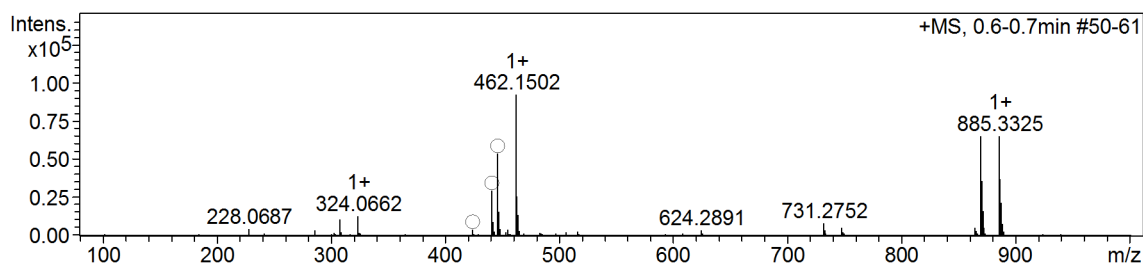




Sample-ID	m_cal_1091_minor	Lab	C13
Submitter	Michael Callingham	Supervisor	Hon Lam
Analysis Name	m_cal_1091_minor_552673_26_01_5889.	Acquisition Date	7/25/2017 10:30:25 AM
Ionisation Mode	ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.6-0.7min #50-61



#	m/z	I %
1	308.0920	12.0
2	324.0662	14.0
3	441.2207	32.3
4	442.2244	9.8
5	446.1745	58.2
6	447.1777	17.1
7	462.1502	100.0
8	463.1532	28.0
9	464.1496	15.0
10	731.2752	9.2
11	747.2524	5.9
12	864.4105	6.0
13	869.3592	70.4
14	870.3629	38.7
15	871.3607	17.4
16	872.3624	5.9
17	885.3325	70.4
18	886.3359	40.3
19	887.3344	23.7
20	888.3369	8.7

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 C₂₅ H₂₉ N₁ O₃ S₁ **Adduct(s):** H, Na, NH₄, C₃H₅N₂, radical

#	meas. m/z	theo. m/z	Err [ppm]	Sigma	Formula	Adduct	Adduct Mass
1	424.1936	424.1941	1.10	0.0182	C ₂₅ H ₃₀ NO ₃ S	M+H	1.0078
1	446.1745	446.1760	3.50	0.0038	C ₂₅ H ₂₉ NNaO ₃ S	M+Na	22.9898
1	441.2207	441.2206	0.00	0.0069	C ₂₅ H ₃₃ N ₂ O ₃ S	M+H ₄ N	18.0344

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