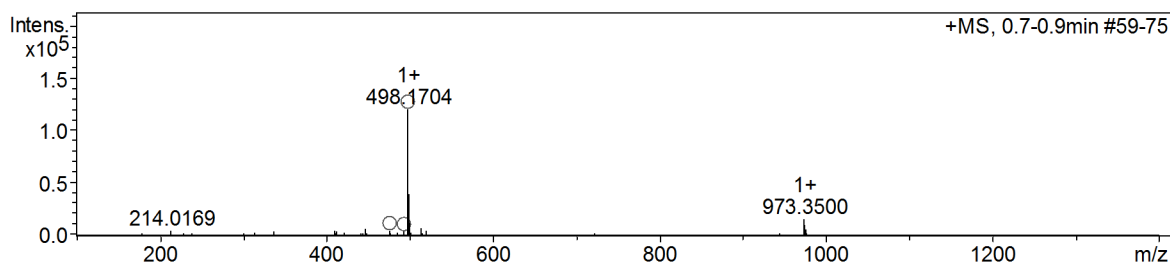




Sample-ID	m_cal_552	Lab	C13
Submitter	Michael Callingham	Supervisor	Hon Lam
Analysis Name	m_cal_552_517789_19_01_13858.d	Acquisition Date	1/28/2016 10:39:15 AM
Ionisation Mode	ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.7-0.9min #59-75



#	m/z	I %
1	214.0169	3.7
2	314.0452	2.5
3	337.0739	2.9
4	411.0934	3.6
5	413.2659	3.2
6	422.1372	2.0
7	447.3424	4.9
8	476.1876	3.6
9	485.1107	2.3
10	493.2145	3.1
11	498.1704	100.0
12	499.1739	32.5
13	500.1703	9.8
14	501.1711	2.2
15	514.1428	5.7
16	515.1455	1.7
17	520.1511	3.5
18	973.3500	13.1
19	974.3498	8.6
20	975.3493	4.2

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		C28 H29 N1 O4 S1		Adduct(s):		H, Na, NH4, radical	
#	meas. m/z	theo. m/z	Err [ppm]	Sigma	Formula	Adduct	Adduct Mass
1	476.1876	476.1890	2.90	0.0102	C28H30NO4S	M+H	1.0078
1	498.1704	498.1710	1.10	0.0036	C28H29NNaO4S	M+Na	22.9898
1	493.2145	493.2156	2.10	0.0552	C28H33N2O4S	M+H4N	18.0344

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