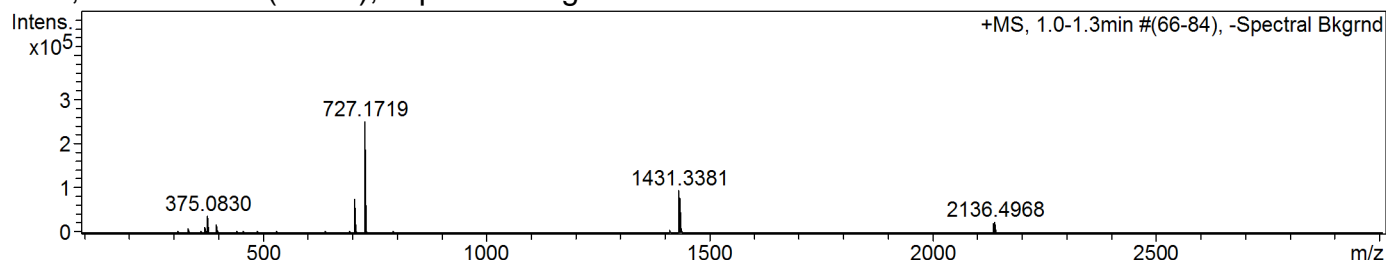


Confirmation of Expected Formula

Sample-ID krt23_32 Submitter krt23 Kate Turner
 Analysis Name krt23_32_356663_45_01_62760.d Supervisor - Tony James
 Method used Confirm Formula Positive 50to1500 loop inj.m Acquisition Date 11/04/2018 15:16:59
 Ionisation Mode positive electrospray (ESI)

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



#	m/z	I	I %	Area	S/N
1	375.0830	37399	15.0	1520	9561.7
2	705.1871	76742	30.7	5044	5188.7
3	706.1870	31652	12.7	2228	2126.5
4	727.1719	249693	100.0	14664	14812.8
5	728.1765	108838	43.6	6704	6420.8
6	729.1732	27869	11.2	2026	1635.0
7	1431.3381	94748	37.9	13560	13518.1
8	1432.3428	78160	31.3	10928	11237.8
9	1433.3452	35219	14.1	5401	5103.3
10	2136.4968	24190	9.7	5999	5228.1

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 C36 H32 O15 **Adduct(s):** H, Na

#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	705.1871	705.1814	8.10	0.0368	C 36 H 33 O 15

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