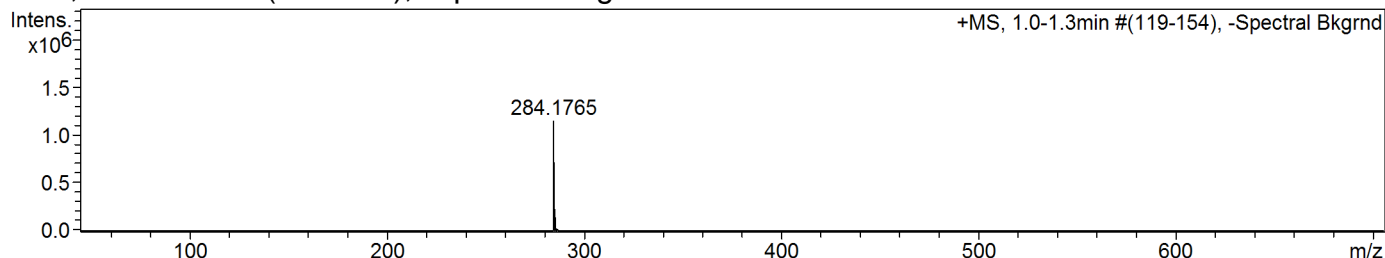


Confirmation of Expected Formula

Sample-ID ug_ja_mo_mlo440
Analysis Name ug_ja_mo_mlo440_360398_35_01_67246.d
Method used Confirm Formula Positive 50to500 loop inj.m
Ionisation Mode positive electrospray (ESI)

Submitter mlo22 Maria Odyniec
Supervisor - Tony James
Acquisition Date 26/04/2019 14:44:37

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



#	m/z	I	I %	Area	S/N
1	130.1619	4885	0.4	131	395.4
2	177.0549	6924	0.6	214	400.5
3	199.0370	7676	0.7	268	374.6
4	214.0953	4819	0.4	83	230.7
5	282.1616	5425	0.5	244	67.6
6	283.2189	4523	0.4	517	55.2
7	284.1765	1157647	100.0	68515	13942.7
8	285.1787	230705	19.9	12594	2729.2
9	286.1814	21294	1.8	1120	247.4
10	353.2680	6066	0.5	326	724.7

Generate Molecular Formula Parameters

Charge	Tolerance	SearchRadius	H/C Ratio min.	H/C Ratio max.	Electron Conf.	Nitrogen Rule	sigma limit
positive	50 ppm	0.05 m/z	0	3	both	true	0.05

Expected Formula C17 H19 N3 O

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

Sample concentration too high! Dilute sample by factor 1000.