Electronic Supplementary Material (ESI) for RSC Advances.

Zirconocene dichloride Catalysed One Pot Synthesis of Pyrroles through Nitroalkene-Enamine Assembly

Sandeep Goyal, Jatinkumar K. Patel, Mukesh Gangar, Kapil Kumar and Vipin A. Nair*

Supporting Information

Contents **Pages**

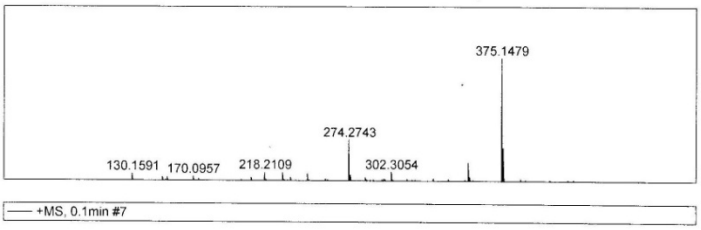
Mass Spectrum List Report

Analysis Info

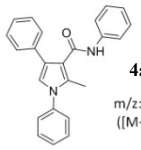
Analysis Name	D:\Data\vipin\13-08-27-MCR-40.d	Acquisition Date	8/29/2013 12:07:41 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MCR-40	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 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	130.1591	17050	423.2	47524	0.0076
2	153.1380	16517	146.8	26840	0.0093
3	170.0957	16598	154.8	27640	0.0102
4	202.2157	18399	40.1	9704	0.0110
5	209.1066	17411	84.9	22553	0.0120
6	218.2109	16964	204.5	61175	0.0129
7	230.2473	17223	168.8	58506	0.0134
8	246.2424	18117	125.9	54311	0.0136
9	274.2743	16800	351.6	298263	0.0163
10	285.1384	18831	31.8	22717	0.0151
11	302.3054	18533	130.7	62190	0.0163
12	353.1654	17877	272.1	134405	0.0198
⇨13	375.1479	16394	1532.6	891742	0.0229
14	376.1509	17323	427.7	241529	0.0217
15	377.1532	17735	43.4	23747	0.0213



4a(i)

m/z: Calc'd for $C_{24}H_{20}N_2NaO$
([M+Na]⁺): 375.1473, found: 375.1479

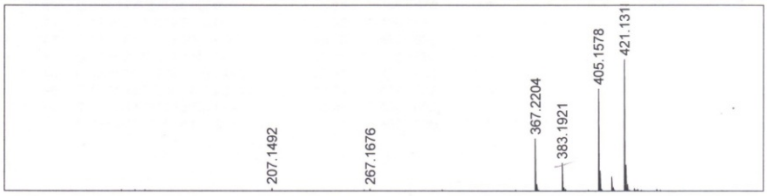
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\vipin\13-01-21-MCR-5.d	Acquisition Date	1/21/2013 10:17:37 AM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MCR-5	Instrument / Ser#	maXis 40
Comment			

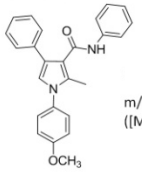
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 l/min
Scan End	500 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



+MS, 0.6min #34

#	m/z	Res.	S/N	I	FWHM
1	116.1180	23474	11.7	347	0.0049
2	124.0755	17906	18.0	583	0.0069
3	130.1592	21898	13.8	404	0.0059
4	177.1380	19480	10.2	148	0.0091
5	207.1492	21316	50.5	964	0.0097
6	256.0790	25702	12.4	217	0.0100
7	263.2116	25677	19.9	371	0.0103
8	267.1676	21863	46.4	891	0.0122
9	311.1579	20531	16.3	264	0.0152
10	316.9829	22213	10.7	167	0.0143
11	332.9560	28057	12.5	179	0.0119
12	355.2816	30744	12.0	295	0.0116
13	367.2204	23312	676.7	21189	0.0158
14	368.2232	24722	88.6	2928	0.0149
15	369.2250	23755	10.2	356	0.0155
16	383.1921	22917	192.1	11314	0.0167
17	384.1937	21671	26.4	1599	0.0177
18	385.1930	17861	10.7	669	0.0216
⇨ 19	405.1578	23088	383.4	41329	0.0175
20	406.1605	24181	73.1	8109	0.0168
21	413.2662	23698	45.1	6029	0.0174
22	414.2690	26842	10.2	1395	0.0154
23	421.1318	22967	334.5	53134	0.0183
24	422.1345	24520	65.0	10525	0.0172
25	423.1327	19596	17.3	2852	0.0216
26	503.1554	25133	11.3	186	0.0200



4a(ii)

m/z: Calc'd for $C_{25}H_{22}N_2NaO_2$ ($[M+Na]^+$): 405.1579, found: 405.1578

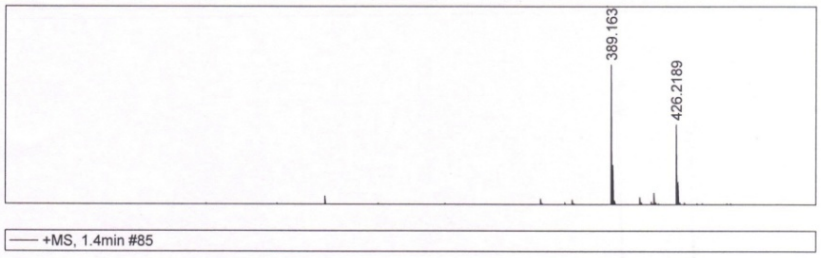
Mass Spectrum List Report

Analysis Info

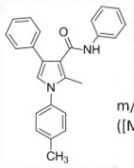
Analysis Name	D:\Data\vipin\13-01-21-MCR-3.d	Acquisition Date	1/21/2013 9:28:01 AM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MCR-3	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 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	389.1637	18999	13875.6	296096	0.0205
2	390.1666	20741	3802.5	83179	0.0188
3	391.1690	23119	338.2	7580	0.0169
4	426.2189	19725	5548.8	168992	0.0216
5	427.2217	22656	1573.1	48162	0.0189
6	428.2237	22737	158.1	4865	0.0188



4a(iii)

m/z: Calc'd for $C_{25}H_{22}N_2NaO$ ([M+Na]$^+$): 389.1630, found: 389.1637

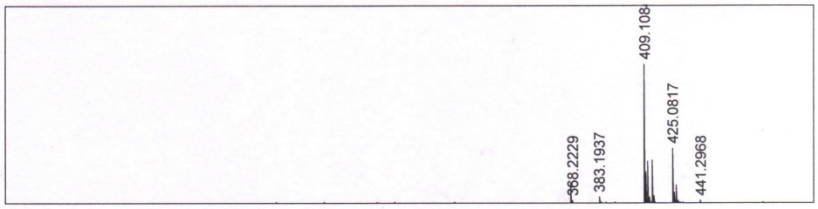
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\vipin\13-01-18-MCR-1.d	Acquisition Date	1/18/2013 4:25:19 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MCR-1	Instrument / Ser#	maXis 40
Comment			

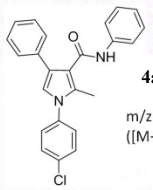
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 l/min
Scan End	500 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



+MS, 0.8min #47

#	m/z	Res.	S/N	I	FWHM
1	256.9614	23184	56.2	1209	0.0111
2	267.1677	22388	38.6	805	0.0119
3	272.9357	27114	19.2	393	0.0101
4	286.9717	21992	14.2	298	0.0130
5	294.9380	24956	19.8	425	0.0118
6	301.1039	21083	50.5	1098	0.0143
7	311.1929	25247	11.0	236	0.0123
8	324.9482	22423	18.3	362	0.0145
9	333.1270	24425	14.0	264	0.0136
10	362.9255	24348	11.8	550	0.0149
11	368.2229	24883	57.8	3253	0.0148
12	383.1937	24264	57.1	6949	0.0158
⇨13	409.1084	20575	851.9	156648	0.0199
14	410.1109	23395	191.2	35131	0.0175
15	411.1057	21774	260.0	47766	0.0189
16	412.1078	22444	40.1	7371	0.0184
17	413.2662	22863	266.3	48856	0.0181
18	414.2689	23673	45.9	8412	0.0175
19	425.0817	22189	339.9	61963	0.0192
20	426.0845	25777	66.1	12044	0.0165
21	427.0793	23699	113.3	20627	0.0180
22	428.0818	22914	19.2	3486	0.0187
23	441.2968	26884	25.2	2991	0.0164
24	460.9235	26649	13.0	412	0.0173
25	466.2881	30913	10.1	317	0.0151
26	477.0948	24422	41.6	1281	0.0195
27	479.0923	25642	14.8	453	0.0187



4a(iv)

m/z: Calc'd for $C_{24}H_{19}ClN_2NaO$ ($[M+Na]^+$): 409.1084, found: 409.1084.

Mass Spectrum List Report

Analysis Info

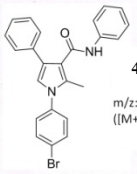
Analysis Name	D:\Data\vipin\13-01-18-MCR-2.d	Acquisition Date	1/18/2013 4:55:17 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MCR-2	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 l/min
Scan End	500 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source

+MS, 0.5min #30

#	m/z	Res.	S/N	I	FWHM
1	301.1042	24302	22.4	460	0.0124
2	317.0761	22641	11.1	231	0.0140
3	349.1147	21031	16.7	485	0.0166
4	365.0905	21109	13.2	514	0.0173
5	367.2202	22542	214.4	8592	0.0163
6	368.2233	22158	32.8	1325	0.0166
7	383.1946	23602	801.8	36303	0.0162
8	384.1975	25122	102.1	4658	0.0153
9	385.1941	21033	36.9	1695	0.0183
10	413.2663	23644	149.8	11373	0.0175
11	414.2692	23432	27.9	2162	0.0177
12	425.0814	23391	14.8	1412	0.0182
13	429.2401	25220	75.6	7770	0.0170
14	430.2435	24586	15.6	1638	0.0175
15	431.0752	26608	12.6	1341	0.0162
16	433.0733	22594	11.3	1249	0.0192
⇨17	453.0576	25116	145.5	21840	0.0180
18	454.0603	23574	23.6	3584	0.0193
19	455.0559	23805	137.5	21183	0.0191
20	456.0587	25172	23.6	3680	0.0181
21	469.0325	21162	1069.9	126989	0.0222
22	470.0349	24958	232.5	26589	0.0188
23	471.0308	20810	1240.2	136480	0.0226
24	472.0331	24477	267.8	28312	0.0193
25	473.0304	22166	67.2	6812	0.0213
26	474.0318	22336	11.7	1134	0.0212
27	490.1124	23335	23.9	701	0.0210
28	492.1110	25777	27.9	817	0.0191
29	493.0122	24236	11.3	332	0.0203



4a(v)

m/z: Calc'd for $C_{24}H_{19}BrN_2NaO$ ([M+Na]$^+$): 453.0578, found: 453.0576.

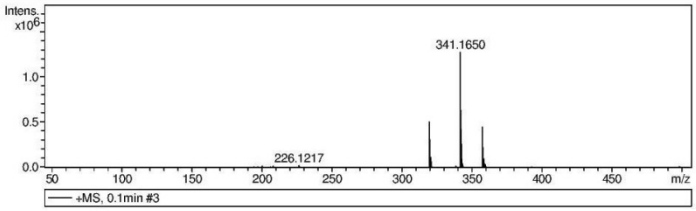
Mass Spectrum List Report

Analysis Info

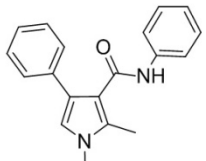
Analysis Name	D:\Data\vipin\14-01-20-SRM-51.d	Acquisition Date	1/20/2014 3:19:41 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	SRM-51	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 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	131.1075	15697	83.5	3595	0.0084
2	194.1148	17424	87.7	11188	0.0111
3	197.0757	16200	52.0	6910	0.0122
4	198.0916	18872	19.9	2678	0.0105
5	200.1411	17475	110.6	15279	0.0115
6	206.0816	18215	44.7	6637	0.0113
7	208.1313	17751	104.8	15949	0.0117
8	226.1217	17469	253.6	29502	0.0129
9	227.1251	17124	24.5	2763	0.0133
10	274.1410	16640	61.0	3182	0.0165
11	319.1819	15150	3823.3	505696	0.0211
12	320.1846	15463	867.4	111977	0.0207
13	321.1867	17139	58.4	7356	0.0187
14	330.1658	17346	41.8	4078	0.0190
15	338.1546	18325	200.6	18339	0.0185
16	338.6561	18049	74.0	7059	0.0188
⇨ 17	341.1650	11514	11110.4	1273847	0.0296
18	341.3031	6607	39.1	4539	0.0517
19	342.1670	14563	3452.8	422649	0.0235
20	343.1692	17787	347.3	45214	0.0193
21	357.1378	15242	1893.7	451111	0.0234
22	358.1404	15976	403.1	99153	0.0224
23	359.1373	16218	126.8	32173	0.0221
24	360.1379	16891	13.4	3517	0.0213
25	392.2330	19552	53.7	6558	0.0201
26	489.2536	18530	46.9	4555	0.0264
27	489.7547	17717	38.1	3734	0.0276
28	497.2428	18415	122.3	11985	0.0270
29	497.7439	18273	82.7	8101	0.0272
30	498.2497	14812	29.8	2920	0.0336



4a(vi)

m/z: Calc'd for $C_{21}H_{22}N_2NaO$ ($[M+Na]^+$): 341.1630, found: 341.1650.

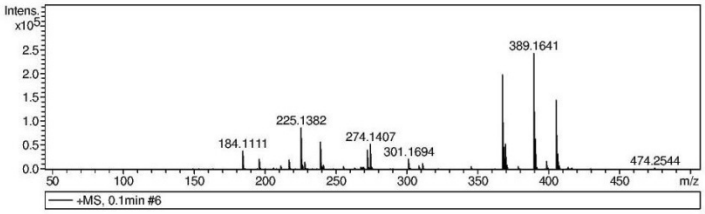
Mass Spectrum List Report

Analysis Info

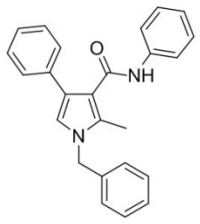
Analysis Name	D:\Data\vipin\14-01-20-SRM-53-A.d	Acquisition Date	1/20/2014 3:32:01 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	SRM-53-A	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 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	184.1111	16828	283.3	38527	0.0109
2	196.1112	17644	152.3	22381	0.0111
3	211.1221	16673	47.3	7605	0.0127
4	217.1690	16858	131.6	21324	0.0129
5	225.1382	15775	545.6	87106	0.0143
6	226.1412	15952	56.7	9038	0.0142
7	228.0986	18038	105.2	16697	0.0126
8	239.1538	16591	376.1	58500	0.0144
9	240.1561	17710	41.8	6493	0.0136
10	241.1328	16615	61.0	9450	0.0145
11	255.1460	16978	39.8	6648	0.0150
12	268.1919	17598	31.6	5775	0.0152
13	272.1429	17629	216.1	40508	0.0154
14	273.1458	17335	28.3	5334	0.0158
15	274.1407	16187	280.4	53239	0.0169
16	301.1694	18141	127.4	22271	0.0166
17	308.1388	17522	48.0	7941	0.0176
18	311.1538	18127	82.7	13006	0.0172
19	345.2532	17941	43.5	5936	0.0192
20	367.1818	15270	783.8	198330	0.0240
21	368.1843	17310	187.9	47603	0.0213
22	369.1960	16446	209.4	53085	0.0224
23	370.2000	17577	35.7	9060	0.0211
24	378.2902	17490	25.3	6468	0.0216
➡ 25	389.1641	14702	939.3	243049	0.0265
26	390.1666	17195	247.6	64122	0.0227
27	398.1873	17201	66.0	17098	0.0231
28	405.1379	15544	645.6	145483	0.0261
29	406.1402	17998	150.6	33206	0.0226
30	407.1383	16223	35.5	7651	0.0251



4a(vii)

m/z: Calc'd for $C_{25}H_{22}N_2NaO$ ($[M+Na]^+$): 389.1630, found: 389.1641

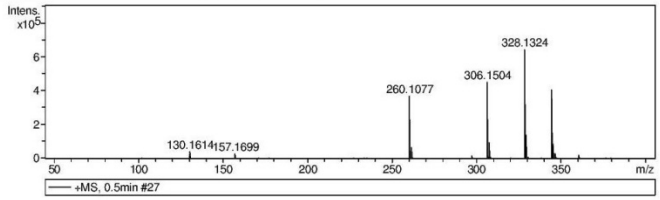
Mass Spectrum List Report

Analysis Info

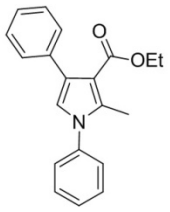
Analysis Name	D:\Data\vipin\14-02-04-SG-4-B-1.d	Acquisition Date	2/4/2014 4:05:53 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	SG-4-B-1	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 l/min
Scan End	400 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



#	m/z	Res.	S/N	I	FWHM
1	102.1349	17305	165.3	5848	0.0059
2	130.1614	15241	358.4	43095	0.0085
3	143.1550	16267	22.5	3010	0.0088
4	157.1699	17245	223.1	29449	0.0091
5	171.1845	15812	54.3	4989	0.0108
6	177.1377	16240	49.3	3708	0.0109
7	191.1530	16588	39.3	2761	0.0115
8	227.1379	17077	29.0	3205	0.0133
9	233.2001	18584	52.1	6642	0.0125
10	235.1217	17300	37.3	4963	0.0136
11	260.1077	14459	1836.5	367896	0.0180
12	261.1106	15880	326.1	66150	0.0164
13	262.1129	17410	17.3	3563	0.0151
14	297.1391	18167	58.4	15650	0.0164
15	306.1504	14808	1648.6	450047	0.0207
16	307.1533	15735	352.9	96538	0.0195
17	308.1575	15982	32.8	8979	0.0193
18	320.1286	17659	11.5	3231	0.0181
➡19	328.1324	14787	2214.2	642727	0.0222
20	329.1356	15170	482.9	140803	0.0217
21	330.1372	17686	35.9	10511	0.0187
22	338.1392	17139	19.8	6013	0.0197
23	344.1064	14821	1302.9	405098	0.0232
24	345.1092	16038	281.4	87592	0.0215
25	346.1058	16124	98.0	30064	0.0215
26	347.1074	16177	10.4	3145	0.0215
27	360.1208	17906	81.7	19924	0.0201
28	361.1235	17066	10.8	2592	0.0212
29	376.1027	9340	29.8	4896	0.0403
30	379.2374	17143	32.4	4762	0.0221



4b(i)

m/z: Calc'd for $C_{20}H_{19}NNaO_2$ ($[M+Na]^+$): 328.1313, found: 328.1324.

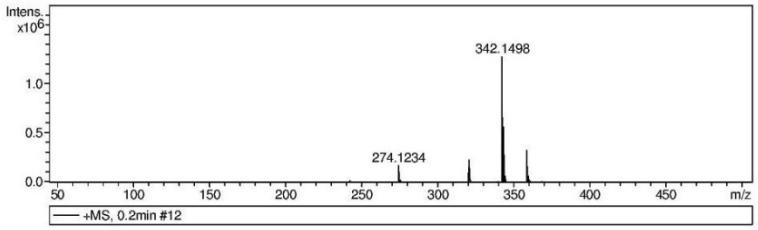
Mass Spectrum List Report

Analysis Info

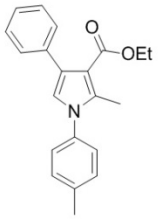
Analysis Name	D:\Data\vipin\14-01-20-SRM-54.d	Acquisition Date	1/20/2014 3:57:00 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	SRM-54	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 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	194.1158	17075	56.8	3319	0.0114
2	208.1316	17497	73.0	4702	0.0119
3	220.1316	16127	39.8	2933	0.0136
4	226.9505	16842	29.9	2420	0.0135
5	234.1263	16773	28.8	2551	0.0140
6	241.0825	16680	34.8	3348	0.0145
7	242.1143	16982	169.8	16511	0.0143
8	274.1234	14899	1824.0	175309	0.0184
9	275.1259	17856	289.6	27804	0.0154
10	302.0999	16531	16.2	1708	0.0183
11	320.1660	15094	2411.8	227007	0.0212
12	321.1684	17130	478.2	44589	0.0187
13	322.1712	16527	32.4	2997	0.0195
14	323.1257	17116	51.6	4727	0.0189
15	339.1389	18697	112.9	10392	0.0181
16	339.6404	17349	42.2	3985	0.0196
17	342.1498	10041	12060.7	1272712	0.0341
18	342.2980	7459	53.7	5706	0.0459
19	343.1511	14961	5099.0	561117	0.0229
20	344.1532	16516	562.2	64420	0.0208
21	345.1553	16697	22.5	2684	0.0207
22	358.1214	14463	1763.1	313102	0.0248
23	359.1240	17067	389.7	70977	0.0210
24	360.1209	16803	115.7	21587	0.0214
25	361.1222	15506	12.0	2300	0.0233
26	368.1462	18477	52.6	11219	0.0199
27	386.1568	16193	24.2	3232	0.0238
28	391.1610	15970	16.9	1879	0.0245
29	400.1706	17846	73.9	5982	0.0224
30	413.2630	17999	64.1	4691	0.0230



4b(ii)

m/z: Calc'd for $C_{21}H_{21}NNaO_2$ ($[M+Na]^+$): 342.1470, found: 342.1498.

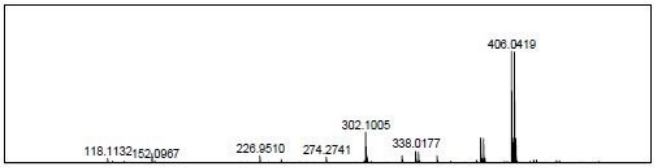
Mass Spectrum List Report

Analysis Info

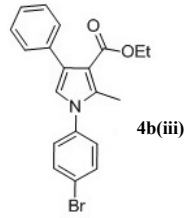
Analysis Name	D:\Data\vipin\813-04-09-MCR-25.d	Acquisition Date	4/9/2013 12:37:21 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MCR-25	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 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	118.1132	17451	6402.5	44520	0.0068
2	152.0967	18577	1884.1	24788	0.0082
3	226.9510	20206	3084.9	70926	0.0112
4	242.0784	19609	1476.2	38926	0.0123
5	274.2741	19983	1910.2	56858	0.0137
6	302.1005	17836	5759.9	304580	0.0169
7	328.1308	20379	1546.8	72830	0.0161
8	338.0177	20060	2647.0	115596	0.0169
9	353.2663	20678	1737.4	72250	0.0171
10	384.0597	18892	1920.0	249855	0.0203
11	406.0419	17851	6774.8	1096810	0.0227
12	406.8610	5212	0.7	105	0.0781
13	407.0449	19001	1595.7	250753	0.0214
14	408.0400	17794	7137.1	1087889	0.0229
15	409.0428	18597	1617.6	238888	0.0220



4b(iii)

m/z: Calc'd for $C_{20}H_{18}BrNNaO_2$ ([M+Na]$^+$): 406.0419, found: 406.0419.

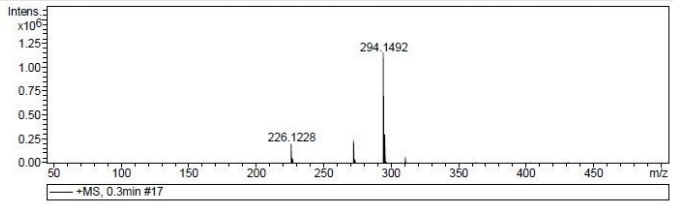
Mass Spectrum List Report

Analysis Info

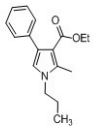
Analysis Name	D:\Data\vipin\13-06-19-MCR-32.d	Acquisition Date	6/19/2013 1:52:16 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MCR-32	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 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	118.1087	16924	65.5	2088	0.0070
2	158.9578	20183	136.7	3508	0.0079
3	184.0721	19094	88.9	1729	0.0096
4	226.1228	15985	5032.4	200971	0.0141
5	226.9510	17453	1153.8	45159	0.0130
6	227.1255	16988	617.9	24080	0.0134
7	240.9668	18025	56.7	1453	0.0134
8	272.1658	15751	2522.2	239196	0.0173
9	273.1687	17148	370.6	36112	0.0159
10	274.1703	19257	17.5	1755	0.0142
11	278.1727	18773	11.5	1506	0.0148
12	284.1638	18876	12.0	2217	0.0151
13	294.1492	11953	4173.1	1139620	0.0246
14	295.1514	15529	1052.9	296927	0.0190
15	296.1531	19757	69.8	20299	0.0150
16	310.1220	16482	191.1	62886	0.0188
17	311.1241	19376	22.7	7253	0.0161
18	326.1364	19993	20.8	3463	0.0163
19	359.2335	18524	27.8	2209	0.0194
20	362.9266	20072	107.1	8778	0.0181
21	381.1958	19331	16.8	1341	0.0197
22	396.1785	19382	24.9	1871	0.0204
23	403.1782	20503	127.9	9374	0.0197
24	404.1802	19780	22.5	1646	0.0204
25	411.2489	18828	21.4	1525	0.0218
26	430.9134	21169	106.3	6801	0.0204
27	498.9011	21791	61.4	1878	0.0229



4b(iv)

m/z: Calc'd for $C_{17}H_{21}NNaO_2$ ($[M+Na]^+$): 294.1470, found: 294.1492.

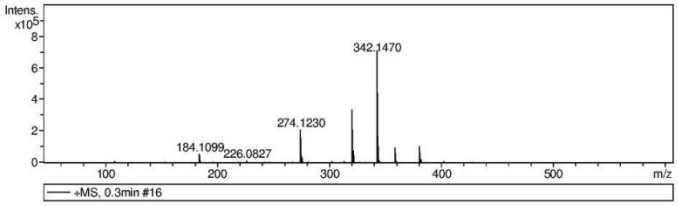
Mass Spectrum List Report

Analysis Info

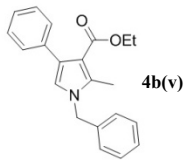
Analysis Name	D:\Data\vipin\14-01-15-BK-74-B.d	Acquisition Date	1/15/2014 9:49:50 AM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	BK-74-B	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 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	108.0730	16542	186.9	9054	0.0065
2	153.1348	15286	58.5	6045	0.0100
3	184.1099	16100	397.0	55954	0.0114
4	185.1128	15328	44.7	6279	0.0121
5	196.1101	16715	39.4	5332	0.0117
6	218.2101	15907	63.2	7732	0.0137
7	220.1318	17113	61.5	7429	0.0129
8	226.0827	17764	124.7	14391	0.0127
9	246.2419	16806	80.7	7856	0.0147
10	267.1848	16921	33.0	5042	0.0158
11	274.1230	14823	1185.0	209893	0.0185
12	274.2739	16122	377.8	67110	0.0170
13	275.1257	16254	204.6	36956	0.0169
14	275.2766	16523	42.2	7650	0.0167
15	281.1338	17708	25.4	5134	0.0159
16	302.3048	17434	66.0	10544	0.0173
17	313.1042	17752	82.8	9226	0.0176
18	320.1651	14262	4096.1	326532	0.0224
19	321.1680	16094	1025.4	77139	0.0200
20	322.1701	16865	80.1	5674	0.0191
21	326.1724	17524	123.2	7862	0.0186
⇨ 22	342.1470	14173	4502.0	684234	0.0241
23	343.1502	15266	1073.9	169174	0.0225
24	344.1521	17486	93.8	15300	0.0197
25	358.1206	15944	400.3	96173	0.0225
26	359.1230	17918	63.8	15692	0.0200
27	380.1859	15800	539.3	107238	0.0241
28	381.1887	18111	113.6	22163	0.0210
29	402.1666	18216	77.7	9529	0.0221
30	427.2371	18315	97.9	7502	0.0233



4b(v)

m/z: Calc'd for $C_{21}H_{21}NNaO_2$ ([M+Na]⁺): 342.1470, found: 342.1470.

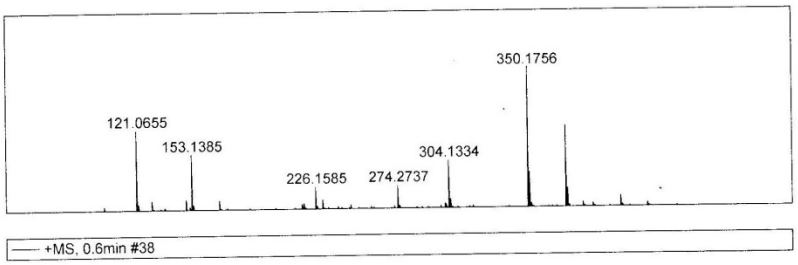
Mass Spectrum List Report

Analysis Info

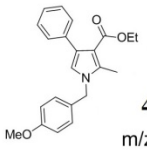
Analysis Name	D:\Data\vipin\13-08-27-MCR-39.d	Acquisition Date	8/29/2013 11:21:04 AM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MCR-39	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 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	121.0655	15077	1715.8	339417	0.0080
2	130.1592	15882	143.8	38386	0.0082
3	153.1385	15779	543.9	234955	0.0097
4	169.1329	15861	118.1	37672	0.0107
5	219.1483	17744	60.7	24747	0.0124
6	226.1585	16800	243.9	93679	0.0135
7	230.2473	17931	103.3	38237	0.0128
8	274.2737	17189	221.3	97163	0.0160
9	304.1334	16666	371.8	200446	0.0182
10	350.1756	16224	1362.2	592239	0.0216
11	351.1787	17665	338.0	147615	0.0199
12	352.1810	18392	35.3	15501	0.0191
⇨13	372.1576	16694	782.5	346882	0.0223
14	373.1604	18048	182.1	79924	0.0207
15	374.1629	18320	17.8	7745	0.0204
16	382.1649	18593	54.6	21733	0.0206
17	388.1331	12073	34.5	12820	0.0321
18	404.1468	18935	162.7	48167	0.0213
19	420.1406	19369	67.5	14679	0.0217
20	437.1932	18468	25.8	3899	0.0237



4b(vi)

m/z: Calc'd for $C_{22}H_{23}NNaO_3$ ($[M+Na]^+$): 372.1576, found: 372.1576

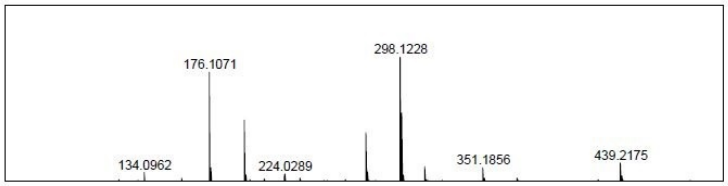
Mass Spectrum List Report

Analysis Info

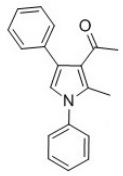
Analysis Name	D:\Data\vipin\13-04-10-MCR-27.d	Acquisition Date	4/10/2013 9:21:42 AM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MCR-27	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 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	134.0962	17896	5864.5	91136	0.0075
2	158.0958	17374	1609.3	33546	0.0091
3	176.1071	15525	31901.4	1120993	0.0113
4	198.0889	16865	17680.0	631911	0.0117
5	224.0289	19320	2517.3	76392	0.0116
6	234.1271	20611	1282.6	38372	0.0114
7	276.1384	17542	9897.3	497247	0.0157
8	298.1228	10174	15843.5	1274989	0.0293
9	314.0942	19136	1962.8	146381	0.0164
10	351.1856	19178	4650.9	143881	0.0183
11	373.1881	20741	1277.1	35422	0.0180
12	425.0695	21423	488.5	18673	0.0198
13	439.2175	19478	6048.3	188984	0.0225



4c(i)

m/z: Calc'd for $C_{19}H_{17}NNaO$ ($[M+Na]^+$): 298.1208, found: 298.1228.

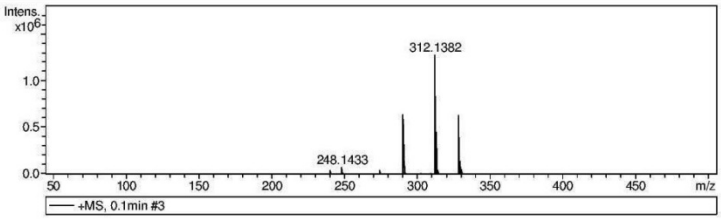
Mass Spectrum List Report

Analysis Info

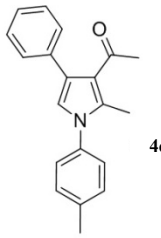
Analysis Name	D:\Data\vipin\14-02-03-BK-76.d	Acquisition Date	2/3/2014 11:11:21 AM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	BK-76	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 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	218.0809	15524	44.3	2674	0.0140
2	218.2107	15917	56.3	3423	0.0137
3	240.0628	16981	320.0	42584	0.0141
4	241.0660	16745	24.0	3276	0.0144
5	246.2425	16877	27.0	3903	0.0146
6	247.1343	17605	13.6	1946	0.0140
7	248.1433	16347	556.4	79054	0.0152
8	249.1461	17725	68.7	9677	0.0141
9	256.0366	18082	17.1	2262	0.0142
10	274.2741	17026	379.9	41355	0.0161
11	275.2770	17503	42.0	4525	0.0157
12	290.1550	15224	6658.2	636854	0.0191
13	291.1581	15479	1507.5	142972	0.0188
14	292.1602	18195	108.3	10192	0.0161
15	302.3053	18912	95.8	8226	0.0160
16	309.1277	18757	63.6	6520	0.0165
17	309.6289	16737	25.4	2683	0.0185
➡18	312.1382	11288	10712.0	1272729	0.0277
19	312.2734	5262	32.4	3886	0.0593
20	313.1403	15215	3602.3	447768	0.0206
21	314.1425	17369	342.3	44436	0.0181
22	315.1447	16155	12.6	1714	0.0195
23	318.2992	17014	11.7	1794	0.0187
24	328.1110	15377	3058.0	630758	0.0213
25	329.1141	15592	651.9	138050	0.0211
26	330.1106	15705	233.7	50764	0.0210
27	330.3365	17168	10.7	2348	0.0192
28	331.1117	16746	24.9	5544	0.0198
29	453.7020	19099	75.8	4334	0.0238
30	454.2030	18548	51.4	2955	0.0245



4c(ii)

m/z: Calc'd for $C_{20}H_{19}NNaO$ ($[M+Na]^+$): 312.1364, found: 312.1382.

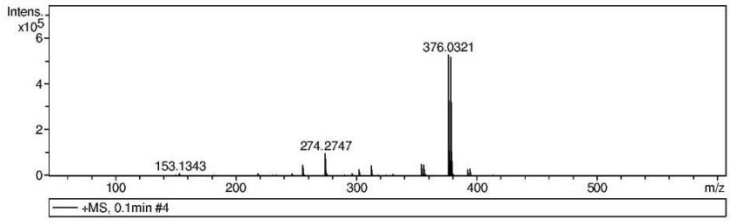
Mass Spectrum List Report

Analysis Info

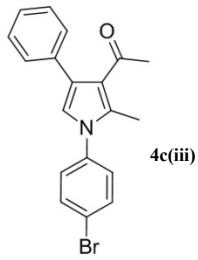
Analysis Name	D:\Data\vipin\14-01-15-BK-77.d	Acquisition Date	1/15/2014 9:42:36 AM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	BK-77	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 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	150.0997	16418	41.9	3332	0.0091
2	153.1343	16428	140.3	11010	0.0093
3	218.2102	16792	86.8	9358	0.0130
4	246.2425	17382	60.8	10445	0.0142
5	255.1469	16689	253.2	46113	0.0153
6	256.1496	15998	24.0	4381	0.0160
7	257.0240	16855	25.4	4639	0.0152
8	274.2747	15596	525.7	97861	0.0176
9	275.2775	17430	67.2	12526	0.0158
10	296.2562	17392	58.1	10840	0.0170
11	302.3056	17877	147.1	27231	0.0169
12	303.3086	17458	19.1	3524	0.0174
13	312.1364	17561	241.5	44064	0.0178
14	313.1394	17109	33.8	6153	0.0183
15	318.3004	17613	24.0	4334	0.0181
16	330.3368	17363	53.6	8796	0.0190
17	354.0494	17222	512.3	49865	0.0206
18	355.0519	18328	70.3	6652	0.0194
19	356.0475	17199	533.3	48906	0.0207
20	357.0503	17624	70.5	6276	0.0203
⇨ 21	376.0321	15061	5851.4	525711	0.0250
22	377.0351	15895	1214.9	110604	0.0237
23	378.0302	15101	5590.4	515513	0.0250
24	379.0330	15921	1134.2	105948	0.0238
25	380.0350	18002	72.9	6902	0.0211
26	392.0050	18440	265.7	28908	0.0213
27	393.0080	16539	32.5	3571	0.0238
28	394.0033	17852	284.2	31588	0.0221
29	395.0056	17867	37.2	4178	0.0221
30	413.2659	17735	47.6	4303	0.0233



4c(iii)

m/z: Calc'd for $C_{19}H_{16}BrNNaO$ ($[M+Na]^+$): 376.0313, found: 376.0321.

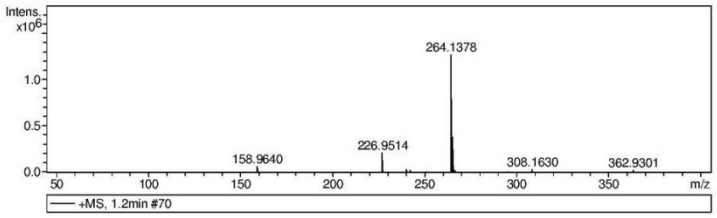
Mass Spectrum List Report

Analysis Info

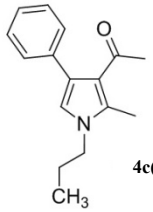
Analysis Name	D:\Data\vipin\14-02-04-SG-252.d	Acquisition Date	2/4/2014 3:26:34 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	SG-252	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 l/min
Scan End	400 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



#	m/z	Res.	S/N	I	FWHM
1	90.9769	17713	127.3	2077	0.0051
2	158.9640	14977	1520.0	63144	0.0106
3	200.1425	15846	77.3	2922	0.0126
4	202.1193	16941	41.0	1656	0.0119
5	219.1346	17134	50.3	3628	0.0128
6	226.9514	13939	2518.8	210950	0.0163
7	227.9538	16862	42.4	3567	0.0135
8	240.0624	17131	385.7	34197	0.0140
9	240.9659	16075	21.5	1911	0.0150
10	241.0654	16642	26.3	2346	0.0145
11	242.1533	17289	254.2	22738	0.0140
12	243.1562	16225	26.4	2373	0.0150
13	251.0856	16690	49.6	6237	0.0150
⇨14	264.1378	10036	3823.8	1271104	0.0263
15	265.1397	14031	1103.0	384138	0.0189
16	266.1419	16955	83.0	30213	0.0157
17	294.9390	18404	52.0	11967	0.0160
18	301.1415	15959	11.2	2079	0.0189
19	308.1630	17514	223.2	33218	0.0176
20	309.1660	15983	25.0	3593	0.0193
21	332.1247	17665	31.2	2052	0.0188
22	362.9301	18232	167.0	28595	0.0199
23	363.1676	18192	35.2	6079	0.0200



4c(iv)

m/z: Calc'd for $C_{16}H_{19}NNaO$ ($[M+Na]^+$): 264.1364, found: 264.1378.

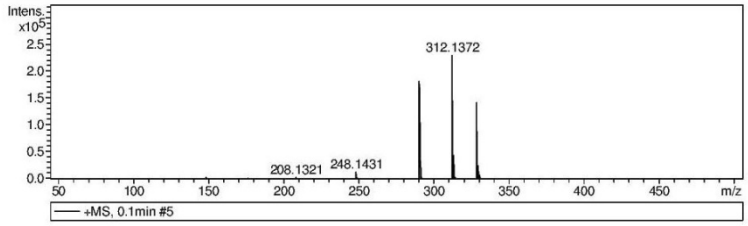
Mass Spectrum List Report

Analysis Info

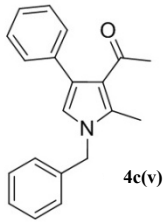
Analysis Name	D:\Data\vipin\14-02-03-SG-249-R.d	Acquisition Date	2/3/2014 10:27:55 AM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	SG-249	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 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	118.1223	15981	24.2	671	0.0074
2	125.1071	16174	12.5	396	0.0077
3	135.0013	13771	13.6	499	0.0098
4	139.0724	13394	16.3	629	0.0104
5	148.1113	15646	71.8	3106	0.0095
6	149.0228	13676	21.1	922	0.0109
7	153.1376	16108	16.0	722	0.0095
8	176.1059	15393	42.2	1678	0.0114
9	182.5635	17117	11.0	420	0.0107
10	186.2205	15485	16.8	634	0.0120
11	194.1168	14754	13.5	498	0.0132
12	208.1321	16419	94.2	3316	0.0127
13	240.0633	15079	11.9	720	0.0159
14	248.1431	17397	204.3	12936	0.0143
15	249.1456	18068	29.9	1883	0.0138
16	250.1433	14866	13.1	819	0.0168
17	290.1549	14965	1912.8	181952	0.0194
18	291.1576	17408	345.7	33804	0.0167
19	292.1600	17414	23.1	2319	0.0168
⇨ 20	312.1372	15076	1832.8	229040	0.0207
21	313.1397	16912	361.6	44571	0.0185
22	314.1426	18047	23.0	2799	0.0174
23	328.1111	15544	1458.1	142725	0.0211
24	329.1135	18403	265.4	25531	0.0179
25	330.1103	16302	79.8	7538	0.0202
26	331.1119	15141	11.0	1023	0.0219
27	356.1625	15700	18.8	882	0.0227
28	372.1368	15836	24.9	645	0.0235
29	413.2668	18320	20.4	461	0.0226
30	429.2391	20830	17.9	426	0.0206



4c(v)

m/z: Calc'd for $C_{20}H_{19}NNaO$ ($[M+Na]^+$): 312.1364, found: 312.1372.

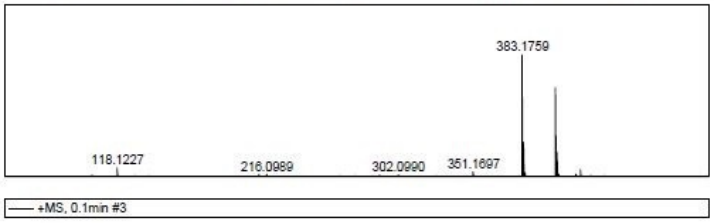
Mass Spectrum List Report

Analysis Info

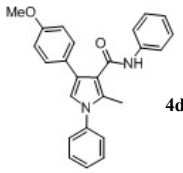
Analysis Name	D:\Data\OUTSIDE\813-04-08-MCR-18.d	Acquisition Date	4/8/2013 9:23:48 AM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MCR-18	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 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	118.1227	15604	5288.9	71074	0.0076
2	211.1225	20087	881.7	19104	0.0105
3	216.0989	20521	920.9	20571	0.0105
4	302.0990	20039	540.0	16955	0.0151
5	351.1697	20946	1078.7	37880	0.0168
6	383.1759	18270	11670.5	1002342	0.0210
7	384.1789	18747	3154.7	280754	0.0205
8	385.1811	20657	360.3	33183	0.0186
⇨ 9	405.1580	18848	6660.8	731678	0.0215
10	406.1611	19324	1852.7	198390	0.0210
11	407.1635	21457	203.0	21175	0.0190



4d(i)

m/z: Calc'd for $C_{25}H_{22}N_2NaO_2$ ($[M+Na]^+$): 405.1579, found: 405.1580.

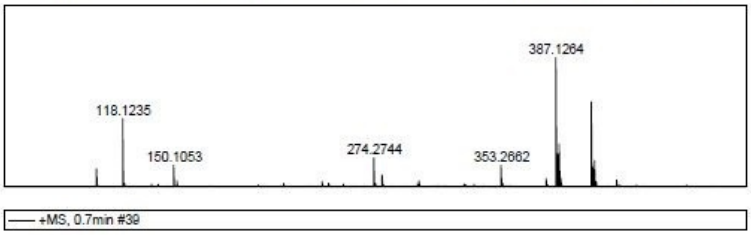
Mass Spectrum List Report

Analysis Info

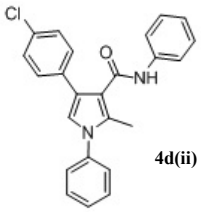
Analysis Name	D:\Data\vipin\813-04-09-MCR-22.d	Acquisition Date	4/9/2013 11:38:05 AM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MCR-22	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 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	102.1282	17142	9369.4	63428	0.0060
2	118.1235	14385	21275.9	237194	0.0082
3	150.1053	17342	4993.5	74833	0.0087
4	274.2744	19155	3310.5	101362	0.0143
5	279.0934	20556	1313.0	39249	0.0136
6	302.3053	20105	837.1	20569	0.0150
7	353.2662	20386	2712.7	73770	0.0173
8	387.1264	18418	7226.7	445223	0.0210
9	388.1292	19763	1795.7	113361	0.0196
10	389.1240	18420	2314.2	149593	0.0211
11	390.1264	20648	436.1	28853	0.0189
12	409.1083	18953	5004.9	292952	0.0216
13	410.1109	20960	1228.1	69843	0.0196
14	411.1058	18801	1641.5	90645	0.0219
15	412.1080	21358	316.9	16971	0.0193
16	425.0818	21475	715.7	22931	0.0198
17	427.0799	19029	238.8	6859	0.0224



4d(ii)

m/z: Calc'd for $C_{24}H_{19}ClN_2NaO$ ($[M+Na]^+$): 409.1084, Found 409.1083.

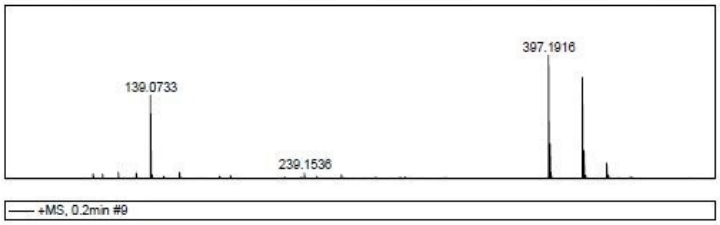
Mass Spectrum List Report

Analysis Info

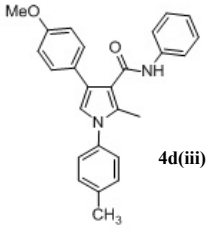
Analysis Name	D:\Data\OUTSIDE\813-04-08-MCR-17.d	Acquisition Date	4/8/2013 9:09:44 AM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MCR-17	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 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	102.1278	17825	2247.8	24568	0.0057
2	108.0807	15571	2095.1	27245	0.0069
3	118.1226	15704	2111.3	34843	0.0075
4	130.1588	16955	1270.2	28342	0.0077
5	139.0733	16330	16101.8	436499	0.0085
6	158.0962	17445	1142.9	35612	0.0091
7	184.1116	19705	715.4	12993	0.0093
8	191.1540	19052	834.4	15641	0.0100
9	239.1536	18953	997.6	30527	0.0126
10	247.2164	20697	437.3	14094	0.0119
11	278.1532	18657	150.1	4267	0.0149
12	397.1916	18637	10780.5	646903	0.0213
13	398.1945	19171	3032.6	184362	0.0208
14	399.1972	21279	352.8	21618	0.0188
15	419.1737	18969	7523.0	534802	0.0221
16	420.1765	20072	2076.4	148628	0.0209
17	421.1790	21063	218.1	15719	0.0200
18	435.1471	20545	1306.5	84132	0.0212
19	436.1498	22393	307.0	19271	0.0195



4d(iii)

m/z: Calc'd for $C_{26}H_{24}N_2NaO_2$ ($[M+Na]^+$): 419.1735, Found 419.1737.

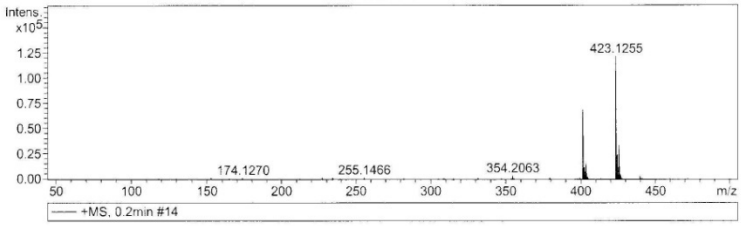
Mass Spectrum List Report

Analysis Info

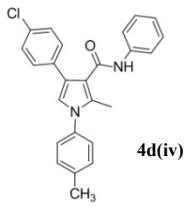
Analysis Name	D:\Data\vipin\13-12-20-AT-71.d	Acquisition Date	12/20/2013 12:07:51 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	AT-71	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 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	118.1169	13225	26.1	1019	0.0089
2	130.1542	15164	15.1	661	0.0086
3	153.1354	12993	32.3	1684	0.0118
4	164.9187	13151	14.8	782	0.0125
5	174.1270	14408	32.5	1726	0.0121
6	212.0779	14588	13.7	729	0.0145
7	226.9505	14092	23.3	1392	0.0161
8	234.0012	15398	24.5	1544	0.0152
9	255.1466	14413	35.3	2053	0.0177
10	282.1039	17042	17.5	750	0.0166
11	305.1571	13776	18.4	907	0.0222
12	308.0831	15471	18.6	911	0.0199
13	315.1929	14682	18.7	896	0.0215
14	331.2164	14096	30.6	1393	0.0235
15	347.2486	14575	18.1	978	0.0238
16	353.2670	15044	17.1	1009	0.0235
17	354.2063	15668	67.0	4009	0.0226
18	355.2104	14488	13.9	843	0.0245
19	379.1942	16310	14.8	1642	0.0232
20	401.1429	16219	397.2	68707	0.0247
21	402.1455	16956	66.7	11577	0.0237
22	403.1404	16175	92.2	16042	0.0249
23	404.1424	15427	16.4	2865	0.0262
⇨ 24	423.1255	14848	654.5	121185	0.0285
25	424.1277	16844	130.4	24213	0.0252
26	424.1870	15623	54.8	10171	0.0272
27	425.1228	16552	180.5	33612	0.0257
28	426.1249	15526	27.1	5059	0.0274
29	439.0982	16383	23.5	3217	0.0268
30	459.1961	14780	15.0	638	0.0311



4d(iv)

m/z: Calc'd for $C_{25}H_{21}ClN_2NaO$ ([M+Na]$^+$): 423.1240, Found 423.1255.

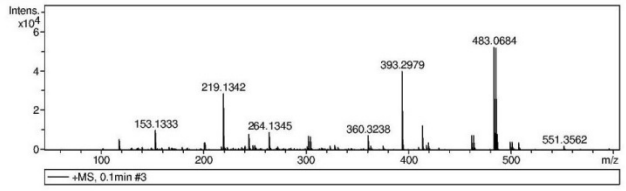
Mass Spectrum List Report

Analysis Info

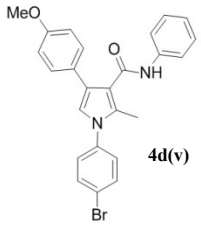
Analysis Name	D:\Data\vipin\14-02-04-SG-251.d	Acquisition Date	2/4/2014 4:15:43 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	SG-251	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 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	118.1131	15252	84.8	5511	0.0077
2	153.1333	17906	125.1	9993	0.0086
3	201.1223	15822	33.3	3743	0.0127
4	219.1342	16739	214.5	28565	0.0131
5	244.2627	17076	57.5	7887	0.0143
6	248.0062	16206	16.6	2284	0.0153
7	250.0043	15646	15.0	2079	0.0160
8	264.1345	17756	68.4	9193	0.0149
9	302.0536	18061	63.2	7184	0.0167
10	304.0524	16047	58.7	6559	0.0189
11	328.1300	16633	25.6	2335	0.0197
12	360.3238	18006	81.2	7497	0.0200
13	363.1642	16235	23.7	2232	0.0224
14	375.2505	16667	17.2	2059	0.0225
15	393.2979	17744	253.4	39766	0.0222
16	394.3006	17101	33.3	5289	0.0231
17	413.2661	18179	98.7	12489	0.0227
18	417.1235	17802	21.4	2449	0.0234
19	419.2769	16522	35.5	3809	0.0254
20	461.0857	18273	75.6	7495	0.0252
21	463.0838	17720	71.3	7343	0.0261
22	463.3029	18568	52.1	5394	0.0250
⇨ 23	483.0684	17817	467.5	52106	0.0271
24	484.0708	18857	80.2	8813	0.0257
25	485.0669	17328	477.2	51726	0.0280
26	486.0691	18283	75.8	8102	0.0266
27	499.0412	18765	47.0	4083	0.0266
28	501.0399	17639	48.5	4069	0.0284
29	507.3295	17577	51.6	3834	0.0289
30	551.3562	17251	69.0	2083	0.0320



4d(v)

m/z: Calc'd for $C_{25}H_{21}BrN_2NaO_2$ ($[M+Na]^+$): 483.0684, Found 483.0684.

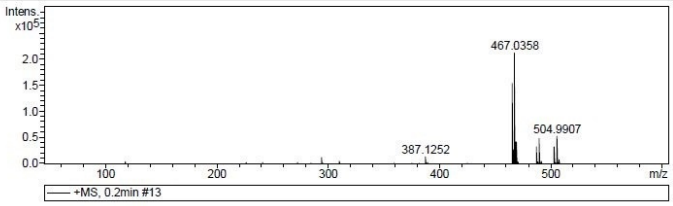
Mass Spectrum List Report

Analysis Info

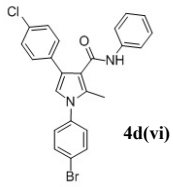
Analysis Name	D:\Data\vipin\13-06-19-MCR-33.d	Acquisition Date	6/19/2013 2:09:18 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MCR-33	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 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	241.7056	19156	17.9	644	0.0126
2	258.1489	18187	13.4	588	0.0142
3	272.1640	19370	47.2	2715	0.0141
4	284.3310	18890	14.8	1029	0.0151
5	311.1233	16050	10.5	600	0.0194
6	354.2837	19117	18.4	825	0.0185
7	359.2395	19787	53.2	2359	0.0182
8	375.2134	20194	21.5	1110	0.0186
9	381.1951	19199	27.1	1495	0.0199
10	387.1252	21709	246.0	14430	0.0178
11	388.1281	19188	32.2	1908	0.0202
12	389.1229	18339	41.3	2469	0.0212
13	409.1070	17414	17.4	992	0.0235
14	425.0811	19098	41.3	1716	0.0223
15	427.0791	16679	14.0	556	0.0256
16	465.0377	16785	994.1	154016	0.0277
17	466.0394	20744	173.9	27720	0.0225
18	467.0358	16776	1300.6	213059	0.0278
19	468.0374	20573	252.0	42411	0.0227
20	469.0329	19699	242.7	41907	0.0238
21	470.0346	20671	25.3	4490	0.0227
22	487.0184	20675	192.5	32341	0.0236
23	488.0205	21850	22.9	3801	0.0223
24	489.0167	19981	299.5	49000	0.0245
25	490.0190	20265	32.8	5289	0.0242
26	491.0139	19770	34.2	5452	0.0248
27	502.9924	21547	249.2	33122	0.0233
28	504.9907	19678	414.9	53331	0.0257
29	505.9932	20439	47.8	6033	0.0248
30	506.9883	21005	66.7	8277	0.0241



4d(vi)

m/z: Calc'd for $C_{24}H_{18}BrClN_2NaO$ ([M+Na]$^+$): 487.0189, Found 487.0184.

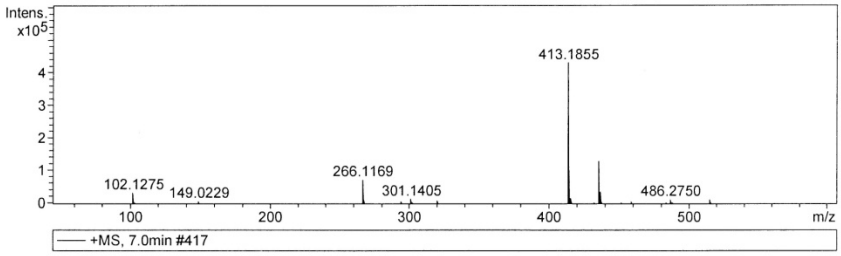
Mass Spectrum List Report

Analysis Info

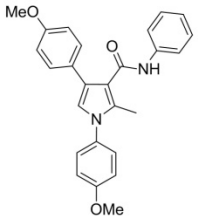
Analysis Name	D:\Data\vipin\SG-292_1-B,1_01_1667.d	Acquisition Date	11/7/2014 4:13:40 PM
Method	HIGH FLOW DIRECT INJECTION LOW MASS.m	Operator	VIKAS GROVER
Sample Name	SG-292	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	600 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	102.1275	12843	1135.6	33350	0.0080
2	103.1307	12440	88.2	2619	0.0083
3	149.0229	14563	169.5	6442	0.0102
4	205.0850	16457	49.1	1664	0.0125
5	253.0854	17503	17.4	1763	0.0145
6	266.1169	17671	748.8	72527	0.0151
7	267.1203	17186	132.8	12823	0.0155
8	288.2893	17197	22.8	2041	0.0168
9	294.1481	18233	56.7	4835	0.0161
10	301.1405	18448	171.1	13763	0.0163
11	302.1435	16986	27.3	2175	0.0178
12	320.1278	18201	115.9	7786	0.0176
13	321.1309	19007	25.6	1702	0.0169
14	413.1855	18716	19693.1	428665	0.0221
15	414.1889	18916	5390.6	116870	0.0219
16	415.1914	18537	803.0	17347	0.0224
17	416.1931	18179	98.2	2122	0.0229
18	432.1596	19861	109.8	2214	0.0218
19	435.1676	19179	6555.9	130002	0.0227
20	436.1710	19763	1846.8	36464	0.0221
21	437.1739	18649	269.4	5357	0.0234
22	451.1422	19010	62.1	3614	0.0237
23	457.1499	19576	21.8	1625	0.0234
24	458.2440	20473	76.1	5904	0.0224
25	459.2468	19865	22.3	1794	0.0231
26	483.1529	19572	28.7	3317	0.0247
27	486.2750	19022	105.4	11939	0.0256
28	487.2785	19373	38.0	4280	0.0252
29	514.3067	19938	117.1	10690	0.0258
30	515.3097	19738	44.4	3991	0.0261



4d(vii)

m/z: Calc'd for $C_{26}H_{25}N_2O_3$ ($[M+H]^+$): 413.1865, found: 413.1855

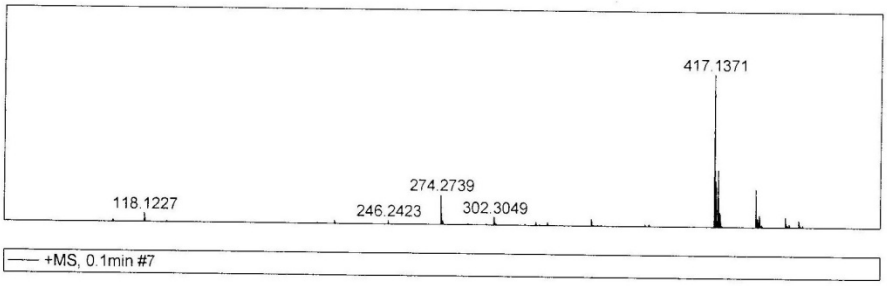
Mass Spectrum List Report

Analysis Info

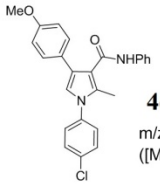
Analysis Name	D:\Data\OUTSIDE\13-04-08-MCR-16.d	Acquisition Date	4/8/2013 8:54:24 AM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MCR-16	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 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	118.1227	16429	399.1	66158	0.0072
2	218.2109	18852	1316.8	25268	0.0116
3	246.2423	20227	1243.6	31115	0.0122
4	274.2739	17969	5199.0	225759	0.0153
5	302.3049	20321	1764.0	59936	0.0149
6	417.1371	17499	10701.7	1156687	0.0238
⇨ 7	439.1188	19144	2528.4	287725	0.0229
8	455.0922	21025	1378.3	75685	0.0216
9	462.1942	22107	1290.3	49957	0.0209



4d(viii)

m/z: Calc'd for $C_{25}H_{21}ClN_2NaO_2$ ($[M+Na]^+$): 439.1189, found: 439.1188

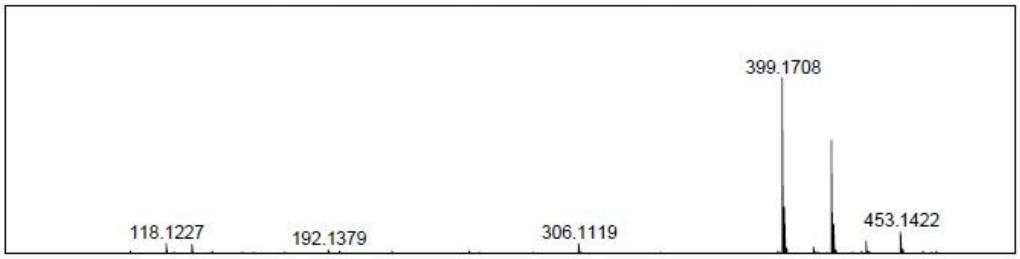
Mass Spectrum List Report

Analysis Info

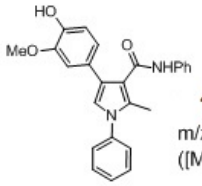
Analysis Name	D:\Data\vipin\13-04-05-MCR-11.d	Acquisition Date	4/5/2013 12:33:30 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MCR-11	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 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	118.1227	15851	3022.8	38824	0.0075
2	130.1590	17833	2268.8	32929	0.0073
3	192.1379	19145	747.4	12440	0.0100
4	197.1070	18807	512.7	8550	0.0105
5	306.1119	20556	1428.9	40973	0.0149
6	399.1708	19099	10890.8	665063	0.0209
➡ 7	421.1529	19419	4727.7	428305	0.0217
8	437.1284	16011	508.2	43344	0.0273
9	453.1422	20773	1417.6	82836	0.0218



4d(ix)

m/z: Calc'd for $C_{25}H_{22}N_2NaO_3$ ($[M+Na]^+$): 421.1528, found: 421.1529

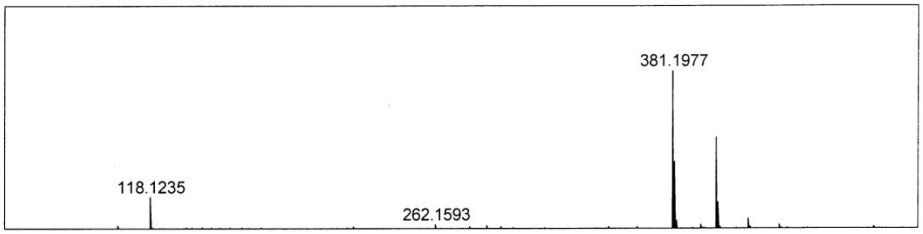
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\vipin\813-04-08-MCR-20.d	Acquisition Date	4/8/2013 9:54:09 AM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MCR-20	Instrument / Ser#	maXis 40
Comment			

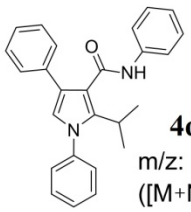
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 l/min
Scan End	500 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



+MS, 0.3min #18

#	m/z	Res.	S/N	I	FWHM
1	118.1235	16069	13918.6	245605	0.0074
2	262.1593	20538	944.1	31017	0.0128
3	381.1977	14276	14624.0	1236302	0.0267
4	382.1998	18392	6149.7	524645	0.0208
5	383.2021	19927	794.1	68364	0.0192
⇨ 6	403.1787	18801	7917.7	709288	0.0214
7	404.1815	18956	2327.4	205294	0.0213
8	405.1840	20651	247.0	21444	0.0196
9	419.1535	18574	1232.1	83384	0.0226
10	435.1665	21156	687.6	33450	0.0206



4d(x)

m/z: Calc'd for $C_{26}H_{24}N_2NaO$ ($[M+Na]^+$): 403.1786, found: 403.1787

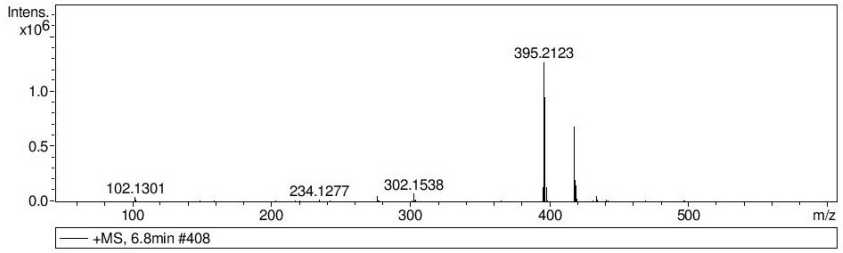
Mass Spectrum List Report

Analysis Info

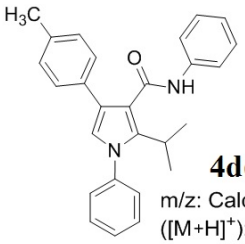
Analysis Name	D:\Data\vipin\SG-287_1-A,4_01_1557.d	Acquisition Date	10/21/2014 4:43:02 PM
Method	HIGH FLOW DIRECT INJECTION LOW MASS.m	Operator	VIKAS GROVER
Sample Name	SG-287	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	600 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	102.1301	13252	1161.3	39177	0.0077
2	149.0242	15001	190.2	11146	0.0099
3	158.9648	15451	223.4	13181	0.0103
4	203.0529	16413	327.1	8160	0.0124
5	217.0688	15721	832.6	10491	0.0138
6	220.1330	17028	556.1	7168	0.0129
7	234.1277	17050	1286.7	18262	0.0137
8	242.1150	17221	714.7	10683	0.0141
9	276.1747	18013	2307.9	52466	0.0153
10	277.1777	16947	480.9	11080	0.0164
11	301.1411	17807	487.4	11934	0.0169
12	302.1538	17865	3055.4	74333	0.0169
13	303.1571	18251	687.4	16672	0.0166
14	365.1055	19102	221.3	7960	0.0191
15	395.2123	11573	11079.7	1265975	0.0342
16	395.4160	12171	76.3	8809	0.0325
17	395.4963	18589	110.6	12779	0.0213
18	395.6704	23017	282.3	32652	0.0172
19	396.2153	18648	8070.3	943244	0.0212
20	397.2185	19790	1109.3	132606	0.0201
21	398.2211	19275	100.6	12337	0.0207
22	417.1938	18680	8403.0	676795	0.0223
23	418.1971	19345	2515.6	196056	0.0216
24	419.2005	19674	369.5	27859	0.0213
25	430.9137	19488	205.7	9228	0.0221
26	433.1682	19418	1316.9	51230	0.0223
27	434.1712	18551	402.2	14604	0.0234
28	440.2700	20009	704.4	19248	0.0220
29	468.3011	20029	420.5	6321	0.0234
30	496.3324	19070	834.9	10782	0.0260



4d(xi)

m/z: Calc'd for $C_{27}H_{27}N_2O$ ($[M+H]^+$): 395.2123, found: 395.2123

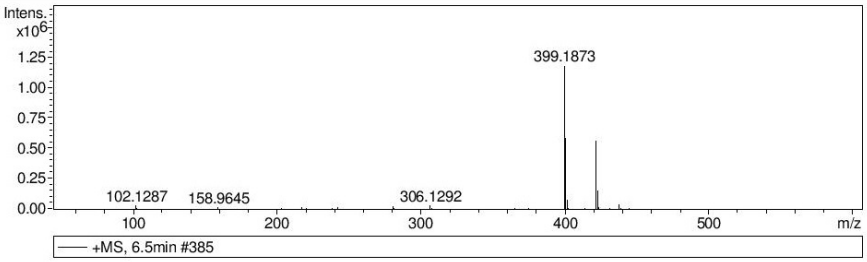
Mass Spectrum List Report

Analysis Info

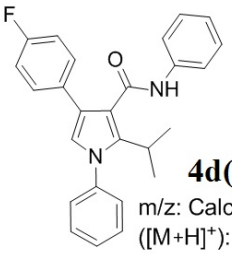
Analysis Name	D:\Data\vipin\SG-291_1-A,5_01_1558.d	Acquisition Date	10/21/2014 4:59:27 PM
Method	HIGH FLOW DIRECT INJECTION LOW MASS.m	Operator	VIKAS GROVER
Sample Name	SG-291	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	600 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	102.1287	13335	910.7	30647	0.0077
2	158.9645	15601	549.6	17548	0.0102
3	203.0530	16256	601.2	9194	0.0125
4	217.0688	16218	910.9	14906	0.0134
5	220.1335	16799	714.0	11795	0.0131
6	238.1029	17161	573.0	9987	0.0139
7	242.1154	16951	1054.7	18590	0.0143
8	280.1500	17621	1060.3	27588	0.0159
9	281.1544	17083	222.2	5855	0.0165
10	306.1292	18034	1117.1	30124	0.0170
11	307.1334	18081	255.5	6892	0.0170
12	362.9267	18243	158.9	5485	0.0199
13	365.1061	18760	248.8	9331	0.0195
14	374.1606	19300	113.1	5720	0.0194
➡ 15	399.1873	13553	13832.5	1184440	0.0295
16	399.4724	14066	59.8	5191	0.0284
17	399.6472	26105	175.6	15197	0.0153
18	400.1905	18986	6784.1	585418	0.0211
19	401.1935	19864	897.2	77239	0.0202
20	402.1963	19201	87.0	7511	0.0209
21	413.2668	18403	83.1	6936	0.0225
22	421.1690	19047	6950.3	563318	0.0221
23	422.1723	19369	1917.1	154924	0.0218
24	423.1757	19070	256.8	20711	0.0222
25	424.0762	18737	65.7	5310	0.0226
26	426.0742	19792	69.4	5571	0.0215
27	430.9141	19370	162.6	12804	0.0222
28	437.1434	19083	561.6	43244	0.0229
29	438.1465	19234	158.7	11980	0.0228
30	444.2451	18510	180.7	11902	0.0240



4d(xii)

m/z: Calc'd for $C_{26}H_{24}FN_2O$ ($[M+H]^+$): 399.1873, found: 399.1873

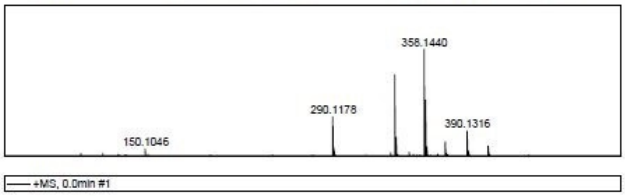
Mass Spectrum List Report

Analysis Info

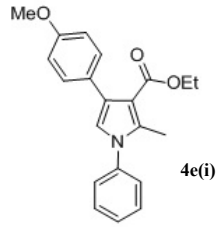
Analysis Name	D:\Data\vipin\813-04-08-MCR-19.d	Acquisition Date	4/8/2013 9:41:08 AM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MCR-19	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 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	150.1046	18137	201.2	83485	0.0083
2	152.1014	17598	47.7	20238	0.0086
3	187.0362	18095	15.1	1953	0.0103
4	199.0573	19865	44.4	6222	0.0100
5	219.0622	20191	13.7	2165	0.0108
6	221.1645	19629	34.2	5470	0.0113
7	236.1070	17860	11.1	1930	0.0132
8	241.0471	19360	13.0	2328	0.0125
9	244.0943	20926	21.7	3943	0.0117
10	245.0789	19800	39.0	7356	0.0124
11	253.0834	18837	12.4	3165	0.0134
12	259.0936	18618	17.0	5225	0.0139
13	275.0918	19454	14.5	6394	0.0141
14	285.1561	21725	11.7	4910	0.0131
15	290.1178	18229	1142.0	470414	0.0159
16	291.1205	18989	205.1	84074	0.0153
17	292.1224	20211	17.4	7108	0.0145
18	306.1317	20434	10.8	4254	0.0150
19	315.0831	21685	22.6	13341	0.0145
20	333.0940	21358	35.4	34770	0.0156
21	336.1599	18463	919.7	965941	0.0182
22	337.1628	18935	200.6	220890	0.0178
23	338.1649	19476	19.2	22157	0.0174
24	347.1097	21641	24.3	39916	0.0160
⇨ 25	358.1440	11321	568.3	1275000	0.0316
26	359.1450	18318	290.2	666792	0.0196
27	360.1462	19145	45.9	107953	0.0188
28	374.1158	18897	73.6	168936	0.0198
29	390.1316	19092	218.8	293596	0.0204
30	406.1254	20390	154.5	112760	0.0199



4e(i)

m/z: Calc'd for $C_{21}H_{21}NNaO_3$ ($[M+Na]^+$): 358.1419, Found 358.1440.

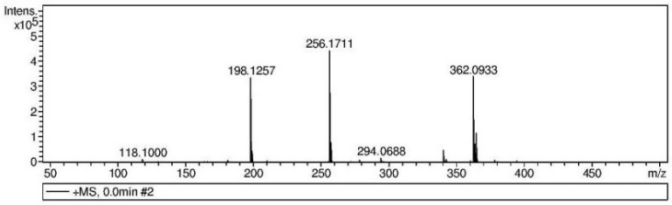
Mass Spectrum List Report

Analysis Info

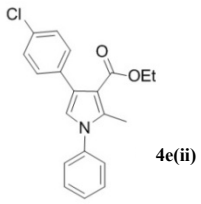
Analysis Name	D:\Data\vipin\14-01-27-AT-73-B.d	Acquisition Date	1/27/2014 2:08:12 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	AT-73-B	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 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	118.1000	15102	127.4	11479	0.0078
2	130.1413	16260	23.4	2181	0.0080
3	139.0581	19575	19.6	1795	0.0071
4	164.0992	15268	24.1	2667	0.0107
5	166.1148	16132	22.3	2546	0.0103
6	176.1013	14810	11.3	1492	0.0119
7	181.0957	17551	67.4	9487	0.0103
8	198.1257	13669	1843.0	335549	0.0145
9	199.1285	16036	252.2	46546	0.0124
10	210.1260	17371	35.0	7427	0.0121
11	255.1467	16374	13.2	2200	0.0156
12	256.1711	14263	2693.8	440878	0.0180
13	257.1738	15816	495.9	79896	0.0163
14	258.1763	17374	24.6	3893	0.0149
15	272.1647	17138	21.8	2678	0.0159
16	278.1520	18009	75.7	9023	0.0154
17	294.0688	17767	138.4	18772	0.0166
18	295.0714	18115	16.4	2235	0.0163
19	296.0662	16966	31.9	4389	0.0175
20	340.1105	17051	223.1	48662	0.0199
21	341.1135	17792	26.6	6058	0.0192
22	342.1078	17124	46.9	11147	0.0200
23	342.2061	18131	19.0	4538	0.0189
24	360.1954	19083	13.8	5689	0.0189
⇨ 25	362.0933	14459	784.8	338226	0.0250
26	363.0959	16672	165.0	72732	0.0218
27	364.0906	15259	257.8	116082	0.0239
28	365.0927	18054	35.8	16469	0.0202
29	378.0655	19141	30.0	10191	0.0198
30	394.0819	17612	42.1	5849	0.0224



4e(ii)

m/z: Calc'd for $C_{20}H_{18}ClNNaO_2$ ($[M+Na]^+$): 362.0924, Found 362.0933.

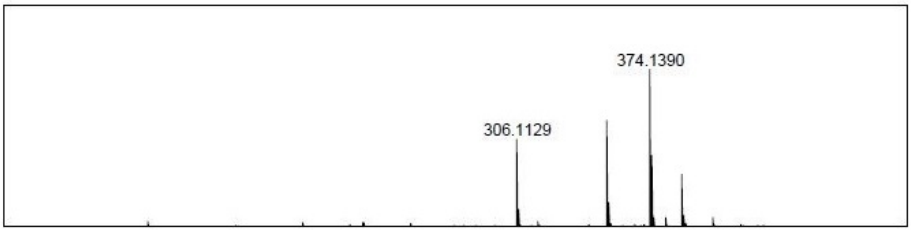
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\vipin\13-04-05-MCR-12.d	Acquisition Date	4/5/2013 1:38:13 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MCR-12	Instrument / Ser#	maXis 40
Comment			

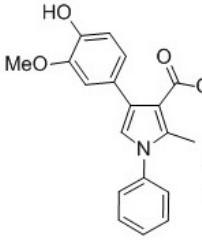
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 l/min
Scan End	500 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



+MS, 0.7min #41

#	m/z	Res.	S/N	I	FWHM
1	306.1129	17945	9952.3	707320	0.0171
2	352.1549	17749	6278.7	864647	0.0198
3	353.1580	18440	1379.6	199244	0.0192
4	354.1598	20371	148.0	22367	0.0174
5	374.1390	12107	6412.7	1274054	0.0309
6	375.1403	18163	2980.2	576385	0.0207
7	376.1427	19759	393.2	73971	0.0190
8	390.1112	18526	3718.4	426160	0.0211



4e(iii)

m/z: Calc'd for $C_{21}H_{21}NNaO_4$ ($[M+Na]^+$): 374.1368, found: 374.1390

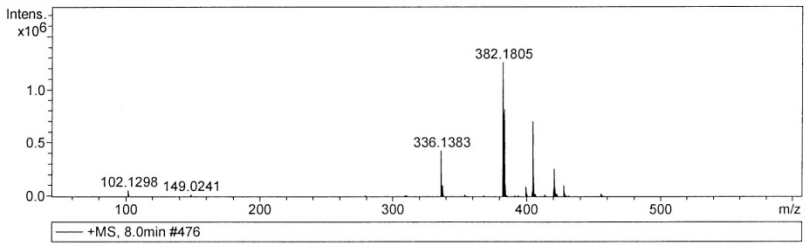
Mass Spectrum List Report

Analysis Info

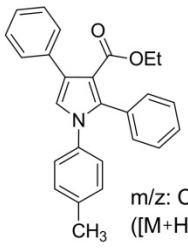
Analysis Name	D:\Data\vipin\SG-243_1-A,6_01_1630.d	Acquisition Date	10/31/2014 10:44:15 AM
Method	HIGH FLOW DIRECT INJECTION LOW MASS.m	Operator	VIKAS GROVER
Sample Name	SG-243	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	600 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	102.1298	12786	2189.4	61587	0.0080
2	149.0241	14923	397.8	19834	0.0100
3	309.1510	18447	221.6	8302	0.0168
4	336.1383	18111	10126.1	430491	0.0186
5	337.1416	17994	2566.0	107990	0.0187
6	338.1450	18343	324.5	13565	0.0184
7	354.1489	18048	448.3	15542	0.0196
8	368.1648	18454	162.0	9419	0.0200
⇨ 9	382.1805	11867	10218.8	1256423	0.0322
10	382.3805	11625	61.6	7692	0.0329
11	382.4598	15623	71.7	8973	0.0245
12	382.6307	23909	220.4	27622	0.0160
13	383.1835	17973	6390.7	815599	0.0213
14	384.1869	18418	900.8	119222	0.0209
15	385.1900	19158	86.8	11951	0.0201
16	391.2844	19244	79.1	13132	0.0203
17	399.2068	19537	447.8	90578	0.0204
18	400.2102	18541	121.1	24601	0.0216
19	404.1620	18476	3761.0	704256	0.0219
20	405.1655	19392	1084.7	198876	0.0209
21	406.1687	19581	151.3	27175	0.0207
22	413.2661	19178	113.6	17250	0.0215
23	420.1361	19101	2074.4	258525	0.0220
24	421.1395	19612	598.5	72250	0.0215
25	422.1373	17238	210.6	24625	0.0245
26	427.2381	18874	1058.9	102494	0.0226
27	428.2413	19454	332.6	30900	0.0220
28	431.1970	18661	80.8	6585	0.0231
29	455.2694	18735	612.8	23039	0.0243
30	456.2727	18802	214.9	7841	0.0243



4e(iv)

m/z: Calc'd for $C_{26}H_{24}NO_2$ ($[M+H]^+$): 382.1807, found: 382.1805

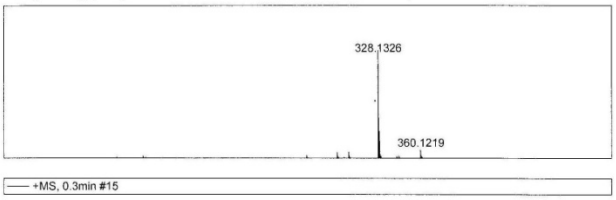
Mass Spectrum List Report

Analysis Info

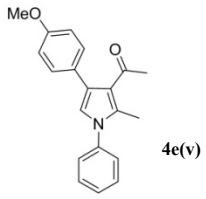
Analysis Name	D:\Data\vipin\13-08-27-MCR-38.d	Acquisition Date	8/29/2013 11:08:16 AM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MCR-38	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 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	226.9512	17337	52.8	4326	0.0131
2	230.2483	17729	49.2	4074	0.0130
3	236.1046	17495	12.7	1069	0.0135
4	246.2427	18023	38.4	3520	0.0137
5	258.2793	20339	11.6	1415	0.0127
6	264.1381	17738	19.1	2609	0.0149
7	268.0945	17874	18.3	2696	0.0150
8	272.2589	19028	12.9	2029	0.0143
9	273.0736	18460	15.4	2458	0.0148
10	274.2744	18556	167.1	27153	0.0148
11	275.2776	18207	24.1	3981	0.0151
12	278.0792	17189	18.2	3155	0.0162
13	297.1580	18234	232.3	53776	0.0163
14	298.1610	18783	31.8	7446	0.0159
15	302.3059	17891	24.0	5920	0.0169
16	306.1495	18655	216.2	56574	0.0164
17	307.1525	18841	36.6	9885	0.0163
⇨ 18	328.1326	14821	2068.0	926672	0.0221
19	329.1355	17139	524.2	239369	0.0192
20	330.1377	18711	45.2	21027	0.0176
21	342.1110	19301	22.7	10907	0.0177
22	344.1252	18295	38.4	17947	0.0188
23	360.1219	18035	208.7	76724	0.0200
24	361.1248	19108	36.7	13260	0.0189
25	376.1160	18514	15.4	3858	0.0203
26	396.1191	18444	14.7	1294	0.0215
27	437.1945	20228	54.6	4404	0.0216
28	438.1978	18417	12.9	1026	0.0238
29	440.1651	20016	23.3	1787	0.0220
30	465.1436	19654	33.5	1686	0.0237



4e(v)

m/z: Calc'd for $C_{20}H_{19}NNaO_2$ ($[M+Na]^+$): 328.1313, Found 328.1326.

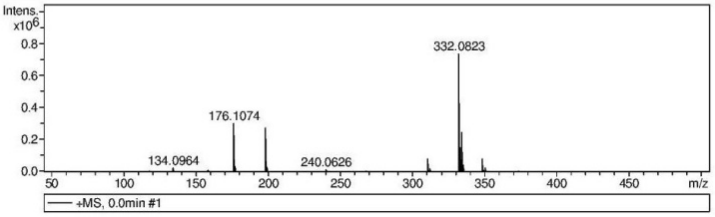
Mass Spectrum List Report

Analysis Info

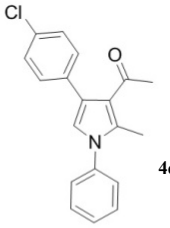
Analysis Name	D:\Data\vipin\14-02-03-SG-250.d	Acquisition Date	2/3/2014 10:36:58 AM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	SG-250	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 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	118.0651	16092	30.9	3886	0.0073
2	134.0964	16657	205.5	25380	0.0081
3	135.0029	15974	19.1	2335	0.0085
4	135.0989	14002	10.7	1304	0.0096
5	139.0729	14632	28.2	3304	0.0095
6	158.0961	16572	97.9	11571	0.0095
7	176.1074	13689	1765.8	303089	0.0129
8	177.1100	16225	196.3	34273	0.0109
9	198.0893	13878	1500.3	276723	0.0143
10	199.0920	16439	152.5	28046	0.0121
11	205.0678	18945	15.0	2711	0.0108
12	240.0626	17379	105.4	13880	0.0138
13	268.0880	17825	40.1	3840	0.0150
14	270.0847	14175	10.5	977	0.0191
15	301.1402	15252	15.8	3128	0.0197
16	310.0996	16497	323.3	83352	0.0188
17	311.1021	18346	41.4	11052	0.0170
18	312.0964	17797	74.2	20471	0.0175
⇨ 19	332.0823	14993	1609.2	737854	0.0221
20	333.0853	14801	318.1	148779	0.0225
21	334.0799	14593	512.9	244538	0.0229
22	335.0822	16896	89.6	43522	0.0198
23	348.0559	16466	235.1	79996	0.0211
24	349.0579	19270	34.6	11325	0.0181
25	350.0531	17849	85.2	26736	0.0196
26	351.0562	17600	10.8	3235	0.0199
27	373.1877	16504	52.0	4296	0.0226
28	374.1919	17136	11.5	942	0.0218
29	393.2970	20214	16.9	1082	0.0195
30	413.2666	17395	42.2	2581	0.0238



4e(vi)

m/z: Calc'd for $C_{19}H_{16}ClNNaO$ ($[M+Na]^+$): 332.0818, Found 332.0823.

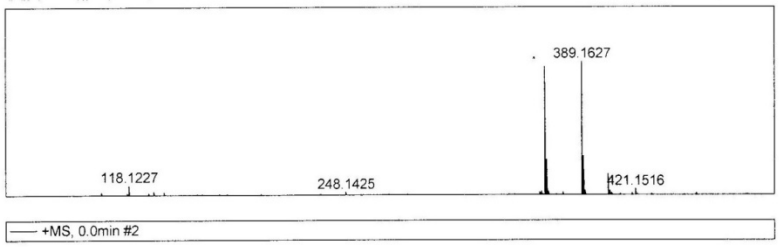
Mass Spectrum List Report

Analysis Info

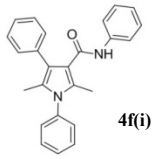
Analysis Name	D:\Data\vipin\13-04-05-MCR-13.d	Acquisition Date	4/5/2013 1:51:38 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MCR-13	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 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	102.1278	15940	1447.6	19223	0.0064
2	118.1227	16217	3195.1	70355	0.0073
3	133.1334	17159	945.7	22979	0.0078
4	139.0726	16579	805.7	19728	0.0084
5	162.1270	19563	260.0	6597	0.0083
6	177.1376	20222	174.8	4560	0.0088
7	197.1067	19044	244.7	6709	0.0103
8	248.1425	19311	486.9	21149	0.0128
9	274.1224	20106	217.3	9187	0.0136
10	285.1559	20679	245.8	9925	0.0138
11	346.1042	21294	146.5	9714	0.0163
12	367.1807	18150	7555.2	906637	0.0202
13	368.1838	18711	2080.1	249679	0.0197
14	369.1867	19758	220.9	26520	0.0187
⇨15	389.1627	17672	7764.0	937673	0.0220
16	421.1516	20995	596.0	41165	0.0201



4f(i)

m/z: Calc'd for $C_{25}H_{22}N_2NaO$
($[M+Na]^+$): 389.1630, Found 389.1627.

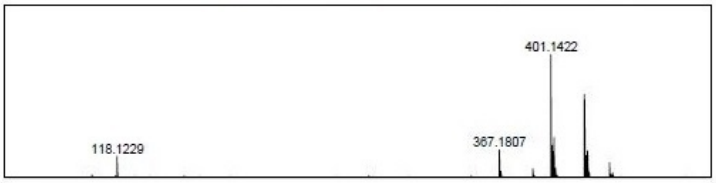
Mass Spectrum List Report

Analysis Info

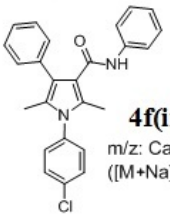
Analysis Name	D:\Data\vipin\13-04-05-MCR-15.d	Acquisition Date	4/5/2013 2:16:55 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MCR-15	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 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	118.1229	16274	8210.9	120130	0.0073
2	367.1807	18950	5199.4	157868	0.0194
3	389.1623	20494	818.1	50377	0.0190
4	401.1422	18619	9336.3	693135	0.0215
5	402.1451	18963	2474.2	184159	0.0212
6	403.1401	17486	3053.1	227833	0.0231
7	404.1422	20459	727.1	54394	0.0198
8	423.1242	18496	5964.1	467893	0.0229
9	424.1270	19465	1563.5	122963	0.0218
10	425.1220	18240	1908.8	150483	0.0233
11	426.1239	20126	407.0	32167	0.0212
12	439.0978	19978	1448.9	84422	0.0220
13	446.1991	21904	132.1	5863	0.0204



4f(ii)

m/z: Calc'd for $C_{25}H_{21}ClN_2NaO$ ($[M+Na]^+$): 423.1240, found: 423.1242

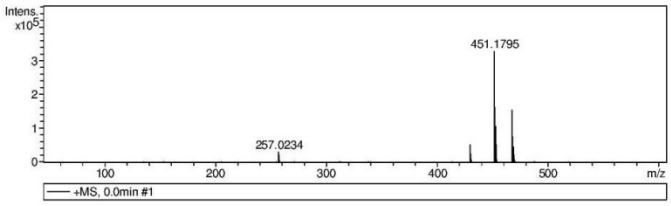
Mass Spectrum List Report

Analysis Info

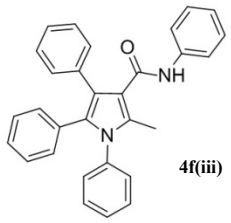
Analysis Name	D:\Data\vipin\14-01-13-SG-239.d	Acquisition Date	1/13/2014 3:12:45 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	SG-239	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 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	102.1267	16291	13.9	602	0.0063
2	116.1429	16875	10.9	635	0.0069
3	135.0022	17088	33.3	2625	0.0079
4	150.9762	18444	10.4	792	0.0082
5	153.1381	16353	45.2	3401	0.0094
6	164.9196	16678	19.7	1373	0.0099
7	205.0673	16841	39.7	3566	0.0122
8	255.1458	18125	16.9	2992	0.0141
9	257.0234	17768	183.4	31637	0.0145
10	258.0267	16841	15.3	2603	0.0153
11	270.9764	17850	12.0	1643	0.0152
12	312.0747	19423	29.3	2910	0.0161
13	314.0703	21219	12.4	1231	0.0148
14	338.1483	19628	21.5	2021	0.0172
15	340.1649	18531	18.2	1688	0.0184
16	375.1454	19787	17.1	1311	0.0190
17	413.2655	17855	14.3	2107	0.0231
18	429.1965	17917	224.6	53506	0.0240
19	430.1992	18512	49.6	12094	0.0232
⇨ 20	451.1795	15585	1177.3	327835	0.0289
21	452.1822	15990	385.7	107269	0.0283
22	453.1846	18703	42.5	11813	0.0242
23	467.1534	15731	567.1	155005	0.0297
24	468.1557	17943	174.1	47533	0.0261
25	469.1544	16382	40.9	11154	0.0286
26	487.2484	19636	10.9	2213	0.0248
27	518.2276	21205	33.7	2343	0.0244



4f(iii)

m/z: Calc'd for $C_{30}H_{24}N_2NaO$ ($[M+Na]^+$): 451.1786, Found 451.1795.

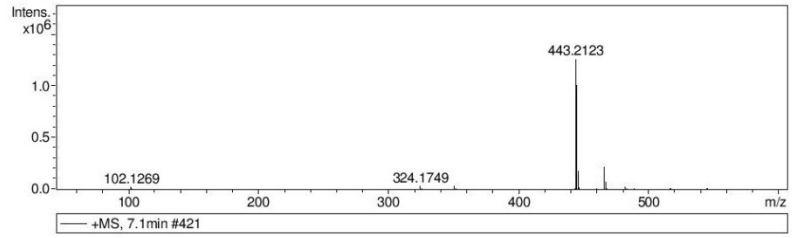
Mass Spectrum List Report

Analysis Info

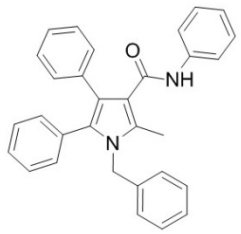
Analysis Name	D:\Data\vipin\SG-240_1-A,6_01_1559.d	Acquisition Date	10/21/2014 5:15:52 PM
Method	HIGH FLOW DIRECT INJECTION LOW MASS.m	Operator	VIKAS GROVER
Sample Name	SG-240	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	600 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	102.1269	13269	1068.7	29234	0.0077
2	158.9638	15804	135.4	5123	0.0101
3	217.0687	16381	100.9	4573	0.0133
4	324.1749	18425	2546.1	37734	0.0176
5	325.1781	18631	648.2	9683	0.0175
6	350.1542	18088	1868.2	31826	0.0194
7	351.1576	19008	510.9	8762	0.0185
8	387.1856	19506	206.0	4163	0.0198
9	441.1964	19008	52.6	4727	0.0232
⇨10	443.2123	11812	14610.8	1259540	0.0375
11	443.4279	12644	101.7	8785	0.0351
12	443.5127	17973	137.0	11798	0.0247
13	443.6976	23734	365.6	31315	0.0187
14	444.2150	18516	11838.4	1003968	0.0240
15	445.2178	19869	2115.2	176458	0.0224
16	446.2212	19819	225.6	18540	0.0225
17	459.2069	19256	96.9	6219	0.0238
18	465.1938	19608	3902.9	216636	0.0237
19	466.1971	20145	1314.3	71123	0.0231
20	467.2001	19813	224.3	11841	0.0236
21	475.2021	18918	113.9	4792	0.0251
22	481.1683	18893	659.3	24407	0.0255
23	482.1716	19457	235.8	8539	0.0248
24	483.1703	17944	107.5	3806	0.0269
25	488.2698	19120	319.3	9938	0.0255
26	501.2648	19187	207.1	4209	0.0261
27	516.3006	20386	309.3	7318	0.0253
28	521.2235	20482	111.7	4102	0.0254
29	544.3323	19942	140.2	13723	0.0273
30	545.3356	20261	57.3	5764	0.0269



4f(iv)

m/z: Calc'd for $C_{31}H_{27}N_2O$ ($[M+H]^+$): 443.2123, found: 443.2123

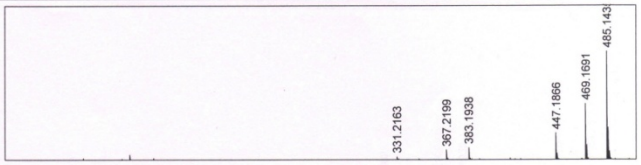
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\vipin\13-01-21-MCR-6.d	Acquisition Date	1/21/2013 2:14:57 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MCR-6	Instrument / Ser#	maXis 40
Comment			

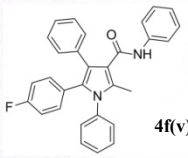
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 l/min
Scan End	500 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



+MS, 0.7min #40

#	m/z	Res.	S/N	I	FWHM
1	281.5948	19485	10.9	326	0.0145
2	331.2163	23457	130.2	4805	0.0141
3	332.2194	22910	26.0	978	0.0145
4	347.2474	23549	28.1	1221	0.0147
5	353.1641	24125	10.4	468	0.0146
6	367.2199	24992	318.3	15606	0.0147
7	368.2226	23425	45.8	2257	0.0157
8	375.1459	23202	16.6	839	0.0162
9	383.1938	23406	378.6	19750	0.0164
10	384.1964	23939	51.0	2670	0.0160
11	385.1940	18938	21.1	1110	0.0203
12	391.1199	22745	35.8	1925	0.0172
13	401.2560	22326	12.9	695	0.0180
14	413.2651	22950	45.6	2278	0.0180
15	414.2692	24718	12.0	597	0.0168
16	417.2295	23421	22.1	1074	0.0178
17	421.1303	23739	19.3	916	0.0177
18	429.2391	24960	16.7	792	0.0172
19	438.1266	21930	10.4	743	0.0200
20	447.1866	22819	441.8	42634	0.0196
21	448.1895	24661	107.9	10712	0.0182
22	449.1924	22882	12.1	1231	0.0196
23	466.1602	24564	13.4	1837	0.0190
⇨ 24	469.1691	22356	635.9	89581	0.0210
25	470.1719	24926	169.6	24090	0.0189
26	471.1747	23475	17.1	2446	0.0201
27	485.1435	21062	1089.3	173871	0.0230
28	486.1462	23100	325.6	52353	0.0210
29	487.1444	22433	85.0	13773	0.0217
30	488.1454	21838	13.7	2231	0.0224



4f(v)

m/z: Calc'd for $C_{30}H_{23}FN_2NaO$ ($[M+Na]^+$): 469.1692, Found 469.1691.

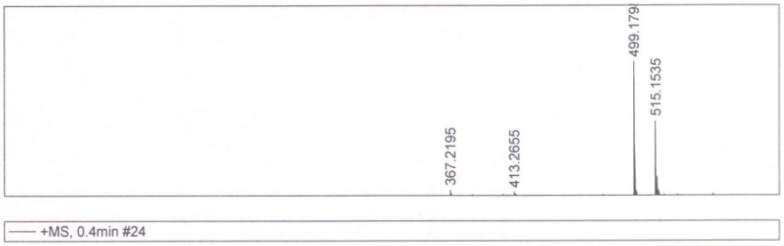
Mass Spectrum List Report

Analysis Info

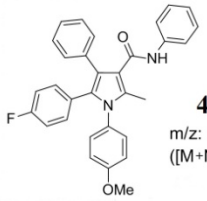
Analysis Name	D:\Data\vipin\13-01-21-MCR-7.d	Acquisition Date	1/21/2013 3:12:14 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MCR-7	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 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	153.1379	21939	14.4	353	0.0070
2	178.8988	20602	18.5	312	0.0087
3	180.8957	23318	15.5	262	0.0078
4	196.8652	18173	16.1	281	0.0108
5	198.8623	20651	16.0	280	0.0096
6	236.8581	26909	13.2	287	0.0088
7	238.8541	22411	10.1	224	0.0107
8	254.8245	20419	14.0	331	0.0125
9	256.8200	26185	20.3	479	0.0098
10	331.2164	24857	15.3	361	0.0133
11	367.2195	25161	162.3	6335	0.0146
12	368.2227	24054	24.8	969	0.0153
13	383.1933	23073	26.7	1072	0.0166
14	405.1567	26595	28.9	1124	0.0152
15	413.2655	23615	115.6	4112	0.0175
16	414.2690	27269	28.6	1006	0.0152
17	421.1310	24982	22.3	720	0.0169
18	441.2968	24145	23.0	597	0.0183
19	443.1372	22910	22.1	576	0.0193
20	468.1367	27685	10.1	271	0.0169
21	469.1665	23818	18.6	498	0.0197
22	477.1959	25736	40.3	1406	0.0185
23	478.1983	22302	10.8	406	0.0214
⇨ 24	499.1798	21328	1645.0	154374	0.0234
25	500.1825	24110	506.8	48924	0.0207
26	501.1849	24938	53.3	5289	0.0201
27	515.1535	22700	722.0	85990	0.0227
28	516.1560	23932	186.4	21786	0.0216
29	517.1544	21693	50.3	5770	0.0238
30	518.1556	21608	10.1	1137	0.0240



4f(vi)

m/z: Calc'd for $C_{31}H_{25}FN_2NaO_2$ ($[M+Na]^+$): 499.1798, found: 499.1798

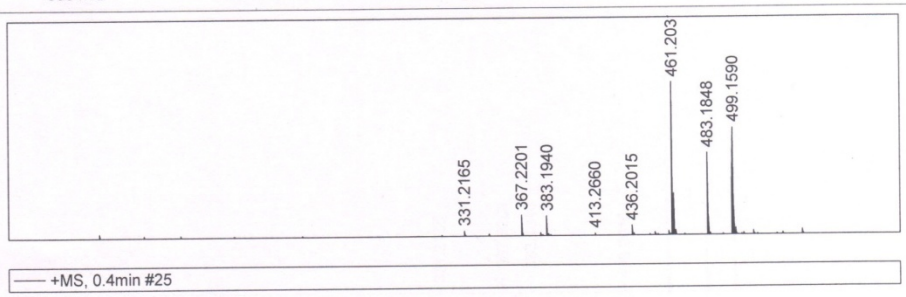
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\vipin\13-01-21-MCR-8.d	Acquisition Date	1/21/2013 3:39:11 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MCR-8	Instrument / Ser#	maXis 40
Comment			

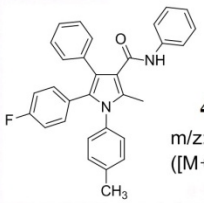
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 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	7.0 l/min
Scan End	600 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



+MS, 0.4min #25

#	m/z	Res.	S/N	I	FWHM
1	200.1640	20608	10.5	228	0.0097
2	229.1132	22086	27.6	572	0.0104
3	245.1854	26903	16.0	324	0.0091
4	267.1673	23147	18.9	387	0.0115
5	277.0961	15537	11.9	247	0.0178
6	289.1756	19673	16.6	355	0.0147
7	317.1642	22139	15.3	437	0.0143
8	331.2165	23119	88.0	3253	0.0143
9	332.2200	23533	18.7	712	0.0141
10	347.2481	21159	23.4	1255	0.0164
11	367.2201	24049	179.1	12196	0.0153
12	368.2231	23283	26.2	1781	0.0158
13	379.1799	26183	32.5	2140	0.0145
14	383.1940	23941	179.8	11694	0.0160
15	384.1967	22961	24.6	1596	0.0167
16	385.1938	20942	10.7	691	0.0184
17	413.2660	22897	23.6	1338	0.0180
18	436.2015	25200	118.9	5682	0.0173
19	437.2050	22802	28.6	1376	0.0192
20	447.1852	23771	12.4	854	0.0188
21	450.2177	22778	23.3	1746	0.0198
22	459.1863	24141	26.6	2478	0.0190
23	461.2031	21724	925.2	90053	0.0212
24	462.2060	24320	247.2	24566	0.0190
25	463.2098	21469	27.2	2763	0.0216
⇨ 26	483.1848	23000	381.2	48273	0.0210
27	484.1877	24257	92.9	11798	0.0200
28	485.1899	23992	11.3	1435	0.0202
29	499.1590	22486	479.0	62920	0.0222
30	500.1615	24461	122.9	16173	0.0204



4f(vii)

m/z: Calc'd for $C_{31}H_{25}FN_2NaO$ ($[M+Na]^+$): 483.1849, found: 483.1848
