

SUPPORTING INFORMATION

Title: Lewis Acid Catalyzed Intermolecular Olefin Hydroamination: Scope, Limitation, and Mechanism

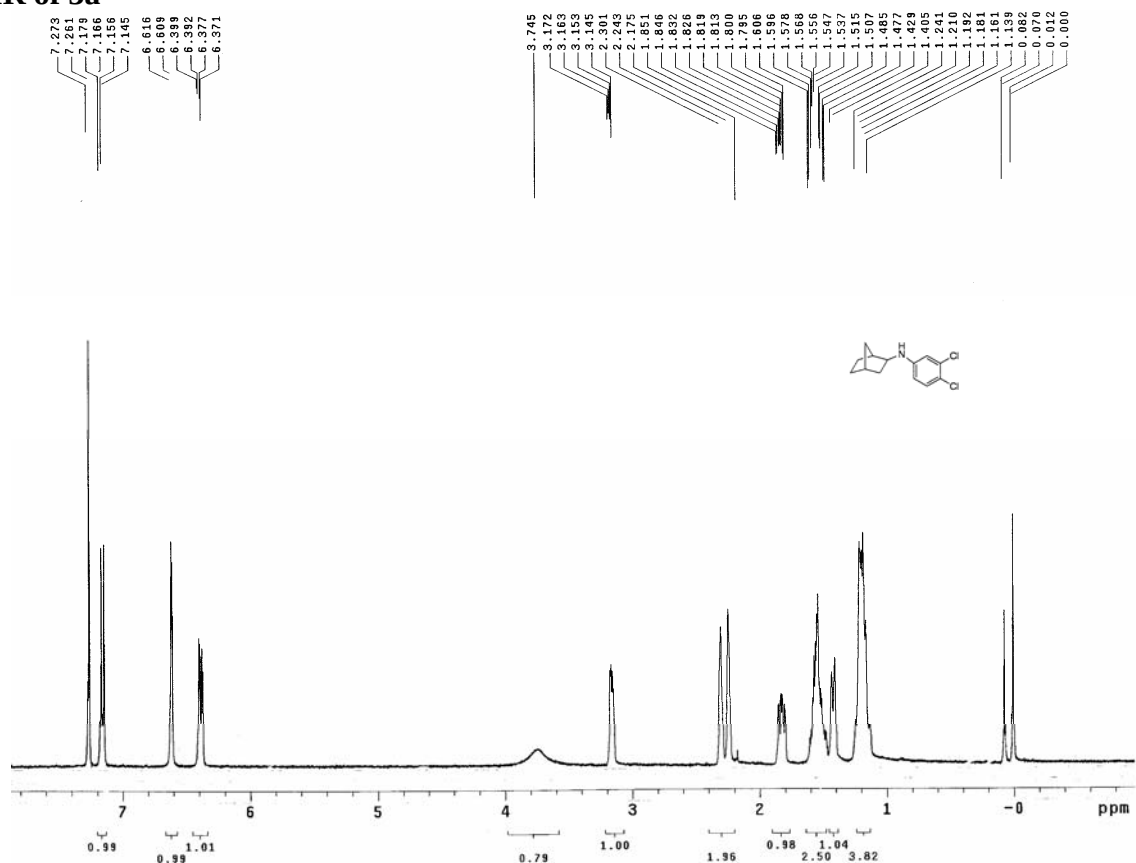
Author(s): Xiaojuan Cheng, Yuanzhi Xia, Hua Wei, Bin Xu, Chongguang Zhang, Yahong Li,* Guimin Qian, Xiaohua Zhang, Kai Li, and Wu Li

Ref. No.: O200701080

***N*-(3, 4-dichlorophenyl)bicyclo[2.2.1]heptan-2-amine (3a)**

¹H NMR (400 MHz, CDCl₃): δ 7.17 (dd, 1H, *J* = 5.2, 4.4 Hz), 6.61 (m, 1H), 6.39 (dd, 1H, *J* = 2.8, 2.4 Hz), 3.74 (s, 1H), 3.16 (m, 1H), 2.30 (s, 1H), 2.24 (s, 1H), 1.83 (m, 1H), 1.61-1.41 (m, 3H), 1.24-1.14 (m, 4H).¹

¹H NMR of 3a

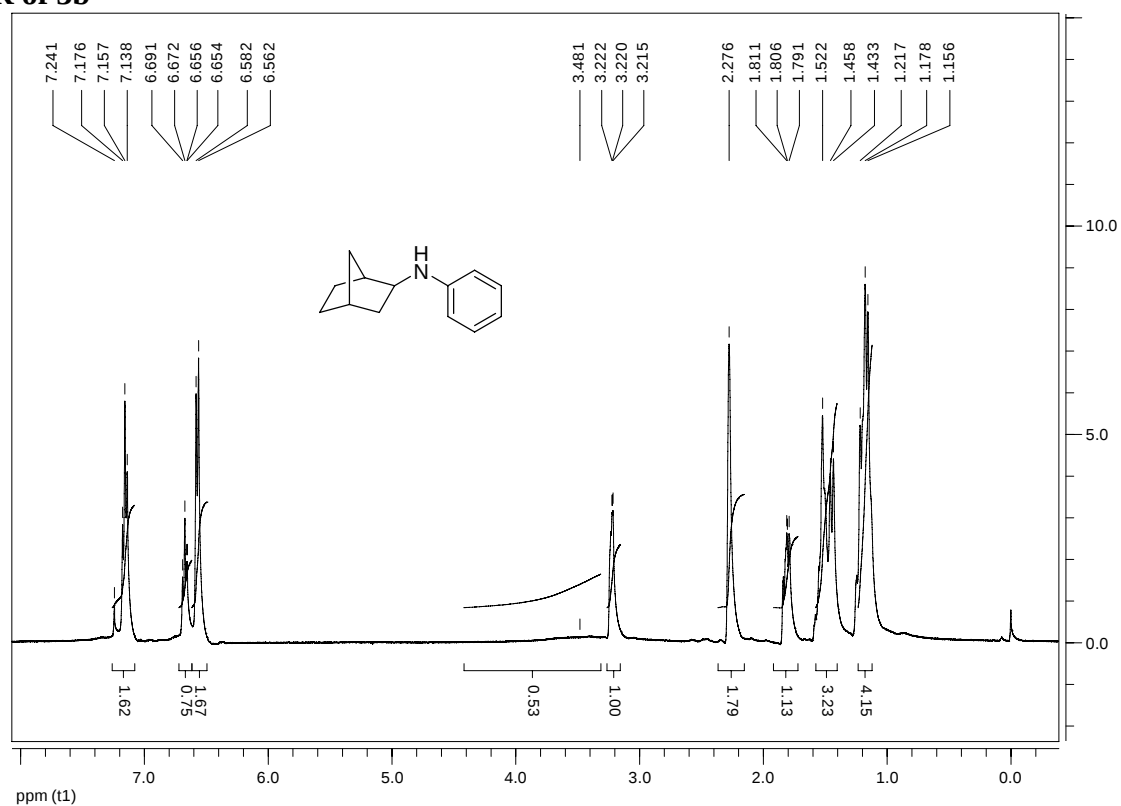


¹ All spectroscopic data of known compounds (**3a-m**) are compared with the reported ones: a) L. Ackermann, L. T. Kaspar, C. J. Gschrei, *Org. Lett.* **2004**, 6, 2515–2518; b) H. Wei, G. Qian, Y. Xia, K. Li, Y. Li, W. Li, *Eur. J. Org. Chem.* **2007**, 4471–4474.

N-phenylbicyclo[2.2.1]heptan-2-amine (3b)

^1H NMR (400 MHz, CDCl_3): δ 7.24-7.14 (m, 2H), 6.69-6.65 (m, 1H), 6.58-6.56 (m, 2H), 3.48 (s, 1H, NH), 3.23-3.22 (m, 1H), 2.27 (s, 2H), 1.84-1.79 (m, 1H), 1.52-1.43 (m, 3H), 1.22-1.16 (m, 4H).

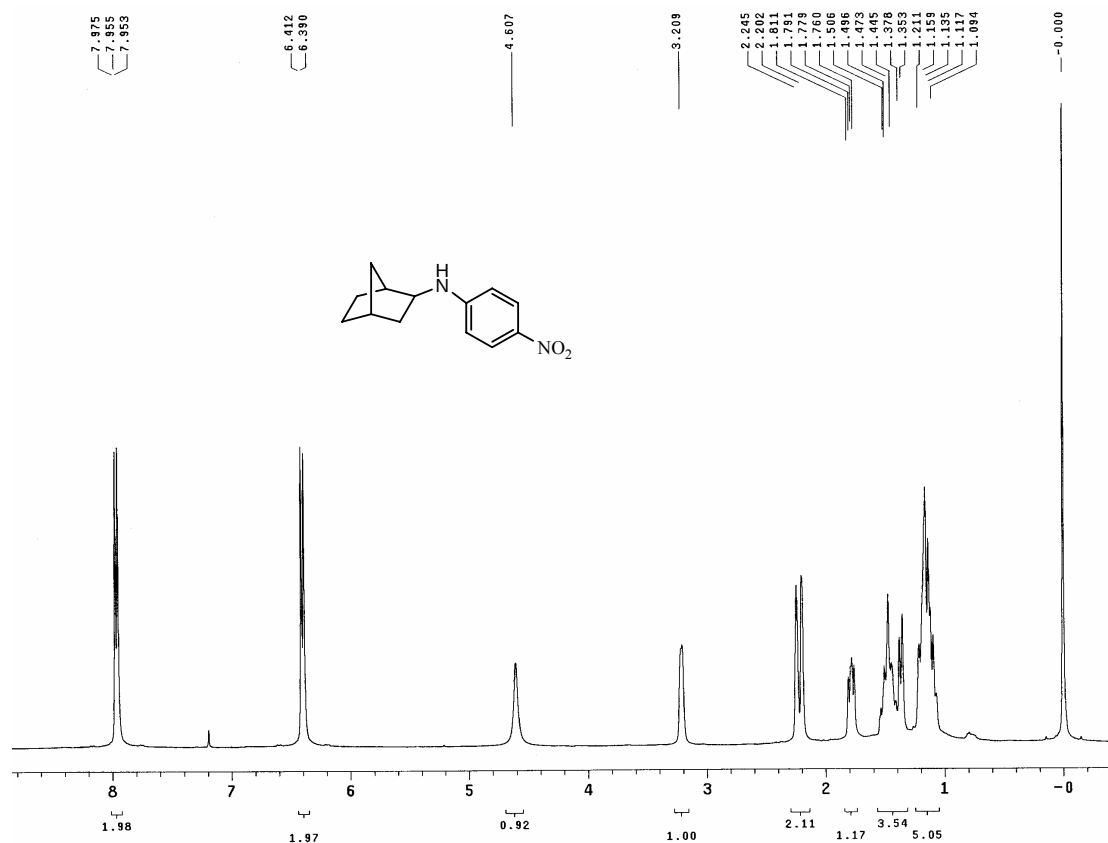
^1H NMR of 3b



***N*-(4-nitrophenyl)bicyclo[2.2.1]heptan-2-amine (3c)**

^1H NMR (400 MHz, CDCl_3): δ 7.86 (t, $J = 8.8$ Hz, 2H), 6.41 (d, $J = 8.8$ Hz, 2H), 4.61 (s, 1H), 3.21 (s, 1H), 2.25 (m, 2H), 1.81-1.76 (dd, $J = 8.0, 7.6$ Hz, 1H), 1.50-1.35 (m, 3H), 1.21-1.09 (m, 4H).

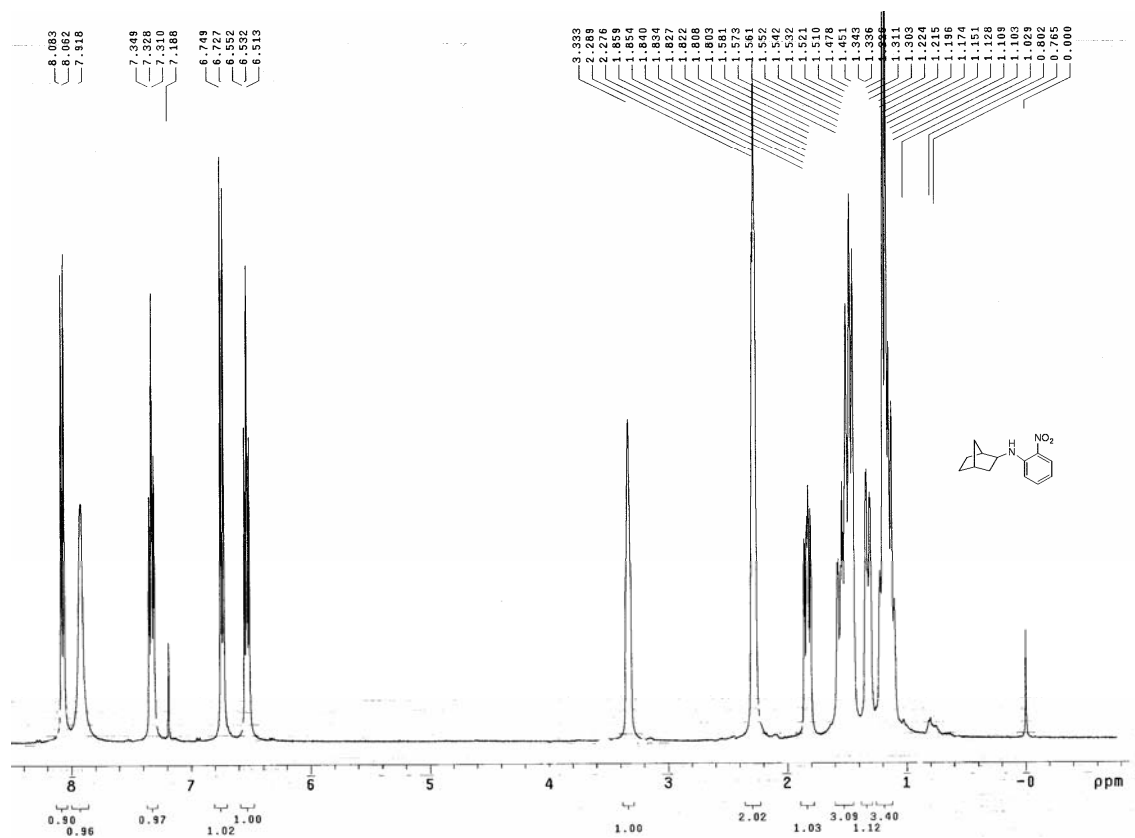
^1H NMR of 3c



***N*-(2-nitrophenyl)bicyclo[2.2.1]heptan-2-amine (3d)**

^1H NMR (400 MHz, CDCl_3): δ 8.06 (d, $J = 8.4$ Hz, 1H), 7.92 (s, 1H), 7.35-7.31 (t, $J = 7.2$ Hz, 1H), 6.75-6.73 (d, $J = 8.8$ Hz, 1H), 6.55-6.51 (t, $J = 8.0$ Hz, 1H), 3.33 (m, 1H), 2.37 (s, 2H), 1.82 (ddd, 1H), 1.58-1.45 (m, 3H), 1.34-1.30 (m, 1H), 1.22-1.10 (m, 3H).

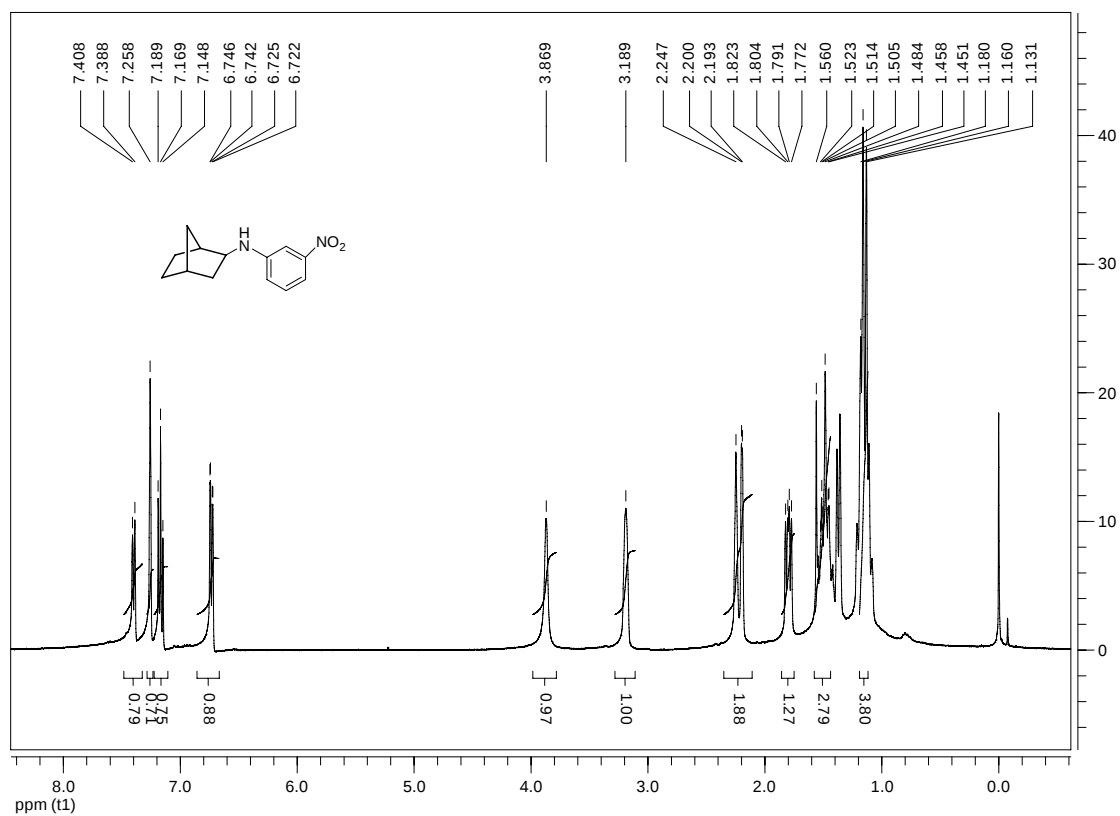
^1H NMR of 3d



***N*-(3-nitrophenyl)bicyclo[2.2.1]heptan-2-amine (3e)**

^1H NMR (400 MHz, CDCl_3): δ 7.41-7.39(d, $J = 8.0$ Hz, 1H), 7.26 (s, 1H), 7.19-7.15 (m, 1H), 6.75-6.72 (m, 1H), 3.87 (s, 1H, NH), 3.19 (s, 1H, CH), 2.19-2.25 (m, 2H, CH_2), 1.82-1.77 (m, 1H, CH), 1.56-1.36 (m, 3H), 1.18-1.13 (m, 4H).

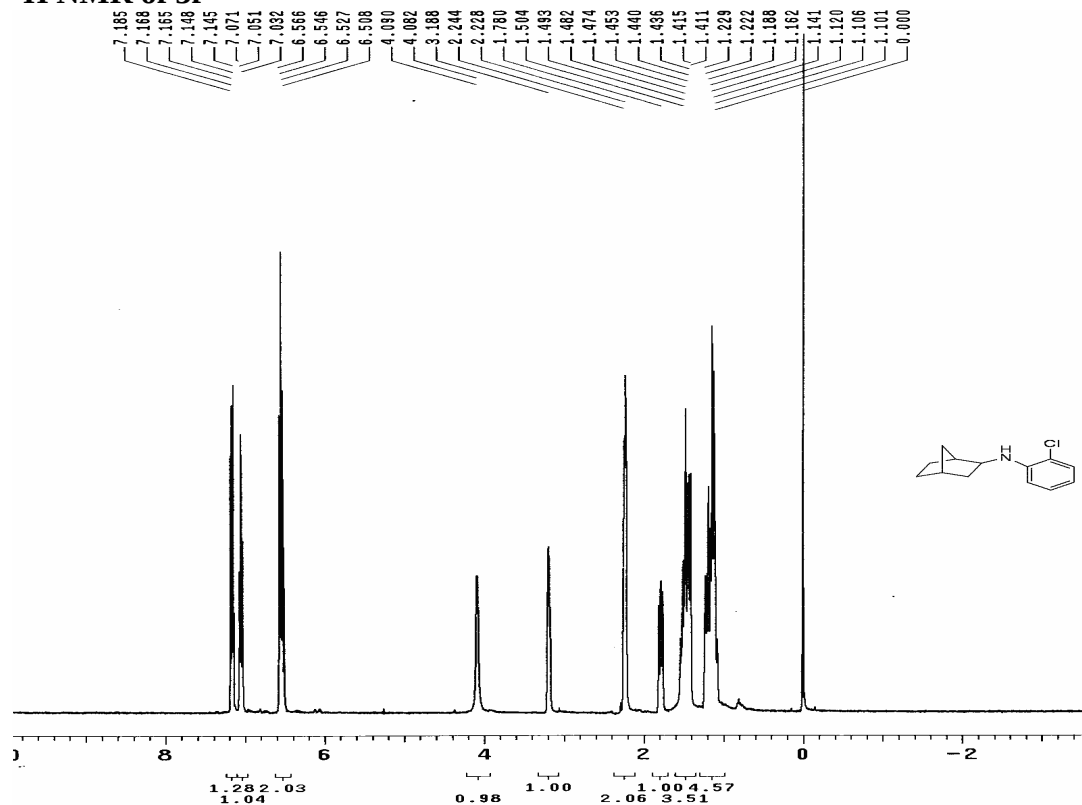
^1H NMR of 3e



***N*-(2-chlorophenyl)bicyclo[2.2.1] heptan-2-amine (3f)**

^1H NMR (400 MHz, CDCl_3): δ 7.19-7.15 (m, 1H), 7.07-7.03 (m, 1H), 6.65-6.57 (m, 2H), 4.09 (s, 1H), 3.19 (m, 1H), 2.23-2.22 (m, 2H), 1.78 (m, 1H), 1.50-1.41 (m, 3H), 1.23-1.10 (m, 4H).

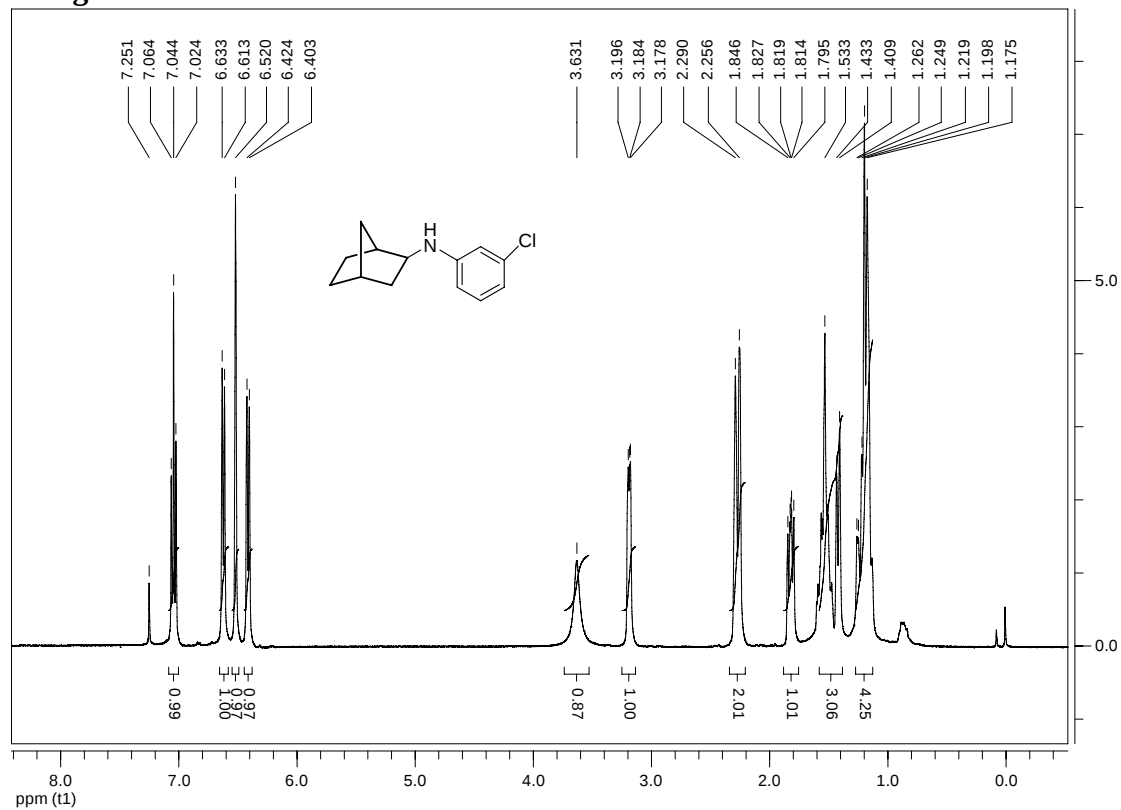
^1H NMR of 3f



***N*-(3-chlorophenyl)bicyclo[2.2.1] heptan-2-amine (3g)**

^1H NMR (400 MHz, CDCl_3): δ 7.06-7.02 (t, $J = 8.0$ Hz, 1H), 6.63-6.61 (d, $J = 8.0$ Hz, 1H), 6.52 (s, 1H), 6.42-6.40 (d, $J = 8.4$ Hz, 1H), 3.63 (s, 1H, NH), 3.20-3.18 (m, 1H), 2.29-2.26 (m, 2H), 1.85-1.80 (m, 1H), 1.53-1.41 (m, 3H), 1.26-1.18 (m, 4H).

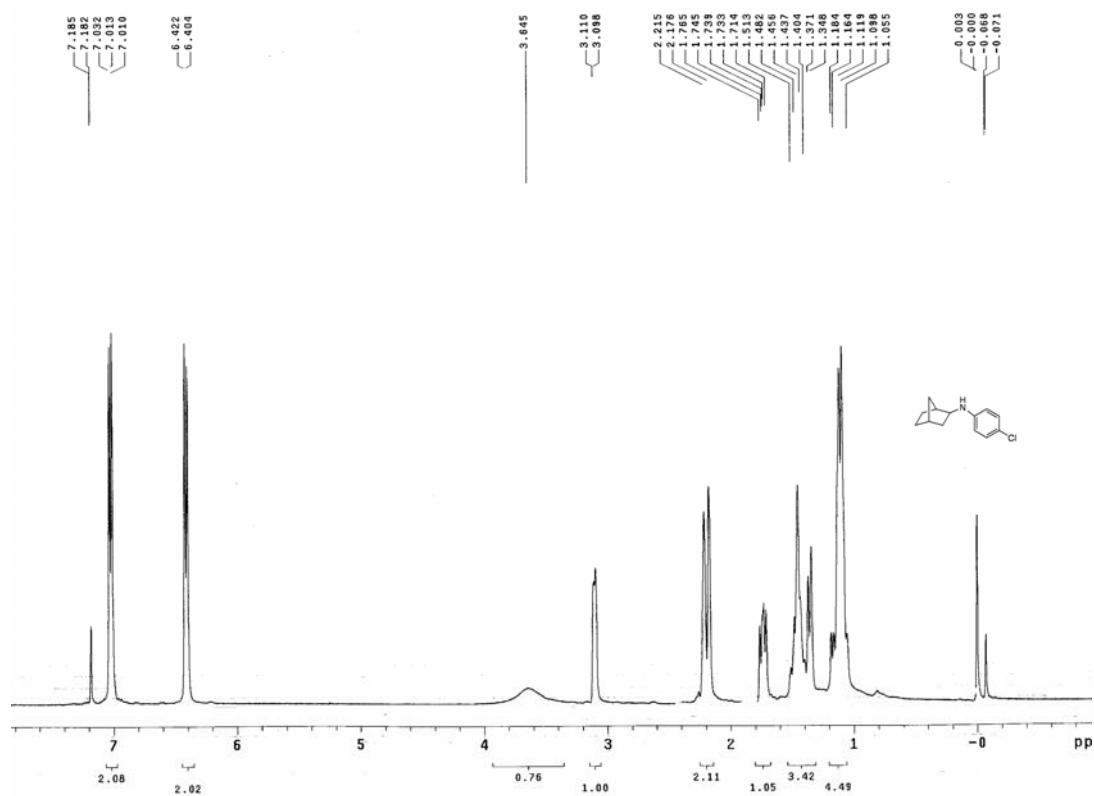
^1H NMR of 3g



***N*-(4-chlorophenyl)bicyclo[2.2.1]heptan-2-amine (3h)**

^1H NMR (400 MHz, CDCl_3): δ 7.03-7.01 (m, 2H), 6.42-6.40 (m, 2H), 3.65 (s, 1H), 3.09 (m, 1H), 2.22 (s, 1H), 2.18 (s, 1H), 1.74 (dd, $J = 8.0, 7.6$, Hz, 1H), 1.51-1.35 (m, 3H), 1.18-1.06 (m, 4H).

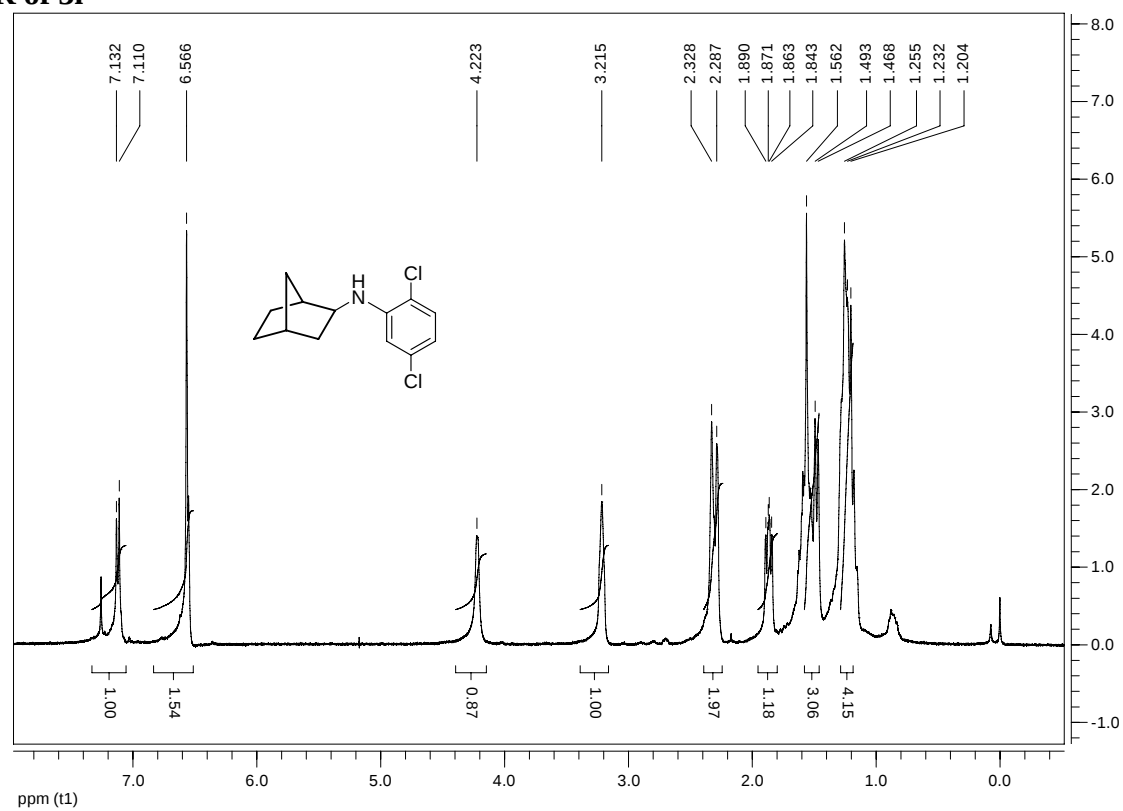
^1H NMR of 3h



***N*-(2,5-dichlorophenyl)bicyclo[2.2.1]heptan-2-amine (3i)**

^1H NMR (400 MHz, CDCl_3): δ 7.26-7.11 (m, 1H), 6.57 (s, 2H), 4.22 (s, 1H, NH), 3.22 (s, 1H), 2.33-2.29 (m, 2H), 1.89-1.84 (m, 1H), 1.56-1.47 (m, 3H), 1.26-1.20 (m, 4H).

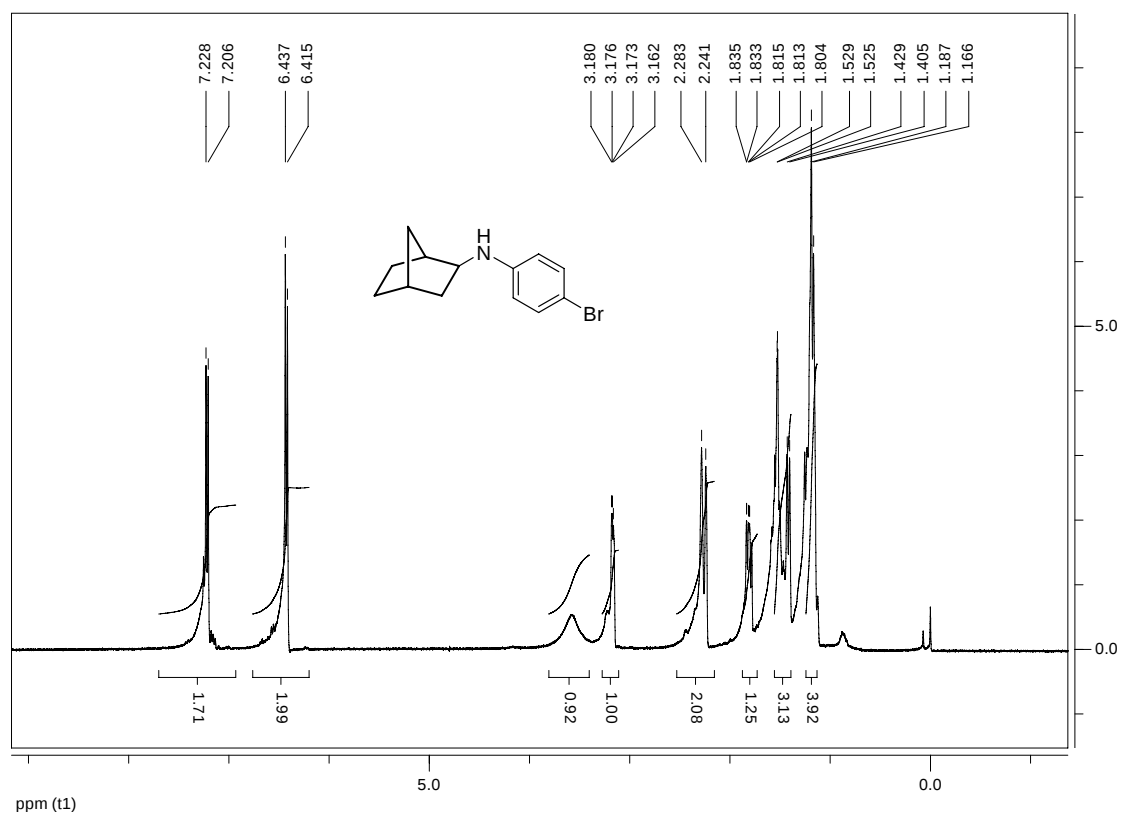
^1H NMR of 3i



***N*-(4-bromophenyl)bicyclo[2.2.1]heptan-2-amine (3j)**

^1H NMR (400 MHz, CDCl_3): δ 7.23-7.21 (d, $J = 8.8$ Hz, 2H), 6.44-6.42 (d, $J = 8.8$ Hz, 2H), 3.62 (s, 1H, NH), 3.16-3.18 (m, 1H, CH), 2.28-2.24 (m, 2H, CH_2), 1.84-1.80 (m, 1H, CH), 1.53-1.41 (m, 3H), 1.19-1.17 (m, 4H).

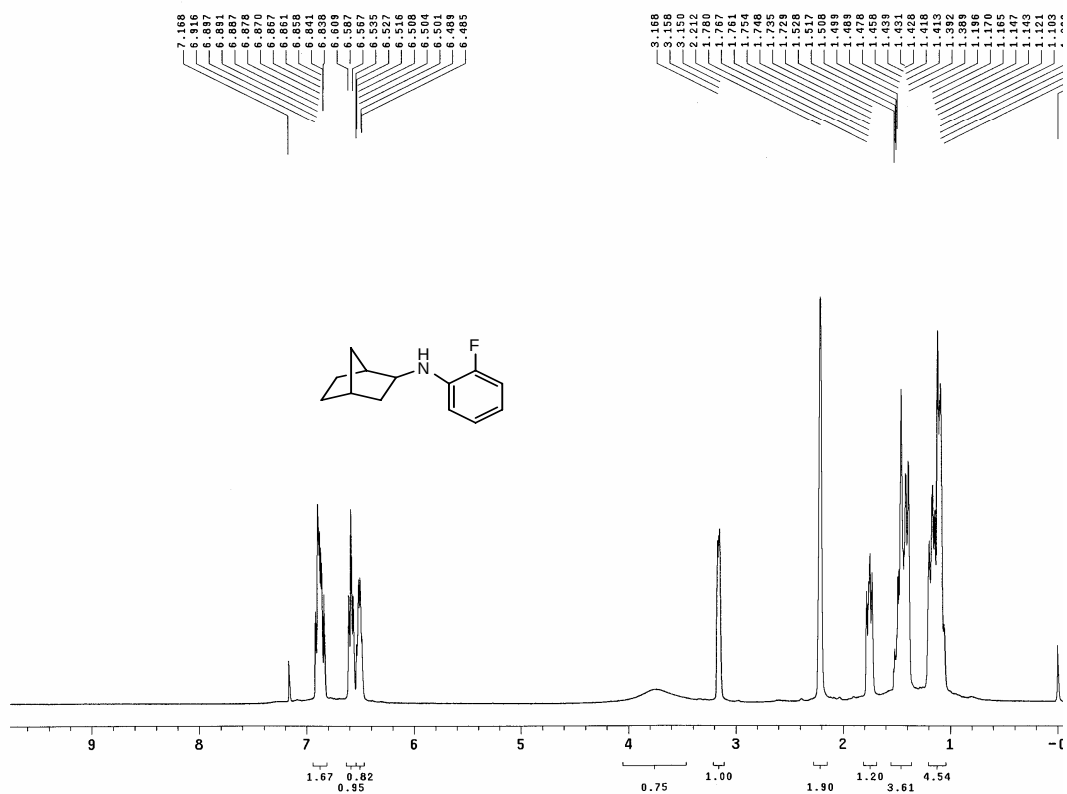
^1H NMR of 3j



***N*-(2-fluorophenyl)bicyclo[2.2.1]heptan-2-amine (3k)**

^1H NMR (400 MHz, CDCl_3): δ 6.92-6.84 (m, 2H), 6.61-6.50 (m, 1H), 6.49-6.48 (d, $J = 1.6$ Hz, 1H), 3.81 (s, 1H, NH), 3.17-3.15 (t, $J = 3.6$ Hz, 1H), 2.21 (s, 2H), 1.78-1.73 (m, 1H), 1.53-1.39 (m, 3H), 1.20-1.06 (m, 4H).

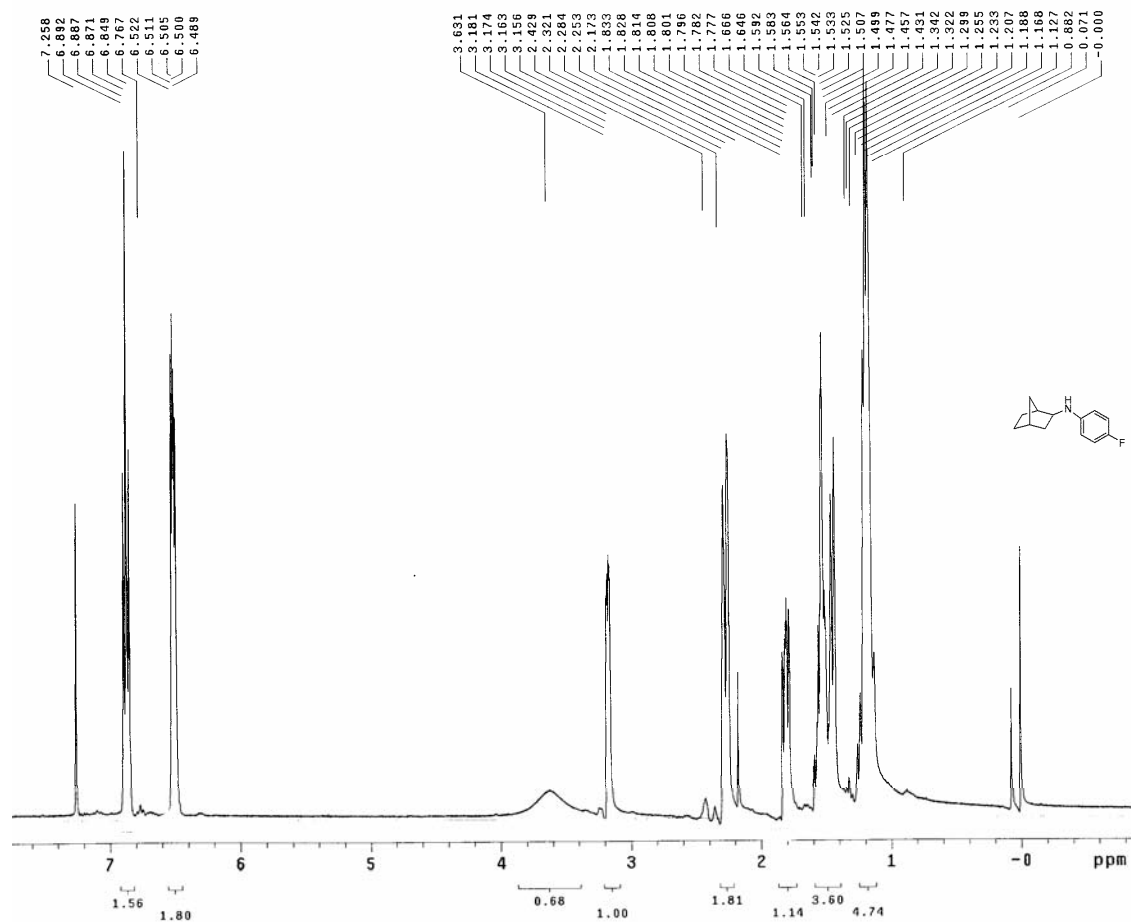
^1H NMR of 3k



***N*-(4-fluorophenyl)bicyclo[2.2.1]heptan-2-amine (3l)**

^1H NMR (400 MHz, CDCl_3): δ 6.87 (dd, $J = 6.4, 8.8$ Hz, 2H), 6.51 (dd, $J = 2.4, 4.4$ Hz, 2H), 3.63 (s, 1H), 3.17 (m, 1H), 2.32 (s, 1H), 2.28 (s, 1H), 1.67-1.43 (m, 3H), 1.34-1.13 (m, 4H).

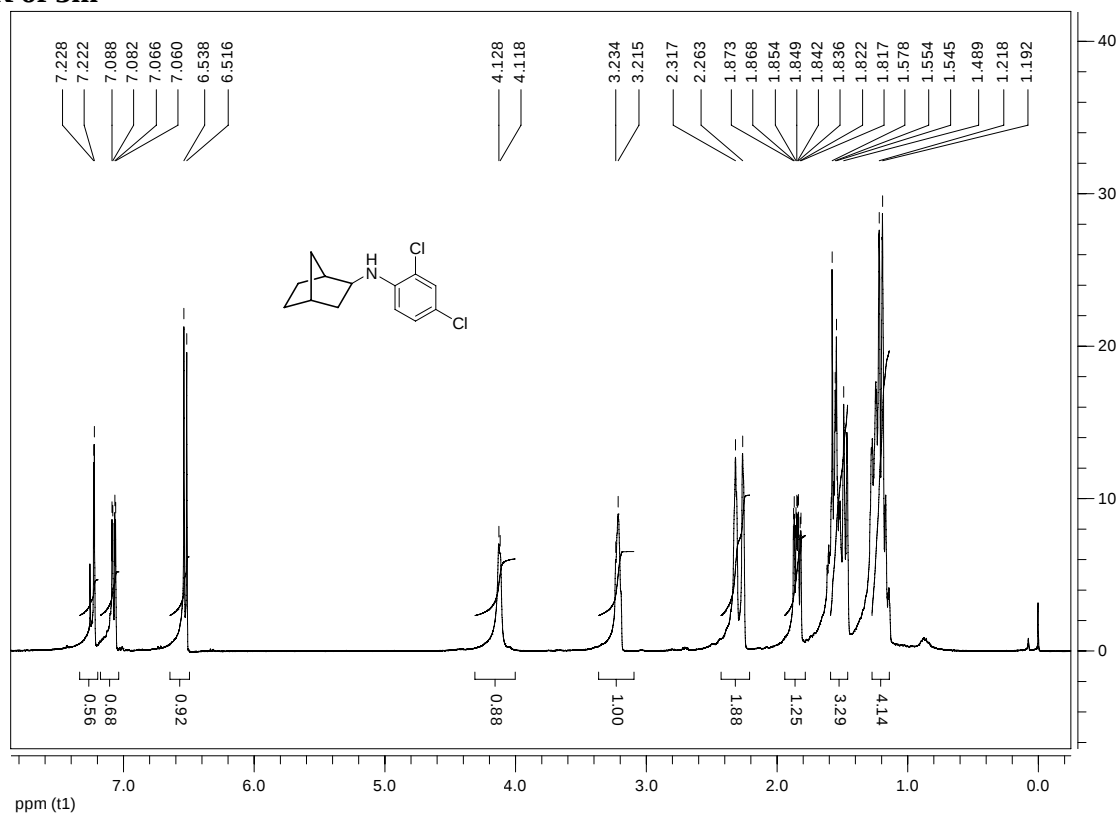
^1H NMR of 3l



***N*-(2,4-dichlorophenyl)bicyclo[2.2.1]heptan-2-amine (3m)**

^1H NMR (400 MHz, CDCl_3): δ 7.23-7.22 (d, $J = 2.4$ Hz, 1H, 3- $\text{C}_6\text{H}_3\text{N}$), 7.09-7.06 (dd, $J = 2.4$, 2.4 Hz, 1H, 5- $\text{C}_6\text{H}_3\text{N}$), 6.54-6.52 (d, $J = 8.8$ Hz, 1H), 4.13 (s, 1H, NH), 3.22 (s, 1H, CH), 2.32-2.26 (d, $J = 21.6$ Hz, 2H), 1.87-1.82 (m, 1H), 1.53-1.40 (m, 3H), 1.22-1.07 (m, 4H).

^1H NMR of 3m

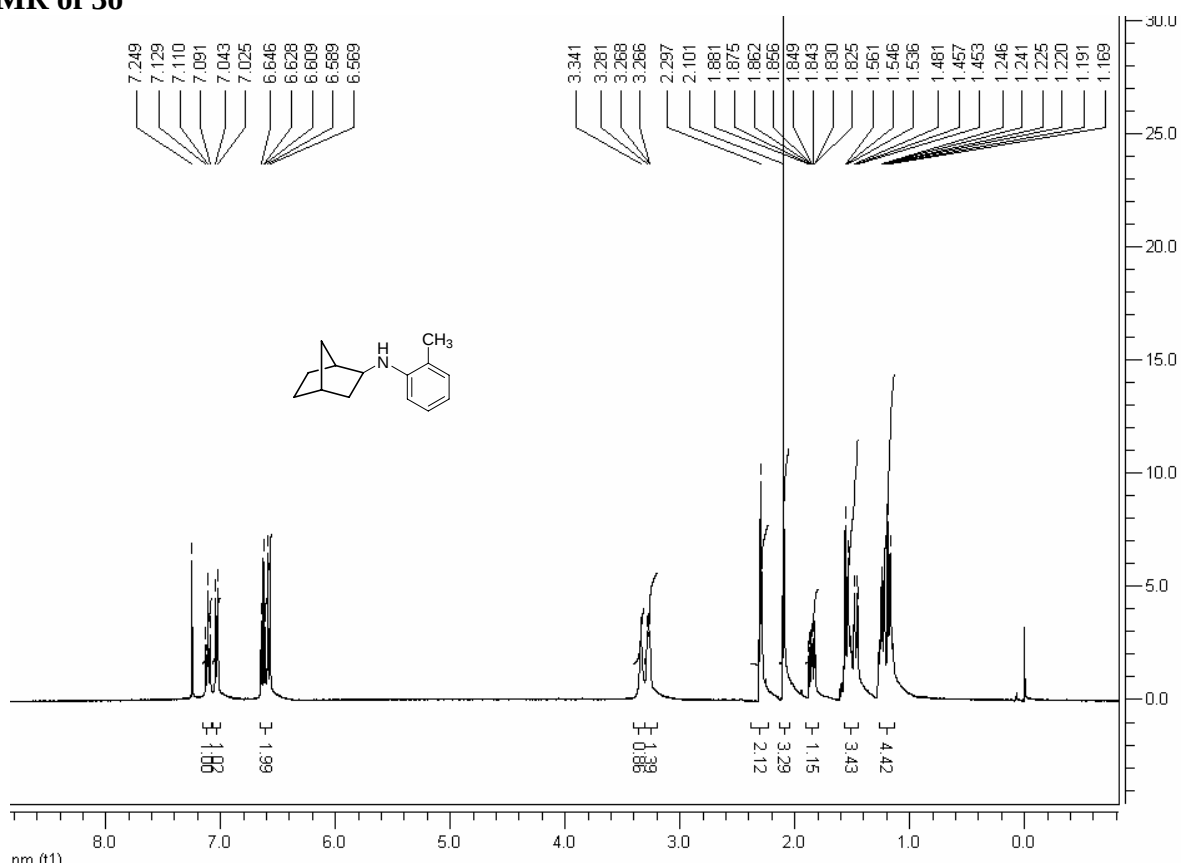


***N*-o-tolybicyclo[2.2.1]heptan-2-amine (3o)**

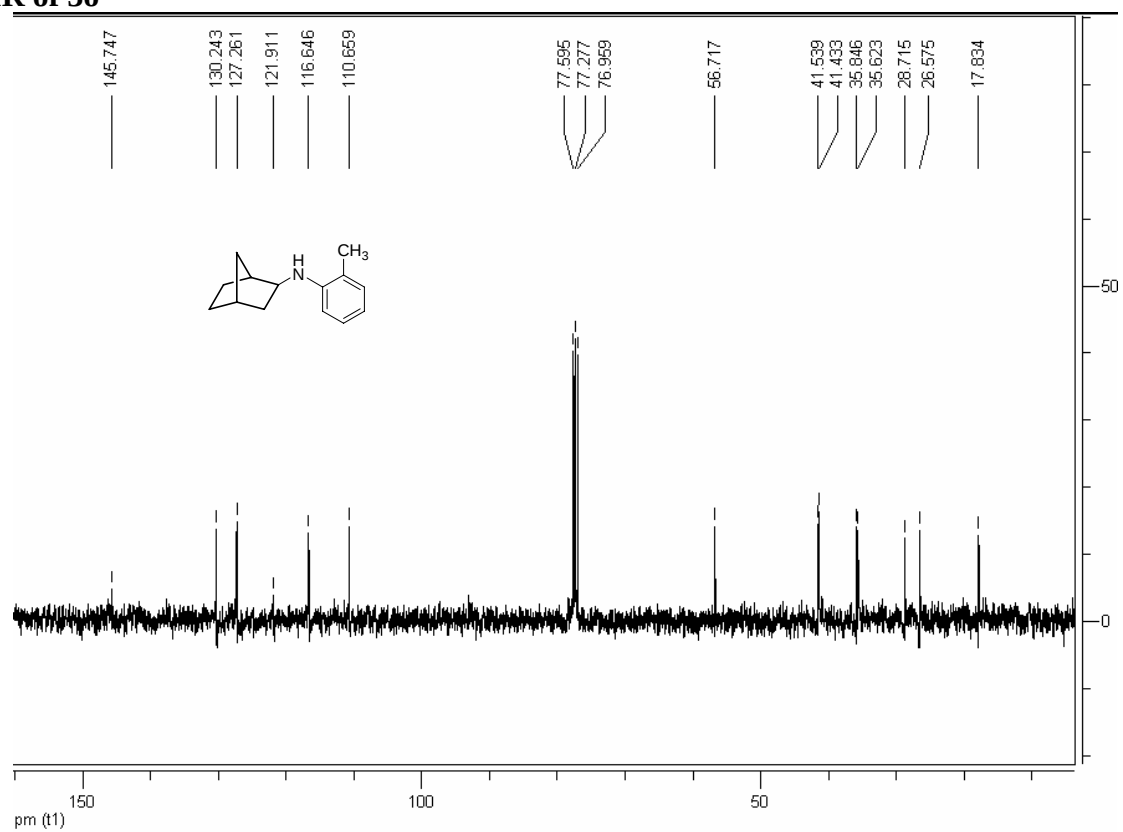
^1H NMR (400 MHz, CDCl_3): δ 7.13-7.09 (t, 1H), 7.04-7.02 (d, 1H, $J = 7.2$ Hz), 6.65-6.56 (m, 2H), 3.34 (s, 1H, NH), 3.28-3.27 (m, 1H, CH), 2.29 (s, 2H, CH_2), 2.10 (s, CH_3), 1.88-1.82 (m, 1H), 1.55-1.45 (m, 3H), 1.24-1.17 (m, 4H).

^{13}C -NMR (100 MHz, CDCl_3): δ 145.75 (C), 130.24 (CH), 127.26 (CH), 121.91 (C), 116.65 (CH), 110.66 (CH), 56.72 (CH), 41.54 (CH), 41.43 (CH_2), 35.85 (CH_2), 35.62 (CH), 28.72 (CH_2), 26.58 (CH_2), 17.83 (CH_3). HR-MS (EI) m/z calcd for $\text{C}_{14}\text{H}_{19}\text{N}$ 201.1517, found 201.1527.

^1H NMR of 3o



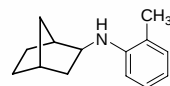
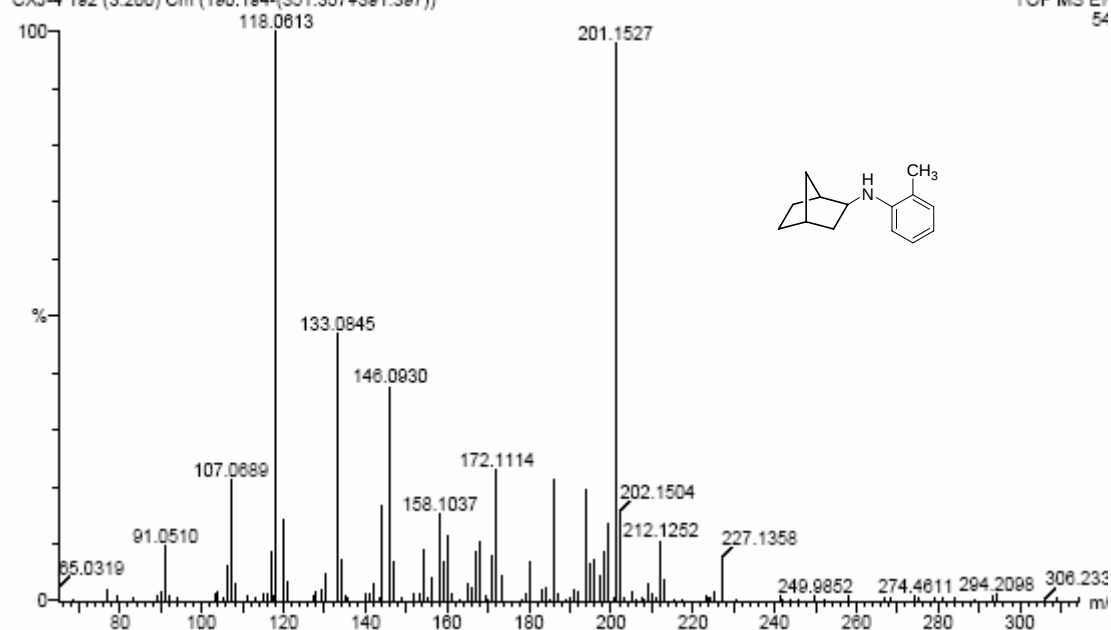
¹³C NMR of 3o



MS of 3o

EI+20071211
CXJ-4 192 (3.200) Cm (190:194-(351:357+391:397))

TOF MS EI
54

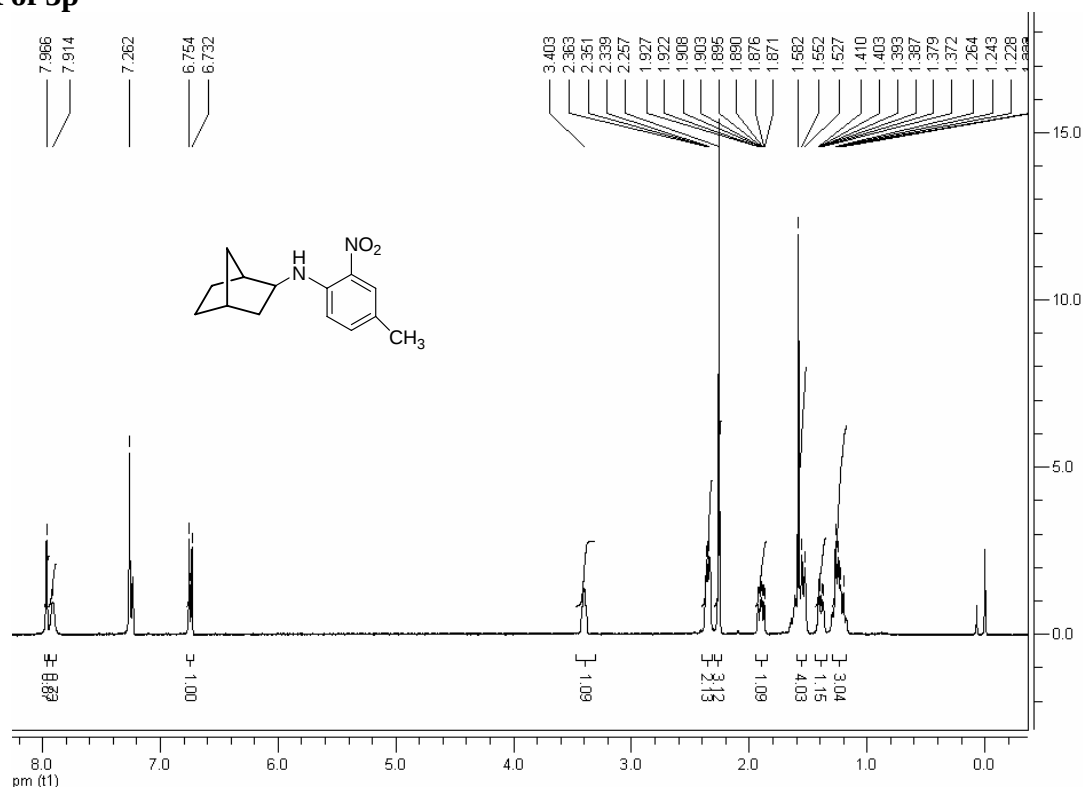


Minimum:	5.00				-1.5		
Maximum:	100.00		10.0	5.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	Score	Formula
91.0510	9.52	91.0548	-3.8	-41.5	4.5	2	C7 H7
		91.0422	8.8	96.7	5.0	1	C6 H5 N
106.0628	6.16	106.0657	-2.9	-27.1	4.5	1	C7 H8 N
107.0689	21.15	107.0735	-4.6	-43.0	4.0	1	C7 H9 N
117.0531	8.40	117.0578	-4.7	-40.6	6.0	1	C8 H7 N
118.0613	100.00	118.0657	-4.4	-37.1	5.5	1	C8 H8 N
133.0845	46.75	133.0891	-4.6	-34.9	5.0	1	C9 H11 N
144.0780	16.60	144.0813	-3.3	-23.1	6.5	1	C10 H10 N
146.0930	37.54	146.0970	-4.0	-27.2	5.5	1	C10 H12 N
154.0632	8.77	154.0657	-2.5	-16.1	8.5	1	C11 H8 N
158.1037	15.31	158.1096	-5.9	-37.0	6.0	1	C12 H14
		158.0970	6.7	42.5	6.5	2	C11 H12 N
159.0998	6.90	159.1048	-5.0	-31.4	6.0	1	C11 H13 N
160.1105	11.21	160.1126	-2.1	-13.3	5.5	1	C11 H14 N
167.0760	8.40	167.0735	2.5	15.0	9.0	1	C12 H9 N
168.0843	10.10	168.0813	3.0	17.7	8.5	1	C12 H10 N
		168.0939	-9.6	-57.1	8.0	2	C13 H12
171.1003	7.65	171.1048	-4.5	-26.3	7.0	1	C12 H13 N
172.1114	22.99	172.1126	-1.2	-7.1	6.5	1	C12 H14 N
180.0939	6.54	180.0939	0.0	0.0	9.0	1	C14 H12
186.1301	21.09	186.1283	1.8	9.8	6.5	1	C13 H16 N
194.0952	19.41	194.0970	-1.8	-9.1	9.5	1	C14 H12 N
196.1059	7.29	196.1126	-6.7	-34.3	8.5	1	C14 H14 N
198.1295	8.40	198.1283	1.2	6.2	7.5	1	C14 H16 N
199.1371	13.47	199.1361	1.0	5.0	7.0	1	C14 H17 N
201.1527	97.84	201.1517	1.0	4.7	6.0	1	C14 H19 N

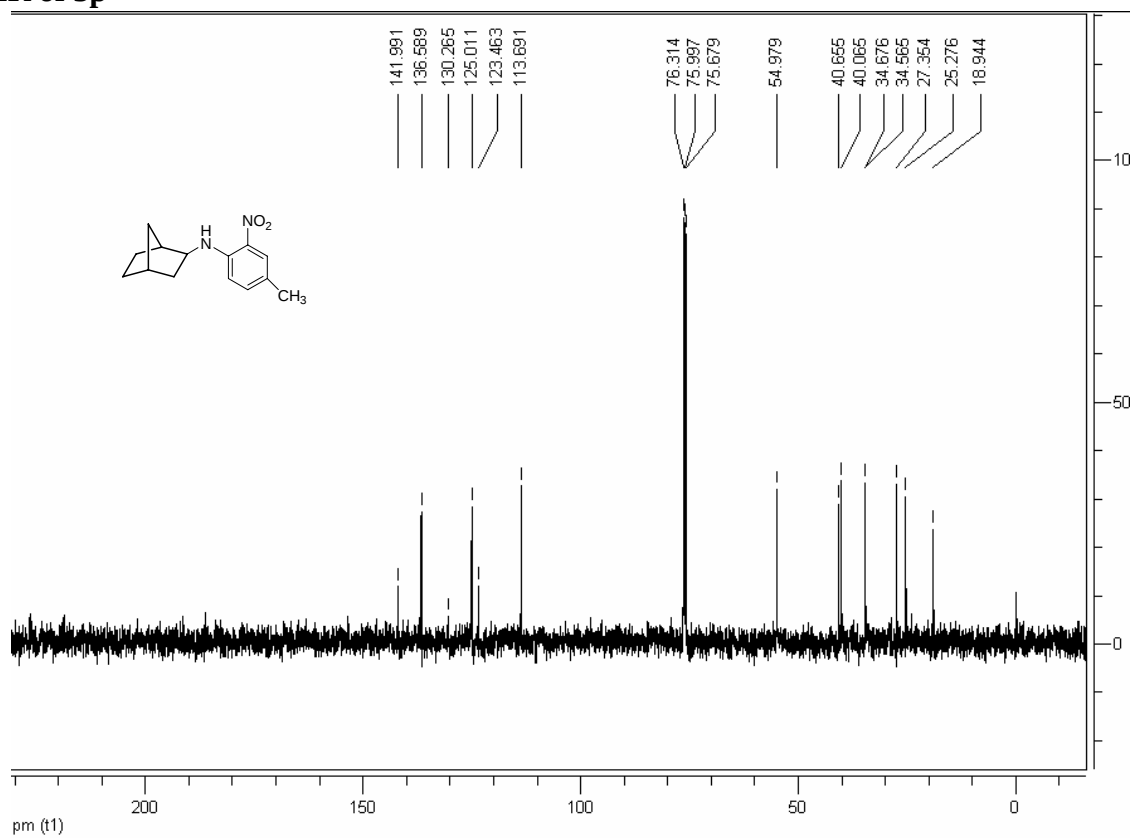
***N*-(4-methyl-2-nitrophenyl)bicyclo[2.2.1]heptan-2-amine (3p)**

^1H NMR (400 MHz, CDCl_3): δ 7.97 (s, 1H), 7.91 (s, 1H), 6.75-6.73 (d, $J = 8.8$ Hz, 1H), 3.40 (s, 1H, NH), 2.36-2.34 (m, 2H), 2.26 (s, 3H, CH_3), 1.93-1.87 (m, 1H, CH), 1.58-1.53 (m, 4H), 1.41-1.37 (m, 1H), 1.26-1.20 (m, 3H). ^{13}C -NMR (100 MHz, CDCl_3): δ 141.99 (CH), 136.59 (C), 130.27 (C), 125.01 (C), 123.46 (CH), 113.69 (CH), 54.98 (CH), 40.66 (CH), 40.07 (CH_2), 34.68 (CH_2), 34.57 (CH), 27.35 (CH_2), 25.28 (CH_2), 18.94 (CH_3). HR-MS (EI) m/z calcd for $\text{C}_{14}\text{H}_{18}\text{N}_2\text{O}_2$ 246.1368, found 246.1376

^1H NMR of 3p



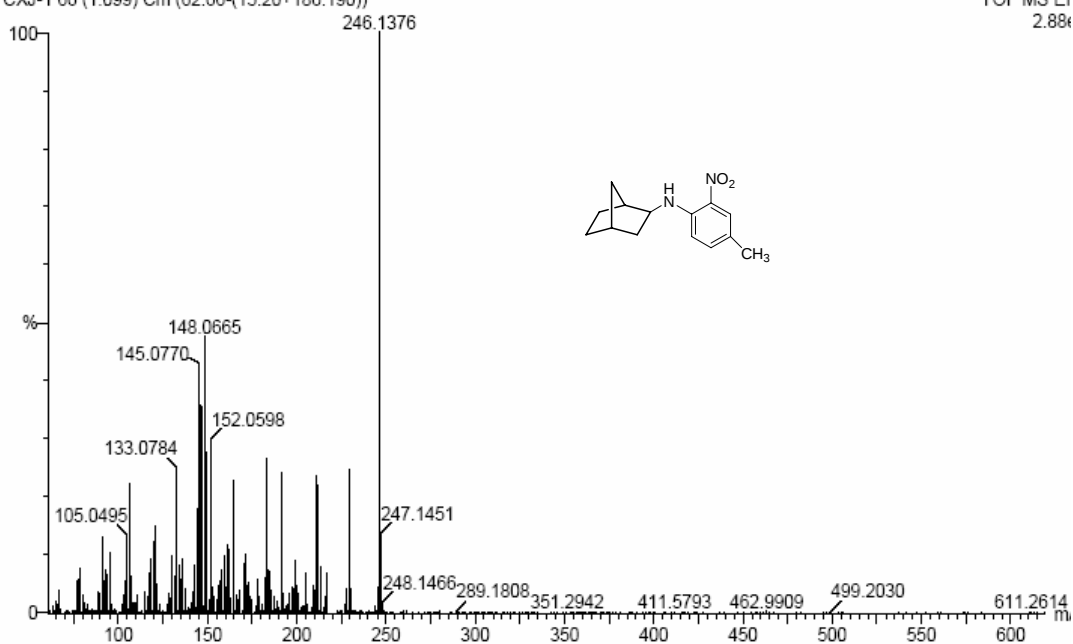
¹³C NMR of 3p



MS of 3p

El+071207
CXJ-1 66 (1.099) Cm (62:66-(15:20+186:190))

TOF MS EI
2.88t



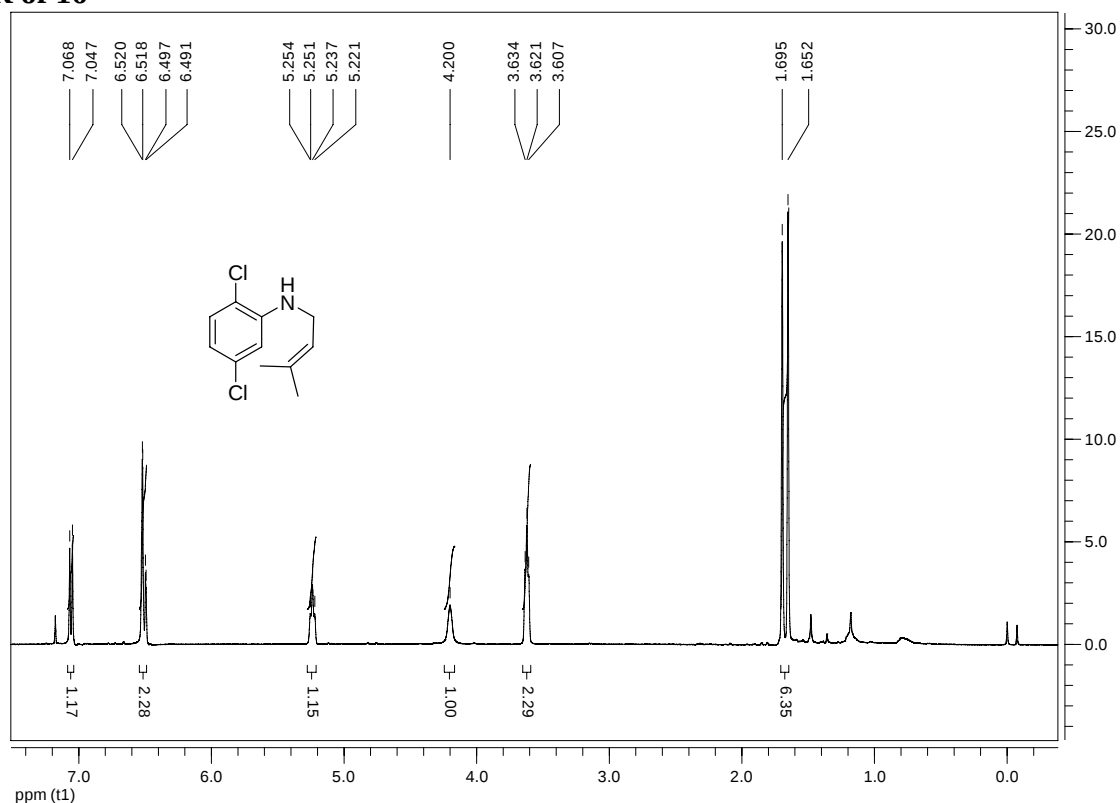
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Maximum:	100.00		5.0	5.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	Score	Formula
133.0784	24.68	133.0766	1.8	13.7	5.5	1	C8 H9 N2
134.0645	8.16	134.0606	3.9	29.2	5.5	1	C8 H8 N O
135.0583	5.65	135.0558	2.5	18.2	5.5	1	C7 H7 N2
							O
136.0653	9.05	136.0637	1.6	12.0	5.0	1	C7 H8 N2
							O
137.0730	4.04	137.0715	1.5	11.0	4.5	1	C7 H9 N2
							O
142.0684	3.52	142.0657	2.7	19.2	7.5	1	C10 H8 N
143.0730	7.90	143.0735	-0.5	-3.5	7.0	1	C10 H9 N
144.0831	17.76	144.0813	1.8	12.3	6.5	1	C10 H10 N
145.0770	42.90	145.0766	0.4	2.9	6.5	1	C9 H9 N2
146.0856	35.78	146.0844	1.2	8.2	6.0	1	C9 H10 N2
148.0665	47.48	148.0637	2.8	19.2	6.0	1	C8 H8 N2
							O
149.0737	27.59	149.0715	2.2	14.8	5.5	1	C8 H9 N2
							O
152.0598	29.69	152.0586	1.2	8.0	5.0	2	C7 H8 N2
							O2
		152.0626	-2.8	-18.4	9.0	1	C12 H8
153.0670	4.16	153.0664	0.6	3.9	4.5	2	C7 H9 N2
							O2
		153.0704	-3.4	-22.4	8.5	1	C12 H9
154.0708	2.62	154.0742	-3.4	-22.2	4.0	1	C7 H10 N2

156.0890	4.59	156.0899	-0.9	-5.6	3.0	2	O2 C7	H12	N2
		156.0939	-4.9	-31.4	7.0	1	O2 C12	H12	
157.0852	5.15	157.0891	-3.9	-25.1	7.0	1	C11	H11	N
158.0962	7.15	158.0970	-0.8	-4.9	6.5	1	C11	H12	N
159.0956	9.67	159.0922	3.4	21.2	6.5	1	C10	H11	N2
160.0842	4.21	160.0888	-4.6	-28.8	6.0	1	C11	H12	O
161.0748	11.46	161.0715	3.3	20.6	6.5	1	C9	H9	N2
							O		
162.0744	10.68	162.0793	-4.9	-30.3	6.0	1	C9	H10	N2
							O		
163.0786	2.30	163.0759	2.7	16.5	5.5	1	C10	H11	O2
165.0688	22.66	165.0704	-1.6	-9.8	9.5	1	C13	H9	
		165.0664	2.4	14.5	5.5	2	C8	H9	N2
							O2		
166.0737	2.90	166.0742	-0.5	-3.2	5.0	2	C8	H10	N2
							O2		
		166.0783	-4.6	-27.4	9.0	1	C13	H10	
167.0799	2.04	167.0821	-2.2	-12.9	4.5	1	C8	H11	N2
							O2		
168.0833	3.83	168.0813	2.0	11.8	8.5	1	C12	H10	N
170.0942	8.36	170.0970	-2.8	-16.3	7.5	1	C12	H12	N
171.1001	10.03	171.1048	-4.7	-27.5	7.0	1	C12	H13	N
172.0992	4.58	172.1000	-0.8	-4.9	7.0	1	C11	H12	N2
173.1114	5.04	173.1079	3.5	20.4	6.5	1	C11	H13	N2
174.0891	2.68	174.0919	-2.8	-16.0	6.5	1	C11	H12	N
							O		
178.0789	5.69	178.0783	0.6	3.6	10.0	1	C14	H10	
		178.0742	4.7	26.2	6.0	2	C9	H10	N2
							O2		
179.0855	2.52	179.0861	-0.6	-3.2	9.5	1	C14	H11	
		179.0821	3.4	19.2	5.5	2	C9	H11	N2
							O2		
183.0951	26.40	183.0922	2.9	15.7	8.5	1	C12	H11	N2
184.1045	7.24	184.1000	4.5	24.2	8.0	1	C12	H12	N2
185.1126	6.81	185.1079	4.7	25.5	7.5	1	C12	H13	N2
186.1149	3.79	186.1157	-0.8	-4.3	7.0	1	C12	H14	N2
187.1006	2.52	187.0997	0.9	4.7	7.0	1	C12	H13	N
							O		
191.0865	23.95	191.0821	4.4	23.3	6.5	1	C10	H11	N2
							O2		
192.0886	3.13	192.0899	-1.3	-6.7	6.0	1	C10	H12	N2
							O2		
197.1115	4.24	197.1079	3.6	18.4	8.5	1	C13	H13	N2
198.1284	3.90	198.1283	0.1	0.6	7.5	1	C14	H16	N
199.1099	8.72	199.1123	-2.4	-12.0	7.5	1	C14	H15	O
200.1286	4.64	200.1313	-2.7	-13.7	7.0	1	C13	H16	N2
201.1416	3.22	201.1392	2.4	12.1	6.5	1	C13	H17	N2
211.1281	23.41	211.1235	4.6	21.7	8.5	1	C14	H15	N2
212.1337	21.82	212.1313	2.4	11.1	8.0	1	C14	H16	N2
213.1435	7.65	213.1392	4.3	20.3	7.5	1	C14	H17	N2
229.1375	24.46	229.1341	3.4	14.9	7.5	1	C14	H17	N2
							O		
230.1410	3.92	230.1419	-0.9	-4.0	7.0	1	C14	H18	N2
							O		
246.1376	100.00	246.1368	0.8	3.1	7.0	1	C14	H18	N2
							O2		

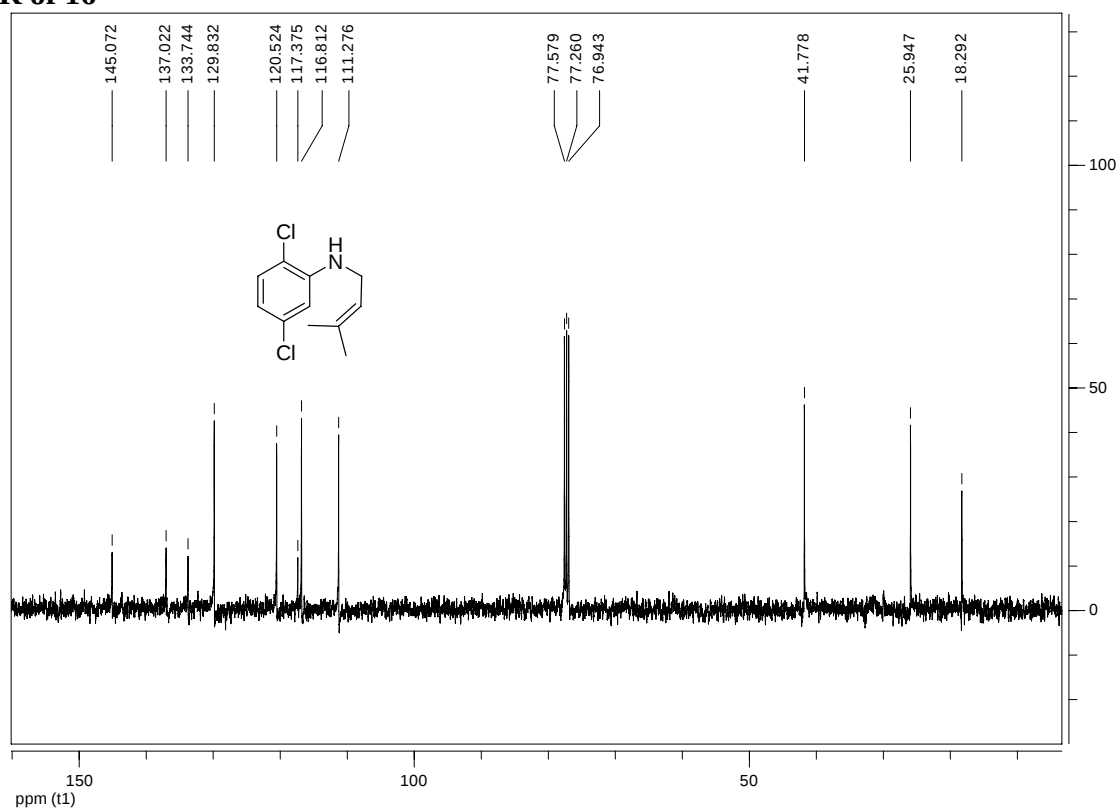
2,5-dichloro-*N*-(2-methylprop-1-enyl)benzenamine (16)

^1H NMR (400 MHz, CDCl_3): δ 7.07-7.05 (d, $J = 8.4$ Hz, 1H), 6.52-6.49 (m, 2H), 5.25-5.22 (t, $J = 6.4$ Hz, 1H), 4.20 (s, 1H, NH), 3.63-3.61 (t, $J = 6.4$ Hz, 2H), 1.70-1.65 (d, $J = 17.2$ Hz, 6H). ^{13}C NMR (100 MHz, CDCl_3): δ 145.07 (1- $\text{C}_6\text{H}_3\text{NCl}_2$), 137.02 (2- $\text{C}_6\text{H}_3\text{NCl}_2$), 133.74 (5- $\text{C}_6\text{H}_3\text{NCl}_2$), 129.83 (6- $\text{C}_6\text{H}_3\text{NCl}_2$), 120.52 (3- $\text{C}_6\text{H}_3\text{NCl}_2$), 117.38 (4- $\text{C}_6\text{H}_3\text{NCl}_2$), 116.81 ($\text{C}_6\text{H}_3\text{NCl}_2\text{NHCH}_2\text{CHC}$), 111.28 ($\text{C}_6\text{H}_3\text{NCl}_2\text{NHCH}_2\text{CH}$), 41.78 ($\text{C}_6\text{H}_3\text{NCl}_2\text{NHCH}_2$), 25.95 ($\text{C}_6\text{H}_3\text{NCl}_2\text{NHCH}_2\text{CHCCH}_3$), 18.29 ($\text{C}_6\text{H}_3\text{NCl}_2\text{NHCH}_2\text{CHCCH}_3$). HR-MS (EI) m/z calcd for $\text{C}_{11}\text{H}_{13}\text{NCl}_2$ 229.0425, found 229.0434.

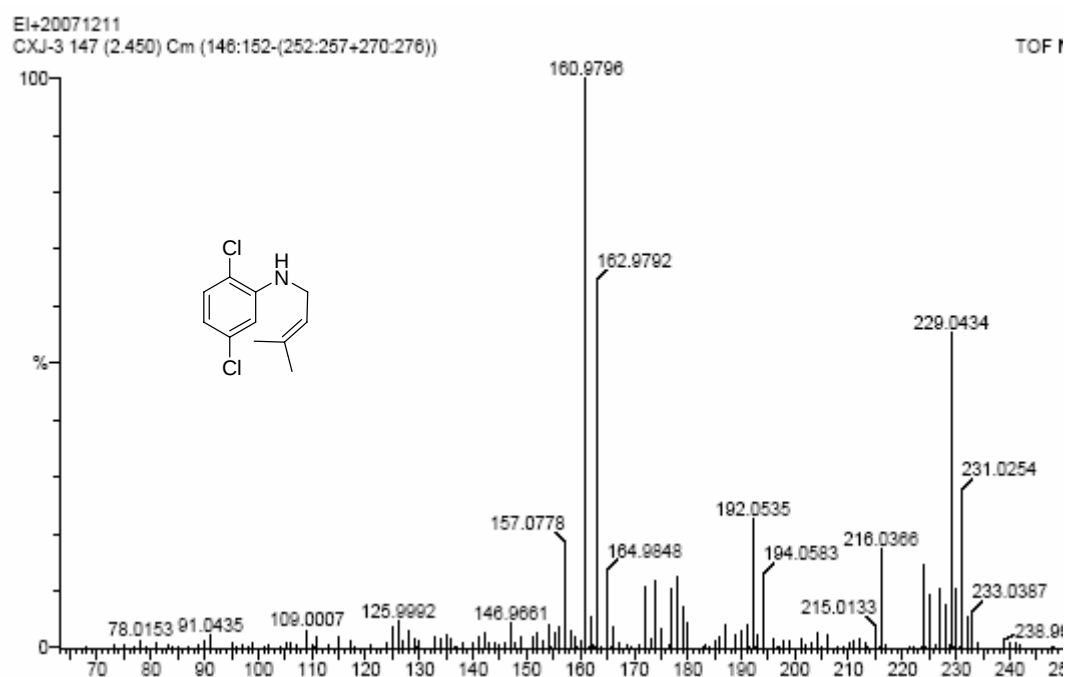
^1H NMR of 16



¹³C NMR of 16



MS of 16



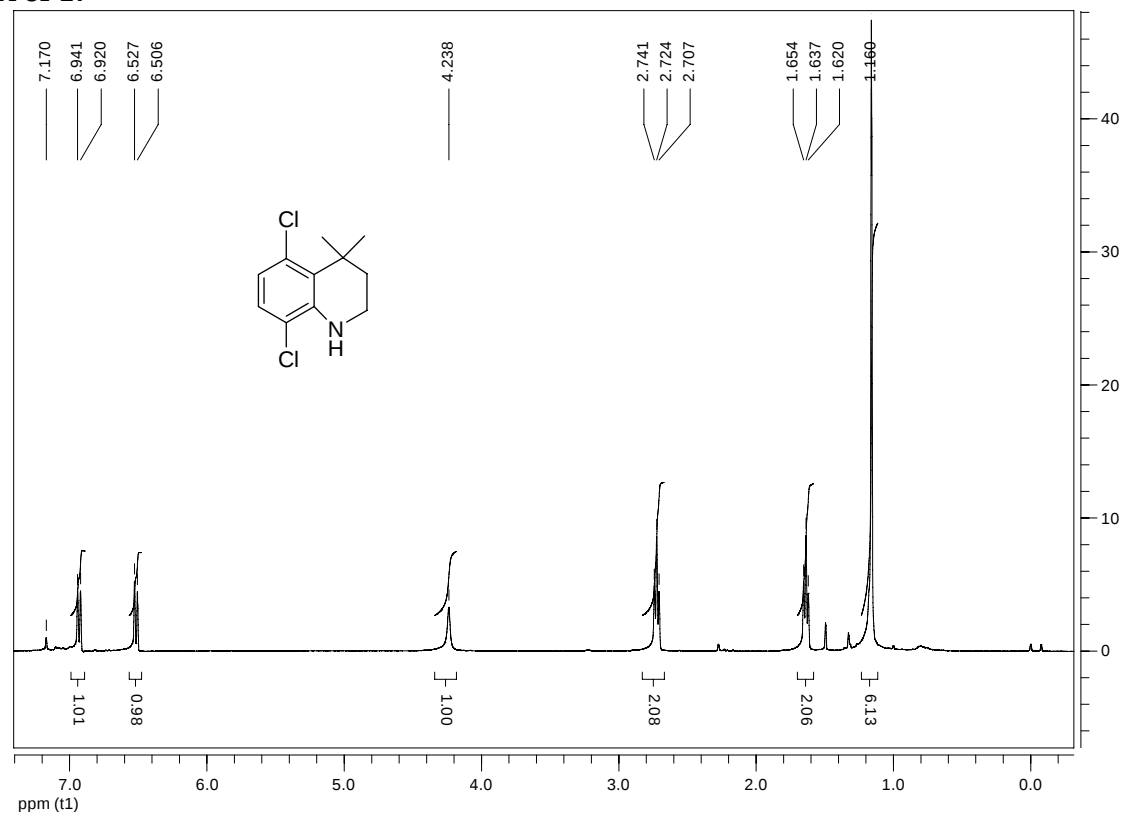
Minimum:	5.00				-1.5		
Maximum:	100.00		5.0	5.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	Score	Formula
160.9796	100.00	160.9799	-0.3	-1.9	4.0	1	C6 H5 N 35Cl2
161.9850	5.31	161.9877	-2.7	-16.9	3.5	1	C6 H6 N 35Cl2
		161.9817	3.3	20.3	4.0	2	C7 H6 3 37Cl
162.9792	64.29	162.9770	2.2	13.8	4.0	1	C6 H5 N 35Cl 37C
164.9848	13.56	164.9866	-1.8	-10.8	3.5	1	C7 H7 37Cl2
		164.9819	2.9	17.8	-1.5	2	C4 H10 35Cl2 37
171.9729	10.50	171.9721	0.8	4.8	5.5	1	C7 H4 N 35Cl2
		171.9768	-3.9	-22.7	10.5	2	C10 H N 37Cl
173.9790	11.53	173.9817	-2.7	-15.6	5.0	1	C8 H6 3 37Cl
177.0379	10.21	177.0345	3.4	19.1	7.0	1	C10 H8 35Cl
178.0364	12.43	178.0363	0.1	0.4	7.0	2	C11 H9 37Cl
		178.0316	4.8	26.9	2.0	1	C8 H12

179.0402	7.15	179.0394	0.8	4.3	1.5	1	35C12
							C8 H13
		179.0442	-4.0	-22.1	6.5	2	35C12
							C11 H10
192.0535	22.41	192.0580	-4.5	-23.4	6.5	1	37C1
							C11 H11 N
194.0583	12.81	194.0551	3.2	16.7	6.5	1	35C1
							C11 H11 N
216.0366	17.14	216.0347	1.9	8.9	4.5	1	37C1
							C10 H12 N
224.0051	14.51	224.0034	1.7	7.7	7.5	1	35C12
							C11 H8 N
229.0434	55.24	229.0425	0.9	3.9	5.0	1	35C12
							C11 H13 N
231.0254	27.62	231.0210	4.4	19.2	6.0	1	35C12
							C11 H11 N
233.0387	6.18	233.0366	2.1	9.0	5.0	1	37C12
							C11 H13 N
							37C12

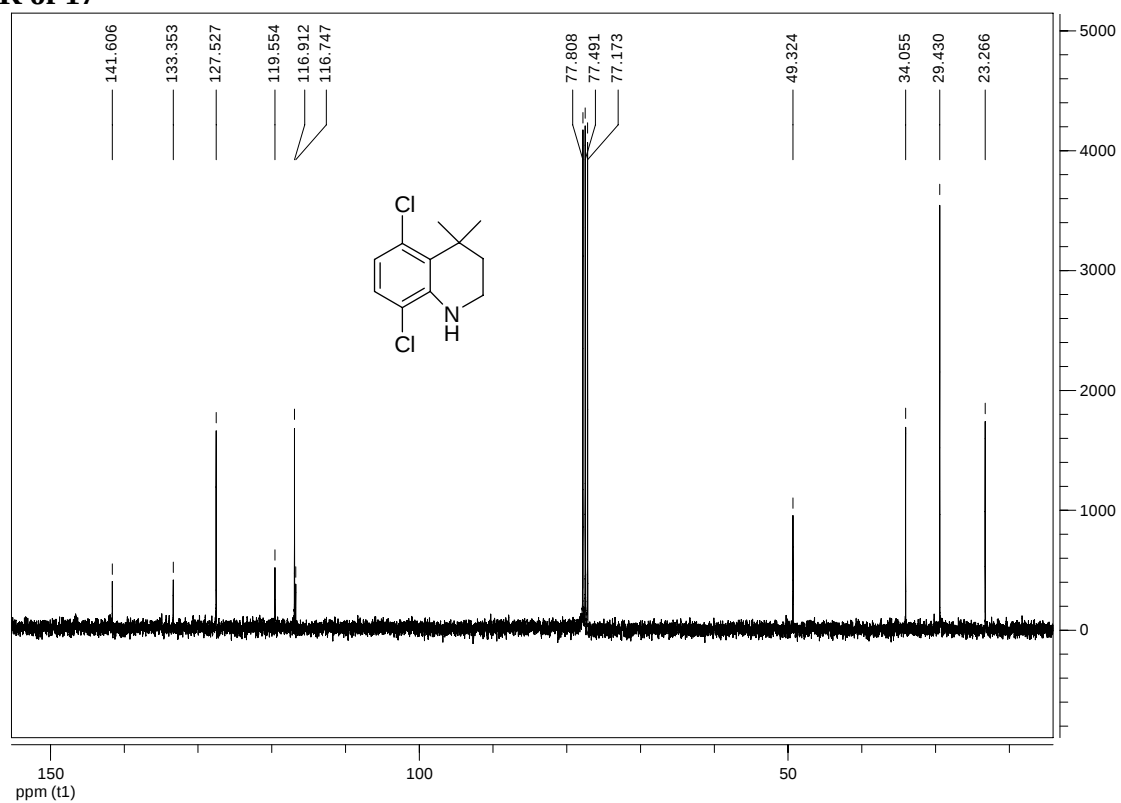
5,8-dichloro-1,2,3,4-tetrahydro-4,4-dimethylquinoline (17)

^1H NMR (400 MHz, CDCl_3): δ 6.94-6.92 (d, $J = 8.4$ Hz, 1H), 6.53-6.51 (d, $J = 8.4$ Hz, 1H), 4.24 (s, 1H, NH), 2.74-2.71 (t, $J = 6.8$ Hz, 2H), 1.65-1.62 (t, $J = 6.8$ Hz, 2H), 1.16 (s, 6H). ^{13}C NMR (100 MHz, CDCl_3): δ 141.61 (C9), 133.36 (C10), 127.53 (C5), 119.55 (C7), 116.91 (C8), 116.75 (C6), 49.32 (C3), 34.06 (C2), 29.43 (C4- CH_3), 23.27 (C4- CH_3). HR-MS (EI) m/z calcd for $\text{C}_{11}\text{H}_{13}\text{NCl}_2$ 229.0425, found 229.0418.

^1H NMR of 17



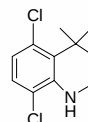
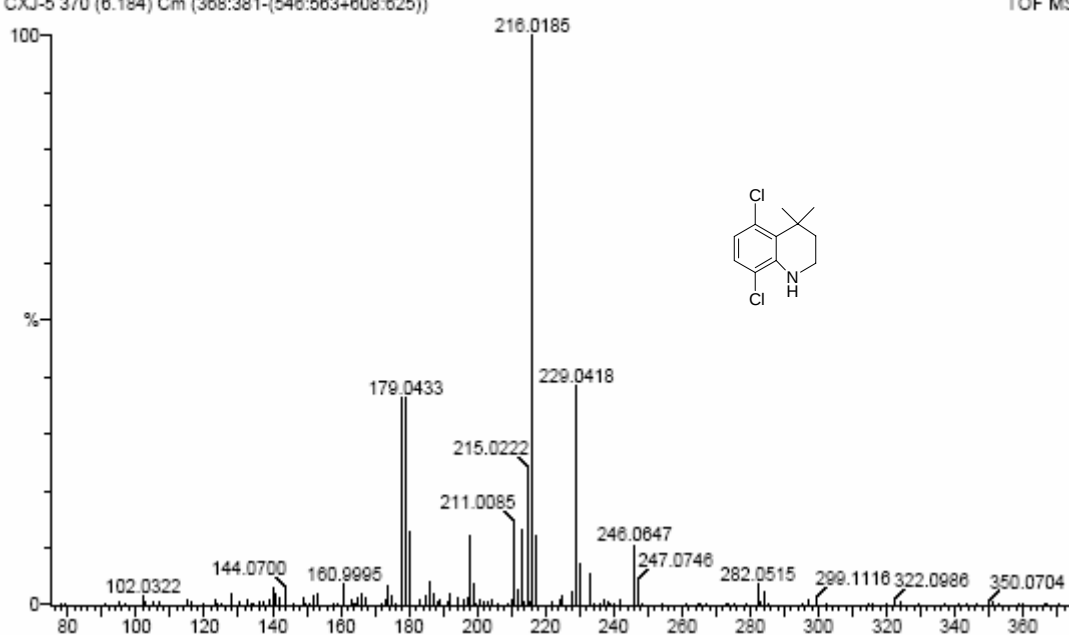
¹³C NMR of 17



MS of 17

El+20071212
CXJ-5 370 (6.184) Cm (368:381-(546:563+608:625))

TOF MS



Minimum:	1.00				-1.5		
Maximum:	100.00		5.0	5.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	Score	Formula
102.0322	1.37	102.0344	-2.2	-21.3	6.5	1	C7 H4 N
128.0518	1.94	128.0500	1.8	13.9	7.5	1	C9 H6 N
140.0378	2.85	140.0393	-1.5	-10.6	4.0	1	C8 H9 35Cl
144.0700	2.96	144.0706	-0.6	-4.0	2.0	1	C8 H13 35Cl
152.0464	1.37	152.0500	-3.6	-23.8	9.5	1	C11 H6 N
153.0119	1.71	153.0112	0.7	4.5	1.0	2	C5 H9 N
		153.0159	-4.0	-26.3	6.0	1	C8 H6 N
160.9995	3.54	160.9972	2.3	14.3	8.5	1	C10 H4 37Cl
		161.0032	-3.7	-23.1	8.0	2	C9 H4 N
165.0207	1.28	165.0238	-3.1	-18.7	1.5	1	C7 H11 35Cl
		165.0159	4.8	28.9	7.0	2	C9 H6 N
166.0546	1.83	166.0549	-0.3	-2.0	5.0	1	C10 H11 35Cl
167.0082	1.03	167.0083	-0.1	-0.3	2.0	1	C6 H9 N
173.9937	3.31	173.9925	1.2	7.2	9.5	1	C10 H3 N

