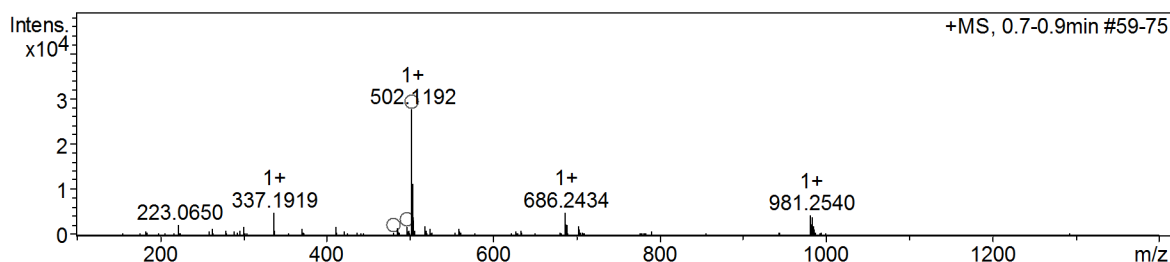




Sample-ID	b_pa1_16_021	Lab	C13
Submitter	Ben Partridge	Supervisor	Hon Lam
Analysis Name	b_pa1_16_021_519773_54_01_16202.d	Acquisition Date	2/17/2016 12:15:07 PM
Ionisation Mode	ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.7-0.9min #59-75



#	m/z	I %
1	223.0650	8.0
2	263.0933	5.6
3	301.1380	6.8
4	337.1919	17.9
5	411.0935	7.0
6	485.1110	6.2
7	497.1650	6.6
8	502.1192	100.0
9	503.1231	32.5
10	504.1184	40.6
11	505.1194	12.5
12	518.0957	7.7
13	686.2434	18.3
14	687.2441	8.7
15	688.2418	8.5
16	702.2164	7.7
17	981.2540	15.8
18	982.2578	9.1
19	983.2495	14.5
20	984.2526	7.8

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		C27 H26 Cl1 N1 O3 S1				Adduct(s):	H, Na, NH4, radical
#	meas. m/z	theo. m/z	Err [ppm]	Sigma	Formula	Adduct	Adduct Mass
1	480.1396	480.1395	0.20	0.0382	C27H27ClNO3S	M+H	1.0078
1	502.1192	502.1214	4.30	0.0096	C27H26ClNNaO3S	M+Na	22.9898

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