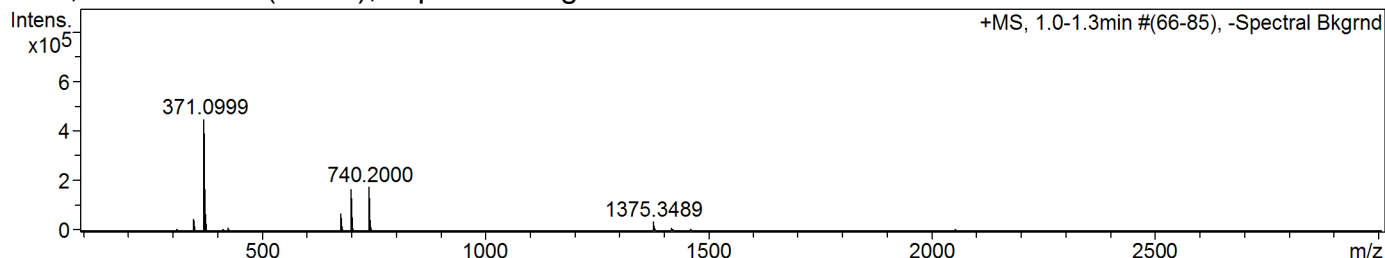


Confirmation of Expected Formula

Sample-ID krt23_37 Submitter krt23 Kate Turner
 Analysis Name krt23_37_356774_50_01_62884.d Supervisor - Tony James
 Method used Confirm Formula Positive 50to1500 loop inj.m Acquisition Date 17/04/2018 15:08:49
 Ionisation Mode positive electrospray (ESI)

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



#	m/z	I	I %	Area	S/N
1	347.0906	49205	11.0	1804	5624.7
2	371.0999	445409	100.0	14973	44675.9
3	372.0976	77406	17.4	3055	7724.7
4	677.1877	68593	15.4	4743	5840.6
5	699.1705	166956	37.5	10480	11827.1
6	700.1728	74922	16.8	5041	5267.0
7	740.2000	175661	39.4	11562	9472.6
8	741.1996	78957	17.7	5934	4233.2
9	1375.3489	36929	8.3	5374	6273.1
10	1376.3482	28976	6.5	4377	4947.0

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 C35 H32 O14

Adduct(s): H, Na

#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	677.1877	677.1865	1.90	0.0135	C 35 H 33 O 14
1	699.1705	699.1684	2.90	0.0310	C 35 H 32 Na 1 O 14

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