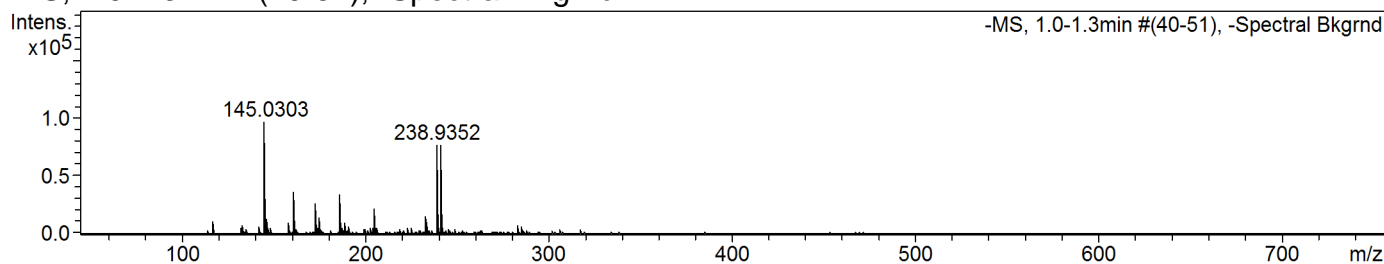


Confirmation of Expected Formula

Sample-ID	ug_ja_mo_mlo344	Submitter	mlo22 Maria Odyniec
Analysis Name	ug_ja_mo_mlo344_357798_68_01_64124.d	Supervisor	- Tony James
Method used	Confirm Formula Negative 50to500 loop inj.m	Acquisition Date	13/07/2018 11:52:42
Ionisation Mode	negative electrospray (ESI)		

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



#	m/z	I	I %	Area	S/N
1	145.0303	96399	100.0	2956	3667.3
2	146.0344	12377	12.8	373	456.9
3	161.0255	36134	37.5	1244	925.2
4	173.0250	25646	26.6	947	618.5
5	175.0410	13396	13.9	457	322.1
6	186.0202	33513	34.8	1332	792.2
7	205.0499	21011	21.8	880	482.7
8	233.0465	14824	15.4	704	256.0
9	238.9352	76849	79.7	3753	1247.7
10	240.9328	76627	79.5	3728	1219.4

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 C14 H12 O6 **Adduct(s):** H, Na

#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
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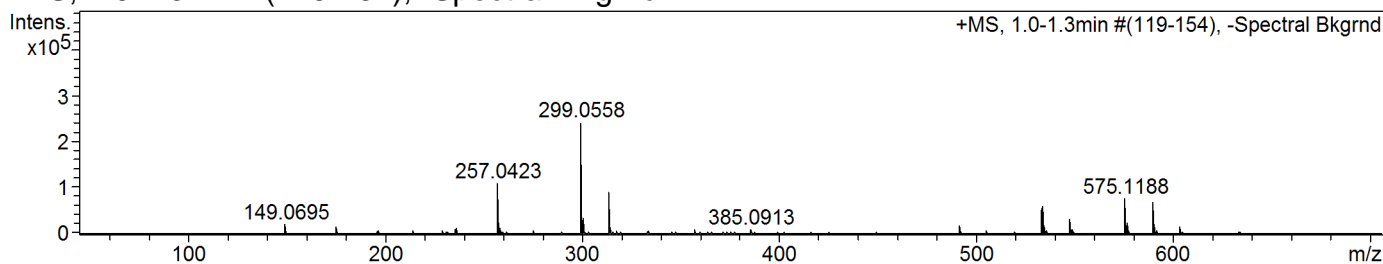
Note: Sigma fits < 0.05 indicates high probability of correct MF.

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

Confirmation of Expected Formula

Sample-ID	ug_ja_mo_mlo344	Submitter	mlo22 Maria Odyniec
Analysis Name	ug_ja_mo_mlo344_357798_68_01_64128.d	Supervisor	- Tony James
Method used	Confirm Formula Positive 50to500 loop inj.m	Acquisition Date	13/07/2018 12:09:54
Ionisation Mode	positive electrospray (ESI)		

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



#	m/z	I	I %	Area	S/N
1	257.0423	108338	44.8	5200	2753.3
2	299.0558	241735	100.0	11729	5138.0
3	300.0598	35187	14.6	1636	750.5
4	313.0720	89396	37.0	4747	2000.4
5	533.1076	60385	25.0	5861	1487.6
6	547.1228	31170	12.9	3102	731.2
7	575.1188	76059	31.5	8277	1363.6
8	576.1222	23789	9.8	2525	422.4
9	589.1341	66979	27.7	7222	1060.8
10	590.1370	21041	8.7	2305	330.4

Generate Molecular Formula Parameters

Charge	Tolerance	SearchRadius	H/C Ratio min.	H/C Ratio max.	Electron Conf.	Nitrogen Rule	sigma limit
positive	25 ppm	0.05 m/z	0	3	both	true	0.05

Expected Formula C₁₄ H₁₂ O₆

Adduct(s): H, Na

#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	299.0558	299.0526	10.80	0.0049	C ₁₄ H ₁₂ Na ₁ O ₆

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