Supporting Information for

Metal-free Tandem Cyclization/Hydrosilylation to Construct Tetrahydroquinoxalines

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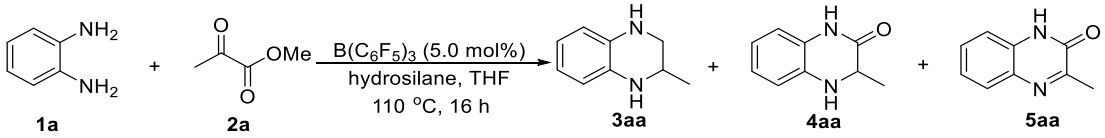
Contents:

1. General information:

Unless otherwise noted, all experiments were carried out in air, and all commercially available chemicals including organic solvents were used as received from Aldrich, Acros or Strem without further purification. ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker Model Avance DMX 400 Spectrometer (^{1}H 400 MHz and ^{13}C 100.6 MHz, respectively). Chemical shifts (δ) are given in ppm and are referenced to residual solvent peaks. 4,5-Dibromobenzene-1,2-diamine (**1m**),[1] 4,5-dimethoxybenzene-1,2-diamine (**1n**),[2] α-ketoesters[3,4a], chiral diene ligands[4b] and $HB(C_6F_5)_2$[4b] were prepared according to the previous reports.

2. Determination of the optimal reaction conditions

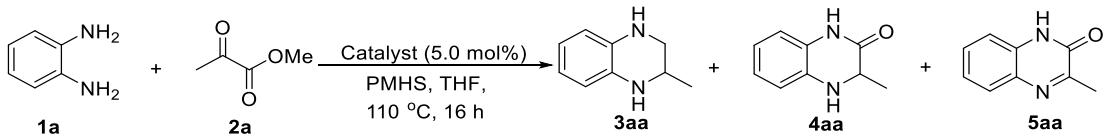
Table S1. Screening of hydrosilanes.[a]

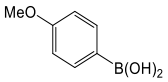
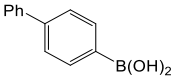
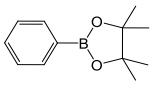
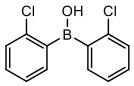


Entry	hydrosilane	**3aa**(%)[b]	**4aa**(%)[b]	**5aa** (%)[b]
1	$PhSiH_3$	67	25	3
2	Ph_2SiH_2	73	20	4
3	Et_3SiH	68	20	8
4	$(EtO)_3SiH$	62	27	10
5	$EtMe_2SiH$	71	23	2
6	Me_2PhSiH	25	60	13
7	TMDS	42	50	2
8	**PMHS**	**80**	**13**	**2**

[a] Reaction conditions: **1a** (0.25 mmol), **2a** (0.275 mmol), $B(C_6F_5)_3$ (5.0 mol%), THF (1.5 mL), hydrosilane (1.0 mmol) at 110 °C for 16 h. [b] Yield determined by ^{1}H NMR with CH_2Br_2 as an internal standard.

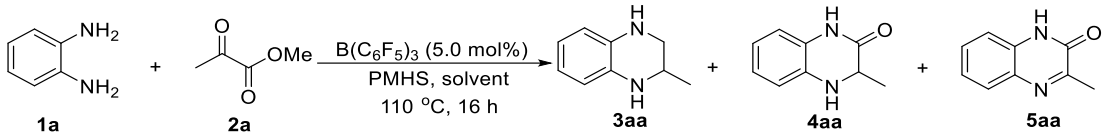
Table S2. Screening of catalysts.[a]



Entry	Catalyst	**3aa** (%)[b]	**4aa** (%)[b]	**5aa** (%)[b]
1	**$B(C_6F_5)_3$**	**80**	**13**	**2**
2	BF_3-OEt_2	12	18	68
3	BEt_3	3	20	73
4	BPh_3	<1	<1	95
5	$InCl_3$	60	25	12
6	$Fe_3(CO)_{12}$	45	35	16
7	$Zn(OAc)_2$	10	15	73
8	$Cu(OTf)_2$	12	15	62
9	$Co(acac)_3$	3	11	82
10	$Co(acac)_2$	2	25	67
11	$Co_2(CO)_8$	23	36	37
12	$Ni(acac)_2$	3	22	71
13		4	12	82
14		3	15	77
15		4	18	75
16		7	41	50

[a] Reaction conditions: **1a** (0.25 mmol), **2a** (0.275 mmol), catalyst (5.0 mol%), THF (1.5 mL), PMHS (1.0 mmol) at 110 °C for 16 h. [b] Yield determined by ^1H NMR with CH_2Br_2 as an internal standard.

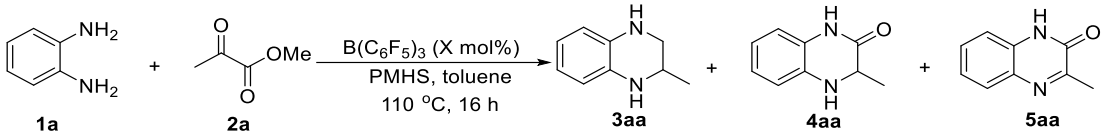
Table S3. Screening of solvents.[a]



Entry	Solvent	**3aa** (%)[b]	**4aa** (%)[b]	**5aa** (%)[c]
1	THF	80	13	2
2	1,4-dioxane	78	12	8
3	dibutyl ether	88	10	<1
4	1,2-dimethoxyl ethane	40	51	4
5	CH_2Cl_2	47	32	18
6	1,2-dichloroethane	53	26	16
7	**toluene**	**94**	**3**	**<1**
8	*p*-xylene	90	5	3
9	PhCl	88	10	<1
10	PhF	86	7	3
11	*tert*-butyl methyl ether	83	10	3
12	MeCN	62	25	10
13	ethanol	36	12	45
14	isopropanol	43	32	20
15	DMSO	4	12	80
16	DMF	4	3	85

[a] Reaction conditions: **1a** (0.25 mmol), **2a** (0.275 mmol), $B(C_6F_5)_3$ (5.0 mol%), solvent (1.5 mL), PMHS (0.06 mL, 1.0 mmol) at 110 °C for 16 h. [b] Yield determined by ^1H NMR with CH_2Br_2 as an internal standard.

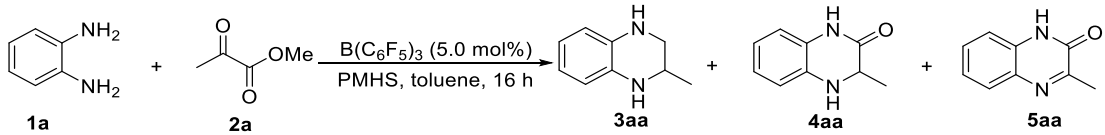
Table S4. Screening of catalyst loadings.[a]



Entry	X (mol%)	**3aa** (%)[b]	**4aa** (%)[b]	**5aa** (%)[b]
1	10	93	2	<1
2	8	92	3	<1
3	6	94	3	<1
4	**5**	**94**	**3**	**<1**
5	4	88	9	<1
6	2	73	23	3
7	1	44	50	4

[a] Reaction conditions: **1a** (0.25 mmol), **2a** (0.275 mmol), $B(C_6F_5)_3$, toluene (1.5 mL), PMHS (0.06 mL, 1.0 mmol) at 110 °C for 16 h. [b] Yield determined by ^1H NMR with CH_2Br_2 as an internal standard.

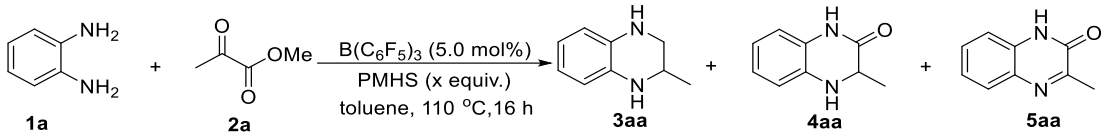
Table S5. Screening of reaction temperature.[a]



Entry	Temperature (°C)	**3aa** (%)[b]	**4aa** (%)[b]	**5aa** (%)[b]
1	140	92	4	<1
2	130	93	3	<1
3	120	94	3	<1
4	**110**	**94**	**3**	**<1**
5	100	91	6	<1
6	80	86	12	<1
7	60	75	15	8

[a] Reaction conditions: **1a** (0.25 mmol), **2a** (0.275 mmol), $B(C_6F_5)_3$ (5.0 mol%), PMHS (0.06 mL, 1.0 mmol), toluene (1.5 mL) at 110 °C for 16 h. [b] Yield determined by ^1H NMR with CH_2Br_2 as an internal standard.

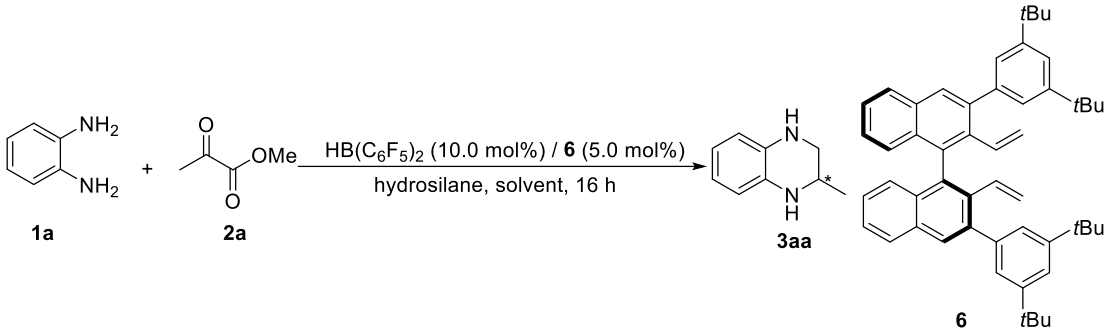
Table S6. Variation of the amount of PMHS.[a]



Entry	X (equiv.)	**3aa** (%)[b]	**4aa** (%)[b]	**5aa** (%)[b]
1	5	92	3	<1
2	**4**	**94**	**4**	**<1**
3	3	83	13	<1
4	2	35	64	<1
5	1.5	20	75	<1
6	1	7	65	25

[a] Reaction conditions: **1a** (0.25 mmol), **2a** (0.275 mmol), $B(C_6F_5)_3$ (5. 0 mol%), toluene (1.5 mL), PMHS (0.06 mL, 1.0 mmol) at 110 °C for 16 h. [b] Yield determined by ^1H NMR with CH_2Br_2 as an internal standard.

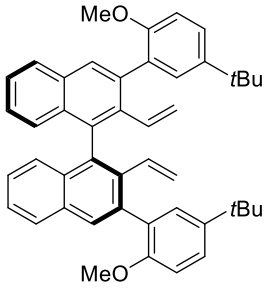
Table S7. Preliminary optimization studies for asymmetric synthesis of **3aa**.[a]



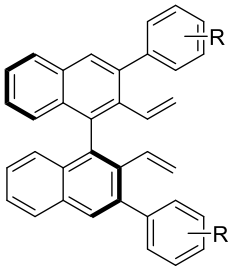
Entry	hydrosilane	solvent	Temp (°C)	**3aa** (%)[b]	ee (%)[c]
1	PMHS	toluene	110	92	racemic
2	PMHS	THF	110	86	18
3	PMHS	*n*Bu_2O	110	88	11
4	PMHS	1,4-dioxane	110	78	6
5	PMHS	1,2-dimethoxyl ethane	110	72	racemic
6	PMHS	*tert*-butyl methyl ether	110	76	11
7	PMHS	CH_2Cl_2	110	43	racemic
8	PMHS	1,2-dichloroethane	110	66	5
9	PMHS	MeCN	110	58	racemic
10	PMHS	*i*PrOH	110	21	racemic
11	PMHS	*p*-xylene	110	88	racemic
12	PMHS	PhCl	110	81	12
13	PMHS	PhF	110	84	13
14	PMHS	THF	90	85	18
15	PMHS	THF	70	84	28
16	PMHS	THF	50	71	28
17	**Ph_2SiH_2**	**THF**	**70**	**87**	**47**
18	Et_3SiH	THF	70	76	32
19	$(EtO)_3SiH$	THF	70	72	27
20	$EtMe_2SiH$	THF	70	68	racemic
21	Me_2PhSiH	THF	70	72	12
22	TMDS	THF	70	52	14
23	Ph_2SiH_2	THF	50	62	47
24[d]	Ph_2SiH_2	THF	70	87	44

25[e]	Ph_2SiH_2	THF	70	85	41
26[f]	Ph_2SiH_2	THF	70	86	42

[a] Reaction conditions: **1a** (0.25 mmol), **2a** (0.275 mmol), $HB(C_6F_5)_2$ (10.0 mol%), **6** (5.0 mol%), solvent (1.5 mL), hydrosilane (1.0 mmol) for 16 h. [b] Isolated yield. [c] The ee values were determined by HPLC using a Chiralcel OD-H column. [d] Chiral diene **7** was employed. [e] Chiral diene **8** was employed. [f] Chiral diene **9** was employed.



7



8, R = 3,5-[3,5-$(TMS)_2C_6H_3]_2$
9, R = 3,5-(3,5-$t Bu_2C_6H_3)_2$

3.General procedure for the synthesis of tetrahydroquinoxalines

(1) General procedure for the synthesis of 2-substituted tetrahydroquinoxalines

To an oven-dried screw-capped pressure tube were sequentially added 1,2-diaminobenzene **1** (0.25 mmol), α-ketoester **2** (0.275 mmol), $B(C_6F_5)_3$ (6.4 mg, 5.0 mol%), PMHS (0.06 mL, 1.0 mmol) and toluene (1.5 mL). Then the reaction mixture was stirred at 110 °C for 16 h. After cooling to ambient temperature, the mixture was diluted with EtOAc (5.0 mL). Then water (5.0 mL) was added to the reaction mixture, which was extracted with EtOAc three times (5.0 mL each). The combined organic phases were dried over Na_2SO_4, then filtered and evaporated under reduced pressure. After the removal of volatile materials by rotary evaporation, the resultant mixture was purified by silica gel column chromatography using a mixture of EtOAc and hexane to give the corresponding pure product.

(2) General procedure for the synthesis of 3,4-dihydroquinoxalin-2(1*H*)-ones

To an oven-dried screw-capped pressure tube were sequentially added 1,2-diaminobenzene **1** (0.25 mmol), α-ketoester **2** (0.275 mmol), $B(C_6F_5)_3$ (6.4 mg, 5.0 mol%), PMHS (22.5 μL, 0.375 mmol) and toluene (1.5 mL). Then the reaction mixture was stirred at 110 °C for 3 h. After cooling to ambient temperature, the mixture was diluted with EtOAc (5.0 mL). Then water (5.0 mL) was added to the reaction mixture, which was then extracted with EtOAc three times (5.0 mL each). The combined organic phases were dried over Na_2SO_4, then filtered and evaporated under reduced pressure.

After the removal of volatile materials by rotary evaporation, the resultant mixture was purified by silica gel column chromatography using a mixture of EtOAc and hexane to give the corresponding pure product.

(3) **General procedure for grammar-scale transformation reaction**

To an oven-dried screw-capped pressure tube were sequentially added 1,2-diaminobenzene **1a** (1.08 g, 10.0 mmol), ethyl 2-oxopropanoate **2a** (1.28 g, 11.0 mmol), $B(C_6F_5)_3$ (250.0 mg, 5.0 mol%), PMHS (2.4 mL, 40.0 mmol) and toluene (60.0 mL). Then the reaction mixture was stirred at 110 °C for 16 h. After cooling to ambient temperature, the mixture was diluted with EtOAc (120.0 mL). Then water (100.0 mL) was added to the reaction mixture, which was extracted with EtOAc five times (30.0 mL each). The combined organic phases were dried over Na_2SO_4, then filtered and evaporated under reduced pressure. After the removal of volatile materials by rotary evaporation, the resultant mixture was purified by silica gel column chromatography using a mixture of EtOAc and hexane to give pure **3aa** (yellow solid, 1.3 g, 90%).

(4) **General procedure for asymmetric synthesis of 2-substituted tetrahydroquinoxalines**

To an oven-dried screw-capped pressure tube were sequentially added 1,2-diaminobenzene **1** (0.25 mmol), α-ketoester **2** (0.275 mmol), $HB(C_6F_5)_2$ (8.67 mg, 10.0 mol%), chiral diene **6** (7.88 mg, 5.0 mol%), Ph_2H_2Si (0.185 mL, 1.0 mmol) and THF (1.5 mL). Then the reaction mixture was stirred at 70 °C for 16 h. After cooling to ambient temperature, the mixture was diluted with EtOAc (5.0 mL). Then water (5.0 mL) was added to the reaction mixture, which was extracted with EtOAc three times (5.0 mL each). The combined organic phases were dried over Na_2SO_4, then filtered and evaporated under reduced pressure. After the removal of volatile materials by rotary evaporation, the resultant mixture was purified by silica gel column chromatography using a mixture of EtOAc and hexane to give the pure product.

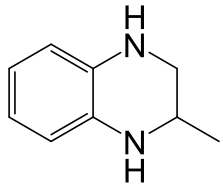
(5) **General procedure for asymmetric synthesis of 3,4-dihydroquinoxalin-2(1*H*)-ones**

To an oven-dried screw-capped pressure tube were sequentially added 1,2-diaminobenzene **1** (0.25 mmol), α-ketoester **2** (0.275 mmol), $HB(C_6F_5)_2$ (8.67 mg, 10.0 mol%), chiral diene **6** (7.88 mg, 5.0 mol%), Ph_2H_2Si (0.069 mL, 0.375 mmol) and THF (1.5 mL). Then the reaction mixture was stirred at 45 °C for 16 h. After cooling to ambient temperature, the mixture was diluted with EtOAc (5.0 mL). Then water (5.0

mL) was added to the reaction mixture, which was extracted with EtOAc five times (5.0 mL each). The combined organic phases were dried over Na_2SO_4, then filtered and evaporated under reduced pressure. After the removal of volatile materials by rotary evaporation, the resultant mixture was purified by silica gel column chromatography using a mixture of EtOAc and hexane to give the pure product.

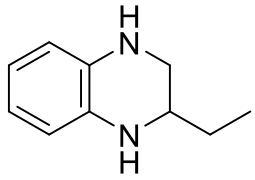
4. Characterization of the products

2-Methyl-1,2,3,4-tetrahydroquinoxaline (**3aa**)[5]



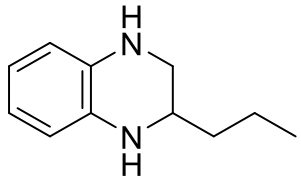
Yellow solid, mp: 71-72 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.99-6.13 (m, 4H), 4.05 (s, 2H), 3.60-3.40 (m, 2H), 3.12-2.89 (m, 1H), 1.15 (dd, *J* = 17.4, 6.5 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 134.37, 133.58, 133.15, 118.81, 118.76, 114.57, 48.23, 45.73, 19.90; HRMS (ESI) calcd. for $C_9H_{13}N_2$ $[M+H]^+$: 149.1073, found: 149.1075.

2-Ethyl-1,2,3,4-tetrahydroquinoxaline (**3ab**)[5]



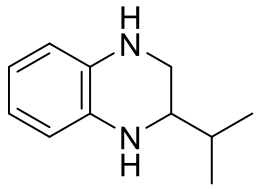
Yellow solid, mp: 67-69 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.59-6.48 (m, 4H), 3.41-3.36 (m, 1H), 3.32 (ddd, *J* = 14.1, 6.7, 2.9 Hz, 1H), 3.08-3.04 (m, 1H), 1.55-1.48 (m, 2H), 1.00 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 133.41, 133.15, 118.97, 118.72, 114.60, 51.71, 46.21, 27.06, 10.03; HRMS (ESI) calcd. for $C_{10}H_{15}N_2$ $[M+H]^+$: 163.1230, found: 163.1227.

2-Propyl-1,2,3,4-tetrahydroquinoxaline (**3ac**)[6]



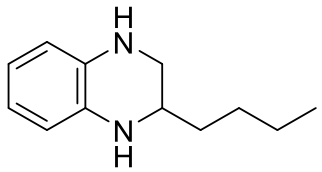
Brown-yellow solid, mp: 66-67 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.60-6.58 (m, 2H), 6.50 (dd, *J* = 8.4, 4.1 Hz, 2H), 3.36-3.34 (m, 2H), 3.08-3.03 (m, 1H), 1.47-1.44 (m, 4H), 0.97 (td, *J* = 6.8, 3.9 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 133.53, 133.41, 118.76, 118.61, 114.49, 114.44, 53.45, 49.99, 36.44, 18.86, 14.16; HRMS (ESI) calcd. for $C_{11}H_{17}N_2$ $[M+H]^+$: 177.1386, found: 177.1388.

2-Isopropyl-1,2,3,4-tetrahydroquinoxaline (**3ad**)[7]



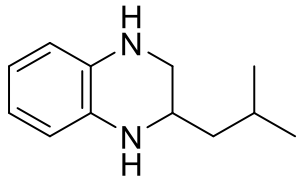
Brown solid, mp: 73-75 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.59-6.48 (m, 4H), 3.37-3.34 (m, 1H), 3.11 (dt, *J* = 14.0, 6.7 Hz, 1H), 1.76-1.67 (m, 1H), 0.98 (ddd, *J* = 21.7, 14.8, 6.9 Hz, 6H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 133.87, 133.36, 118.84, 118.39, 114.37, 114.32, 56.00, 53.44, 31.03, 18.73; HRMS (ESI) calcd. for $C_{11}H_{17}N_2$ $[M+H]^+$: 177.1386, found: 177.1395.

2-Butyl-1,2,3,4-tetrahydroquinoxaline (**3ae**)[7]



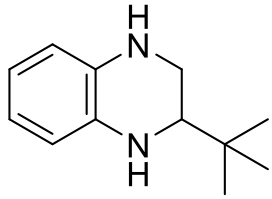
Brown solid; mp: 58-59°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.59-6.53 (m, 2H), 6.52-6.51 (m, 2H), 3.38 (d, *J* = 8.5 Hz, 2H), 3.07 (dd, *J* = 17.8, 6.9 Hz, 1H), 1.51-1.36 (m, 6H), 0.95 (dd, *J* =9.1, 5.0 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 134.37, 133.58, 133.15, 118.79, 118.62, 114.47, 50.24, 46.66, 33.98, 31.68, 27.82, 21.05, 14.20; HRMS (ESI) calcd. for $C_{12}H_{19}N_2$ $[M+H]^+$: 191.1543, found: 191.1548.

2-Isobutyl-1,2,3,4-tetrahydroquinoxaline (**3af**)[8]



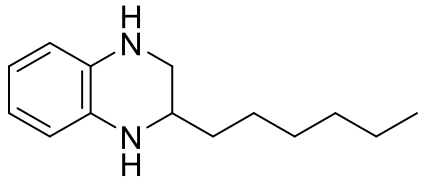
Yellow solid, mp: 69-70°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.65-6.40 (m, 4H), 3.62 (s, 2H), 3.43 (qd, *J* = 7.8, 2.8 Hz, 1H), 3.33 (dd, *J* = 10.7, 2.8 Hz, 1H), 3.14-2.85 (m, 1H), 1.74 (dp, *J* = 13.3, 6.7 Hz, 1H), 1.44-1.24 (m, 3H), 0.99-0.90 (m, 6H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 133.57, 133.52, 118.77, 118.69, 114.60, 114.49, 48.18, 47.09, 43.41, 24.53, 23.24, 22.59; HRMS (ESI) calcd. for $C_{12}H_{19}N_2$ $[M+H]^+$: 191.1543, found: 191.1550.

2-(Tert-butyl)-1,2,3,4-tetrahydroquinoxaline (**3ag**)[8]



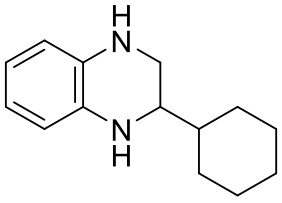
Yellow solid, mp: 82-83°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.656.44 (m, 4H), 3.80-3.47 (m, 1H), 3.45-3.23 (m, 1H), 3.23-2.88 (m, 2H), 0.98 (s, 9H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 134.57, 133.36, 118.85, 118.24, 114.32, 114.25, 59.02, 42.52, 32.79, 26.05; HRMS (ESI) calcd. for $C_{12}H_{19}N_2[M+H]^+$: 191.1543, found: 191.1546.

2-Hexyl-1,2,3,4-tetrahydroquinoxaline (**3ah**)[8]



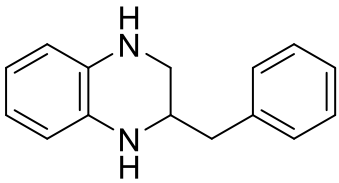
Yellow solid, mp: 74-76°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.54 (dq, *J* = 29.5, 4.6 Hz, 4H), 3.62 (s, 1H), 3.40-3.25 (m, 1H), 3.04 (dd, *J* = 11.1, 8.4 Hz, 1H), 1.59-1.16 (m, 10H), 0.89 (t, *J* = 6.5 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 133.58, 133.47, 118.72, 118.59, 114.47, 114.42, 50.27, 46.72, 34.34, 31.81, 29.41, 25.64, 22.65, 14.13; HRMS (ESI) calcd. for $C_{14}H_{23}N_2[M+H]^+$: 219.1856, found: 219.1866.

2-Cyclohexyl-1,2,3,4-tetrahydroquinoxaline (**3ai**)[8]



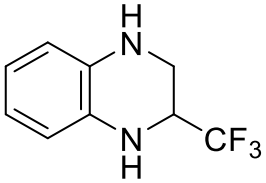
Yellow solid, mp: 105-106°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.63-6.53 (m, 2H), 6.52-6.42 (m, 2H), 3.67 (s, 2H), 3.36 (dd, *J* = 10.4, 2.3 Hz, 1H), 3.24-3.03 (m, 2H), 1.92-1.63 (m, 5H), 1.54-1.36 (m, 1H), 1.33-0.95 (m, 6H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 133.77, 133.42, 118.69, 118.28, 114.26, 55.12, 43.90, 40.65, 29.11, 28.88, 26.39, 26.12, 26.07; HRMS (ESI) calcd. for $C_{14}H_{21}N_2$ $[M+H]^+$: 217.1699, found: 217.1705.

2-Benzyl-1,2,3,4-tetrahydroquinoxaline (**3aj**)[6]



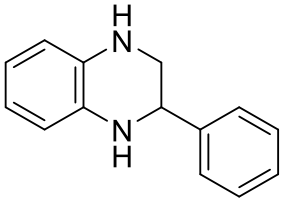
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37-7.17 (m, 5H), 6.62-6.35 (m, 4H), 3.65-3.53 (m, 1H), 3.37 (dd, *J* = 10.8, 2.8 Hz, 1H), 3.15 (dd, *J* = 10.7, 7.1 Hz, 1H), 2.89-2.75 (m, 1H), 2.75-2.59 (m, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 138.05, 133.29, 133.07, 129.33, 128.72, 126.67, 118.87, 118.79, 114.64, 114.49, 51.29, 46.29, 40.58, 29.76; HRMS (ESI) calcd. for $C_{15}H_{17}N_2$ $[M+H]^+$: 225.1386, found: 225.1379.

2-(Trifluoromethyl)-1,2,3,4-tetrahydroquinoxaline (**3ak**)



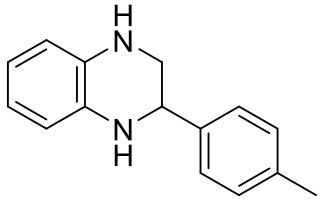
Pale-yellow oil; ^{1}H NMR (400 MHz, DMSO) δ 7.92 (d, *J* = 8.0 Hz, 1H), 7.73 (t, *J* = 7.3 Hz, 1H), 7.42 (t, *J* = 7.9 Hz, 2H), 4.38 (t, *J* = 4.8 Hz, 1H), 3.44 (tt, *J* = 17.0, 8.5 Hz, 2H); ^{13}C NMR (100.6 MHz, DMSO) δ 152.17, 134.20, 133.96, 130.34, 124.63, 116.33, 56.48, 55.38, 19.02; HRMS (ESI) calcd. for $C_9H_{10}F_3N_2$ $[M+H]^+$: 203.0791, found: 203.0793.

2-Phenyl-1,2,3,4-tetrahydroquinoxaline (**3al**)[9]



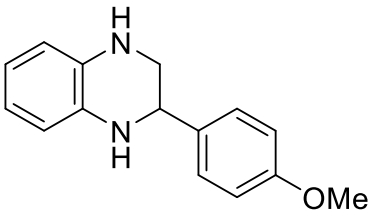
Yellow solid, mp: 121-123 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43-7.28 (m, 5H), 6.70-6.53 (m, 4H), 4.48 (dd, *J* = 8.2, 3.1 Hz, 1H), 3.46 (dd, *J* = 11.0, 3.1 Hz, 1H), 3.32 (dd, *J* = 11.0, 8.2 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 134.13, 132.82, 128.65, 127.91, 127.01, 118.90, 118.78, 114.70, 114.43, 53.46, 49.15; HRMS (ESI) calcd. for $C_{14}H_{15}N_2$ $[M+H]^+$: 211.1230, found 211.1233.

2-(*p*-Tolyl)-1,2,3,4-tetrahydroquinoxaline (3am)[9]



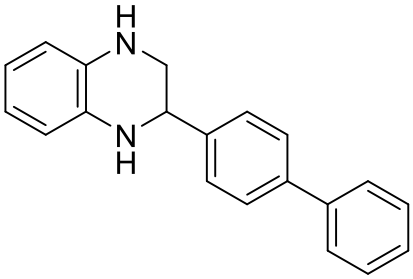
Yellow solid, mp: 120-121°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35-7.17 (m, 4H), 6.69-6.55 (m, 4H), 4.48 (dd, *J* = 8.2, 3.0 Hz, 1H), 3.88 (t, *J* = 18.3 Hz, 2H), 3.46 (dd, *J* = 11.0, 3.1 Hz, 1H), 3.34 (dd, *J* = 11.0, 8.2 Hz, 1H), 2.38 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 137.63, 129.32, 126.89, 118.88, 118.72, 114.68, 114.39, 54.44, 49.20, 21.15; HRMS (ESI) calcd for $C_{15}H_{17}N_2$ $[M+H]^+$: 225.1386, found 225.1384.

2-(4-Methoxyphenyl)-1,2,3,4-tetrahydroquinoxaline (3an)[9]



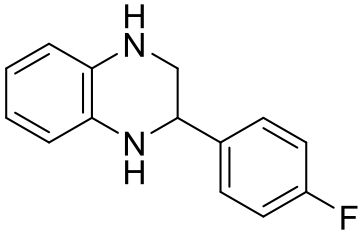
Yellow solid, mp: 63-65 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34-7.28 (m, 2H), 6.94-6.91 (m, 2H), 6.67-6.57 (m, 4H), 4.45 (ddd, *J* = 11.3, 8.2, 3.0 Hz, 1H), 3.84 (s, 3H), 3.45-3.42 (m, 1H), 3.34-3.29 (m, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 159.29, 134.22, 133.92, 132.85, 128.12, 118.84, 118.75, 114.65, 114.41, 114.01, 55.34, 54.09, 49.29; HRMS (ESI) calcd for $C_{15}H_{17}ON_2$ $[M+H]^+$: 241.1335, found 242.1339.

2-([1,1'-Biphenyl]-4-yl)-1,2,3,4-tetrahydroquinoxaline (3ao)[10]



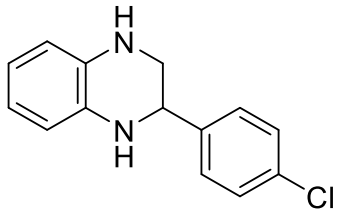
White solid, mp: 118-120 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (ddd, *J* = 5.8, 5.1, 4.3 Hz, 4H), 7.46-7.43 (m, 4H), 6.67-6.58 (m, 5H), 4.54 (dd, *J* = 8.0, 3.0 Hz, 1H), 3.51 (dd, *J* = 11.0, 3.1 Hz, 1H), 3.37 (dd, *J* = 11.0, 8.1 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 140.92, 132.83, 128.82, 127.40, 127.12, 118.98, 118.84, 114.76, 114.47, 54.45, 49.09; HRMS (ESI) calcd for $C_{20}H_{19}N_2$ $[M+H]^+$: 287.1543 found: 287.1547.

2-(4-Fluorophenyl)-1,2,3,4-tetrahydroquinoxaline (3ap)[9]



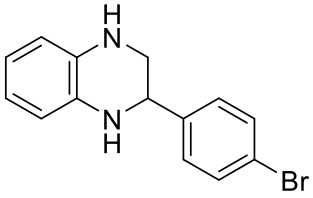
Yellow solid, mp: 103-104°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37-7.02 (m, 4H), 6.65-6.57 (m, 4H), 4.47 (dd, *J* = 8.1, 3.0 Hz, 1H), 3.42 (dd, *J* = 11.0, 3.1 Hz, 1H), 3.28 (dd, *J* = 11.0, 8.1 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 150.80, 142.98, 130.47, 129.65, 129.17, 128.62, 128.54, 118.95, 116.39, 115.59, 114.71, 54.02, 49.18; HRMS (ESI) calcd. for $C_{14}H_{14}FN_2$ $[M+H]^+$: 229.1136, found: 229.1131.

2-(4-Chlorophenyl)-1,2,3,4-tetrahydroquinoxaline (**3aq**)[9]



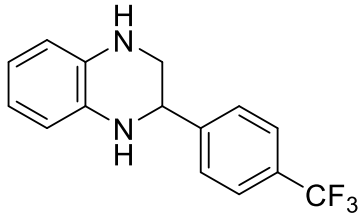
Yellow solid, mp 104-105°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33-7.29 (m, 4H), 6.65-6.55 (m, 4H), 4.45 (dd, *J* = 8.0, 3.1 Hz, 1H), 3.42 (dd, *J* = 11.1, 3.1 Hz, 1H), 3.26 (dd, *J* = 11.1, 8.0 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 140.45, 133.79, 132.75, 128.81, 128.36, 119.03, 118.99, 114.77, 114.53, 54.09, 49.00; HRMS (ESI) calcd. for $C_{14}H_{14}ClN_2$ $[M+H]^+$: 245.0840, found: 245.0833.

2-(4-Bromophenyl)-1,2,3,4-tetrahydroquinoxaline (**3ar**)[9]



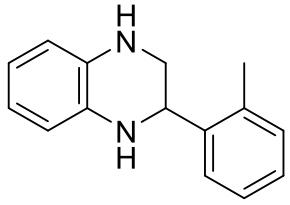
Yellow solid, mp: 144-146°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53-7.50 (m, 2H), 7.29-7.27 (m, 2H), 6.68-6.58 (m, 4H), 4.48 (dd, *J* = 8.0, 3.0 Hz, 1H), 3.46 (dt, *J* = 4.8, 2.4 Hz, 1H), 3.31 (ddd, *J* = 11.1, 8.0, 5.6 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 140.99, 133.77, 132.75, 131.76, 128.73, 121.68, 119.04, 119.00, 114.78, 114.55, 54.15, 48.93; HRMS (ESI) calcd for $C_{14}H_{14}BrN_2$ $[M+H]^+$: 289.0335, found: 285.0329.

2-(4-(Trifluoromethyl)phenyl)-1,2,3,4-tetrahydroquinoxaline (**3as**)[11]



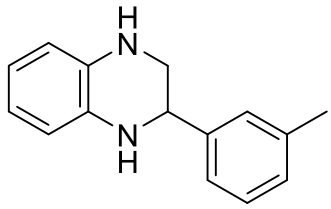
White solid, mp: 143-144 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68-7.49 (m, 4H), 6.77-6.50 (m, 4H), 4.58 (dd, J = 7.7, 3.0 Hz, 1H), 3.96 (d, J = 8.7 Hz, 2H), 3.50 (dd, J = 11.1, 3.1 Hz, 1H), 3.33 (dd, J = 11.1, 7.7 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100.6 MHz): δ 146.08, 133.60, 132.74, 127.88, 127.35, 126.09, 125.60, 119.15, 119.10, 114.67, 114.60, 54.36, 48.77; HRMS (ESI) calcd for $C_{15}H_{14}F_3N_2$ $[M+H]^+$: 279.1104, found: 279.1108.

2-(*o*-Tolyl)-1,2,3,4-tetrahydroquinoxaline (**3at**)[9]



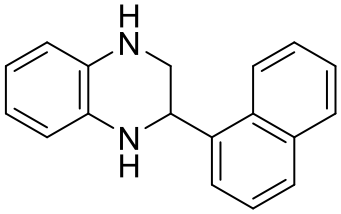
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55-7.45 (m, 1H), 7.33-7.16 (m, 3H), 6.76-6.52 (m, 4H), 4.75 (dd, J = 8.2, 2.9 Hz, 1H), 3.84 (d, J = 7.3 Hz, 1H), 3.48 (dd, J = 11.1, 3.0 Hz, 1H), 3.29 (dt, J = 21.6, 10.8 Hz, 1H), 2.45 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 139.55, 135.28, 134.47, 132.84, 130.47, 127.50, 126.66, 126.54, 118.91, 118.79, 114.72, 114.54, 77.42, 77.10, 76.78, 50.57, 47.81, 19.27; HRMS (ESI) calcd for $C_{15}H_{17}N_2$ $[M+H]^+$: 225.1386, found 225.1381.

2-(*m*-Tolyl)-1,2,3,4-tetrahydroquinoxaline (**3au**)[9]



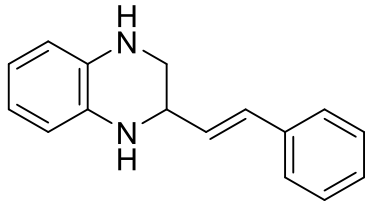
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26-7.10 (m, 4H), 6.63-6.54 (m, 4H), 4.42 (dd, *J* = 8.3, 3.0 Hz, 1H), 3.90-3.79 (m, 2H), 3.42 (dd, *J* = 11.0, 3.1 Hz, 1H), 3.30 (dd, *J* = 11.0, 8.3 Hz, 1H), 2.27-2.35(s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 141.75, 138.36, 134.20, 132.86, 128.67, 128.57, 127.69, 124.10, 118.90, 118.78, 114.72, 114.45, 54.72, 49.23, 21.49; HRMS (ESI) calcd. for $C_{15}H_{17}N_2$ $[M+H]^+$: 225.1386, found 225.1396.

2-(Naphthalen-1-yl)-1,2,3,4-tetrahydroquinoxaline (**3av**)[11]



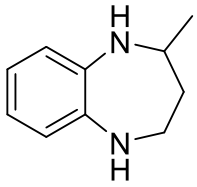
White solid, mp: 108-110 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01-7.96 (m, 1H), 7.89-7.78 (m, 1H), 7.54-7.53 (m, 1H), 7.51-7.44 (m, 4H), 6.67-6.58 (m, 4H), 5.30 (dd, *J* = 7.9, 2.9 Hz, 1H), 4.05-3.75 (m, 2H), 3.65 (dd, *J* = 11.2, 3.0 Hz, 1H), 3.44-3.39 (m,1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 137.17, 134.37, 134.06, 132.97, 130.49, 130.20, 129.71, 129.14, 128.21, 126.36, 125.74, 125.67, 124.12, 122.62, 119.06, 118.89, 114.89, 114.67, 50.71, 48.14; HRMS (ESI) calcd. for $C_{18}H_{17}N_2$ $[M+H]^+$: 261.1386, found 261.1379.

(*E*)-2-Styryl-1,2,3,4-tetrahydroquinoxaline (**3aw**)[10]



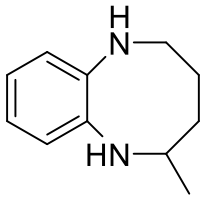
Red solid, mp: 104-105 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43-7.23 (m, 6H), 6.67-6.49 (m, 6H), 4.50 (dt, *J* = 11.5, 5.8 Hz, 1H), 3.48 (dd, *J* = 11.0, 3.1 Hz, 1H), 3.35 (dd, *J* = 11.0, 8.2 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 134.14, 132.83, 128.65, 128.55, 128.36, 127.91, 127.01, 118.89, 118.77, 114.70, 114.43, 114.32, 53.47, 49.15; HRMS (ESI) calcd. for $C_{16}H_{17}N_2$ $[M+H]^+$: 237.1386, found: 233.1379.

2-Methyl-2,3,4,5-tetrahydro-1H-benzo[b] [1, 4] diazepine (**3ax**)[12]



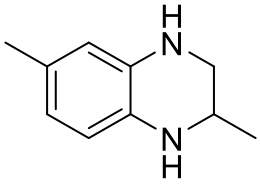
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.76-6.69 (m, 2H), 6.44-6.37 (m, 2H), 3.51-3.45 (m, 1H), 3.31-3.27 (m, 1H), 3.04-2.99 (m, 1H), 1.83-1.79 (m,1H), 1.64-1.57 (m,1H), 1.17 (d, *J* = 3.5 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 121.64, 120.69, 120.13, 114.97, 52.67, 45.91, 39.48, 19.74; HRMS (ESI) calcd. for $C_{10}H_{15}N_2$ $[M+H]^+$: 163.1230, found: 163.1234.

2-Methyl-1,2,3,4,5,6-hexahydrobenzo[b] [1, 4]diazocine (**3ay**)



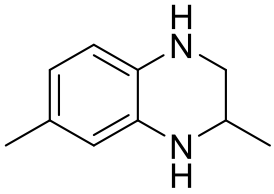
White solid, mp: 112-114 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (dd, *J* = 5.7, 3.3 Hz, 2H), 7.53 (dd, *J* = 5.7, 3.3 Hz, 2H), 4.22 (qd, *J* = 10.9, 6.0 Hz, 3H), 1.72-1.65 (m, 2H), 1.46-1.39 (m, 2H), 1.31 (d, *J* = 3.0 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 119.64, 118.13, 117.68, 111.96, 53.67, 46.91, 31.48, 29.48, 22.75; HRMS (ESI) calcd. for $C_{11}H_{17}N_2$ $[M+H]^+$: 177.1386, found: 177.1397.

2,6-Dimethyl-1,2,3,4-tetrahydroquinoxaline (**3ba$_1$**)



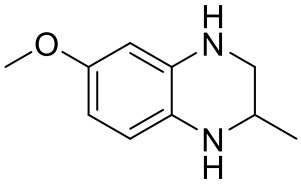
Yellow solid, mp: 77-79 °C;^{1}H NMR (400 MHz, $CDCl_3$) δ 6.39 (ddd, *J* = 27.3, 13.5, 4.7 Hz, 3H), 3.50 (ddd, *J* = 12.0, 6.0, 2.8 Hz, 1H), 3.29 (dt, *J* = 10.7, 3.3 Hz, 1H), 3.07-2.93 (m, 1H), 2.17 (s, 3H), 1.17 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 131.06, 130.64, 119.05, 115.20, 114.73, 48.42, 45.94, 45.87, 20.68, 19.94; HRMS (ESI) calcd. for $C_{10}H_{15}N_2$ $[M+H]^+$: 163.1230, found: 163.1233.

2,7-Dimethyl-1,2,3,4-tetrahydroquinoxaline (**3ba$_2$**)



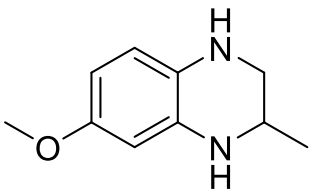
Yellow solid, mp: 75-76 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.44 (m, 3H), 3,91(s, 3H), 3.50 (m, 1H), 3.29 (dt, *J* = 10.3, 3.6 Hz, 1H), 3.04-2.97 (m, 1H), 2.17 (s, 3H), 1.18 (d, *J* = 6.7 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 130.61, 127.92, 118.65, 114.82, 114.35, 48.08, 45.51, 20.32, 19.58; HRMS (ESI) calcd. for $C_{10}H_{15}N_2$ $[M+H]^+$:163.1230, found: 163.1238.

6-Methoxy-2-methyl-1,2,3,4-tetrahydroquinoxaline (**3ca$_1$**)[6]



White solid, mp: 90-91 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.39 (ddd, *J* = 27.3, 13.5, 4.7 Hz, 3H), 3.91 (s, 3H), 3.56-3.42 (m, 2H), 3.29 (dt, *J* = 10.7, 3.3 Hz, 1H), 3.05-2.96 (m, 1H), 1.17 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 153.17, 134.64, 127.88, 114.76, 102.90, 100.74, 55.62, 48.01, 45.53, 19.64; HRMS (ESI) calcd. for $C_{10}H_{15}N_2O$ $[M+H]^+$:179.1179, found: 179.1185.

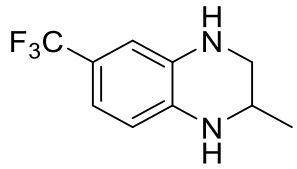
7-Methoxy-2-methyl-1,2,3,4-tetrahydroquinoxaline (**3ca$_2$**)



White solid, mp: 94-96 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.39 (ddd, *J* = 27.3, 13.5, 4.7 Hz, 3H), 3.91 (s, 3H), 3.56-3.42 (m, 2H), 3.29 (dt, *J* = 10.7, 3.3 Hz, 1H), 3.05-2.96 (m, 1H), 1.17 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 153.17, 134.64, 127.88, 114.76, 102.90, 100.74, 55.62, 48.01, 45.53, 19.64; HRMS (ESI) calcd. for $C_{10}H_{15}N_2O$

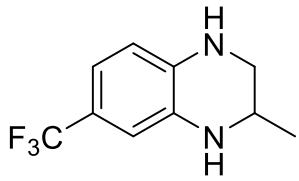
$[M+H]^+$:179.1179, found: 179.1175.

2-Methyl-6-(trifluoromethyl)-1,2,3,4-tetrahydroquinoxaline (**3da$_1$**) [13]



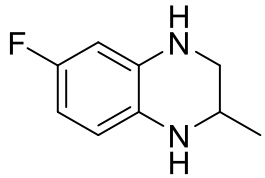
Brown solid, mp: 112-113 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.84 (d, *J* = 8.1 Hz, 1H), 6.71 (s, 1H), 6.49 (dd, *J* = 8.1, 2.7 Hz, 1H), 3.83 (s, 1H), 3.62-3.45 (m, 1H), 3.36 (ddd, *J* = 10.8, 7.8, 3.0 Hz, 1H), 3.06 (ddd, *J* = 16.2, 10.8, 8.0 Hz, 1H), 1.22 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 136.38, 132.60, 123.60, 115.81, 112.94, 110.54, 47.57, 45.54, 19.70; HRMS (ESI) calcd. for $C_{10}H_{12}F_3N_2$ $[M+H]^+$:217.0947, found: 217.0953.

2-Methyl-7-(trifluoromethyl)-1,2,3,4-tetrahydroquinoxaline (**3da$_2$**)



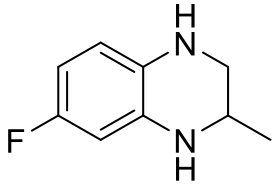
White solid, mp: 101-103 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.95 (d, *J* = 8.3 Hz, 1H), 6.95 (s, 1H), 6.59 (dd, *J* = 8.1, 2.4 Hz, 1H), 3.69-3.60 (m, 1H), 3.50 (ddd, *J* = 11.2, 7.3, 3.3 Hz, 1H), 3.15 (ddd, *J* = 16.2, 11.8, 8.1 Hz, 1H), 1.34 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 136.86, 133.08, 124.08, 120.53, 116.29, 113.42, 111.03, 48.06, 45.67, 21.53; HRMS (ESI) calcd. for $C_{10}H_{12}F_3N_2$ $[M+H]^+$: 217.0947, found: 217.0945.

6-Fluoro-2-methyl-1,2,3,4-tetrahydroquinoxaline (**3ea$_1$**)



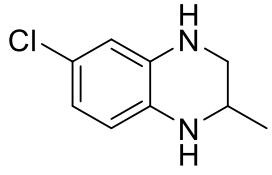
White solid, mp: 84-85 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.48-6.11 (m, 3H), 3.63-3.18 (m, 3H), 3.11-2.90 (m, 1H), 1.18 (d, *J* = 6.2 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 114.84, 103.94, 103.72, 101.15, 100.89, 48.11, 45.81, 45.51, 19.77; HRMS (ESI) calcd. for $C_9H_{12}FN_2$ $[M+H]^+$: 167.0979, found: 167.0977.

7-Fluoro-2-methyl-1,2,3,4-tetrahydroquinoxaline (**3ea$_2$**)



Yellow solid, mp: 92-93 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.45-6.22 (m, 3H), 3.56-3.51 (m, 1H), 3.32-2.97 (m, 1H), 1.21 (d, *J* = 6.2 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 128.99, 115.11, 104.21, 103.99, 101.42, 101.16, 48.38, 46.08, 20.04; HRMS (ESI) calcd. for $C_9H_{12}FN_2$ $[M+H]^+$:167.0985, found: 167.0979.

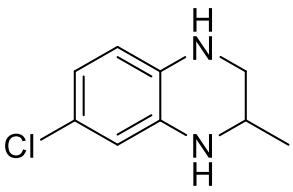
6-Chloro-2-methyl-1,2,3,4-tetrahydroquinoxaline (**3fa$_1$**)[6]



Yellow solid, mp: 86-87 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.52-6.38 (m, 3H), 3.52-3.45(m, 1H), 3.33-3.30 (m, 1H), 3.04-2.96 (m, 1H), 1.17 (d, *J* = 6.2 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 131.53, 130.00, 117.92, 114.94, 113.76, 47.91, 45.55, 19.78; HRMS (ESI) calcd. for

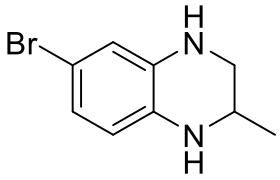
$C_9H_{12}ClN_2$ $[M+H]^+$:183.0684, found: 183.0681.

7-Chloro-2-methyl-1,2,3,4-tetrahydroquinoxaline (**3fa$_2$**)



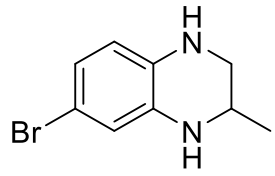
White solid, mp: 77-78 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.45-6.22 (m, 3H), 3.55-3.44(m, 1H), 3.35-3.29 (m, 1H), 3.07-2.99 (m, 1H), 1.21 (d, *J* = 6.2 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 134.36, 131.65, 130.12, 118.03, 115.05, 113.87, 48.02, 45.67, 19.90; HRMS (ESI) calcd. for $C_9H_{12}ClN_2$ $[M+H]^+$: 183.0684, found: 183.0687.

6-Bromo-2-methyl-1,2,3,4-tetrahydroquinoxaline (**3ga$_1$**)



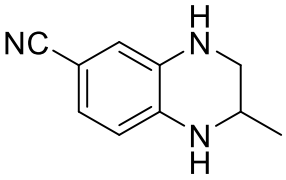
Dark brown solid, mp: 88-90 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.67-6.23 (m, 3H), 3.54-3.33 (m, 1H), 3.30 (dd, *J* = 10.8, 2.7 Hz, 1H), 3.08-2.88 (m, 1H),1.17 (d, *J* = 6.3 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 120.76, 116.45, 116.35, 115.34, 115.26, 110.09, 47.81, 45.48, 19.73; HRMS (ESI) calcd. for $C_9H_{12}BrN_2$ $[M+H]^+$: 227.0178, found: 227.0171.

7-Bromo-2-methyl-1,2,3,4-tetrahydroquinoxaline (**3ga$_2$**)



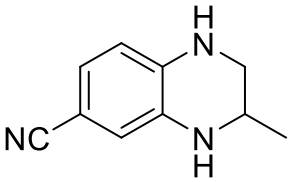
Brown solid, mp: 77-80 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.60-6.29 (m, 3H), 3.46-3.40 (m, 2H), 3.27 (dd, *J* = 9.8, 2.5 Hz, 1H), 2.99-2.92 (m, 1H),1.14 (d, *J* = 6.6 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 134.98, 132.46, 120.76, 116.45, 115.34, 110.09, 47.83, 45.48, 19.73; HRMS (ESI) calcd. for $C_9H_{12}BrN_2$ $[M+H]^+$: 227.0178, found: 227.0185.

2-Methyl-1,2,3,4-tetrahydroquinoxaline-6-carbonitrile (**3ha$_1$**)



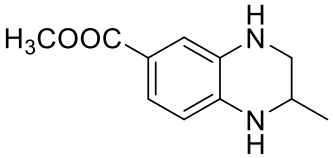
Grey solid, mp: 100-101°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.47-6.33 (m, 3H), 3.53-3.44 (m, 1H), 3.33-3.24 (m, 1H), 3.04-2.94 (m, 1H), 1.17 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 131.06, 123.84, 119.08, 116.30, 115.17, 114.74, 112.99, 48.42, 45.87, 19.87; HRMS (ESI) calcd. for $C_{10}H_{12}N_3$ $[M+H]^+$:174.1026, found: 174.1037.

2-Methyl-1,2,3,4-tetrahydroquinoxaline-7-carbonitrile (**3ha$_2$**)



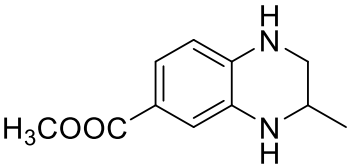
White solid, mp: 95-96 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.44-6.37 (m, 3H), 3.51-3.44 (m, 3H), 3.32-3.27 (m, 1H), 3.04-2.99 (m, 1H), 1.17 (d, *J* = 6.2 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 130.86, 123.64, 118.88, 116.20, 114.96, 114.53, 112.79, 48.22, 45.67, 20.48; HRMS (ESI) calcd. for $C_{10}H_{12}N_3$ $[M+H]^+$:174.1026, found: 174.1029.

Methyl 2-methyl-1,2,3,4-tetrahydroquinoxaline-6-carboxylate (**3ia$_1$**)



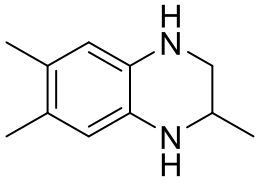
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33-7.19 (m, 2H), 6.43 (d, *J* = 8.2 Hz, 1H), 3.83 (s, 3H), 3.62-3.57 (m, 2H), 3.47-3.06 (m, 1H), 1.23-1.16 (m, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 167.54, 138.32, 131.91, 121.69, 119.05, 115.18, 112.52, 51.51, 47.44, 45.86, 44.90, 19.83; HRMS (ESI) calcd. for $C_{11}H_{15}N_2O_2$ $[M+H]^+$:207.1128, found: 207.1131.

Methyl 2-methyl-1,2,3,4-tetrahydroquinoxaline-7-carbo-xylate (**3ia$_2$**)



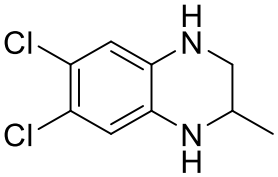
Colourless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33-7.19 (m, 2H), 6.43 (d, *J* = 7.8 Hz, 1H), 3.82 (s, 3H), 3.62-3.57 (m, 2H), 3.47-3.06 (m, 1H), 1.23-1.16 (m, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 167.54, 138.32, 131.91, 121.69, 119.05, 115.18, 112.52, 51.51, 47.44, 45.86, 44.90, 19.83; HRMS (ESI) calcd. for $C_{11}H_{15}N_2O_2$ $[M+H]^+$:207.1128, found: 207.1133.

2,6,7-Trimethyl-1,2,3,4-tetrahydroquinoxaline (**3ja**)[8]



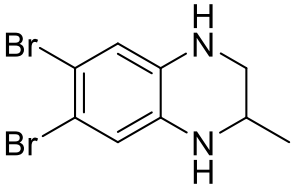
White solid, mp: 105-106 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.33 (d, *J* = 4.9 Hz, 2H), 3.27 (m, 2H), 3.07-2.89 (m, 1H), 2.04 (s, 6H), 1.14 (dd, *J* = 21.9, 8.0 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 131.43, 130.97, 126.42, 116.37, 48.61, 46.07, 21.04, 19.88, 18.87; HRMS (ESI) calcd. for $C_{11}H_{17}N_2$ $[M+H]^+$: 177.1386, found: 177.1381.

6,7-Dichloro-2-methyl-1,2,3,4-tetrahydroquinoxaline (**3ka**)[6]



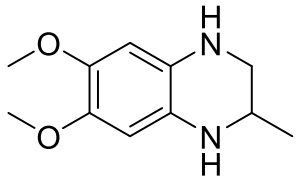
White solid, mp: 101-102 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.52 (t, *J* = 3.7 Hz, 2H), 3.53-3.37 (m, 1H), 3.30 (dd, *J* = 10.8, 3.0 Hz, 1H), 2.99 (dd, *J* = 10.7, 8.1 Hz, 1H), 1.18 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 133.15, 132.84, 120.27, 114.68, 114.57, 47.57, 45.35, 19.68; HRMS (ESI) calcd. for $C_9H_{11}Cl_2N_2$ $[M+H]^+$: 217.0294, found: 217.0299.

6,7-Dibromo-2-methyl-1,2,3,4-tetrahydroquinoxaline (**3la**)



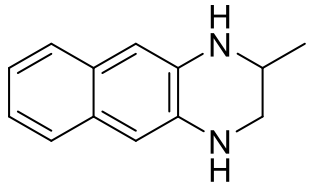
Brown solid, mp: 112-114 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.56 (d, *J* = 3.7 Hz, 2H), 3.53-3.49 (m, 1H), 3.36 (dd, *J* = 10.8, 3.0 Hz, 1H), 3.01 (dd, *J* = 10.7, 8.1 Hz, 1H), 1.23 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 133.14, 132.86, 118.28, 114.69, 1114.57, 47.57, 45.33, 19.77; HRMS (ESI) calcd. for $C_9H_{11}Br_2N_2$ $[M+H]^+$: 304.9283, found: 304.9291.

6,7-Dimethoxy-2-methyl-1,2,3,4-tetrahydroquinoxaline (**3ma**)



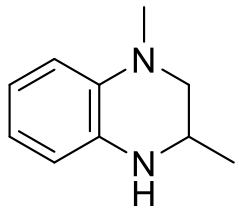
White solid, mp: 131-132 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.25 (d, *J* = 4.9 Hz, 2H), 4.04 (d, *J* = 7.1 Hz, 6H), 3.38 (s, 2H), 3.20 (d, *J* = 8.8 Hz, 1H), 2.89 (d, *J* = 14.6 Hz, 1H), 1.09 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 139.55, 139.09, 125.53, 100.48, 59.50, 47.72, 45.19, 17.99; HRMS (ESI) calcd. for $C_{11}H_{17}O_2N_2$ $[M+H]^+$: 209.1285, found: 209.1277.

2-Methyl-1,2,3,4-tetrahydrobenzo[g]quinoxaline (**3na**)



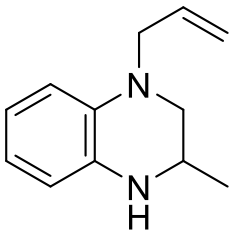
White solid, mp: 173-175 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (dd, *J* = 5.9, 3.3 Hz, 2H), 7.14 (dd, *J* = 6.2, 3.3 Hz, 2H), 6.82 (s, 2H), 3.72-3.55 (m, 1H), 3.39 (d, *J* = 3.1 Hz, 1H), 3.16 (d, *J* = 8.5 Hz, 1H), 1.26 (d, *J* = 3.8 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 134.80, 134.46, 129.08, 125.20, 125.12, 122.57, 122.49, 107.96, 107.73, 47.87, 45.76, 19.75; HRMS (ESI) calcd. for $C_{13}H_{15}N_2$ $[M+H]^+$: 199.1230, found: 199.1226.

1,3-Dimethyl-1,2,3,4-tetrahydroquinoxaline (**3oa**)



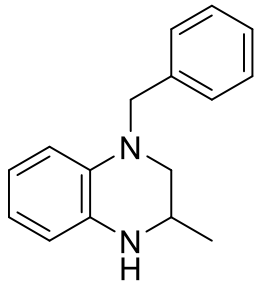
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.69-6.65 (m, 1H), 6.58-6.55 (m, 2H), 6.48 (dd, *J* = 7.5, 1.4 Hz, 1H), 3.62 (s, 1H), 3.15 (dd, *J* = 10.6, 2.4 Hz, 1H), 2.94 (t, *J* = 8.8 Hz, 1H), 2.85 (s, 3H), 1.17 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 129.33, 126.91, 118.19, 114.42, 113.47, 111.56, 56.97, 45.67, 39.11, 20.08; HRMS (ESI) calcd. for $C_{10}H_{15}N_2$ $[M+H]^+$: 163.1230, found: 163.1238.

1-Allyl-3-methyl-1,2,3,4-tetrahydroquinoxaline (**3pa**)



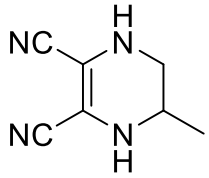
Pale-yellow oil; ^{1}H NMR (400 MHz, CDCl3) δ 6.72-6.48 (m, 4H), 5.93-5.83 (m, 1H), 5.28-5.17 (m, 2H), 3.86 (dtd, J = 20.8, 16.7, 8.7 Hz, 2H), 3.57 (d, J = 6.2 Hz, 1H), 3.22 (dd, J = 10.7, 2.6 Hz, 1H), 3.04 (dd, J = 13.1, 6.0 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 135.79, 134.48, 133.65, 119.15, 118.15, 117.55, 113.97, 111.53, 59.71, 55.15, 45.27, 19.91; HRMS (ESI) calcd. for $C_{12}H_{17}N_2$ $[M+H]^+$: 189.1286, found: 189.1282.

1-Benzyl-3-methyl-1,2,3,4-tetrahydroquinoxaline (**3qa**)



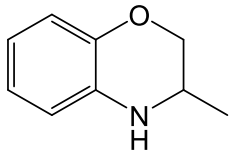
Colourless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32-7.28 (m, 5H), 6.60-6.51 (m, 4H), 4.72 (s, 1H), 4.43 (s, 1H), 3.58-3.55 (m, 1H), 3.26-3.23 (m, 1H), 3.11-3.07 (m, 1H), 1.17 (d, *J* = 6.3 Hz, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 138.77, 134.93, 133.70, 128.57, 126.99, 126.87, 119.15, 117.59, 113.97, 111.51, 55.28, 55.16, 45.31, 19.91; HRMS (ESI) calcd. for $C_{16}H_{19}N_2$ $[M+H]^+$: 239.1543, found: 239.1547.

5-Methyl-1,4,5,6-tetrahydropyrazine-2,3-dicarbonitrile (**3ra**)



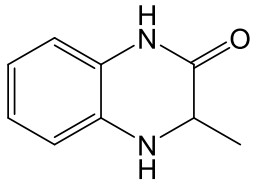
White solid, mp: 101-102 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.348-3.44 (m, 1H), 3.31- 3.28 (m, 1H), 3.00-2.96 (m, 1H), 1.18 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 120.34, 120.27, 114.70, 114.58, 47.56, 45.35, 19.65; HRMS (ESI) calcd. for $C_7H_9N_4$ $[M+H]^+$: 149.0822, found: 149.0826.

3-Methyl-3,4-dihydro-2H-benzo[b][1,4]oxazine (**3sa**)[14]



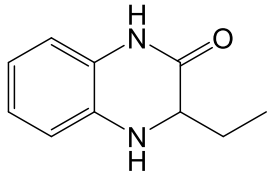
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.76-6.48 (m, 4H), 4.28 (m, 1H), 3.69-3.62 (m, 1H), 3.50-3.45 (m, 1H), 1.27 (dd, *J* = 17.4, 6.3 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 143.75, 132.14, 121.20, 118.87, 116.20, 113.53, 45.87, 19.88; HRMS (ESI) calcd. for $C_9H_{12}NO$ $[M+H]^+$: 150.0913, found: 150.0921.

3-Methyl-3,4-dihydroquinoxalin-2(1H)-one (**4aa**)[8]



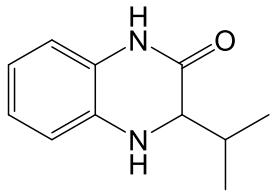
White solid, mp:136-136 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47(s, 1H), 6.94-6.70 (m, 4H), 4.06(m, 1H), 1.49 (d, *J* = 10.6 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 170.25, 133.92, 123.94, 121.52, 119.66, 115.43, 114.15, 51.92, 17.827; HRMS (ESI) calcd. for $C_9H_{11}N_2O$ $[M+H]^+$: 163.0866, found: 163.0869.

3-Ethyl-3,4-dihydroquinoxalin-2(1H)-one (**4ab**)[8]



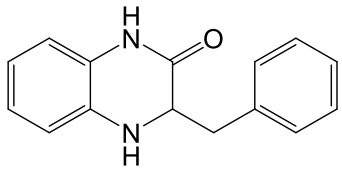
Yellow solid, mp: 77-78 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86-7.24 (m, 4H), 2.95(m, 2H), 1.89(m, 2H), 1.09 (t, *J* = 10.6 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 169.41, 133.41, 125.17, 122.15, 118.97, 116.71, 114.60, 51.71, 27.06, 10.03; HRMS (ESI) calcd. for $C_{10}H_{13}N_2O$ $[M+H]^+$: 177.1022, found: 177.1029.

3-Isopropyl-3,4-dihydroquinoxalin-2(1H)-one (**4ad**)[8]



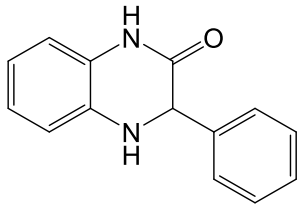
Yellow solid, mp: 121-123°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.76(s, 1H), 7.29-6.67 (m, 4H), 4.09(s, 1H), 3.81(s, 1H), 2.28 (d, *J* = 10.6 Hz, 1H), 1.08-1.01(dd, *J* = 17.4, 16.3 Hz, 6H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 168.83, 133.31, 124.89, 123.91, 118.79, 115.51, 113.39, 81.77, 30.83, 20.23, 19.04, 17.508; HRMS (ESI) calcd. for $C_{11}H_{15}N_2O$ $[M+H]^+$: 191.1179, found: 191.1181.

3-Benzyl-3,4-dihydroquinoxalin-2(1H)-one (**4aj**)[15]



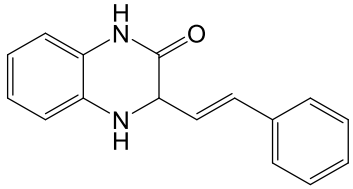
Yellow solid, mp: 188-189 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.04(s, 1H), 7.40-7.25 (m, 5H), 6.93-6.61(m, 4H), 4.12 (d, *J* = 10.6 Hz, 1H), 3.95 (s, 1H), 3.32(m, 1H), 2.93 (m, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 169.28, 136.91, 132.43, 129.49, 128.99, 127.09, 125.56, 124.12, 119.60, 115.82, 114.59, 57.82, 37.57; HRMS (ESI) calcd. for $C_{15}H_{15}N_2O$ $[M+H]^+$: 239.1179, found: 239.1177.

3-Phenyl-3,4-dihydroquinoxalin-2(1H)-one (**4al**)[16]



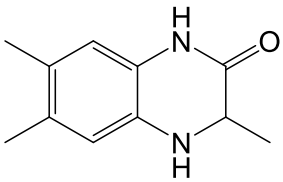
White solid, mp: 79-81 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39-7.25 (m, 5H), 6.84 (m, 1H), 6.63-6.56(m, 3H), 5.09 (s, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 177.13, 139.13, 132.82, 129.91, 127.00, 122.90, 118.78, 115.70,114.42, 53.46; HRMS (ESI) calcd. for $C_{14}H_{13}N_2O$ $[M+H]^+$: 225.1022, found: 225.1017.

(E)-3-styryl-3,4-dihydroquinoxalin-2(1H)-one (**4aw**)[17]



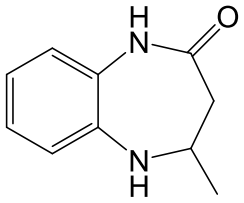
White solid, mp: 134-136ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24-8.20 (m, 1H), 7.92-7.74 (m, 4H), 7.52-7.41(m, 6H), 4.42 (d, *J* = 6.3 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 169.78, 140.77, 133.06, 131.76, 127.58, 126.83, 125.93, 117.82, 117.70, 117.27, 113.62, 113.35, 113.25, 61.14; HRMS (ESI) calcd. for $C_{16}H_{15}N_2O$ $[M+H]^+$: 251.1179, found: 251.1173.

3,6,7-Trimethyl-3,4-dihydroquinoxalin-2(1*H*)-one (**4ja**)[16]



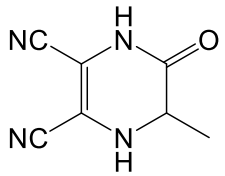
Yellow solid, mp: 125-127°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.33-6.32 (m, 2H), 3.99 (s, 1H), 3.79 (s, 1H), 2.14 (s, 6H), 1.32 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 170.43, 133.97, 126.47, 123.42, 117.79, 116.38, 51.62, 19.89, 18.87; HRMS (ESI) calcd. for $C_{11}H_{15}N_2O$ $[M+H]^+$: 191.1179, found: 191.1183.

4-Methyl-1,3,4,5-tetrahydro-2H-benzo[b][1,4]diazepin-2-one (**4ax**)[18]



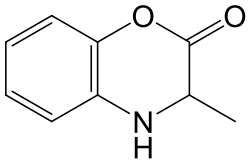
Yellow solid, mp: 110-113°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33-7.07 (m, 4H), 3.26 (m, 1H), 2.66 (m, 1H), 2.28 (m, 1H), 1.24 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 170.43, 138.99, 133.98, 126.47, 123.42, 117.79, 116.38, 51.62, 41.38, 23.89; HRMS (ESI) calcd. for $C_{10}H_{13}N_2O$ $[M+H]^+$: 177.1022, found: 177.1028.

5-Methyl-6-oxo-1,4,5,6-tetrahydropyrazine-2,3-dicarbonitrile (**4ua**)[19]



White solid, mp: 239-240 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.55 (m, 1H), 1.60 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 151.56, 116.02, 115.70, 111.74, 100.41, 55.34, 14.35; HRMS (ESI) calcd. for $C_7H_7N_4O$ $[M+H]^+$: 163.0614, found: 163.0621.

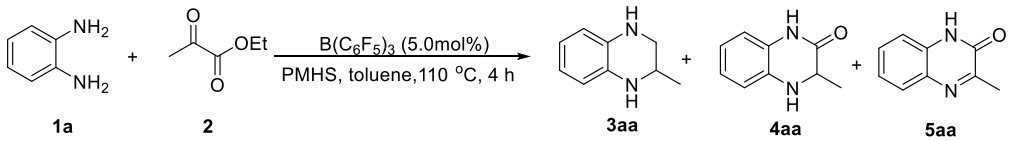
3-Methyl-3,4-dihydro-2H-benzo[b] [1,4] oxazin-2-one (**4ya**)[20]

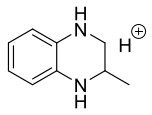


Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.03-6.76 (m, 4H), 3.99 (m, 1H), 1.55 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 166.14, 144.55, 137.11, 123.60, 120.44, 116.38, 114.38, 50.85, 21.31; HRMS (ESI) Calcd for $C_9H_{10}NO_2$ $[M+H]^+$: 164.0706, found: 164.0710.

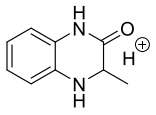
5. The mechanistic study

1) ESI-MS Study

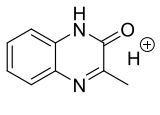




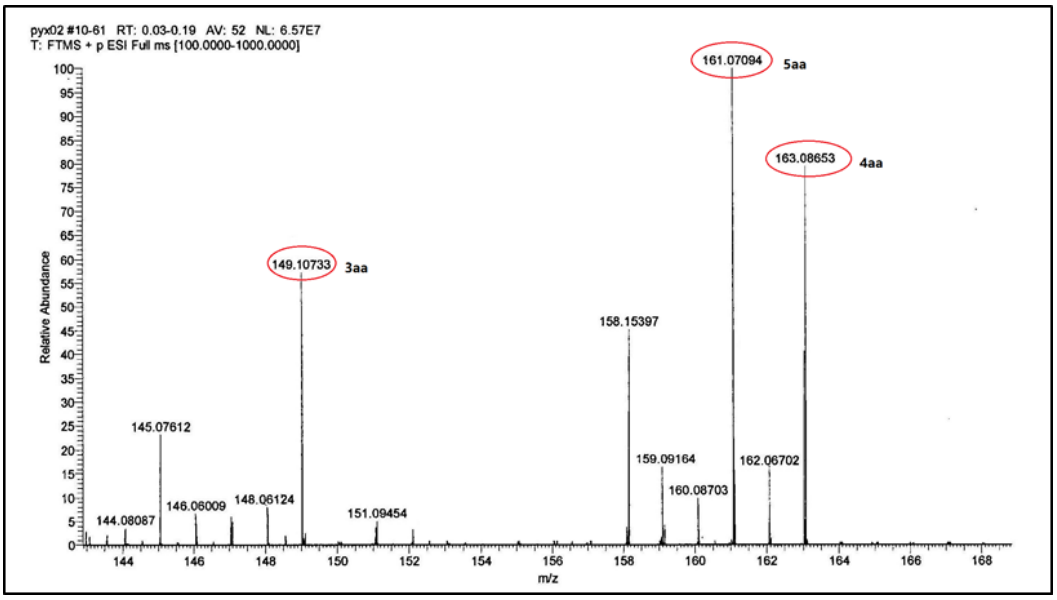
Chemical Formula: $C_9H_{13}N_2^+$
Exact Mass: 149.1073



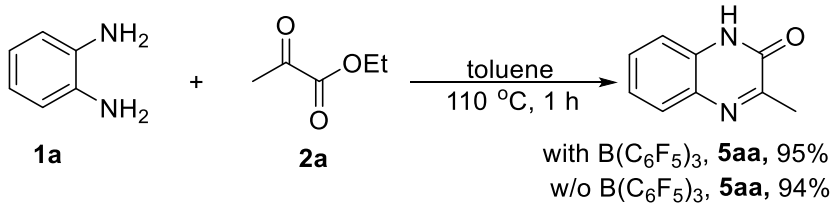
Chemical Formula: $C_9H_{11}N_2O^+$
Exact Mass: 163.0866



Chemical Formula: $C_9H_9N_2O^+$
Exact Mass: 161.0709

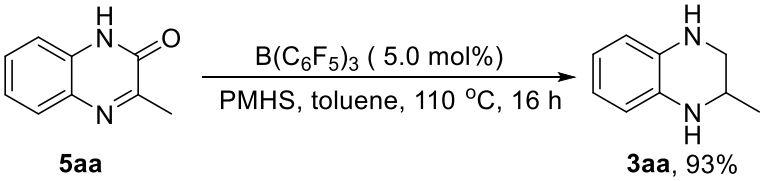


2) General procedure for the reaction of 1a with 2a



A mixture of *o*-phenylenediamine **1a** (27.5 mg, 0.25 mmol), ethyl 2-oxopropanoate **2a** (31.93 mg, 0.275 mmol) and toluene (1.5 mL) with or without $B(C_6F_5)_3$ (6.4 mg, 5.0 mol%) in an oven-dried screw-capped pressure tube was stirred at 110 °C for 1 h. After cooling to ambient temperature, the volatiles were removed under reduced pressure, and the reaction mixture was purified by column chromatography on silica gel using a mixture of ethyl acetate and hexane to give the target compound **5aa** as a light solid.

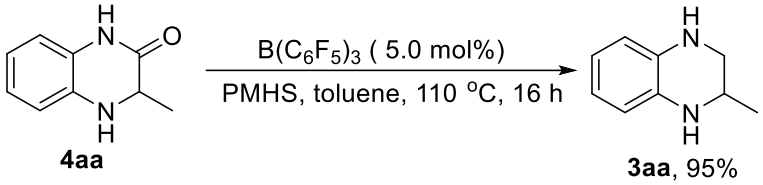
3) General procedure for the synthesis 3aa from 5aa



A mixture of 3-methylquinoxalin-2(1*H*)-one **5aa** (40.04 mg, 0.25 mmol), $B(C_6F_5)_3$ (6.4 mg, 5.0 mol%) and PMHS (0.06 mL, 1.0 mmol) in toluene (1.5 mL) in an oven-dried screw-capped pressure tube was stirred at 110 °C for 16 h. After cooling to ambient temperature, the mixture was diluted with EtOAc (5.0 mL). Then water (5.0 mL) was added to the reaction mixture, which was extracted with EtOAc three times (5.0 mL each). The combined organic phases were dried over Na_2SO_4, filtered and evaporated

under reduced pressure. After the removal of volatile materials by rotary evaporation, the resultant mixture was purified by column chromatography on silica gel using a mixture of ethyl acetate and hexane to give the target compound **3aa** as a light yellow oil.

4) General procedure for the synthesis 3aa from 4aa



4aa **3aa**, 95%

A mixture of **4aa** (40.55 mg, 0.25 mmol), $B(C_6F_5)_3$ (6.4 mg, 5.0 mol%) and PMHS (0.06 mL, 1.0 mmol) in toluene (1.5 mL) in an oven-dried screw-capped pressure tube was stirred at 110 °C for 16 h. After cooling to ambient temperature, the mixture was diluted with EtOAc (5.0 mL). Then water (5.0 mL) was added to the reaction mixture, which was extracted with EtOAc three times (5.0 mL each). The combined organic phases were dried over Na_2SO_4, filtered and evaporated under reduced pressure. After the removal of volatile materials by rotary evaporation, the resultant mixture was purified by column chromatography on silica gel using a mixture of ethyl acetate and hexane to give the target compound **3aa** as a light yellow oil.

6. References:

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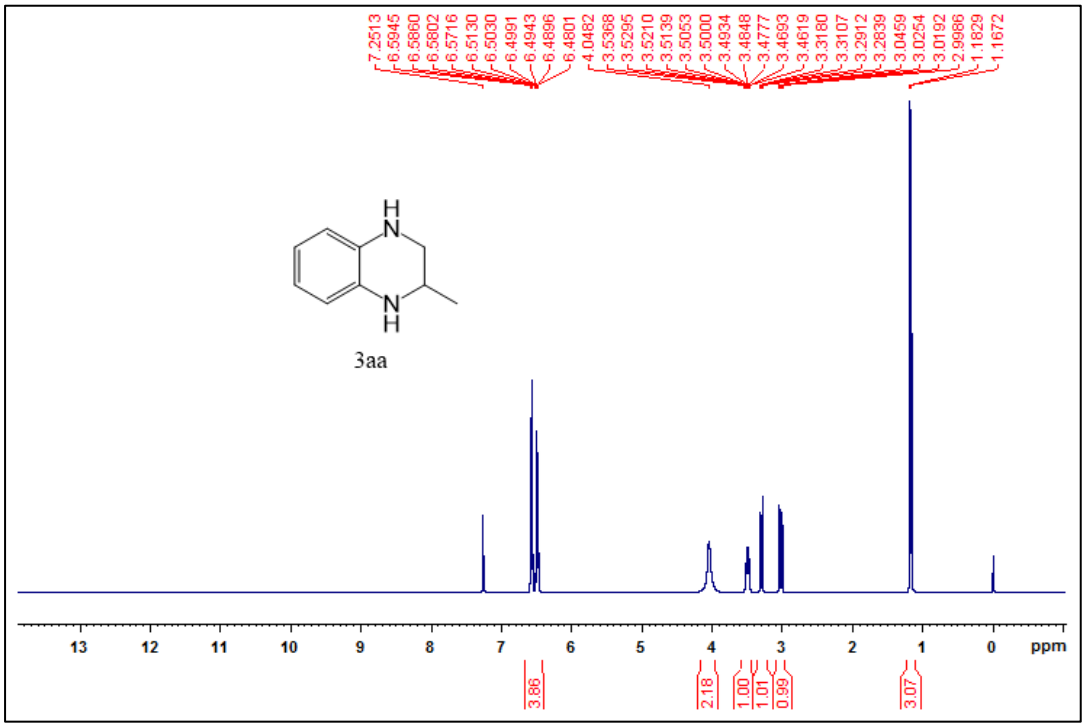
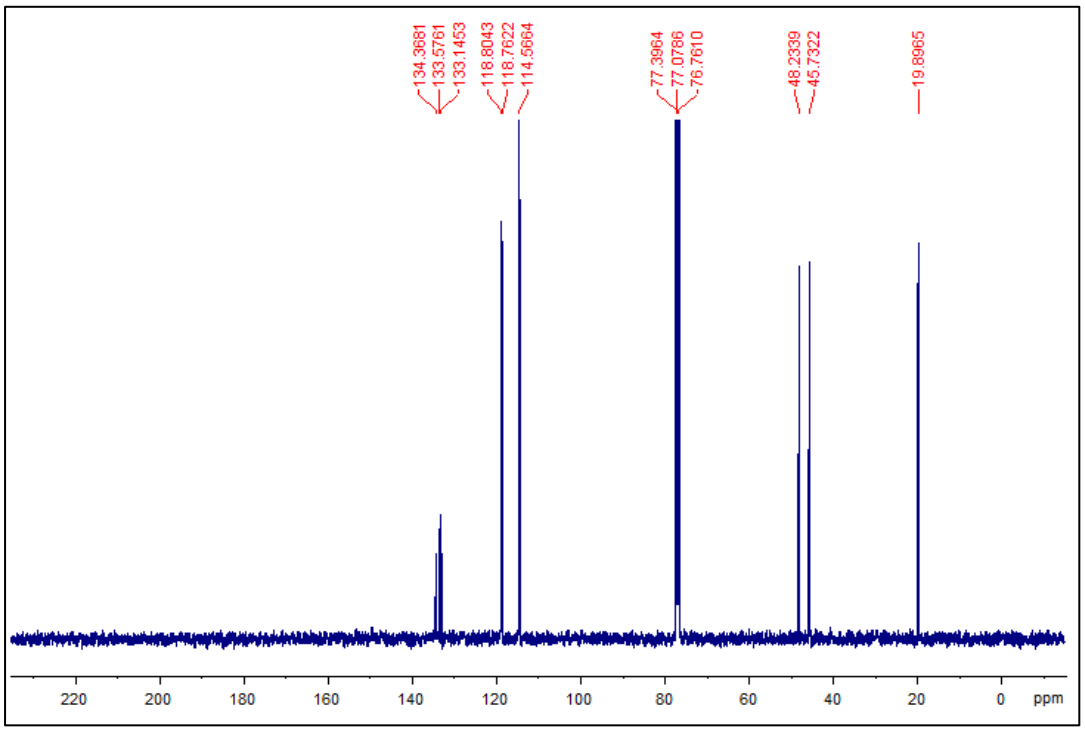
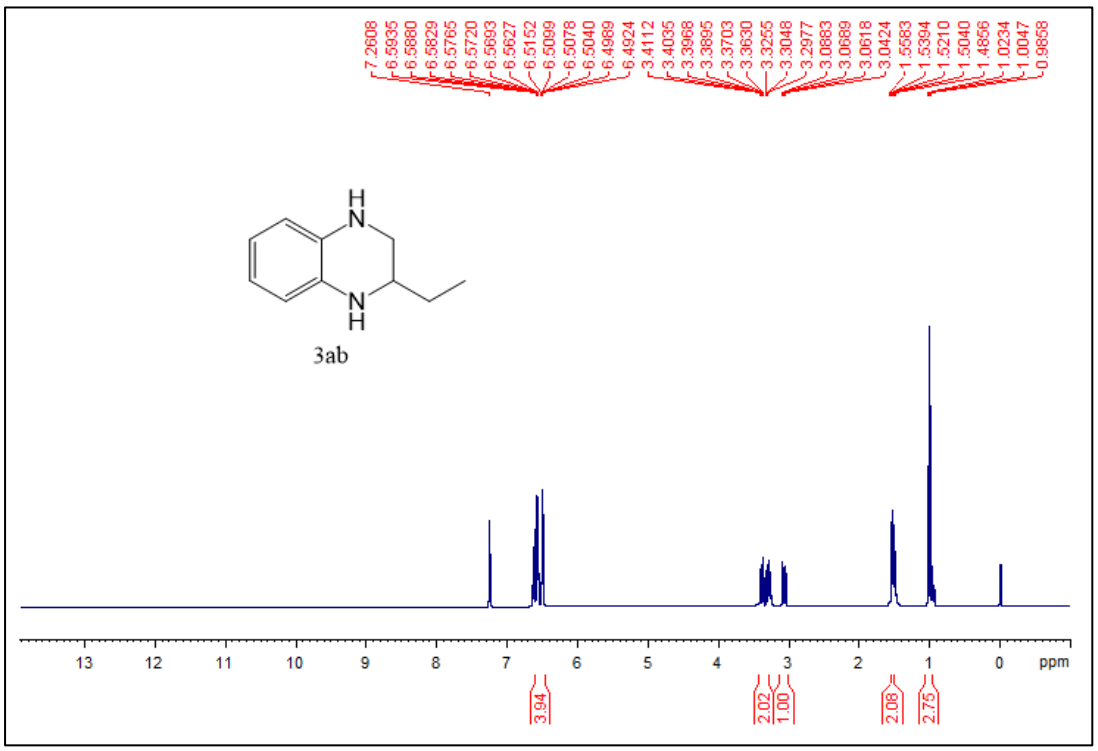
7. ^{1}H and ^{13}C NMR spectra of the products



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N
N
H
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12
11
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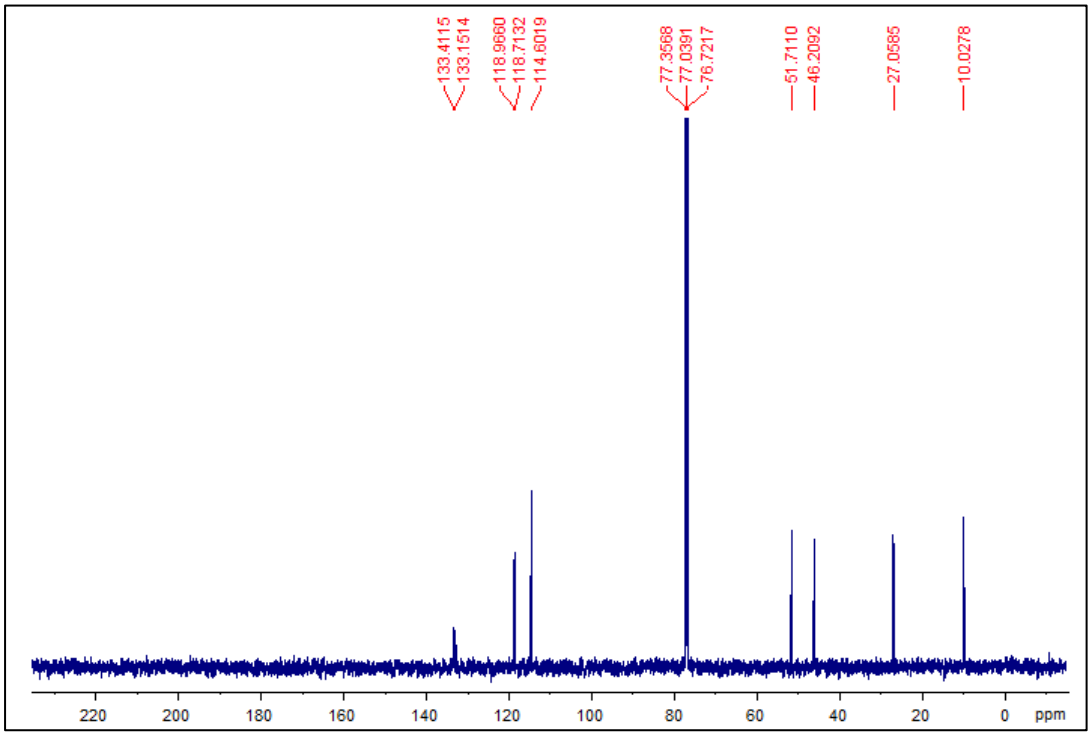
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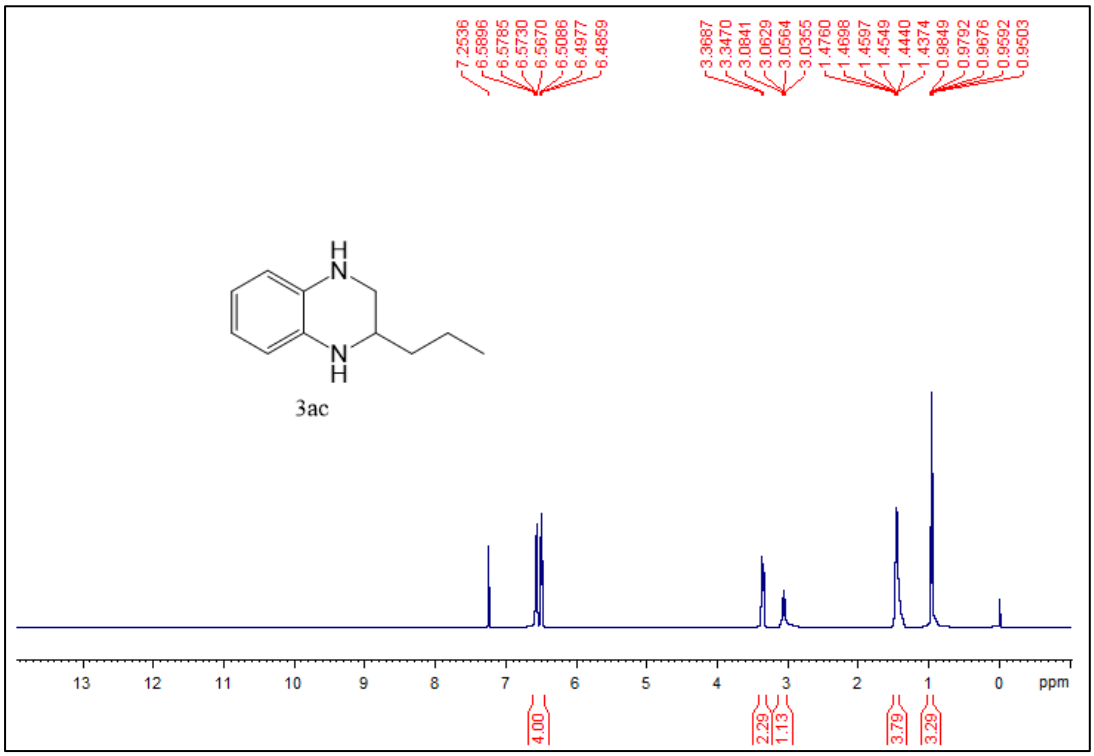
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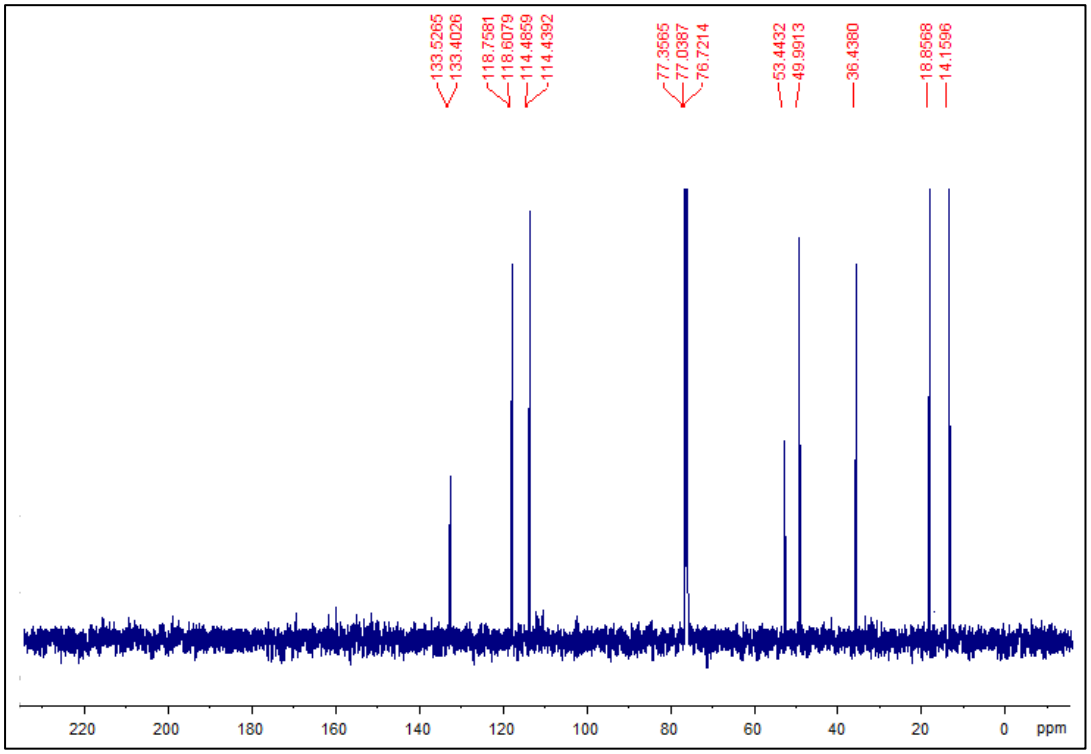
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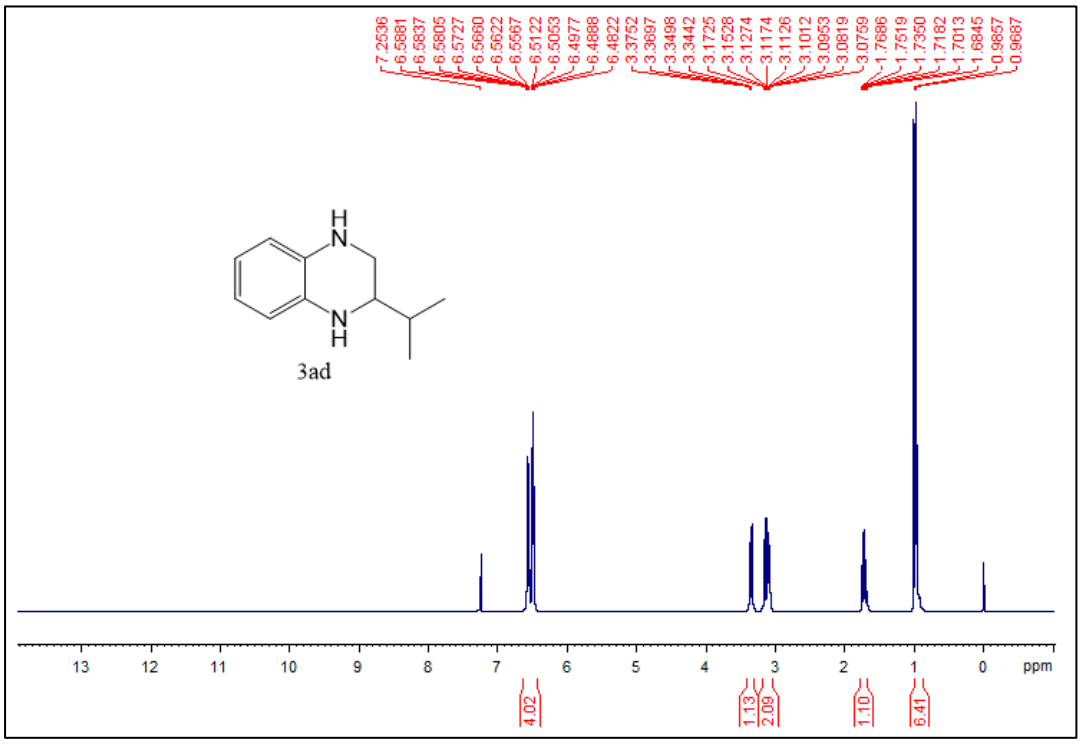
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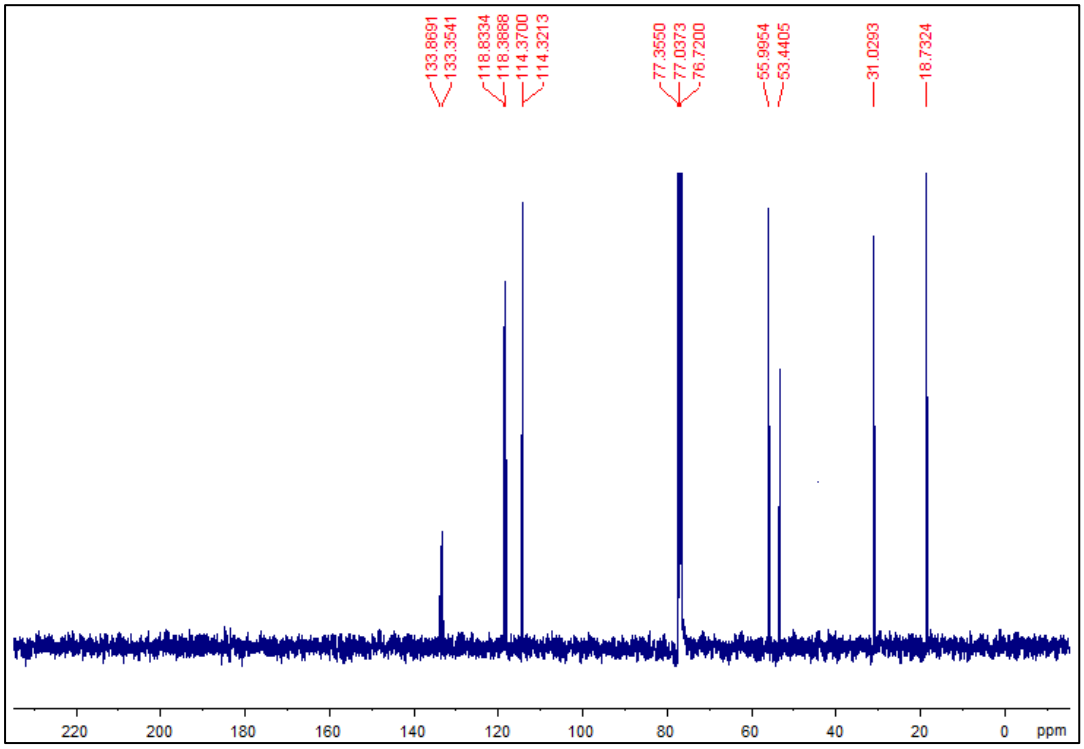
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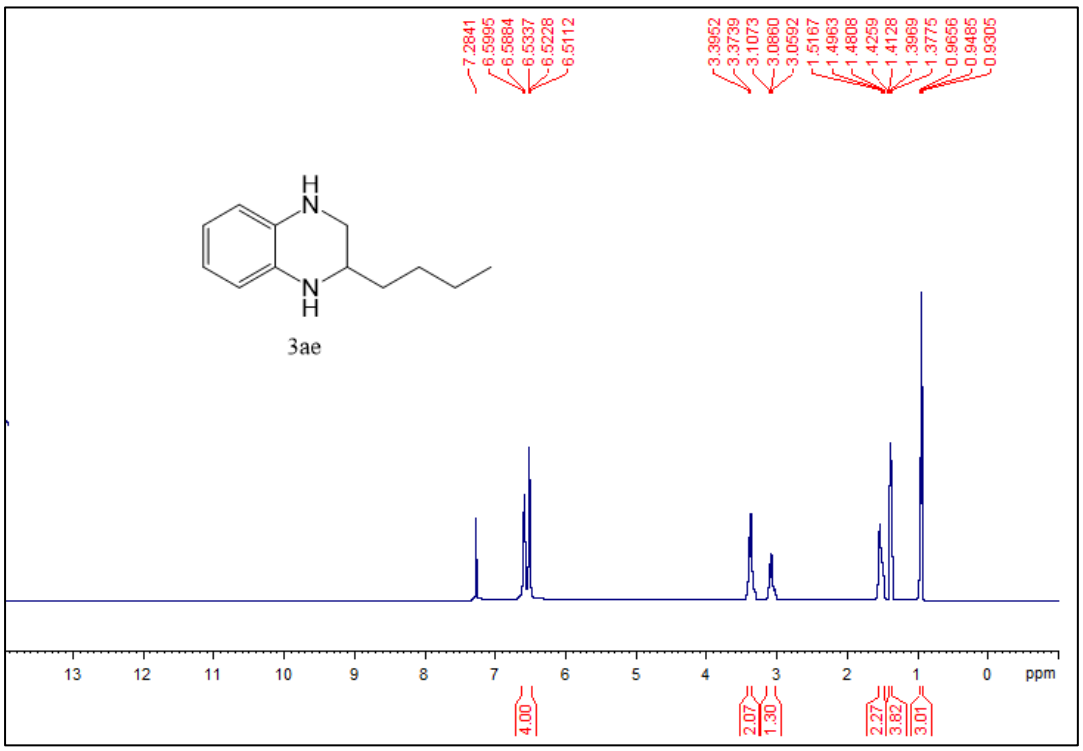
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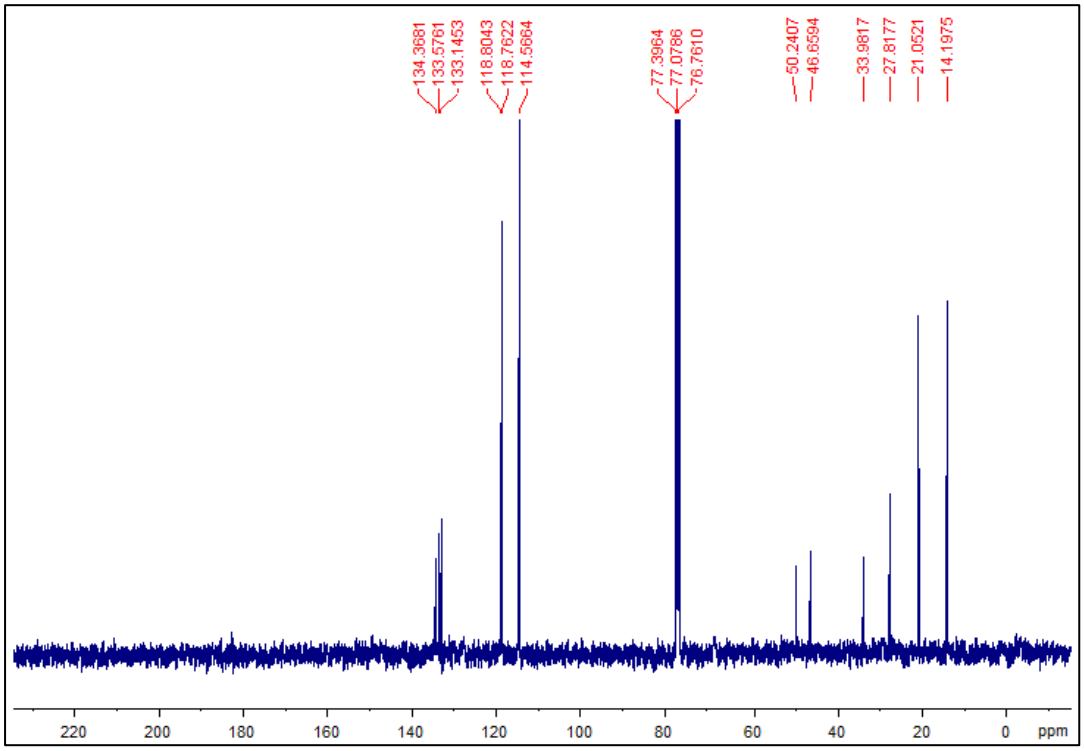
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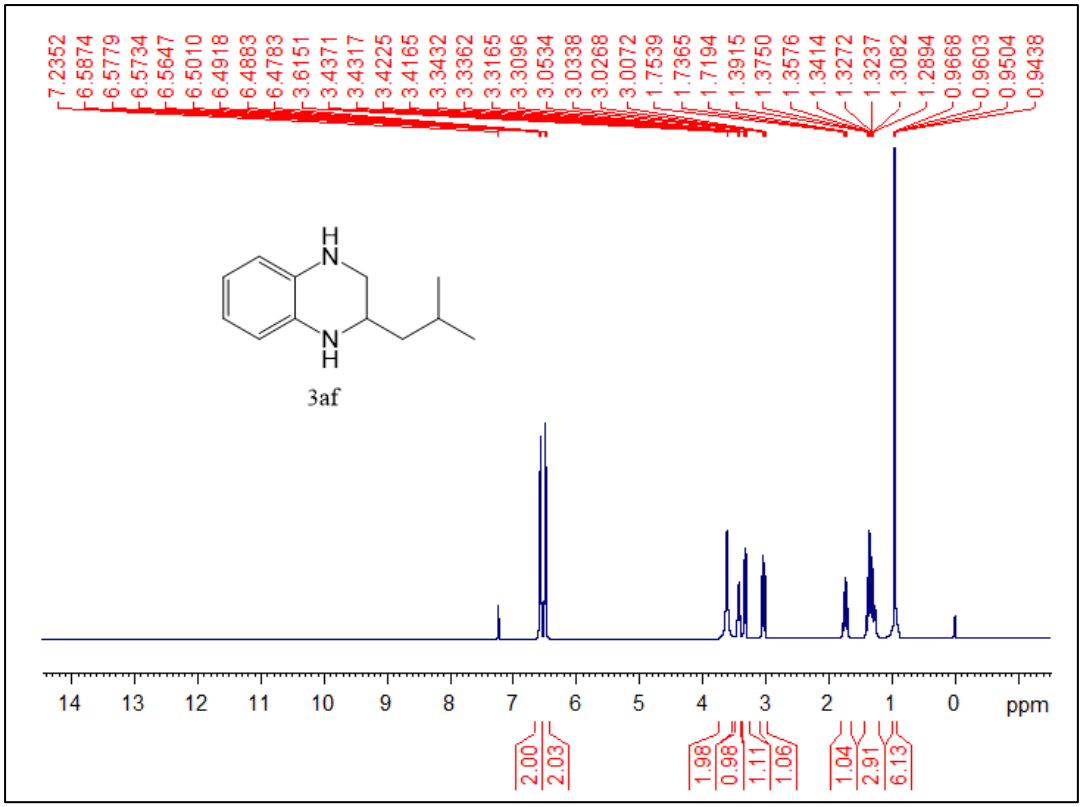
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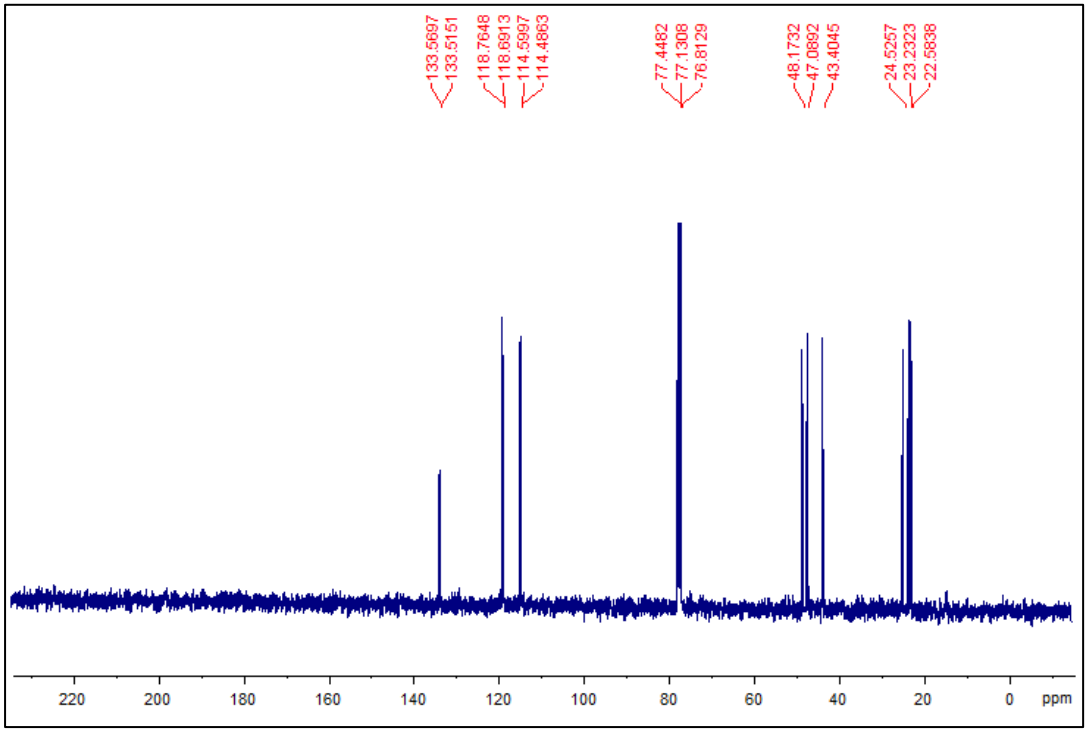
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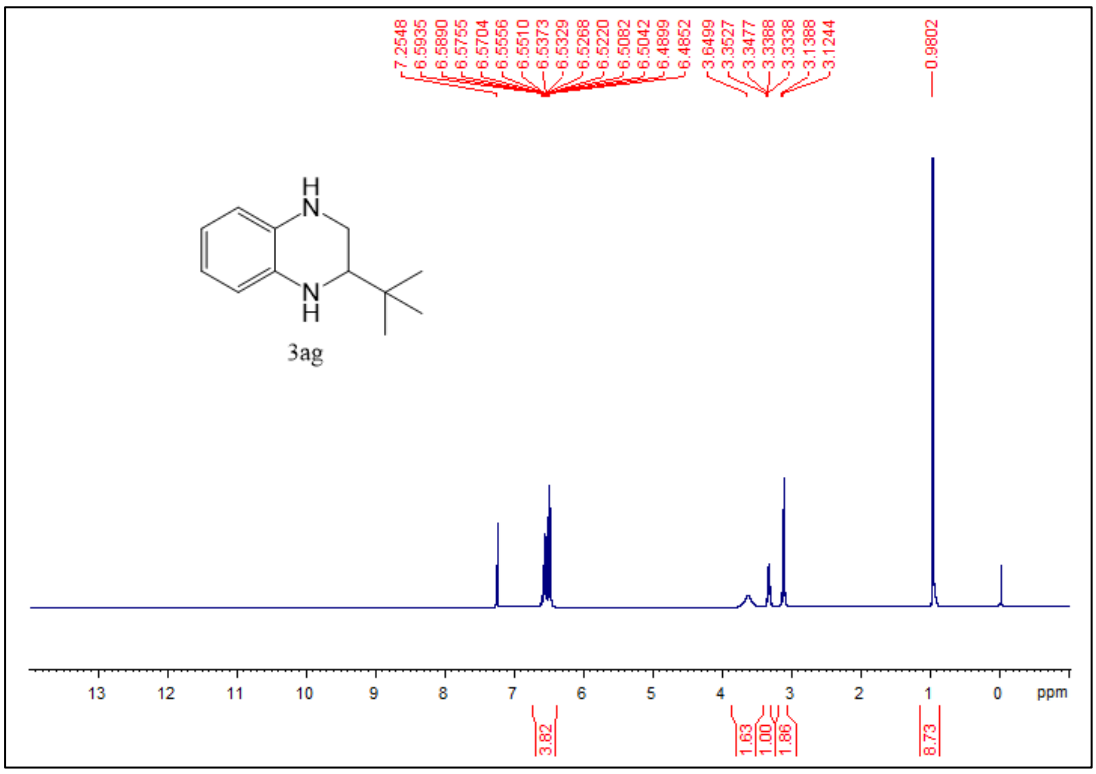
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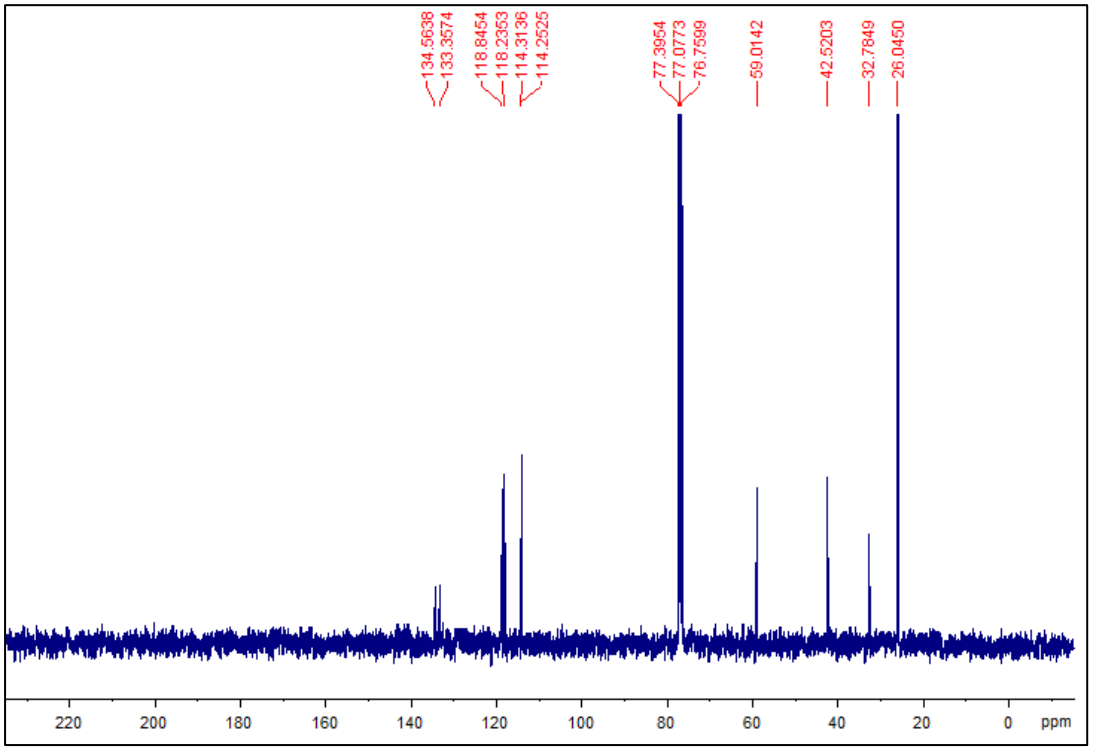
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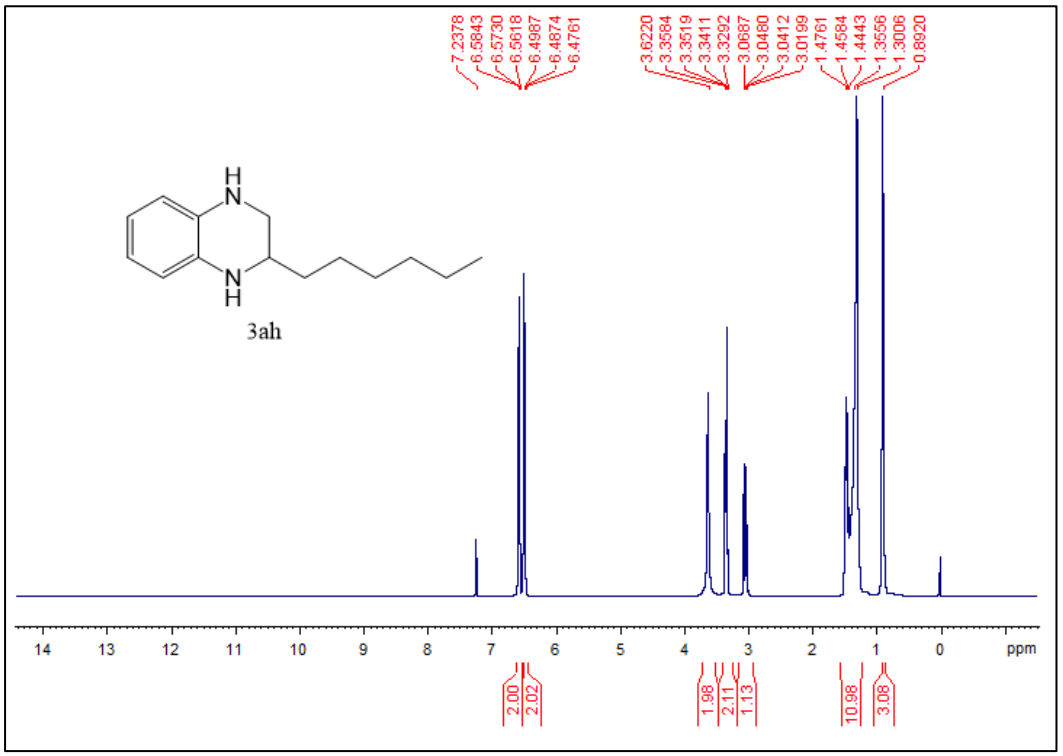
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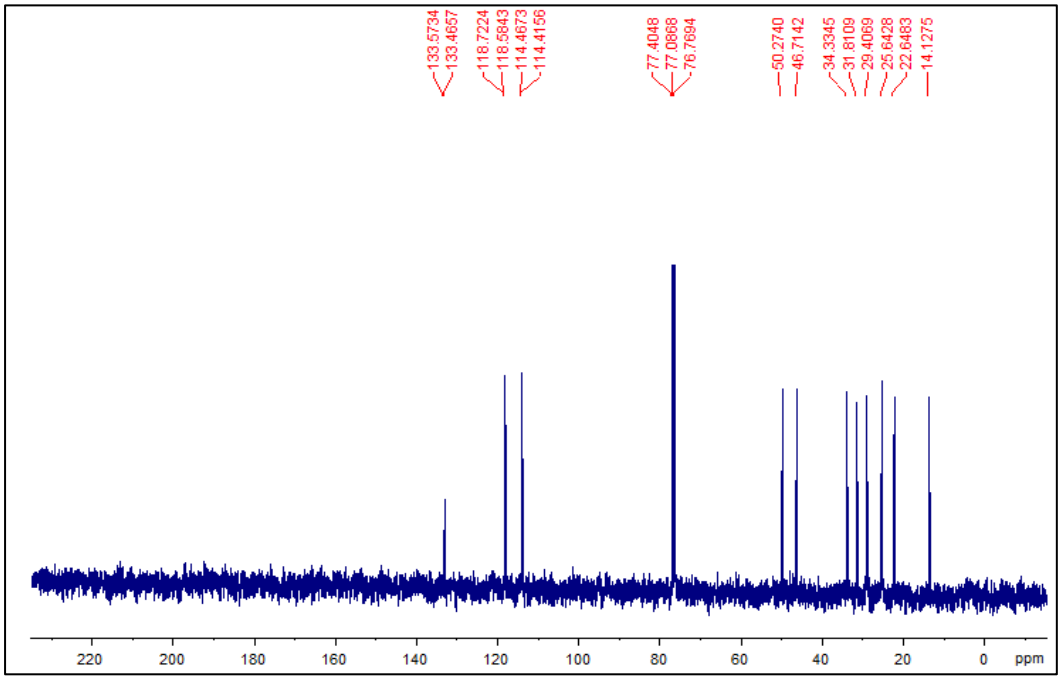
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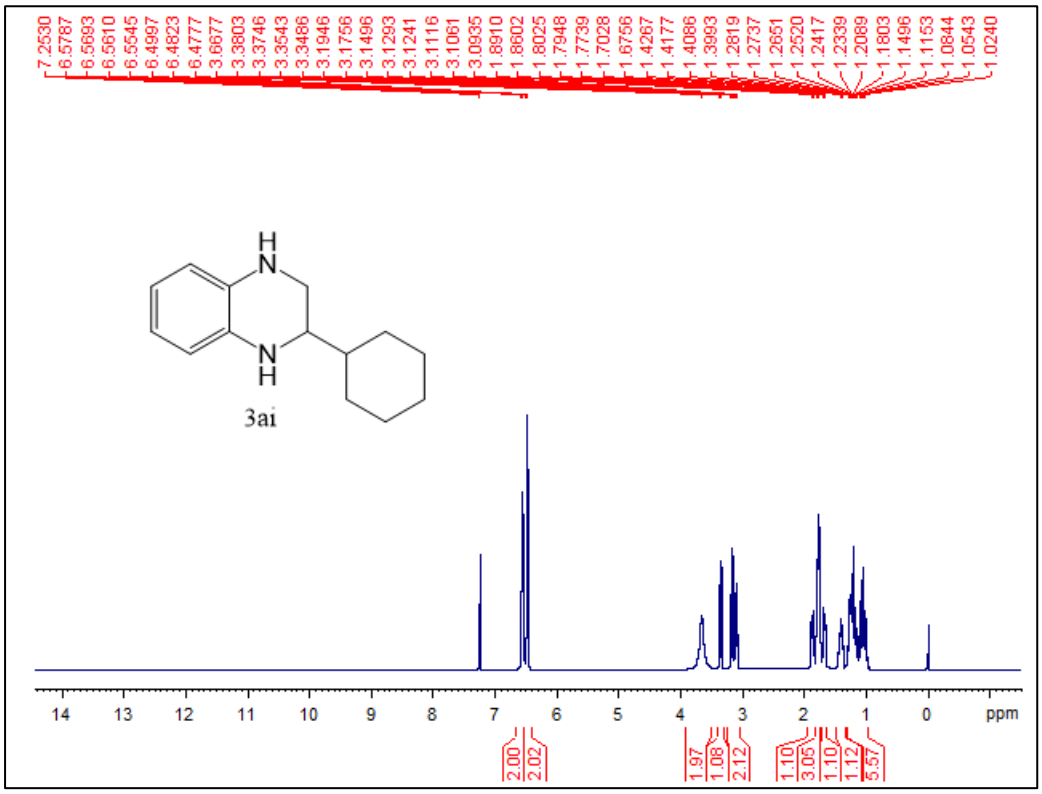
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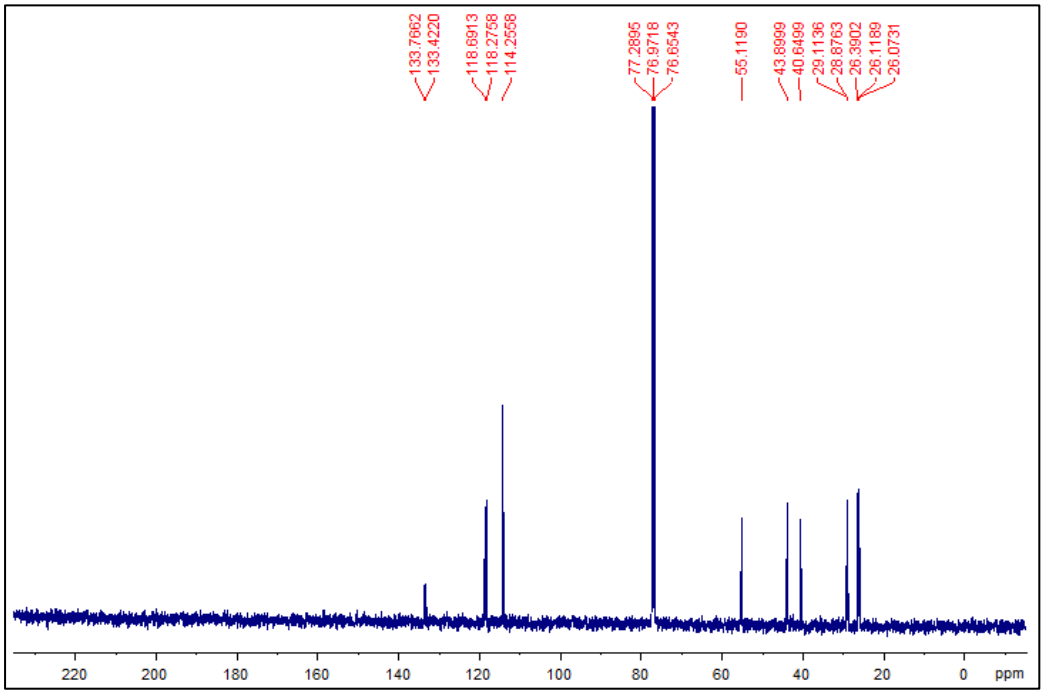
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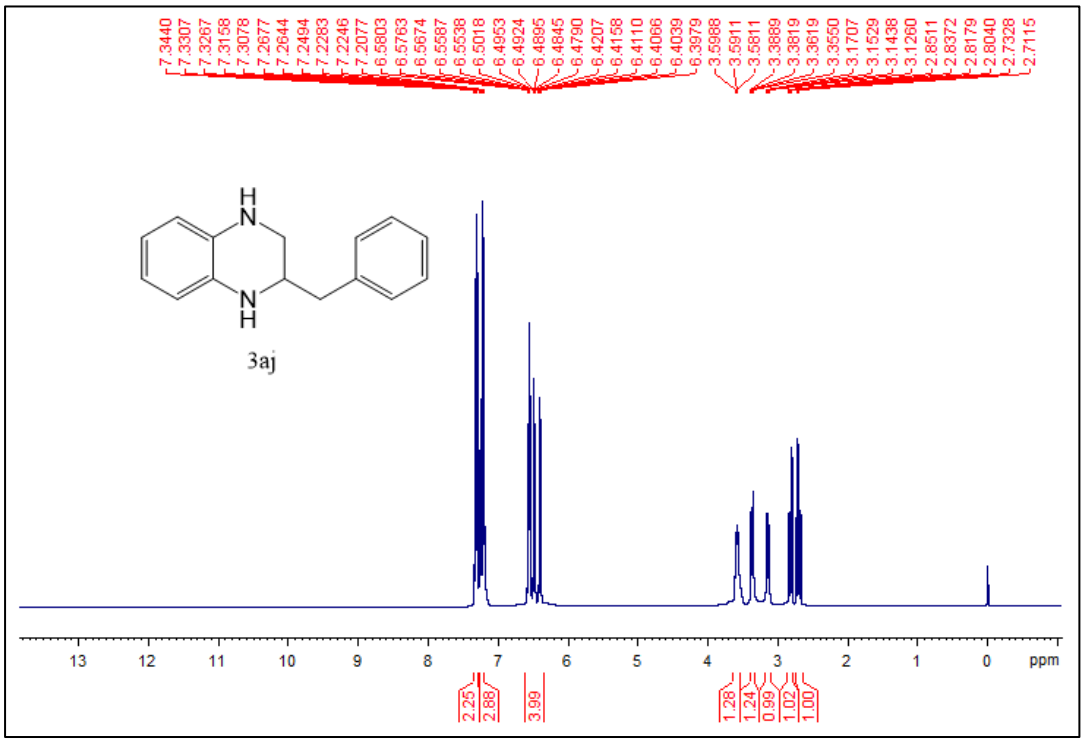
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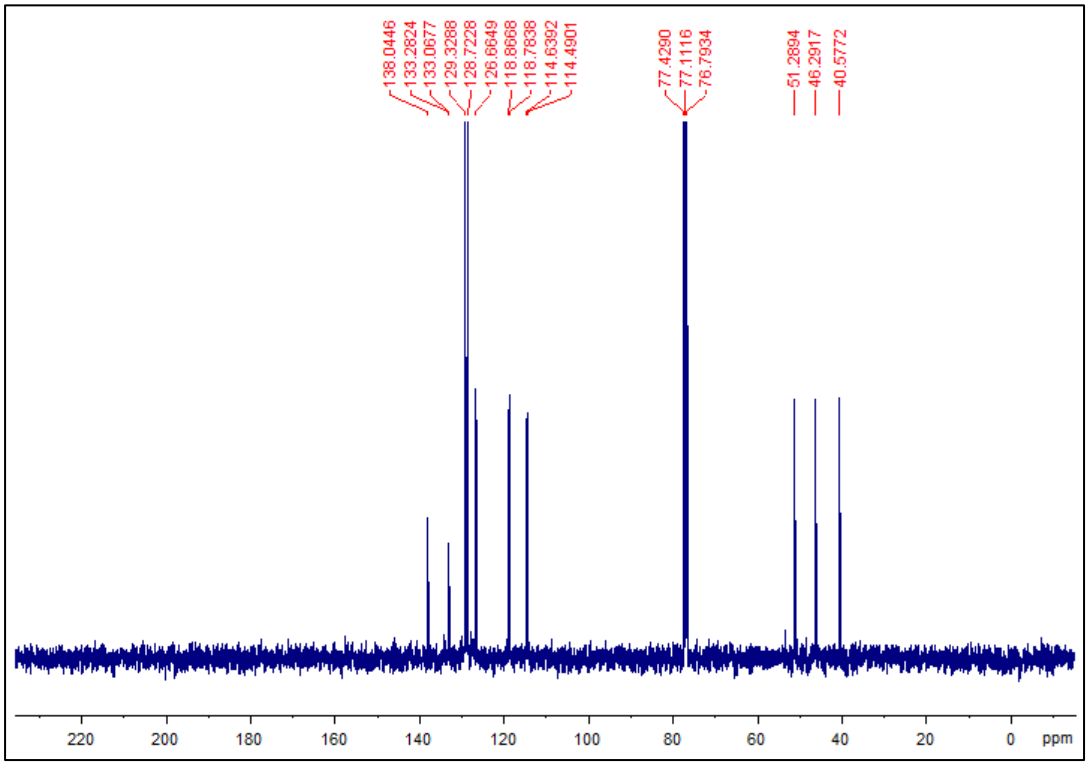
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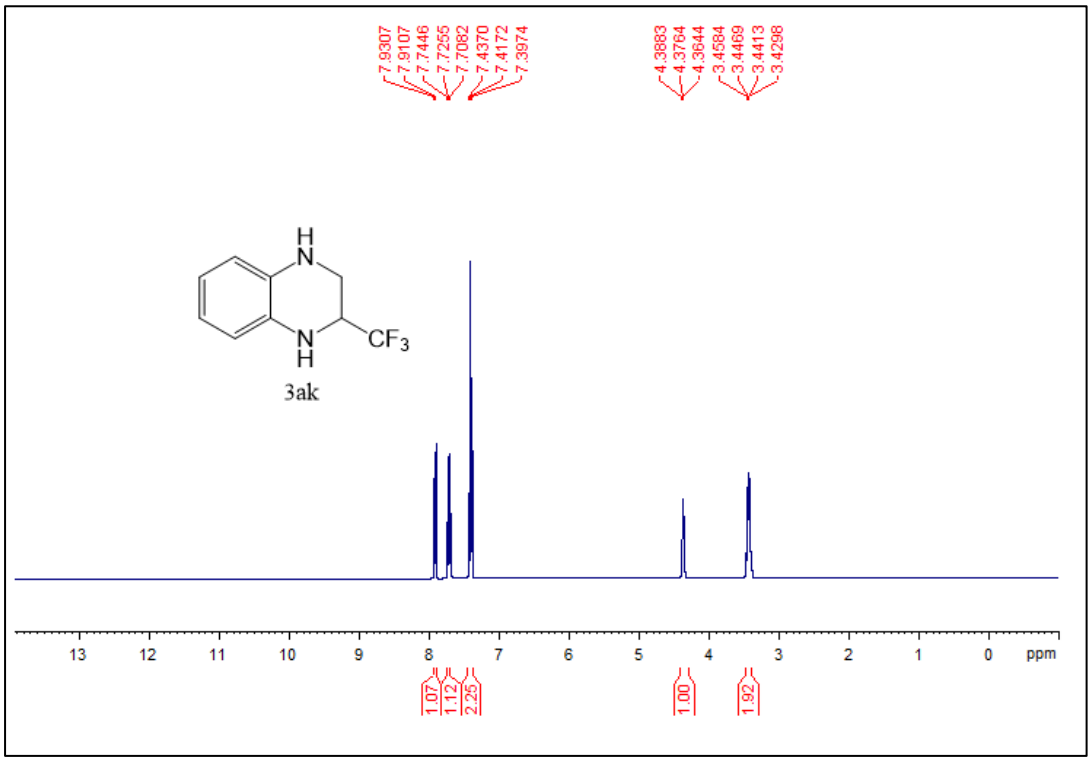
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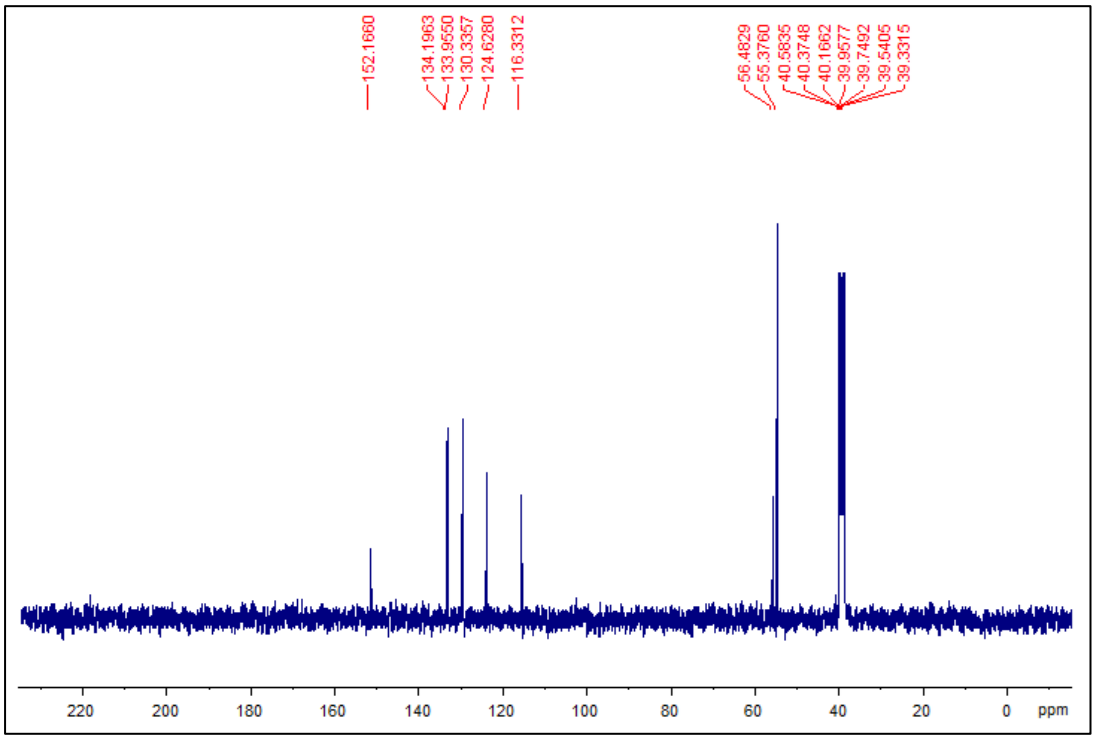
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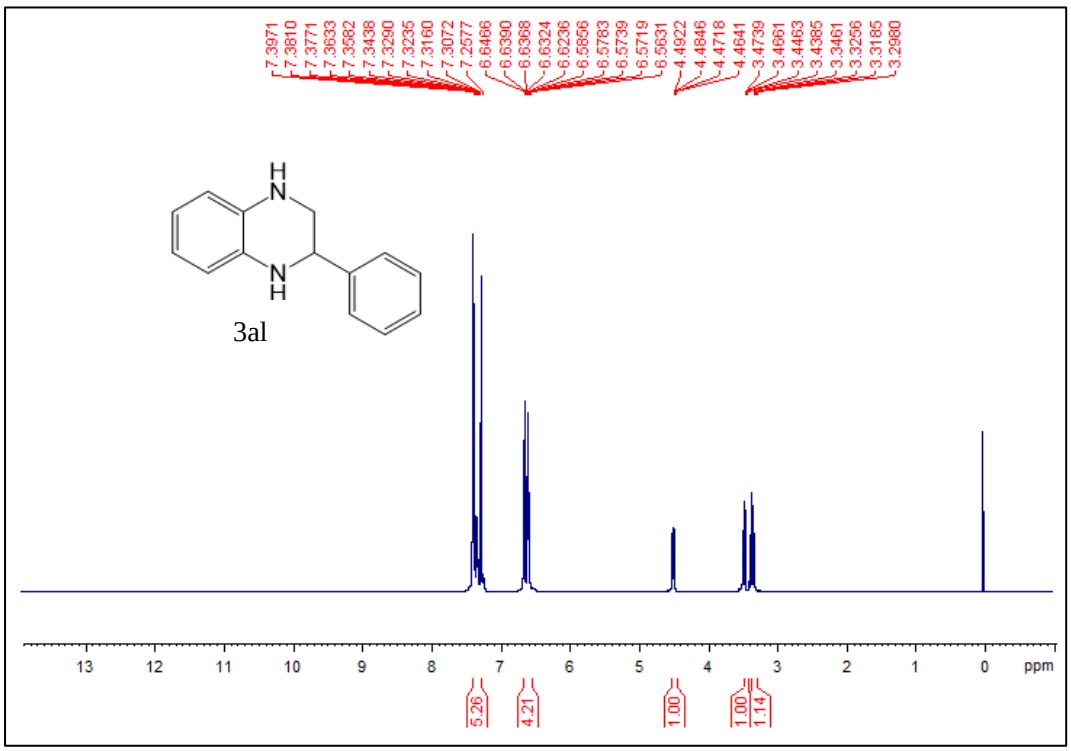
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H
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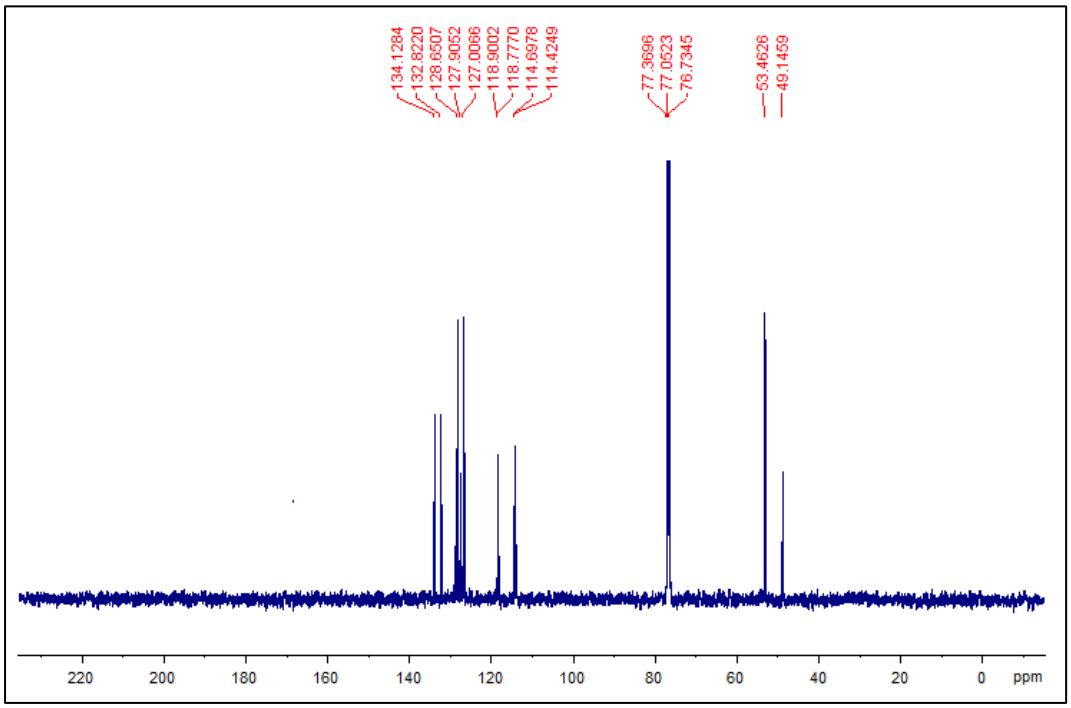
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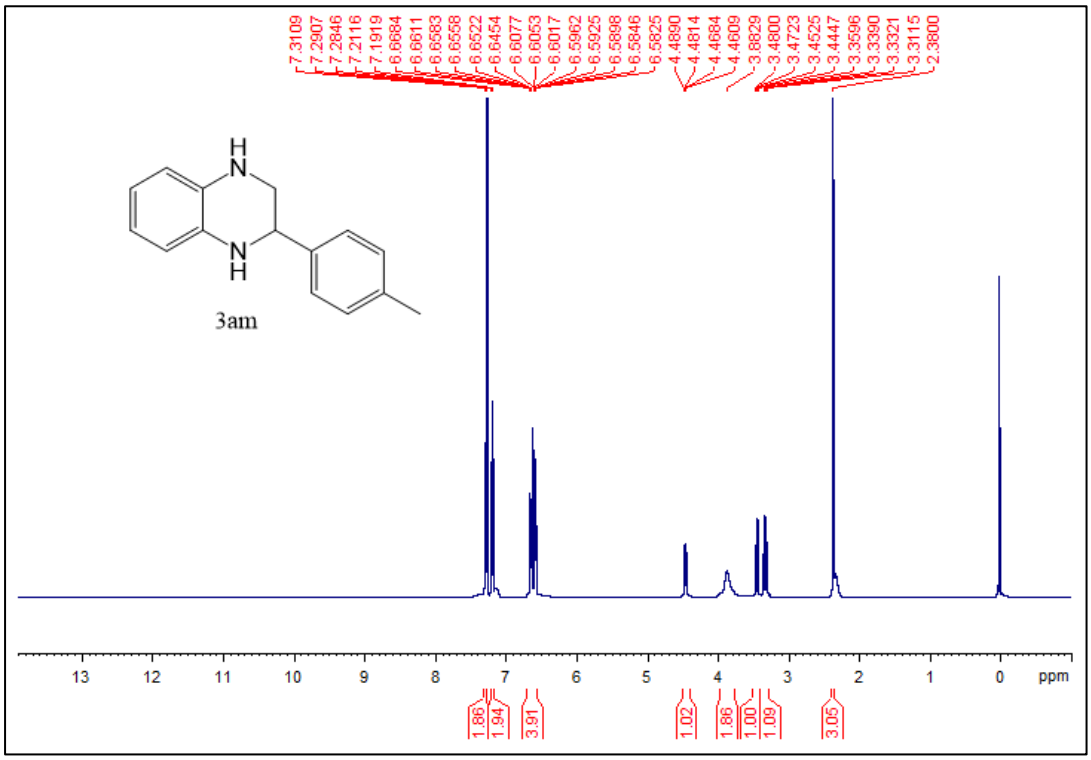
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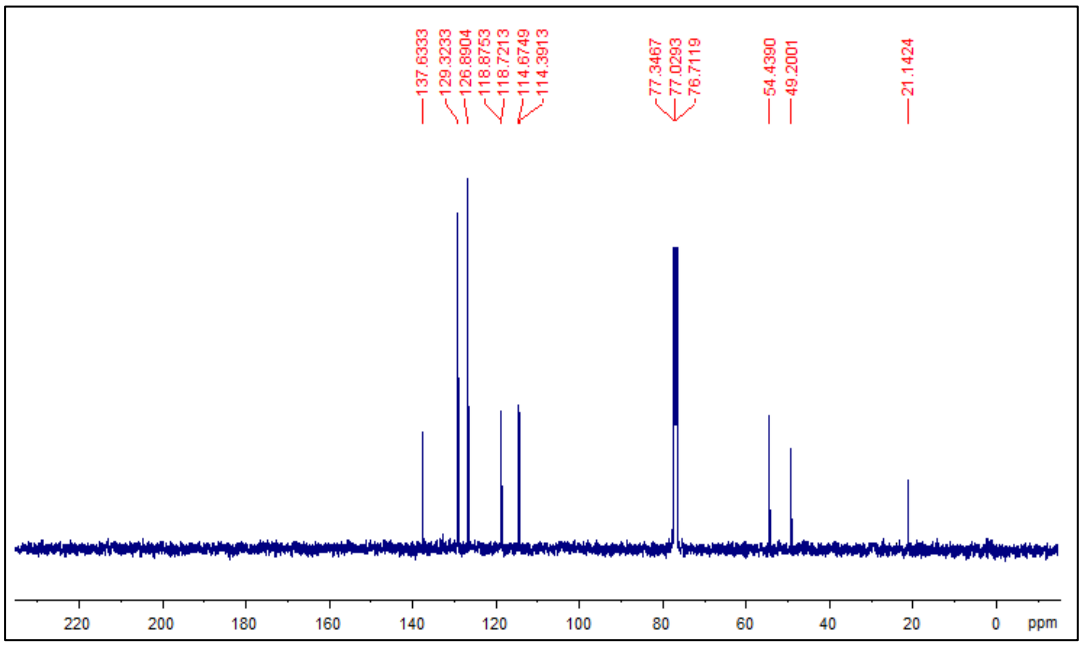
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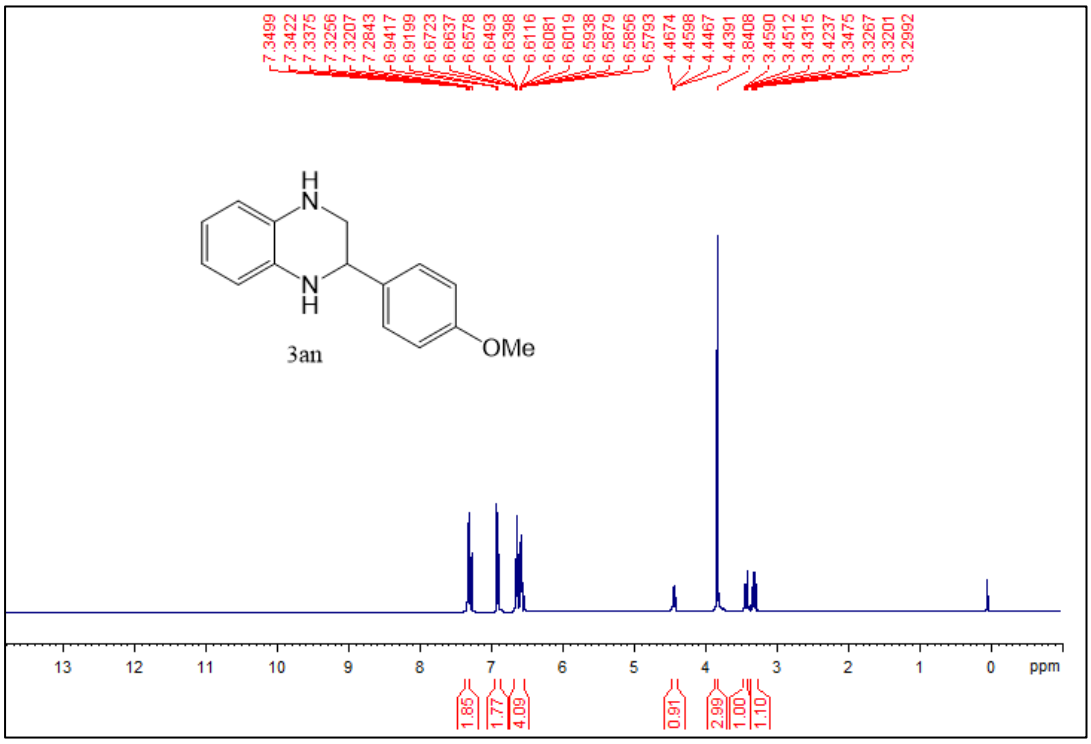
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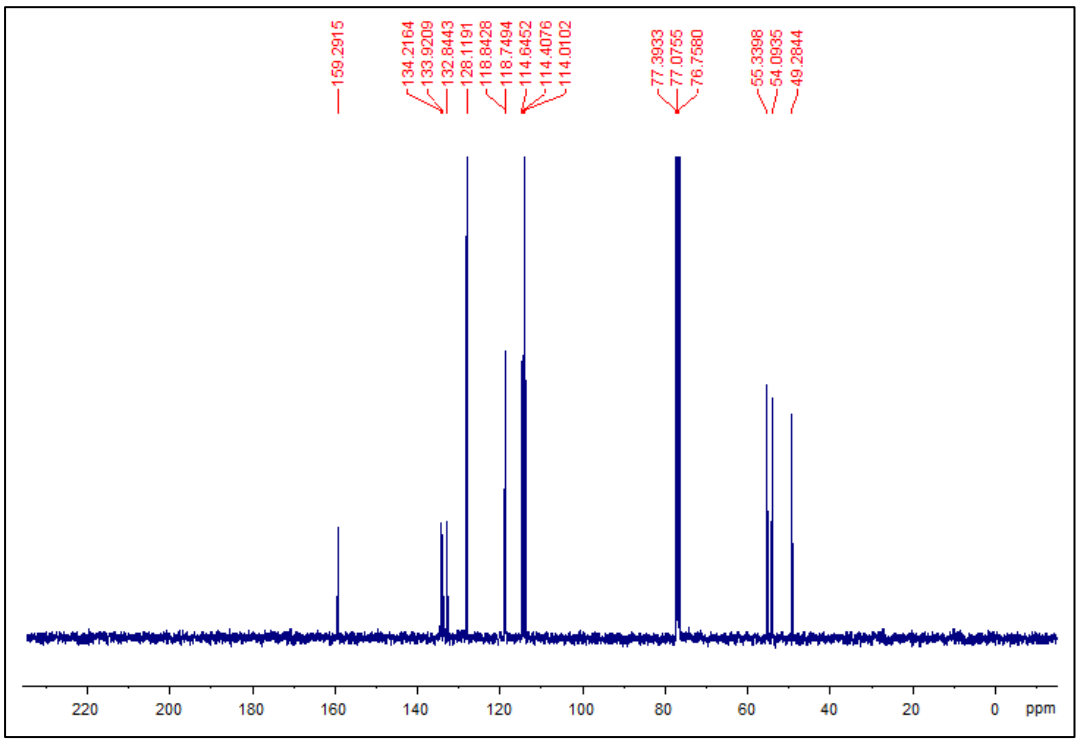
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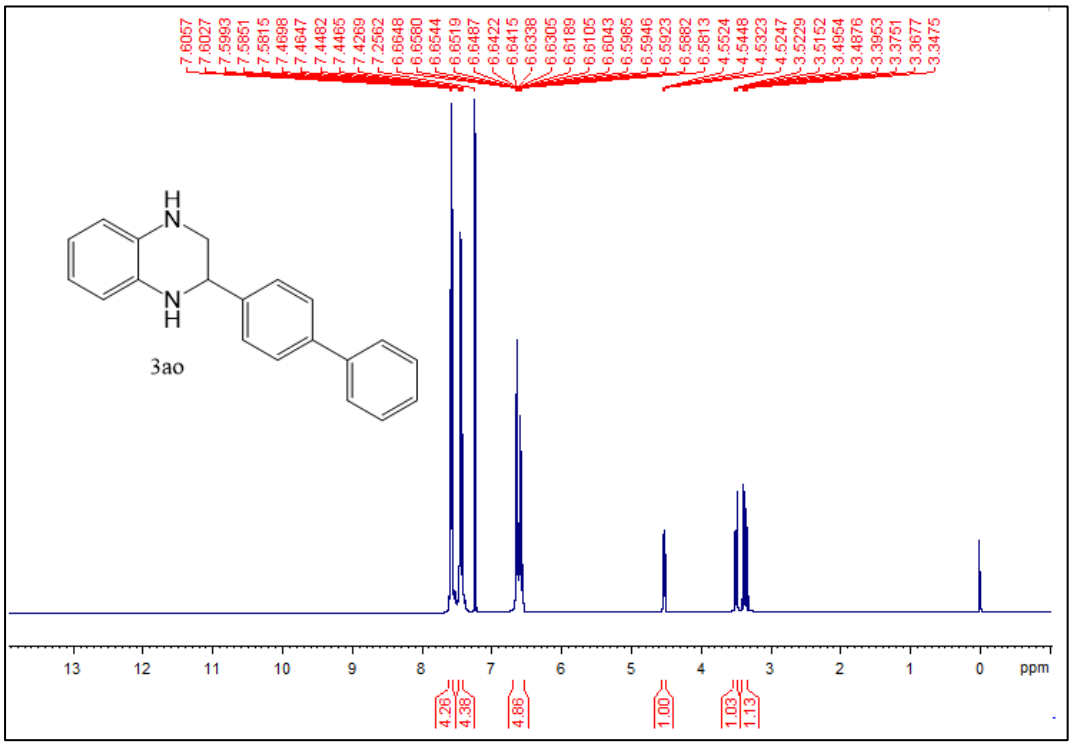
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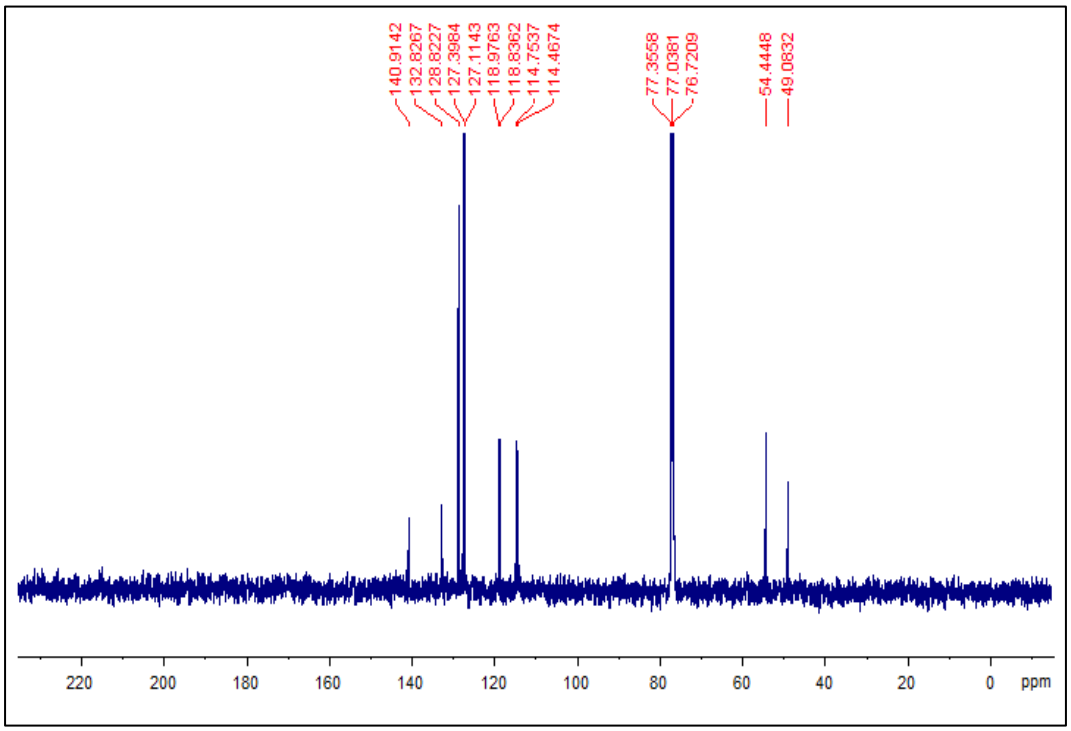
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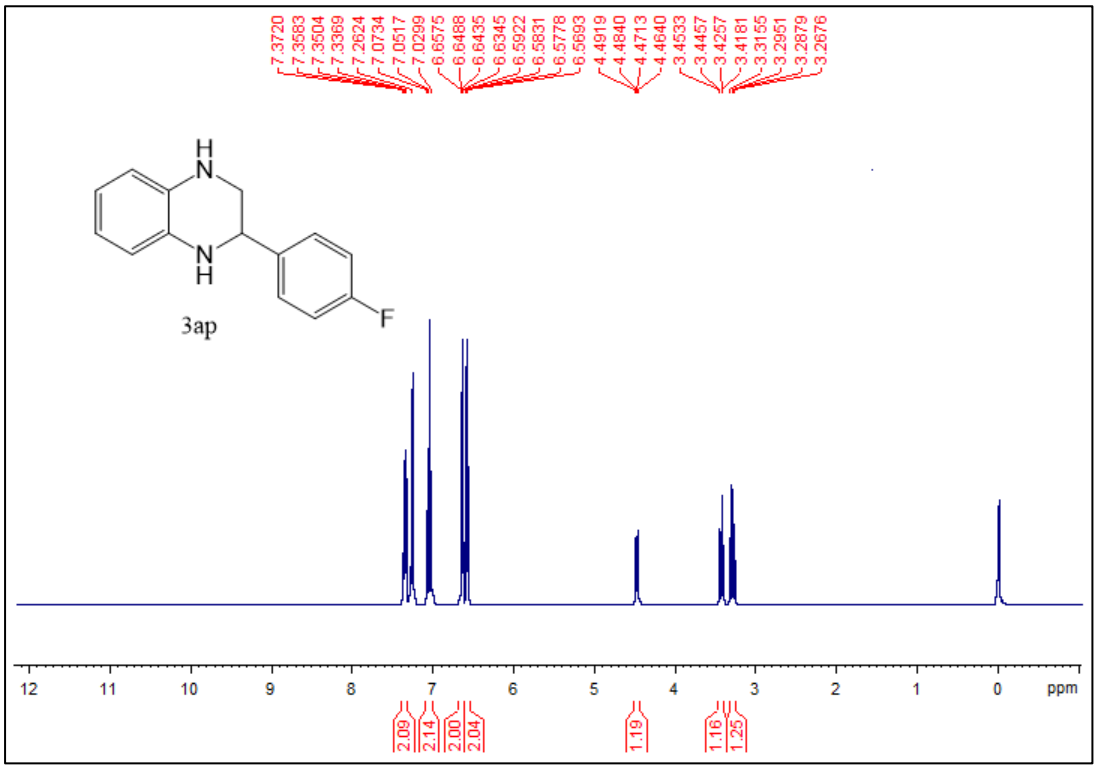
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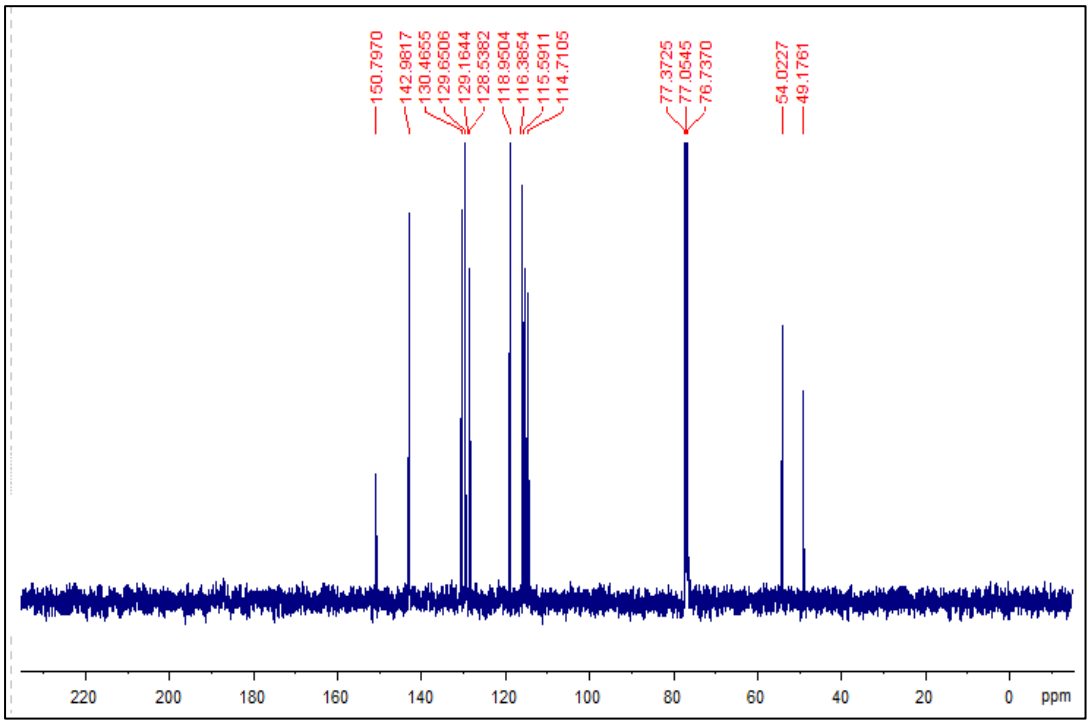
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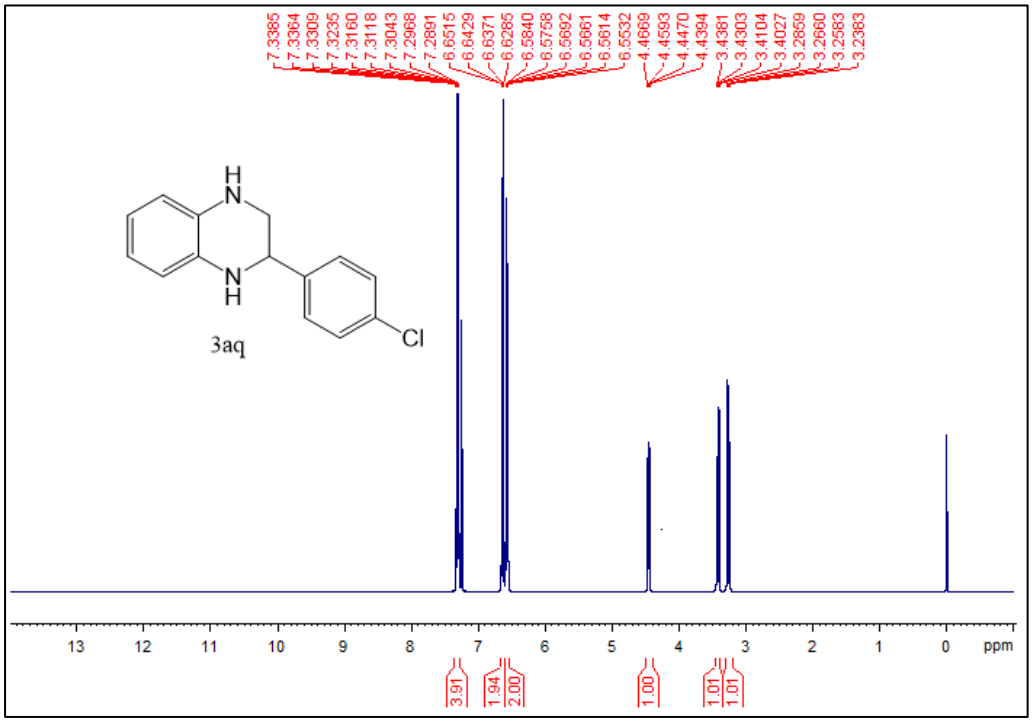
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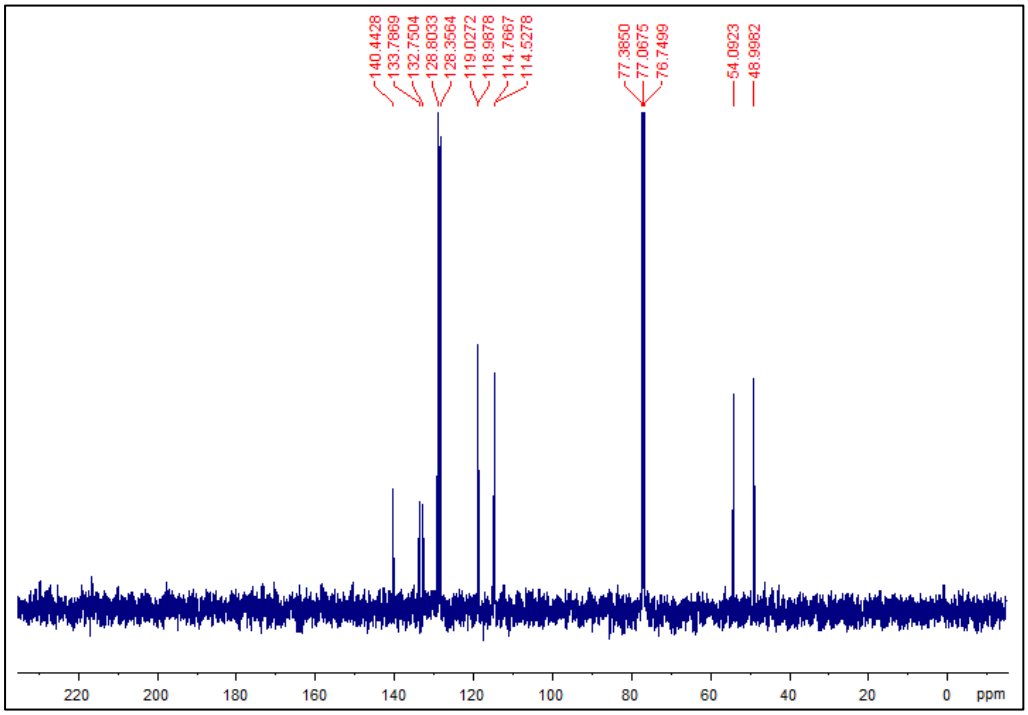
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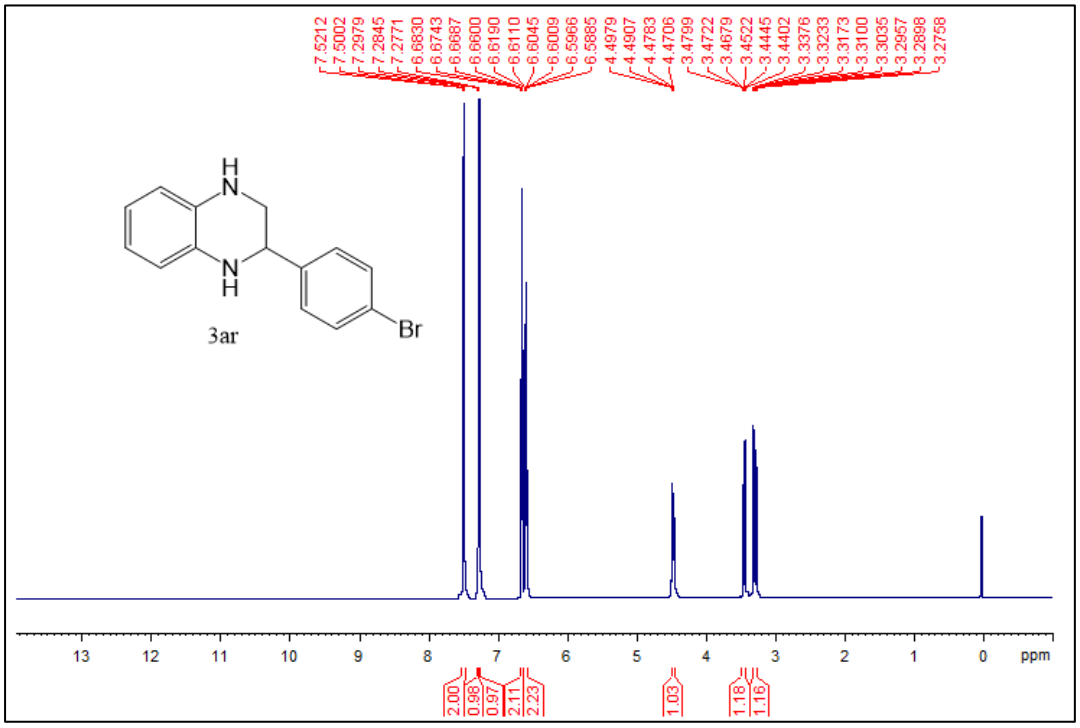
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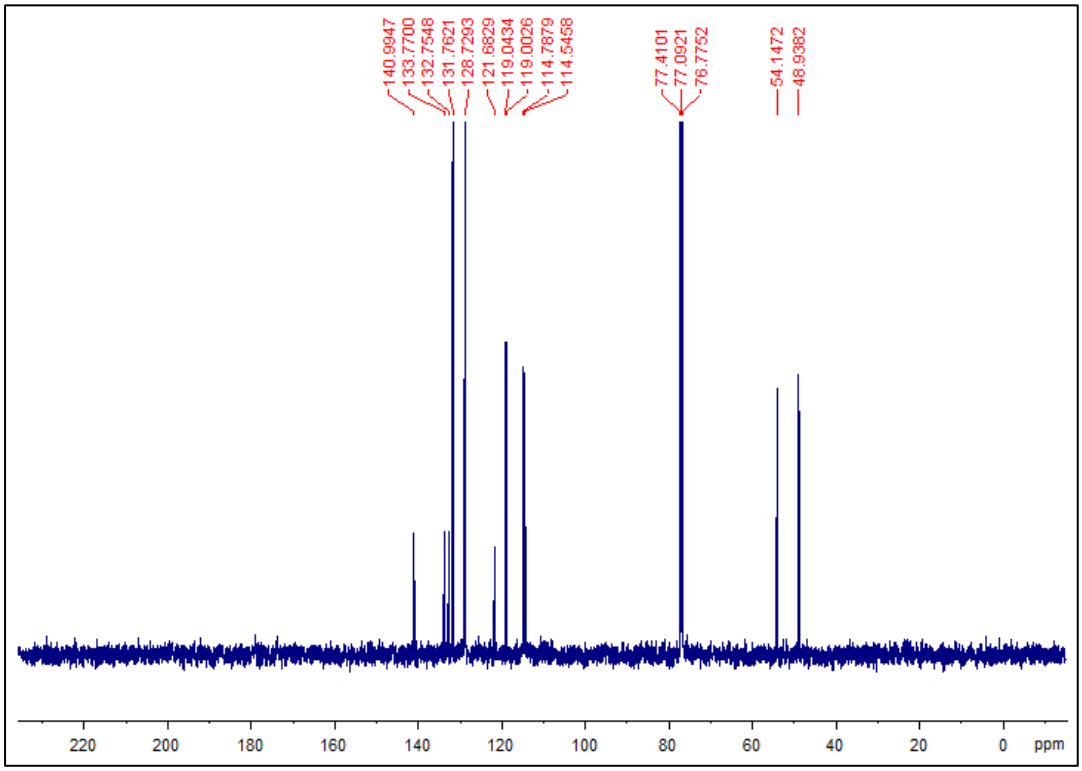
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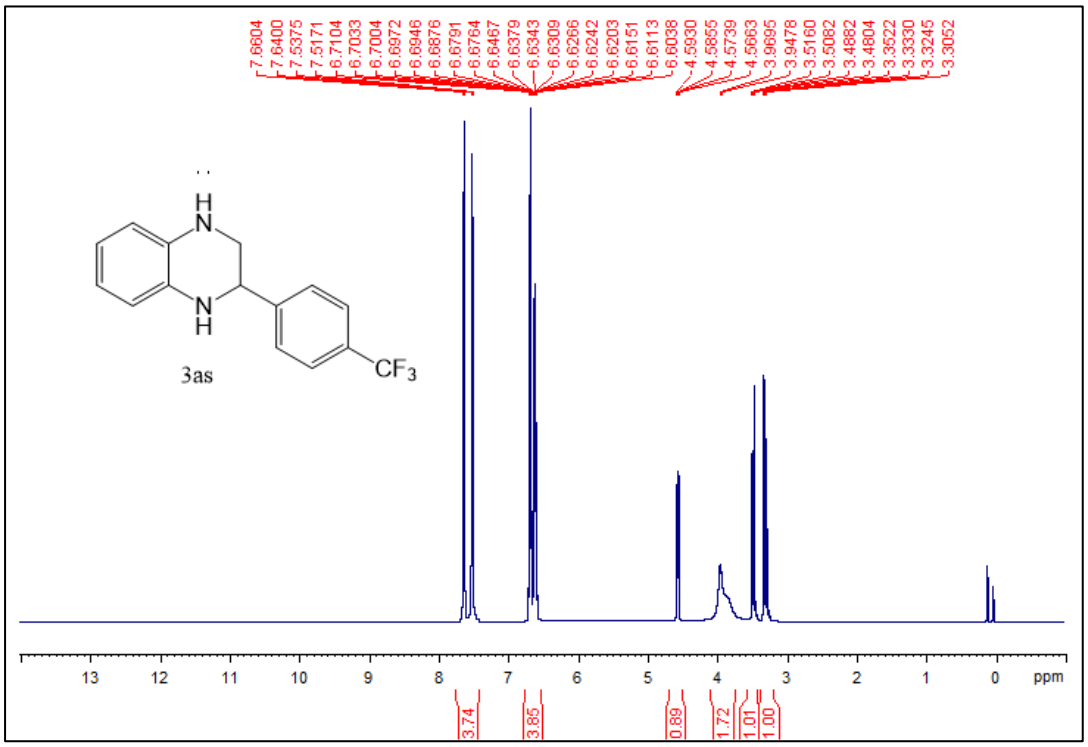
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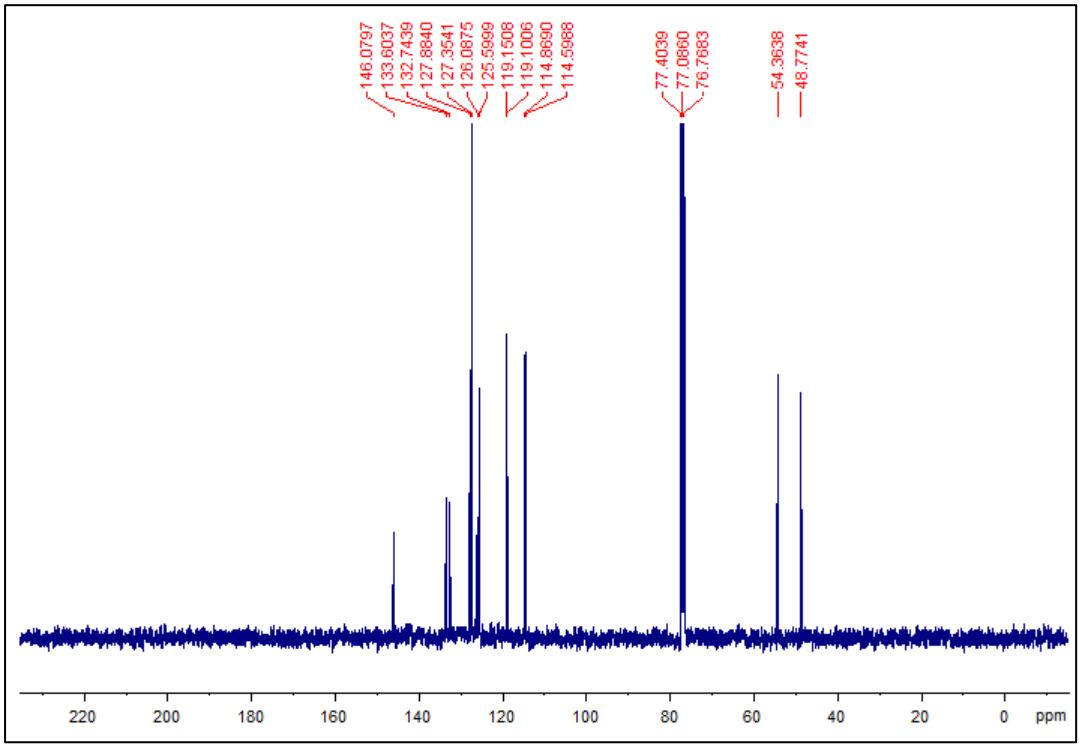
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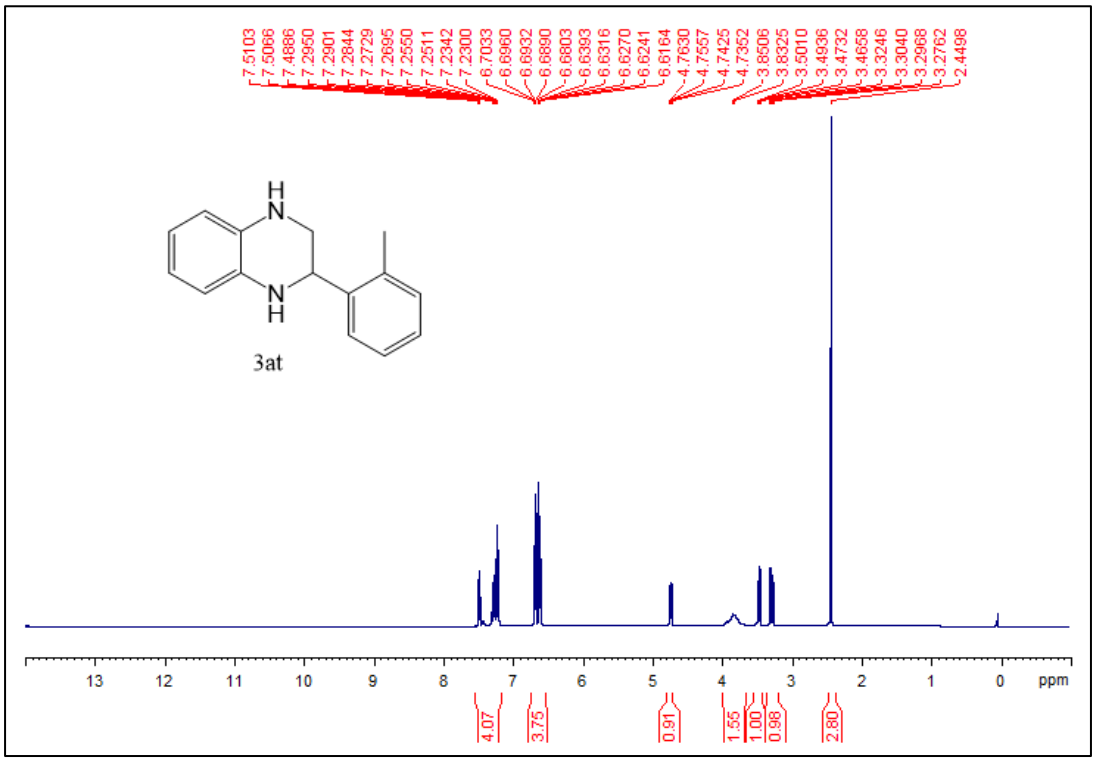
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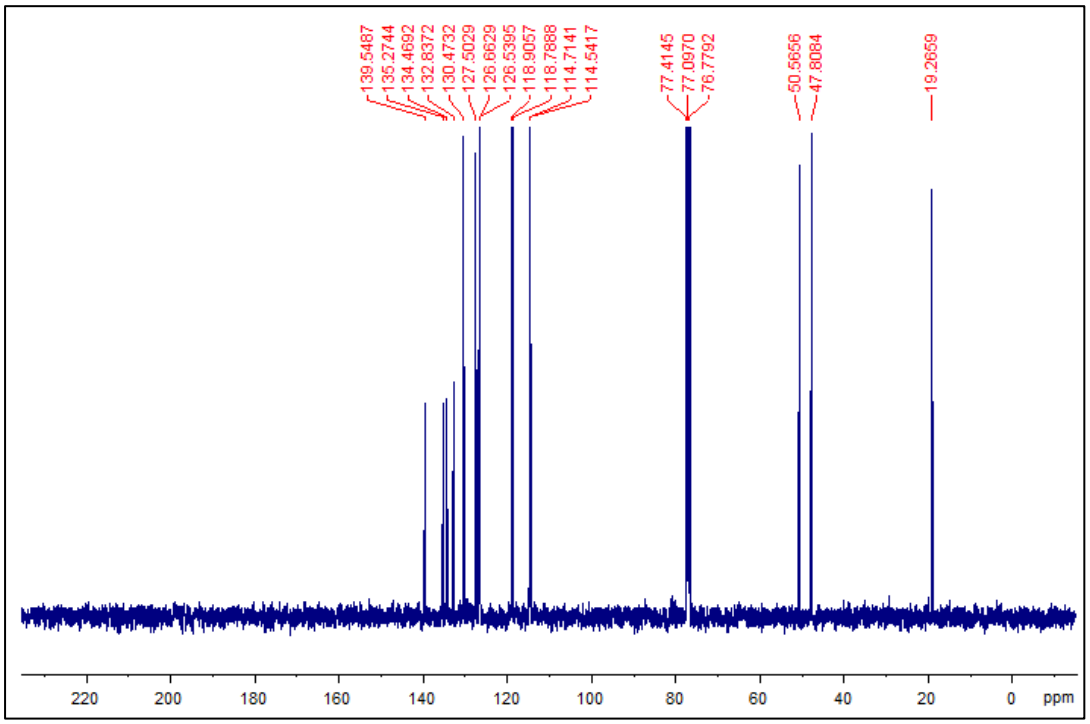
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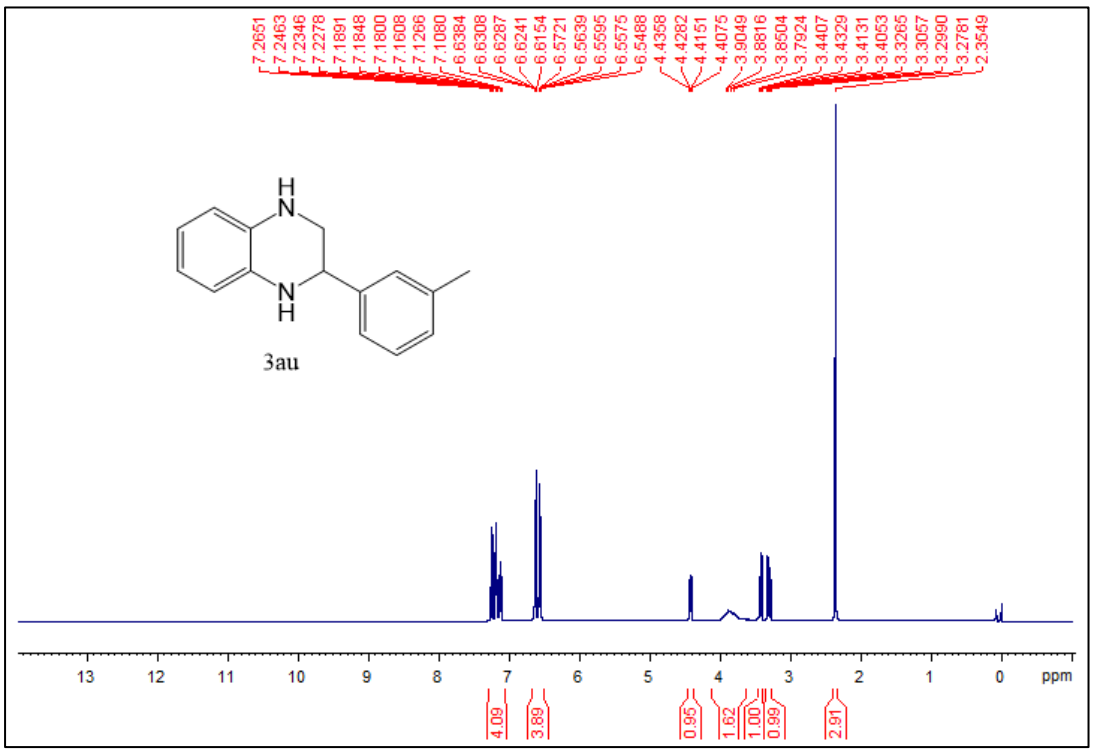
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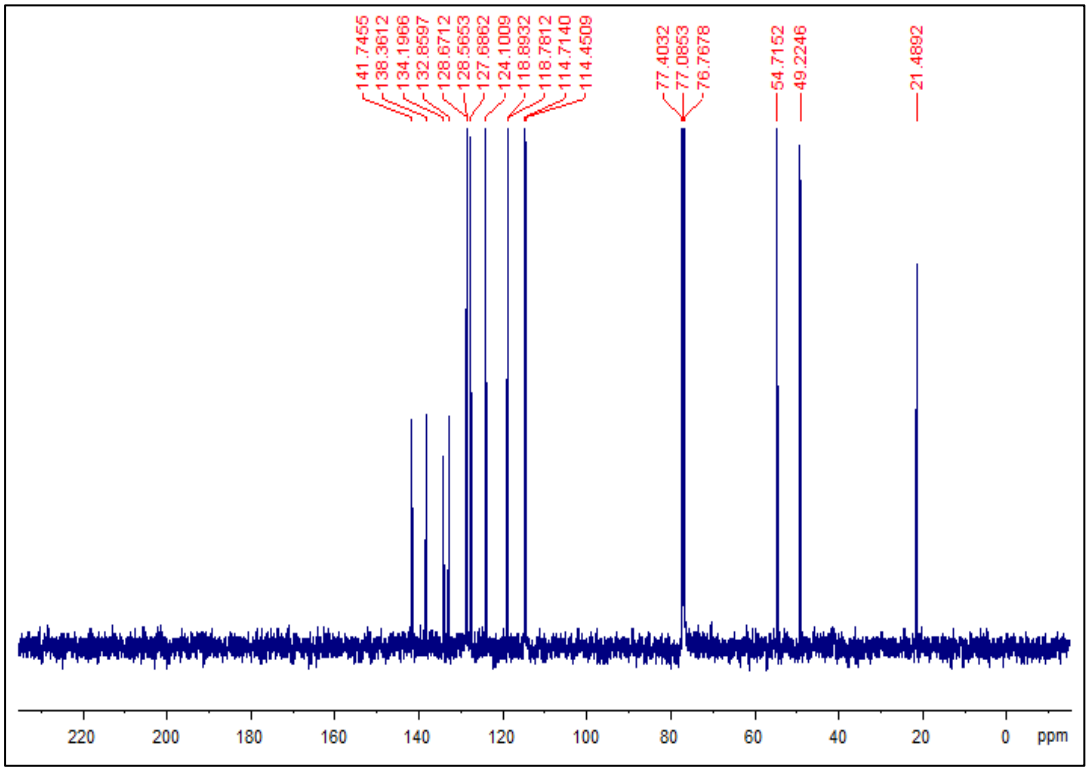
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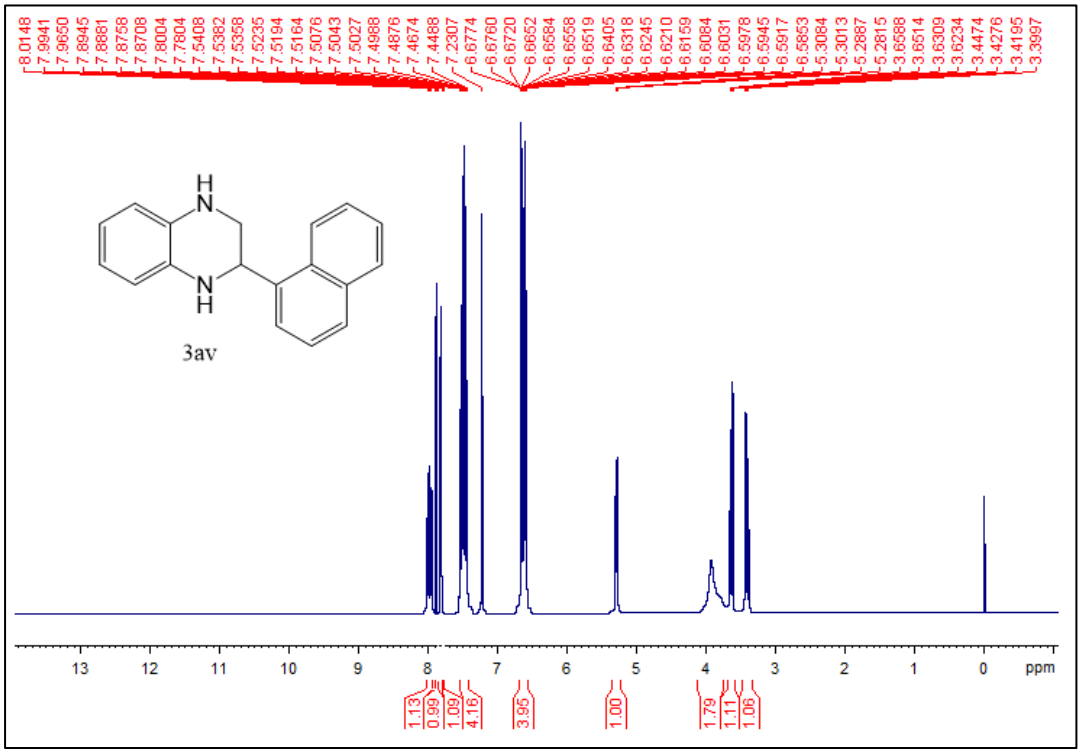
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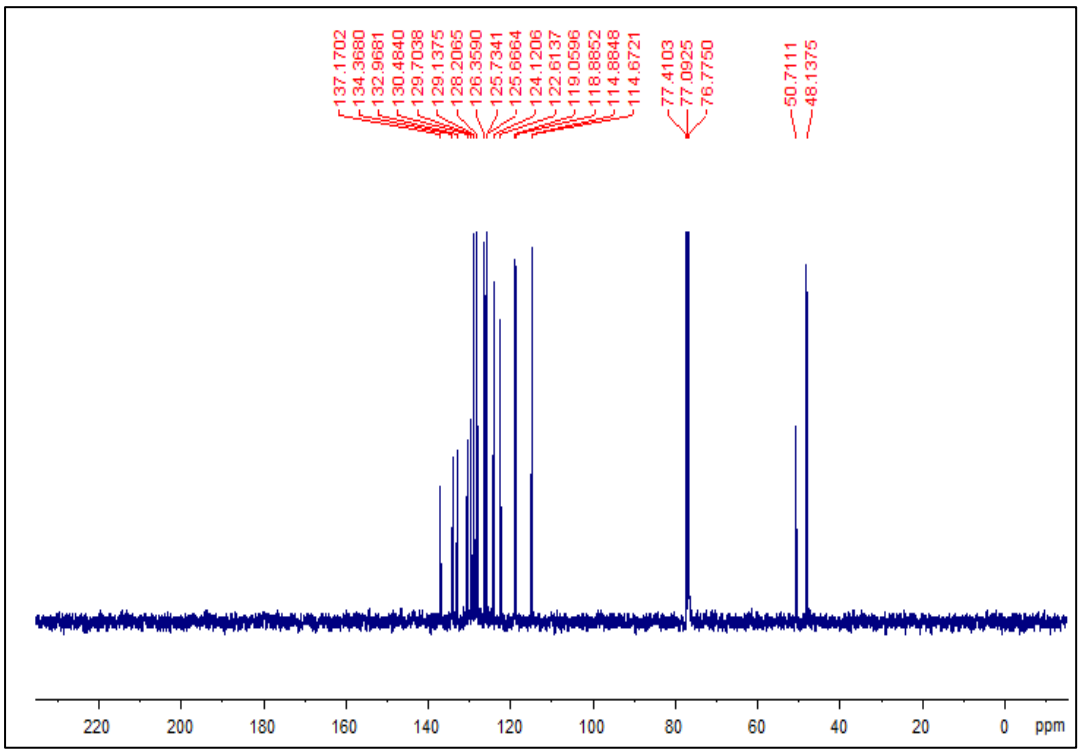
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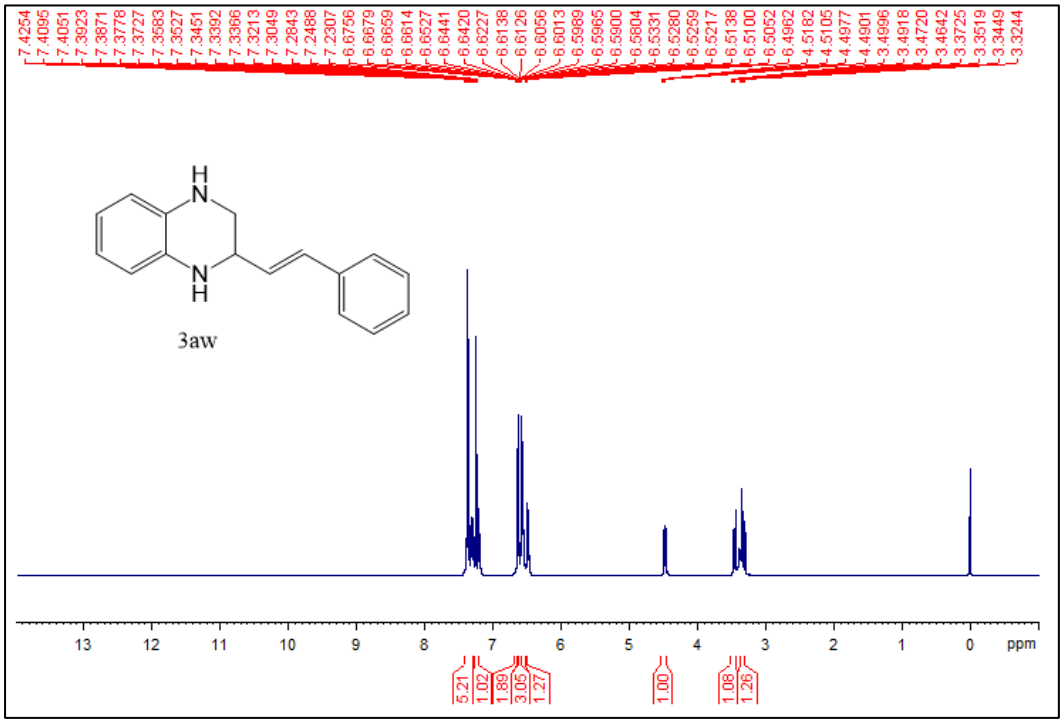
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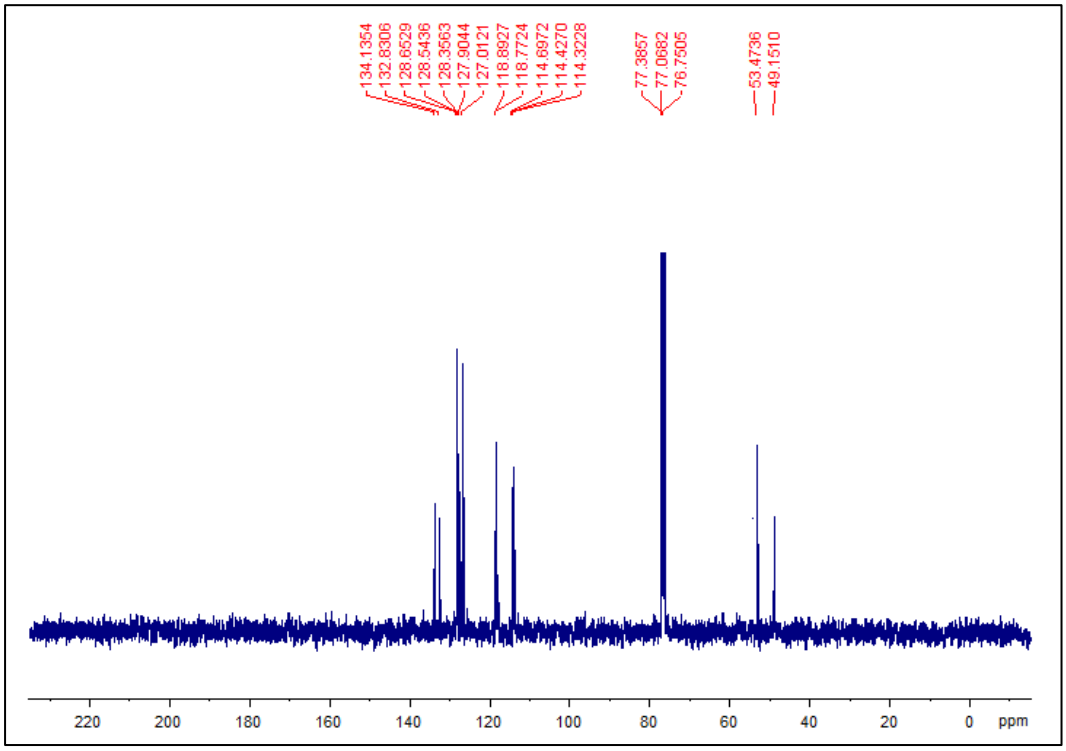
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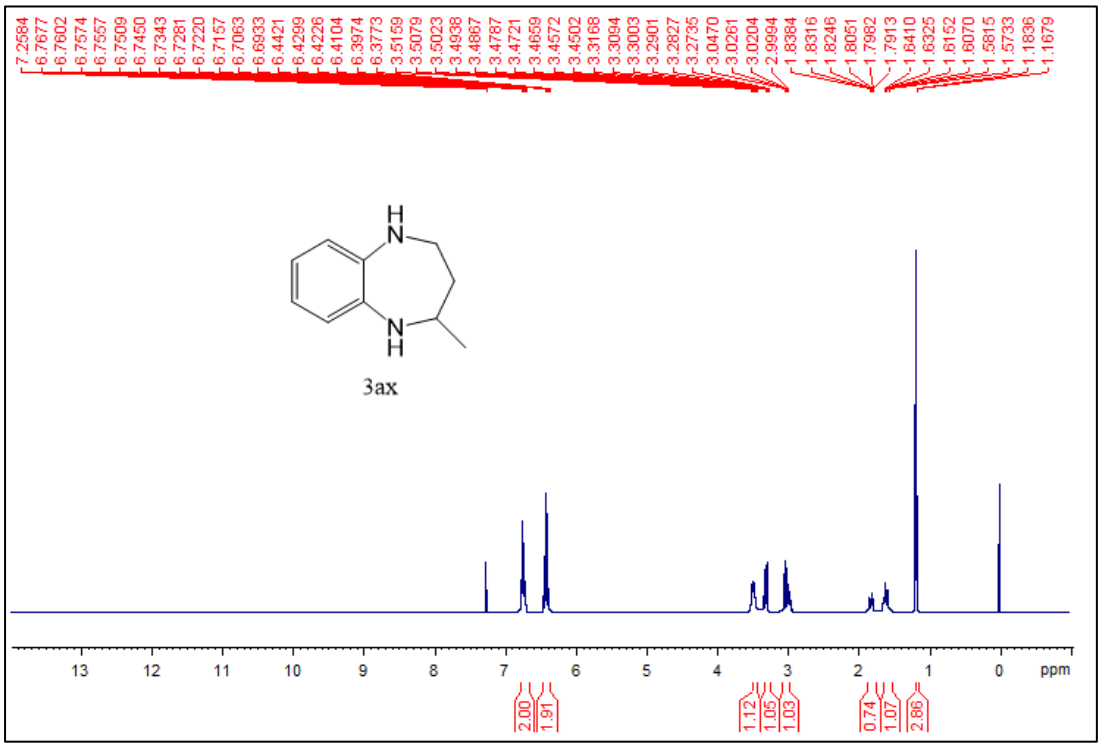
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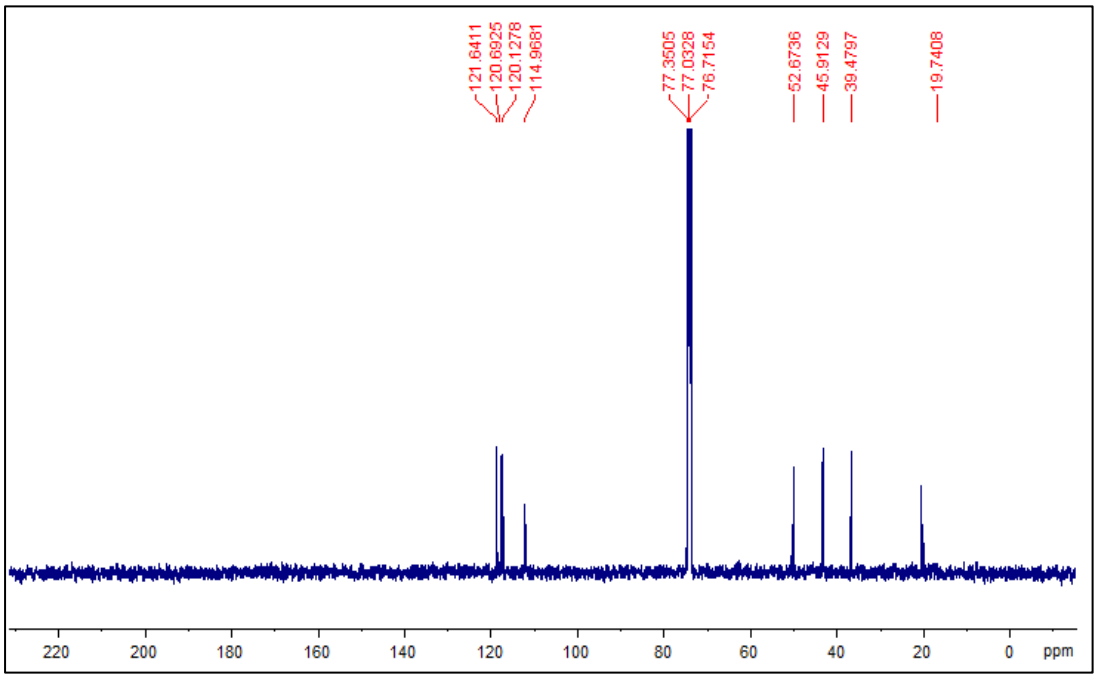
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19.7408
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120
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20
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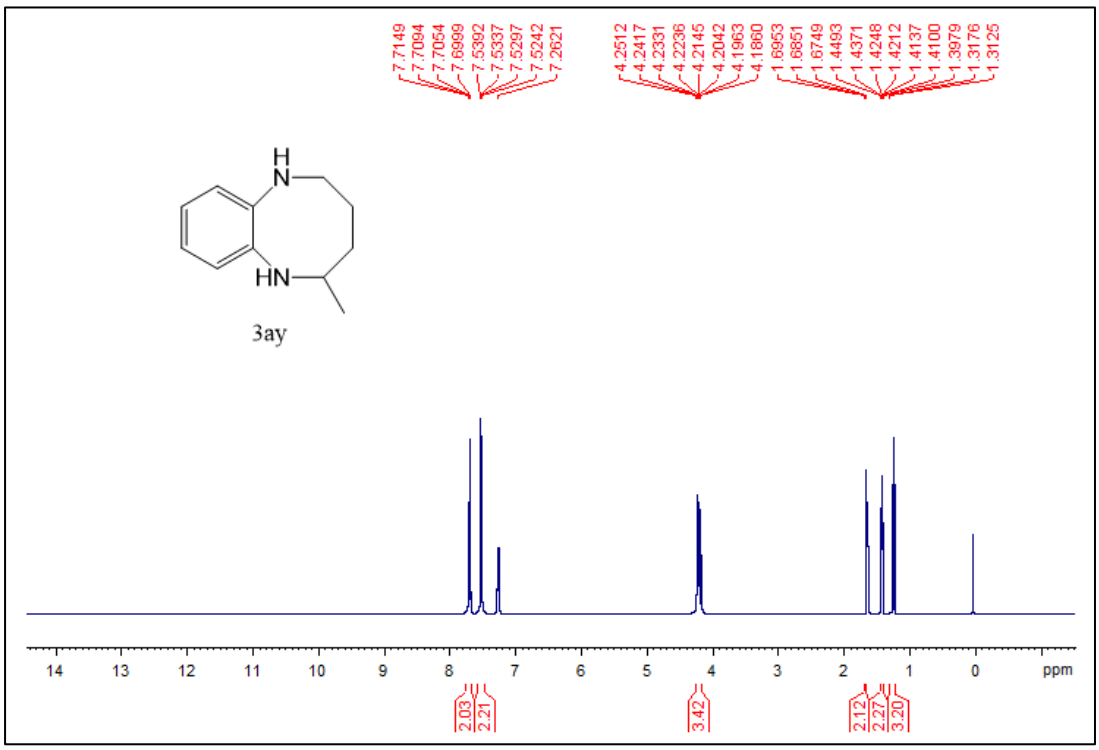
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4.2331
4.2236
4.2145
4.2042
4.1963
4.1860
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1.6851
1.6749
1.4493
1.4371
1.4248
1.4212
1.4137
1.4100
1.3979
1.3176
1.3125
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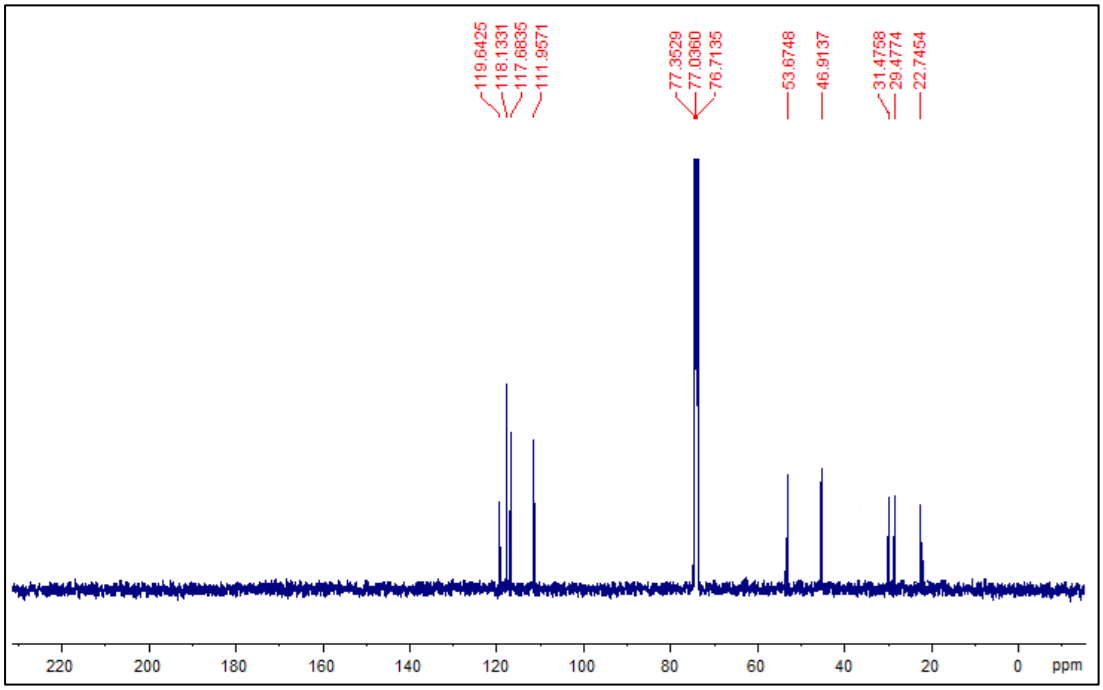
2.12
2.27
3.20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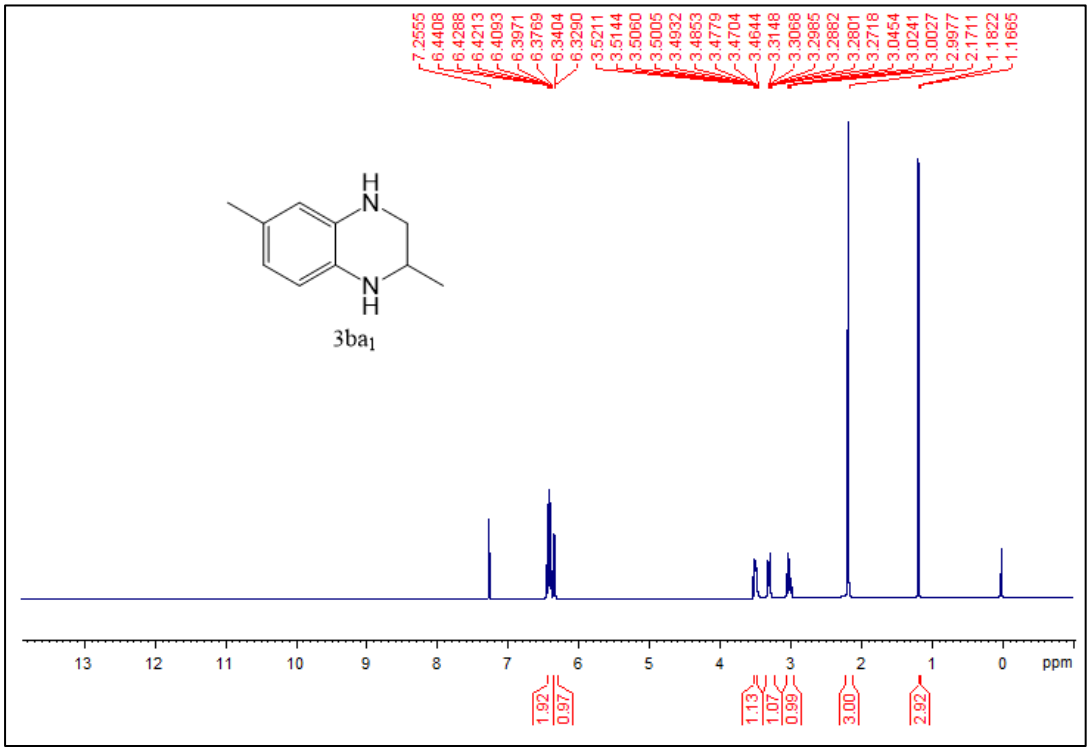
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6.3769
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3.5144
3.5060
3.5005
3.4932
3.4853
3.4779
3.4704
3.4644
3.3148
3.3068
3.2985
3.2882
3.2801
3.2718
3.0454
3.0241
3.0027
2.9977
2.1711
1.1822
1.1665
H
N
N
H
3ba1
13
12
11
10
9
8
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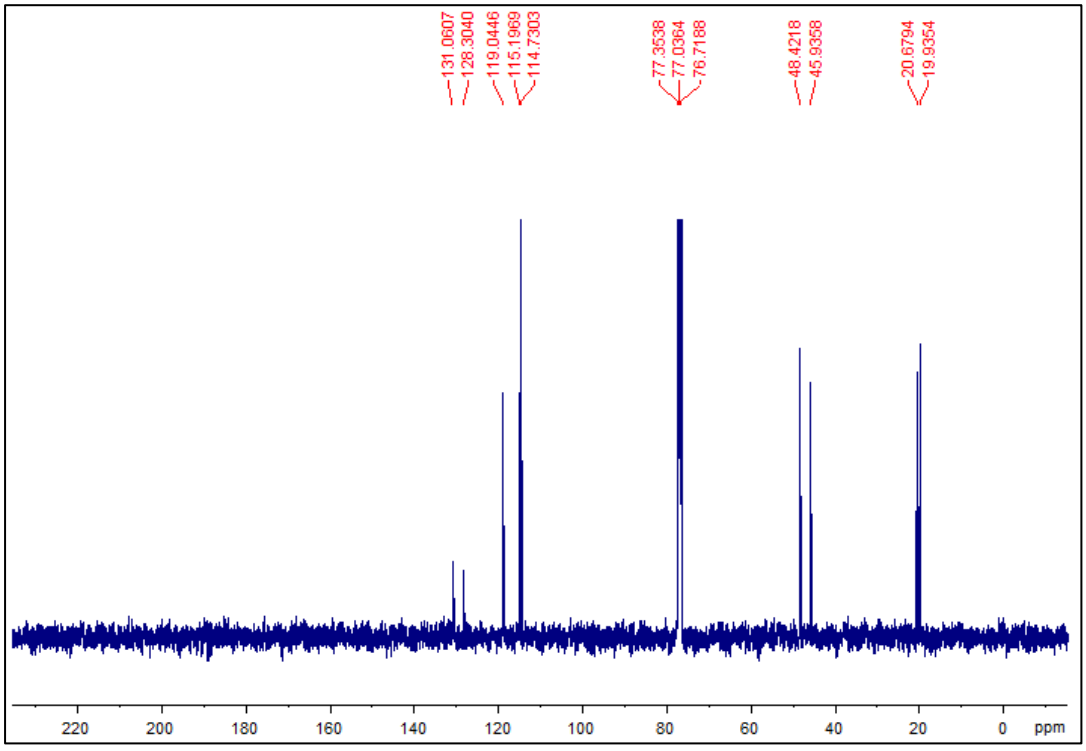
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19.9354
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200
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140
120
100
80
60
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20
0
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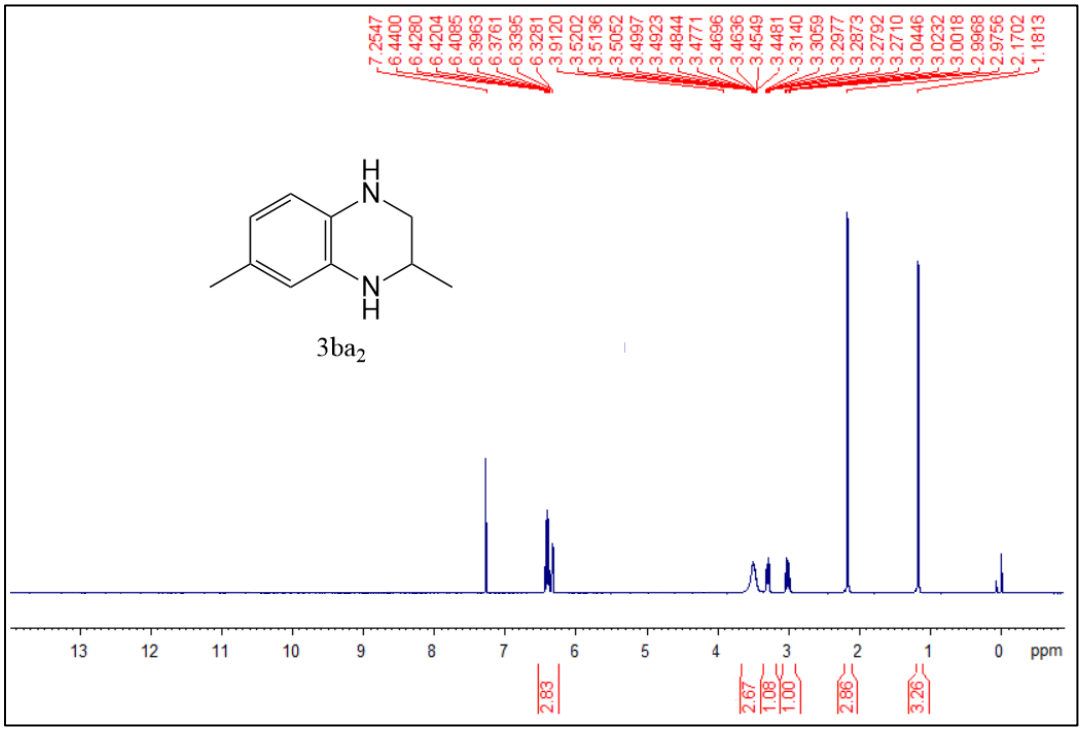
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3.5136
3.5052
3.4997
3.4923
3.4844
3.4771
3.4696
3.4636
3.4549
3.4481
3.3140
3.3059
3.2977
3.2873
3.2792
3.2710
3.0446
3.0232
3.0018
2.9968
2.9756
2.1702
1.1813
H
N
N
H
13
12
11
10
9
8
7
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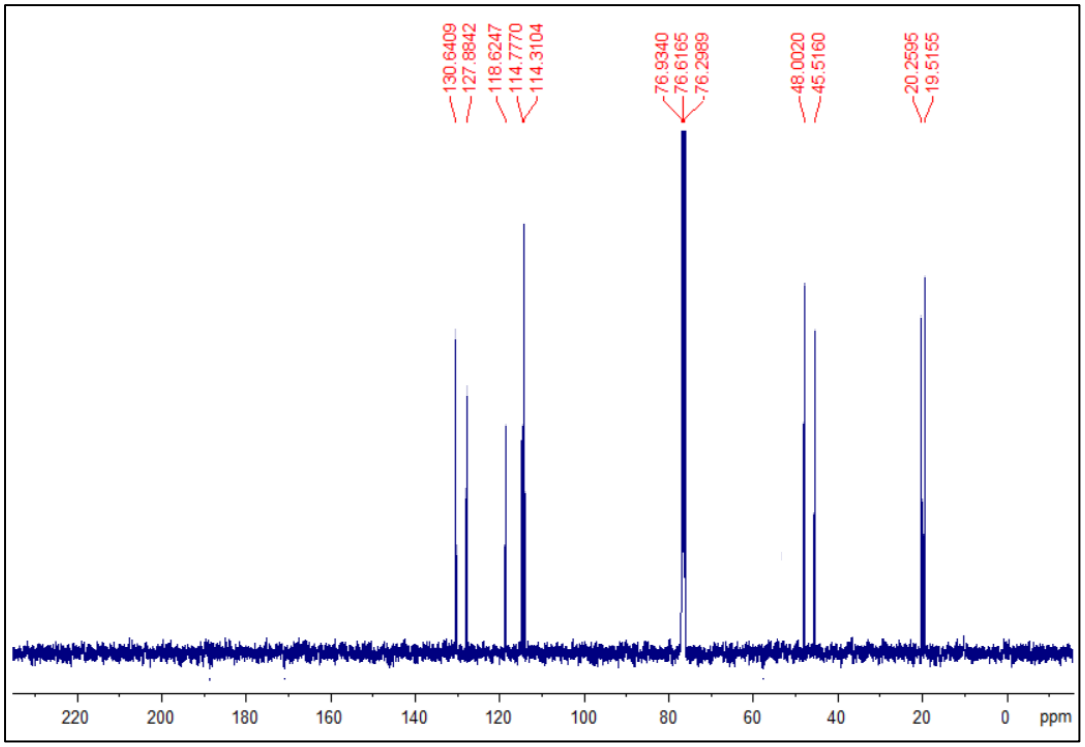
3.26

$3ba_2$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118.6247
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114.3104
76.9340
76.6165
76.2989
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19.5155
220
200
180
160
140
120
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80
60
40
20
0
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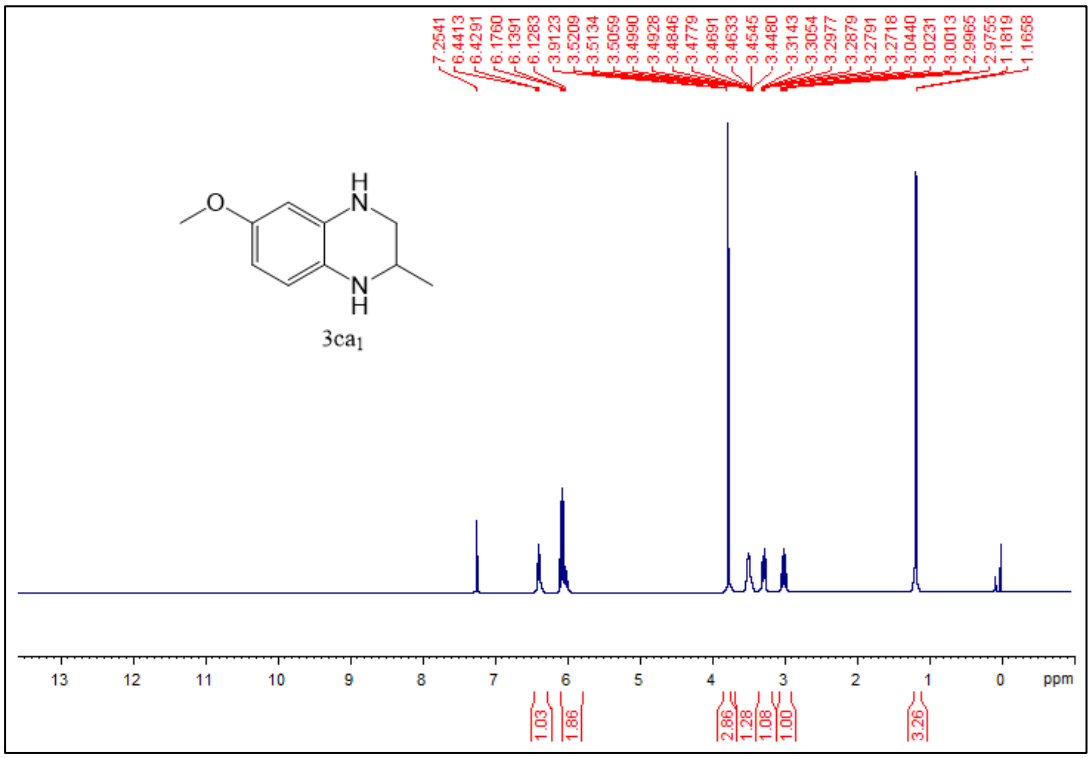
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3.4928
3.4846
3.4779
3.4691
3.4633
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3.3143
3.3054
3.2977
3.2879
3.2791
3.2718
3.0440
3.0231
3.0013
2.9965
2.9755
1.1819
1.1658
H
N
O
N
H
13
12
11
10
9
8
7
6
5
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0
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1.86
2.86
1.28
1.08
1.00
3.26

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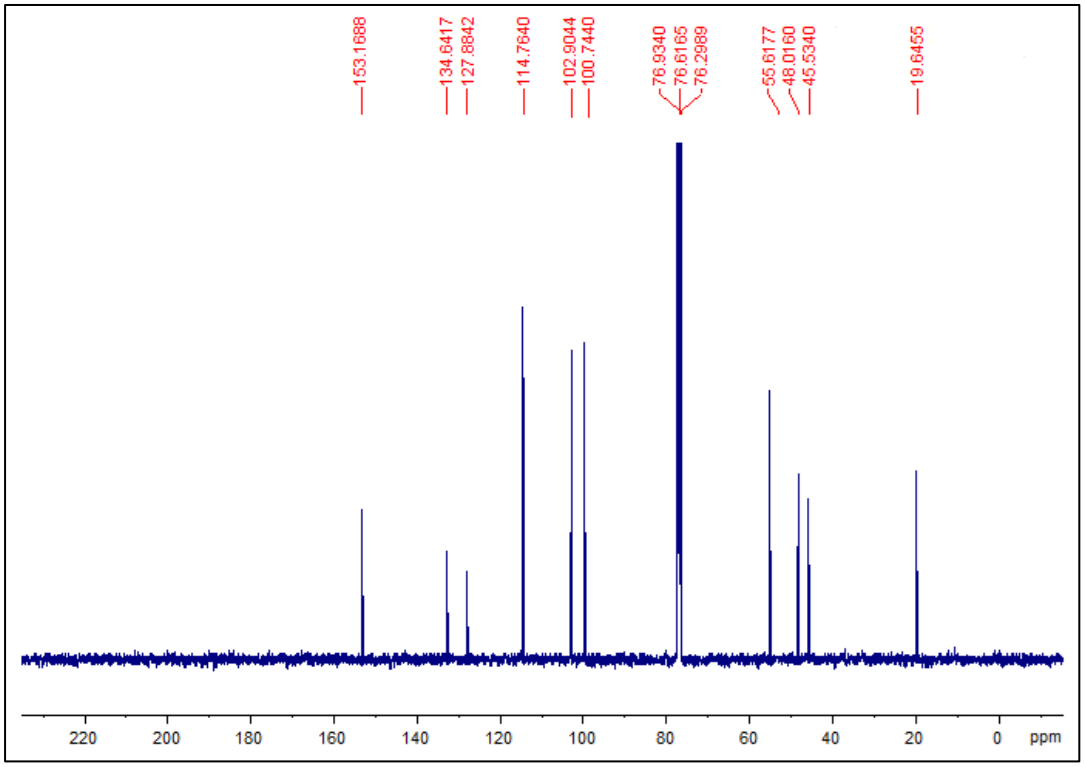
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102.9044
100.7440
76.9340
76.6165
76.2989
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48.0160
45.5340
19.6455
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200
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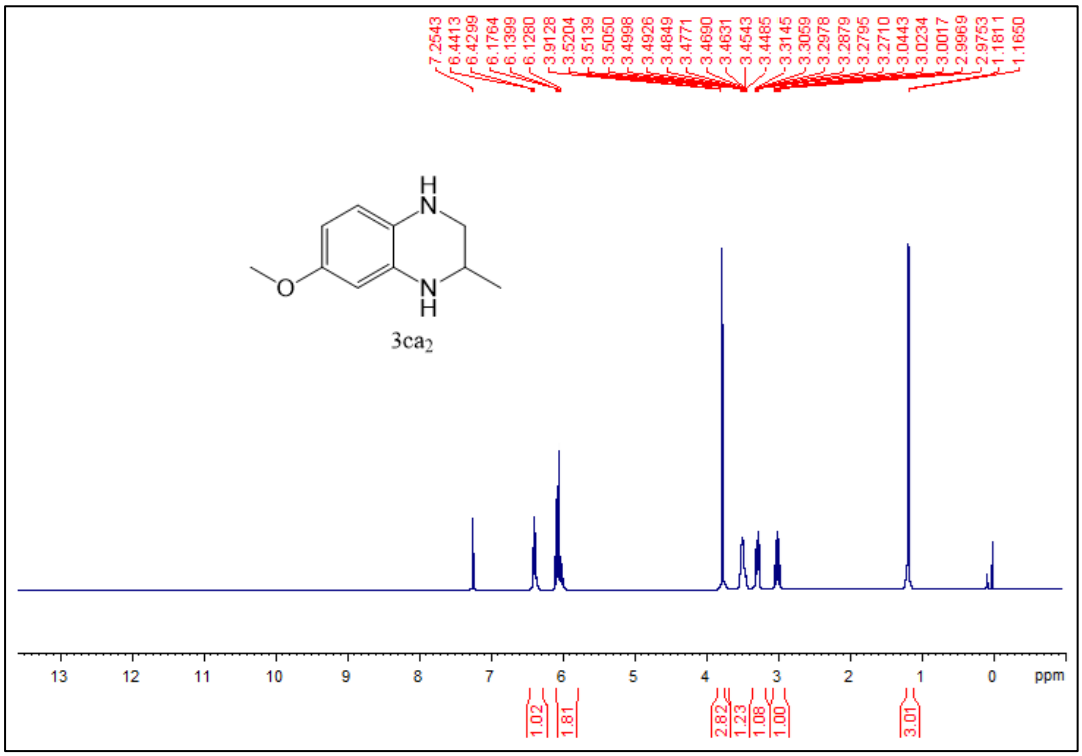
140
120
100
80
60
40
20
0
ppm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6.1764
6.1399
6.1280
3.9128
3.5204
3.5139
3.5050
3.4998
3.4926
3.4849
3.4771
3.4690
3.4631
3.4543
3.4485
3.3145
3.3059
3.2978
3.2879
3.2795
3.2710
3.0443
3.0234
3.0017
2.9969
2.9753
1.1811
1.1650
H
N
O
N
H
13
12
11
10
9
8
7
6
5
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3
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0
ppm
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1.81
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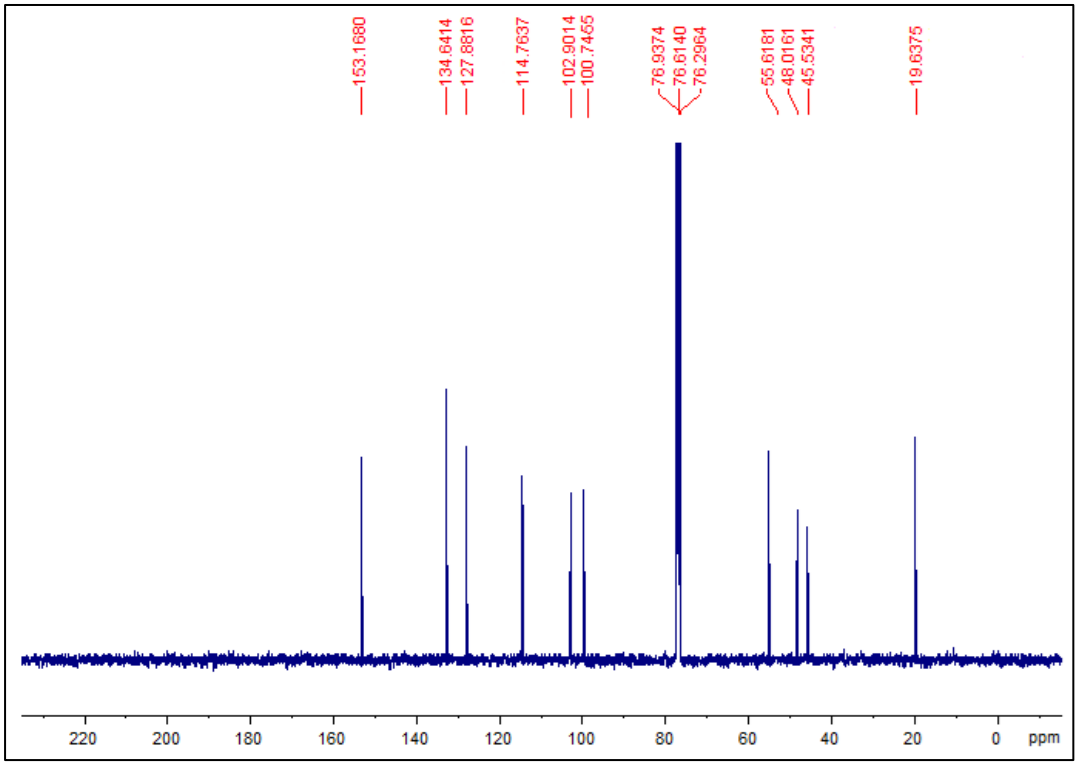
1.08
1.00
3.01

3ca$_2$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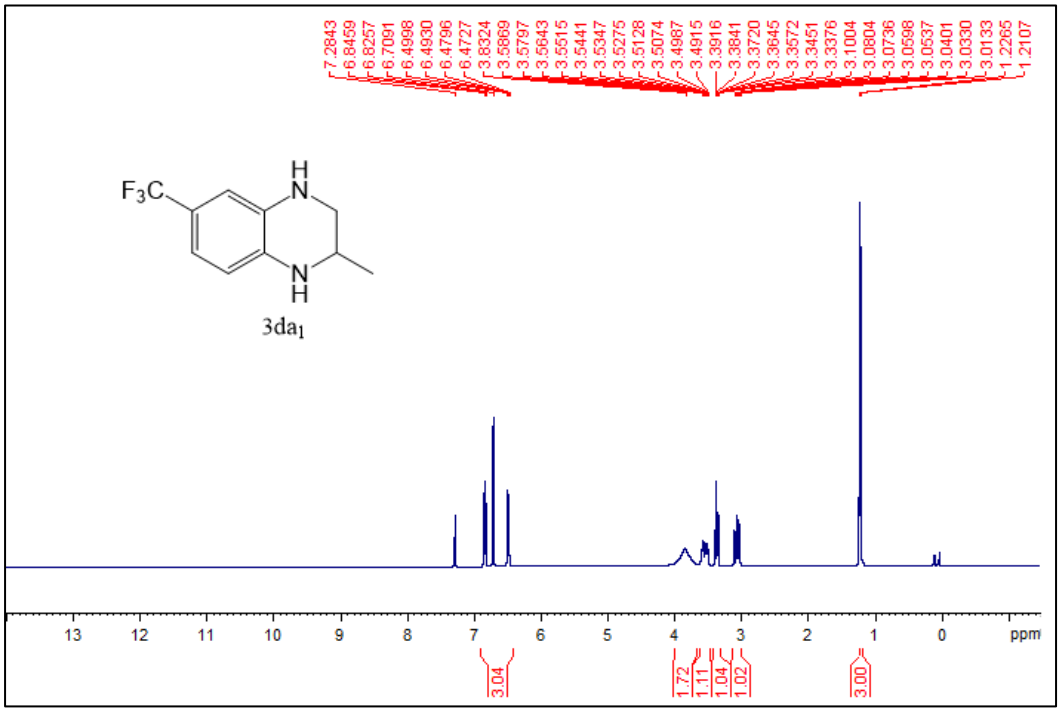
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6.4796
6.4727
3.8324
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3.5797
3.5643
3.5515
3.5441
3.5347
3.5275
3.5128
3.5074
3.4987
3.4915
3.3916
3.3841
3.3720
3.3645
3.3572
3.3451
3.3376
3.1004
3.0804
3.0736
3.0598
3.0537
3.0401
3.0330
3.0133
1.2265
1.2107
F3C
H
N
N
H
3da1
13
12
11
10
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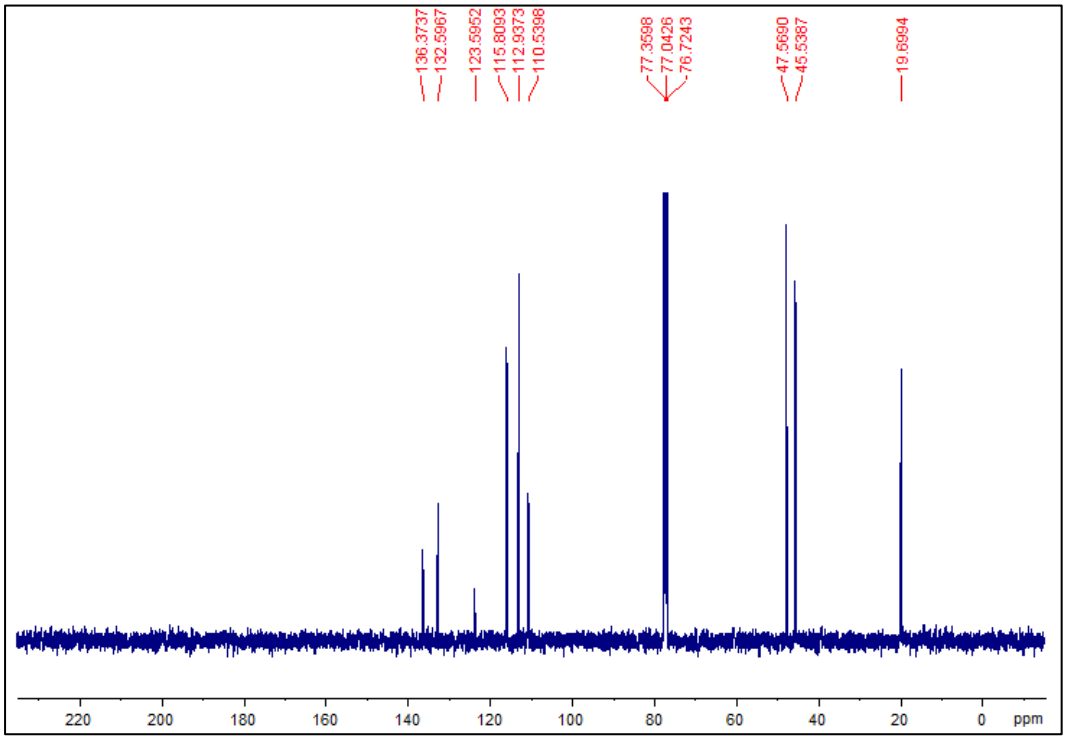
1.11
1.04
1.02
3.00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19.6994
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200
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120
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20
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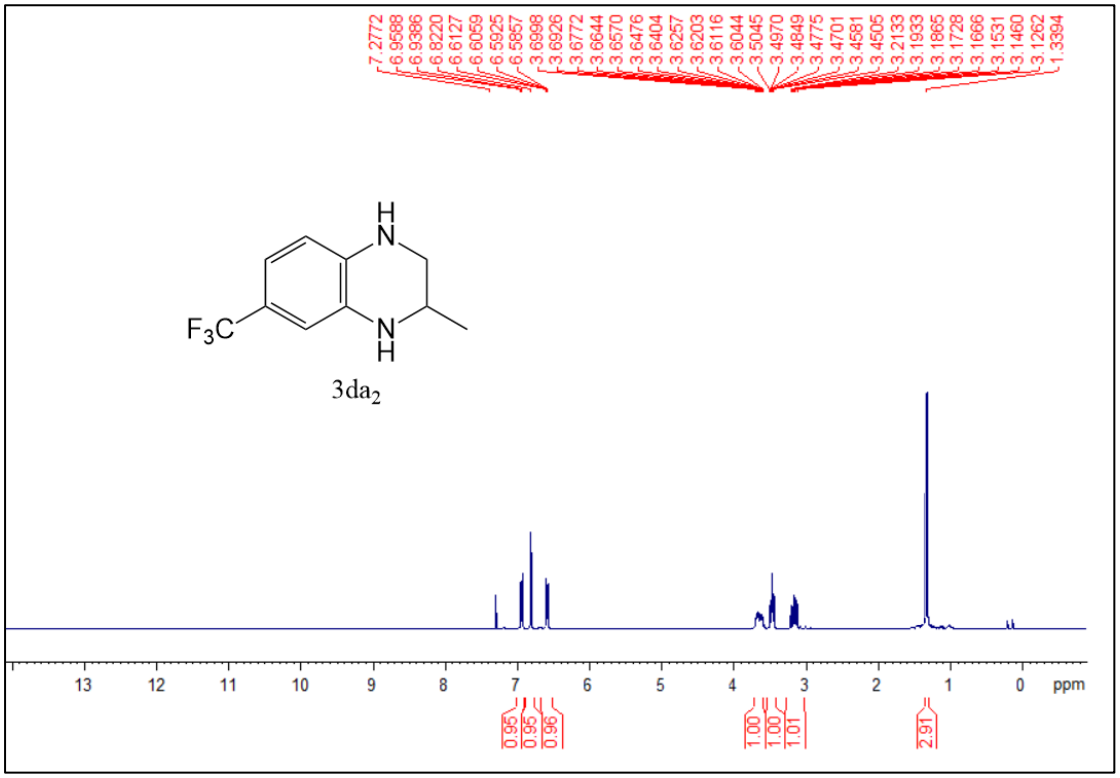
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3.6644
3.6570
3.6476
3.6404
3.6257
3.6203
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3.6044
3.5045
3.4970
3.4849
3.4775
3.4701
3.4581
3.4505
3.2133
3.1933
3.1865
3.1728
3.1666
3.1531
3.1460
3.1262
1.3394
H
N
F3C
N
H
3da2
13
12
11
10
9
8
7
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4
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2
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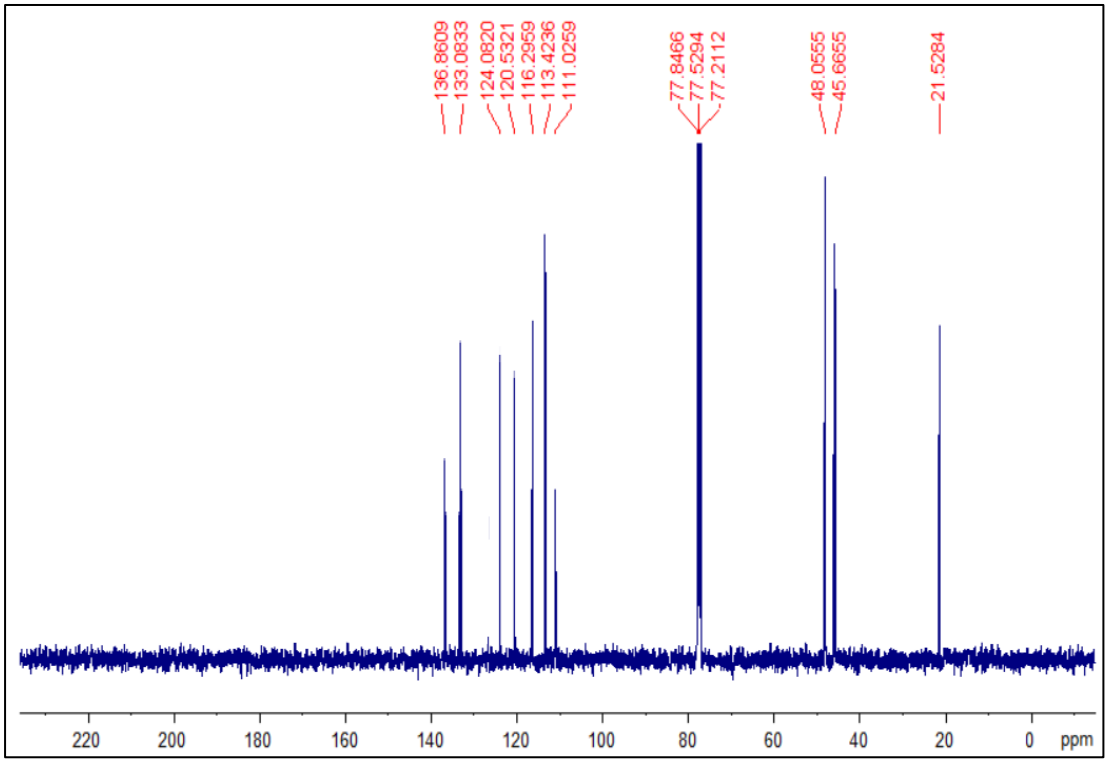
1.00
1.01
2.91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120.5321
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111.0259
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77.5294
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21.5284
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200
180
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140
120
100
80
60
40
20
0
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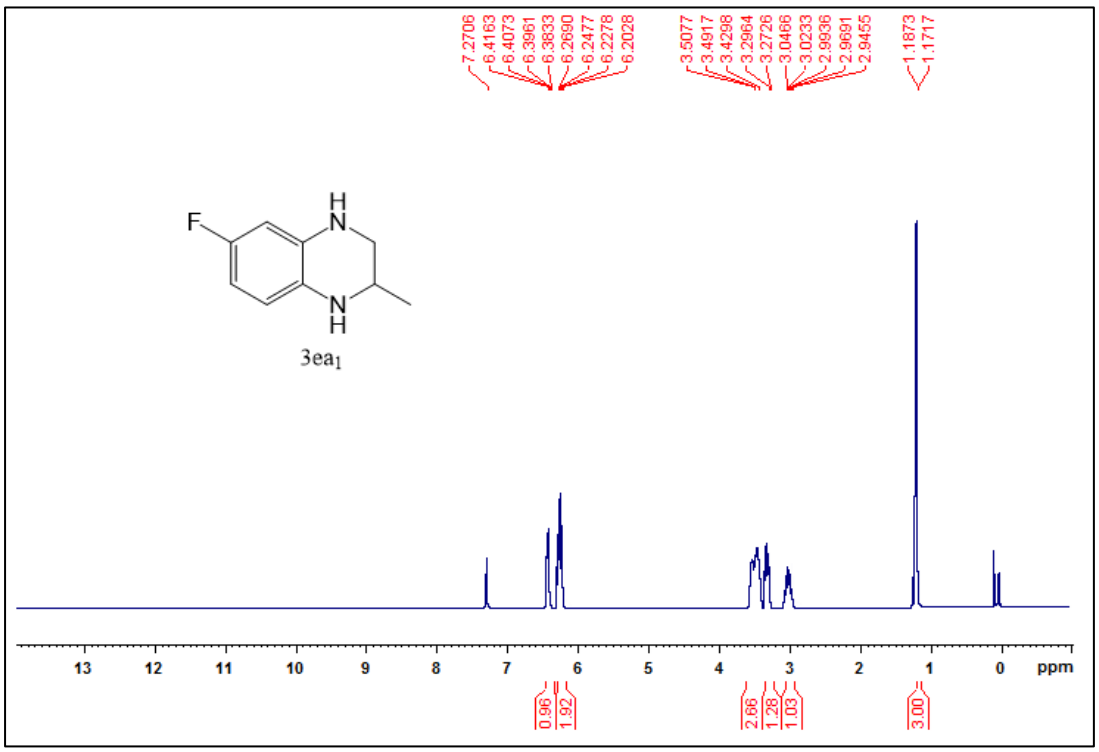
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6.2028
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3.4917
3.4298
3.2964
3.2726
3.0466
3.0233
2.9936
2.9691
2.9455
1.1873
1.1717
F
H
N
N
H
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1.28
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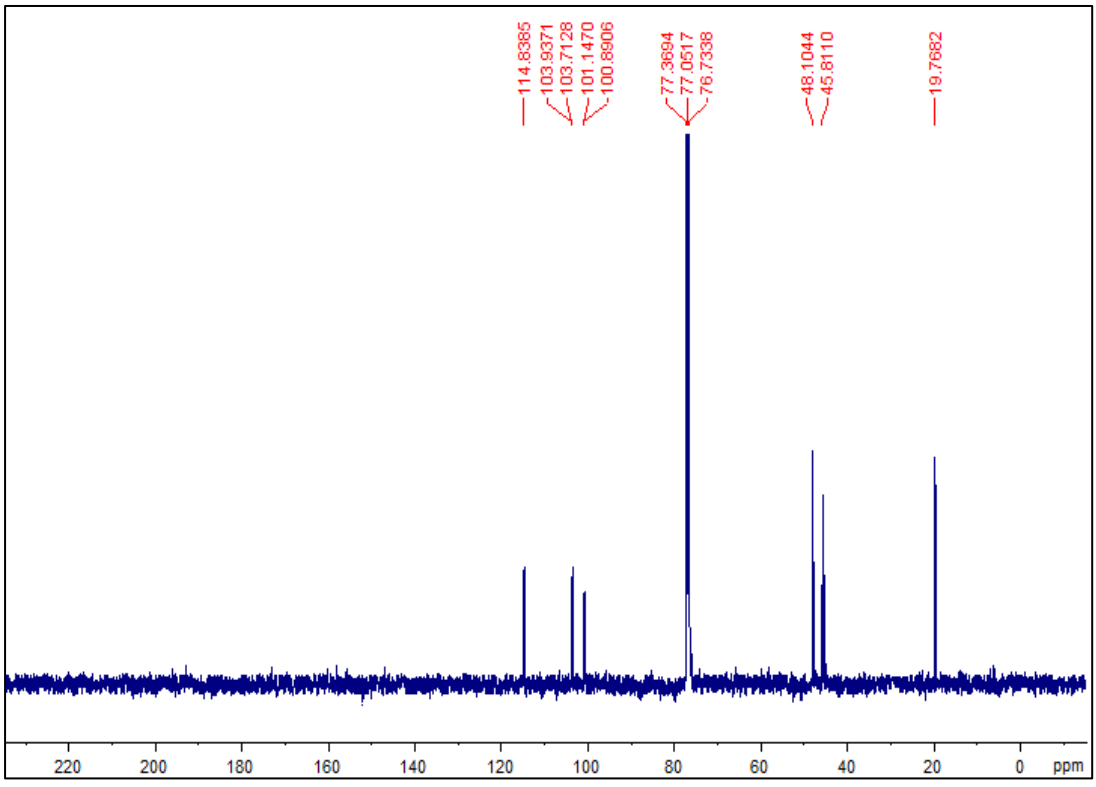
3.00

$3ea_1$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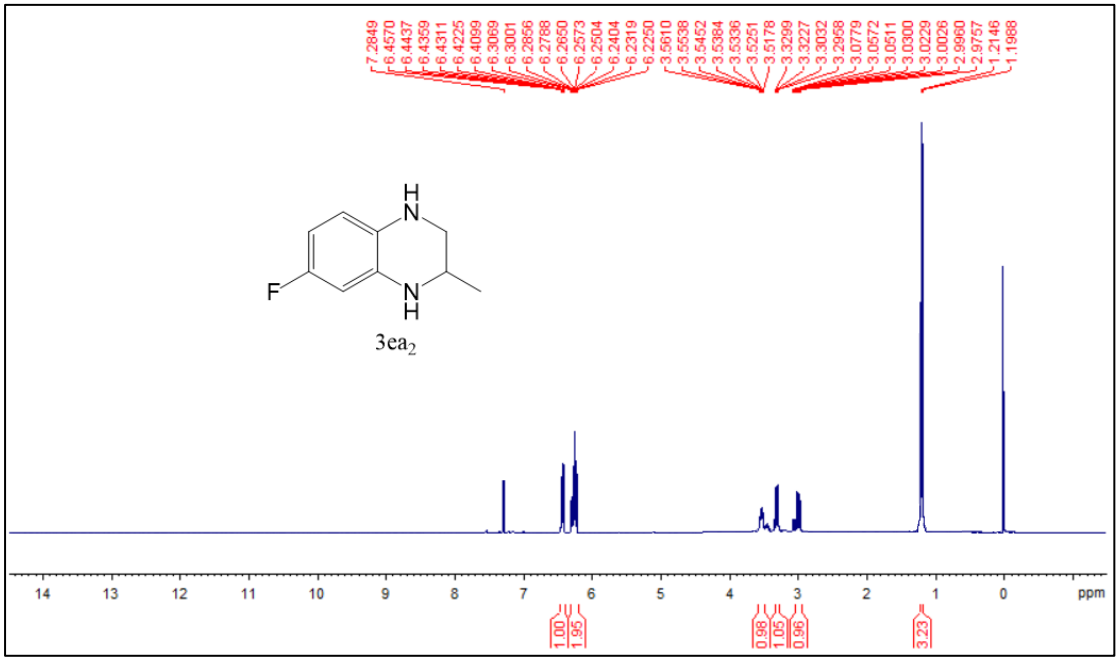
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6.2650
6.2573
6.2504
6.2404
6.2319
6.2250
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3.5538
3.5452
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3.5336
3.5251
3.5178
3.3299
3.3227
3.3032
3.2958
3.0779
3.0572
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3.0300
3.0229
3.0026
2.9960
2.9757
1.2146
1.1988
H
N
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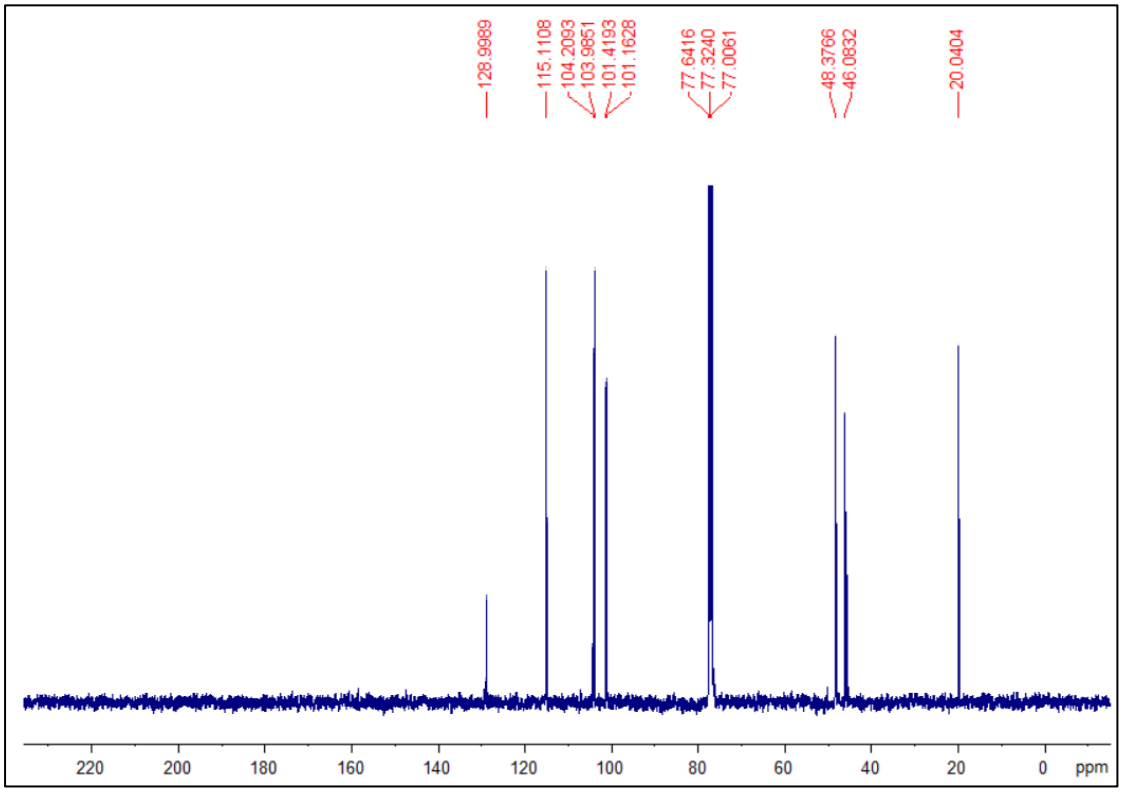
3.23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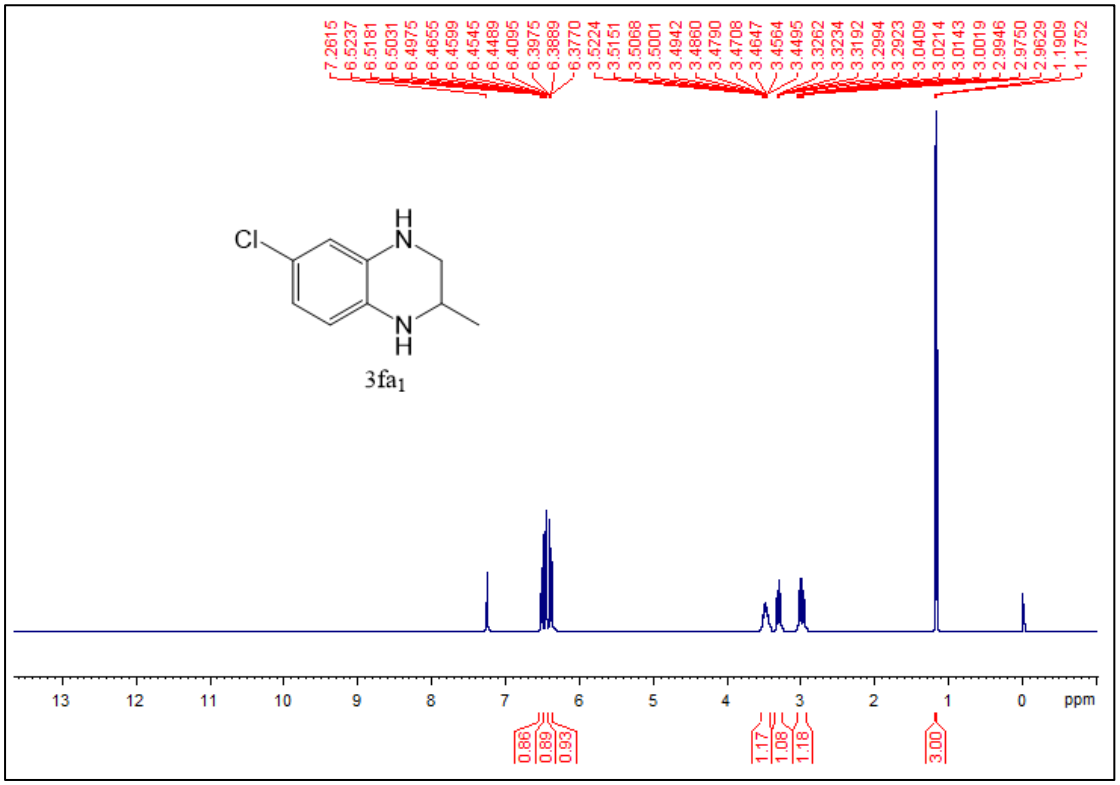
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6.3770
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3.4495
3.3262
3.3234
3.3192
3.2994
3.2923
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3.0214
3.0143
3.0019
2.9946
2.9750
2.9629
1.1909
1.1752
Cl
H
N
N
H
13
12
11
10
9
8
7
6
5
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1.08
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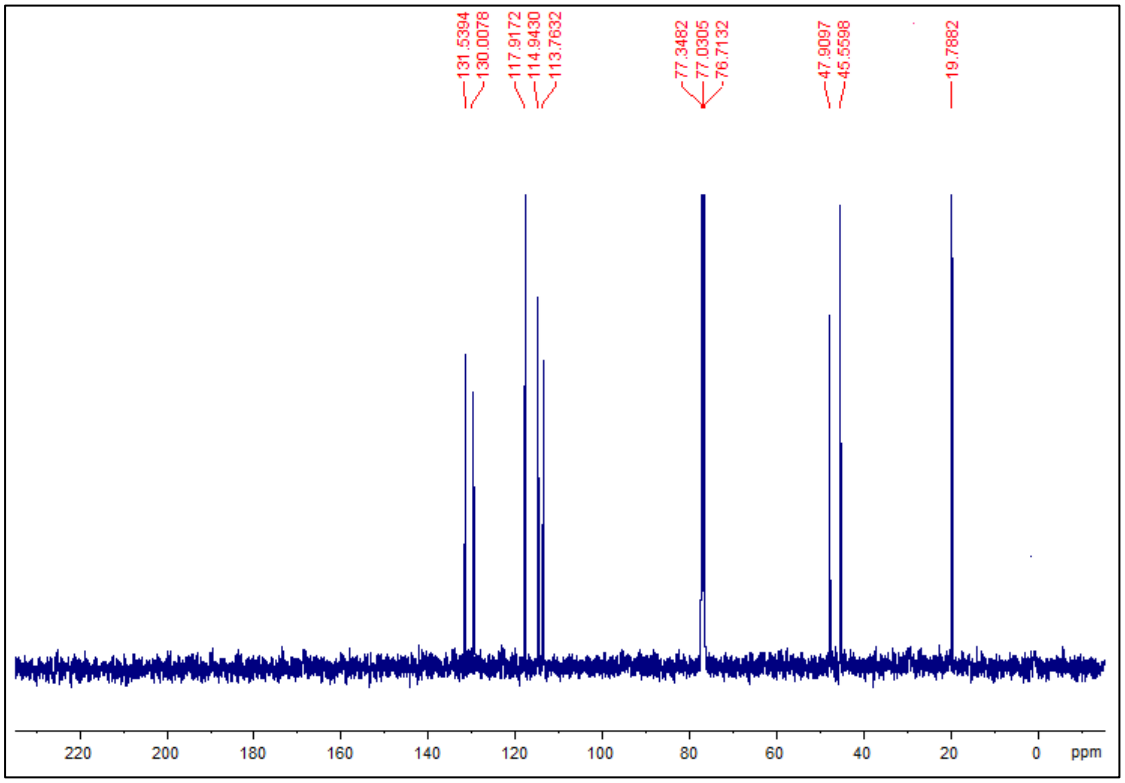
$3fa_1$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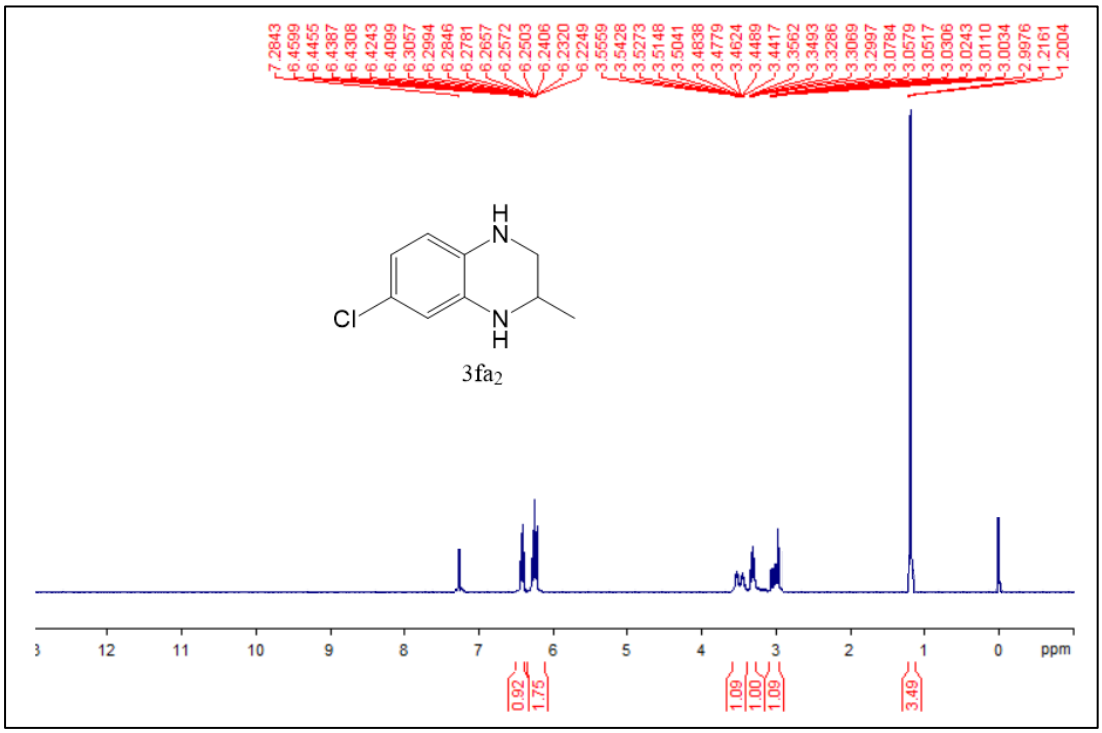
200
180
160
140
120
100
80
60
40
20
0
ppm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6.2994
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6.2781
6.2657
6.2572
6.2503
6.2406
6.2320
6.2249
3.5559
3.5428
3.5273
3.5148
3.5041
3.4838
3.4779
3.4624
3.4489
3.4417
3.3562
3.3493
3.3286
3.3069
3.2997
3.0784
3.0579
3.0517
3.0306
3.0243
3.0110
3.0034
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1.2161
1.2004
H
N
Cl
N
H
12
11
10
9
8
7
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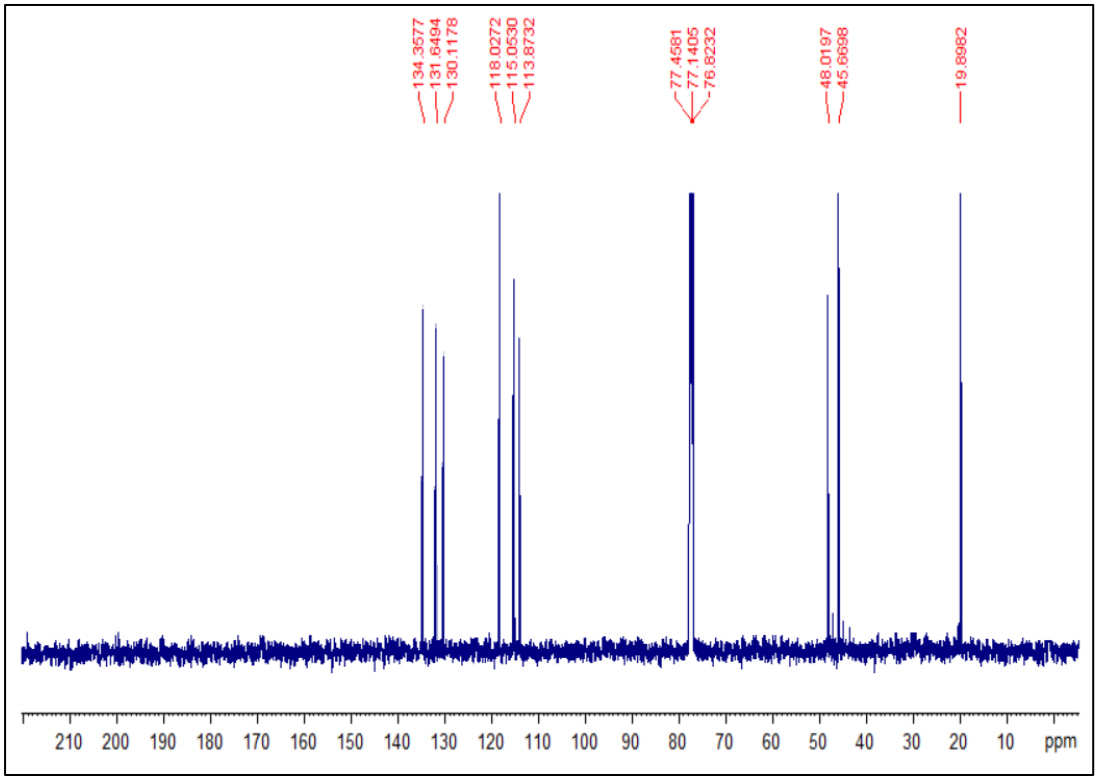
3.49

3fa$_2$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76.8232
48.0197
45.6698
19.8982
210
200
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150
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120
110
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90
80
70
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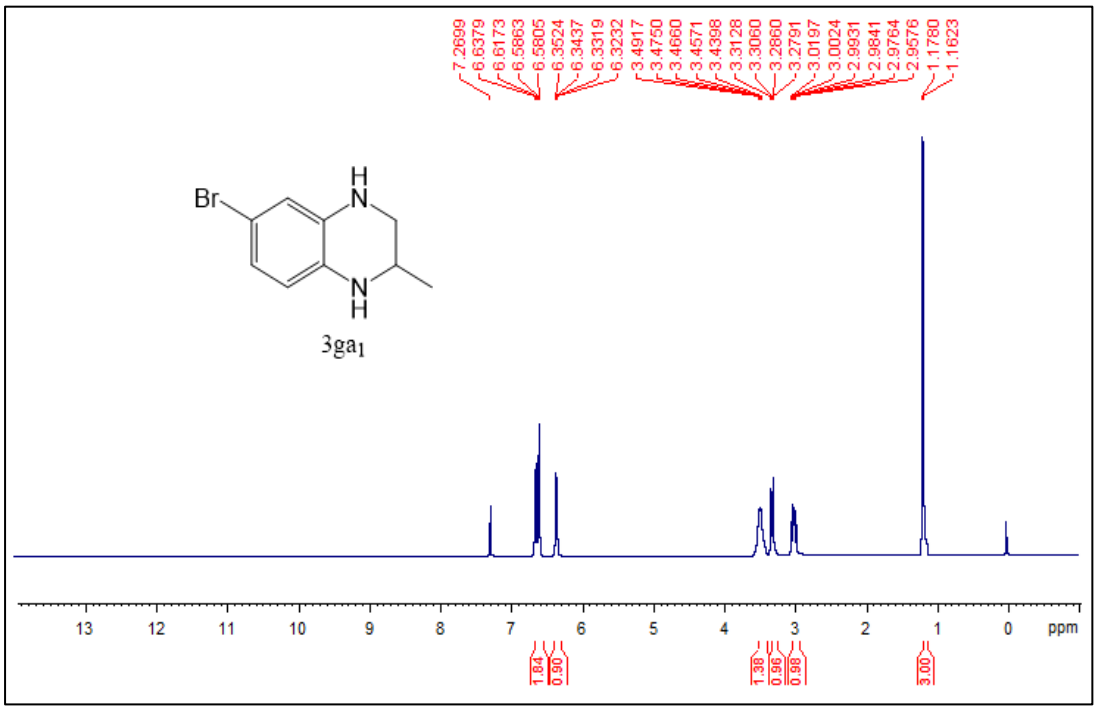
10
ppm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6.6173
6.5863
6.5805
6.3524
6.3437
6.3319
6.3232
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3.4750
3.4660
3.4571
3.4398
3.3128
3.3060
3.2860
3.2791
3.0197
3.0024
2.9931
2.9841
2.9764
2.9576
1.1780
1.1623
Br
H
N
N
H
13
12
11
10
9
8
7
6
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4
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1
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0.96
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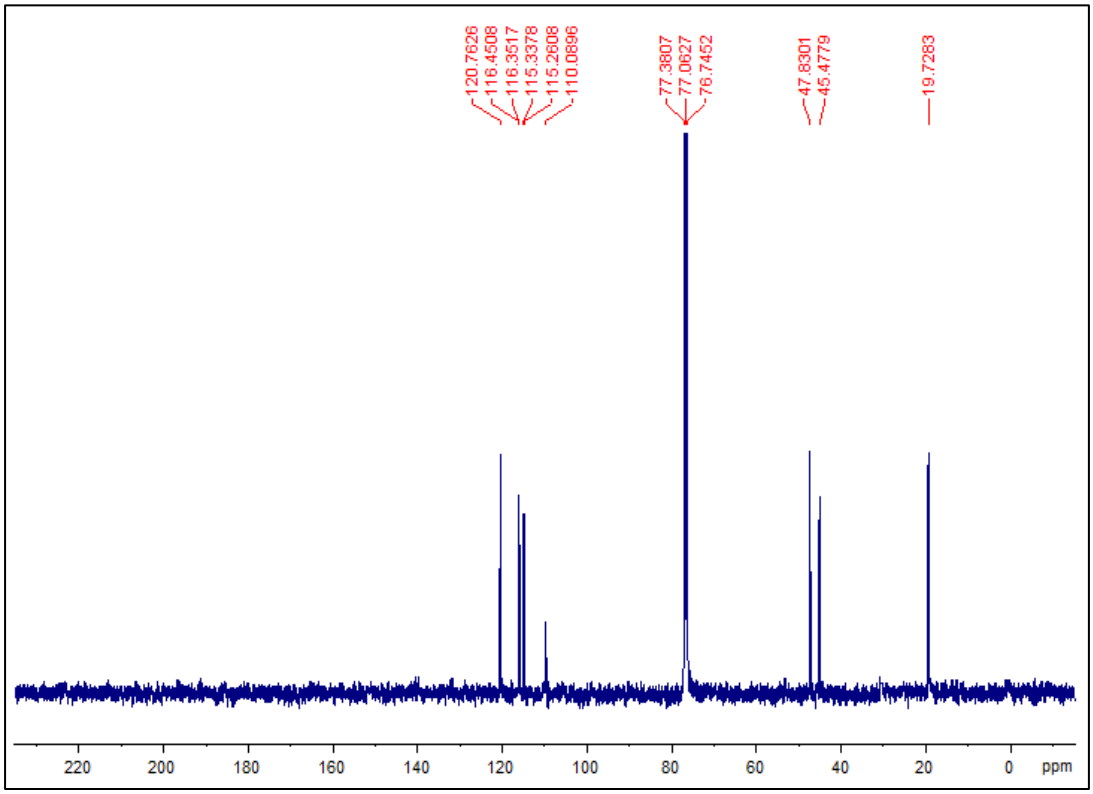
3.00

$3ga_1$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77.3807
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76.7452
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45.4779
19.7283
220
200
180
160
140
120
100
80
60
40
20
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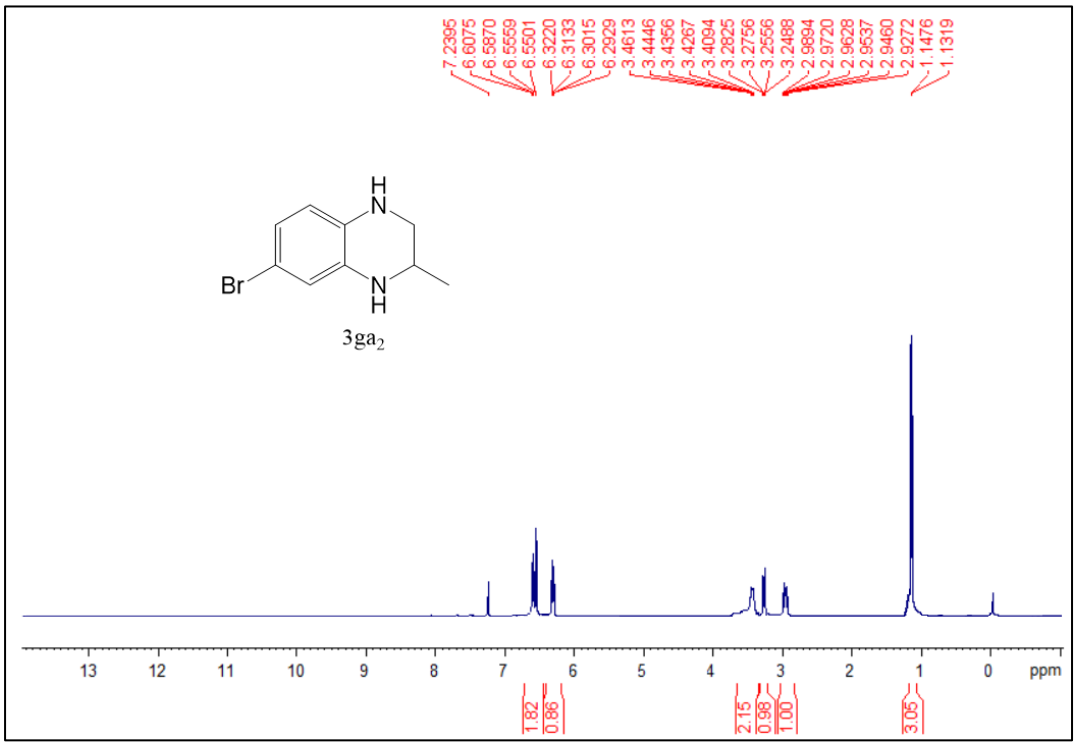
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3.4356
3.4267
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3.2756
3.2556
3.2488
2.9894
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2.9460
2.9272
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1.1319
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N
Br
N
H
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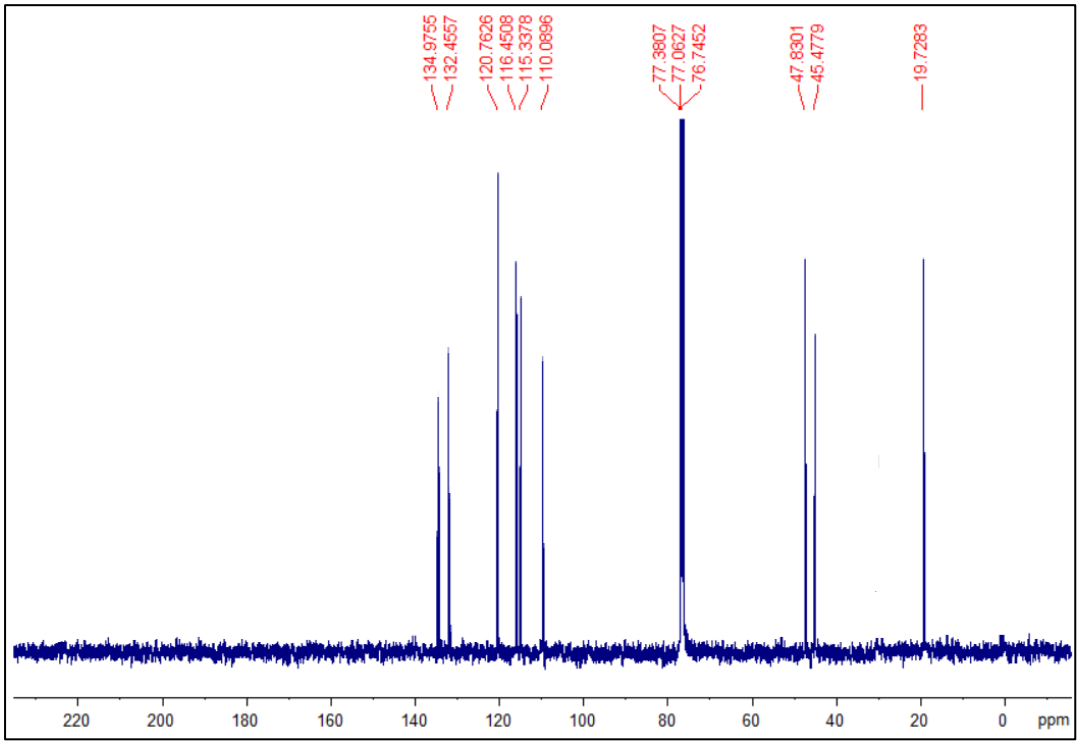
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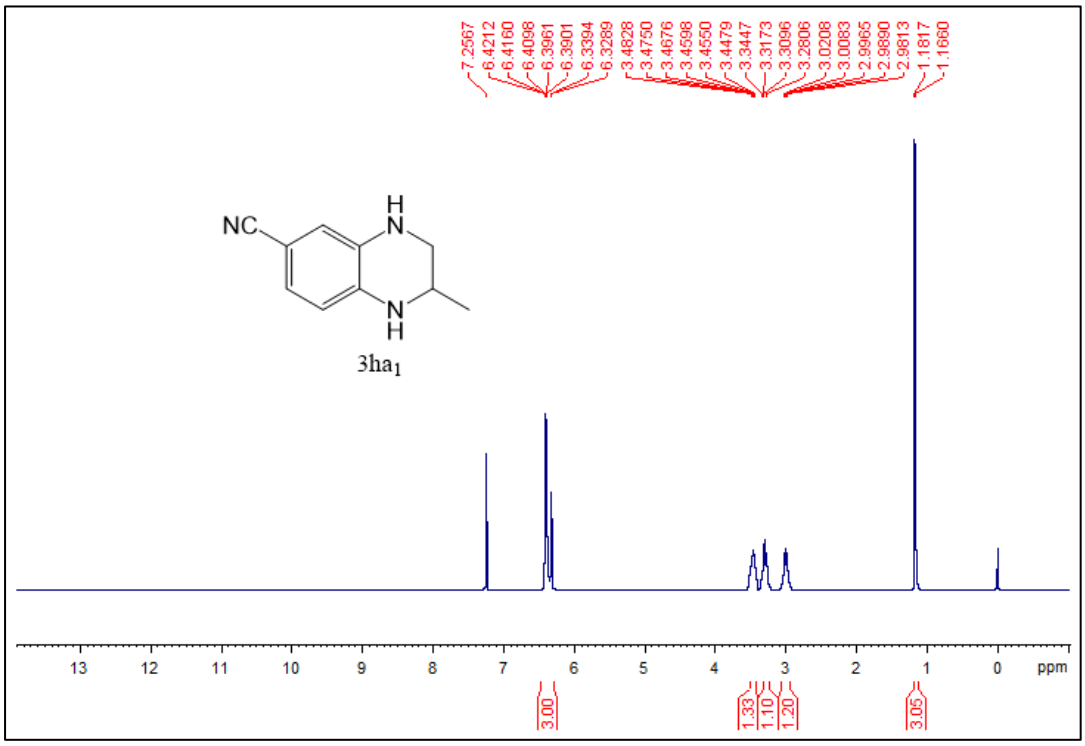
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3.4550
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3.3173
3.3096
3.2806
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3.0083
2.9965
2.9890
2.9813
1.1817
1.1660
NC
H
N
N
H
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12
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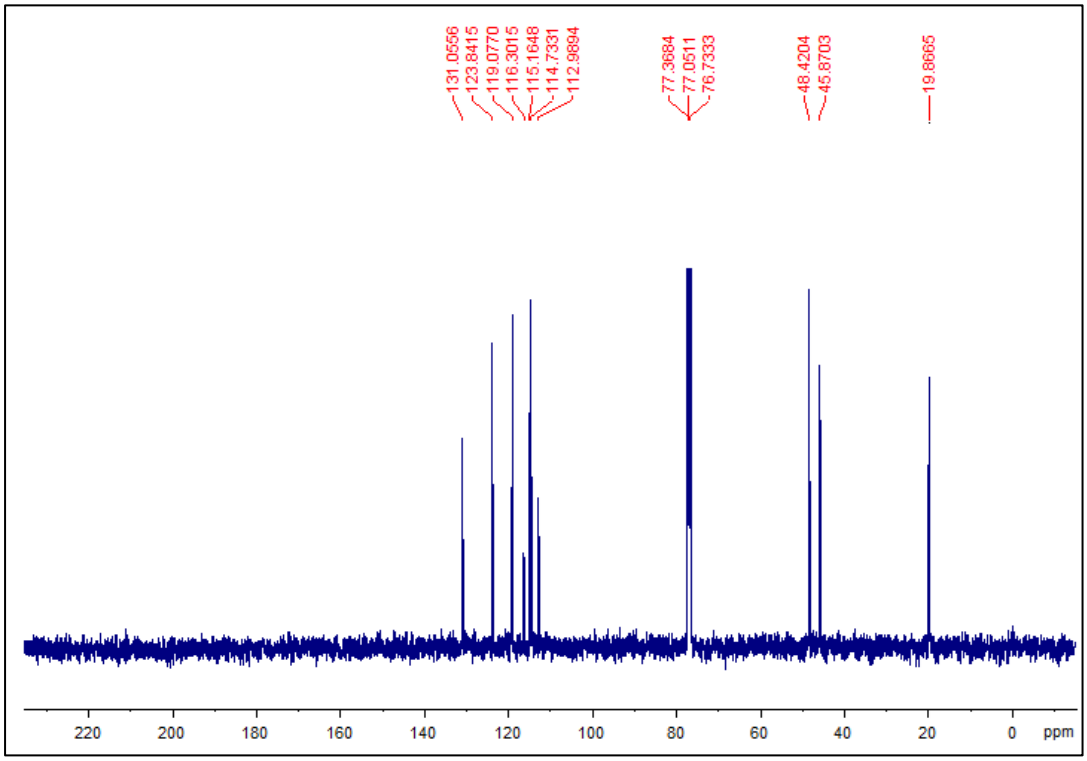
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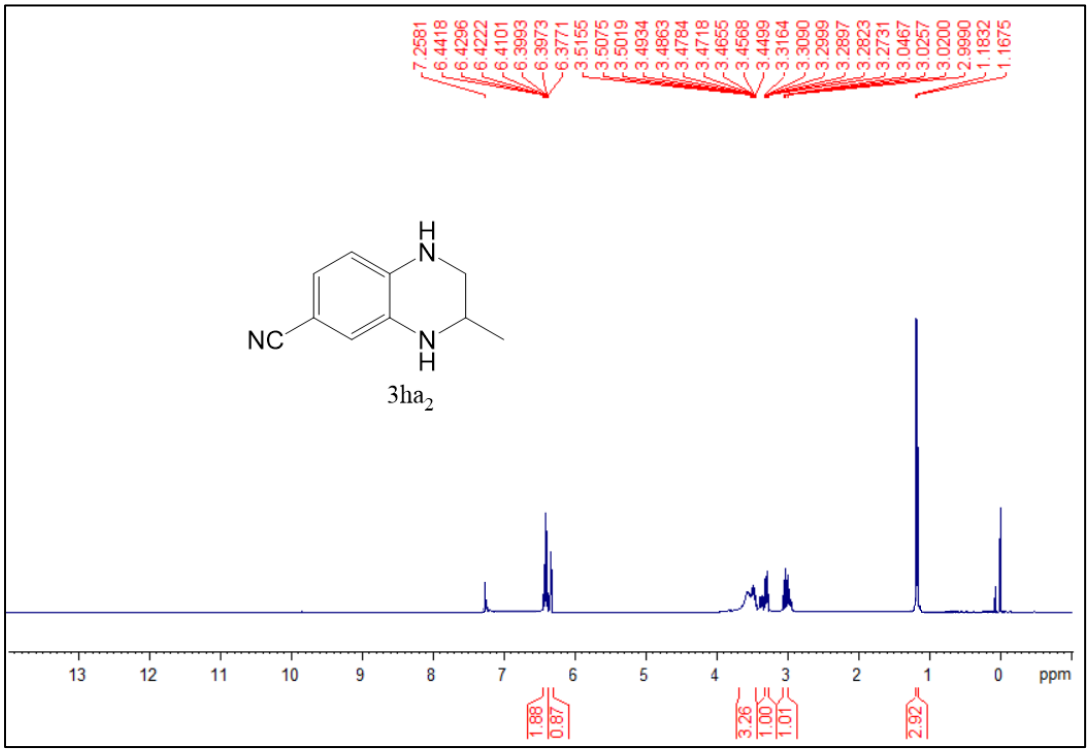
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3.0257
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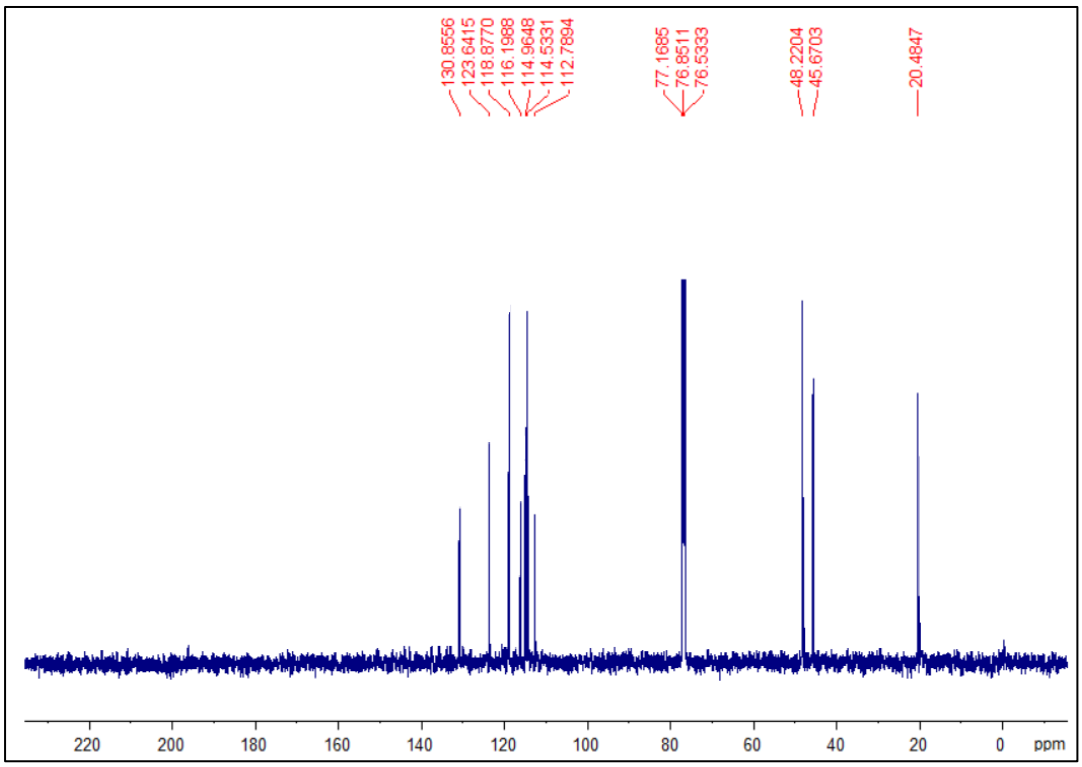
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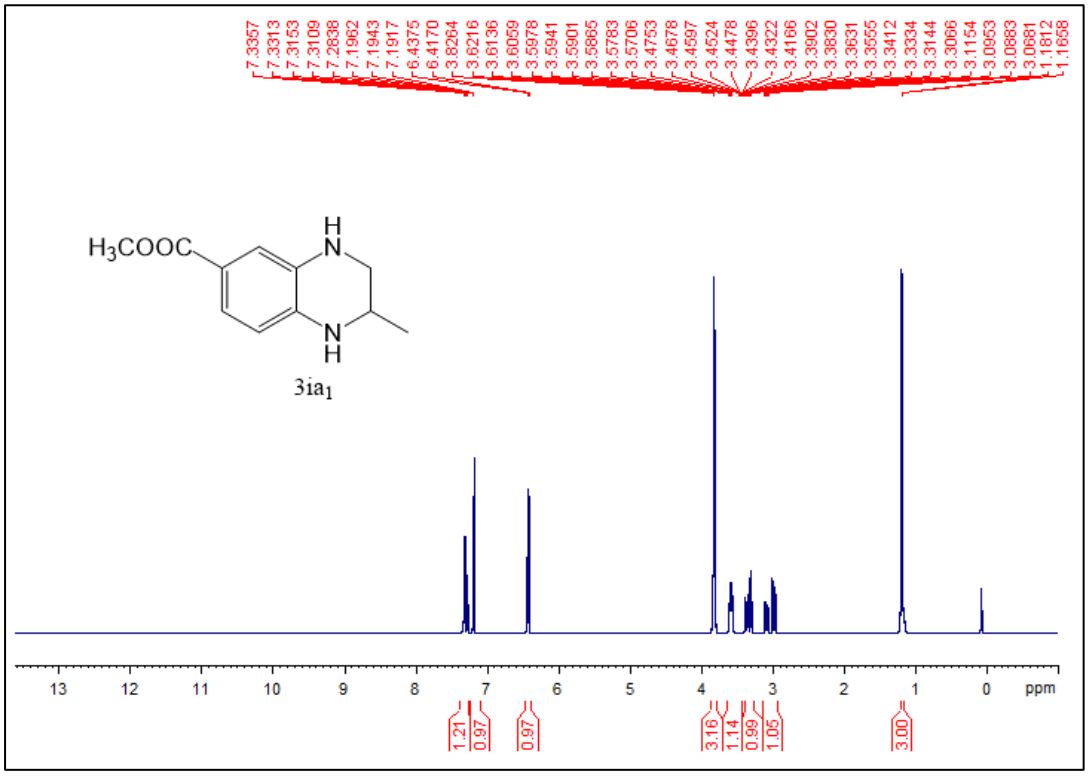
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3.6136
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3.5978
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3.5901
3.5665
3.5783
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3.4524
3.4478
3.4396
3.4322
3.4166
3.3902
3.3830
3.3631
3.3555
3.3412
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3.3144
3.3066
3.1154
3.0953
3.0883
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12
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10
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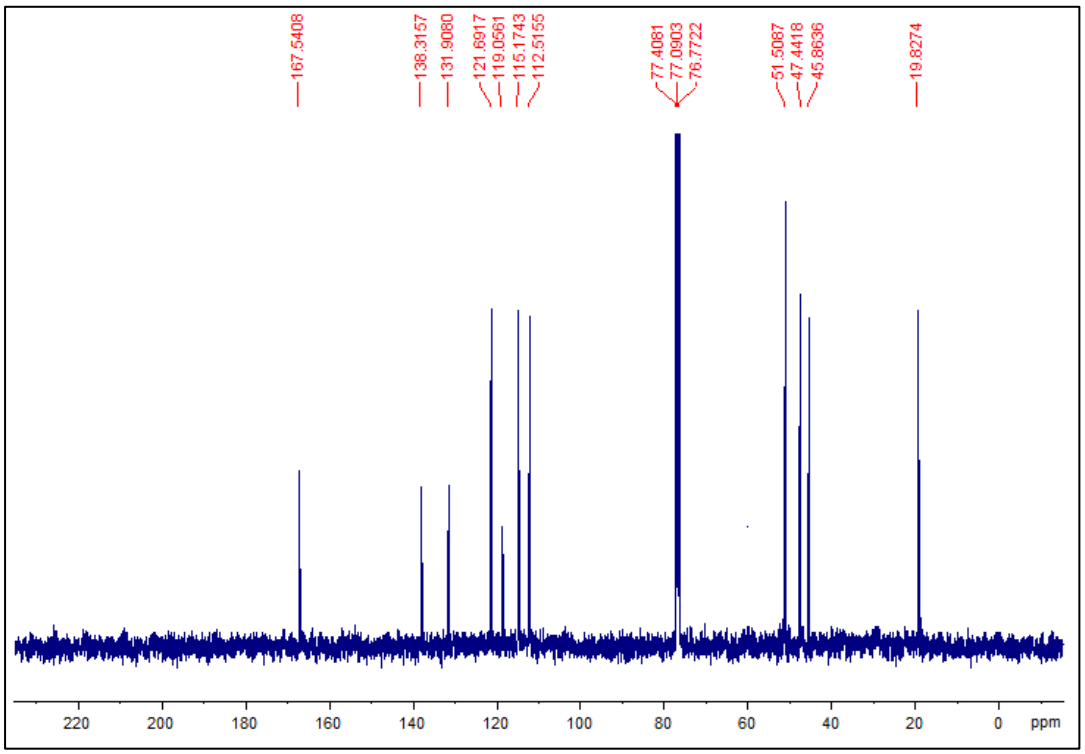
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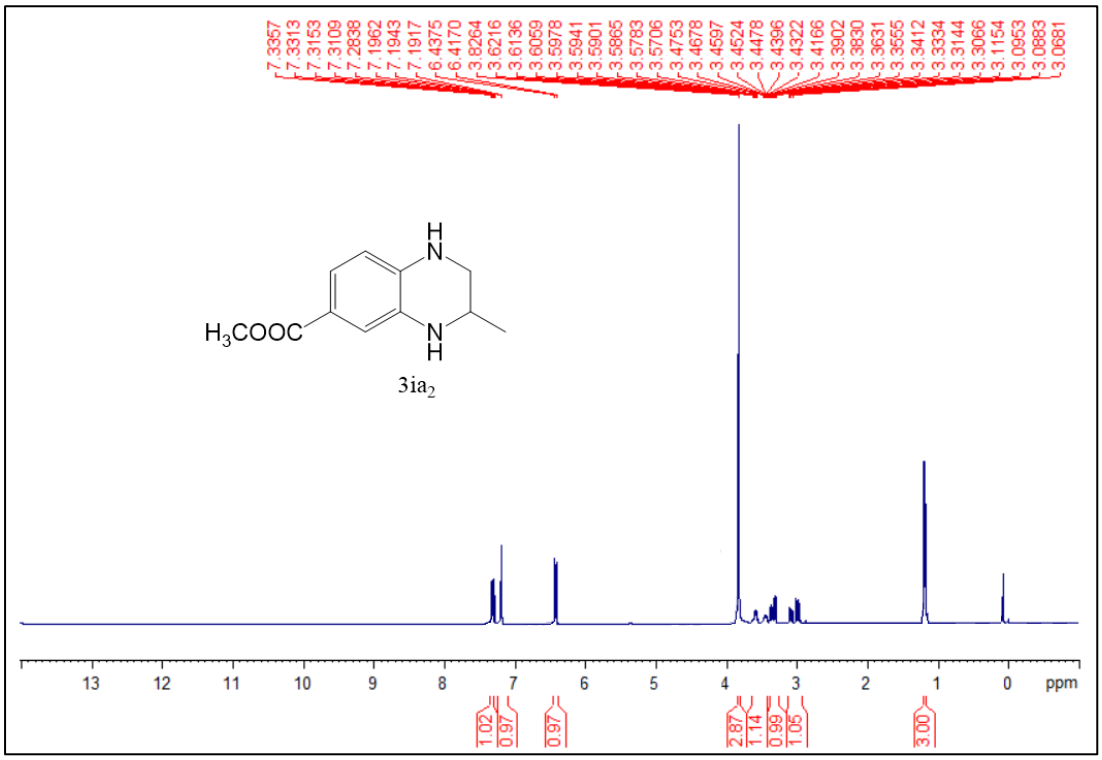
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9
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7
6
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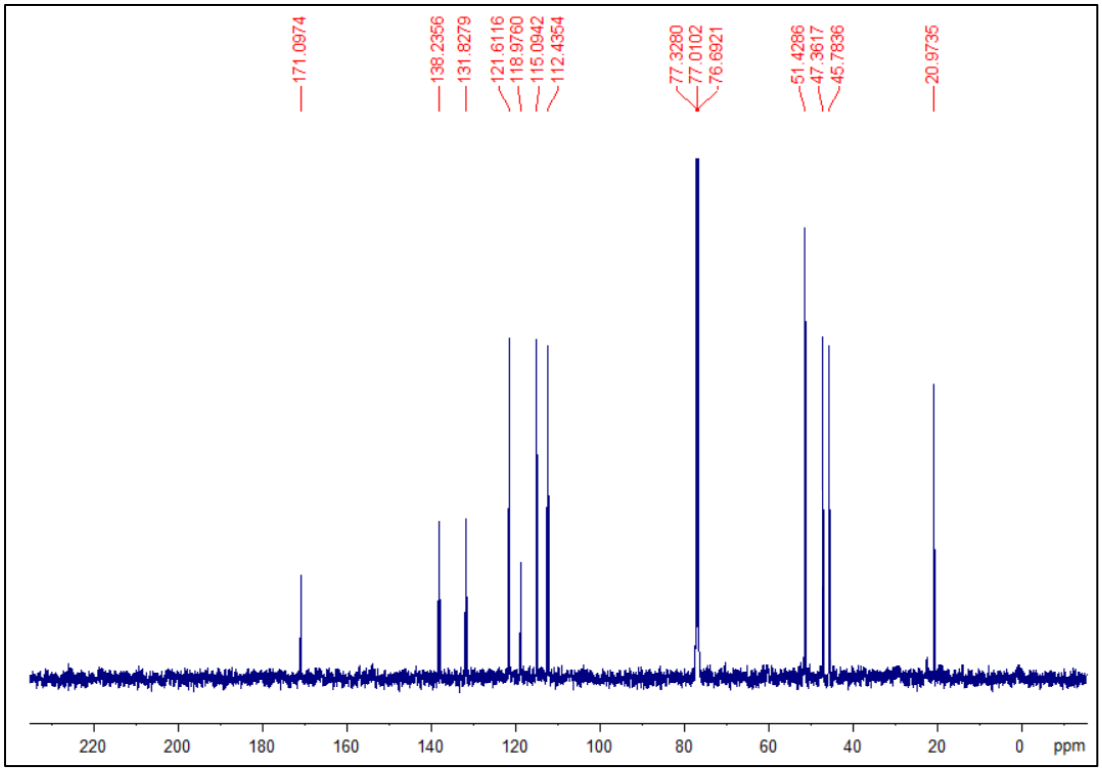
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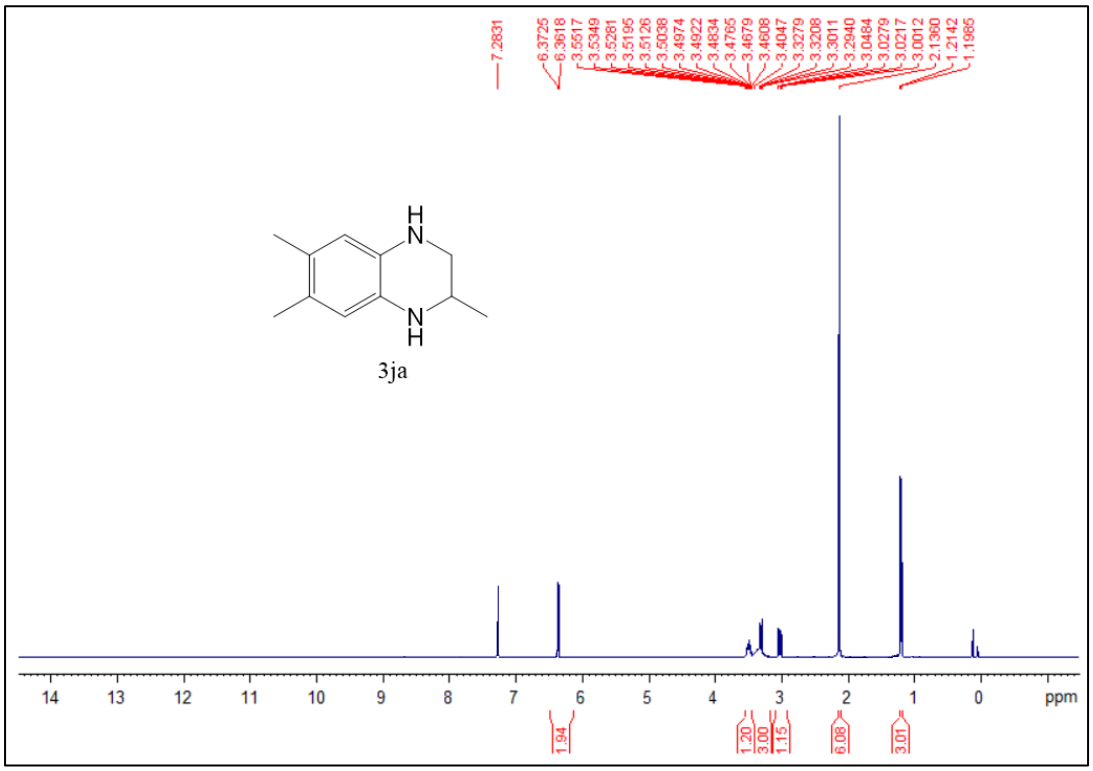
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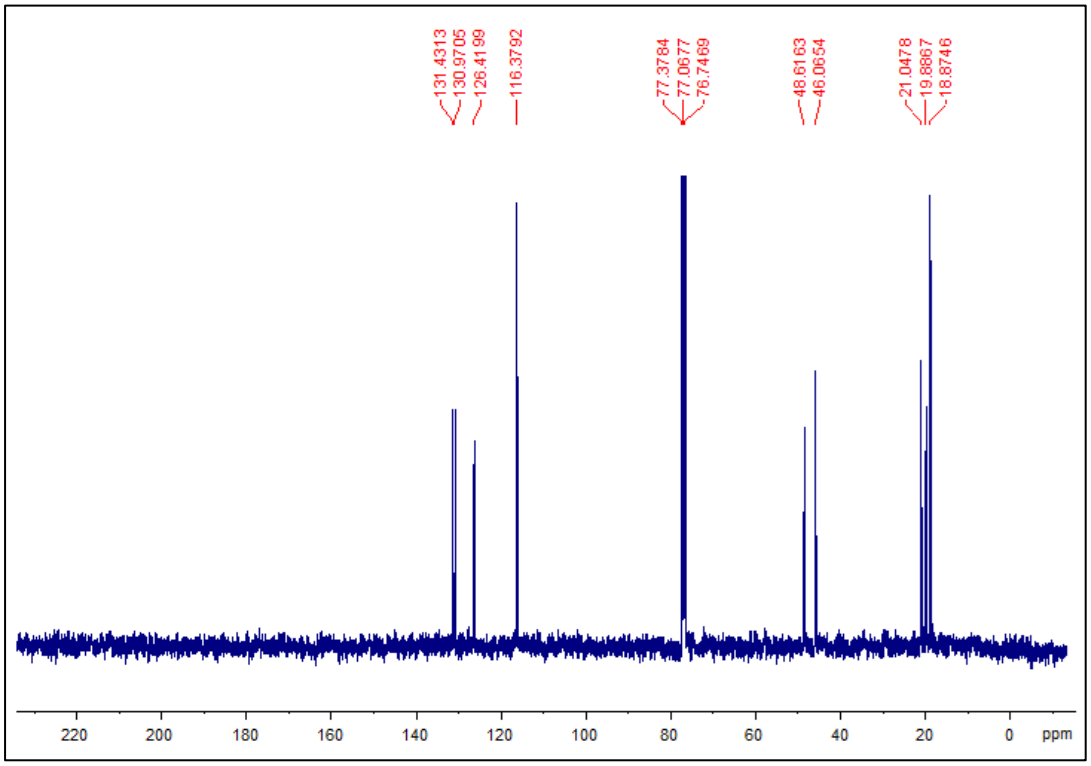
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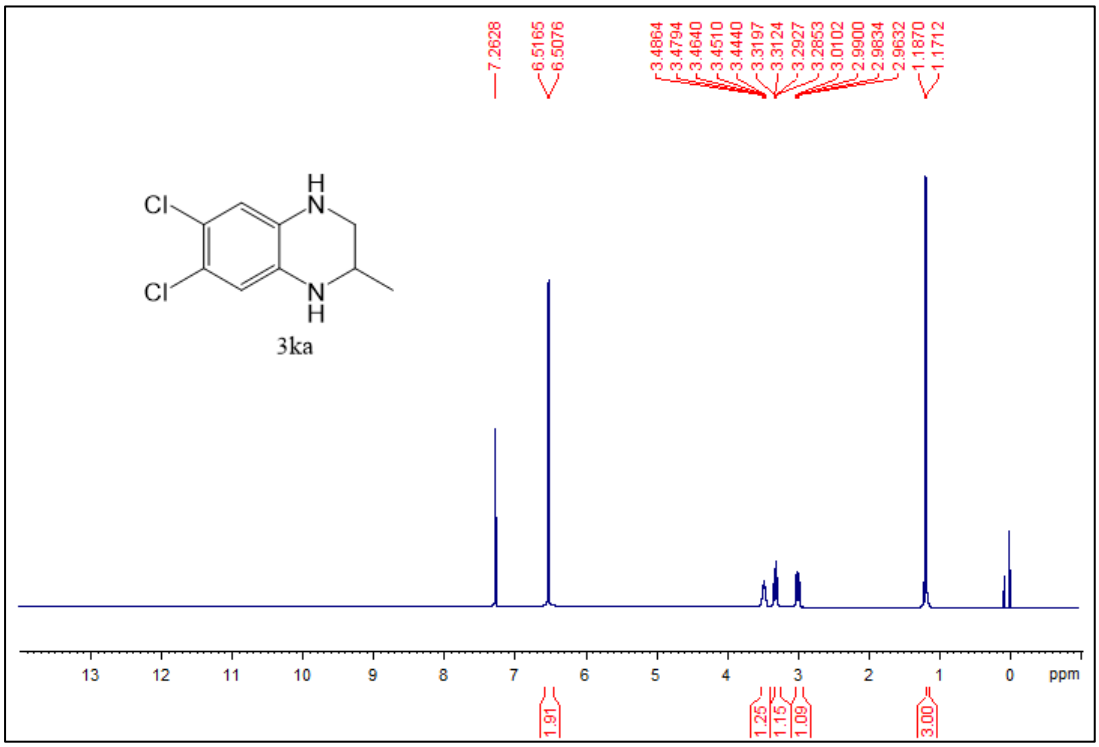
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3.2927
3.2853
3.0102
2.9900
2.9834
2.9632
1.1870
1.1712
Cl
Cl
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H
3ka
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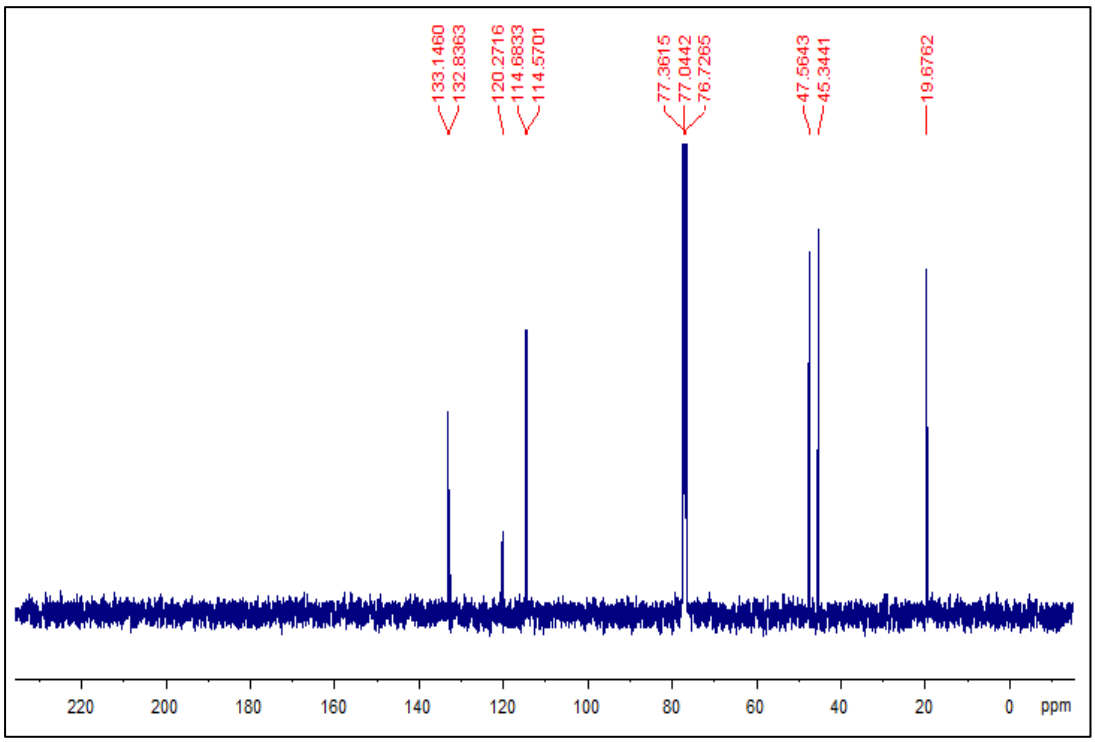
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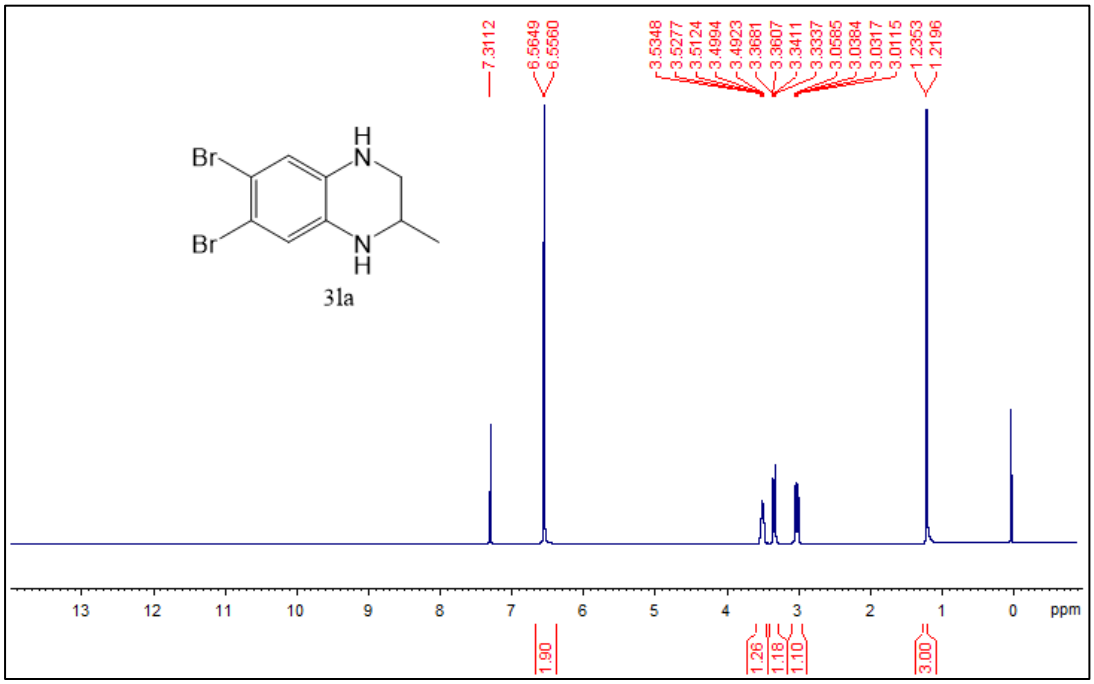
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3.0317
3.0115
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1.2196
Br
Br
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N
N
H
3la
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12
11
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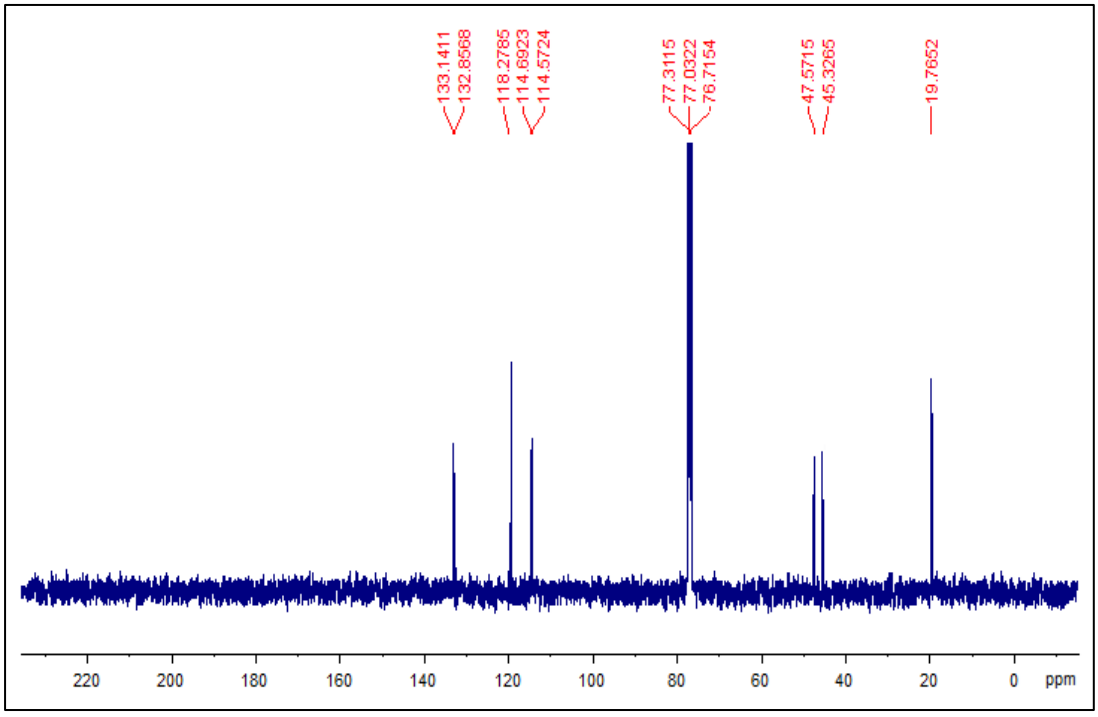
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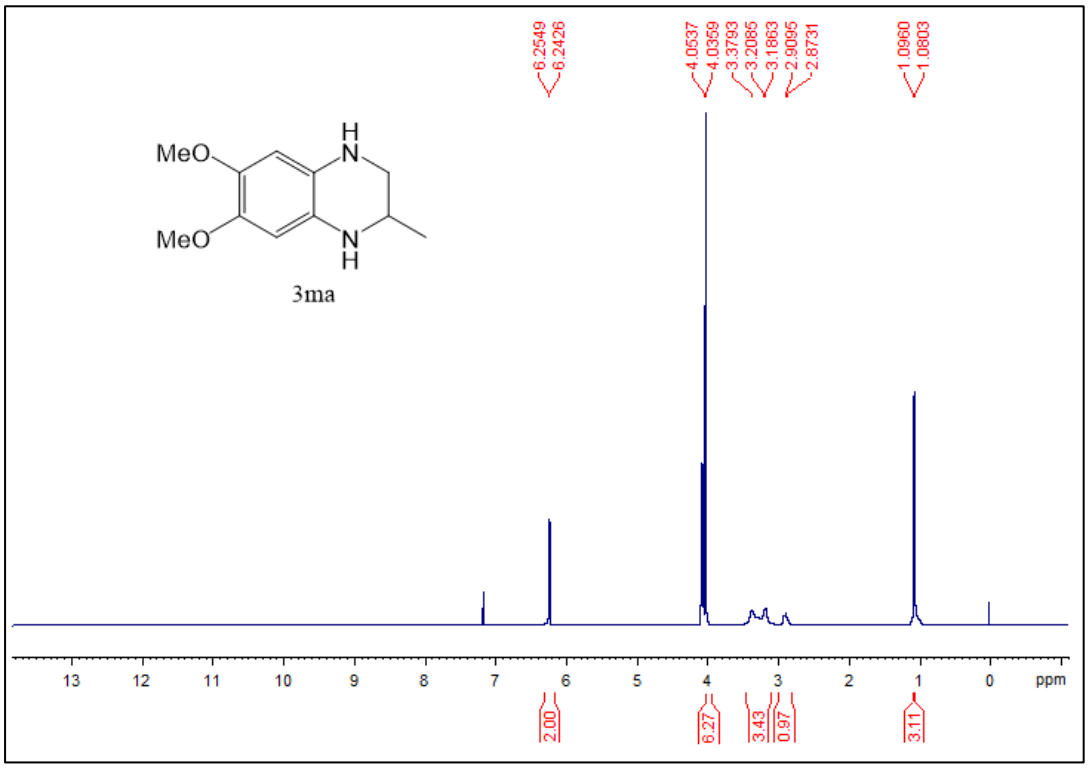
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MeO
H
N
N
H
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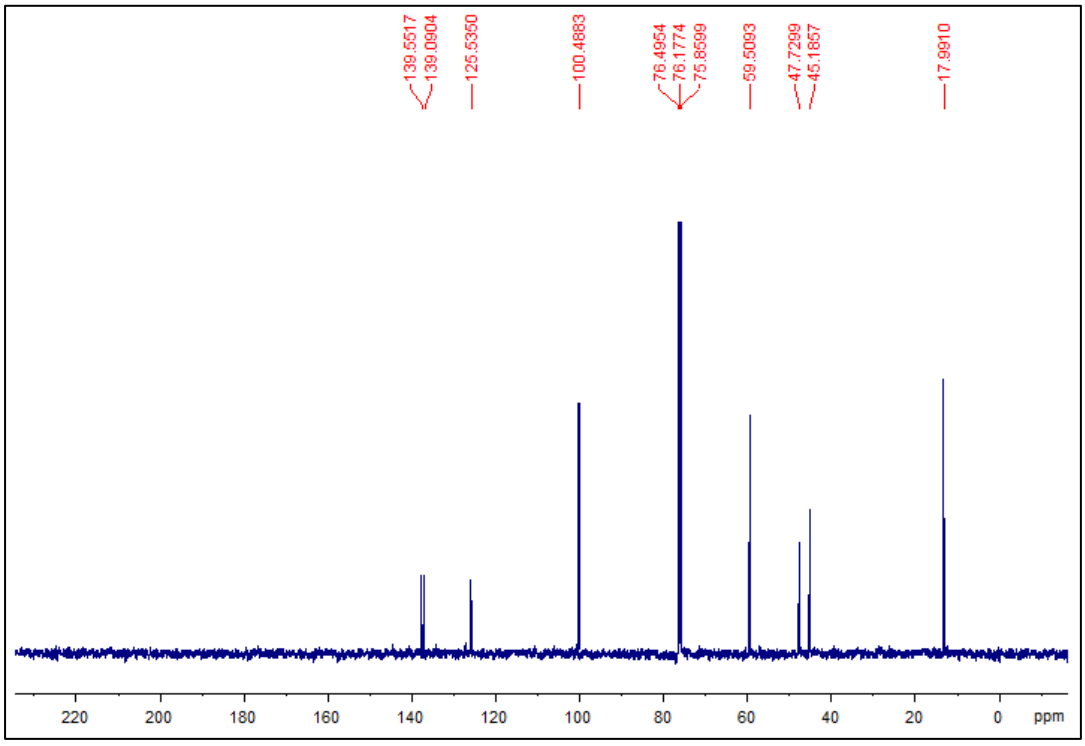
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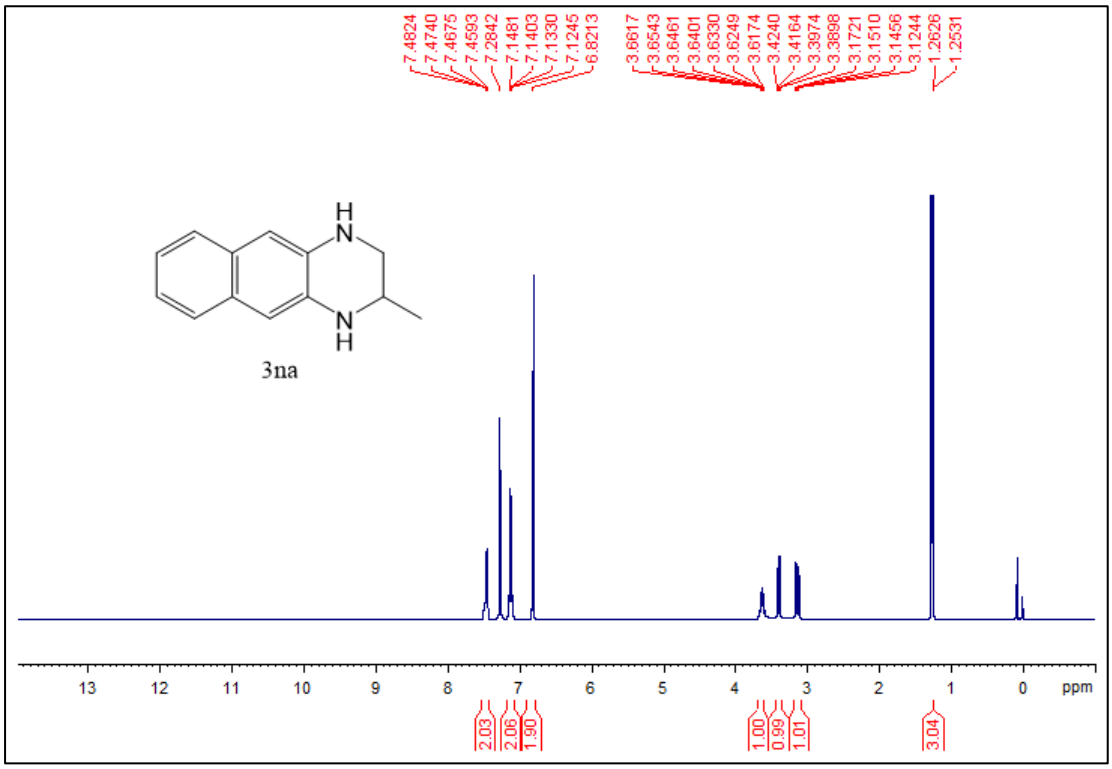
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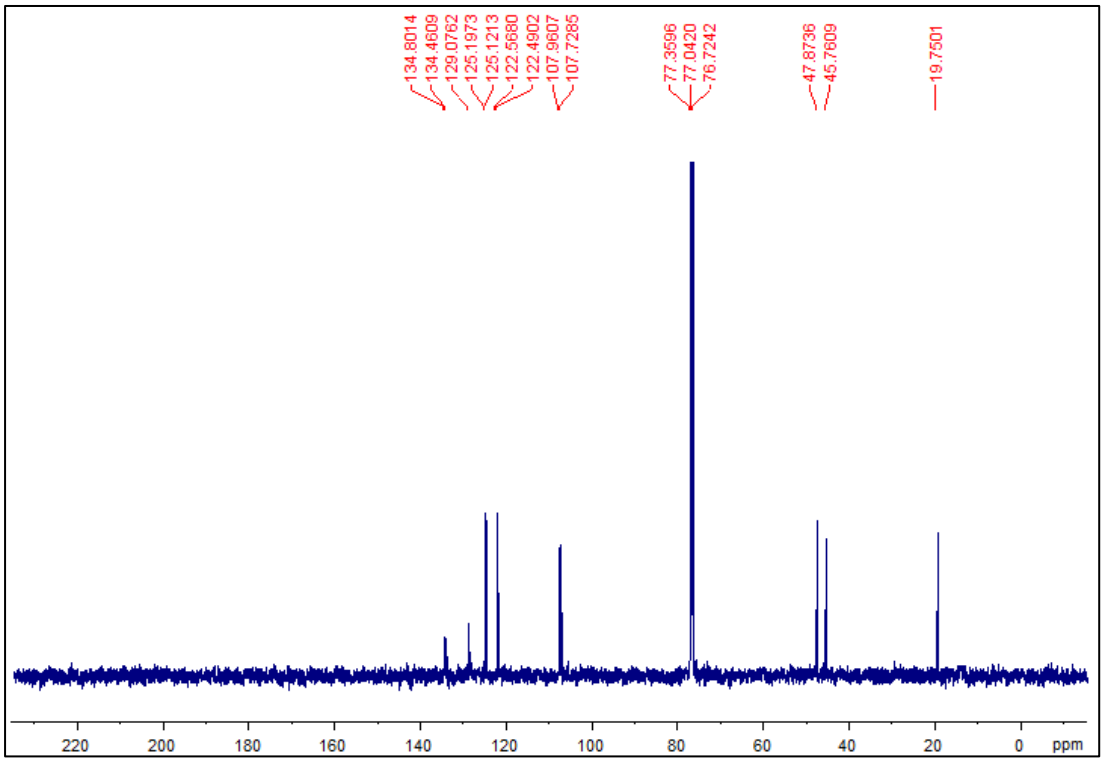
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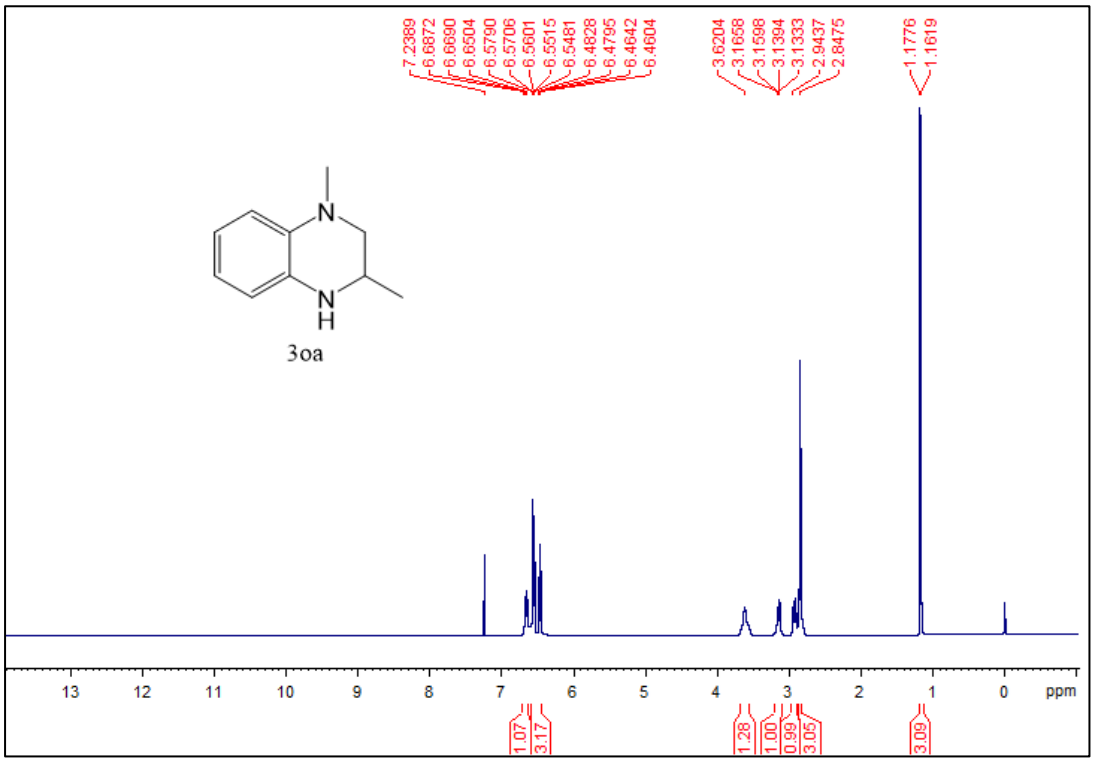
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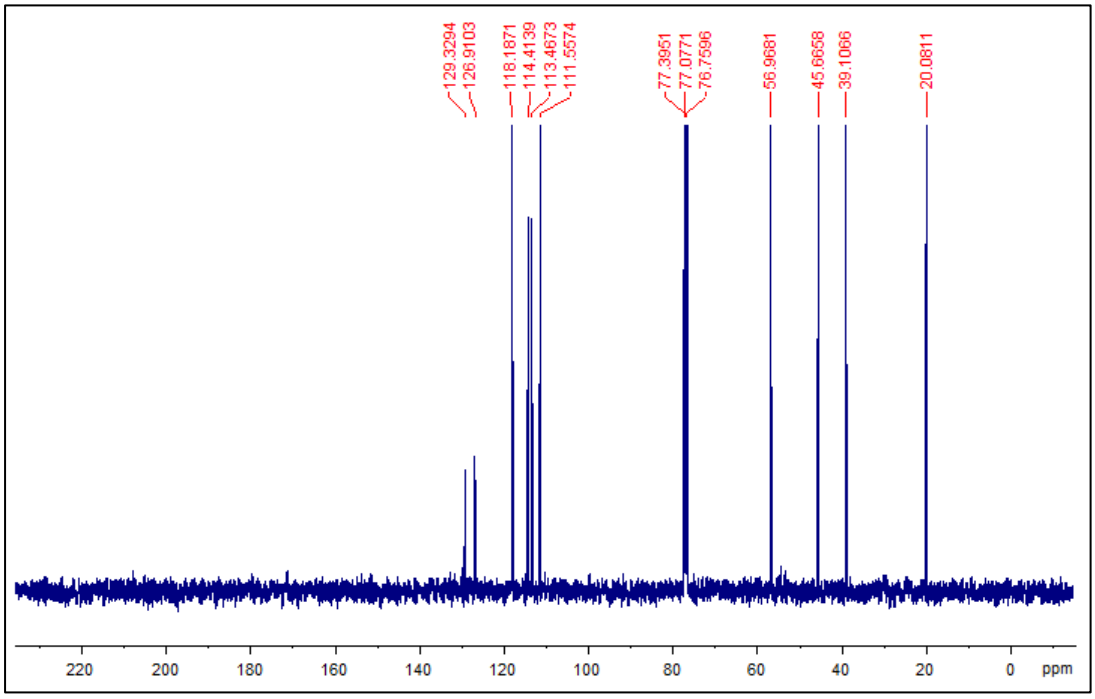
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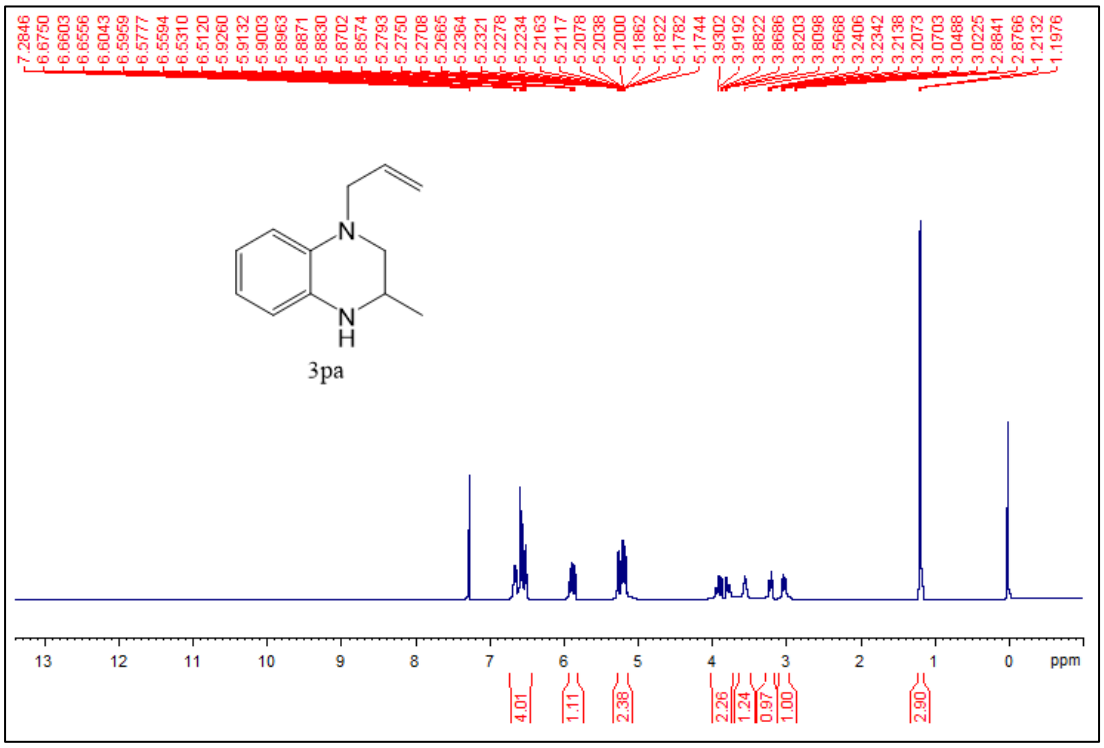
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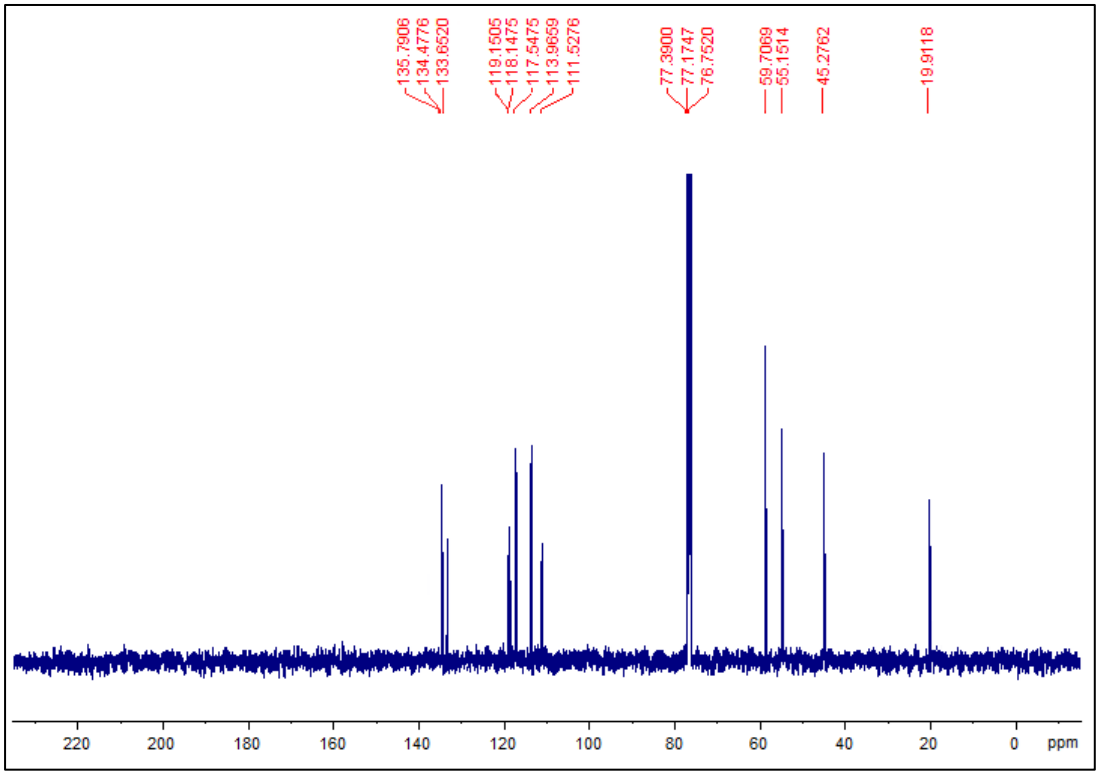
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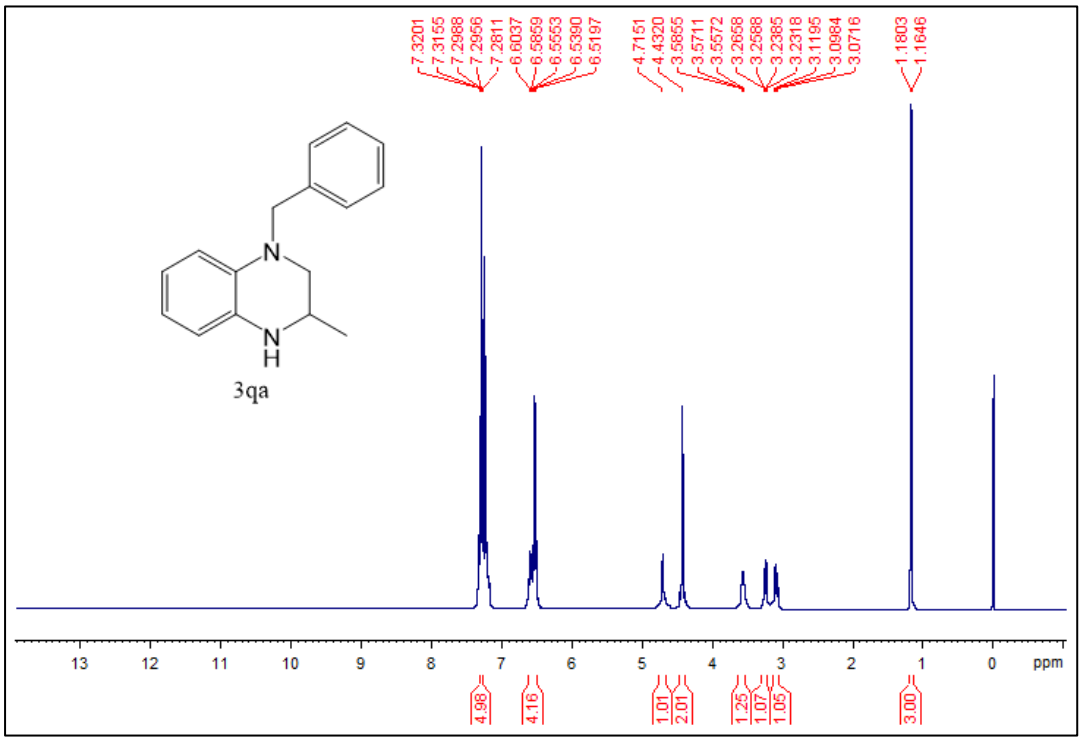
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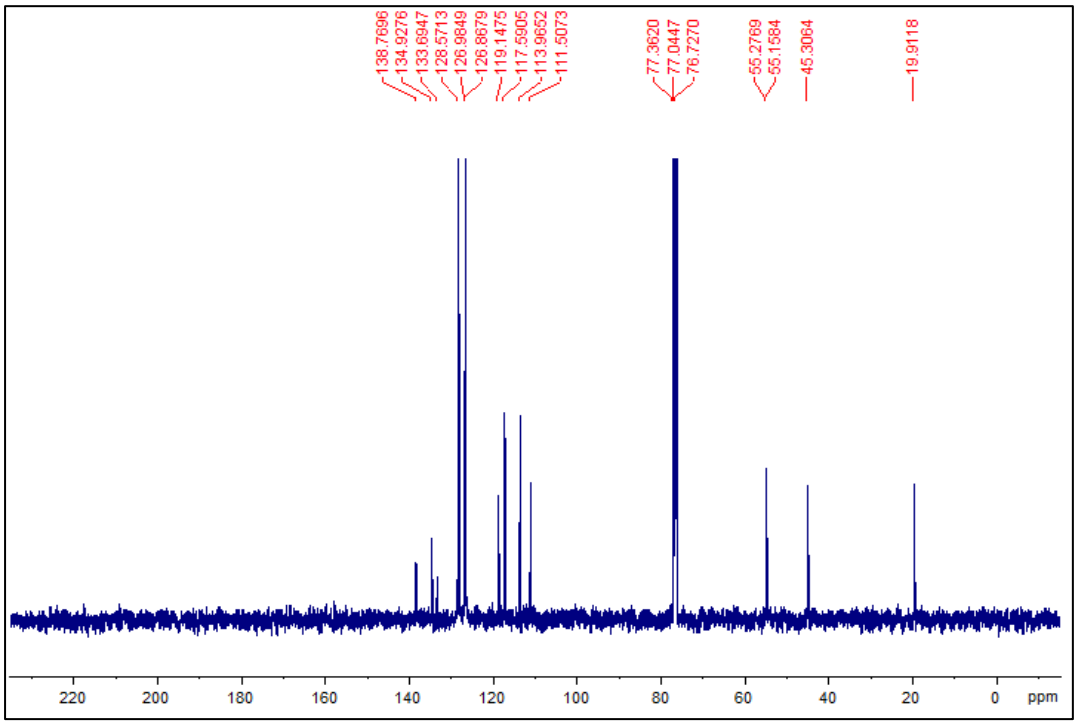
1.05
3.00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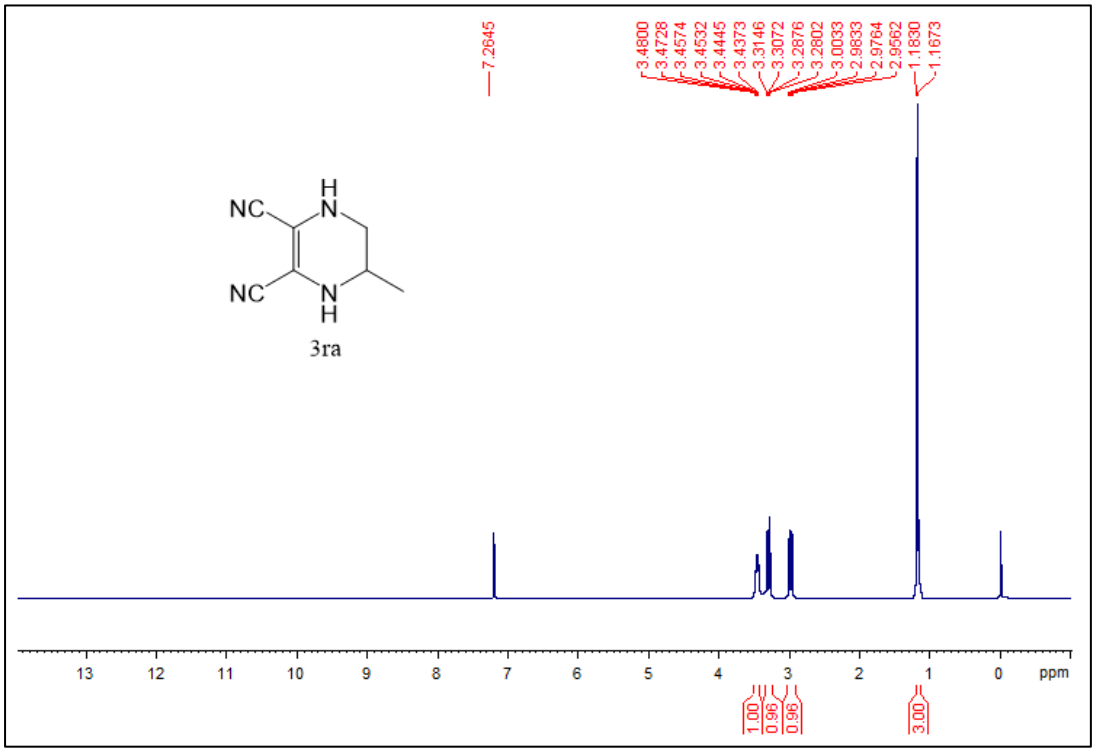
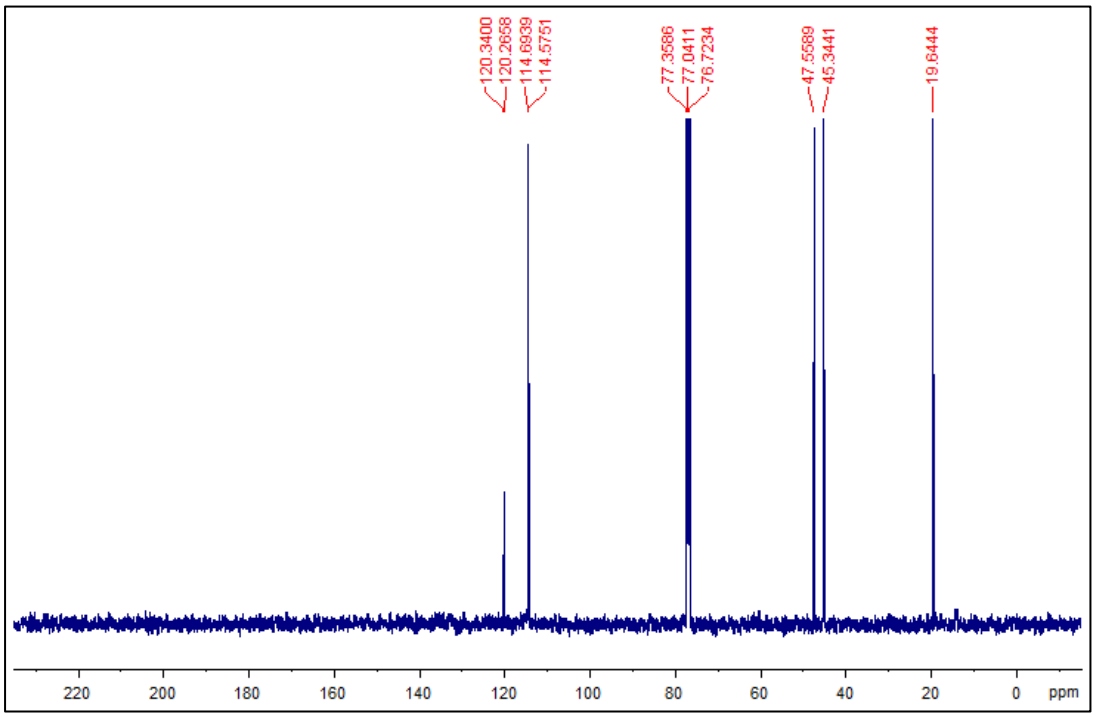
134.9276
133.6947
128.5713
126.9849
126.8679
119.1475
117.5905
113.9652
111.5073
77.3620
77.0447
76.7270
55.2769
55.1584
45.3064
19.9118
220
200
180
160
140
120
100
80
60
40
20
0
ppm


7.2645
3.4800
3.4728
3.4574
3.4532
3.4445
3.4373
3.3146
3.3072
3.2876
3.2802
3.0033
2.9833
2.9764
2.9562
1.1830
1.1673
NC
NC
H
N
N
H
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
0.96
0.96
3.00

3ra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120.2658
114.6939
114.5751
77.3586
77.0411
76.7234
47.5589
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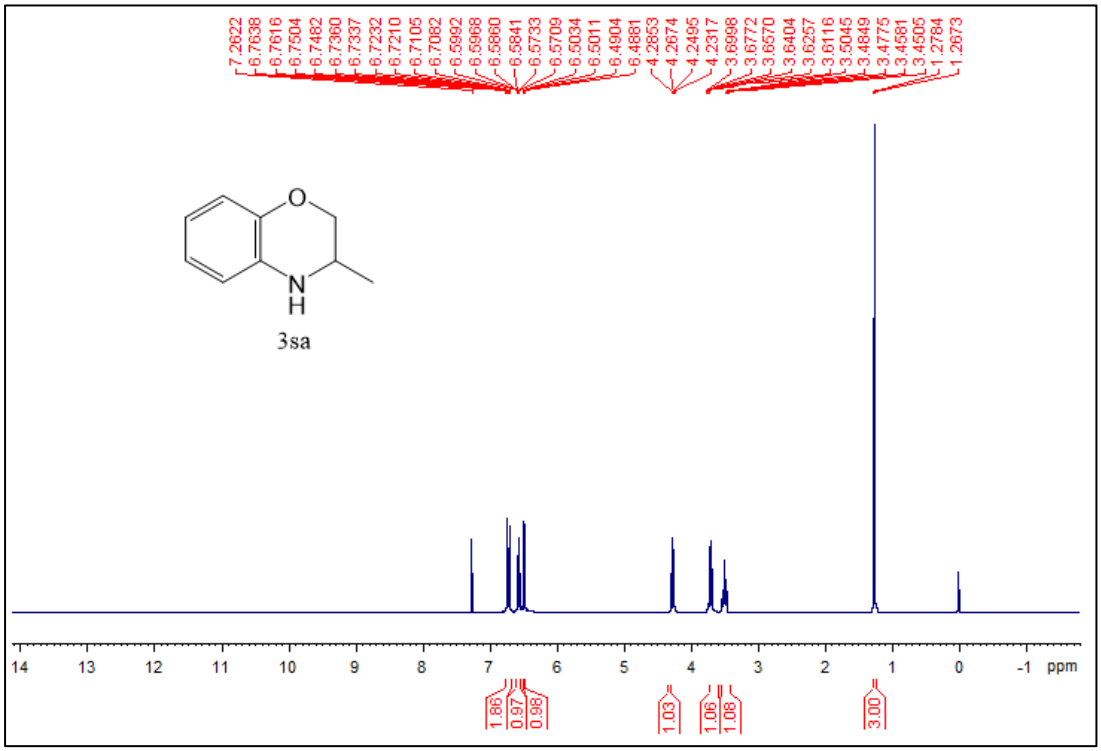
19.6444
220
200
180
160
140
120
100
80
60
40
20
0
ppm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6.7616
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6.7360
6.7337
6.7232
6.7210
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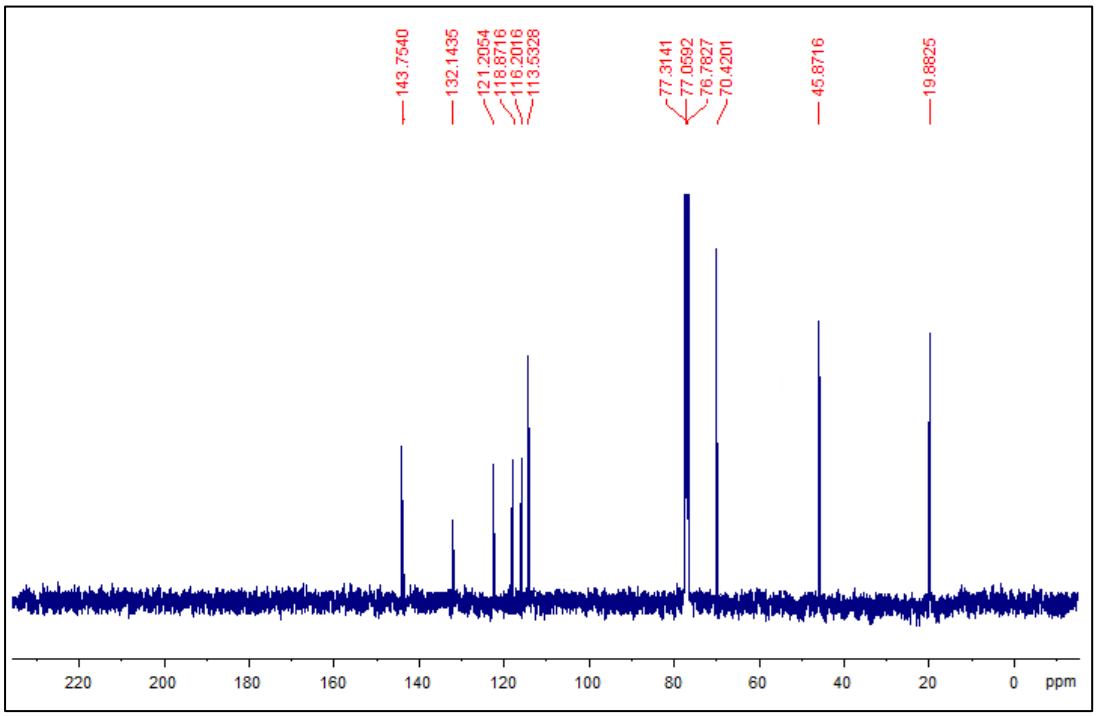
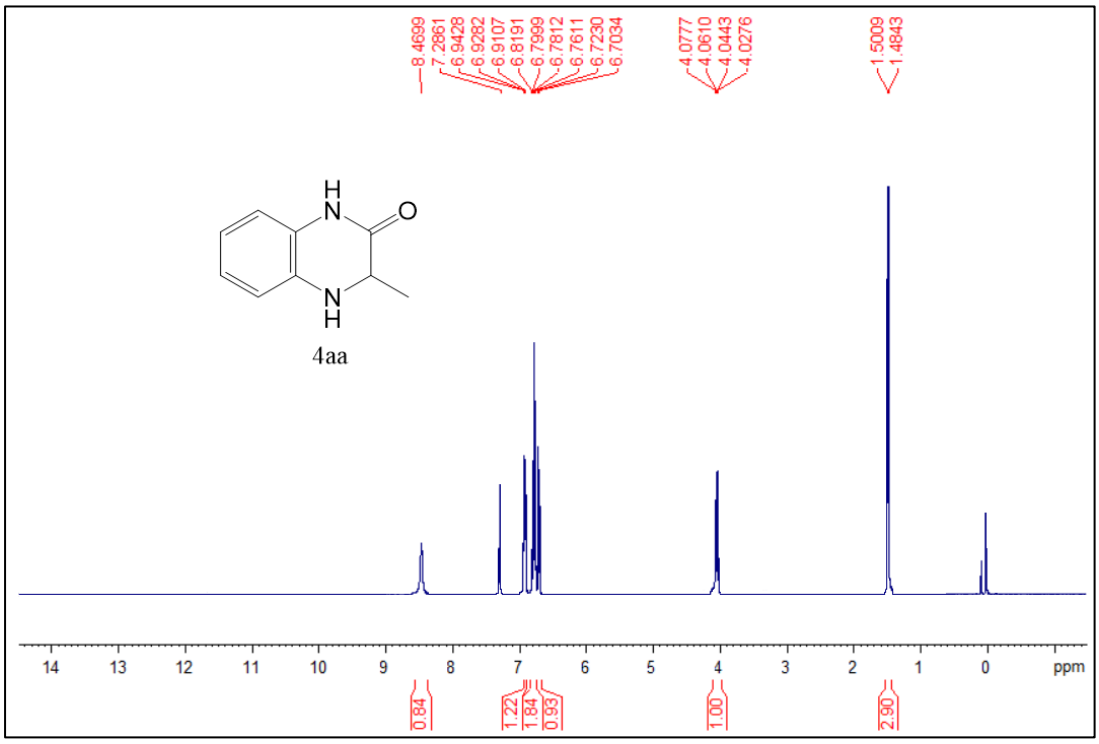
6.7082
6.5992
6.5968
6.5860
6.5841
6.5733
6.5709
6.5034
6.5011
6.4904
6.4881
4.2853
4.2674
4.2495
4.2317
3.6998
3.6772
3.6570
3.6404
3.6257
3.6116
3.5045
3.4849
3.4775
3.4581
3.4505
1.2784
1.2673
O
N
H
3sa
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 ppm
1.86
0.97
0.98
1.03
1.06
1.06
3.00


143.7540
132.1435
121.2054
118.8716
116.2016
113.5328
77.3141
77.0592
76.7827
70.4201
45.8716
19.8825
220 200 180 160 140 120 100 80 60 40 20 0 ppm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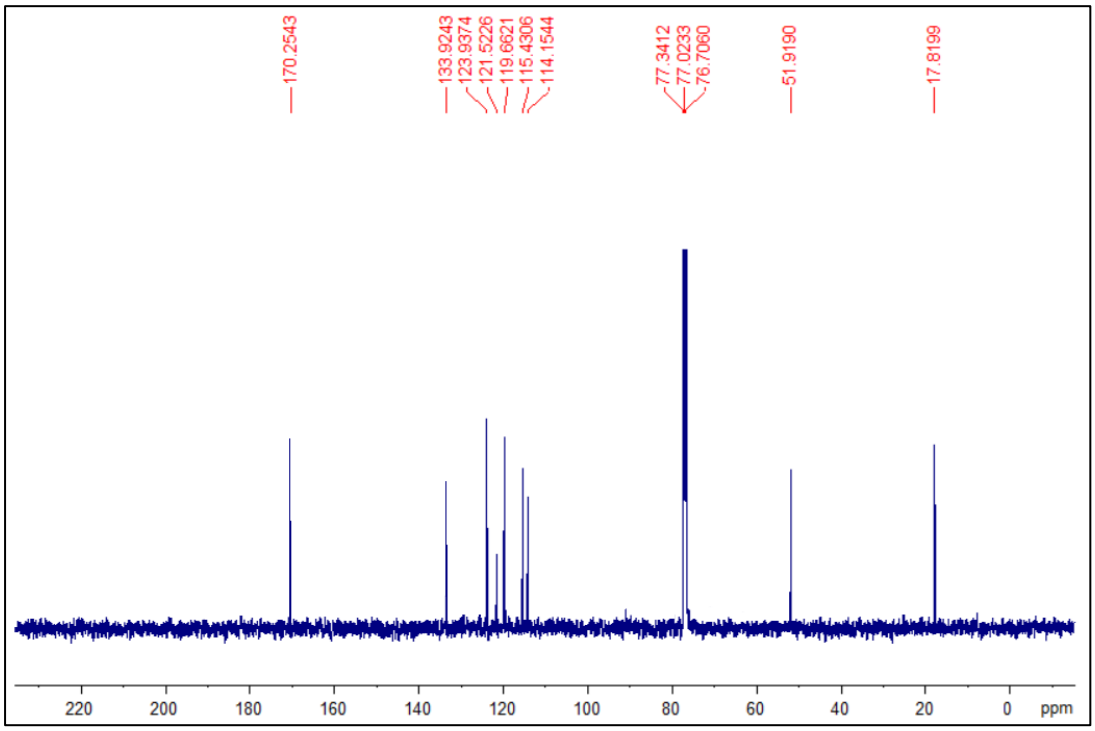
7.2861
6.9428
6.9282
6.9107
6.8191
6.7999
6.7812
6.7611
6.7230
6.7034
4.0777
4.0610
4.0443
4.0276
1.5009
1.4843
H
N
O
N
H
4aa
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.84
1.22
1.84
0.93
1.00
2.90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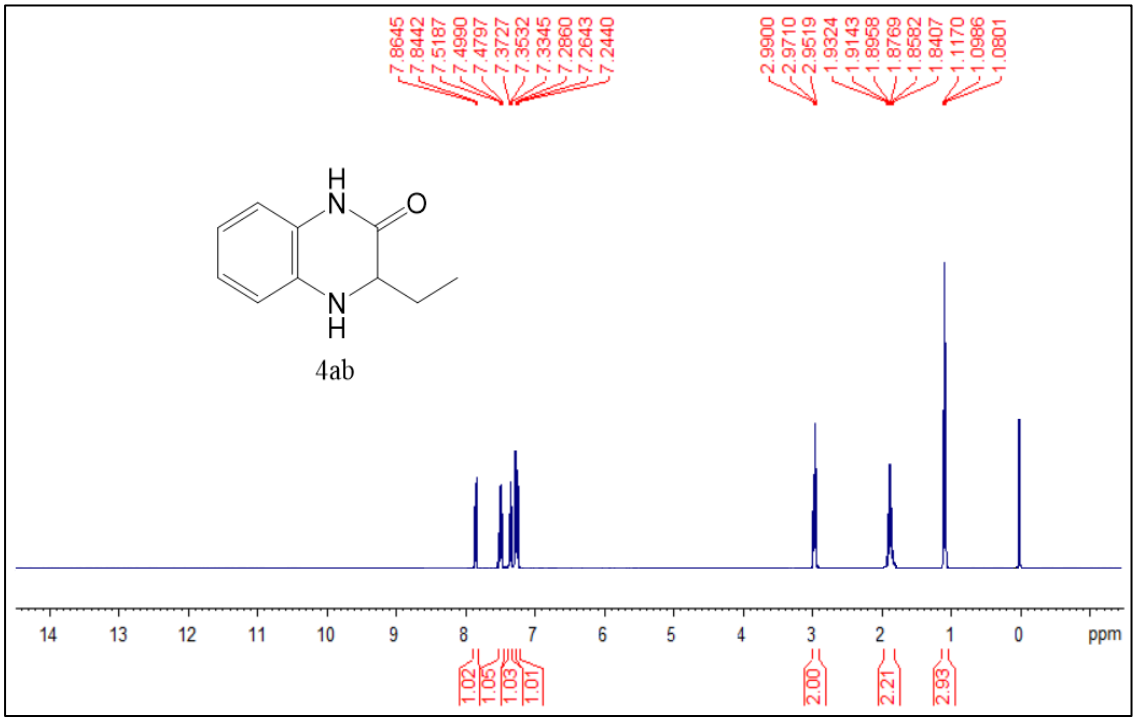
123.9374
121.5226
119.6621
115.4306
114.1544
77.3412
77.0233
76.7060
51.9190
17.8199
220
200
180
160
140
120
100
80
60
40
20
0
ppm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7.5187
7.4990
7.4797
7.3727
7.3532
7.3345
7.2860
7.2643
7.2440
2.9900
2.9710
2.9519
1.9324
1.9143
1.8958
1.8769
1.8582
1.8407
1.1170
1.0986
1.0801
H
N
O
N
H
4ab
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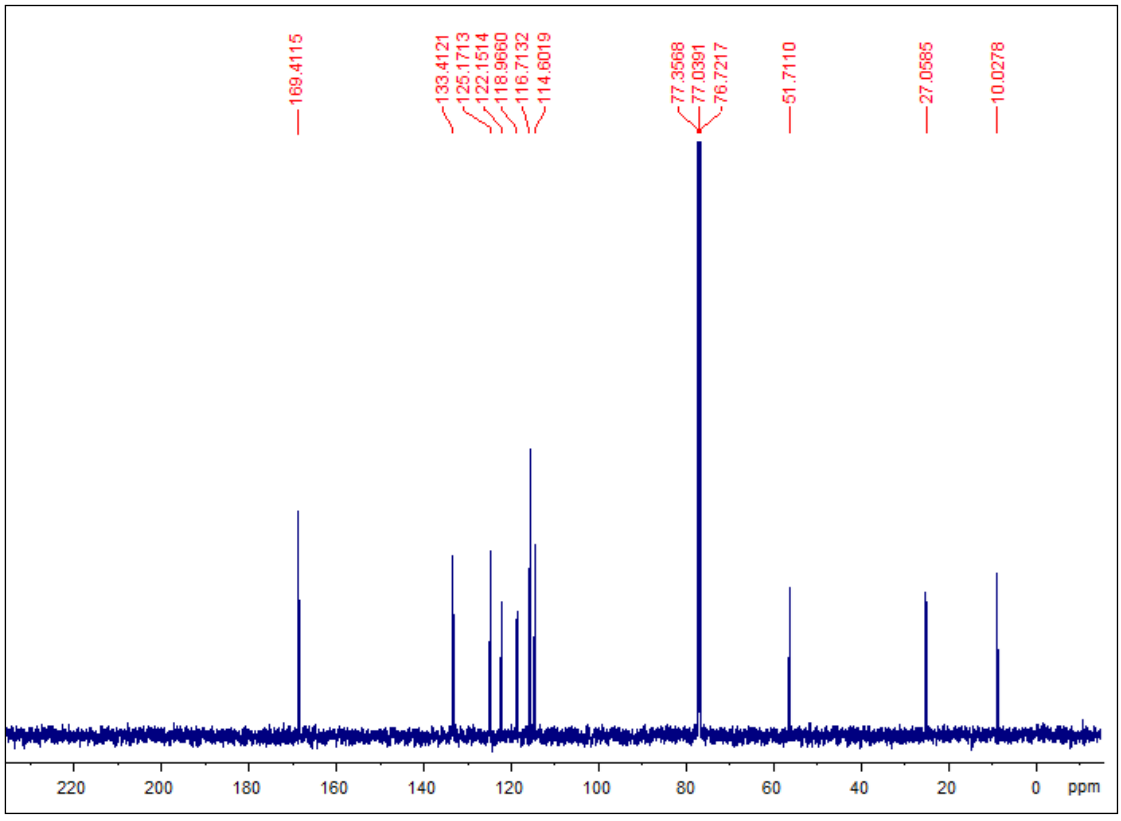
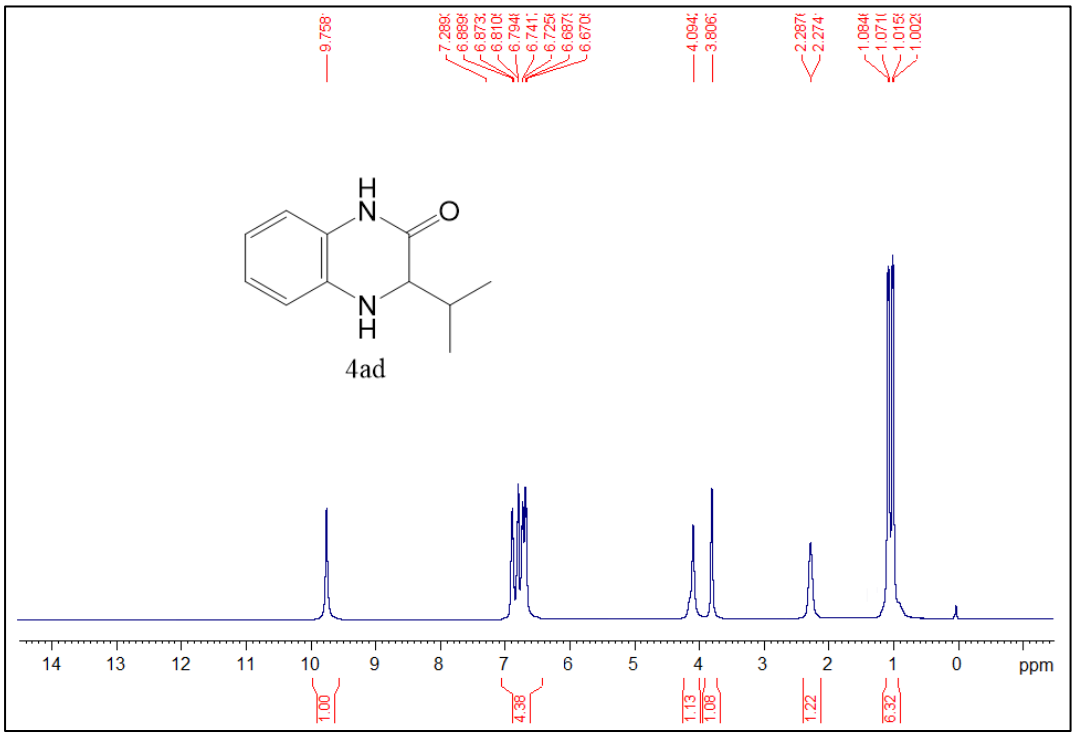
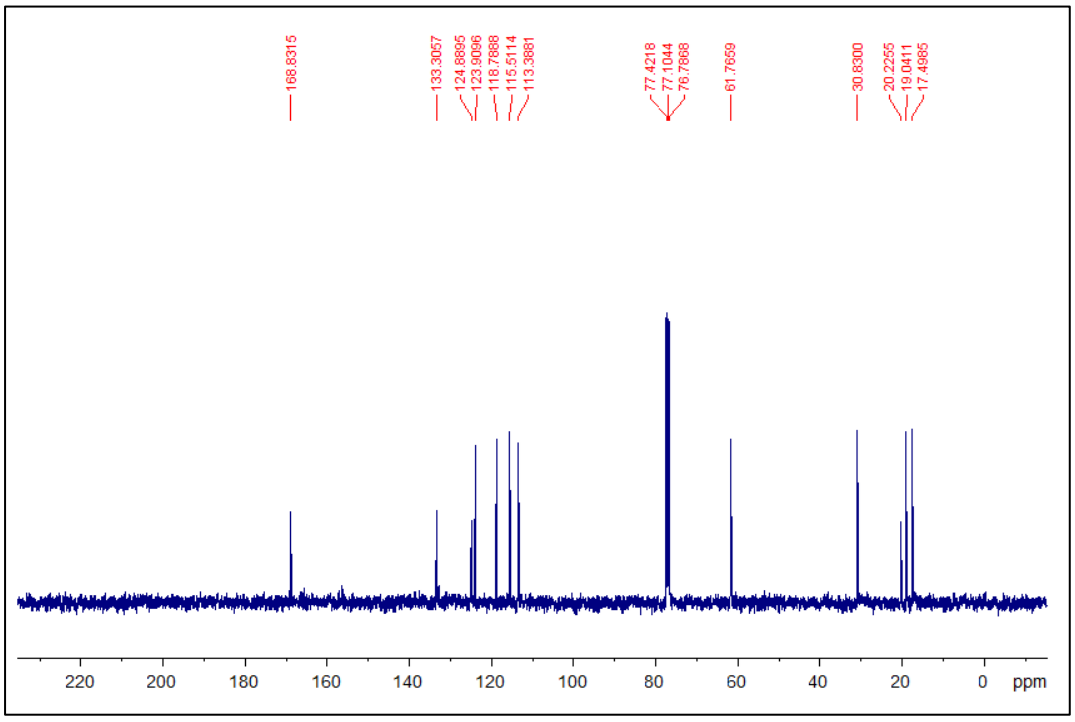
1.02
1.05
1.03
1.01
2.00
2.21
2.93


169.4115
133.4121
125.1713
122.1514
118.9660
116.7132
114.6019
77.3568
77.0391
76.7217
51.7110
27.0585
10.0278
220 200 180 160 140 120 100 80 60 40 20 0 ppm


9.758
7.289
6.889
6.873
6.810
6.794
6.741
6.725
6.687
6.670
4.094
3.806
2.287
2.274
1.094
1.071
1.015
1.002
H
N
O
N
H
4ad
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.00
4.38
1.13
1.06
1.22
6.32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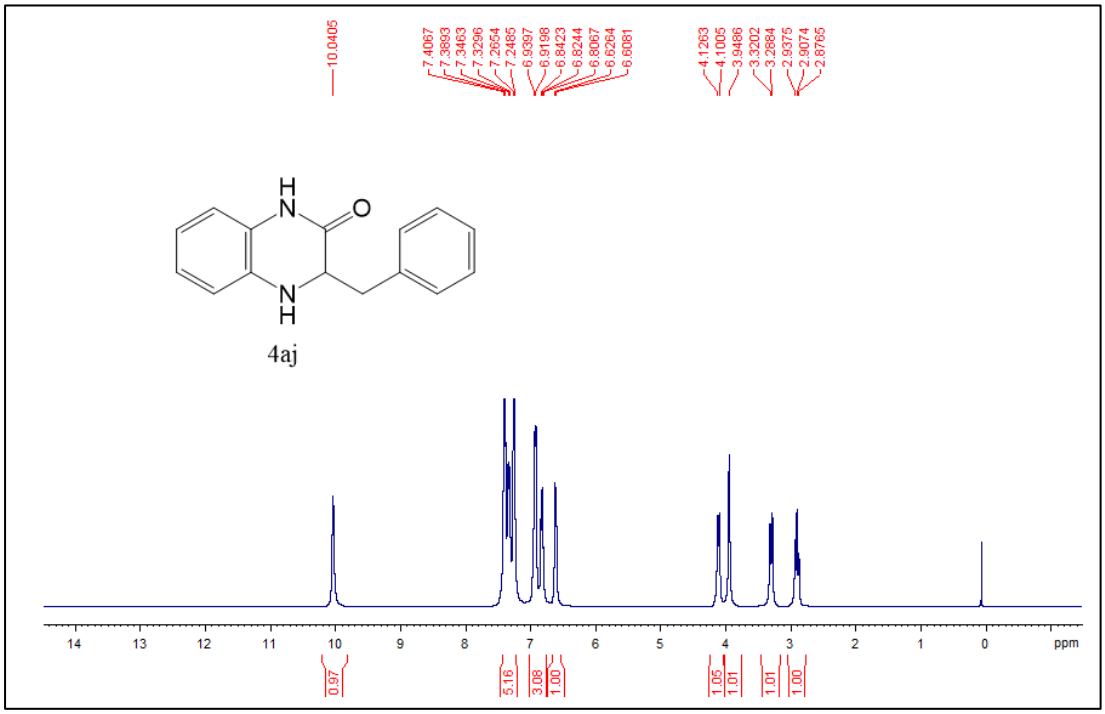
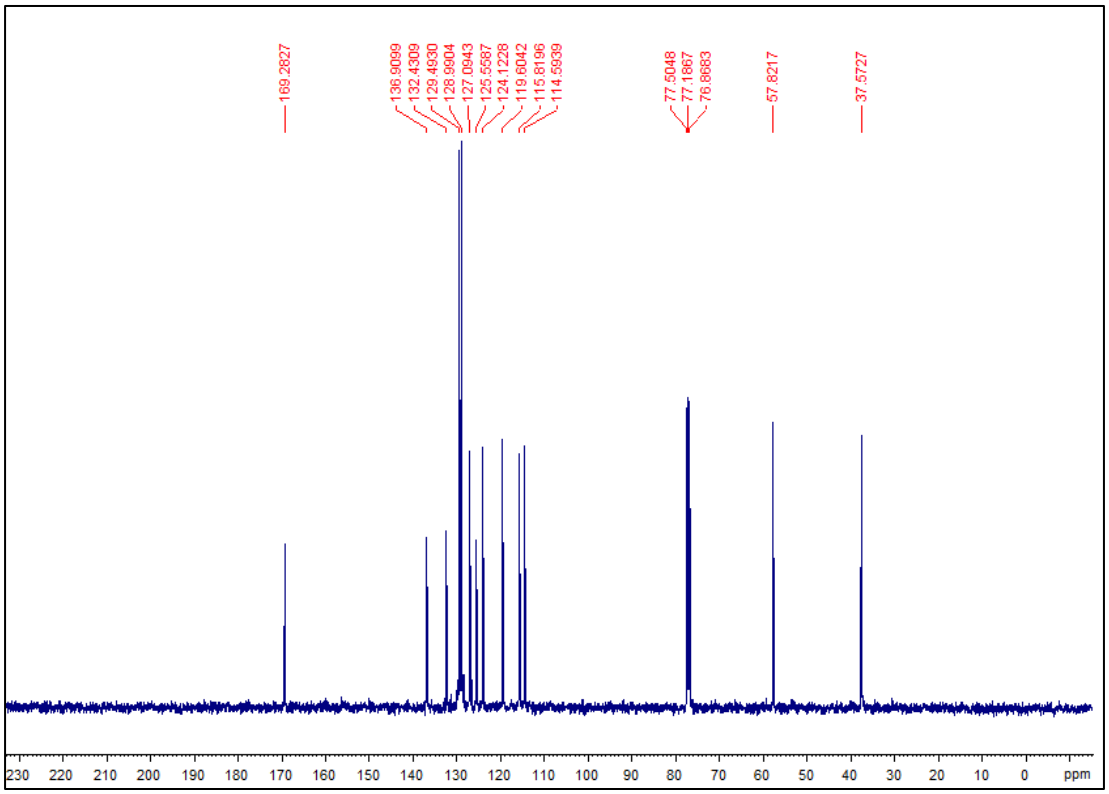
133.3057
124.8895
123.9096
118.7888
115.5114
113.3881
77.4218
77.1044
76.7868
61.7659
30.8300
20.2255
19.0411
17.4985
220 200 180 160 140 120 100 80 60 40 20 0 ppm


10.0405
7.4067
7.3893
7.3463
7.3296
7.2654
7.2485
6.9397
6.9198
6.8423
6.8244
6.8067
6.6264
6.6081
4.1263
4.1005
3.9486
3.3202
3.2884
2.9375
2.9074
2.8765
4aj
ppm
0.97
5.16
3.08
1.00
1.05
1.01
1.01
1.00


169.2827
136.9099
132.4309
129.4930
128.9904
127.0943
125.5587
124.1228
119.6042
115.8196
114.5939
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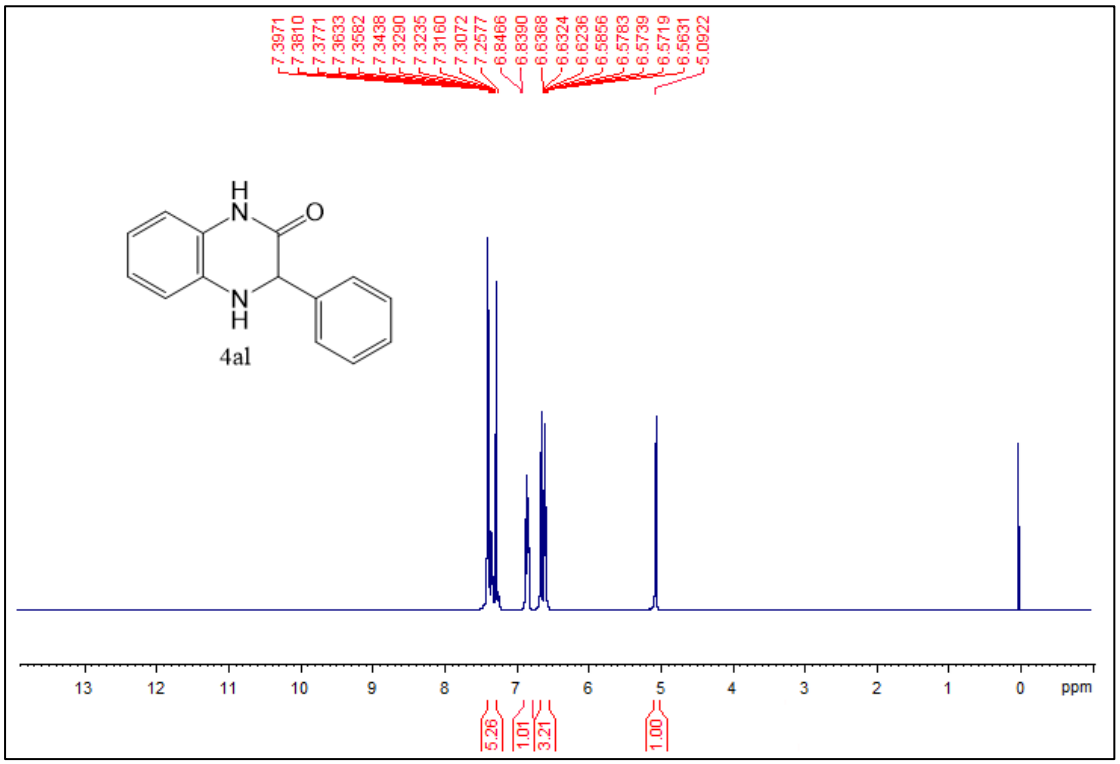
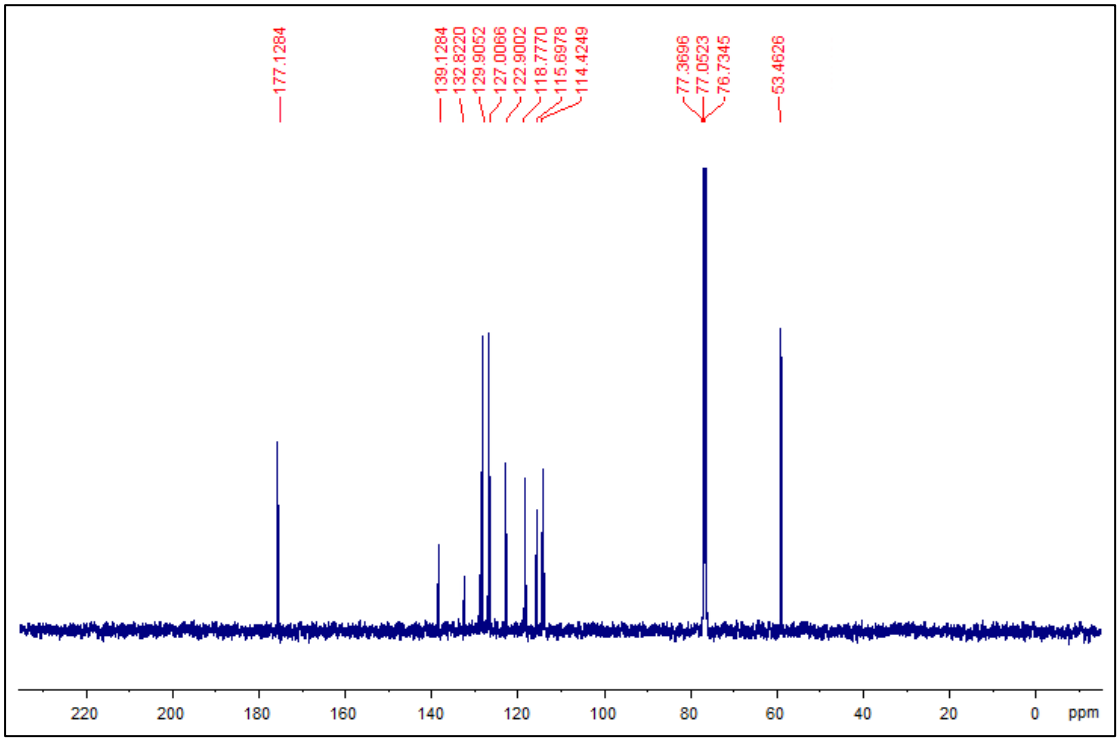
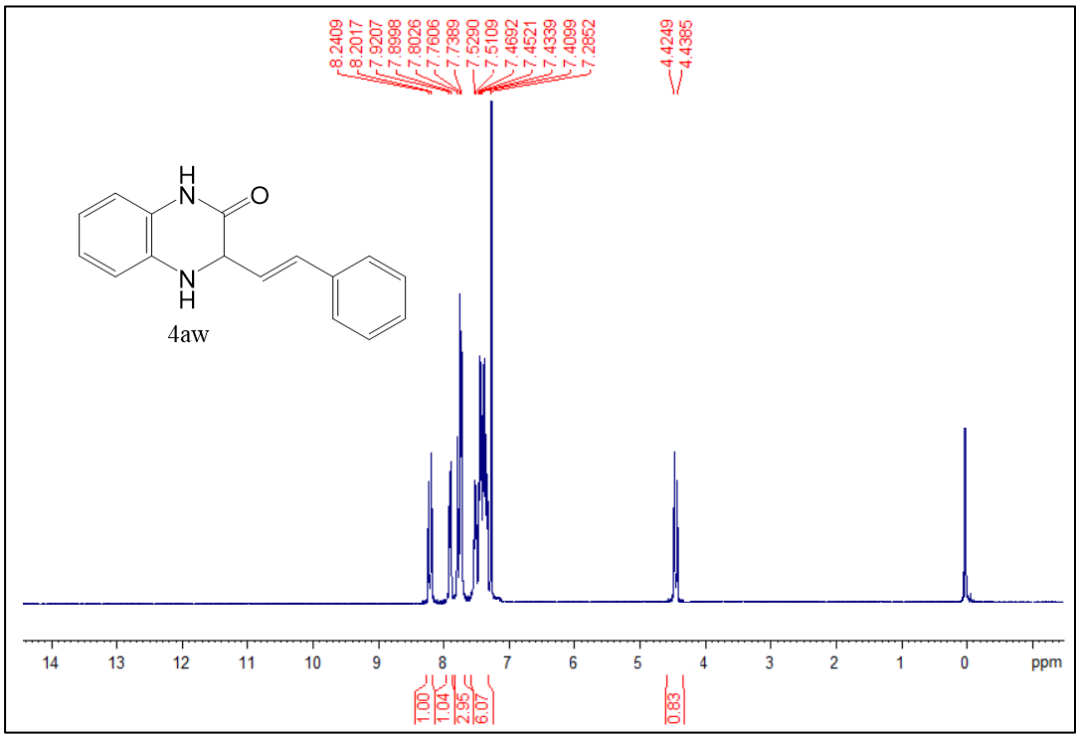
77.1867
76.8683
57.8217
37.5727
ppm


7.3971
7.3810
7.3771
7.3633
7.3582
7.3438
7.3290
7.3235
7.3160
7.3072
7.2577
6.8466
6.8390
6.6368
6.6324
6.6236
6.5856
6.5783
6.5739
6.5719
6.5631
5.0922
H
N
O
N
H
4al
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
5.26
1.01
3.21
1.00


177.1284
139.1284
132.8220
129.9052
127.0066
122.9002
118.7770
115.6978
114.4249
77.3696
77.0523
76.7345
53.4626
220
200
180
160
140
120
100
80
60
40
20
0
ppm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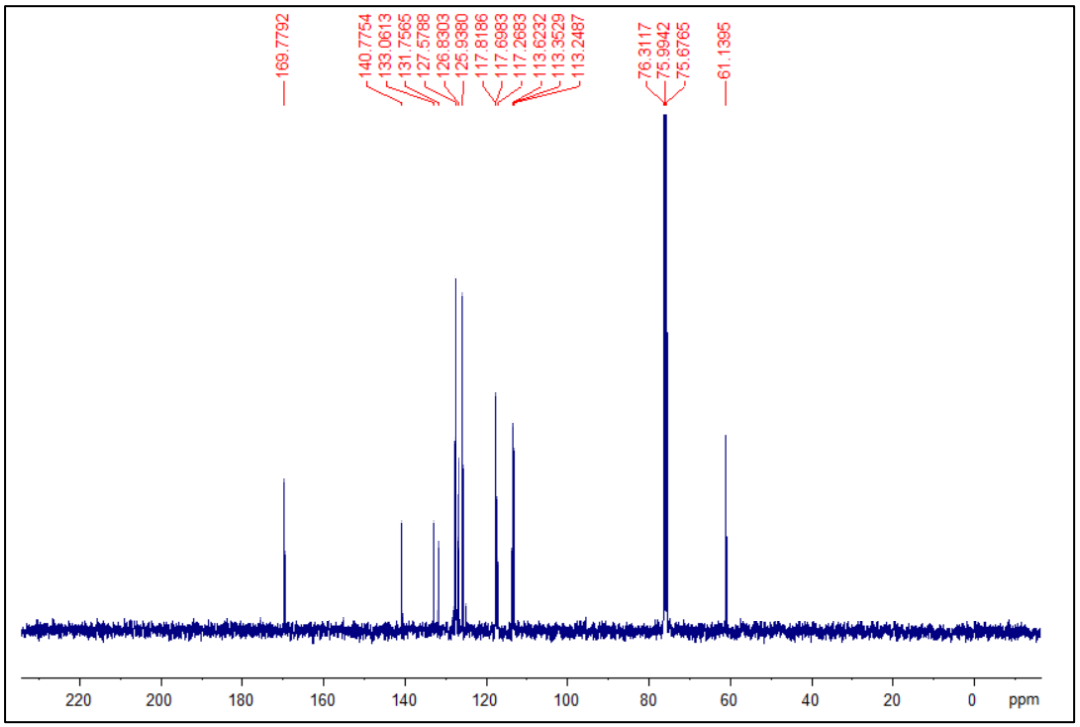
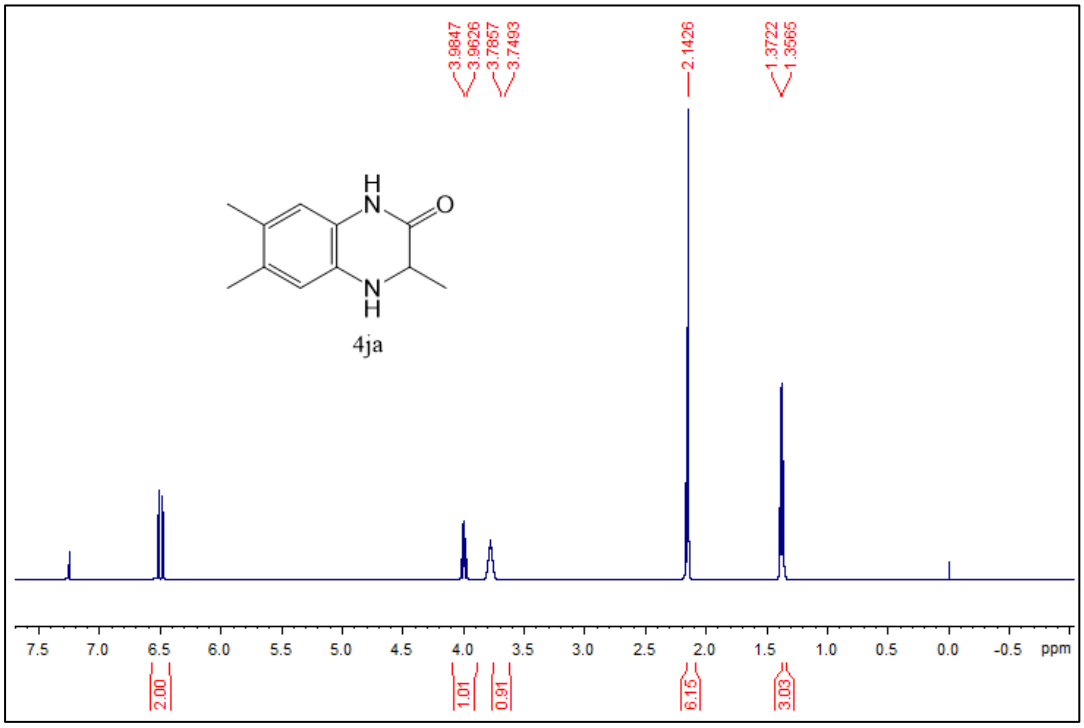
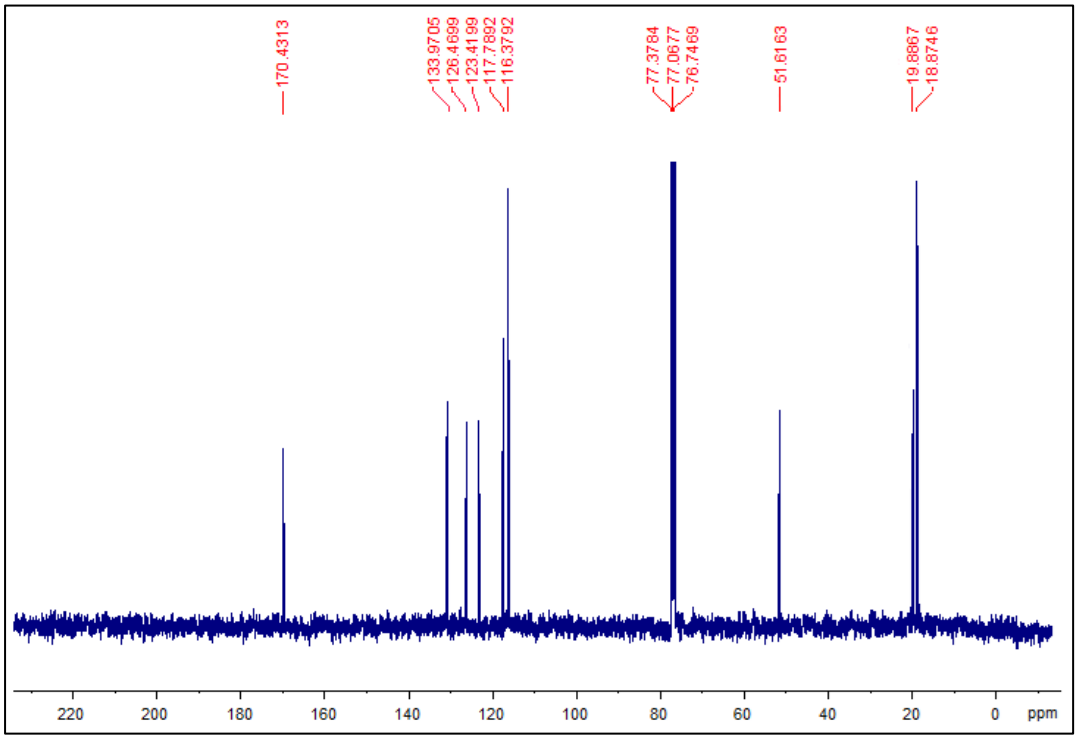
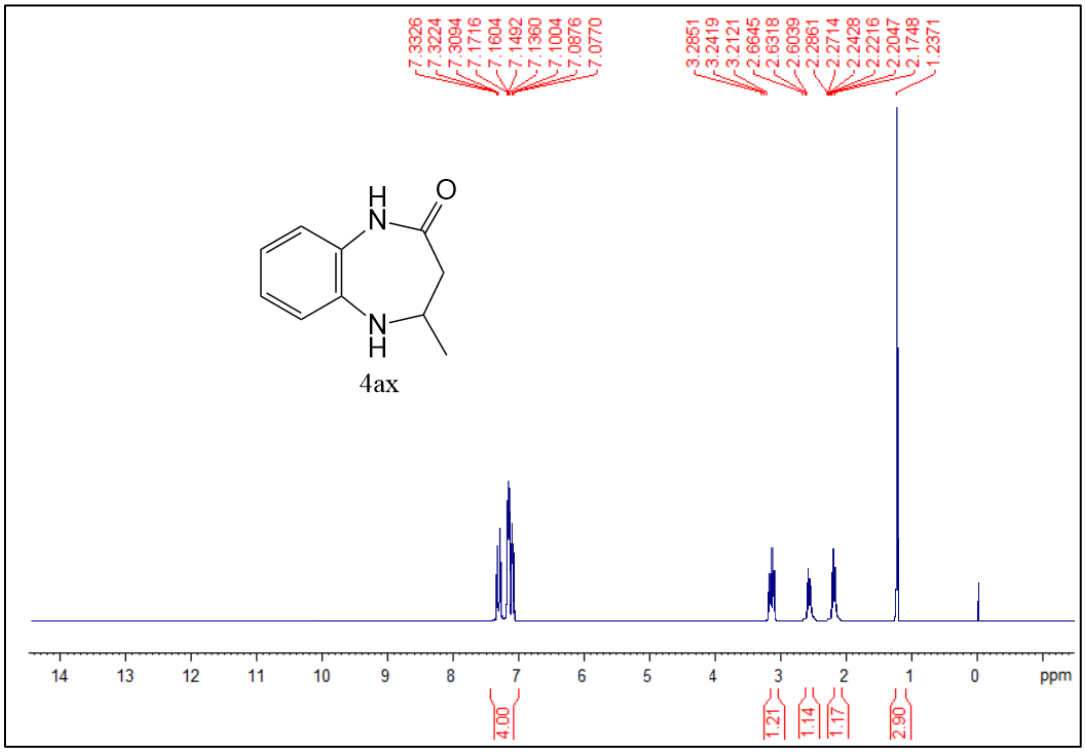
8.2017
7.9207
7.8998
7.8026
7.7606
7.7389
7.5290
7.5109
7.4692
7.4521
7.4339
7.4099
7.2852
4.4249
4.4385
H
N
O
N
H
4aw
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.04
2.95
6.07
0.83


169.7792
140.7754
133.0613
131.7565
127.5788
126.8303
125.9380
117.8186
117.6983
117.2683
113.6232
113.3529
113.2487
76.3117
75.9942
75.6765
61.1395
220
200
180
160
140
120
100
80
60
40
20
0
ppm


3.9847
3.9626
3.7857
3.7493
2.1426
1.3722
1.3565
H
N
O
N
H
4ja
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 ppm
2.00
1.01
0.91
6.15
3.03


170.4313
133.9705
126.4699
123.4199
117.7892
116.3792
77.3784
77.0677
76.7469
51.6163
19.8867
18.8746
220 200 180 160 140 120 100 80 60 40 20 0 ppm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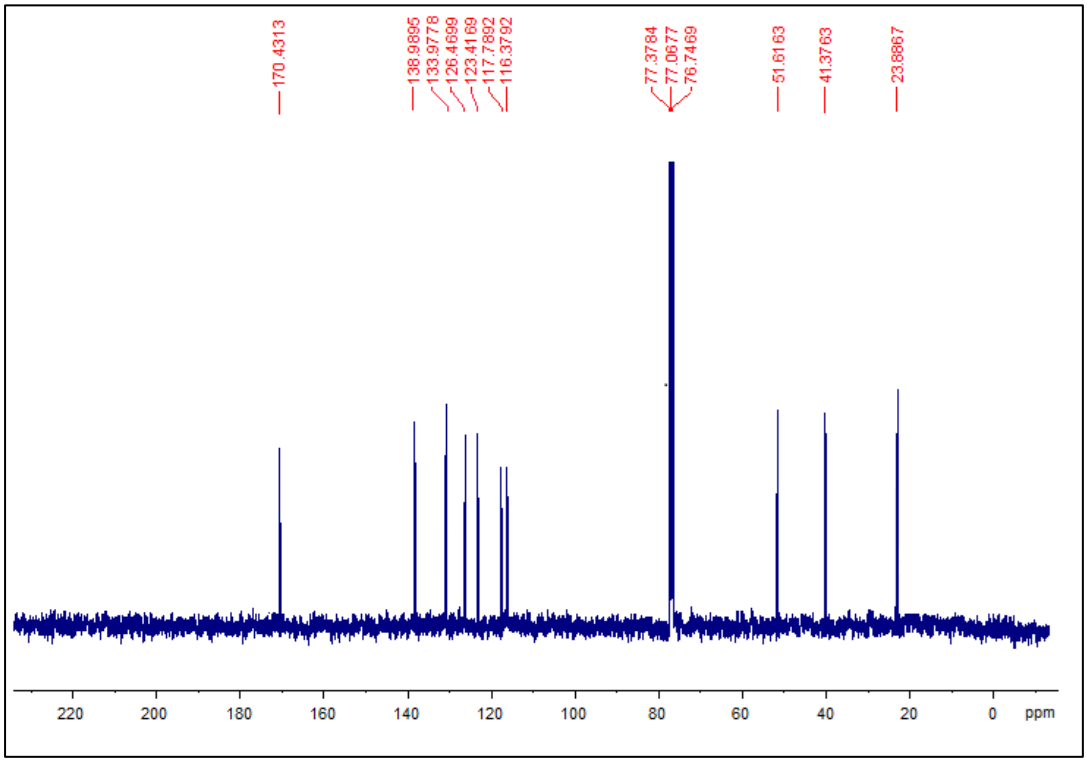
7.3224
7.3094
7.1716
7.1604
7.1492
7.1360
7.1004
7.0876
7.0770
3.2851
3.2419
3.2121
2.6645
2.6318
2.6039
2.2861
2.2714
2.2428
2.2216
2.2047
2.1748
1.2371
H
N
O
N
H
4ax
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
4.00
1.21
1.14
1.17
2.90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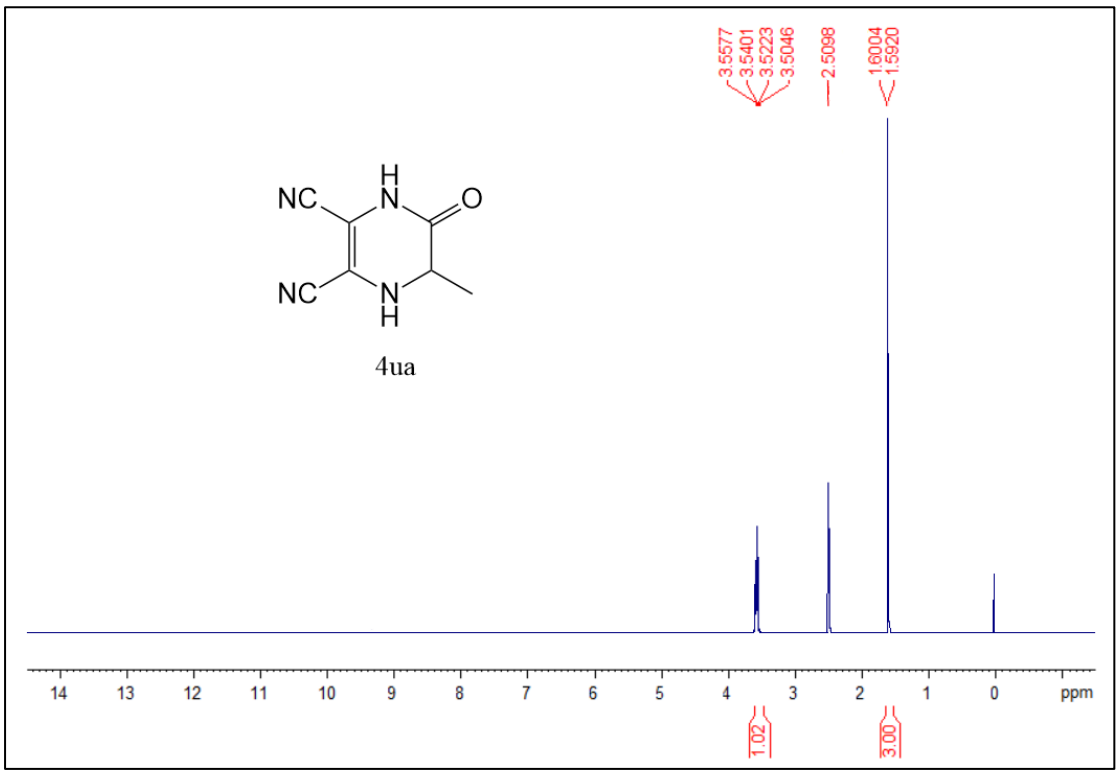
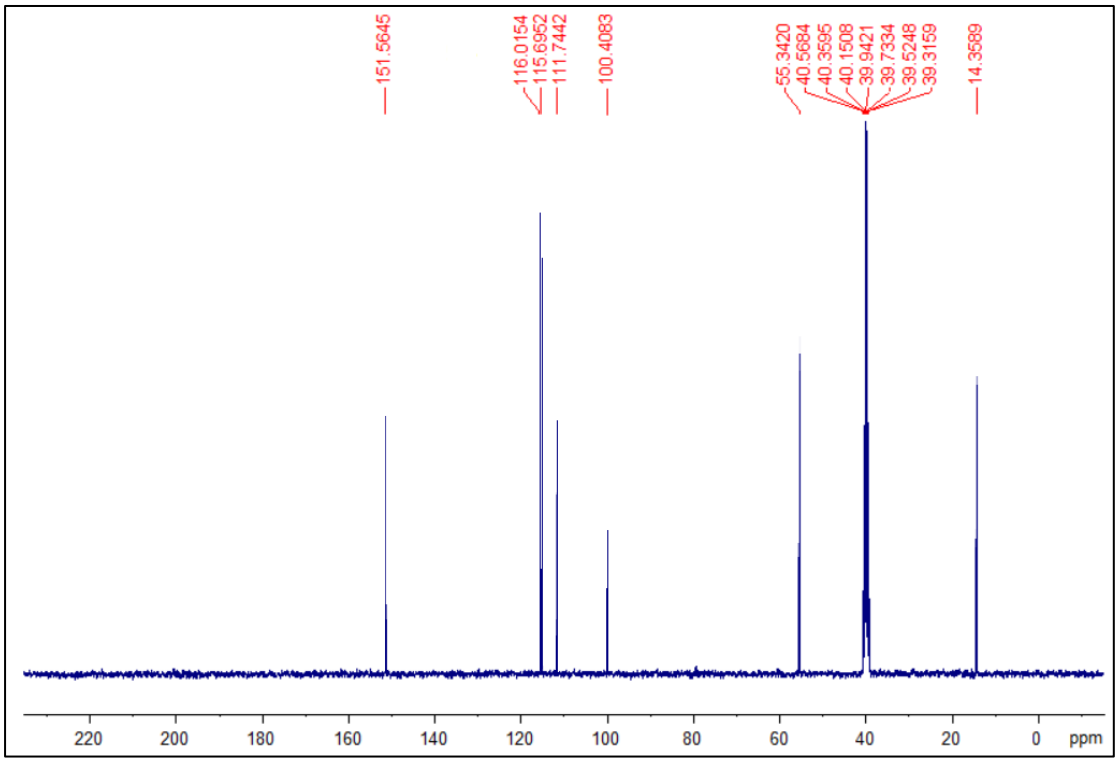
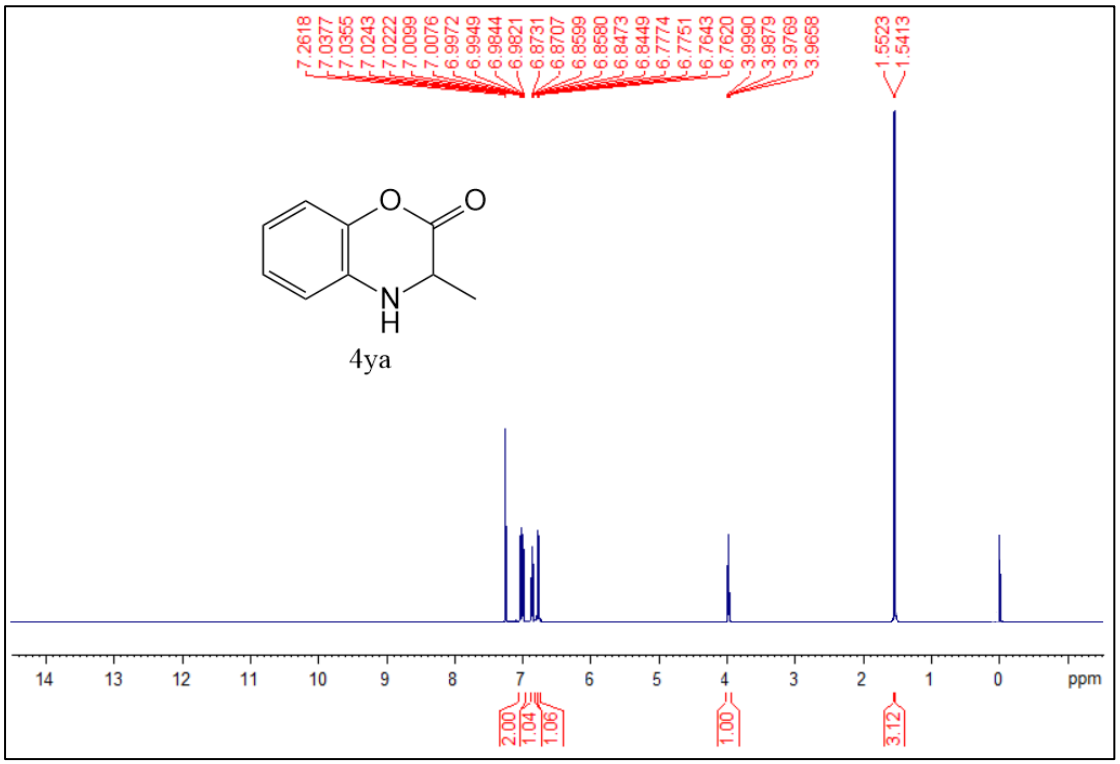
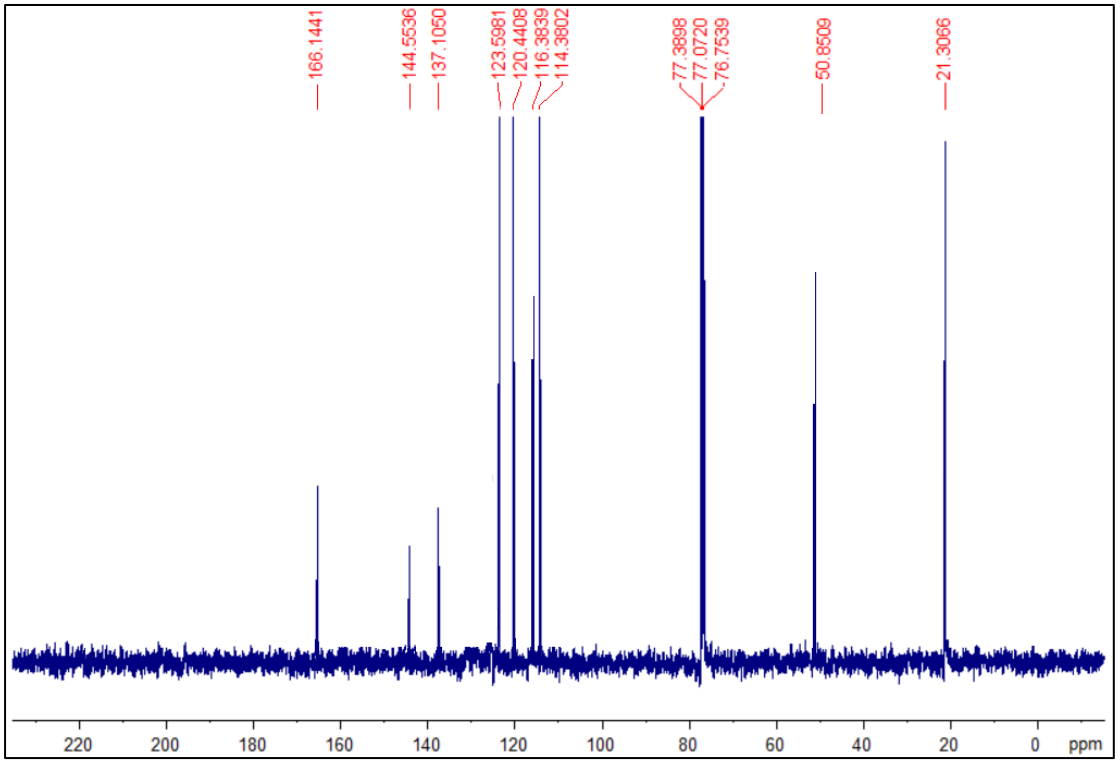
138.9895
133.9778
126.4699
123.4169
117.7892
116.3792
77.3784
77.0677
76.7469
51.6163
41.3763
23.8867
220 200 180 160 140 120 100 80 60 40 20 0 ppm


3.5577
3.5401
3.5223
3.5046
2.5098
1.6004
1.5920
NC
NC
H
N
O
N
H
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.02
3.00

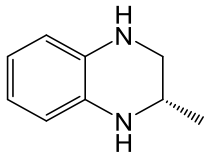
4ua


151.5645
116.0154
115.6952
111.7442
100.4083
55.3420
40.5684
40.3595
40.1508
39.9421
39.7334
39.5248
39.3159
14.3589
220
200
180
160
140
120
100
80
60
40
20
0
ppm

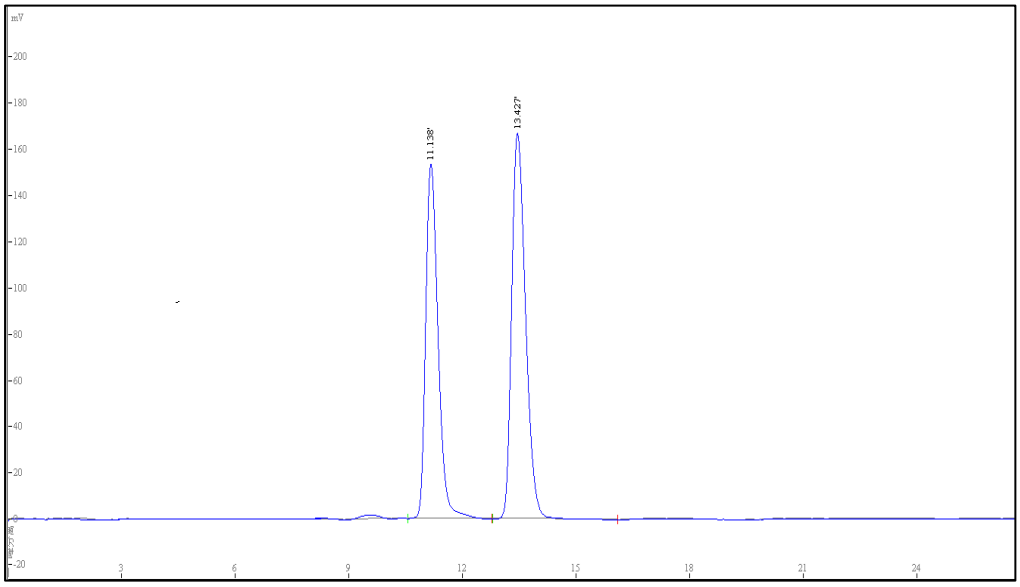

7.2618
7.0377
7.0355
7.0243
7.0222
7.0099
7.0076
6.9972
6.9949
6.9844
6.9821
6.8731
6.8707
6.8599
6.8580
6.8473
6.8449
6.7774
6.7751
6.7643
6.7620
3.9990
3.9879
3.9769
3.9658
1.5523
1.5413
O
O
N
H
4ya
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.00
1.04
1.06
1.00
3.12


166.1441
144.5536
137.1050
123.5981
120.4408
116.3839
114.3802
77.3898
77.0720
76.7539
50.8609
21.3066
220 200 180 160 140 120 100 80 60 40 20 0 ppm

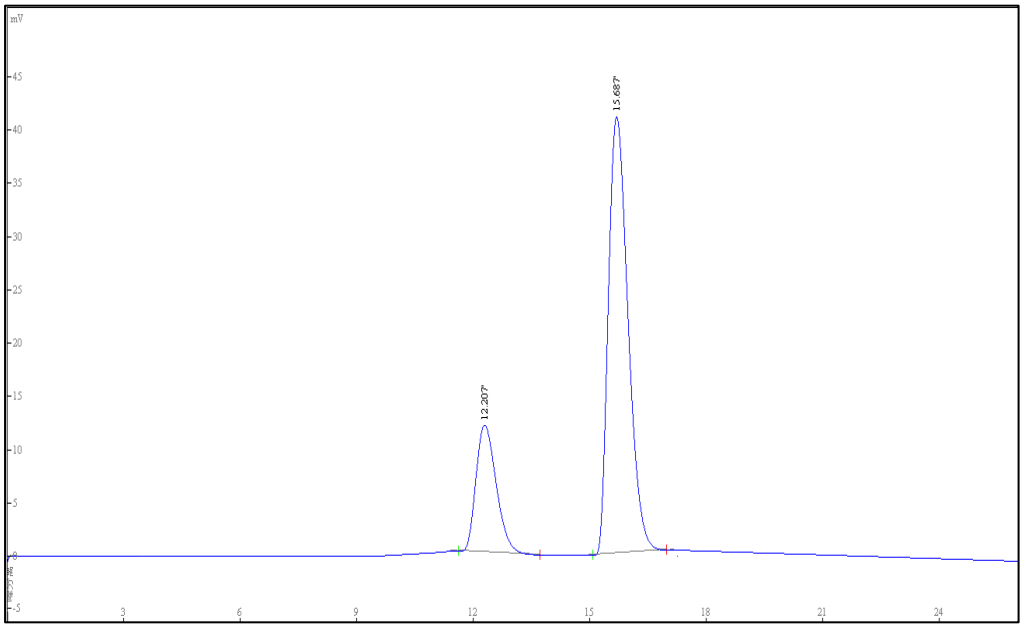
8.HPLC CHART



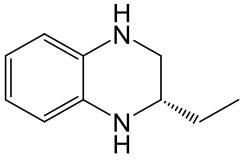
(S)-2-methyl-1,2,3,4-tetrahydroquinoxaline
Chiralcel OD-H
Hexane / i-PrOH = 95/5 0.5ml/min, 230 nm
tr = 12.207 (S) and 15.687 (R)
ee = 47.76 $[\alpha]_D^{25}$= -15.8 (c 1.06, EtOH)



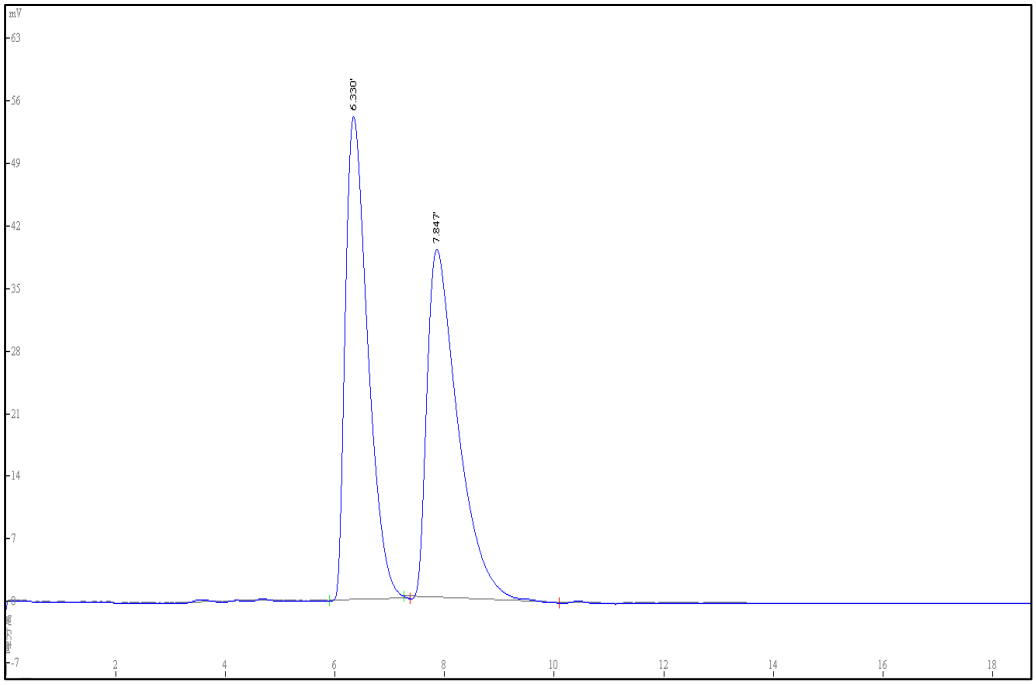
	保留时间	组份名称	校正因子	浓度	峰面积	峰高	半高峰宽	峰标志
1	11.138			45.02	3494384	153778	21.340	
2	13.427			54.98	4267952	167054	23.993	RM



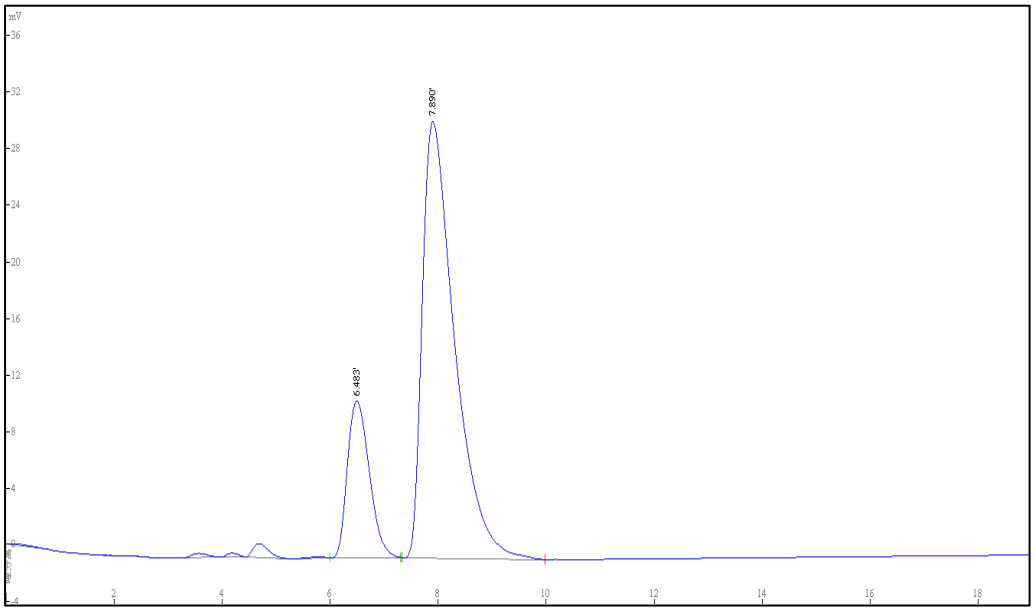
	保留时间	组份名称	校正因子	浓度	峰面积	峰高	半高峰宽	峰标志
1	12.207			26.12	434839	11936	33.039	RM
2	15.687			73.88	1235623	41091	34.213	



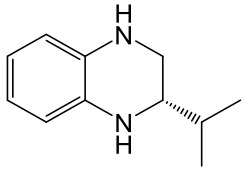
(S)-2-ethyl-1,2,3,4-tetrahydroquinoxaline
Chiralcel OD-H
Hexane / i-PrOH = 95/5 1ml/min, 230 nm
t_r = 6.483 (*S*) and 7.890 (*R*)
ee = 52.56 $[\alpha]_D^{25}$= -13.1 (c 1.00, EtOH)



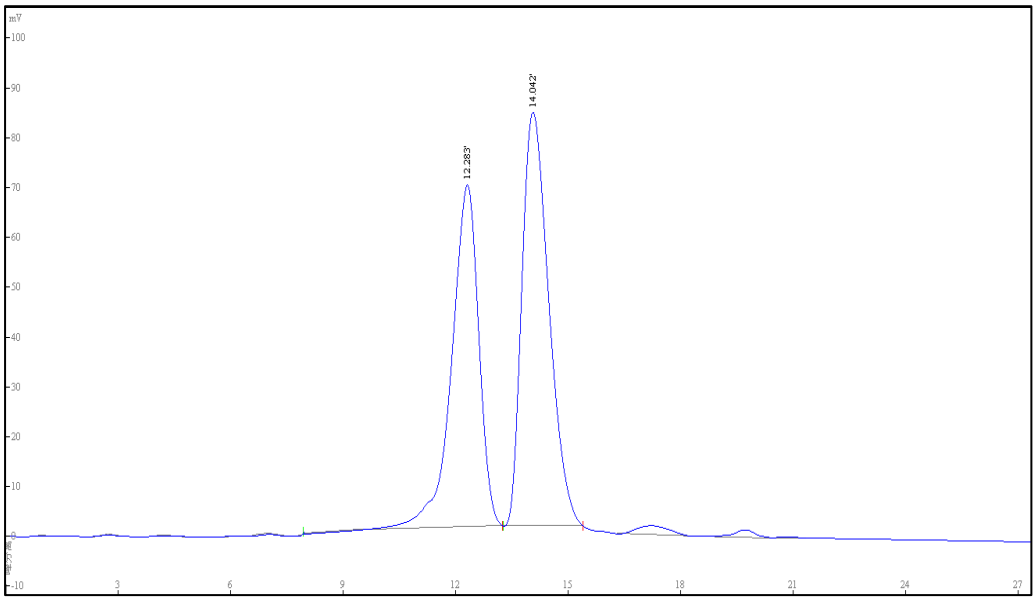
	保留时间	組份名称	校正因子	浓度	峰面积	峰高	半高峰宽	峰标志
1	6.330			50.14	1544736	54151	26.789	
2	7.847			49.86	1535886	38997	36.987	R



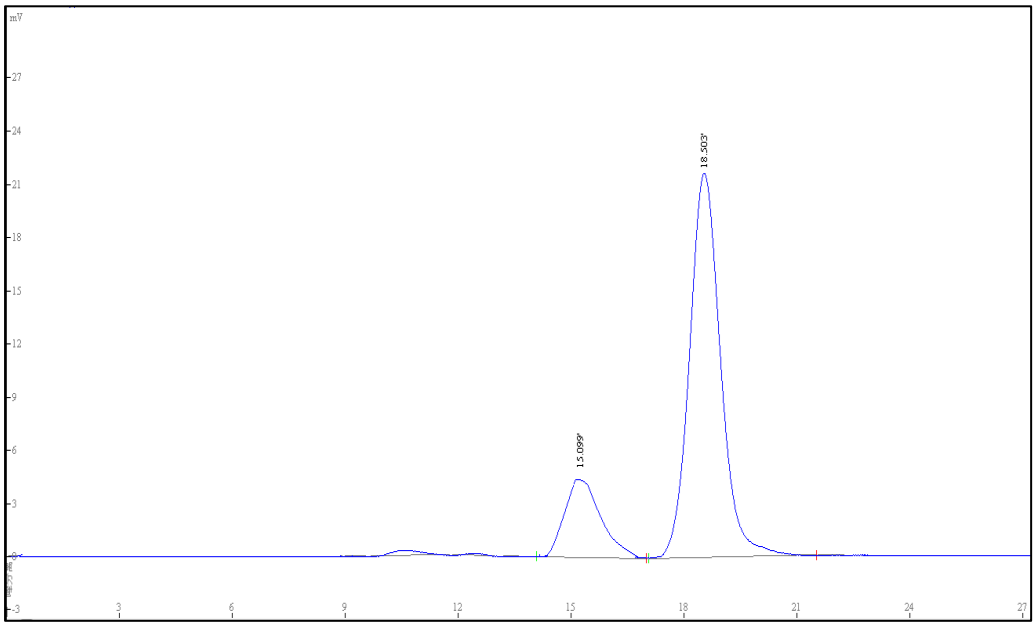
	保留时间	組份名称	校正因子	浓度	峰面积	峰高	半高峰宽	峰标志
1	6.483			23.72	315556	10150	26.578	
2	7.890			76.28	1015008	30865	39.098	R



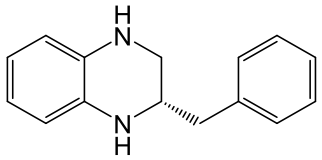
(S)-2-isopropyl-1,2,3,4-tetrahydroquinoxaline
Chiralcel OD-H
Hexane / i-PrOH = 95/5 0.5ml/min, 230 nm
t_r = 15.009 (*S*) and 18.503 (*R*)
ee = 51.74 $[\alpha]_D^{25}$= -13.8 (c 1.06, EtOH)



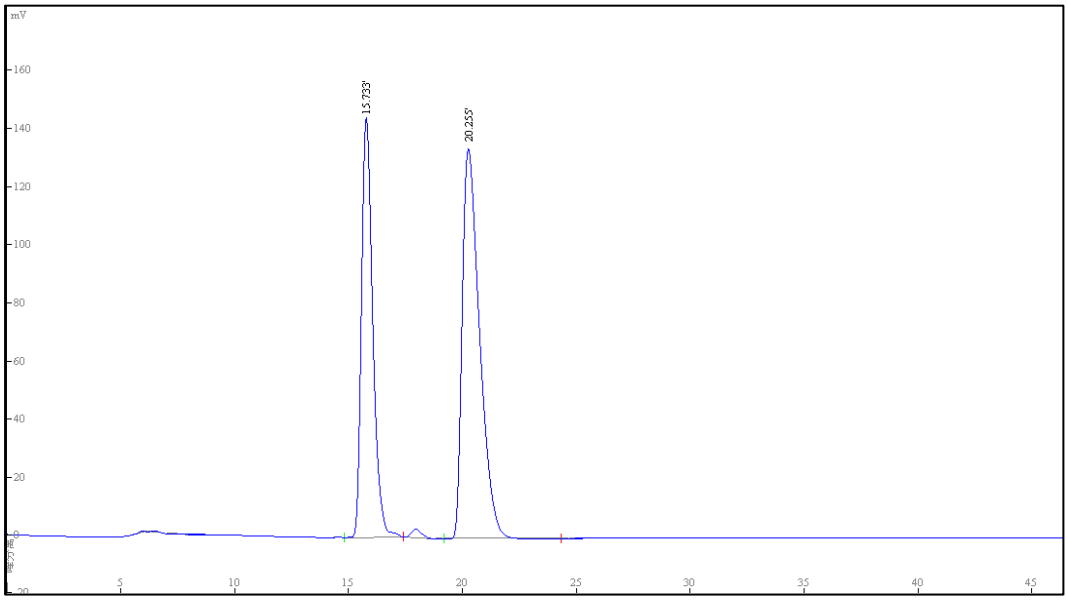
	保留时间	組份名称	校正因子	浓度	峰面积	峰高	半高峰宽	峰标志
1	12.283			49.43	4050312	68690	55.375	
2	14.042			50.57	4143650	83052	46.854	R



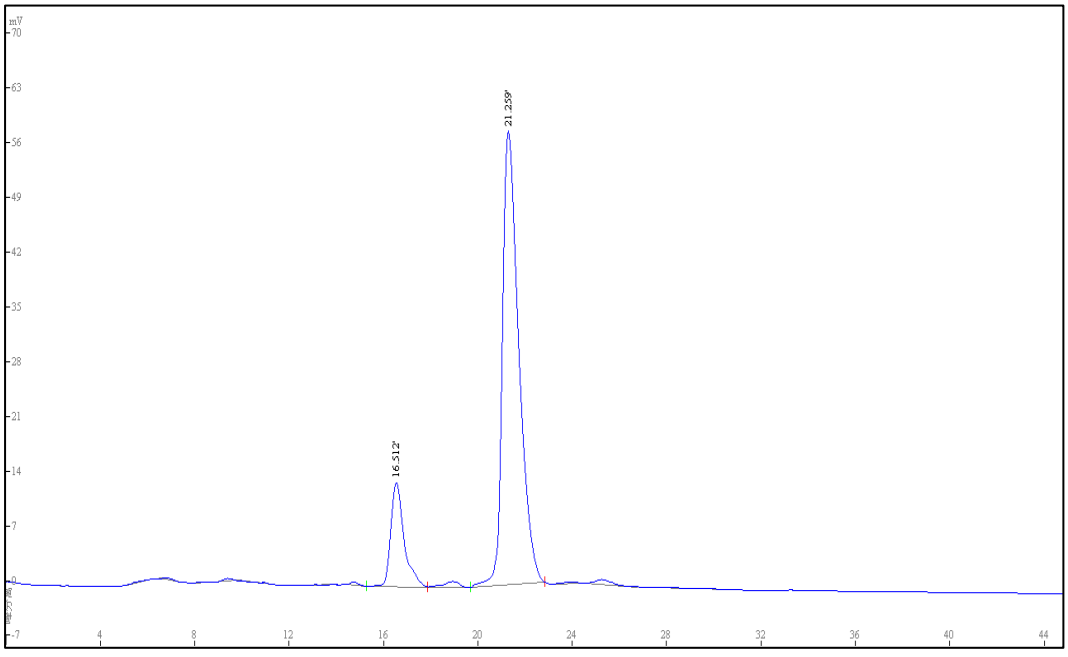
	保留时间	組份名称	校正因子	浓度	峰面积	峰高	半高峰宽	峰标志
1	15.099			24.13	375764	5823	57.059	
2	18.503			75.87	1180705	21691	54.149	



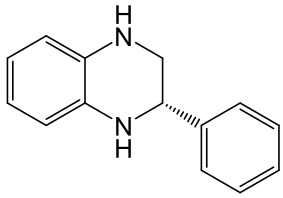
(S)-2-benzyl-1,2,3,4-tetrahydroquinoxaline
Chiralcel OD-H
Hexane / i-PrOH = 95/5 0.5 ml/min, 230 nm
t_r = 16.512 (*S*) and 21.259 (*R*)
ee = 58.72 $[\alpha]_D^{25}$ = -14.7 (c 1.06, EtOH)



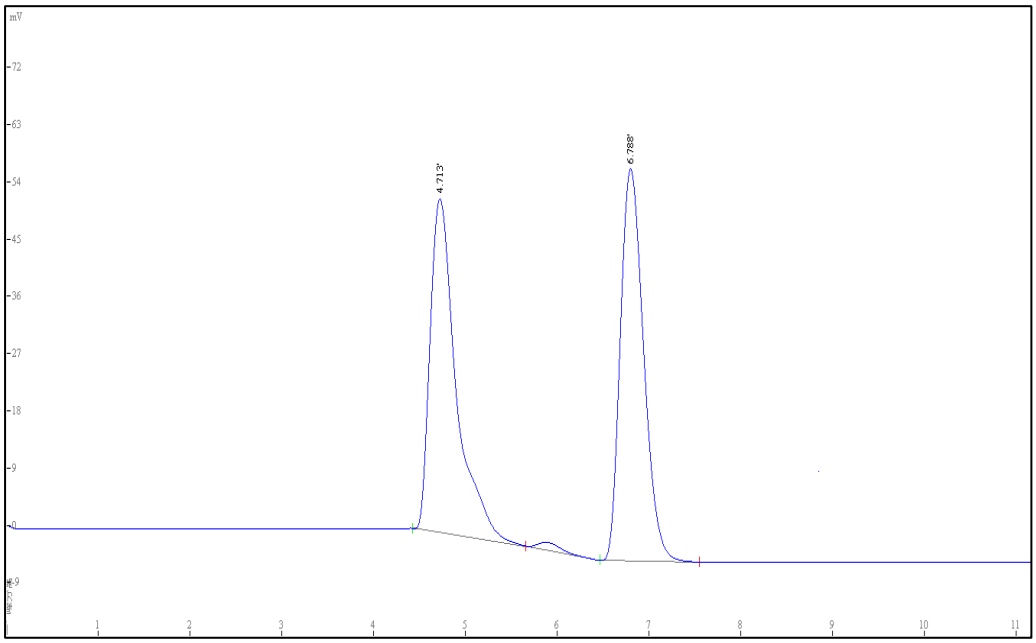
	保留时间	組份名称	校正因子	浓度	峰面积	峰高	半高峰宽	峰标志
1	15.733			49.88	5020836	145073	32.502	R
2	20.255			50.12	5064528	131702	37.459	



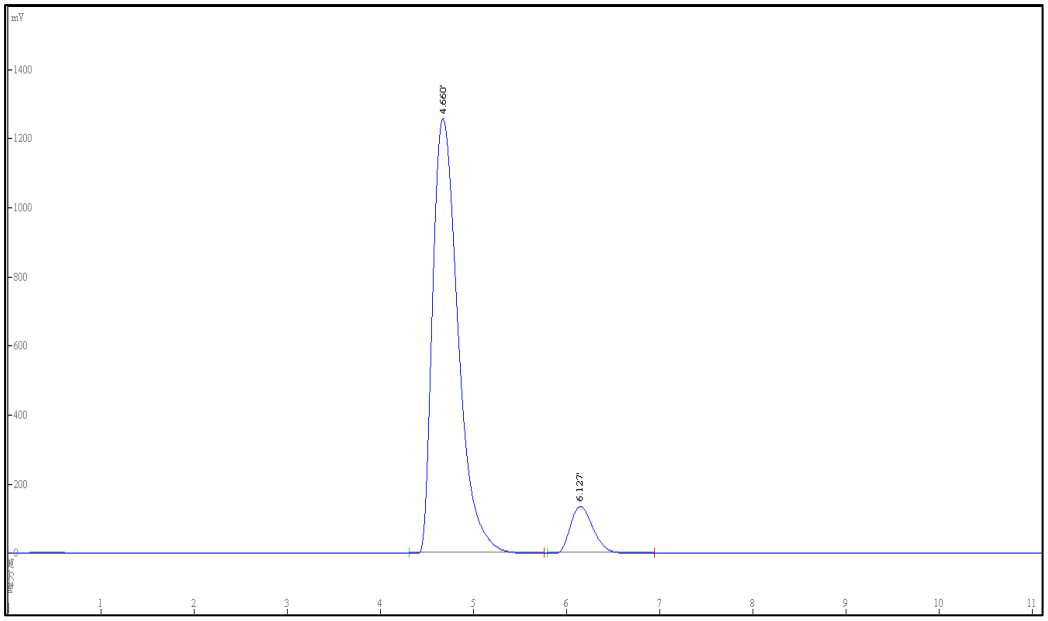
	保留时间	組份名称	校正因子	浓度	峰面积	峰高	半高峰宽	峰标志
1	16.512			20.64	527768	13377	37.051	LR
2	21.259			79.36	2076275	57996	37.813	



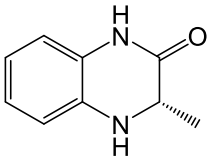
(S)-2-phenyl-1,2,3,4-tetrahydroquinoxaline
Chiralcel OD-H
Hexane / i-PrOH = 99/1 1 ml/min, 230 nm
t_r = 4.660 (*S*) and 6.127 (*R*)
ee = 76.28 $[\alpha]_D^{25}$ = +75.8 (c 1.06, EtOH)



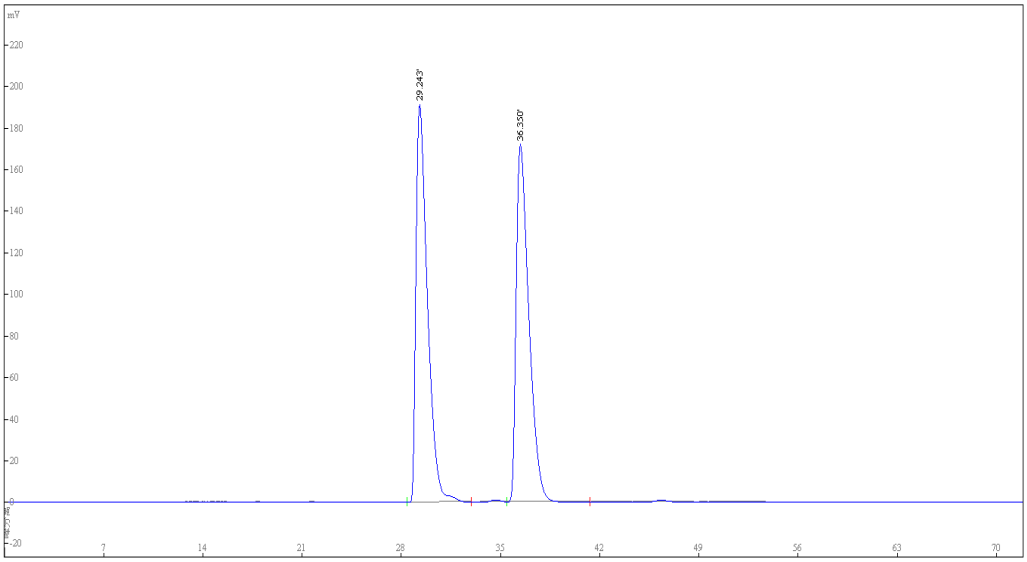
	保留时间	組份名称	校正因子	浓度	峰面积	峰高	半高峰宽	峰标志
1	4.713			48.79	1036583	52401	18.577	R
2	6.788			51.21	1087889	61699	16.559	



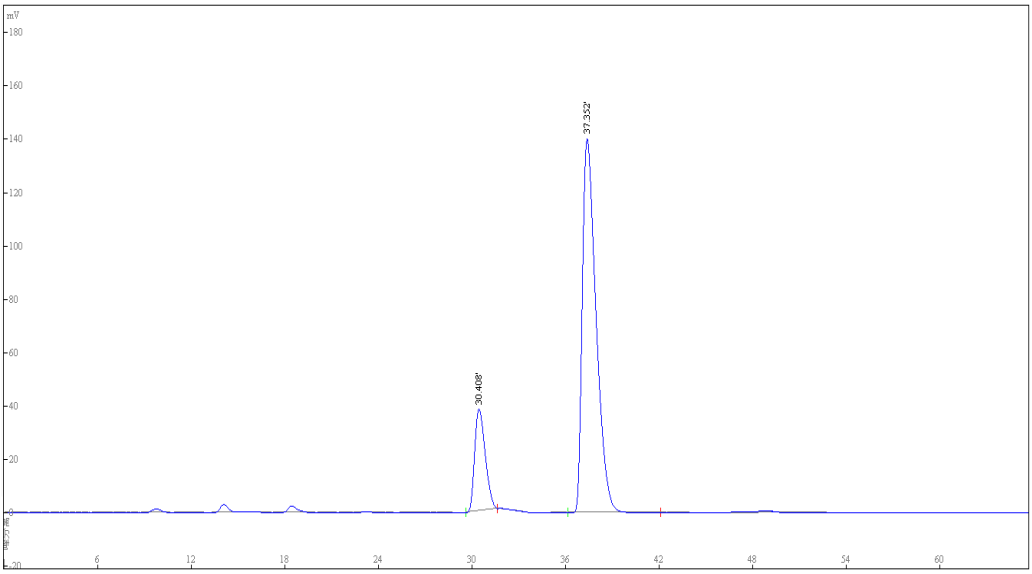
	保留时间	組份名称	校正因子	浓度	峰面积	峰高	半高峰宽	峰标志
1	4.660			88.14	23794880	1258552	17.755	
2	6.127			11.86	3201136	135575	16.009	R



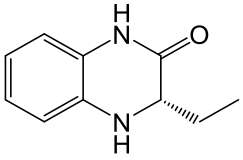
(S)-3-methyl-3,4-dihydroquinoxalin-2(1H)-one
Chiralcel OD-H
Hexane / i-PrOH = 99/1 1 ml/min, 230 nm
t_r = 30.480 (*S*) and 37.352 (*R*)
ee = 57.38 $[\alpha]_D^{25}$ = -18.7 (c 1.06, EtOH)



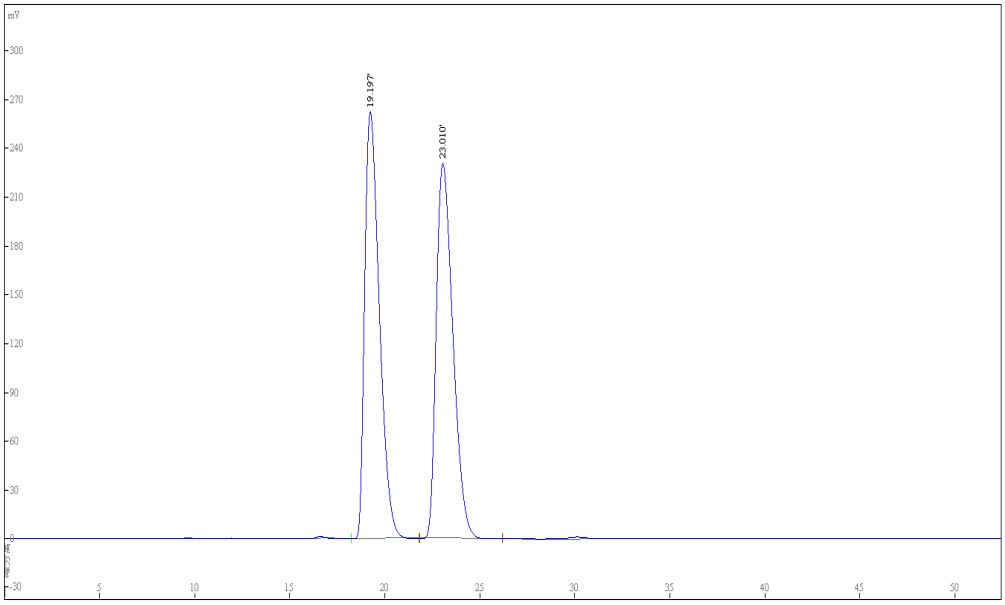
	保留时间	組份名称	校正因子	浓度	峰面积	峰高	半高峰宽	峰标志
1	29.243			50.26	10814813	191644	52.996	LRM
2	36.350			49.74	10701593	172107	58.394	RM



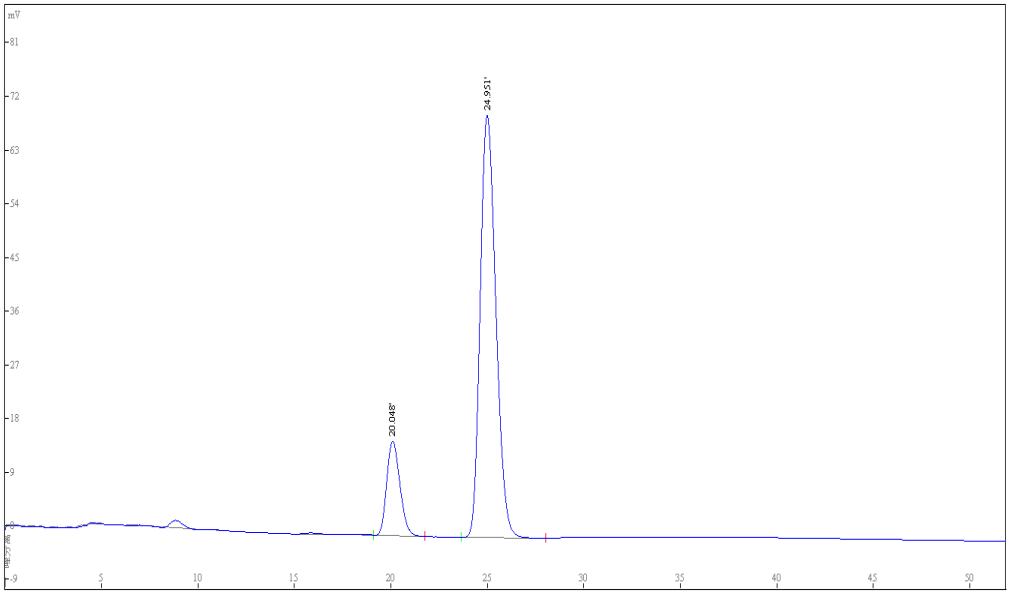
	保留时间	組份名称	校正因子	浓度	峰面积	峰高	半高峰宽	峰标志
1	30.408			21.31	1804163	38161	44.399	
2	37.352			78.69	6617117	140402	57.638	RM



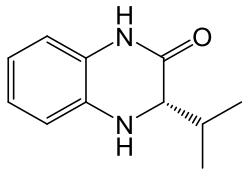
(S)-3-ethyl-3,4-dihydroquinoxalin-2(1H)-one
Chiralcel OD-H
Hexane / i-PrOH = 97/3 1 ml/min, 230 nm
t_r = 20.048 (*S*) and 24.951 (*R*)
ee = 61.88 $[\alpha]_D^{25}$ = -13.2(c 1.06, EtOH)



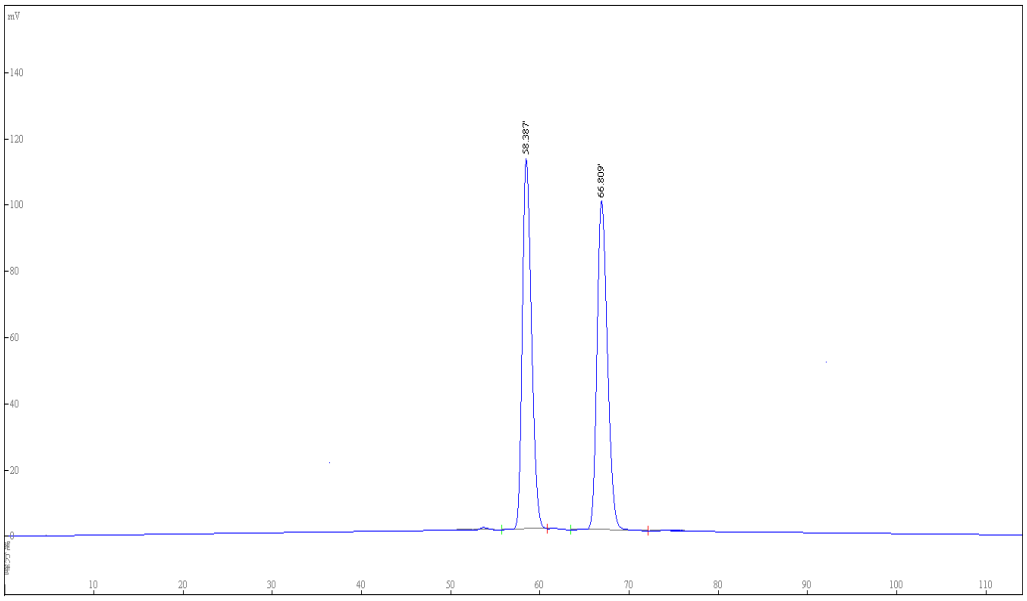
	保留时间	組份名称	校正因子	浓度	峰面积	峰高	半高峰宽	峰标志
1	19.197			49.95	14083683	262609	50.364	
2	23.010			50.05	14113923	230927	57.397	



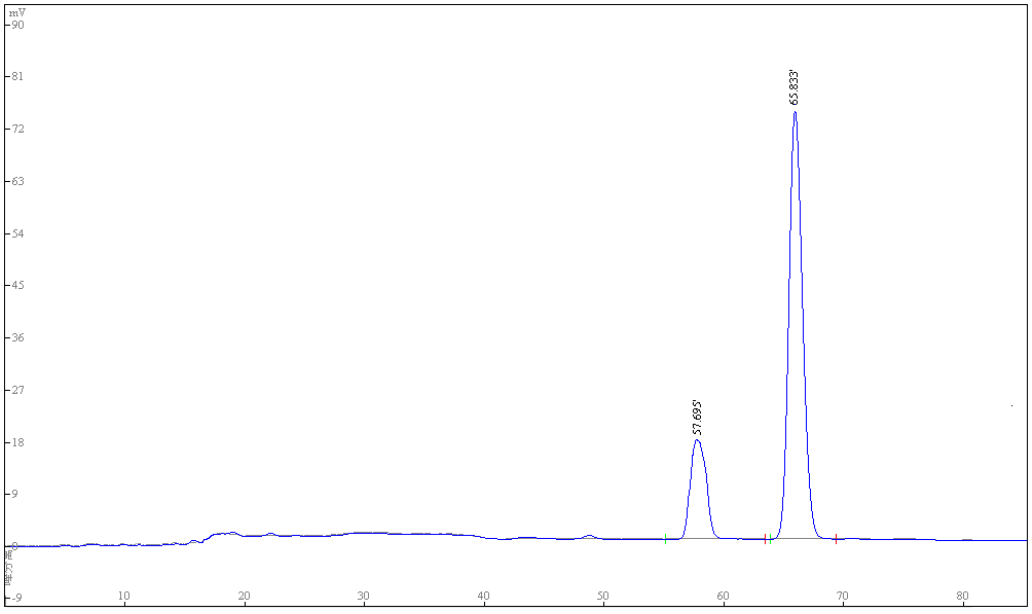
	保留时间	組份名称	校正因子	浓度	峰面积	峰高	半高峰宽	峰标志
1	20.048			19.06	789367	16012	45.124	RM
2	24.951			80.94	3319737	71007	53.163	RM



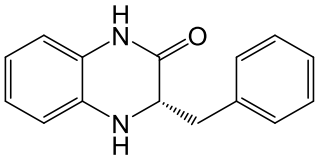
(S)-3-isopropyl-3,4-dihydroquinoxalin-2(1H)-one
Chiralcel OD-H
Hexane / i-PrOH = 99/1 0.5 ml/min, 230 nm
t_r = 57.695 (*S*) and 65.833 (*R*)
ee = 60.96 $[\alpha]_D^{25}$ = -18.4 (c 1.06, EtOH)



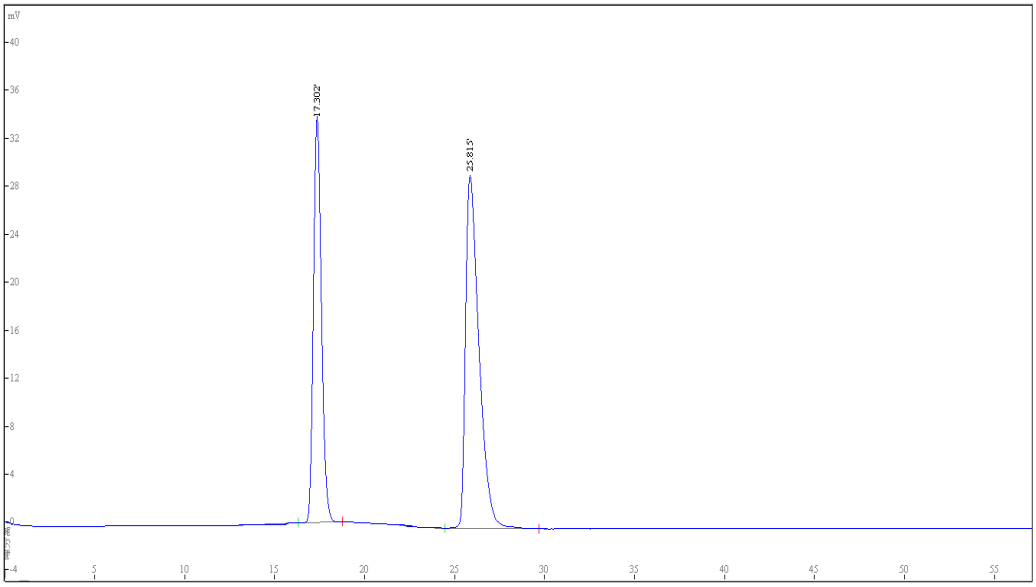
	保留时间	組份名称	校正因子	浓度	峰面积	峰高	半高峰宽	峰标志
1	58.387			49.71	7982398	112013	66.924	LM
2	66.809			50.29	8074100	99588	76.138	LRM



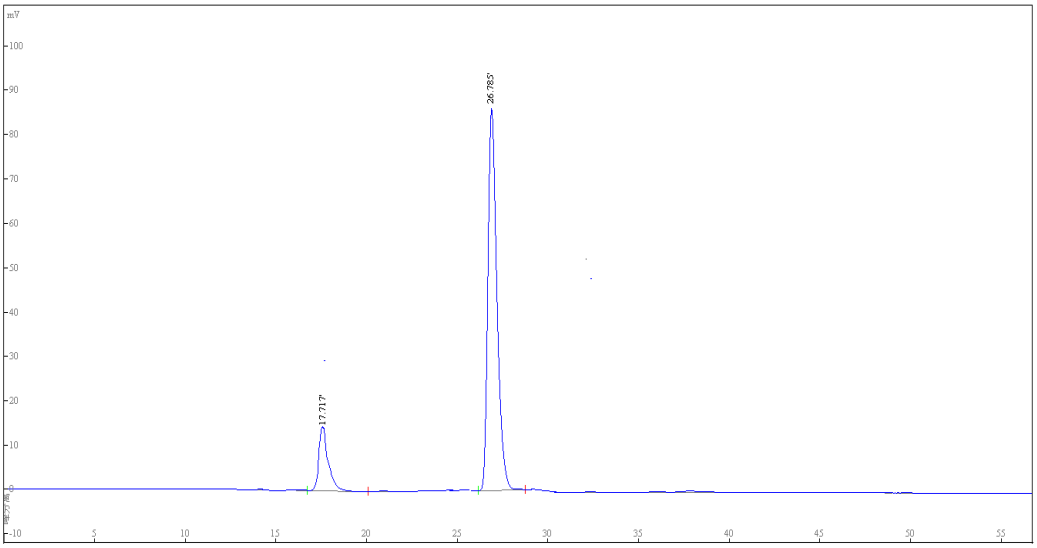
	保留时间	組份名称	校正因子	浓度	峰面积	峰高	半高峰宽	峰标志
1	57.695			19.52	2458331	19511	66.896	LRM
2	65.833			80.48	5869866	73805	74.689	



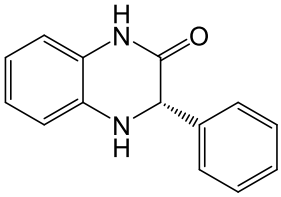
(S)-3-benzyl-3,4-dihydroquinoxalin-2(1H)-one
Chiralcel OD-H
Hexane / i-PrOH = 98/2 1 ml/min, 230 nm
t_r = 17.717(*S*) and 26.785 (*R*)
ee = 71.00 $[\alpha]_D^{25}$ = -20.7 (c 1.06, EtOH)



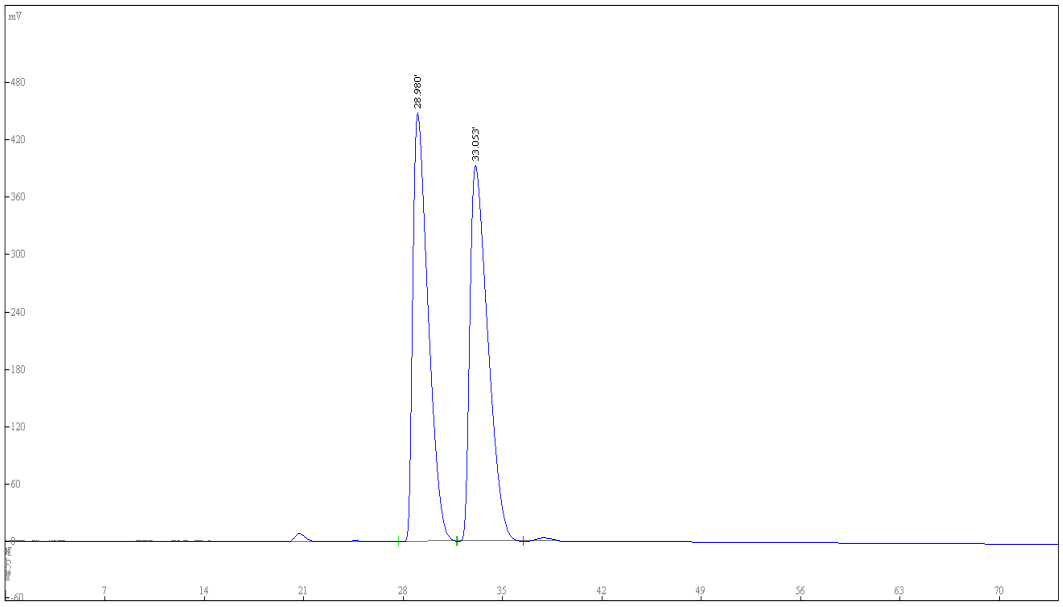
	保留时间	組份名称	校正因子	浓度	峰面积	峰高	半高峰宽	峰标志
1	17.302			49.67	1053552	33902	29.184	L
2	25.815			50.33	1538864	29484	48.951	RM



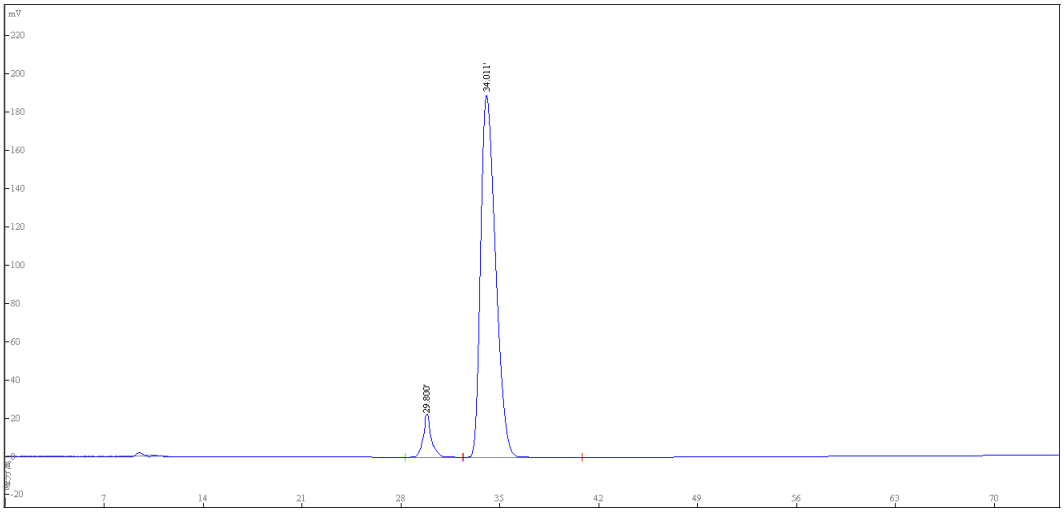
	保留时间	組份名称	校正因子	浓度	峰面积	峰高	半高峰宽	峰标志
1	17.717			14.5	510535	14054	44.802	RM
2	26.785			85.5	3011201	86558	32.670	RM



(S)-3-phenyl-3,4-dihydroquinoxalin-2(1H)-one
Chiralcel OD-H
Hexane / i-PrOH = 99/1 1 ml/min, 230 nm
t_r = 29.800 (*R*) and 34.011 (*S*)
ee = 82.24 $[\alpha]_D^{25}$ = +73.8 (c 1.06, EtOH)



	保留时间	組份名称	校正因子	浓度	峰面积	峰高	半高峰宽	峰标志
1	28.980			49.36	33671818	448267	70.542	
2	33.053			50.64	34545638	392887	82.574	



	保留时间	組份名称	校正因子	浓度	峰面积	峰高	半高峰宽	峰标志
1	29.800			8.881	126896	21624	57.918	R
2	34.011			91.12	13970650	189487	69.239	RM