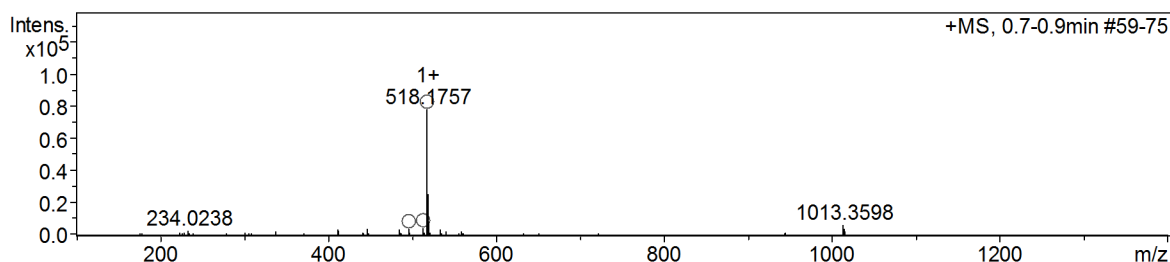




Sample-ID	m_cal_553	Lab	C13
Submitter	Michael Callingham	Supervisor	Hon Lam
Analysis Name	m_cal_553_517790_20_01_13859.d	Acquisition Date	1/28/2016 10:40:56 AM
Ionisation Mode	ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.7-0.9min #59-75



#	m/z	I %
1	234.0238	4.0
2	301.1317	2.6
3	337.0746	3.3
4	411.0936	4.6
5	413.2665	4.1
6	441.2953	2.4
7	447.3440	5.6
8	485.1115	4.3
9	496.1929	5.4
10	513.2197	5.9
11	518.1757	100.0
12	519.1795	32.8
13	520.1767	10.4
14	534.1508	4.7
15	540.1578	3.2
16	559.1299	3.2
17	944.0763	2.6
18	1013.3598	8.0
19	1014.3591	5.5
20	1015.3614	2.7

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		C31 H29 N1 O3 S1		Adduct(s):		H, Na, NH4, radical	
#	meas. m/z	theo. m/z	Err [ppm]	Sigma	Formula	Adduct	Adduct Mass
1	496.1929	496.1941	2.40	0.0466	C31H30NO3S	M+H	1.0078
1	518.1757	518.1760	0.60	0.0120	C31H29NNaO3S	M+Na	22.9898
1	513.2197	513.2206	1.90	0.0186	C31H33N2O3S	M+H4N	18.0344

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