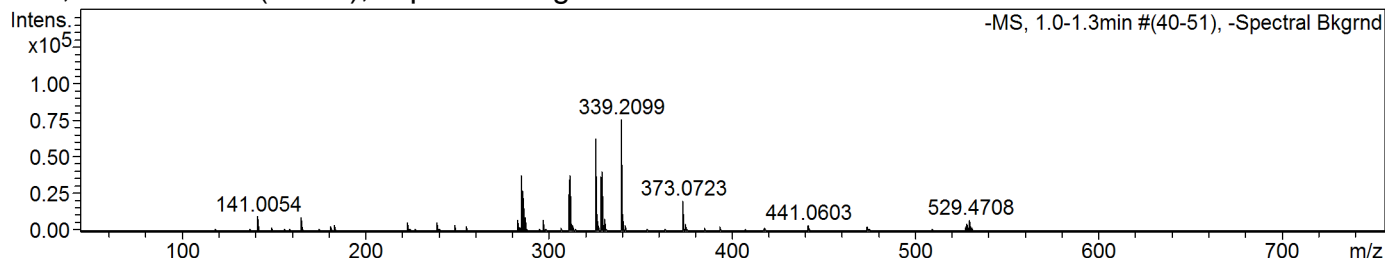


Confirmation of Expected Formula

Sample-ID krt23_34 Submitter krt23 Kate Turner
Analysis Name krt23_34_356693_72_01_62791.d Supervisor - Tony James
Method used Confirm Formula Negative 50to500 loop inj.m Acquisition Date 12/04/2018 14:37:49
Ionisation Mode negative electrospray (ESI)

-MS, 1.0-1.3min #(40-51), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	285.0558	37760	50.1	2048	1130.9
2	286.0624	27462	36.5	1408	796.9
3	311.1834	37586	49.9	1026	721.9
4	325.1992	62446	82.9	1864	1377.8
5	326.2003	11626	15.4	371	259.3
6	328.0741	36941	49.1	2079	840.7
7	329.0813	40415	53.7	2387	930.0
8	339.2099	75306	100.0	1997	1951.7
9	340.2197	11586	15.4	338	304.1
10	373.0723	20528	27.3	1368	927.7

Generate Molecular Formula Parameters

Charge	Tolerance	SearchRadius	H/C Ratio min.	H/C Ratio max.	Electron Conf.	Nitrogen Rule	sigma limit
negative	10 ppm	0.05 m/z	0	3	both	true	0.05

Expected Formula C22 H14 O6 Adduct(s): H, Na

#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	373.0723	373.0718	1.50	0.0030	C 22 H 13 O 6

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