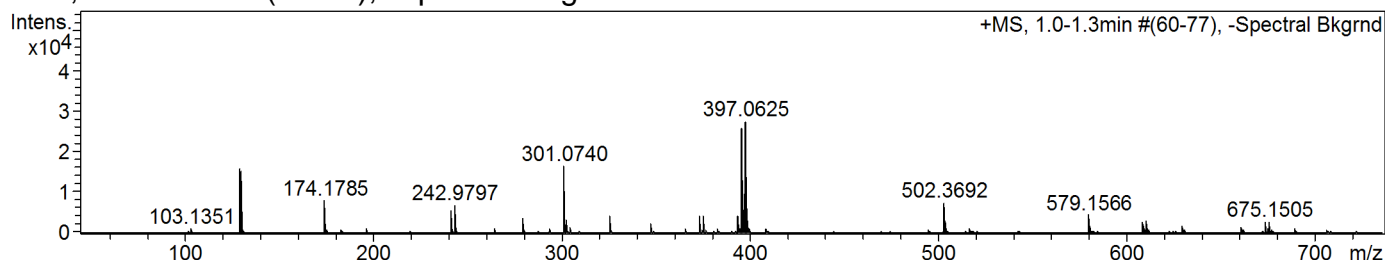


Confirmation of Expected Formula

Sample-ID acs_sdb_acs116 Submitter Adam Sedgwick
 Analysis Name acs_sdb_acs116_342782_2_01_47064.d Supervisor Steve Bull
 Method used Confirm Formula Positive 50to500 loop inj.m Acquisition Date 24/02/2015 10:08:06
 Ionisation Mode positive electrospray (ESI)

+MS, 1.0-1.3min #(60-77), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	129.1117	15805	57.8	116	79497.8
2	130.1675	15162	55.4	184	76105.4
3	174.1785	7941	29.0	69	39232.7
4	242.9797	6807	24.9	284	6930.3
5	301.0740	16365	59.8	974	4666.4
6	395.0651	25900	94.7	2053	1616.2
7	396.0669	5854	21.4	444	373.3
8	397.0625	27363	100.0	2120	1783.7
9	398.0654	6174	22.6	444	411.7
10	502.3692	7436	27.2	888	1834.1

Generate Molecular Formula Parameters

Charge	Tolerance	SearchRadius	H/C Ratio min.	H/C Ratio max.	Electron Conf.	Nitrogen Rule	sigma limit
positive	10 ppm	0.05 m/z	0	3	both	true	0.05

Expected Formula C12 H25 Br O3 Si **Adduct(s):** H, Na

#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
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Note: Sigma fits < 0.05 indicates high probability of correct MF, and mass accuracy of 5ppm or better is generally acceptable for publication