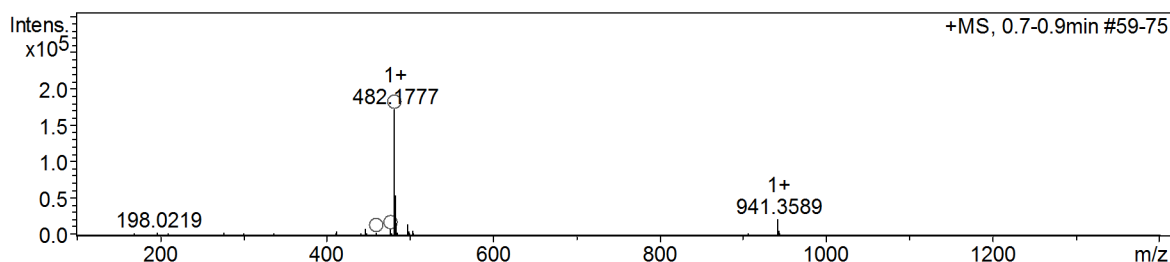




Sample-ID	m_cal_550	Lab	C13
Submitter	Michael Callingham	Supervisor	Hon Lam
Analysis Name	m_cal_550_517787_17_01_13856.d	Acquisition Date	1/28/2016 10:36:00 AM
Ionisation Mode	ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.7-0.9min #59-75



#	m/z	I %
1	170.0964	1.6
2	198.0219	2.6
3	210.0896	1.5
4	276.9884	2.4
5	411.0939	1.7
6	413.2660	3.2
7	447.3437	5.1
8	460.1928	2.3
9	477.2195	4.3
10	482.1777	100.0
11	483.1788	31.5
12	484.1763	9.7
13	485.1631	2.2
14	498.1483	9.0
15	499.1508	2.9
16	500.1477	1.5
17	504.1573	4.0
18	941.3589	12.9
19	942.3641	8.5
20	943.3686	4.1

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		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	460.1928	460.1941	2.80	0.0213	C28H30NO3S	M+H	1.0078
1	482.1777	482.1760	3.40	0.0107	C28H29NNaO3S	M+Na	22.9898
1	477.2195	477.2206	2.30	0.0520	C28H33N2O3S	M+H4N	18.0344

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