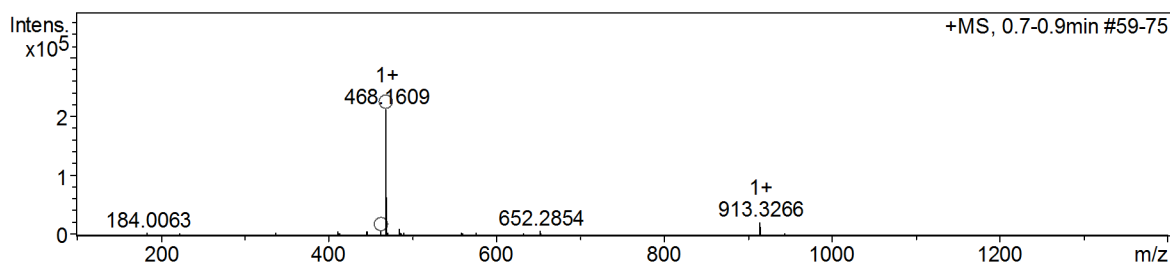




Sample-ID	m_cal_555	Lab	C13
Submitter	Michael Callingham	Supervisor	Hon Lam
Analysis Name	m_cal_555_517791_21_01_13860.d	Acquisition Date	1/28/2016 10:42:34 AM
Ionisation Mode	ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.7-0.9min #59-75



#	m/z	I %
1	184.0063	2.4
2	337.0737	2.4
3	411.0929	3.3
4	446.1756	3.1
5	447.3406	2.7
6	463.2032	3.0
7	468.1609	100.0
8	469.1638	30.5
9	470.1612	8.6
10	471.1604	1.9
11	484.1336	4.9
12	485.1204	3.9
13	486.1201	2.0
14	490.1405	2.4
15	559.1295	2.4
16	576.2509	2.4
17	652.2854	3.8
18	913.3266	10.4
19	914.3301	6.6
20	915.3292	3.0

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		C27 H27 N1 O3 S1				Adduct(s): H, Na, NH4, radical	
#	meas. m/z	theo. m/z	Err [ppm]	Sigma	Formula	Adduct	Adduct Mass
1	468.1609	468.1604	1.20	0.0056	C27H27NNaO3S	M+Na	22.9898
1	463.2032	463.2050	3.90	0.0503	C27H31N2O3S	M+H4N	18.0344

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