found:444.1141.

1-benzyl-3-(5-chloro-2-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)phenyl)pyrrolidine-2,5-dione (5de)



It was obtained as white solid having melting point 178-180^{o}C with 66% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 6.52 (d, *J* = 8.0 Hz, 1H), 6.43 (d, *J* = 8.4 Hz, 1H), 6.33 (t, *J* = 7.9 Hz, 1H), 6.11-6.07 (m, 3H), 6.03 (d, *J* = 5.8 Hz, 2H), 5.98-5.96 (m, 3H), 5.88 (s, 1H), 3.17 (d, *J* = 14.0 Hz, 1H), 3.04 (d, *J* = 14.0 Hz, 1H), 2.96 (dd, *J* = 9.5, 5.7 Hz, 1H), 2.47 (s, 3H), 1.97 (dd, *J* = 18.4, 9.5 Hz, 1H), 1.76 (dd, *J* = 18.4, 5.8 Hz, 1H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 177.22, 175.70, 155.39, 154.41, 138.64, 136.05, 135.72, 134.05, 133.61, 132.53,132.35, 131.33, 130.37, 128.92, 128.70, 128.06, 127.61, 124.12, 113.98, 44.51, 42.50, 38.62, 29.64.
HRMS (ESI$^+$): m/z [M+H]$^+$ calculated for C:458.1266; found:458.1273.

Important Crystal Data of Compound 3aa

CCDC deposition number	2441948
Empirical Formula	$C_{20}H_{17}N_3O_3$
Formula weight	347.36
Temperature (K)	256(60)
Crystal System	orthorhombic
Space Group	Pbca
Unit Cell Dimension	a/Å = 13.3576(15) b/Å = 9.1052(6) c/Å = 27.6587(18) α/° = 90 β/° = 90 γ/° = 90
Volume Å^3	3364.0(5)
Z	8
Density Calculated g/cm^3	1.372
Absorption coefficient (μ) mm^{-1}	0.094
F (000)	1456.0
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.944 to 62.212

Index ranges	$-17 \leq h \leq 16$ $-11 \leq k \leq 10$ $-38 \leq l \leq 34$
Reflection Collected	18468
Independent Reflections	4324 [R_{int} = 0.1300, R_{sigma} = 0.0893]
Data/Restraints/parameter s	4324/0/237
Goodness of fit on F^2	1.208
Final R indices [I>=2sigma(I)]	R_1 = 0.0874, wR_2 = 0.2527
R indices (all data)	R_1 = 0.1496, wR_2 = 0.3501
Largest difference peak and hole [e Å^{-3}]	0.62/-0.65

Important Crystal Data of Compound 5ca

CCDC deposition number	2441949
Empirical Formula	$C_{20}H_{16}FN_3O_3$
Formula weight	365.36
Temperature (K)	224(100)
Crystal System	orthorhombic
Space Group	$Pna2_1$
Unit Cell Dimension	a/Å = 14.9270(8) b/Å = 11.3024(5) c/Å = 20.4930(9) α/° = 90 β/° = 90 γ/° = 90
Volume Å^3	3457.4(3)
Z	8
Density Calculated g/cm^3	1.404
Absorption coefficient (μ) mm^{-1}	0.104
F (000)	1520.0
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.976 to 62.394

Index ranges	$-18 \leq h \leq 13$ $-14 \leq k \leq 16$ $-29 \leq l \leq 26$
Reflection Collected	20086
Independent Reflections	7915 [R_{int} = 0.1005, R_{sigma} = 0.0822]
Data/Restraints/parameter s	7915/1/491
Goodness of fit on F^2	1.072
Final R indices [I>=2sigma(I)]	R_1 = 0.0657, wR_2 = 0.1701
R indices (all data)	R_1 = 0.1026, wR_2 = 0.1935
Largest difference peak and hole [e Å^{-3}]	0.39/-0.31

Copies of ^{1}H NMR and ^{13}C NMR Spectra

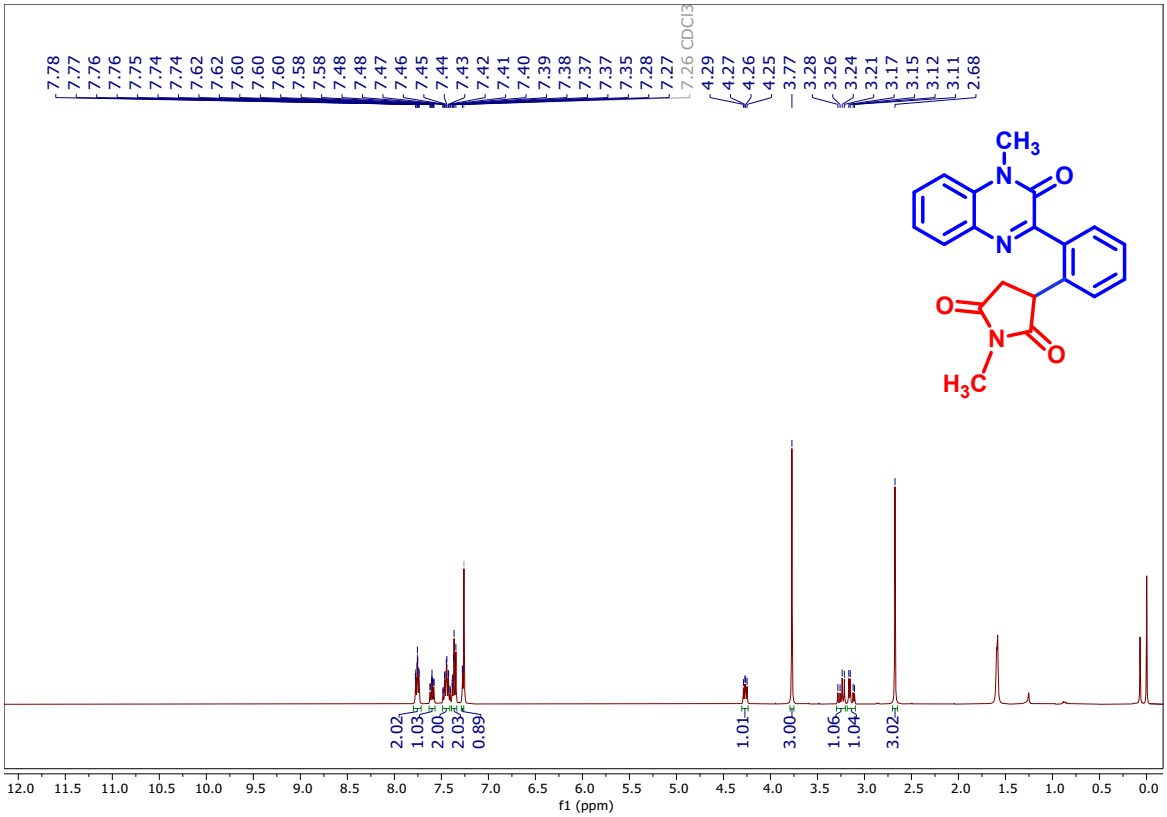


Figure 1: ^{1}H NMR spectrum of compound **3aa** (400 MHz, $CDCl_3$).

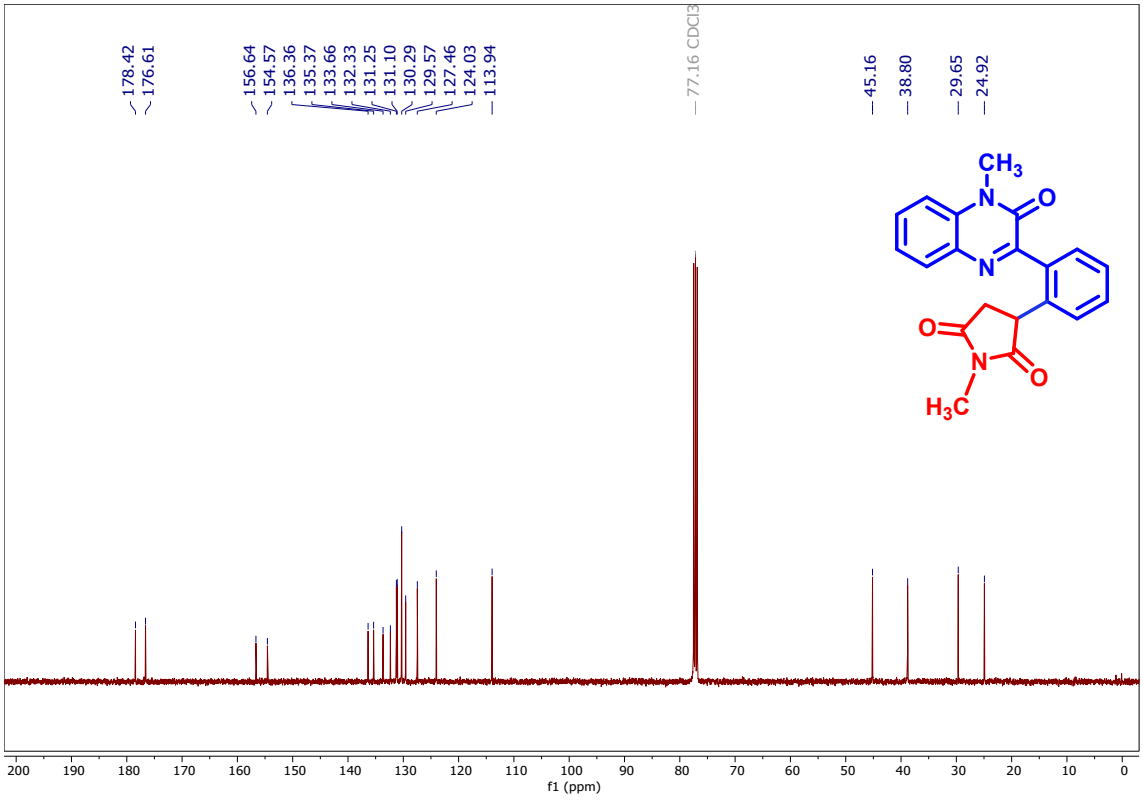


Figure 2: ^{13}C{1H} NMR spectrum of compound **3aa** (100 MHz, $CDCl_3$).

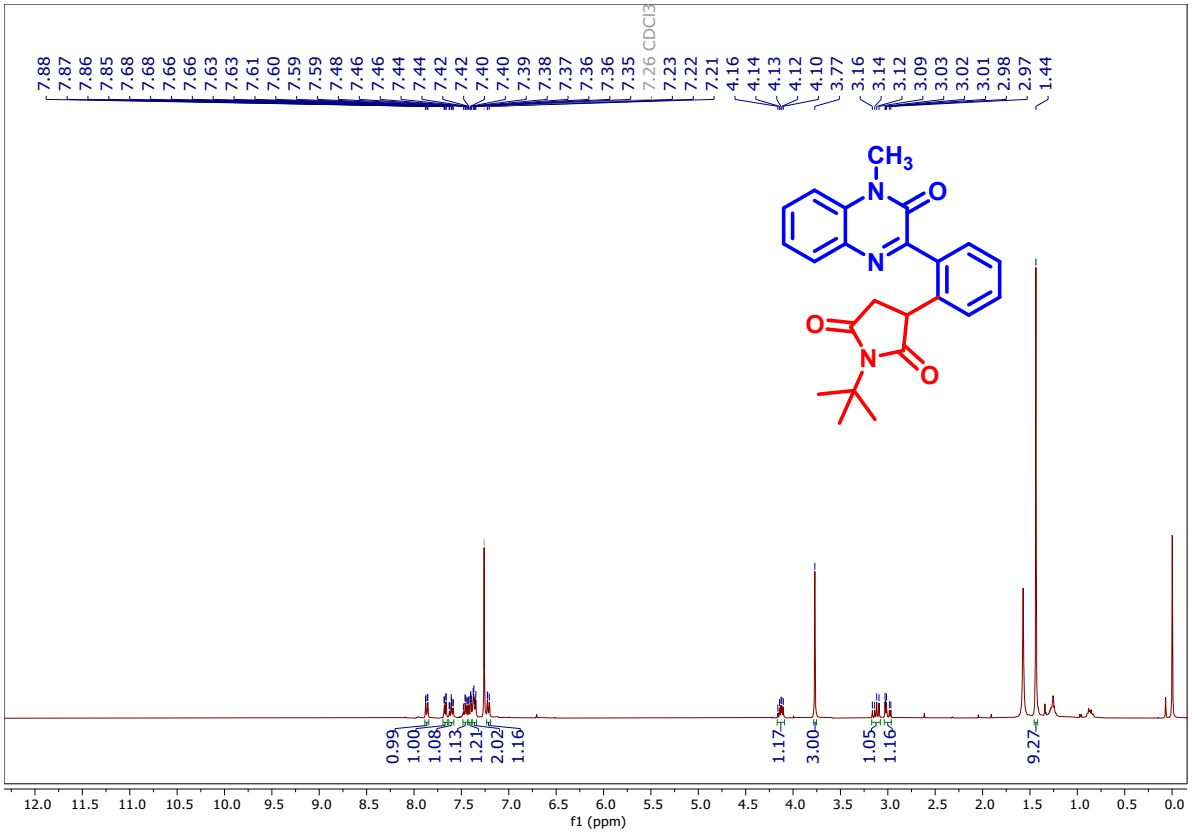


Figure 3: ^{1}H NMR spectrum of compound **3ab** (400 MHz, $CDCl_3$).

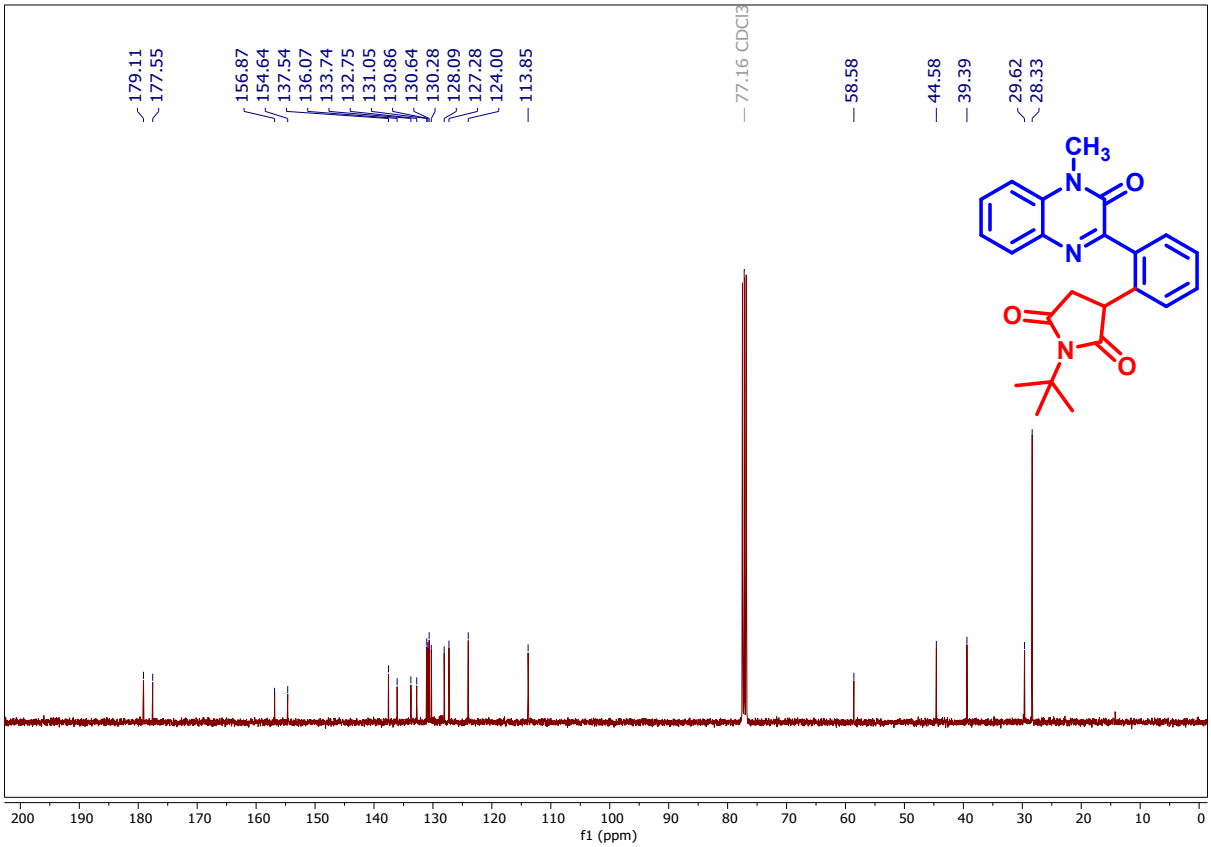


Figure 4: ^{13}C{1H} NMR spectrum of compound **3ab** (100 MHz, $CDCl_3$).

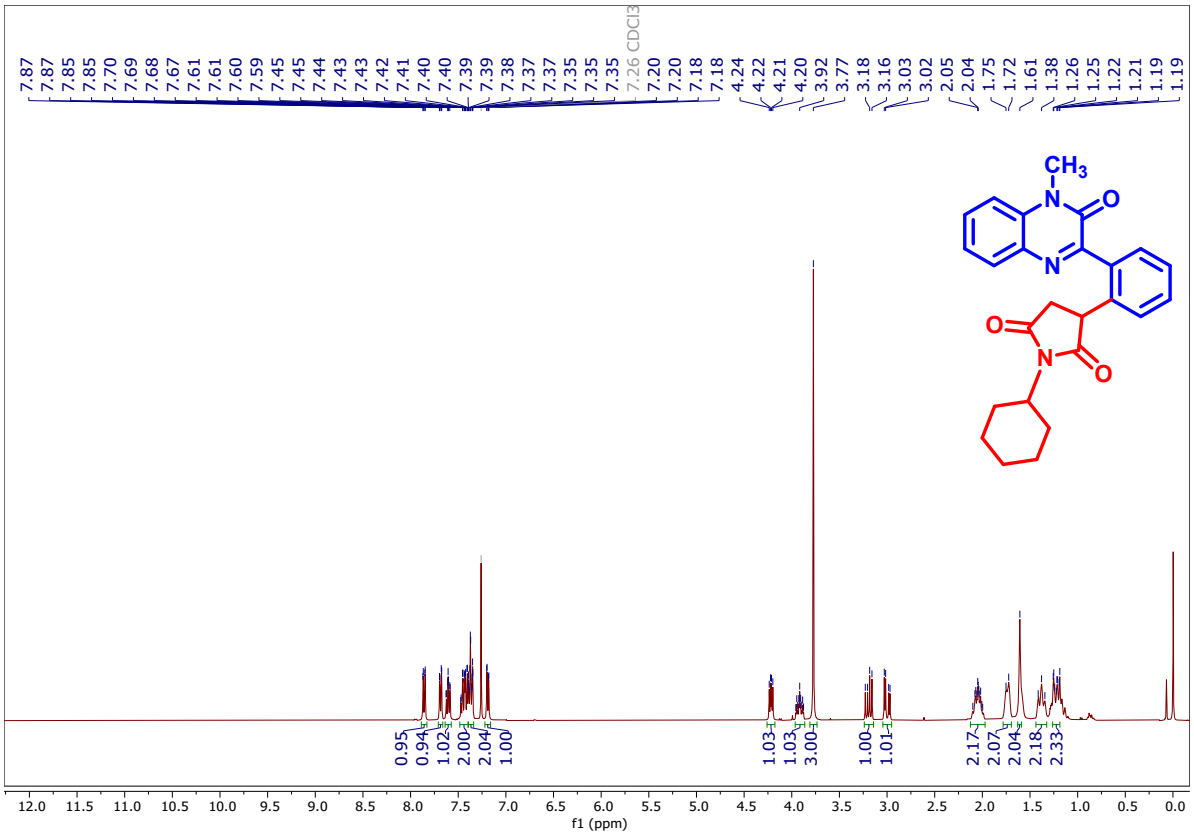


Figure 5: ^{1}H NMR spectrum of compound **3ac** (400 MHz, $CDCl_3$).

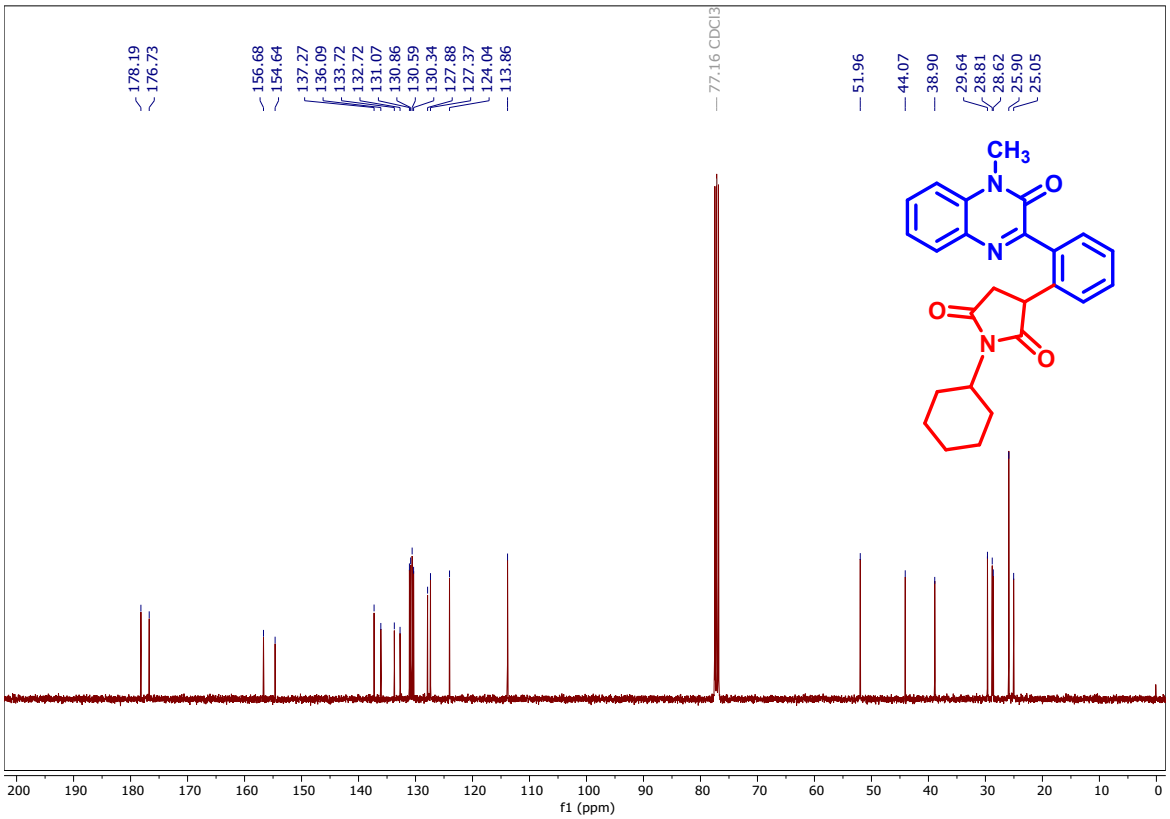


Figure 6: ^{13}C{1H} NMR spectrum of compound **3ac** (100 MHz, $CDCl_3$).

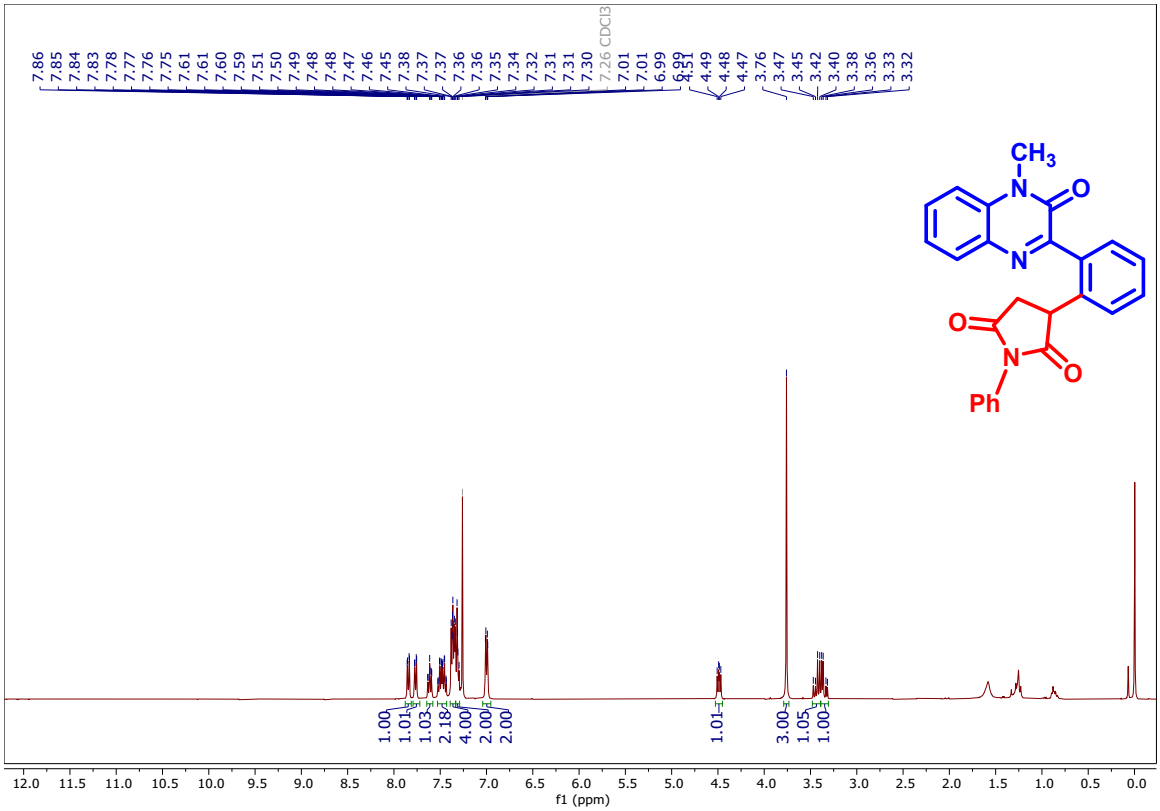


Figure 7: ^{1}H NMR spectrum of compound **3ad** (400 MHz, $CDCl_3$).

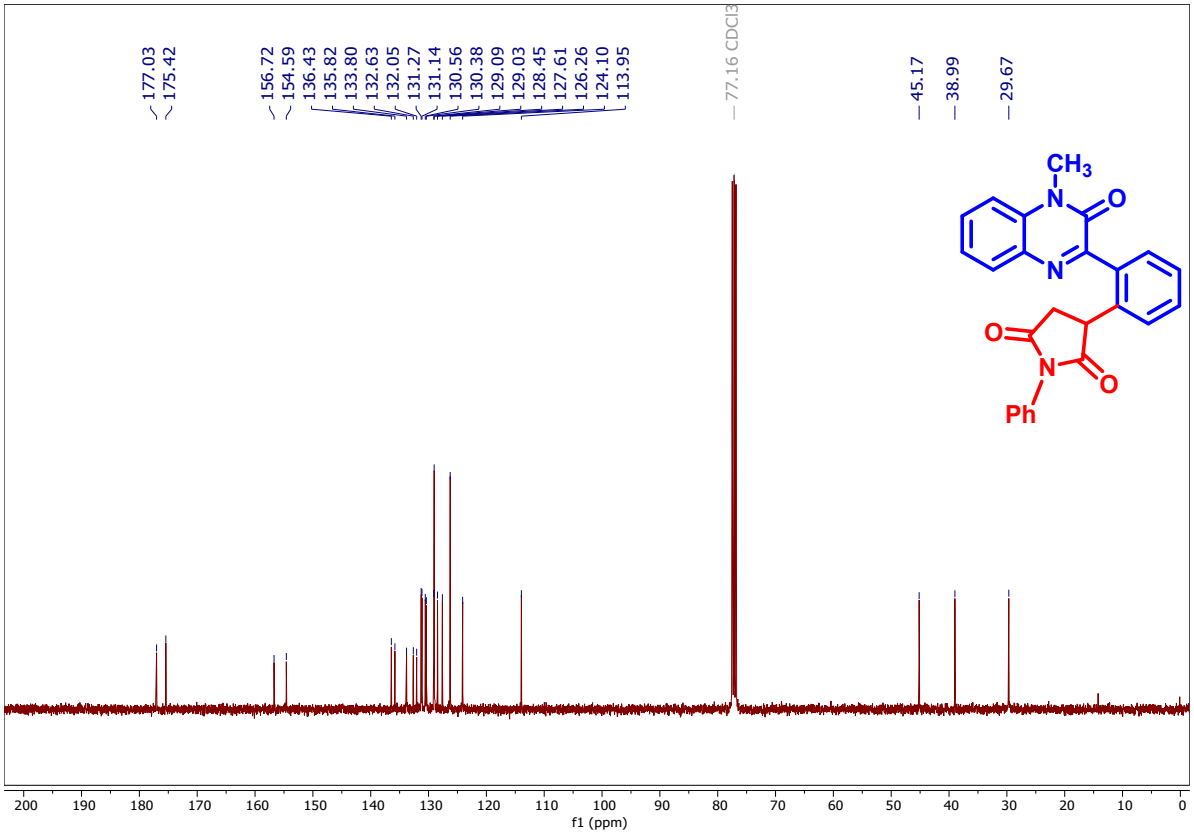


Figure 8: ^{13}C{1H} NMR spectrum of compound **3ad** (100 MHz, $CDCl_3$).

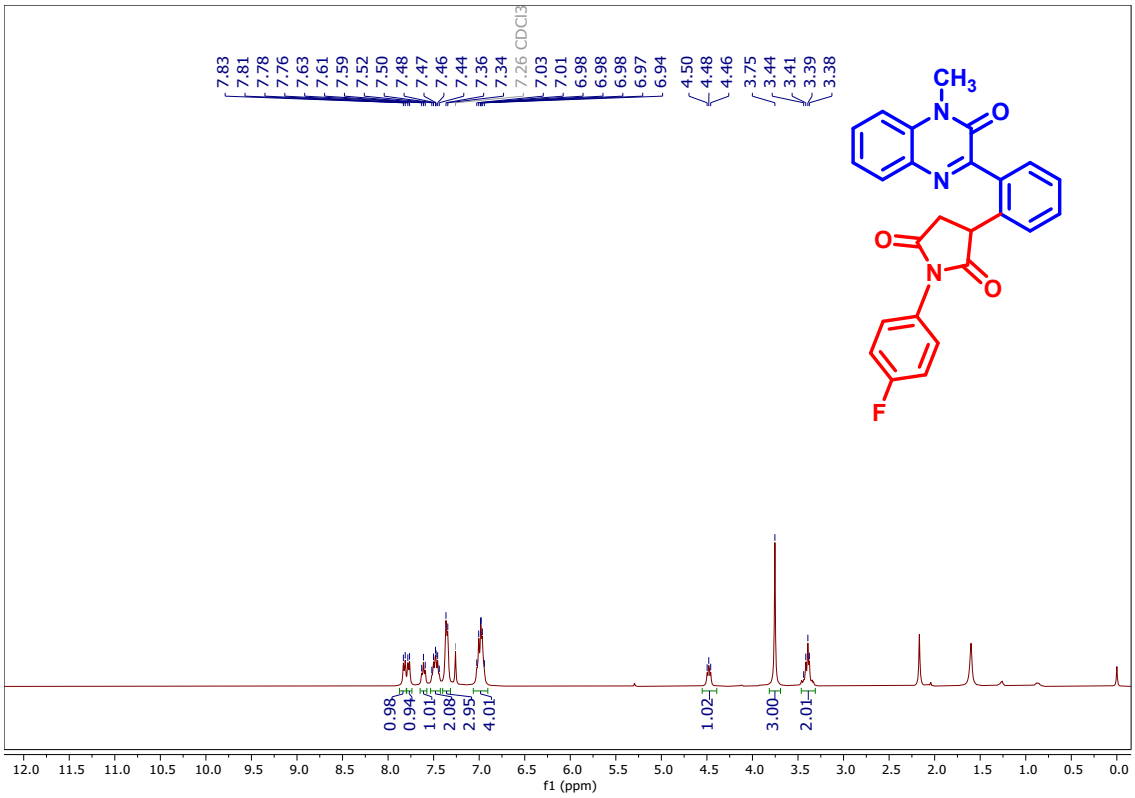


Figure 9: ^{1}H NMR spectrum of compound **3ae** (400 MHz, $CDCl_3$).

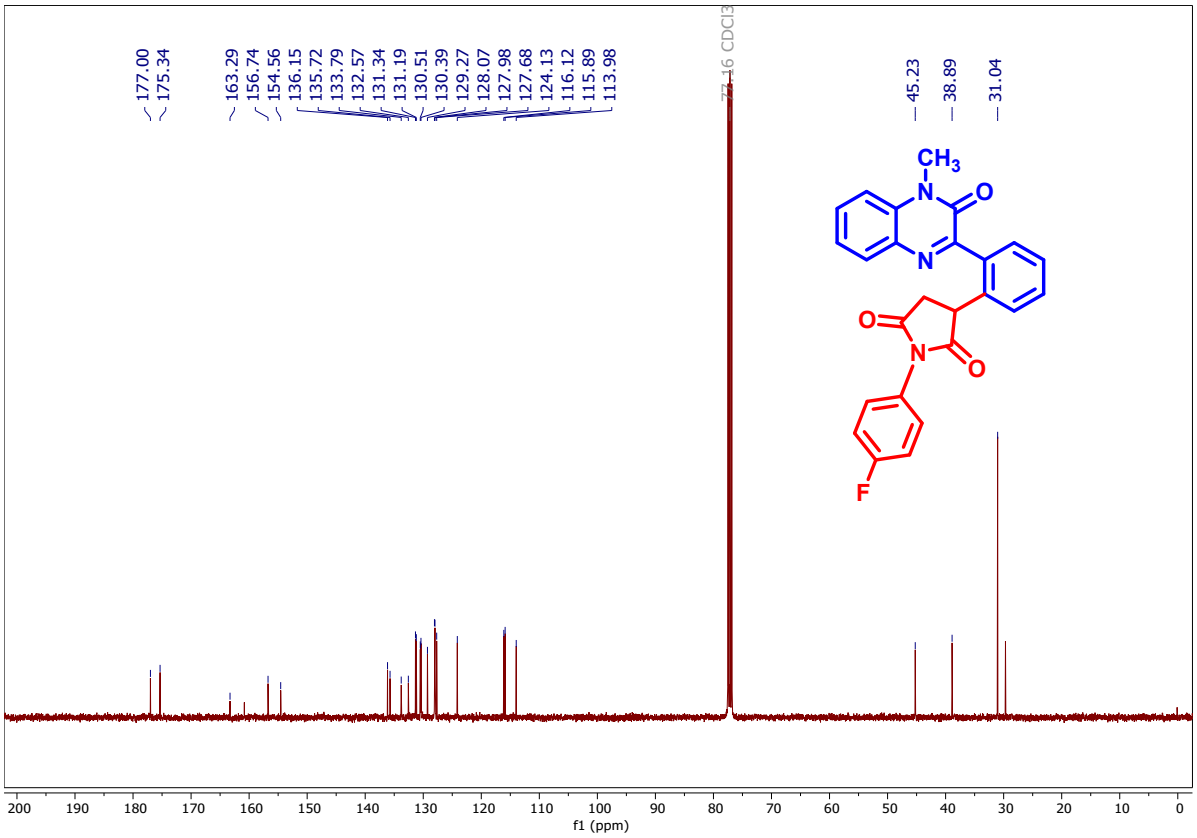


Figure 10: ^{13}C{1H} NMR spectrum of compound **3ae** (100 MHz, $CDCl_3$).

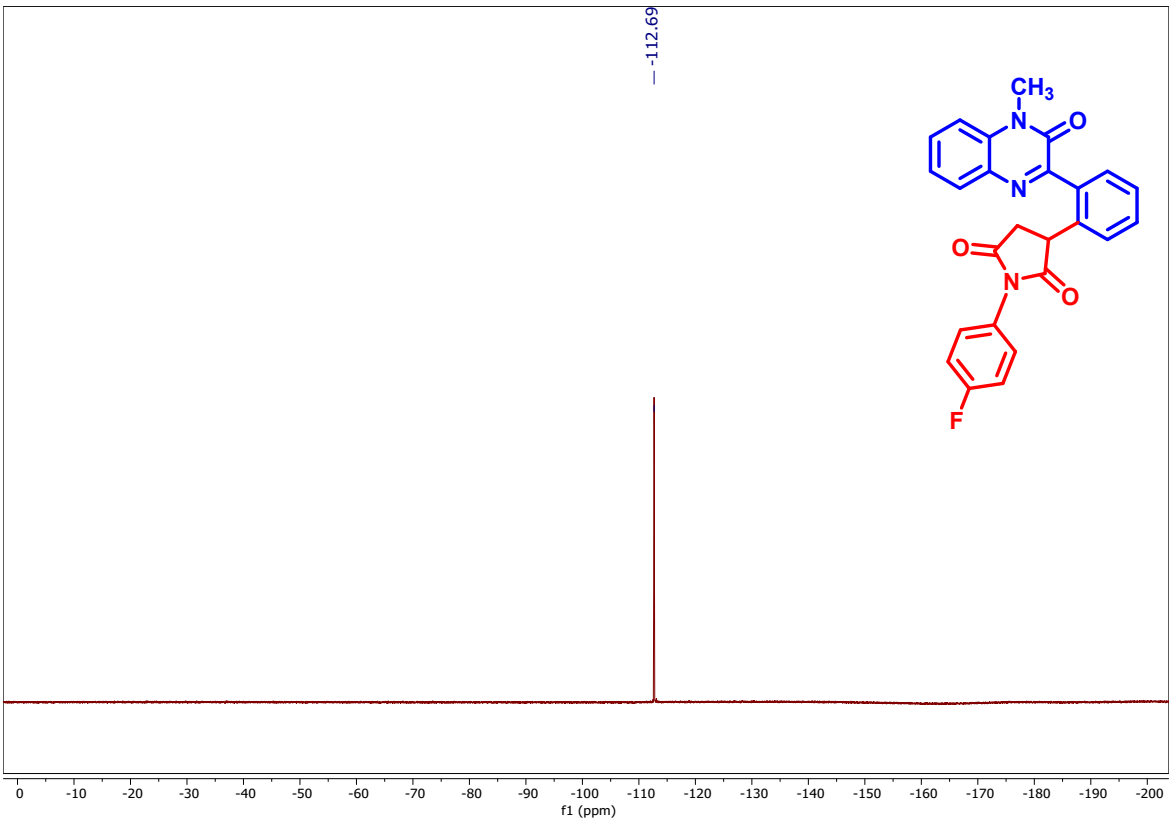


Figure 11: ^{19}F NMR spectrum of compound **3ae** (377 MHz, $CDCl_3$).

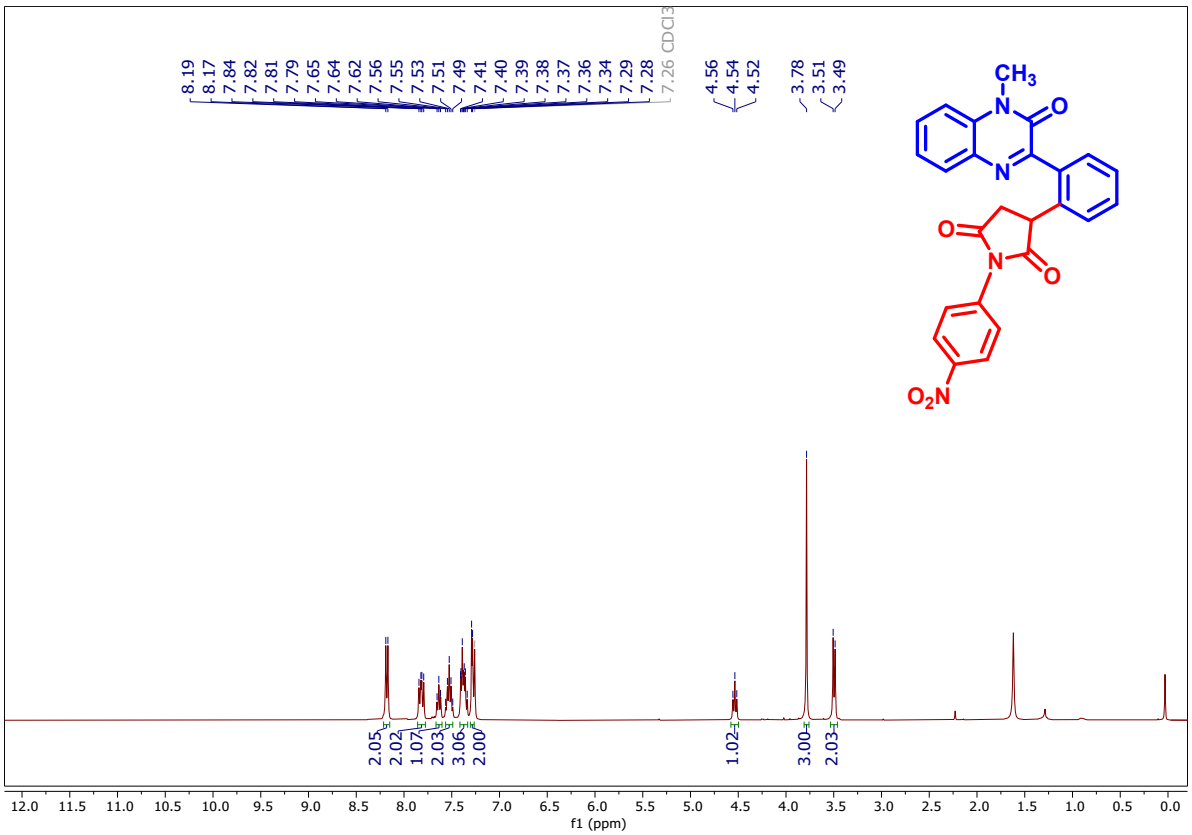


Figure 12: ^{1}H NMR spectrum of compound **3af** (400 MHz, $CDCl_3$).

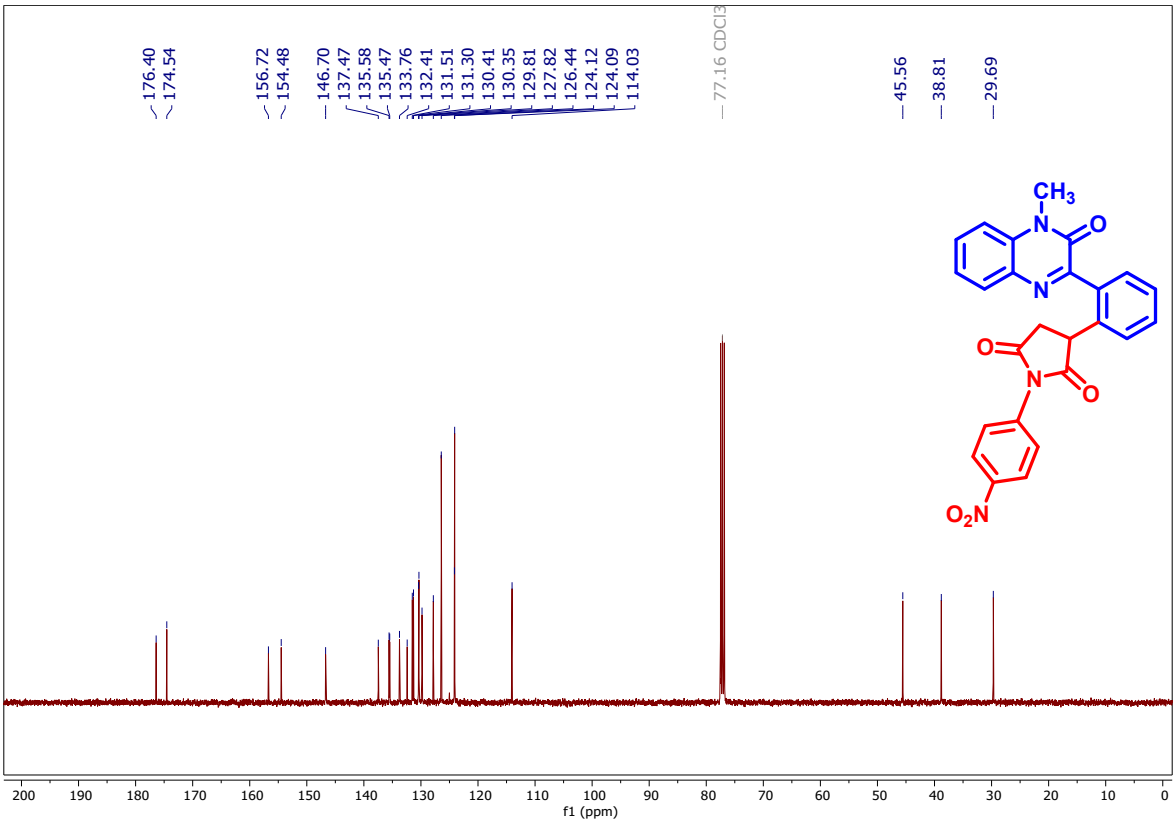


Figure 13: ^{13}C{1H} NMR spectrum of compound **3af** (100 MHz, $CDCl_3$).

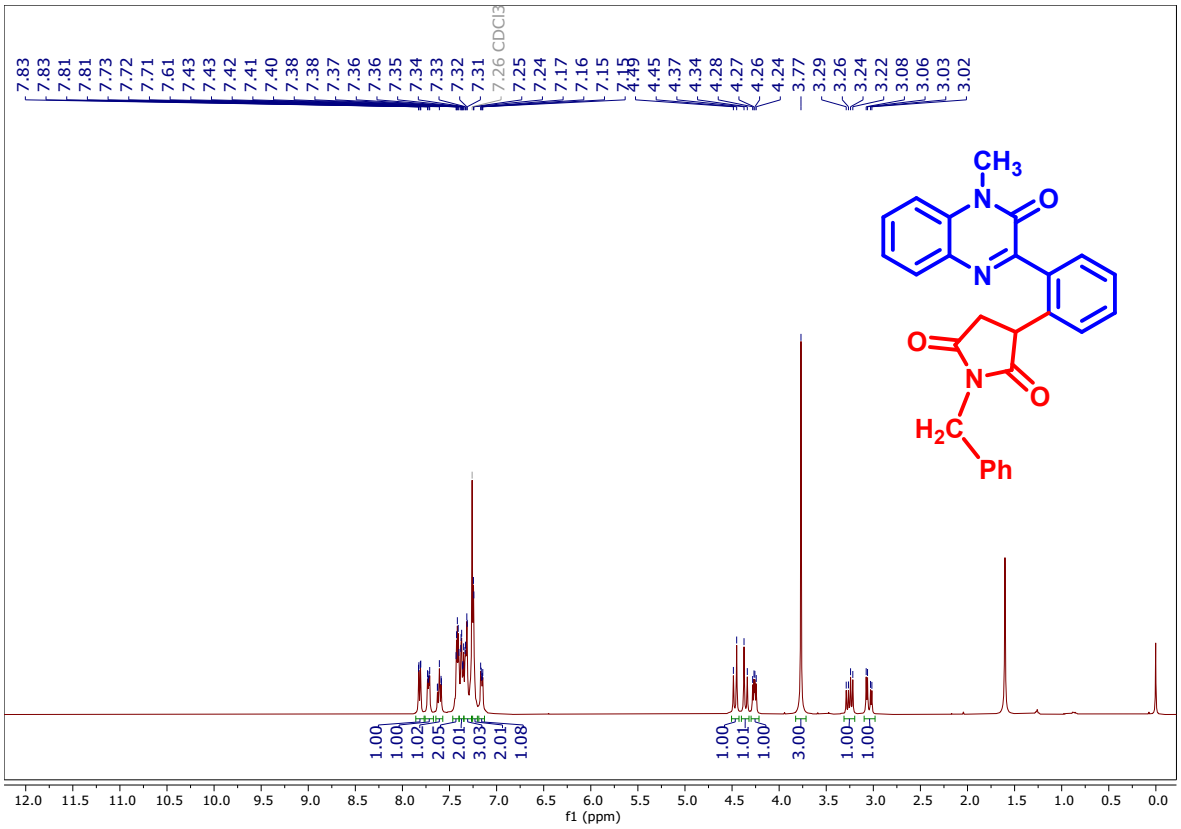


Figure 14: ^{1}H NMR spectrum of compound **3ag** (400 MHz, $CDCl_3$).

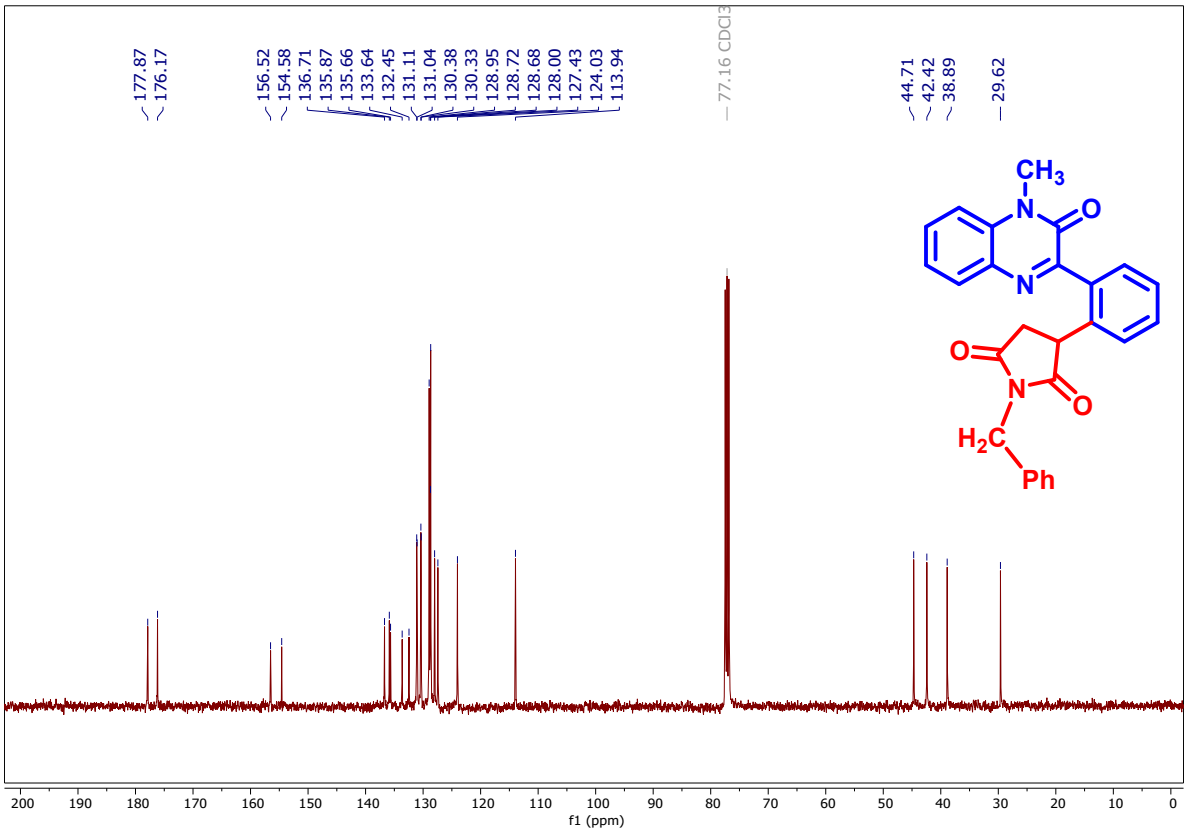


Figure 15: ^{13}C{1H} NMR spectrum of compound **3ag** (100 MHz, $CDCl_3$).

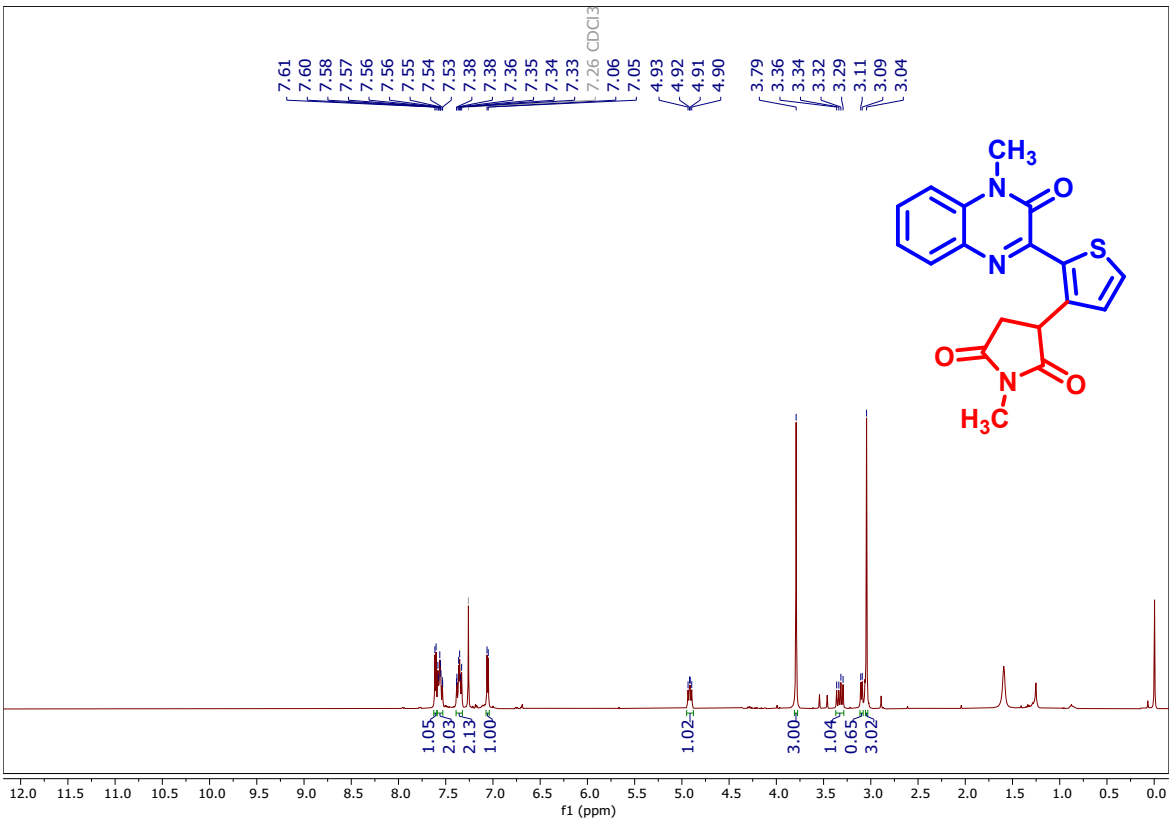


Figure 16: ^{1}H NMR spectrum of compound **3da** (400 MHz, $CDCl_3$).

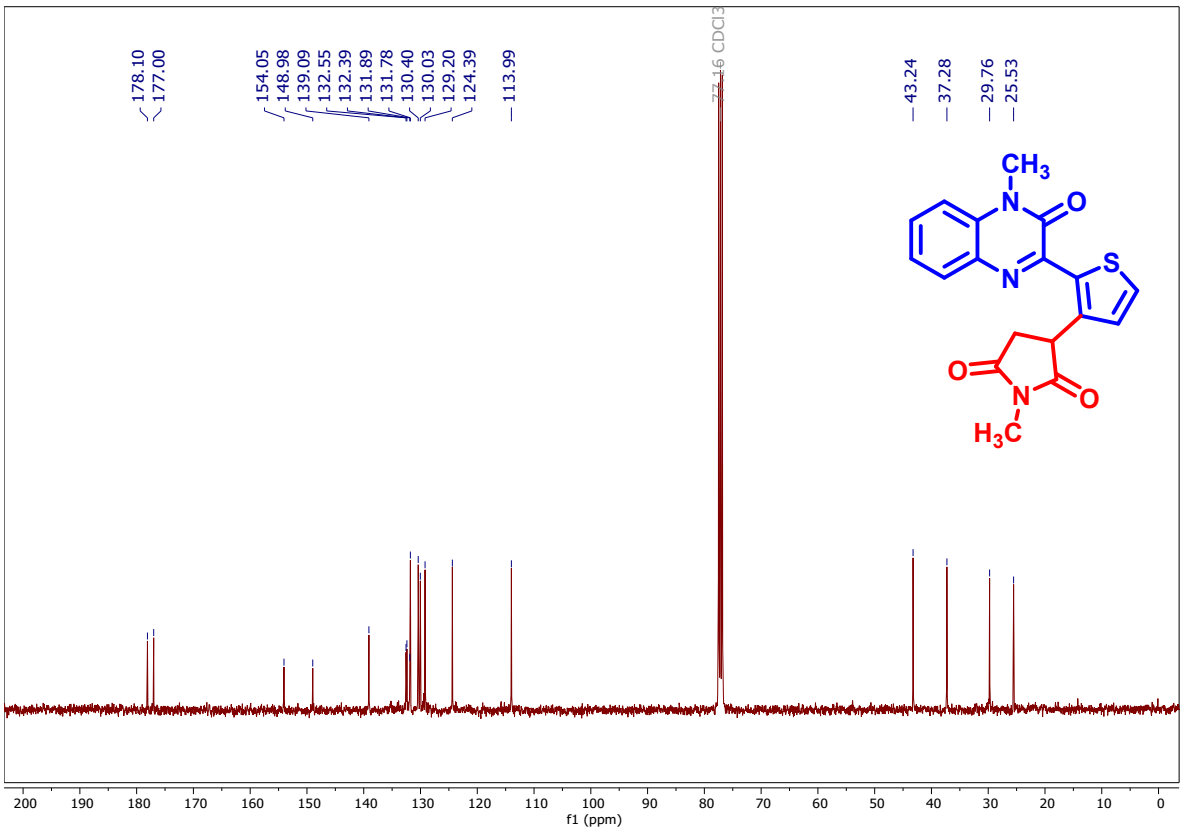


Figure 17: ^{13}C{1H} NMR spectrum of compound **3da** (100 MHz, $CDCl_3$).

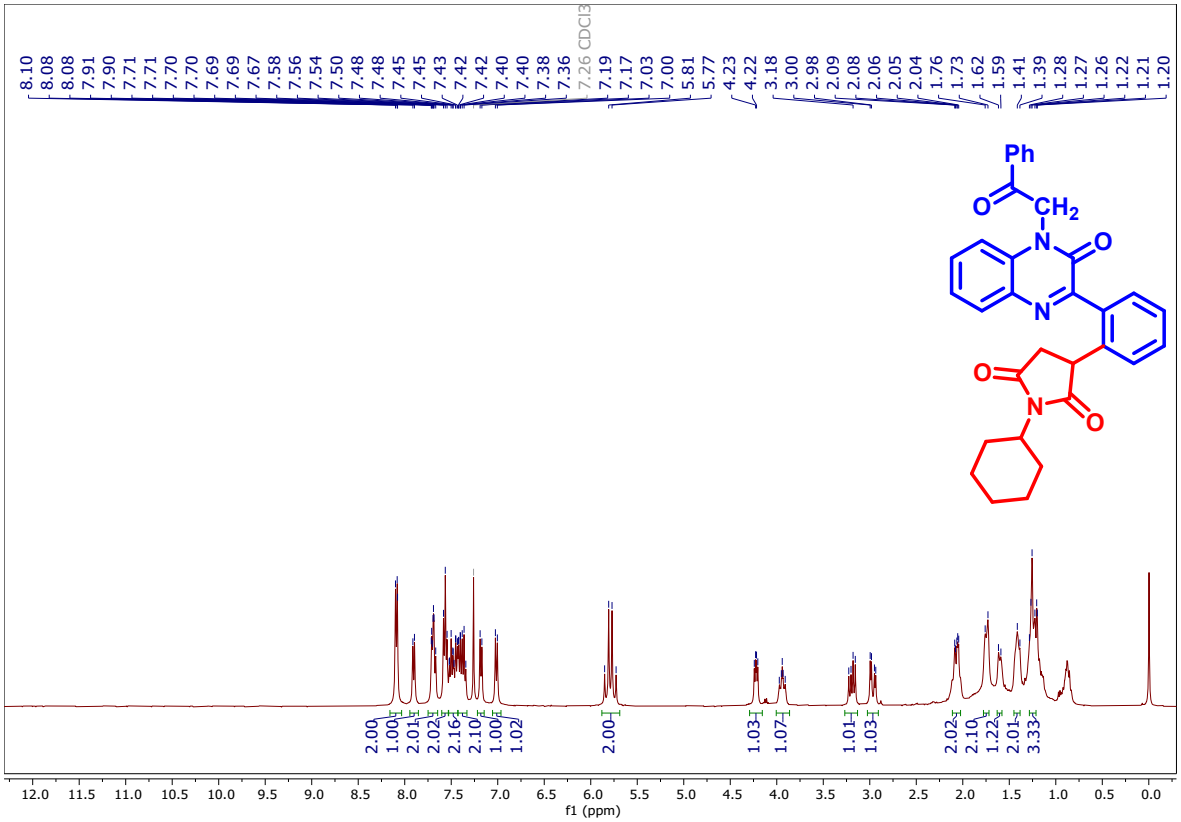


Figure 18: ^{1}H NMR spectrum of compound **3fc** (400 MHz, $CDCl_3$).

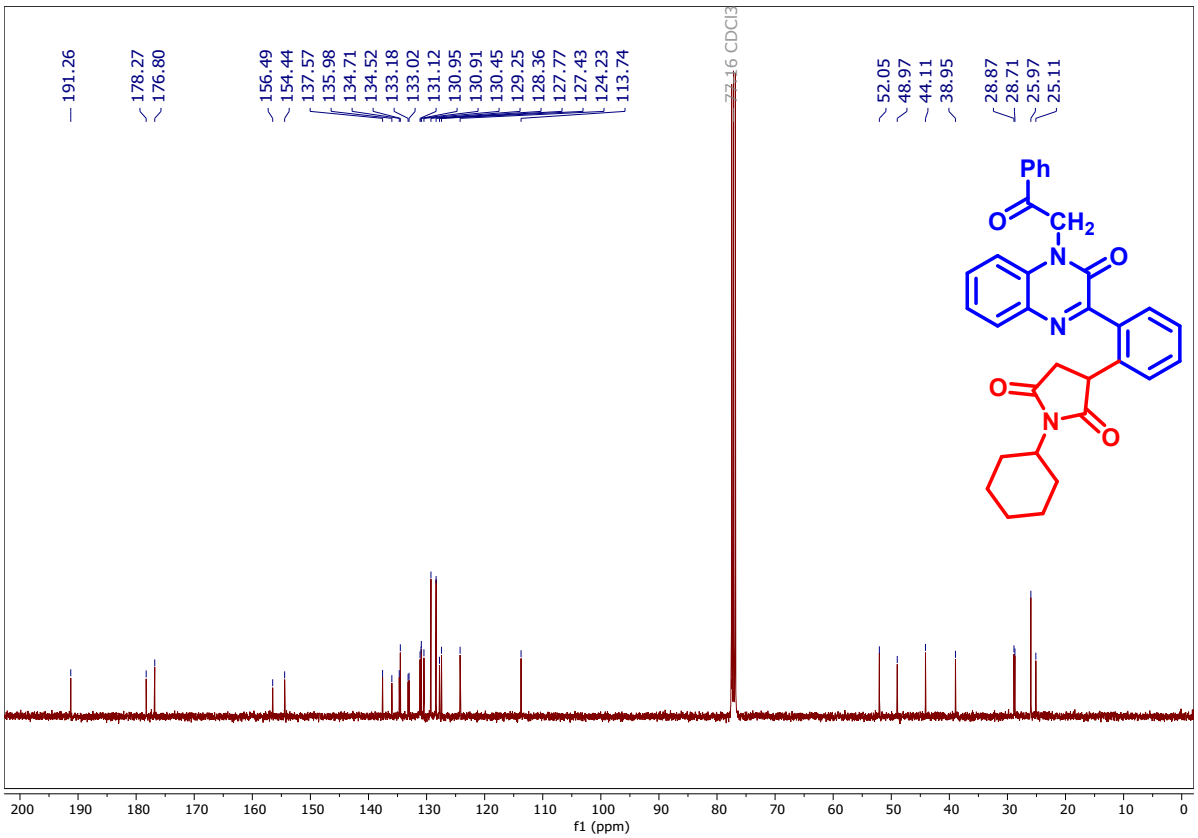


Figure 19: ^{13}C{1H} NMR spectrum of compound **3fc** (100 MHz, $CDCl_3$).

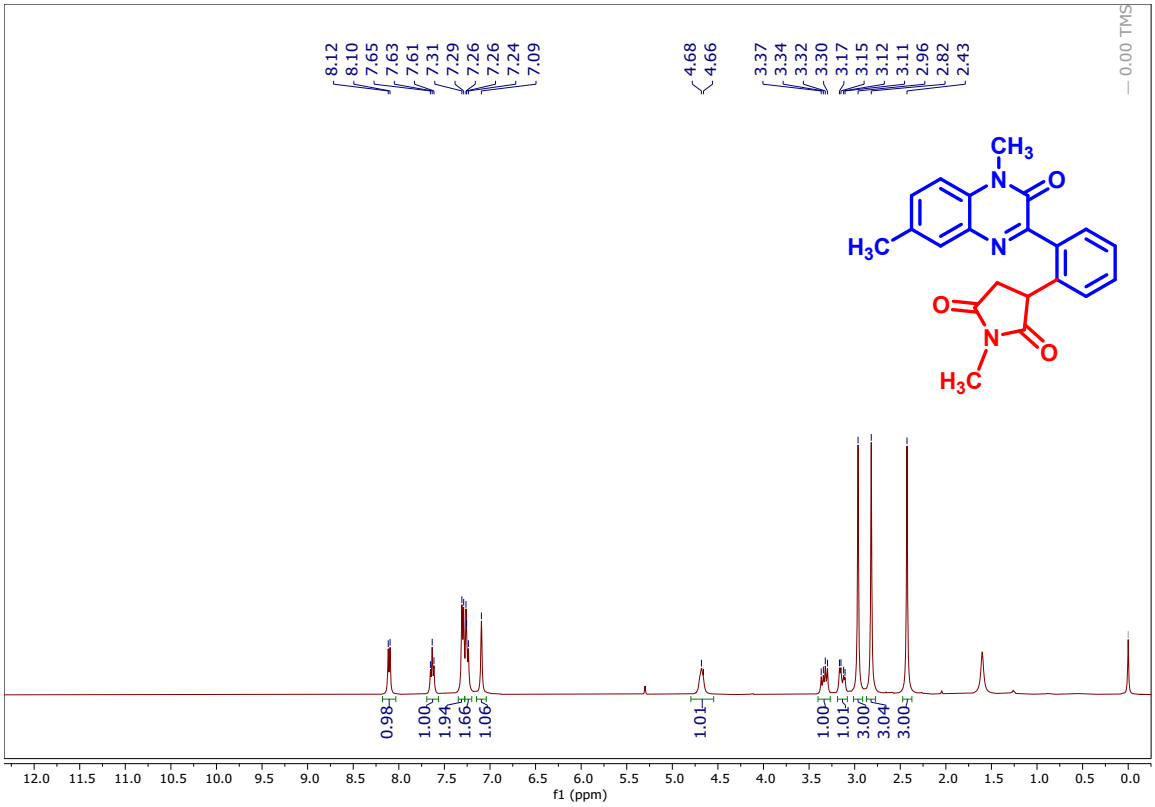


Figure 20: ^{1}H NMR spectrum of compound **4aa** (400 MHz, $CDCl_3$).

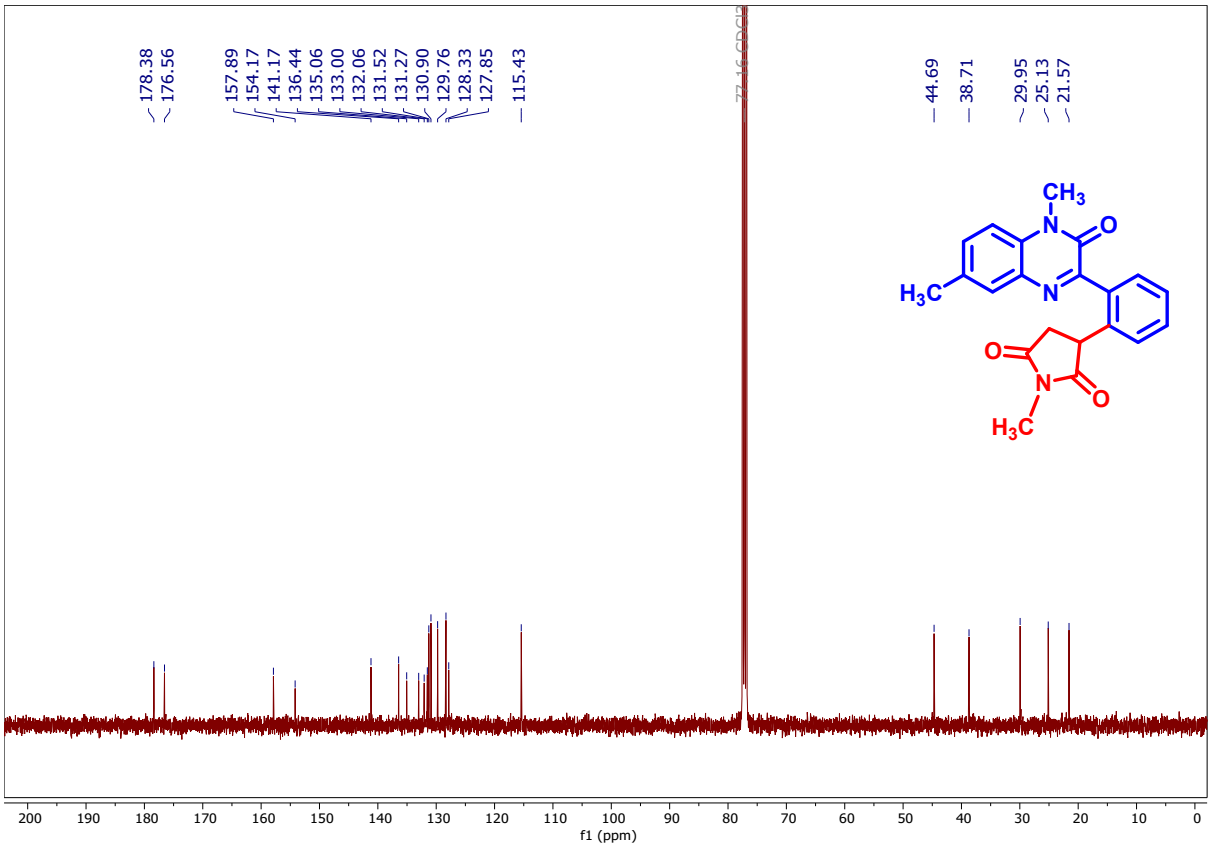


Figure 21: ^{13}C{1H} NMR spectrum of compound **4aa** (100 MHz, $CDCl_3$).

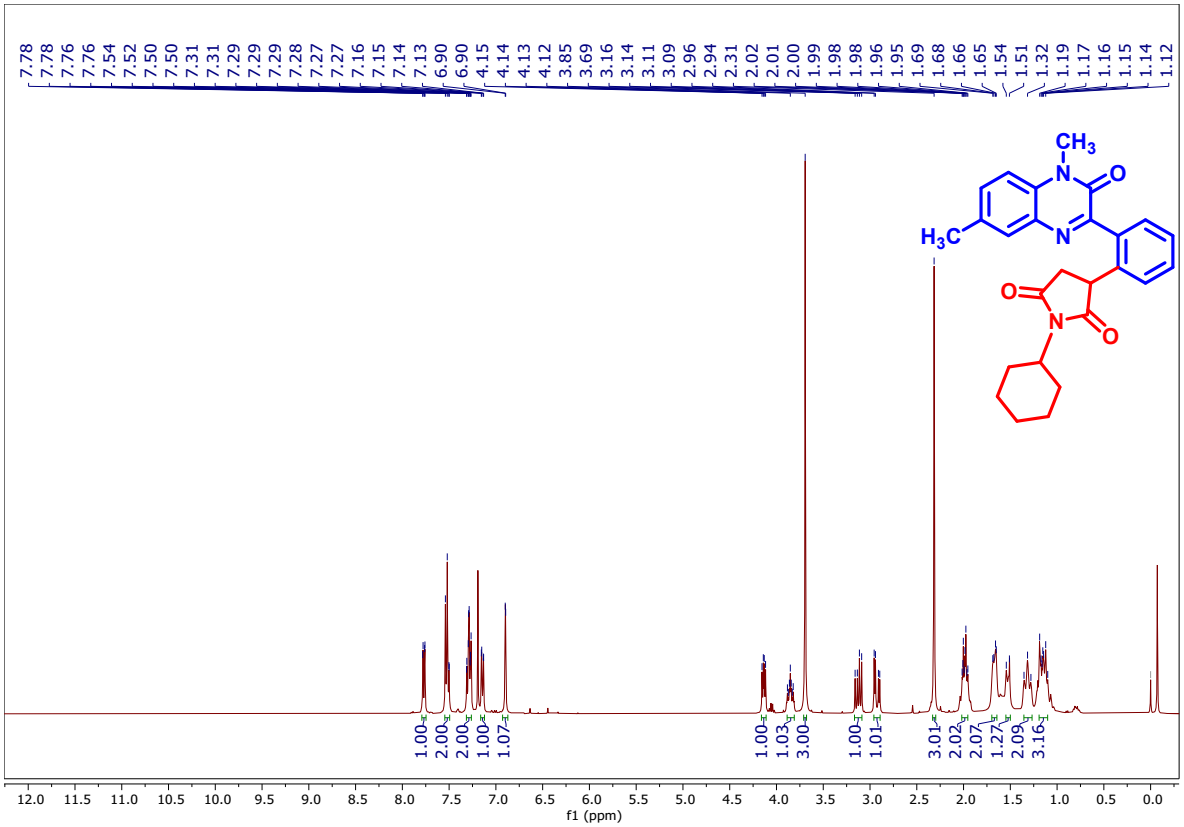


Figure 22: ^{1}H NMR spectrum of compound **4ab** (400 MHz, $CDCl_3$).

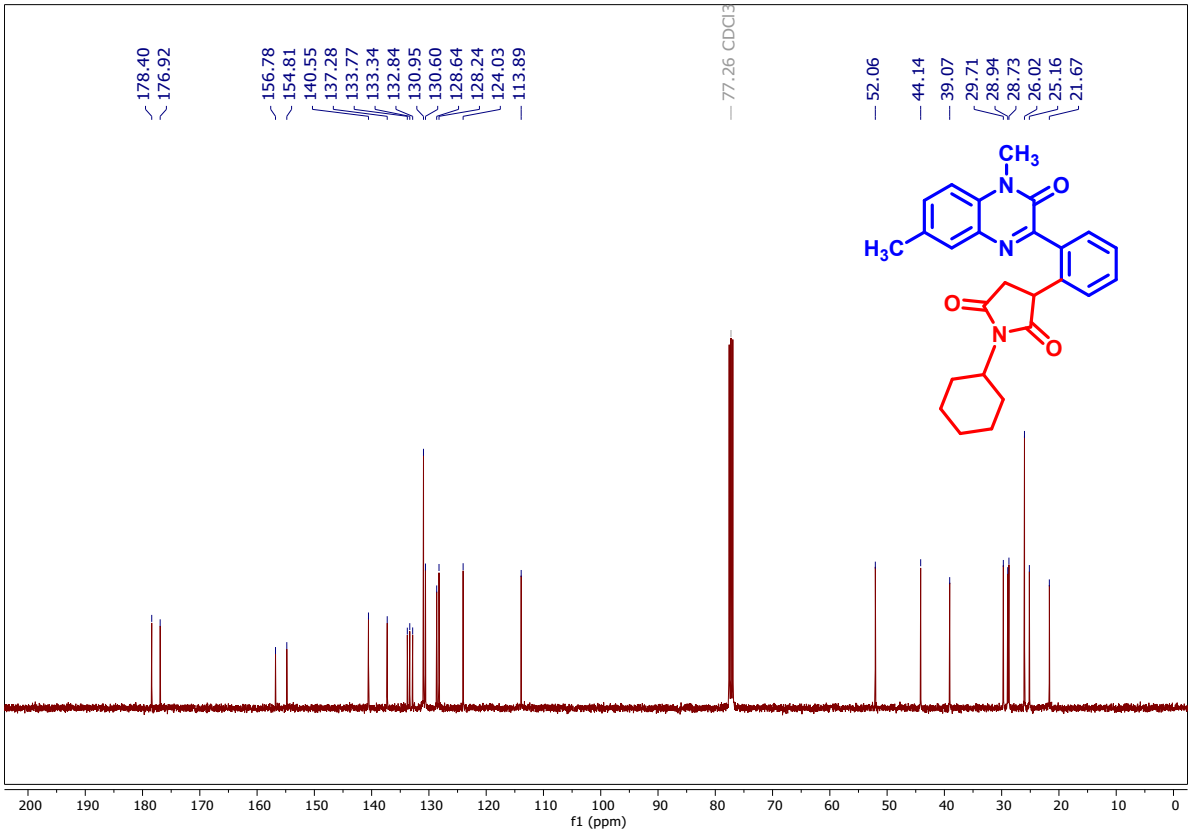


Figure 23: ^{13}C{1H} NMR spectrum of compound **4ab** (100 MHz, $CDCl_3$).

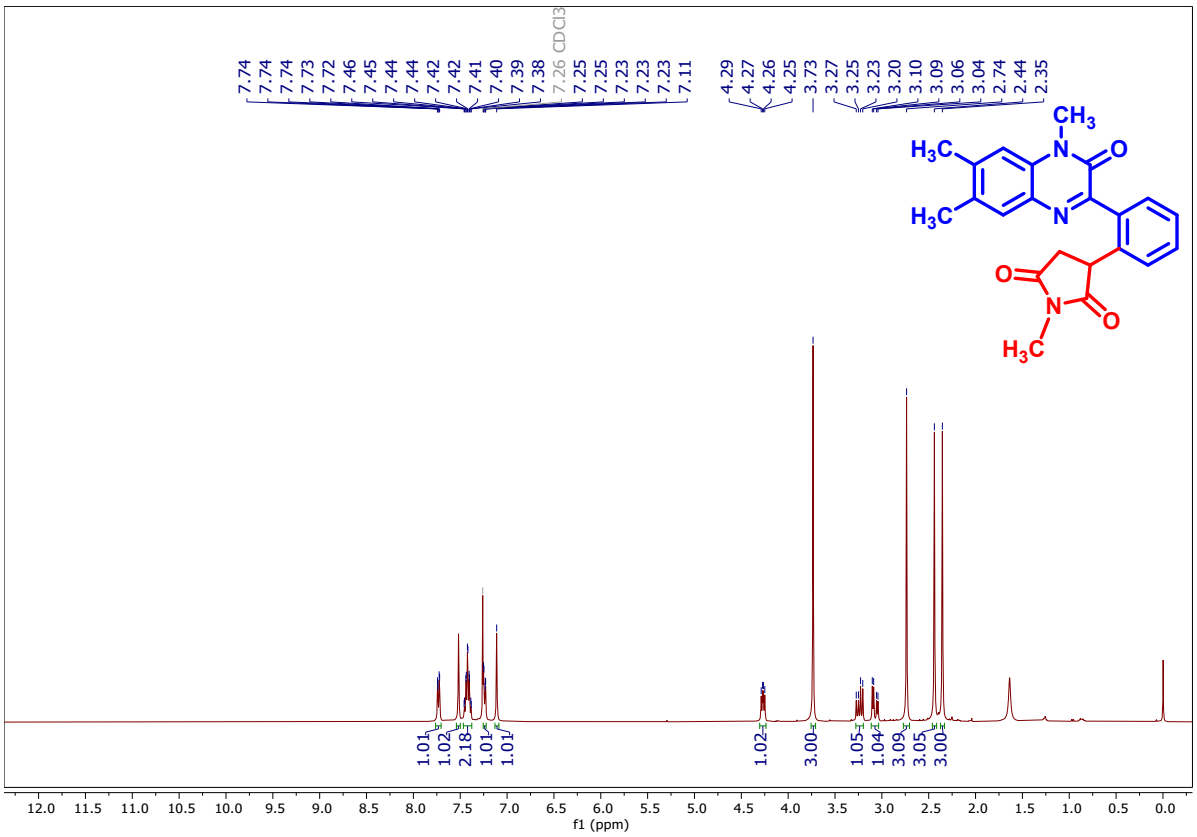


Figure 24: ^{1}H NMR spectrum of compound **4ba** (400 MHz, $CDCl_3$).

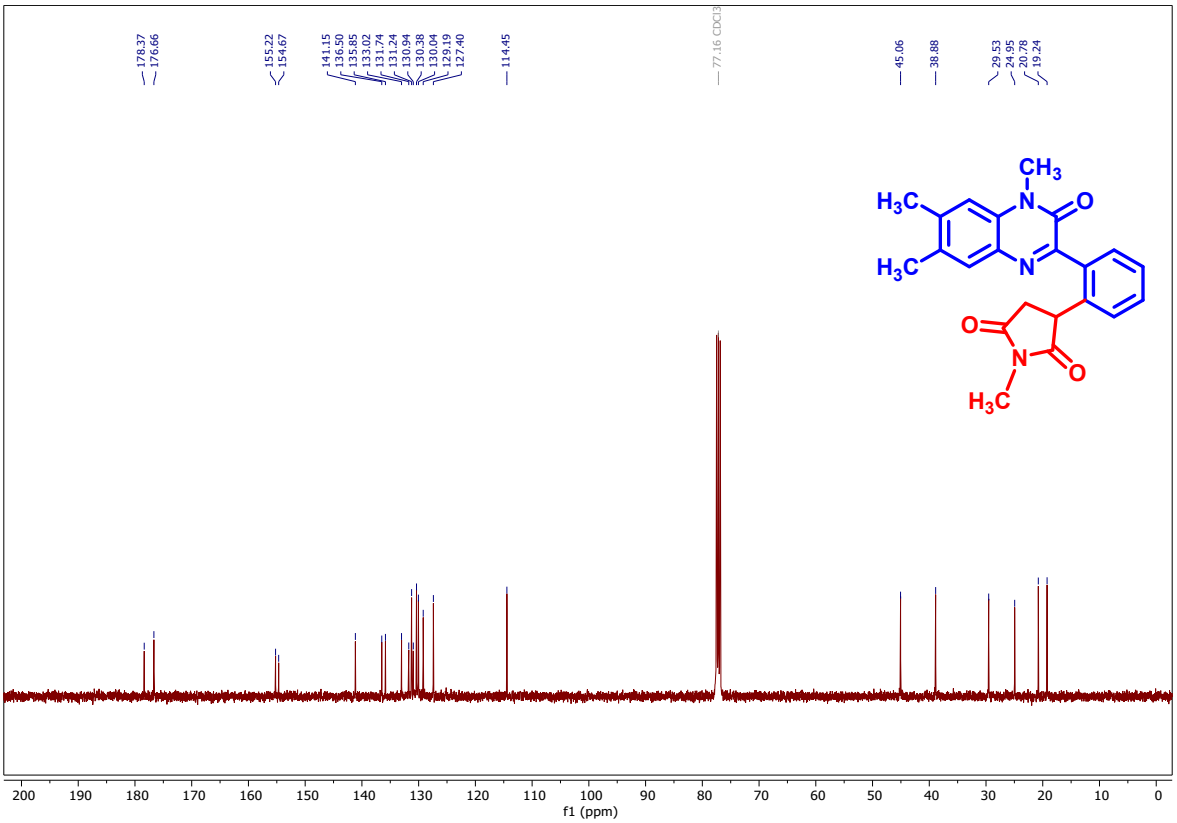


Figure 25: ^{13}C{1H} NMR spectrum of compound **4ba** (100 MHz, $CDCl_3$).

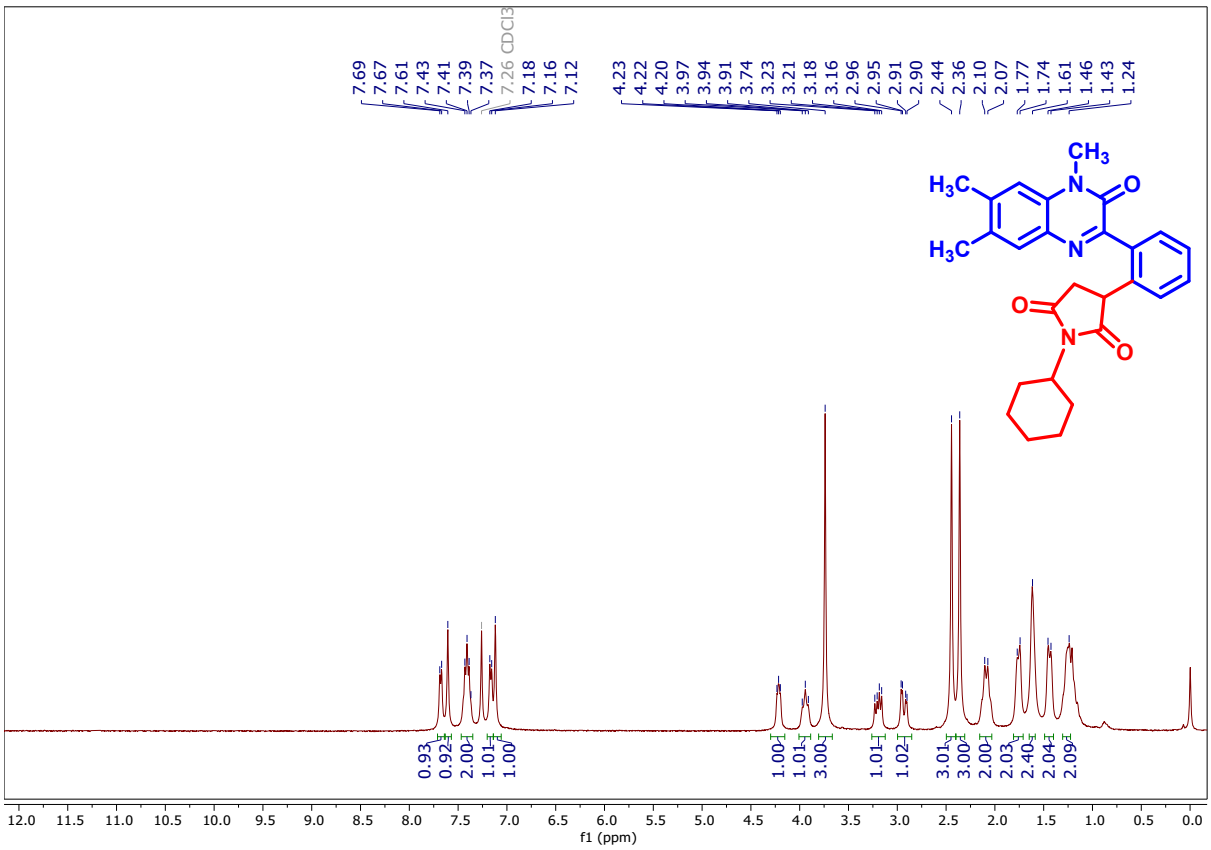


Figure 26: ^{1}H NMR spectrum of compound **4bb** (400 MHz, $CDCl_3$).

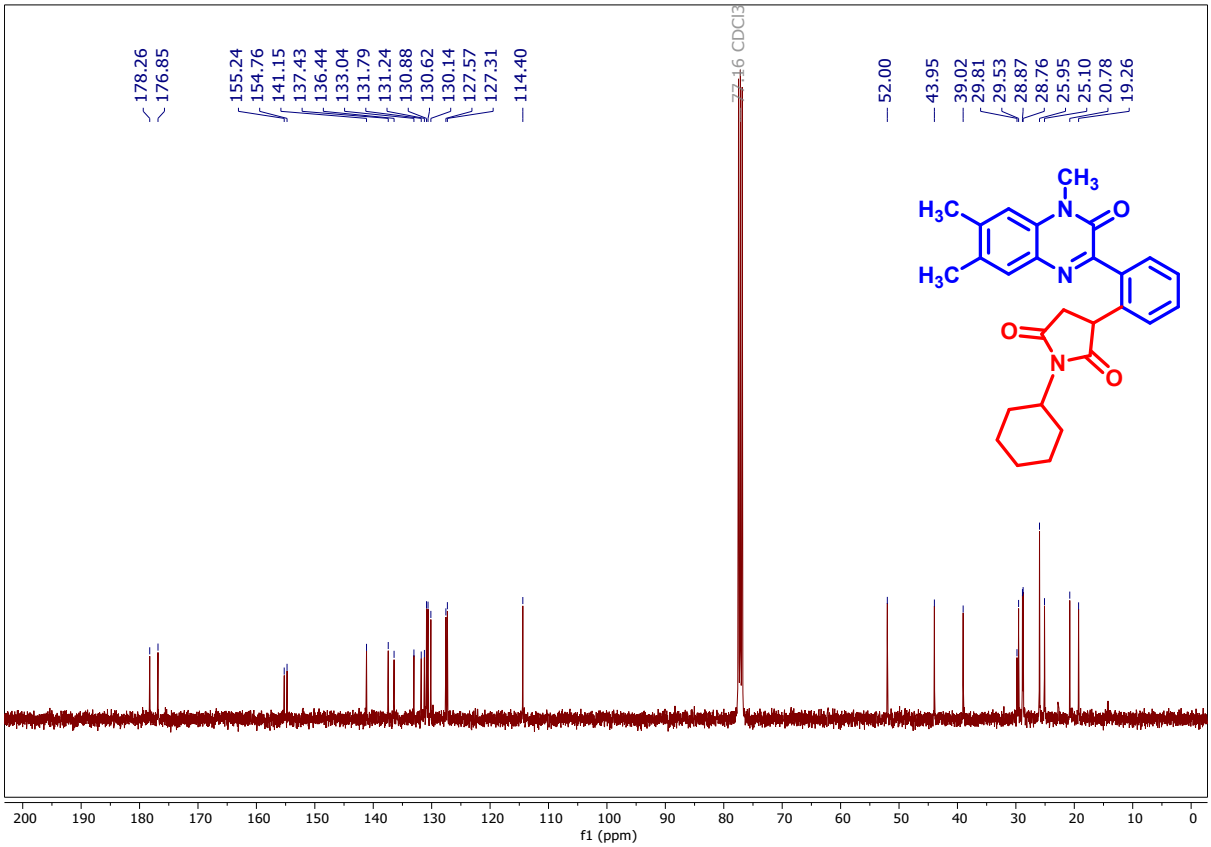


Figure 27: ^{13}C{1H} NMR spectrum of compound **4bb** (100 MHz, $CDCl_3$).

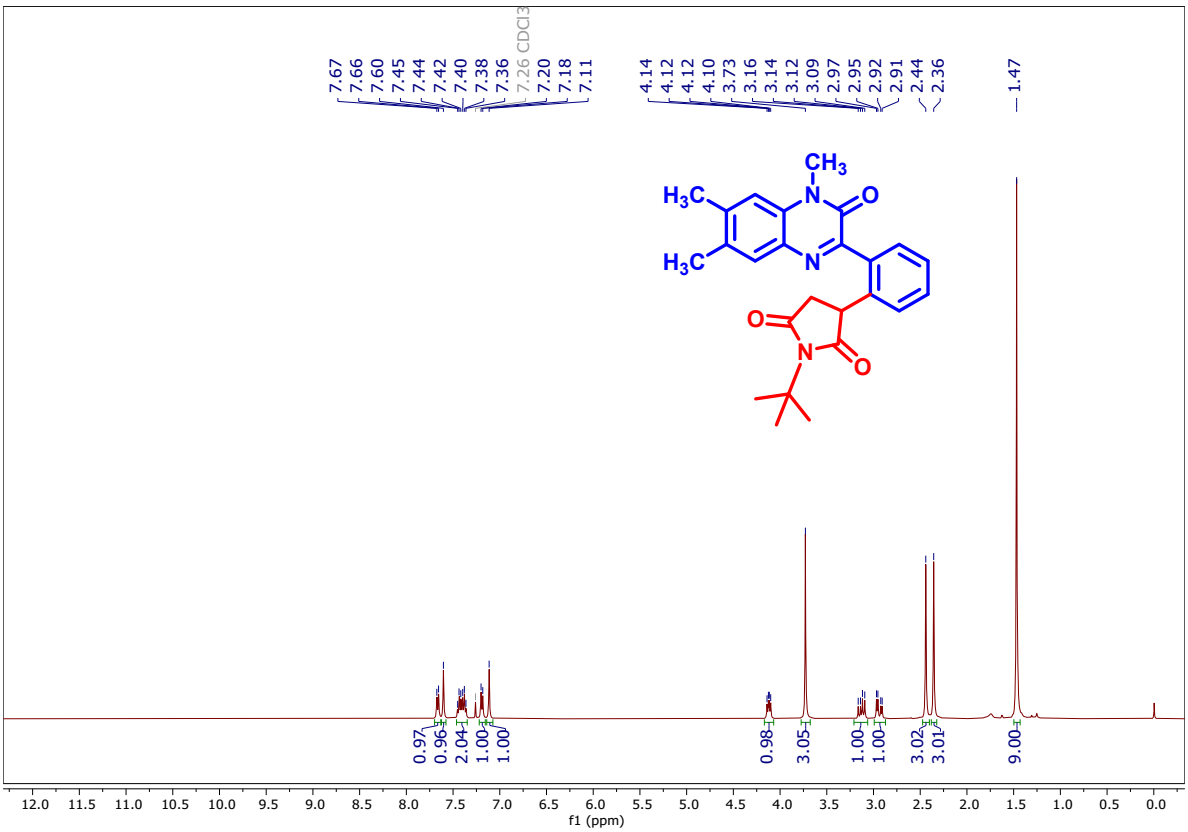


Figure 28: ^{1}H NMR spectrum of compound **4bc** (400 MHz, $CDCl_3$).

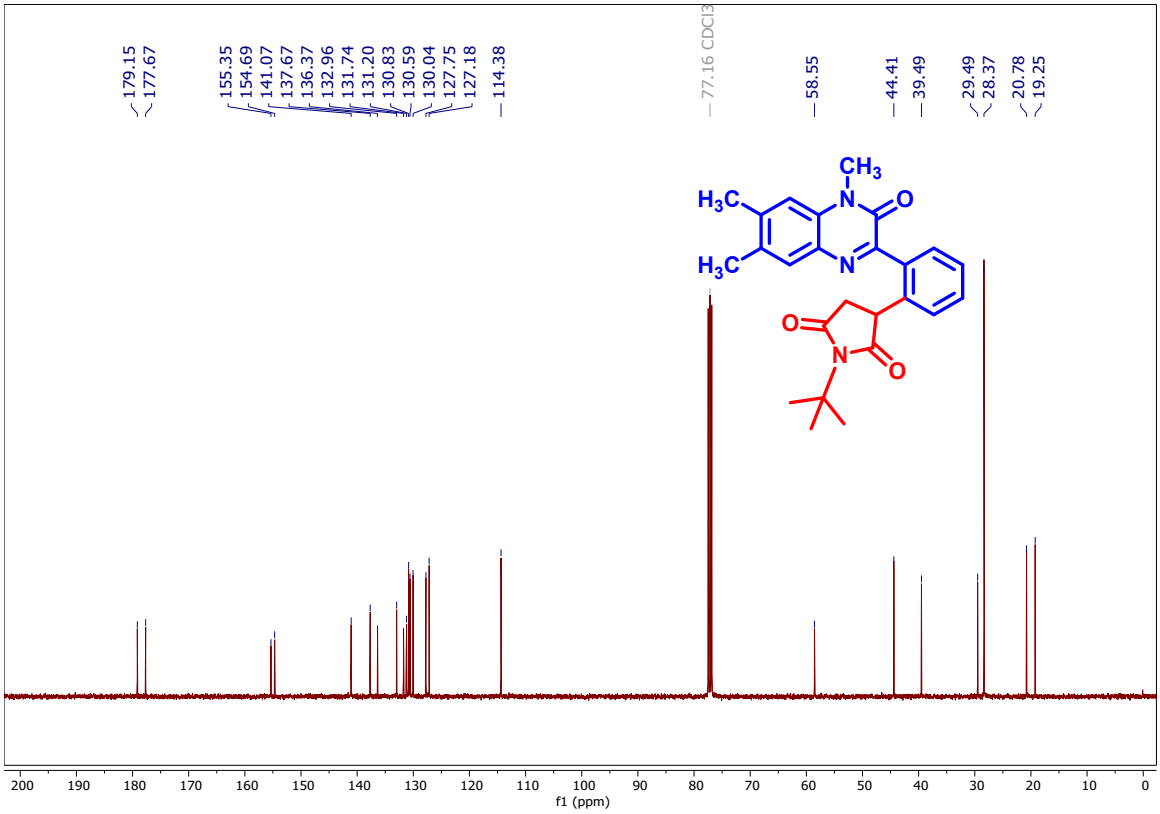


Figure 29: ^{13}C{1H} NMR spectrum of compound **4bc** (100 MHz, $CDCl_3$).

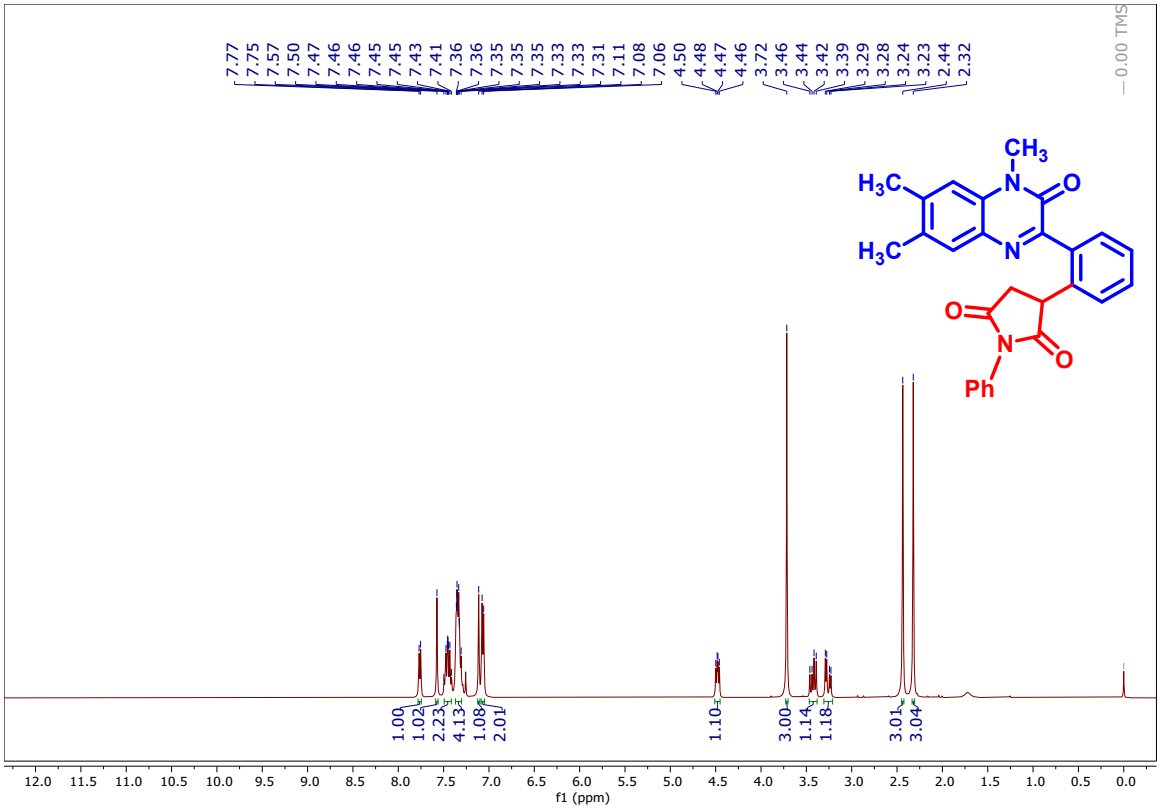


Figure 30: ^{1}H NMR spectrum of compound **4bd** (400 MHz, $CDCl_3$).

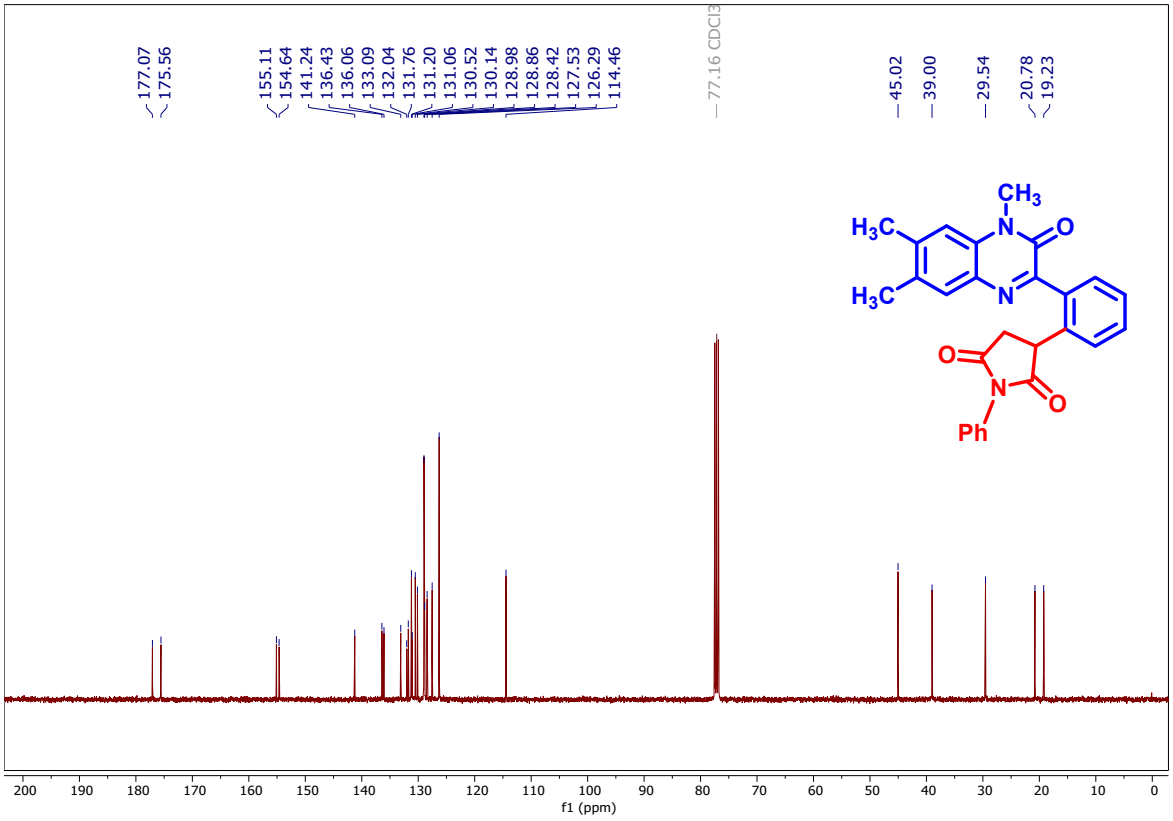


Figure 31: ^{13}C{1H} NMR spectrum of compound **4bd** (100 MHz, $CDCl_3$).

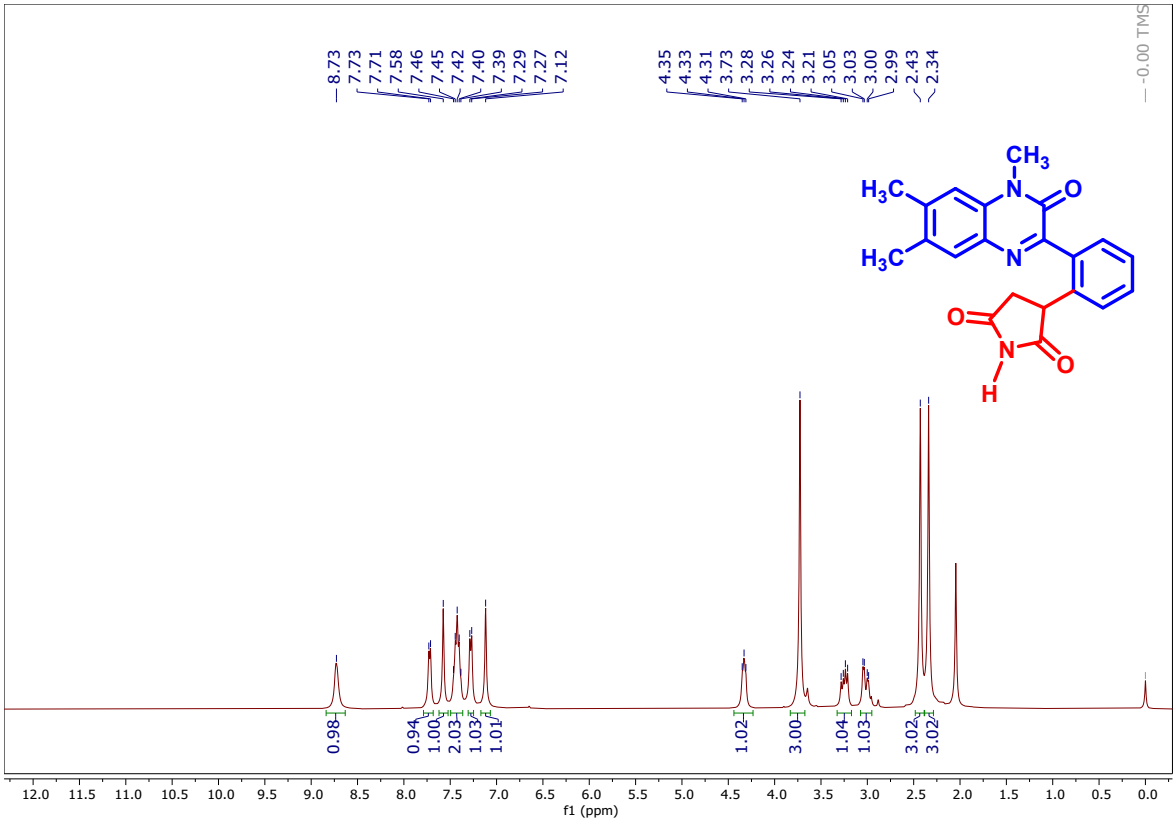


Figure 32: ^{1}H NMR spectrum of compound **4bf** (400 MHz, $CDCl_3$).

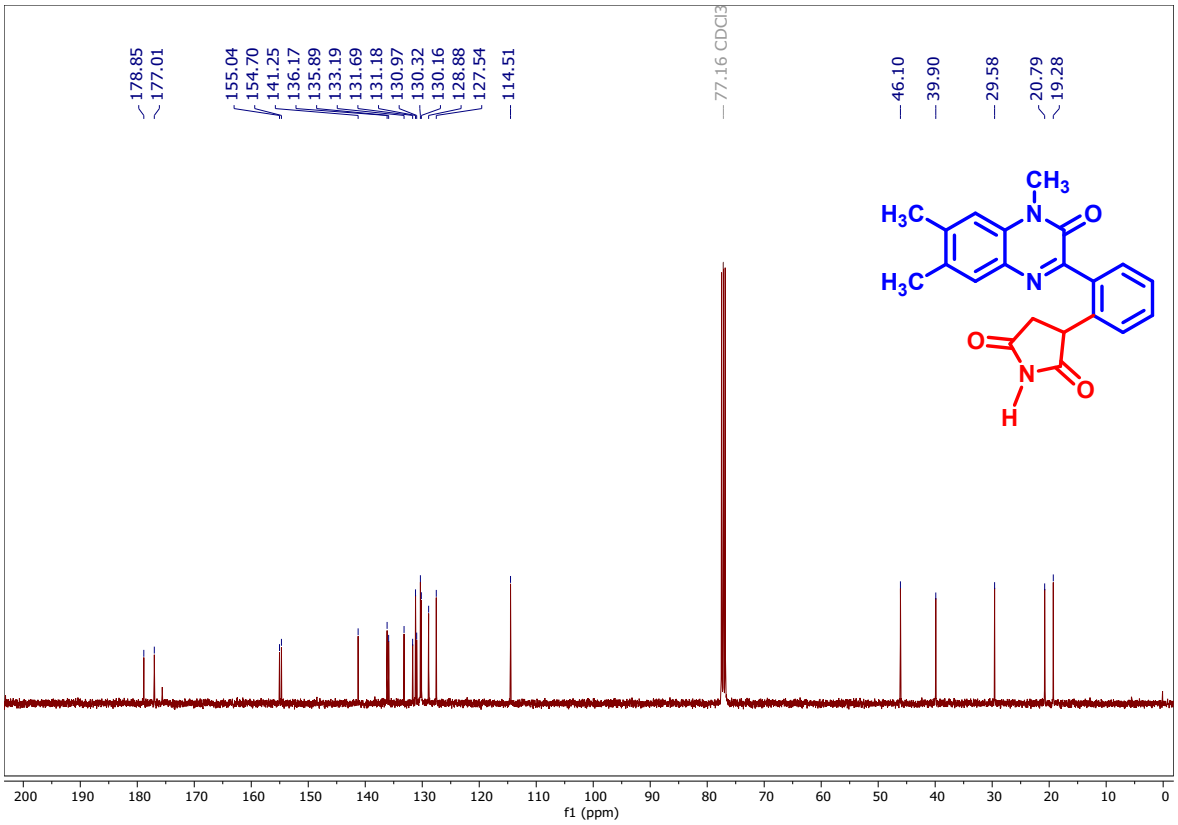


Figure 33: ^{13}C{1H} NMR spectrum of compound **4bf** (100 MHz, $CDCl_3$).

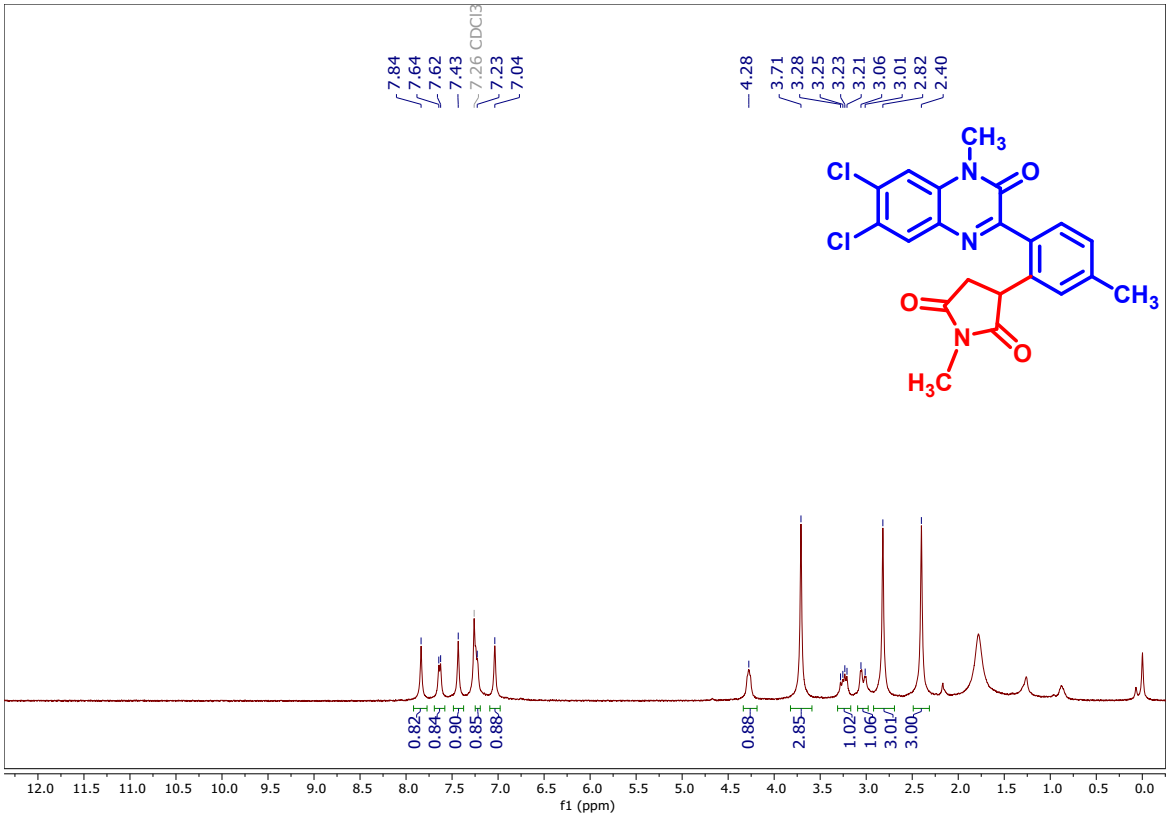


Figure 34: ^{1}H NMR spectrum of compound **4ca** (400 MHz, $CDCl_3$).

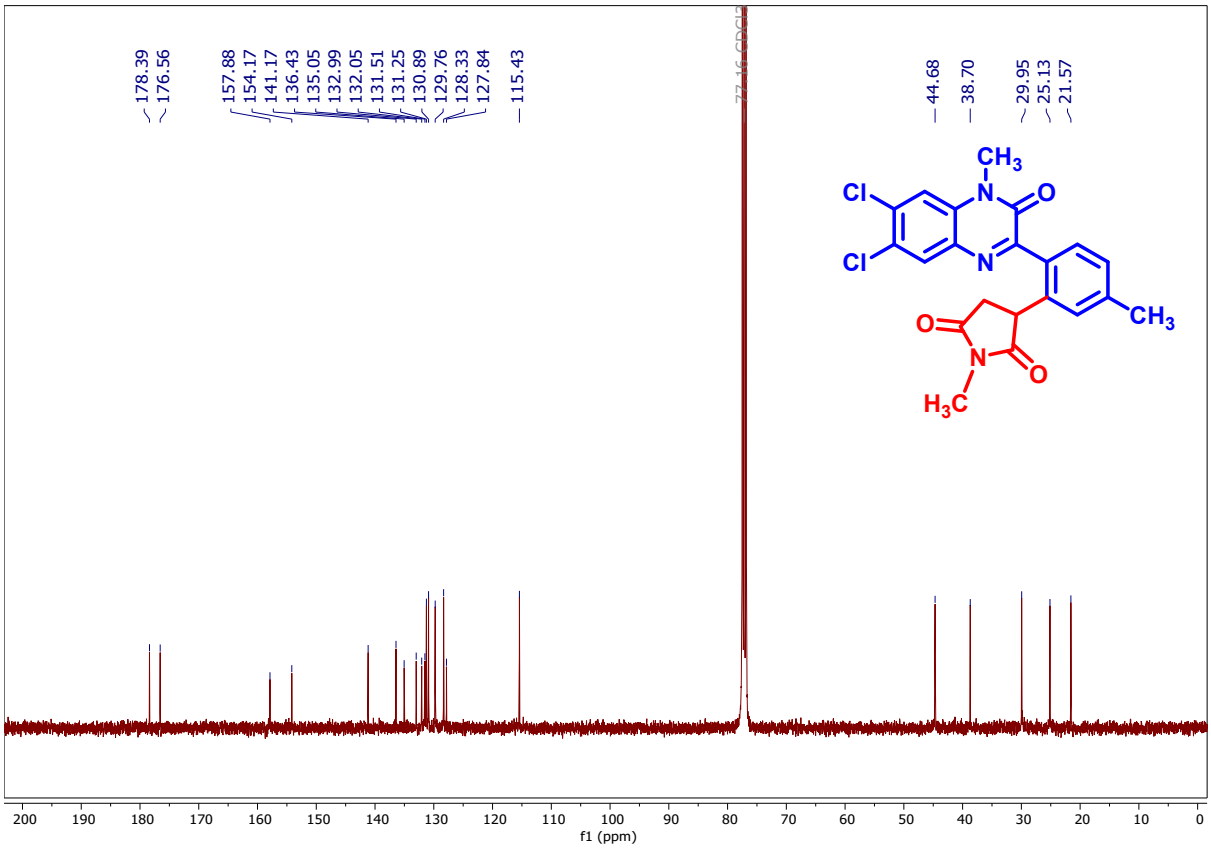


Figure 35: ^{13}C{1H} NMR spectrum of compound **4ca** (100 MHz, $CDCl_3$).

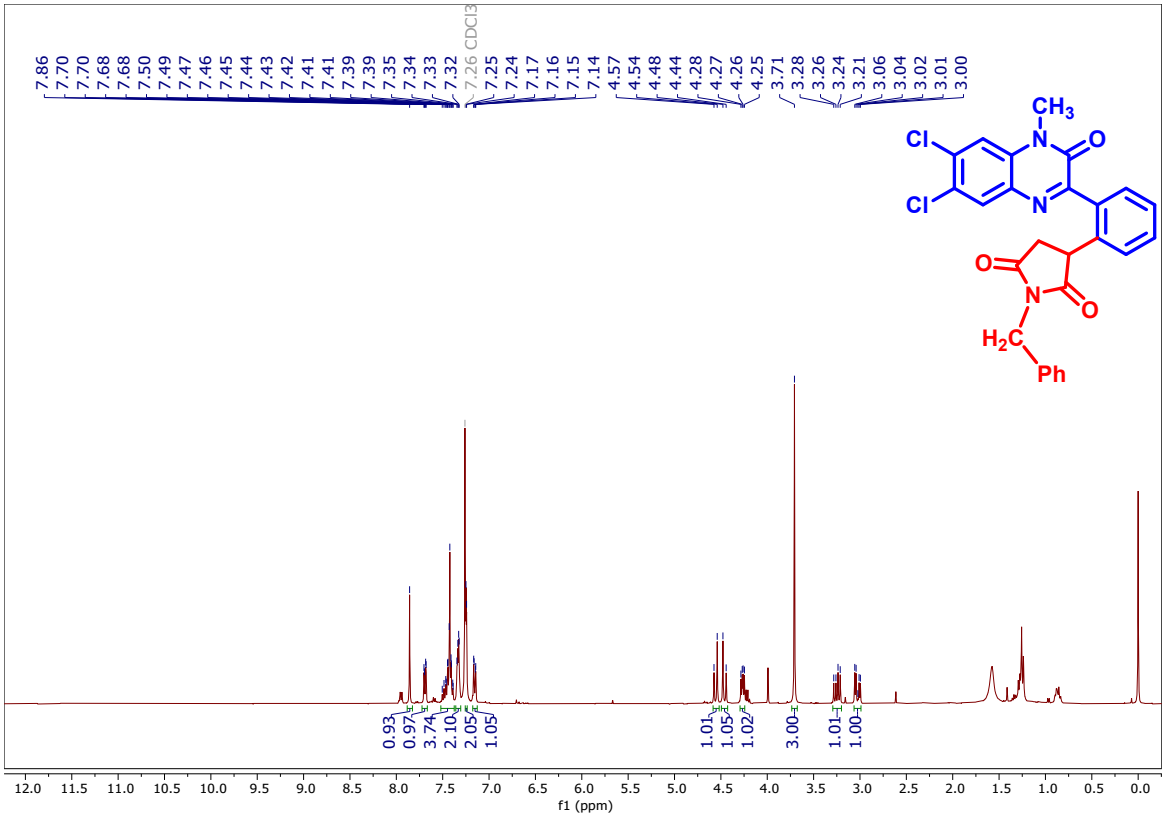


Figure 36: ^{1}H NMR spectrum of compound **4de** (400 MHz, $CDCl_3$).

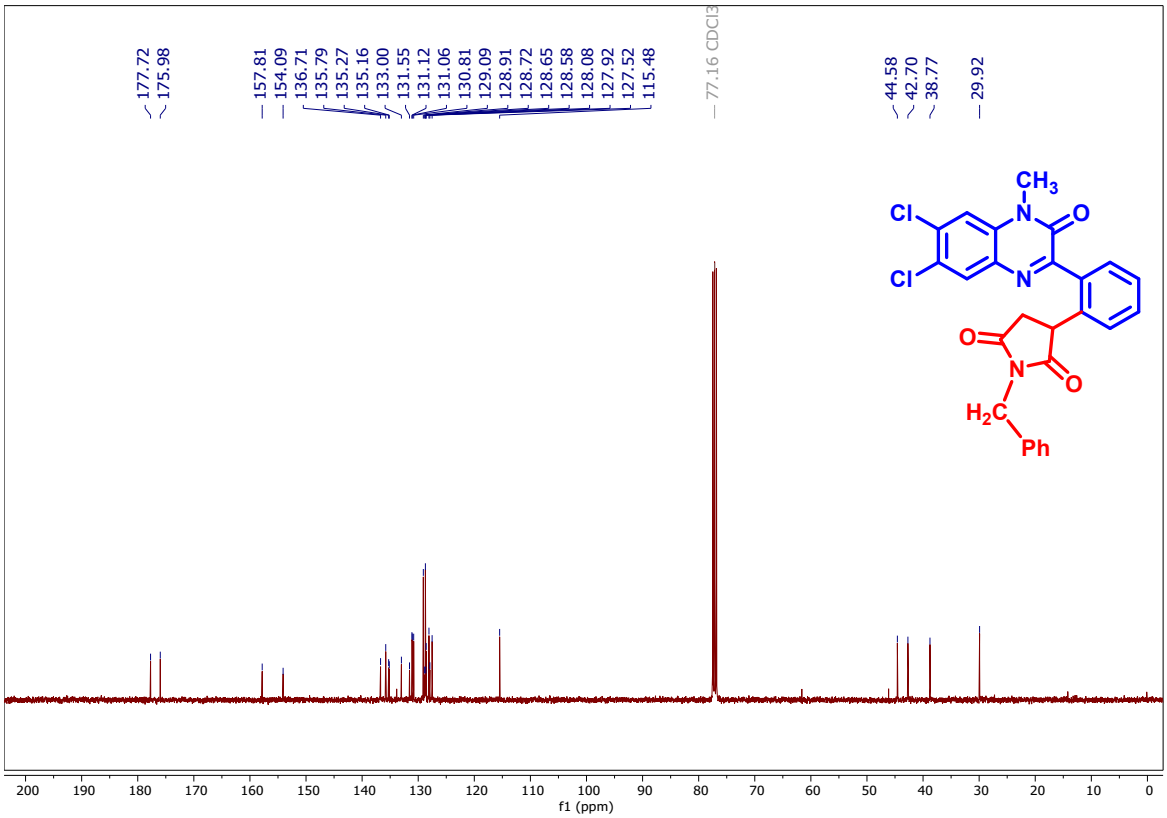


Figure 37: ^{13}C{1H} NMR spectrum of compound **4de** (100 MHz, $CDCl_3$).

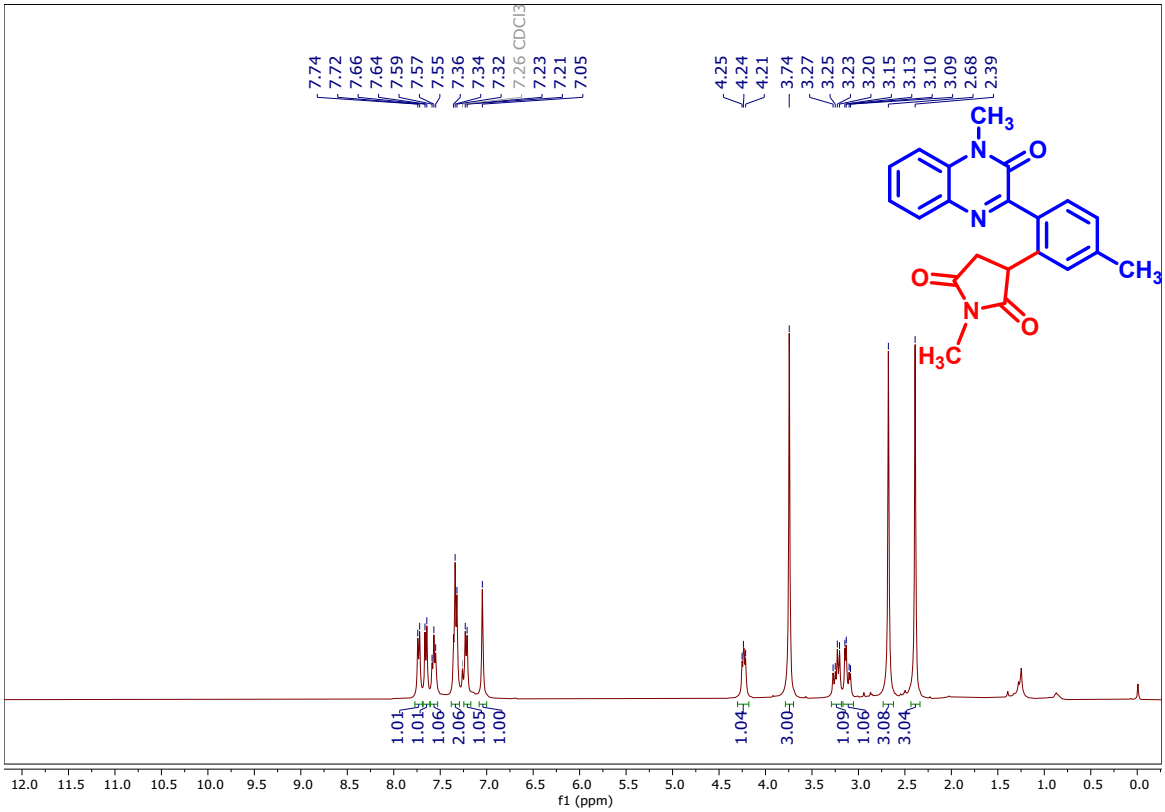


Figure 38: ^{1}H NMR spectrum of compound **5aa** (400 MHz, $CDCl_3$).

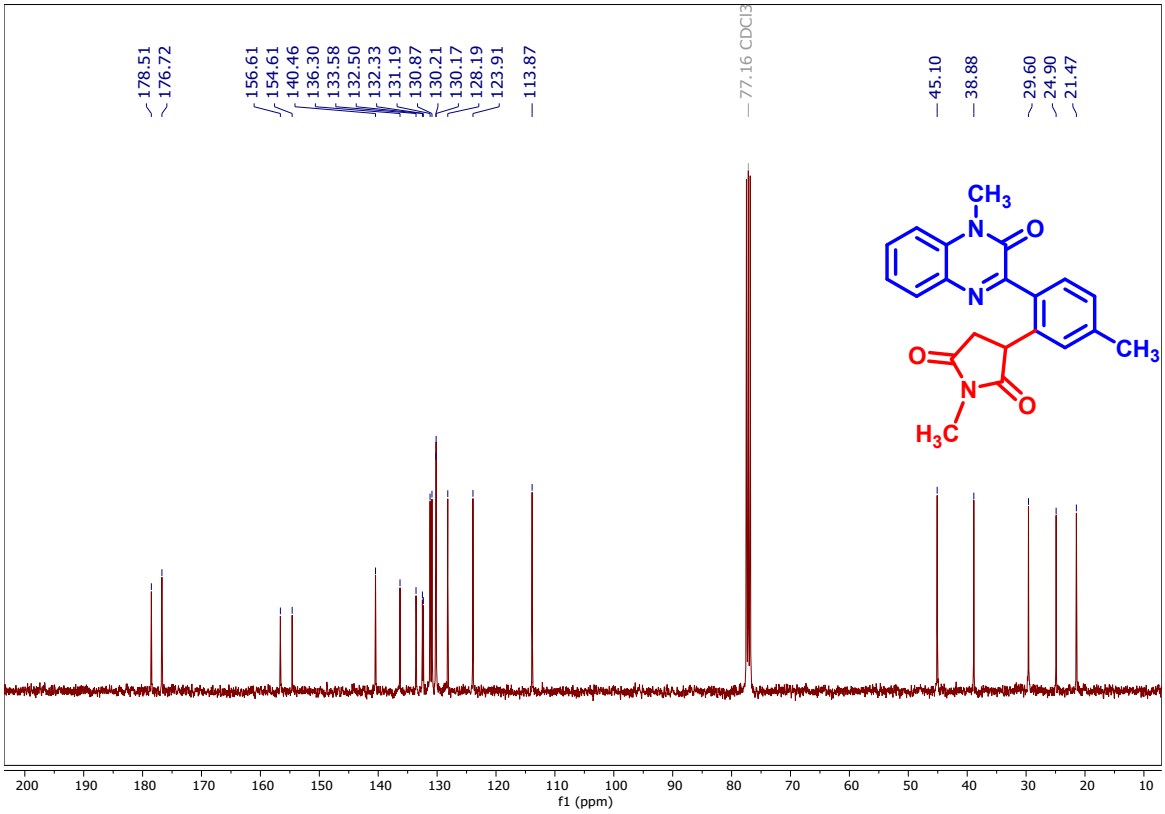


Figure 39: ^{13}C{1H} NMR spectrum of compound **5aa** (100 MHz, $CDCl_3$).

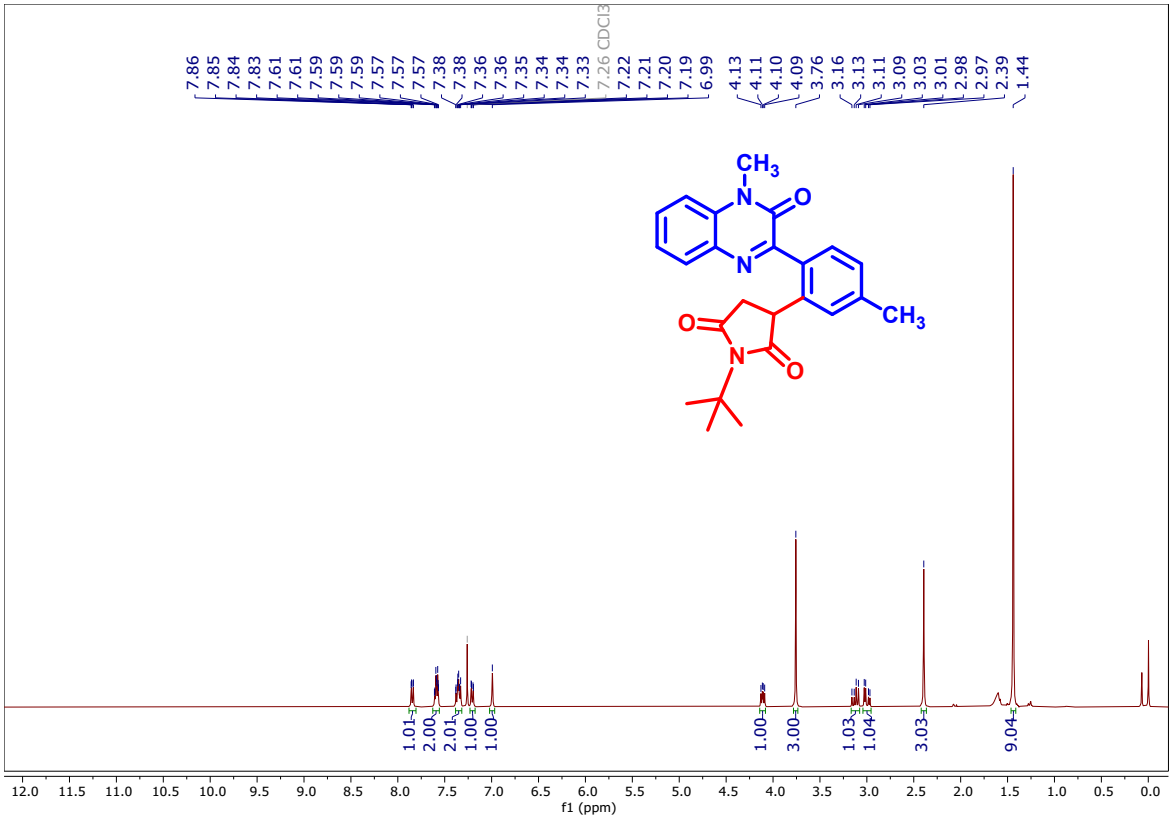


Figure 40: ^{1}H NMR spectrum of compound **5ab** (400 MHz, $CDCl_3$).

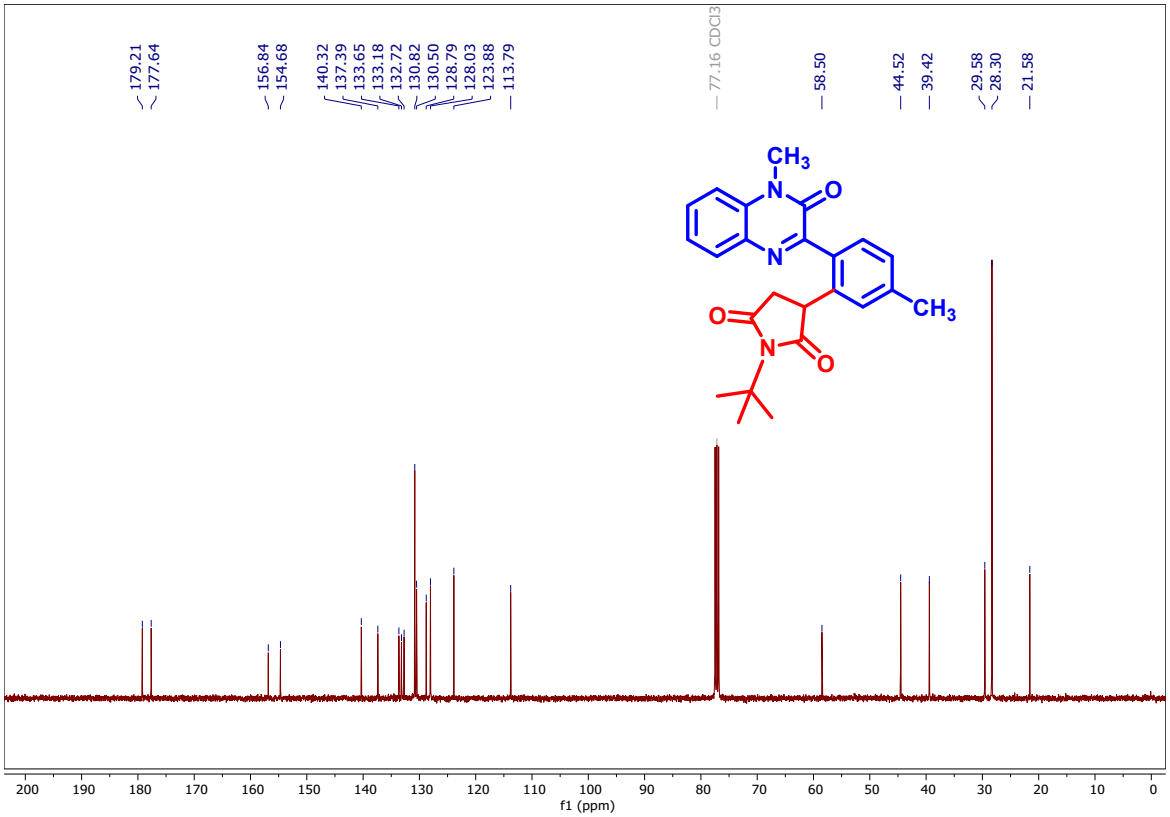


Figure 41: ^{13}C{1H} NMR spectrum of compound **5ab** (100 MHz, $CDCl_3$).

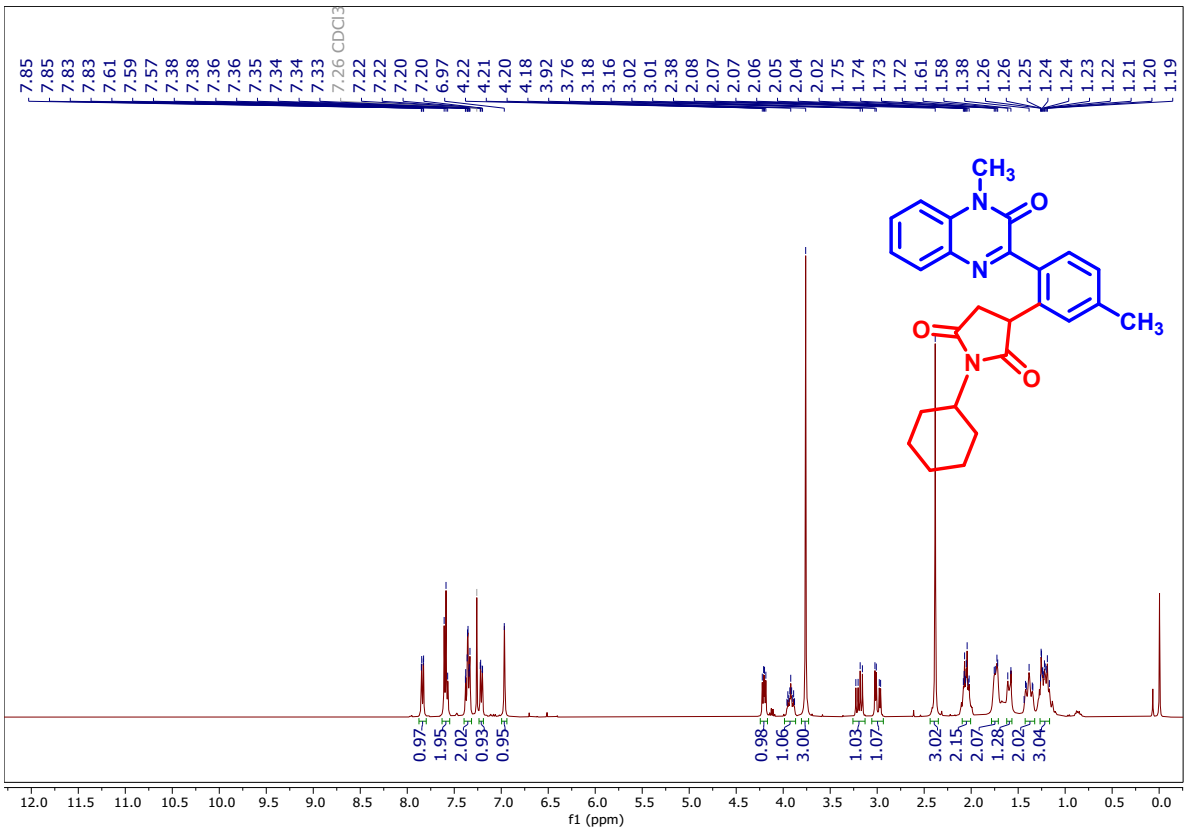


Figure 42: ^{1}H NMR spectrum of compound **5ac** (400 MHz, $CDCl_3$).

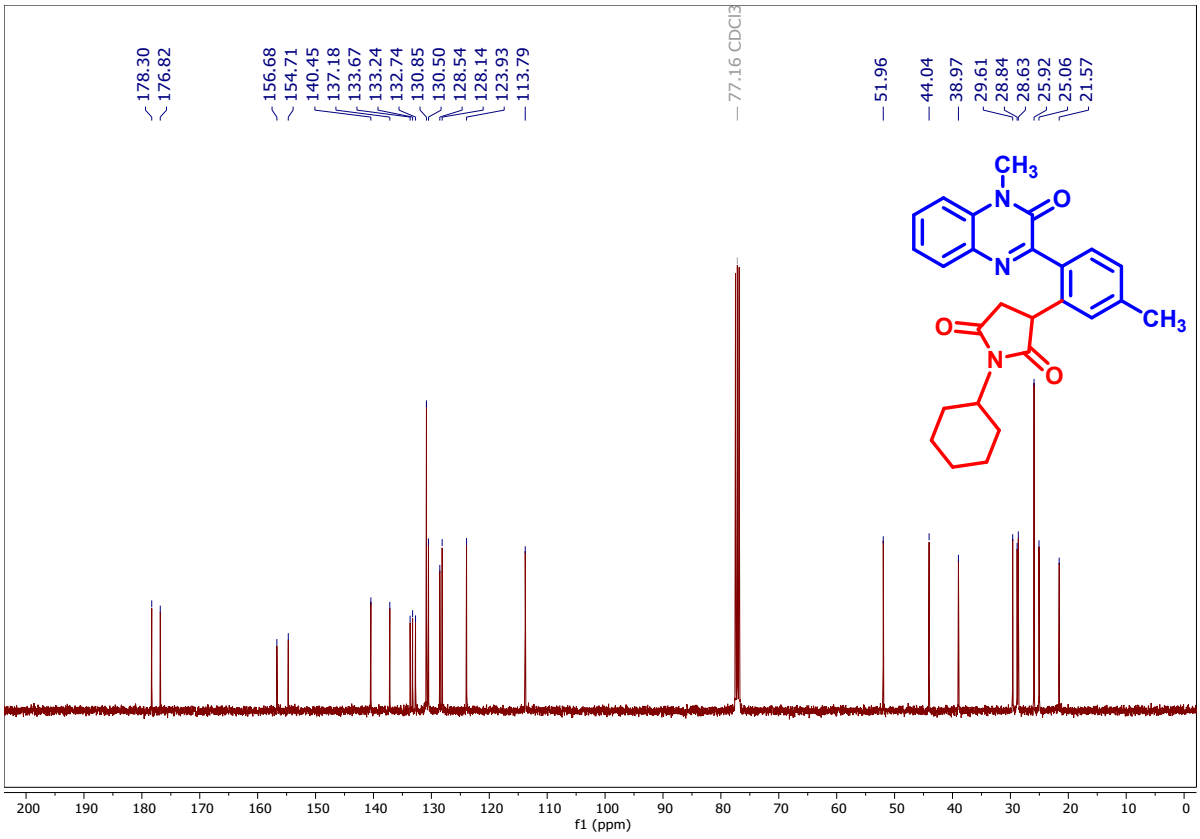


Figure 43: ^{13}C{1H} NMR spectrum of compound **5ac** (100 MHz, $CDCl_3$).

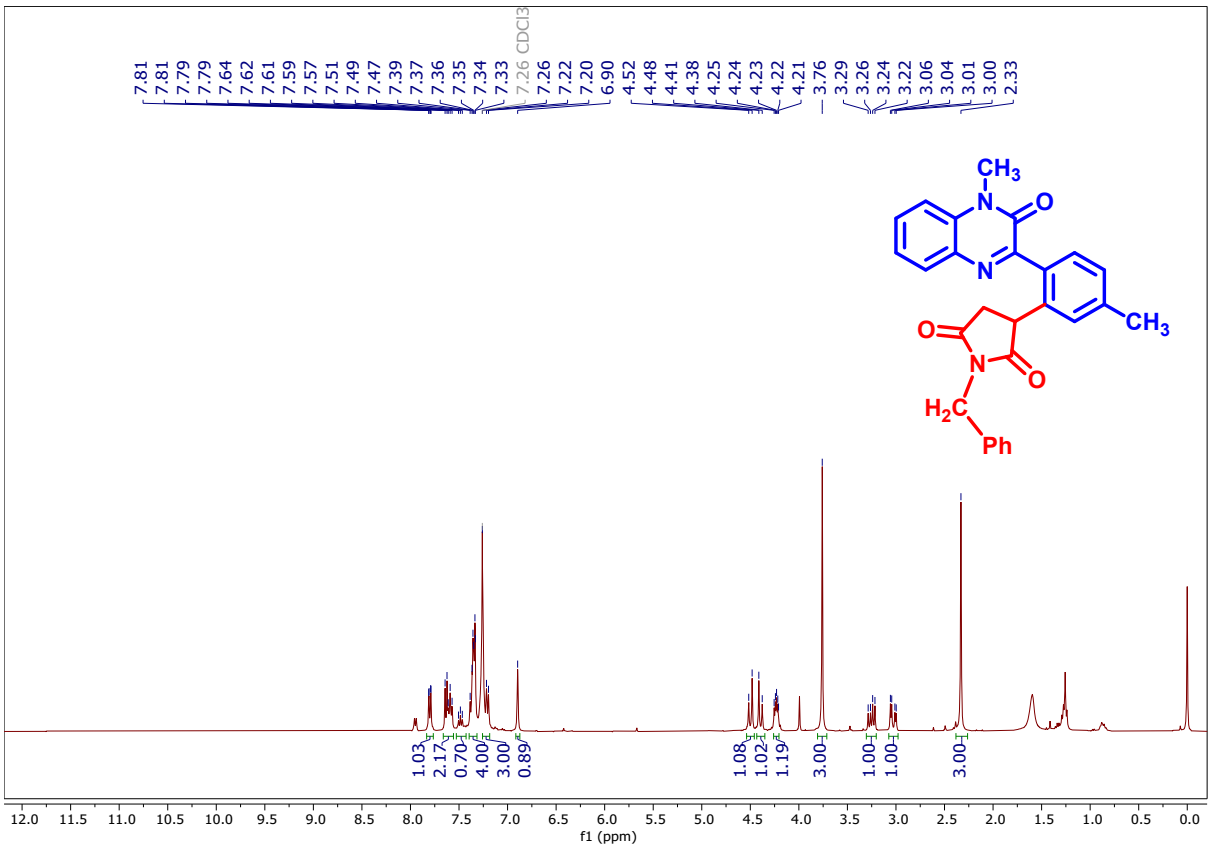


Figure 44: ^{1}H NMR spectrum of compound **5ae** (400 MHz, $CDCl_3$).

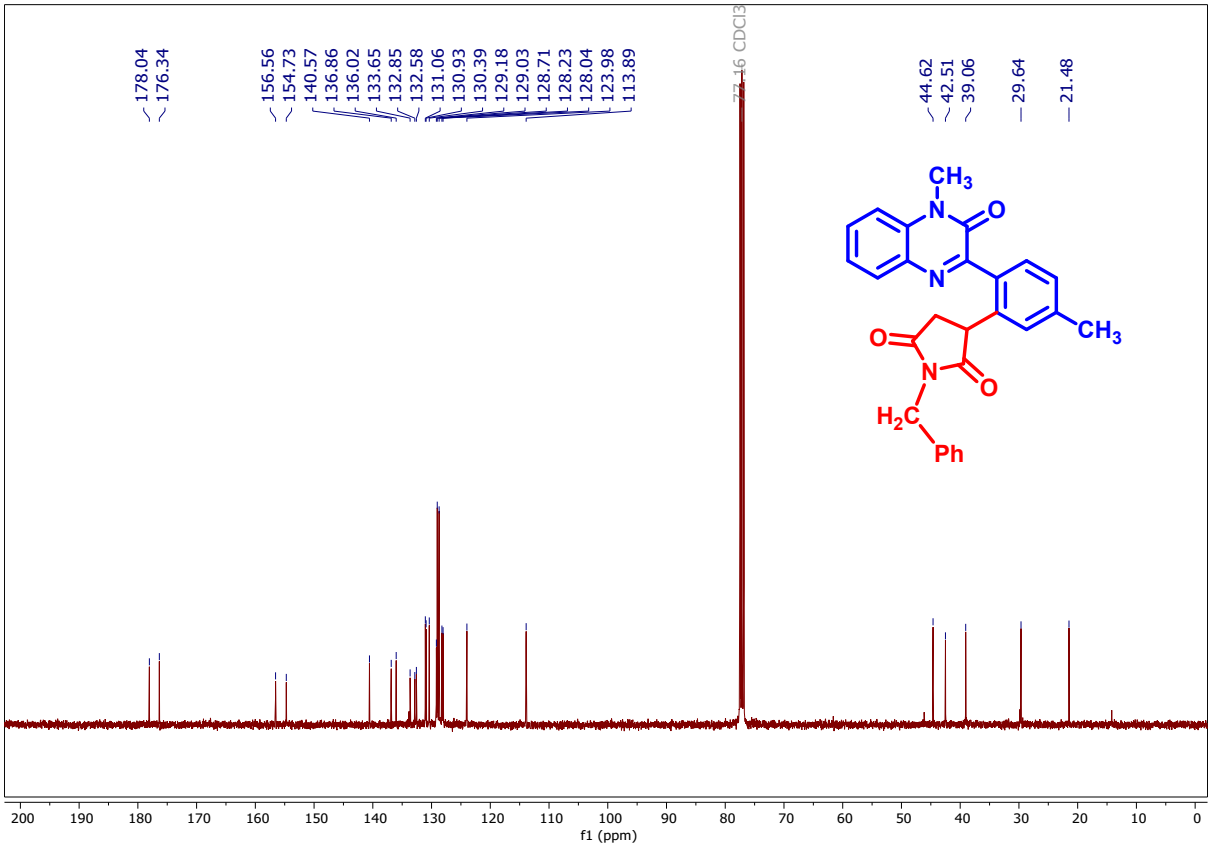


Figure 45: ^{13}C{1H} NMR spectrum of compound **5ae** (100 MHz, $CDCl_3$).

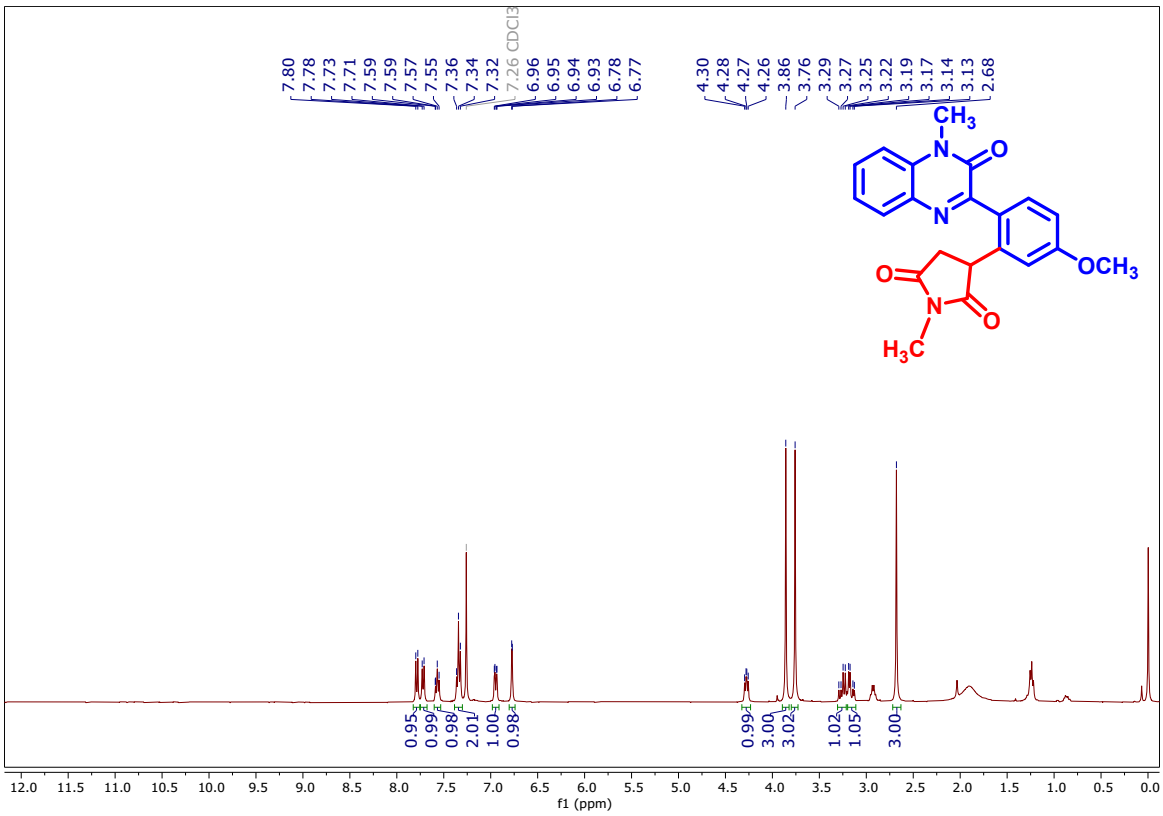


Figure 46: ^{1}H NMR spectrum of compound **5ba** (400 MHz, $CDCl_3$).

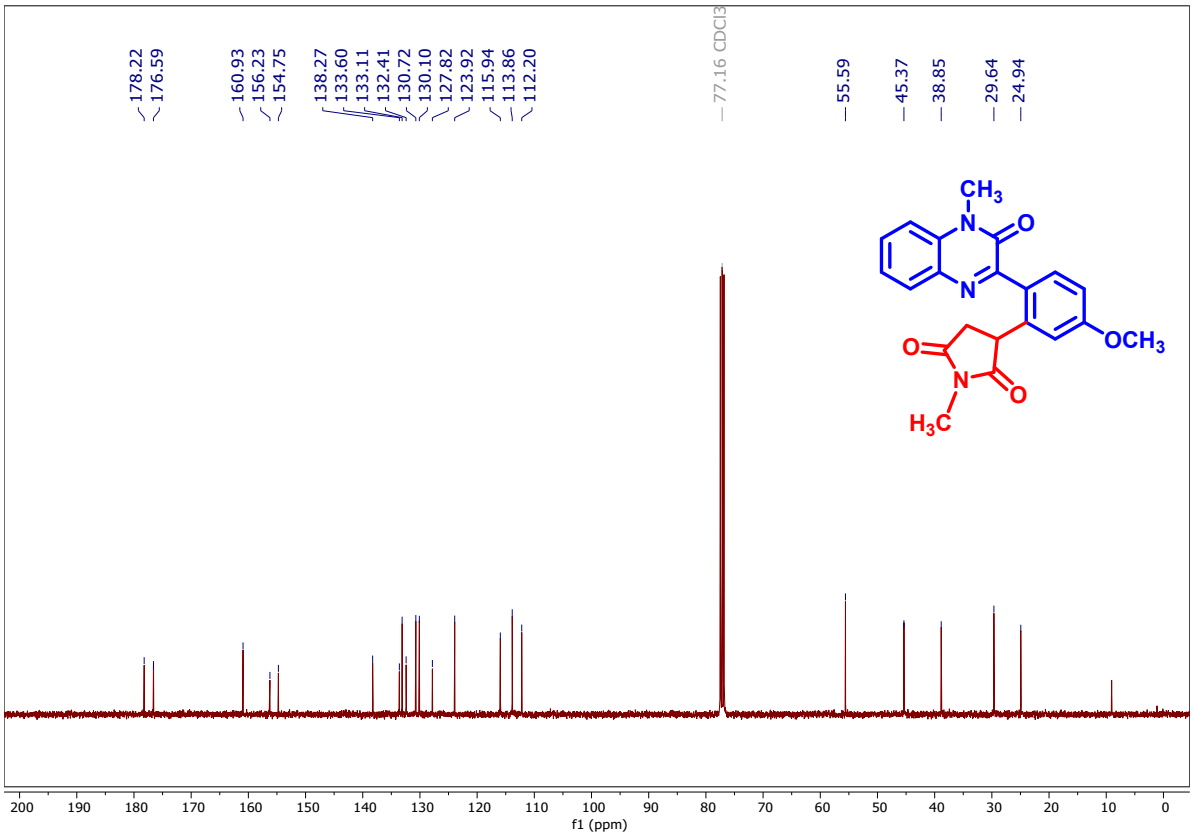


Figure 47: ^{13}C{1H} NMR spectrum of compound **5ba** (100 MHz, $CDCl_3$).

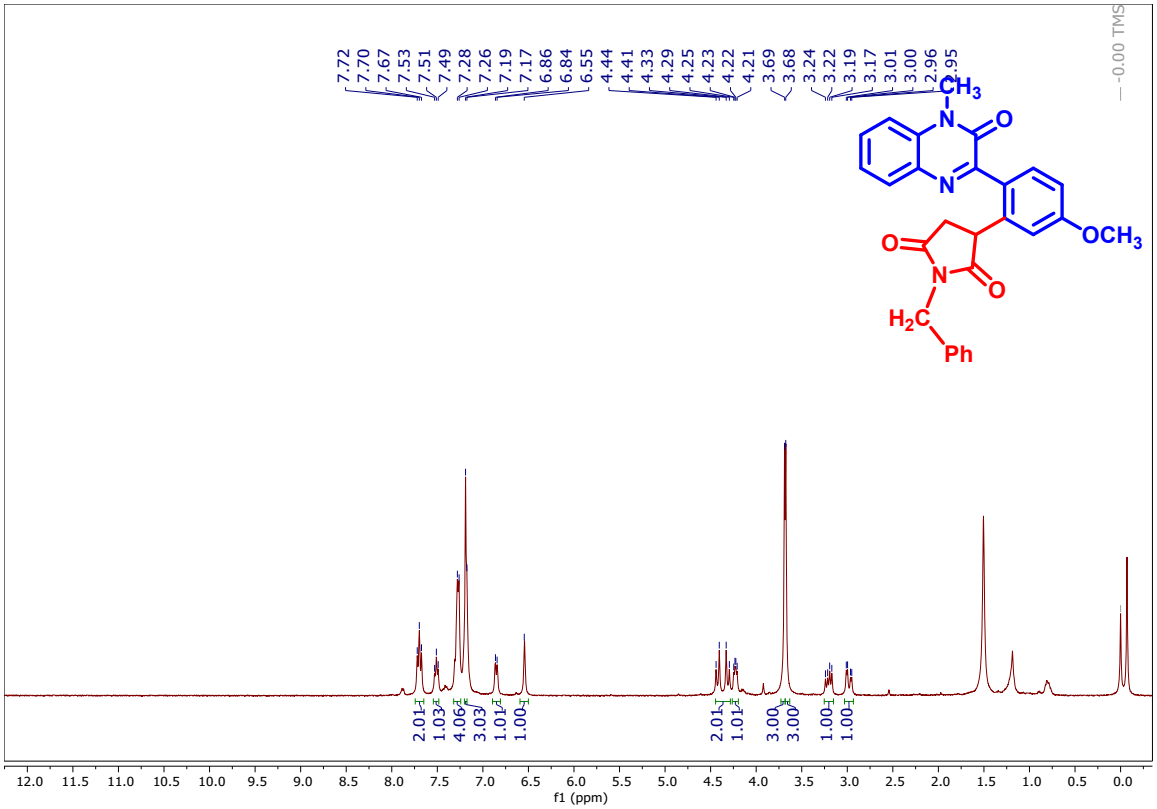


Figure 48: ^{1}H NMR spectrum of compound **5be** (400 MHz, $CDCl_3$).

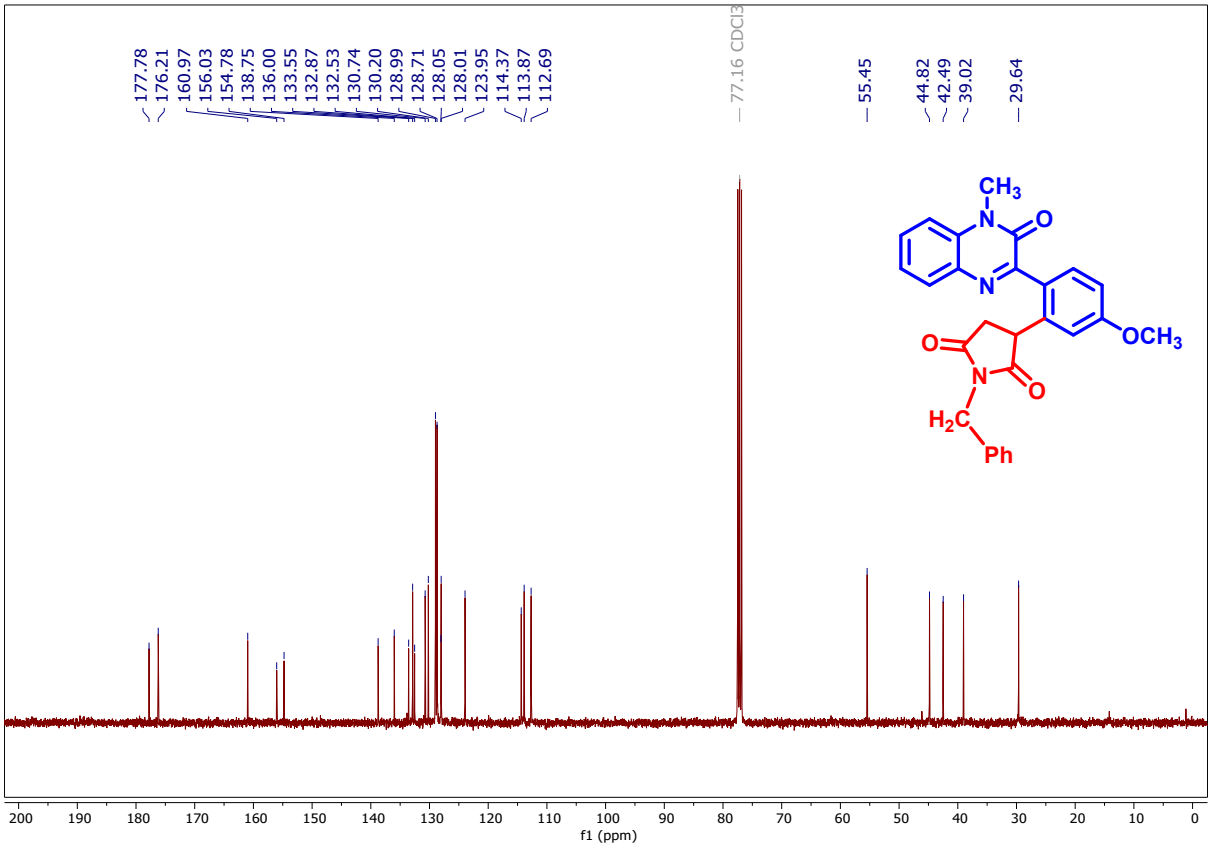


Figure 49: ^{13}C{1H} NMR spectrum of compound **5be** (100 MHz, $CDCl_3$).

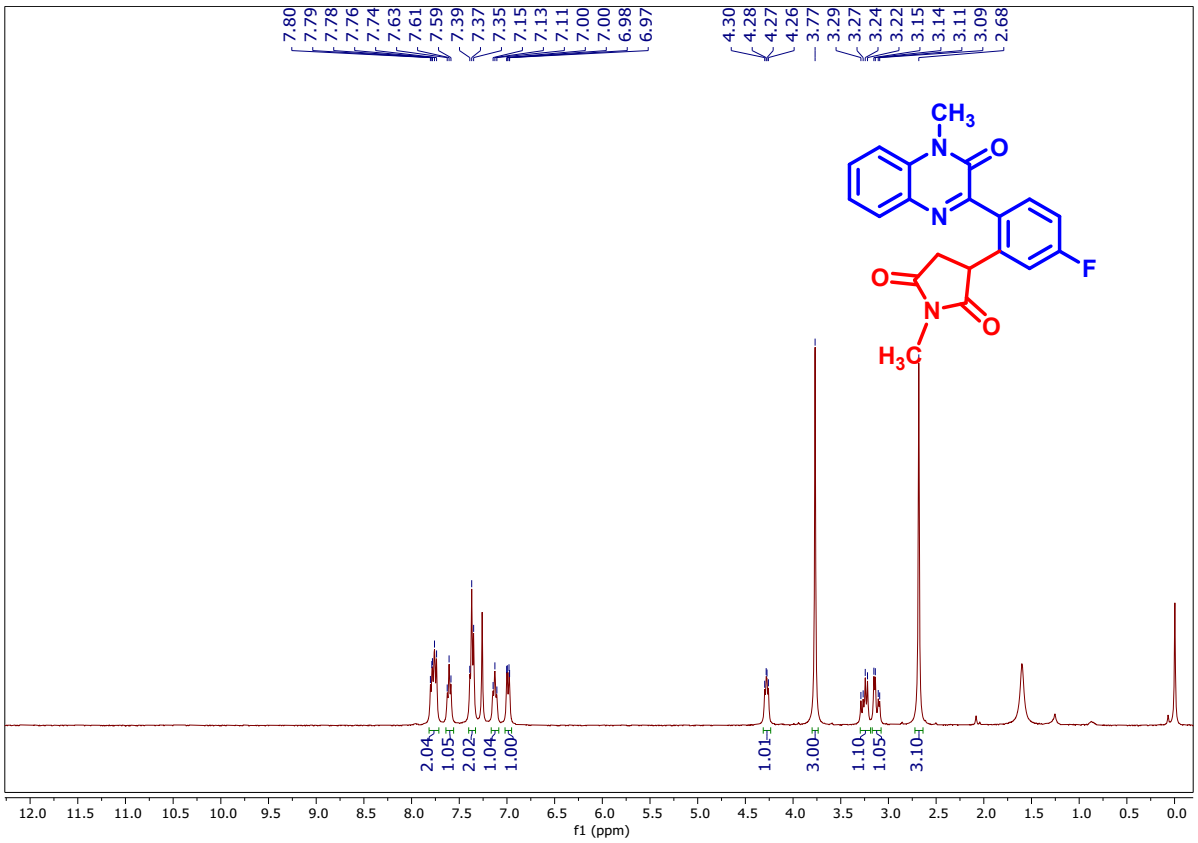


Figure 50: ^{1}H NMR spectrum of compound **5ca** (400 MHz, $CDCl_3$).

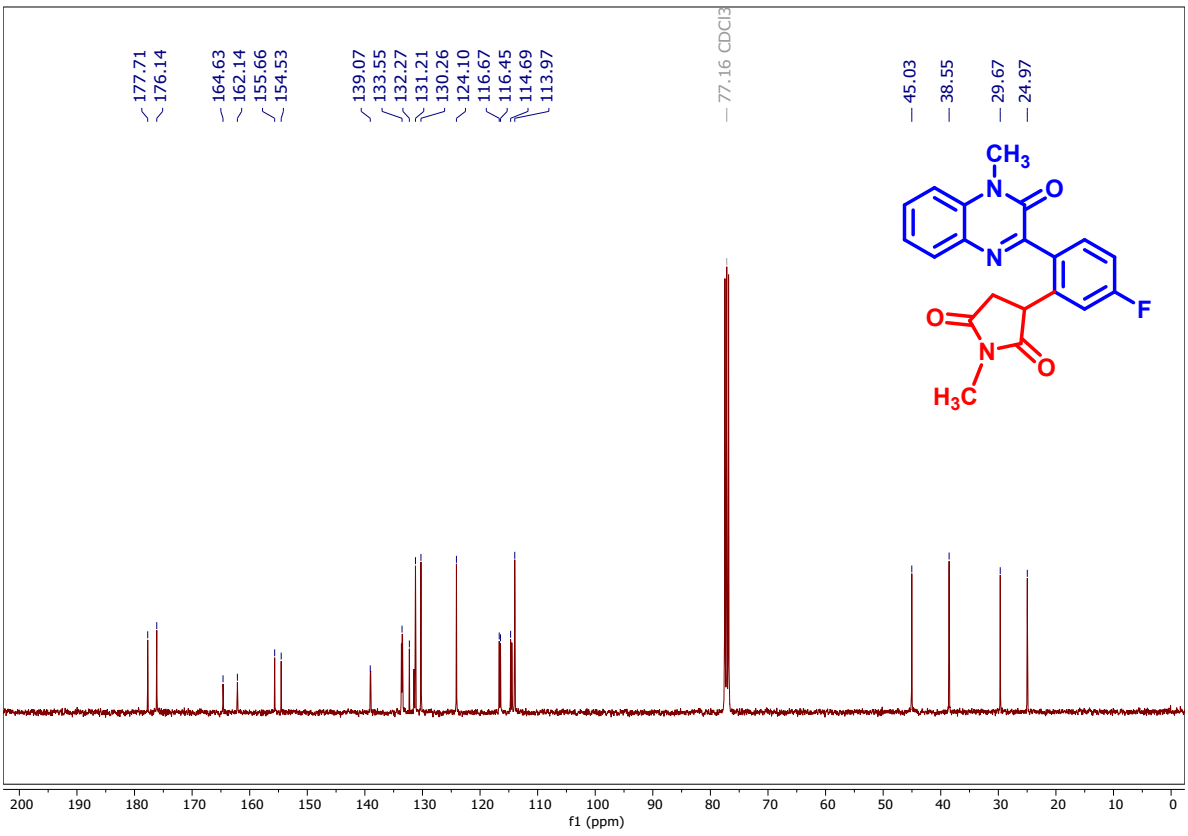


Figure 51: ^{13}C{1H} NMR spectrum of compound **5ca** (100 MHz, $CDCl_3$).

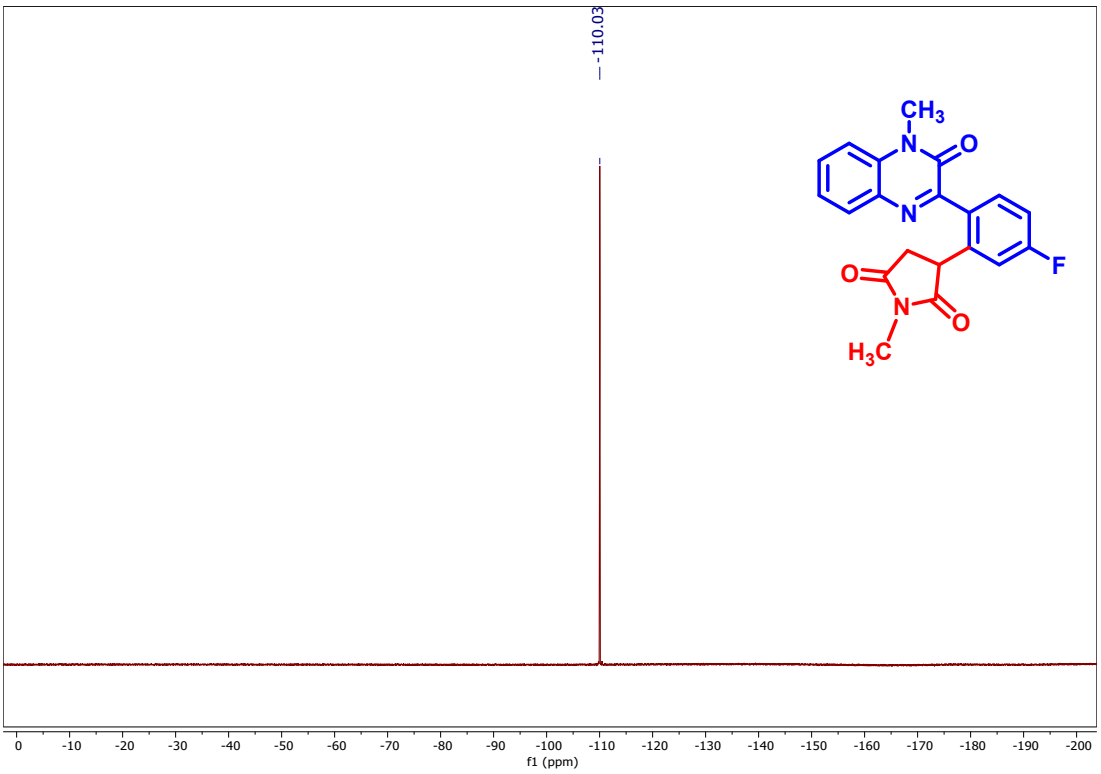


Figure 52: ^{19}F NMR spectrum of compound **5ca** (377 MHz, $CDCl_3$).

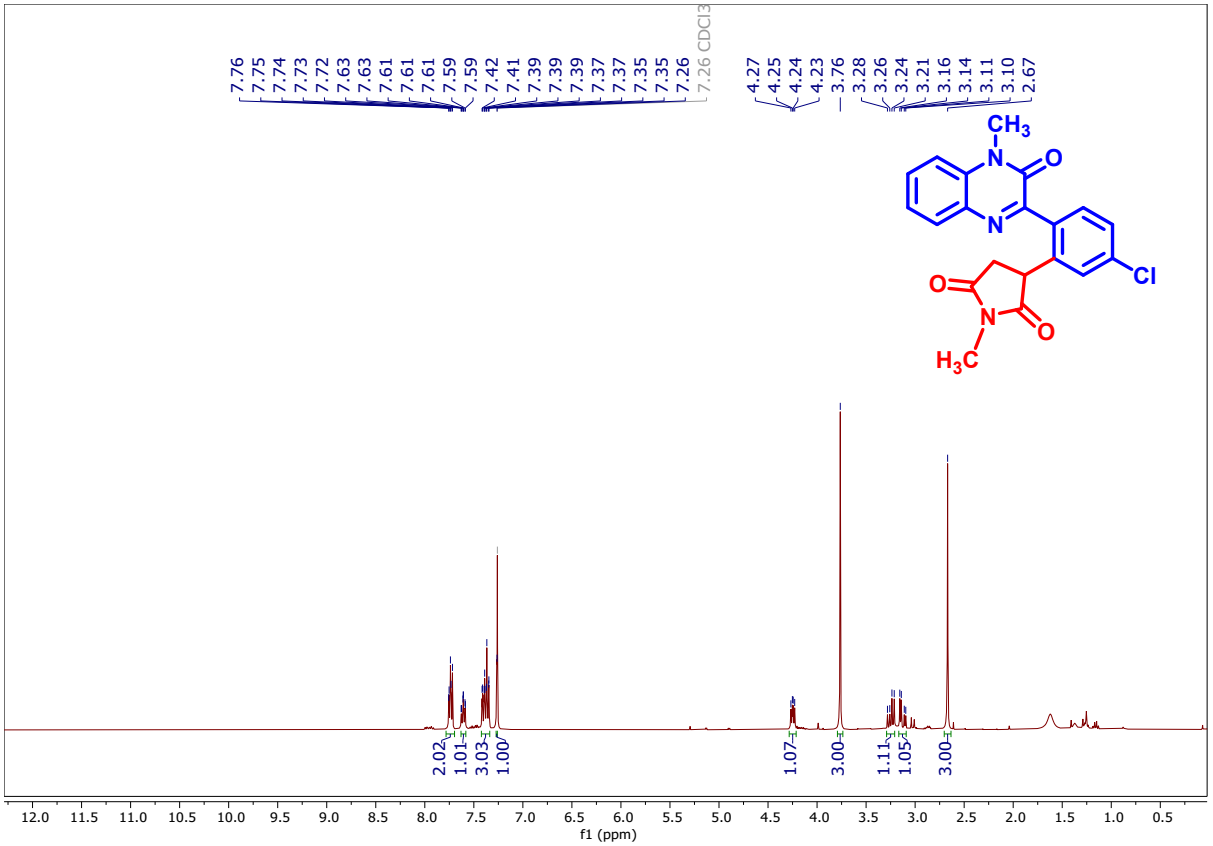


Figure 53: ^{1}H NMR spectrum of compound **5da** (400 MHz, $CDCl_3$).

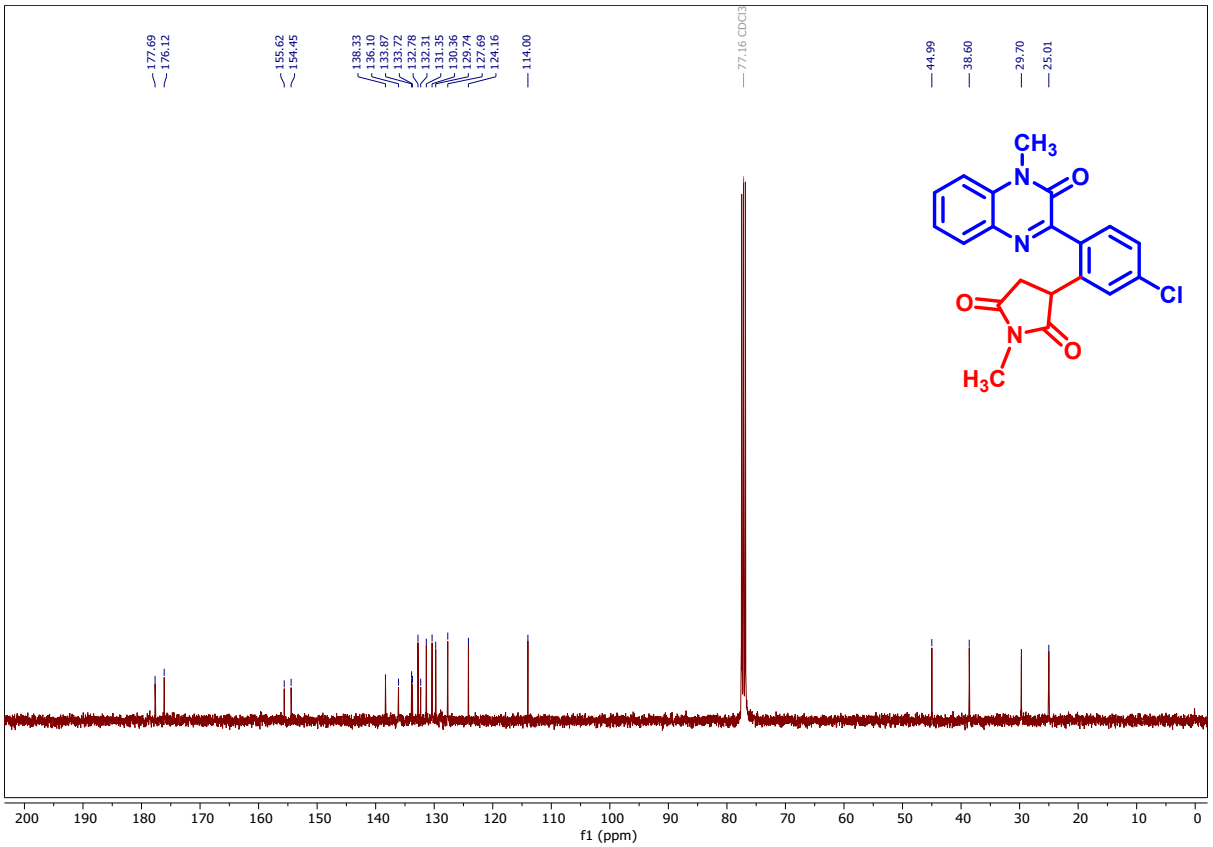


Figure 54: ^{13}C{1H} NMR spectrum of compound **5da** (100 MHz, $CDCl_3$).

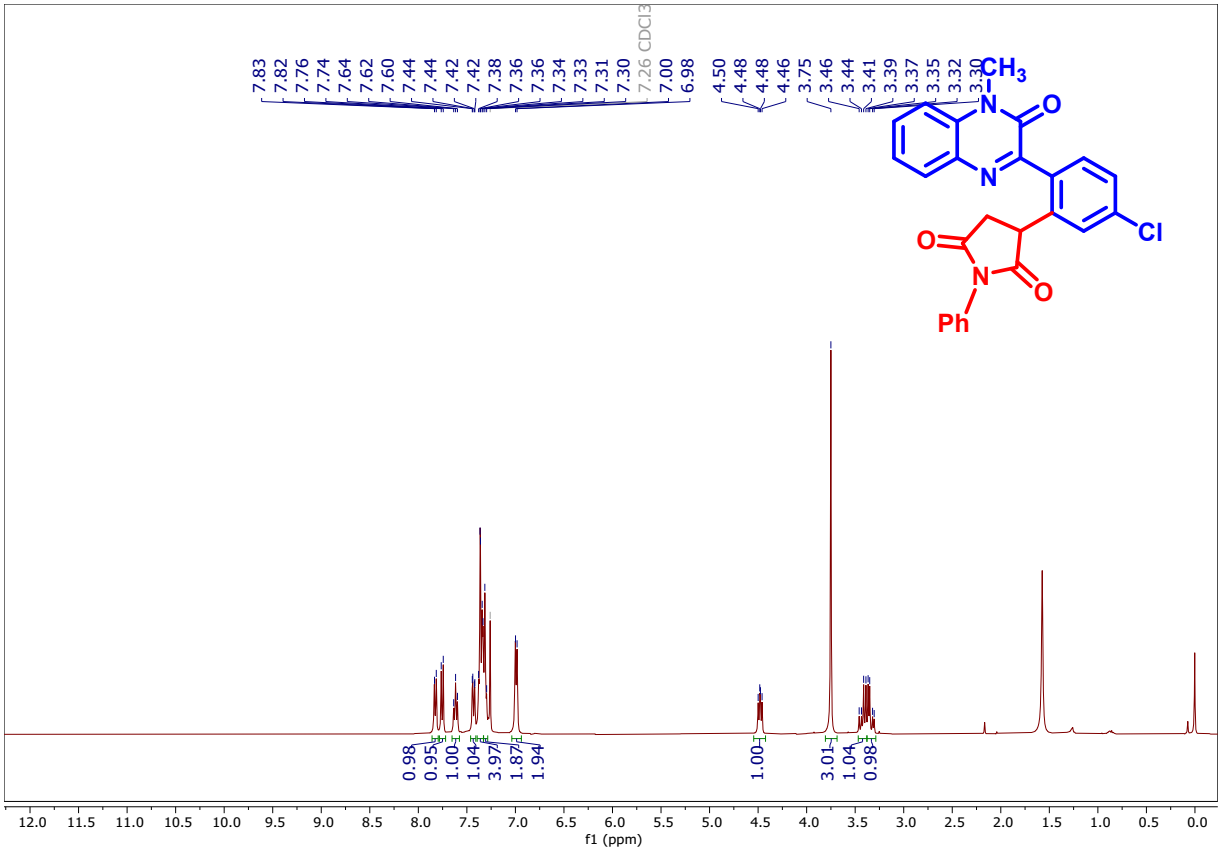


Figure 55: ^{1}H NMR spectrum of compound **5dd** (400 MHz, $CDCl_3$).

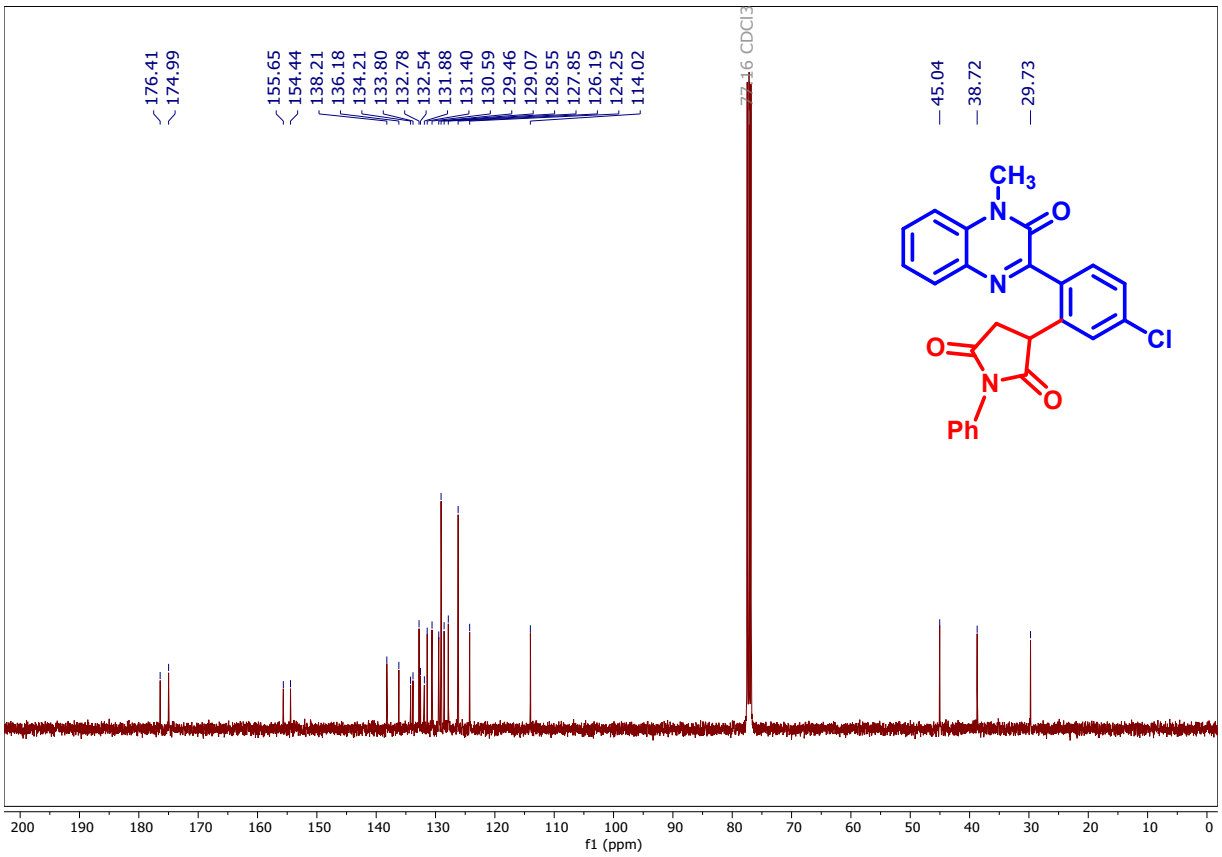


Figure 56: $^{13}C\{1H\}$ NMR spectrum of compound **5dd** (100 MHz, $CDCl_3$).

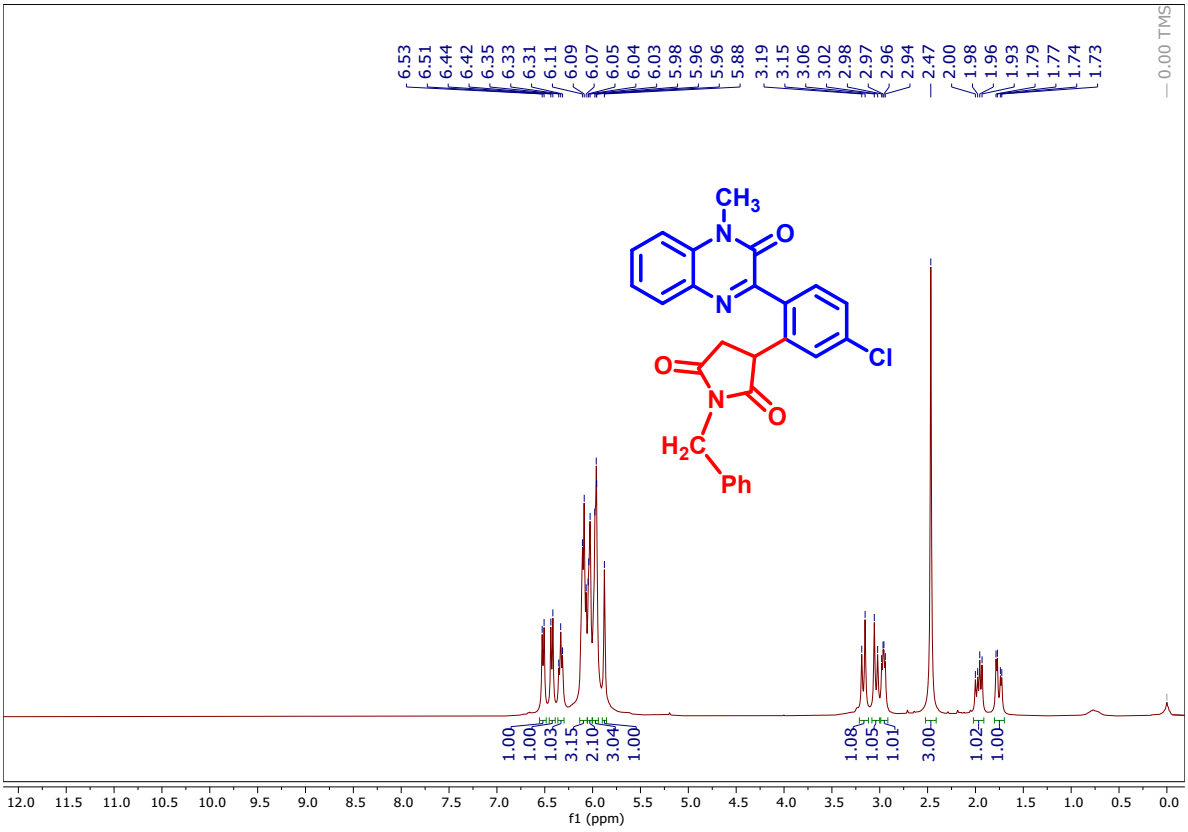


Figure 57: ^{1}H NMR spectrum of compound **5de** (400 MHz, $CDCl_3$).

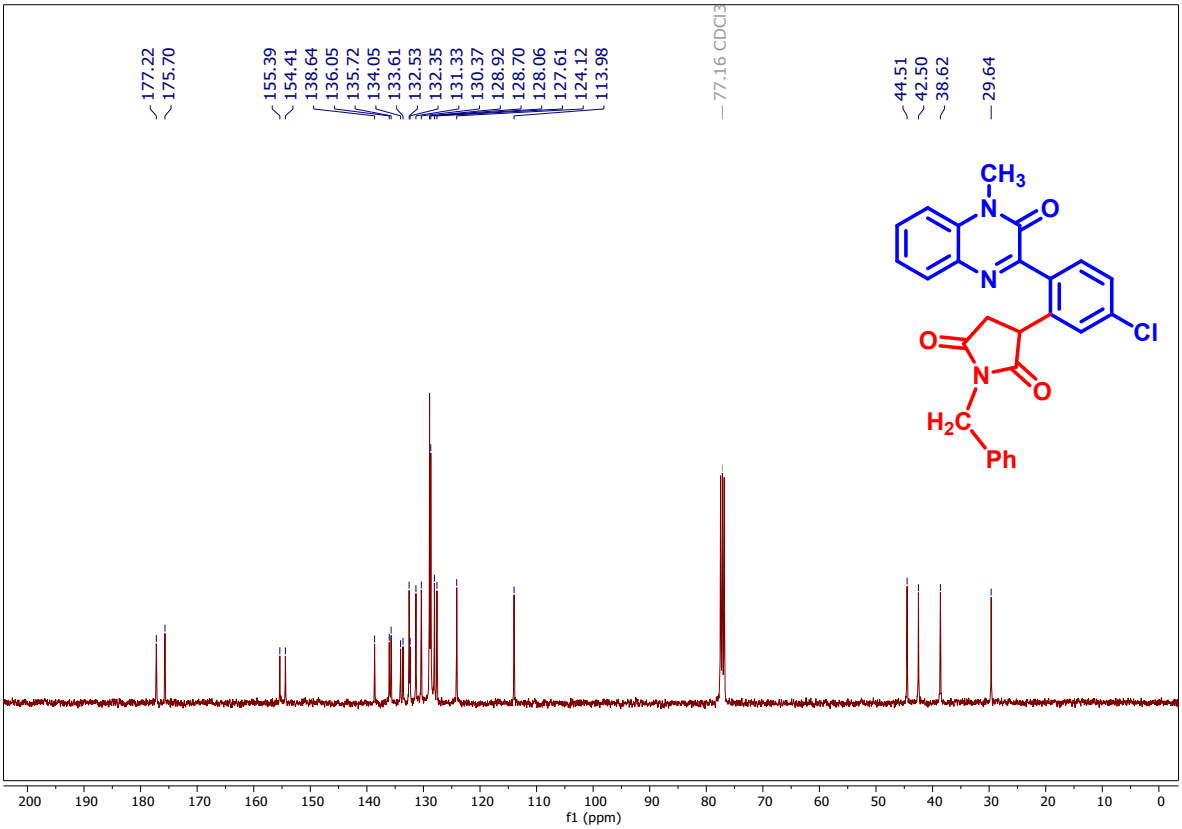


Figure 58: $^{13}C\{1H\}$ NMR spectrum of compound **5de** (100 MHz, $CDCl_3$).