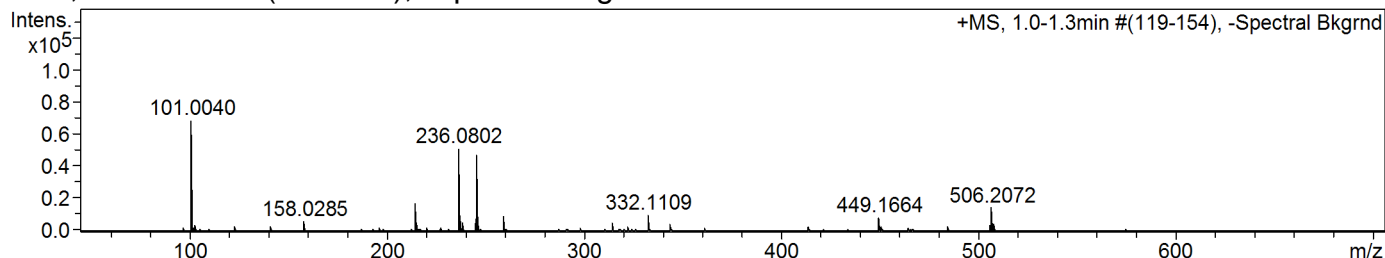


# Confirmation of Expected Formula

Sample-ID rslc20\_rslc-5-082  
 Analysis Name rslc20\_rslc-5-082\_352881\_16\_01\_58459.d  
 Method used Confirm Formula Positive 50to500 loop inj.m  
 Ionisation Mode positive electrospray (ESI)

Submitter rslc20 Robert Chapman  
 Supervisor  
 Acquisition Date 17/08/2017 14:28:44

## +MS, 1.0-1.3min #(119-154), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	101.0040	68697	100.0	1557	10216.9
2	158.0285	6052	8.8	171	1128.1
3	214.0905	17280	25.2	673	1033.5
4	236.0802	51029	74.3	1817	1867.6
5	237.0776	8732	12.7	218	314.1
6	245.1357	47170	68.7	2233	1592.1
7	259.1020	8814	12.8	217	381.1
8	332.1109	9928	14.5	575	560.3
9	449.1664	8225	12.0	445	822.5
10	506.2072	14297	20.8	1270	1269.2

## Generate Molecular Formula Parameters

Charge	Tolerance	SearchRadius	H/C Ratio min.	H/C Ratio max.	Electron Conf.	Nitrogen Rule	sigma limit
positive	10 ppm	0.05 m/z	0	3	both	true	0.05

**Expected Formula** C25 H28 B1 F2 N3 O4

**Adduct(s):** H, Na

#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	484.2252	484.2218	6.90	0.0363	C 25 H 29 B 1 F 2 N 3 O 4
1	506.2072	506.2038	6.90	0.0056	C 25 H 28 B 1 F 2 N 3 Na 1 O 4

Note: Sigma fits < 0.05 indicates high probability of correct MF, and mass accuracy of 5ppm or better is generally acceptable for publication