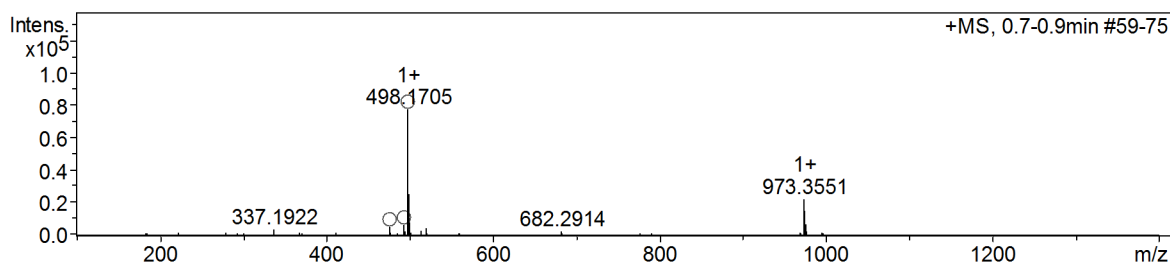




Sample-ID	b_pa1_16_009	Lab	C13
Submitter	Ben Partridge	Supervisor	Hon Lam
Analysis Name	b_pa1_16_009_519774_53_01_16201.d	Acquisition Date	2/17/2016 12:13:30 PM
Ionisation Mode	ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.7-0.9min #59-75



#	m/z	I %
1	223.0653	2.1
2	279.0969	2.2
3	337.1922	4.2
4	368.1330	2.0
5	476.1888	6.8
6	477.1910	2.3
7	493.2158	8.3
8	494.2164	2.9
9	498.1705	100.0
10	499.1739	32.8
11	500.1714	10.2
12	501.1724	2.3
13	514.1428	3.5
14	520.1512	5.7
15	682.2914	2.8
16	973.3551	28.9
17	974.3529	19.6
18	975.3540	9.3
19	976.3589	3.3
20	995.3342	2.5

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	476.1888	476.1890	0.50	0.0107	C28H30NO4S	M+H	1.0078
1	498.1705	498.1710	0.90	0.0043	C28H29NNaO4S	M+Na	22.9898
1	493.2158	493.2156	0.50	0.0148	C28H33N2O4S	M+H4N	18.0344

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