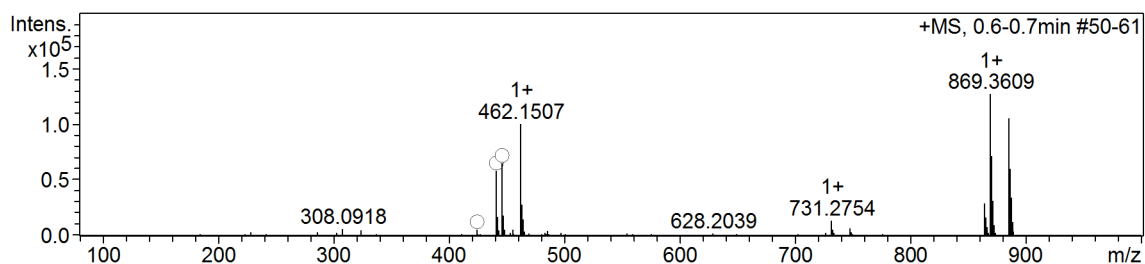




Sample-ID	m_cal_1091_major	Lab	C13
Submitter	Michael Callingham	Supervisor	Hon Lam
Analysis Name	m_cal_1091_major_552672_25_01_5888.	Acquisition Date	7/25/2017 10:27:58 AM
Ionisation Mode	ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.6-0.7min #50-61



#	m/z	I %
1	441.2211	46.1
2	442.2250	13.4
3	446.1749	51.5
4	447.1779	14.3
5	462.1507	79.1
6	463.1534	22.1
7	464.1497	11.7
8	731.2754	10.9
9	747.2527	5.5
10	864.4071	22.9
11	865.4099	13.3
12	866.4056	6.4
13	869.3609	100.0
14	870.3642	56.5
15	871.3625	24.7
16	872.3607	7.8
17	885.3340	83.3
18	886.3366	47.4
19	887.3344	27.1
20	888.3359	10.1

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 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	424.1935	424.1941	1.40	0.0106	C ₂₅ H ₃₀ NO ₃ S	M+H	1.0078
1	446.1749	446.1760	2.50	0.0049	C ₂₅ H ₂₉ NNaO ₃ S	M+Na	22.9898
1	441.2211	441.2206	1.10	0.0021	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