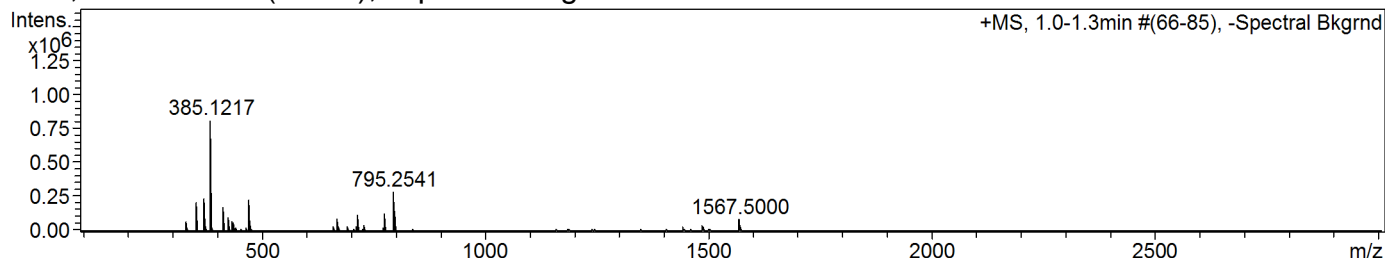


Confirmation of Expected Formula

Sample-ID ug_ja_mo_MLO162 Submitter mlo22 Maria Odyniec
 Analysis Name ug_ja_mo_MLO162_352876_12_01_58452.d Supervisor - Tony James
 Method used Confirm Formula Positive 50to1500 loop inj.m Acquisition Date 17/08/2017 12:15:17
 Ionisation Mode positive electrospray (ESI)

+MS, 1.0-1.3min #(66-85), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	353.0860	205327	25.3	7363	1831.2
2	371.0981	242031	29.9	9750	2027.4
3	385.1217	810266	100.0	28424	6480.8
4	386.1149	164379	20.3	6879	1313.1
5	412.1237	151586	18.7	6553	1343.1
6	413.1108	167809	20.7	6500	1493.0
7	471.1874	228125	28.2	11782	2687.4
8	773.2674	120894	14.9	9361	1179.0
9	795.2541	286885	35.4	20931	3032.8
10	796.2523	143679	17.7	11737	1525.0

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 C40 H41 B O15

Adduct(s): H, Na

#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	773.2674	773.2618	7.20	0.0163	C 40 H 42 B 1 O 15

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