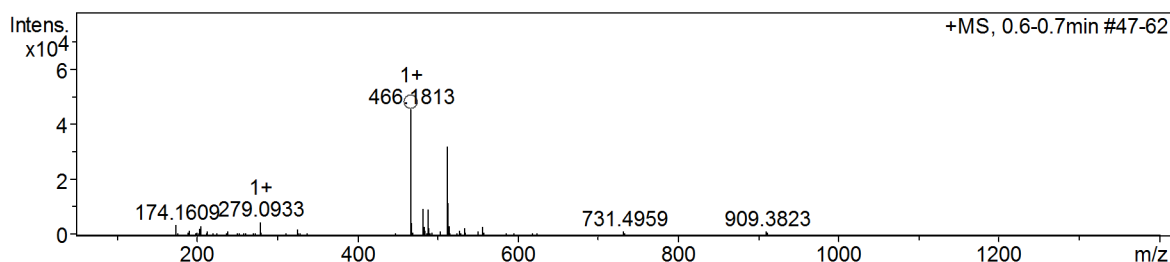




Sample-ID	m_cal_598	Lab	C13
Submitter	Michael Callingham	Supervisor	Hon Lam
Analysis Name	m_cal_598_524778_88_01_21532.d	Acquisition Date	4/22/2016 5:08:52 PM
Ionisation Mode	ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.6-0.7min #47-62



#	m/z	I %
1	174.1609	8.3
2	191.0076	3.6
3	204.0273	5.6
4	205.0242	7.7
5	279.0933	10.9
6	326.2115	4.6
7	466.1813	100.0
8	467.1839	31.3
9	468.1822	9.6
10	482.1551	21.5
11	483.1578	6.6
12	484.1537	3.5
13	488.1627	20.1
14	489.1656	6.2
15	512.2367	70.4
16	513.2399	26.0
17	514.2373	7.7
18	528.1519	3.7
19	534.1682	5.8
20	556.1505	7.0

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 O2 S1		Adduct(s):		H, Na, NH4, radical	
#	meas. m/z	theo. m/z	Err [ppm]	Sigma	Formula	Adduct	Adduct Mass
1	466.1813	466.1811	0.40	0.0032	C28H29NNaO2S	M+Na	22.9898

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