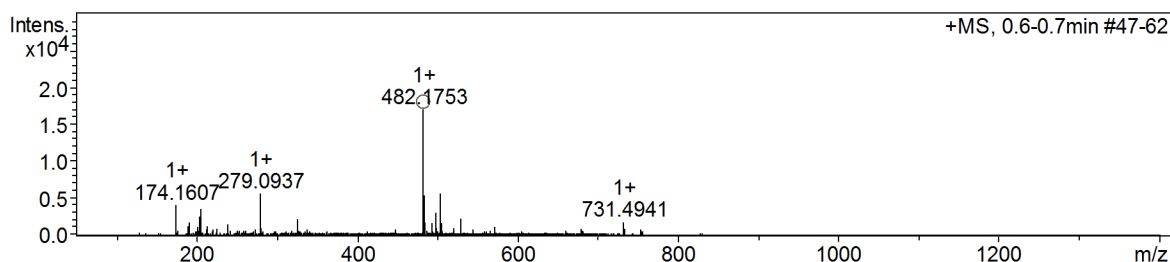




Sample-ID	m_cal_602	Lab	C13
Submitter	Michael Callingham	Supervisor	Hon Lam
Analysis Name	m_cal_602_524780_90_01_21534.d	Acquisition Date	4/22/2016 5:12:05 PM
Ionisation Mode	ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.6-0.7min #47-62



#	m/z	I %
1	174.1607	24.2
2	190.0112	7.2
3	191.0078	10.8
4	201.0105	6.5
5	204.0274	15.5
6	205.0243	21.4
7	212.9913	7.6
8	238.9946	8.7
9	279.0937	33.6
10	326.2104	13.1
11	482.1753	100.0
12	483.1784	31.9
13	484.1764	10.4
14	493.3993	9.5
15	498.1478	17.8
16	504.1574	33.5
17	505.1611	10.0
18	528.2287	13.9
19	572.1433	7.1
20	731.4941	10.2

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 O3 S1		Adduct(s):		H, Na, NH4, radical	
#	meas. m/z	theo. m/z	Err [ppm]	Sigma	Formula	Adduct	Adduct Mass
1	482.1753	482.1760	1.50	0.0106	C28H29NNaO3S	M+Na	22.9898

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