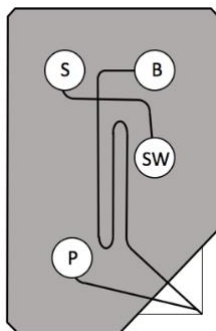
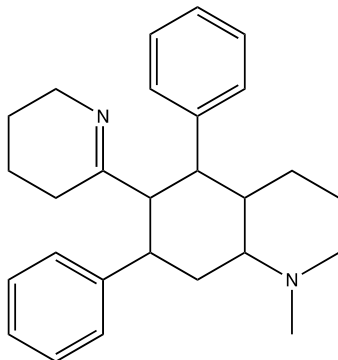


Supplemental Data

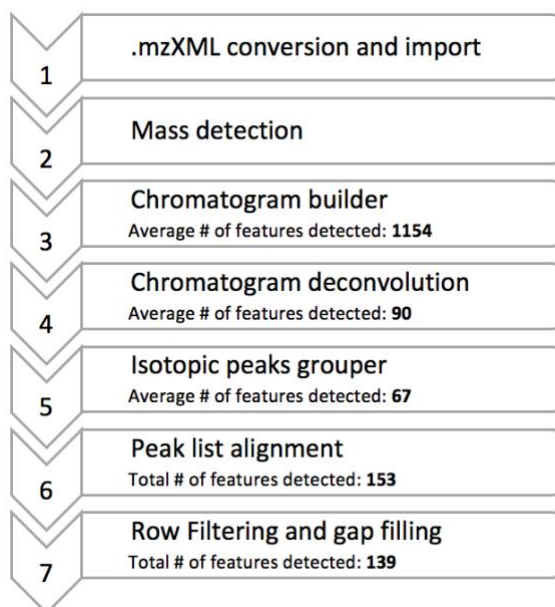
S1: Schematic of the 908 Devices ZipChip displaying the sample well (S), the background electrolyte well (B), the sample waste well (SW), the well in which the bulk flow pressure is provided to produce the spray (P), and the channels that connect the wells. Analyte separation occurs in the serpentine channel.



S2: Lobinaline, the primary alkaloid produced by *Lobelia Cardinalis*.



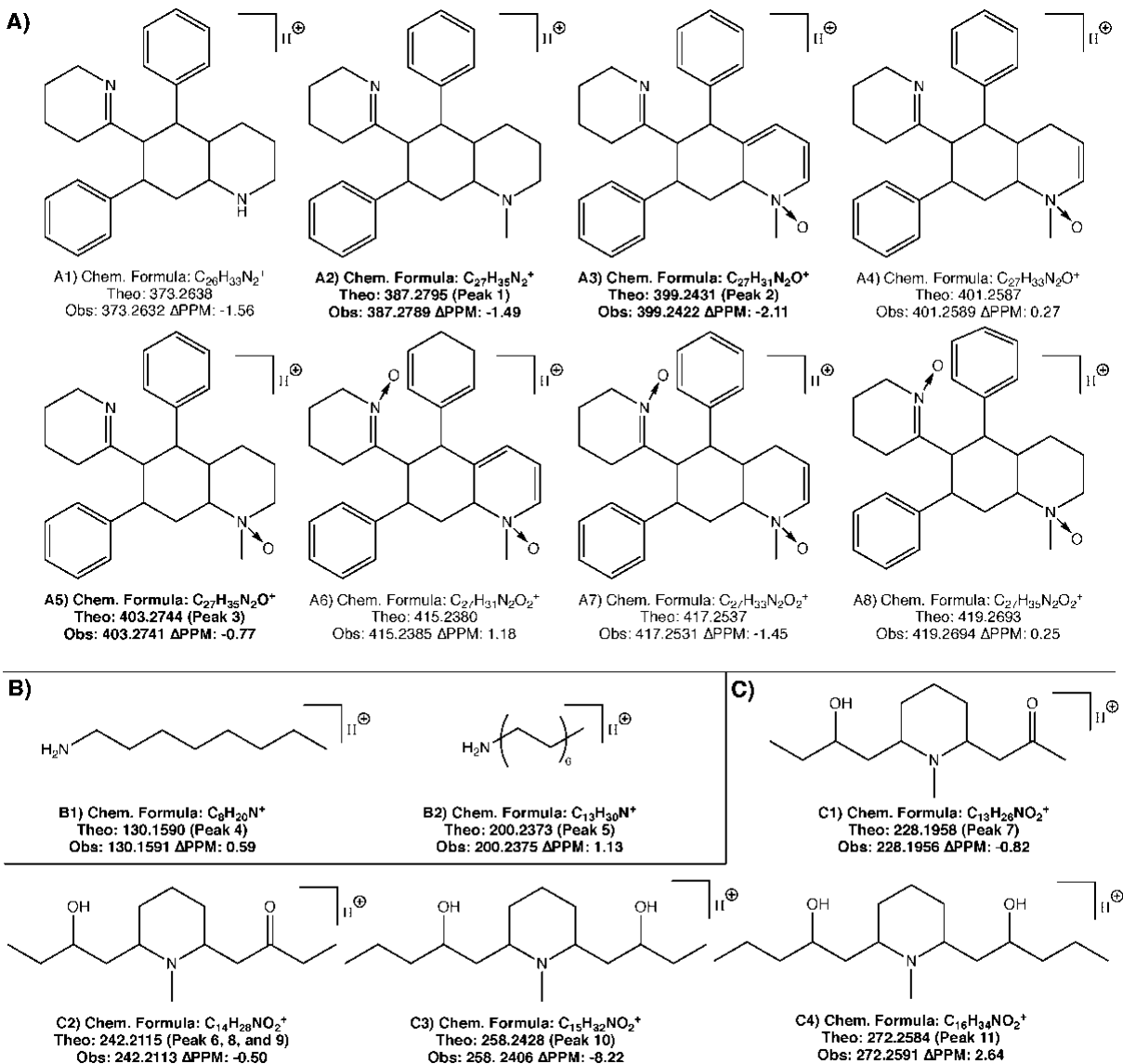
S3: Flow-chart displaying the processing steps of the mass spectral data using MZmine2.



S4: Average area counts and %RSD for each of the selected ions of interest. Corresponding putative structures can be found in supplementary figure S4.

	Feature(m/z)(charge)	Putative Formula	Avg Area Count WT	RSD	Avg Area Count DAT	RSD	Avg Area Count Mutant	RSD	NOTES
A1	373.2638(z=1), 387.1359(z=2)	C ₂₇ H ₃₃ N ₂	8.16E+07	9%	9.09E+07	17%	1.79E+08	16%	lob. derivative
A2	387.2795(z=1), 394.1415(z=2)	C ₂₇ H ₃₅ N ₂	1.75E+09	7%	3.45E+09	11%	5.23E+09	11%	Peak 1
A3	399.2822(z=1), 400.1446(z=2)	C ₂₇ H ₃₁ N ₂ O	7.28E+07	23%	1.57E+08	24%	1.60E+08	24%	Peak 2
A4	401.2587(z=1), 401.1284(z=2)	C ₂₇ H ₃₃ N ₂ O	9.42E+06	19%	4.61E+07	21%	6.53E+07	25%	lob. derivative
A5	403.2740(z=1), 402.1410(z=2)	C ₂₇ H ₃₅ N ₂ O	8.38E+07	11%	3.84E+08	19%	5.31E+08	20%	Peak 3
A6	415.2749(z=1), 408.1415(z=2)	C ₂₇ H ₃₁ N ₂ O ₂	1.42E+07	17%	6.94E+07	23%	3.09E+07	23%	lob. derivative
A7	417.2537(z=1), 409.1308(z=2)	C ₂₇ H ₃₃ N ₂ O ₂	6.61E+06	21%	2.35E+06	33%	3.91E+06	25%	lob. derivative
A8	419.2693(z=1), 410.1383(z=2)	C ₂₇ H ₃₅ N ₂ O ₂	7.50E+05	16%	8.21E+06	20%	1.23E+07	30%	lob. derivative
B1	130.1595(z=1)	C ₈ H ₂₀ N	1.43E+08	25%	1.51E+08	23%	1.72E+08	23%	Peak 4
B2	200.2363(z=1)	C ₁₃ H ₃₀ N	1.78E+08	22%	2.03E+08	24%	2.19E+08	26%	Peak 5
C1	228.1967(z=1)	C ₁₃ H ₂₆ NO ₂	7.17E+07	25%	1.77E+08	22%	3.03E+08	22%	Peak 6
C2	242.2115(z=1) isomer	C ₁₄ H ₂₈ NO ₂	8.49E+07	29%	1.69E+08	25%	4.09E+08	25%	Peak 7
C2	242.2115(z=1) isomer	C ₁₄ H ₂₈ NO ₂	5.60E+07	24%	1.00E+08	21%	2.58E+08	25%	Peak 8
C2	242.2115(z=1) isomer	C ₁₄ H ₂₈ NO ₂	3.24E+08	20%	5.22E+08	21%	1.43E+09	21%	Peak 9
C3	258.2437(z=1)	C ₁₅ H ₃₂ NO ₂	1.03E+08	28%	8.22E+08	23%	1.28E+09	24%	Peak 10
C4	272.2574(z=1)	C ₁₆ H ₃₄ NO ₂	6.82E+07	25%	3.82E+08	24%	1.15E+09	25%	Peak 11
Note: Peaks corresponding to A1, A4, and A6-A8 are not visible in the base peak electropherogram, however they are molecules of interest due to their lobinaline-like structure									

S5: Structures of interest. Group A represents lobinaline and lobinaline-like molecules. Group B consists of conjugated monoamines. Structures shown are putative as multiple varying chain lengths are possible for both molecules. Group C consists of lobeline-like molecules which are consistent with similar molecules found in other *Lobelia* species.¹⁶



S6: Feature list with area counts

row m/z	WT-1	WT-2	WT-3	DAT-1	DAT-2	DAT-3	Mutant-1	Mutant-2	Mutant-3
90.0918	3.46E+06	3.55E+06	2.63E+06	1.41E+06	1.52E+06	1.24E+06	1.63E+06	1.91E+06	1.49E+06
91.0542	3.59E+06	1.70E+06	1.47E+06	5.87E+06	1.16E+06	3.20E+06	4.96E+06	6.29E+06	3.32E+06
97.0079	1.89E+07	4.10E+07	3.24E+07	2.67E+07	3.31E+07	3.83E+07	2.19E+07	3.36E+07	4.86E+07
99.0037	2.39E+06	4.87E+06	4.12E+06	2.61E+06	3.91E+06	5.36E+06	2.38E+06	4.23E+06	6.45E+06
102.0915	2.53E+07	1.86E+07	1.35E+07	2.45E+07	1.76E+07	1.76E+07	2.28E+07	1.94E+07	2.14E+07
102.9705	9.27E+06	3.50E+07	1.93E+07	1.14E+07	2.71E+07	3.98E+07	7.39E+06	1.63E+07	6.14E+07
104.0708	3.19E+06	2.29E+06	1.73E+06	1.27E+06	8.22E+05	1.14E+06	9.19E+05	1.65E+05	9.09E+05
104.1073	4.71E+06	2.87E+06	2.25E+06	9.10E+06	4.84E+06	5.66E+06	5.36E+06	3.08E+06	5.23E+06
105.0036	1.15E+07	1.96E+07	1.68E+07	1.22E+07	1.64E+07	2.46E+07	1.05E+07	1.96E+07	2.49E+07
106.0500	9.36E+05	4.52E+05	4.30E+05	8.85E+05	3.79E+06	5.05E+06	6.40E+05	2.64E+05	3.26E+05
111.0233	1.66E+07	2.29E+07	1.95E+07	2.07E+07	1.88E+07	2.28E+07	2.05E+07	2.13E+07	2.81E+07
113.0190	6.35E+06	6.47E+06	6.45E+06	7.43E+06	4.53E+06	6.24E+06	8.10E+06	5.41E+06	8.02E+06
120.9808	9.10E+06	5.99E+07	3.75E+07	1.22E+07	4.36E+07	6.54E+07	8.91E+06	2.74E+07	8.67E+07
121.0075	9.44E+06	3.81E+06	5.30E+06	7.17E+06	5.18E+06	2.79E+06	1.13E+07	5.44E+06	7.23E+06
122.0812	4.50E+06	1.41E+06	1.13E+06	1.51E+06	2.66E+05	3.93E+05	8.65E+06	2.15E+06	3.49E+06
125.0026	3.41E+06	1.61E+07	1.27E+07	4.54E+06	1.12E+07	1.34E+07	8.73E+06	1.18E+07	1.67E+07
126.9984	2.03E+06	4.94E+06	4.93E+06	2.46E+06	4.04E+06	4.39E+06	2.11E+06	4.79E+06	6.73E+06
132.1015	2.28E+06	2.46E+06	1.34E+06	4.32E+06	3.57E+06	4.78E+06	1.52E+06	1.23E+06	1.16E+06
133.0610	2.80E+06	1.15E+06	6.17E+05	5.06E+06	1.98E+06	2.30E+06	5.94E+06	2.19E+06	3.54E+06
134.9869	6.22E+06	7.92E+06	6.71E+06	7.44E+06	7.05E+06	8.44E+06	6.87E+06	5.27E+06	1.04E+07
136.0426					2.72E+07	3.55E+07			
139.0182	1.71E+07	1.89E+07	1.53E+07	2.60E+07	1.56E+07	1.64E+07	2.07E+07	1.36E+07	1.88E+07
140.1437	6.10E+05	4.12E+05	3.33E+05	6.54E+06	3.61E+06	4.61E+06	6.93E+05	3.03E+05	5.71E+05
141.0139	2.42E+07	1.61E+07	1.55E+07	2.47E+07	1.19E+07	1.92E+07	2.48E+07	1.22E+07	2.11E+07
142.1577	2.41E+06	1.27E+06	8.11E+05	2.67E+06	1.00E+06	1.55E+06	4.34E+06	2.81E+06	4.85E+06
144.0478	5.10E+07	3.37E+07	2.86E+07	3.71E+07	2.19E+07	2.64E+07	6.81E+07	4.36E+07	6.40E+07
144.1383	1.86E+06	1.38E+06	1.07E+06	1.92E+07	1.26E+07	1.52E+07	1.56E+06	8.20E+05	1.34E+06
148.9756	6.29E+06	1.38E+07	7.61E+06	8.48E+06	9.34E+06	1.41E+07	5.75E+06	5.63E+06	1.76E+07
149.0026	8.75E+07	4.25E+07	3.71E+07	1.07E+08	3.61E+07	4.26E+07	4.80E+07	3.90E+07	5.23E+07
151.0541		5.18E+05	1.26E+06		2.71E+06	3.73E+06		4.43E+06	7.16E+06
151.0971	1.93E+06	1.57E+06	1.19E+06	1.09E+06	1.08E+06	1.26E+06	1.47E+06	1.09E+06	1.74E+06
152.9974	1.54E+07	3.07E+07	2.55E+07	2.25E+07	2.33E+07	2.78E+07	1.92E+07	2.47E+07	3.26E+07
155.0299	1.45E+07	8.23E+06	6.00E+06	1.78E+07	6.36E+06	8.67E+06	1.73E+07	5.64E+06	9.25E+06
156.0766	6.23E+05	1.96E+05	2.36E+05	3.62E+05	3.41E+06	3.69E+06	8.35E+05	2.64E+05	4.09E+05
158.1175	8.08E+05	4.81E+05	1.74E+05	4.58E+05	2.12E+05	3.12E+05	2.91E+06	1.75E+06	2.37E+06
158.1539	1.03E+07	7.20E+06	6.95E+06	8.59E+07	5.52E+07	7.07E+07	1.15E+07	6.96E+06	1.11E+07
167.0130	5.99E+07	4.36E+07	3.87E+07	8.51E+07	3.44E+07	4.21E+07	3.76E+07	3.26E+07	4.57E+07
170.1539	9.36E+05	6.32E+05	5.95E+05	1.38E+06	6.62E+05	1.29E+06	2.88E+06	9.93E+05	3.77E+06

172.1692	2.43E+06	2.05E+06	2.09E+06	8.10E+07	5.62E+07	7.34E+07	3.89E+07	2.77E+07	4.46E+07
174.1605	3.94E+06	3.35E+06	3.09E+06	1.62E+06	9.28E+05	1.28E+06	2.70E+04	1.79E+05	1.18E+05
180.1272	1.87E+06	1.97E+06	2.76E+06	5.23E+06	1.58E+06	5.22E+06	8.30E+06	6.57E+06	6.44E+06
181.0289	2.13E+07	1.01E+07	7.89E+06	8.50E+06	8.66E+06	1.01E+07	2.70E+07	6.62E+06	9.09E+06
181.0453	2.81E+05	7.68E+05	1.80E+06	2.77E+05	2.75E+06	4.95E+06	4.35E+05	3.87E+06	5.58E+06
186.1276	8.16E+06	1.43E+07	7.58E+06	7.38E+07	3.51E+07	1.76E+07	3.61E+07	6.38E+07	7.53E+07
186.1277	1.71E+07	7.91E+06	1.19E+07	1.86E+07	4.27E+07	5.32E+07	1.02E+08	2.40E+07	7.75E+07
186.1855	2.00E+05	1.15E+05	1.06E+05	1.53E+07	3.86E+06	1.22E+07	1.12E+06	2.25E+06	3.25E+06
189.0335	2.17E+05	1.74E+06	5.13E+06	1.42E+05	1.42E+07	2.08E+07	6.91E+04	1.76E+07	2.89E+07
193.1356	3.58E+06	2.78E+06	5.30E+05	2.65E+07	1.22E+07	1.65E+07	2.93E+07	2.24E+07	2.81E+07
193.1360	4.44E+06	9.15E+05	5.20E+05	1.57E+07	6.58E+06	2.94E+06	1.13E+07	7.58E+05	5.91E+06
199.0942	8.79E+06	3.11E+06	8.90E+06	6.87E+06	2.53E+06	9.15E+06	1.67E+07	2.69E+06	5.66E+06
200.1253	2.11E+05	1.18E+06	1.01E+06	2.16E+07	1.66E+07	2.44E+07	4.06E+06	4.13E+06	6.60E+06
200.1254	1.05E+06	1.18E+06	1.01E+06	2.40E+07	1.09E+07	2.30E+07	3.87E+06	4.13E+06	6.78E+06
201.0442	1.82E+05	1.87E+05	3.42E+05	2.83E+06	2.79E+06	3.70E+06	3.12E+06	2.91E+06	4.39E+06
201.1500	3.19E+06	2.26E+06	7.06E+05	1.11E+07	5.19E+06	3.28E+06	6.58E+06	4.17E+06	4.90E+06
201.1508	3.29E+06	1.54E+05	4.85E+05	5.01E+06	1.90E+06	3.71E+06	6.73E+06	7.30E+05	2.08E+06
207.0443	1.45E+05	8.17E+05	1.60E+06	2.02E+05	4.61E+06	7.89E+06	2.73E+05	3.57E+06	9.55E+06
213.1099	6.54E+07	8.23E+07	1.10E+08	4.13E+07	3.74E+07	5.18E+07	3.45E+07	8.30E+07	2.52E+07
214.1134	1.22E+06	8.31E+06	7.40E+06	1.79E+07	8.75E+06	5.10E+06	3.68E+06	8.21E+06	4.06E+06
216.0431				7.31E+05	2.84E+05	3.96E+05	6.25E+06	3.41E+06	4.89E+06
216.1569	1.46E+05	2.39E+06	1.76E+06	5.92E+06	4.11E+06	4.60E+06	2.12E+04	3.91E+06	5.43E+06
216.1959	1.93E+07	1.55E+07	1.29E+07	6.07E+06	7.82E+06	4.37E+06	9.01E+05	1.60E+06	2.78E+06
216.1962	5.38E+05	1.62E+07	1.33E+07	1.25E+07	3.60E+06	1.09E+07	4.78E+05	1.60E+06	2.78E+06
219.1357	3.58E+05	3.47E+05	7.51E+05	2.07E+07	9.01E+06	1.76E+07	9.85E+05	5.87E+05	1.64E+06
224.1539	5.12E+05	2.04E+06	2.06E+06	6.25E+06	1.06E+07	1.49E+07	9.88E+06	7.07E+06	1.20E+07
229.1985	7.75E+06	5.57E+06	5.08E+06	2.31E+07	1.35E+07	1.91E+07	3.79E+07	2.66E+07	4.08E+07
230.2113	9.03E+07	6.71E+07	5.14E+07	7.12E+07	2.78E+07	1.21E+07	6.78E+06	2.88E+07	4.69E+07
230.2113	8.33E+07	6.89E+06	7.84E+05	3.99E+07	1.00E+07	5.56E+07	1.33E+07	7.96E+06	1.17E+07
230.2116	7.16E+07	1.89E+07	8.14E+06	1.78E+07	4.24E+07	3.41E+07	3.81E+07	5.36E+06	1.66E+07
232.1524	1.19E+05	3.42E+05	1.90E+05	3.98E+06	8.98E+05	1.12E+06	1.69E+05	4.41E+05	5.78E+05
235.0928	3.86E+06	1.56E+06	1.33E+06	4.43E+06	1.16E+06	1.87E+06	4.78E+06	1.16E+06	2.00E+06
240.1955	4.25E+06	2.90E+06	2.76E+06	3.39E+06	1.86E+06	4.98E+05	6.01E+06	3.22E+06	6.96E+06
242.2830	7.61E+06	1.43E+05	2.45E+06	1.18E+07	1.27E+05	1.83E+06	6.50E+08	4.26E+08	7.17E+08
244.1908	8.72E+06	6.62E+06	6.07E+06	6.39E+06	4.74E+06	1.54E+07	1.37E+07	1.07E+07	4.82E+07
244.1909	3.87E+05	5.28E+06	4.64E+06	1.72E+07	1.20E+07	5.18E+06	4.08E+07	3.12E+07	1.59E+07
244.2268	1.38E+07	4.46E+07	9.84E+06	1.83E+08	5.01E+07	1.43E+08	9.23E+07	1.36E+08	3.37E+08
244.2270	7.30E+07	5.58E+07	4.65E+07	1.61E+08	1.14E+08	6.74E+07	2.79E+08	6.09E+07	1.01E+08
244.2271	3.70E+07	2.65E+07	2.41E+07	6.48E+07	9.46E+07	1.28E+08	5.19E+07	2.15E+08	2.95E+08
245.1883	1.09E+07	4.09E+06	2.30E+06	1.76E+07	3.86E+06	2.07E+06	2.03E+06	5.74E+06	7.27E+06
247.0756	1.68E+07	9.31E+06	7.57E+06	2.25E+07	7.64E+06	9.33E+06	2.40E+07	4.42E+06	1.09E+07

254.2111	6.05E+05	2.53E+05	2.86E+05	1.99E+06	3.84E+05	2.19E+05	1.40E+07	9.01E+06	1.45E+07
256.2269	2.40E+07	9.38E+07	9.13E+07	2.79E+08	1.77E+08	5.95E+07	8.97E+08	6.52E+08	1.02E+09
256.2270	2.40E+07	1.63E+07	3.63E+07	7.13E+07	4.61E+07	2.26E+08	1.90E+08	1.32E+08	7.37E+08
258.2068	3.69E+06	5.37E+07	5.03E+07	4.67E+07	2.68E+07	1.34E+07	8.62E+06	3.59E+07	5.79E+07
259.2076	2.75E+07	8.08E+05	1.13E+06	3.91E+06	1.13E+06	5.79E+05	2.13E+06	6.37E+05	1.45E+06
259.2454	1.64E+07	8.39E+06	5.88E+06	1.26E+08	4.77E+07	6.26E+07	1.56E+08	8.35E+07	1.79E+08
259.6726	9.65E+04	4.73E+05	5.12E+05	6.65E+06	4.77E+06	4.06E+06	3.25E+07	2.32E+07	3.53E+07
260.2224	2.28E+07	1.54E+07	1.26E+07	1.57E+07	8.01E+06	1.00E+07	5.87E+06	3.58E+06	6.58E+06
260.2487	3.75E+05	1.09E+06	4.20E+05	6.86E+05	5.89E+06	9.20E+06	1.03E+06	2.08E+06	1.65E+07
261.0914	1.00E+07	3.07E+06	2.79E+06	1.53E+07	3.14E+06	3.85E+06	6.11E+06	3.34E+06	3.05E+06
270.2428	4.58E+06	2.68E+06	2.80E+06	1.56E+07	9.36E+06	1.15E+07	4.88E+07	4.44E+07	4.44E+07
270.3152	3.83E+07	2.59E+07	1.88E+07	3.30E+07	1.54E+07	2.65E+07	3.59E+07	2.46E+07	3.38E+07
272.2217	2.98E+07	2.22E+07	1.94E+07	3.11E+07	1.95E+07	2.59E+07	8.40E+07	5.37E+07	8.76E+07
273.1904	3.88E+06	1.42E+06	2.46E+06	1.64E+06	5.90E+05	3.70E+06	8.96E+06	1.65E+06	1.25E+06
273.2177	3.83E+06	5.65E+05	1.14E+06	2.70E+06	1.05E+06	2.46E+06	1.50E+06	8.89E+05	3.36E+06
273.2252	5.46E+06	4.57E+06	4.95E+06	6.61E+06	7.45E+06	7.43E+06	1.84E+07	8.93E+06	1.97E+07
273.2617	4.57E+06	4.05E+05	1.50E+06	6.90E+07	4.34E+07	7.71E+05	1.78E+08	1.60E+06	2.21E+08
274.2370	9.28E+06	2.23E+06	4.42E+05	6.38E+07	3.55E+07	4.53E+07	3.14E+07	1.62E+07	3.06E+07
281.1882	1.53E+05	6.32E+04	8.17E+04	9.63E+04	2.90E+05	4.90E+05	1.89E+06	7.01E+04	3.27E+05
282.2791	1.18E+07	7.71E+06	7.13E+06	8.04E+06	4.48E+06	5.63E+06	7.17E+04	1.35E+05	2.46E+05
286.2381	1.35E+06	1.53E+06	6.55E+05	2.19E+07	1.32E+07	1.57E+07	2.04E+07	1.45E+07	2.77E+07
288.2179	1.26E+07	9.19E+06	7.19E+06	4.12E+05	2.70E+06	4.00E+06	1.18E+06	7.31E+06	8.07E+06
288.2529	1.81E+07	1.31E+07	2.44E+05	1.24E+08	7.44E+07	1.30E+06	7.56E+07	5.26E+07	8.16E+07
288.5204	1.23E+06	8.27E+05	6.02E+05	7.28E+06	6.06E+06	6.42E+06	7.87E+06	6.44E+06	9.81E+06
289.2040	2.55E+04	6.99E+05	1.90E+06	2.71E+05	9.75E+05	1.28E+06	8.55E+06	3.56E+06	9.97E+05
289.2561	2.66E+06	1.86E+06	1.95E+06	2.76E+07	1.42E+07	1.99E+07	1.39E+07	9.09E+06	1.28E+07
293.1343	2.44E+04	2.33E+05	1.89E+05	9.16E+06	1.67E+06	4.48E+06	7.78E+06	3.41E+06	5.29E+06
296.2948	3.84E+05	2.10E+06	1.30E+06	5.80E+06	8.30E+05	3.51E+06	6.36E+05	1.04E+05	2.05E+05
299.1612	1.39E+07	1.10E+07	1.79E+07	1.38E+07	6.75E+06	6.72E+06	1.10E+07	3.73E+06	2.70E+06
302.2324	2.94E+06	5.16E+05	5.55E+05	2.52E+06	5.52E+05	2.77E+05	4.53E+06	2.20E+05	1.45E+06
302.2694	3.88E+05	6.74E+04	2.03E+05	6.29E+06	5.52E+05	6.16E+05	3.01E+05	3.92E+05	4.63E+05
306.2129	3.53E+06	5.67E+05	4.91E+04	5.48E+06	2.59E+06	3.36E+06	5.93E+06	9.47E+05	2.72E+06
310.1655	2.37E+06	7.27E+06	1.22E+06	8.16E+05	4.89E+05	2.53E+05	1.03E+07	2.67E+06	3.97E+06
313.1913	1.08E+05	2.20E+04	1.92E+04	4.12E+05	6.16E+05	1.03E+06	1.32E+07	5.21E+05	1.04E+07
322.2371	1.59E+05	2.50E+05	2.90E+05	4.46E+06	1.86E+06	2.71E+06	5.37E+06	2.50E+06	8.27E+06
324.2076		6.28E+04	2.08E+05		2.06E+04	3.42E+05	2.63E+04	3.85E+04	4.11E+06
325.1336	1.44E+07	6.82E+06	2.15E+05	3.15E+06	2.44E+05				
344.2389	2.48E+05	2.23E+05	2.21E+05	3.05E+05	4.01E+06	6.26E+05	1.20E+07	1.27E+07	7.06E+06
349.2278	7.08E+05	3.46E+05	1.09E+06	5.49E+06	1.08E+05	4.77E+06	2.83E+05	5.03E+05	1.49E+05
366.3362				1.25E+06	4.40E+05	3.03E+05	8.41E+06	3.80E+05	1.39E+06
367.3323	6.12E+06	8.23E+05	4.19E+06	1.20E+07	6.94E+06	8.75E+06	2.33E+05	1.67E+05	3.68E+05

381.3479	2.62E+05	7.74E+05	7.13E+05	1.24E+07	2.48E+06	3.75E+05	1.40E+05	2.32E+05	3.68E+05
432.2771	1.37E+06	1.28E+06	1.14E+06	1.28E+07	9.18E+06	1.39E+07	1.09E+07	9.22E+06	1.67E+07
451.3899	1.33E+05	2.03E+05	8.10E+04		2.98E+05	2.20E+05	2.18E+07	8.88E+06	1.35E+07
373.2638, 187.1359	8.83E+07	8.30E+07	7.34E+07	1.05E+08	7.42E+07	9.33E+07	1.81E+08	1.50E+08	2.07E+08
387.2795, 194.1415	1.89E+09	1.75E+09	1.63E+09	3.78E+09	3.05E+09	3.52E+09	5.35E+09	4.62E+09	5.72E+09
399.2822, 200.1446	9.19E+07	6.64E+07	6.01E+07	1.96E+08	1.21E+08	1.54E+08	1.76E+08	1.16E+08	1.89E+08
401.2587, 201.1284	1.03E+07	1.06E+07	7.39E+06	5.30E+07	3.51E+07	5.03E+07	6.66E+07	4.85E+07	8.09E+07
403.2740, 202.1410	9.36E+07	8.29E+07	7.49E+07	4.45E+08	3.03E+08	4.03E+08	5.57E+08	4.14E+08	6.21E+08
415.2749, 208.1415	1.65E+07	1.43E+07	1.17E+07	8.21E+07	5.16E+07	7.45E+07	3.19E+07	2.34E+07	3.74E+07
417.2537, 209.1308	8.03E+06	6.53E+06	5.25E+06	3.25E+06	1.81E+06	2.00E+06	4.37E+06	2.80E+06	4.56E+06
419.2693, 210.1383	8.82E+05	7.24E+05	6.44E+05	7.61E+06	6.93E+06	1.01E+07	1.05E+07	9.87E+06	1.66E+07
130.1595	1.80E+08	1.39E+08	1.10E+08	1.78E+08	1.12E+08	1.62E+08	1.82E+08	1.28E+08	2.06E+08
200.2363	2.21E+08	1.65E+08	1.48E+08	2.44E+08	1.50E+08	2.14E+08	2.27E+08	1.60E+08	2.71E+08
228.1967	9.22E+07	6.57E+07	5.74E+07	2.18E+08	1.40E+08	1.74E+08	3.24E+08	2.27E+08	3.57E+08
242.2115 isomer	1.11E+08	7.91E+07	6.41E+07	2.15E+08	1.32E+08	1.60E+08	4.28E+08	2.98E+08	5.02E+08
242.2115 isomer	7.14E+07	5.09E+07	4.56E+07	1.20E+08	7.73E+07	1.03E+08	2.73E+08	1.86E+08	3.14E+08
242.2115 isomer	3.94E+08	3.12E+08	2.67E+08	6.36E+08	4.14E+08	5.17E+08	1.50E+09	1.09E+09	1.69E+09
258.2437	1.34E+08	9.53E+07	7.79E+07	1.01E+09	6.28E+08	8.27E+08	1.35E+09	9.50E+08	1.55E+09
272.2574	8.76E+07	6.08E+07	5.61E+07	4.69E+08	2.87E+08	3.91E+08	1.25E+09	8.25E+08	1.36E+09

S7: Confidence interval calculation for error in lobinaline concentration from calibration curve

$$\mu_{C_A} = C_A \pm t(s_{C_A})$$

C_A = analyte concentration from the regression equation ($y = b_1x + b_0$)

t = t value based on the desired level of confidence and $n-2$ degrees of freedom (in this case, at 95% confidence and $n-2 = 8$; $t = 2.306$)

$$s_{C_A} = \frac{(stdev_{reg})}{b_1} \sqrt{\left(\frac{1}{m}\right) + \left(\frac{1}{n}\right) + \frac{(\bar{Y} - \bar{y})^2}{(b_1)^2 \sum_i (x_i - \bar{x})^2}}$$

$(stdev_{reg}) = \sqrt{\frac{\sum (y_i - \hat{y}_i)^2}{n-2}}$ where y_i = average response for the i^{th} standard and \hat{y}_i = the calculated response for that standard using the regression equation

m = number of internal standard replicates

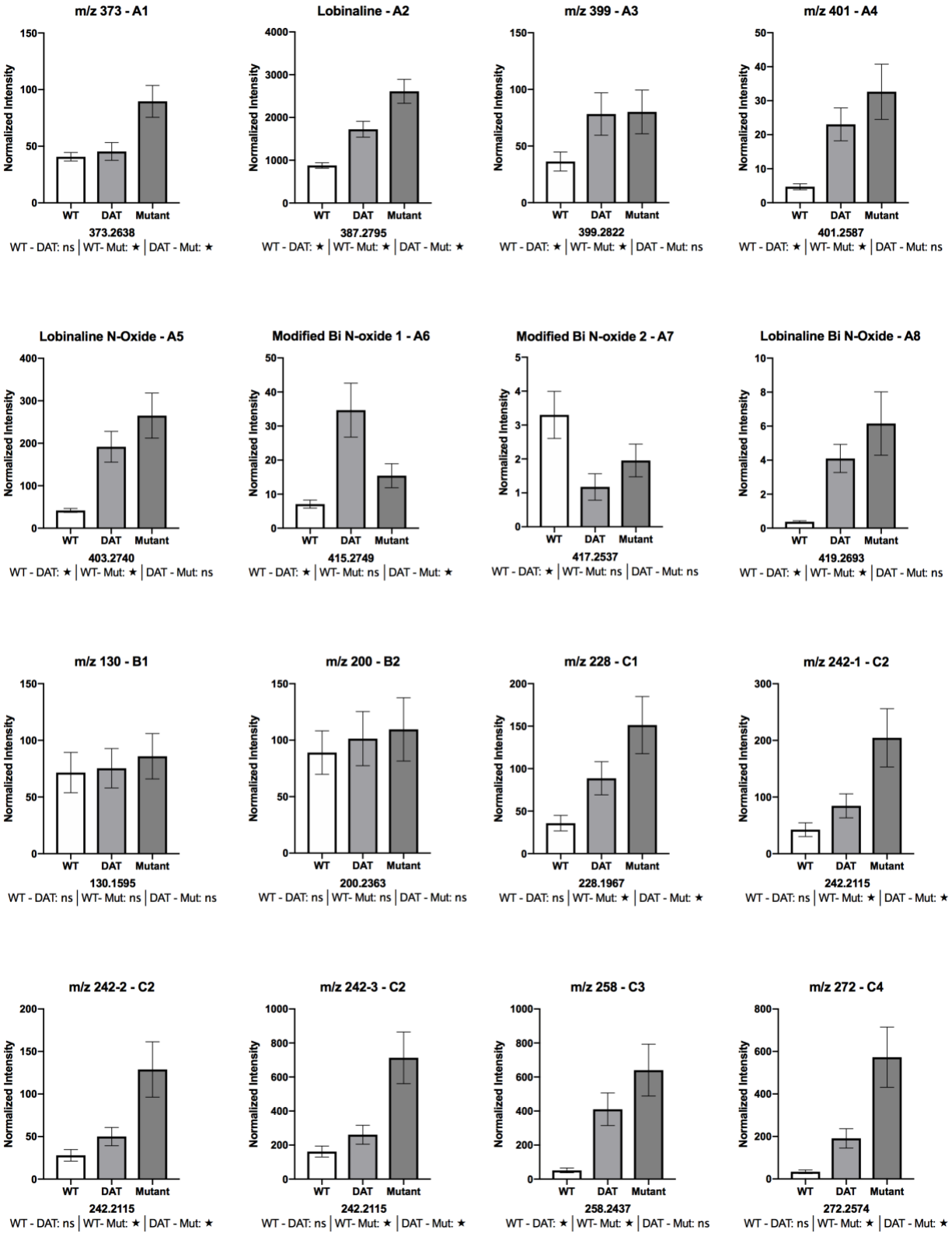
n = number of points in the curve

\bar{Y} = response for analyte in sample

\bar{y} = average response for analyte in all standards

$\sum_i (x_i - \bar{x})^2$ = standard sum of squares for concentration range of internal standards.

S8: Expanded version of figure 8 displaying bar graphs of the normalized area counts for the prioritized list



S9: Normalized feature list

Normalized Data set for all 139 features - average area count for m/z 200.2363: 2.00E+08									
row m/z	WT-1	WT-2	WT-3	DAT-1	DAT-2	DAT-3	Mutant-1	Mutant-2	Mutant-3
90.0918	1.728	1.771	1.316	0.706	0.757	0.622	0.815	0.957	0.742
91.0542	1.794	0.847	0.735	2.932	0.579	1.597	2.481	3.145	1.661
97.0079	9.462	20.465	16.211	13.363	16.523	19.122	10.964	16.763	24.292
99.0037	1.196	2.435	2.058	1.302	1.952	2.680	1.187	2.114	3.221
102.0915	12.642	9.273	6.738	12.253	8.813	8.800	11.387	9.687	10.696
102.9705	4.632	17.499	9.649	5.682	13.559	19.904	3.692	8.162	30.668
104.0708	1.592	1.142	0.866	0.634	0.410	0.567	0.459	0.082	0.454
104.1073	2.356	1.436	1.123	4.546	2.418	2.827	2.677	1.541	2.612
105.0036	5.764	9.814	8.382	6.118	8.204	12.292	5.255	9.777	12.460
106.0500	0.468	0.226	0.215	0.442	1.893	2.524	0.320	0.132	0.163
111.0233	8.294	11.457	9.733	10.362	9.416	11.399	10.263	10.660	14.062
113.0190	3.175	3.234	3.222	3.712	2.264	3.118	4.049	2.702	4.007
120.9808	4.545	29.947	18.714	6.086	21.789	32.652	4.452	13.668	43.338
121.0075	4.716	1.906	2.649	3.585	2.590	1.392	5.649	2.716	3.612
122.0812	2.248	0.704	0.567	0.756	0.133	0.196	4.324	1.073	1.742
125.0026	1.704	8.068	6.349	2.267	5.619	6.685	4.364	5.880	8.319
126.9984	1.015	2.466	2.462	1.229	2.018	2.193	1.054	2.392	3.363
132.1015	1.138	1.229	0.672	2.159	1.781	2.388	0.761	0.612	0.578
133.0610	1.400	0.574	0.308	2.529	0.992	1.149	2.967	1.097	1.767
134.9869	3.109	3.956	3.350	3.716	3.524	4.217	3.431	2.631	5.175
136.0426	0.000	0.000	0.000	0.000	13.609	17.726	0.000	0.000	0.000
139.0182	8.566	9.429	7.652	12.969	7.782	8.194	10.354	6.777	9.385
140.1437	0.305	0.206	0.167	3.269	1.805	2.302	0.346	0.152	0.285
141.0139	12.077	8.022	7.750	12.335	5.926	9.598	12.379	6.111	10.559
142.1577	1.205	0.632	0.405	1.332	0.500	0.775	2.167	1.405	2.423
144.0478	25.481	16.857	14.289	18.516	10.959	13.213	34.047	21.760	31.975
144.1383	0.929	0.691	0.535	9.601	6.301	7.589	0.781	0.410	0.668
148.9756	3.144	6.908	3.802	4.237	4.668	7.049	2.872	2.814	8.808
149.0026	43.735	21.255	18.548	53.391	18.030	21.279	24.006	19.510	26.110
151.0541	0.000	0.259	0.627	0.000	1.354	1.861	0.000	2.216	3.579
151.0971	0.965	0.783	0.594	0.545	0.538	0.627	0.732	0.544	0.867
152.9974	7.705	15.315	12.723	11.253	11.632	13.879	9.616	12.353	16.311
155.0299	7.231	4.112	3.000	8.916	3.176	4.331	8.659	2.820	4.622
156.0766	0.311	0.098	0.118	0.181	1.705	1.842	0.417	0.132	0.204
158.1175	0.404	0.241	0.087	0.229	0.106	0.156	1.455	0.874	1.186
158.1539	5.131	3.599	3.473	42.927	27.603	35.305	5.768	3.476	5.557
167.0130	29.913	21.806	19.312	42.521	17.182	21.018	18.762	16.264	22.823

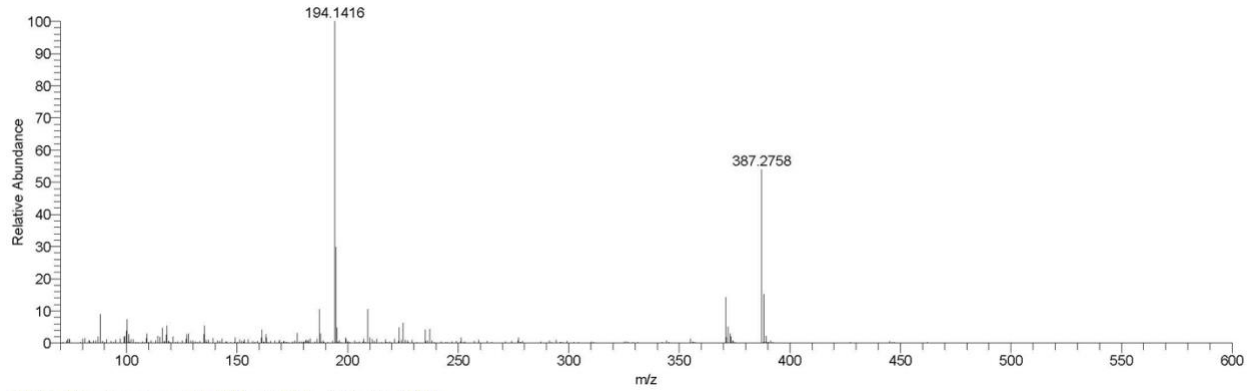
170.1539	0.468	0.316	0.297	0.692	0.331	0.643	1.439	0.496	1.883
172.1692	1.213	1.025	1.047	40.483	28.069	36.687	19.447	13.831	22.302
174.1605	1.969	1.674	1.543	0.808	0.464	0.640	0.013	0.090	0.059
180.1272	0.934	0.985	1.381	2.615	0.788	2.609	4.147	3.283	3.218
181.0289	10.658	5.063	3.944	4.246	4.329	5.028	13.483	3.309	4.540
181.0453	0.141	0.384	0.901	0.138	1.376	2.473	0.217	1.934	2.786
186.1276	4.075	7.167	3.787	36.859	17.513	8.811	18.041	31.881	37.636
186.1277	8.532	3.952	5.938	9.315	21.347	26.559	50.975	11.999	38.745
186.1855	0.100	0.057	0.053	7.632	1.928	6.090	0.558	1.122	1.624
189.0335	0.109	0.869	2.563	0.071	7.093	10.390	0.035	8.807	14.455
193.1356	1.788	1.387	0.265	13.241	6.099	8.246	14.637	11.186	14.036
193.1360	2.220	0.457	0.260	7.844	3.287	1.469	5.621	0.379	2.955
199.0942	4.391	1.553	4.444	3.434	1.263	4.570	8.334	1.342	2.830
200.1253	0.105	0.591	0.506	10.802	8.283	12.192	2.029	2.064	3.297
200.1254	0.526	0.591	0.506	12.012	5.464	11.487	1.936	2.064	3.386
201.0442	0.091	0.094	0.171	1.415	1.393	1.849	1.558	1.453	2.193
201.1500	1.593	1.128	0.353	5.549	2.594	1.639	3.289	2.086	2.448
201.1508	1.643	0.077	0.242	2.504	0.947	1.852	3.361	0.365	1.040
207.0443	0.072	0.408	0.798	0.101	2.305	3.944	0.136	1.785	4.770
213.1099	32.693	41.099	54.816	20.652	18.685	25.870	17.252	41.486	12.591
214.1134	0.608	4.151	3.695	8.954	4.373	2.548	1.839	4.104	2.031
216.0431	0.000	0.000	0.000	0.365	0.142	0.198	3.125	1.704	2.444
216.1569	0.073	1.192	0.879	2.957	2.052	2.299	0.011	1.955	2.712
216.1959	9.662	7.719	6.427	3.031	3.910	2.184	0.450	0.797	1.388
216.1962	0.269	8.105	6.633	6.259	1.801	5.441	0.239	0.797	1.388
219.1357	0.179	0.173	0.375	10.339	4.501	8.786	0.492	0.293	0.820
224.1539	0.256	1.021	1.030	3.122	5.307	7.462	4.938	3.532	5.976
229.1985	3.874	2.783	2.540	11.518	6.751	9.539	18.929	13.287	20.405
230.2113	45.103	33.506	25.683	35.586	13.878	6.021	3.387	14.406	23.443
230.2113	41.613	3.440	0.391	19.957	5.019	27.799	6.640	3.976	5.831
230.2116	35.774	9.463	4.067	8.912	21.184	17.021	19.014	2.677	8.316
232.1524	0.059	0.171	0.095	1.991	0.449	0.557	0.085	0.220	0.289
235.0928	1.931	0.782	0.667	2.213	0.581	0.935	2.390	0.578	1.001
240.1955	2.124	1.448	1.377	1.694	0.929	0.249	3.002	1.609	3.477
242.2830	3.803	0.072	1.222	5.874	0.063	0.916	324.881	212.834	358.452
244.1908	4.354	3.305	3.033	3.190	2.367	7.705	6.866	5.341	24.076
244.1909	0.193	2.637	2.319	8.597	6.009	2.590	20.361	15.593	7.957
244.2268	6.883	22.296	4.917	91.322	25.048	71.450	46.134	68.169	168.396
244.2270	36.450	27.869	23.256	80.592	56.830	33.658	139.165	30.407	50.558
244.2271	18.463	13.233	12.061	32.359	47.246	63.846	25.941	107.265	147.217
245.1883	5.426	2.043	1.149	8.789	1.928	1.033	1.017	2.866	3.632

247.0756	8.402	4.652	3.781	11.253	3.819	4.663	12.009	2.210	5.456
254.2111	0.302	0.126	0.143	0.995	0.192	0.109	7.004	4.500	7.220
256.2269	11.987	46.881	45.641	139.518	88.195	29.752	448.349	325.985	509.560
256.2270	11.987	8.139	18.135	35.645	23.049	112.926	94.704	66.141	368.145
258.2068	1.844	26.814	25.124	23.323	13.409	6.712	4.309	17.925	28.931
259.2076	13.753	0.404	0.564	1.954	0.565	0.289	1.062	0.318	0.725
259.2454	8.178	4.194	2.939	62.951	23.810	31.293	77.747	41.737	89.402
259.6726	0.048	0.237	0.256	3.321	2.383	2.027	16.244	11.602	17.638
260.2224	11.367	7.710	6.315	7.869	4.004	5.017	2.935	1.786	3.288
260.2487	0.187	0.545	0.210	0.343	2.942	4.598	0.516	1.039	8.262
261.0914	5.016	1.535	1.396	7.632	1.571	1.922	3.053	1.668	1.526
270.2428	2.290	1.340	1.398	7.779	4.675	5.728	24.366	22.203	22.171
270.3152	19.125	12.958	9.396	16.507	7.689	13.256	17.929	12.297	16.884
272.2217	14.888	11.080	9.676	15.551	9.744	12.936	41.945	26.808	43.752
273.1904	1.936	0.710	1.231	0.821	0.295	1.851	4.477	0.824	0.625
273.2177	1.913	0.282	0.571	1.351	0.527	1.229	0.747	0.444	1.677
273.2252	2.726	2.281	2.474	3.305	3.723	3.714	9.201	4.462	9.844
273.2617	2.282	0.203	0.751	34.493	21.662	0.385	89.116	0.800	110.284
274.2370	4.639	1.112	0.221	31.875	17.750	22.624	15.687	8.082	15.298
281.1882	0.077	0.032	0.041	0.048	0.145	0.245	0.944	0.035	0.163
282.2791	5.876	3.852	3.562	4.019	2.236	2.815	0.036	0.067	0.123
286.2381	0.674	0.766	0.327	10.925	6.602	7.868	10.193	7.230	13.856
288.2179	6.298	4.589	3.592	0.206	1.347	1.996	0.591	3.651	4.030
288.2529	9.034	6.543	0.122	61.936	37.181	0.648	37.792	26.301	40.748
288.5204	0.613	0.413	0.301	3.639	3.029	3.205	3.934	3.220	4.900
289.2040	0.013	0.349	0.948	0.135	0.487	0.639	4.272	1.780	0.498
289.2561	1.327	0.929	0.973	13.767	7.072	9.935	6.955	4.540	6.417
293.1343	0.012	0.116	0.095	4.578	0.837	2.240	3.889	1.703	2.645
296.2948	0.192	1.050	0.651	2.899	0.415	1.753	0.318	0.052	0.102
299.1612	6.945	5.493	8.938	6.901	3.370	3.356	5.495	1.861	1.350
302.2324	1.471	0.258	0.277	1.261	0.276	0.139	2.265	0.110	0.724
302.2694	0.194	0.034	0.101	3.142	0.276	0.308	0.150	0.196	0.232
306.2129	1.764	0.283	0.025	2.736	1.295	1.679	2.961	0.473	1.360
310.1655	1.184	3.631	0.609	0.408	0.244	0.126	5.171	1.333	1.983
313.1913	0.054	0.011	0.010	0.206	0.308	0.514	6.620	0.260	5.197
322.2371	0.080	0.125	0.145	2.227	0.927	1.352	2.684	1.251	4.133
324.2076	0.000	0.031	0.104	0.000	0.010	0.171	0.013	0.019	2.055
325.1336	7.176	3.407	0.108	1.576	0.122	0.000	0.000	0.000	0.000
344.2389	0.124	0.112	0.111	0.152	2.004	0.313	6.004	6.370	3.525
349.2278	0.354	0.173	0.546	2.744	0.054	2.382	0.142	0.251	0.075
366.3362	0.000	0.000	0.000	0.623	0.220	0.152	4.202	0.190	0.694

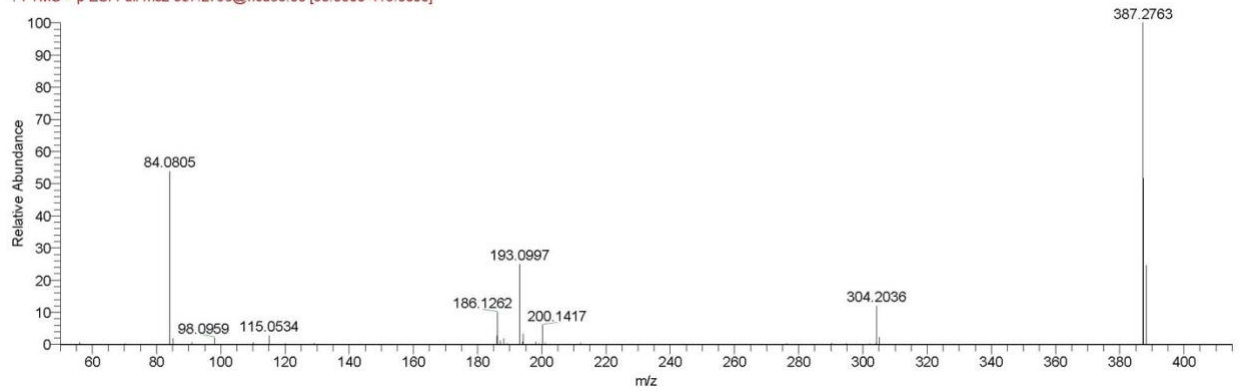
367.3323	3.057	0.411	2.091	6.011	3.467	4.374	0.116	0.084	0.184
381.3479	0.131	0.387	0.356	6.180	1.239	0.187	0.070	0.116	0.184
432.2771	0.684	0.637	0.568	6.401	4.587	6.950	5.447	4.606	8.354
451.3899	0.067	0.101	0.040	0.000	0.149	0.110	10.884	4.438	6.723
373.2638, 187.1359	44.100	41.468	36.693	52.606	37.050	46.629	90.543	75.096	103.226
387.2795, 194.1415	942.501	872.394	815.170	1891.060	1524.384	1759.488	2670.708	2308.580	2858.175
399.2822, 200.1446	45.905	33.176	30.042	97.719	60.264	76.876	87.888	58.198	94.319
401.2587, 201.1284	5.141	5.290	3.694	26.461	17.515	25.144	33.295	24.223	40.417
403.2740, 202.1410	46.761	41.434	37.410	222.112	151.634	201.371	278.414	206.729	310.481
415.2749, 208.1415	8.236	7.163	5.850	41.007	25.798	37.216	15.961	11.667	18.680
417.2537, 209.1308	4.012	3.265	2.624	1.622	0.904	1.001	2.186	1.400	2.278
419.2693, 210.1383	0.441	0.362	0.322	3.804	3.460	5.039	5.237	4.932	8.298
130.1595	90.164	69.670	54.757	89.153	55.952	81.086	91.112	63.845	102.822
200.2363	110.668	82.611	73.881	122.000	75.040	107.166	113.176	79.865	135.593
228.1967	46.077	32.804	28.658	108.946	69.950	87.033	161.838	113.509	178.310
242.2115 isomer	55.703	39.533	32.039	107.643	65.919	79.901	213.728	149.076	250.758
242.2115 isomer	35.687	25.427	22.774	59.843	38.608	51.578	136.577	93.104	156.852
242.2115 isomer	196.865	155.823	133.270	317.947	206.694	258.134	748.534	546.598	843.107
258.2437	67.182	47.603	38.916	505.039	313.575	413.151	674.147	474.522	773.172
272.2574	43.757	30.395	28.012	234.213	143.189	195.592	625.380	412.413	681.683

S10: MS/MS spectra for: 1) m/z 387, 2) m/z 403, 3) m/z 419, 4) m/z 228, 5) m/z 242-1, 6) m/z 242-2, 7) m/z 242-3, 8) m/z 258, and 9) m/z 272

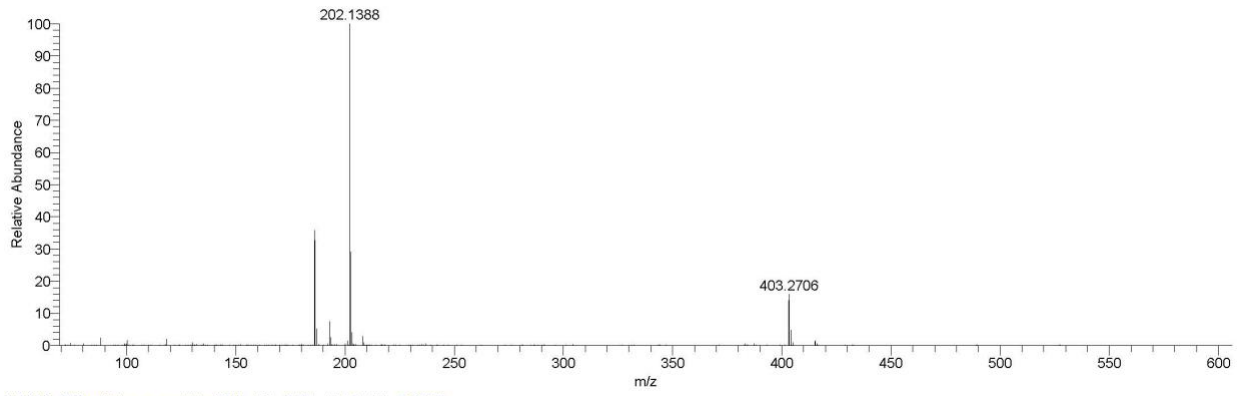
S10-1) m/z 387



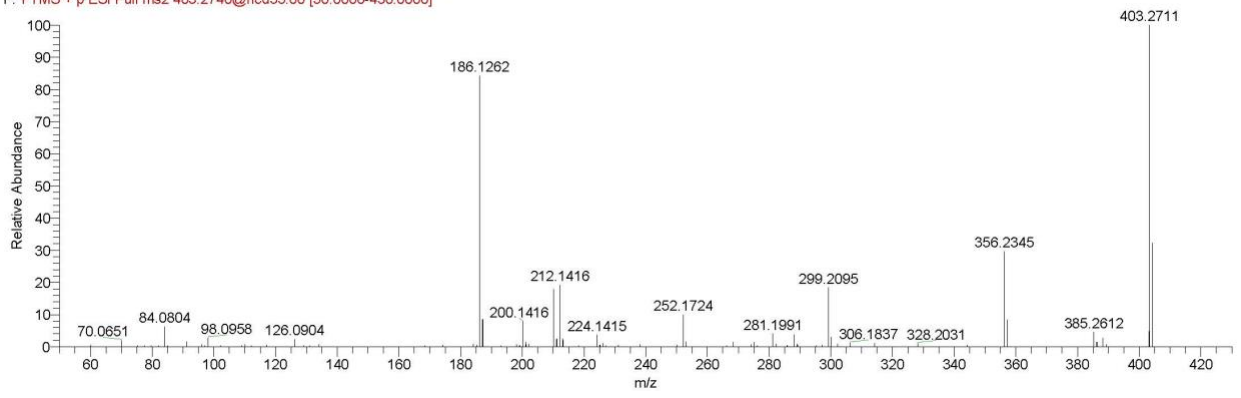
041919_479multiplexprmandda#900 RT: 2.01 AV: 1 NL: 5.11E8
=: FTMS + p ESI Full ms2 387.2795@hcd35.00 [50.0000-415.0000]



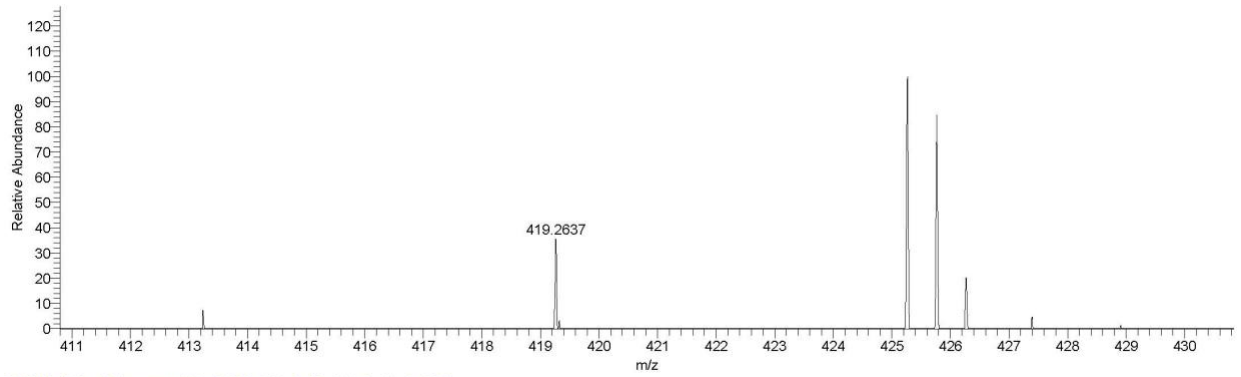
S10-2) m/z 403



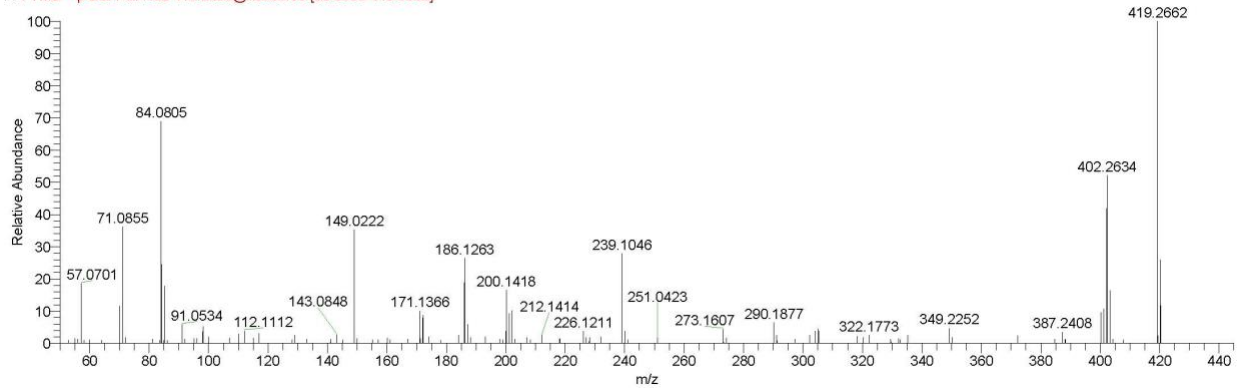
041919_479multiplexprmandda#919 RT: 2.05 AV: 1 NL: 6.85E6
F: FTMS + p ESI Full ms2 403.2740@hcd35.00 [50.0000-430.0000]



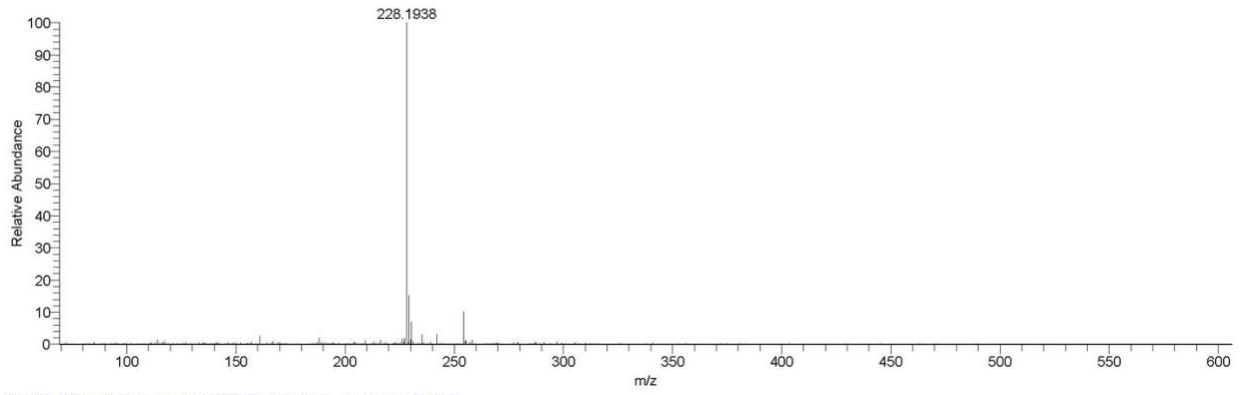
S10-3) m/z 419



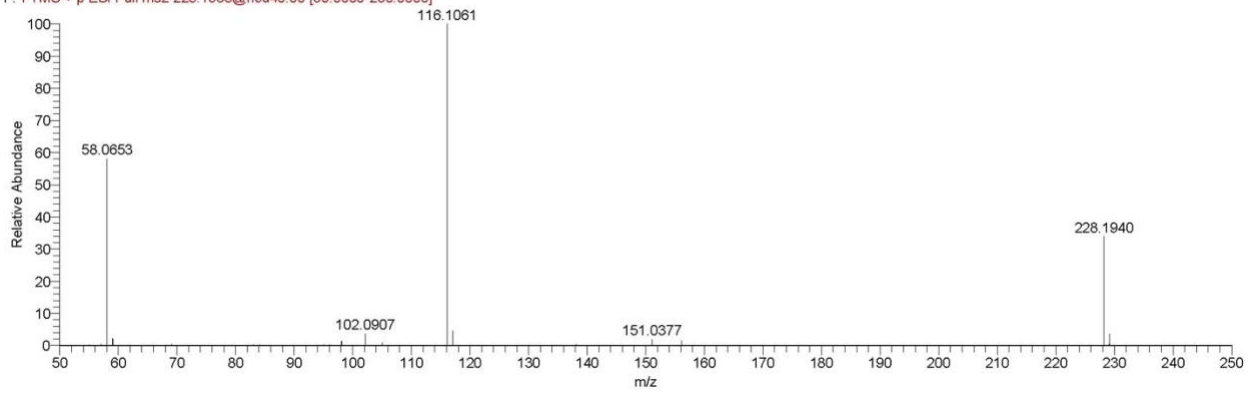
041919_479multiplexprmandda2#972 RT: 2.15 AV: 1 NL: 1.80E5
F: FTMS + p ESI Full ms2 419.2693@hed35.00 [50.0000-445.0000]



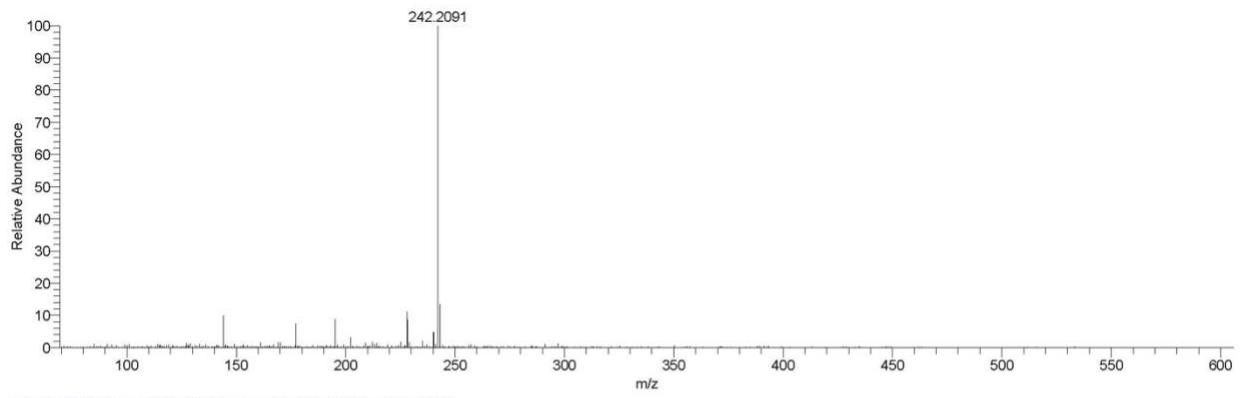
S10-4) m/z 228



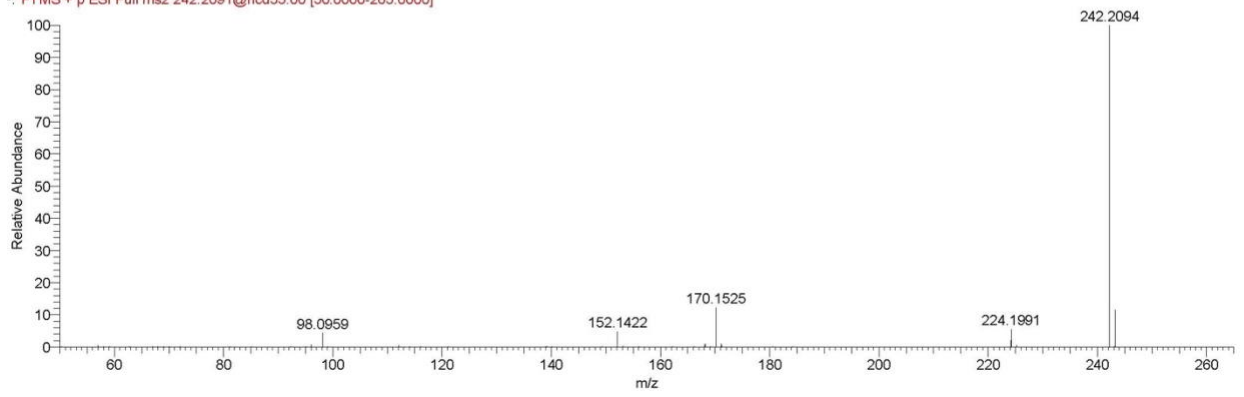
041919_479multiplexprmandda2#1170 RT: 2.52 AV: 1 NL: 5.19E7
F: FTMS + p ESI Full ms2 228.1938@hcd40.00 [50.0000-250.0000]



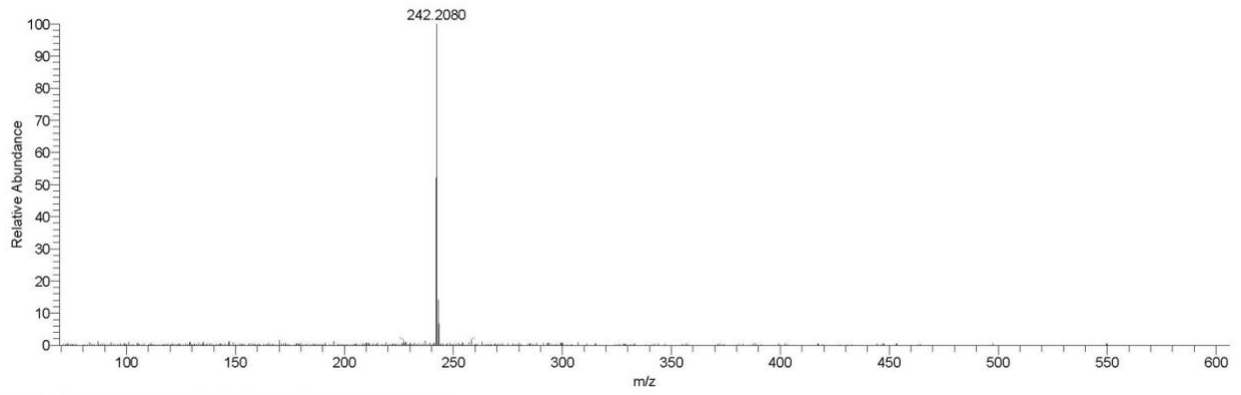
S10-5) m/z 242



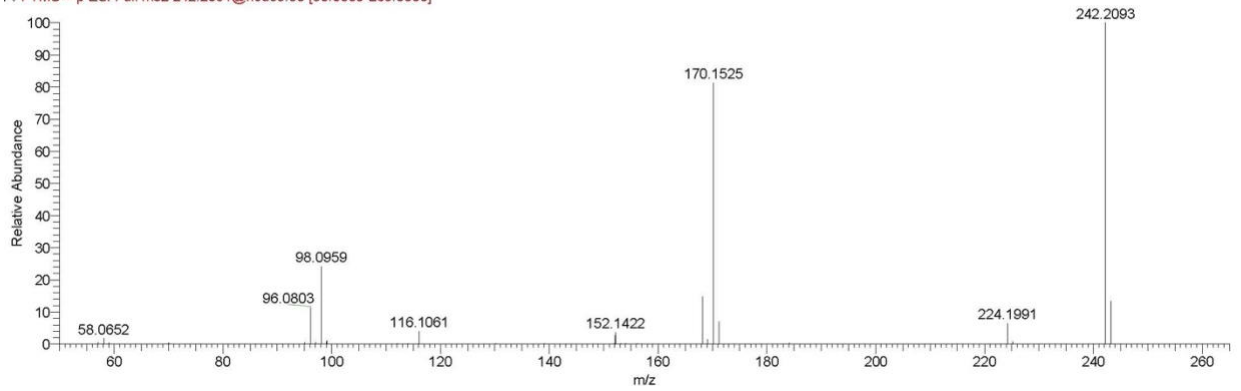
J41919_479multiplexprmanddda #1134 RT: 2.48 AV: 1 NL: 1.57E8
=: FTMS + p ESI Full ms2 242.2091@hcd35.00 [50.0000-265.0000]



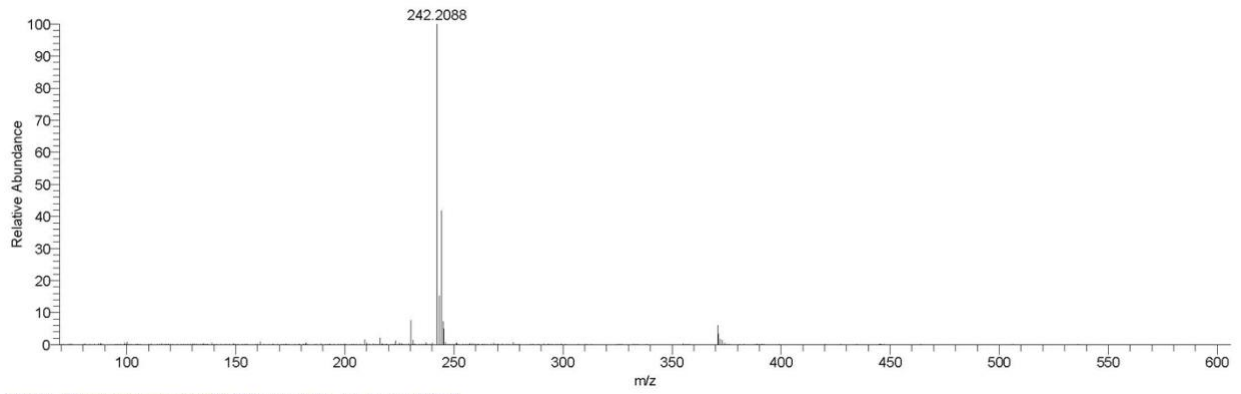
S10-6) m/z 242



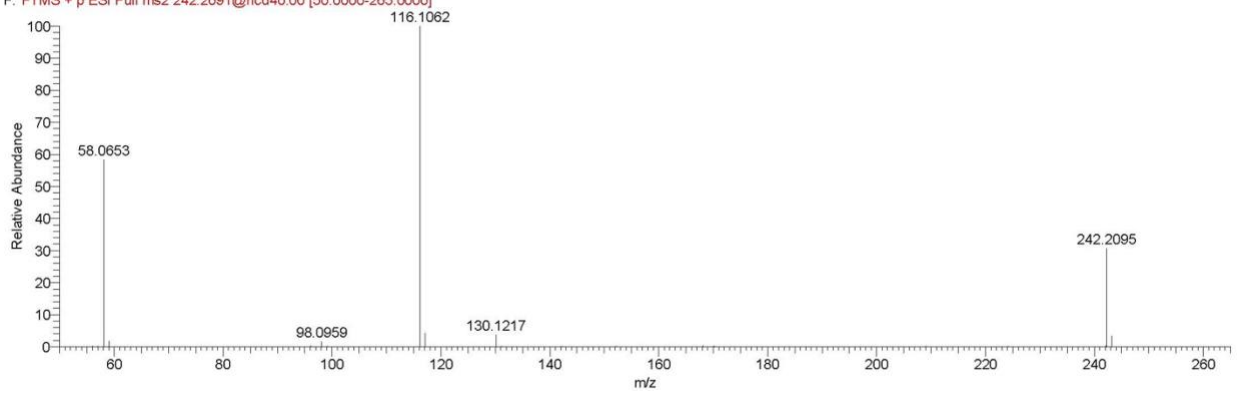
041919_479multiplexprmandda#1166 RT: 2.52 AV: 1 NL: 5.31E7
F: FTMS + p ESI Full ms2 242.2091@hcd35.00 [50.0000-265.0000]



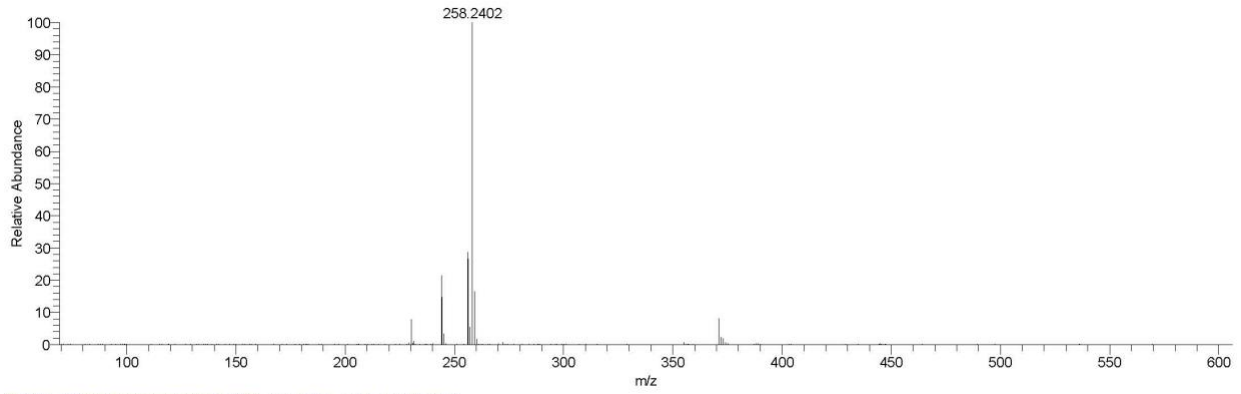
S10-7) m/z 242



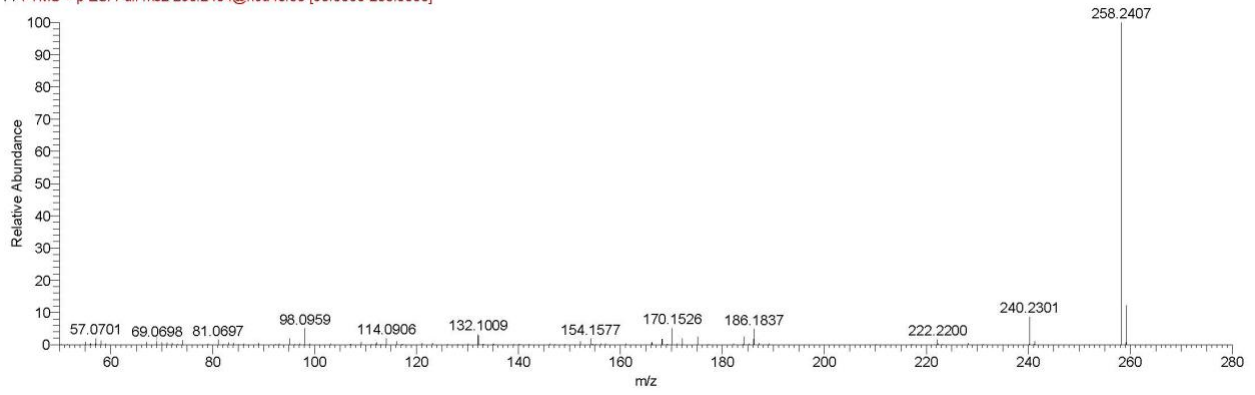
041919_479multiplexprmandda2#1207 RT: 2.57 AV: 1 NL: 1.25E8
F: FTMS + p ESI Full ms2 242.2091@hcd40.00 [50.0000-265.0000]



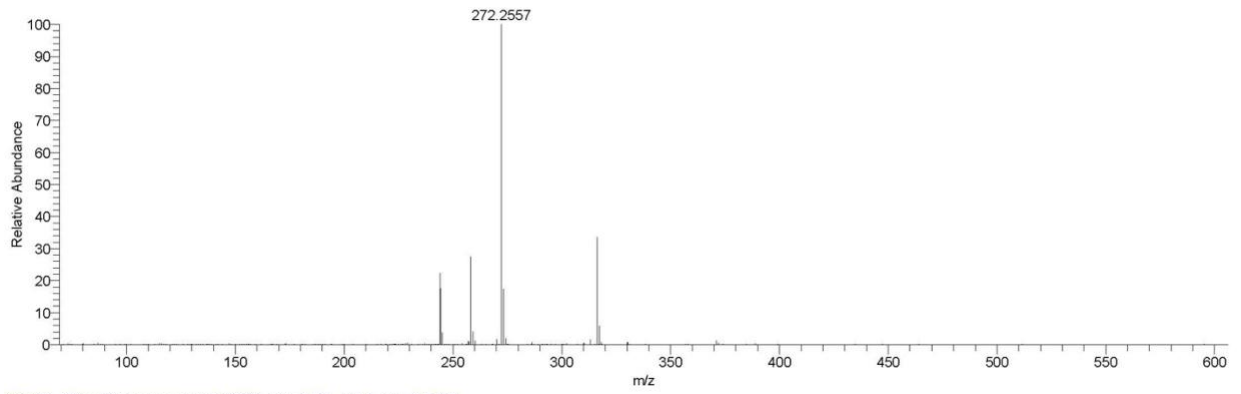
S10-8) m/z 258



041919_479multiplexprmanddda3#1215 RT: 2.63 AV: 1 NL: 7.92E6
F: FTMS + p ESI Full ms2 258.2404@hcd40.00 [50.0000-280.0000]



S10-9) m/z 272



041919_479multiplexprmanddda2#1295 RT: 2.72 AV: 1 NL: 2.50E7
F: FTMS + p ESI Full ms2 272.2558@hcd40.00 [50.0000-295.0000]

