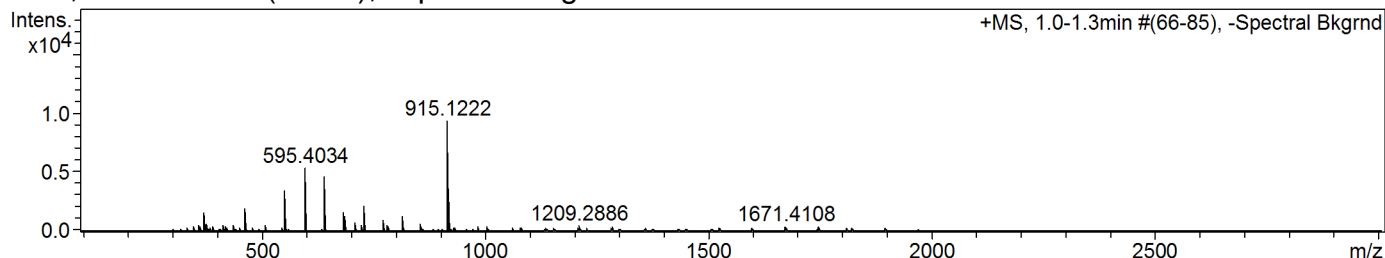


# Confirmation of Expected Formula

Sample-ID krt23\_8 Submitter krt23 Kate Turner  
 Analysis Name krt23\_8\_356012\_5\_01\_61998.d Supervisor - Tony James  
 Method used Confirm Formula Positive 50to1500 loop inj.m Acquisition Date 23/02/2018 12:29:24  
 Ionisation Mode positive electrospray (ESI)

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



#	m/z	I	I %	Area	S/N
1	371.0999	1539	16.4	36	2548.3
2	463.3021	1872	20.0	26	2593.2
3	551.3822	3391	36.2	56	4234.6
4	595.4034	5308	56.6	96	6027.0
5	639.4133	4547	48.5	78	4397.9
6	683.4383	1590	17.0	43	1338.7
7	727.4601	2106	22.5	46	1570.4
8	728.4853	1786	19.1	36	1328.8
9	915.1222	9371	100.0	922	4262.8
10	916.1195	3603	38.4	300	1635.4

## 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 C40 H32 N2 O20 S Adduct(s): H, Na

#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	915.1222	915.1161	6.60	0.0433	C 40 H 32 N 2 Na 1 O 20 S 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