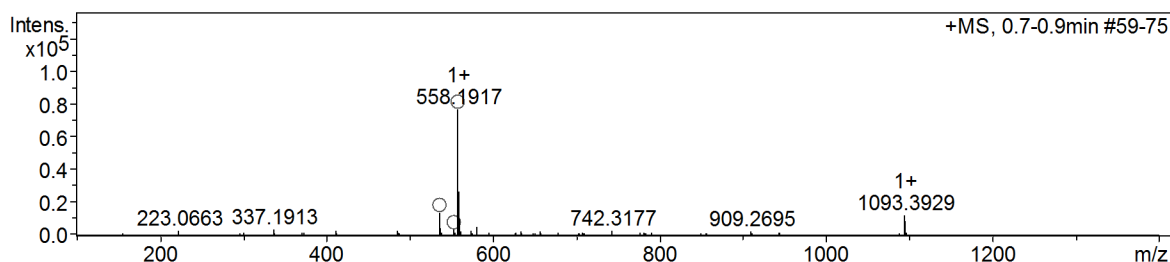




Sample-ID	b_pa1_16_024	Lab	C13
Submitter	Ben Partridge	Supervisor	Hon Lam
Analysis Name	b_pa1_16_024_519858_49_01_16197.d	Acquisition Date	2/17/2016 12:06:45 PM
Ionisation Mode	ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.7-0.9min #59-75



#	m/z	I %
1	223.0663	3.5
2	337.0776	2.7
3	337.1913	4.7
4	411.0950	4.1
5	485.1131	3.9
6	536.2106	17.9
7	537.2109	6.3
8	553.2368	4.9
9	558.1917	100.0
10	559.1933	35.1
11	560.1893	12.9
12	561.1697	3.1
13	574.1641	3.9
14	580.1736	6.6
15	656.1880	3.3
16	742.3177	3.9
17	909.2695	3.0
18	1093.3929	16.0
19	1094.3979	11.5
20	1095.3961	5.7

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		C30 H33 N1 O6 S1		Adduct(s):		H, Na, NH4, radical	
#	meas. m/z	theo. m/z	Err [ppm]	Sigma	Formula	Adduct	Adduct Mass
1	536.2106	536.2101	0.80	0.0061	C30H34NO6S	M+H	1.0078
1	558.1917	558.1921	0.70	0.0155	C30H33NNaO6S	M+Na	22.9898

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