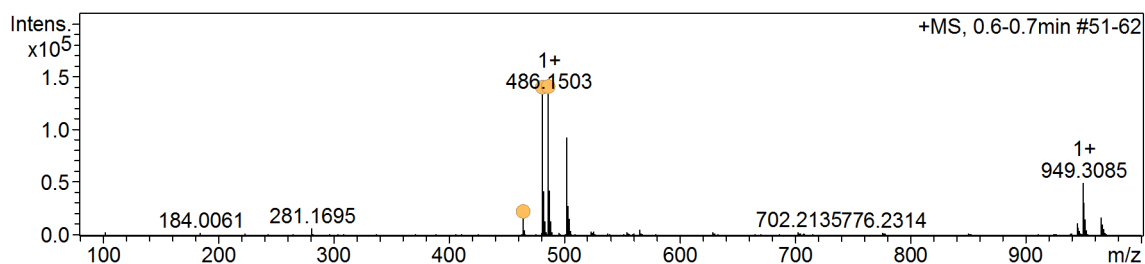




Sample-ID	m_cal_1082_c	Lab	C13
Submitter	Michael Callingham	Supervisor	Hon Lam
Analysis Name	m_cal_1082_c_551560_21_01_5550.d	Acquisition Date	7/3/2017 10:40:49 AM
Ionisation Mode	ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.6-0.7min #51-62



#	m/z	I %
1	281.1695	4.7
2	464.1680	11.7
3	481.1947	99.9
4	482.1983	31.5
5	483.1933	10.1
6	486.1503	100.0
7	487.1535	31.9
8	488.1519	9.7
9	502.1243	69.2
10	503.1273	21.2
11	504.1245	11.6
12	565.2886	4.0
13	944.3533	8.7
14	945.3555	5.3
15	949.3085	37.6
16	950.3112	23.6
17	951.3121	11.1
18	965.2838	12.6
19	966.2847	7.6
20	967.2846	4.6

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 H26 F1 N1 O3 S1 **Adduct(s):** H, Na, NH4, C3H5N2, radical

#	meas. m/z	theo. m/z	Err [ppm]	Sigma	Formula	Adduct	Adduct Mass
1	464.1680	464.1690	2.30	0.0059	C27H27FNO3S	M+H	1.0078
1	486.1503	486.1510	1.30	0.0057	C27H26FNNaO3S	M+Na	22.9898
1	481.1947	481.1956	1.70	0.0028	C27H30FN2O3S	M+H4N	18.0344

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