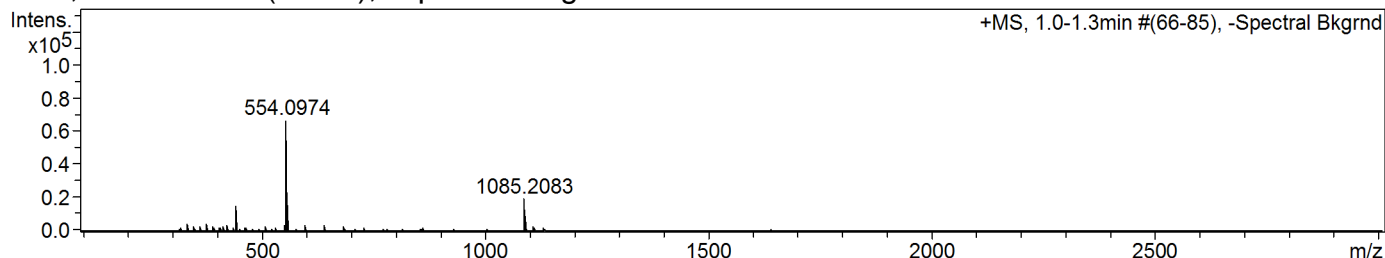


Confirmation of Expected Formula

Sample-ID ug_ja_mo_mlo386 Submitter mlo22 Maria Odyniec
 Analysis Name ug_ja_mo_mlo386_358973_87_01_65434.d Supervisor - Tony James
 Method used Confirm Formula Positive 50to1500 loop inj.m Acquisition Date 28/09/2018 15:14:05
 Ionisation Mode positive electrospray (ESI)

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



#	m/z	I	I %	Area	S/N
1	441.3030	15020	22.5	336	4533.7
2	554.0974	66662	100.0	3617	13949.8
3	555.1029	18900	28.4	981	3944.3
4	556.0984	19541	29.3	1134	4067.0
5	557.0978	5362	8.0	271	1112.9
6	1085.2083	19391	29.1	2225	5559.9
7	1086.2106	12040	18.1	1410	3428.4
8	1087.2068	16775	25.2	2005	4743.8
9	1088.2087	8951	13.4	1022	2514.0
10	1089.2065	4858	7.3	503	1355.1

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 C₂₉H₂₂ClN₇O Adduct(s): H, Na

#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	554.0974	554.0977	-0.60	0.0454	C ₂₉ H ₂₂ ClN ₇ O

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