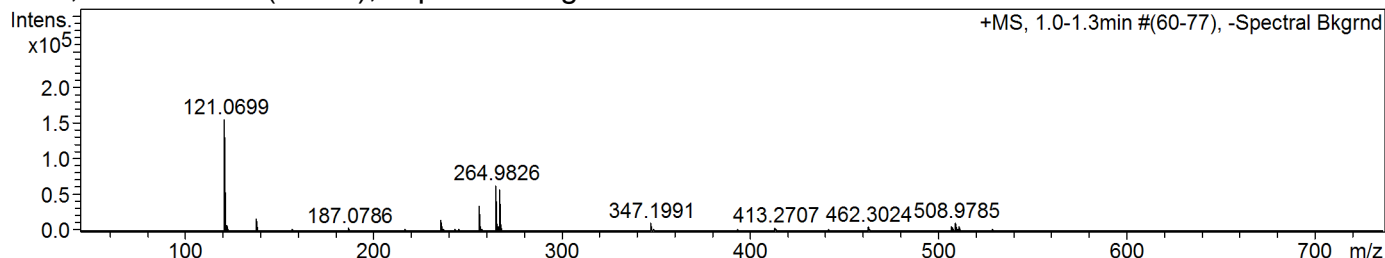


# Confirmation of Expected Formula

Sample-ID acs\_sdb\_acs88 Submitter Adam Sedgwick  
 Analysis Name acs\_sdb\_acs88\_342544\_64\_01\_46806.d Supervisor Steve Bull  
 Method used Confirm Formula Positive 50to500 loop inj.m Acquisition Date 27/01/2015 10:04:56  
 Ionisation Mode positive electrospray (ESI)

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



#	m/z	I	I %	Area	S/N
1	121.0699	154581	100.0	1586	49031.5
2	122.0764	8332	5.4	108	2657.8
3	138.0952	16380	10.6	346	5736.1
4	236.0822	14901	9.6	523	852.7
5	256.1439	35128	22.7	666	1485.5
6	264.9826	63250	40.9	3102	3235.8
7	265.9868	5939	3.8	345	311.2
8	266.9806	56929	36.8	2995	3057.4
9	347.1991	10891	7.0	803	1366.9
10	508.9785	10585	6.8	1116	739.7

## 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 C10 H11 Br O2 Adduct(s): H, Na

#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	264.9826	264.984012	3.10	0.0377	C 10 H 11 Br 1 Na 1 O 2

Note: Sigma fits < 0.05 indicates high probability of correct MF, and mass accuracy of 5ppm or better is generally acceptable for publication