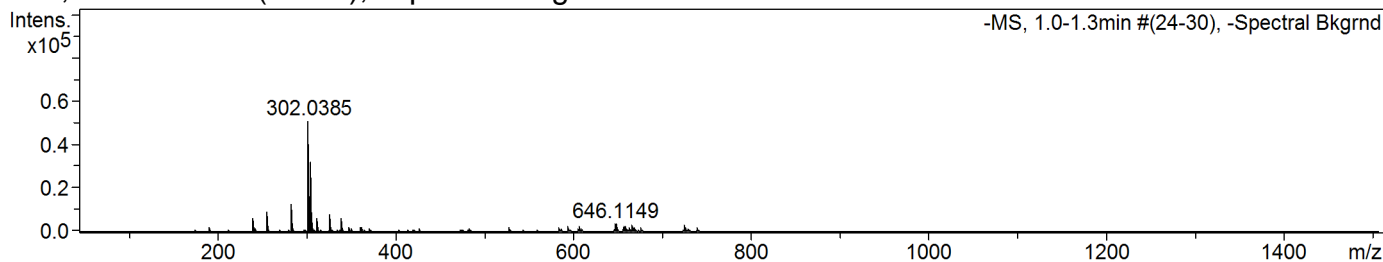


Confirmation of Expected Formula

Sample-ID	ug_ja_mo_mlo347	Submitter	mlo22 Maria Odyniec
Analysis Name	ug_ja_mo_mlo347_357865_39_01_64200.d	Supervisor	- Tony James
Method used	Confirm Formula Negative 50to1500 loop inj.m	Acquisition Date	18/07/2018 14:52:53
Ionisation Mode	negative electrospray (ESI)		

-MS, 1.0-1.3min #(24-30), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	240.0446	6273	12.3	165	868.0
2	255.1994	8840	17.3	267	941.5
3	283.2304	12765	25.0	382	953.3
4	302.0385	51049	100.0	2027	3808.5
5	303.0423	8198	16.1	294	613.9
6	304.0359	32022	62.7	1342	2406.8
7	305.0381	5500	10.8	203	415.0
8	311.1371	5864	11.5	164	452.8
9	325.1523	8169	16.0	284	666.9
10	339.1679	5835	11.4	220	505.2

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 C37 H42 B Cl2 N O7 **Adduct(s):** H, Na

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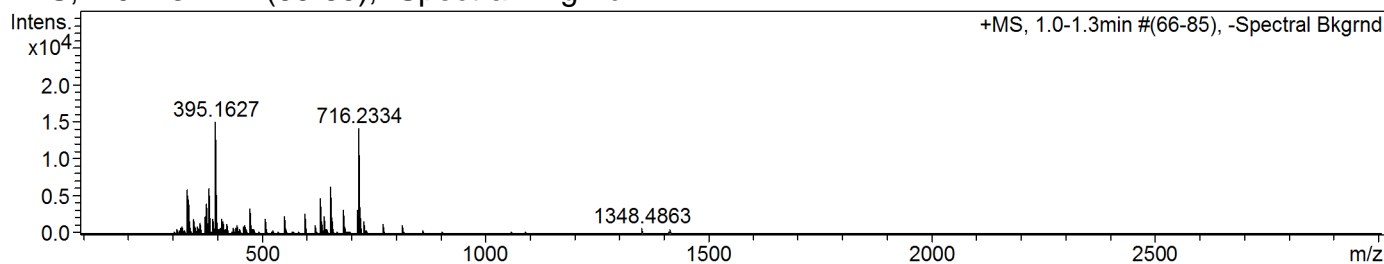
Note: Sigma fits < 0.05 indicates high probability of correct MF.

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_mlo347	Submitter	mlo22 Maria Odyniec
Analysis Name	ug_ja_mo_mlo347_357865_39_01_64205.d	Supervisor	- Tony James
Method used	Confirm Formula Positive 50to1500 loop inj.m	Acquisition Date	18/07/2018 15:13:24
Ionisation Mode	positive electrospray (ESI)		

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



#	m/z	I	I %	Area	S/N
1	333.1732	5932	39.6	255	1177.0
2	337.2026	4513	30.1	162	871.7
3	381.1092	6044	40.4	240	905.7
4	395.1627	14968	100.0	668	2228.2
5	397.1589	10973	73.3	478	1639.6
6	632.2587	4676	31.2	283	1057.0
7	654.2393	6310	42.2	360	1420.3
8	716.2334	14138	94.4	1036	3144.0
9	717.2333	7030	47.0	484	1563.2
10	718.2274	9487	63.4	675	2108.9

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 C37 H42 B Cl2 N O7 **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