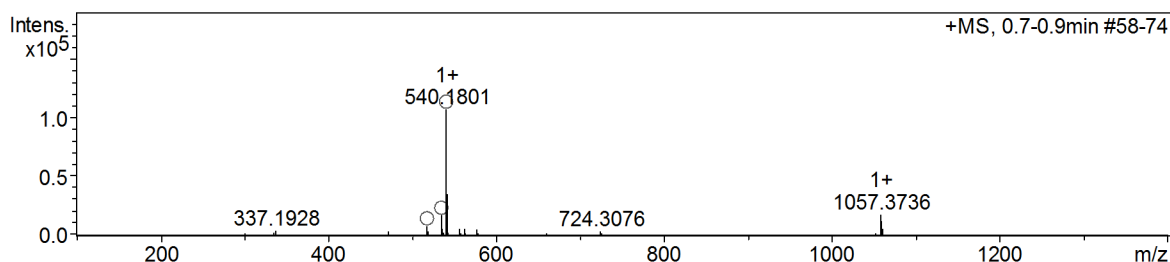




Sample-ID	b_pa1_16_014	Lab	C13
Submitter	Ben Partridge	Supervisor	Hon Lam
Analysis Name	b_pa1_16_014_519855_51_01_16199.d	Acquisition Date	2/17/2016 12:10:10 PM
Ionisation Mode	ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.7-0.9min #58-74



#	m/z	I %
1	335.2019	2.5
2	337.1928	3.5
3	472.1578	3.0
4	518.1971	7.8
5	519.2018	2.8
6	535.2259	15.6
7	536.2289	5.7
8	537.2250	1.9
9	540.1801	100.0
10	541.1848	32.7
11	542.1825	10.6
12	543.1827	2.4
13	556.1556	5.1
14	562.1605	5.1
15	577.2721	4.5
16	724.3076	3.3
17	1057.3736	16.7
18	1058.3764	11.4
19	1059.3783	5.4
20	1060.3772	2.1

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 H31 N1 O5 S1		Adduct(s):		H, Na, NH4, radical	
#	meas. m/z	theo. m/z	Err [ppm]	Sigma	Formula	Adduct	Adduct Mass
1	518.1971	518.1996	4.80	0.0077	C30H32NO5S	M+H	1.0078
1	540.1801	540.1815	2.60	0.0079	C30H31NNaO5S	M+Na	22.9898
1	535.2259	535.2261	0.30	0.0110	C30H35N2O5S	M+H4N	18.0344

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