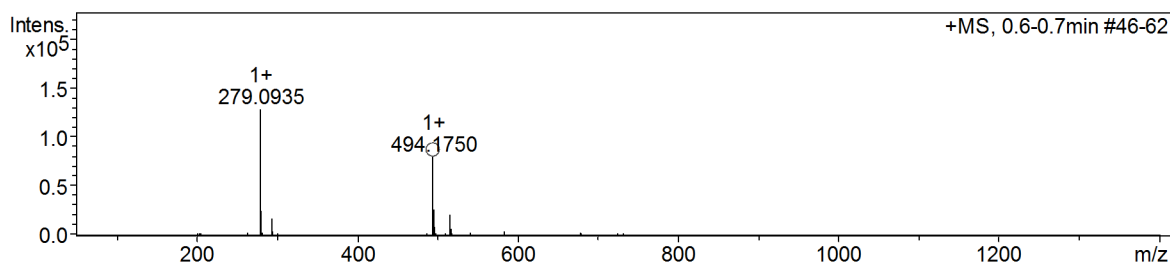




Sample-ID	b_pa1_16_068	Lab	C13
Submitter	Ben Partridge	Supervisor	Hon Lam
Analysis Name	b_pa1_16_068_525598_22_01_22471.d	Acquisition Date	5/6/2016 11:51:02 AM
Ionisation Mode	ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.6-0.7min #46-62



#	m/z	I %
1	201.0450	1.7
2	205.0240	1.8
3	264.1744	2.5
4	279.0935	100.0
5	280.0969	19.9
6	281.0999	2.1
7	293.1087	13.8
8	294.1119	2.8
9	301.0752	1.5
10	494.1750	62.1
11	495.1782	20.7
12	496.1765	6.6
13	510.1472	1.5
14	516.1572	16.4
15	517.1610	5.4
16	518.1582	1.7
17	540.2291	2.5
18	584.1432	2.7
19	678.3022	2.5
20	724.3589	1.8

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		C29 H29 N1 O3 S1				Adduct(s):	H, Na, NH4, radical
#	meas. m/z	theo. m/z	Err [ppm]	Sigma	Formula	Adduct	Adduct Mass
1	494.1750	494.1760	2.10	0.0025	C29H29NNaO3S	M+Na	22.9898

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