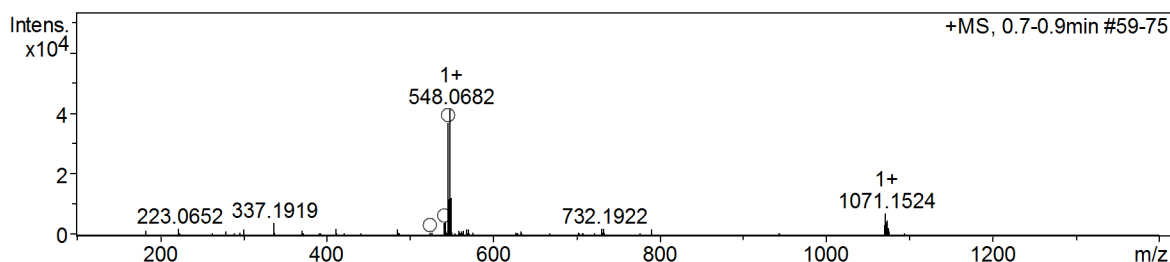




Sample-ID	b_pa1_16_008	Lab	C13
Submitter	Ben Partridge	Supervisor	Hon Lam
Analysis Name	b_pa1_16_008_516955_55_01_16203.d	Acquisition Date	2/17/2016 12:16:47 PM
Ionisation Mode	ESI Positive	Instrument	Bruker MicroTOF

+MS, 0.7-0.9min #59-75



#	m/z	I %
1	223.0652	5.2
2	337.1919	9.9
3	411.0946	5.3
4	541.1134	9.8
5	543.1133	10.9
6	546.0700	89.2
7	547.0734	28.7
8	548.0682	100.0
9	549.0699	29.6
10	550.0703	8.8
11	568.0522	4.7
12	570.0481	4.9
13	730.1931	4.9
14	732.1922	5.6
15	1069.1536	8.0
16	1070.1507	5.1
17	1071.1524	17.5
18	1072.1487	10.9
19	1073.1515	12.1
20	1074.1487	6.3

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	524.0884	524.0890	1.10	0.0210	C27H27BrNO3S	M+H	1.0078
1	546.0700	546.0709	1.70	0.0177	C27H26BrNNaO3S	M+Na	22.9898
1	541.1134	541.1155	3.90	0.0212	C27H30BrN2O3S	M+H4N	18.0344

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