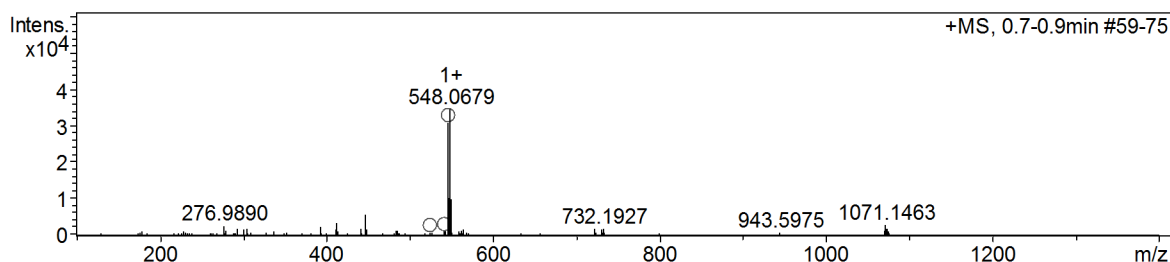




Sample-ID	m_cal_551	Lab	C13
Submitter	Michael Callingham	Supervisor	Hon Lam
Analysis Name	m_cal_551_517788_18_01_13857.d	Acquisition Date	1/28/2016 10:37:39 AM
Ionisation Mode	ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.7-0.9min #59-75



#	m/z	I %
1	276.9890	7.6
2	292.9841	5.5
3	301.1334	4.6
4	305.1618	5.6
5	393.2943	6.9
6	413.2660	9.8
7	441.2953	5.0
8	447.3423	16.3
9	448.3444	4.8
10	546.0699	89.4
11	547.0734	29.1
12	548.0679	100.0
13	549.0701	28.9
14	550.0684	8.8
15	722.5253	5.2
16	730.1931	4.7
17	732.1927	5.4
18	1071.1463	8.0
19	1072.1444	5.1
20	1073.1458	5.5

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 Br1 N1 O3 S1				Adduct(s):	H, Na, NH4, radical
#	meas. m/z	theo. m/z	Err [ppm]	Sigma	Formula	Adduct	Adduct Mass
1	524.0872	524.0890	3.40	0.0275	C27H27BrNO3S	M+H	1.0078
1	546.0699	546.0709	1.90	0.0176	C27H26BrNNaO3S	M+Na	22.9898

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