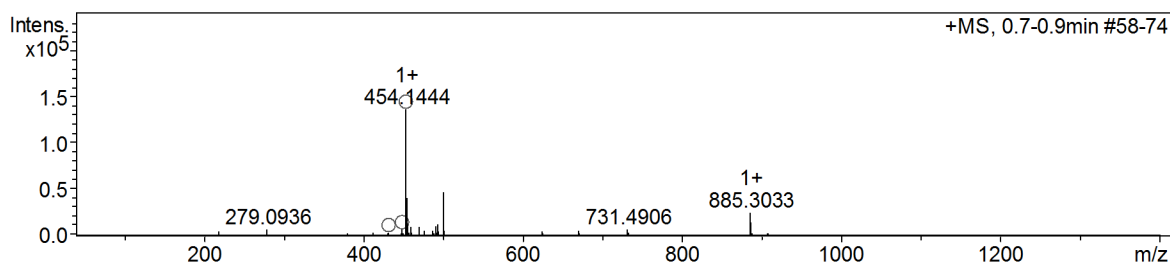




Sample-ID	m_cal_721	Lab	C13
Submitter	Michael Callingham	Supervisor	Hon Lam
Analysis Name	m_cal_721_527759_31_01_24960.d	Acquisition Date	6/14/2016 2:16:21 PM
Ionisation Mode	ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.7-0.9min #58-74



#	m/z	I %
1	279.0936	4.7
2	449.1895	4.3
3	454.1444	100.0
4	455.1475	29.4
5	456.1458	9.1
6	459.3216	7.0
7	470.1177	7.0
8	476.1262	3.8
9	487.3527	3.7
10	491.2355	7.3
11	493.3988	9.2
12	494.4019	3.1
13	500.1993	34.2
14	501.2023	11.6
15	502.2012	3.7
16	670.3089	3.8
17	731.4906	4.7
18	885.3033	17.8
19	886.3062	10.4
20	887.3062	4.7

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		C26 H25 N1 O3 S1		Adduct(s):		H, Na, NH4, radical	
#	meas. m/z	theo. m/z	Err [ppm]	Sigma	Formula	Adduct	Adduct Mass
1	432.1630	432.1628	0.50	0.0146	C26H26NO3S	M+H	1.0078
1	454.1444	454.1447	0.80	0.0019	C26H25NNaO3S	M+Na	22.9898
1	449.1895	449.1893	0.30	0.0098	C26H29N2O3S	M+H4N	18.0344

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