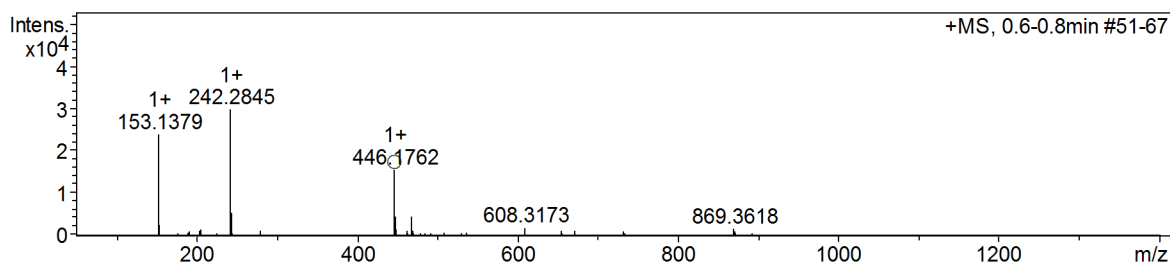




Sample-ID	b_pa1_16_038	Lab	C13
Submitter	Ben Partridge	Supervisor	Hon Lam
Analysis Name	b_pa1_16_038_523333_70_01_19911.d	Acquisition Date	4/1/2016 3:06:34 PM
Ionisation Mode	ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.6-0.8min #51-67



#	m/z	I %
1	153.1379	80.2
2	154.1410	8.3
3	191.0076	3.2
4	204.0274	3.7
5	205.0243	4.5
6	242.2845	100.0
7	243.2878	17.9
8	279.0938	3.6
9	446.1762	52.5
10	447.1794	14.8
11	448.1786	4.8
12	462.1657	3.6
13	468.1580	14.9
14	469.1619	4.1
15	608.3173	6.2
16	654.3698	4.1
17	670.3633	3.5
18	731.4885	3.2
19	869.3618	5.3
20	870.3636	3.1

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		C25 H29 N1 O3 S1		Adduct(s):		H, Na, NH4, radical	
#	meas. m/z	theo. m/z	Err [ppm]	Sigma	Formula	Adduct	Adduct Mass
1	446.1762	446.1760	0.30	0.0022	C25H29NNaO3S	M+Na	22.9898

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