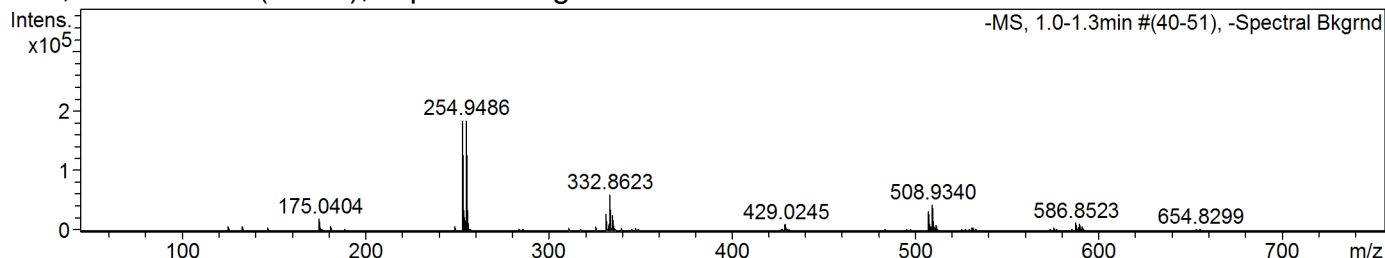


Confirmation of Expected Formula

Sample-ID ug_ja_mo_mlo381 Submitter mlo22 Maria Odyniec
 Analysis Name ug_ja_mo_mlo381_358868_72_01_65293.d Supervisor - Tony James
 Method used Confirm Formula Negative 50to500 loop inj.m Acquisition Date 19/09/2018 14:26:30
 Ionisation Mode negative electrospray (ESI)

-MS, 1.0-1.3min #(40-51), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	175.0404	20260	11.0	694	4252.8
2	252.9507	184708	99.8	9616	6404.2
3	253.9657	25367	13.7	1833	861.4
4	254.9486	184990	100.0	9276	6158.3
5	255.9520	19987	10.8	1014	652.3
6	330.8606	28852	15.6	1638	1161.5
7	332.8623	60747	32.8	4062	2360.7
8	334.8647	26598	14.4	1709	999.0
9	506.9343	33709	18.2	3396	1137.5
10	508.9340	43871	23.7	4454	1517.8

Generate Molecular Formula Parameters

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

Expected Formula C₁₀ H₇ Br O₃

Adduct(s): H, Na

#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	252.9507	252.9506	0.50	0.0148	C ₁₀ H ₆ Br O ₃

Note: Sigma fits < 0.05 indicates high probability of correct MF.

For formula confirmation the mass error / accuracy at 200 Da should be better than 25 ppm, for 500 Da better than 10 ppm and for 1000 Da better than 5 ppm