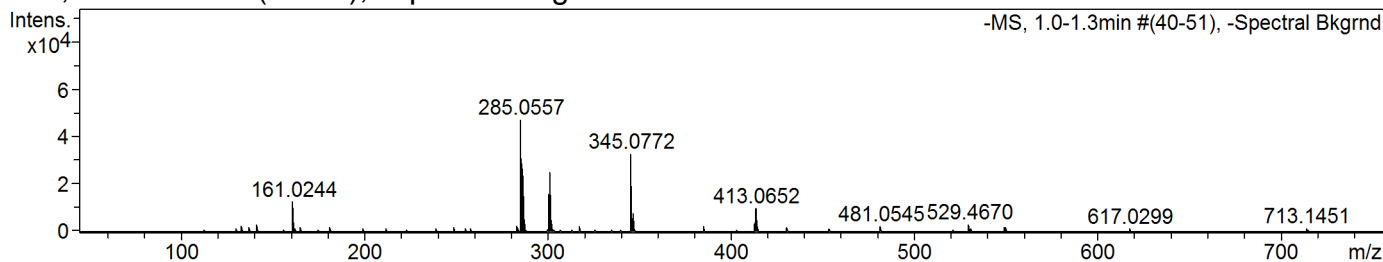


Confirmation of Expected Formula

Sample-ID	ug_ja_mo_mlo330	Submitter	mlo22 Maria Odyniec
Analysis Name	ug_ja_mo_mlo330_357543_18_01_63804.d	Supervisor	- Tony James
Method used	Confirm Formula Negative 50to500 loop inj.m	Acquisition Date	11/06/2018 09:56:48
Ionisation Mode	negative electrospray (ESI)		

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



#	m/z	I	I %	Area	S/N
1	161.0244	12601	26.9	398	7749.9
2	285.0557	46889	100.0	2381	4197.9
3	286.0614	29001	61.8	1494	2519.1
4	287.0657	5250	11.2	252	442.9
5	300.0796	16061	34.3	820	986.1
6	301.0859	25183	53.7	1298	1514.2
7	302.0901	5002	10.7	252	294.7
8	345.0772	32665	69.7	1940	3495.0
9	346.0811	7768	16.6	440	851.1
10	413.0652	9733	20.8	680	2409.1

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	C21 H14 O5	Adduct(s):	H, Na
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#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	345.0772	345.0768	1.10	0.0064	C 21 H 13 O 5

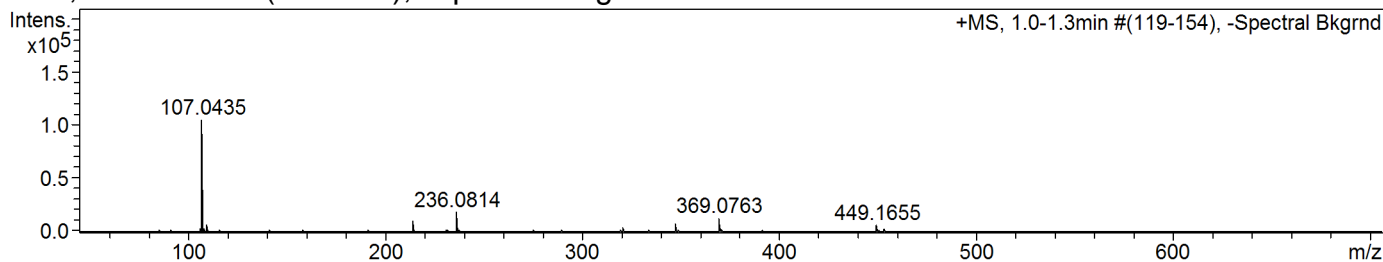
Note: Sigma fits < 0.05 indicates high probability of correct MF.

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_mlo330	Submitter	mlo22 Maria Odyniec
Analysis Name	ug_ja_mo_mlo330_357543_18_01_63806.d	Supervisor	- Tony James
Method used	Confirm Formula Positive 50to500 loop inj.m	Acquisition Date	11/06/2018 10:06:50
Ionisation Mode	positive electrospray (ESI)		

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



#	m/z	I	I %	Area	S/N
1	106.0397	3028	2.9	38	507.9
2	107.0435	104487	100.0	1228	17101.8
3	108.0453	2891	2.8	32	462.1
4	109.0424	6036	5.8	79	942.7
5	214.0906	9851	9.4	374	1970.4
6	236.0814	18182	17.4	376	2728.3
7	320.1342	3870	3.7	80	646.3
8	347.0954	7080	6.8	375	1014.7
9	369.0763	12482	11.9	752	1618.7
10	449.1655	6109	5.8	405	1310.6

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 C₂₁ H₁₄ O₅ **Adduct(s):** H, Na

#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	347.0954	347.0914	11.50	0.0243	C ₂₁ H ₁₅ O ₅
1	369.0763	369.0733	8.10	0.0130	C ₂₁ H ₁₄ Na O ₅

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