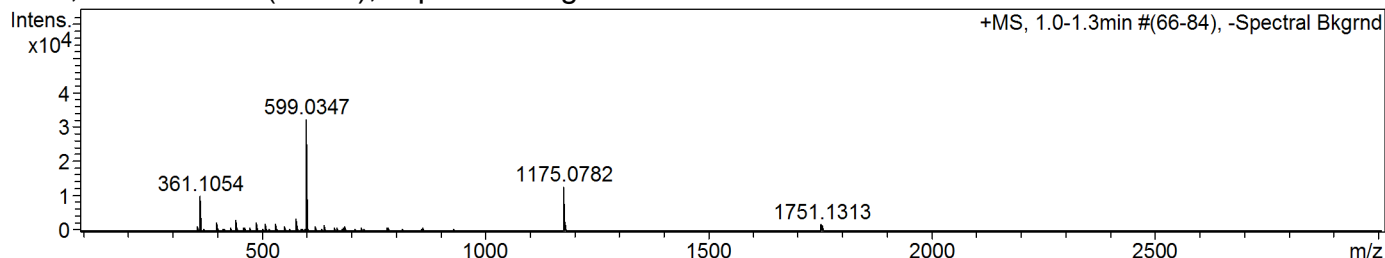


Confirmation of Expected Formula

Sample-ID krt23_31 Submitter krt23 Kate Turner
 Analysis Name krt23_31_356640_24_01_62740.d Supervisor - Tony James
 Method used Confirm Formula Positive 50to1500 loop inj.m Acquisition Date 10/04/2018 16:55:02
 Ionisation Mode positive electrospray (ESI)

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



#	m/z	I	I %	Area	S/N
1	361.1054	9948	30.9	379	9475.3
2	399.3085	2361	7.3	86	1734.9
3	443.3348	3161	9.8	126	1680.9
4	487.3625	2436	7.6	119	1015.1
5	577.0555	3397	10.6	167	982.2
6	599.0347	32159	100.0	1815	9729.6
7	600.0390	8284	25.8	412	2513.6
8	1175.0782	12793	39.8	1338	11148.7
9	1176.0906	6655	20.7	710	5830.6
10	1177.0940	2367	7.4	289	2084.7

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 H16 N2 O11 S Adduct(s): H, Na

#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	577.0555	577.0548	1.30	0.0479	C 27 H 17 N 2 O 11 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