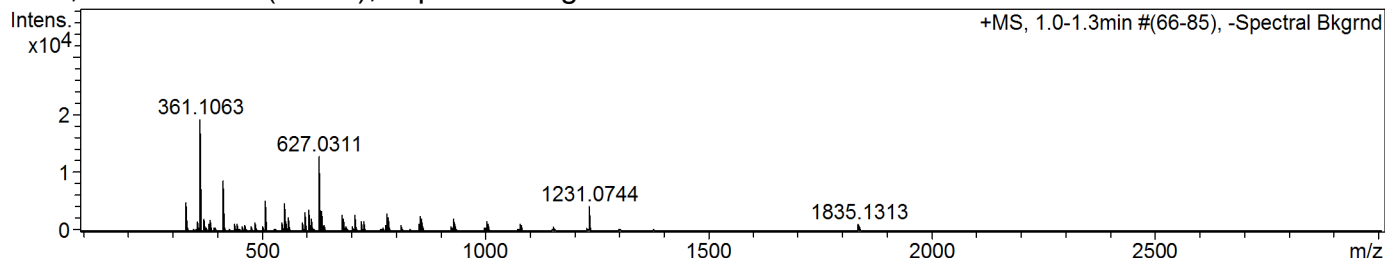


Confirmation of Expected Formula

Sample-ID krt23_36 Submitter krt23 Kate Turner
 Analysis Name krt23_36_356772_40_01_62872.d Supervisor - Tony James
 Method used Confirm Formula Positive 50to1500 loop inj.m Acquisition Date 17/04/2018 11:14:21
 Ionisation Mode positive electrospray (ESI)

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



#	m/z	I	I %	Area	S/N
1	331.2264	4877	25.5	74	3104.4
2	361.1063	19123	100.0	808	10039.2
3	362.1098	4229	22.1	153	2207.3
4	413.2711	8640	45.2	244	3633.5
5	507.3421	5128	26.8	73	1680.3
6	551.3813	4609	24.1	69	1368.7
7	605.0458	3594	18.8	209	988.1
8	627.0311	12803	66.9	830	3464.6
9	634.4599	3328	17.4	119	896.0
10	1231.0744	4219	22.1	468	2882.8

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 C28 H16 N2 O12 S **Adduct(s):** H, Na

#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
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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