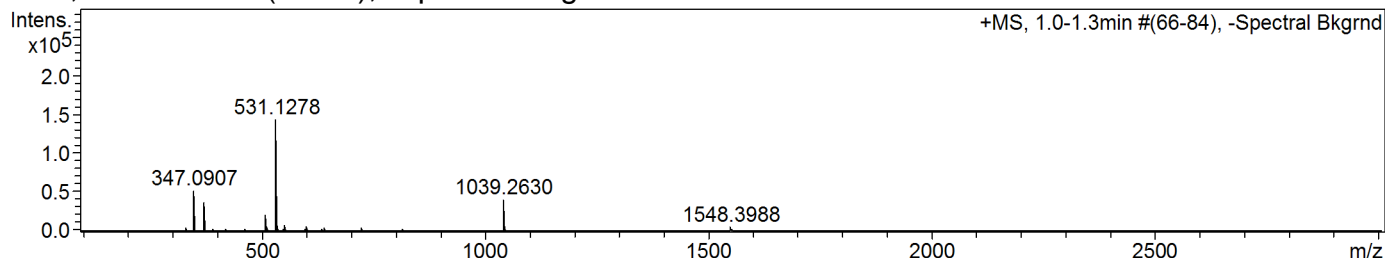


Confirmation of Expected Formula

Sample-ID krt23_38 Submitter krt23 Kate Turner
 Analysis Name krt23_38_356795_70_01_62909.d Supervisor - Tony James
 Method used Confirm Formula Positive 50to1500 loop inj.m Acquisition Date 18/04/2018 12:15:24
 Ionisation Mode positive electrospray (ESI)

+MS, 1.0-1.3min #(66-84), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	347.0907	51853	36.2	1806	18276.7
2	348.0938	8972	6.3	285	3143.0
3	369.0728	37619	26.3	1398	11674.8
4	509.1449	19956	13.9	928	3526.6
5	531.1278	143128	100.0	7317	23693.9
6	532.1296	39890	27.9	2395	6584.5
7	533.1330	8545	6.0	424	1406.4
8	551.3737	7883	5.5	122	1233.2
9	1039.2630	40281	28.1	4348	15688.9
10	1040.2663	21241	14.8	2488	8319.6

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 C27 H24 O10 Adduct(s): H, Na

#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	509.1449	509.1442	1.30	0.0340	C 27 H 25 O 10
1	531.1278	531.1262	3.00	0.0091	C 27 H 24 Na 1 O 10

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