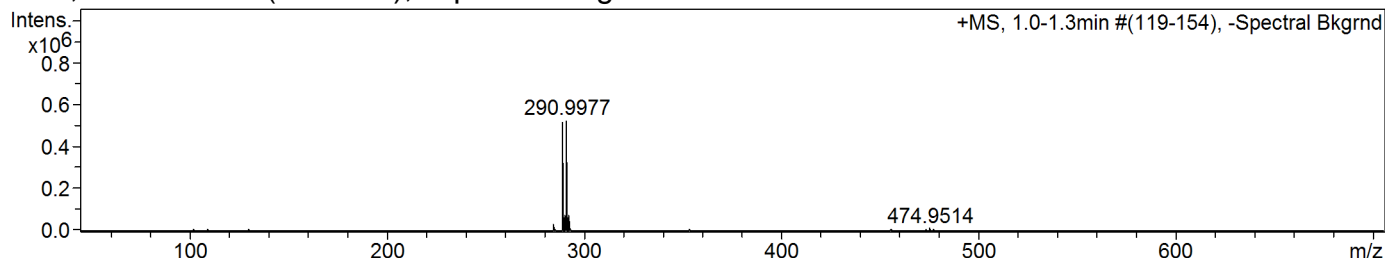


Confirmation of Expected Formula

Sample-ID ug_ja_mo_mlo434 Submitter mlo22 Maria Odyniec
 Analysis Name ug_ja_mo_mlo434_360397_34_01_67239.d Supervisor - Tony James
 Method used Confirm Formula Positive 50to500 loop inj.m Acquisition Date 26/04/2019 14:13:48
 Ionisation Mode positive electrospray (ESI)

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



#	m/z	I	I %	Area	S/N
1	109.0783	6756	1.3	136	737.8
2	284.1763	32370	6.2	1719	332.4
3	289.0000	518819	98.9	28368	5306.7
4	290.0021	76247	14.5	4065	797.7
5	290.9977	524552	100.0	29211	5617.6
6	291.9999	74314	14.2	3928	814.9
7	293.0107	16513	3.1	909	185.5
8	455.2185	7707	1.5	538	702.1
9	474.9514	13274	2.5	1100	1331.3
10	476.9506	6840	1.3	575	718.3

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 C13 H9 Br N2 O **Adduct(s):** H, Na

#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	289.0000	288.9971	10.10	0.0133	C 13 H 10 Br 1 N 2 O 1

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