Supporting Information

Stereoregulations of Pyrimidinone Based Chiral Auxiliary in Aldol and Alkylation Reactions: A Convenient Route to Oxyneolignans

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Copies of HRMS spectra

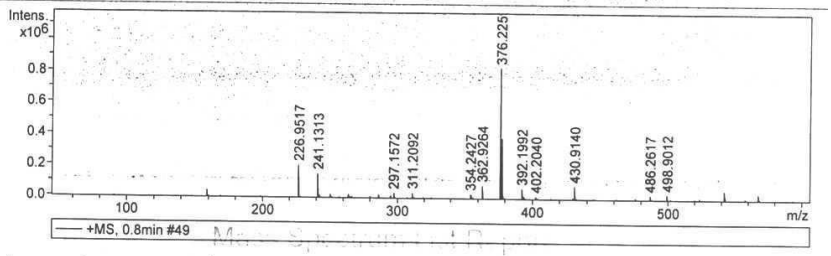
Mass Spectrum List Report

Analysis Info

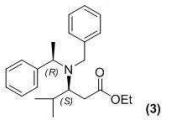
Analysis Name	D:\Data\vipin\12-02-09-MC-121.d	Acquisition Date	2/9/2012 10:20:38 AM
Method	sodium formate tune_low.m		
Sample Name	12-02-09-MC-121	Operator	VIKAS GROVER
Comment		Instrument / Ser#	maXis 40

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	226.9517	21417	6728.1	203827	0.0106
2	241.1313	22644	4499.9	151815	0.0106
3	297.1572	23642	953.1	32195	0.0126
4	311.2092	23407	1046.4	34786	0.0133
5	354.2427	24118	353.3	27138	0.0147
6	362.9264	24716	935.4	82228	0.0147
→ 7	376.2259	16813	4770.6	825595	0.0224
8	377.2286	23352	5748.2	382325	0.0162
9	378.2313	23535	676.4	43974	0.0161
10	392.1992	24619	1458.1	64320	0.0159
11	402.2040	25642	463.6	15371	0.0157
12	430.9140	25473	2354.6	81326	0.0169
13	475.3253	26363	411.0	12481	0.0180
14	486.2617	25327	850.5	26813	0.0192
15	498.9012	25923	997.5	32782	0.0192



(3)

m/z: Calc'd for $C_{23}H_{31}NNaO_2$ ($[M+Na]^+$): 376.2252, found: 376.2259.

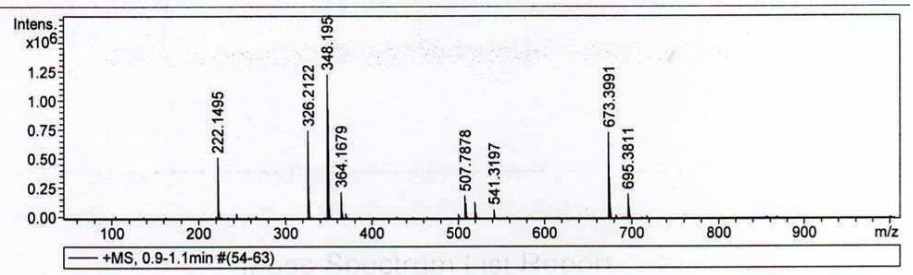
Mass Spectrum List Report

Analysis Info

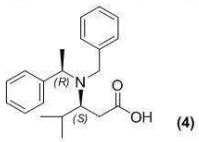
Analysis Name	D:\Data\vipin\11-01-04-MC-TP-IP-1.d	Acquisition Date	1/4/2011 2:18:44 PM
Method	tune_low.m		
Sample Name	MC-TP-IP-1	Operator	VIKAS GROVER
Comment		Instrument / Ser#	maXis 40

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	222.1495	19629	64775.5	514386	0.0113
→ 2	326.2122	21235	21063.1	742439	0.0154
3	348.1958	11780	39702.6	1219774	0.0296
4	364.1679	21666	9684.7	218068	0.0168
5	507.7878	25287	9749.6	182800	0.0201
6	519.3379	24417	6041.0	133938	0.0213
7	541.3197	25738	3800.8	70631	0.0210
8	673.3991	22721	30995.5	728483	0.0296
9	695.3811	23908	9971.2	202072	0.0291



(4)

m/z: Calc'd for $C_{21}H_{28}NO_2$ ([M+H]+): 326.2120, found: 326.2122.

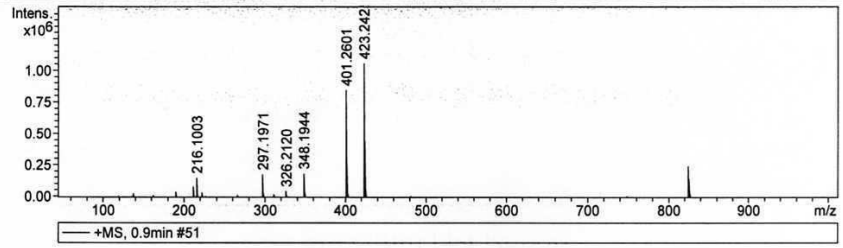
Mass Spectrum List Report

Analysis Info

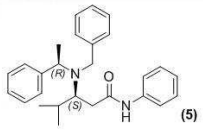
Analysis Name	D:\Data\vipin\11-01-04-MC-TP-IP-2.d	Acquisition Date	1/5/2011 9:47:55 AM
Method	tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-TP-IP-2	Instrument / Ser#	maXis 40
Comment			

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	216.1003	20998	1030.4	153941	0.0103
2	297.1971	21372	1411.8	181147	0.0139
3	311.2122	26341	150.8	19739	0.0118
4	326.2120	24316	345.4	46198	0.0134
5	348.1944	21731	1298.4	187070	0.0160
6	401.2601	21139	5075.9	843326	0.0190
→ 7	423.2425	17982	8054.6	1059349	0.0235



(5)

m/z: Calc'd for $C_{27}H_{32}N_2NaO$ ($[M+Na]^+$): 423.2412, found: 423.2425.

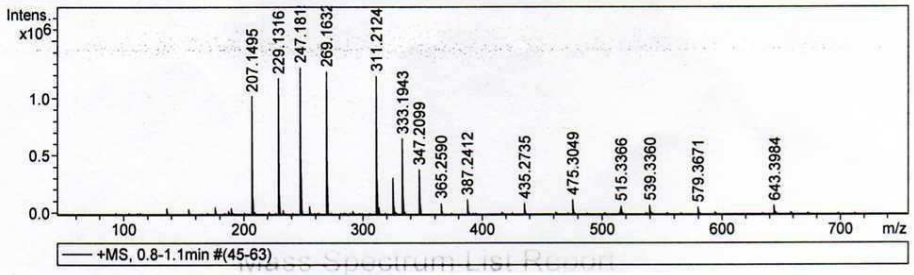
Mass Spectrum List Report

Analysis Info

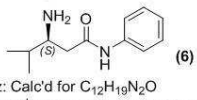
Analysis Name	D:\Data\vipin\11-01-04-MC-TP-IP-3.d	Acquisition Date	1/5/2011 5:04:12 PM
Method	tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-TP-IP-3	Instrument / Ser#	maXis 40
Comment			

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	750 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



#	m/z	Res.	S/N	I	FWHM
→ 1	207.1495	18453	27156.5	1015976	0.0112
2	229.1316	18366	24311.8	1170743	0.0125
3	247.1815	13763	22514.3	1267034	0.0180
4	269.1632	16960	20659.7	1235515	0.0159
5	311.2124	19391	22516.1	1191610	0.0160
6	325.2279	20633	6619.9	308618	0.0158
7	333.1943	21181	15114.1	650465	0.0157
8	347.2099	21197	10320.7	379121	0.0164
9	365.2590	23741	3042.8	88167	0.0154
10	387.2412	23443	6087.2	119988	0.0165
11	435.2735	24589	6079.1	84936	0.0177
12	475.3049	24051	7932.5	116246	0.0198
13	515.3366	25008	4554.8	63667	0.0206
14	539.3360	25272	5450.0	68364	0.0213
15	579.3671	27091	5509.6	53066	0.0214
16	643.3984	26984	7794.1	70702	0.0238



(6)

m/z: Calc'd for $C_{12}H_{19}N_2O$ ($[M+H]^+$): 207.1497, found: 207.1495.

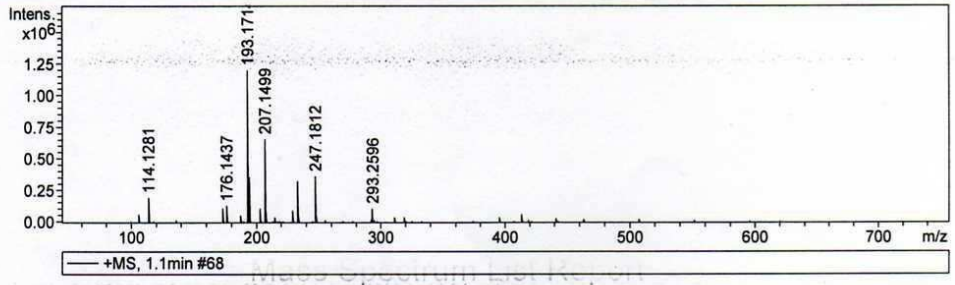
Mass Spectrum List Report

Analysis Info

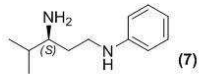
Analysis Name	D:\Data\vipin\11-01-06-MC-TP-IP-4.d	Acquisition Date	1/6/2011 10:04:27 AM
Method	tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-TP-IP-4	Instrument / Ser#	maXis 40
Comment			

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	750 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



#	m/z	Res.	S/N	I	FWHM
1	114.1281	17304	14476.9	194953	0.0066
2	176.1437	19031	3670.2	130913	0.0093
→ 3	193.1714	12114	5855.8	1197198	0.0159
4	207.1499	19395	8061.0	660559	0.0107
5	233.2019	19721	5491.9	327229	0.0118
6	247.1812	18924	8592.0	365717	0.0131
7	293.2596	22157	3606.3	110167	0.0132



(7)

m/z: Calc'd for $C_{12}H_{21}N_2$
($[M+H]^+$): 193.1705, found: 193.1714.

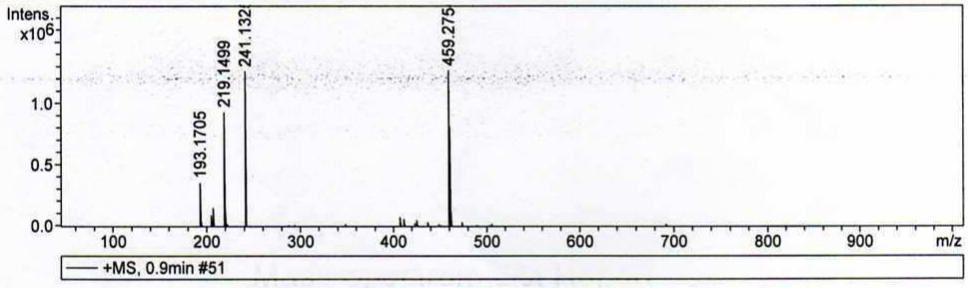
Mass Spectrum List Report

Analysis Info

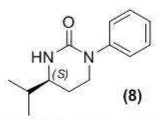
Analysis Name	D:\Data\vipin\11-01-06-MC-TP-IP-5.d	Acquisition Date	1/6/2011 11:39:51 AM
Method	tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-TP-IP-5	Instrument / Ser#	maXis 40
Comment			

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	193.1705	18464	10805.2	354242	0.0105
2	207.1496	19904	3486.0	145638	0.0104
→ 3	219.1499	19039	13831.8	930582	0.0115
4	241.1325	14048	11051.0	1259704	0.0172
5	459.2754	13824	3343.1	1264709	0.0332



(8)

m/z: Calc'd for $C_{13}H_{19}N_2O$
($[M+H]^+$): 219.1497, found: 219.1499.

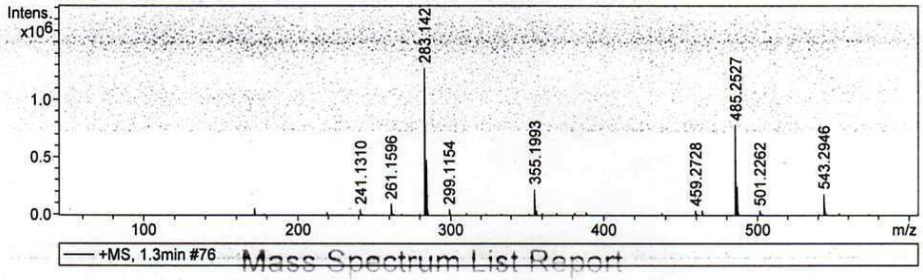
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\vipin\12-02-08-MC-101.d	Acquisition Date	2/8/2012 11:31:35 AM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	12-02-08-MC-101	Instrument / Ser#	maXis 40
Comment			

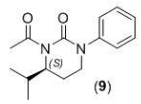
Acquisition Parameter

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



Mass Spectrum List Report

#	m/z	Res.	S/N	I	FWHM
1	241.1310	24149	1593.6	52138	0.0100
2	261.1596	22455	2179.2	97129	0.0116
→ 3	283.1427	14357	19636.2	1274942	0.0197
4	284.1450	20894	7275.1	479103	0.0136
5	285.1473	22597	707.3	47236	0.0126
6	299.1154	24635	938.3	51349	0.0121
7	355.1993	23827	6748.1	226535	0.0149
8	459.2728	26306	792.6	39542	0.0175
9	463.2701	25682	722.1	39397	0.0180
10	485.2527	23731	13692.5	777885	0.0204
11	501.2262	25660	982.5	40716	0.0195
12	543.2946	25608	4861.6	186205	0.0212



(**9**)

m/z: Calc'd for $C_{15}H_{20}N_2NaO_2$
([M+Na]+): 283.1422, found: 283.1427

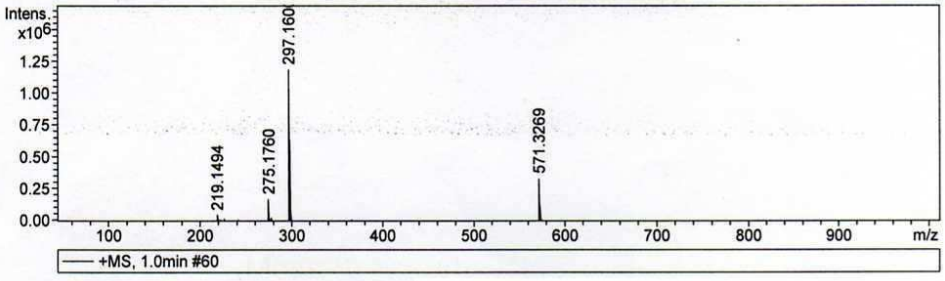
Mass Spectrum List Report

Analysis Info

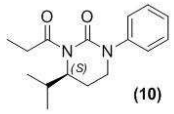
Analysis Name	D:\Data\vipin\11-01-11-MC-TP-IP6.d	Acquisition Date	1/12/2011 10:31:46 AM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-TP-IP6	Instrument / Ser#	maXis 40
Comment			

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	400.0 Vpp	Set Divert Valve	Source



#	m/z	Res.	S/N	I	FWHM
1	219.1494	23229	2202.3	46603	0.0094
→ 2	275.1760	20730	3822.0	170436	0.0133
3	297.1600	10969	29798.1	1183900	0.0271
4	365.1448	29248	426.5	12968	0.0125
5	571.3269	22049	4815.8	330017	0.0259



(**10**)

m/z: Calc'd for $C_{16}H_{23}N_2O_2$
([M+H]$^+$) requires 275.1760; found 275.1760.

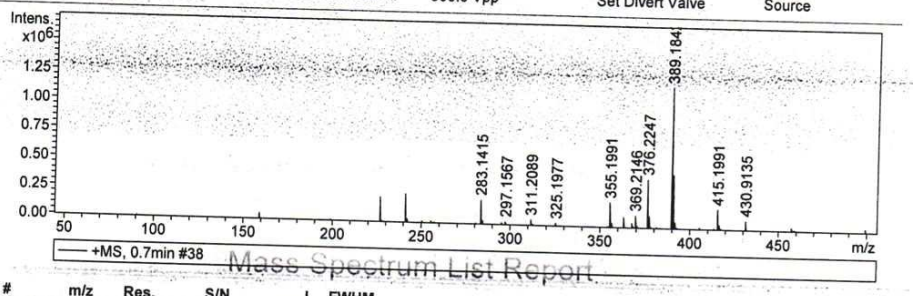
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\vipin\12-02-09-MC-108.d	Acquisition Date	2/9/2012 4:44:00 PM
Method	sodium formate tune_low.m		
Sample Name	12-02-09-MC-108	Operator	VIKAS GROVER
Comment		Instrument / Ser#	maXis 40

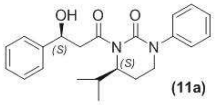
Acquisition Parameter

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



Mass Spectrum List Report

#	m/z	Res.	S/N	I	FWHM
1	283.1415	23154	4772.8	206387	0.0122
2	297.1567	23762	708.3	28178	0.0125
3	311.2089	24528	1293.2	47910	0.0127
4	325.1977	24731	651.5	23081	0.0131
5	355.1991	24296	2350.3	210294	0.0146
6	362.9260	25395	749.1	83933	0.0143
7	369.2146	24427	862.2	106160	0.0151
8	376.2247	23036	3425.1	415736	0.0163
→ 9	389.1842	18355	10184.5	1203280	0.0212
10	415.1991	24840	2190.0	271151	0.0167
11	430.9135	25479	206.0	79878	0.0169



(11a)

m/z: Calc'd for $C_{22}H_{26}N_2NaO_3$ ([M+Na]$^+$): 389.1841, found: 389.1842.

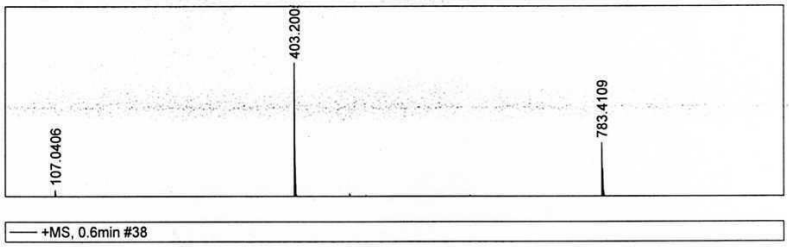
Mass Spectrum List Report

Analysis Info

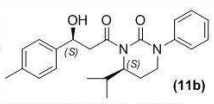
Analysis Name	D:\Data\vipin\11-03-09-MC-IP-AA1.d	Acquisition Date	3/9/2011 12:08:38 PM
Method	tune_low.m		
Sample Name	MC-IP-AA1	Operator	VIKAS GROVER
Comment		Instrument / Ser#	maXis 40

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	107.0406	23086	4298.4	39673	0.0046
→ 2	403.2005	21014	62150.1	822612	0.0192
3	404.2035	21523	15961.9	210540	0.0188
4	783.4109	21891	22869.3	330833	0.0358



(11b)

m/z: Calc'd for $C_{23}H_{28}N_2NaO_3$ ([M+Na]$^+$): 403.1998, found: 403.2005.

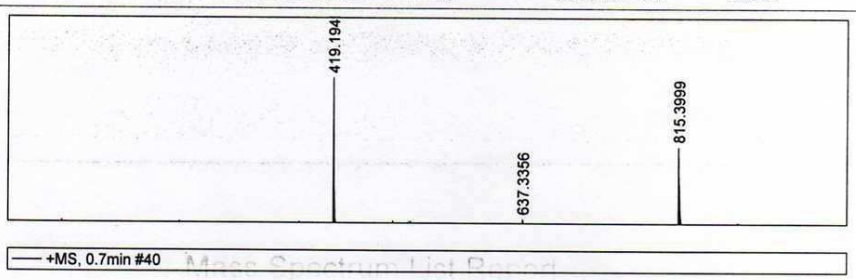
Mass Spectrum List Report

Analysis Info

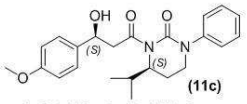
Analysis Name	D:\Data\vipin\11-03-09-MC-IP-AA2.d	Acquisition Date	3/9/2011 12:22:01 PM
Method	tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-IP-AA2	Instrument / Ser#	maXis 40
Comment			

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	379.2014	34704	614.4	4883	0.0109
→ 2	419.1949	21641	84915.6	650013	0.0194
3	420.1978	22089	21443.0	162970	0.0190
4	421.1998	29658	1541.5	11631	0.0142
5	480.3221	33061	421.2	2288	0.0145
6	487.1815	34997	1564.8	8526	0.0139
7	507.2823	31825	1338.7	7360	0.0159
8	637.3356	33454	3280.8	18246	0.0191
9	815.3999	21562	42386.1	344539	0.0378



(11c)

m/z: Calc'd for $C_{23}H_{28}N_2NaO_4$ ($[M+Na]^+$): 419.1947, found: 419.1949.

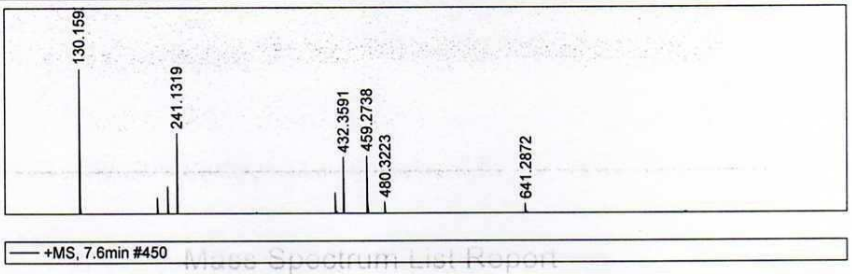
Mass Spectrum List Report

Analysis Info

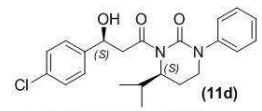
Analysis Name	D:\Data\vipin\11-03-09-MC-IP-AA3.d	Acquisition Date	3/9/2011 1:57:59 PM
Method	tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-IP-AA3	Instrument / Ser#	maXis 40
Comment			

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	130.1593	16466	29591.8	269538	0.0079
2	219.1496	22902	3102.7	29085	0.0096
3	231.1861	23333	5255.1	50264	0.0099
4	241.1319	19879	15283.2	148587	0.0121
→ 5	423.1448	27991	3404.2	37867	0.0151
6	432.3591	22971	9096.7	103767	0.0188
7	459.2738	23739	8718.6	106678	0.0193
8	480.3223	32309	1826.6	20901	0.0149
9	641.2872	31413	1742.2	17006	0.0204



(11d)

m/z: Calc'd for $C_{22}H_{25}ClN_2NaO_3$ ($[M+Na]^+$): 423.1451, found: 423.1448.

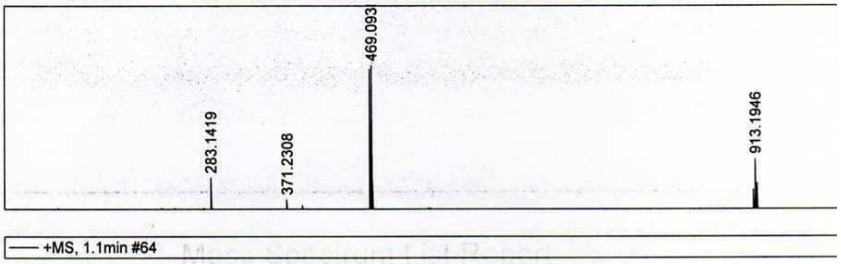
Mass Spectrum List Report

Analysis Info

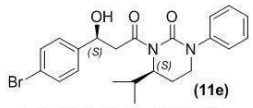
Analysis Name	D:\Data\vipin\11-03-09-MC-IP-AA4.d	Acquisition Date	3/9/2011 3:04:00 PM
Method	tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-IP-AA4	Instrument / Ser#	maXis 40
Comment			

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	283.1419	25328	3391.7	55056	0.0112
2	371.2308	30994	1031.5	16608	0.0120
3	389.1842	26217	376.7	6093	0.0148
→ 4	467.0955	21436	12508.4	245804	0.0218
5	468.0981	26259	2849.9	55809	0.0178
6	469.0938	21812	12884.9	251516	0.0215
7	470.0961	26353	2685.7	52257	0.0178
8	911.1956	27704	1803.2	34373	0.0329
9	912.1985	32063	524.9	9982	0.0284
10	913.1946	22729	4620.7	87659	0.0402
11	914.1970	27498	1769.9	33495	0.0332
12	915.1933	26061	2392.6	45171	0.0351
13	916.1949	29912	511.6	9636	0.0306



(11e)

m/z: Calc'd for $C_{22}H_{25}BrN_2NaO_3$ ($[M+Na]^+$): 467.0946, found: 467.0955.

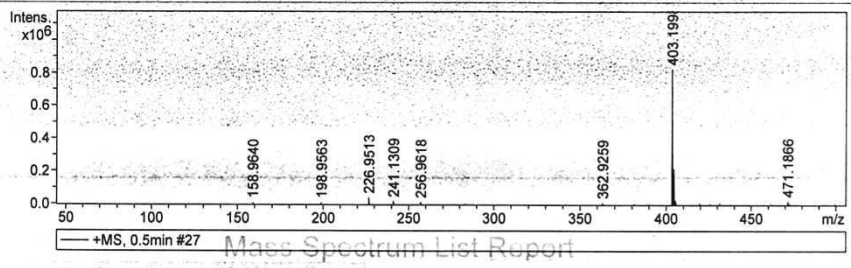
Mass Spectrum List Report

Analysis Info

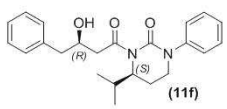
Analysis Name	D:\Data\vipin\12-03-14-MC-128.d	Acquisition Date	3/14/2012 11:35:49 AM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	12-03-14-MC-128	Instrument / Ser#	maXis 40
Comment			

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	158.9640	21343	1278.2	14582	0.0074
2	198.9563	23120	828.5	13799	0.0086
3	226.9513	22026	2017.3	43569	0.0103
4	228.0962	24133	164.5	3565	0.0095
5	241.1309	24190	933.3	21010	0.0100
6	256.9618	23710	643.5	14679	0.0108
7	362.9259	24575	427.3	12319	0.0148
→ 8	403.1998	22935	10032.8	823330	0.0176
9	404.2027	23772	3782.9	217624	0.0170
10	405.2050	24338	522.9	29276	0.0166
11	419.1729	24575	311.9	10764	0.0171
12	430.9136	25919	564.7	11478	0.0166
13	460.9240	26620	278.2	5213	0.0173
14	471.1866	25770	1312.1	22905	0.0183



(11f)

m/z: Calc'd for $C_{23}H_{28}N_2NaO_3$ ($[M+Na]^+$): 403.1998, found: 403.1998.

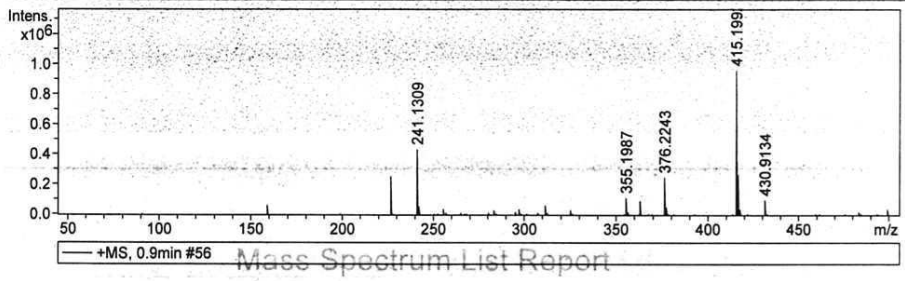
Mass Spectrum List Report

Analysis Info

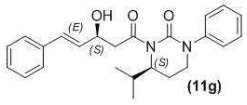
Analysis Name	D:\Data\vipin\12-02-09-MC-107.d	Acquisition Date	2/9/2012 3:35:24 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	12-02-09-MC-107	Instrument / Ser#	maXis 40
Comment			

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	241.1309	21057	9473.3	434185	0.0115
2	355.1987	24460	1769.4	115572	0.0145
3	362.9258	24289	1203.5	96495	0.0149
4	376.2243	23821	3622.8	249897	0.0158
→ 5	415.1992	22868	14235.4	958811	0.0182
6	430.9134	25541	973.8	99572	0.0169



(11g)

m/z: Calc'd for $C_{24}H_{28}N_2NaO_3$ ([M+Na]$^+$): 415.1998, found: 415.1992.

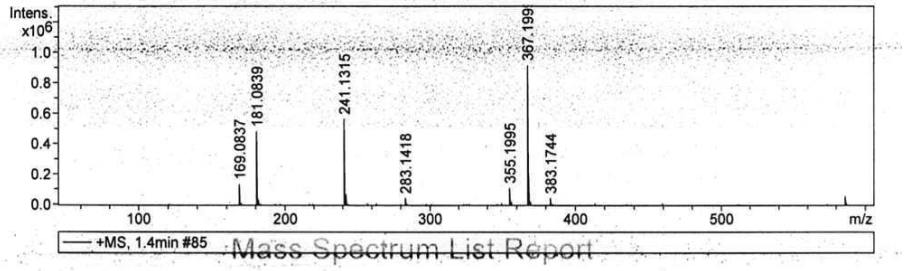
Mass Spectrum List Report

Analysis Info

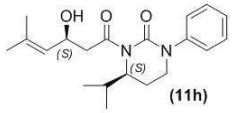
Analysis Name	D:\Data\vipin\12-02-08-MC-106a.d	Acquisition Date	2/8/2012 3:09:20 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	12-02-08-MC-106	Instrument / Ser#	maXis 40
Comment			

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	169.0837	19178	4387.5	137719	0.0088
2	181.0839	21148	14786.2	484650	0.0086
3	241.1315	21045	16067.0	565881	0.0115
4	283.1418	25030	1546.6	47511	0.0113
5	355.1995	23471	1721.6	116171	0.0151
→ 6	367.1999	23127	13036.3	916107	0.0159
7	383.1744	25312	973.3	48133	0.0151



(11h)

m/z: Calc'd for $C_{20}H_{28}N_2NaO_3$ ([M+Na]$^+$): 367.1998, found: 367.1999.

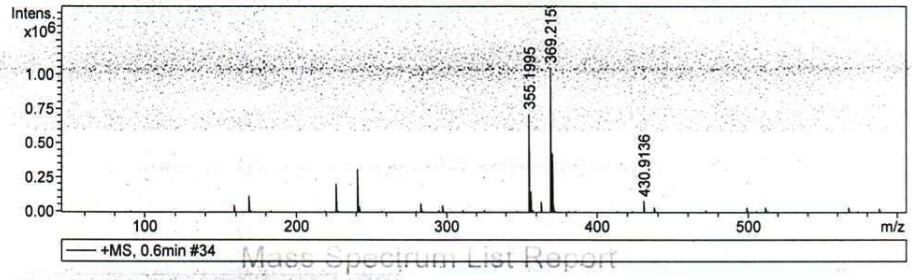
Mass Spectrum List Report

Analysis Info

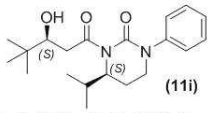
Analysis Name	D:\Data\vipin\12-02-08-MC-105.d	Acquisition Date	2/8/2012 1:54:21 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	12-02-08-MC-105	Instrument / Ser#	maXis 40
Comment			

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	355.1995	22123	7100.9	714559	0.0161
2	356.2025	23267	1471.3	151402	0.0153
3	362.9262	24005	667.8	76719	0.0151
→ 4	369.2159	16650	10692.5	1047862	0.0222
5	370.2184	23073	4506.0	429465	0.0160
6	371.2228	20577	606.6	56179	0.0180
7	430.9136	25412	3503.7	82083	0.0170



(11i)

m/z: Calc'd for $C_{20}H_{30}N_2NaO_3$ ($[M+Na]^+$): 369.2154, found: 369.2159.

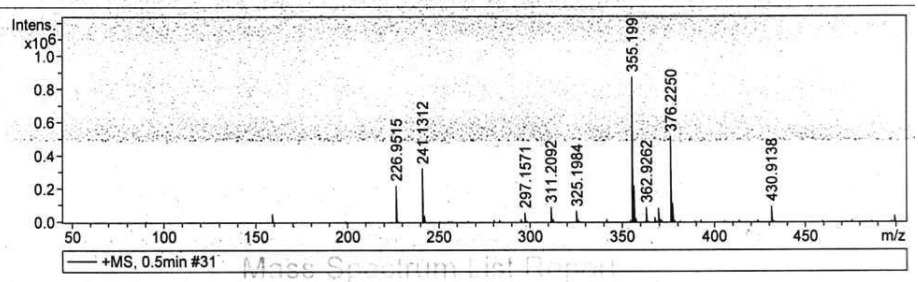
Mass Spectrum List Report

Analysis Info

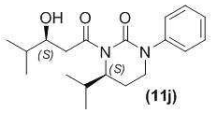
Analysis Name	D:\Data\vipin\12-02-09-MC-110.d	Acquisition Date	2/9/2012 2:41:54 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	12-02-09-MC-110	Instrument / Ser#	maXis 40
Comment			

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	226.9515	21152	6519.4	221084	0.0107
2	241.1312	21422	8203.1	322826	0.0113
3	297.1571	24077	1591.4	59228	0.0123
4	311.2092	23761	2254.4	88441	0.0131
5	325.1984	24823	1785.5	66046	0.0131
→ 6	355.1997	19739	6866.1	869098	0.0180
7	356.2025	22894	1672.3	219761	0.0156
8	357.2049	23893	194.0	26433	0.0150
9	362.9262	24436	551.0	90278	0.0149
10	367.1989	25139	164.1	29797	0.0146
11	369.2146	24702	512.7	87768	0.0149
12	376.2250	23564	3800.0	512552	0.0160
13	430.9138	25770	3016.3	98288	0.0167



(11j)

m/z: Calc'd for $C_{19}H_{28}N_2NaO_3$ ($[M+Na]^+$): 355.1998, found: 355.1997.

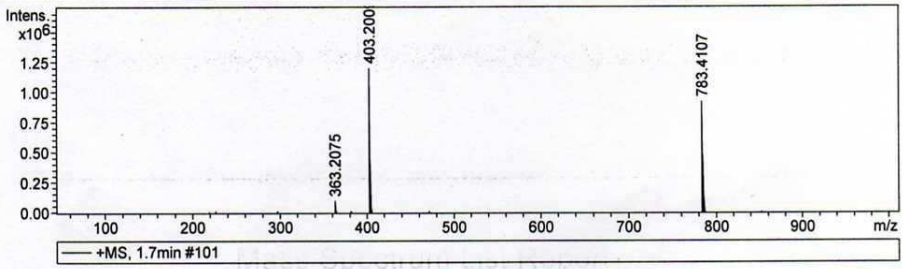
Mass Spectrum List Report

Analysis Info

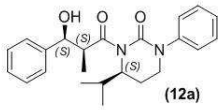
Analysis Name	D:\Data\vipin\11-01-11-MC-TP-IP7.d	Acquisition Date	1/12/2011 2:08:24 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-TP-IP7	Instrument / Ser#	maXis 40
Comment			

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	400.0 Vpp	Set Divert Valve	Source



#	m/z	Res.	S/N	I	FWHM
1	363.2075	22621	1753.9	98967	0.0161
2	403.2009	16995	12855.3	1199408	0.0237
3	783.4107	22255	7340.2	916030	0.0352



(12a)

m/z: Calc'd for $C_{23}H_{28}N_2NaO_3$ ($[M+Na]^+$): 403.1998, found: 403.2009.

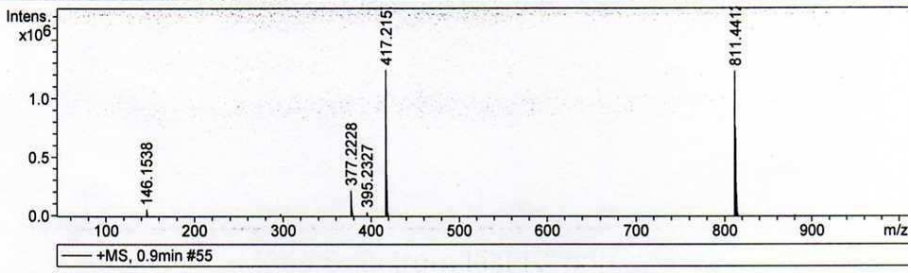
Mass Spectrum List Report

Analysis Info

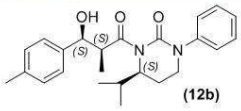
Analysis Name	D:\Data\vipin\11-01-11-MC-TP-IP8.d	Acquisition Date	1/12/2011 3:15:19 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-TP-IP8	Instrument / Ser#	maXis 40
Comment			

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	400.0 Vpp	Set Divert Valve	Source



#	m/z	Res.	S/N	I	FWHM
1	146.1538	20572	1345.0	55605	0.0071
2	297.1572	27329	1441.2	16821	0.0109
3	377.2228	21875	4571.9	220229	0.0172
4	395.2327	27868	557.9	35510	0.0142
5	417.2157	20075	19357.8	1242507	0.0208
6	811.4412	20565	10779.0	1230558	0.0395



(12b)

m/z: Calc'd for $C_{24}H_{30}N_2NaO_3$ ($[M+Na]^+$): 417.2154, found: 417.2157.

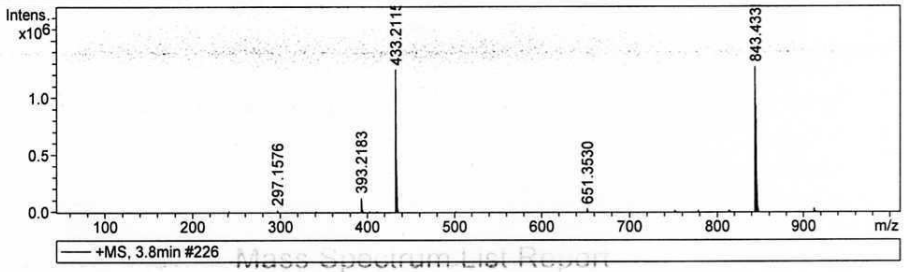
Mass Spectrum List Report

Analysis Info

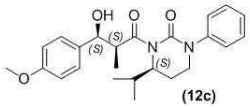
Analysis Name	D:\Data\vipin\11-01-11-MC-TP-IP9.d	Acquisition Date	1/12/2011 4:24:14 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-TP-IP9	Instrument / Ser#	maXis 40
Comment			

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	400.0 Vpp	Set Divert Valve	Source



#	m/z	Res.	S/N	I	FWHM
1	297.1576	26326	1386.0	22176	0.0113
2	393.2183	23222	4648.8	127042	0.0169
→ 3	433.2115	20584	17317.9	1243601	0.0210
4	651.3530	29896	845.7	30853	0.0218
5	843.4335	18581	5481.8	1264753	0.0454



(12c)

m/z: Calc'd for $C_{24}H_{30}N_2NaO_4$ ($[M+Na]^+$): 433.2103, found: 433.2115.

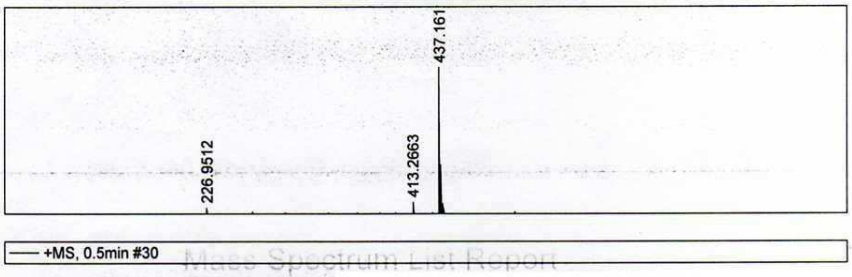
Mass Spectrum List Report

Analysis Info

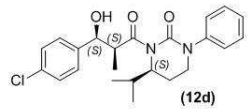
Analysis Name	D:\Data\vipin\11-02-25-MC-TPO-AK-5.d	Acquisition Date	3/3/2011 4:21:51 PM
Method	tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-TPO-AK-5	Instrument / Ser#	maXis 40
Comment			

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	800 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



#	m/z	Res.	S/N	I	FWHM
1	226.9512	23464	2647.7	24786	0.0097
2	413.2663	27202	1980.6	47262	0.0152
→ 3	437.1611	20983	24821.9	583051	0.0208



(12d)

m/z: Calc'd for $C_{23}H_{27}ClN_2NaO_3$ ($[M+Na]^+$): 437.1608, found: 437.1611.

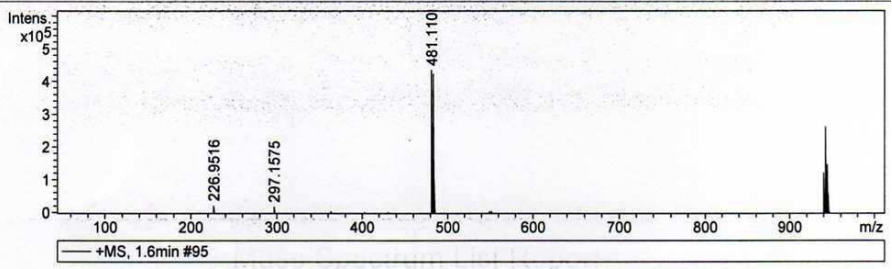
Mass Spectrum List Report

Analysis Info

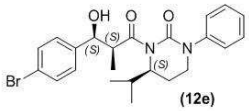
Analysis Name	D:\Data\vipin\11-02-08-MC-IP-IP-14.d	Acquisition Date	2/9/2011 11:09:36 AM
Method	tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-IP-IP-14	Instrument / Ser#	maXis 40
Comment			

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	226.9516	27773	497.2	23955	0.0082
2	297.1575	27497	713.8	19657	0.0108
3	362.9263	31866	452.8	6099	0.0114
4	403.1994	27624	159.1	3589	0.0146
→ 5	481.1108	22673	5094.5	433149	0.0212
6	482.1137	24994	1290.6	108638	0.0193
7	483.1091	21917	5078.5	423235	0.0220
8	484.1117	23905	1214.9	100221	0.0203



(12e)

m/z: Calc'd for $C_{23}H_{27}BrN_2NaO_3$ ($[M+Na]^+$): 481.1103, found: 481.1108.

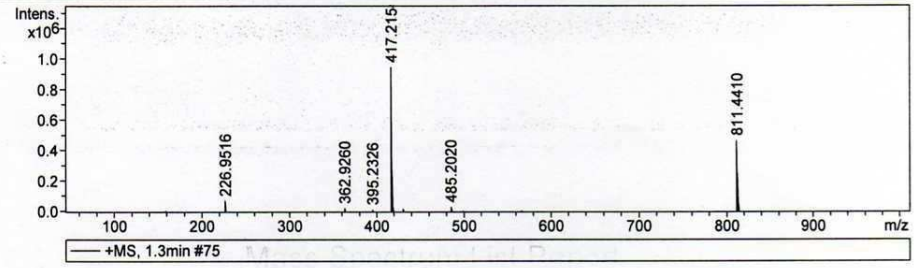
Mass Spectrum List Report

Analysis Info

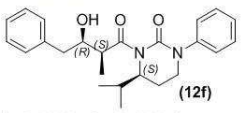
Analysis Name	D:\Data\vipin\11-02-08-MC-IP-IP-13.d	Acquisition Date	2/9/2011 9:47:28 AM
Method	tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-IP-IP-13	Instrument / Ser#	maXis 40
Comment			

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	226.9516	21513	2549.8	72578	0.0105
2	362.9260	28949	641.4	23651	0.0125
3	395.2326	32122	249.3	15612	0.0123
→ 4	417.2154	21016	16014.5	943910	0.0199
5	430.9135	30542	386.3	21444	0.0141
6	485.2020	29976	828.8	32258	0.0162
7	811.4410	23207	6600.9	463632	0.0350



(12f)

m/z: Calc'd for $C_{24}H_{30}N_2NaO_3$ ($[M+Na]^+$): 417.2154, found: 417.2154.

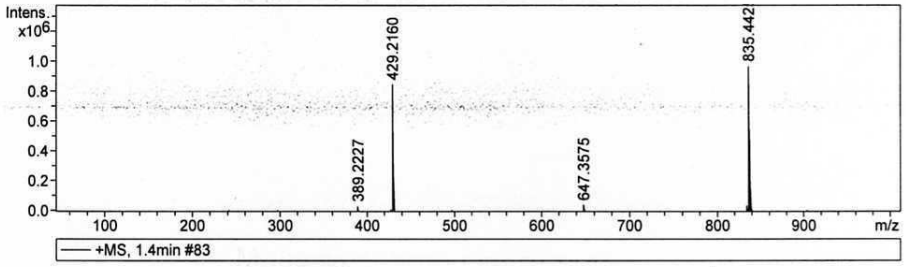
Mass Spectrum List Report

Analysis Info

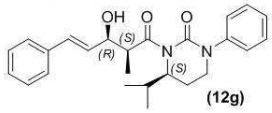
Analysis Name	D:\Data\vipin\11-02-08-MC-IP-IP-12.d	Acquisition Date	2/8/2011 1:46:28 PM
Method	tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-IP-IP-12	Instrument / Ser#	maXis 40
Comment			

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	389.2227	29374	1075.2	32745	0.0133
→ 2	429.2160	22092	9394.1	844698	0.0194
3	647.3575	30455	1459.0	44403	0.0213
4	835.4425	23807	6551.4	966920	0.0351



(12g)

m/z: Calc'd for $C_{25}H_{30}N_2NaO_3$ ($[M+Na]^+$): 429.2154, found: 429.2160.

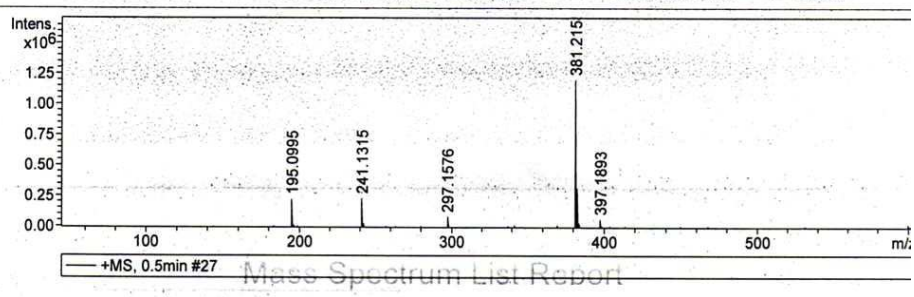
Mass Spectrum List Report

Analysis Info

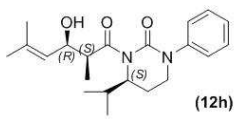
Analysis Name	D:\Data\vipin\12-02-08-MC-103a.d	Acquisition Date	2/8/2012 12:13:59 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	12-02-08-MC-103	Instrument / Ser#	maXis 40
Comment			

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	195.0995	21438	5334.1	226657	0.0091
2	241.1315	22101	8421.5	235993	0.0109
3	297.1576	23907	2818.5	83299	0.0124
4	298.1602	24621	441.1	13003	0.0121
→ 5	381.2158	21043	21759.0	1197234	0.0181
6	382.2187	23220	5614.1	317000	0.0165
7	397.1893	25483	824.6	64316	0.0156



(12h)

m/z: Calc'd for $C_{21}H_{30}N_2NaO_3$ ($[M+Na]^+$): 381.2154, found: 381.2158.

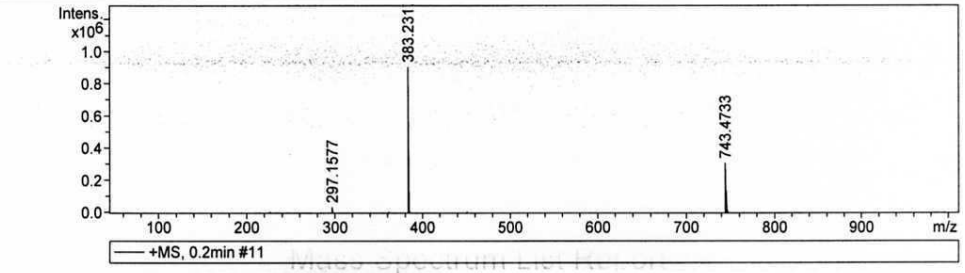
Mass Spectrum List Report

Analysis Info

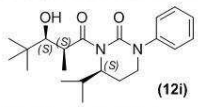
Analysis Name	D:\Data\vipin\11-02-08-MC-IP-IP-11.d	Acquisition Date	2/8/2011 11:41:58 AM
Method	tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-IP-IP-11	Instrument / Ser#	maXis 40
Comment			

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	297.1577	28471	1732.3	35556	0.0104
→ 2	383.2317	21378	14223.2	902904	0.0179
3	743.4733	23344	11589.0	306898	0.0318



(12i)

m/z: Calc'd for $C_{21}H_{32}N_2NaO_3$ ([M+Na]$^+$): 383.2311, found: 383.2317.

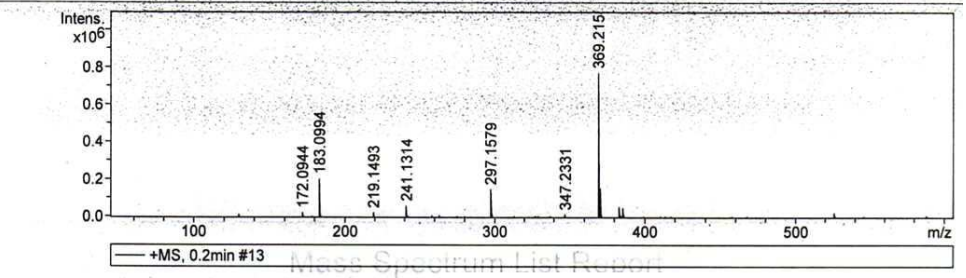
Mass Spectrum List Report

Analysis Info

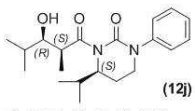
Analysis Name	D:\Data\vipin\12-02-08-MC-102A.d	Acquisition Date	2/8/2012 11:41:34 AM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	12-02-08-MC-102	Instrument / Ser#	maXis 40
Comment			

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	172.0944	21622	256.8	24288	0.0080
2	183.0994	19808	10595.0	204959	0.0092
3	219.1493	23891	1467.3	24896	0.0092
4	241.1314	23863	3341.6	62376	0.0101
5	297.1579	23337	5445.9	149185	0.0127
6	347.2331	25929	482.4	15620	0.0134
→ 7	369.2158	23258	20655.1	768150	0.0159



(12j)

m/z: Calc'd for $C_{20}H_{30}N_2NaO_3$ ([M+Na]$^+$): 369.2154, found: 369.2158.

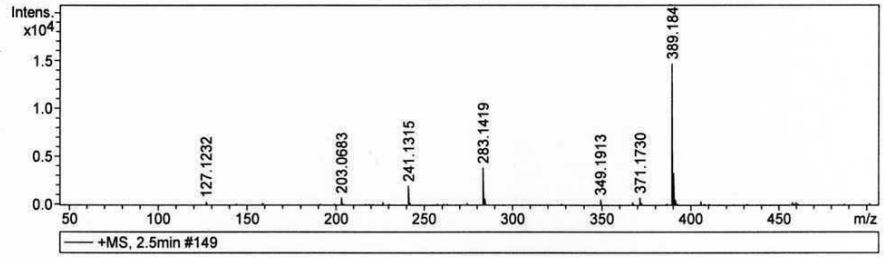
Mass Spectrum List Report

Analysis Info

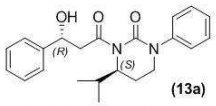
Analysis Name	D:\Data\vipin\12-05-22-MC-LAA1.d	Acquisition Date	5/22/2012 10:47:22 AM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-LAA1	Instrument / Ser#	maXis 40
Comment			

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	127.1232	18144	10.5	345	0.0070
2	203.0683	24939	15.7	745	0.0081
3	241.1315	24333	33.8	1984	0.0099
4	283.1419	25092	62.1	3847	0.0113
5	284.1447	25231	10.6	640	0.0113
6	349.1913	27062	15.0	583	0.0129
7	371.1730	30488	15.4	739	0.0122
→ 8	389.1841	24909	184.6	14625	0.0156
9	390.1873	23686	40.8	3307	0.0165



(13a)

m/z: Calc'd for $C_{22}H_{26}N_2NaO_3$ ($[M+Na]^+$): 389.1841, found: 389.1841.

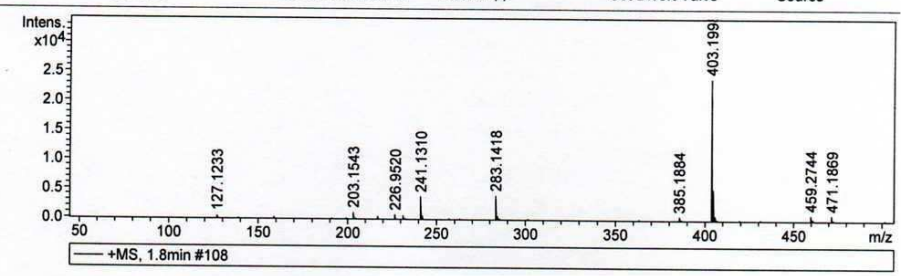
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\vipin\12-05-22-MC-LAA2.d	Acquisition Date	5/22/2012 10:58:34 AM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-LAA2	Instrument / Ser#	maXis 40
Comment			

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	127.1233	17683	16.6	521	0.0072
2	203.1543	20969	24.8	1126	0.0097
3	217.0833	22811	10.1	549	0.0095
4	226.9520	19504	13.2	735	0.0116
5	231.0985	20368	10.6	593	0.0113
6	241.1310	20943	67.6	3890	0.0115
7	242.1340	21002	10.5	608	0.0115
8	283.1418	23235	81.3	4081	0.0122
9	284.1447	23645	14.7	724	0.0120
10	385.1884	25205	11.1	654	0.0153
→ 11	403.1998	25590	331.0	24013	0.0158
12	404.2030	23161	73.5	5229	0.0175
13	405.2056	25320	11.6	811	0.0160
14	459.2744	25709	16.6	996	0.0179
15	471.1869	26172	18.8	905	0.0180

(13b)

m/z: Calc'd for $C_{23}H_{28}N_2NaO_3$ ($[M+Na]^+$): 403.1998, found: 403.1998.

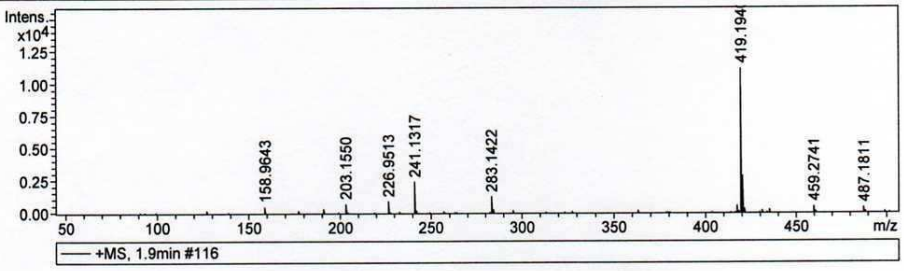
Mass Spectrum List Report

Analysis Info

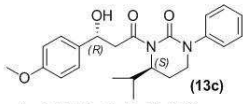
Analysis Name	D:\Data\vipin\12-05-22-MC-LAA3.d	Acquisition Date	5/22/2012 11:11:40 AM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-LAA3	Instrument / Ser#	maXis 40
Comment			

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	158.9643	18827	14.4	538	0.0084
2	203.1550	22739	13.3	748	0.0089
3	226.9513	21024	13.7	938	0.0108
4	241.1317	21865	35.0	2439	0.0110
5	283.1422	22785	28.1	1300	0.0124
→ 6	419.1940	25220	105.8	11141	0.0166
7	420.1975	25479	26.7	2906	0.0165
8	459.2741	24040	13.4	535	0.0191
9	487.1811	26614	10.7	438	0.0183



m/z: Calc'd for $C_{23}H_{28}N_2NaO_4$ ($[M+Na]^+$): 419.1947, found: 419.1940.

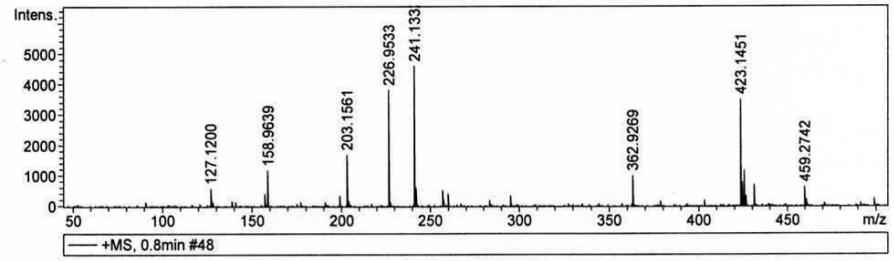
Mass Spectrum List Report

Analysis Info

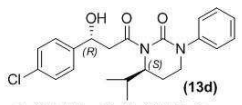
Analysis Name	D:\Data\vipin\12-05-22-MC-LAA4.d	Acquisition Date	5/22/2012 12:19:54 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-LAA4	Instrument / Ser#	maXis 40
Comment			

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	127.1200	17578	13.9	597	0.0072
2	158.9639	18422	24.0	1186	0.0086
3	203.1561	22385	24.1	1693	0.0091
4	226.9533	20882	46.3	3815	0.0109
5	241.1332	23170	60.3	4603	0.0104
6	362.9269	24449	20.7	1021	0.0148
→ 7	423.1451	24791	34.6	3509	0.0171
8	425.1419	21174	11.2	1194	0.0201
9	459.2742	28368	14.1	650	0.0162



m/z: Calc'd for $C_{22}H_{25}ClN_2NaO_3$ ($[M+Na]^+$): 423.1451, found: 423.1451.

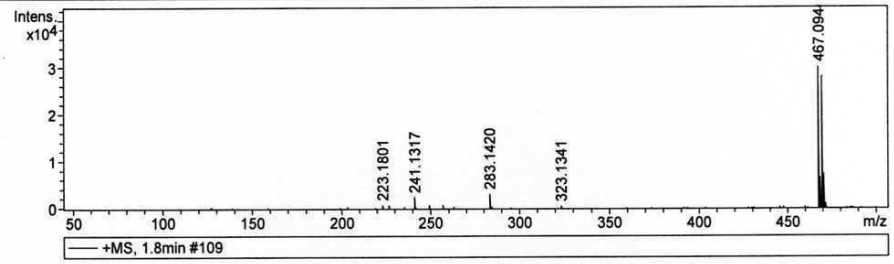
Mass Spectrum List Report

Analysis Info

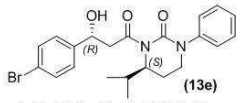
Analysis Name	D:\Data\vipin\12-05-22-MC-LAA5.d	Acquisition Date	5/22/2012 2:00:00 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-LAA5	Instrument / Ser#	maXis 40
Comment			

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	223.1801	21211	11.3	904	0.0105
2	226.9514	21537	10.0	844	0.0105
3	241.1317	21696	25.3	2552	0.0111
4	283.1420	23554	42.9	3158	0.0120
5	323.1341	22648	12.1	573	0.0143
6	467.0944	25116	203.9	29986	0.0186
7	468.0975	25429	46.7	6688	0.0184
8	469.0927	24463	200.5	27944	0.0192
9	470.0958	24524	55.0	7455	0.0192
10	471.0980	27556	8.6	1127	0.0171



(13e)

m/z: Calc'd for $C_{22}H_{25}BrN_2NaO_3$
($[M+Na]^+$): 467.0946, found: 467.0944.

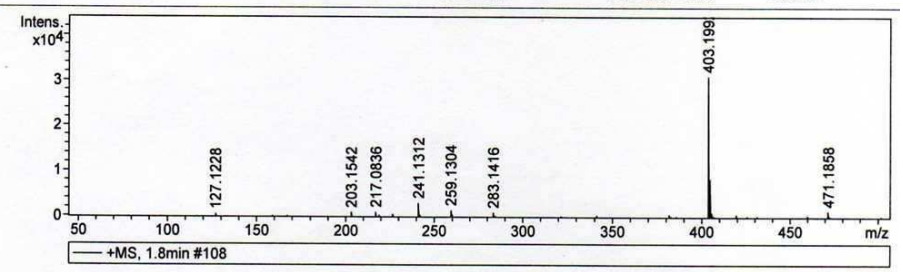
Mass Spectrum List Report

Analysis Info

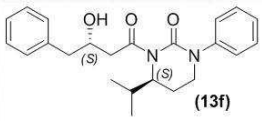
Analysis Name	D:\Data\vipin\12-05-22-MC-LAA6.d	Acquisition Date	5/22/2012 2:25:42 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-LAA6	Instrument / Ser#	maXis 40
Comment			

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	127.1228	22264	16.1	576	0.0057
2	203.1542	23265	19.4	1001	0.0087
3	217.0836	21973	16.5	1055	0.0099
4	226.9517	25700	10.8	665	0.0088
5	241.1312	21605	52.6	3042	0.0112
6	259.1304	25635	27.0	1447	0.0101
7	260.0894	24253	13.7	733	0.0107
8	283.1416	24038	22.1	997	0.0118
9	341.1836	24755	10.5	411	0.0138
10	403.1992	24248	326.5	30988	0.0166
11	404.2027	24312	89.9	8368	0.0166
12	405.2042	23056	11.8	1079	0.0176
13	471.1858	26353	24.3	1403	0.0179



(13f)

m/z: Calc'd for $C_{23}H_{28}N_2NaO_3$
($[M+Na]^+$): 403.1998, found: 403.1992.

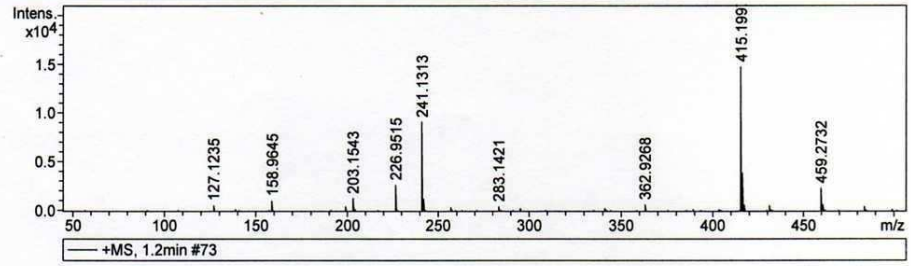
Mass Spectrum List Report

Analysis Info

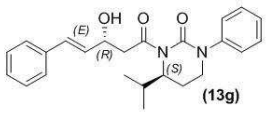
Analysis Name	D:\Data\vipin\12-05-22-MC-LAA7.d	Acquisition Date	5/22/2012 2:32:24 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-LAA7	Instrument / Ser#	maXis 40
Comment			

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	127.1235	17932	14.8	620	0.0071
2	158.9645	24104	24.7	1074	0.0066
3	203.1543	22094	19.9	1310	0.0092
4	226.9515	22415	26.8	2692	0.0101
5	241.1313	22032	76.4	9079	0.0109
6	242.1339	20083	10.4	1244	0.0121
7	283.1421	22804	13.4	532	0.0124
8	362.9268	25709	20.1	728	0.0141
→ 9	415.1997	25069	219.2	14751	0.0166
10	416.2024	24567	56.7	3913	0.0169
11	459.2732	24110	32.9	2369	0.0190
12	460.2757	25340	10.2	726	0.0182



(13g)

m/z: Calc'd for $C_{24}H_{28}N_2NaO_3$ ($[M+Na]^+$): 415.1998, found: 415.1997.

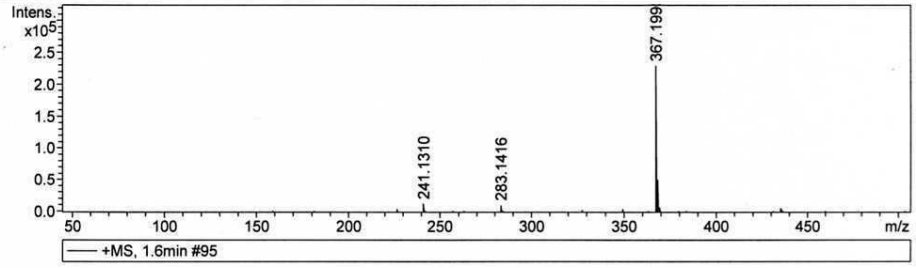
Mass Spectrum List Report

Analysis Info

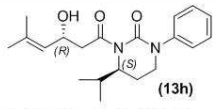
Analysis Name	D:\Data\vipin\12-09-24-MC-LI-AA10.d	Acquisition Date	9/24/2012 4:26:26 PM
Method	tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-LI-AA10	Instrument / Ser#	maXis 40
Comment			

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	241.1310	20785	405.7	13482	0.0116
2	283.1416	20123	284.7	11206	0.0141
→ 3	367.1990	21248	1776.4	228254	0.0173
4	368.2021	20975	394.7	49474	0.0176
5	369.2047	22165	63.0	7703	0.0167



(13h)

m/z: Calc'd for $C_{20}H_{26}N_2NaO_3$ ($[M+Na]^+$): 367.1998, found: 367.1990.

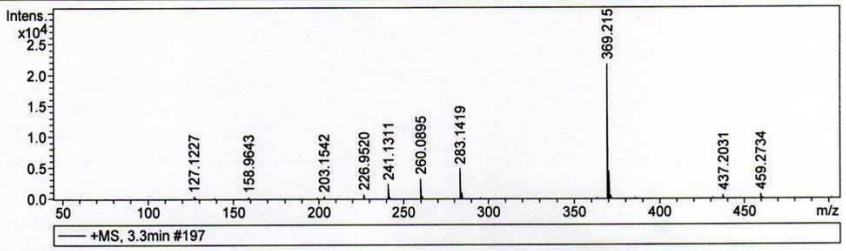
Mass Spectrum List Report

Analysis Info

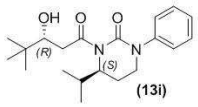
Analysis Name	D:\Data\vipin\12-05-22-MC-LAA8.d	Acquisition Date	5/22/2012 3:15:43 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-LAA8	Instrument / Ser#	maXis 40
Comment			

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	127.1227	22255	14.2	431	0.0057
2	158.9643	26881	12.2	343	0.0059
3	203.1542	19709	13.7	440	0.0103
4	226.9520	23877	18.5	752	0.0095
5	241.1311	20425	53.1	2346	0.0118
6	260.0895	21502	64.2	3287	0.0121
7	283.1419	22640	100.1	4901	0.0125
8	284.1455	24834	20.9	1002	0.0114
→ 9	369.2151	24912	323.0	21679	0.0148
10	370.2179	23094	68.6	4517	0.0160
11	437.2031	27227	16.1	633	0.0161
12	459.2734	23015	17.3	669	0.0200



(13i)

m/z: Calc'd for $C_{20}H_{30}N_2NaO_3$ ($[M+Na]^+$): 369.2154, found: 369.2151.

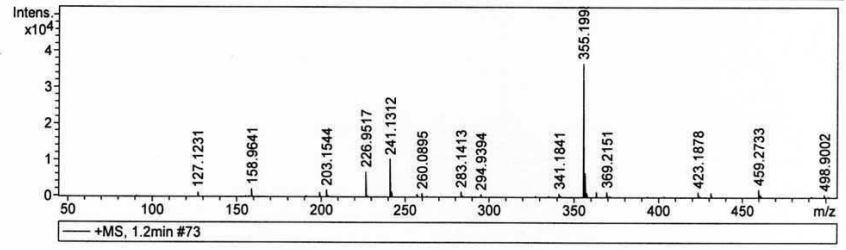
Mass Spectrum List Report

Analysis Info

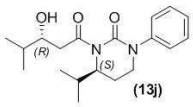
Analysis Name	D:\Data\vipin\12-05-22-MC-LAA9.d	Acquisition Date	5/22/2012 3:27:01 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-LAA9	Instrument / Ser#	maXis 40
Comment			

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	127.1231	19205	31.2	1331	0.0066
2	158.9641	20086	50.3	2137	0.0079
3	198.9567	22869	21.8	1139	0.0087
4	203.1544	20416	34.2	1917	0.0100
5	226.9517	23542	101.9	6949	0.0096
6	241.1312	21714	147.3	10384	0.0111
7	242.1343	19569	21.4	1511	0.0124
8	256.9625	24191	13.1	873	0.0106
9	260.0895	23001	16.5	1081	0.0113
10	283.1413	21676	25.0	1381	0.0131
11	294.9394	24378	15.6	750	0.0121
12	341.1841	22989	17.1	1069	0.0148
→ 13	355.1998	24188	396.5	36713	0.0147
14	356.2029	21915	71.3	6751	0.0163
15	357.2052	25068	13.1	1267	0.0142
16	362.9261	20701	12.4	1358	0.0175
17	369.2151	23835	12.5	1406	0.0155
18	423.1878	27351	23.1	1462	0.0155
19	430.9130	25660	17.5	1177	0.0168
20	459.2733	24672	35.2	2214	0.0186
21	460.2756	24877	11.9	740	0.0185
22	498.9002	37520	13.9	653	0.0133



(13j)

m/z: Calc'd for $C_{19}H_{28}N_2NaO_3$ ($[M+Na]^+$): 355.1995, found: 355.1998.

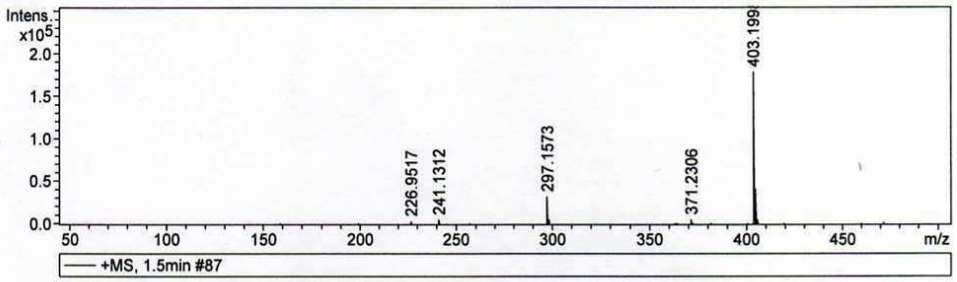
Mass Spectrum List Report

Analysis Info

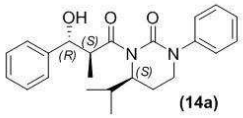
Analysis Name	D:\Data\vipin\12-05-01-MC-LP-1.d	Acquisition Date	5/1/2012 4:06:49 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-LP-1	Instrument / Ser#	maXis 40
Comment			

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	143.1046	19035	21.5	598	0.0075
2	158.9644	19320	38.6	1102	0.0082
3	198.9570	25251	45.6	1531	0.0079
4	226.9517	23770	81.6	3856	0.0095
5	241.1312	22244	105.5	5461	0.0108
6	242.1339	23057	16.2	845	0.0105
7	256.9622	22701	33.2	1405	0.0113
8	263.1137	22706	17.6	656	0.0116
9	294.9381	28141	11.2	451	0.0105
10	297.1573	23162	781.3	32460	0.0128
11	298.1605	22408	129.7	5473	0.0133
12	299.1637	26786	15.9	681	0.0112
13	334.9319	28268	10.3	333	0.0118
14	337.1499	28827	15.3	493	0.0117
15	344.1948	22856	17.0	630	0.0151
16	362.9268	23831	14.9	749	0.0152
17	363.2068	24155	28.5	1436	0.0150
18	364.1512	25980	17.6	898	0.0140
19	365.1470	19845	14.2	733	0.0184
20	371.2306	24693	96.3	5997	0.0150
21	372.2346	24562	20.2	1306	0.0152
22	381.2175	24088	14.9	1255	0.0158
→ 23	403.1998	24714	1637.2	178523	0.0163
24	404.2029	24551	390.8	41759	0.0165
25	405.2056	22018	54.4	5698	0.0184
26	419.1730	25335	16.3	1210	0.0165
27	430.9136	22586	10.8	589	0.0191
28	459.2735	26466	14.9	896	0.0174
29	471.1879	24980	47.5	2342	0.0189
30	472.1904	22258	12.0	579	0.0212



(14a)

m/z: Calc'd for $C_{23}H_{28}N_2NaO_3$ ($[M+Na]^+$): 403.1998, found: 403.1998.

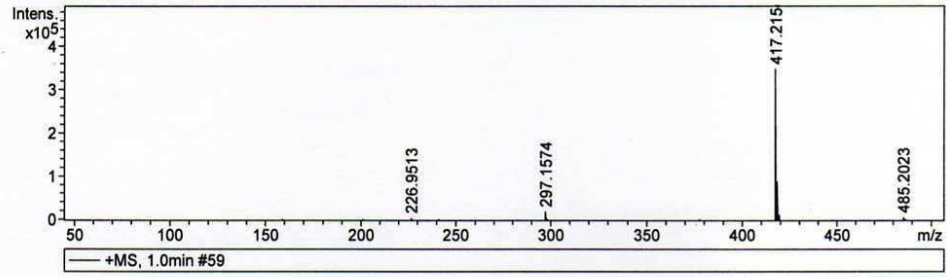
Mass Spectrum List Report

Analysis Info

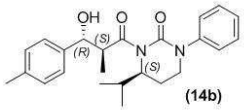
Analysis Name	D:\Data\vipin\12-05-01-MC-LP-2.d	Acquisition Date	5/1/2012 4:33:43 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-LP-2	Instrument / Ser#	maXis 40
Comment			

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	143.1043	18878	45.9	1413	0.0076
2	158.9640	19549	62.5	1903	0.0081
3	198.9561	19828	23.7	748	0.0100
4	201.0884	19670	51.8	1707	0.0102
5	226.9513	22912	122.7	5022	0.0099
6	241.1309	21897	64.7	2642	0.0110
7	256.9625	22198	26.5	940	0.0116
8	263.1136	22658	17.2	566	0.0116
9	294.9385	22701	15.3	548	0.0130
10	297.1574	22860	555.2	20341	0.0130
11	298.1606	22020	92.2	3416	0.0135
12	299.1635	23291	11.8	443	0.0128
13	337.1496	24007	18.5	668	0.0140
14	344.1955	24222	14.3	545	0.0142
15	362.9262	25891	33.5	1464	0.0140
16	364.1521	22155	18.7	825	0.0164
17	377.2227	23928	74.5	3255	0.0158
18	378.2251	22307	19.8	861	0.0170
19	387.1263	25892	18.9	801	0.0150
20	395.2331	24802	35.8	1479	0.0159
21	396.2369	21799	10.8	443	0.0182
→ 22	417.2154	24121	1383.3	346923	0.0173
23	418.2184	24355	342.9	89702	0.0172
24	419.2214	24534	48.9	13320	0.0171
25	468.3228	24817	10.8	634	0.0189
26	485.2023	25061	78.4	6573	0.0194
27	486.2063	26627	21.4	1825	0.0183



(14b)

m/z: Calc'd for $C_{24}H_{30}N_2NaO_3$ ($[M+Na]^+$): 417.2154, found: 417.2154.

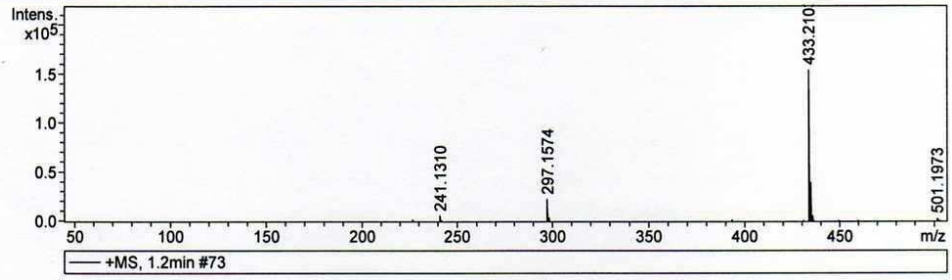
Mass Spectrum List Report

Analysis Info

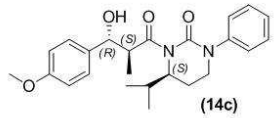
Analysis Name	D:\Data\vipin\12-05-01-MC-LP-3.d	Acquisition Date	5/1/2012 4:43:53 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-LP-3	Instrument / Ser#	maXis 40
Comment			

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	102.1277	17617	10.6	234	0.0058
2	143.1045	20406	20.4	541	0.0070
3	158.9642	19337	23.8	643	0.0082
4	198.9572	24422	24.4	657	0.0081
5	226.9517	27119	45.0	1938	0.0084
6	241.1310	23338	106.4	5751	0.0103
7	242.1337	21679	15.5	849	0.0112
8	256.9620	21637	15.1	666	0.0119
9	263.1136	22673	16.8	640	0.0116
10	297.1574	22527	622.5	22529	0.0132
11	298.1608	23099	107.4	3936	0.0129
12	299.1635	23675	14.8	549	0.0126
13	337.1507	21672	17.5	479	0.0156
14	344.1940	26742	16.7	469	0.0129
15	362.9270	23964	16.0	476	0.0151
16	364.1523	24551	20.1	599	0.0148
17	365.1472	18538	16.8	503	0.0197
18	387.1264	26180	13.4	468	0.0148
19	393.2177	25342	52.7	1917	0.0155
20	394.2219	22711	15.4	564	0.0174
→ 21	433.2103	24938	1283.8	153621	0.0174
22	434.2134	25279	340.3	39844	0.0172
23	435.2161	23916	51.9	5938	0.0182
24	449.1832	24465	11.5	905	0.0184
25	459.2734	21345	15.3	820	0.0215
26	501.1973	24961	49.6	3073	0.0201
27	502.2013	21471	14.1	871	0.0234



(14c)

m/z: Calc'd for $C_{24}H_{30}N_2NaO_4$ ($[M+Na]^+$): 433.2103, found: 433.2103.

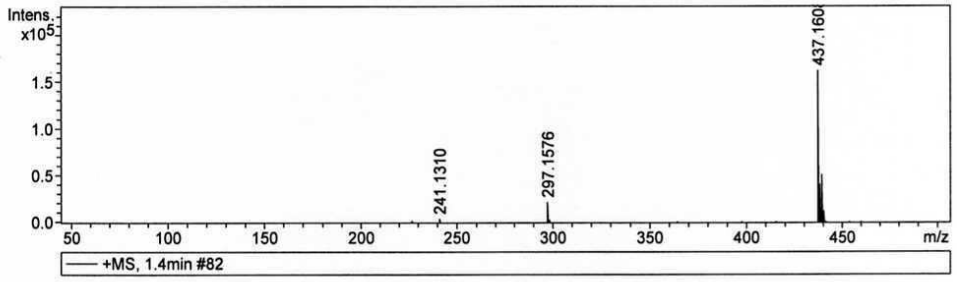
Mass Spectrum List Report

Analysis Info

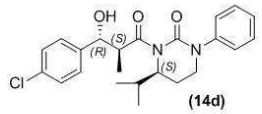
Analysis Name	D:\Data\vipin\12-05-01-MC-LP-4.d	Acquisition Date	5/1/2012 4:51:27 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-LP-4	Instrument / Ser#	maXis 40
Comment			

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	108.0803	17853	11.6	265	0.0061
2	143.1044	18655	14.4	387	0.0077
3	158.9641	19021	25.7	699	0.0084
4	226.9519	23349	50.0	2158	0.0097
5	241.1310	23299	80.5	4256	0.0103
6	242.1346	20337	12.4	666	0.0119
7	256.9620	21140	11.4	511	0.0122
8	263.1133	22095	11.9	475	0.0119
9	297.1576	23152	593.4	21666	0.0128
10	298.1608	23377	105.0	3866	0.0128
11	299.1648	26389	11.3	420	0.0113
12	337.1492	23989	18.2	544	0.0141
13	362.9265	22126	14.0	447	0.0164
14	364.1528	23550	25.7	824	0.0155
15	365.1492	15918	10.6	340	0.0229
16	387.1275	23312	10.3	353	0.0166
17	397.1674	23507	37.3	1323	0.0169
18	398.1705	22078	10.2	385	0.0180
19	399.1657	25302	10.1	426	0.0158
20	415.1786	24915	10.9	1254	0.0167
→ 21	437.1608	24457	1147.3	161894	0.0179
22	438.1640	24801	300.1	41179	0.0177
23	439.1586	22738	382.5	51028	0.0193
24	440.1614	23665	98.7	12783	0.0186
25	441.1639	23346	14.2	1783	0.0189
26	453.1369	26214	12.5	990	0.0173
27	459.2718	25948	15.4	869	0.0177



(14d)

m/z: Calc'd for $C_{23}H_{27}ClN_2NaO_3$ ($[M+Na]^+$): 437.1608, found: 437.1608.

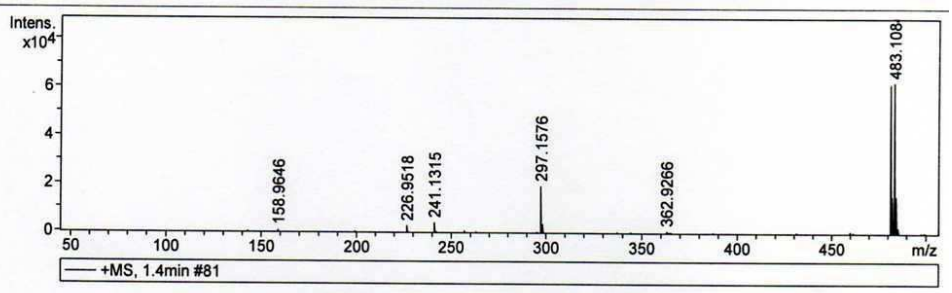
Mass Spectrum List Report

Analysis Info

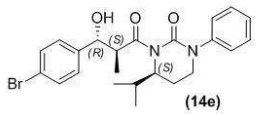
Analysis Name	D:\Data\vipin\12-05-02-MC-LP-5.d	Acquisition Date	5/2/2012 11:20:10 AM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-LP-5	Instrument / Ser#	maXis 40
Comment			

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	143.1046	19134	23.4	635	0.0075
2	158.9646	20968	34.5	945	0.0076
3	198.9569	21171	23.9	599	0.0094
4	226.9518	22673	88.6	2747	0.0100
5	241.1315	23043	135.6	4203	0.0105
6	242.1346	21468	19.5	606	0.0113
7	256.9623	23234	23.6	703	0.0111
8	263.1129	21782	12.6	370	0.0121
9	294.9391	24597	14.0	538	0.0120
10	297.1576	23569	488.4	19348	0.0126
11	298.1608	24328	88.3	3543	0.0123
12	337.1494	23834	16.5	438	0.0141
13	344.1954	22748	16.0	432	0.0151
14	362.9266	25798	32.6	931	0.0141
15	364.1521	24244	15.8	454	0.0150
16	365.1473	18150	12.5	359	0.0201
17	387.1266	23431	18.2	477	0.0165
18	430.9145	26753	23.1	616	0.0161
19	459.2736	25890	29.4	884	0.0177
→ 20	481.1103	25185	586.9	61416	0.0191
21	482.1132	24958	141.1	15250	0.0193
22	483.1084	24968	559.4	62358	0.0193
23	484.1115	25835	134.8	15487	0.0187
24	485.1148	25042	19.5	2304	0.0194



(14e)

m/z: Calc'd for $C_{23}H_{27}BrN_2NaO_3$ ($[M+Na]^+$): 481.1103, found: 481.1103.

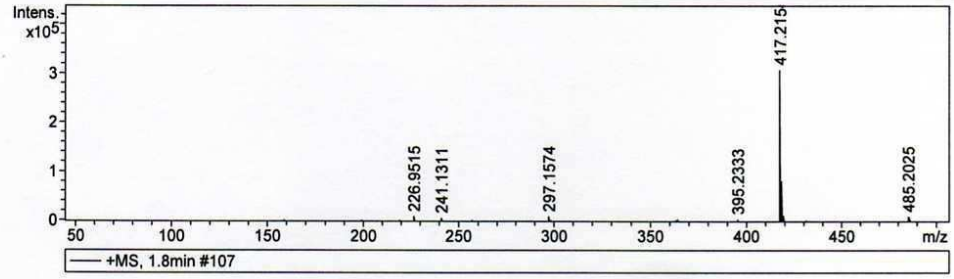
Mass Spectrum List Report

Analysis Info

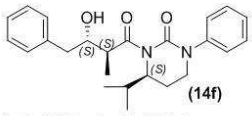
Analysis Name	D:\Data\vipin\12-05-02-MC-LP-6.d	Acquisition Date	5/2/2012 11:49:18 AM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-LP-6	Instrument / Ser#	maXis 40
Comment			

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	219.1491	23421	33.2	1600	0.0094
2	226.9515	23312	184.2	9424	0.0097
3	235.1046	24594	13.4	726	0.0096
4	241.1311	22320	115.3	6532	0.0108
5	242.1330	20582	14.7	838	0.0118
6	256.9625	22240	36.4	1732	0.0116
7	263.1132	25144	17.2	729	0.0105
8	264.9285	23941	10.3	421	0.0111
9	270.1564	27085	13.7	503	0.0100
10	294.9390	21914	21.5	915	0.0135
11	297.1574	24174	230.8	10098	0.0123
12	298.1609	22328	34.9	1544	0.0134
13	334.9309	23155	10.3	383	0.0145
14	337.1497	23856	12.2	451	0.0141
15	344.1940	27342	17.8	710	0.0126
16	362.9264	24028	49.8	2359	0.0151
17	364.1521	24607	76.4	3658	0.0148
18	365.1551	21950	20.0	965	0.0166
19	387.1270	25102	20.1	971	0.0154
20	392.9370	25920	11.5	556	0.0152
21	393.2989	26925	14.4	694	0.0146
22	395.2333	23530	93.1	4477	0.0168
23	396.2372	24978	26.0	1250	0.0159
→ 24	417.2154	24029	1361.3	307934	0.0174
25	418.2185	24309	344.9	81174	0.0172
26	419.2212	25535	49.1	12013	0.0164
27	460.9240	27788	19.4	878	0.0166
28	485.2025	24797	104.9	9969	0.0196
29	486.2051	25831	26.6	2579	0.0188
30	498.9015	28341	10.6	1101	0.0176



(14f)

m/z: Calc'd for $C_{24}H_{30}N_2NaO_3$ ($[M+Na]^+$): 417.2154, found: 417.2154.

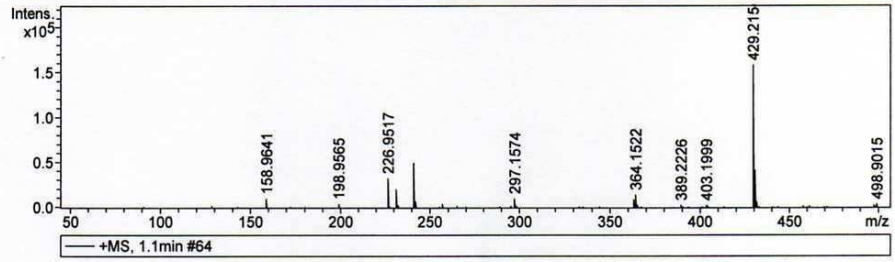
Mass Spectrum List Report

Analysis Info

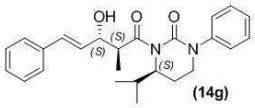
Analysis Name	D:\Data\vipin\12-05-02-MC-LP-7.d	Acquisition Date	5/2/2012 12:27:37 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-LP-7	Instrument / Ser#	maXis 40
Comment			

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	158.9641	20914	247.9	10704	0.0076
2	198.9565	20967	98.7	4558	0.0095
3	226.9517	22436	446.2	32856	0.0101
4	297.1574	23430	145.6	10576	0.0127
5	332.9161	25695	13.9	784	0.0130
6	334.9317	25012	22.2	1209	0.0134
7	344.1941	24568	17.2	1121	0.0140
8	362.9267	24551	102.5	9693	0.0148
9	364.1522	25070	153.7	14837	0.0145
10	365.1555	23037	33.4	3279	0.0159
11	367.1423	23886	13.5	1358	0.0154
12	389.2226	25815	40.2	3209	0.0151
13	390.2264	25765	12.0	949	0.0151
14	392.9374	23888	14.4	1096	0.0164
15	393.2983	24377	17.9	1361	0.0161
16	400.9038	26177	12.7	1129	0.0153
17	402.9190	24675	13.6	1359	0.0163
18	403.1999	25053	31.3	3165	0.0161
→ 19	429.2154	24789	679.9	157516	0.0173
20	430.2187	25076	184.6	41822	0.0172
21	430.9138	25597	39.2	8730	0.0168
22	431.2215	23206	28.0	6195	0.0186
23	457.2098	26138	20.2	1782	0.0175
24	459.2730	26706	12.0	951	0.0172
25	460.9249	24694	23.3	1837	0.0187
26	468.8909	26183	14.9	1170	0.0179
27	470.9066	26849	11.4	899	0.0175
28	497.2030	24694	39.6	3091	0.0201
29	498.2058	26198	12.8	1000	0.0190
30	498.9015	26415	48.7	3805	0.0189



(14g)

m/z: Calc'd for $C_{25}H_{30}N_2NaO_3$ ($[M+Na]^+$): 429.2154, found: 429.2154.

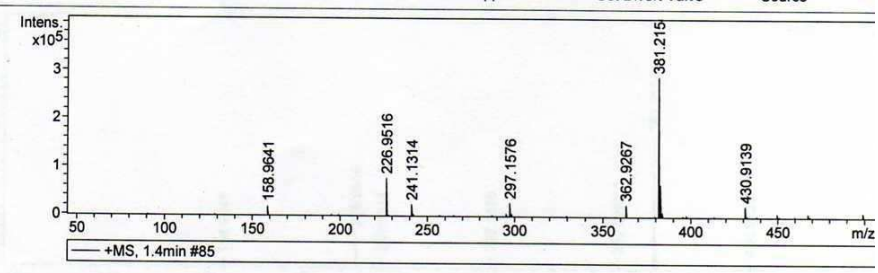
Mass Spectrum List Report

Analysis Info

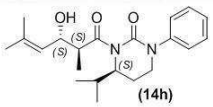
Analysis Name	D:\Data\vipin\12-09-24-MC-LI-PA10.d	Acquisition Date	9/24/2012 4:16:51 PM
Method	tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-LI-PA10	Instrument / Ser#	maXis 40
Comment			

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	158.9641	17415	2681.0	19341	0.0091
2	226.9516	20728	7227.6	77651	0.0109
3	241.1314	20567	2378.0	24421	0.0117
4	297.1576	21472	2280.2	27598	0.0138
5	362.9267	21988	889.9	25061	0.0165
→ 6	381.2154	21912	5306.7	288279	0.0174
7	382.2183	21844	3107.5	66503	0.0175
8	383.2211	21326	444.9	9247	0.0180
9	430.9139	22670	1880.5	22398	0.0190



(14h)

m/z: Calc'd for $C_{21}H_{30}N_2NaO_3$ ($[M+Na]^+$): 381.2154, found: 381.2154.

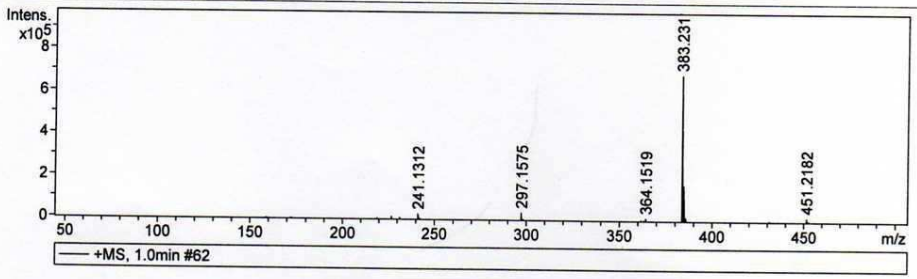
Mass Spectrum List Report

Analysis Info

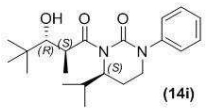
Analysis Name	D:\Data\vipin\12-05-02-MC-LP-8.d	Acquisition Date	5/2/2012 2:53:30 PM
Method	sodium formate tune_low.m		
Sample Name	MC-LP-8	Operator	VIKAS GROVER
Comment		Instrument / Ser#	maXis 40

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	241.1312	23619	334.3	25598	0.0102
2	242.1345	21680	46.4	3561	0.0112
3	256.9622	22368	53.2	2843	0.0115
4	263.1134	23054	64.1	2693	0.0114
5	270.1581	23122	53.6	1548	0.0117
6	294.9390	23798	96.3	2119	0.0124
7	296.1827	24290	32.3	719	0.0122
8	297.1575	23058	1609.4	35692	0.0129
9	298.1606	22965	268.8	5996	0.0130
10	337.1490	23153	63.1	1466	0.0146
11	343.2379	23441	79.8	1946	0.0146
12	344.1947	30982	31.5	780	0.0111
13	361.2487	24695	206.9	5750	0.0146
14	362.2520	22598	36.4	1026	0.0160
15	362.9263	24588	162.3	4566	0.0148
16	364.1519	25203	446.1	12633	0.0144
17	365.1558	23936	105.3	3010	0.0153
18	367.1420	23825	52.0	1589	0.0154
19	369.2169	19373	21.8	1262	0.0191
→ 20	383.2311	23119	2850.1	687666	0.0166
21	384.2341	24303	658.6	167582	0.0158
22	385.2366	23148	74.5	19939	0.0166
23	430.9136	24496	50.3	3853	0.0176
24	451.2182	25625	185.4	20141	0.0176
25	452.2210	24342	45.1	4974	0.0186
26	460.9240	25970	13.8	1610	0.0177
27	481.2283	23816	12.0	832	0.0202
28	498.9007	27304	42.3	2097	0.0183



(14i)

m/z: Calc'd for $C_{21}H_{32}N_2NaO_3$ ($[M+Na]^+$): 383.2311, found: 383.2311.

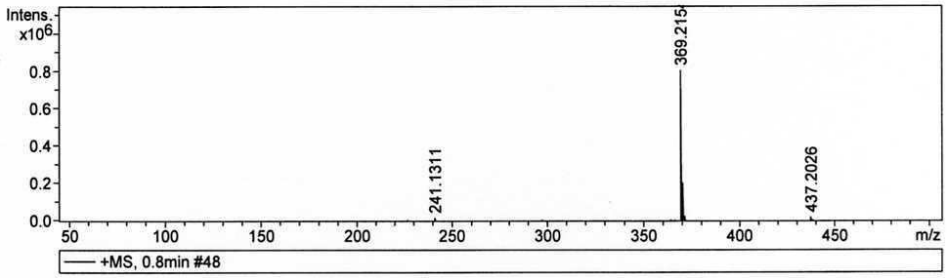
Mass Spectrum List Report

Analysis Info

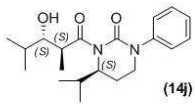
Analysis Name	D:\Data\vipin\12-05-02-MC-LP-9.d	Acquisition Date	5/2/2012 3:31:21 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-LP-9	Instrument / Ser#	maXis 40
Comment			

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	231.0992	23360	68.8	3158	0.0099
2	241.1311	22621	629.4	17123	0.0107
3	242.1347	21786	89.3	2269	0.0111
4	256.9625	24178	119.7	2552	0.0106
5	263.1130	24584	130.4	2781	0.0107
6	270.1576	22637	47.2	1012	0.0119
7	294.9390	21878	50.5	1133	0.0135
8	296.1826	22773	45.1	1016	0.0130
9	297.1574	21787	306.0	6864	0.0136
10	298.1609	24621	61.4	1386	0.0121
11	329.2223	26095	58.7	1463	0.0126
12	337.1489	23987	48.7	1649	0.0141
13	347.2327	23193	20.4	2853	0.0150
14	364.1519	24632	27.1	8617	0.0148
15	366.2064	26544	13.8	4699	0.0138
→ 16	369.2154	22378	2438.1	801121	0.0165
17	370.2183	23819	629.8	201344	0.0155
18	371.2211	23811	81.1	25196	0.0156
19	385.1886	23483	12.8	2381	0.0164
20	387.1270	25595	11.8	1997	0.0151
21	437.2026	25052	161.9	21533	0.0175
22	438.2057	25375	39.1	5073	0.0173
23	460.9248	25945	20.0	1191	0.0178
24	467.2128	25277	42.6	2575	0.0185
25	485.2527	25277	24.6	1543	0.0192
26	497.2997	26013	16.5	1049	0.0191
27	503.3086	23719	12.8	814	0.0212



(14j)

m/z: Calc'd for $C_{20}H_{30}N_2NaO_3$ ($[M+Na]^+$): 369.2154, found: 369.2154.

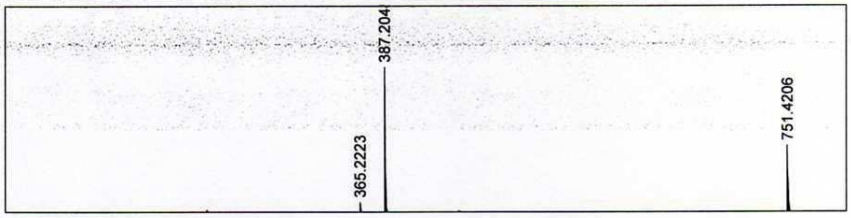
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\vipin\11-02-25-MC-TPO-AK-2.d	Acquisition Date	3/3/2011 11:23:39 AM
Method	tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-TPO-AK-2	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

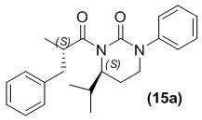
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	800 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



+MS, 1.4min #82

Mass Spectrum List Report

#	m/z	Res.	S/N	I	FWHM
1	365.2223	24604	2883.1	77862	0.0148
→ 2	387.2048	20572	42220.4	1179209	0.0188
3	751.4206	22411	19313.2	538884	0.0335



(15a)

m/z: Calc'd for $C_{23}H_{28}N_2NaO_2$ ([M+Na]$^+$): 387.2048, found: 387.2048.

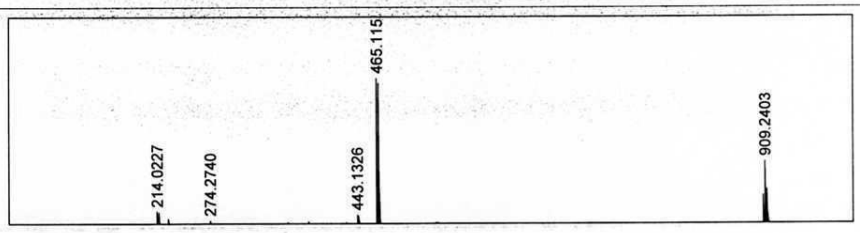
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\vipin\11-03-09-MC-IP-AA5.d	Acquisition Date	3/9/2011 4:29:43 PM
Method	tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-IP-AA5	Instrument / Ser#	maXis 40
Comment			

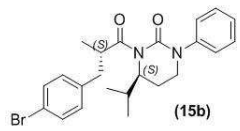
Acquisition Parameter

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



+MS, 2.2min #129

#	m/z	Res.	S/N	I	FWHM
1	214.0227	25575	1457.1	26317	0.0084
2	226.9516	30865	624.2	11256	0.0074
3	274.2740	28231	397.3	7131	0.0097
4	443.1326	31749	805.0	19512	0.0140
→ 5	465.1155	22188	12159.6	320241	0.0210
6	466.1182	25330	2999.4	78582	0.0184
7	467.1138	21100	11889.1	309962	0.0221
8	468.1164	25055	2954.2	76636	0.0187
9	907.2412	26430	2524.9	61716	0.0343
10	909.2403	22334	5519.3	135585	0.0407



(15b)

m/z: Calc'd for $C_{23}H_{27}BrN_2NaO_2$ ([M+Na]$^+$): 465.1154, found: 465.1155.

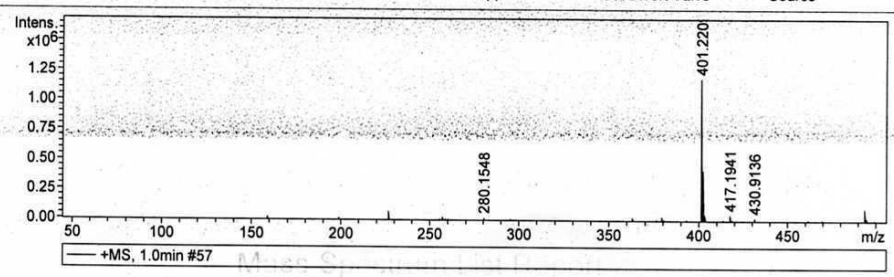
Mass Spectrum List Report

Analysis Info

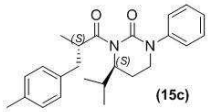
Analysis Name	D:\Data\vipin\12-02-08-MC-1123.d	Acquisition Date	2/8/2012 10:16:16 AM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	12-02-08-MC-1123	Instrument / Ser#	maXis 40
Comment			

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	280.1548	23738	865.3	20168	0.0118
→ 2	401.2209	19803	13044.2	1186599	0.0203
3	402.2238	23635	6584.9	424274	0.0170
4	403.2263	24094	803.3	50626	0.0167
5	417.1941	25769	1135.0	49255	0.0162
6	430.9136	25728	833.3	22801	0.0167



(15c)

m/z: Calc'd for $C_{24}H_{30}N_2NaO_2$
($[M+Na]^+$): 401.2205, found: 401.2109.

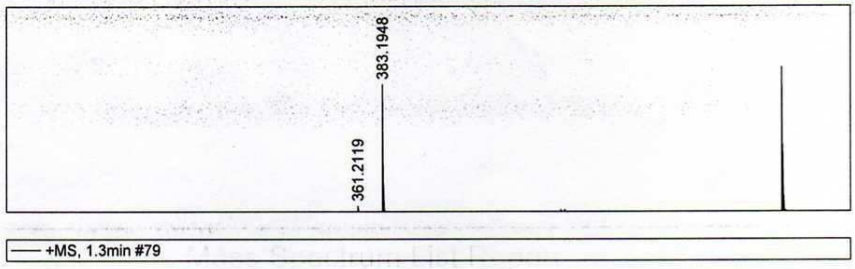
Mass Spectrum List Report

Analysis Info

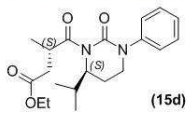
Analysis Name	D:\Data\vipin\11-02-25-MC-TPO-AK-4.d	Acquisition Date	3/3/2011 2:17:55 PM
Method	tune_low.m	Operator	VIKAS GROVER
Sample Name	MC-TPO-AK-4	Instrument / Ser#	maXis 40
Comment			

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	800 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



#	m/z	Res.	S/N	I	FWHM
1	361.2119	27062	3824.7	48525	0.0133
→ 2	383.1948	21595	70730.5	1024292	0.0177



(15d)

m/z: Calc'd for $C_{20}H_{28}N_2NaO_4$
($[M+Na]^+$): 383.1947, found: 383.1948.

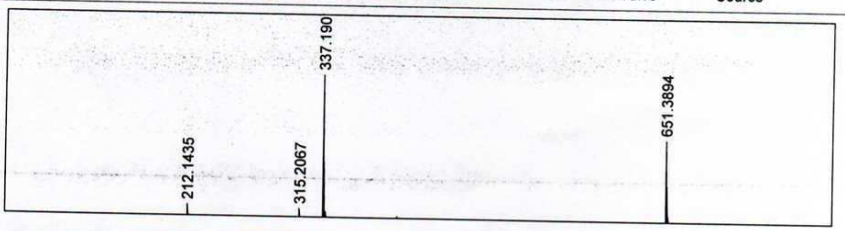
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\vipin\11-02-25-MC-TPO-AK-3.d	Acquisition Date	3/3/2011 12:44:05 PM
Method	tune_low.m		
Sample Name	MC-TPO-AK-3	Operator	VIKAS GROVER
Comment		Instrument / Ser#	maXis 40

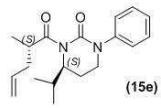
Acquisition Parameter

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	800 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



+MS, 0.6min #36

#	m/z	Res.	S/N	I	FWHM
1	212.1435	21033	12224.9	97154	0.0101
2	315.2067	23713	4155.2	72034	0.0133
→ 3	337.1901	14249	79005.8	1270066	0.0237
4	651.3894	22186	68553.1	730346	0.0294



(15e)

m/z: Calc'd for $C_{19}H_{26}N_2NaO_2$ ($[M+Na]^+$): 337.1892, found: 337.1901.

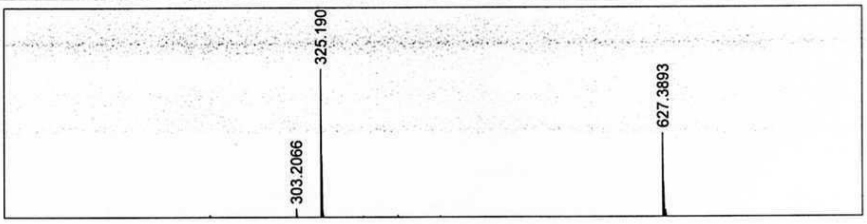
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\vipin\11-02-25-MC-TPO-AK-1.d	Acquisition Date	3/3/2011 10:12:11 AM
Method	tune_low.m		
Sample Name	MC-TPO-AK-1	Operator	VIKAS GROVER
Comment		Instrument / Ser#	maXis 40

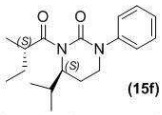
Acquisition Parameter

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	800 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



+MS, 1.0min #60

#	m/z	Res.	S/N	I	FWHM
1	303.2066	24382	4187.3	72229	0.0124
→ 2	325.1901	13378	53058.8	1264854	0.0243
3	627.3893	22723	41884.4	717755	0.0276



(15f)

m/z: Calc'd for $C_{18}H_{26}N_2NaO_2$ ($[M+Na]^+$): 325.1892, found: 325.1901.

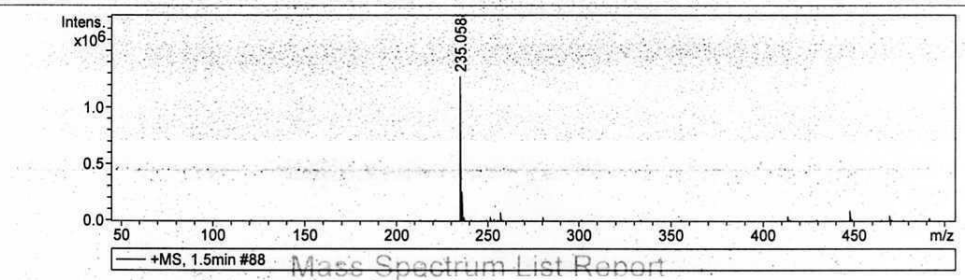
Mass Spectrum List Report

Analysis Info

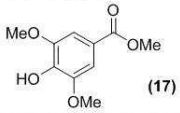
Analysis Name	D:\Data\vipin\12-02-08-MC-116.d	Acquisition Date	2/8/2012 11:08:56 AM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	12-02-08-MC-116	Instrument / Ser#	maXis 40
Comment			

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	235.0588	15425	3920.9	1273247	0.0152
2	236.0616	21417	3577.1	258052	0.0110
3	237.0629	22276	427.2	31729	0.0106



(17)

m/z: Calc'd for $C_{10}H_{12}NaO_5$
($[M+Na]^+$): 235.0582, found: 235.0588.

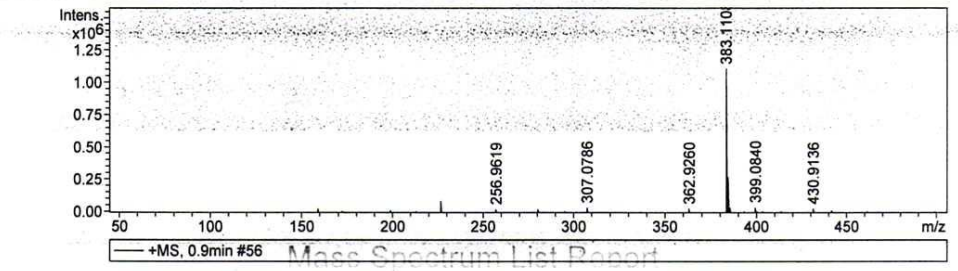
Mass Spectrum List Report

Analysis Info

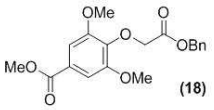
Analysis Name	D:\Data\vipin\12-02-08-MC-[redacted].d	Acquisition Date	2/8/2012 10:27:05 AM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	12-02-08-MC-114	Instrument / Ser#	maXis 40
Comment			

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	256.9619	24626	1166.4	25612	0.0104
2	307.0786	25081	1409.9	36444	0.0122
3	362.9260	24677	1081.3	29906	0.0147
4	383.1108	20578	4061.8	1103987	0.0186
5	384.1138	23298	4674.5	270371	0.0165
6	385.1160	25330	683.3	40694	0.0152
7	399.0840	25039	499.1	38955	0.0159
8	430.9136	26141	1387.4	27551	0.0165
9	441.1156	26937	722.0	13354	0.0164



(18)

m/z: Calc'd for $C_{19}H_{20}NaO_7$
($[M+Na]^+$): 383.1107, found: 383.1108.

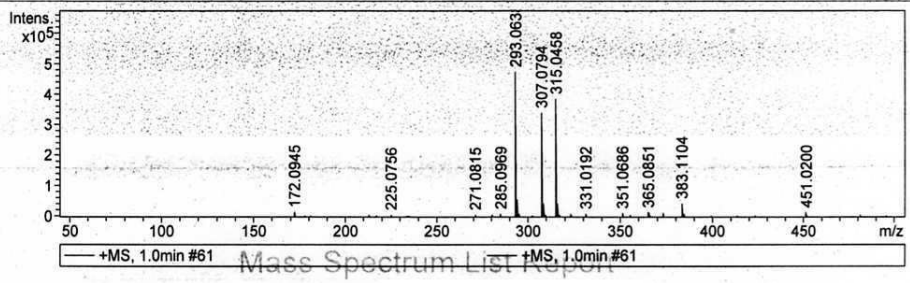
Mass Spectrum List Report

Analysis Info

Analysis Name	D:\Data\vipin\12-02-08-MC-[redacted]d MC-116	Acquisition Date	2/8/2012 10:33:10 AM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	12-02-08-MC-115	Instrument / Ser#	maXis 40
Comment			

Acquisition Parameter

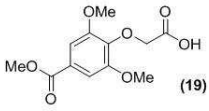
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	500 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



Mass Spectrum List Report

#	m/z	Res.	S/N	I	FWHM
1	293.0638	22358	8463.3	473892	0.0131
2	307.0794	22978	4446.5	338601	0.0134
3	315.0458	22747	6363.0	384810	0.0138
4	351.0686	24870	583.0	12505	0.0141
5	365.0851	25700	638.8	15366	0.0142
6	373.0507	25468	555.9	13610	0.0146
7	383.1104	24883	1798.8	44292	0.0154

#	m/z	Res.	S/N	I	FWHM
1	172.0945	23336	817.5	14689	0.0074
2	213.0757	23088	301.1	6019	0.0092
3	225.0756	23976	346.4	7075	0.0094
4	235.0572	21872	190.7	3967	0.0107
5	271.0815	24808	318.7	7182	0.0109
6	280.1548	25058	175.2	5666	0.0112
7	285.0969	24485	256.2	10607	0.0116
→ 8	293.0638	22358	8463.3	473892	0.0131
9	294.0668	23019	942.1	54498	0.0128
10	295.0682	23808	141.3	8446	0.0124
11	302.1236	25780	62.2	4526	0.0117
12	307.0794	22978	4118.8	338611	0.0134
13	308.0823	23898	509.7	43012	0.0129
14	309.0364	23278	64.3	5569	0.0133
15	309.0839	22682	71.8	6220	0.0136
16	315.0458	22747	3871.1	384818	0.0138
17	316.0488	24097	441.3	44834	0.0131
18	317.0505	25057	65.2	6774	0.0127
19	323.0527	24332	88.8	10367	0.0133
20	331.0192	25240	79.3	10617	0.0131
21	351.0686	24866	79.0	12507	0.0141
22	355.0376	24788	38.8	6280	0.0143
23	365.0851	25695	90.1	15369	0.0142
24	373.0507	25463	74.5	13614	0.0147
25	383.1104	24882	221.3	44296	0.0154
26	384.1137	25227	41.7	8413	0.0152
27	413.2657	25996	25.8	4209	0.0159
28	451.0200	26507	123.3	14689	0.0170



(19)

m/z: Calc'd for $C_{12}H_{14}NaO_7$ ($[M+Na]^+$): 293.0637, found: 293.0638.

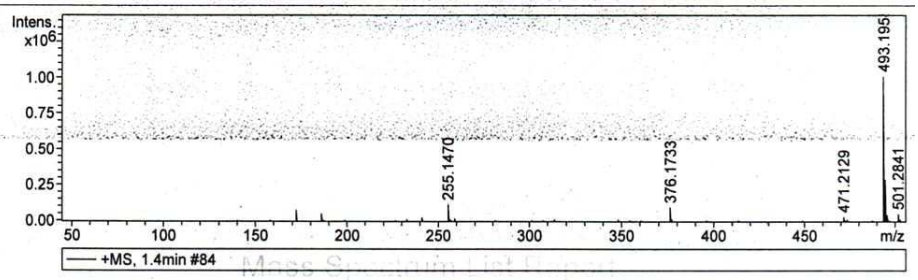
Mass Spectrum List Report

Analysis Info

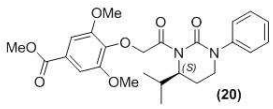
Analysis Name	D:\Data\vipin\12-02-08-MC-117.d	Acquisition Date	2/8/2012 11:16:30 AM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	12-02-08-MC-117	Instrument / Ser#	maXis 40
Comment			

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	255.1470	22569	4649.1	116898	0.0113
2	376.1733	24258	2690.6	96352	0.0155
3	471.2129	26092	439.2	32135	0.0181
→ 4	493.1958	22817	8052.3	1008706	0.0216
5	494.1988	24272	2365.2	296285	0.0204
6	494.7793	7434	0.3	33	0.0666
7	495.2010	25552	382.9	47971	0.0194
8	495.2010	25552	382.9	47971	0.0194
9	501.2841	25941	402.3	50400	0.0193



(20)

m/z: Calc'd for $C_{25}H_{30}N_2NaO_7$ ($[M+Na]^+$): 493.1951, found: 493.1958.

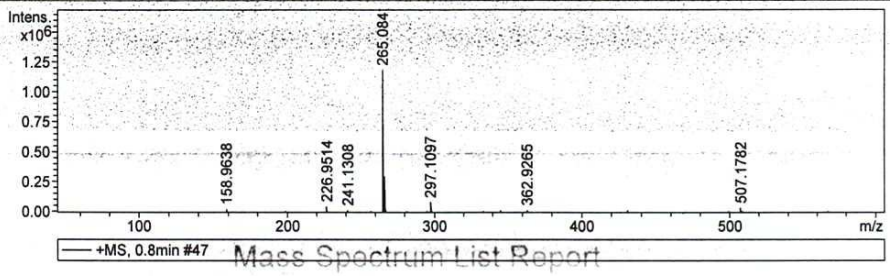
Mass Spectrum List Report

Analysis Info

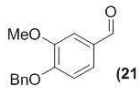
Analysis Name	D:\Data\vipin\12-03-14-MC-122.d	Acquisition Date	3/14/2012 10:06:50 AM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	12-03-14-MC-122	Instrument / Ser#	maXis 40
Comment			

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	158.9638	22231	893.5	28075	0.0072
2	226.9514	24167	1106.9	51000	0.0094
3	241.1308	23586	328.6	18362	0.0102
4	256.9617	23177	209.0	11516	0.0111
→ 5	265.0841	17877	13704.8	1182541	0.0148
6	266.0871	22409	6526.2	295766	0.0119
7	267.0894	22345	609.2	26955	0.0120
8	297.1097	23374	4171.0	84938	0.0127
9	333.0708	24761	876.4	13319	0.0135
10	345.1460	24766	897.0	13980	0.0139
11	362.9265	26005	1236.8	19951	0.0140
12	430.9137	26117	952.8	14573	0.0165
13	507.1782	27041	1587.6	39222	0.0188



(21)

m/z: Calc'd for $C_{15}H_{14}NaO_3$ ($[M+Na]^+$): 265.0841, found: 265.0841.

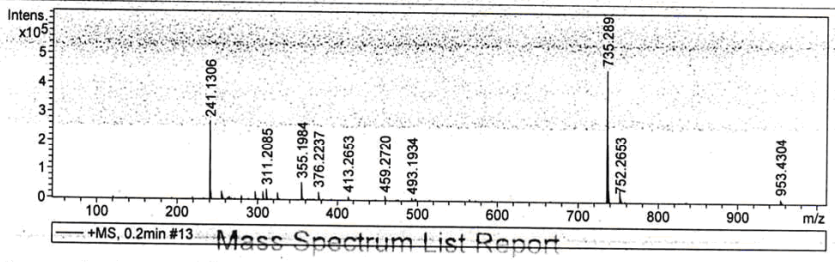
Mass Spectrum List Report

Analysis Info

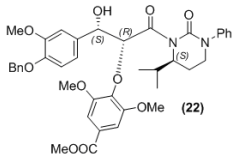
Analysis Name	D:\Data\vipin\12-02-09-MC-118B.d	Acquisition Date	2/9/2012 3:24:28 PM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	12-02-09-MC-118	Instrument / Ser#	maXis 40
Comment			

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	241.1306	21607	10502.8	268721	0.0112
2	280.1540	25757	401.2	13097	0.0109
3	297.1564	24738	813.9	26606	0.0120
4	311.2085	24984	1074.1	35156	0.0125
5	325.1977	25250	708.6	23222	0.0129
6	355.1984	24786	1966.8	59188	0.0143
7	376.2237	25845	991.6	27309	0.0146
8	413.2653	25737	531.6	13504	0.0161
9	459.2720	26580	572.3	15157	0.0173
10	493.1934	27100	318.7	9181	0.0182
→ 11	735.2893	24949	13288.6	455486	0.0295
12	736.2925	25726	5868.5	200450	0.0286
13	737.2945	27085	1360.3	46302	0.0272
14	752.2653	28013	534.2	17241	0.0269
15	953.4304	26719	868.3	16478	0.0357



(22)

m/z: Calc'd for $C_{40}H_{44}N_2NaO_{10}$ ($[M+Na]^+$): 735.2894, found: 735.2893.

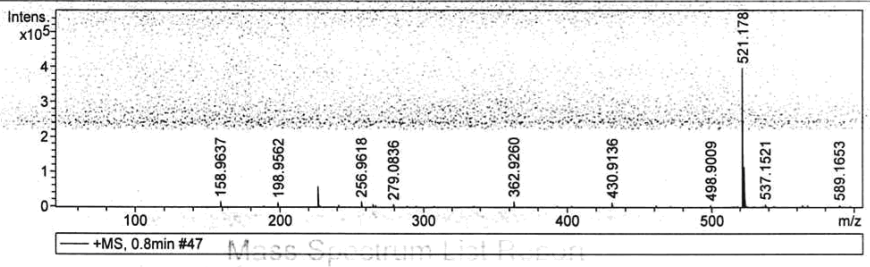
Mass Spectrum List Report

Analysis Info

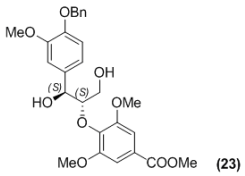
Analysis Name	D:\Data\vipin\12-03-14-MC-126.d	Acquisition Date	3/14/2012 10:24:02 AM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	12-03-14-MC-126	Instrument / Ser#	maXis 40
Comment			

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	158.9637	19504	1571.1	15304	0.0082
2	198.9562	21336	11109.4	131296	0.0093
3	256.9618	24451	1247.4	15317	0.0105
4	279.0836	24851	607.3	7602	0.0112
5	362.9260	25444	1208.7	16889	0.0143
6	402.9187	26216	253.7	3941	0.0154
7	430.9136	26301	819.8	14099	0.0164
8	460.9238	27408	275.7	5340	0.0168
9	498.9009	27543	169.4	5862	0.0181
→ 10	521.1788	24575	6143.0	395702	0.0212
11	522.1820	26054	3210.6	115029	0.0200
12	523.1840	27077	591.8	20860	0.0193
13	537.1521	26420	343.7	9329	0.0203
14	589.1653	25668	441.5	6611	0.0230



(23)

m/z: Calc'd for $C_{27}H_{30}NaO_9$ ($[M+Na]^+$): 521.1788, found: 521.1788.

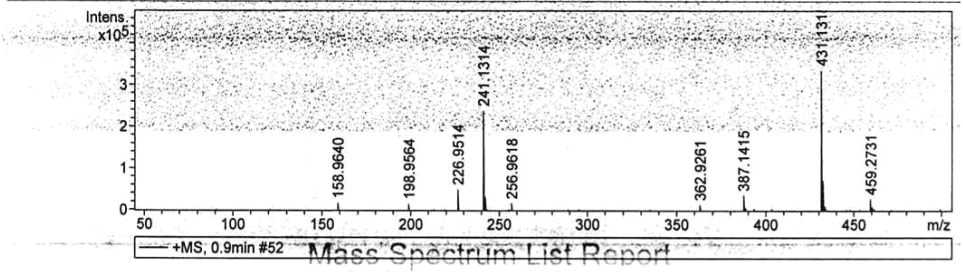
Mass Spectrum List Report

Analysis Info

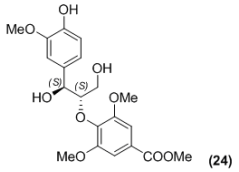
Analysis Name	D:\Data\vipin\12-03-14-MC-127.d	Acquisition Date	3/14/2012 11:23:16 AM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	12-03-14-MC-127	Instrument / Ser#	maXis 40
Comment			

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	158.9640	22046	1106.4	18037	0.0072
2	198.9564	23601	884.9	16589	0.0084
3	219.1489	21557	111.8	2447	0.0102
4	226.9514	21901	2203.5	50349	0.0104
5	241.1314	23031	2348.3	238752	0.0105
6	256.9618	24019	811.7	16922	0.0107
7	362.9261	25467	731.5	14389	0.0143
8	387.1415	25433	1652.2	36561	0.0152
9	431.1318	24451	9506.3	335928	0.0176
10	432.1349	25627	2088.7	72679	0.0169
11	433.1369	25201	360.8	12358	0.0172
12	459.2731	26287	1390.6	28182	0.0175
13	460.2760	26034	414.3	8306	0.0177



(24)

m/z: Calc'd for $C_{20}H_{24}NaO_9$ ($[M+Na]^+$): 431.1318, found: 431.1318.

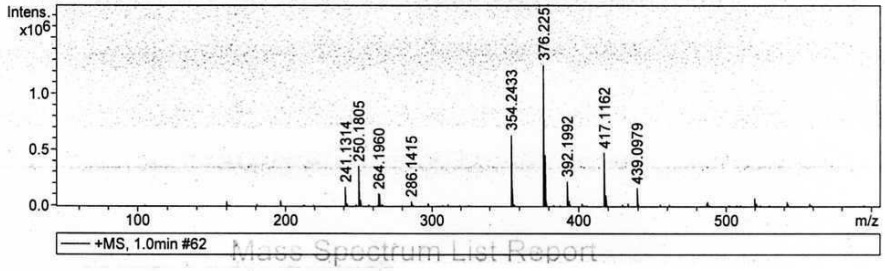
Mass Spectrum List Report

Analysis Info

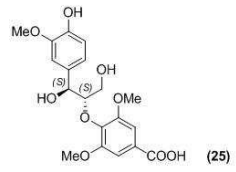
Analysis Name	D:\Data\vipin\12-02-09-MC-120.d	Acquisition Date	2/9/2012 9:53:40 AM
Method	sodium formate tune_low.m	Operator	VIKAS GROVER
Sample Name	12-02-09-MC-120	Instrument / Ser#	maXis 40
Comment			

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	241.1314	22374	2755.0	174340	0.0108
2	250.1805	20906	4918.4	354433	0.0120
3	264.1960	21814	1811.5	112298	0.0121
4	286.1415	23847	1001.3	46022	0.0120
5	354.2433	21894	5795.8	632529	0.0162
6	376.2257	18307	11011.8	1255624	0.0206
7	392.1992	24114	2224.0	221779	0.0163
8	417.1162	23321	5961.8	477219	0.0179
9	439.0979	24519	2490.7	160553	0.0179



(25)

m/z: Calc'd for $C_{19}H_{22}NaO_9$ ($[M+Na]^+$): 417.1162, found: 417.1162.
