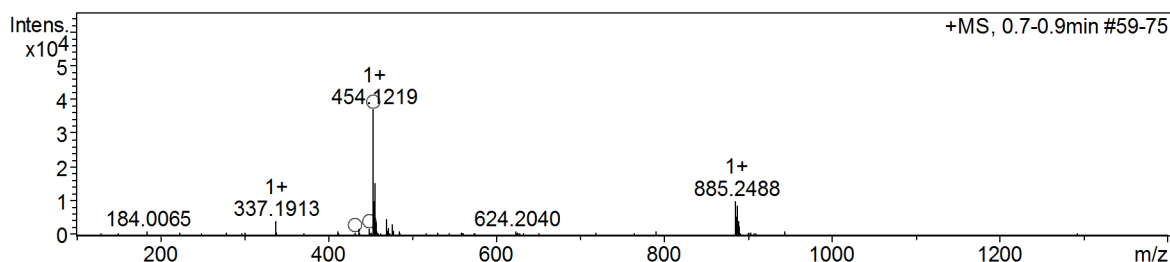




Sample-ID	b_pa1_16_032	Lab	C13
Submitter	Ben Partridge	Supervisor	Hon Lam
Analysis Name	b_pa1_16_032_519876_68_01_16220.d	Acquisition Date	2/17/2016 1:19:52 PM
Ionisation Mode	ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.7-0.9min #59-75



#	m/z	I %
1	184.0065	3.3
2	337.1913	11.1
3	437.2435	5.2
4	449.1650	5.0
5	454.1219	100.0
6	455.1239	27.6
7	456.1176	41.8
8	457.1200	10.7
9	470.0936	12.9
10	471.0983	3.6
11	472.0926	6.2
12	476.1030	8.8
13	478.0988	3.5
14	485.1103	3.2
15	624.2040	3.2
16	885.2488	27.4
17	886.2520	14.9
18	887.2495	23.3
19	888.2515	11.7
20	889.2488	7.9

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		C23 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	432.1404	432.1395	2.20	0.0225	C23H27ClNO3S	M+H	1.0078
1	454.1219	454.1214	1.10	0.0084	C23H26ClNNaO3S	M+Na	22.9898
1	449.1650	449.1660	2.20	0.0399	C23H30ClN2O3S	M+H4N	18.0344

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