Supporting Information

Selective Electrochemical Oxidation of Tetrahydroquinolines to 3,4-Dihydroquinolones

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Contents

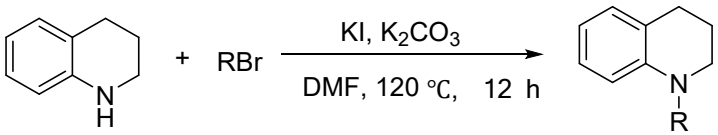
1. General methods

Unless otherwise noted, all reagents were purchased from commercial suppliers and used without further purification. Reactions were monitored by thin-layer chromatography (TLC) with Haiyang GF 254 silica gel plates (Qingdao Haiyang chemical industry Co Ltd, Qingdao, China) using UV light and vanillic aldehyde or phosphomolybdic acid as visualizing agents. Flash column chromatography was performed using 200-300 mesh silica gel at increased pressure. ^{1}H NMR spectra, ^{13}C NMR spectra and ^{19}F NMR spectra were respectively recorded on 600 MHz, 565 MHz, 400 MHz, 151 MHz and 101MHz NMR spectrometers. Chemical shifts (δ) were expressed in ppm with TMS as the internal standard, and coupling constants (*J*) were reported in Hz. High-resolution mass spectra were obtained by using ESI ionization sources (quadrupole time-of-flight mass spectrometer, Bruker Impact II, Bremen, Germany).

2. Experimental procedures

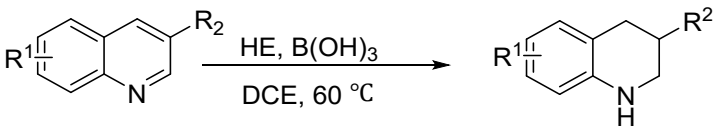
2.1. General procedure for the preparation of substrates

2.1.1. Method A[1] (preparation of substrates 1c-1k)



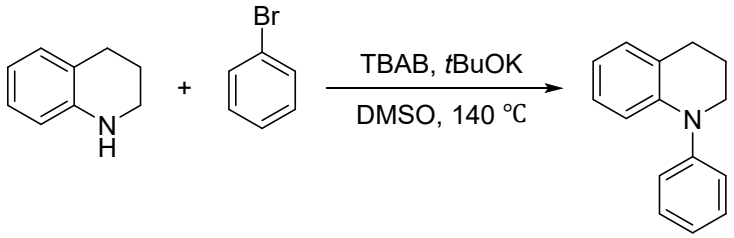
Anhydrous potassium carbonate (691.1 mg, 5 mmol) and potassium iodide (1037.5 mg, 6.25 mmol) were added to a solution of 1,2,3,4-tetrahydroquinoline (333 mg, 2.5 mmol) and corresponding RBr (5 mmol) in DMF (50 mL). The mixture was stirred at 120 °C. After completion of the reaction (detected by TLC), the reaction mixture was cooled to room temperature, extracted with EtOAc and H_2O. The combined organic layers were dried over anhydrous Na_2SO_4 and evaporated in vacuo. The residue was purified by flash chromatography on silica gel using petroleum ether/ethyl acetate as the eluent to give desired product.

2.1.2. Method B[2] (preparation of substrate 1m, 1p, 1aj)



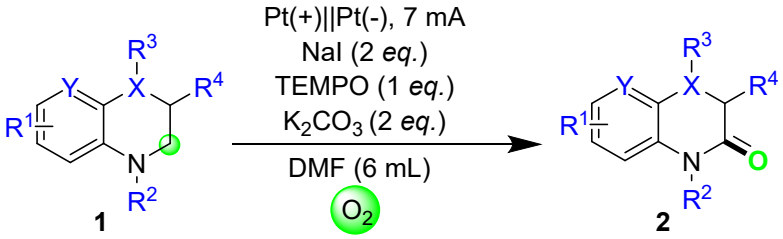
In a 50 mL round-bottomed flask, 8-quinoline (5 mmol), Hantzsch ester (2.5 equiv.), $B(OH)_3$ (15 mol%) and dichloroethane (20 mL) were charged. The reaction mixture was stirred at 60 °C (in a preheated oil bath). After completion of the reaction (detected by TLC), the reaction mixture was cooled to room temperature, extracted with EtOAc and H_2O. The combined organic layers were dried over anhydrous Na_2SO_4 and evaporated in vacuo. The residue was purified by flash chromatography on silica gel using petroleum ether/ethyl acetate as the eluent to give desired product.

2.1.3. Method C[3] (preparation of substrate 1l)



To a dry round-bottom flask 1,2,3,4-tetrahydroquinoline was added bromobenzene (2.0 mmol) and 1,2,3,4-tetrahydroquinoline (3.0 mmol) in 3 mL of DMSO, followed by TBAB (32.0 mg, 5 mol%) and potassium tert-butoxide (337.0 mg, 3.0 mmol). The reaction mixture was heated at 130 °C and monitored by TLC at frequent time intervals. After completion, the reaction mixture was cooled to room temperature, diluted with water, and extracted with ethyl acetate. The organic layers were combined, washed with brine, dried over $MgSO_4$, filtered, and concentrated in vacuo. The crude reaction mixture was purified by column chromatography (petroleum ether/ethyl acetate) to provide the desired product.

2.2. General procedure for the electrochemical oxidation of tetrahydroquinolines



Substrate **1** (0.3 mmol, 1 equiv.), NaI (0.6 mmol, 2 equiv.), TEMPO (0.3 mmol, 1 equiv.), K_2CO_3 (0.6 mmol, 2 equiv.) and DMF (6 mL) were added to a three-necked flask (10 mL) equipped with a magnetic stir bar. Two platinum plates (1 cm x 1 cm x 0.2 mm each) were used as anode and cathode respectively (the electrodes were immersed 1 cm in the reaction solution). The reaction mixture was stirred and electrolyzed at a constant current of 7 mA at RT under O_2 atmosphere. After reaction completion (monitored by TLC), the reaction mixture was diluted with water, and extracted with ethyl acetate. The organic layers were combined, washed with brine, and concentrated under reduced pressure. The crude reaction mixture was purified by flash column chromatography on silica gel with petroleum ether/ethyl acetate as the eluent to obtain the target product **2**.

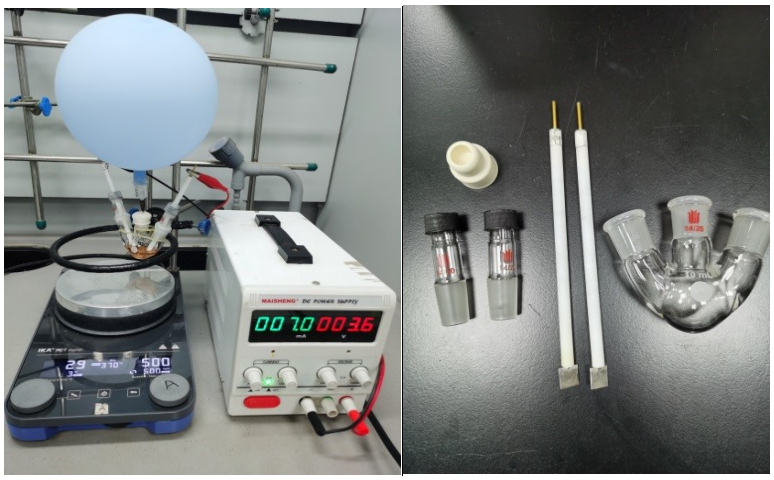
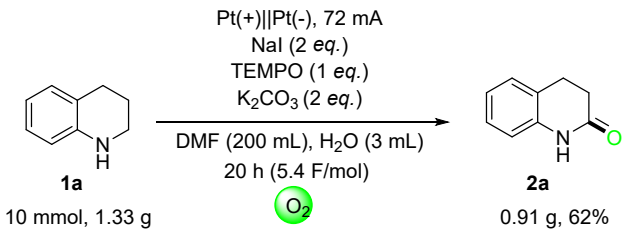


Figure S1 Electrochemical setup used.

The experimental setup consisted of two platinum sheet electrodes (10 mm × 10 mm × 0.2 mm each), a three-necked flask (10 mL), an adjustable DC regulated power supply (MS-150V 100 mA), a magnetic stirrer and an oxygen balloon.

2.3. Gram-scale experiment for the synthesis of 2a



Substrate **1a** (10 mmol, 1 equiv.), NaI (20 mmol, 2 equiv.), TEMPO (10 mmol, 1 equiv.), K_2CO_3 (20 mmol, 2 equiv.), 3 mL H_2O and DMF (200 mL) were added to a three-necked flask (250 mL) equipped with a magnetic stir bar. Two platinum plates (3 cm x 3 cm x 0.2 mm each) were used as anode and cathode respectively (the electrodes were immersed 3 cm in the reaction solution). The reaction mixture was stirred and electrolyzed at a constant current of 72 mA at RT under O_2 atmosphere. After reaction completion (monitored by TLC), the reaction mixture was diluted with water, and extracted with ethyl acetate. The organic layers were combined, washed with brine, and concentrated under reduced pressure. The crude reaction mixture was purified by flash column chromatography on silica gel with petroleum ether/ethyl acetate as the eluent to obtain the target product **2a** (0.91 g, 62% yield).

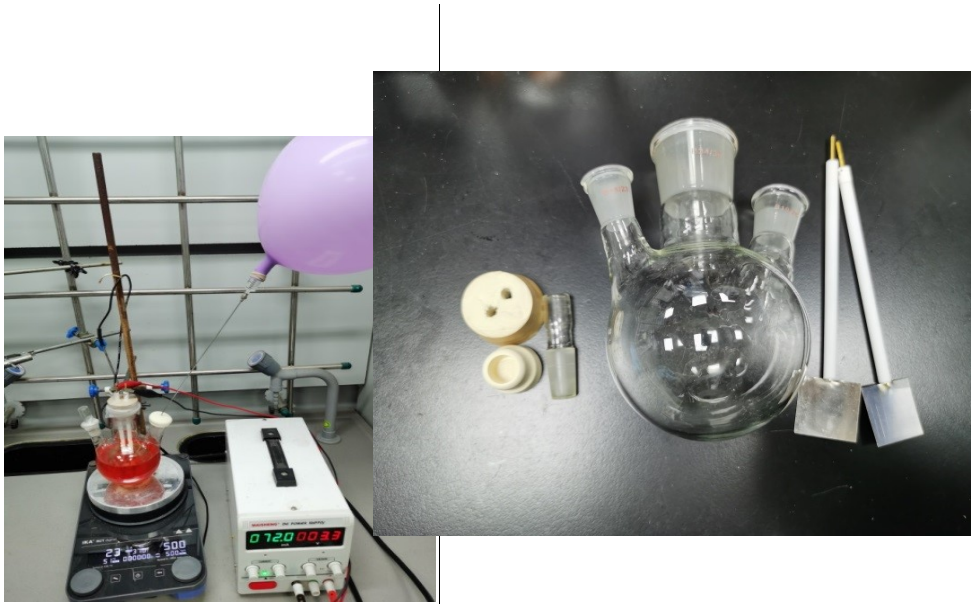
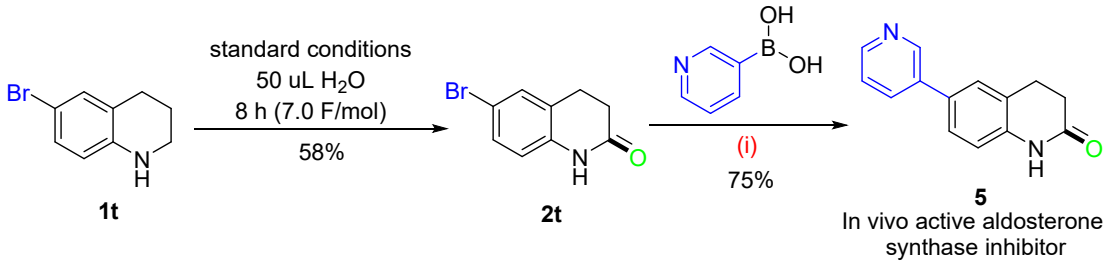


Figure S2 Electrochemical setup for the scale-up experiment.

The electrochemical setup for the scale-up experiment consisted of two platinum sheet electrodes (30 mm × 30 mm × 0.2 mm each), a three-necked flask (250 mL), an adjustable DC regulated power supply (MS-150V 100 mA), a magnetic stirrer and an oxygen balloon.

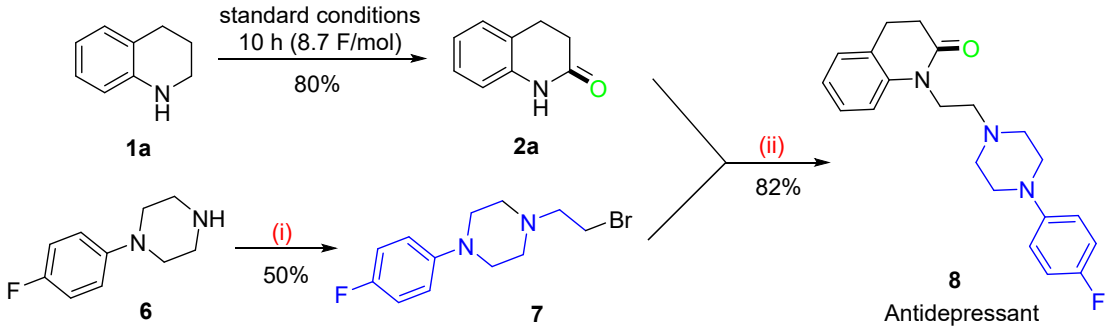
2.4. Synthesis of bioactive molecules containing 3,4-dihydroquinolone moieties



Reagents and conditions: (i) $Pd[P(C_6H_5)_3]$ (5 mol%), K_2CO_3 aqueous solution (2 mol/L), toluene/ethanol, at 80 °C under Ar for 24 h.

6-bromo-3,4-dihydro-2-quinolone **2t** was prepared from **1t** following the general procedure (§2.2. Electrochemical oxidation of tetrahydroquinolines).

A round bottom flask was charged with **2t** (1130 mg, 5 mmol), 3-pyridinylboronic acid (800 mg, 6.5 mmol), K_2CO_3 aqueous solution (2.0 mol/L) and 50 mL of toluene/ethanol (4/1), followed by $Pd[P(C_6H_5)_3]$ (228 mg, 5 mol%). The reaction mixture was heated at 80 °C under Ar and monitored by TLC at frequent time intervals. After completion, the reaction mixture was cooled to room temperature, diluted with water, and extracted with ethyl acetate. The organic layers were combined, washed with brine, dried over $MgSO_4$, filtered, and concentrated in vacuo. The crude reaction mixture was purified by column chromatography (petroleum ether/ethyl acetate) to provide the white soild **5** (840 mg, 75% yield).



Reagents and conditions: (i) Cs_2CO_3 (3 *equiv.*), 1,2-dibromoethane, 35 °C for 48 h.; (ii) Cs_2CO_3 (3 *equiv.*), MeCN, rt for 4 h.

3,4-dihydro-2-quinolone **2a** was prepared from **1a** following the general procedure (§2.2. Electrochemical oxidation of tetrahydroquinolines).

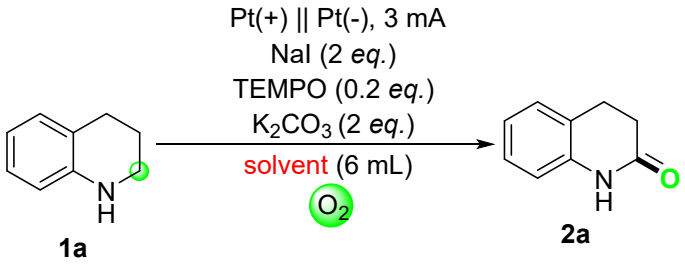
To the mixture of 1,2-dibromoethane (20 mL, 230 mmol) and $CsCO_3$ (7494 mg, 23.3 mmol) was added 1-(4-fluorophenyl)piperazine **6** (4200 mg, 23.3 mmol), and the resulting mixture

was stirred at 35 °C for 48 h. The reaction mixture was concentrated in vacuum, and the residue was purified by column chromatography on silica gel (PE/EA = 2:1) to give compound **7** as a white solid (3180 mg, 50% yield).

To the mixture of **7** (29 mg, 0.1 mmol) and $CsCO_3$ (116.1 mg, 0.3 mmol) in acetonitrile (1.0 mL) was added **2a** (28 mg, 0.2 mmol), and the resulting mixture was stirred at rt for 4 h. The precipitate was filtered and the filtrate was concentrated in vacuum. The residue was purified by column chromatography on silica gel (PE/EA = 2:1) to give the antidepressant **8** as a white powder (28.9 mg, 82% yield).

3. Optimization of reaction conditions

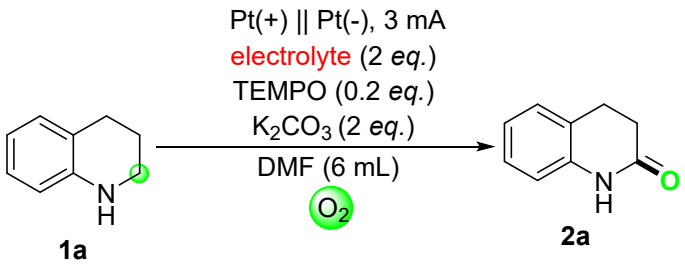
Table S1. Solvent screening [a]



Entry	Solvent	Yield (%) [b]
1	**DMF**	**44**
2	DMA	10
3	THF	9
4	DMSO	Trace
5	MeOH	Trace
6	CH_3CH_2OH	Trace
7	MeCN	Trace

[a] Reaction conditions: A mixture of **1a** (0.3 mmol), NaI (0.6 mmol, 2 *equiv.*), TEMPO (0.06 mmol, 0.2 *equiv.*) and K_2CO_3 (0.6 mmol, 2 *equiv.*) in a solvent (6 mL) under a constant current of 3 mA (Pt anode: 1 cm x 1 cm x 0.2 mm; Pt cathode: 1 cm x 1 cm x 0.2 mm) in an undivided cell at RT under O_2 for 10 h (3.7 F/mol). [b] Isolated yield.

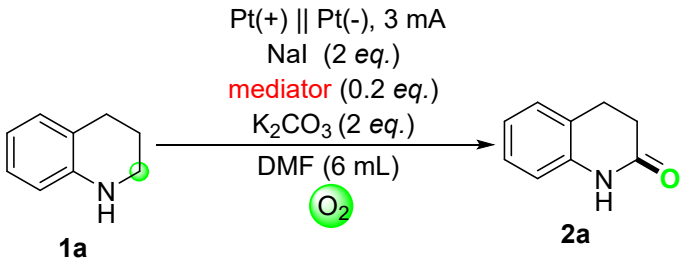
Table S2. Electrolyte screening



Entry	Electrolyte	Yield (%) [b]
1	--	Trace
2	**NaI**	**44**
3	nBu$_4$NCl	Trace
4	nBu$_4$NBr	10
5	nBu$_4$NI	26
6	NH$_4$I	30
7	nBu$_4$NBF$_4$	Trace
8	KClO$_4$	Trace
9	nBu$_4$NPF$_6$	Trace
10	nBu$_4$NClO$_4$	Trace
11	nEt$_4$NBF$_4$	Trace
12	LiBr	Trace

[a] Reaction conditions: A mixture of **1a** (0.3 mmol), electrolyte (0.6 mmol, 2 *equiv.*), TEMPO (0.06 mmol, 0.2 *equiv.*) and K_2CO_3 (0.6 mmol, 2 *equiv.*) in a DMF (6 mL) under a constant current of 3 mA (Pt anode: 1 cm x 1 cm x 0.2 mm; Pt cathode: 1 cm x 1 cm x 0.2 mm) in an undivided cell at RT under O_2 for 10 h (3.7 F/mol), 8.7 F/mol·h^{-1}. [b] Isolated yield.

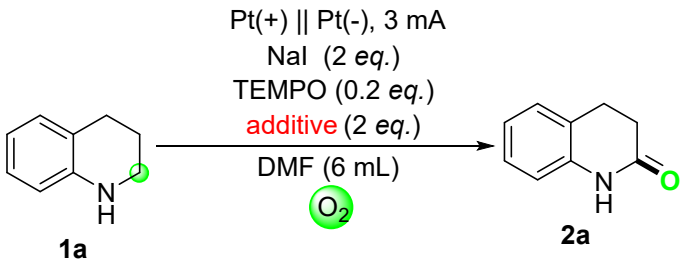
Table S3. Mediator screening [a]



Entry	Mediator	Yield (%) [b]
1	--	Trace
2	**TEMPO**	**44**
3	Ferrocene	27
4	*N*,*N*,*N*-Triphenylamine	30
5	*N*,*N*-Bis(4-bromophenyl)-4-bromoaniline	35
6	NaBr	18
7	9-Azabicyclo[3.3.1]nonane *N*-oxyl	30

[a] Reaction conditions: A mixture of **1a** (0.3 mmol), NaI (0.6 mmol, 2 *equiv.*), mediator (0.06 mmol, 0.2 *equiv.*) and K_2CO_3 (0.6 mmol, 2 *equiv.*) in a DMF (6 mL) under a constant current of 3 mA (Pt anode: 1 cm x 1 cm x 0.2 mm; Pt cathode: 1 cm x 1 cm x 0.2 mm) in an undivided cell at RT under O_2 for 10 h (3.7 F/mol). [b] Isolated yield.

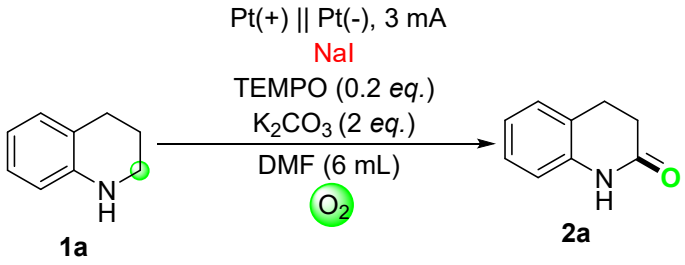
Table S4. Additive screening [a]



Entry	Additive	Yield (%) [b]
1	--	19
2	**K_2CO_3**	**44**
3	Na_2CO_3	33
4	Cs_2CO_3	19
5	KOH	Trace
6	CsF	19
7	NaOH	10
8	K_3PO_4	Trace
9	*t*BuOK	Trace
10	DBU	Trace
11	DMAP	25
12	Et_3N	39

[a] Reaction conditions: A mixture of **1a** (0.3 mmol), NaI (0.6 mmol, 2 *equiv.*), TEMPO (0.06 mmol, 0.2 *equiv.*) and additive (0.6 mmol, 2 *equiv.*) in a DMF (6 mL) under a constant current of 3 mA (Pt anode: 1 cm x 1 cm x 0.2 mm; Pt cathode: 1 cm x 1 cm x 0.2 mm) in an undivided cell at RT under O_2 for 10 h (3.7 F/mol). [b] Isolated yield.

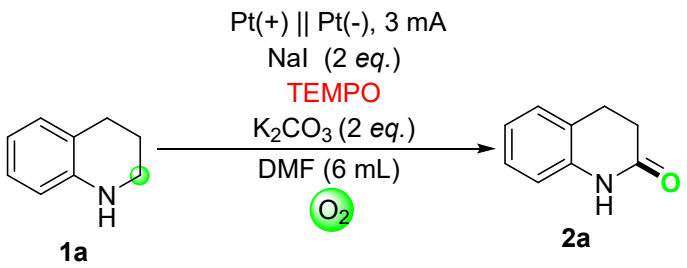
Table S5. Screening of the amount of NaI [a]



Entry	Amount of NaI (*equiv.*)	Yield (%) [b]
1	1	30
2	**2**	**44**
3	3	37
4	4	25

[a] Reaction conditions: A mixture of **1a** (0.3 mmol), NaI (x mmol), TEMPO (0.06 mmol, 0.2 *equiv.*) and K_2CO_3 (0.6 mmol, 2 *equiv.*) in a DMF (6 mL) under a constant current of 3 mA (Pt anode: 1 cm x 1 cm x 0.2 mm; Pt cathode: 1 cm x 1 cm x 0.2 mm) in an undivided cell at RT under O_2 for 10 h (3.7 F/mol). [b] Isolated yield.

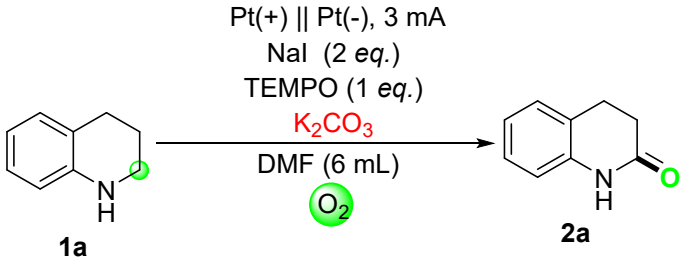
Table S6. Screening of the amount of TEMPO [a]



Entry	Amount of TEMPO (*equiv.*)	Yield (%) [b]
1	0.2	44
2	0.4	54
3	0.6	56
4	**1**	**65**
5	2	60

[a] Reaction conditions: A mixture of **1a** (0.3 mmol), NaI (0.6 mmol, 2 *equiv.*), TEMPO (x mmol) and K_2CO_3 (0.6 mmol, 2 *equiv.*) in a DMF (6 mL) under a constant current of 3 mA (Pt anode: 1 cm x 1 cm x 0.2 mm; Pt cathode: 1 cm x 1 cm x 0.2 mm; Pt cathode : 1 cm x 1 cm x 0.2 mm) in an undivided cell at RT under O_2 for 10 h (3.7 F/mol). [b] Isolated yield.

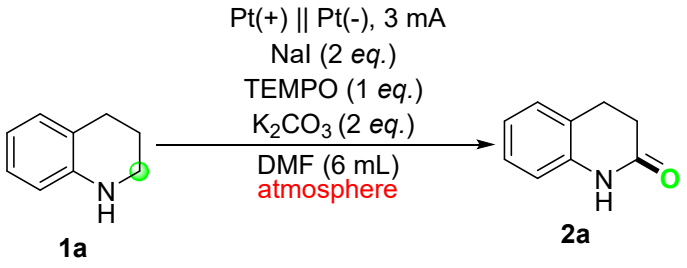
Table S7. Screening of the amount of K_2CO_3 [a]



Entry	Amount of K_2CO_3 (*equiv.*)	Yield (%) [b]
1	0	32
2	1	54
3	**2**	**65**
4	3	58
5	4	46

[a] Reaction conditions: A mixture of **1a** (0.3 mmol), NaI (0.6 mmol, 2 *equiv.*), TEMPO (0.3 mmol, 1 *equiv.*) and K_2CO_3 (x mmol) in a DMF (6 mL) under a constant current of 3 mA (Pt anode: 1 cm x 1 cm x 0.2 mm; Pt cathode: 1 cm x 1 cm x 0.2 mm) in an undivided cell at RT under O_2 for 10 h (3.7 F/mol). [b] Isolated yield.

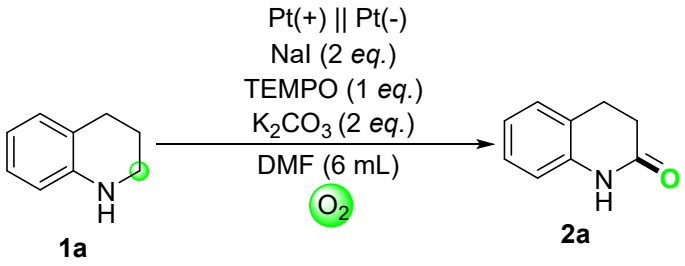
Table S8. Atmosphere screening [a]



Entry	Atmosphere	Yield (%) [b]
1	Air	60
2	**O_2**	**65**
3	Ar	N.D.

[a] Reaction conditions: A mixture of **1a** (0.3 mmol), NaI (0.6 mmol, 2 *equiv.*), TEMPO (0.3 mmol, 1 *equiv.*) and K_2CO_3 (0.6 mmol, 2 *equiv.*) in a DMF (6 mL) under a constant current of 3 mA (Pt anode: 1 cm x 1 cm x 0.2 mm; Pt cathode: 1 cm x 1 cm x 0.2 mm) in an undivided cell at RT under atmosphere for 10 h (3.7 F/mol) [b] Isolated yield.

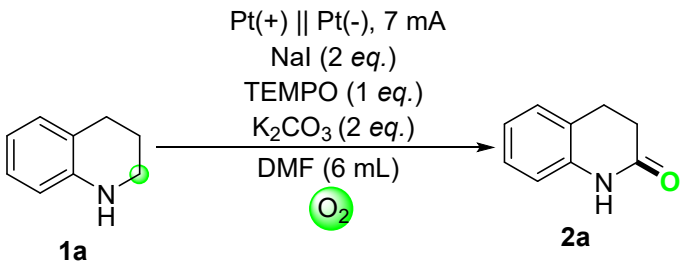
Table S9. Current screening [a]



Entry	Current (mA)	Yield (%) [b]
1	0	N.D.
2	1	18
3	2	27
4	3	65
5	5	64
6	6	71
7	**7**	**80**
8	8	60
9	9	54

[a] Reaction conditions: A mixture of **1a** (0.3 mmol), NaI (0.6 mmol, 2 *equiv.*), TEMPO (0.3 mmol, 1 *equiv.*) and K_2CO_3 (0.6 mmol, 2 *equiv.*) in a DMF (6 mL) under a constant current (Pt anode: 1 cm x 1cm x 0.2 mm; Pt cathode: 1 cm x 1 cm x 0.2 mm) in an undivided cell at RT in O_2 for 10 h. [b] Isolated yield.

Table S10. Electrode material screening [a]



Entry	Electrode material	Yield (%) [b]
1	C(+) || Pt(-)	45
2	C(+) || C(-)	Voltage overload
3	**Pt(+) || Pt(-)**	**80**

4	Pt(+) || C(-)	47

[a] Reaction conditions: A mixture of **1a** (0.3 mmol), NaI (0.6 mmol, 2 *equiv.*), TEMPO (0.3 mmol, 1 *equiv.*) and K_2CO_3 (0.6 mmol, 2 *equiv.*) in a DMF (6 mL) under a constant current of 7 mA (x anode, x cathode) in an undivided cell at RT under O_2 for 10 h (8.7 F/mol). [b] Isolated yield.

4. Mechanistic investigation

4.1. Cyclic voltammetry experiments

The electrochemical measurement was performed by a computer-controlled electrochemical analyzer. Cyclic voltammetry performed in a three-electrode cell was carried out in a three-electrode battery (volume 15 mL; DMF as solvent, nBu$_4$NClO$_4$ 0.05 M as supporting electrolyte, 2 mM concentration of test compound), and glassy carbon (diameter 3 mm) as working electrode, platinum wire as auxiliary electrode, Hg/Hg_2Cl_2 (3 M KCl) as reference electrode. The scanning speed is 100 $mV \cdot s^{-1}$. For 1,2,3,4-tetrahydroquinoline (**1a**), NaI, and TEMPO, the oxidation potential range studied was 0.0 V to +1.8 V, relative to Hg/Hg_2Cl_2 (3 M KCl). The oxidation potential of 1,2,3,4-tetrahydroquinoline (**1a**), NaI and TEMPO was determined as: 1,2,3,4-tetrahydroquinoline (**1a**) (Eox = +0.837 V *vs* SCE in DMF); NaI (Eox = +0.692 V *vs* SCE in DMF); TEMPO (Eox = +0.757 V *vs* SCE in DMF). The result indicates that NaI has a lower oxidation potential than TEMPO and can be oxidized preferentially. NaI and TEMPO may circulate in the system as a dual mediator, and finally, 1,2,3,4-tetrahydroquinoline (**1a**) is oxidized to a product.

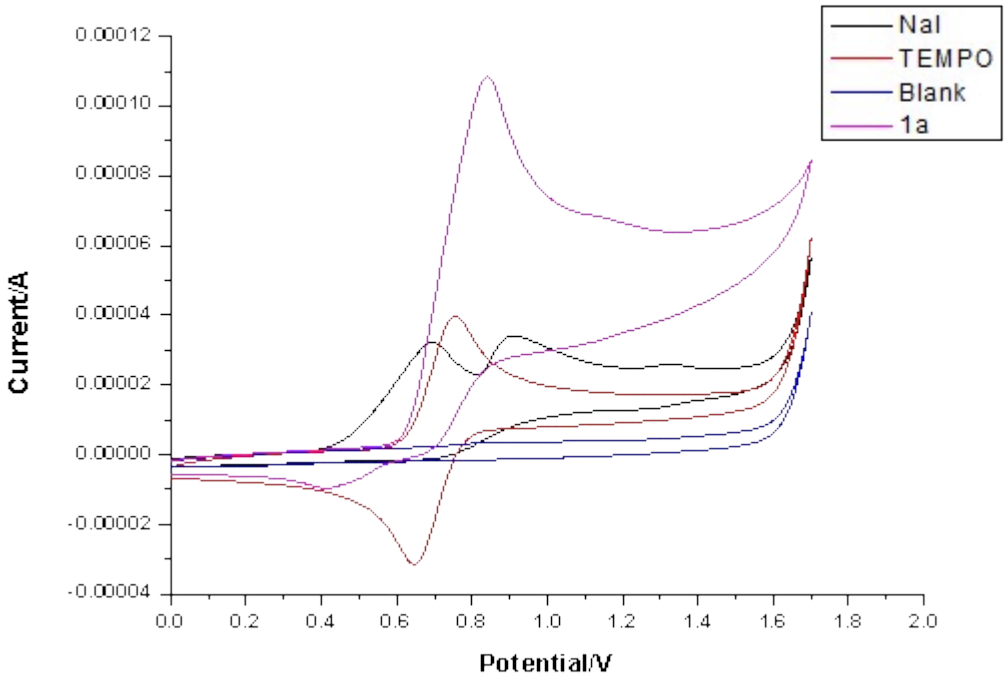
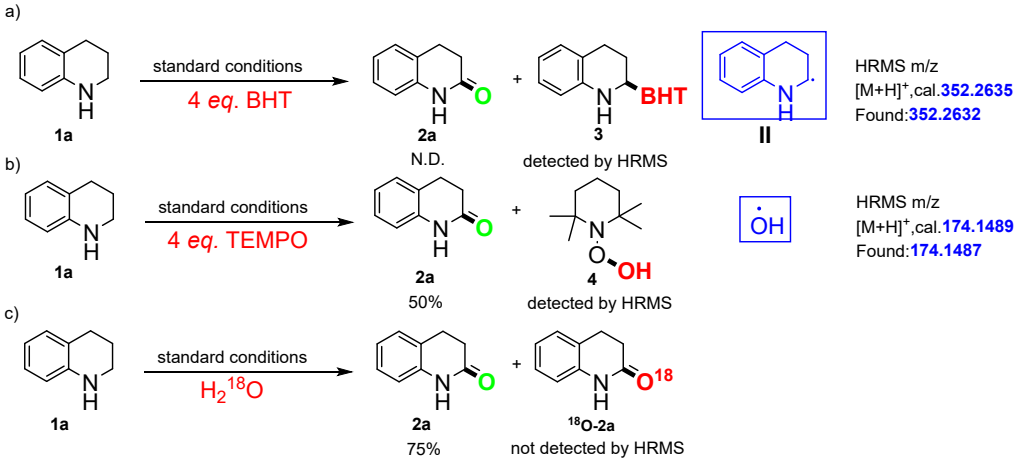


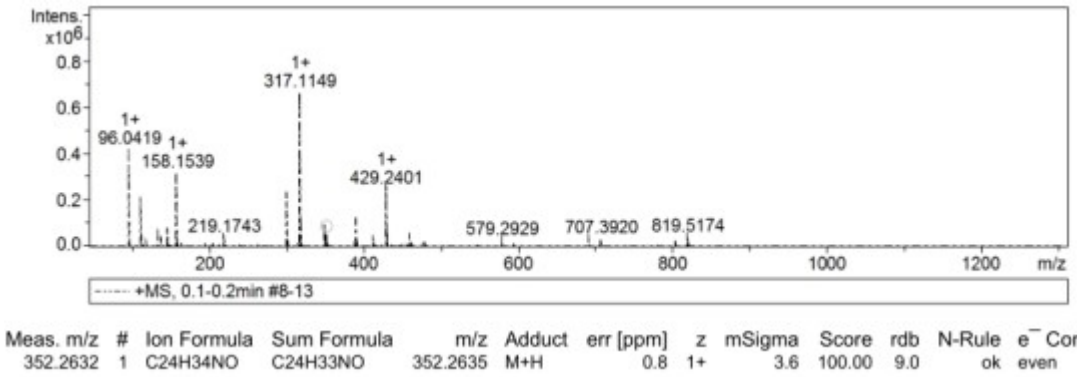
Figure S3. Cyclic voltammetry of NaI, TEMPO, **1a** in DMF and blank.

4.2. Radical trapping and isotope labeling experiments

In order to confirm whether the reaction undergoes a radical mechanism, commonly used radical scavengers, 2,6-di-tert-butyl-4-methylphenol (BHT) and 2,2,6,6-tetramethylpiperidinooxy (TEMPO) were used in radical capture and suppression experiments. Under standard conditions, BHT (4.0 *equiv.* to **1a**) and TEMPO (4.0 *equiv.* to **1a**) were added to the model reaction system at the beginning of the reaction, respectively. After 2 h, a small amount of reaction mixture was taken out for high-resolution mass spectrometry (HRMS) measurement. When 50 uL $H_2{}^{18}O$ was added to the model reaction system under standard reaction conditions, product **2a** was obtained in 75% yield, and the ^{18}O-containing product (compound **^{18}O-2a**) was not detected by HRMS.

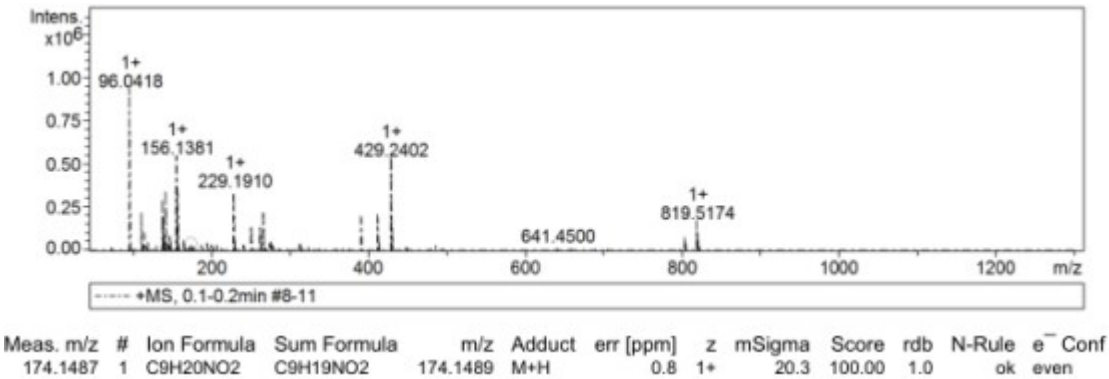


Scheme S1. Radical trapping and isotope labeling experiments.



Meas. m/z	#	Ion Formula	Sum Formula	m/z	Adduct	err [ppm]	z	mSigma	Score	rdb	N-Rule	e⁻ Conf
352.2632	1	C24H34NO	C24H33NO	352.2635	M+H	0.8	1+	3.6	100.00	9.0	ok	even

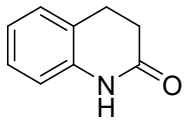
Figure S4. Mass spectrometry (HRMS) data of the radical trapping experiments (with BHT).



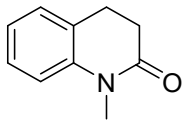
Meas. m/z	#	Ion Formula	Sum Formula	m/z	Adduct	err [ppm]	z	mSigma	Score	rdb	N-Rule	e⁻ Conf
174.1487	1	C9H20NO2	C9H19NO2	174.1489	M+H	0.8	1+	20.3	100.00	1.0	ok	even

Figure S5. Mass spectrometry (HRMS) data of possible intermediate (with TEMPO).

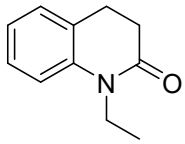
5. Characterization data of the products



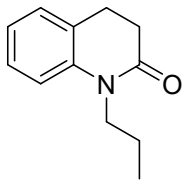
3,4-dihydro-2-quinolone (2a)[4]: R_f = 0.25 (Petroleum ether/EtOAc, 2:1). 35.3 mg, 80% yield. White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.56 (s, 1H), 7.21 – 7.12 (m, 2H), 6.97 (t, *J* = 7.4 Hz, 1H), 6.87 (d, *J* = 7.8 Hz, 1H), 2.96 (t, *J* = 7.6 Hz, 2H), 2.70 – 2.59 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.5, 137.4, 127.9, 127.5, 123.6, 123.0, 115.7, 30.7, 25.3.



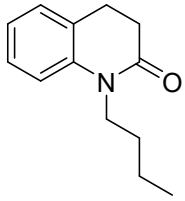
1-methyl-3,4-dihydro-2-quinolone (2b)[5]: R_f = 0.25 (Petroleum ether/EtOAc, 15:1). 36.3 mg, 75% yield. Light yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 (t, *J* = 7.6 Hz, 1H), 7.16 (d, *J* = 7.2 Hz, 1H), 7.07 – 6.94 (m, 2H), 3.36 (s, 3H), 2.90 (t, *J* = 6.9 Hz, 2H), 2.69 – 2.58 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.5, 140.6, 127.7, 127.4, 126.2, 122.8, 114.7, 31.7, 29.5, 25.4.



1-ethyl-3,4-dihydro-2-quinolone (2c)[5]: R_f = 0.25 (Petroleum ether/EtOAc, 15:1). 36.8 mg, 70% yield. Light yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24 (t, *J* = 7.8 Hz, 1H), 7.16 (d, *J* = 7.3 Hz, 1H), 7.00 (m, 2H), 3.99 (q, *J* = 7.1 Hz, 2H), 2.89 (t, *J* = 6.9 Hz, 2H), 2.69 – 2.58 (m, 2H), 1.26 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.5, 140.1, 128.6, 128.0, 127.1, 123.2, 115.2, 37.9, 32.5, 26.2, 13.4.

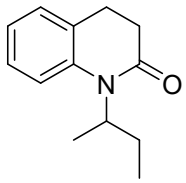


1-propyl-3,4-dihydro-2-quinolone (2d)[5]: R_f = 0.25 (Petroleum ether/EtOAc, 15:1). 34.6 mg, 61% yield. Light yellow liquid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.23 (t, *J* = 8.4 Hz, 1H), 7.16 (d, *J* = 6.9 Hz, 1H), 7.03 – 6.95 (m, 2H), 3.90 (t, *J* = 7.7 Hz, 2H), 2.89 (t, *J* = 6.9 Hz, 2H), 2.68 – 2.61 (m, 2H), 1.71 – 1.63 (m, 2H), 0.96 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.2, 139.6, 128.0, 127.4, 126.6, 122.6, 114.9, 43.65, 32.0, 25.6, 20.4, 11.2.

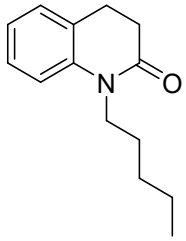


1-butyl-3,4-dihydro-2-quinolone (2e): R_f = 0.25 (Petroleum ether/EtOAc, 15:1). 42.0 mg, 69% yield. Light yellow liquid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.23 (t, *J* = 7.8 Hz, 1H), 7.15 (d, *J* = 7.3 Hz, 1H), 7.02 – 6.97 (m, 2H), 3.93 (t, *J* = 7.7 Hz, 2H), 2.89 (t, *J* = 7.0 Hz, 2H), 2.65 – 2.60

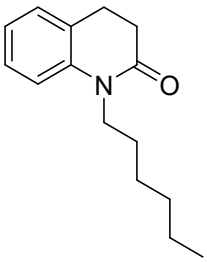
(m, 2H), 1.68 – 1.59 (m, 2H), 1.43 – 1.34 (m, 2H), 0.96 (t, J = 7.4 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.1, 139.7, 128.0, 127.4, 126.6, 122.6, 114.8, 41.9, 32.0, 29.3, 25.6, 20.2, 13.8. HRMS (ESI): m/z: calcd for $C_{13}H_{17}NO$ $(M+H)^+$ 204.1383; found 204.1379. $(M+Na)^+$ 226.1202; found 226.1200.



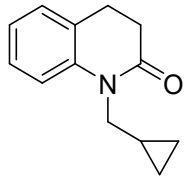
1-isobutyl-3,4-dihydro-2-quinolone (2f): R_f = 0.25 (Petroleum ether/EtOAc, 15:1). 37.8 mg, 61% yield. Light yellow liquid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.22 (t, J = 7.8 Hz, 1H), 7.16 (d, J = 7.3 Hz, 1H), 7.02 – 6.97 (m, 2H), 3.87 – 3.83 (d, J = 5.0 Hz, 2H), 2.90 (t, J = 7.0 Hz, 2H), 2.68 – 2.61 (m, 2H), 2.08 – 1.99 (m, 1H), 0.92 (d, J = 6.7 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.5, 139.5, 128.0, 127.2, 126.9, 122.6, 115.4, 47.96, 32.1, 26.1, 25.6, 20.0. HRMS (ESI): m/z: calcd for $C_{13}H_{17}NO$ $(M+H)^+$ 204.1383; found 204.1381. $(M+Na)^+$ 226.1202; found 226.1201.



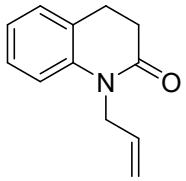
1-pentyl-3,4-dihydro-2-quinolone (2g): R_f = 0.25 (Petroleum ether/EtOAc, 15:1). 41.7 mg, 64% yield. Light yellow liquid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.23 (t, J = 7.8 Hz, 1H), 7.15 (d, J = 7.3 Hz, 1H), 7.02 – 6.96 (m, 2H), 3.93 (t, J = 7.7 Hz, 2H), 2.88 (t, J = 6.9 Hz, 2H), 2.65 – 2.60 (m, 2H), 1.68 – 1.60 (m, 2H), 1.39 – 1.31 (m, 4H), 0.90 (t, J = 6.9 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.0, 139.7, 128.0, 127.4, 126.6, 122.6, 114.8, 42.1, 32.0, 29.1, 26.9, 25.6, 22.4, 14.0. HRMS (ESI): m/z: calcd for $C_{14}H_{19}NO$ $(M+H)^+$ 218.1539; found 218.1537. $(M+Na)^+$ 240.1359; found 240.1356.



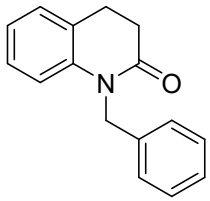
1-hexyl-3,4-dihydro-2-quinolone (2h)[7]: R_f = 0.25 (Petroleum ether/EtOAc, 15:1). 47.2 mg, 68% yield. Light yellow liquid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.23 (t, J = 7.8 Hz, 1H), 7.15 (d, J = 7.4 Hz, 1H), 7.02 – 6.96 (m, 2H), 3.92 (t, J = 7.7 Hz, 2H), 2.87 (t, J = 7.1 Hz, 2H), 2.66 – 2.60 (m, 2H), 1.67 – 1.59 (m, 2H), 1.42 – 1.28 (m, 6H), 0.88 (t, J = 6.9 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.0, 139.7, 128.0, 127.4, 126.6, 122.6, 114.8, 42.2, 32.0, 31.5, 27.2, 26.6, 25.6, 22.6, 14.0.



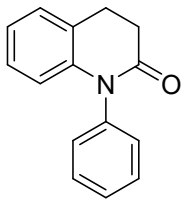
1-methylcyclopropane-3,4-dihydro-2-quinolone (2i): R_f = 0.25 (Petroleum ether/EtOAc, 15:1). 36.2 mg, 60% yield. Light yellow liquid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.25 (t, *J* = 13.4 Hz, 1H), 7.15 (dd, *J* = 19.8, 7.7 Hz, 2H), 7.00 (t, *J* = 7.3 Hz, 1H), 3.88 (d, *J* = 6.7 Hz, 4H), 2.90 (t, *J* = 7.0 Hz, 2H), 2.80 – 2.63 (m, 2H), 1.1 – 1.2 (m, 1H), 0.51 – 0.48 (m, 2H), 0.44 – 0.40 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.3, 138.0, 128.0, 127.3, 126.6, 122.6, 115.2, 45.8, 32.0, 25.7, 9.9, 4.1. HRMS (ESI): m/z: calcd for $C_{13}H_{15}NO$ $(M+H)^+$ 202.1226; found 202.1224. $(M+Na)^+$ 224.1046; found 224.1044.



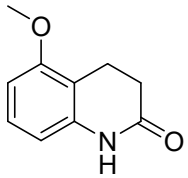
1-allyl-3,4-dihydro-2-quinolone (2j): R_f = 0.25 (Petroleum ether/EtOAc, 15:1). 37.0 mg, 66% yield. Light yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) 7.20 (t, *J* = 7.8 Hz, 1H), δ 7.16 (d, *J* = 7.0 Hz, 2H), 7.05 – 6.95 (m, 2H), 5.94 – 5.85 (m, 1H), 5.24 – 5.09 (m, 2H), 4.60 – 4.52 (m, 2H), 2.93 (t, *J* = 6.7 Hz, 2H), 2.73 – 2.66 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.1, 139.9, 132.7, 127.8, 127.4, 126.3, 122.9, 116.3, 115.4, 45.1, 31.8, 25.6. HRMS (ESI): m/z: calcd for $C_{12}H_{13}NO$ $(M+H)^+$188.1070; found 188.1066. $(M+Na)^+$ 210.0889; found 210.0887.



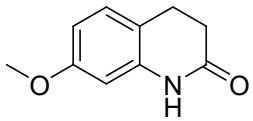
1-benzyl-3,4-dihydro-2-quinolone (2k)[5]: R_f = 0.25 (Petroleum ether/EtOAc, 15:1). 54.1 mg, 76% yield. Light yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.26 (m, 2H), 7.23 – 7.18 (m, 3H), 7.16 (d, *J* = 6.8 Hz, 1H), 7.12 – 7.06 (m, 1H), 6.96 (td, *J* = 7.4, 0.9 Hz, 1H), 6.86 (d, *J* = 8.1 Hz, 1H), 5.18 (s, 2H), 2.97 (*J* = 7.0 Hz, 2H), 2.84 – 2.74 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.5, 139.9, 137.0, 128.8, 127.9, 127.4, 127.1, 126.4, 123.0, 115.6, 46.2, 31.9, 25.6.



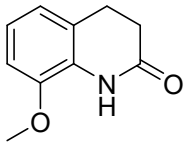
1-phenyl-3,4-dihydro-2-quinolone (2l)[4]: R_f = 0.25 (Petroleum ether/EtOAc, 15:1). 15.8 mg, 25% yield. White solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.50 (t, *J* = 7.7 Hz, 2H), 7.45 – 7.39 (m, 1H), 7.26–7.19 (m, 3H), 7.04 (t, *J* = 7.4 Hz, 1H), 6.98 (t, *J* = 7.3 Hz, 1H), 6.36 (d, *J* = 8.0 Hz, 1H), 3.07 (t, *J* = 6.9 Hz, 2H), 2.85 – 2.78 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.2, 141.7, 138.5, 129.8, 129.0, 128.2, 127.8, 127.1, 125.7, 123.0, 117.0, 32.3, 25.7.



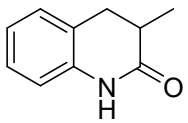
5-methoxy-3,4-dihydro-2-quinolone (2m)[17]**:** R_f = 0.25 (Petroleum ether/EtOAc, 2:1). 37.7 mg, 71% yield. Light yellow solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.80 (s, 1H), 7.12 (t, *J* = 8.1 Hz, 1H), 6.57 (d, *J* = 8.3 Hz, 1H), 6.46 (d, *J* = 7.9 Hz, 1H), 3.83 (s, 3H), 2.95 (t, *J* = 7.7 Hz, 2H), 2.58–2.62 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.9, 156.9, 138.4, 127.9, 111.7, 108.4, 105.4, 55.5, 30.2, 18.5.



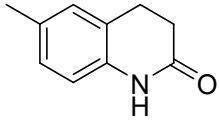
7-methoxy-3,4-dihydro-2-quinolone (2n)[6]**:** R_f = 0.25 (Petroleum ether/EtOAc, 2:1). 47.8 mg, 90% yield. Light yellow solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.82 (s, 1H), 6.90 – 6.95 (m, 1H), 6.80 – 6.74 (m, 2H), 3.85 (s, 3H), 2.97 – 2.92 (m, 2H), 2.62 – 2.59 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.2, 145.8, 126.6, 124.0, 122.6, 120.0, 109.1, 55.8, 30.6, 25.4.



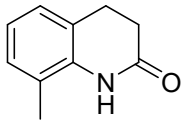
8-methoxy-3,4-dihydro-2-quinolone (2o)[6] **:** R_f = 0.25 (Petroleum ether/EtOAc, 2:1). 34.5 mg, 65% yield. Light yellow solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.77 (s, 1H), 7.07 – 6.97 (m, 2H), 6.90 (t, *J* = 7.5 Hz, 1H), 3.85 (s, 3H), 2.99 – 2.92 (m, 2H), 2.65 – 2.59 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.2, 145.8, 126.6, 124.0, 122.6, 120.0, 109.1, 55.8, 30.7, 25.4.



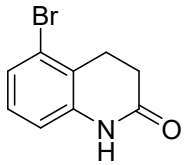
3-methyl-3,4-dihydro-2-quinolone (2p)[6] **:** R_f = 0.25 (Petroleum ether/EtOAc, 2:1). 25.6 mg, 53% yield. Light yellow solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.76 (s, 1H), 7.12 – 7.19 (m, 2H), 6.97 (t, *J* = 7.5 Hz, 1H), 6.82 (d, *J* = 7.8 Hz, 1H), 2.96 – 3.02 (m, 1H), 2.76 – 2.62 (m, 2H), 1.29 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 174.6, 137.2, 128.0, 127.4, 123.54 , 122.9, 115.1, 35.0, 33.5, 15.3.



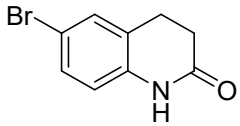
6-methyl-3,4-dihydro-2-quinolone (2q)[8]: R_f = 0.25 (Petroleum ether/EtOAc, 2:1). 38.2 mg, 79% yield. Light yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.62 (s, 1H), 6.99 – 6.94 (m, 2H), 6.73 – 6.67 (m, 1H), 2.93 (t, *J* = 7.2 Hz, 2H), 2.65 – 2.59 (m, 2H), 2.29 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.8, 134.8, 132.6, 128.6, 127.9, 123.5, 115.3, 30.8, 25.4, 20.7.



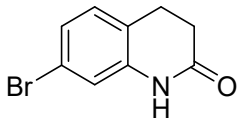
8-methyl-3,4-dihydro-2-quinolone (2r)[8]: R_f = 0.25 (Petroleum ether/EtOAc, 2:1). 35.3 mg, 73% yield. Light yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (s, 1H), 7.07 – 6.97 (m, 2H), 6.90 (t, *J* = 7.5 Hz, 1H), 2.96 (t, *J* = 7.0 Hz, 2H), 2.65 – 2.59 (m, 2H), 2.25 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.6, 135.6, 129.1, 125.8, 123.8, 122.8, 122.7, 30.8, 25.7, 16.7.



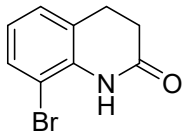
5-bromo-3,4-dihydro-2-quinolone (2s)[17]: R_f = 0.25 (Petroleum ether/EtOAc, 2:1). 47.2 mg, 70% yield. White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.40 (s, 1H), 7.25 (d, *J* = 9.8 Hz, 1H), 7.03 (t, *J* = 8.0 Hz, 1H), 6.82 (d, *J* = 7.9 Hz, 1H), 3.09 (t, *J* = 7.4 Hz, 2H), 2.69 – 2.63 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.0, 138.6, 128.6, 127.1, 123.8, 123.5, 114.9, 30.1, 25.5.



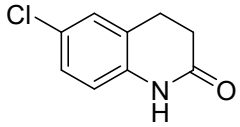
6-bromo-3,4-dihydro-2-quinolone (2t)[8]: R_f = 0.25 (Petroleum ether/EtOAc, 2:1). 39.1 mg, 58% yield. White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.03 (s, 1H), 7.36 – 7.25 (m, 2H), 6.71 (d, *J* = 8.1 Hz, 1H), 2.96 (t, *J* = 8.3 Hz, 2H), 2.67 – 2.59 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.7, 136.4, 130.8, 130.4, 125.7, 117.0, 115.5, 30.3, 25.2.



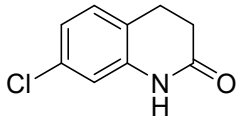
7-**bromo-3,4-dihydro-2-quinolone (2u)**: R_f = 0.25 (Petroleum ether/EtOAc, 2:1). 52.0 mg, 77% yield. White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.99 (s, 1H), 7.13 – 7.10 (m, 1H), 7.05 – 6.97 (m, 2H), 2.92 (t, *J* = 7.2 Hz, 2H), 2.67 – 2.61 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.9, 138.7, 129.3, 125.9, 122.6, 120.7, 118.4, 30.5, 24.9. HRMS (ESI): m/z: calcd for C_9H_8BrNO $(M+Na)^+$ 247.9681; found 247.9679.



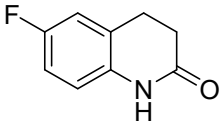
8-bromo-3,4-dihydro-2-quinolone (2v)[8]: R_f = 0.25 (Petroleum ether/EtOAc, 2:1). 54.7 mg, 81% yield. White solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.81 (s, 1H), 7.40 (d, *J* = 8.1 Hz, 1H), 7.12 (d, *J* = 7.2 Hz, 1H), 6.88 (t, *J* = 7.8 Hz, 1H), 2.99 (t, *J* = 7.2 Hz, 2H), 2.70 – 2.60 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.5, 135.2, 130.9, 127.5, 125.6, 123.8, 109.6, 30.6, 26.0.



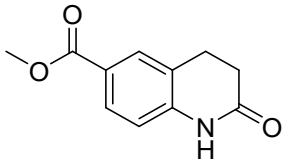
6-chloro-3,4-dihydro-2-quinolone (2w)[8]: R_f = 0.25 (Petroleum ether/EtOAc, 2:1). 33.1 mg, 61% yield. White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.12 (s, 1H), 7.18 – 7.12 (m, 2H), 6.77 (d, *J* = 8.9 Hz, 1H), 2.95 (t, *J* = 7.6 Hz, 2H), 2.66 – 2.60 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.9, 136.0, 128.0, 127.9, 127.5, 125.3, 116.7, 30.3, 25.2.



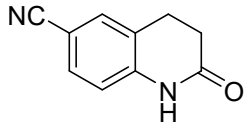
7-chloro-3,4-dihydro-2-quinolone (2x)[10]: R_f = 0.25 (Petroleum ether/EtOAc, 2:1). 35.8 mg, 66% yield. White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.28 (s, 1H), 7.07 (d, *J* = 8.0 Hz, 1H), 6.95 (dd, *J* = 8.0, 1.8 Hz, 1H), 6.86 (d, *J* = 1.7 Hz, 1H), 2.94 (t, *J* = 7.6 Hz, 2H), 2.67 – 2.61 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.1, 138.5, 133.0, 128.9, 123.0, 122.0, 115.6, 30.5, 24.9.



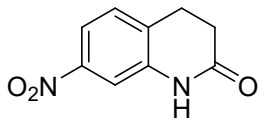
6-fluoro-3,4-dihydro-2-quinolone (2y)[8]: R_f = 0.25 (Petroleum ether/EtOAc, 2:1). 31.2 mg, 63% yield. White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.93 – 6.72 (m, 3H), 2.95 (t, *J* = 7.5 Hz, 2H), 2.68 – 2.56 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.9, 158.7 (d, *J* = 240 Hz), 133.5 (d, *J* = 2 Hz), 125.4 (d, *J* = 8 Hz), 116.5 (d, *J* = 8 Hz), 114.9 (d, *J* = 23 Hz), 114.0 (d, *J* = 23 Hz), 30.27, 25.42. ^{19}F NMR (565 MHz, $CDCl_3$) δ -120.2.



6-methylformate-3,4-dihydro-2-quinolone (2z)[9]: R_f = 0.25 (Petroleum ether/EtOAc, 2:1). 31.4 mg, 57% yield. White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 – 7.84 (m, 2H), 6.92 – 6.86 (m, 1H), 3.90 (s, 3H), 3.03 (t, *J* = 7.6 Hz, 2H), 2.71 – 2.65 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.1, 166.6, 141.3, 129.6, 129.5, 124.9, 123.3, 115.2, 52.0, 30.5, 25.1.

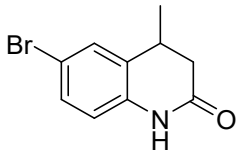


6-cyano-3,4-dihydro-2-quinolone (2aa)[9]: R_f = 0.25 (Petroleum ether/EtOAc, 2:1). 34.1 mg, 66% yield. White solid. ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.49 (s, 1H), 7.65 (s, 1H), 7.60 (dd, *J* = 8.2, 1.9 Hz, 1H), 6.98 (d, *J* = 8.2 Hz, 1H), 2.93 (t, *J* = 7.6 Hz, 2H), 2.60 – 2.46 (m, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 175.5, 147.8, 136.9, 136.8, 128.0, 124.4, 120.8, 108.9, 34.9, 29.4.

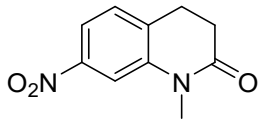


7-nitro-3,4-dihydro-2-quinolone (2ab): R_f = 0.25 (Petroleum ether/EtOAc, 2:1). 36.3 mg, 63% yield. Light yellow solid. ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.44 (s, 1H), 7.78 (dt, *J* = 8.2, 2.1

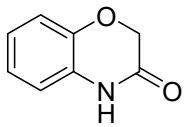
Hz, 1H), 7.71 – 7.68 (m, 1H), 7.45 (d, *J* = 8.2 Hz, 1H), 3.02 (t, *J* = 7.6 Hz, 2H), 2.56 – 2.47 (m, 5H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 175.2, 151.9, 144.7, 136.9, 134.1, 121.8, 114.4, 44.8, 34.7, 30.1. HRMS (ESI): m/z: calcd for $C_9H_8N_2O_3$ $(M+H)^+$ 193.0608; found 193.0605. $(M+Na)^+$ 215.0427; found 215.0425.



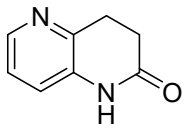
4-methyl-6-bromo-3,4-dihydro-2-quinolone (2ac): R_f = 0.25 (Petroleum ether/EtOAc, 2:1). 51.6 mg, 72% yield. Light yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.95 (s, 1H), 7.34 – 7.25 (m, 2H), 6.72 (d, *J* = 8.3 Hz, 1H), 3.18 – 3.07 (m, 1H), 2.71 (dd, *J* = 16.2, 5.8 Hz, 1H), 2.41 (dd, *J* = 16.2, 7.4 Hz, 1H), 1.31 (d, *J* = 7.0 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.2, 135.6, 130.8, 130.4, 129.5, 117.2, 115.8, 38.0, 30.7, 19.5. HRMS (ESI): m/z: calcd for $C_{10}H_{10}BrNO$ $(M+Na)^+$ 261.9838; found 261.9836.



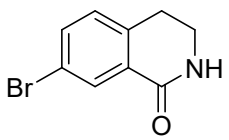
1-methyl-7-nitro-3,4-dihydro-2-quinolone (2ad): R_f = 0.25 (Petroleum ether/EtOAc, 2:1). 35.3 mg, 57% yield. Light yellow solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.90 (dd, *J* = 8.2, 2.0 Hz, 1H), 7.83 (d, *J* = 1.9 Hz, 1H), 7.33 (d, *J* = 8.2 Hz, 1H), 3.43 (s, 3H), 3.03 (t, *J* = 7.0 Hz, 2H), 2.77 – 2.69 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.6, 147.7, 141.7, 133.3, 128.3, 117.7, 109.5, 30.8, 29.7, 25.5. HRMS (ESI): m/z: calcd for $C_{10}H_{10}N_2O_3$ $(M+Na)^+$ 229.0584; found 229.0583.



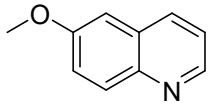
2H-1,4-benzoxazin-3(4H)-one (2ae)[11]: R_f = 0.25 (Petroleum ether/EtOAc, 2:1). 15.6 mg, 35% yield. Light yellow solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.88 (s, 1H), 6.98 – 6.95 (m, 3H), 6.87 – 6.82 (m, 1H), 4.62 (s, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.9, 143.7, 126.1, 124.2, 122.7, 116.8, 115.9, 67.2.



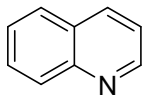
3,4-dihydro-1,5-naphthyridin-2(1H)-one (2af) [12]: R_f = 0.25 (Petroleum ether/EtOAc, 2:1). 32.0 mg, 72% yield. Light yellow solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.09 (s, 1H), 8.20 (t, *J* =2.9, 1H), 7.14 (d, *J* = 2.9 Hz, 2H), 3.20 (t, *J* = 7.8 Hz, 2H), 2.78 (t, *J* = 7.8 Hz, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.50, 144.95, 143.60, 133.39, 122.43, 30.21, 28.05.



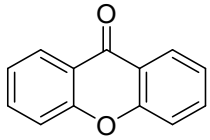
7-bromo-3, 4-dihydro-2-isoquinolone (2ah)[13]: R_f = 0.25 (Petroleum ether/EtOAc, 2:1). 47.9 mg, 71% yield. White solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.30 (s, 1H), 7.49 (dd, J = 8.2, 2.2 Hz, 1H), 7.43 (d, *J* = 2.2 Hz, 1H), 7.06 (d, *J* = 8.7 Hz, 1H), 3.83 – 3.78 (m, 2H), 2.72 (t, *J* = 8.4 Hz, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.5, 135.2, 130.9, 127.1, 125.6, 123.8, 109.6, 30.6, 26.0.



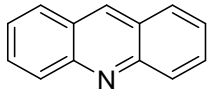
6-methoxy-quinoline (2ai)[14]: R_f = 0.25 (Petroleum ether/EtOAc, 2:1). 38.2 mg, 80% yield. Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.76 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.07 – 7.98 (m, 2H), 7.38–7.32 (m, 2H), 7.06 (d, *J* = 2.8 Hz, 1H), 3.92 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.8, 147.8, 144.3, 134.8, 130.8, 129.3, 122.3, 121.3, 105.2, 55.5.



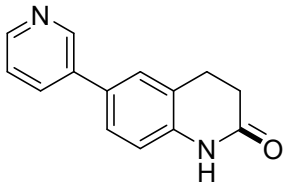
Quinoline (2aj)[14] : R_f = 0.25 (Petroleum ether/EtOAc, 5:1). 32.3 mg, 50% yield. Yellow liquid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.95 – 8.90 (m, 1H), 8.16 (d, *J* = 8.2 Hz, 1H), 8.12 (d, *J* = 8.5 Hz, 1H), 7.82 (d, *J* = 8.1 Hz, 1H), 7.72 (t, *J* = 7.6 Hz, 1H), 7.55 (t, *J* = 7.5 Hz, 1H), 7.40 (dd, *J* = 8.2, 4.2 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 150.3, 148.3, 136.1, 129.5, 129.4, 128.3, 127.8, 126.5, 121.0.



Xanthene (2ak)[15]: R_f= 0.25 (Petroleum ether/EtOAc, 50:1). 50.0 mg, 85% yield. White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (dd, *J* = 8.0, 1.1 Hz, 2H), 7.75 – 7.69 (m, 2H), 7.48 (d, *J* = 8.4 Hz, 2H), 7.39 – 7.35 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 177.2, 156.2, 134.8, 126.8, 123.9, 121.9, 118.0.

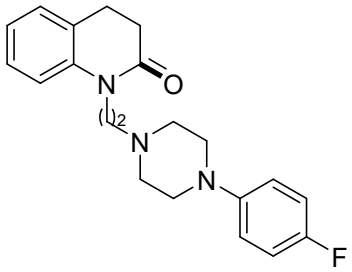


10-azaanthracene (2al)[16]: R_f = 0.25 (Petroleum ether/EtOAc, 50:1). 50.0 mg, 93% yield. Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.74 – 8.67 (m, 1H), 8.24 (d, *J* = 8.8 Hz, 2H), 7.99 – 7.90 (m, 2H), 7.79 – 7.71 (m, 2H), 7.54 – 7.46 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.1, 136.0, 130.3, 129.4, 128.2, 126.6, 125.7.



In vivo active aldosterone synthase inhibitor (5)[18]: R_f = 0.25 (Petroleum ether/EtOAc, 2:1). 840.4 mg. White solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.83 (s, 1H), 8.58 (d, *J* = 4.3 Hz, 1H), 7.85 (d, *J* = 7.9 Hz, 1H), 7.40 (d, *J* = 7.4 Hz, 2H), 7.36 (dd, *J* = 7.8, 4.9 Hz, 1H), 6.93 (d,

J = 8.2 Hz, 1H), 3.06 (t, J = 7.6 Hz, 2H), 2.75 – 2.60 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.5, 147.9, 147.7, 137.5, 136.1, 134.1, 132.6, 126.8, 126.3, 124.5, 123.6, 116.0, 30.7, 25.5.



Antidepressant (8)[19]: R_f = 0.25 (Petroleum ether/EtOAc, 2:1). 28.9 mg. White solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.27 – 7.23 (m, 1H), 7.16 (d, J = 7.4 Hz, 1H), 7.09 (d, J = 8.2 Hz, 1H), 7.01 (t, J = 7.5 Hz, 1H), 6.95 (t, J = 8.7 Hz, 2H), 6.89 – 6.83 (m, 2H), 4.13 (t, J = 7.4 Hz, 2H), 3.12 (t, J = 4.9 Hz, 4H), 2.89 (t, J = 6.2 Hz, 2H), 2.71 (t, J = 4.9 Hz, 4H), 2.62 – 2.69 (m, 4H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.2, 157.2 (d, J = 239 Hz), 147.9, 139.7, 128.0, 127.5, 126.7, 122.9, 117.8 (d, J = 7 Hz), 115.5 (d, J = 22 Hz), 114.9, 54.9, 53.4, 50.1, 39.9, 31.9, 25.6. ^{19}F NMR (565 MHz, $CDCl_3$) δ -124.7.

6. References

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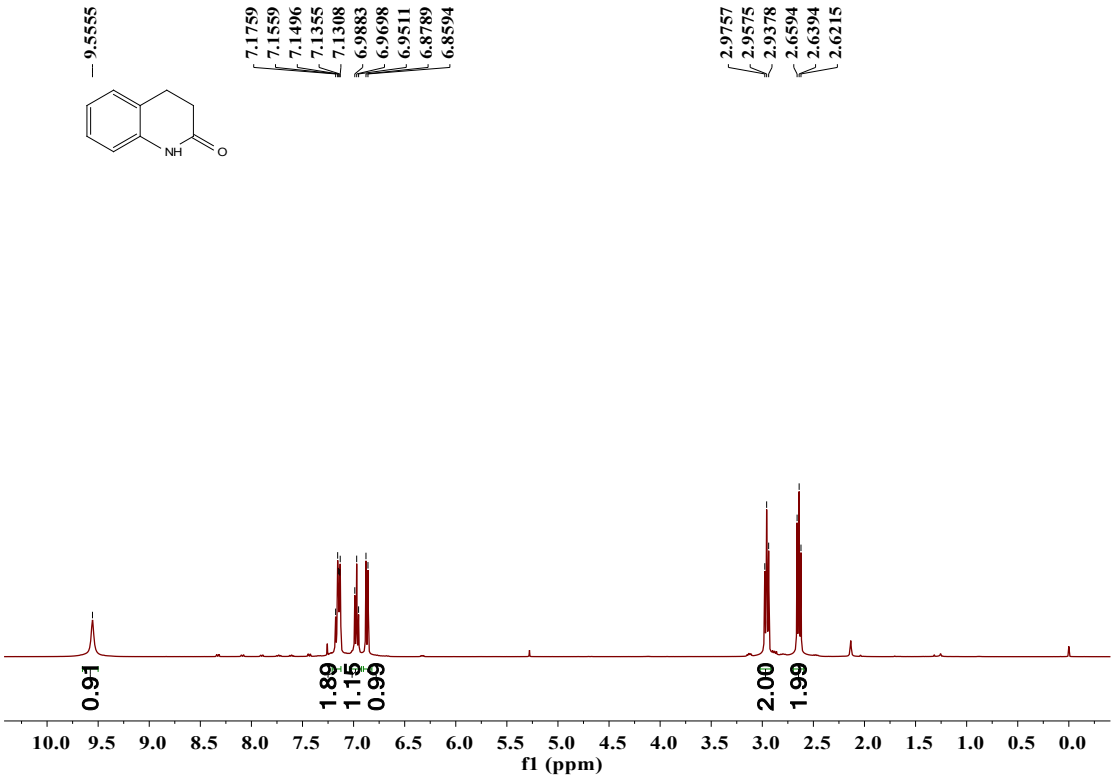
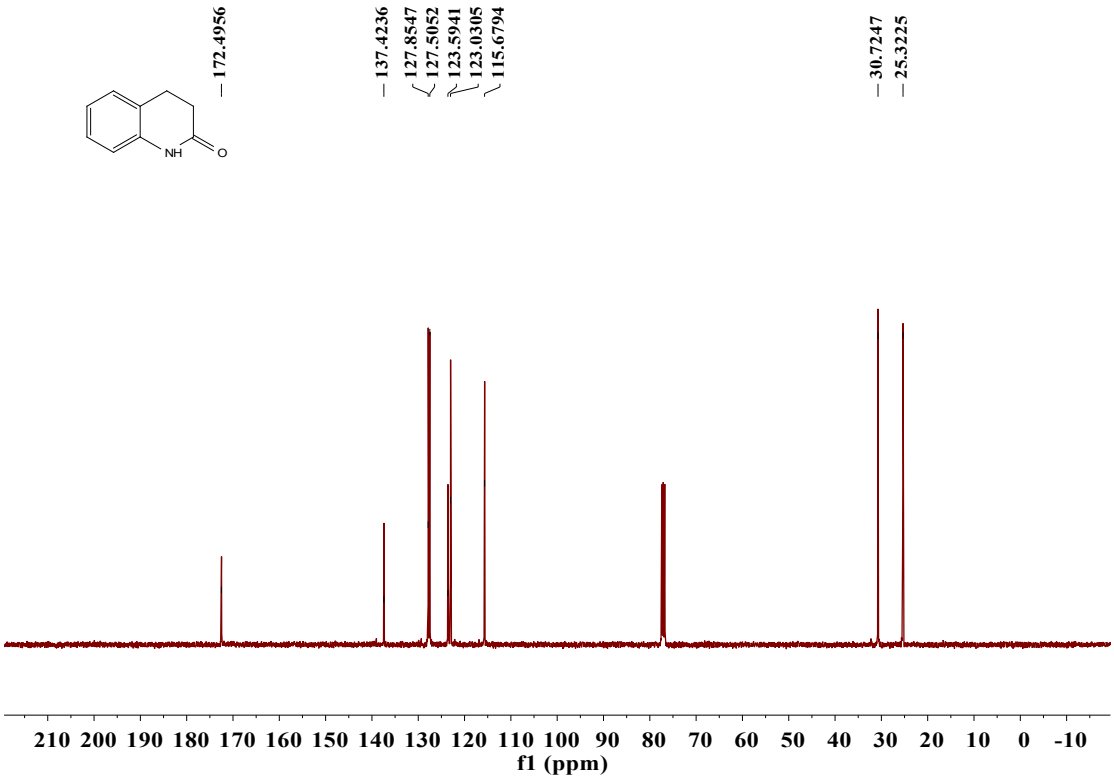
7. NMR of Products

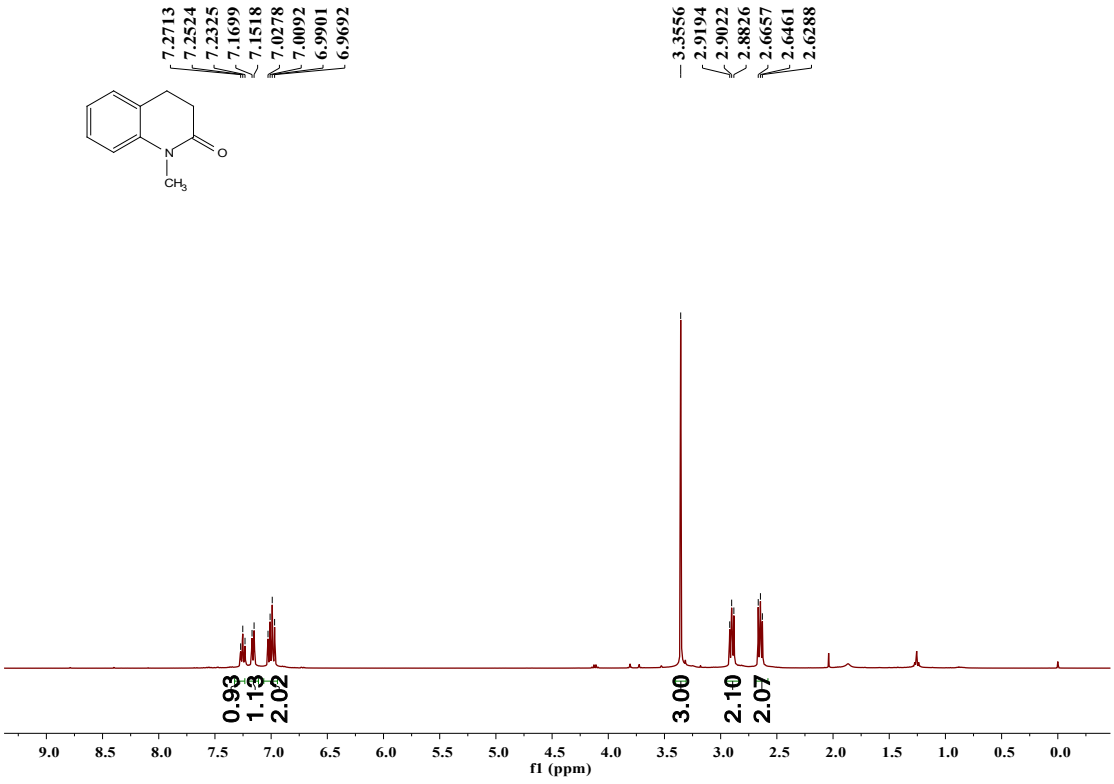
^{1}H-NMR Spectrum ($CDCl_3$) of 2a



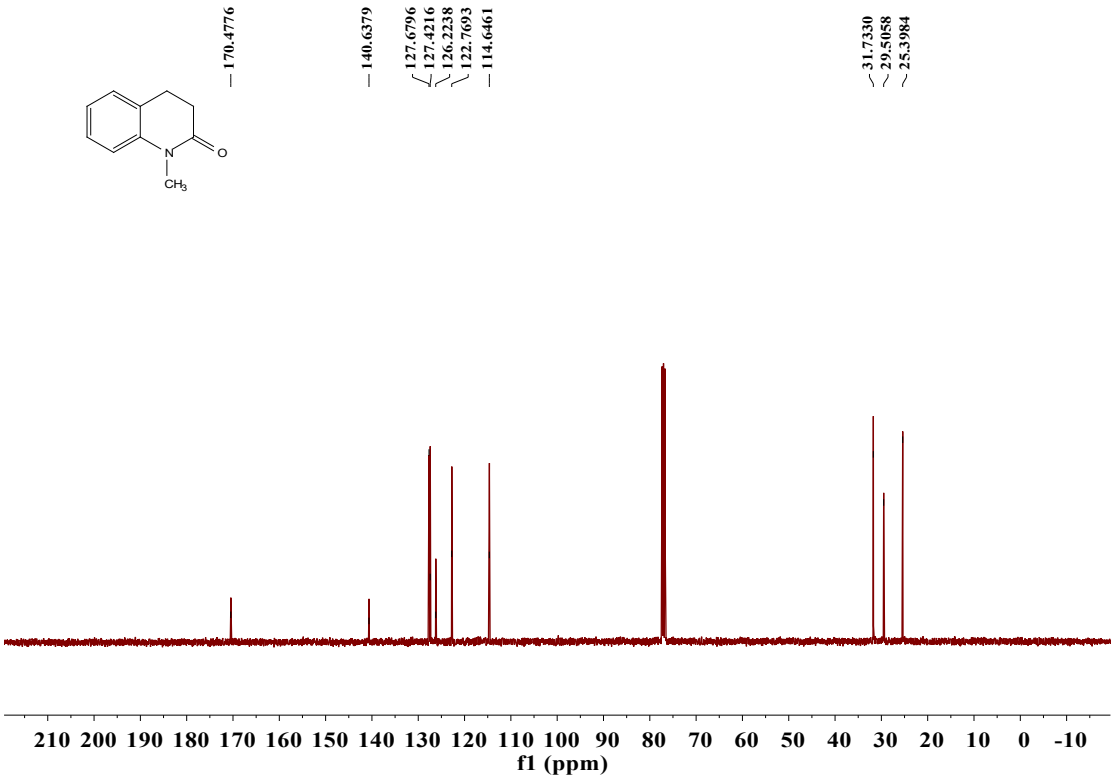
^{13}C-NMR Spectrum ($CDCl_3$) of 2a



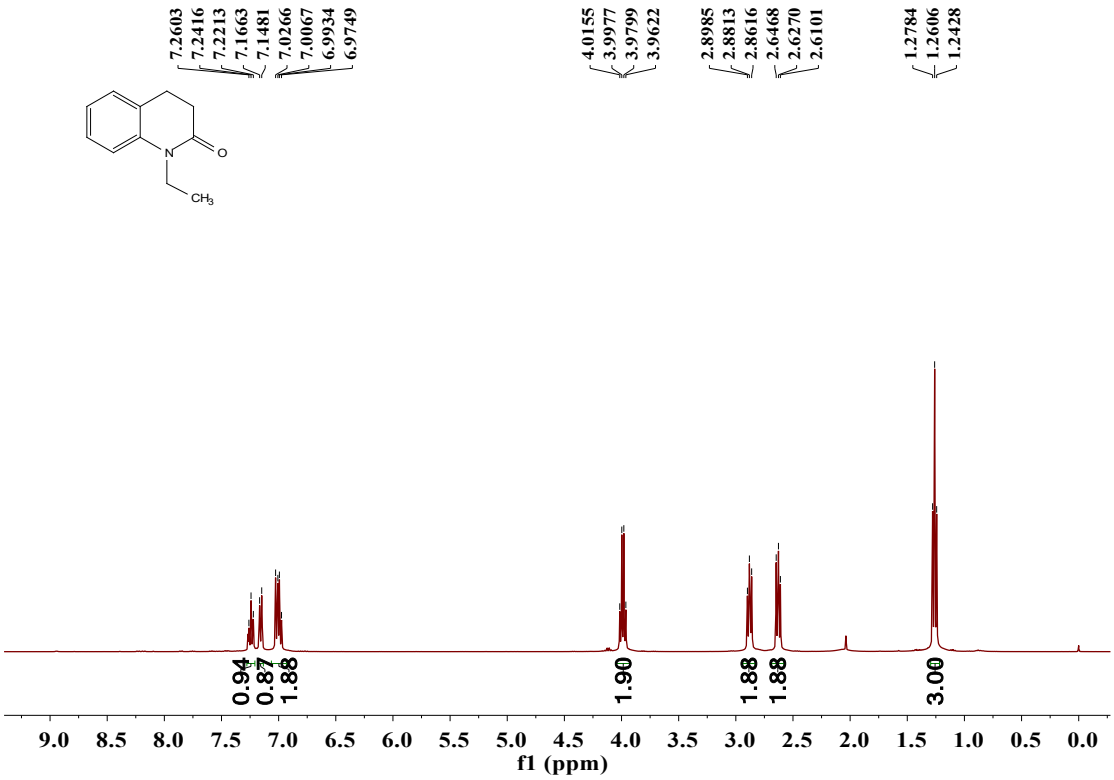
^{1}H-NMR Spectrum ($CDCl_3$) of 2b



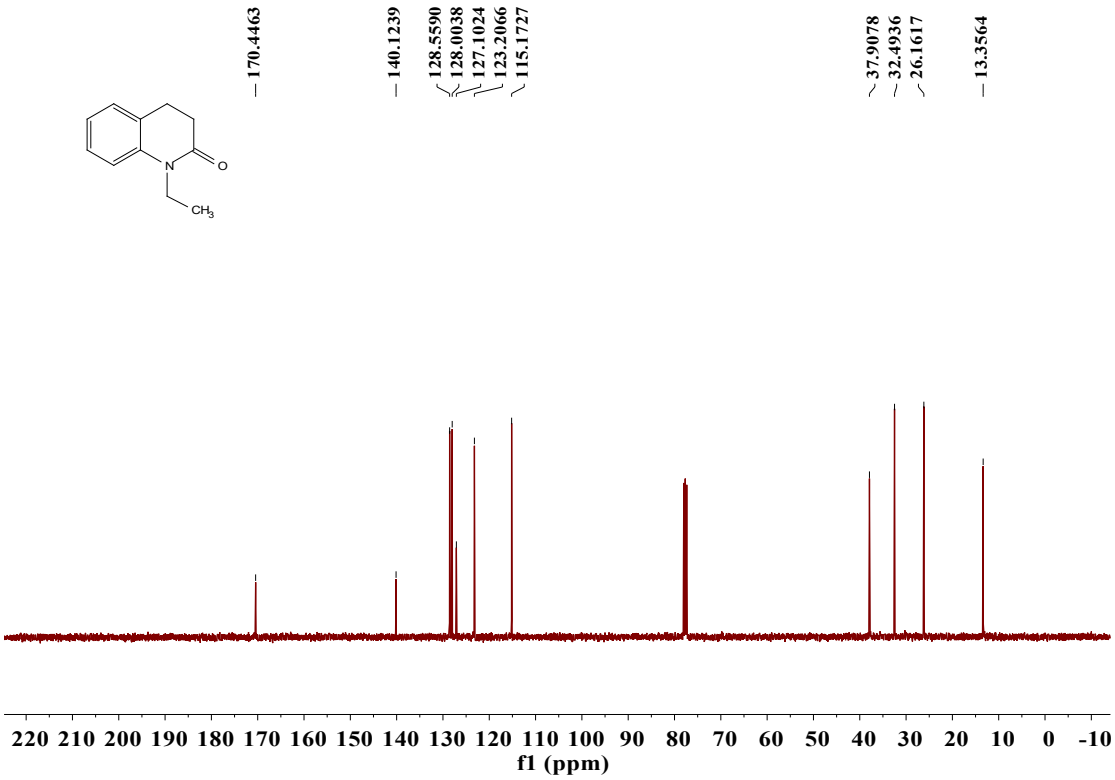
^{13}C-NMR Spectrum ($CDCl_3$) of 2b



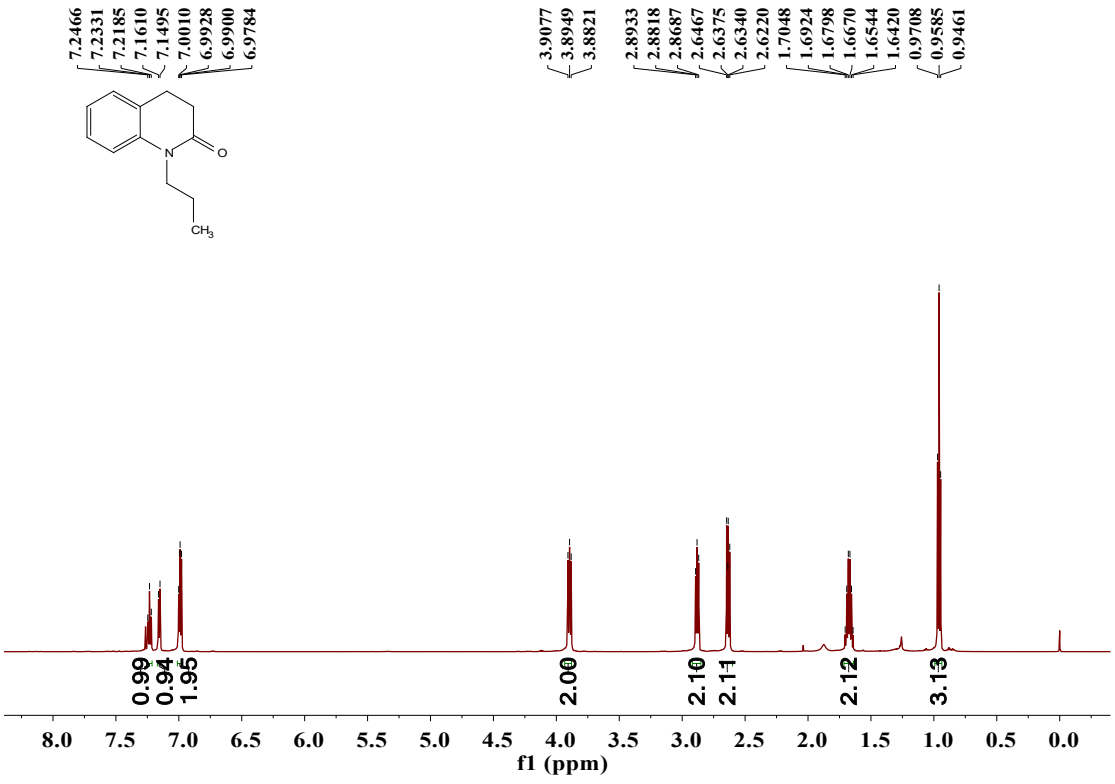
^{1}H-NMR Spectrum ($CDCl_3$) of 2c



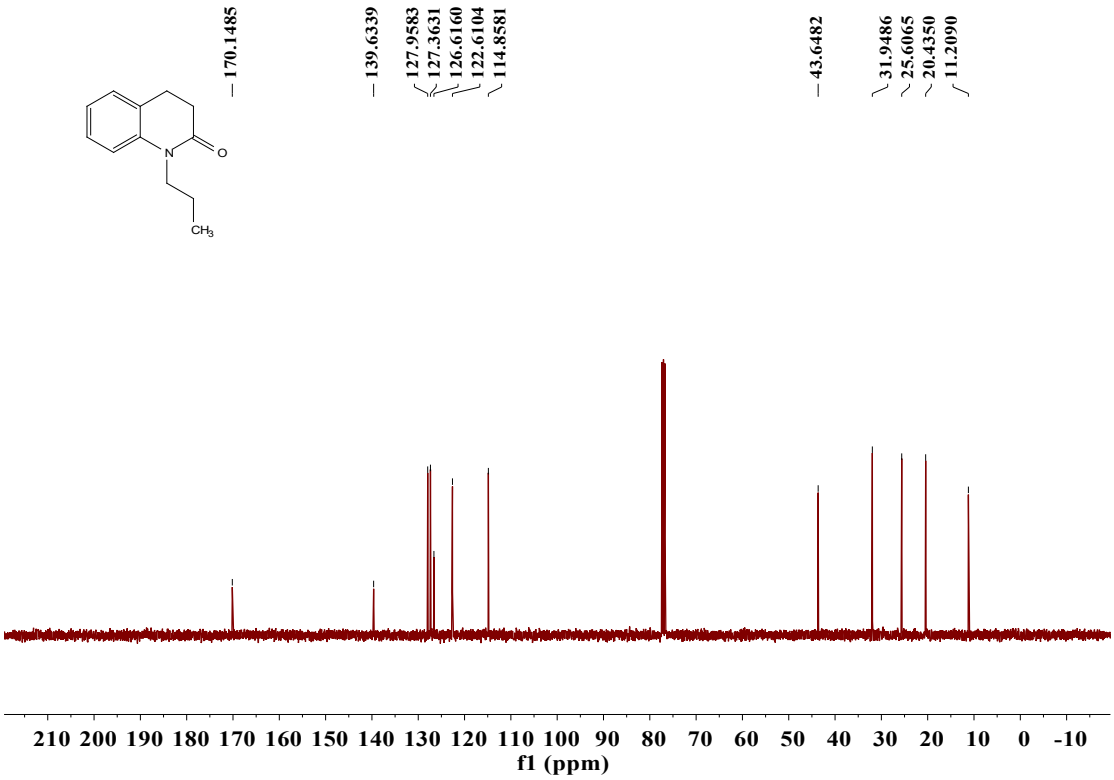
^{13}C-NMR Spectrum ($CDCl_3$) of 2c



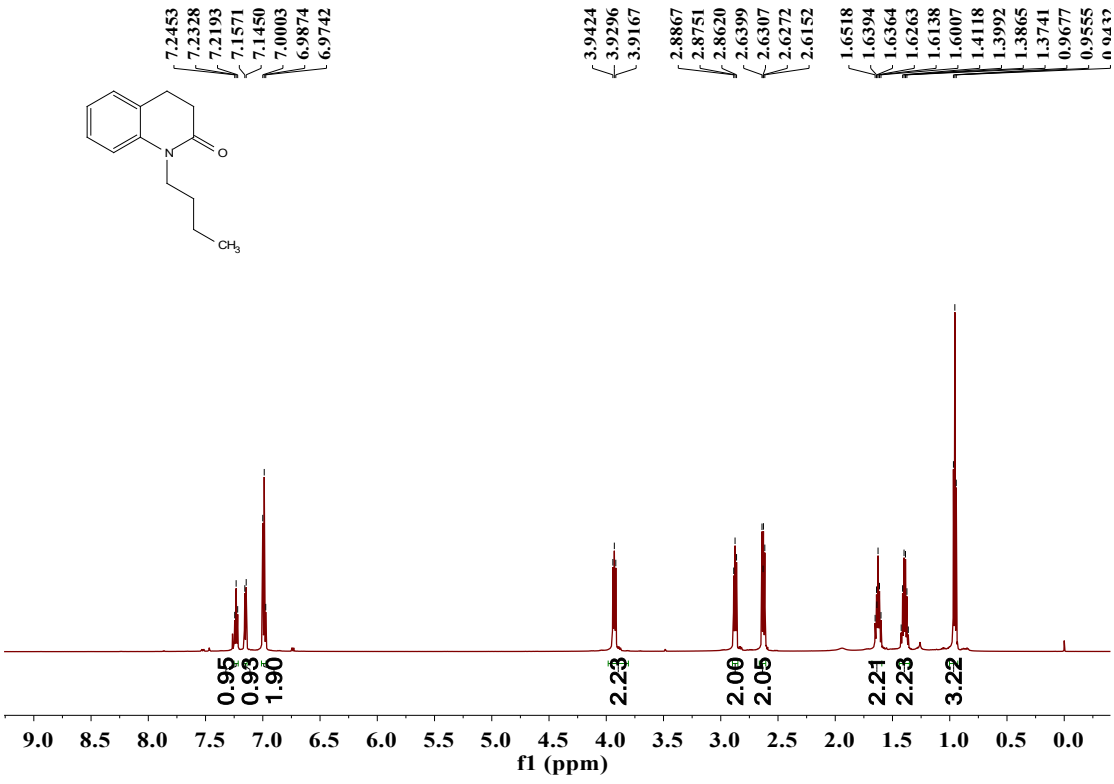
^{1}H-NMR Spectrum ($CDCl_3$) of 2d



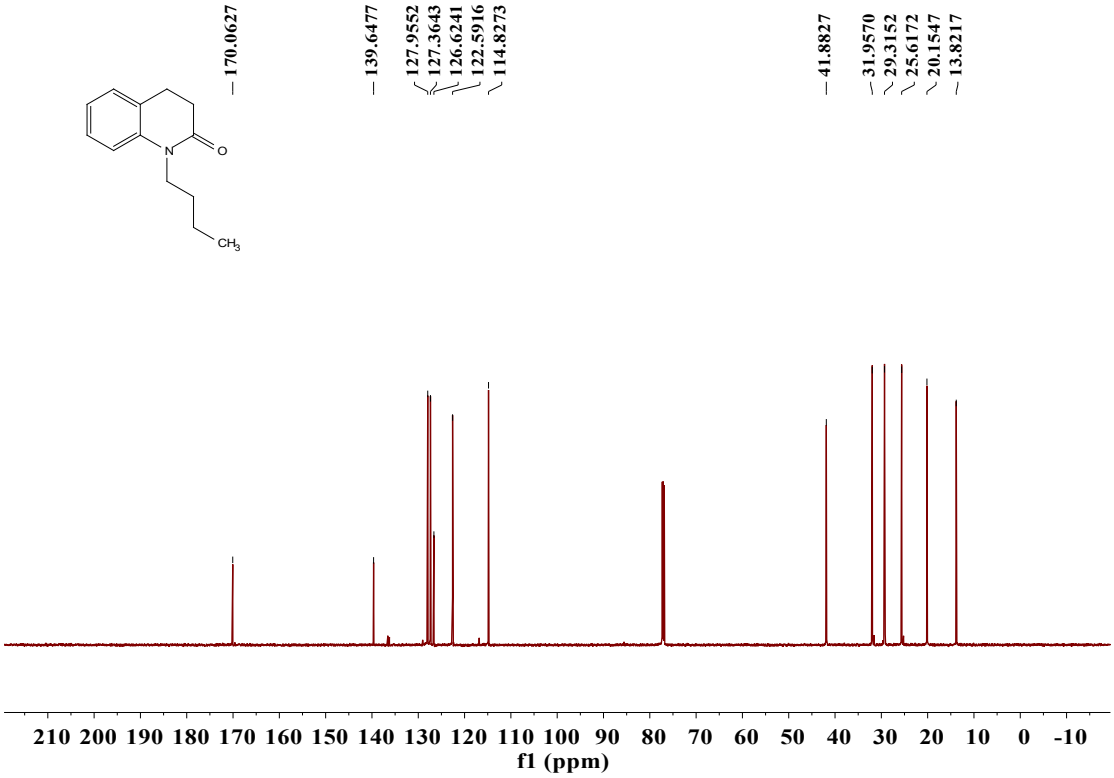
^{13}C-NMR Spectrum ($CDCl_3$) of 2d



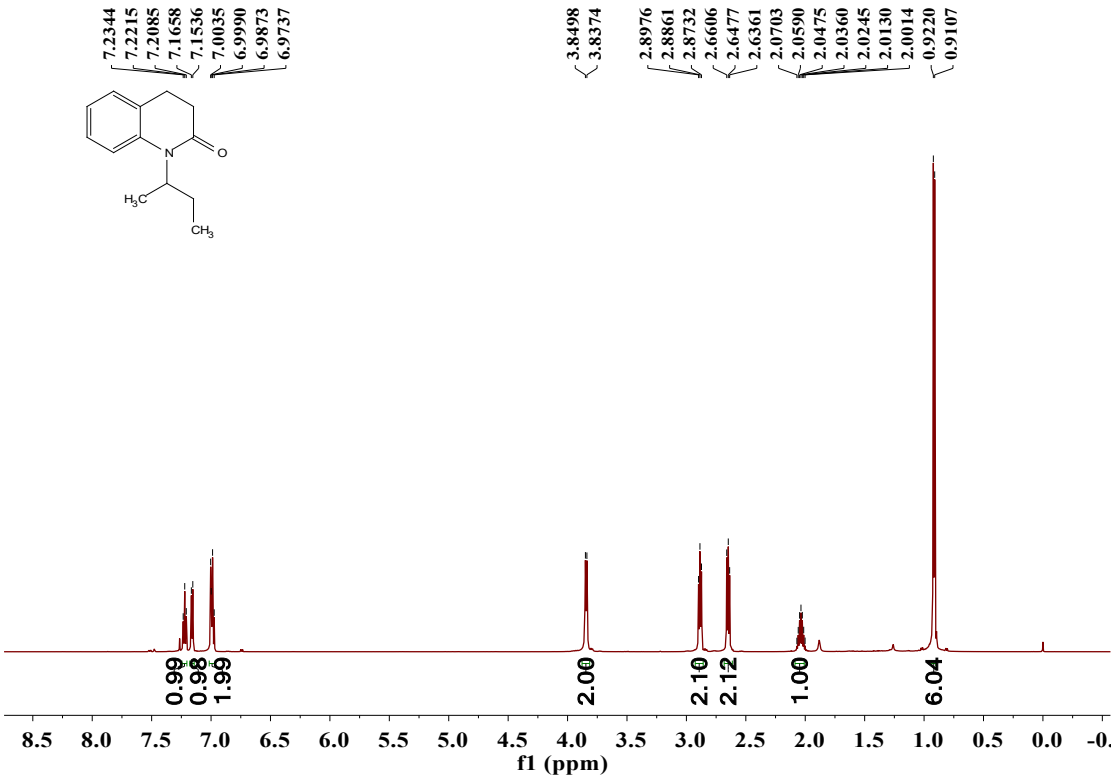
^{1}H-NMR Spectrum ($CDCl_3$) of 2e



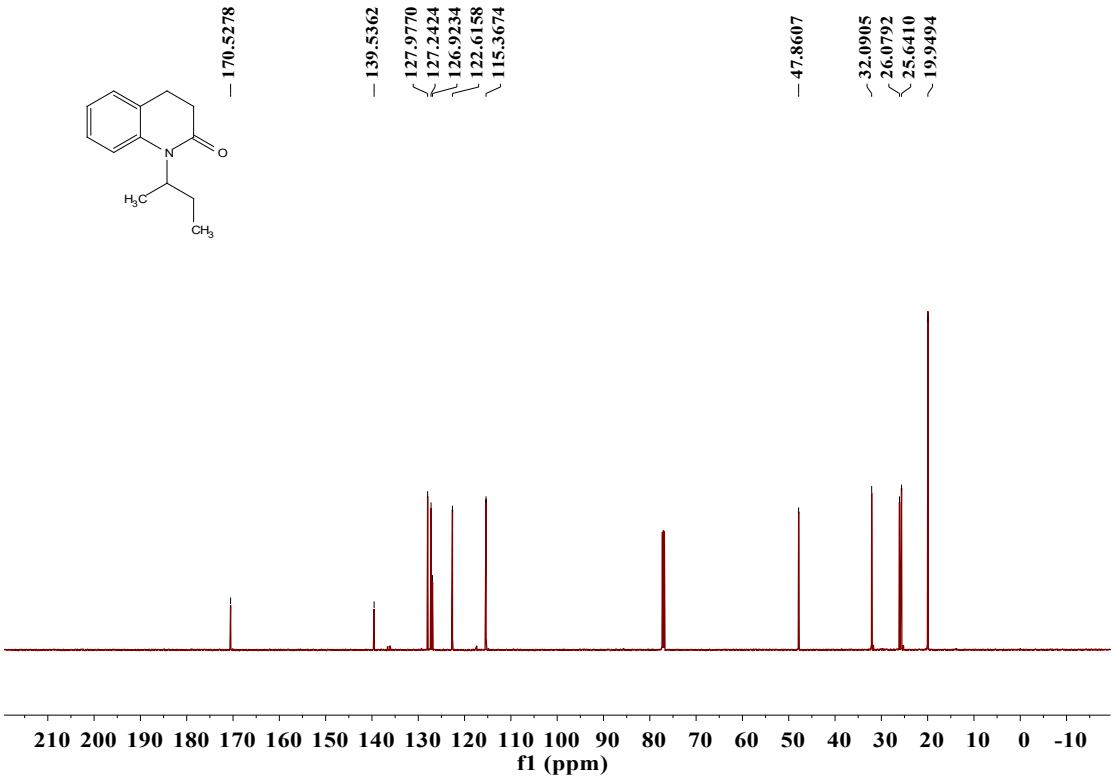
^{13}C-NMR Spectrum ($CDCl_3$) of 2e



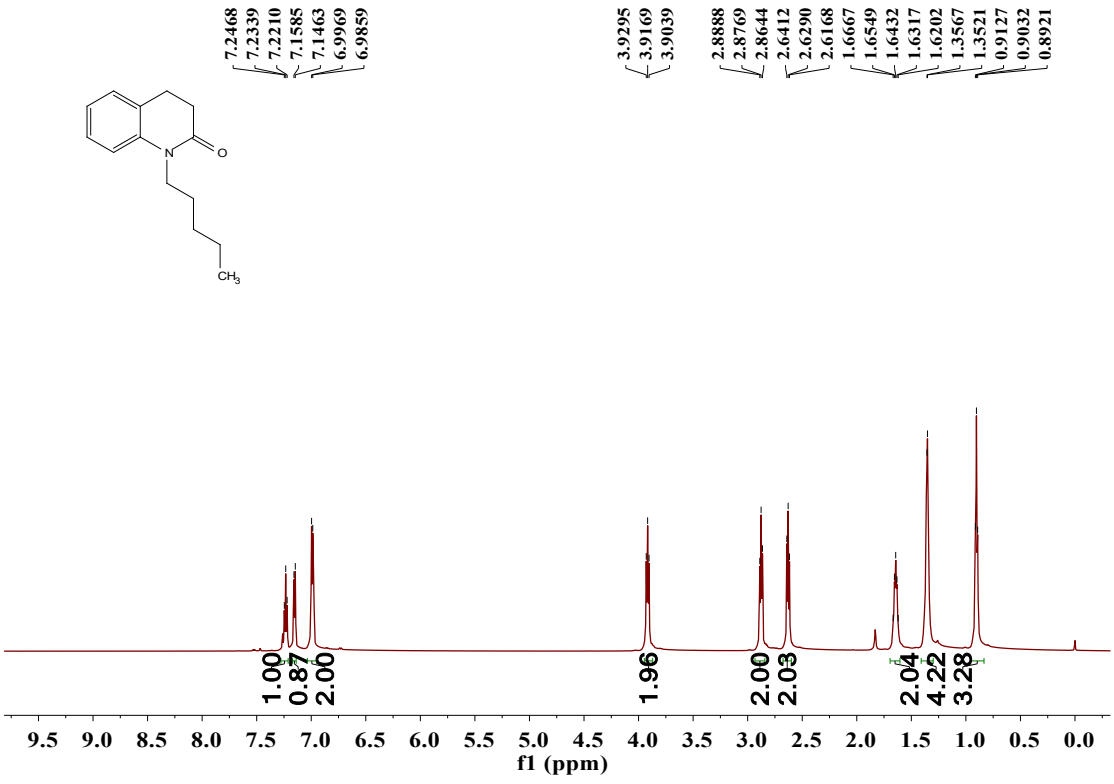
^{1}H-NMR Spectrum ($CDCl_3$) of 2f



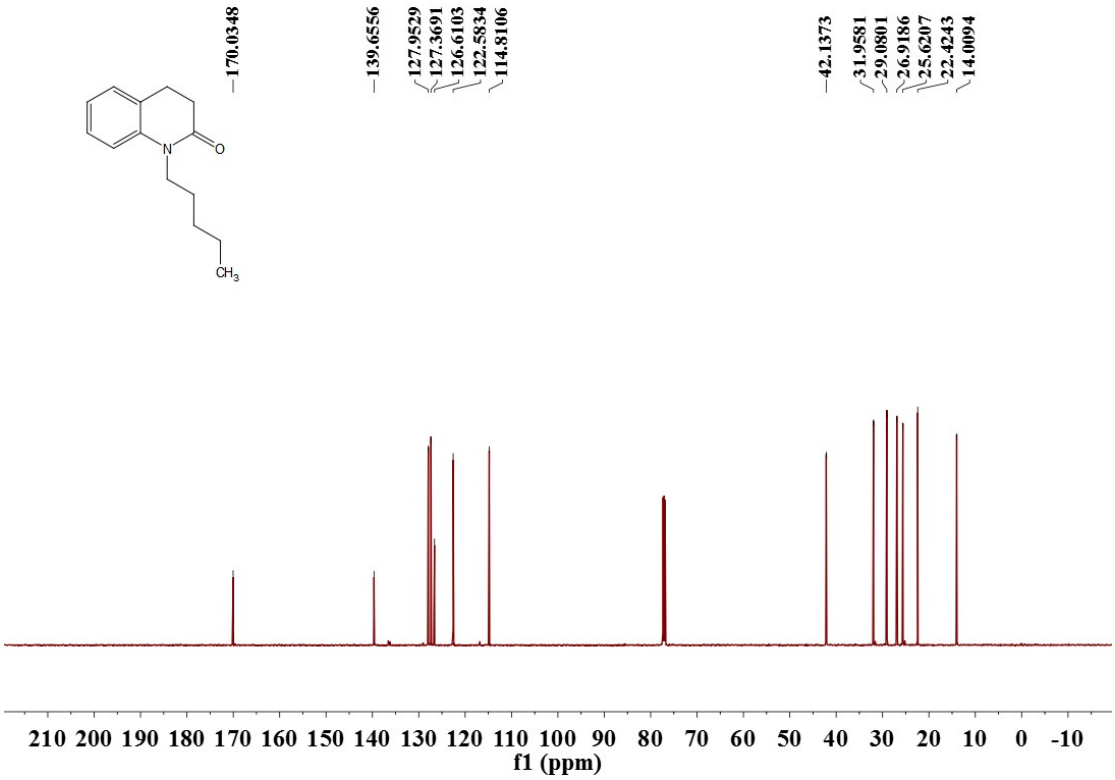
^{13}C-NMR Spectrum ($CDCl_3$) of 2f



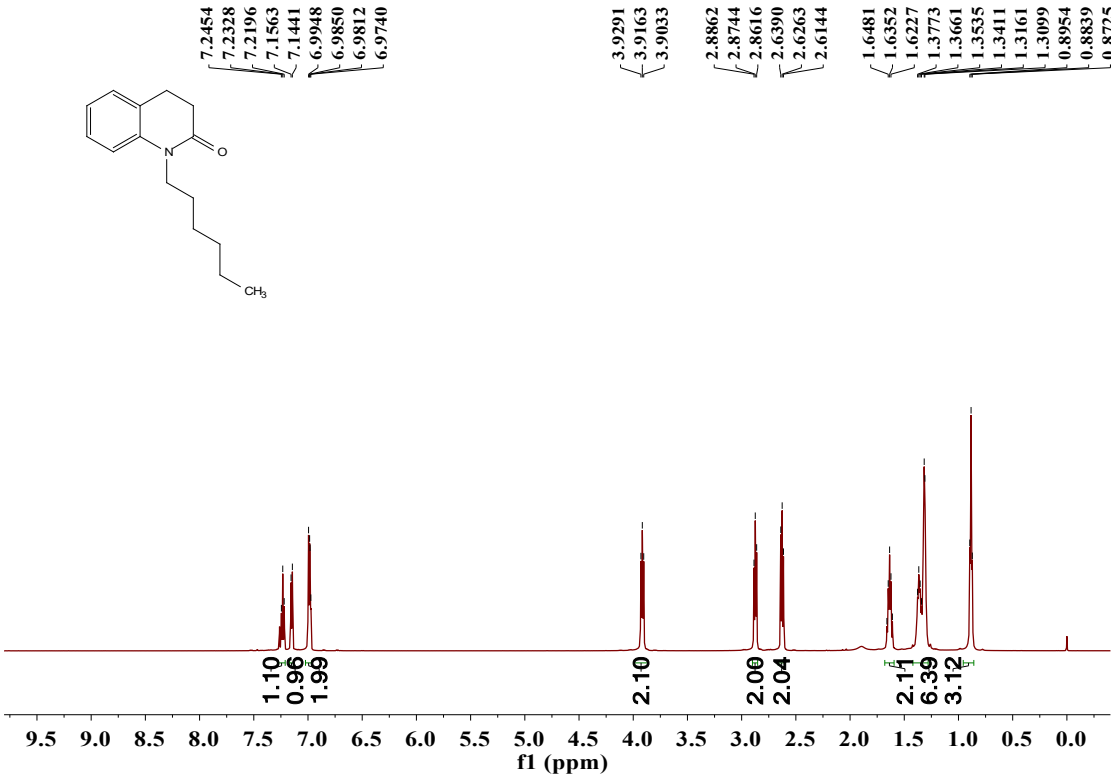
^{1}H-NMR Spectrum ($CDCl_3$) of 2g



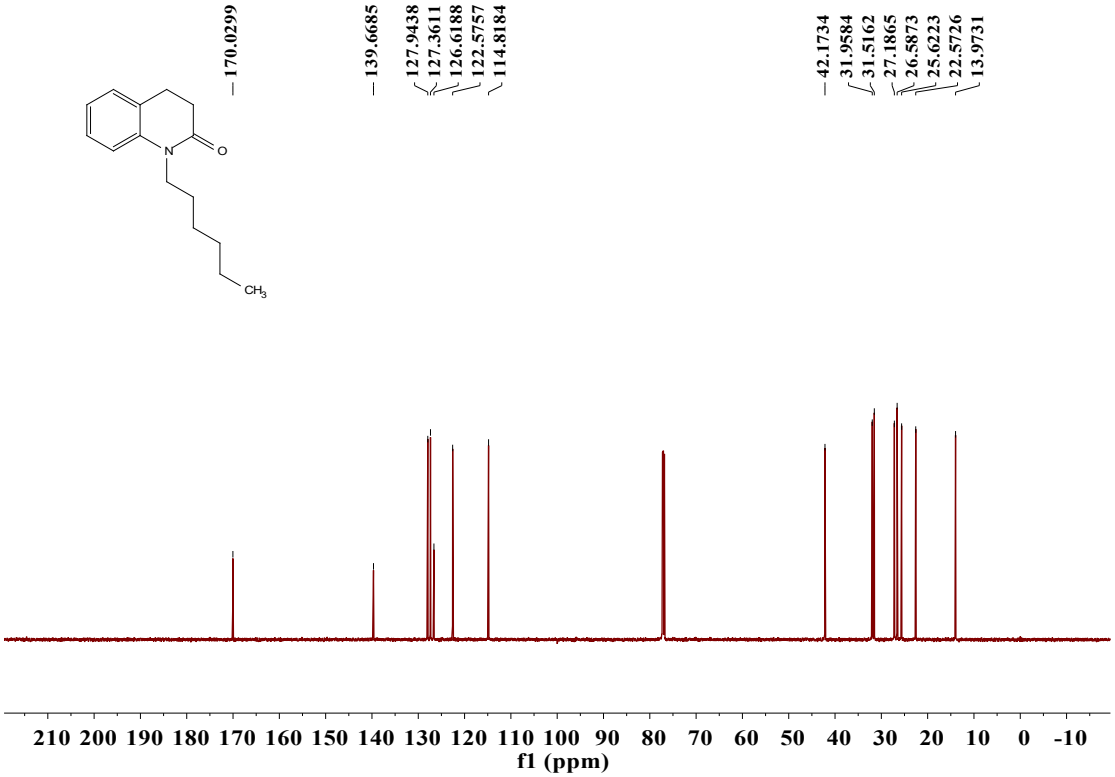
^{13}C-NMR Spectrum ($CDCl_3$) of 2g



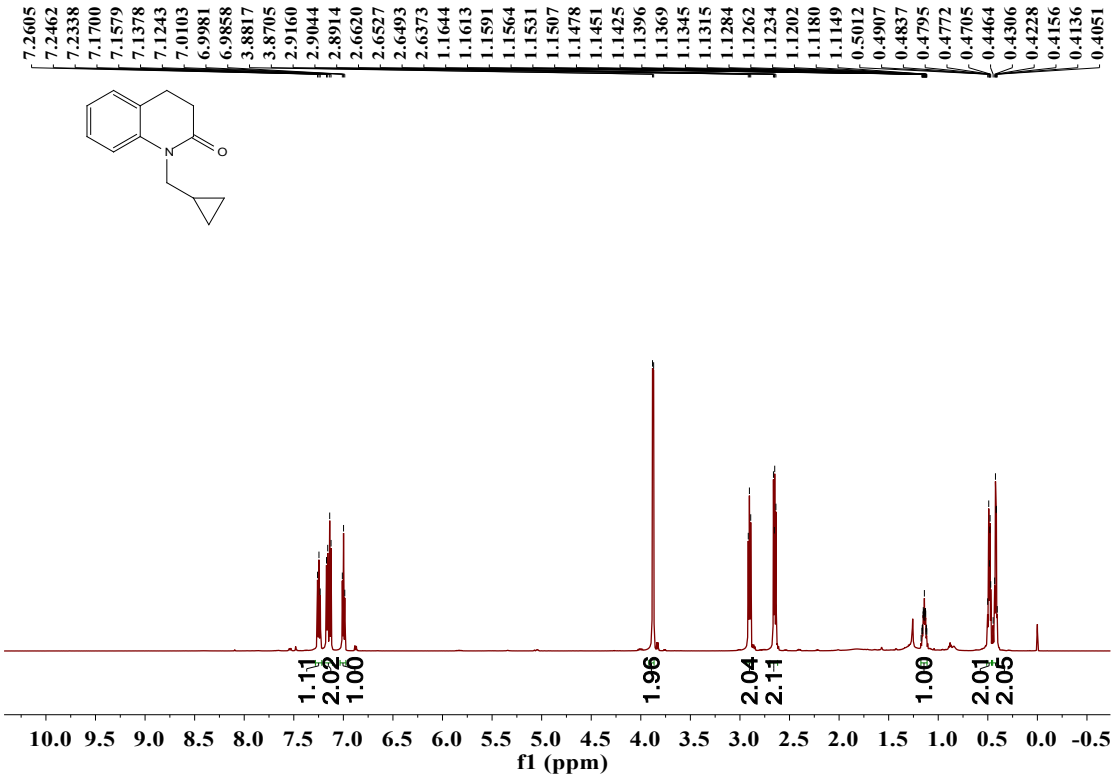
^{1}H-NMR Spectrum ($CDCl_3$) of 2h



^{13}C-NMR Spectrum ($CDCl_3$) of 2h



^{1}H-NMR Spectrum ($CDCl_3$) of 2i



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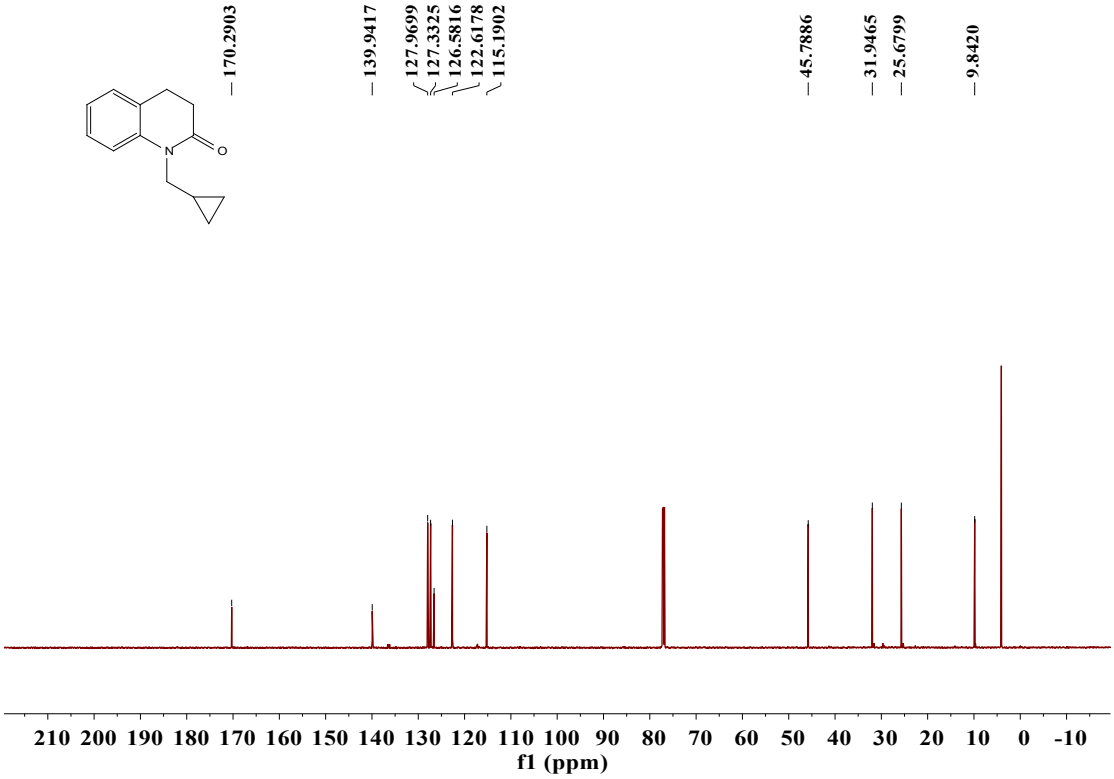

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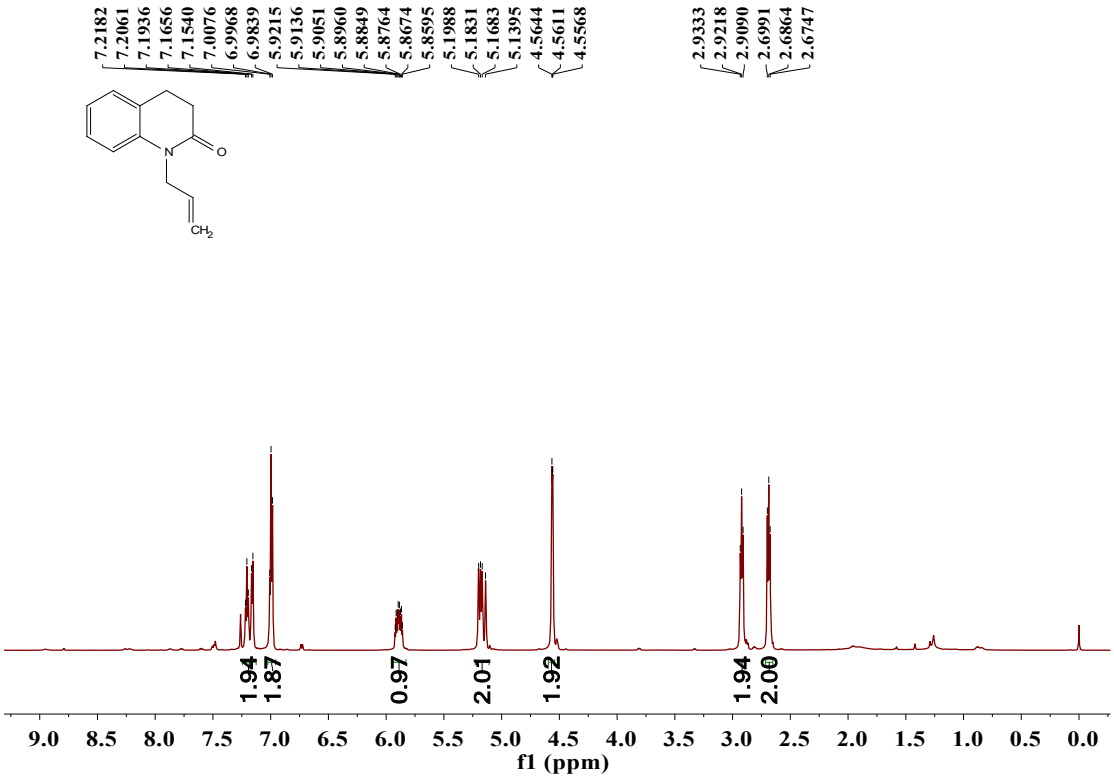

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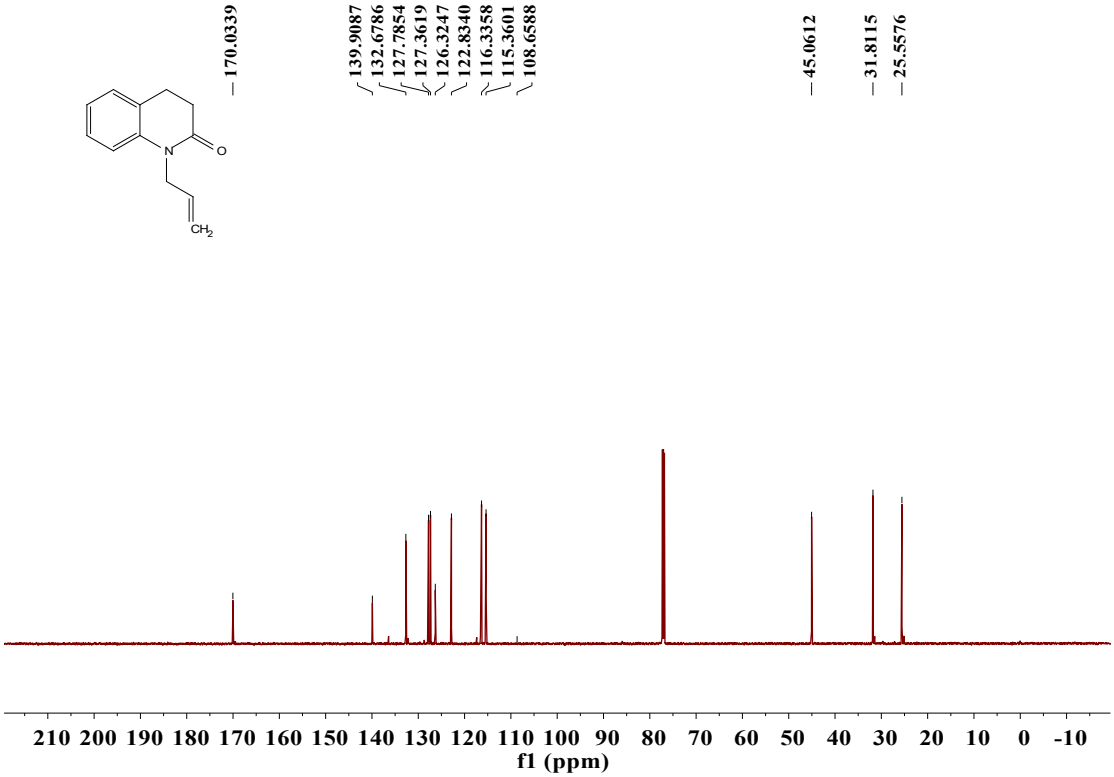

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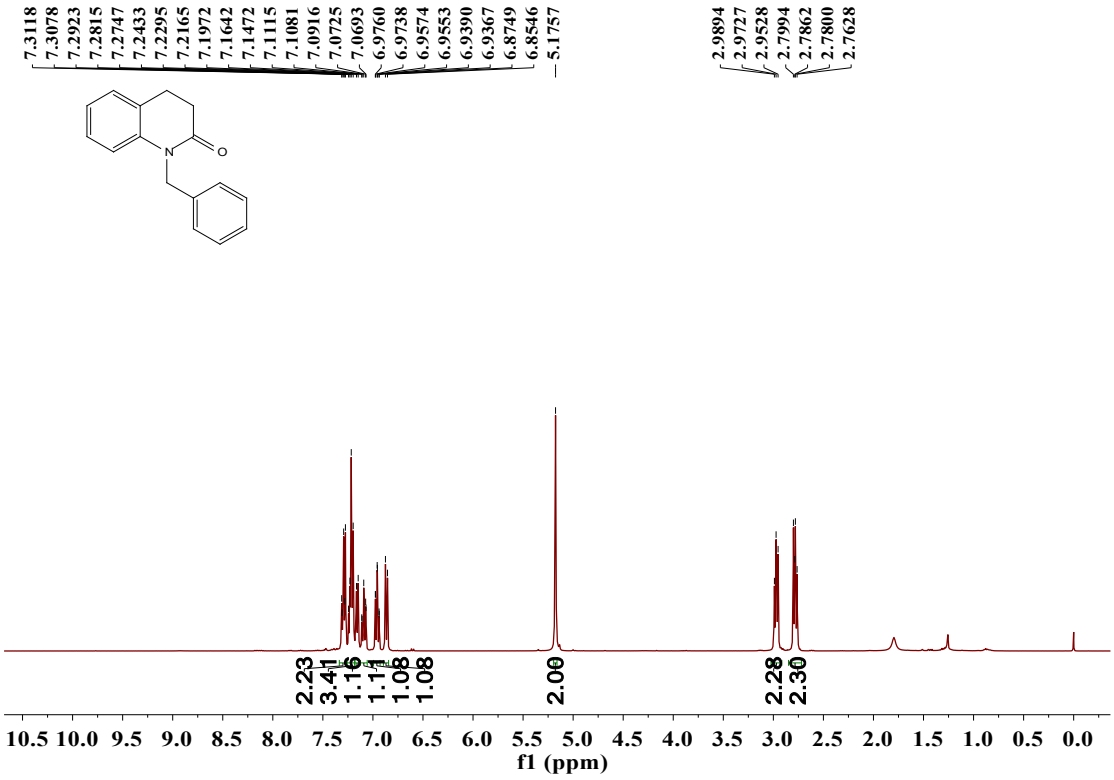

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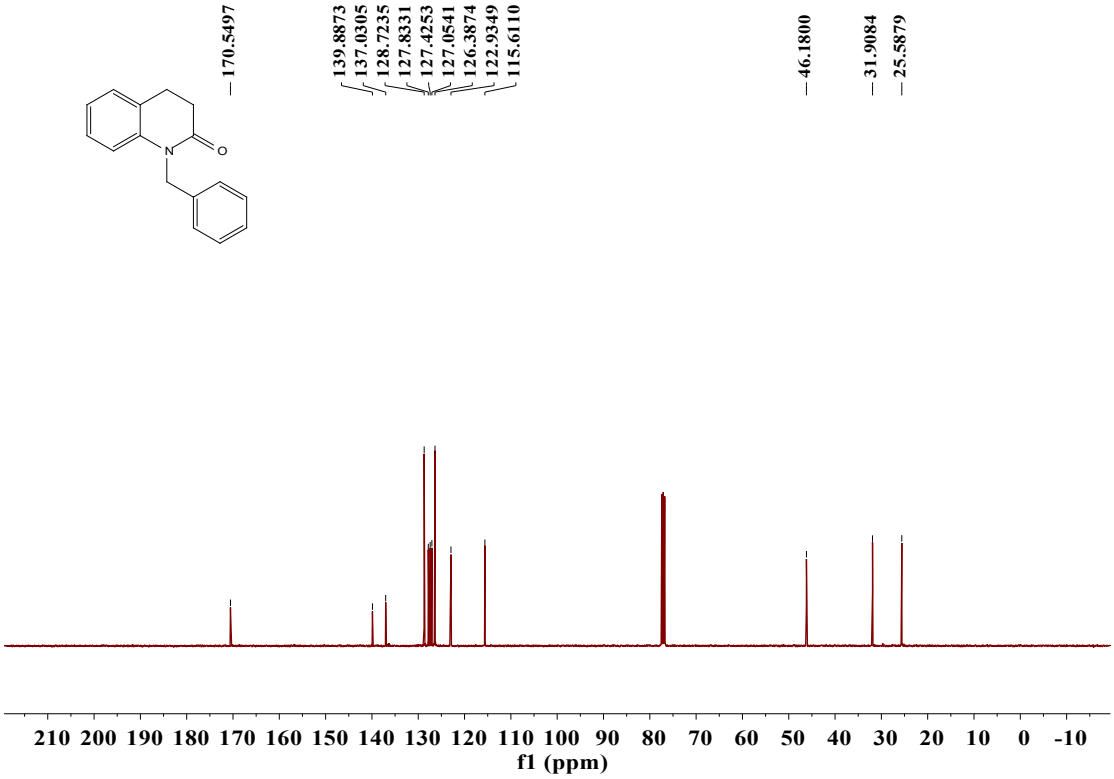
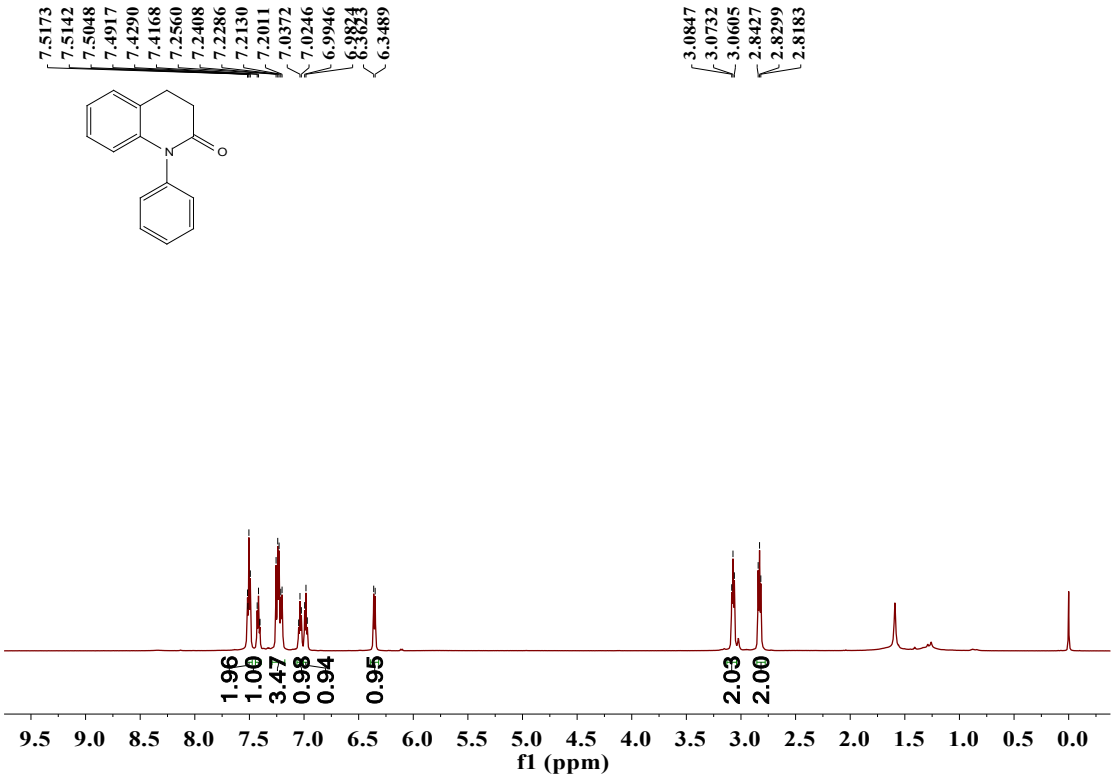
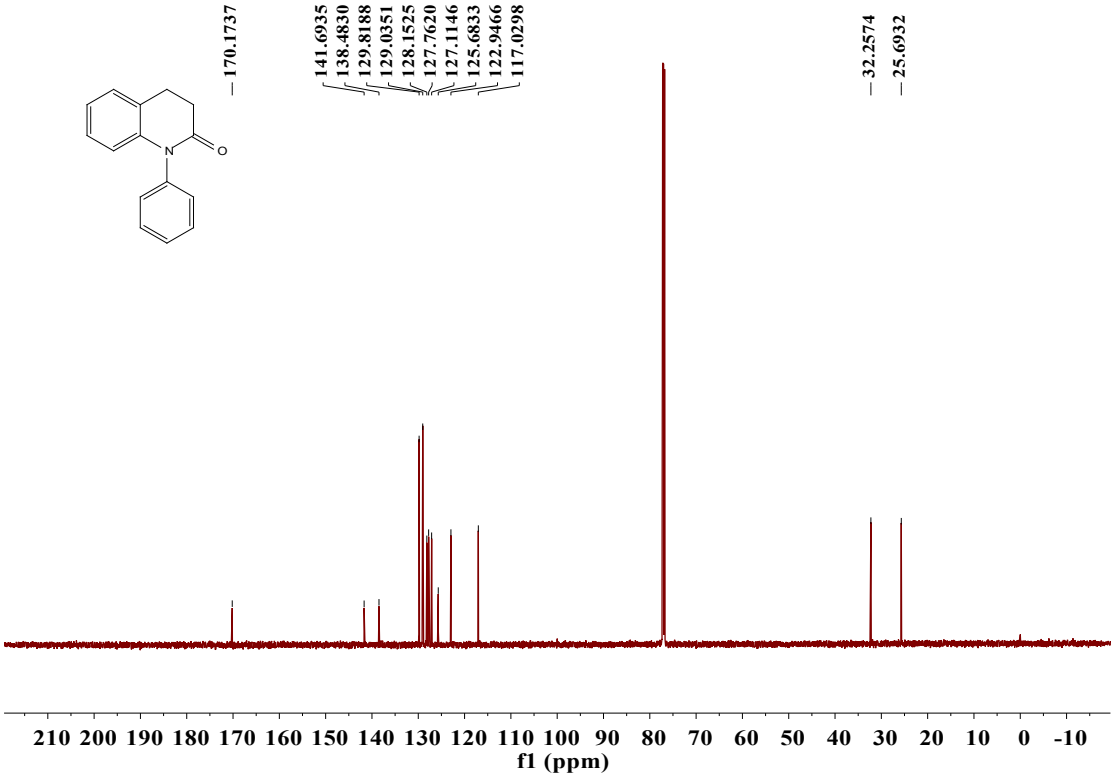


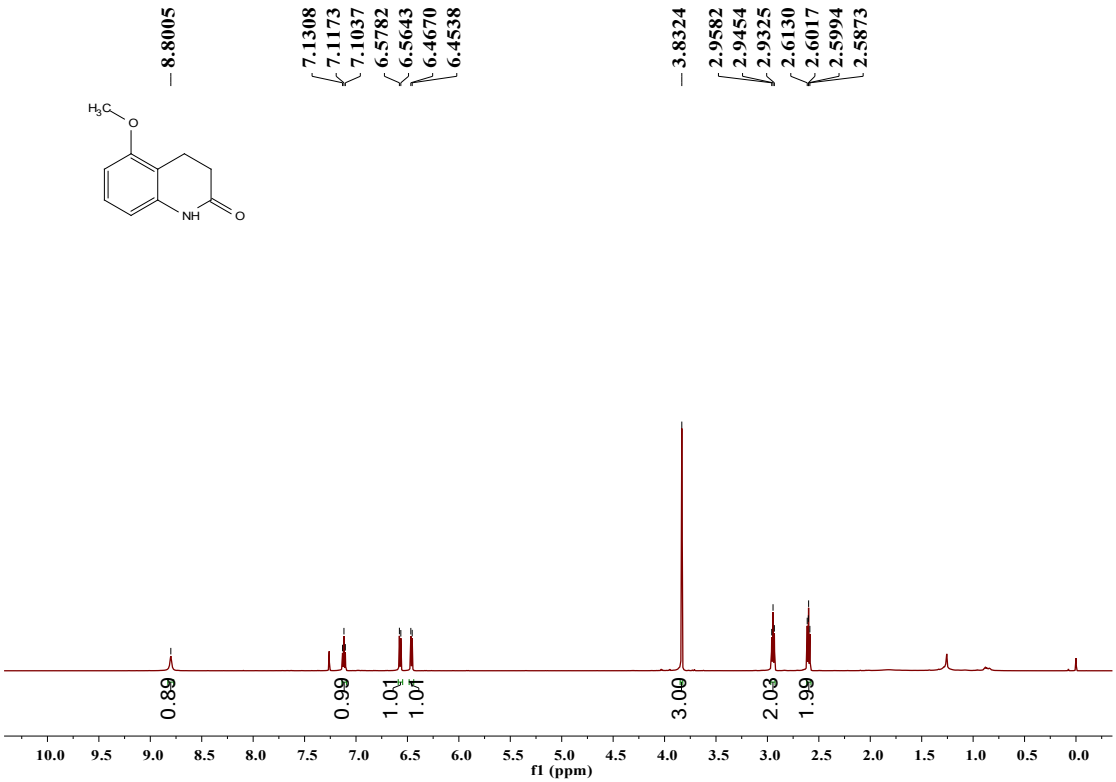
^{1}H-NMR Spectrum ($CDCl_3$) of 2l



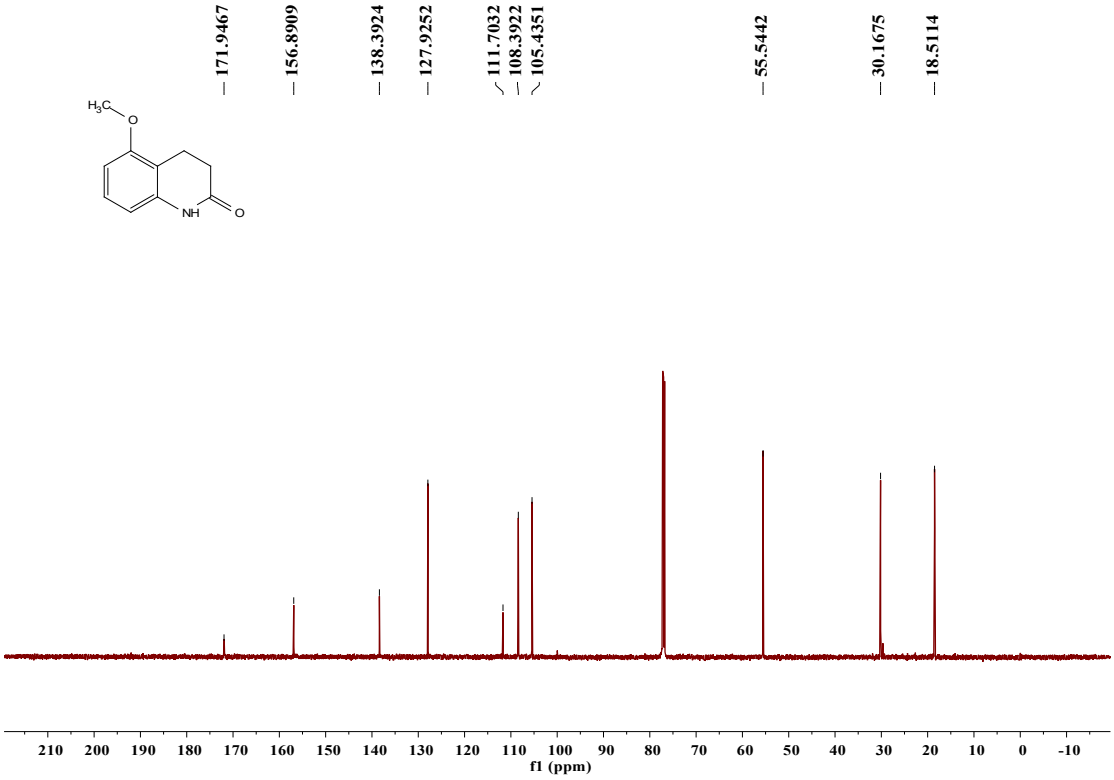
^{13}C-NMR Spectrum ($CDCl_3$) of 2l



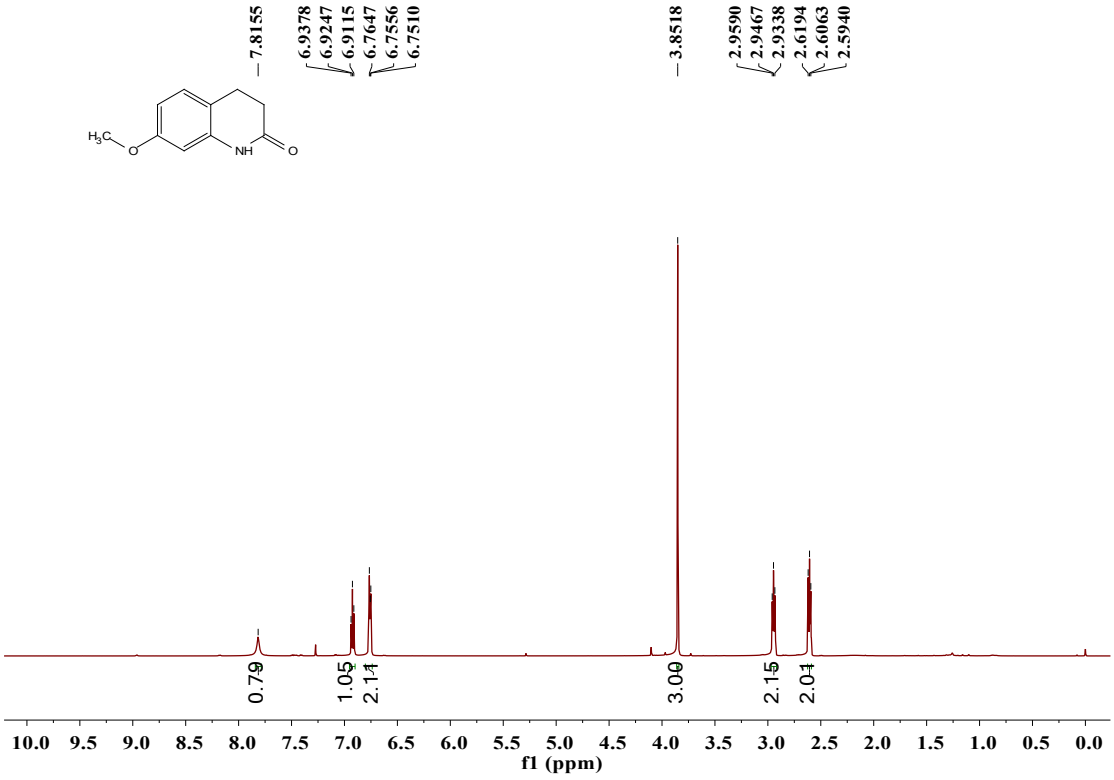
^{1}H-NMR Spectrum ($CDCl_3$) of 2m



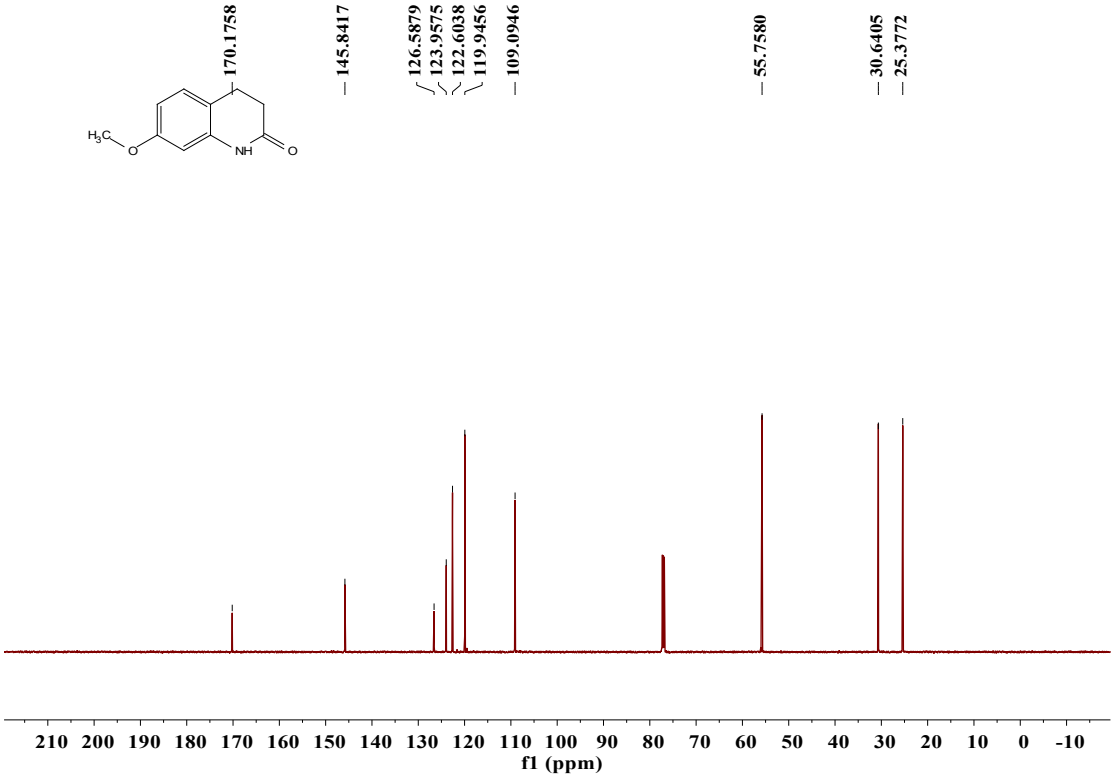
^{13}C-NMR Spectrum ($CDCl_3$) of 2m



^{1}H-NMR Spectrum ($CDCl_3$) of 2n



^{13}C-NMR Spectrum ($CDCl_3$) of 2n



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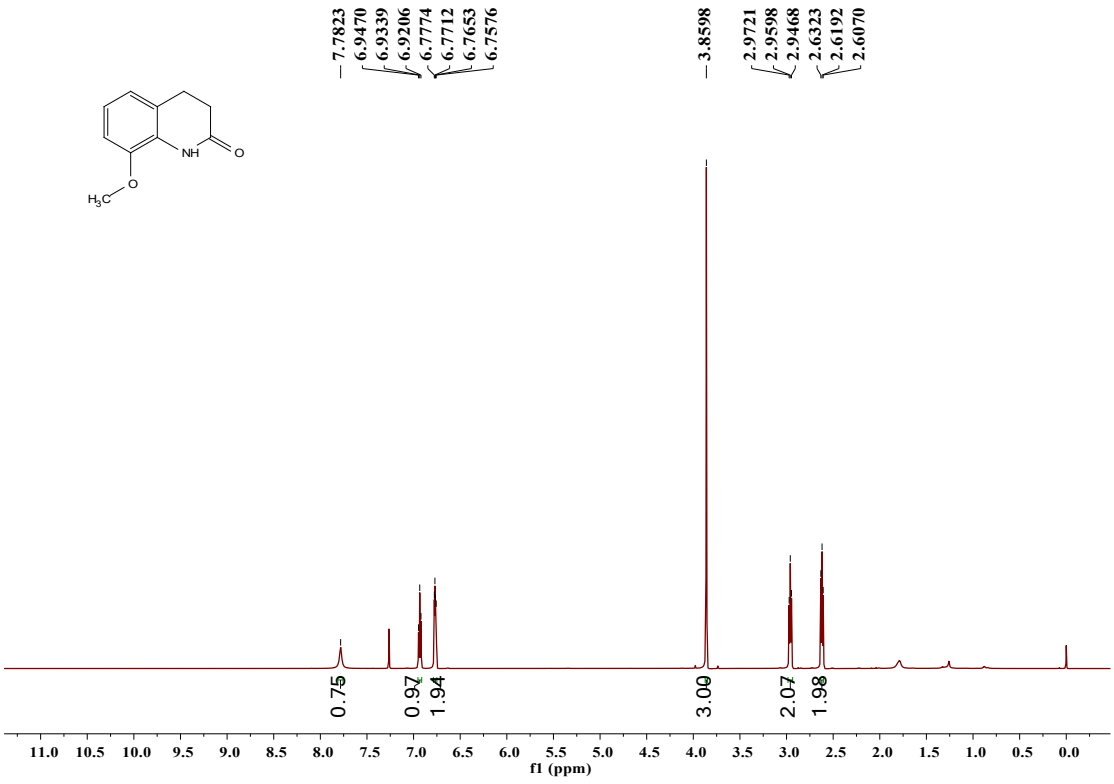
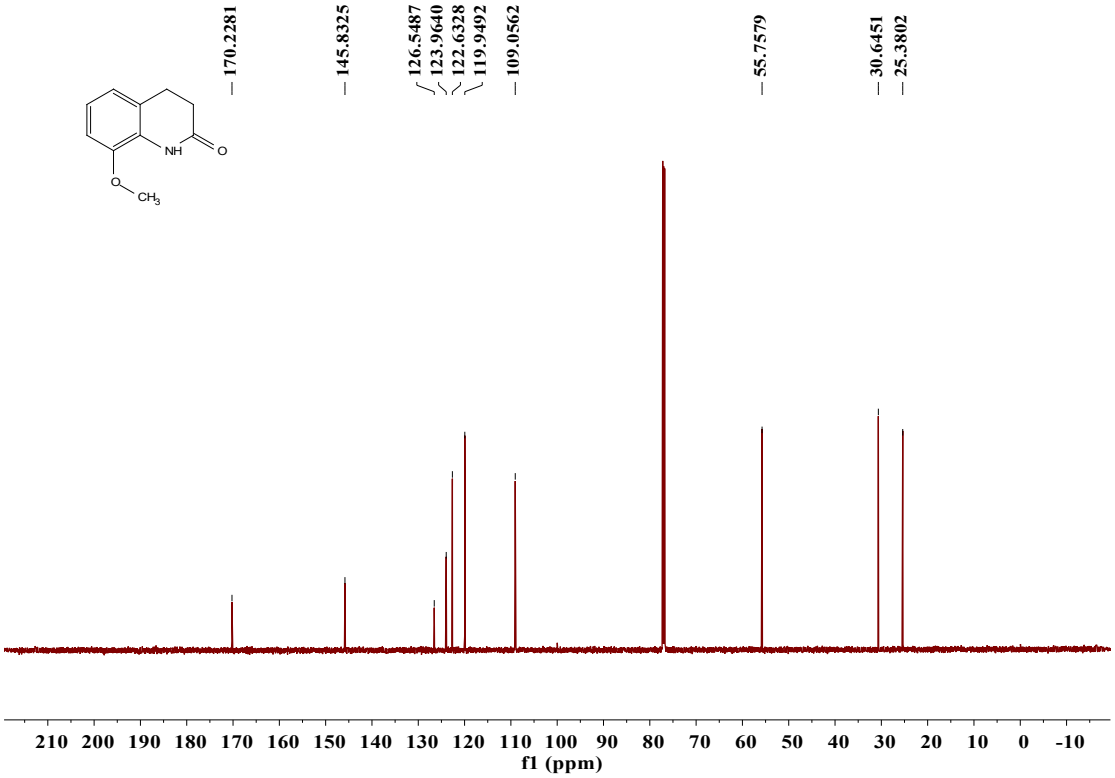
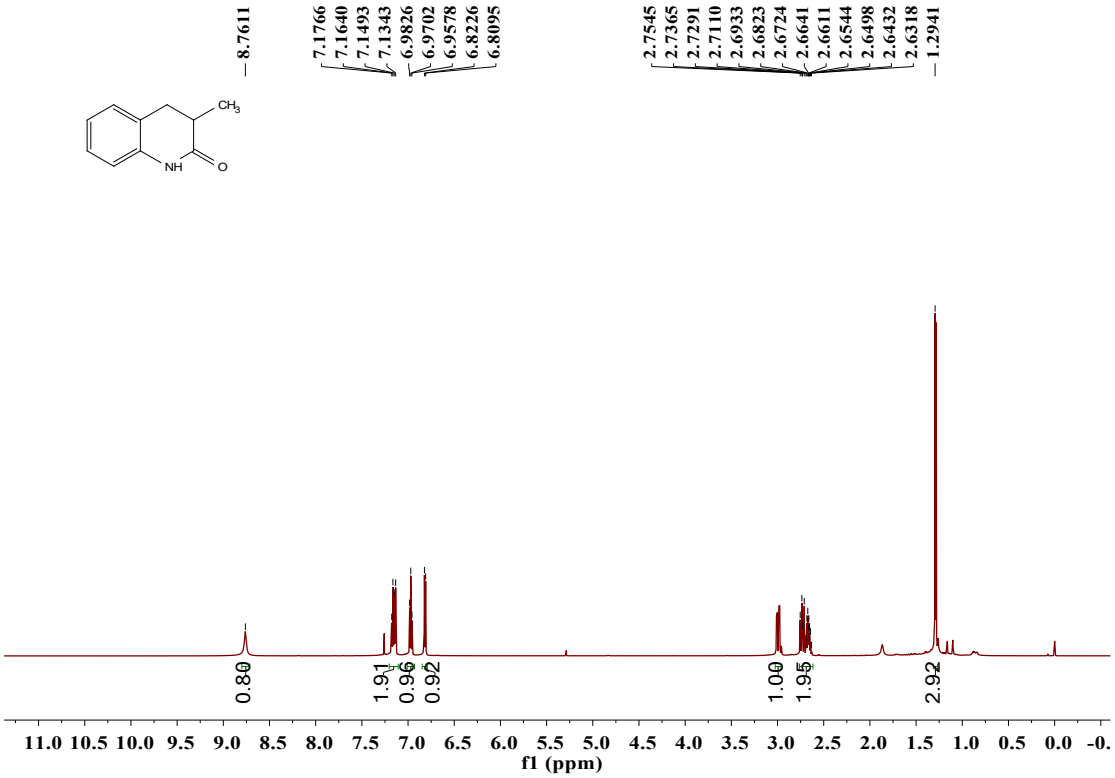


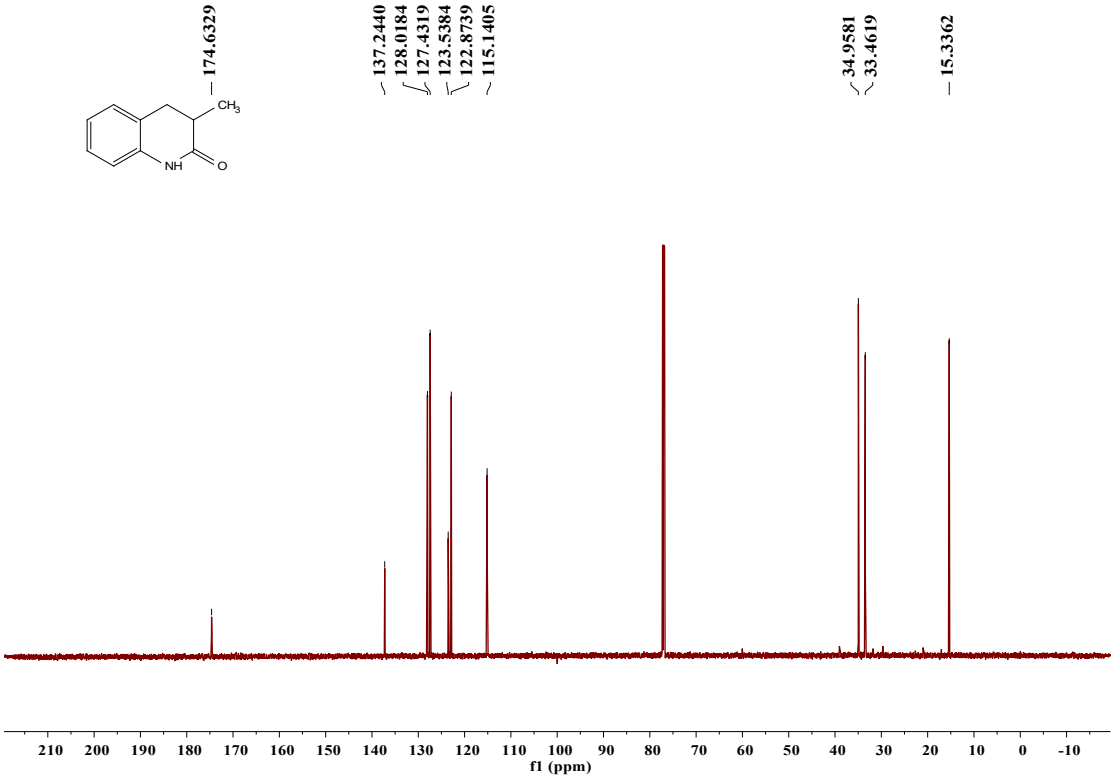
^{13}C-NMR Spectrum ($CDCl_3$) of 2o



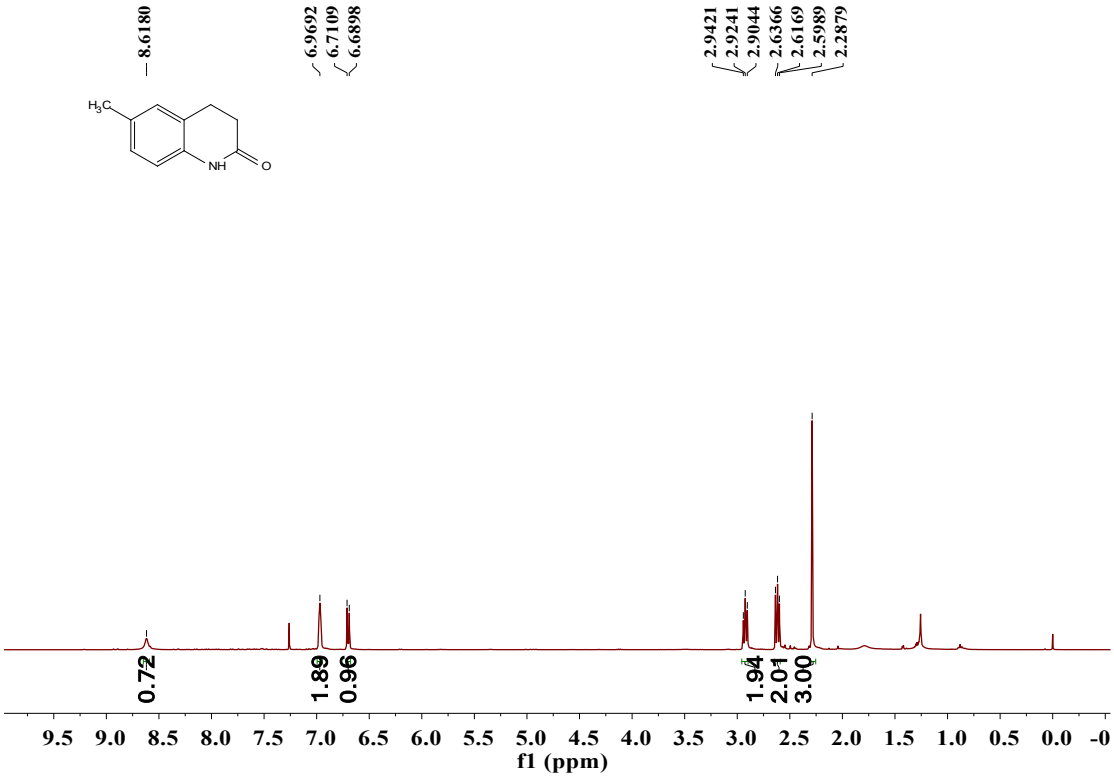
^{1}H-NMR Spectrum ($CDCl_3$) of 2p



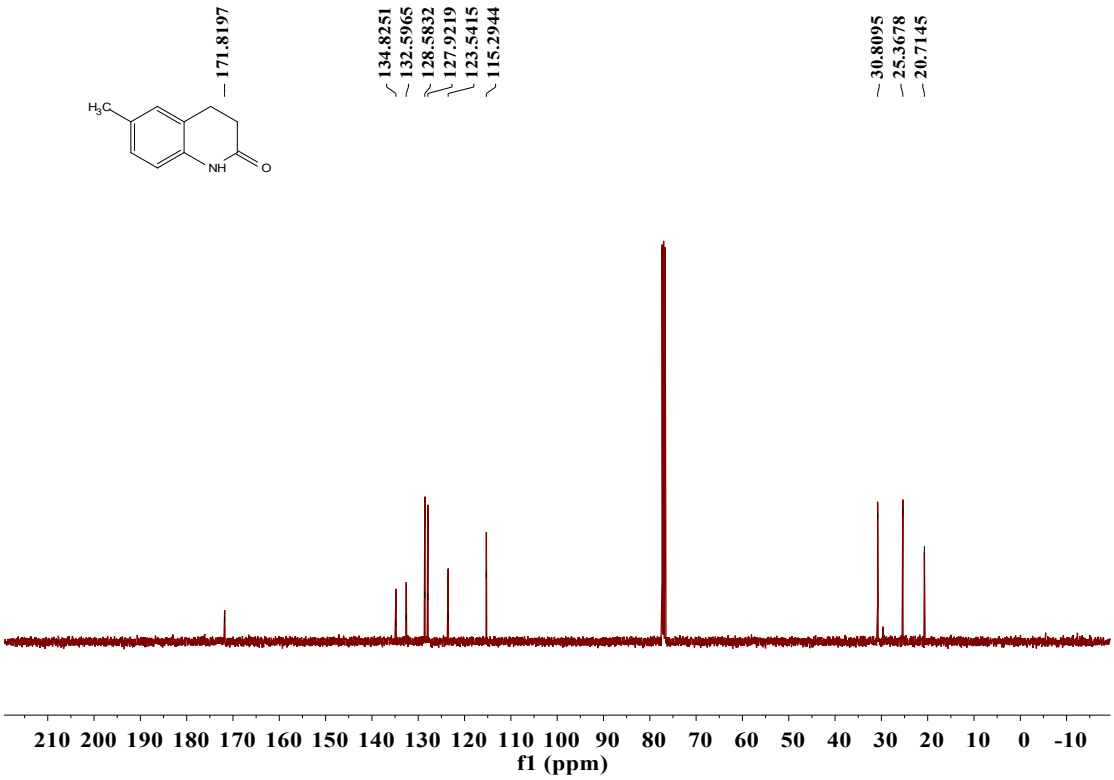
^{13}C-NMR Spectrum ($CDCl_3$) of 2p



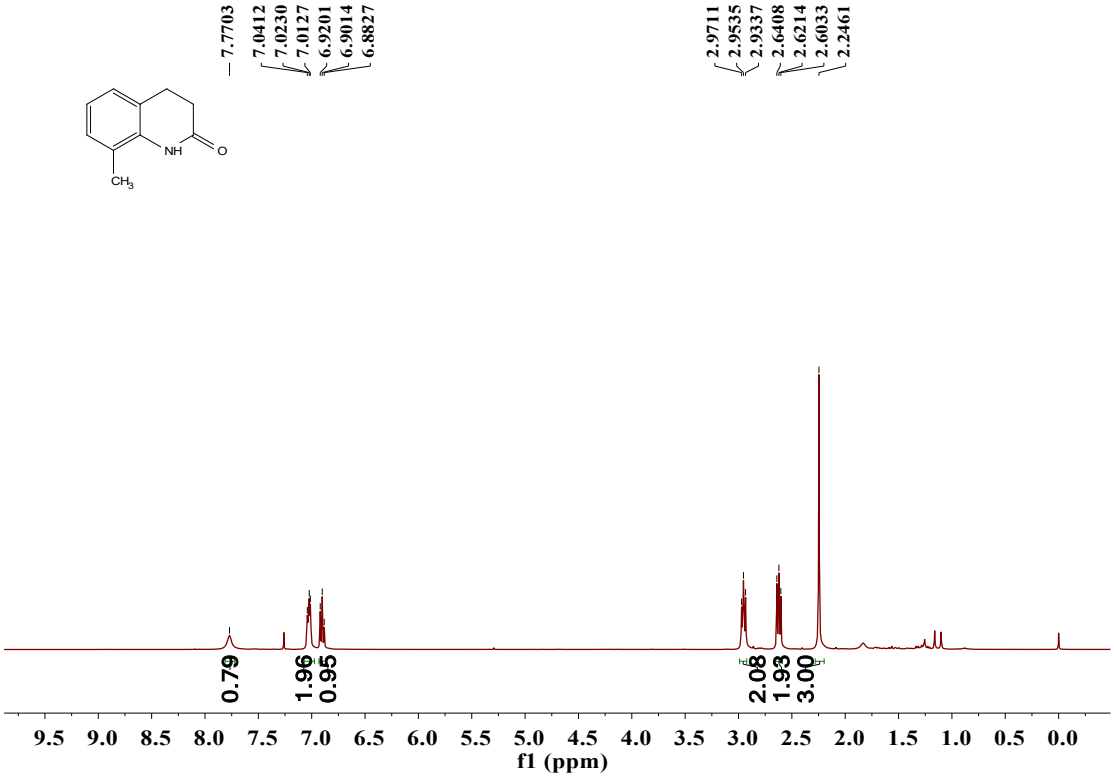
^{1}H-NMR Spectrum ($CDCl_3$) of 2q



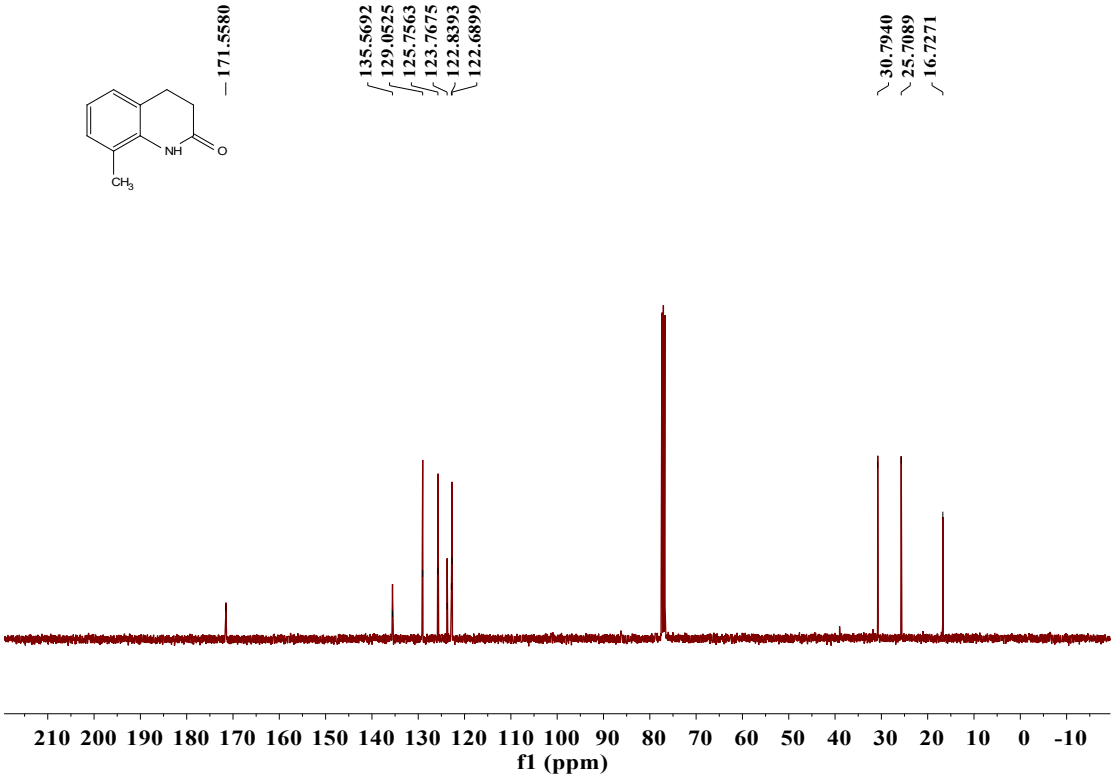
^{13}C-NMR Spectrum ($CDCl_3$) of 2q



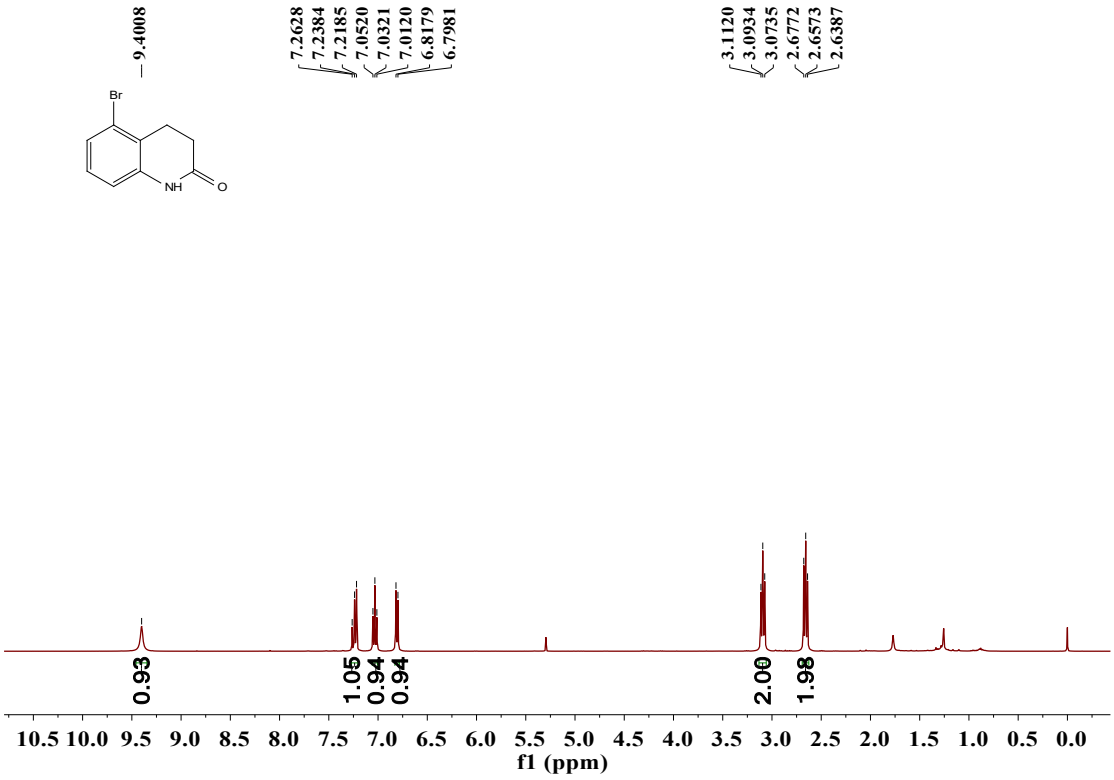
^{1}H-NMR Spectrum ($CDCl_3$) of 2r



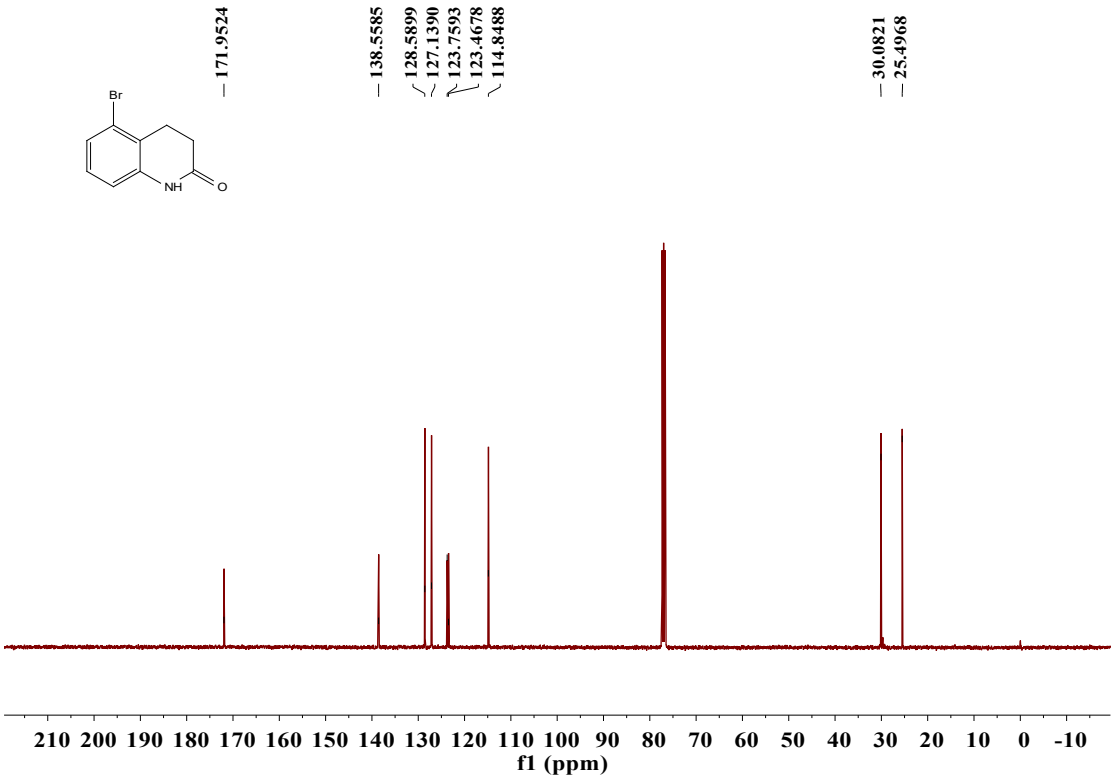
^{13}C-NMR Spectrum ($CDCl_3$) of 2r



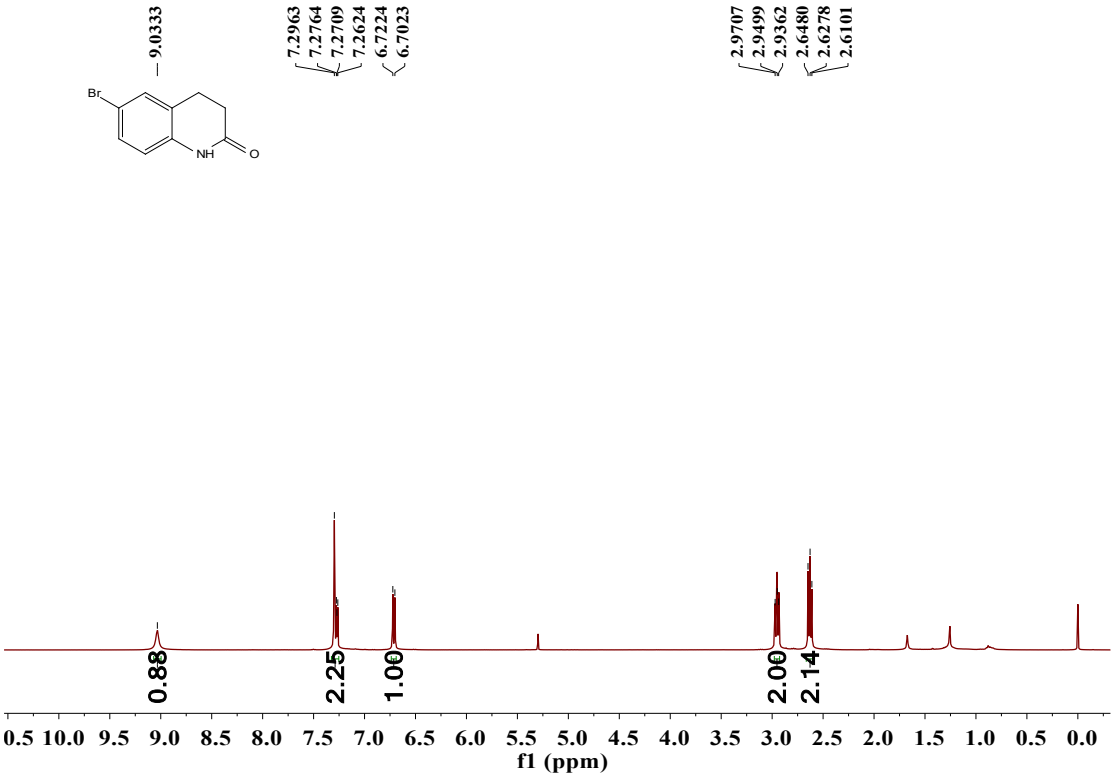
^{1}H-NMR Spectrum ($CDCl_3$) of 2s



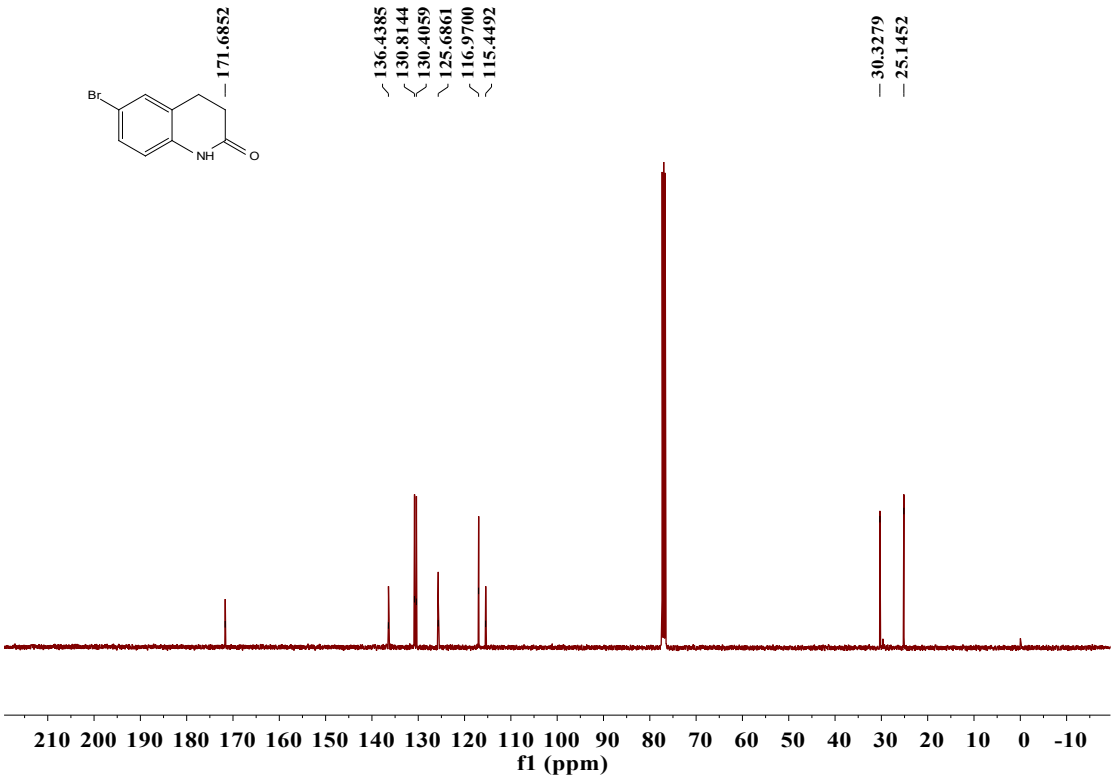
^{13}C-NMR Spectrum ($CDCl_3$) of 2s



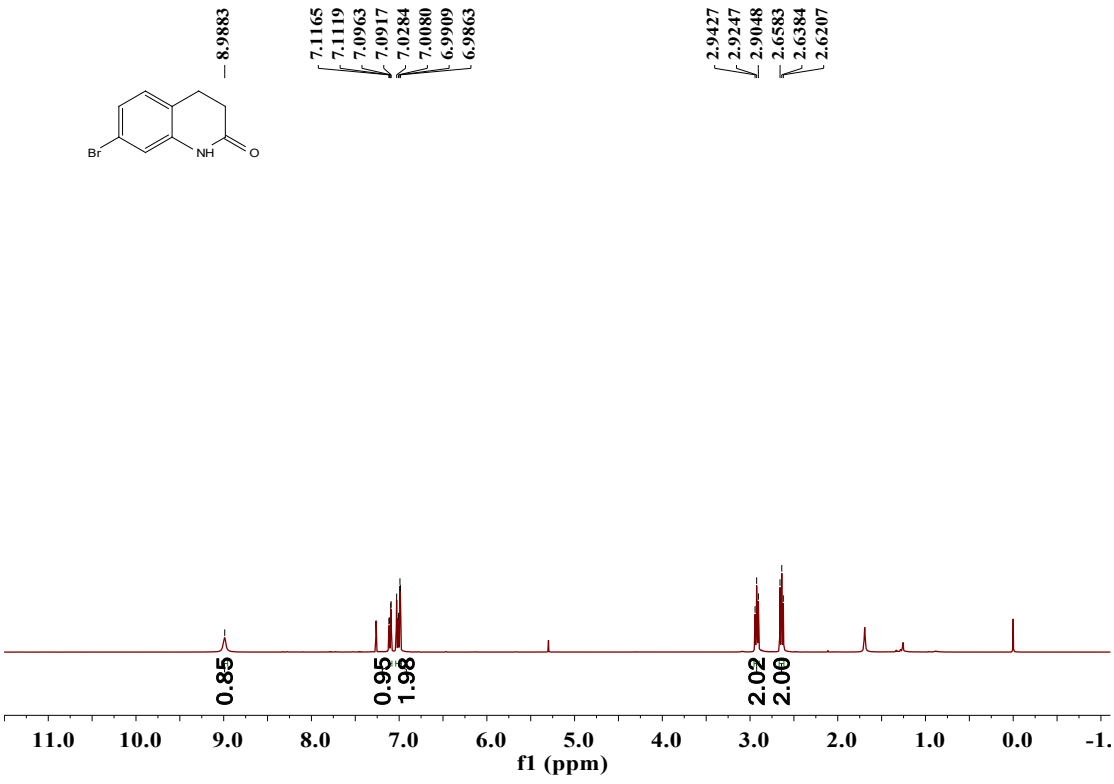
^{1}H-NMR Spectrum ($CDCl_3$) of 2t



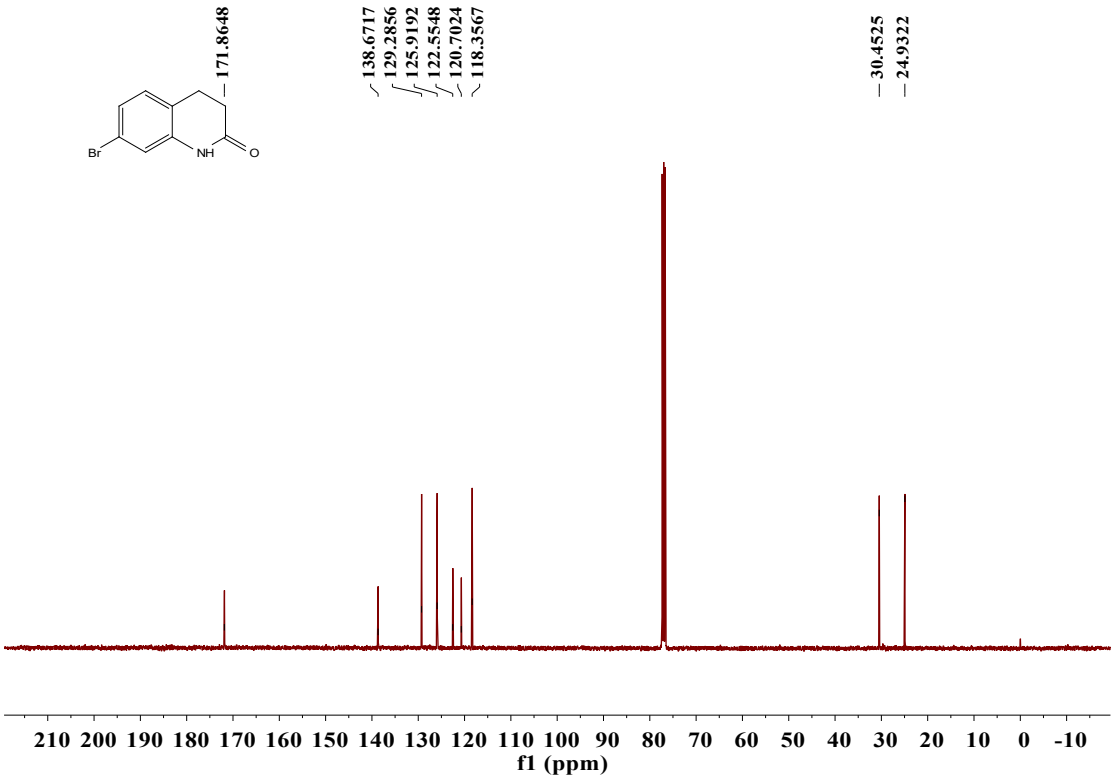
^{13}C-NMR Spectrum ($CDCl_3$) of 2t



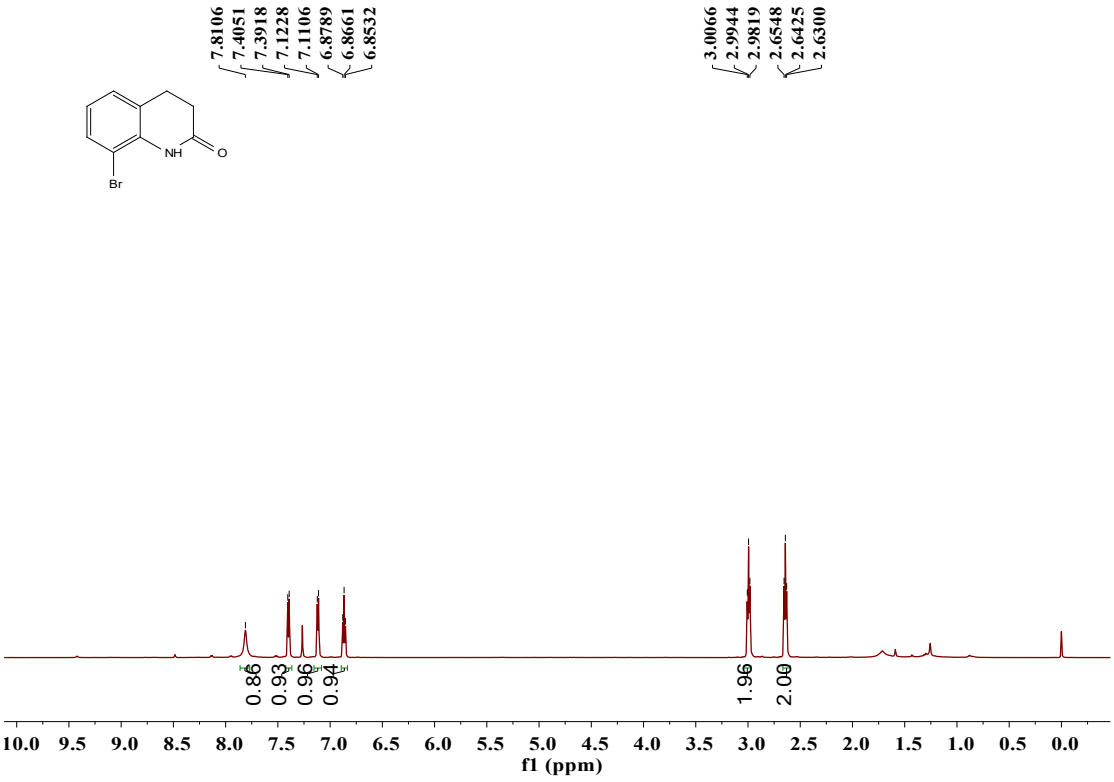
^{1}H-NMR Spectrum ($CDCl_3$) of 2u



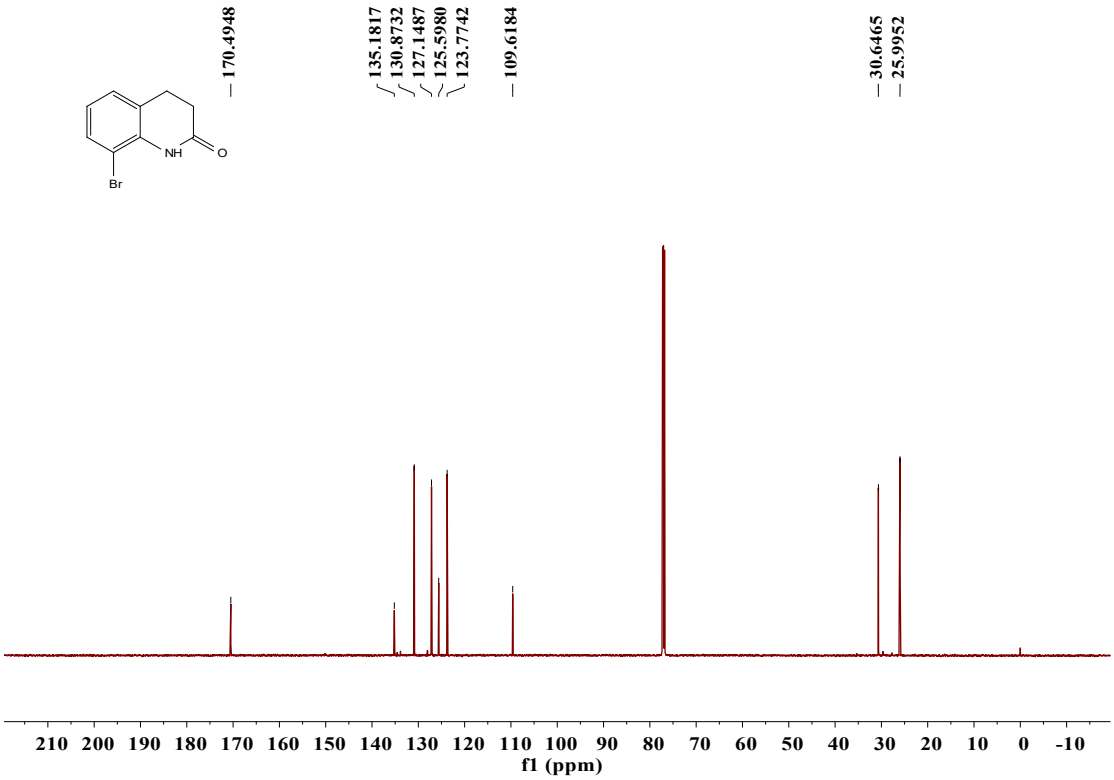
^{13}C-NMR Spectrum ($CDCl_3$) of 2u



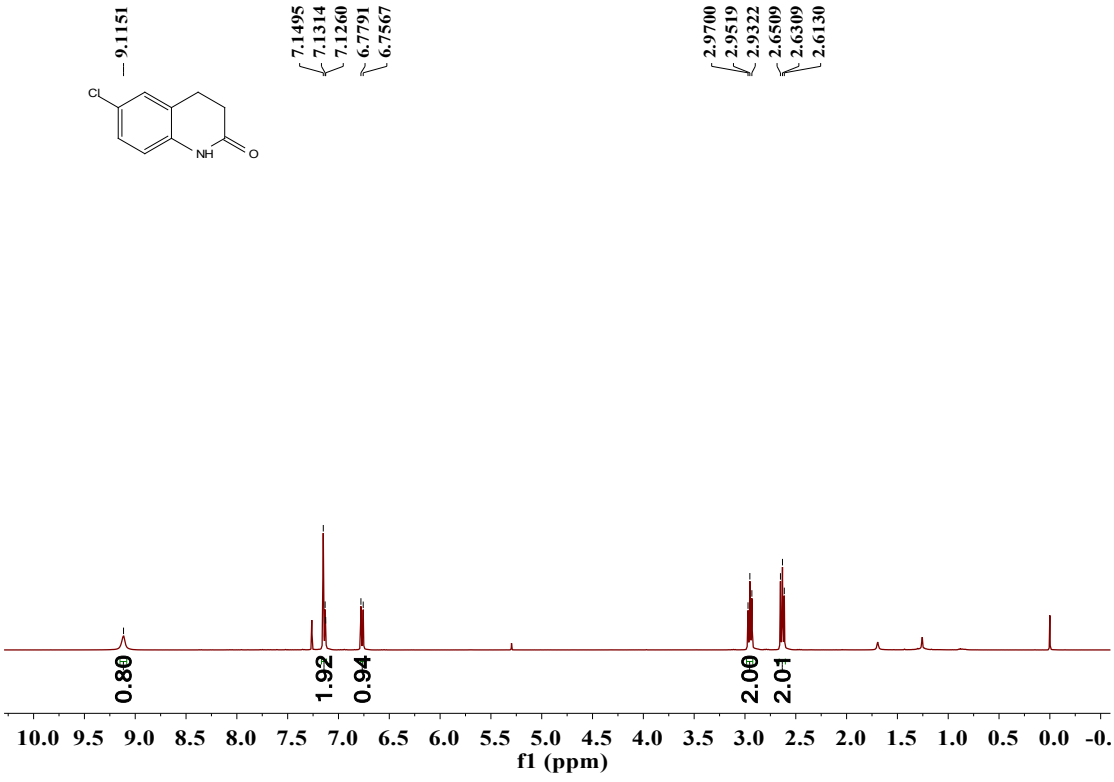
^{1}H-NMR Spectrum ($CDCl_3$) of 2v



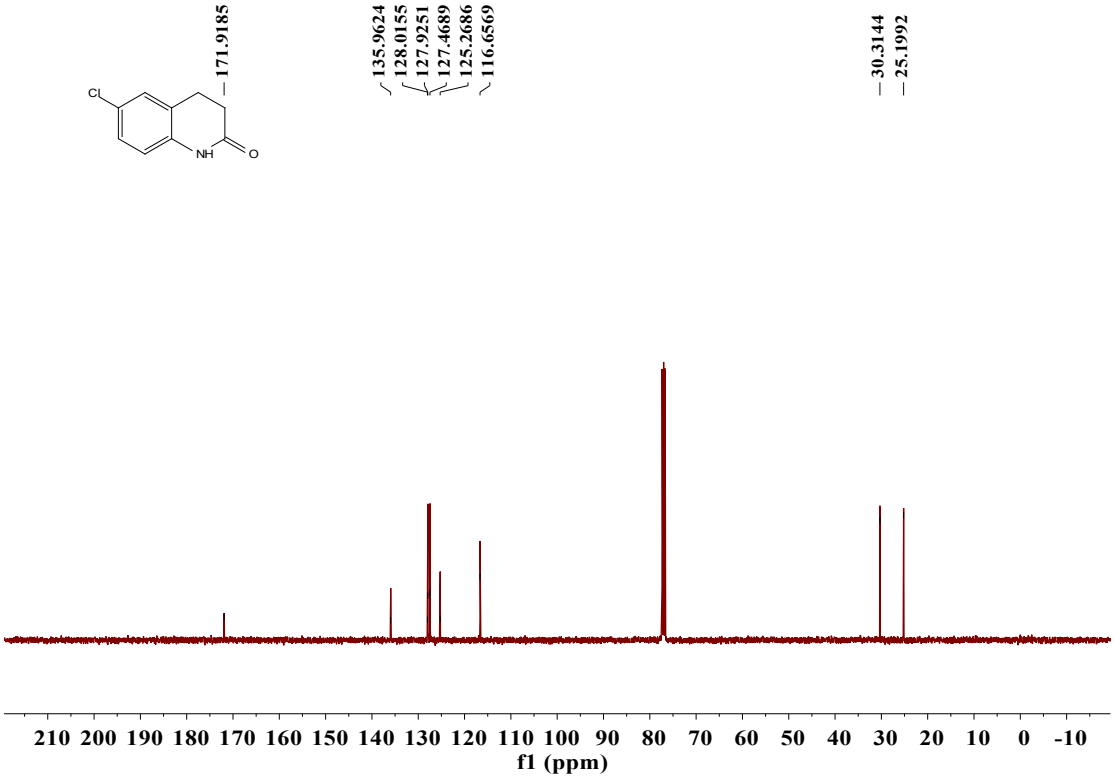
^{13}C-NMR Spectrum ($CDCl_3$) of 2v



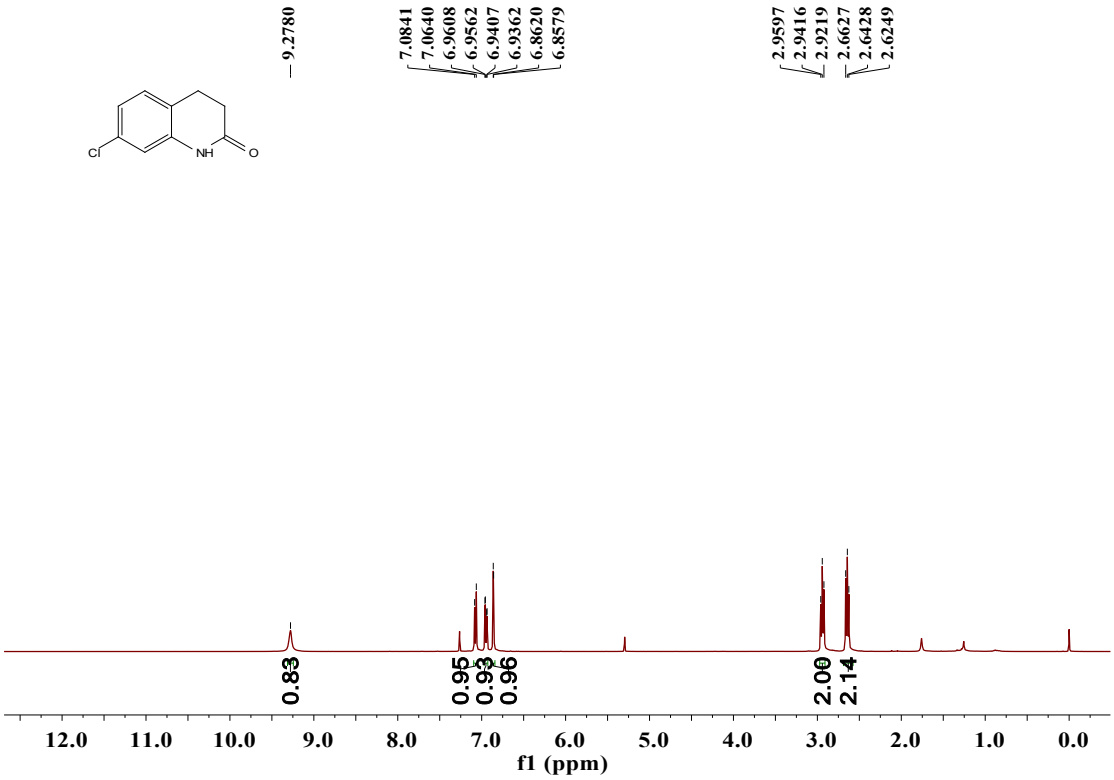
^{1}H-NMR Spectrum ($CDCl_3$) of 2w



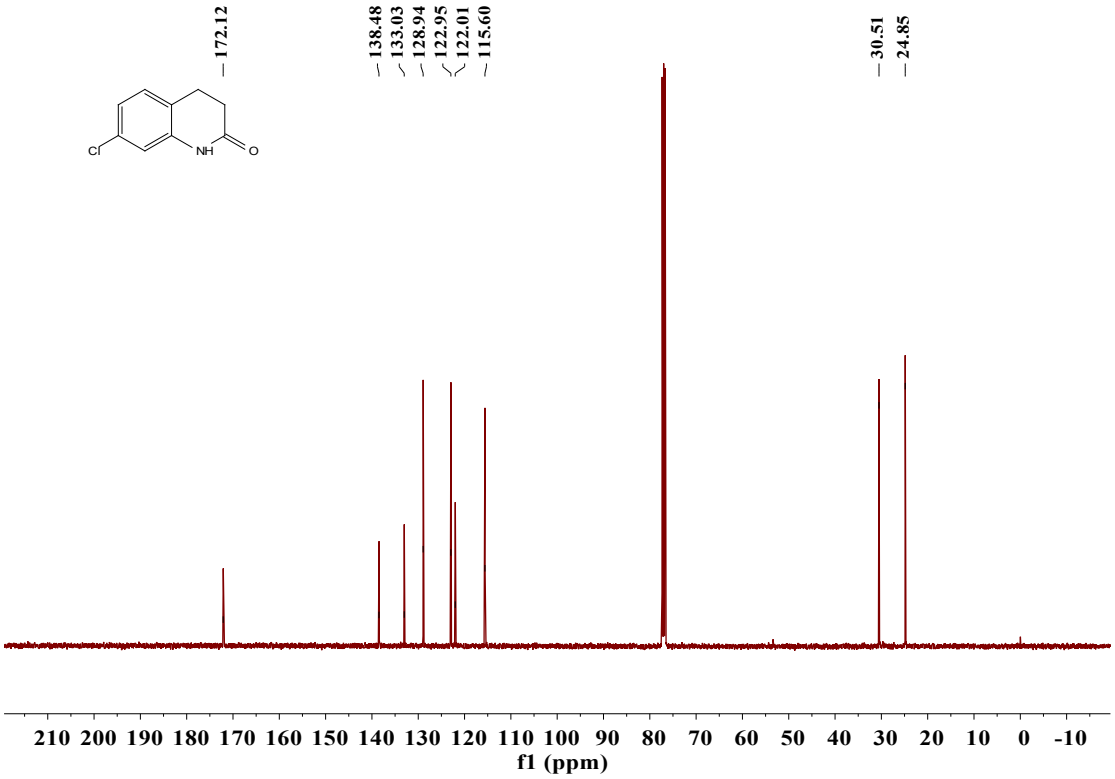
^{13}C-NMR Spectrum ($CDCl_3$) of 2w



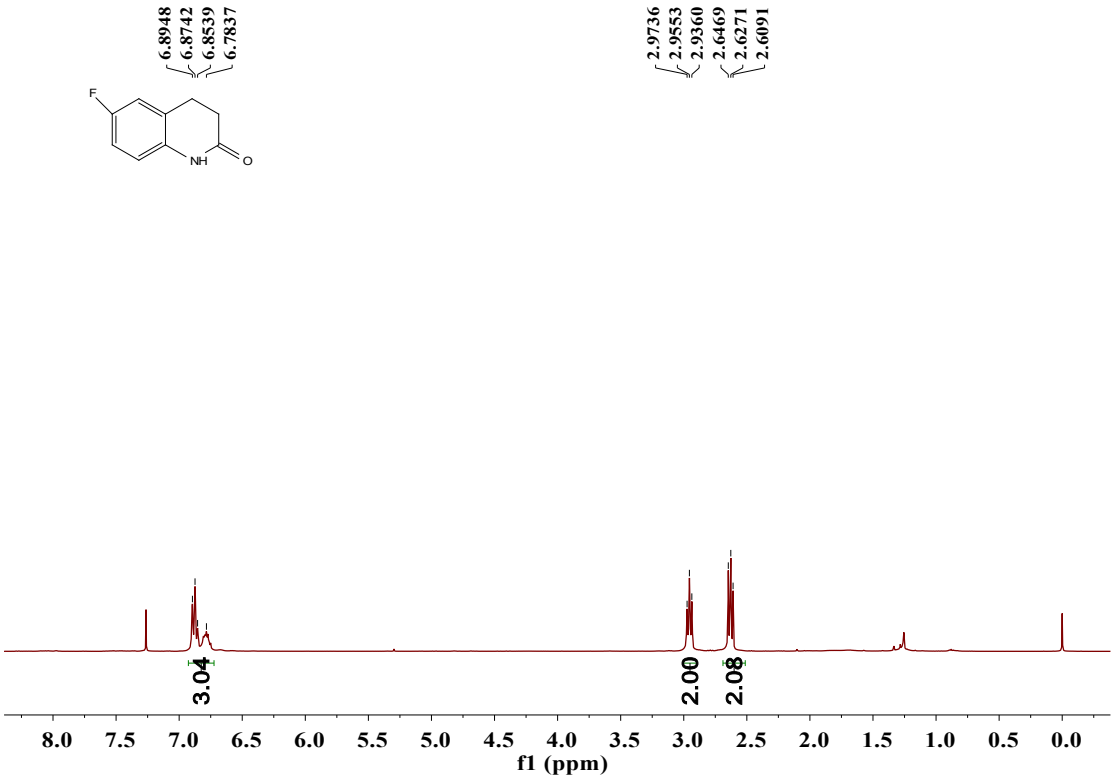
^{1}H-NMR Spectrum ($CDCl_3$) of 2x



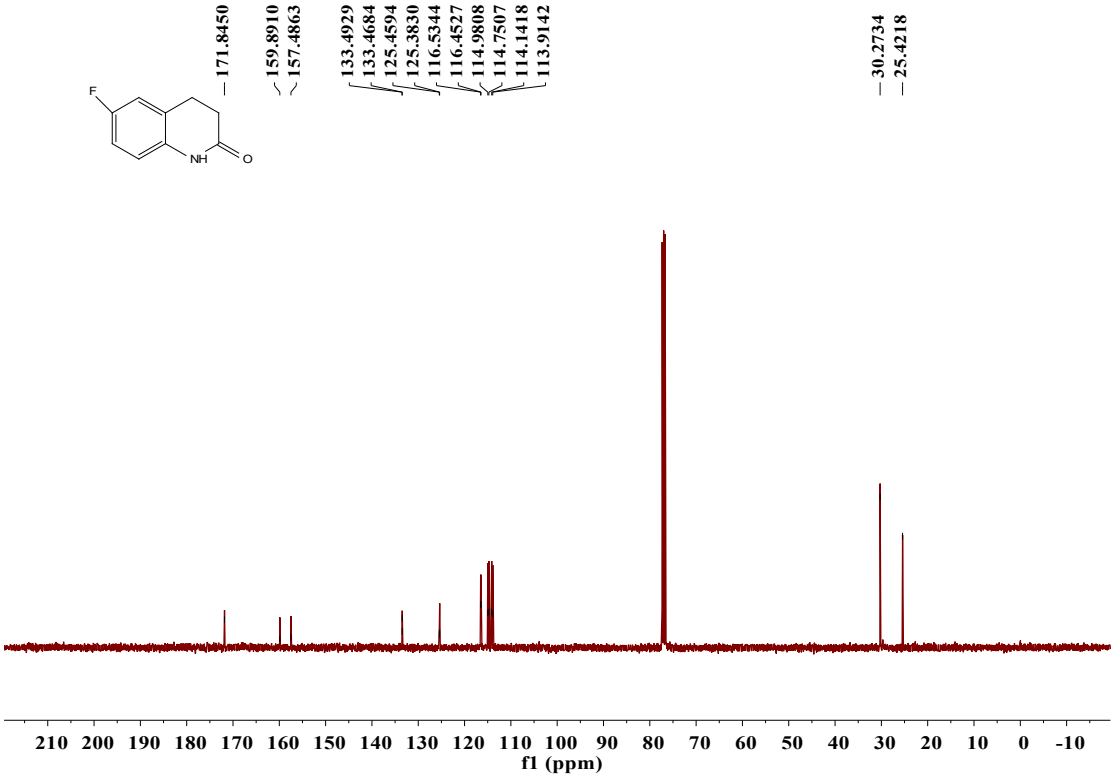
^{13}C-NMR Spectrum ($CDCl_3$) of 2x



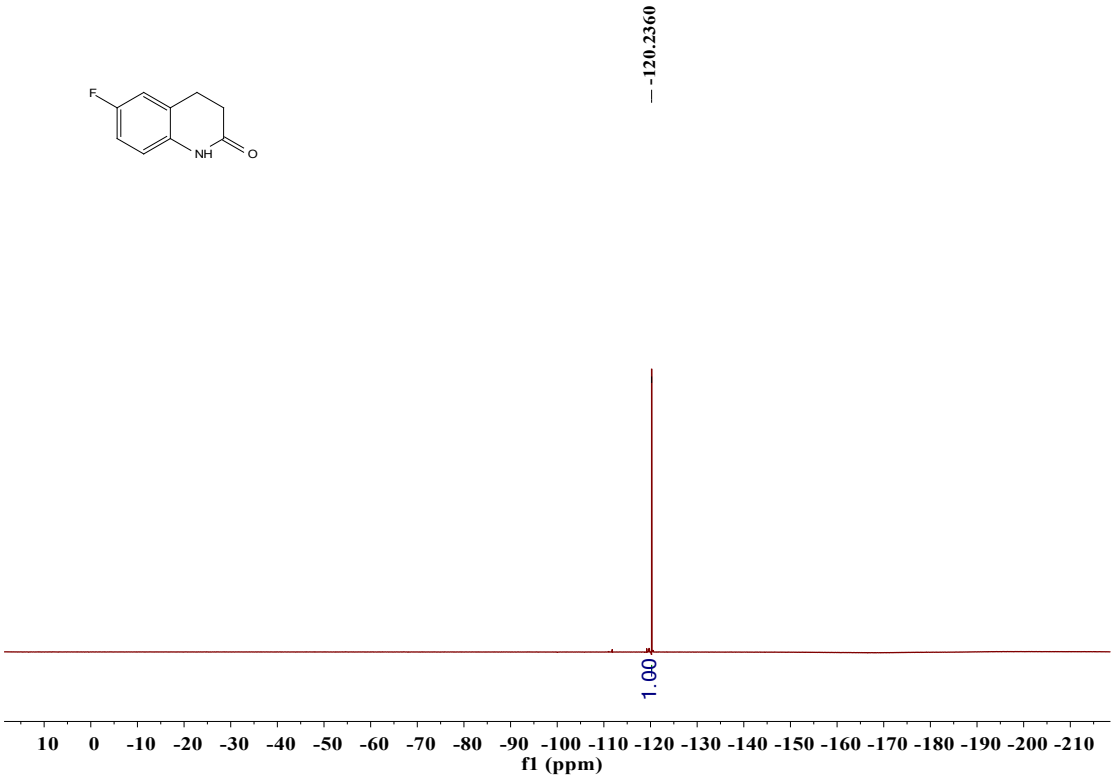
^{1}H-NMR Spectrum ($CDCl_3$) of 2y



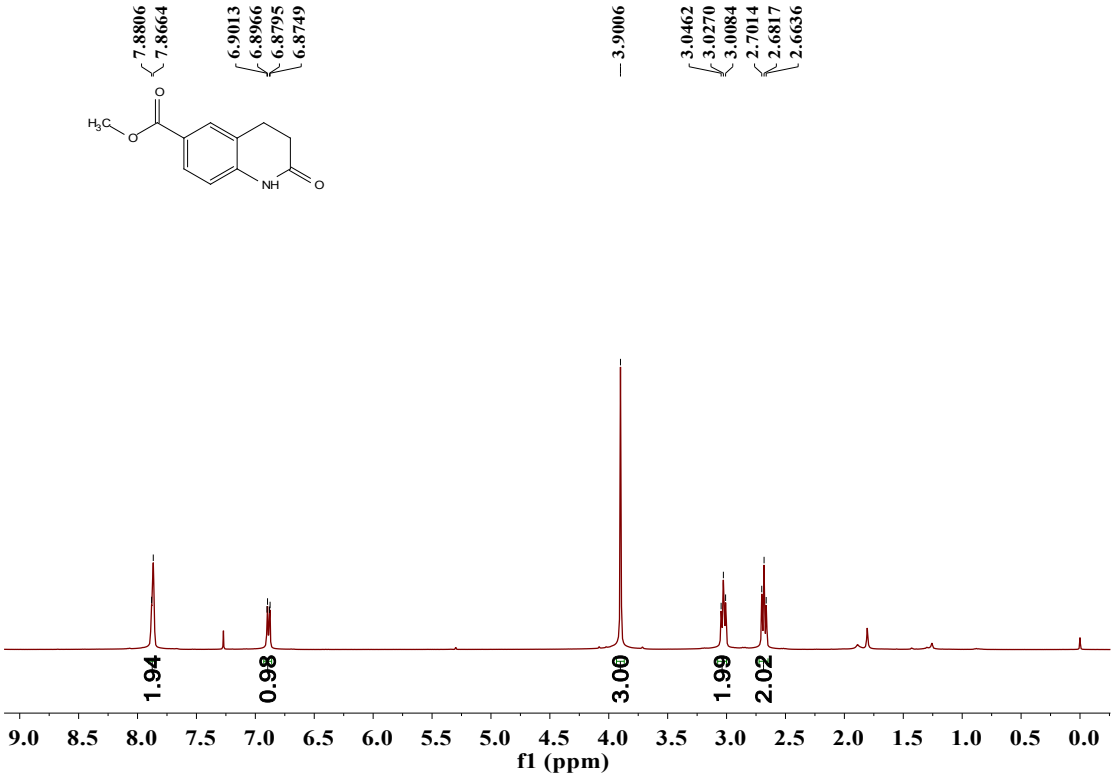
^{13}C-NMR Spectrum ($CDCl_3$) of 2y



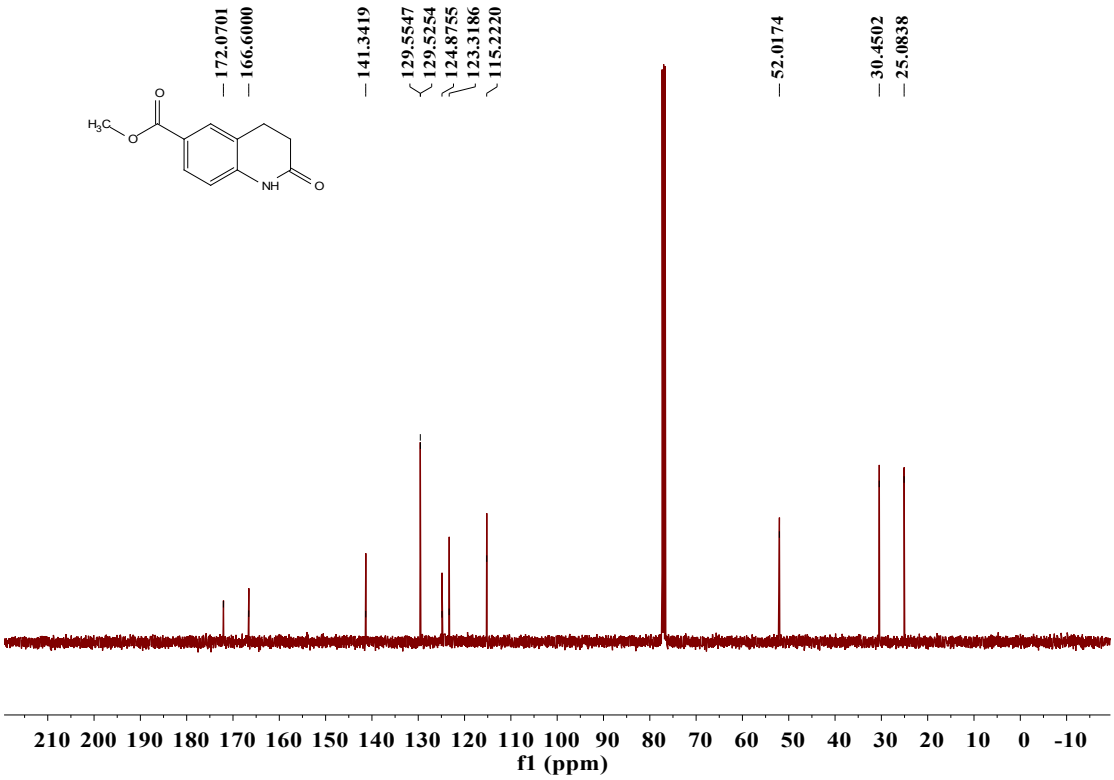
^{19}F-NMR Spectrum ($CDCl_3$) of 2y



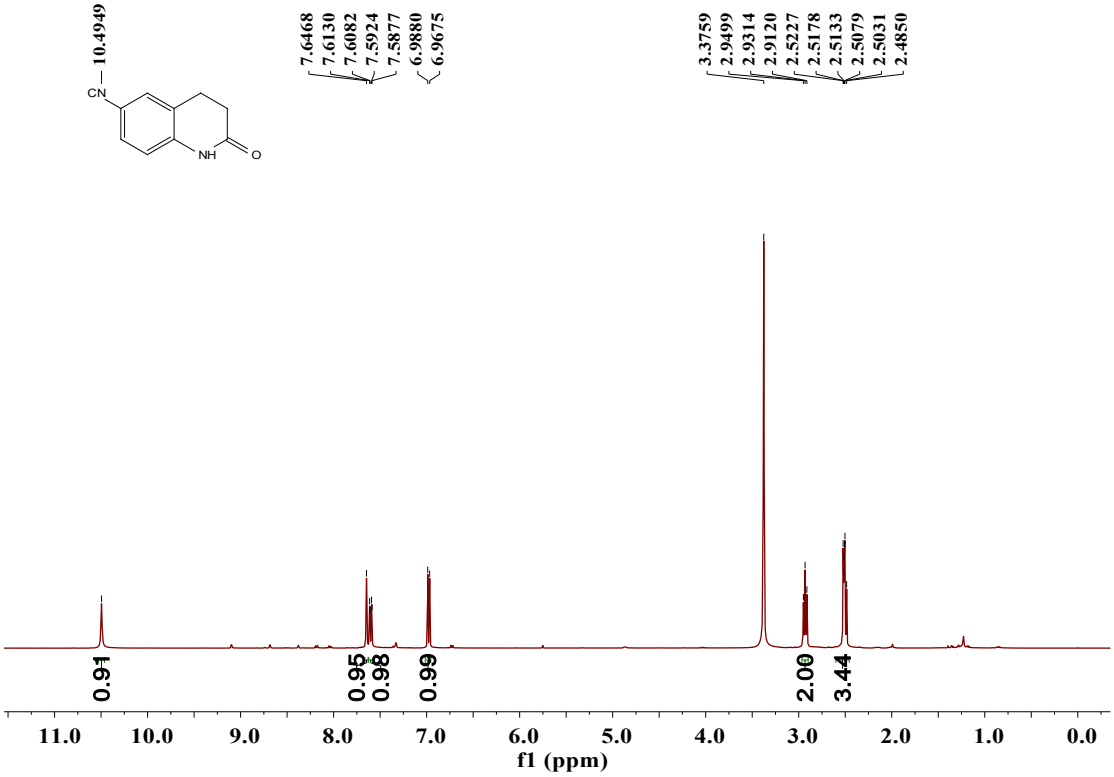
^{1}H-NMR Spectrum ($CDCl_3$) of 2z



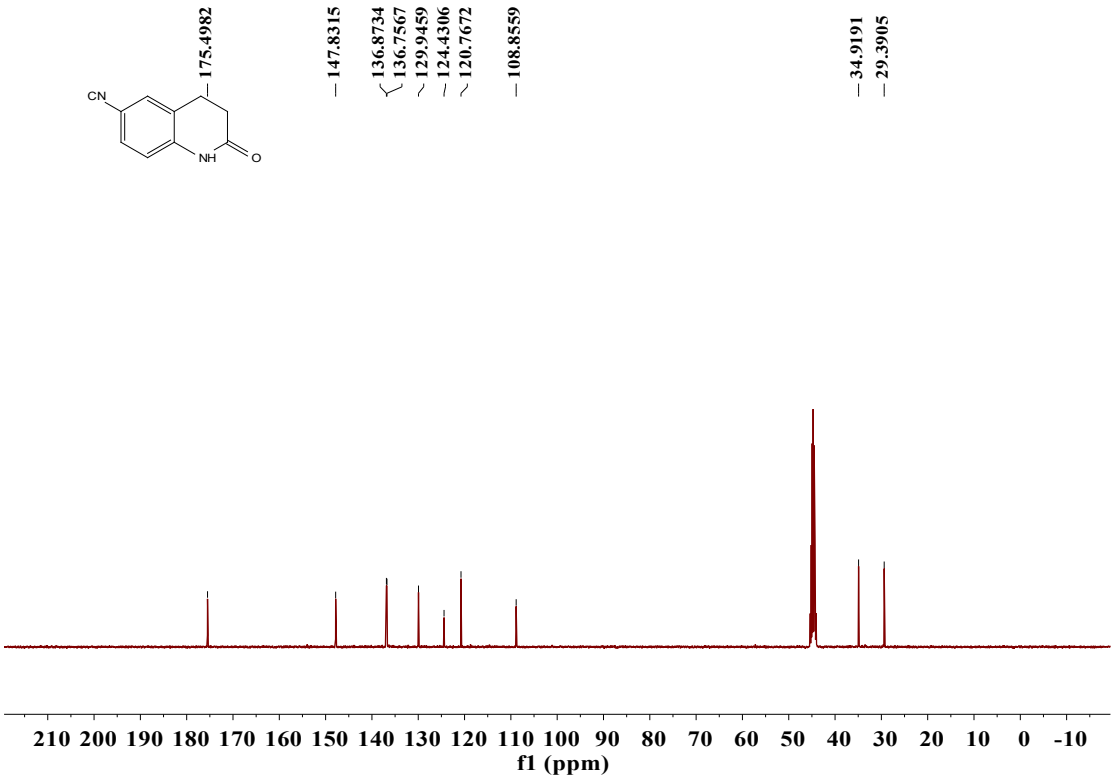
^{13}C-NMR Spectrum ($CDCl_3$) of 2z



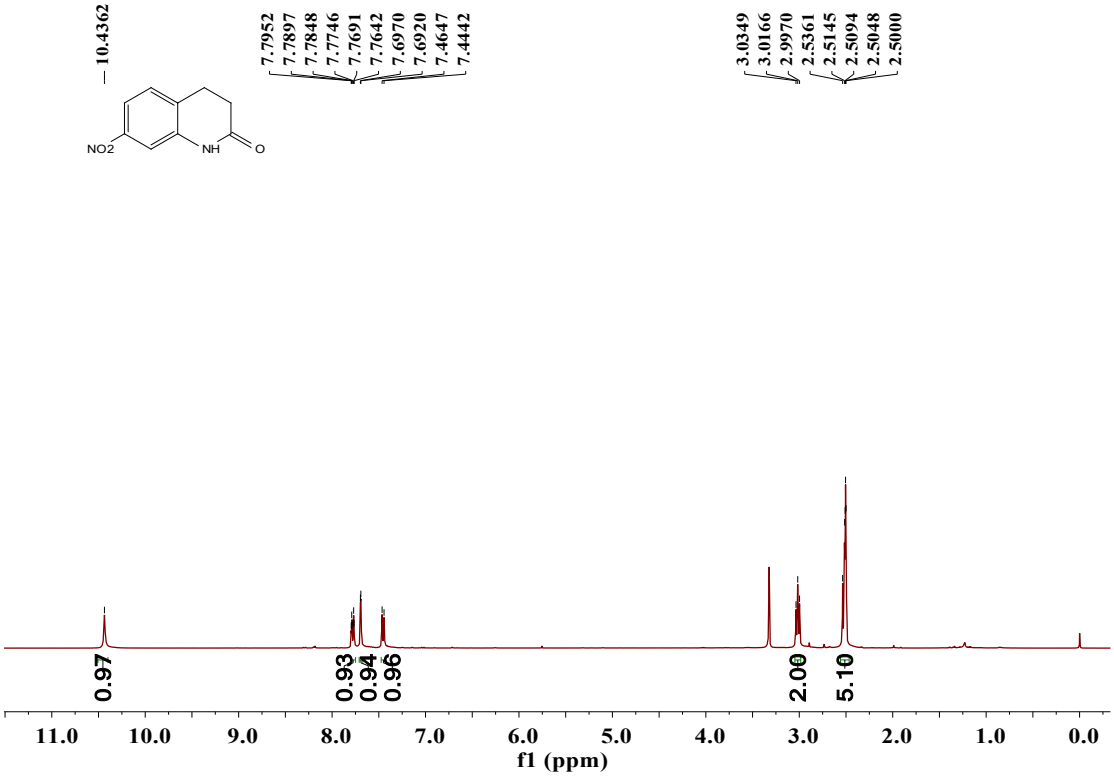
^{1}H-NMR Spectrum (DMSO-d_6) of 2aa



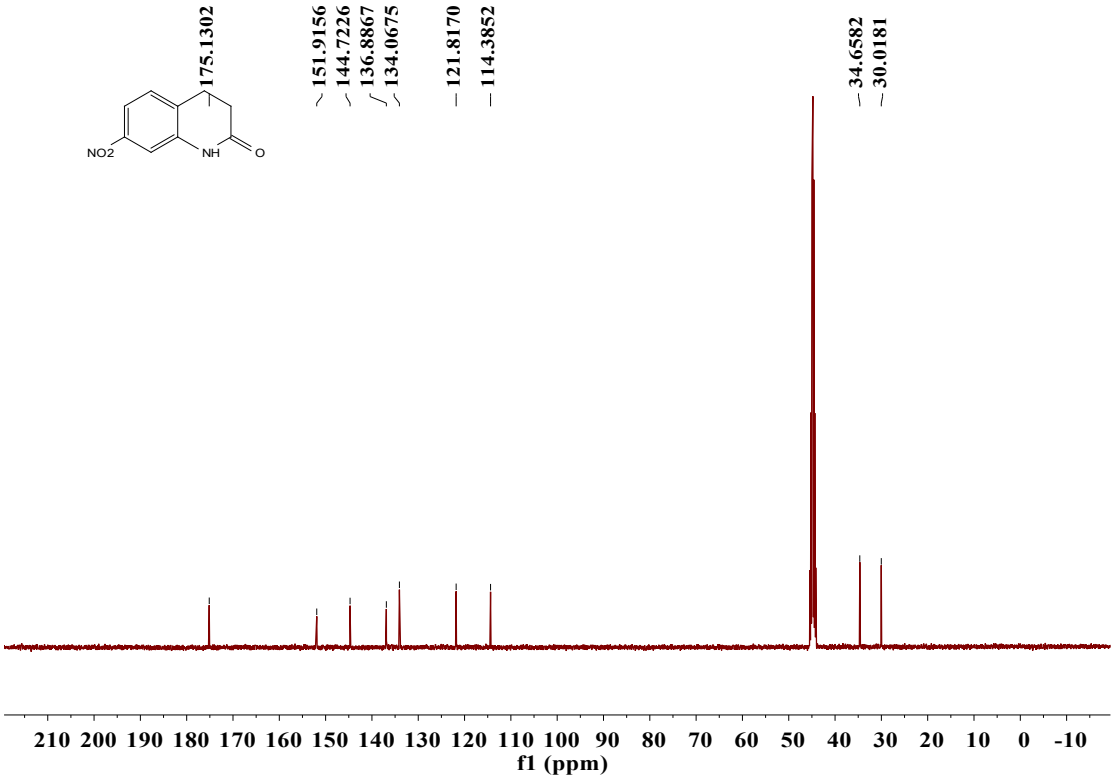
^{13}C-NMR Spectrum (DMSO-d_6) of 2aa



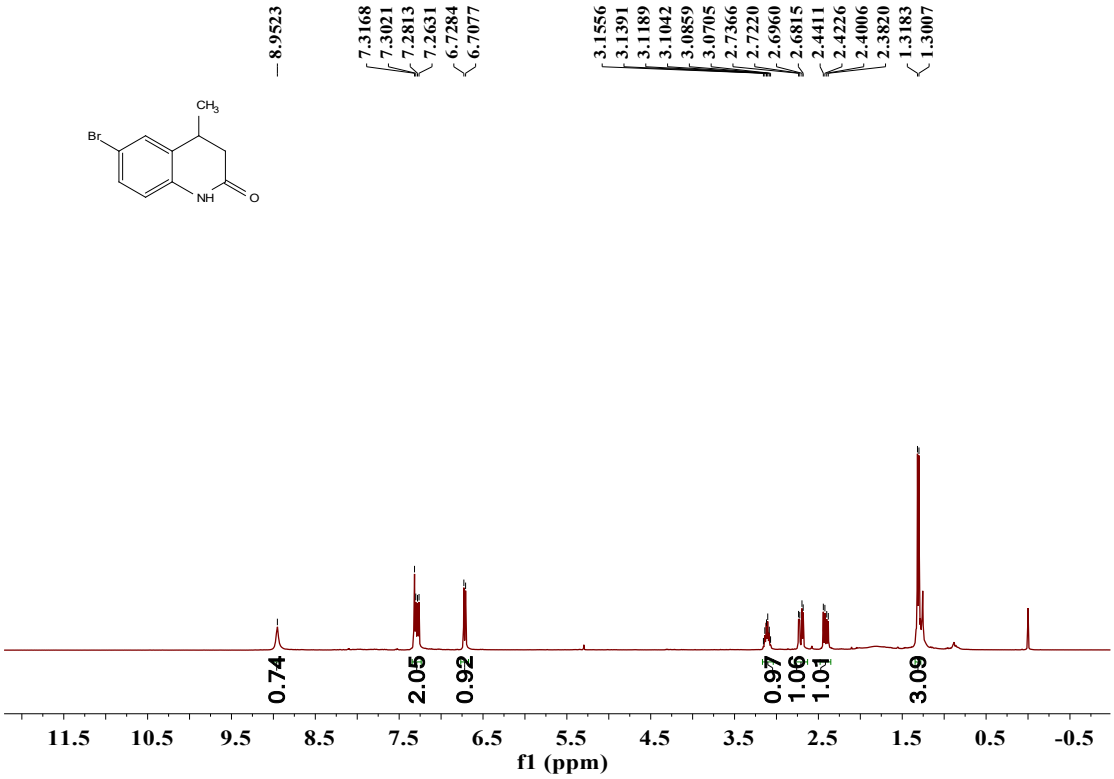
^{1}H-NMR Spectrum (DMSO-d_6) of 2ab



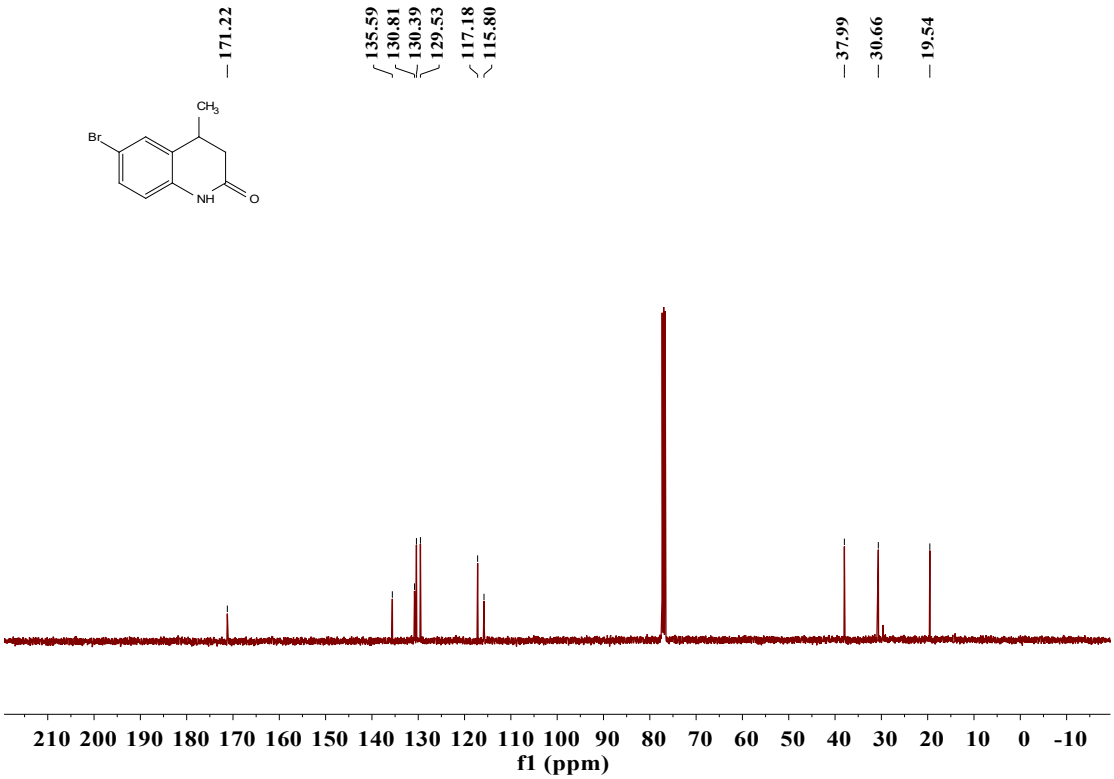
^{13}C-NMR Spectrum (DMSO-d_6) of 2ab



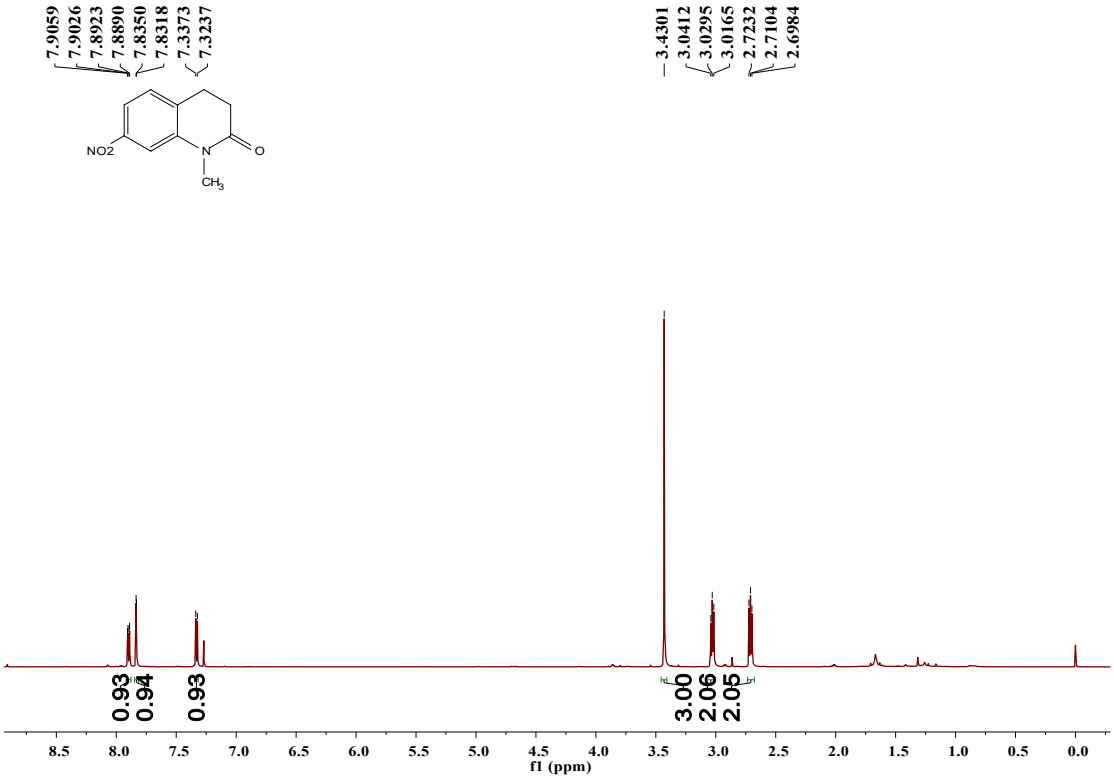
^{1}H-NMR Spectrum ($CDCl_3$) of 2ac



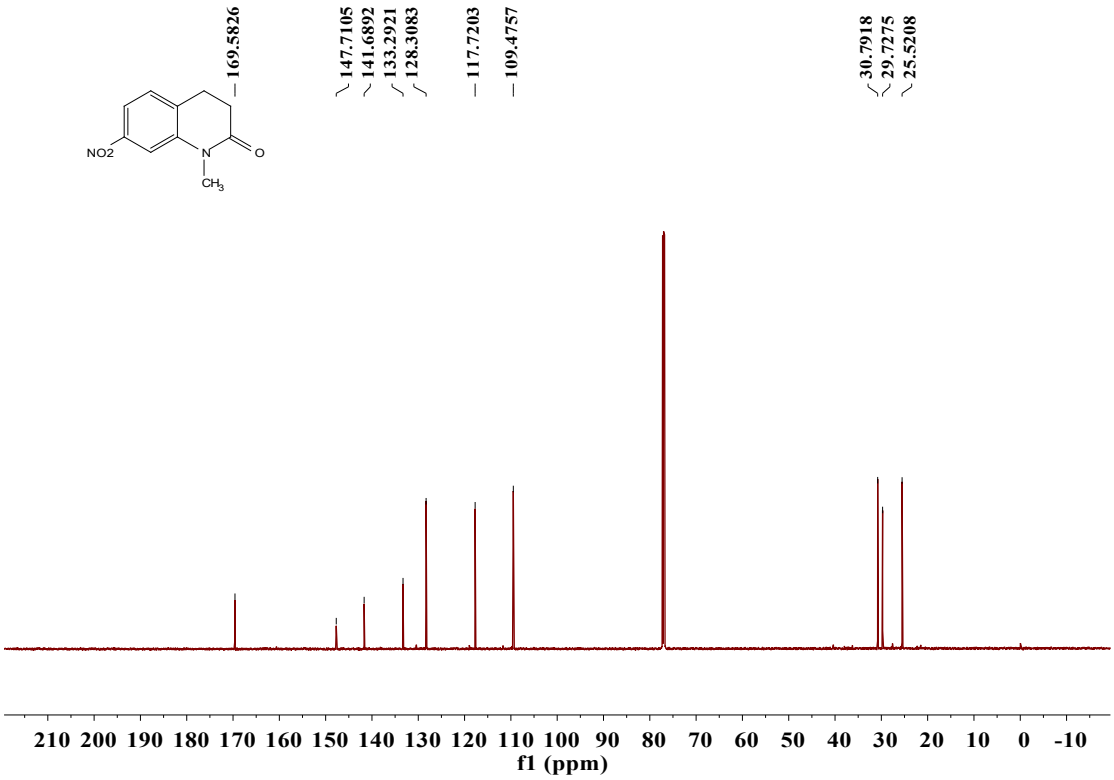
^{13}C-NMR Spectrum ($CDCl_3$) of 2ac



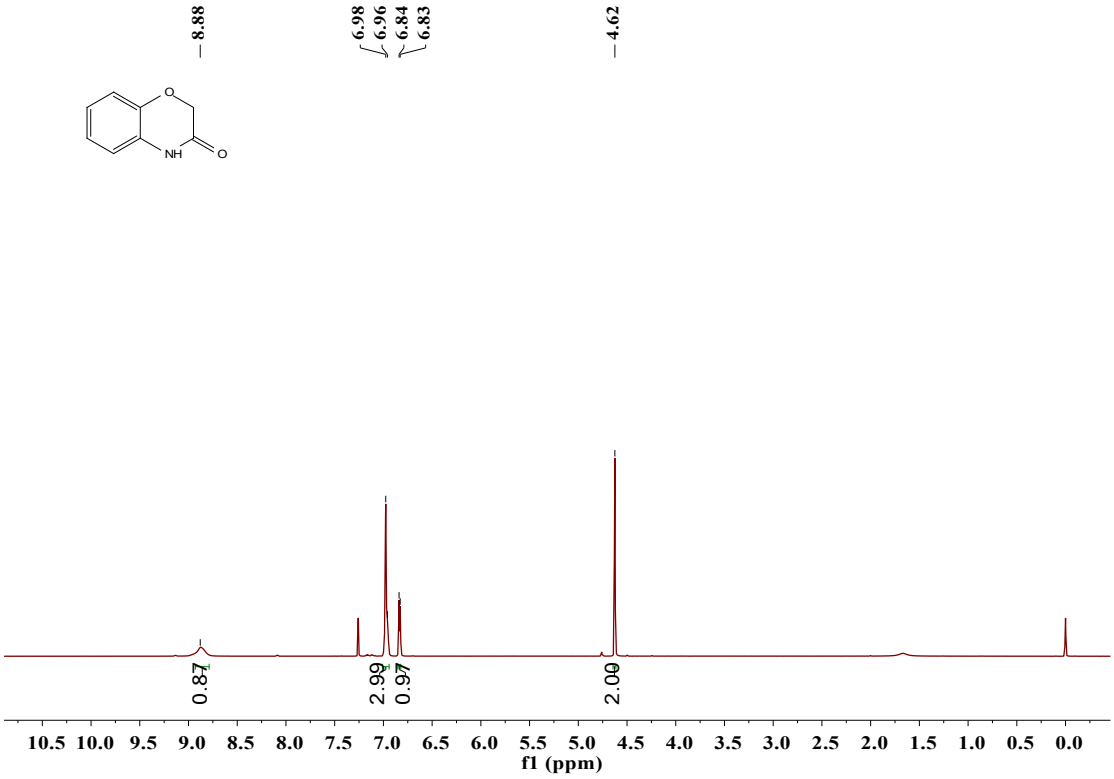
^{1}H-NMR Spectrum ($CDCl_3$) of 2ad



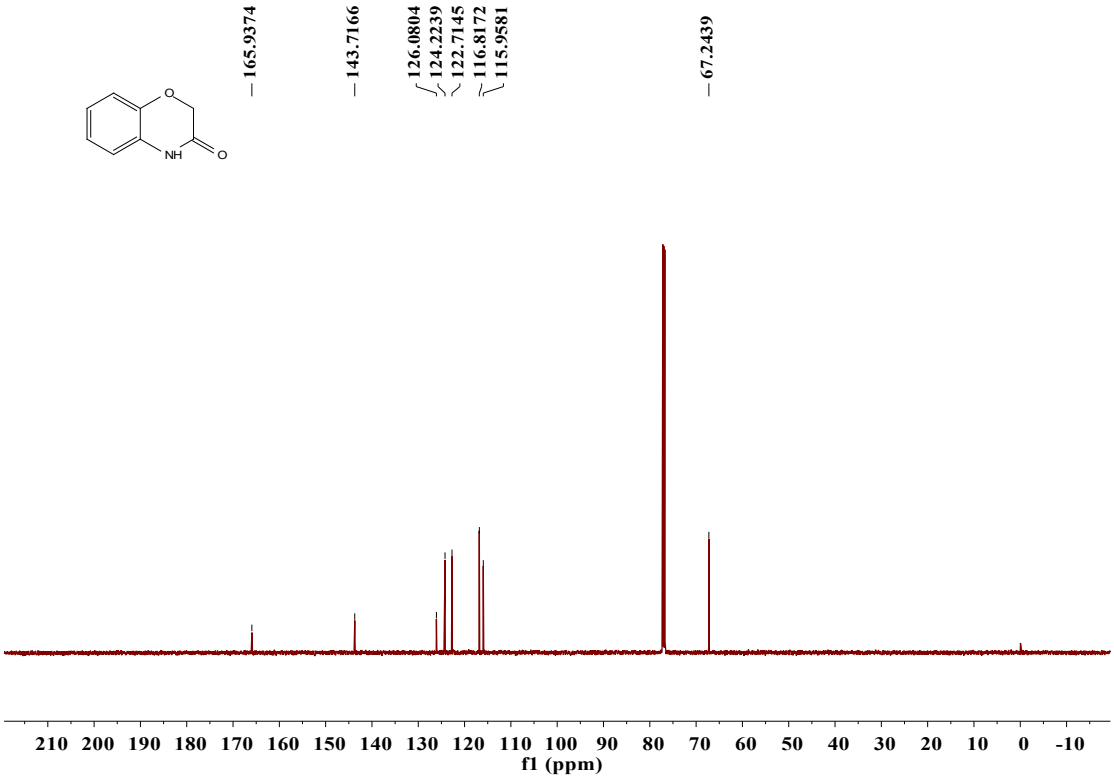
^{13}C-NMR Spectrum ($CDCl_3$) of 2ad



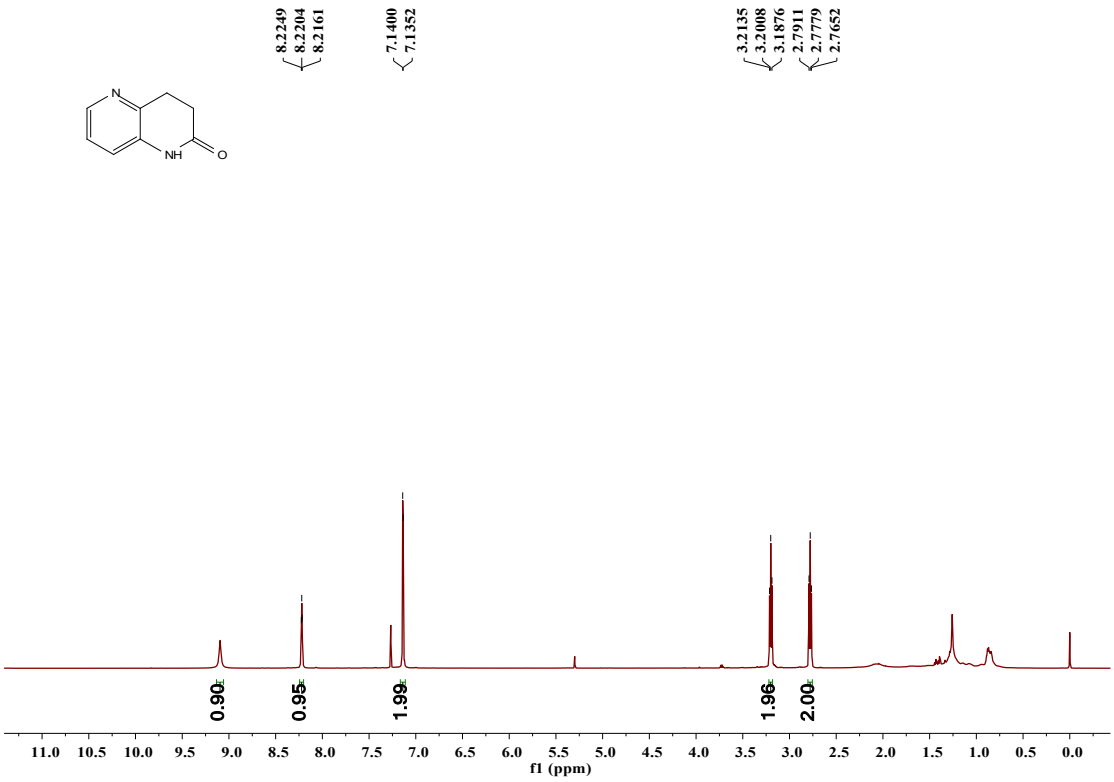
^{1}H-NMR Spectrum ($CDCl_3$) of 2ae



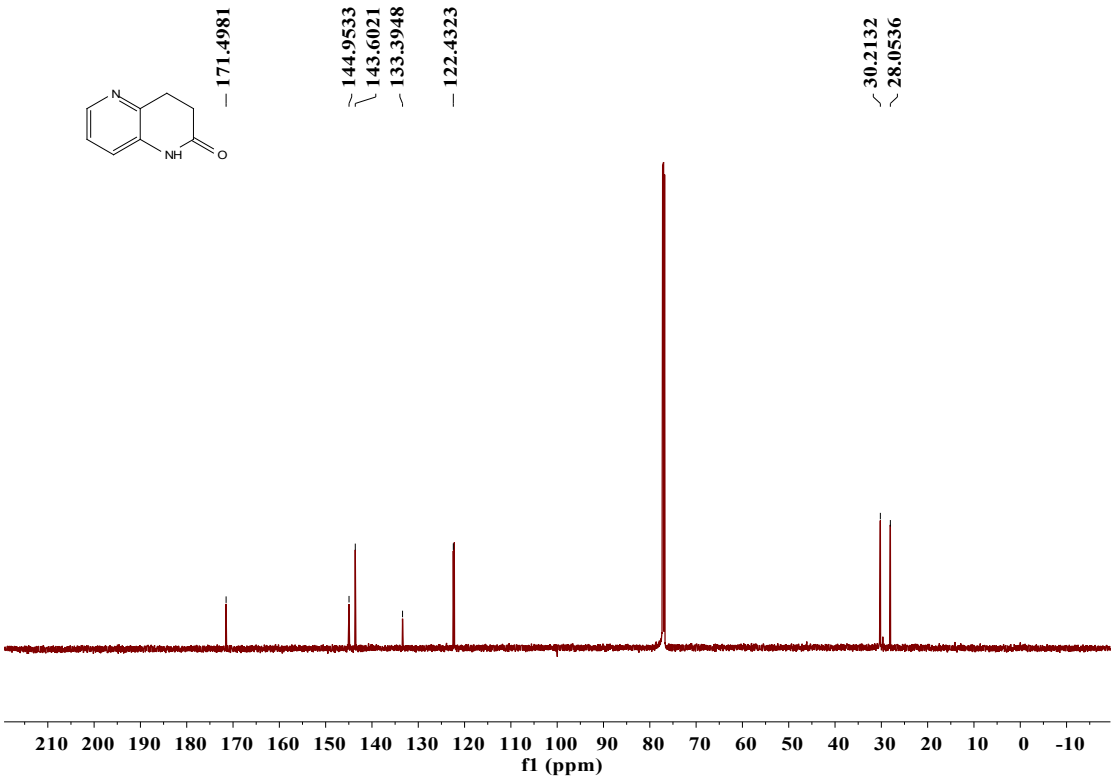
^{13}C-NMR Spectrum ($CDCl_3$) of 2ae



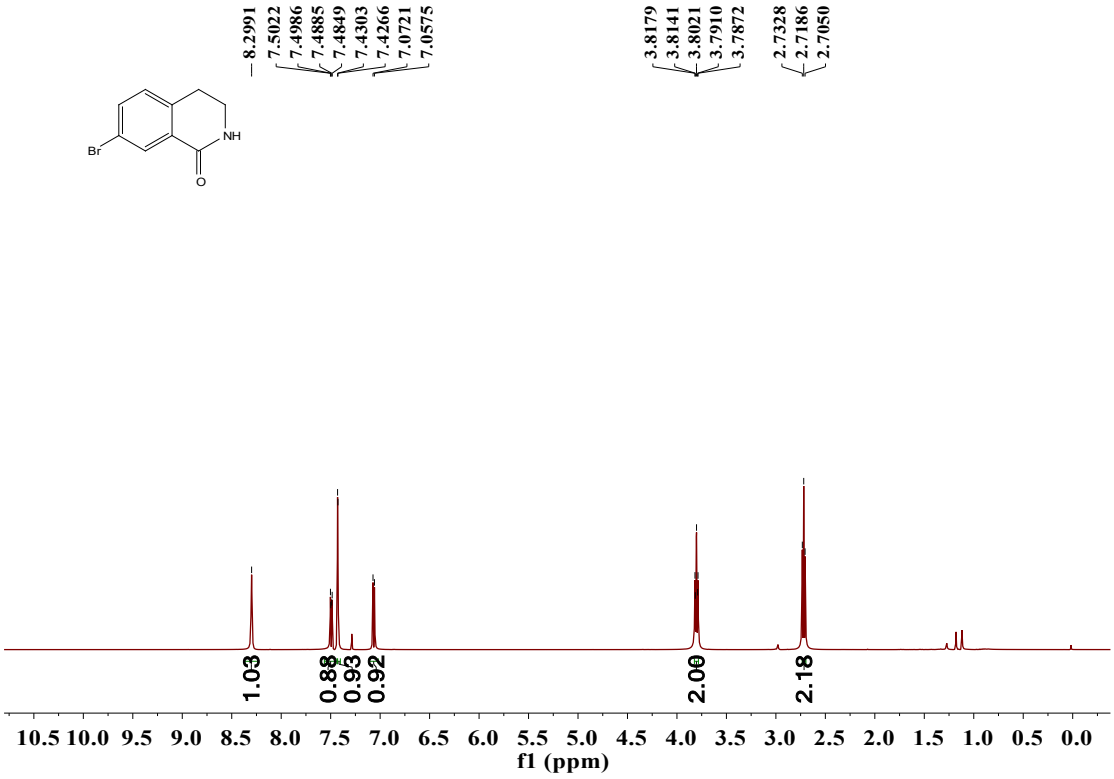
^{1}H-NMR Spectrum ($CDCl_3$) of 2af



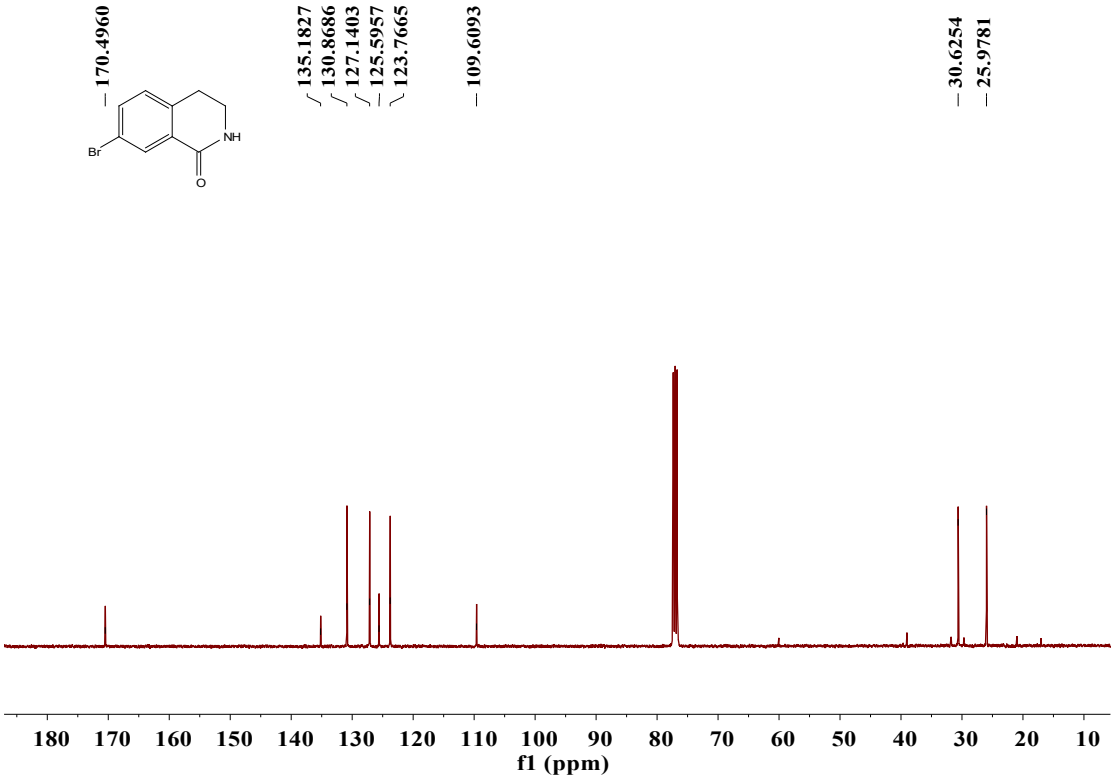
^{13}C-NMR Spectrum ($CDCl_3$) of 2af



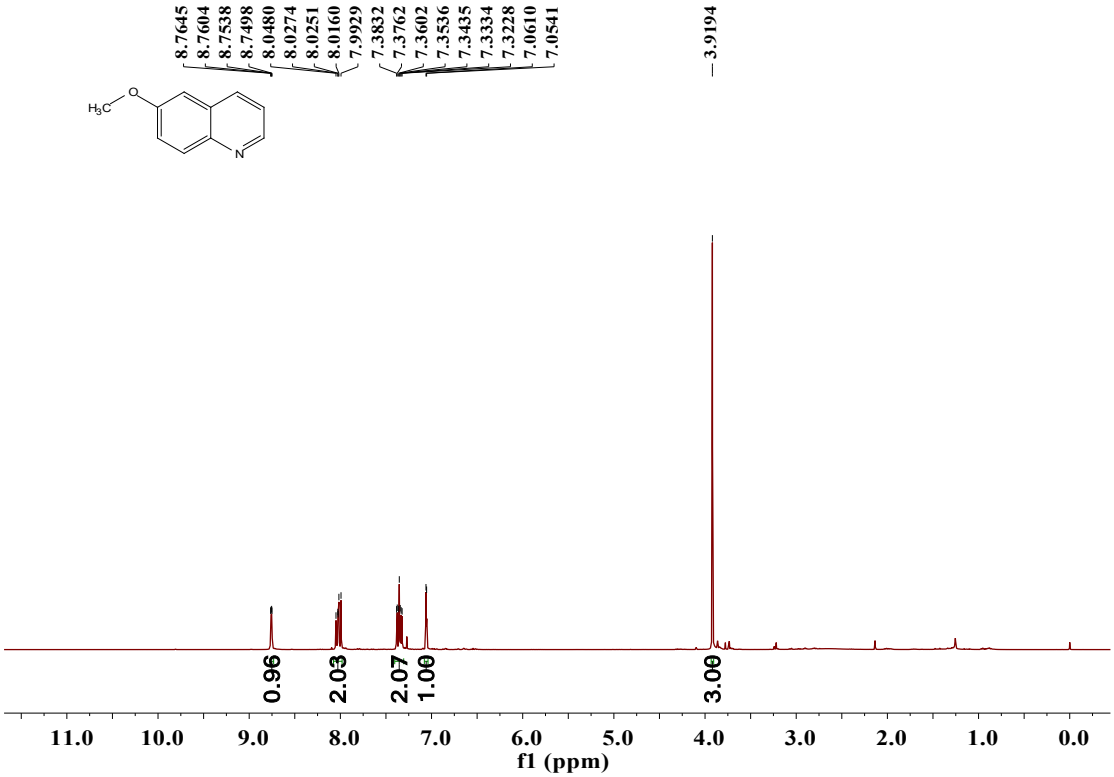
^{1}H-NMR Spectrum ($CDCl_3$) of 2ah



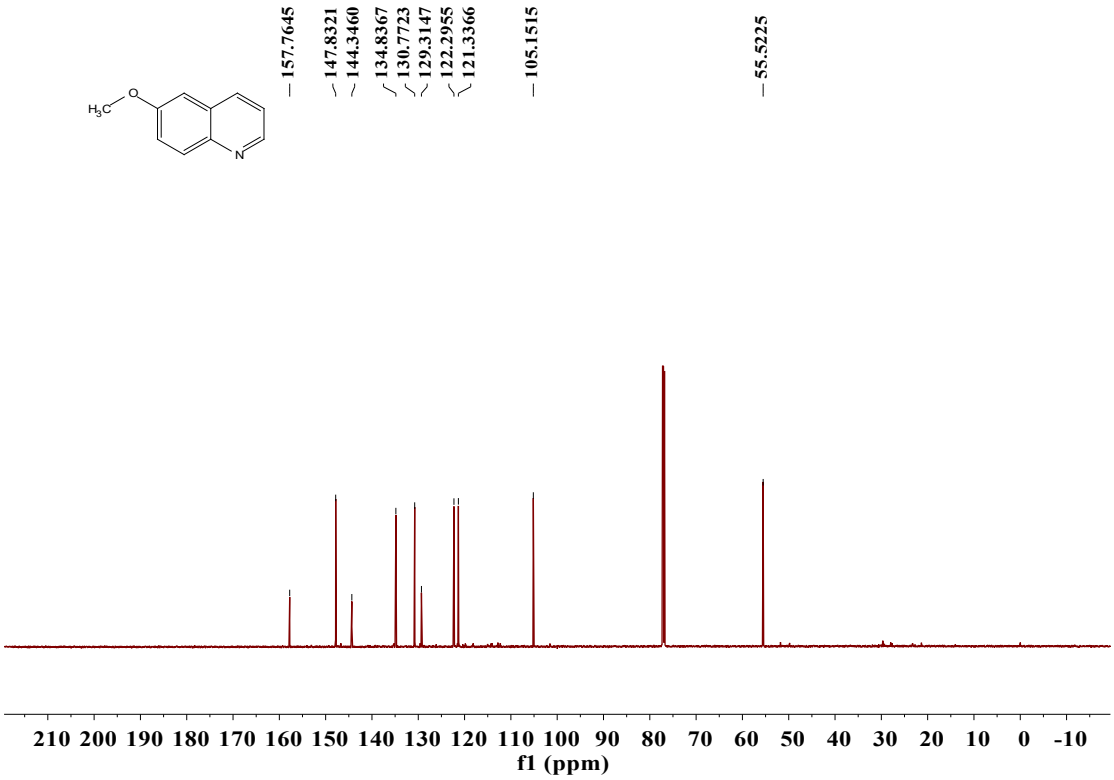
^{13}C-NMR Spectrum ($CDCl_3$) of 2ah



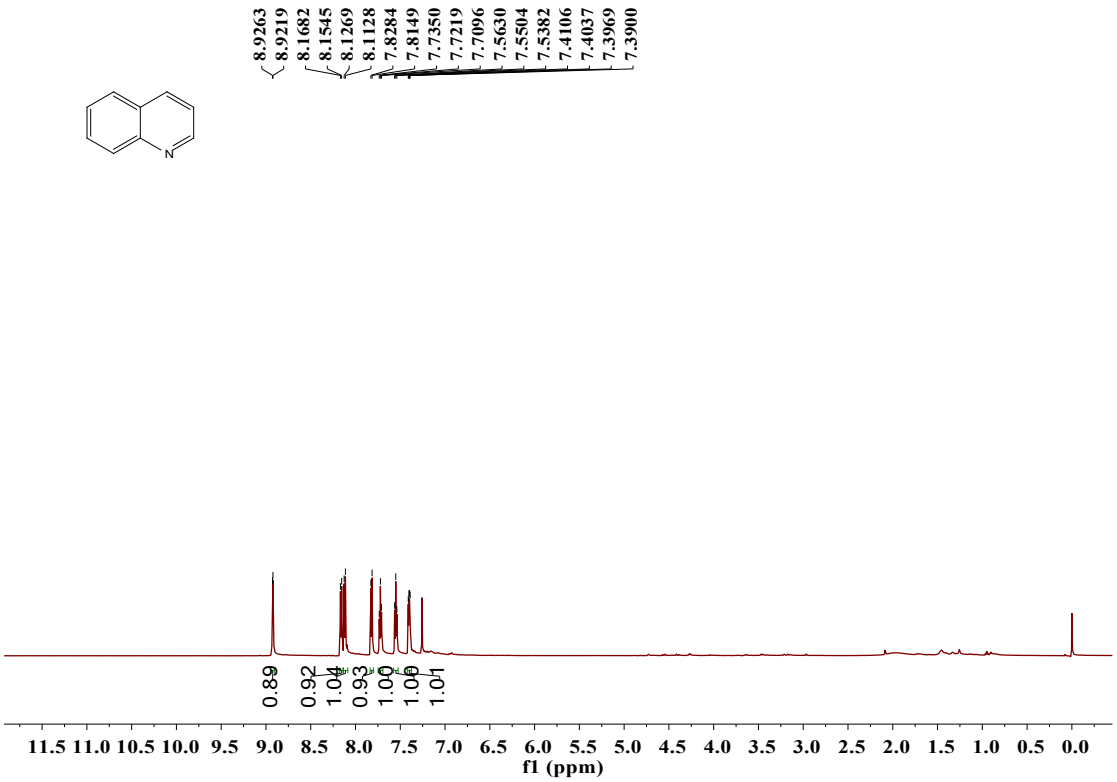
^{1}H-NMR Spectrum ($CDCl_3$) of 2ai



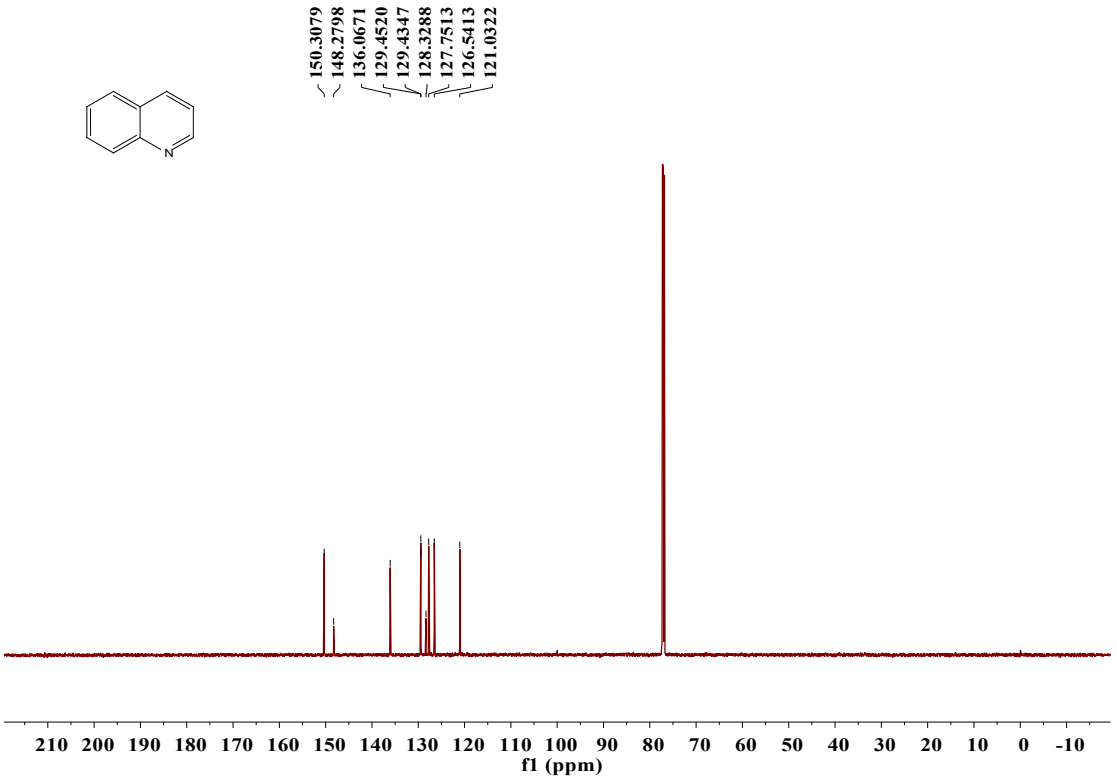
^{13}C-NMR Spectrum ($CDCl_3$) of 2ai



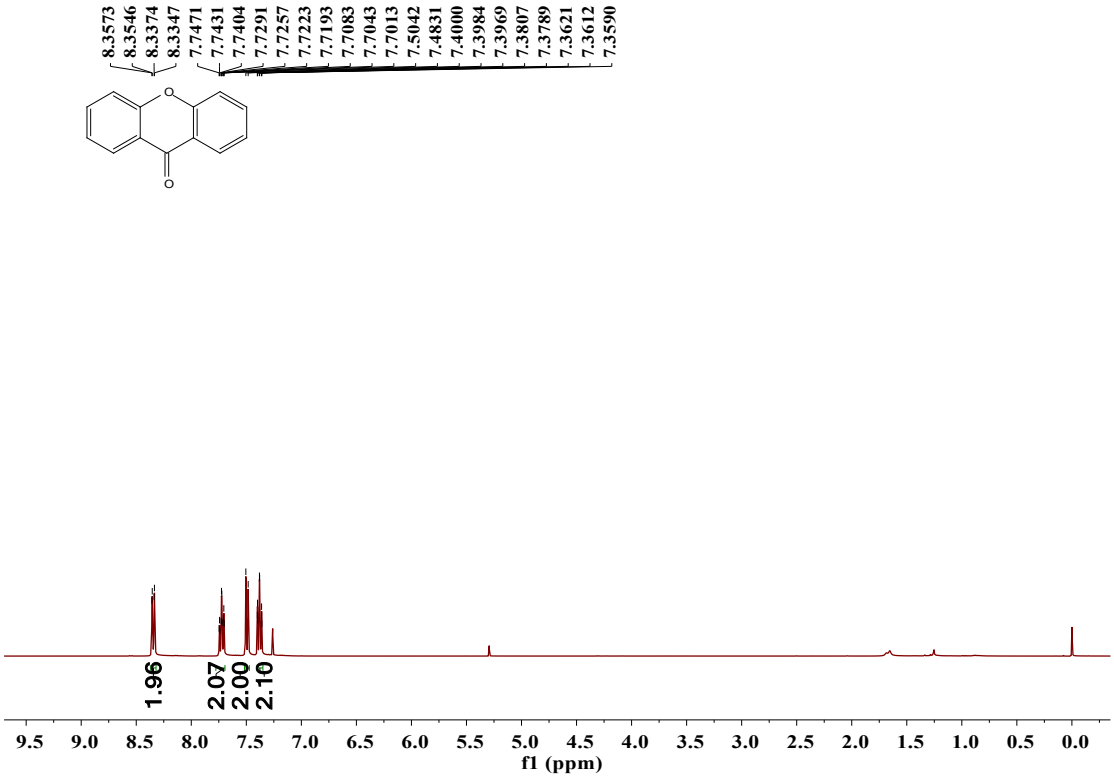
^{1}H-NMR Spectrum ($CDCl_3$) of 2aj



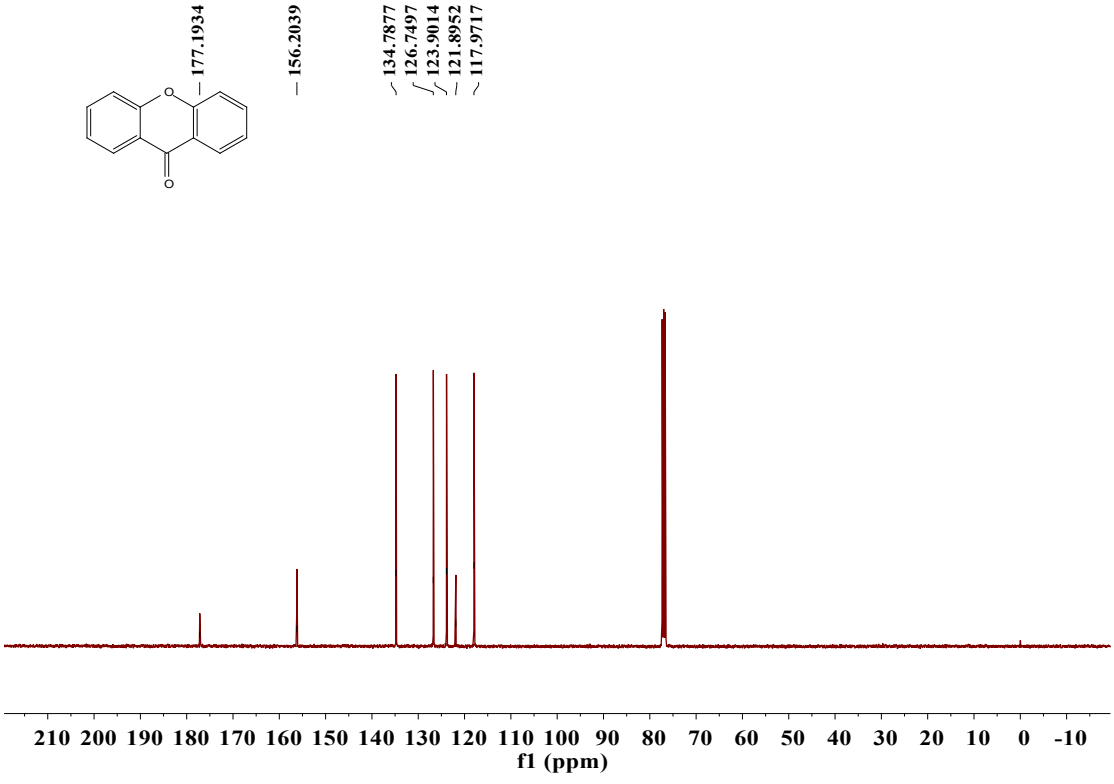
^{13}C-NMR Spectrum ($CDCl_3$) of 2aj



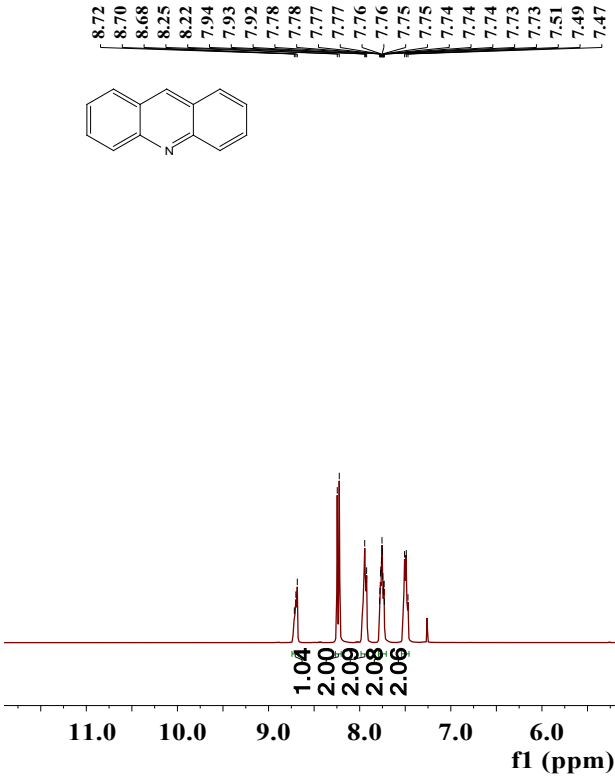
^{1}H-NMR Spectrum ($CDCl_3$) of 2ak



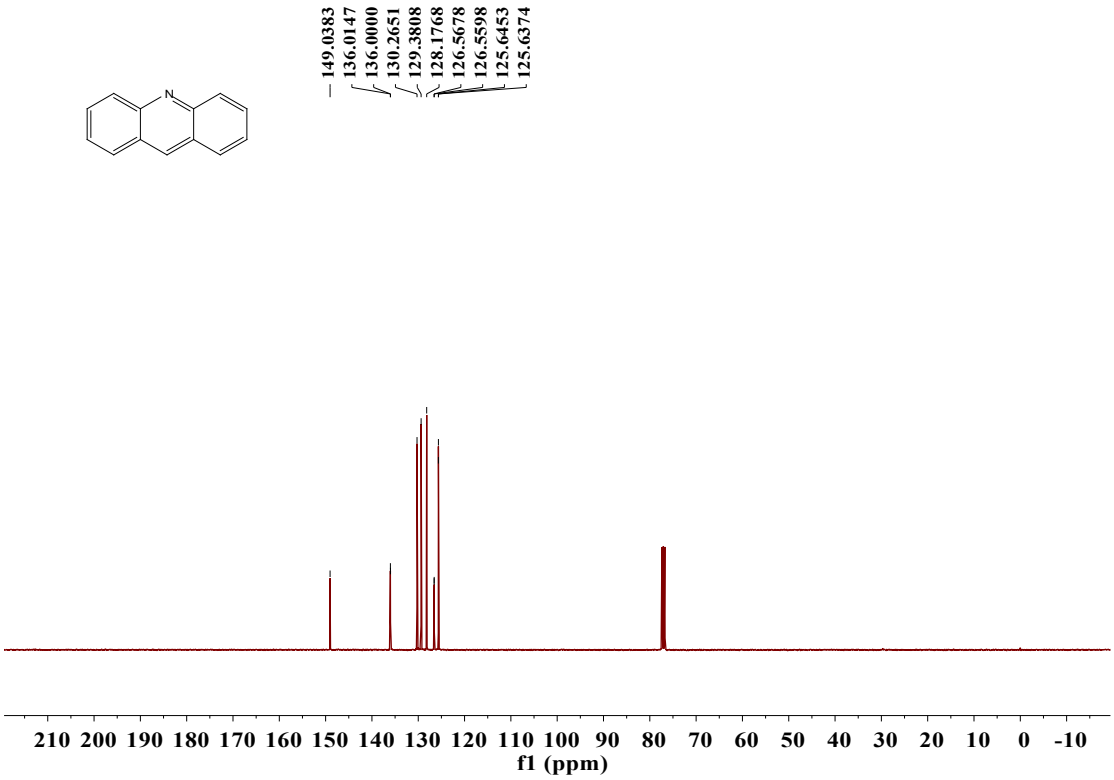
^{13}C-NMR Spectrum ($CDCl_3$) of 2ak



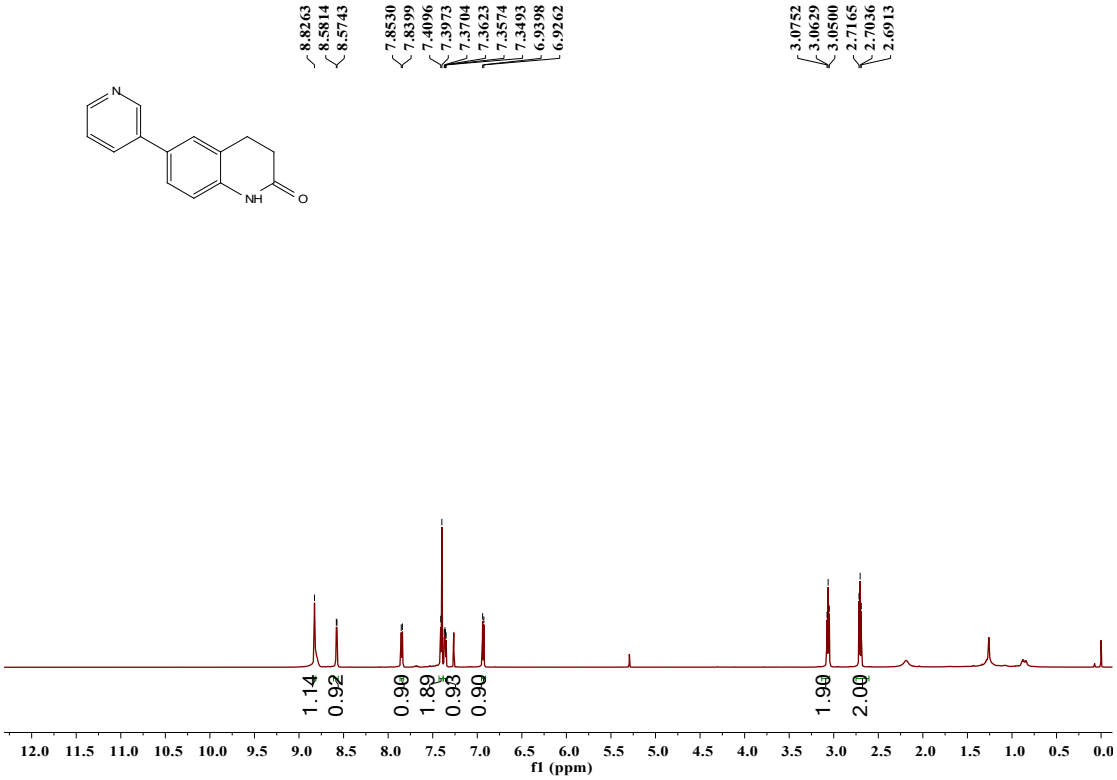
^{1}H-NMR Spectrum ($CDCl_3$) of 2al



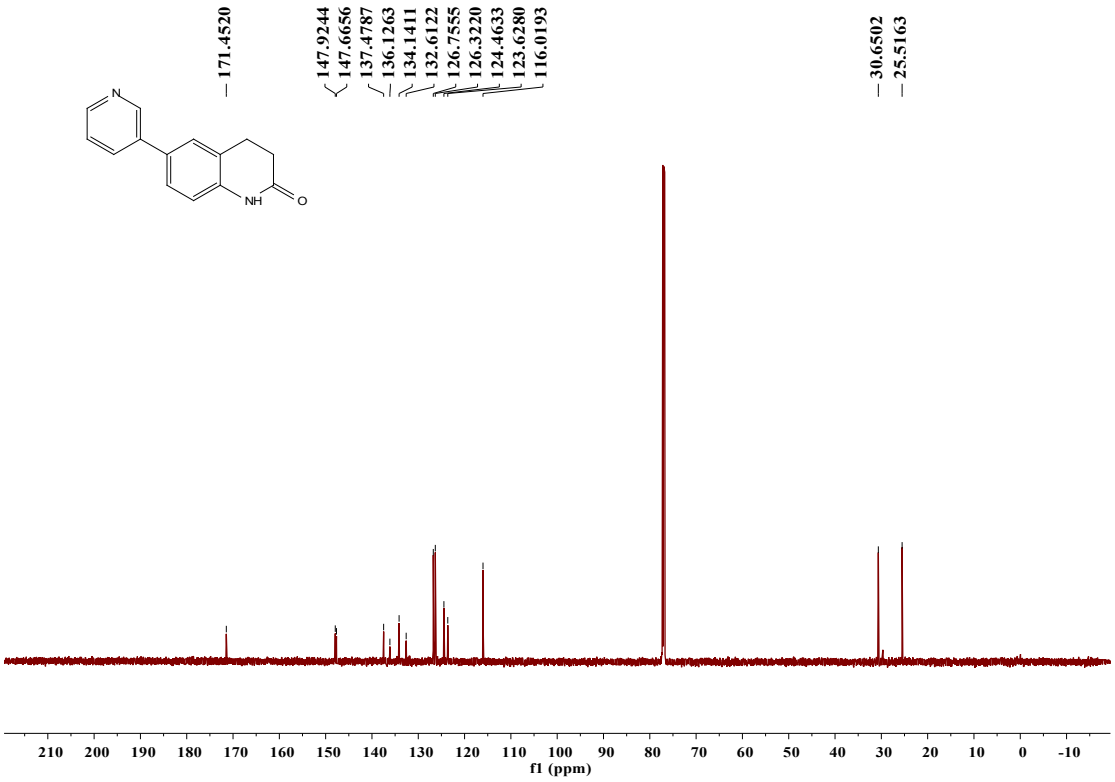
^{13}C-NMR Spectrum ($CDCl_3$) of 2al



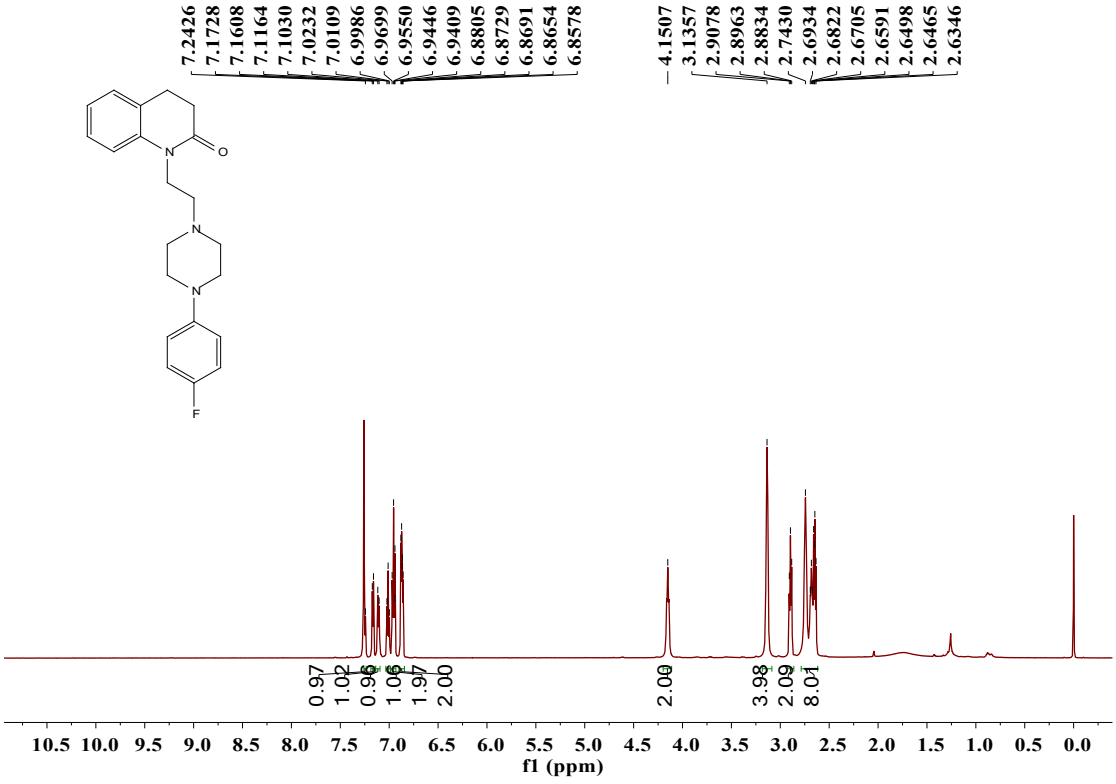
^{1}H-NMR Spectrum ($CDCl_3$) of 5



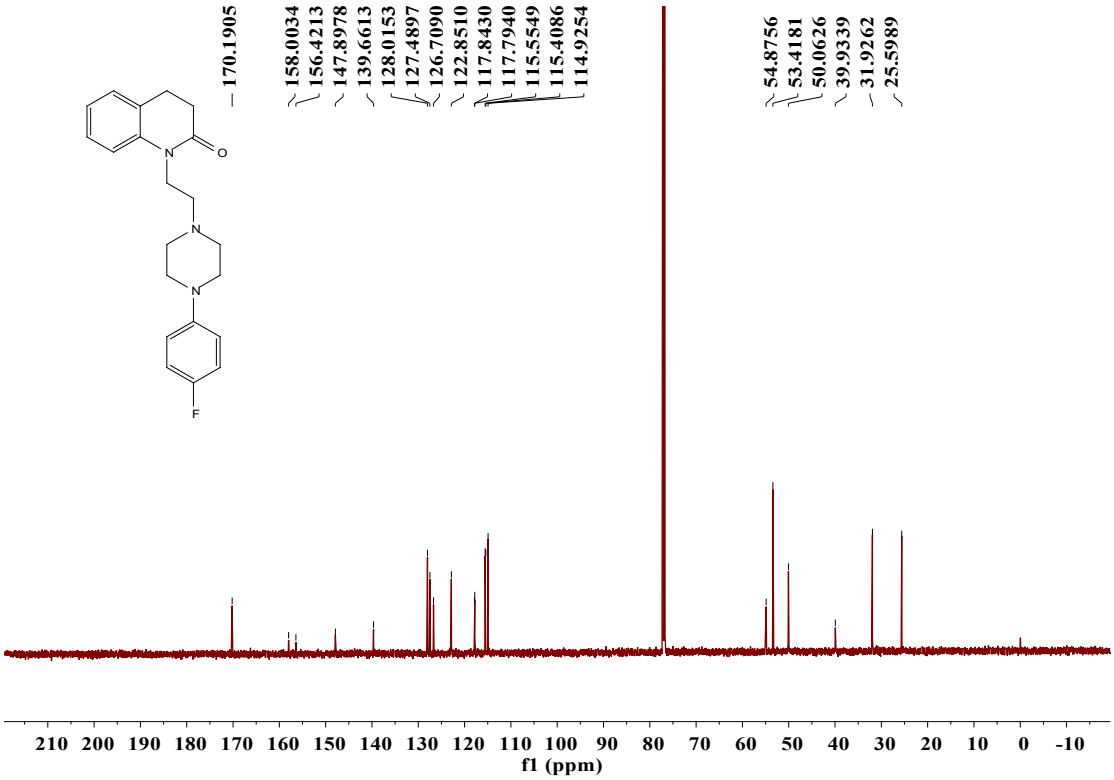
^{13}C-NMR Spectrum ($CDCl_3$) of 5



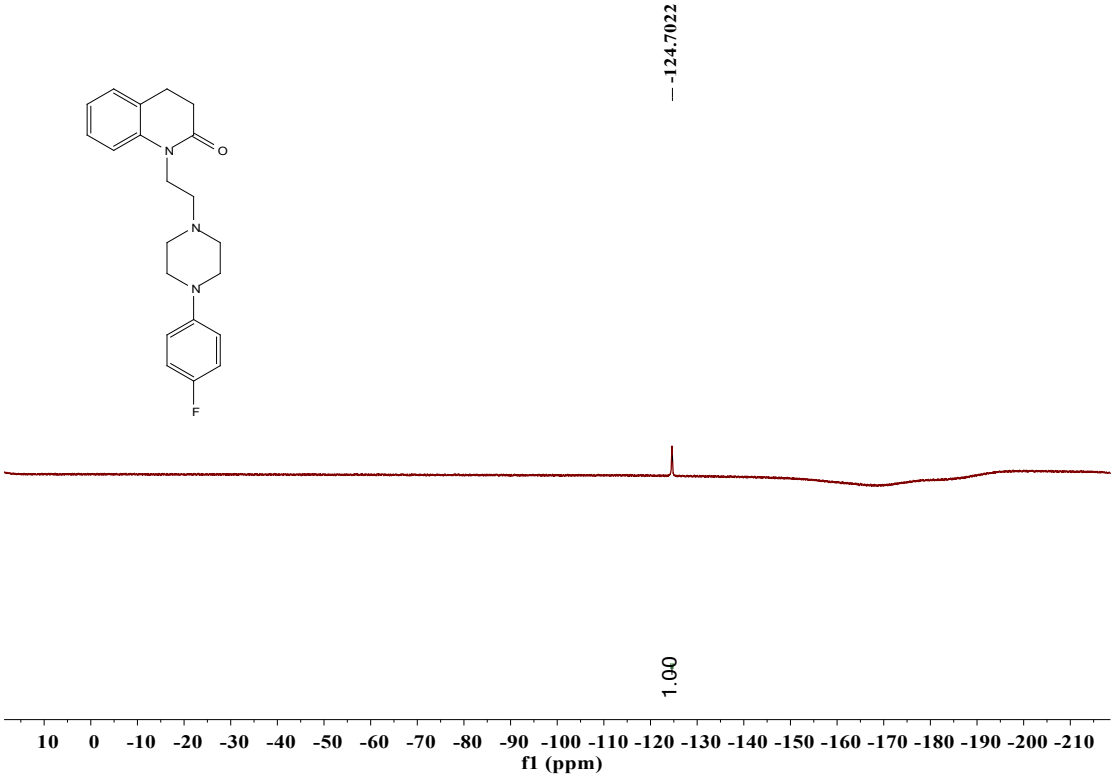
^{1}H-NMR Spectrum ($CDCl_3$) of 8



^{13}C-NMR Spectrum ($CDCl_3$) of 8

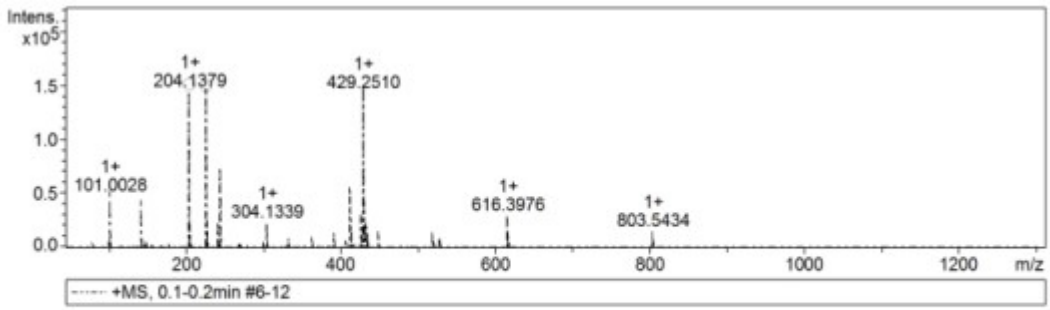


^{19}F-NMR Spectrum ($CDCl_3$) of 8



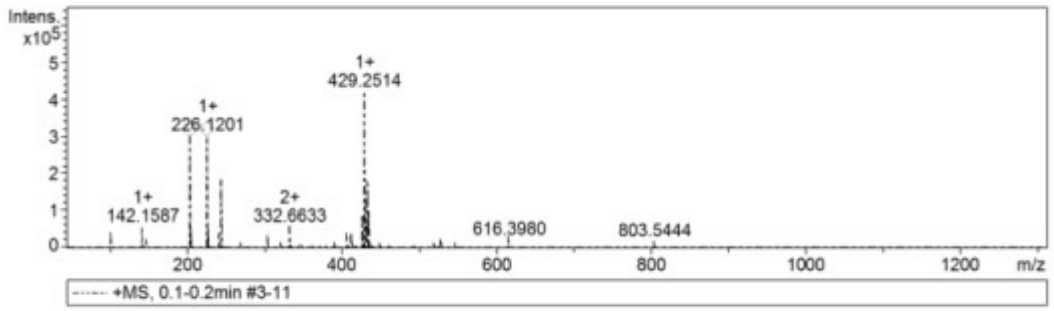
8. HRMS of Products

HRMS of 2e



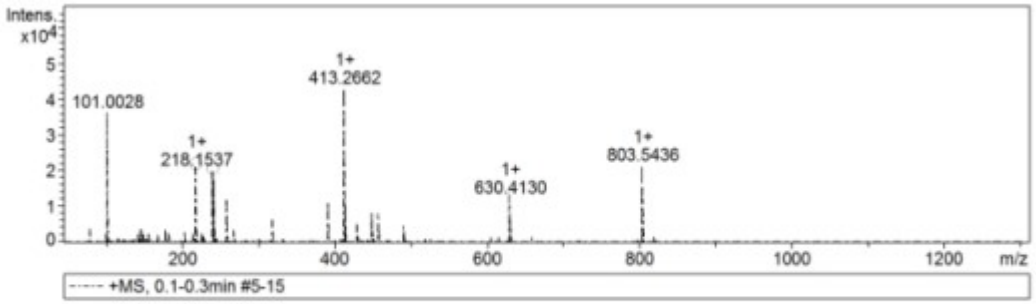
Meas. m/z	#	Ion Formula	Sum Formula	m/z	Adduct	err [ppm]	z	mSigma	Score	rdb	N-Rule	e¯ Conf
204.1379	1	C13H18NO	C13H17NO	204.1383	M+H	1.7	1+	3.8	100.00	6.0	ok	even
226.1200	1	C13H17NNaO		226.1202	M+Na	1.0	1+	0.5	100.00	6.0	ok	even

HRMS of 2f



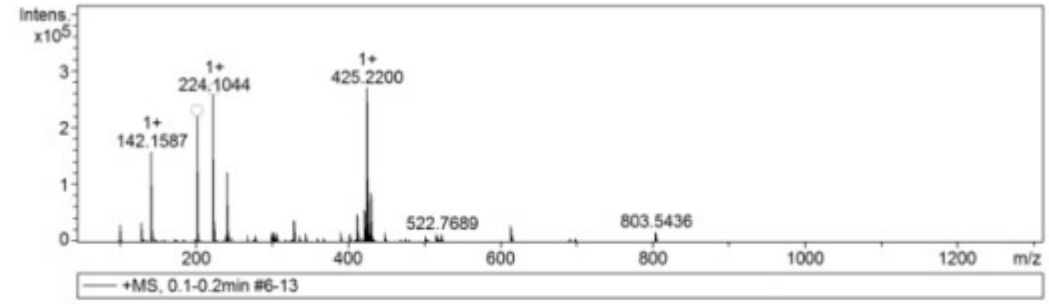
Meas. m/z	#	Ion Formula	Sum Formula	m/z	Adduct	err [ppm]	z	mSigma	Score	rdb	N-Rule	e¯ Conf
204.1381	1	C13H18NO	C13H17NO	204.1383	M+H	1.0	1+	0.5	100.00	6.0	ok	even
226.1201	1	C13H17NNaO		226.1202	M+Na	0.5	1+	0.5	100.00	6.0	ok	even

HRMS of 2g



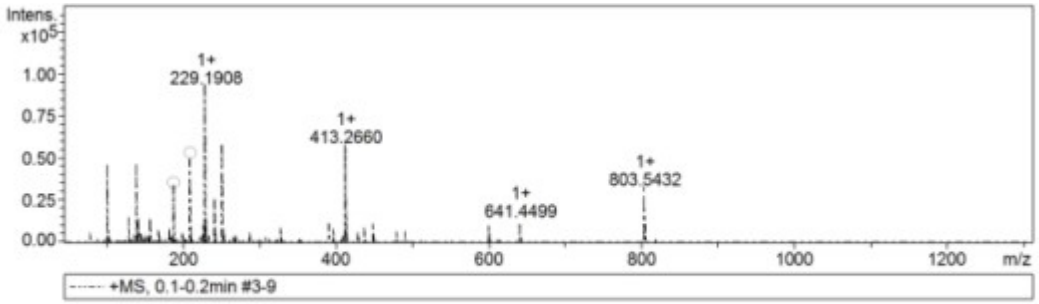
Meas. m/z	#	Ion Formula	Sum Formula	m/z	Adduct	err [ppm]	z	mSigma	Score	rdb	N-Rule	e⁻ Conf
218.1537	1	C14H20NO	C14H19NO	218.1539	M+H	1.1	1+	7.2	100.00	6.0	ok	even
240.1356	1	C14H19NNaO		240.1359	M+Na	1.1	1+	0.6	100.00	6.0	ok	even

HRMS of 2i



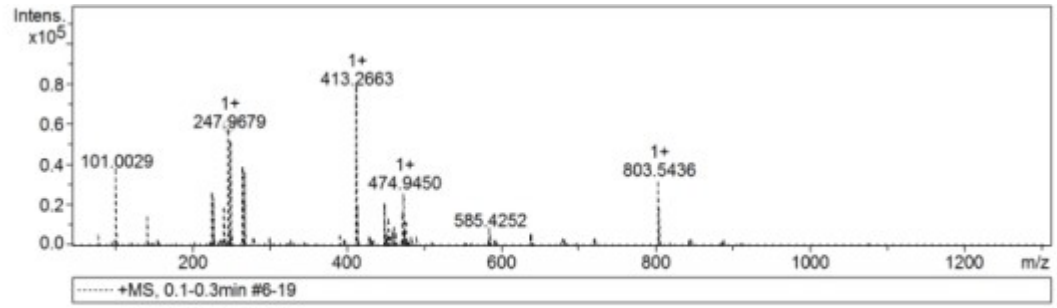
Meas. m/z	#	Ion Formula	Sum Formula	m/z	Adduct	err [ppm]	z	mSigma	Score	rdb	N-Rule	e⁻ Conf
202.1224	1	C13H16NO	C13H15NO	202.1226	M+H	1.2	1+	1.2	100.00	7.0	ok	even
224.1044	1	C13H15NNaO		224.1046	M+Na	1.0	1+	4.3	100.00	7.0	ok	even

HRMS of 2j



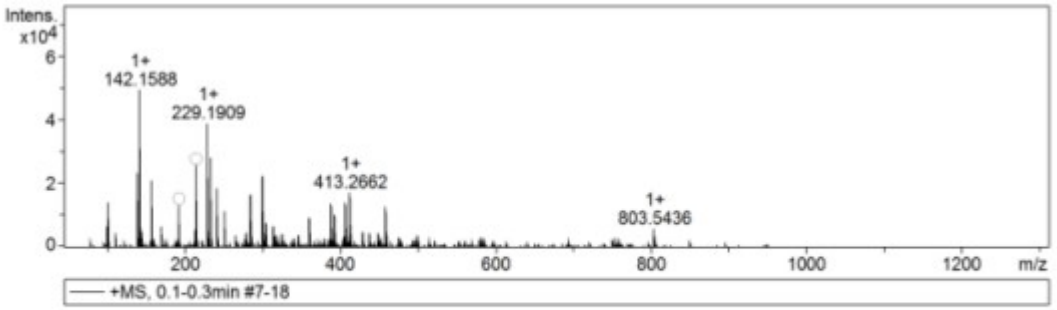
Meas. m/z	#	Ion Formula	Sum Formula	m/z	Adduct	err [ppm]	z	mSigma	Score	rdb	N-Rule	e⁻ Conf
188.1066	1	C12H14NO	C12H13NO	188.1070	M+H	1.8	1+	1.5	100.00	7.0	ok	even
210.0887	1	C12H13NNaO		210.0889	M+Na	1.3	1+	5.5	100.00	7.0	ok	even

HRMS of 2u



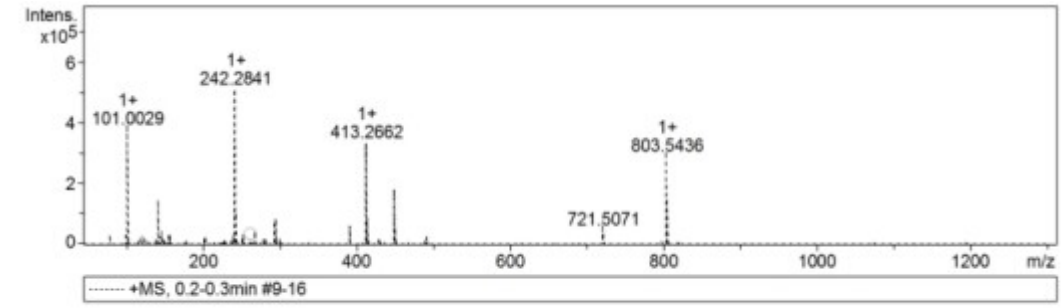
Meas. m/z	#	Ion Formula	Sum Formula	m/z	Adduct	err [ppm]	z	mSigma	Score	rdb	N-Rule	e⁻ Conf
247.9679	1	C9H8BrNNaO	C9H8BrNO	247.9681	M+Na	0.8	1+	24.6	100.00	6.0	ok	even

HRMS of 2ab



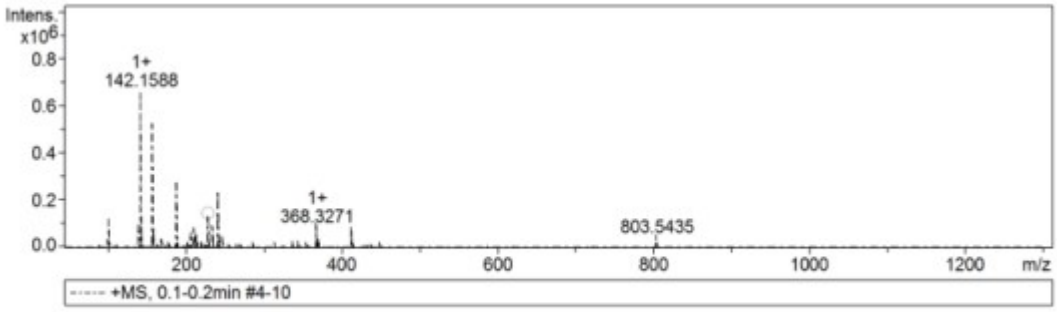
Meas. m/z	#	Ion Formula	Sum Formula	m/z	Adduct	err [ppm]	z	mSigma	Score	rdb	N-Rule	e⁻ Conf
193.0605	1	C9H9N2O3	C9H8N2O3	193.0608	M+H	1.3	1+	6.5	100.00	7.0	ok	even
215.0425	1	C9H8N2NaO3		215.0427	M+Na	0.8	1+	7.4	100.00	7.0	ok	even

HRMS of 2ac



Meas. m/z	#	Ion Formula	Sum Formula	m/z	Adduct	err [ppm]	z	mSigma	Score	rdb	N-Rule	e⁻ Conf
261.9836	1	C10H10BrNNaO	C10H10BrNO	261.9838	M+Na	0.7	1+	10.2	100.00	6.0	ok	even

HRMS of 2ad



Meas. m/z	#	Ion Formula	Sum Formula	m/z	Adduct	err [ppm]	z	mSigma	Score	rdb	N-Rule	e⁻ Conf
229.0583	1	C10H10N2NaO3	C10H10N2O3	229.0584	M+Na	0.5	1+	2.9	100.00	7.0	ok	even