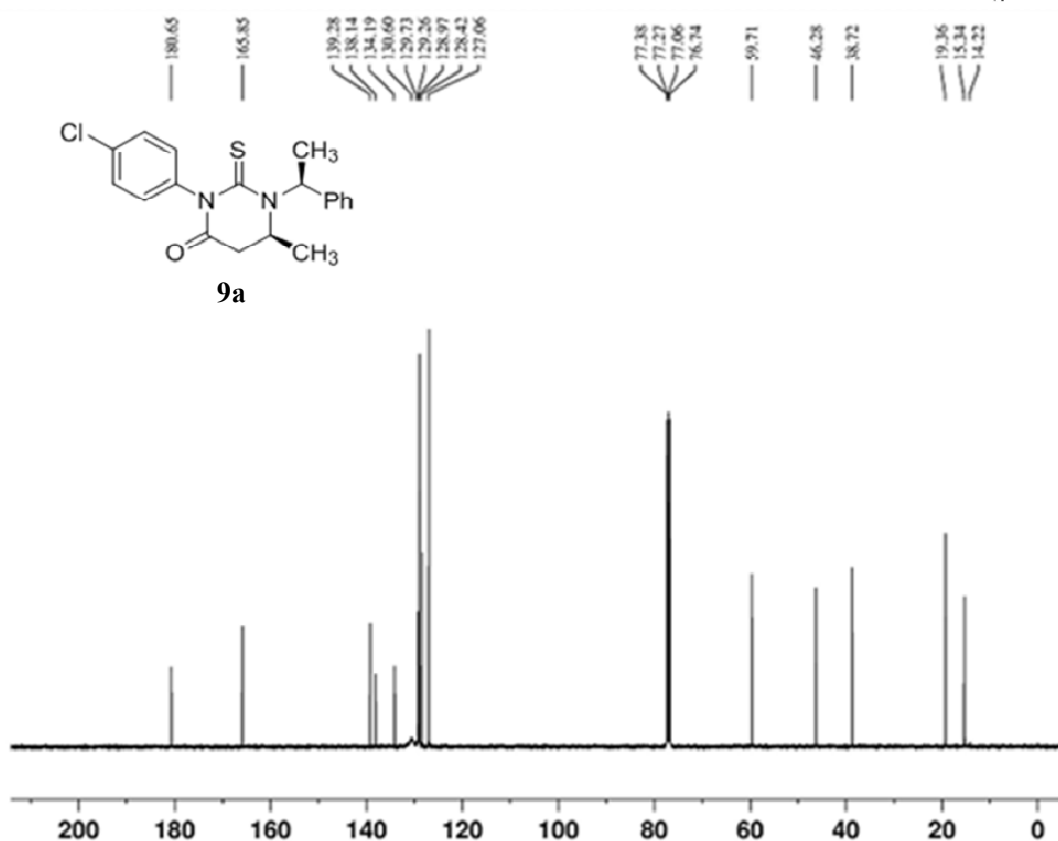
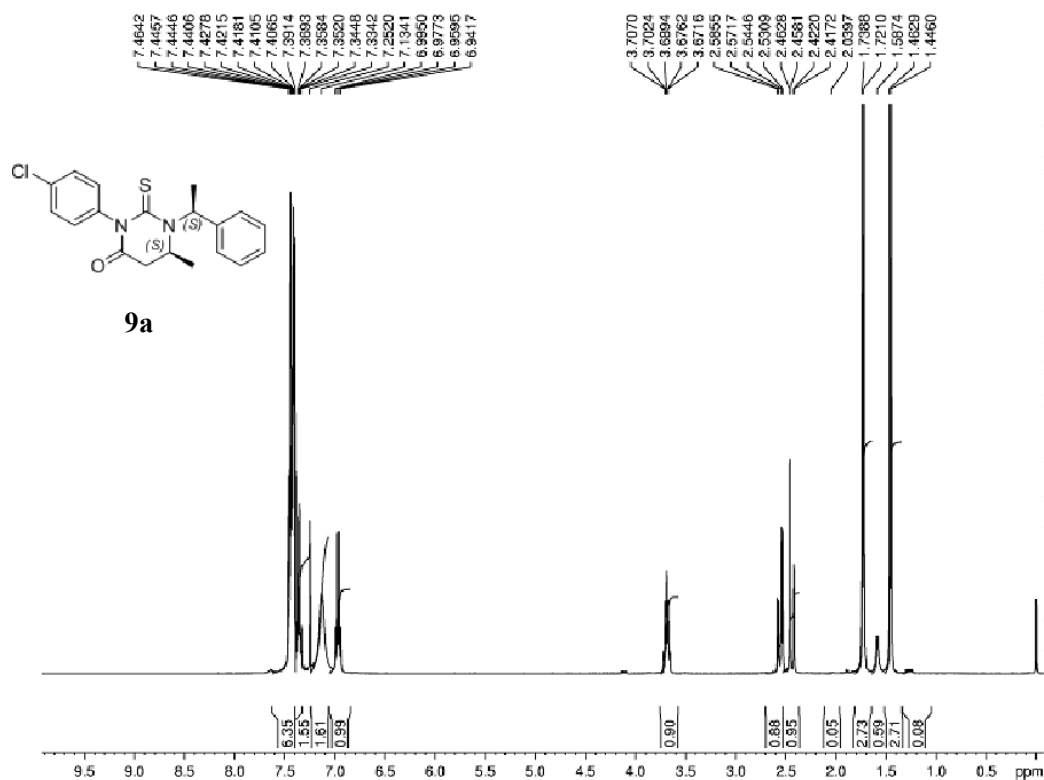


Supporting Information

Design And Synthesis of Optically Pure 3-Aryl-6-methyl-2-thioxotetrahydropyrimidin-4(1*H*)-ones as Anti-prostate Cancer Agents

Varun Kumar,* Mahesh Rachamalla, Prajwal Nandekar, Gopal L. Khatik, Abhay T. Sangamwar, Kulbhushan Tikoo, and Vipin A. Nair*

Sr. No.	Contents
Page 1	Table of Contents
Page 2 to Page 25	¹ H, ¹³ C NMR and HRMS spectra of 3-aryl-6(<i>R/S</i>)-methyl-1-((<i>R/S</i>)-1-phenylethyl)-2-thioxotetrahydropyrimidin-4(1 <i>H</i>)-ones (9a-9f , 9'a-9'f)
Page 25 to Page 49	¹ H, ¹³ C NMR and HRMS spectra of 3-aryl-6(<i>R/S</i>)-methyl-2-thioxotetrahydropyrimidin-4(1 <i>H</i>)-ones (10a-10f , 10'a-10'f)
Page 50 to Page 52	¹ H, ¹³ C NMR spectra of compounds 4, 6 and 7



Mass Spectrum List Report

Analysis Info

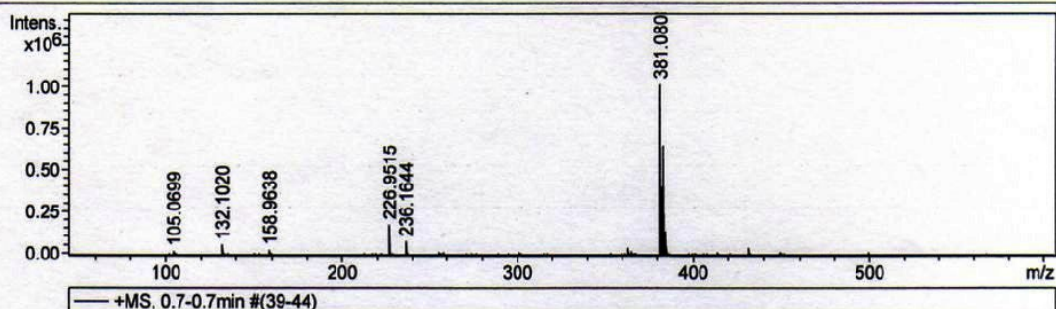
Analysis Name D:\Data\vipin\10-05-18-VK-8A.d
Method tune_low.m
Sample Name VK-8A
Comment

Acquisition Date 5/18/2010 11:20:28 AM

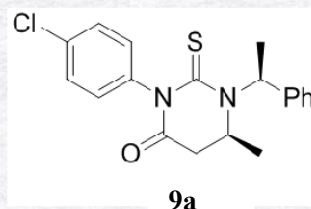
Operator VIKAS GROVER
Instrument / Ser# maXis 40

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



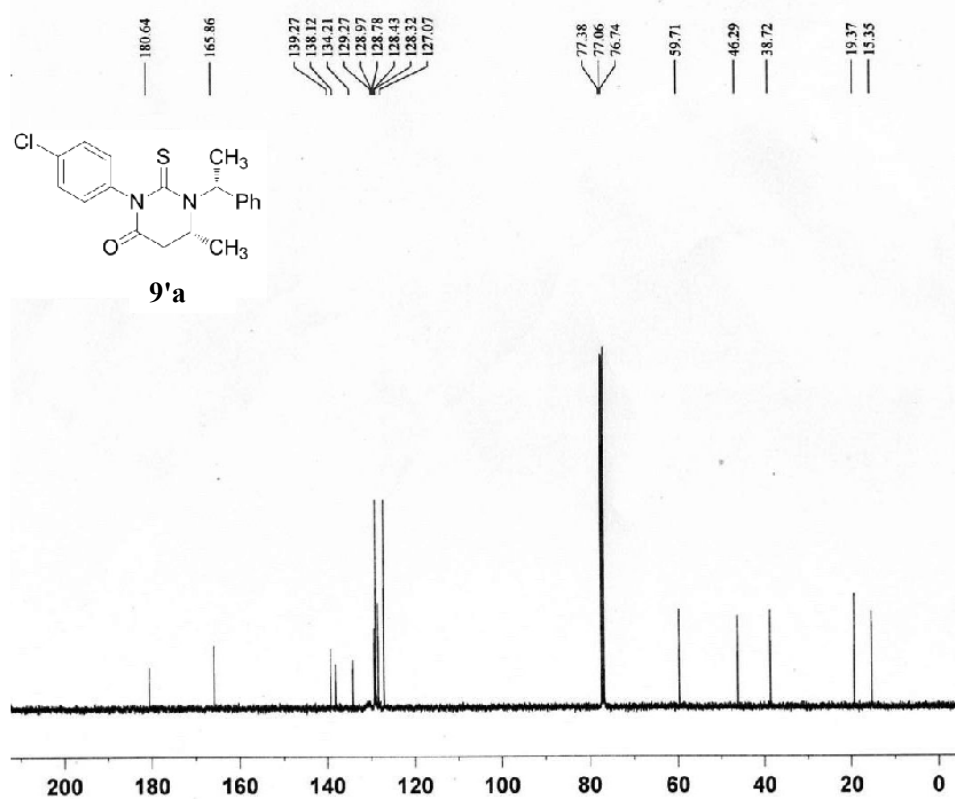
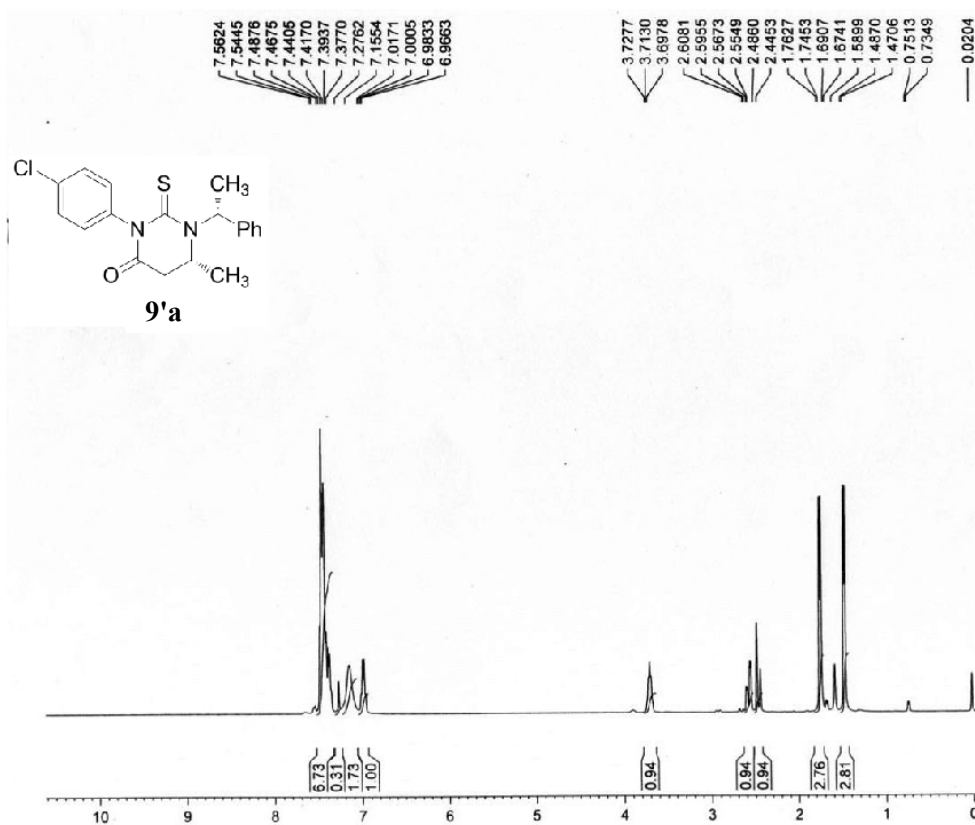
#	m/z	Res.	S/N	I	FWHM
1	105.0699	22485	14985.7	17886	0.0047
2	132.1020	21091	19221.6	53716	0.0063
3	158.9638	20022	7052.5	24794	0.0079
4	226.9515	21127	17351.7	174327	0.0107
5	236.1644	21732	7108.3	76277	0.0109
6	381.0808	15636	22423.0	1011544	0.0244
7	382.0833	21791	8751.8	400401	0.0175
8	383.0776	20273	13848.9	642375	0.0189
9	384.0802	21153	2917.8	137207	0.0182



$[M+Na]^+$

Calcd.: 381.0805

Found: 381.0808



Mass Spectrum List Report

Analysis Info

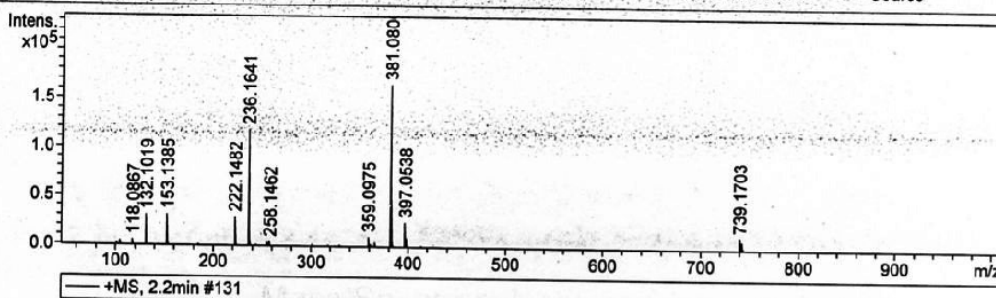
Analysis Name D:\Data\vipin\11-07-04-VN-3133-7.d
Method sodium formate tune_low.m
Sample Name VN-3133-7
Comment I

Acquisition Date 7/4/2011 3:26:01 PM

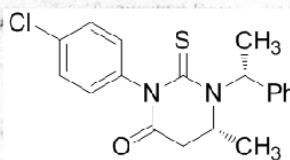
Operator VIKAS GROVER
Instrument / Ser# maXis 40

Acquisition Parameter

Source Type ESI Ion Polarity Positive Set Nebulizer 0.4 Bar
Focus Not active Set Capillary 4500 V Set Dry Heater 180 °C
Scan Begin 50 m/z Set End Plate Offset -500 V Set Dry Gas 4.0 l/min
Scan End 1000 m/z Set Collision Cell RF 300.0 Vpp Set Divert Valve Source

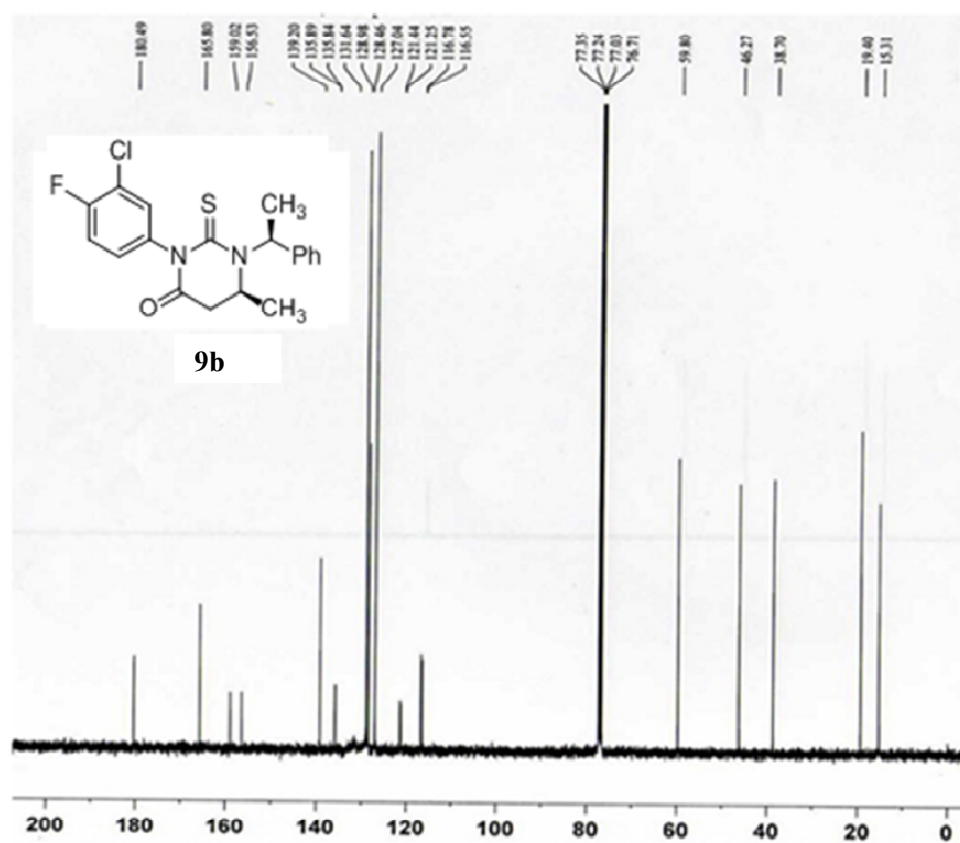
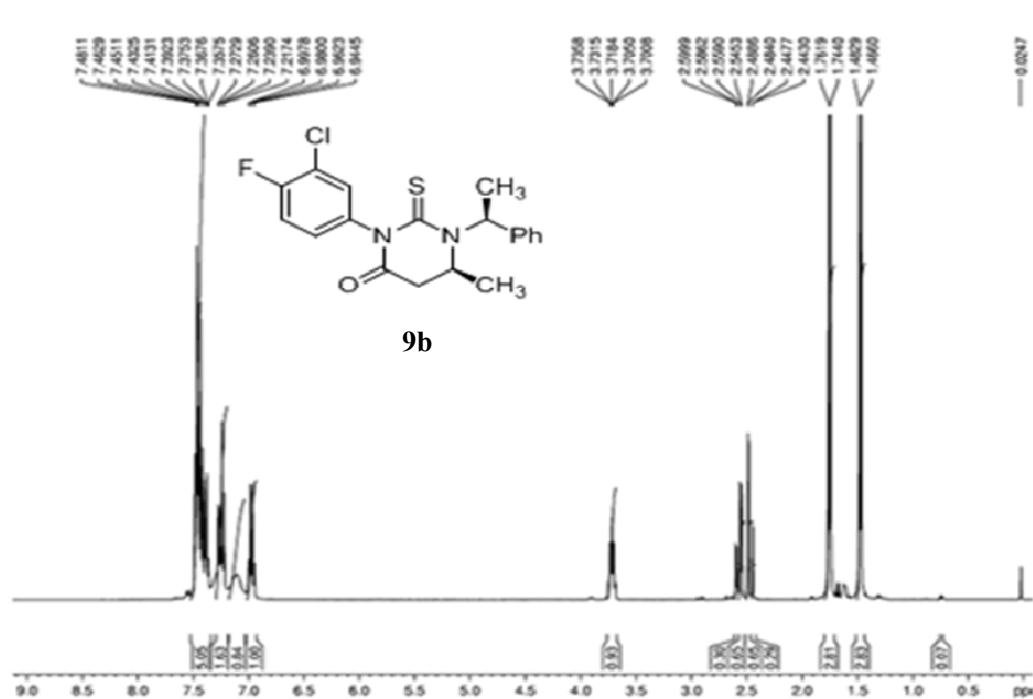


#	m/z	Res.	S/N	I	FWHM
1	118.0857	19850	61.7	5076	0.0059
2	132.1019	19371	305.8	31035	0.0068
3	153.1385	19532	294.3	31234	0.0078
4	222.1482	20871	394.1	29062	0.0106
5	236.1641	19394	1659.1	117933	0.0122
6	258.1462	21579	59.8	4005	0.0119
7	359.0975	23542	109.0	9853	0.0153
8	380.1151	16827	0.3	27	0.0226
9	381.0800	20369	1559.9	165092	0.0187
10	382.0825	24625	173.7	18501	0.0155
11	383.0771	22838	444.1	47625	0.0168
12	384.0811	21647	35.4	3820	0.0177
13	397.0538	22456	211.9	24767	0.0177
14	399.0516	23234	74.3	8474	0.0172
15	739.1703	27958	221.1	12721	0.0264



9'a

[M+Na]⁺ Calcd.: 381.0805
Found: 381.0800



Mass Spectrum List Report

Analysis Info

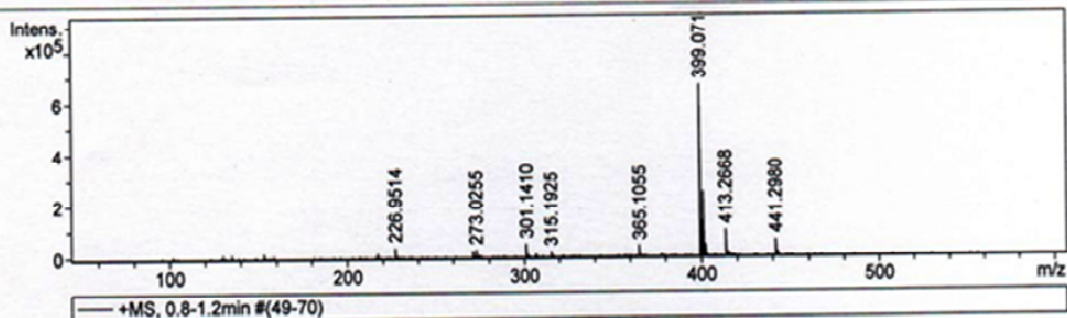
Analysis Name D:\Data\vipin\10-05-18-VK-7A.d
Method tune_low.m
Sample Name VK-7A
Comment

Acquisition Date 5/18/2010 9:28:38 AM

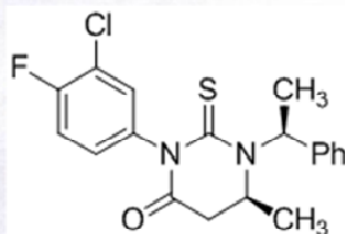
Operator VIKAS GROVER
Instrument / Ser# maXis 40

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source

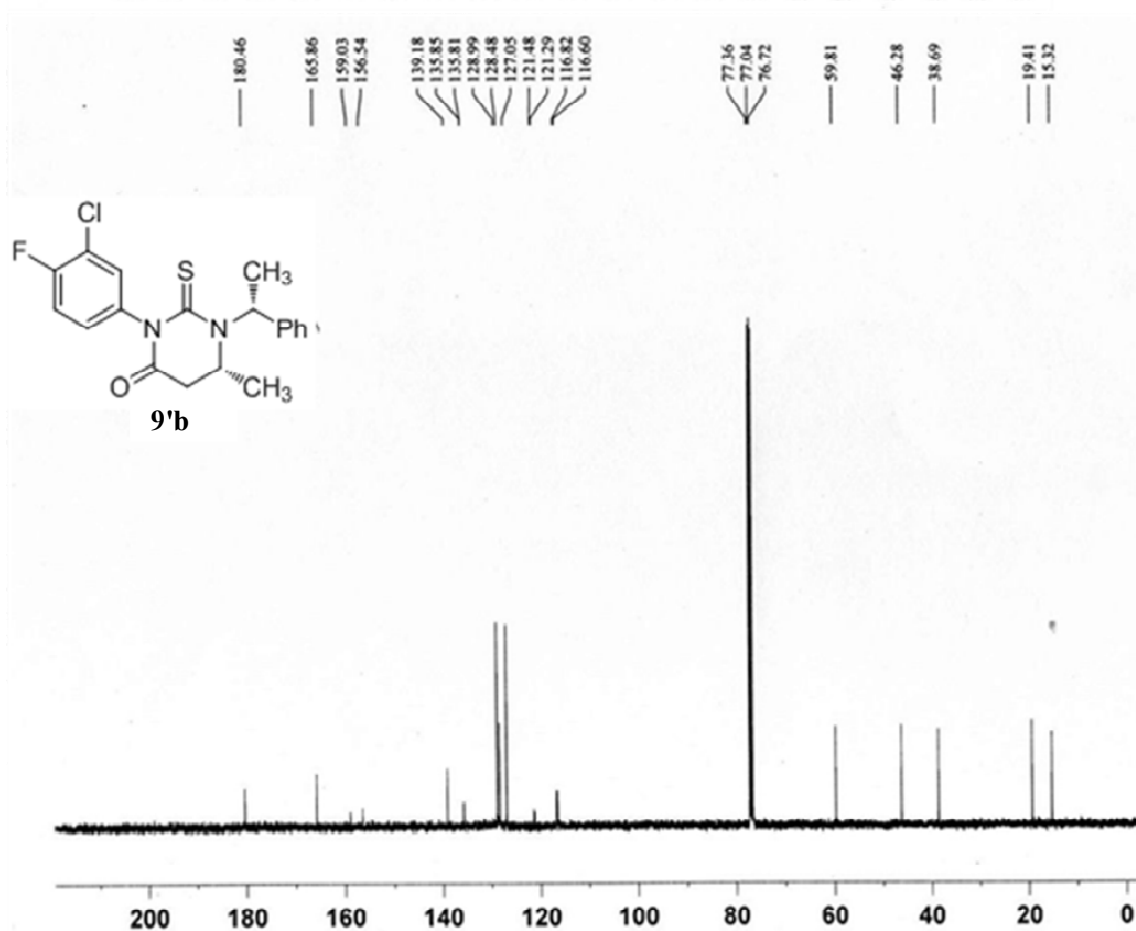
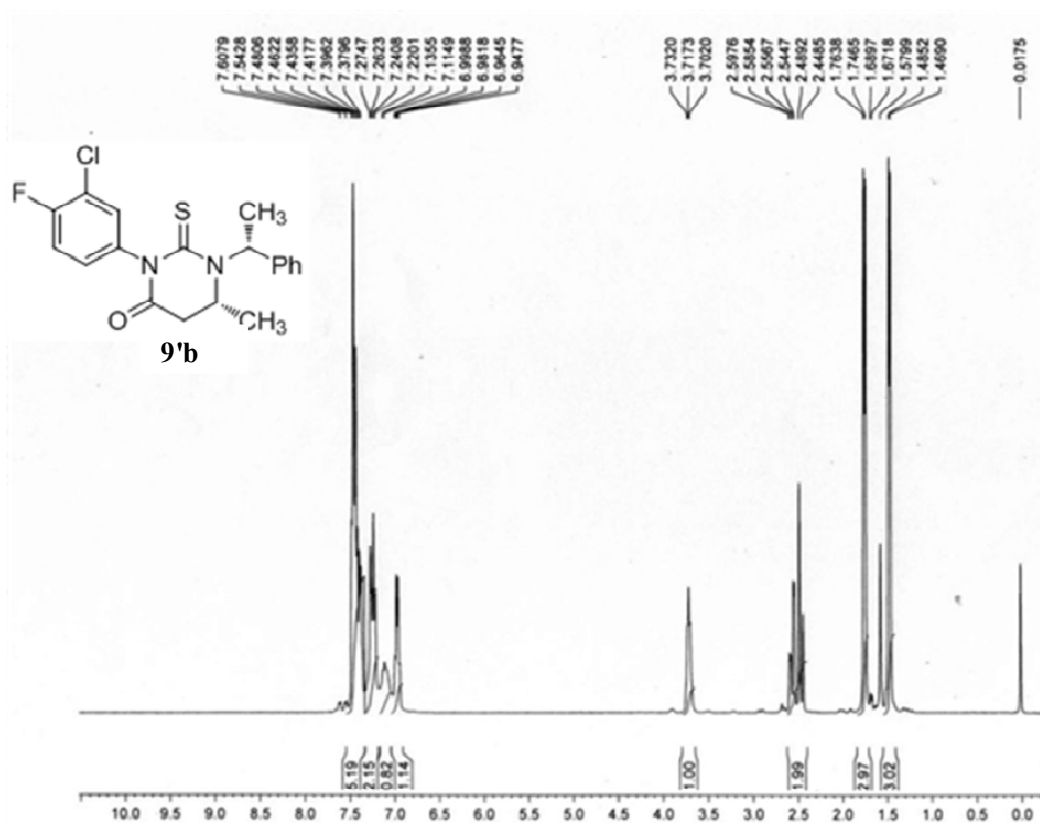


#	m/z	Res.	S/N	I	FWHM
1	216.9224	24162	997.9	14650	0.0090
2	226.9514	21619	2589.2	38926	0.0105
3	273.0255	23866	944.4	26389	0.0114
4	301.1410	23823	1527.6	50307	0.0126
5	306.2786	25800	322.1	10247	0.0119
6	315.1925	25230	602.3	17992	0.0125
7	365.1055	24714	1189.5	40844	0.0148
8	399.0714	22088	8970.9	663240	0.0181
9	400.0741	21798	1828.3	136265	0.0184
10	401.0687	21351	3405.0	249804	0.0188
11	402.0708	24055	646.5	46671	0.0167
12	413.2668	23115	1680.9	99251	0.0179
13	441.2980	23977	2093.6	62927	0.0184



9b

[M+Na]⁺ Calcd.: 399.0710
found: 399.0714



Mass Spectrum List Report

Analysis Info

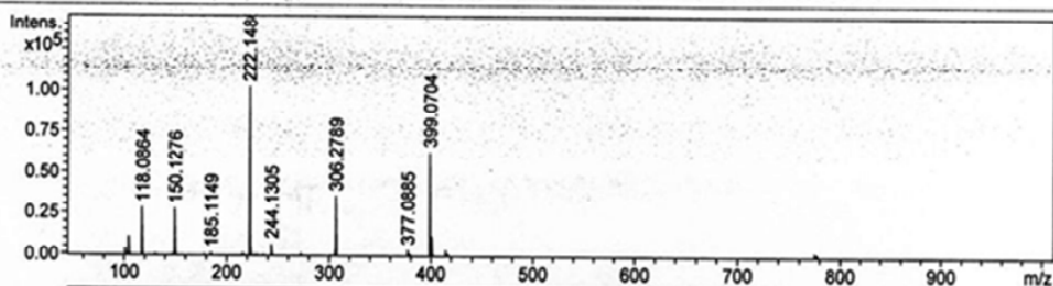
Analysis Name D:\Data\vipin\11-07-05-VN-3137-7.d
Method sodium formate tune_low.m
Sample Name VN-3137-7
Comment

Acquisition Date 7/5/2011 9:15:19 AM

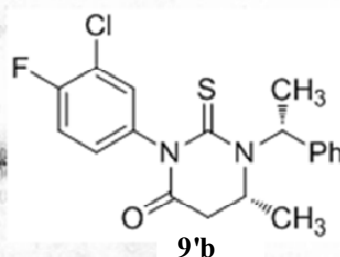
Operator VIKAS GROVER
Instrument / Ser# maXis 40

Acquisition Parameter

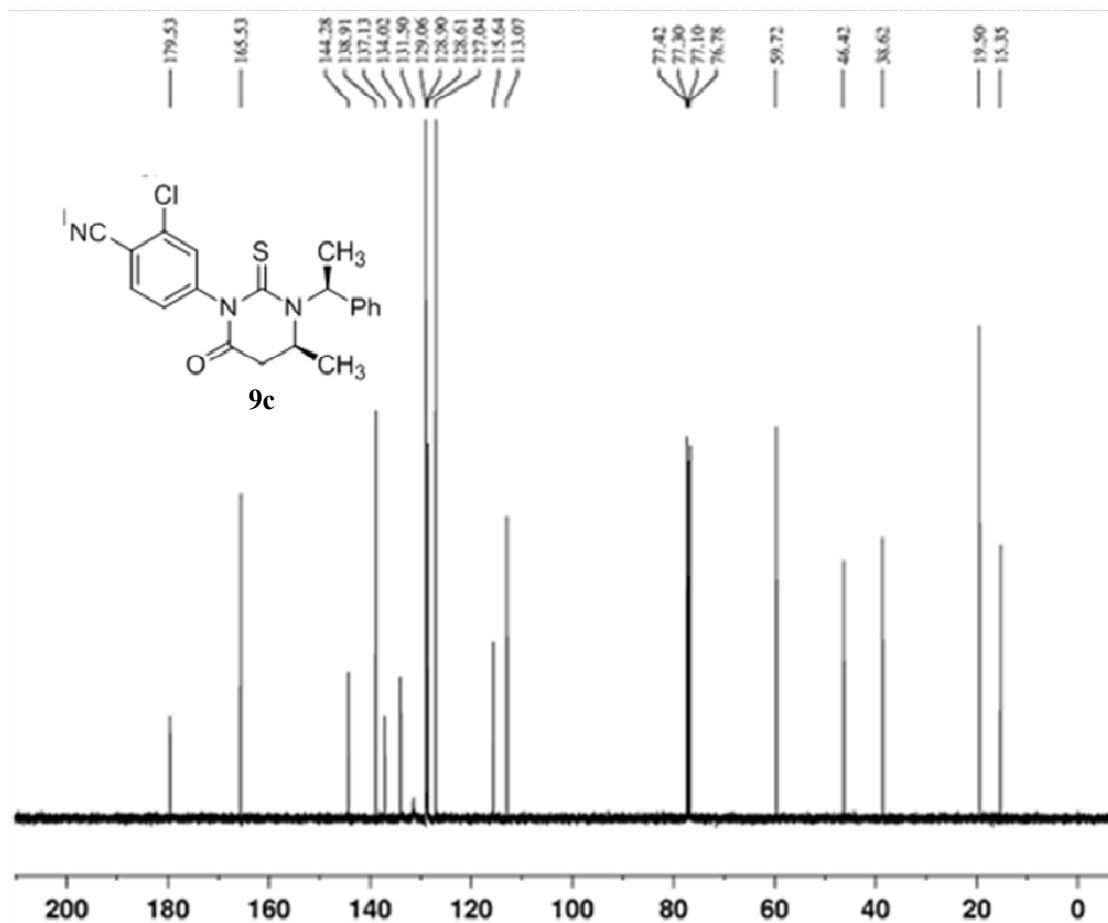
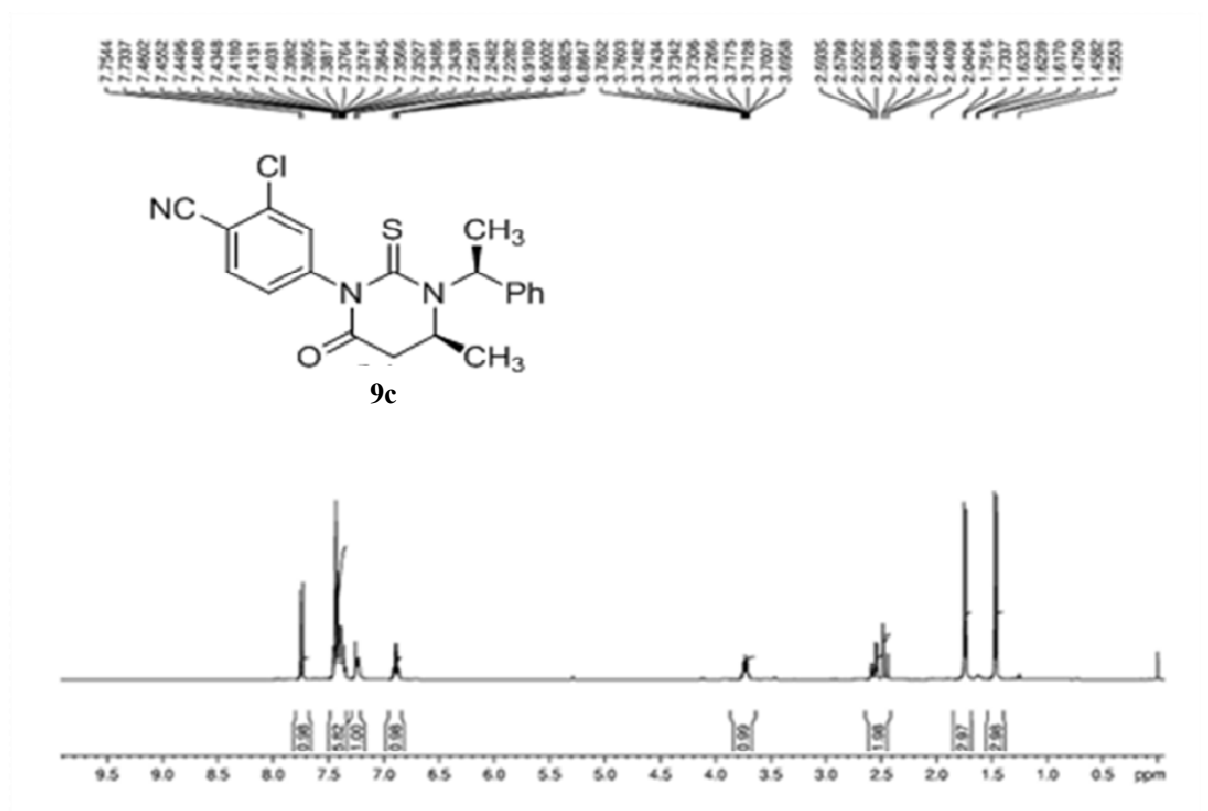
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



#	m/z	Res.	S/N	I	FWHM
1	102.1283	17941	81.4	4189	0.0057
2	105.0703	17298	211.6	11486	0.0061
3	106.0739	16714	11.6	643	0.0063
4	118.0864	17903	423.7	28341	0.0066
5	130.1593	17119	10.4	821	0.0076
6	148.1121	22076	10.9	948	0.0067
7	150.1276	21746	317.5	27569	0.0069
8	151.1313	17293	13.8	1196	0.0087
9	178.1594	18348	11.0	884	0.0097
10	185.1149	19736	21.0	1652	0.0094
11	216.0995	20073	21.0	1452	0.0108
12	222.1486	18170	1534.4	101987	0.0122
13	223.1518	22238	97.9	6464	0.0100
14	228.1571	21680	12.4	794	0.0105
15	230.1151	23410	13.2	832	0.0098
16	236.1646	23660	17.1	1032	0.0100
17	244.1305	22235	123.4	7018	0.0110
18	245.1343	19080	11.0	619	0.0128
19	273.0252	22264	27.5	1268	0.0123
20	301.1416	21528	11.3	526	0.0140
21	306.2789	23193	766.6	35713	0.0132
22	307.2823	23639	72.6	3384	0.0130
23	377.0885	23373	36.2	3702	0.0161
24	379.0863	22346	11.0	1151	0.0170
25	399.0704	24392	509.5	62924	0.0164
26	400.0738	24139	41.6	5073	0.0166
27	401.0883	23620	99.0	11891	0.0170
28	402.0713	20298	11.1	1320	0.0198
29	415.0447	25650	32.6	3155	0.0162



[M+Na]⁺ Calcd.: 399.0710
Found: 399.0704



Mass Spectrum List Report

Analysis Info

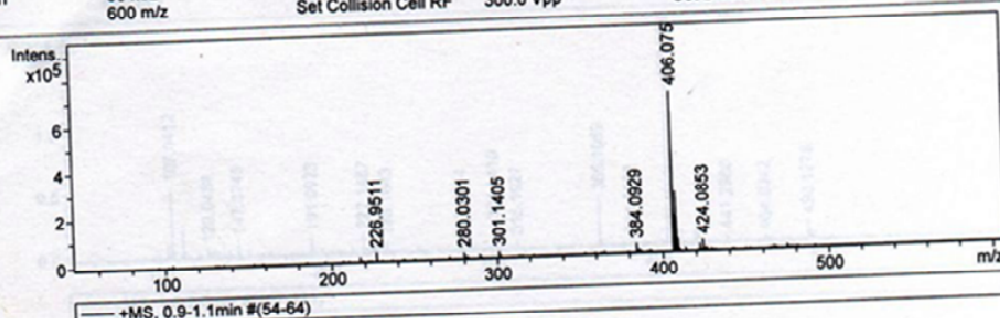
Analysis Name D:\Data\vipin\10-05-18-VK-6A.d
Method tune_low.m
Sample Name VK-6A
Comment

Acquisition Date 5/18/2010 11:12:47 AM

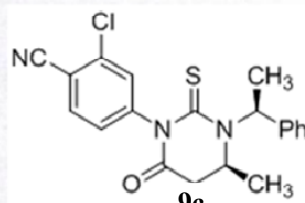
Operator VIKAS GROVER
Instrument / Ser# maXis 40

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



#	m/z	Res.	S/N	I	FWHM
1	216.9221	24549	1830.2	13953	0.0088
2	226.9511	23652	4330.9	32076	0.0096
3	270.9769	26339	728.6	8057	0.0103
4	280.0301	24934	1611.5	20773	0.0112
5	289.1533	25799	692.1	9898	0.0112
6	301.1405	26219	1723.8	22378	0.0115
7	384.0929	25068	912.5	34735	0.0153
8	406.0757	22348	13085.1	679592	0.0182
9	407.0785	22022	2940.1	150213	0.0185
10	407.5373	20028	0.2	9	0.0203
11	408.0731	21015	4947.9	248640	0.0194
12	409.0752	24048	1034.8	51124	0.0170
13	424.0853	25477	1171.9	43064	0.0166



[m+Na]⁺ calcd.: 406.0757
Found: 406.0757

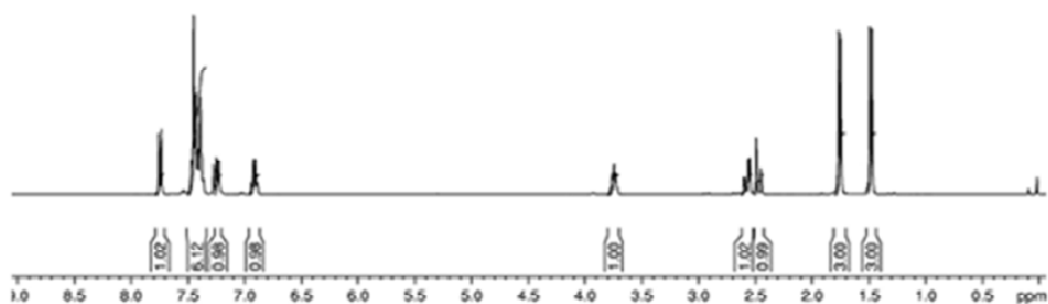
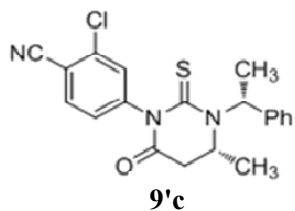
7.7571
7.7365
7.5000
7.5060
7.4700
7.4512
7.4333
7.4142
7.3952
7.3809
7.3663
7.3629
7.2728
7.2509
7.2305
6.9419
6.9241
6.9064
6.8890

3.7762
3.7638
3.7470
3.7331
3.7170

2.6037
2.5902
2.5627
2.5491
2.4832
2.4523

1.7864
1.7486
1.6875
1.6700
1.4907
1.4759

0.7588
0.7421
0.6920



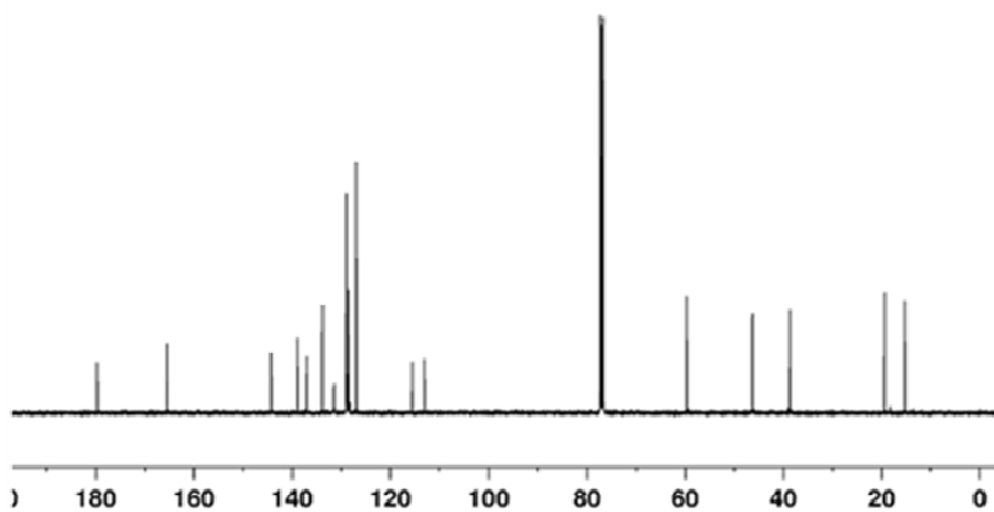
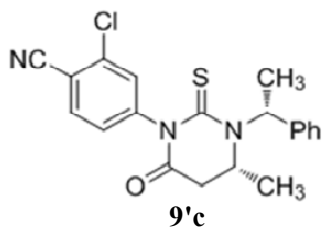
179.64
165.40
144.29
138.99
137.08
133.92
131.52
129.03
128.86
128.57
128.28
127.03
115.53
113.10

77.33
77.22
77.01
76.70

59.73

46.38
39.12
38.65

19.46
18.22
15.32



Mass Spectrum List Report

Analysis Info

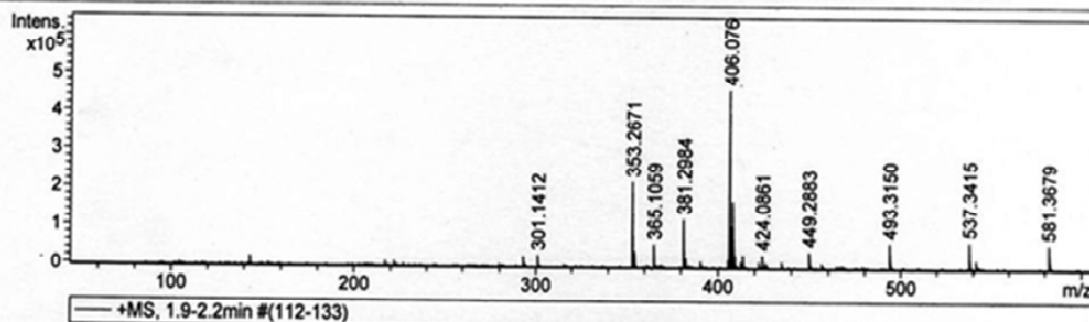
Analysis Name D:\Data\vipin\10-05-18-VK-6C.d
Method tune_low.m
Sample Name VK-6C
Comment

Acquisition Date 5/18/2010 9:12:31 AM

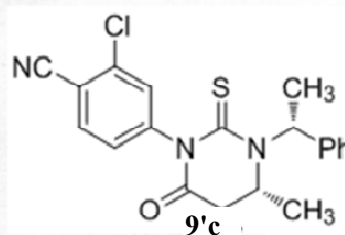
Operator VIKAS GROVER
Instrument / Ser# maXis 40

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source

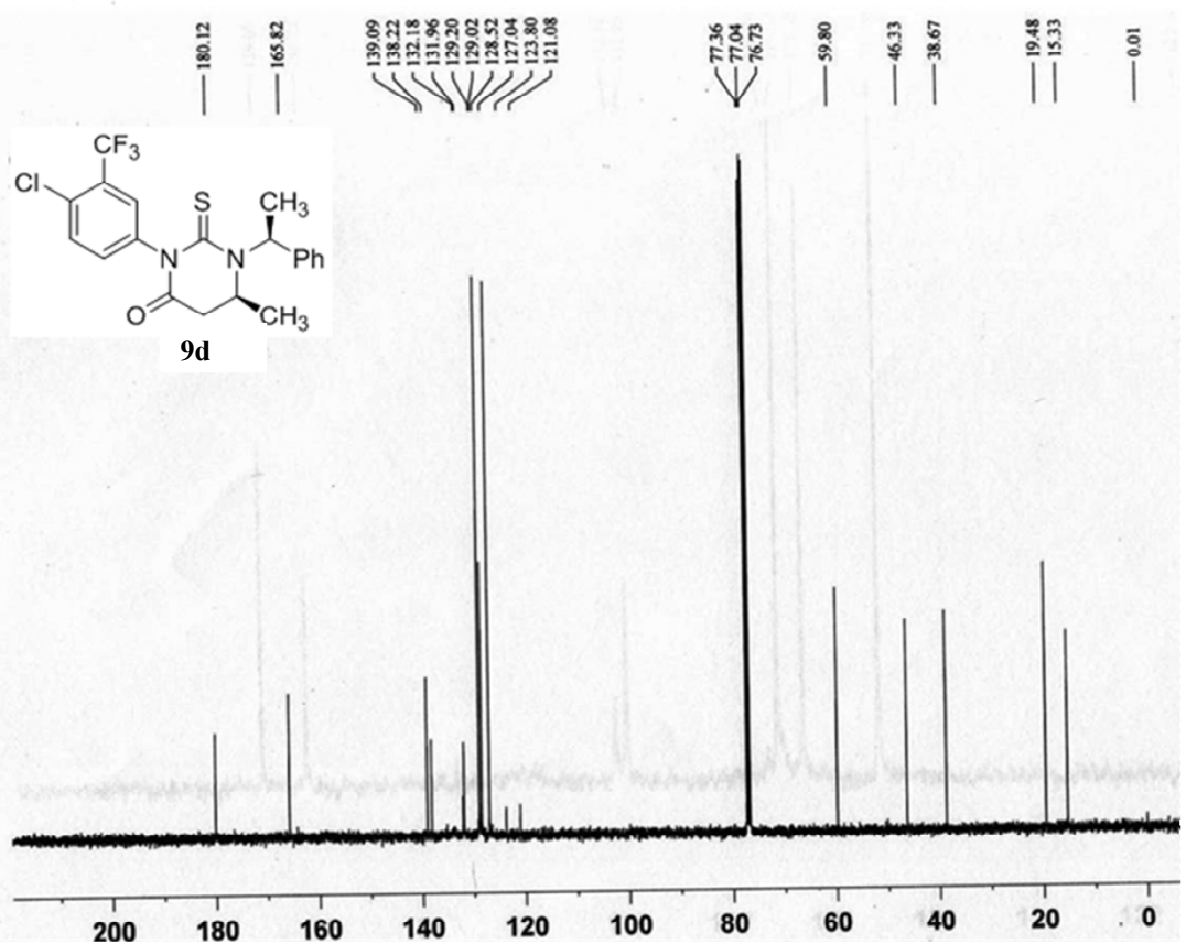
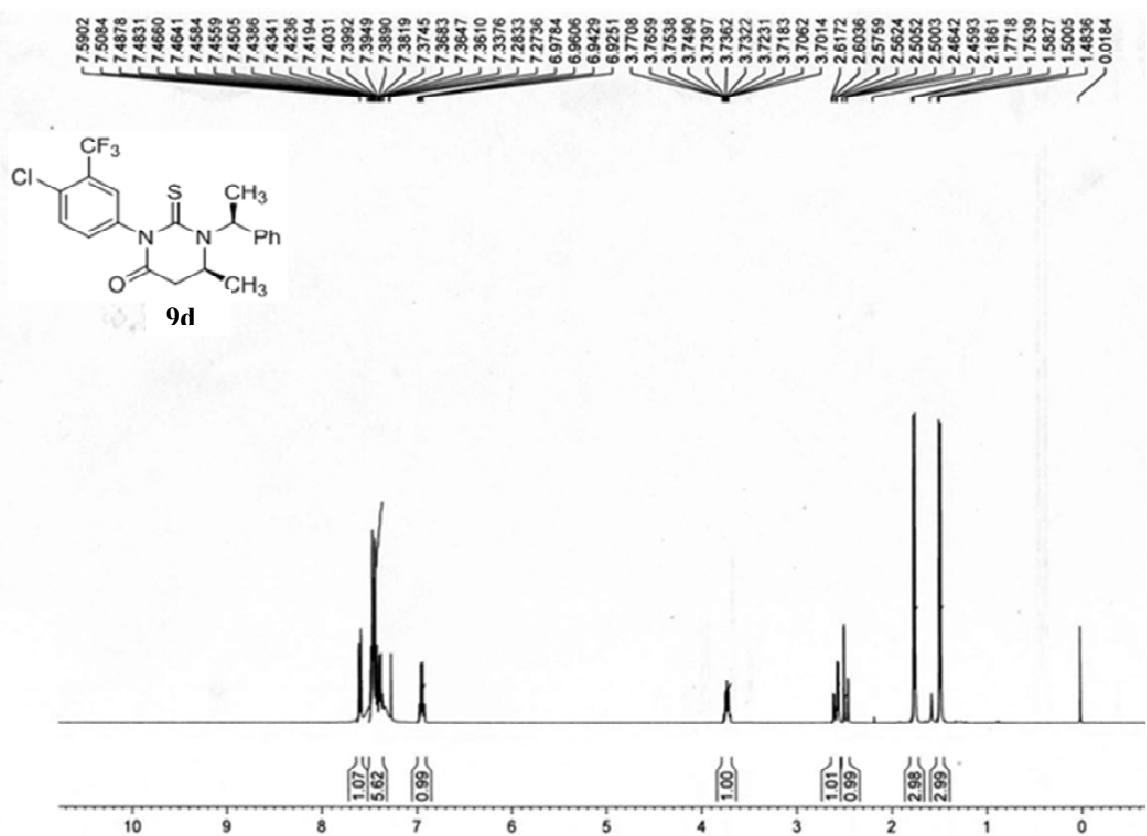


#	m/z	Res.	S/N	I	FWHM
1	301.1412	25222	1721.1	28534	0.0119
2	353.2671	21332	8035.1	219458	0.0166
3	365.1059	23981	1662.4	57945	0.0152
4	381.2984	22623	2268.6	122849	0.0169
5	406.0766	22036	6780.4	460465	0.0184
6	407.0791	23017	1565.9	104244	0.0177
7	408.0738	21600	2592.2	169127	0.0189
8	424.0861	25886	746.2	32726	0.0164
9	434.2567	27256	436.5	13216	0.0159
10	449.2883	24885	1637.2	41502	0.0181
11	493.3150	24964	3193.3	63447	0.0198
12	537.3415	24270	3458.3	66391	0.0221
13	581.3679	25384	3856.7	60525	0.0229



[M+Na]⁺

Calcd.: 406.0757
Found: 406.0766



Mass Spectrum List Report

Analysis Info

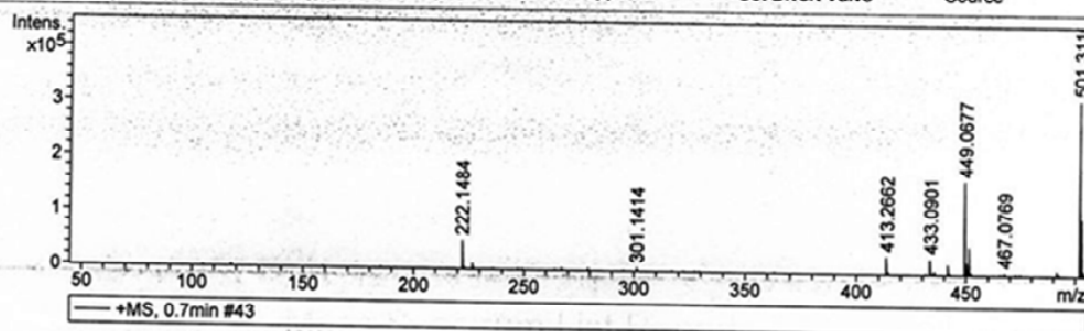
Analysis Name D:\Data\vipin\11-06-28-VN-3127-7.d
Method sodium formate tune_low.m
Sample Name VN-3127-7
Comment I

Acquisition Date 6/28/2011 2:23:08 PM

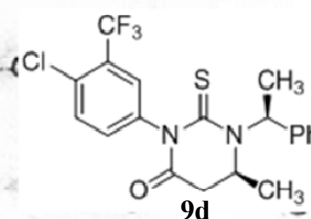
Operator VIKAS GROVER
Instrument / Ser# maXis 40

Acquisition Parameter

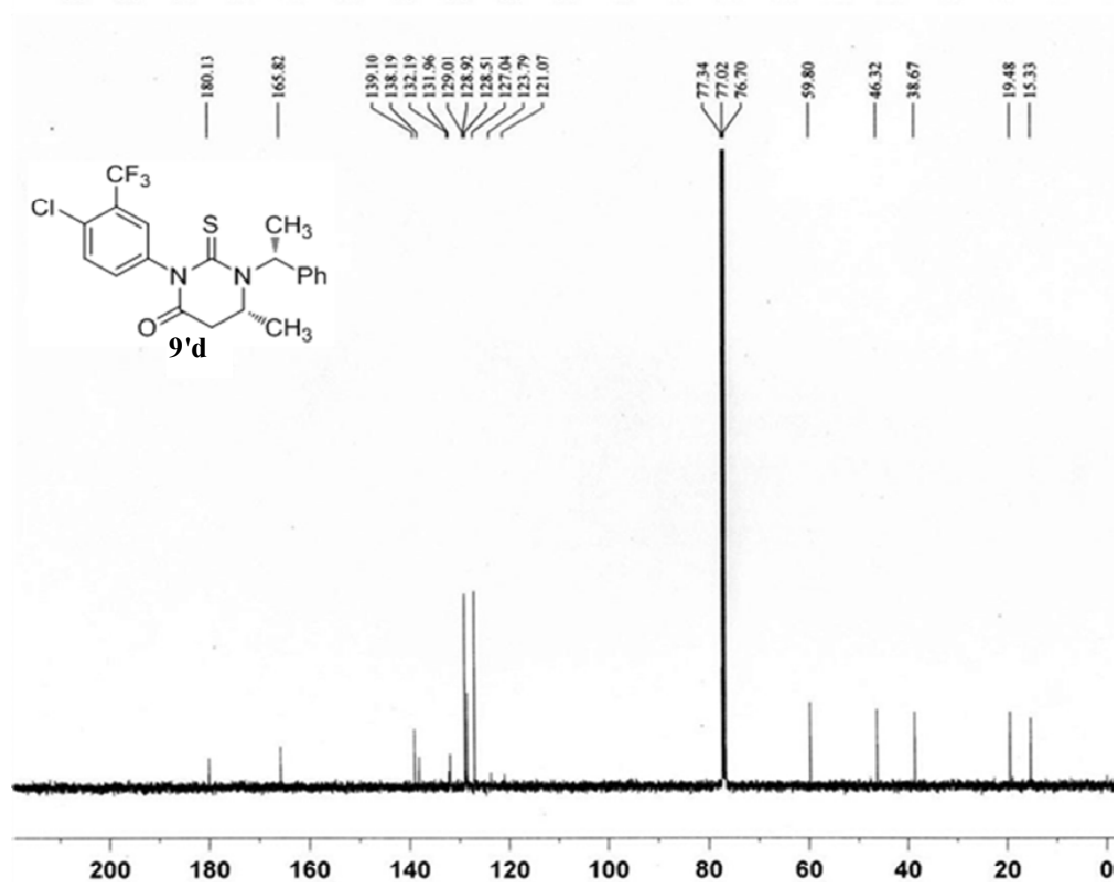
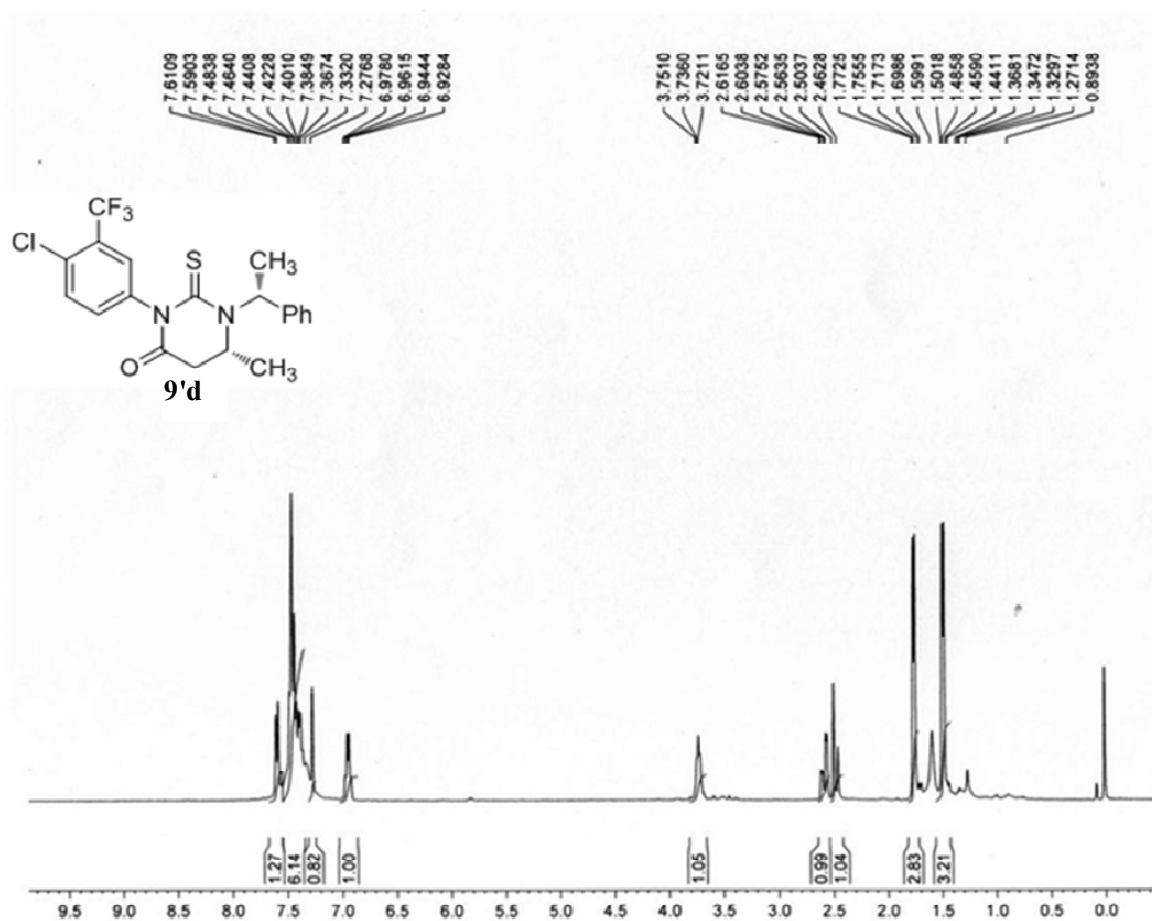
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	500 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



#	m/z	Res.	S/N	I	FWHM
1	222.1484	20054	417.3	50850	0.0111
2	223.1522	21282	25.8	3083	0.0105
3	226.9512	21184	91.2	10131	0.0107
4	236.1645	22411	31.5	2854	0.0105
5	244.1308	19936	10.4	755	0.0122
6	247.1783	21575	30.8	2334	0.0115
7	249.0559	20492	22.1	1722	0.0122
8	301.1414	22148	59.1	5922	0.0136
9	312.1579	23083	15.5	1408	0.0135
10	317.0643	21831	36.7	3112	0.0145
11	319.0618	23959	12.5	1028	0.0133
12	322.2020	22676	27.3	2147	0.0142
13	326.9668	23109	30.3	2206	0.0141
14	328.9647	20940	30.9	2174	0.0157
15	362.9267	22577	54.3	2682	0.0161
16	413.2662	24876	251.5	32633	0.0166
17	414.2701	22988	29.5	3995	0.0180
18	433.0901	25680	129.9	29236	0.0169
19	434.0937	24708	12.3	2799	0.0176
20	435.0979	13220	31.8	7286	0.0329
21	441.2976	25248	80.8	19443	0.0175
22	442.3016	20579	10.3	2495	0.0215
23	449.0677	20830	660.7	168639	0.0216
24	450.0702	25431	85.5	21992	0.0177
25	451.0650	24479	196.9	50996	0.0184
26	452.0679	23508	16.0	4169	0.0192
27	465.0432	24293	10.6	2909	0.0191
28	467.0769	23958	16.8	4601	0.0195
29	472.0788	22166	10.8	2968	0.0213
30	501.3116	19264	1147.4	316670	0.0260



$[M+Na]^+$ Calcd.: 449.0678
Found: 449.0677



Mass Spectrum List Report

Analysis Info

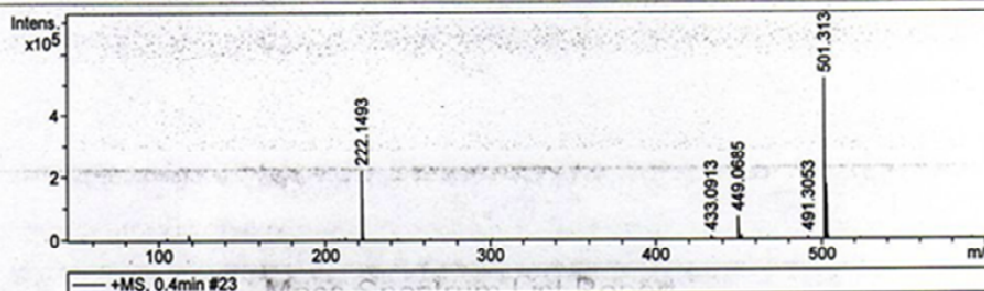
Analysis Name D:\Data\vipin\11-07-05-VN-3138-7-a.d
Method sodium formate tune_low.m
Sample Name VN-3138-7
Comment I

Acquisition Date 7/5/2011 10:34:49 AM

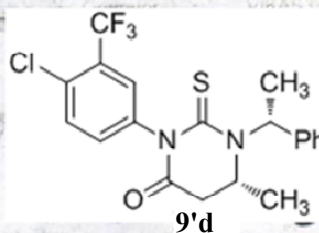
Operator VIKAS GROVER
Instrument / Ser# maXis 40

Acquisition Parameter

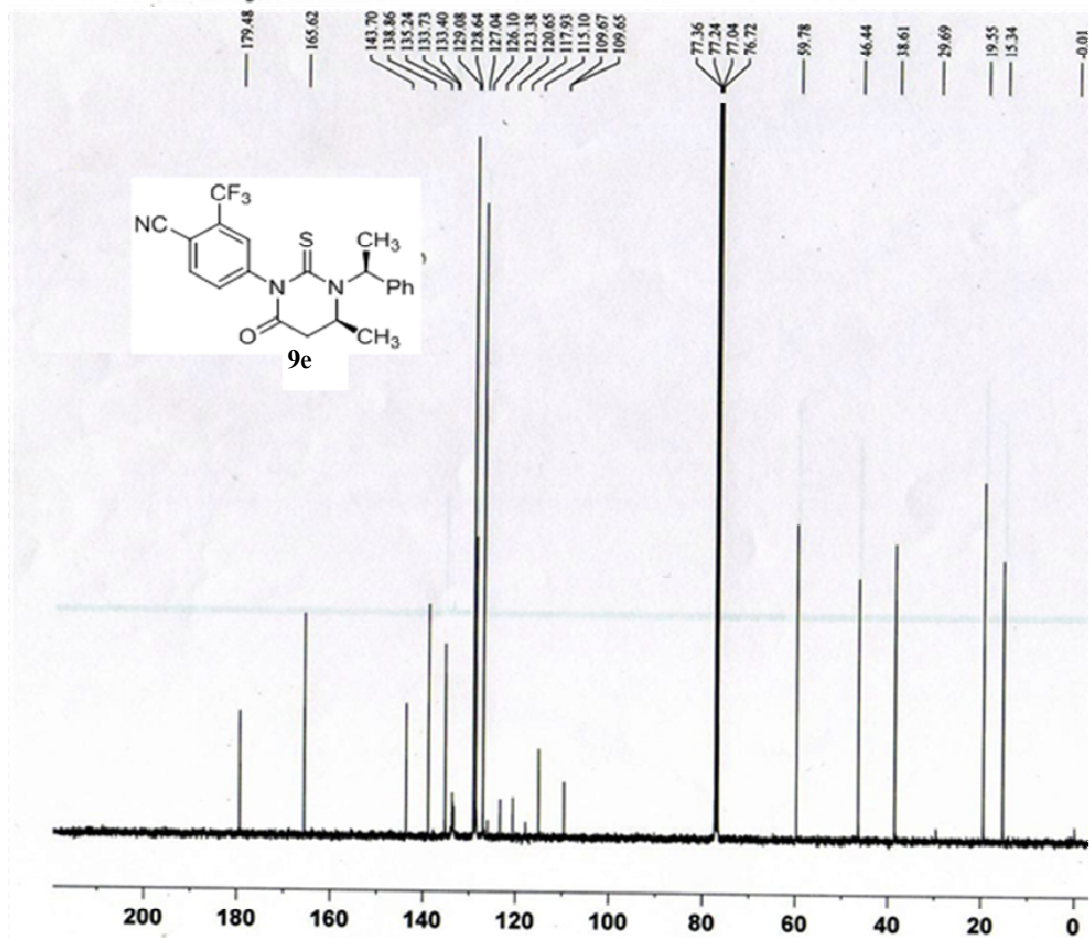
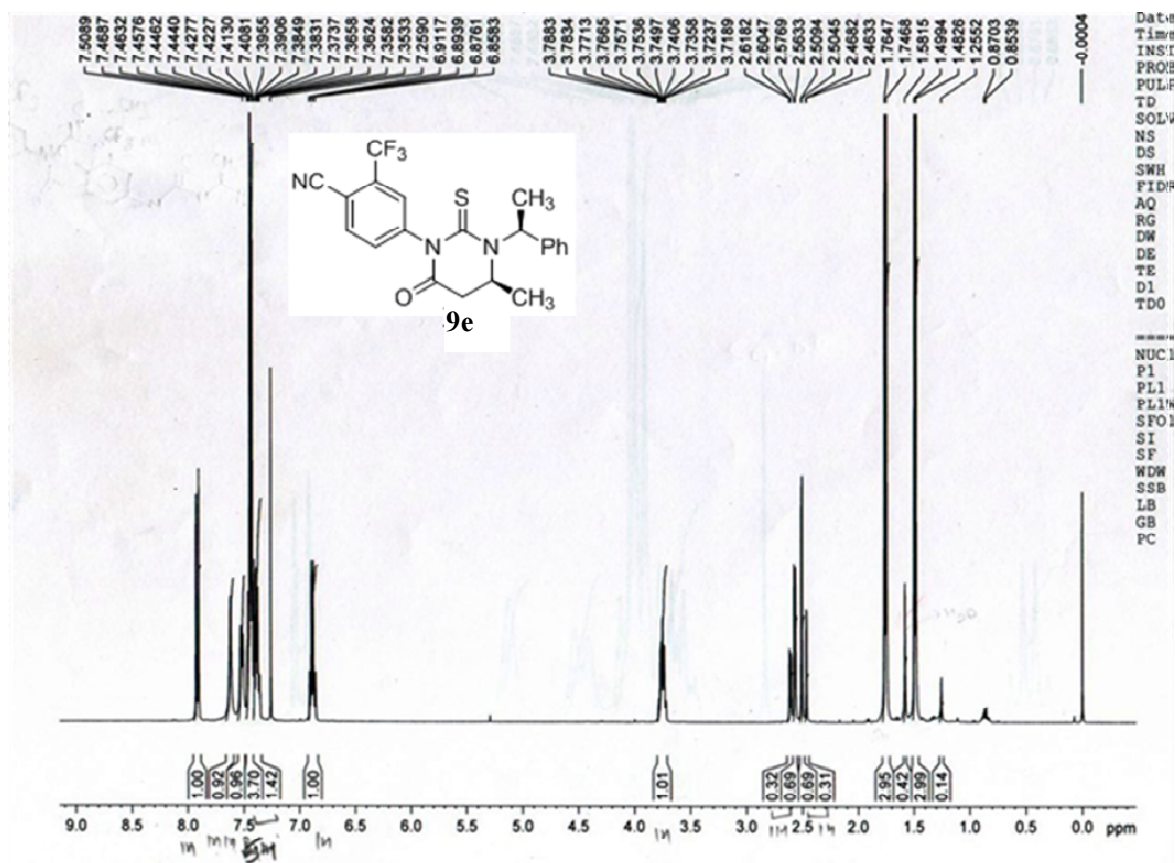
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



#	m/z	Res.	S/N	I	FWHM
1	212.1435	20802	50.9	6259	0.0102
2	222.1493	17058	1961.8	219007	0.0130
3	223.1522	21607	131.9	14535	0.0103
4	226.9517	22181	11.4	1190	0.0102
5	236.1651	20740	21.4	1958	0.0114
6	244.1314	21455	49.2	3932	0.0114
7	264.1963	21580	42.2	2993	0.0122
8	279.0871	21565	25.5	1806	0.0129
9	292.2280	22055	21.1	1471	0.0132
10	301.1420	23033	47.4	3226	0.0131
11	312.1582	23821	18.3	1206	0.0131
12	317.0654	23136	23.3	1513	0.0137
13	322.2023	22465	55.9	3583	0.0143
14	399.0728	22625	21.4	1192	0.0176
15	401.2612	21425	13.7	806	0.0187
16	427.0871	23353	13.8	1486	0.0183
17	433.0913	24559	81.4	9669	0.0176
18	434.0952	21838	10.2	1232	0.0199
19	435.0996	13055	25.1	3083	0.0333
20	449.0685	22812	614.6	69780	0.0197
21	450.0717	24382	52.3	5881	0.0185
22	451.0663	25424	136.1	15175	0.0177
23	452.0695	20923	13.0	1441	0.0216
24	467.0785	20766	13.1	1246	0.0225
25	469.2866	19954	10.4	968	0.0235
26	472.0794	24330	21.7	1946	0.0194
27	474.0772	23004	12.3	1077	0.0206
28	491.3053	24469	61.9	8178	0.0201
29	492.3088	23690	15.2	2047	0.0208
30	501.3134	18834	3232.4	511476	0.0266



[M+Na]⁺ Calcd.: 449.0678
Found: 449.0685



Mass Spectrum List Report

Analysis Info

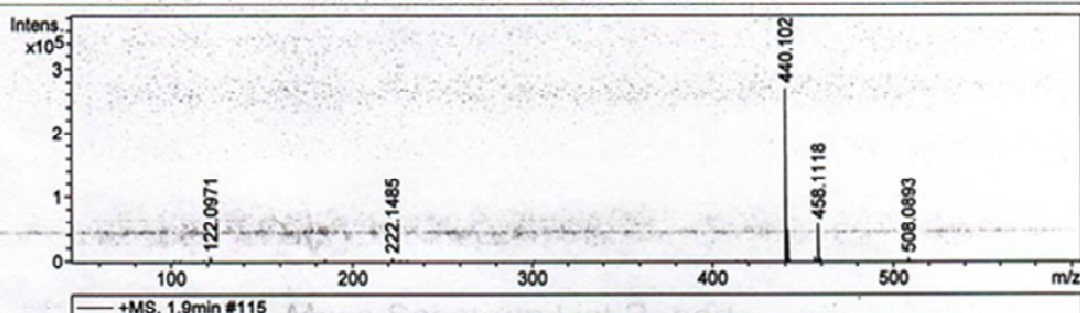
Analysis Name D:\Data\vipin\11-06-28-VN-3131-7.d
Method sodium formate tune_low.m
Sample Name VN-3131-7
Comment I

Acquisition Date 6/28/2011 3:50:38 PM

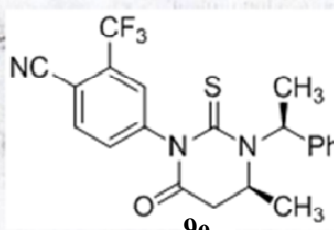
Operator VIKAS GROVER
Instrument / Ser# maXis 40

Acquisition Parameter

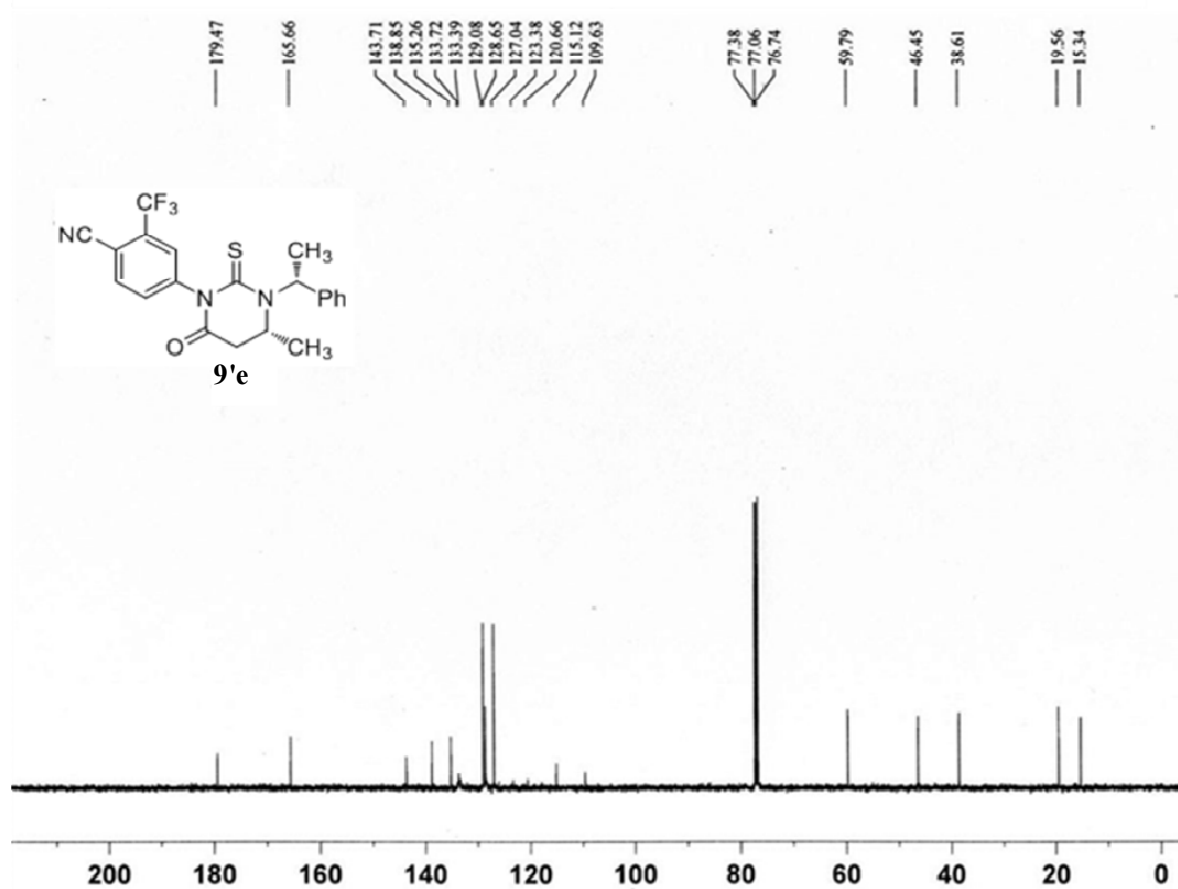
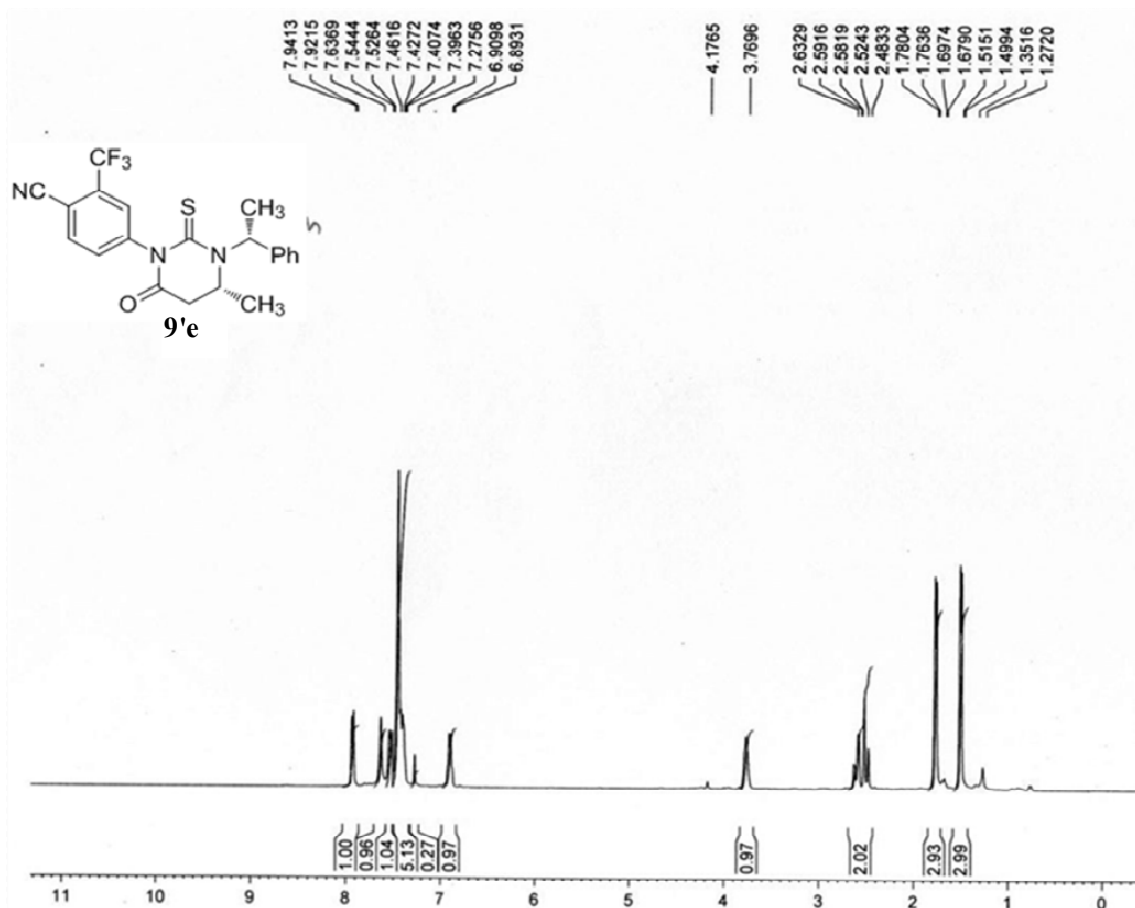
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



#	m/z	Res.	S/N	I	FWHM
1	102.1288	16977	18.7	1347	0.0060
2	105.0709	17491	24.6	1776	0.0060
3	118.0870	17606	35.9	2602	0.0067
4	122.0971	18433	95.6	6936	0.0066
5	158.9647	15296	10.5	632	0.0104
6	185.1149	21236	56.9	3324	0.0087
7	222.1485	21027	67.3	5162	0.0106
8	226.9517	19097	22.1	1604	0.0119
9	230.1150	19514	41.8	2929	0.0118
10	249.0555	23871	20.2	1088	0.0104
11	267.0459	21157	16.2	760	0.0126
12	301.1419	18828	33.5	1356	0.0160
13	328.9641	24077	16.0	677	0.0137
14	360.3236	20879	17.2	687	0.0173
15	365.2230	20800	15.6	636	0.0176
16	382.1615	23104	18.1	840	0.0165
17	389.1951	22825	17.0	829	0.0171
18	413.2659	22851	32.3	2713	0.0181
19	418.1200	24070	17.0	1620	0.0174
20	440.1021	19669	1990.3	269625	0.0224
21	441.1043	24385	361.7	48595	0.0181
22	442.1018	18717	39.4	5252	0.0236
23	456.0756	26113	69.1	8120	0.0175
24	457.0785	24518	10.2	1182	0.0186
25	458.1118	23630	502.4	57885	0.0194
26	459.1148	23067	51.2	5845	0.0199
27	460.1061	11700	11.3	1280	0.0393
28	508.0893	24974	98.1	4971	0.0203
29	509.0938	20335	17.4	859	0.0250
30	576.0778	21672	35.4	784	0.0266



$[M+Na]^+$ Calcd.: 440.1021
Found: 440.1021



Mass Spectrum List Report

Analysis Info

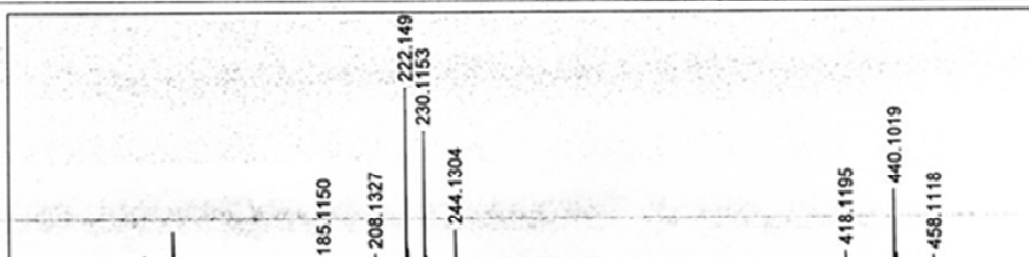
Analysis Name D:\Data\vipin\11-07-15-VN-3139-7.d
Method sodium formate tune_low.m
Sample Name VN-3139-7
Comment

Acquisition Date 7/15/2011 2:36:31 PM

Operator VIKAS GROVER
Instrument / Ser# maXis 40

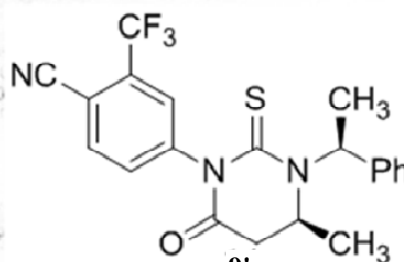
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	500 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source

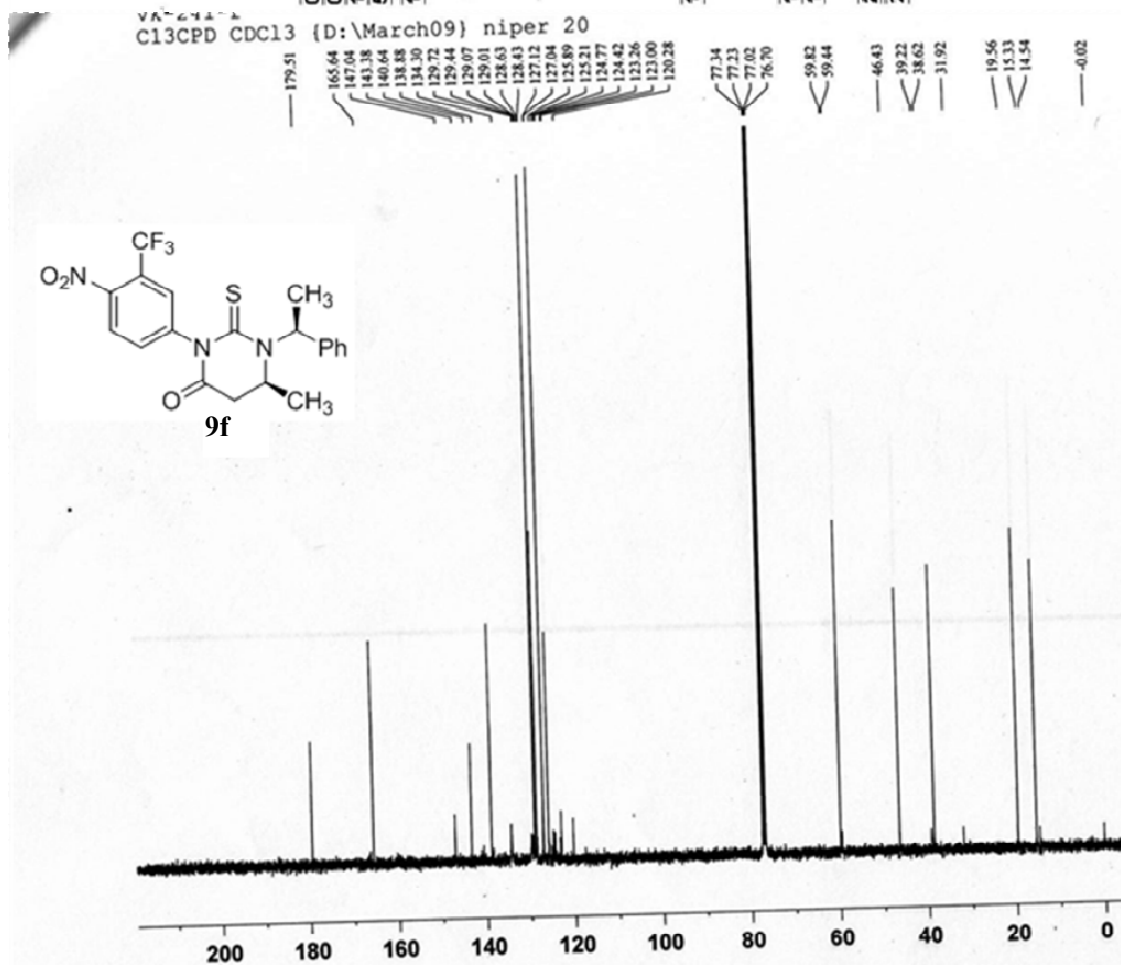
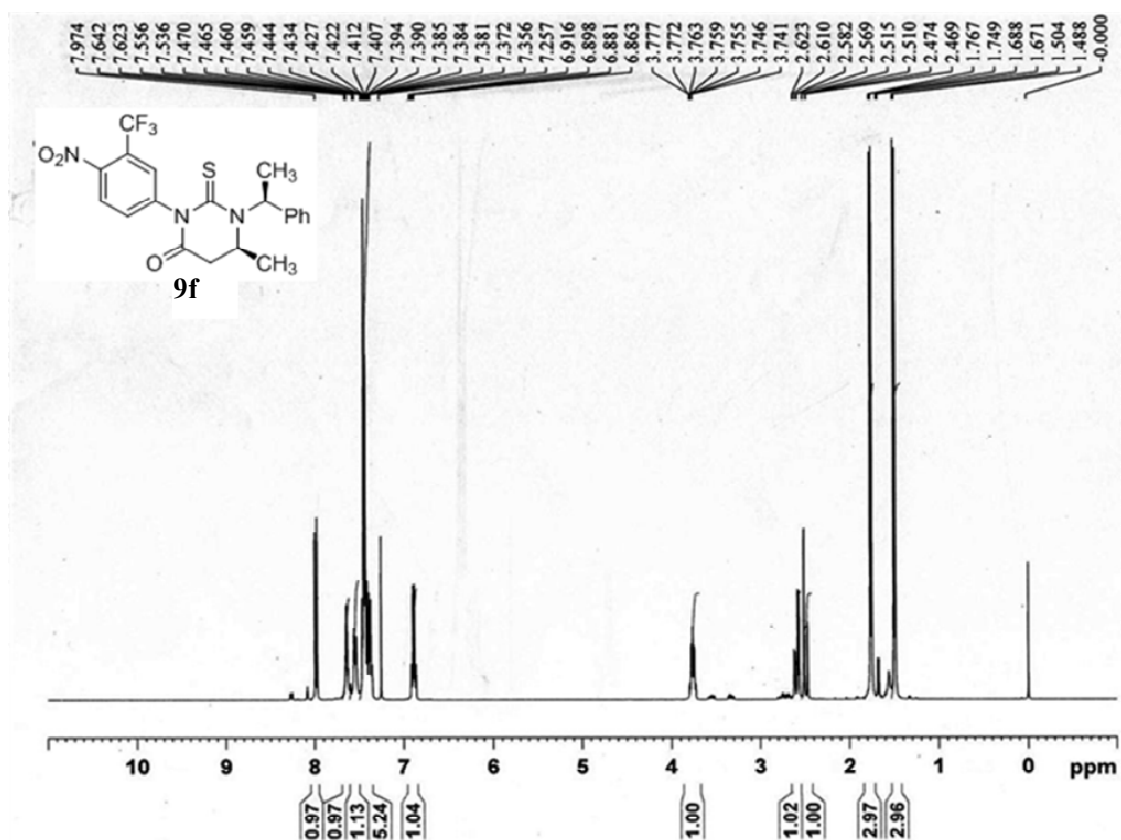


+MS, 2.7min #161

#	m/z	Res.	S/N	I	FWHM
1	185.1150	18942	109.8	6303	0.0098
2	208.1327	22290	204.5	20760	0.0093
3	209.0300	21151	13.6	1400	0.0099
4	222.1491	15701	2744.1	360048	0.0141
5	223.1516	20051	249.9	33349	0.0111
6	230.1153	15837	1809.7	269884	0.0145
7	231.1179	20309	115.4	17464	0.0114
8	244.1304	19094	378.4	68370	0.0128
9	245.1340	20217	20.0	3553	0.0121
10	252.0971	22979	22.4	3448	0.0110
11	274.0623	19218	13.9	1067	0.0143
12	283.0123	21752	49.5	3829	0.0130
13	296.0438	21539	29.4	2445	0.0137
14	301.1413	18126	22.4	1915	0.0166
15	305.1007	19575	15.4	1345	0.0156
16	314.0568	22034	29.3	2428	0.0143
17	327.0347	19747	29.4	2229	0.0166
18	333.1320	20728	35.3	2556	0.0161
19	413.2665	22011	33.5	3990	0.0188
20	418.1195	24093	157.9	22678	0.0174
21	419.1225	21176	14.1	2092	0.0198
22	440.1019	18060	910.5	147114	0.0244
23	441.1045	23914	127.2	20188	0.0184
24	442.1039	15271	14.2	2211	0.0290
25	456.0772	20315	11.5	1337	0.0225
26	458.1118	23294	127.3	14064	0.0197
27	459.1147	23170	16.0	1726	0.0198
28	472.1276	22119	26.9	2264	0.0213
29	474.1430	20768	17.3	1291	0.0228
30	499.1610	17748	19.9	809	0.0281



$[M+Na]^+$ Calcd : 440.1021
Found : 440.1029



Mass Spectrum List Report

Analysis Info

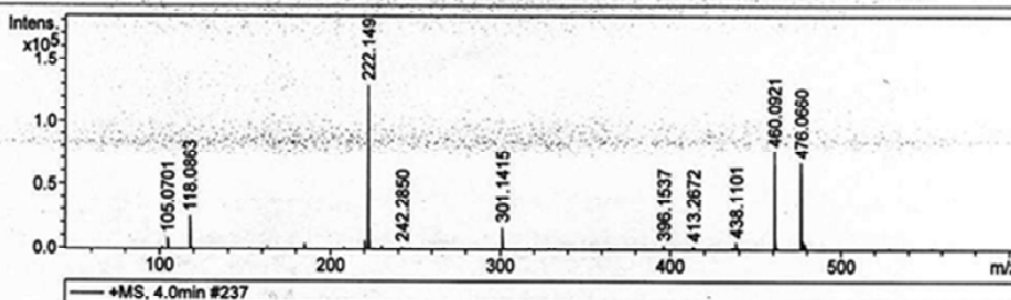
Analysis Name D:\Data\vipin\11-06-28-VN-3129-7.d
Method sodium formate tune_low.m
Sample Name VN-3129-7
Comment I

Acquisition Date 6/28/2011 2:39:42 PM

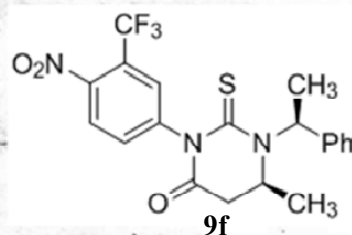
Operator VIKAS GROVER
Instrument / Ser# maXis 40

Acquisition Parameter

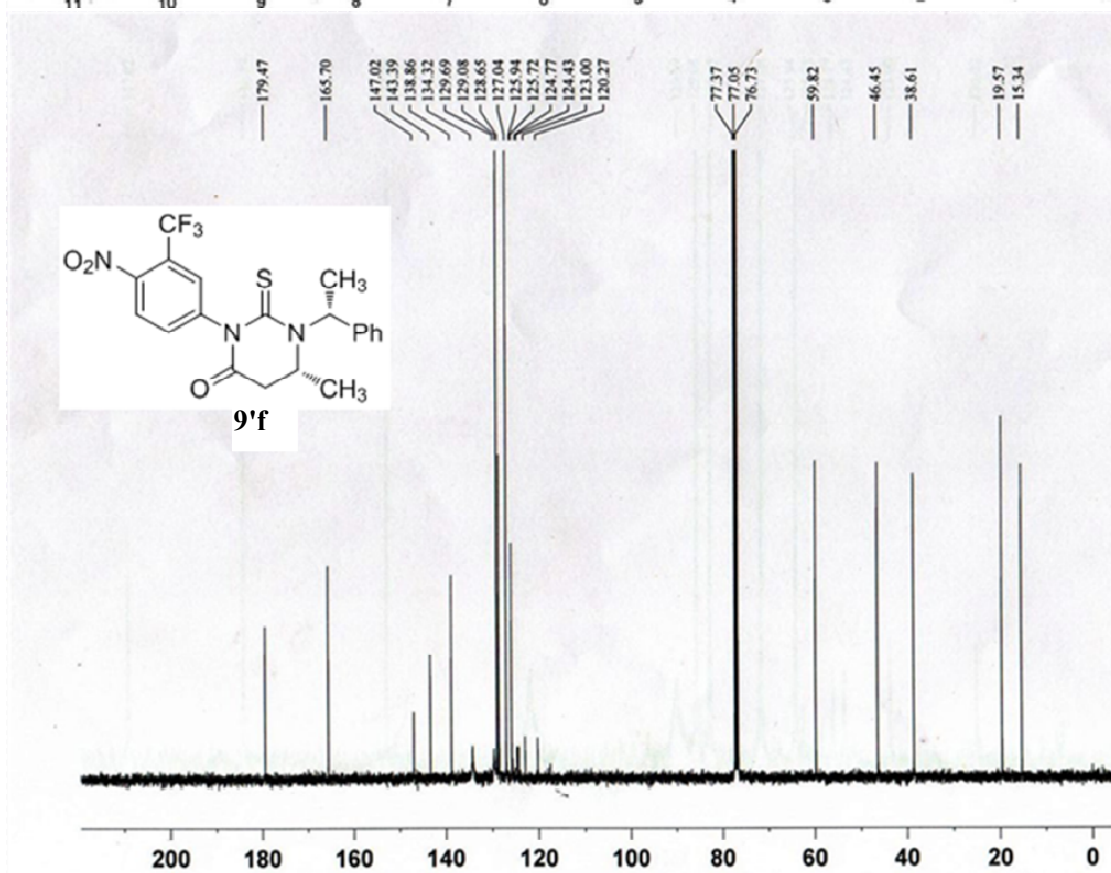
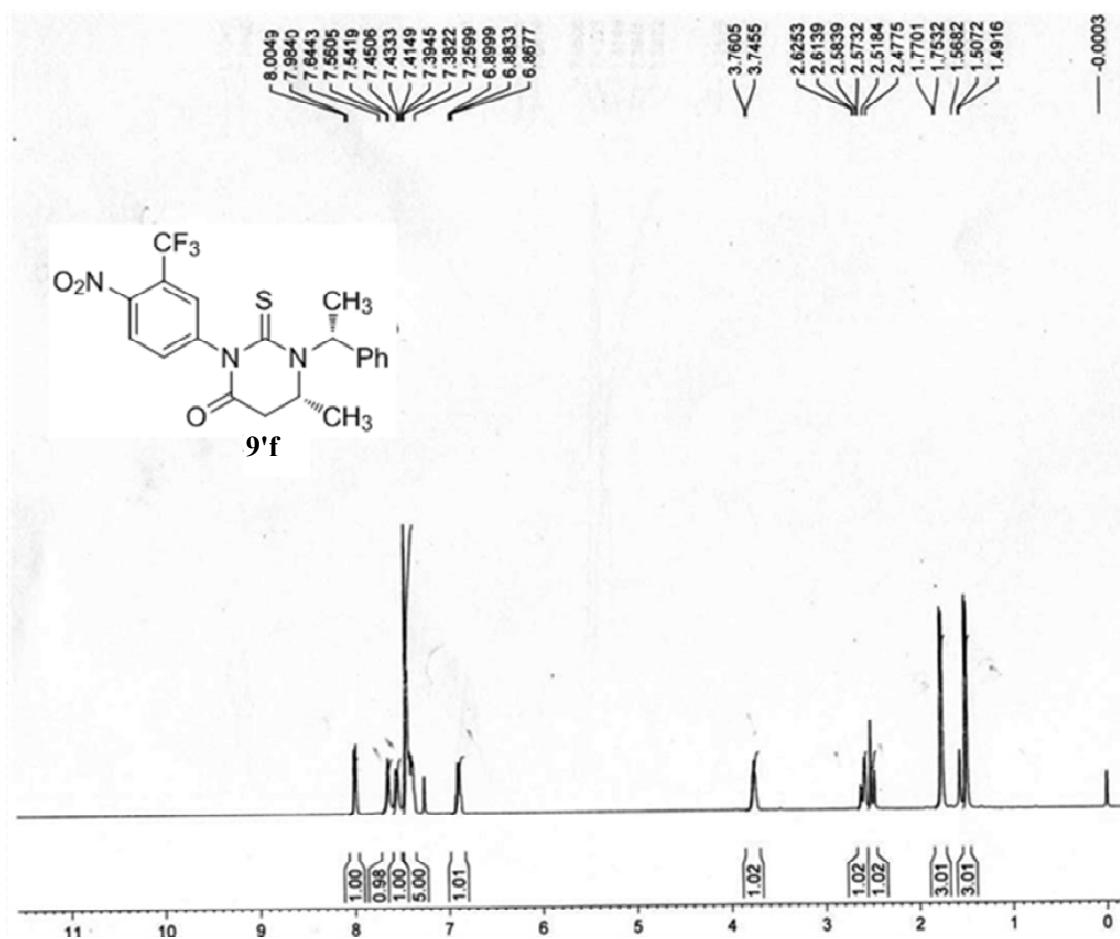
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



#	m/z	Res.	S/N	I	FWHM
1	105.0701	19133	130.7	8470	0.0055
2	118.0863	17857	145.4	24746	0.0066
3	220.1336	20969	70.7	7030	0.0105
4	222.1493	17663	1340.3	129055	0.0126
5	223.1527	21908	88.7	8396	0.0102
6	230.1159	20222	30.8	2578	0.0114
7	242.2850	20389	29.1	1870	0.0119
8	244.1316	21479	19.1	1171	0.0114
9	247.1792	20149	18.7	1056	0.0123
10	267.0478	22537	20.0	1195	0.0118
11	301.1415	23098	273.8	17157	0.0130
12	302.1455	20228	22.7	1409	0.0149
13	317.1160	22993	17.4	938	0.0138
14	326.9675	24594	11.8	580	0.0133
15	364.0594	25764	25.4	989	0.0141
16	365.1070	20993	10.8	426	0.0174
17	396.1537	22825	63.5	3283	0.0174
18	397.1578	19743	10.1	526	0.0201
19	413.2672	22948	51.0	2781	0.0180
20	414.2703	21362	10.3	564	0.0194
21	429.2420	22102	10.2	572	0.0194
22	436.0953	24398	27.0	1537	0.0179
23	438.1101	25297	101.2	5901	0.0173
24	439.1134	20410	12.9	765	0.0215
25	460.0921	23004	910.2	76669	0.0200
26	461.0949	25953	92.8	7929	0.0178
27	462.0945	15324	15.6	1349	0.0302
28	476.0660	24101	684.7	67018	0.0198
29	477.0694	25838	69.7	6697	0.0185
30	478.0992	22880	59.3	5595	0.0209



$[M+Na]^+$ Calcd.: 460.0919
found: 460.0921



Mass Spectrum List Report

Analysis Info

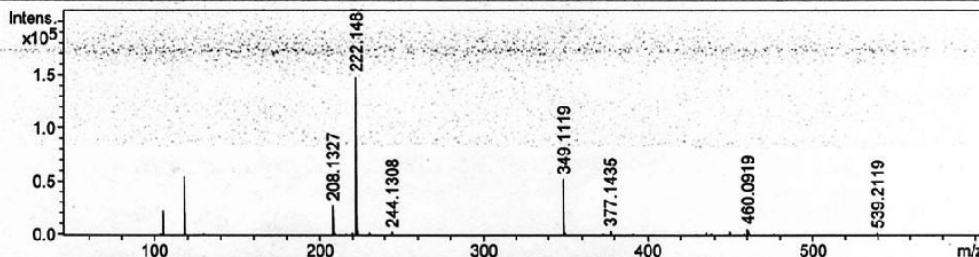
Analysis Name D:\Data\vipin\11-07-05-VN-3140-7.d
Method sodium formate tune_low.m
Sample Name VN-3140-7
Comment

Acquisition Date 7/5/2011 11:25:24 AM

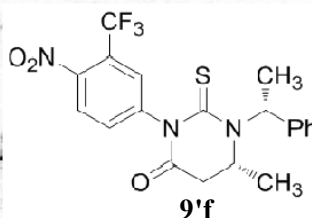
Operator VIKAS GROVER
Instrument / Ser# maxis 40

Acquisition Parameter

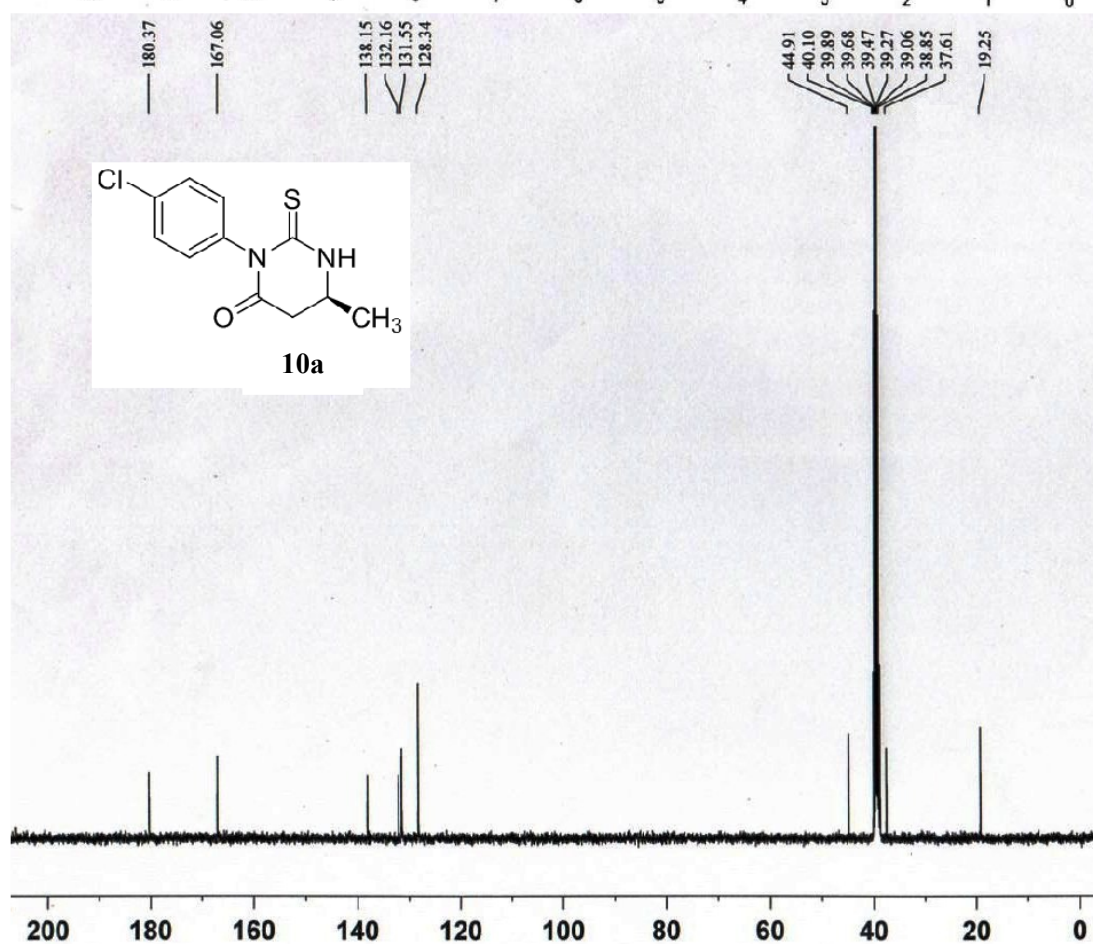
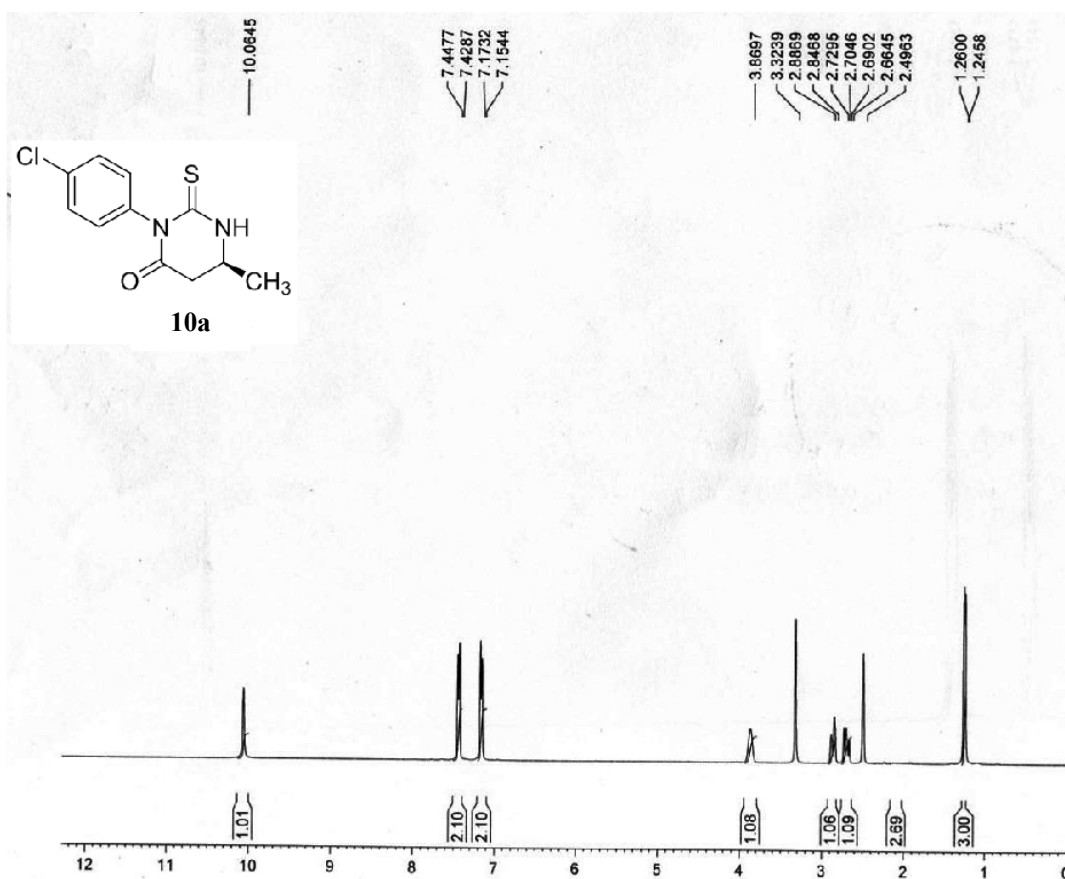
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



#	m/z	Res.	S/N	I	FWHM
1	119.0915	16499	13.2	947	0.0072
2	130.1607	19773	17.6	843	0.0066
3	153.1395	18683	10.3	269	0.0082
4	208.1327	21302	204.2	27389	0.0098
5	209.1366	20554	11.1	1525	0.0102
6	220.1335	20841	20.0	2613	0.0106
7	222.1488	18039	1185.1	148290	0.0123
8	223.1519	20526	63.6	7756	0.0109
9	230.1155	20836	18.0	1845	0.0110
10	244.1308	21624	45.4	2869	0.0113
11	292.0899	22917	16.7	390	0.0127
12	301.1418	17735	12.3	301	0.0170
13	319.1012	23470	10.0	265	0.0136
14	349.1119	23145	549.0	52565	0.0151
15	350.1153	21871	26.4	2599	0.0160
16	377.1435	23136	39.2	3777	0.0163
17	391.1599	24393	25.4	1568	0.0160
18	403.1607	23772	15.4	668	0.0170
19	419.1562	19860	11.9	634	0.0211
20	435.1497	22313	30.8	1948	0.0195
21	438.1109	23963	13.3	853	0.0183
22	449.1653	25609	53.9	3504	0.0175
23	458.1137	21865	21.0	1378	0.0210
24	460.0919	25078	93.5	6141	0.0183
25	461.0954	21878	12.7	836	0.0211
26	476.0692	18423	12.7	814	0.0258
27	525.1962	25165	15.3	380	0.0209
28	539.2119	24397	73.6	2133	0.0221
29	540.2160	20992	16.9	495	0.0257
30	604.7986	88349	0.2	2	0.0068



$[M+Na]^+$ Calcd.: 460.0919
Found: 460.0919



Mass Spectrum List Report

Analysis Info

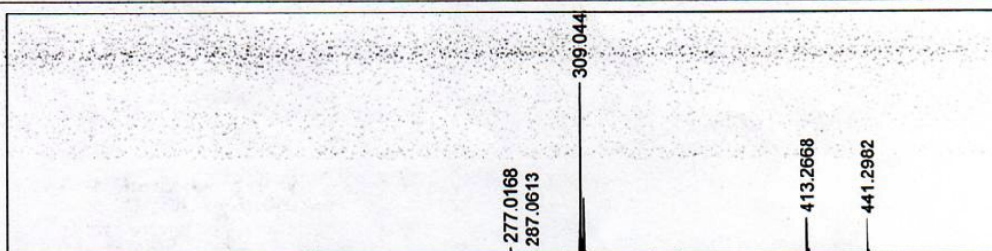
Analysis Name D:\Data\vipin\11-07-07-VN-3151-8.d
Method sodium-formate tune_low.m
Sample Name VN-3151-8
Comment I

Acquisition Date 7/7/2011 11:00:31 AM

Operator VIKAS GROVER
Instrument / Ser# maXis 40

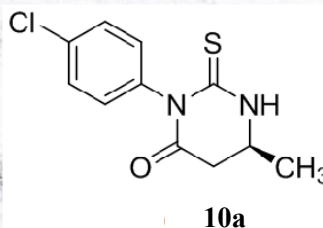
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	500 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



+MS, 15.2min #908

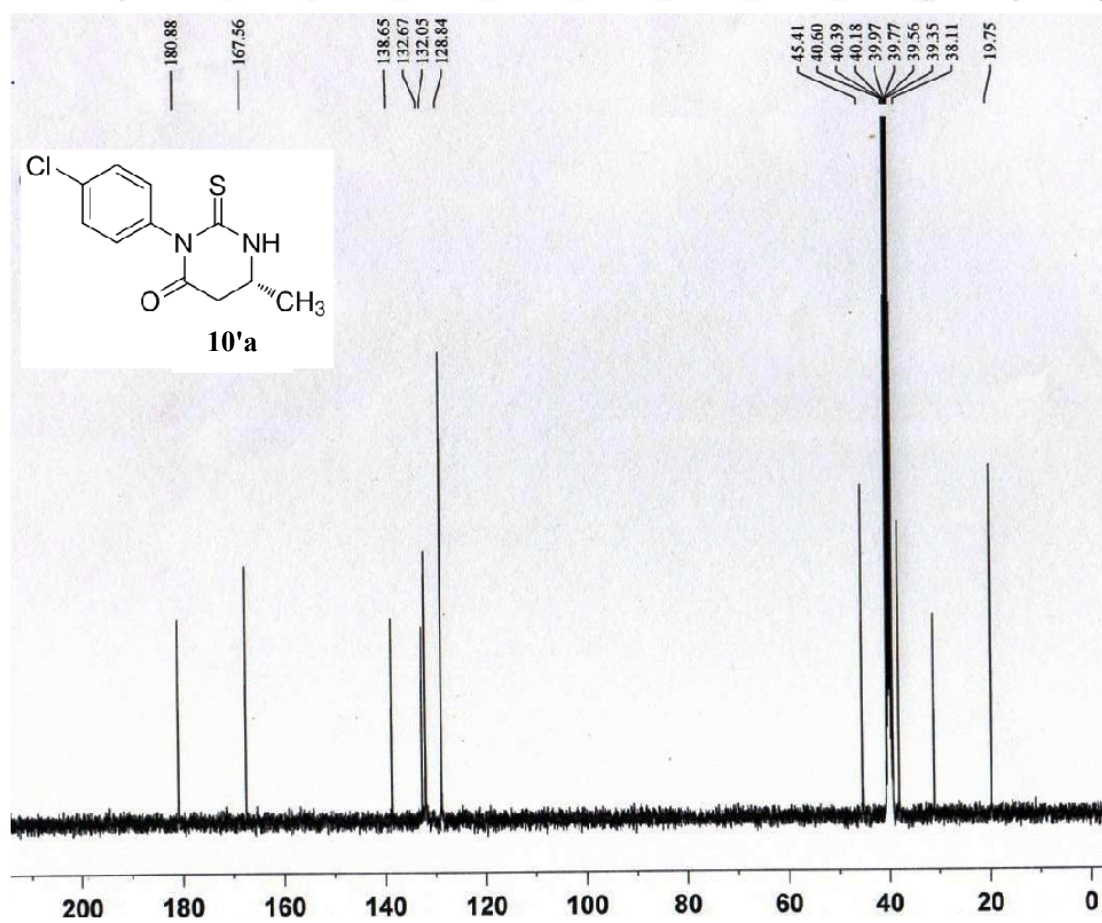
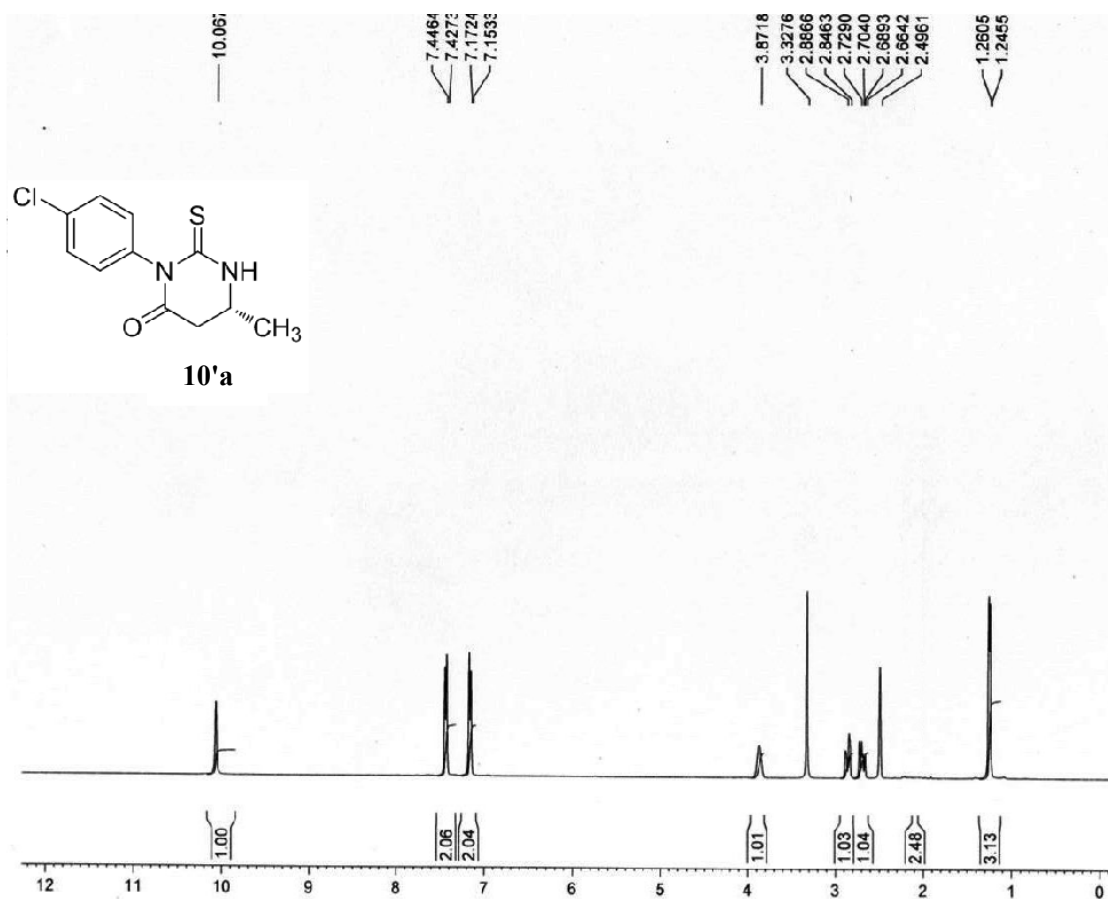
#	m/z	Res.	S/N	I	FWHM
1	217.1697	21720	80.6	4114	0.0100
2	222.1492	19759	22.0	1096	0.0112
3	255.0357	22177	36.4	2801	0.0115
4	277.0168	21668	207.1	29864	0.0128
5	278.0205	21511	11.3	1665	0.0129
6	279.0142	21427	41.9	6320	0.0130
7	287.0613	23890	71.3	12730	0.0120
8	289.0591	21803	14.8	2741	0.0133
9	301.1413	23367	23.4	5299	0.0129
10	309.0442	17393	2692.3	604242	0.0178
11	310.0462	21427	323.7	71006	0.0145
12	311.0409	17296	949.9	203536	0.0180
13	312.0433	22814	64.4	13471	0.0137
14	313.0387	17460	11.0	2240	0.0179
15	325.0187	19962	14.1	2020	0.0163
16	343.1994	23287	78.7	6725	0.0147
17	353.2668	21484	39.1	3305	0.0164
18	355.1061	21584	31.3	2615	0.0169
19	380.0816	21378	12.1	827	0.0178
20	381.2980	21241	29.4	1965	0.0180
21	391.2850	22351	18.4	1015	0.0175
22	413.2668	20479	1215.5	130378	0.0202
23	414.2699	24894	169.0	18767	0.0166
24	415.2745	21822	11.1	1271	0.0190
25	441.2982	21220	1114.2	124950	0.0208
26	442.3011	23998	164.0	17735	0.0184
27	443.3055	21492	13.7	1428	0.0206
28	457.2725	20895	28.0	1361	0.0219
29	489.0898	23828	34.1	1416	0.0205
30	491.0881	20438	20.6	856	0.0240



[M+Na]⁺

Calcd.: 277.0179

Found: 277.0168



Mass Spectrum List Report

Analysis Info

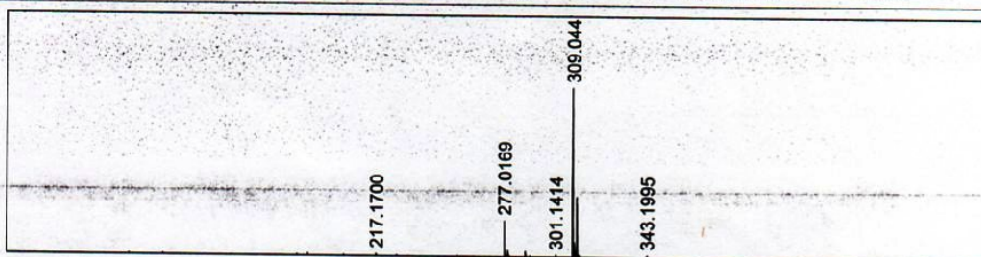
Analysis Name D:\Data\vipin\11-07-07-VN-3152-8.d
Method sodium formate tune_low.m
Sample Name VN-3152-8
Comment I

Acquisition Date 7/7/2011 12:06:45 PM

Operator VIKAS GROVER
Instrument / Ser# maXis 40

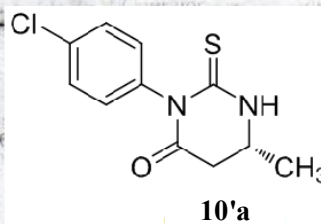
Acquisition Parameter

Source Type ESI Ion Polarity Positive
Focus Not active Set Capillary 4500 V Set Nebulizer 0.4 Bar
Scan Begin 50 m/z Set End Plate Offset -500 V Set Dry Heater 180 °C
Scan End 500 m/z Set Collision Cell RF 300.0 Vpp Set Dry Gas 4.0 l/min
Set Divert Valve Source



+MS, 4.0min #237

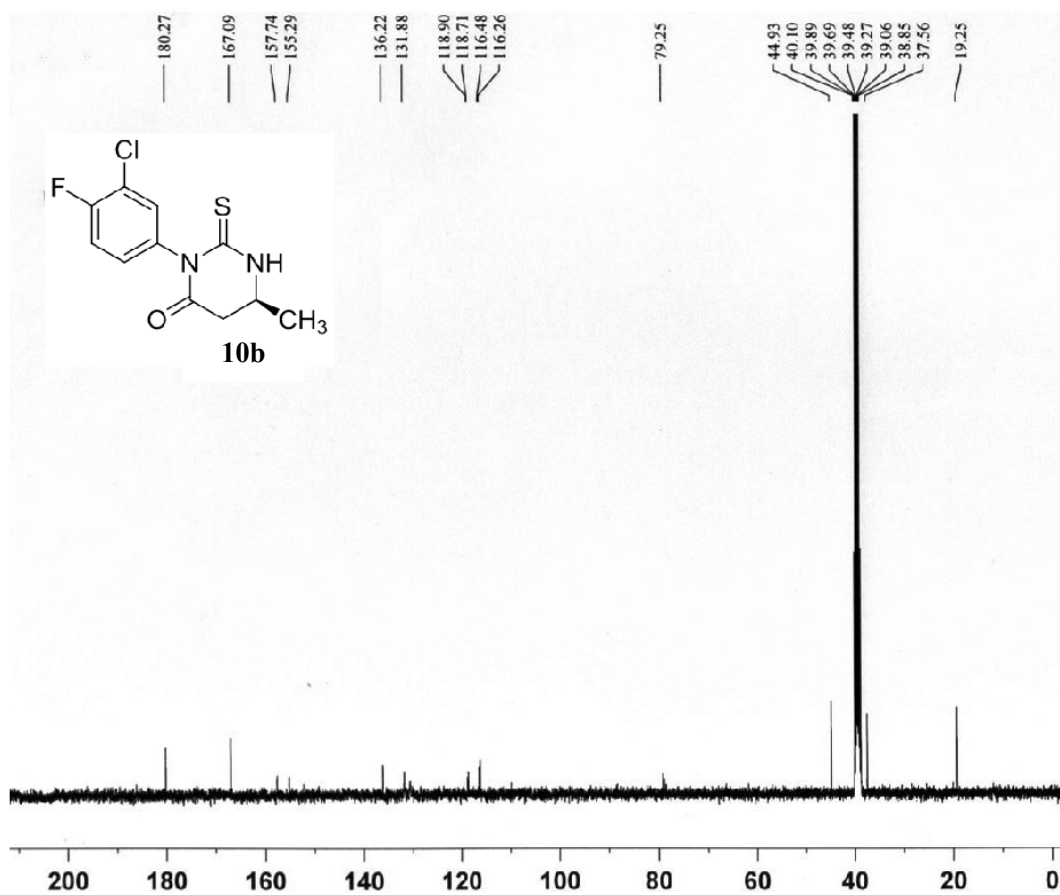
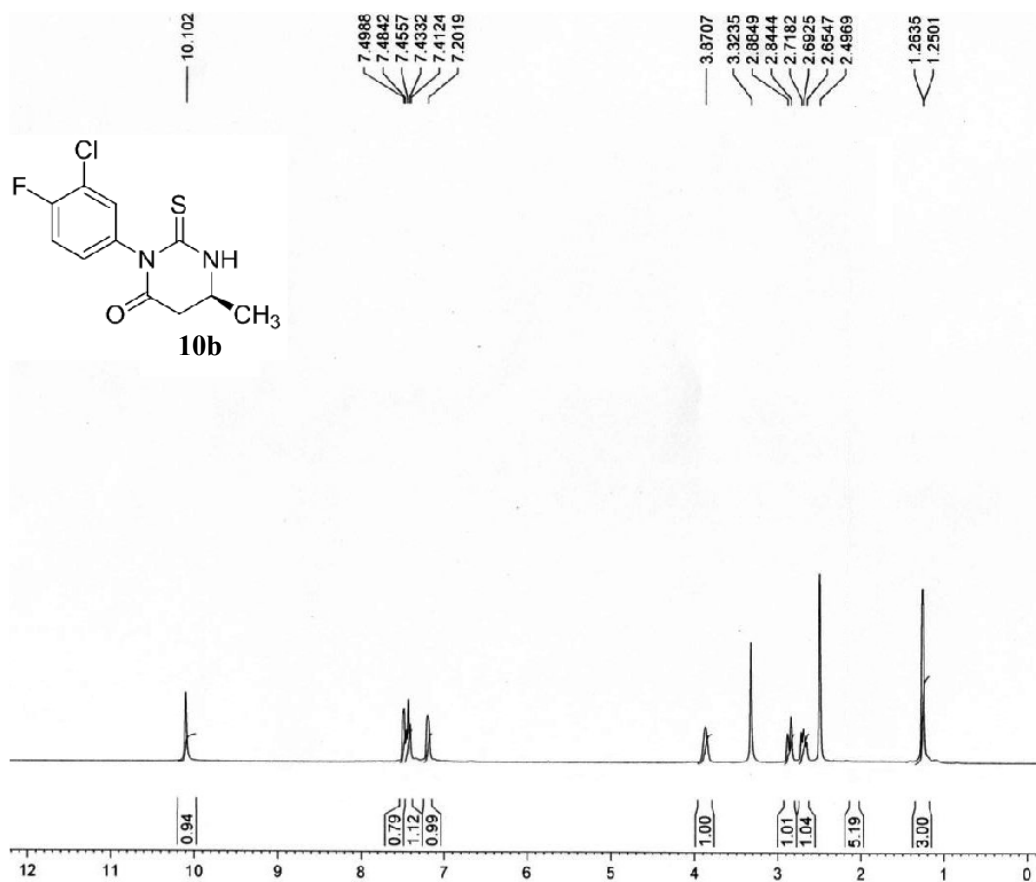
#	m/z	Res.	S/N	I	FWHM
1	118.0884	21870	37.9	2370	0.0054
2	130.1608	17343	10.2	598	0.0075
3	135.0699	17327	10.5	561	0.0078
4	158.9648	18314	37.0	1454	0.0087
5	180.1261	20069	33.6	1788	0.0090
6	185.1150	21182	78.6	4383	0.0087
7	202.1075	18679	24.5	1513	0.0108
8	217.1700	21664	74.8	4813	0.0100
9	226.9516	20283	40.2	2405	0.0112
10	255.0351	21898	38.1	3397	0.0116
11	277.0169	21011	415.0	66896	0.0132
12	278.0202	21819	16.0	2611	0.0127
13	279.0142	23052	80.1	13154	0.0121
14	287.0613	22308	64.0	11307	0.0129
15	289.0589	22188	15.8	2842	0.0130
16	301.1414	22105	22.6	4471	0.0136
17	309.0441	17016	1642.1	311743	0.0182
18	310.0452	23893	151.6	28114	0.0130
19	311.0408	19457	612.0	110818	0.0160
20	312.0437	23106	30.7	5430	0.0135
21	343.1995	22346	68.5	4554	0.0154
22	345.0055	22304	12.4	809	0.0155
23	362.9263	23877	18.4	1024	0.0152
24	377.0319	20588	16.2	759	0.0183
25	413.2667	23814	72.6	2962	0.0174
26	414.2707	21915	13.2	542	0.0189
27	430.9146	20022	13.2	604	0.0215
28	441.2980	20112	24.2	955	0.0219
29	489.0904	20887	13.3	415	0.0234
30	491.0832	19229	11.0	344	0.0255



[m+H]⁺

Calcd.: 277.0179

Found: 277.0169



Mass Spectrum List Report

Analysis Info

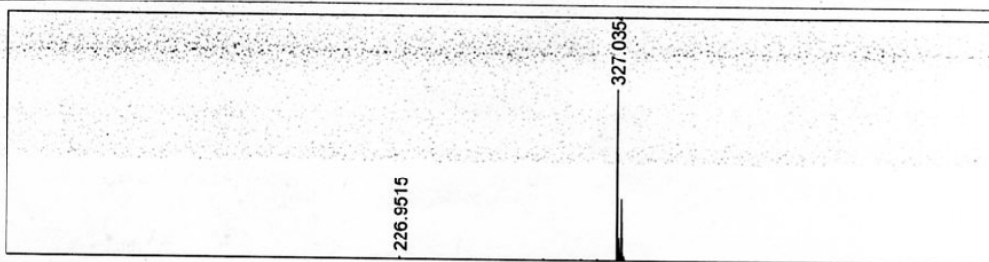
Analysis Name D:\Data\vipin\11-07-18-VN-3155-8P.d
Method sodium formate tune_low.m
Sample Name VN-3155-8P
Comment

Acquisition Date 7/18/2011 4:05:28 PM

Operator VIKAS GROVER
Instrument / Ser# maXis 40

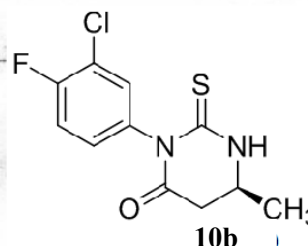
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	500 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source

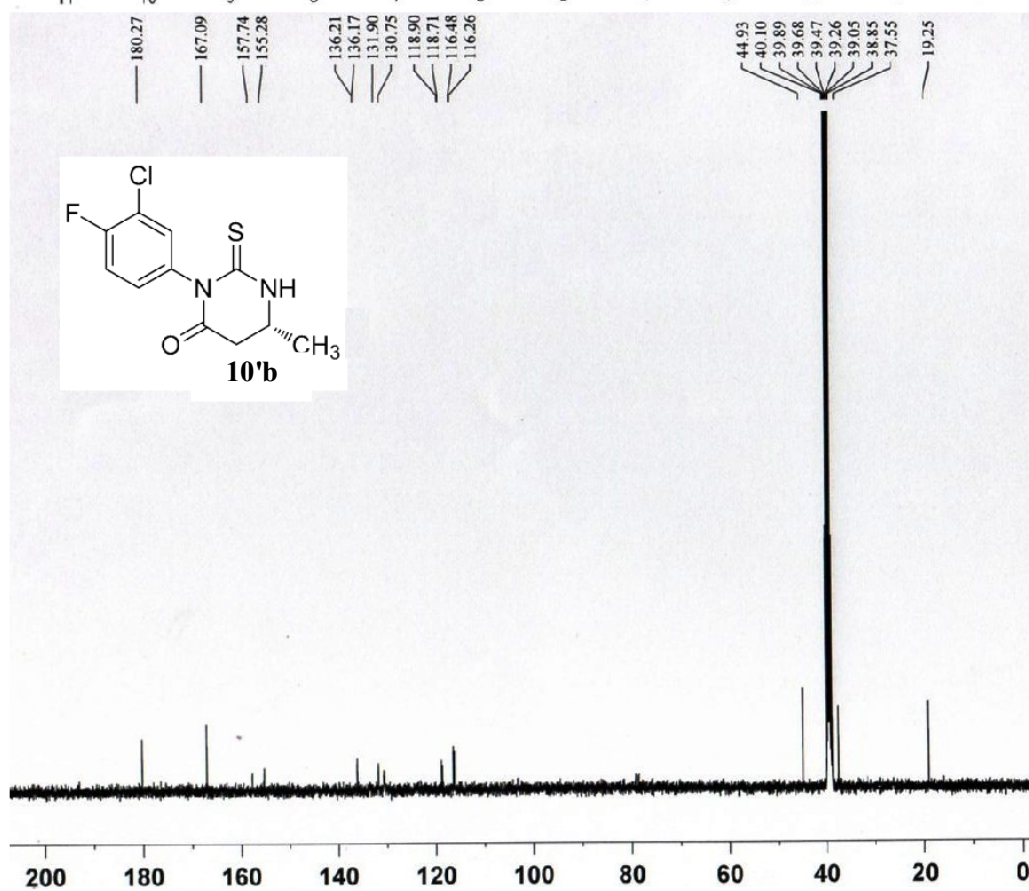
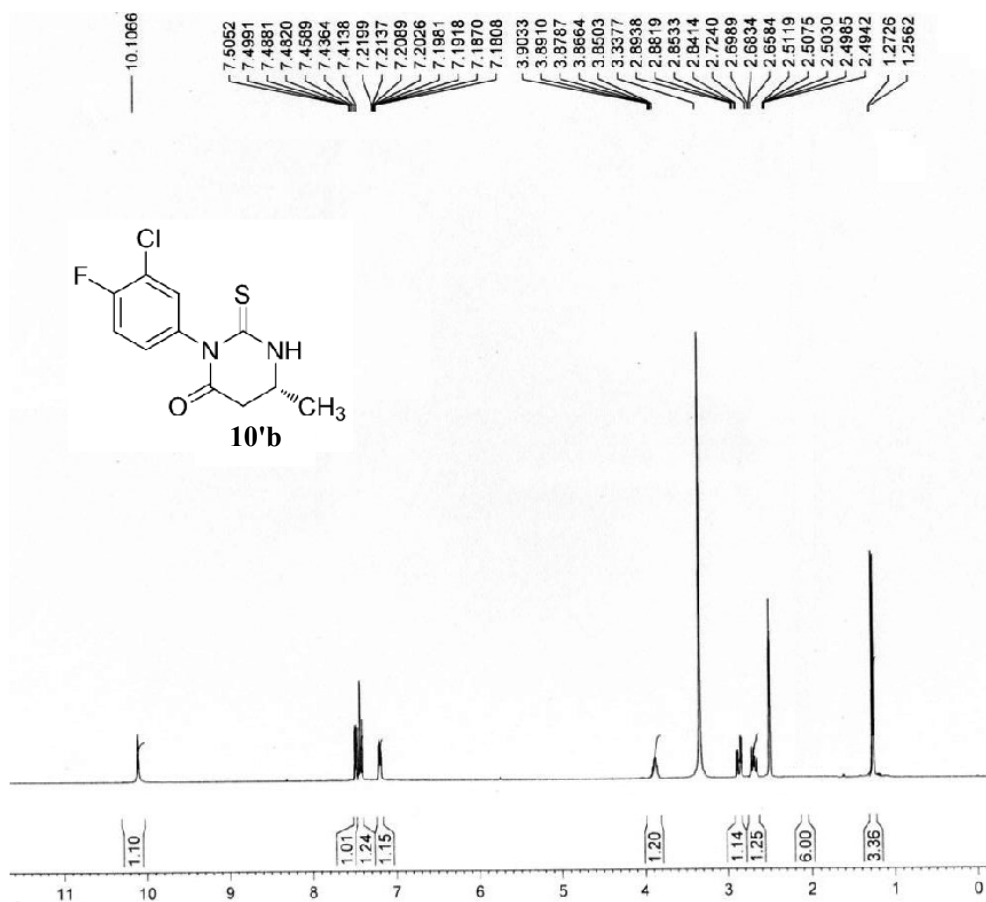


+MS, 1.6min #96

#	m/z	Res.	S/N	I	FWHM
1	118.0869	16827	24.6	880	0.0070
2	158.9644	18365	59.9	2795	0.0087
3	185.1155	18630	70.0	2982	0.0099
4	226.9515	20530	254.0	10557	0.0111
5	273.0812	20600	33.5	1253	0.0133
6	293.0726	18696	51.5	4845	0.0157
7	294.9395	19593	16.4	1635	0.0151
8	300.1003	21201	15.9	1836	0.0142
9	301.1412	21669	18.0	2146	0.0139
10	305.0529	21261	22.1	2903	0.0143
11	311.0573	22486	22.0	3610	0.0138
12	318.0904	22081	40.1	8220	0.0144
13	325.1894	20863	10.7	2634	0.0156
14	327.0354	16095	2847.2	730778	0.0203
15	328.0376	18255	363.5	95401	0.0180
16	329.0324	16463	996.5	267273	0.0200
17	330.0340	22232	81.0	22180	0.0148
18	331.0298	18289	11.9	3316	0.0181
19	362.9271	22391	22.8	1878	0.0162
20	395.0217	21262	26.2	1251	0.0186
21	399.0714	18932	16.3	787	0.0211
22	413.2668	22506	28.2	1572	0.0184
23	416.0749	19083	19.2	1099	0.0218
24	417.0812	22714	17.4	1004	0.0184
25	430.9150	19233	16.9	1015	0.0224
26	431.0982	20136	19.9	1192	0.0214



[M+H]⁺ Calcd.: 373.0265
Found: 373.0812



Mass Spectrum List Report

Analysis Info

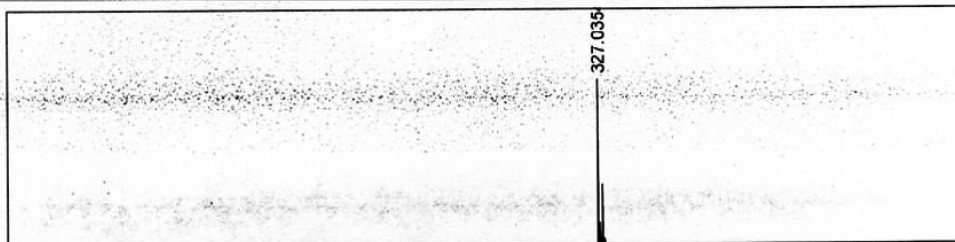
Analysis Name D:\Data\vipin\11-07-07-VN-3156-8.d
Method sodium formate tune_low.m
Sample Name VN-3156-8
Comment

Acquisition Date 7/7/2011 3:45:57 PM

Operator VIKAS GROVER
Instrument / Ser# maXis 40

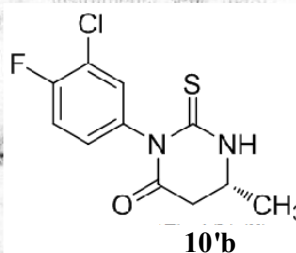
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	500 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source

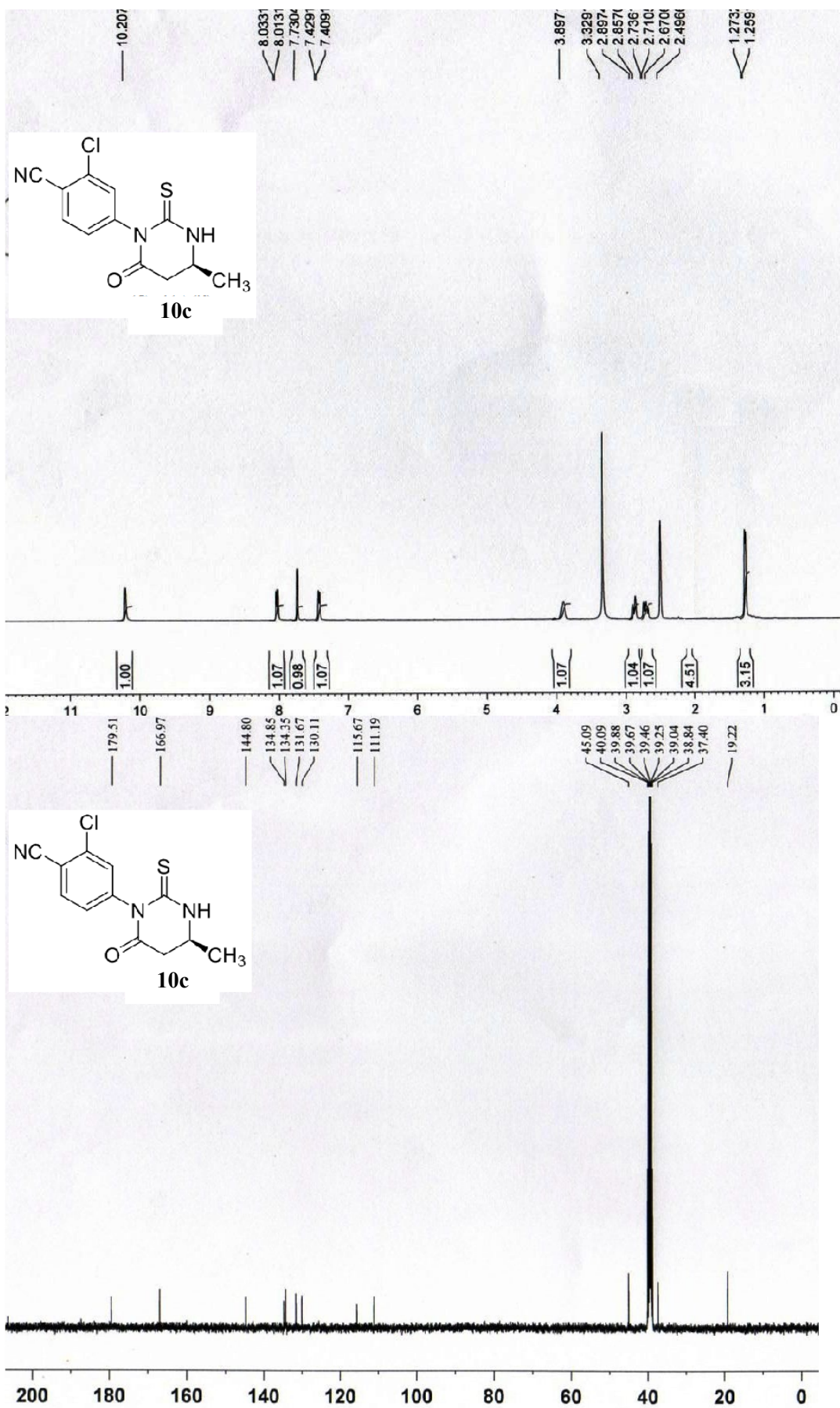


+MS, 1.4min #85

#	m/z	Res.	S/N	I	FWHM
1	132.1030	16821	33.0	1662	0.0079
2	158.9648	17544	27.6	1101	0.0091
3	185.1152	18969	59.6	2062	0.0098
4	226.9515	19685	98.1	4432	0.0115
5	236.1649	20410	100.3	4682	0.0116
6	264.1978	18002	30.6	1156	0.0147
7	293.0724	19137	53.8	3487	0.0153
8	294.9400	20500	26.7	1817	0.0144
9	295.0093	19232	15.3	1042	0.0153
10	301.1418	21047	26.3	2082	0.0143
11	305.0527	21754	37.9	3270	0.0140
12	327.0354	16675	5165.1	1013259	0.0198
13	328.0376	18494	657.2	132264	0.0177
14	329.0324	16741	1772.1	365612	0.0197
15	330.0343	22320	151.9	32108	0.0148
16	331.0302	17411	21.6	4878	0.0190
17	349.0166	23462	23.9	4059	0.0149
18	360.1733	21514	44.8	4764	0.0167
19	362.1711	20332	12.2	1153	0.0178
20	362.9272	22094	23.7	2148	0.0164
21	395.0227	21794	44.9	3158	0.0181
22	399.0714	22068	28.9	2039	0.0181
23	409.1164	20947	14.8	1052	0.0195
24	413.2675	21153	34.6	2469	0.0195
25	417.0826	23250	43.3	3100	0.0179
26	430.9147	21557	17.3	1193	0.0200
27	441.2969	23257	21.0	1167	0.0190
28	463.0098	22030	42.2	1429	0.0210
29	499.1618	22838	32.7	1236	0.0219



[M+Na]⁺ Calcd.: 345.0084
Found: 345.0093



Mass Spectrum List Report

Analysis Info

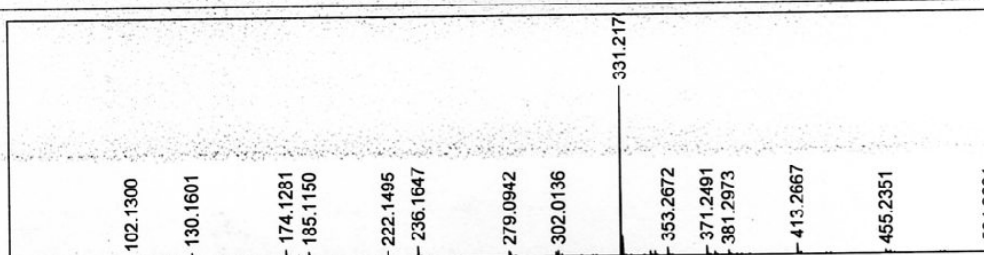
Analysis Name D:\Data\vipin\11-07-15-VN-3153-8.d
Method sodium formate tune_low.m
Sample Name VN-3153-8
Comment

Acquisition Date 7/15/2011 2:14:02 PM

Operator VIKAS GROVER
Instrument / Ser# maXis 40

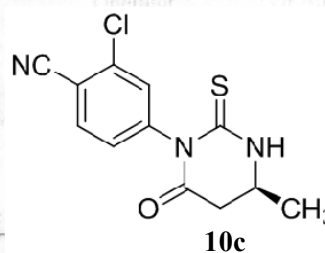
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	500 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source

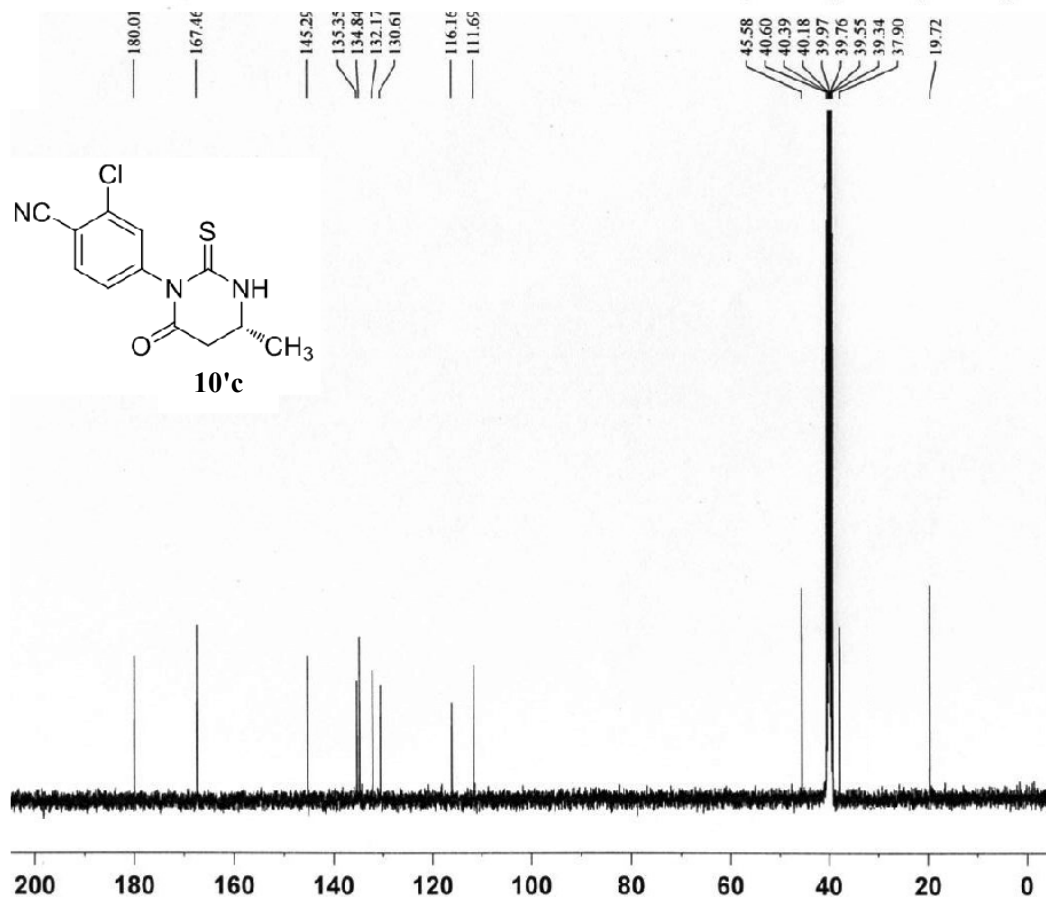
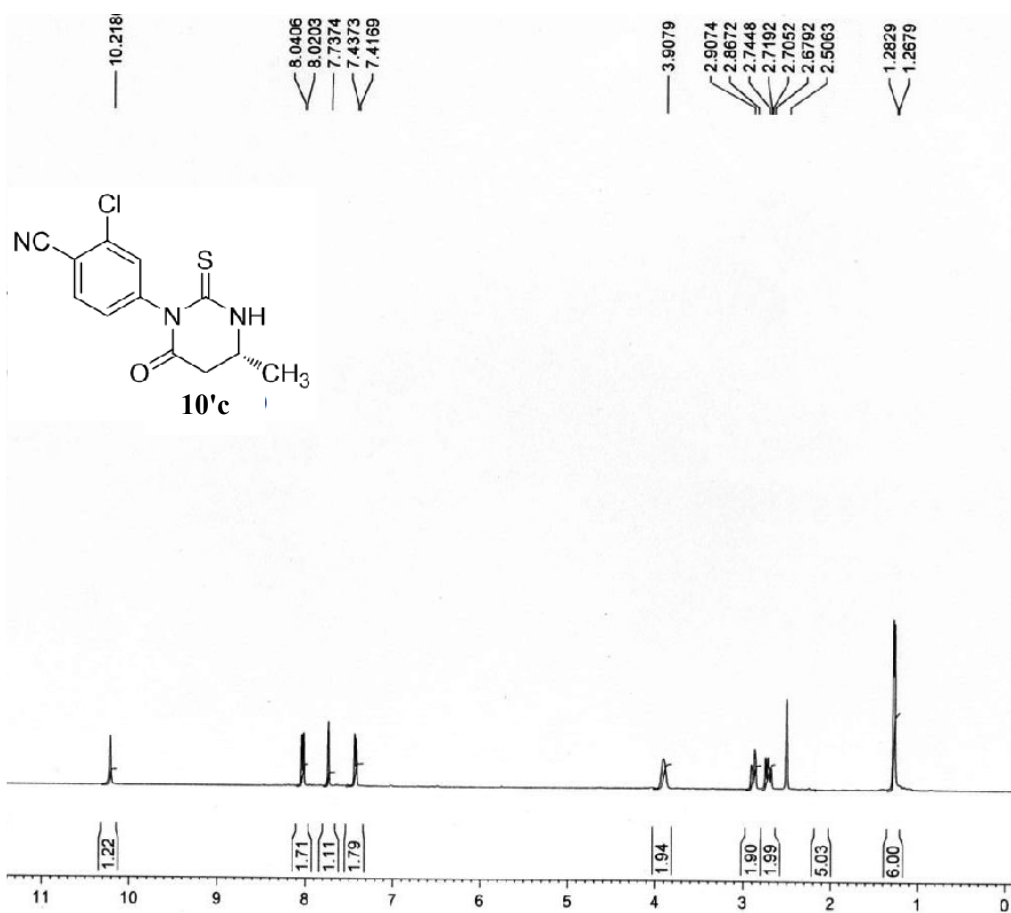


— +MS, 7.5min #445

#	m/z	Res.	S/N	I	FWHM
1	102.1300	19272	23.5	713	0.0053
2	130.1601	16700	41.9	1516	0.0078
3	132.1031	17980	16.7	599	0.0073
4	153.1390	18807	14.3	461	0.0081
5	158.0972	16565	12.9	447	0.0095
6	174.1281	17422	46.8	2003	0.0100
7	180.1264	15655	16.6	760	0.0113
8	185.1150	18760	32.5	1526	0.0099
9	222.1495	19034	31.3	1358	0.0117
10	236.1647	19695	55.8	2427	0.0120
11	279.0942	21290	32.1	1355	0.0131
12	280.0308	19492	22.3	947	0.0144
13	301.1419	17715	22.6	1111	0.0170
14	302.0136	19416	25.5	1260	0.0156
15	331.2170	22922	422.7	36697	0.0144
16	332.2203	22666	46.2	4078	0.0147
17	345.2330	23567	13.0	1079	0.0146
18	347.2487	17729	11.4	925	0.0196
19	353.2672	21226	23.8	1750	0.0156
20	371.2491	24146	34.8	1910	0.0154
21	375.2446	20462	15.2	802	0.0183
22	381.2973	21102	19.1	949	0.0181
23	413.2667	21257	47.0	2103	0.0194
24	415.2753	20286	12.7	575	0.0205
25	455.2351	19065	17.0	756	0.0239
26	457.2357	18756	10.4	457	0.0244
27	504.3381	20948	29.5	1119	0.0241



$[M+Na]^+$ calcd.: 302.0131
Found: 302.0136



Mass Spectrum List Report

Analysis Info

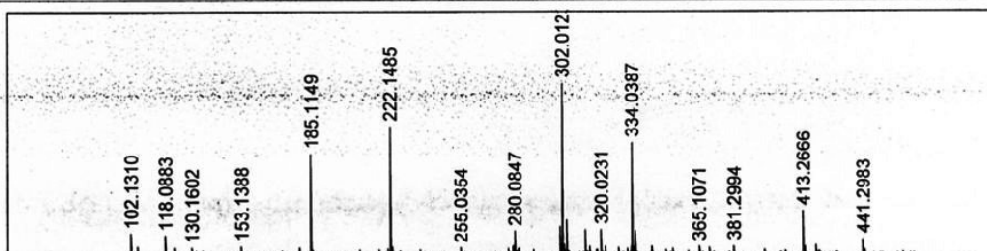
Analysis Name D:\Data\vipin\11-07-07-VN-3154-8.d
Method sodium formate tune_low.m
Sample Name VN-3154-8
Comment

Acquisition Date 7/7/2011 12:49:28 PM

Operator VIKAS GROVER
Instrument / Ser# maXis 40

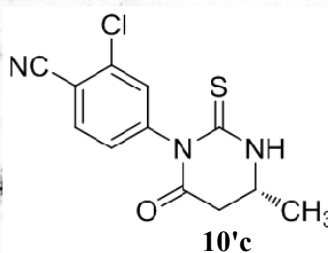
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	500 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source

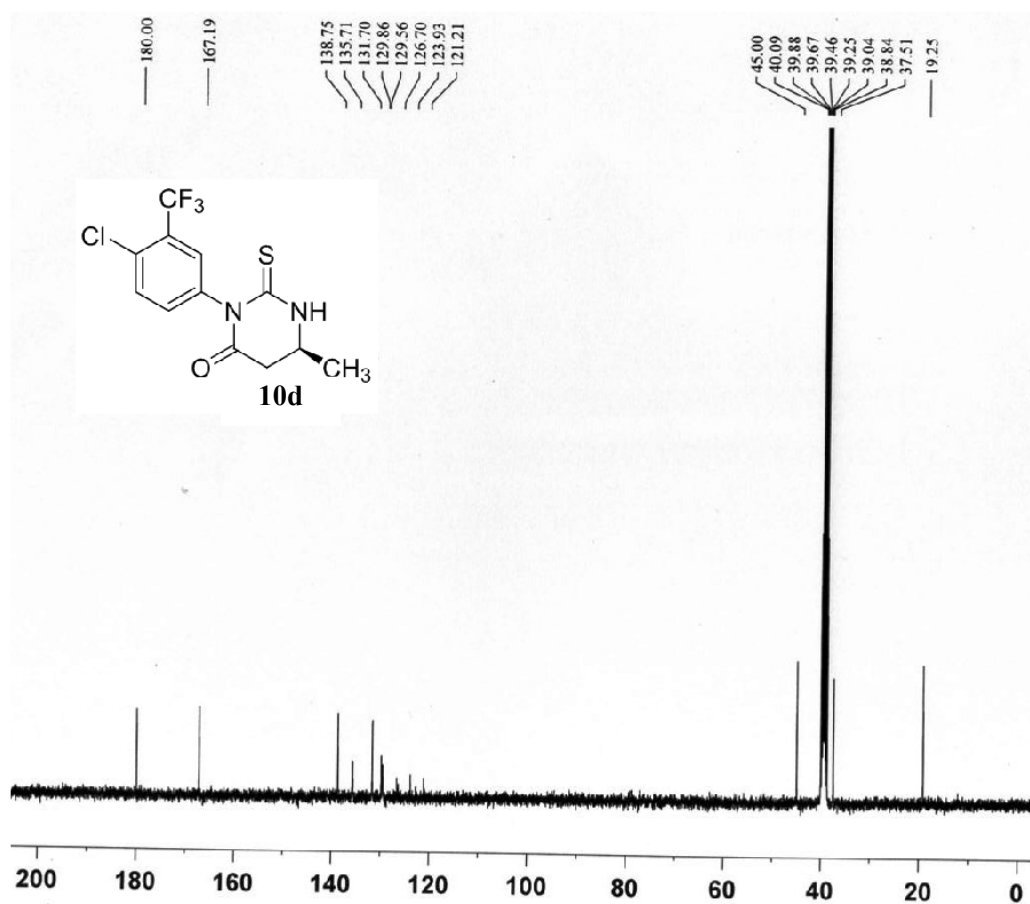
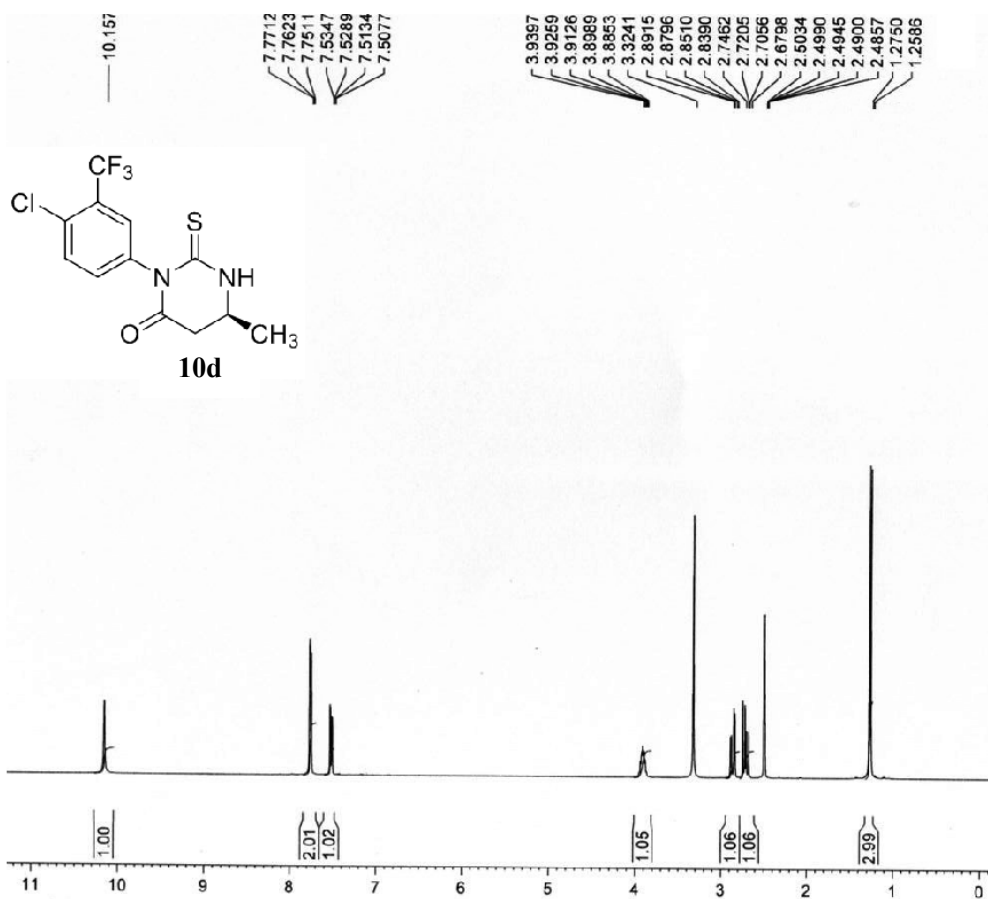


+MS, 9.5min #569

#	m/z	Res.	S/N	I	FWHM
1	102.1310	17033	39.5	1903	0.0060
2	105.0729	15253	15.7	757	0.0069
3	118.0883	18038	35.6	1710	0.0065
4	122.0980	19978	12.2	583	0.0061
5	130.1602	20681	13.3	594	0.0063
6	153.1388	18330	20.2	754	0.0084
7	185.1149	21035	133.9	9226	0.0088
8	222.1485	23194	145.4	11705	0.0096
9	255.0354	22900	11.5	616	0.0111
10	280.0847	20420	10.9	856	0.0137
11	280.0847	20943	26.8	2101	0.0134
12	301.1417	20645	19.1	2578	0.0146
13	302.0123	22863	114.3	15652	0.0132
14	304.0104	19607	21.8	3107	0.0155
15	313.0774	21597	16.5	2227	0.0145
16	320.0231	22156	18.0	2254	0.0144
17	334.0387	24169	98.1	10206	0.0138
18	336.0367	20130	20.7	2092	0.0167
19	365.1071	20547	12.4	699	0.0178
20	370.0020	17739	11.3	593	0.0209
21	381.2994	19218	15.3	737	0.0198
22	413.2666	23119	76.8	3934	0.0179
23	414.2706	20263	13.6	706	0.0204
24	419.0930	22040	15.3	836	0.0190
25	441.2983	21440	28.5	1367	0.0206



$[M+Na]^+$ Calcd.: 302.0131
Found: 302.0123



Mass Spectrum List Report

Analysis Info

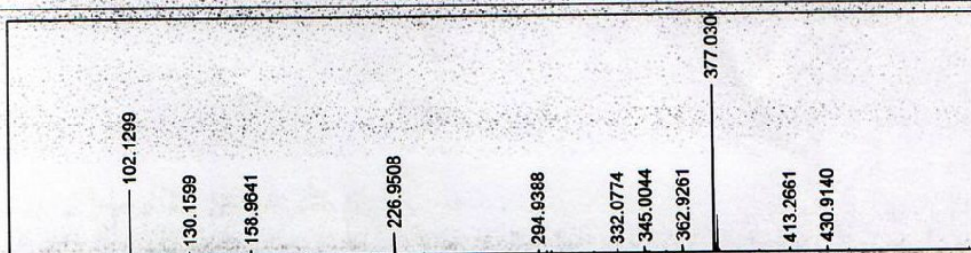
Analysis Name D:\Data\vipin\11-07-08-VN-3157-8.d
Method sodium formate tune_low.m
Sample Name VN-3157-8
Comment I

Acquisition Date 7/8/2011 9:46:26 AM

Operator VIKAS GROVER
Instrument / Ser# maXis 40

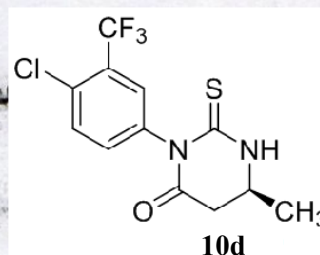
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	500 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source

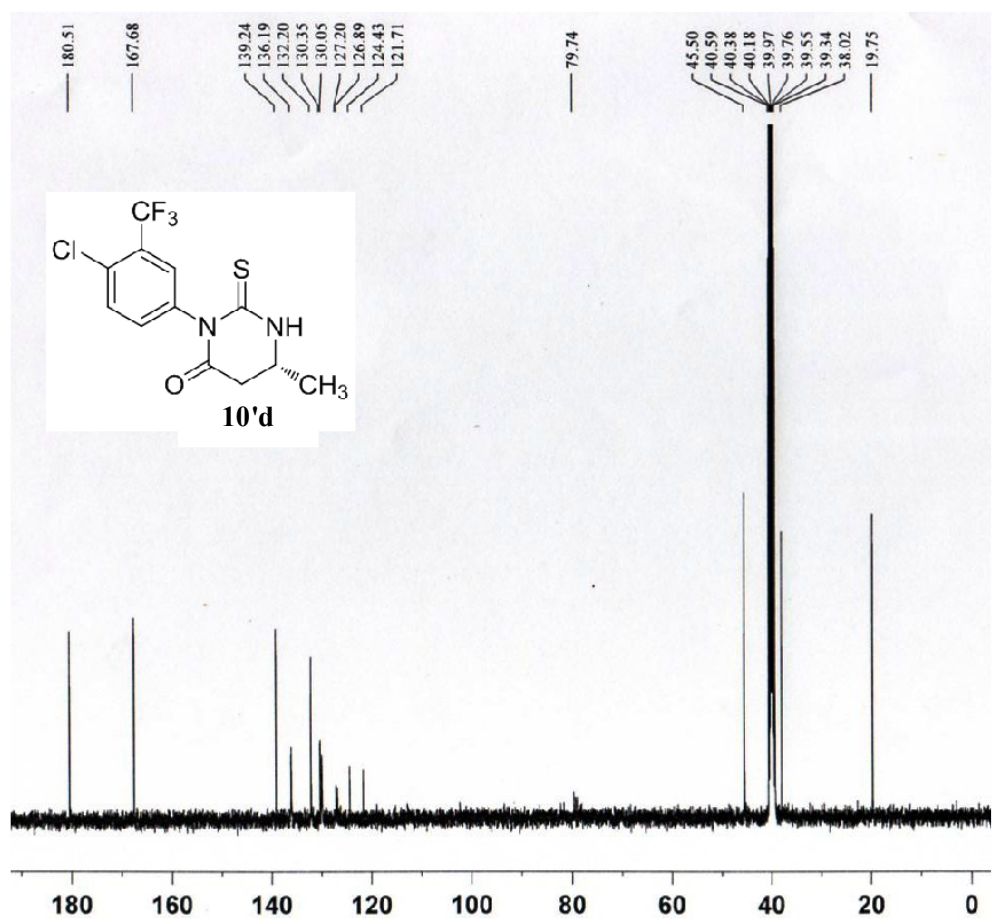
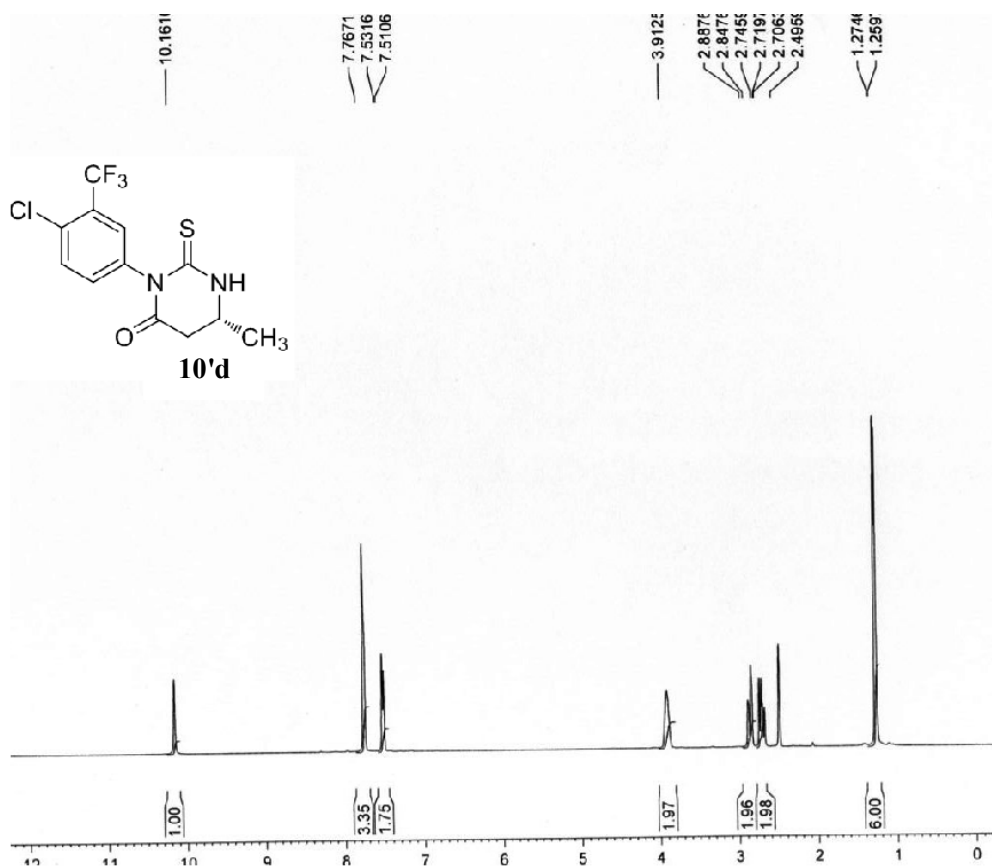


+MS, 1.7min #102

#	m/z	Res.	S/N	I	FWHM
1	102.1299	19020	417.7	40605	0.0054
2	103.1335	18253	10.8	1035	0.0057
3	130.1599	18535	46.1	2732	0.0070
4	153.1397	16374	10.5	522	0.0094
5	158.9641	18679	69.8	3244	0.0085
6	185.1146	21634	24.2	895	0.0086
7	226.9508	20770	218.8	13111	0.0109
8	240.9669	19300	19.7	805	0.0125
9	294.9388	20074	40.5	2154	0.0147
10	299.1104	20747	22.0	1256	0.0144
11	301.1410	22276	20.9	1235	0.0135
12	321.2409	20723	10.5	740	0.0155
13	332.0774	22771	24.4	1843	0.0146
14	345.0044	23582	36.3	3494	0.0146
15	362.9261	23725	28.4	3844	0.0153
16	377.0306	20765	926.4	100775	0.0182
17	378.0337	24658	51.1	5384	0.0153
18	379.0274	23063	218.2	22219	0.0164
19	380.0314	20006	13.5	1332	0.0190
20	399.0133	21906	24.7	944	0.0182
21	413.2661	23550	41.1	2061	0.0175
22	430.9140	21561	42.7	2675	0.0200
23	441.2982	19744	17.4	871	0.0224
24	498.9012	20133	49.1	1218	0.0248



[M+H]⁺ Calcd.: 345.0052
Found: 345.0044



Mass Spectrum List Report

Analysis Info

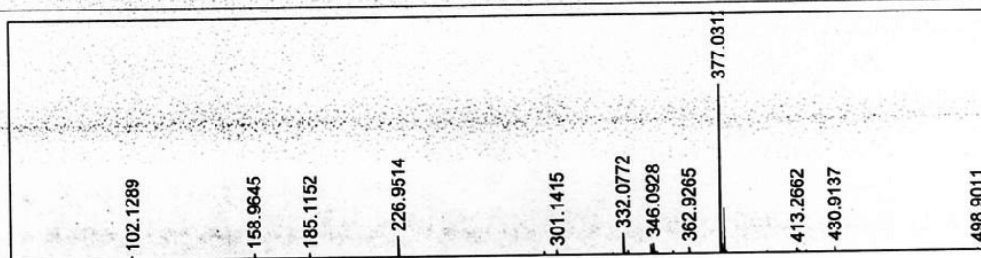
Analysis Name D:\Data\vipin\11-07-08-VN-3158-8.d
Method sodium formate tune_low.m
Sample Name VN-3158-8
Comment I

Acquisition Date 7/8/2011 1:19:00 PM

Operator VIKAS GROVER
Instrument / Ser# maXis 40

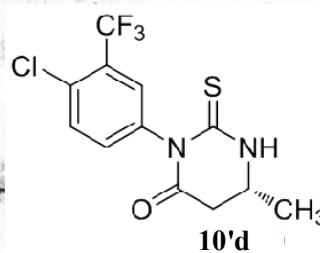
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	500 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source

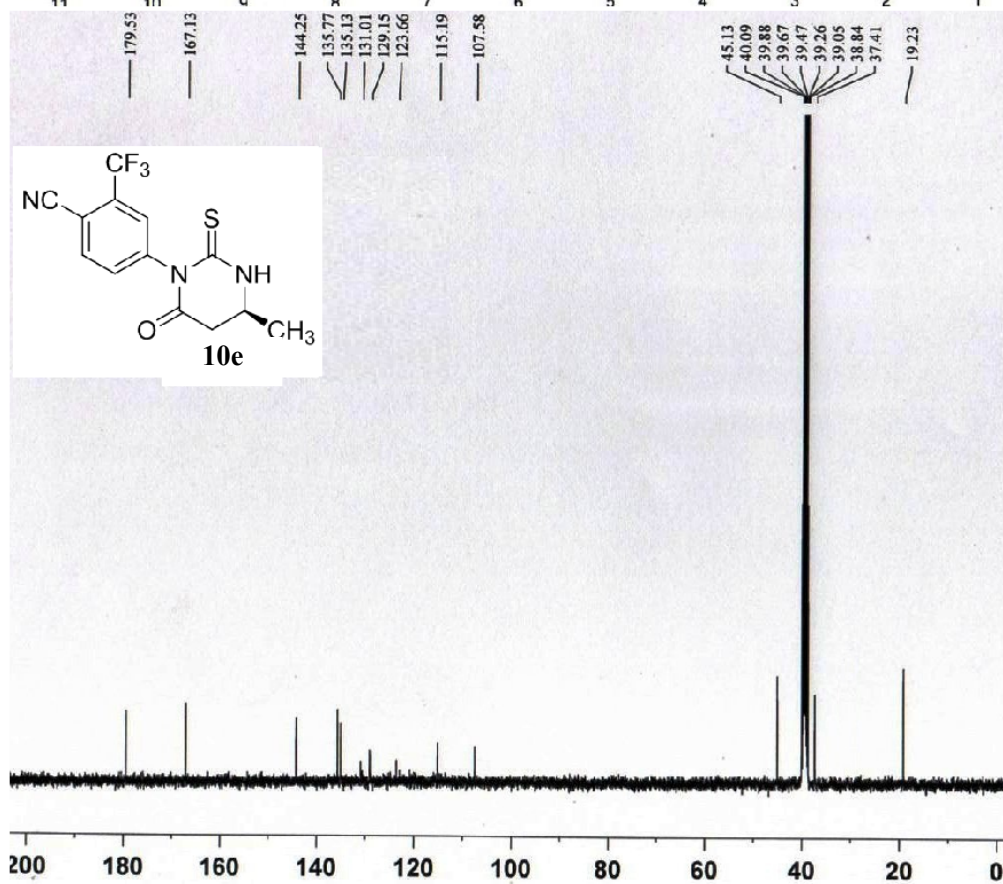
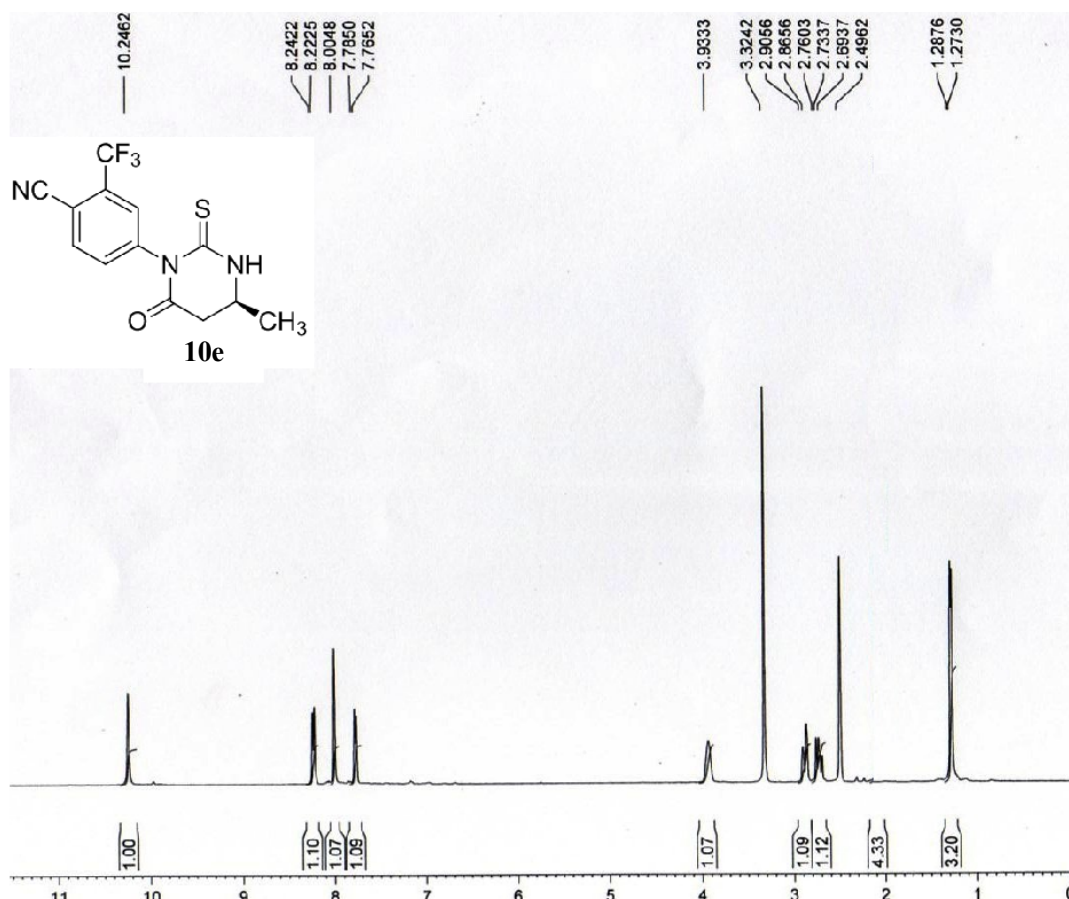


+MS, 2.1min #126

#	m/z	Res.	S/N	I	FWHM
1	102.1289	18027	39.4	2605	0.0057
2	130.1596	23275	10.6	460	0.0056
3	158.9645	18385	65.7	3501	0.0086
4	185.1152	22467	84.0	3547	0.0082
5	226.9514	21973	269.8	15921	0.0103
6	294.9393	22041	52.6	2655	0.0134
7	301.1415	22552	60.7	3409	0.0134
8	332.0772	23941	92.4	16139	0.0139
9	334.0752	22039	16.2	2968	0.0152
10	345.0048	24904	41.9	7877	0.0139
11	346.0928	24521	47.3	8851	0.0141
12	355.0496	22585	11.0	1998	0.0157
13	362.9265	24495	31.7	5649	0.0148
14	377.0312	20481	998.2	130176	0.0184
15	378.0339	24420	62.2	7832	0.0155
16	379.0280	23894	288.3	34993	0.0159
17	380.0310	25887	19.2	2241	0.0147
18	399.0140	21728	34.5	1357	0.0184
19	413.2662	23703	69.9	3967	0.0174
20	414.2703	24661	12.2	705	0.0168
21	417.1300	24315	11.0	675	0.0172
22	430.9137	24554	63.4	4531	0.0175
23	498.9011	23431	69.5	2264	0.0213



[M+Na]⁺ Calcd.: 345.0052
Found: 345.0048



Mass Spectrum List Report

Analysis Info

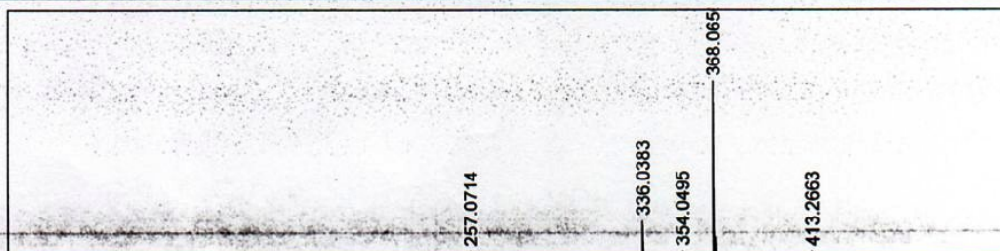
Analysis Name D:\Data\vipin\11-07-08-VN-3159-8.d
Method sodium formate tune_low.m
Sample Name VN-3159-8
Comment I

Acquisition Date 7/8/2011 1:47:41 PM

Operator VIKAS GROVER
Instrument / Ser# maXis 40

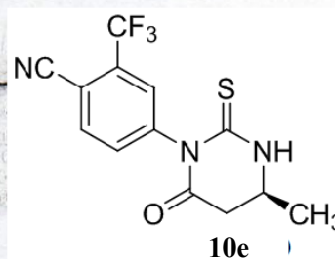
Acquisition Parameter

Source Type ESI Ion Polarity Positive Set Nebulizer 0.4 Bar
Focus Not active Set Capillary 4500 V Set Dry Heater 180 °C
Scan Begin 50 m/z Set End Plate Offset -500 V Set Dry Gas 4.0 l/min
Scan End 500 m/z Set Collision Cell RF 300.0 Vpp Set Divert Valve Source

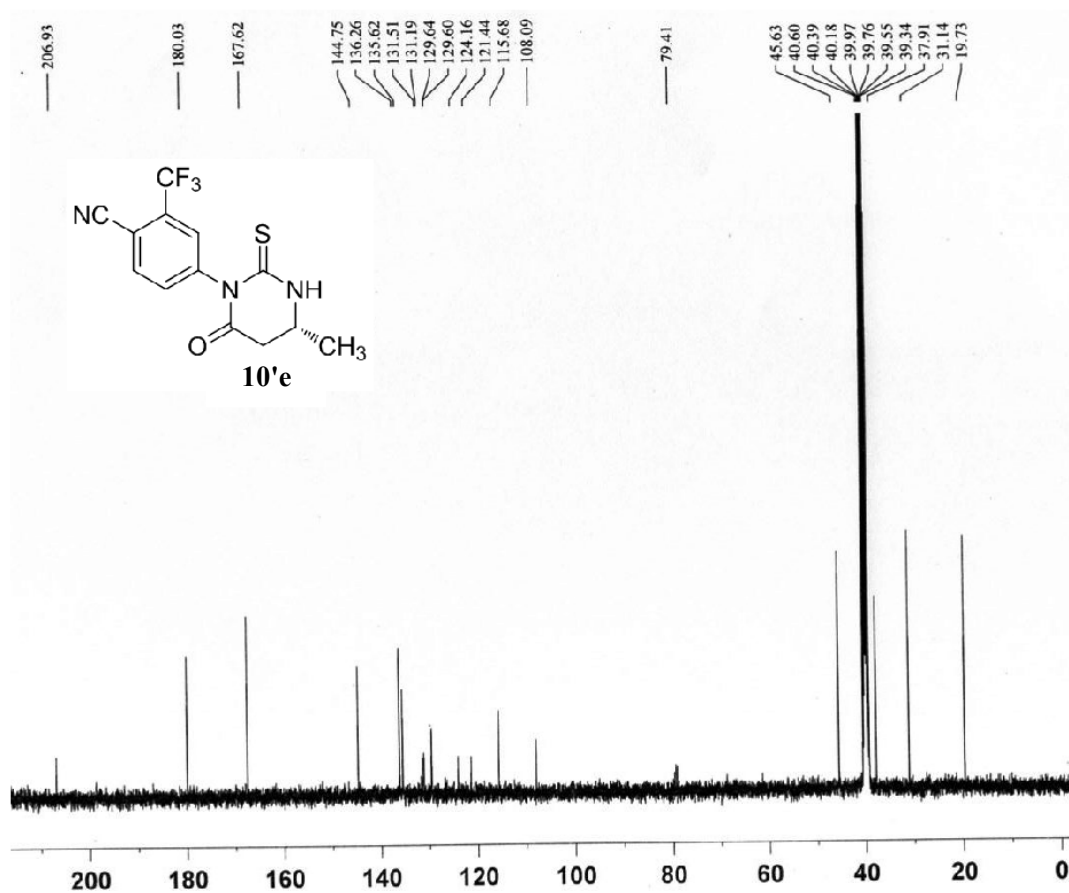
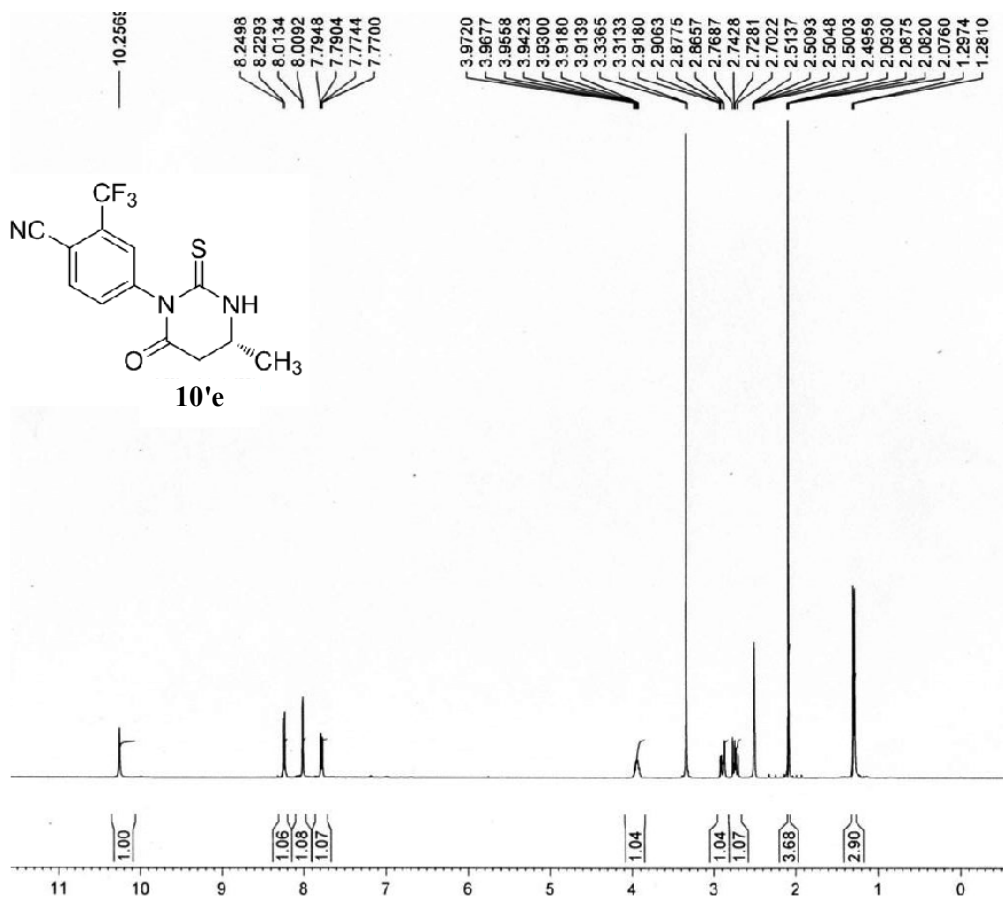


— +MS, 2.0min #117

#	m/z	Res.	S/N	I	FWHM
1	122.0985	15388	12.1	745	0.0079
2	123.0932	15327	18.5	1124	0.0080
3	130.1603	17387	14.3	803	0.0075
4	132.1032	18282	14.6	802	0.0072
5	146.1180	20615	12.6	573	0.0071
6	158.9645	18804	35.8	1516	0.0085
7	185.1147	20498	57.5	2797	0.0090
8	208.1329	19622	32.2	2530	0.0106
9	225.1961	20626	22.9	1950	0.0109
10	226.9513	19988	40.8	3461	0.0114
11	247.1779	20527	43.6	3495	0.0120
12	257.0714	21678	84.2	5715	0.0119
13	294.9392	19883	20.8	1181	0.0148
14	301.1411	22551	54.6	3284	0.0134
15	336.0383	21362	416.3	60940	0.0157
16	337.0416	22600	23.6	3492	0.0149
17	354.0495	24183	40.2	6883	0.0146
18	368.0656	18181	1779.3	312290	0.0202
19	369.0675	23000	187.3	32131	0.0160
20	370.0632	19243	30.0	5029	0.0192
21	390.0484	21114	10.5	929	0.0185
22	404.0271	23220	27.5	1789	0.0174
23	413.2663	22937	79.5	5857	0.0180
24	414.2710	17926	13.0	968	0.0231
25	435.0652	22484	28.3	2213	0.0194
26	441.2977	22299	26.8	1856	0.0198
27	468.3834	21118	13.7	606	0.0222
28	488.0915	22393	31.6	1380	0.0218
29	498.9019	21255	11.5	502	0.0235
30	504.0389	26945	11.3	495	0.0187



[M+Na]⁺ Calcd.: 336.0395
Found: 336.0383



Mass Spectrum List Report

Analysis Info

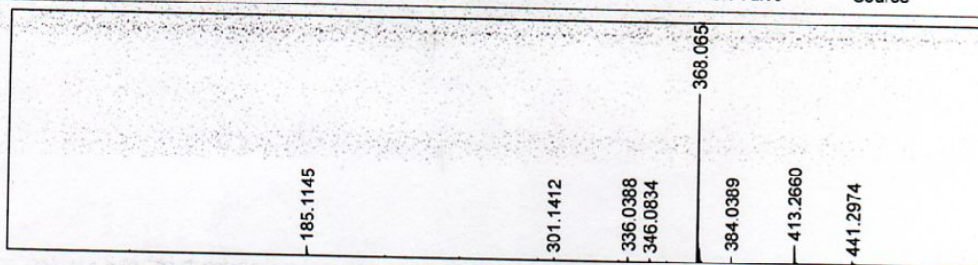
Analysis Name D:\Data\vipin\11-07-15-VN-3160-8.d
Method sodium formate tune_low.m
Sample Name VN-3160-8
Comment

Acquisition Date 7/15/2011 2:03:37 PM

Operator VIKAS GROVER
Instrument / Ser# maXis 40

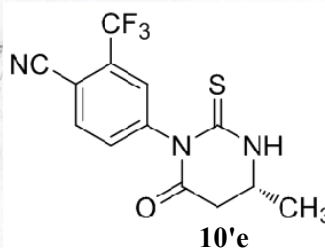
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	500 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source

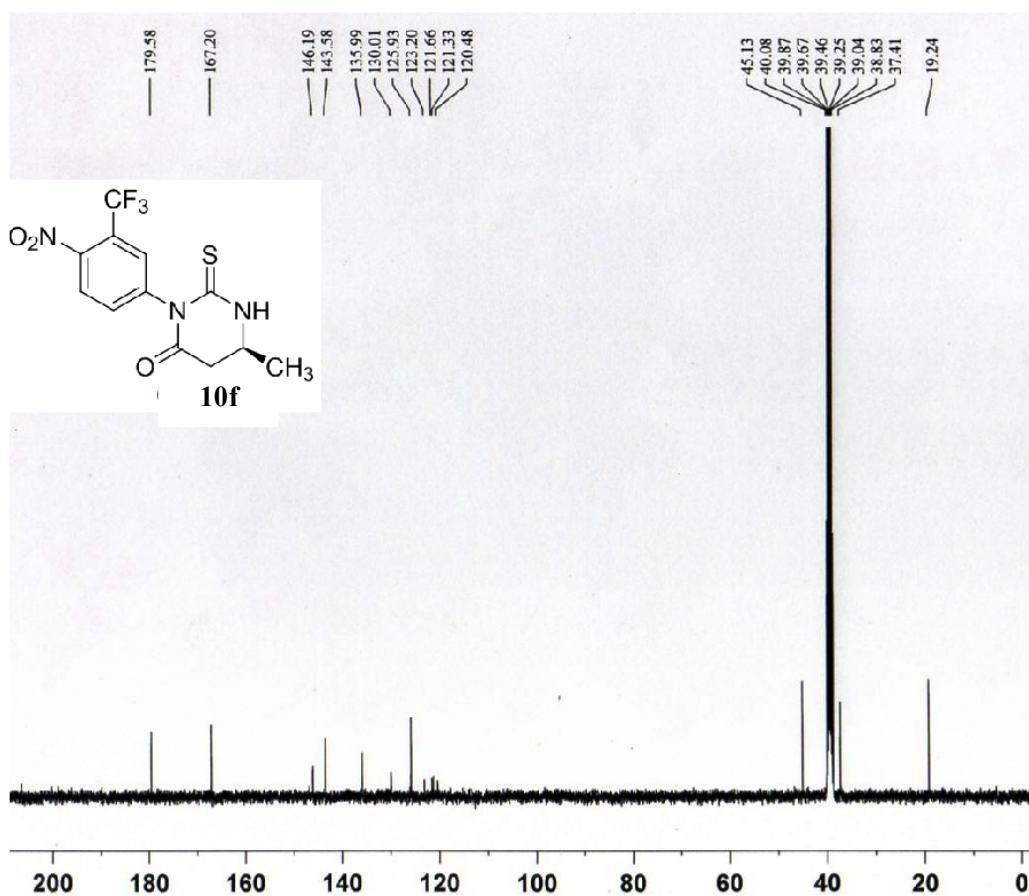
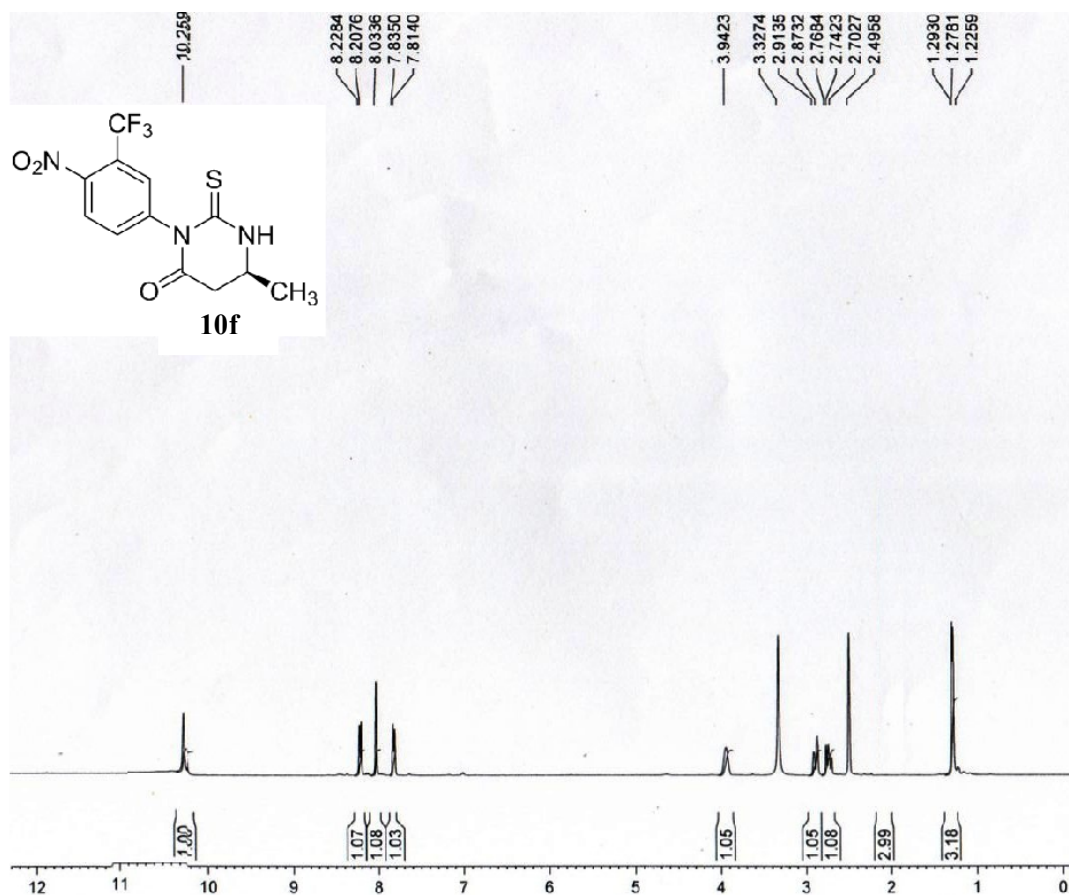


+MS, 3.6min #217

#	m/z	Res.	S/N	I	FWHM
1	102.1302	17721	39.1	1167	0.0058
2	118.0887	16844	12.6	428	0.0070
3	130.1604	17532	22.8	788	0.0074
4	149.0244	15452	13.6	459	0.0056
5	174.1277	19690	11.0	630	0.0088
6	185.1145	20078	155.4	10099	0.0092
7	222.1489	18773	25.4	989	0.0118
8	257.0719	19332	34.3	1312	0.0133
9	294.0515	20027	23.6	1080	0.0147
10	301.1412	20593	59.0	2916	0.0146
11	314.0565	19376	10.8	637	0.0162
12	331.2170	20887	17.5	1302	0.0159
13	336.0388	21265	76.5	6017	0.0159
14	346.0834	20326	36.3	3658	0.0170
15	368.0654	17297	1390.0	201734	0.0213
16	369.0677	23669	117.1	15693	0.0156
17	370.0635	18950	21.0	2935	0.0195
18	384.0389	22745	83.6	3621	0.0169
19	413.2660	24364	273.8	22725	0.0170
20	414.2694	22040	30.7	2575	0.0188
21	441.2974	22060	73.5	5204	0.0200
22	442.3007	21363	14.3	980	0.0207
23	488.0904	25338	12.8	373	0.0193



[M+Na]⁺ Calcd.: 336.0395
Found: 336.0388



Mass Spectrum List Report

Analysis Info

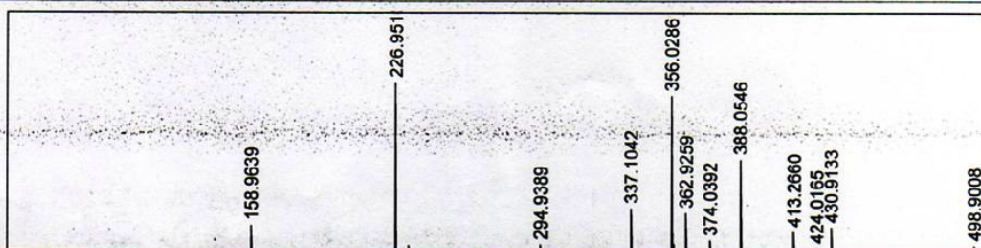
Analysis Name D:\Data\vipin\11-07-11-VN-3161-8.d
Method sodium formate tune_low.m
Sample Name VN-3161-8
Comment I

Acquisition Date 7/11/2011 11:04:43 AM

Operator VIKAS GROVER
Instrument / Ser# maXis 40

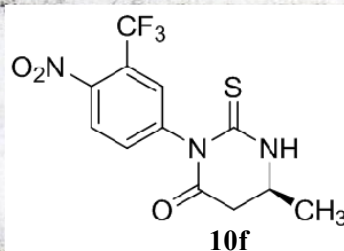
Acquisition Parameter

Source Type ESI Ion Polarity Positive Set Nebulizer 0.4 Bar
Focus Not active Set Capillary 4500 V Set Dry Heater 180 °C
Scan Begin 50 m/z Set End Plate Offset -500 V Set Dry Gas 4.0 l/min
Scan End 500 m/z Set Collision Cell RF 300.0 Vpp Set Divert Valve Source



+MS, 1.5min #88

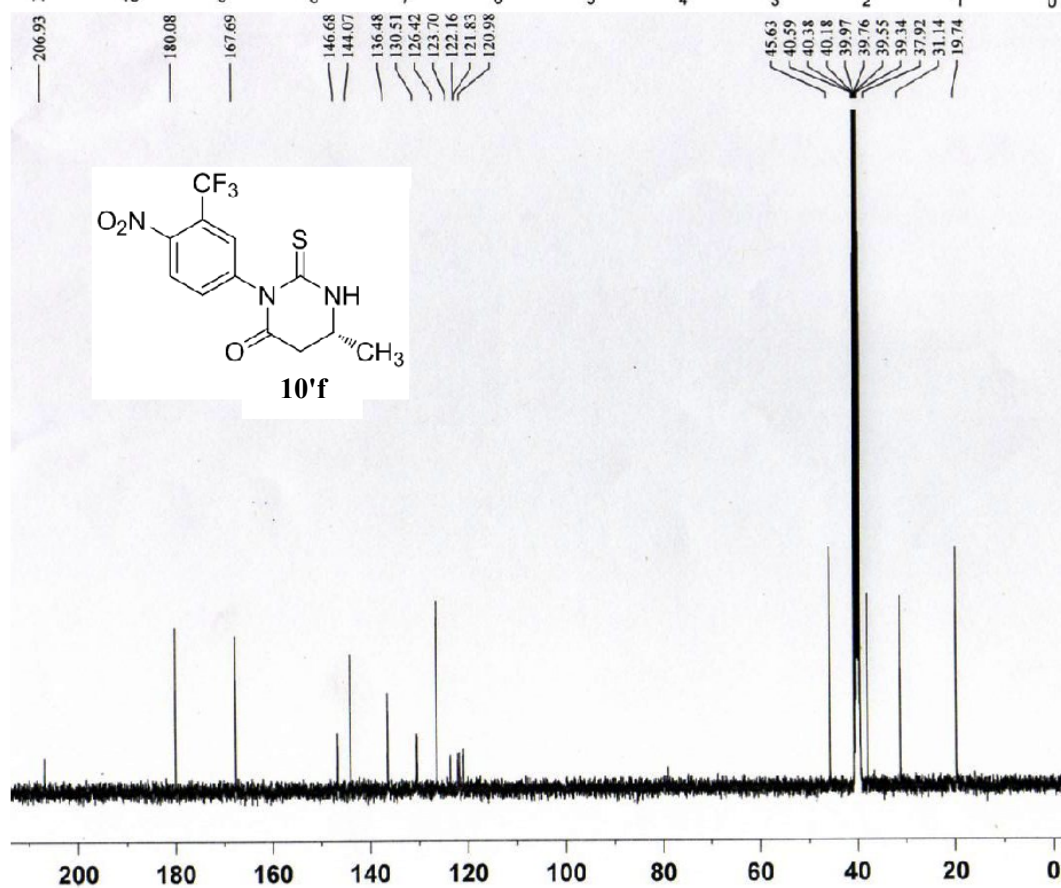
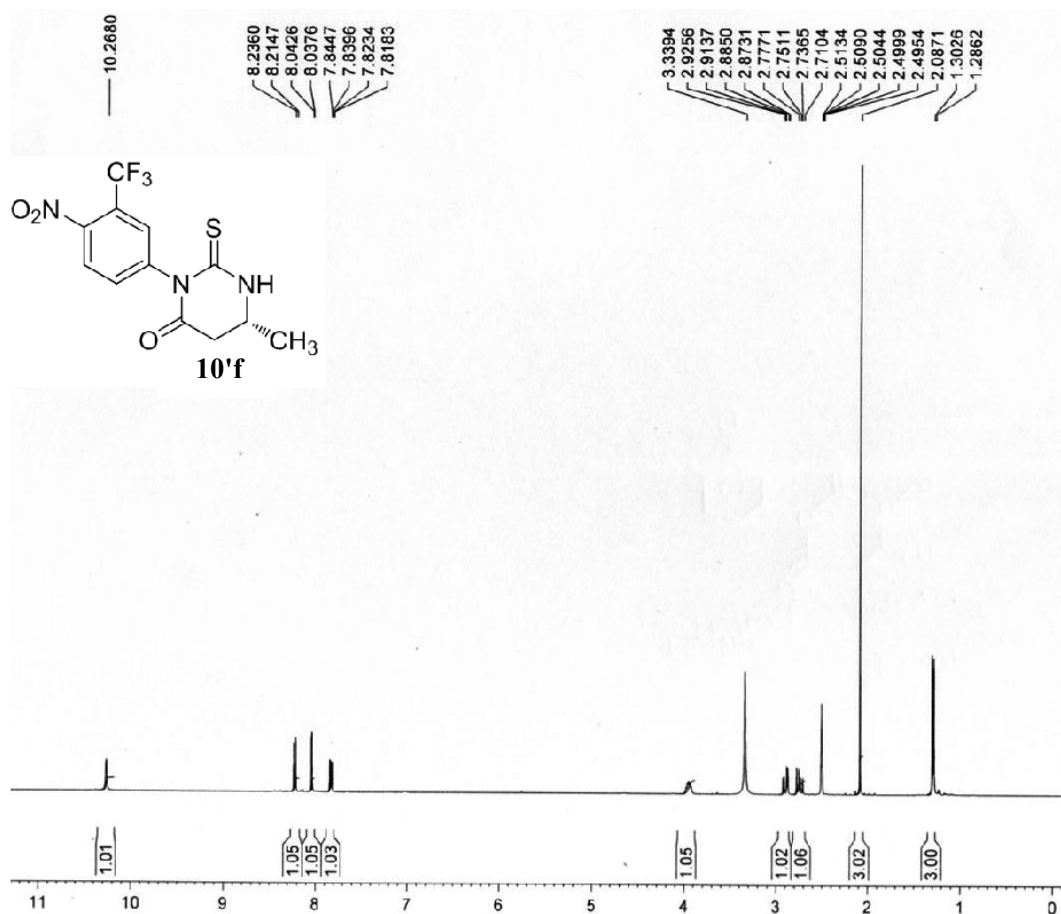
#	m/z	Res.	S/N	I	FWHM
1	90.9795	15712	23.2	633	0.0058
2	158.9639	19542	261.4	16071	0.0081
3	226.9510	18025	1742.9	103862	0.0126
4	227.9548	17938	13.6	801	0.0127
5	233.0780	21106	72.8	4093	0.0110
6	294.9389	22569	116.0	4504	0.0131
7	337.1042	24735	245.6	27020	0.0136
8	338.1081	23458	21.4	2403	0.0144
9	342.0499	23085	13.0	1589	0.0148
10	356.0286	20223	618.1	95840	0.0176
11	357.0316	22931	33.5	5279	0.0156
12	362.9259	25064	140.5	24092	0.0145
13	374.0392	24837	47.0	7316	0.0151
14	388.0546	22999	542.4	57082	0.0169
15	389.0575	21945	30.3	3081	0.0177
16	413.2660	26355	168.8	12758	0.0157
17	414.2699	22344	24.2	1833	0.0185
18	424.0165	21982	32.8	2582	0.0193
19	430.9133	24954	203.8	15385	0.0173
20	464.9077	25120	18.4	555	0.0185
21	473.1080	19084	12.0	404	0.0248
22	498.9008	24905	103.3	4260	0.0200



[M+Na]⁺

Calcd : 356.0293

Found : 356.0286



Mass Spectrum List Report

Analysis Info

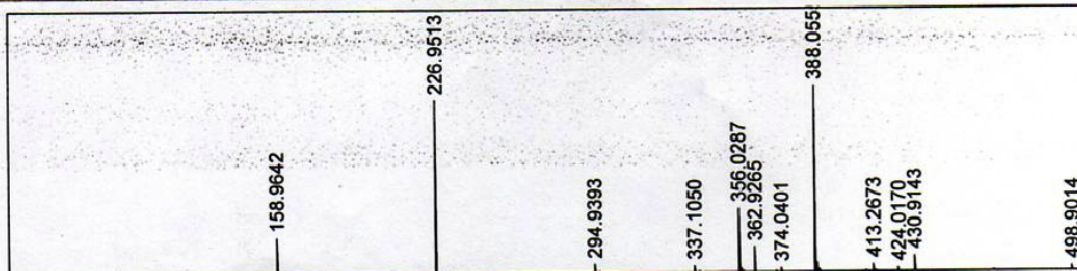
Analysis Name D:\Data\vipin\11-07-11-VN-3162-8.d
Method sodium formate tune_low.m
Sample Name VN-3162-8
Comment I

Acquisition Date 7/11/2011 11:49:51 AM

Operator VIKAS GROVER
Instrument / Ser# maXis 40

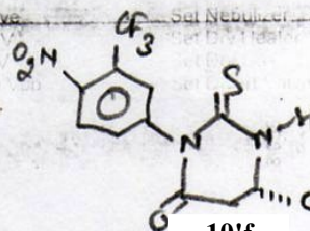
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	500 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



+MS, 1.2min #74

#	m/z	Res.	S/N	I	FWHM
1	90.9797	17839	28.4	681	0.0051
2	158.9642	19878	513.4	20358	0.0080
3	185.1155	18968	13.2	264	0.0098
4	226.9513	18232	2172.7	96605	0.0124
5	227.9557	17557	19.3	840	0.0130
6	233.0796	18735	15.1	576	0.0124
7	261.0472	16854	10.9	269	0.0155
8	294.9393	21471	105.2	4642	0.0137
9	297.0470	24614	13.7	634	0.0121
10	337.1050	22595	72.1	3520	0.0149
11	339.1589	20743	10.1	557	0.0164
12	356.0287	23082	327.9	35598	0.0154
13	357.0324	21559	16.8	1881	0.0166
14	362.9265	23348	106.8	13920	0.0155
15	374.0401	22753	16.7	2371	0.0164
16	388.0555	21017	739.7	103736	0.0185
17	389.0582	21955	37.9	5316	0.0177
18	413.2673	24599	37.3	4215	0.0168
19	424.0170	21274	26.1	2483	0.0199
20	430.9143	23643	109.3	9064	0.0182
21	464.9088	21082	17.1	537	0.0221
22	473.1106	17849	13.7	471	0.0265
23	478.0244	28575	11.1	402	0.0167
24	498.9014	21695	75.9	3089	0.0230



[M+Na]⁺ Calcd.: 356.0293
Found: 356.0287

