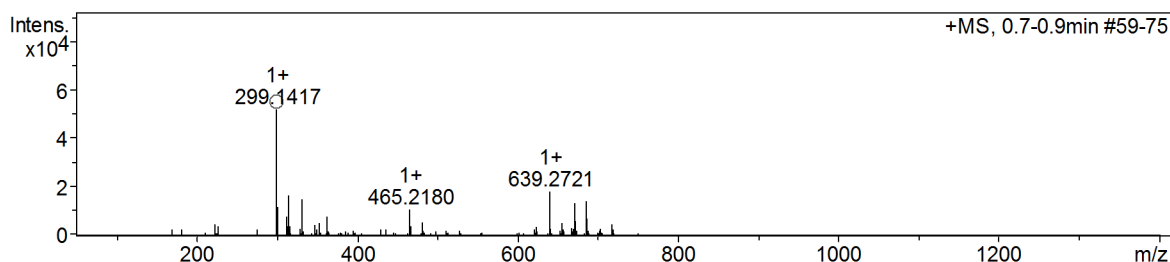




Sample-ID	m_cal_659	Lab	C13
Submitter	Michael Callingham	Supervisor	Hon Lam
Analysis Name	m_cal_659_526336_90_01_23302.d	Acquisition Date	5/18/2016 6:37:41 PM
Ionisation Mode	ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.7-0.9min #59-75



#	m/z	I %
1	223.0735	8.9
2	299.1417	100.0
3	300.1456	22.3
4	313.1208	15.0
5	314.1268	7.6
6	315.1364	31.6
7	331.1310	28.7
8	347.1245	8.4
9	353.1143	10.0
10	363.1212	14.8
11	465.2180	20.5
12	481.2081	10.4
13	639.2721	34.7
14	640.2754	15.3
15	655.2648	9.5
16	671.2625	26.0
17	672.2662	11.4
18	685.3267	26.9
19	686.3299	13.4
20	717.3168	9.1

Generate Molecular Formula Parameters

Charge	Tolerance	sigma limit	H/C Ratio	Electron Conf.	Nitrogen Rule	Chrom.BackGround	Calibration
+1	6 ppm	0.08	3 - 0	both	false	false	TRUE
Expected Formula		C20 H20 O1		Adduct(s):		H, Na, NH4, radical	
#	meas. m/z	theo. m/z	Err [ppm]	Sigma	Formula	Adduct	Adduct Mass
1	299.1417	299.1406	3.50	0.0034	C20H20NaO	M+Na	22.9898

Note: Sigma fits < 0.05 indicates high probability of correct MF