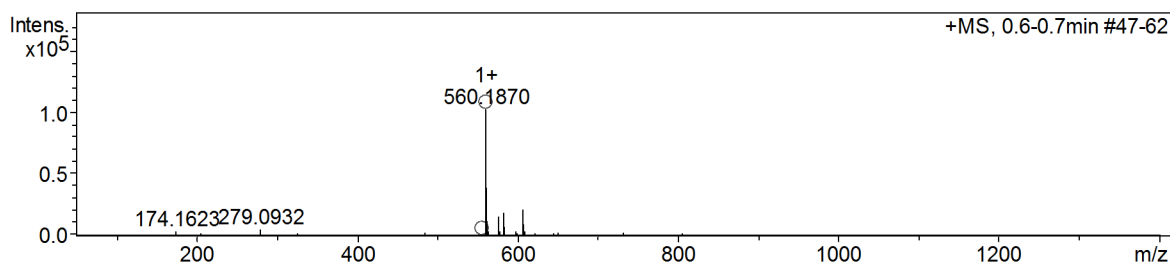




Sample-ID	m_cal_666	Lab	C13
Submitter	Michael Callingham	Supervisor	Hon Lam
Analysis Name	m_cal_666_524782_2_01_21536.d	Acquisition Date	4/22/2016 5:15:23 PM
Ionisation Mode	ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.6-0.7min #47-62



#	m/z	I %
1	174.1623	3.4
2	279.0932	4.6
3	484.1538	2.5
4	560.1870	100.0
5	561.1902	37.6
6	562.1895	11.5
7	563.1906	2.7
8	576.1602	15.2
9	577.1632	5.8
10	578.1615	2.8
11	582.1688	18.6
12	583.1724	7.0
13	584.1708	2.3
14	598.1442	2.9
15	606.2401	20.6
16	607.2431	8.8
17	608.2404	3.1
18	644.1410	1.7
19	650.1589	2.1
20	731.4958	2.0

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		C33 H31 N1 O4 S1				Adduct(s):	H, Na, NH4, radical
#	meas. m/z	theo. m/z	Err [ppm]	Sigma	Formula	Adduct	Adduct Mass
1	560.1870	560.1866	0.60	0.0031	C33H31NNaO4S	M+Na	22.9898

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