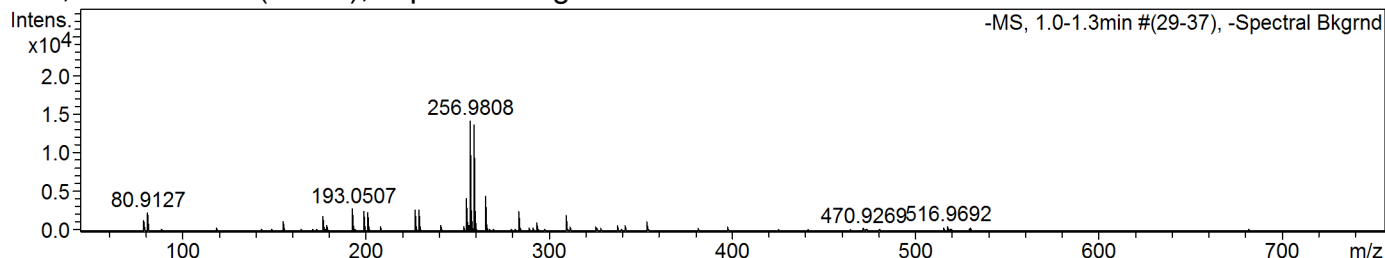


# Confirmation of Expected Formula

Sample-ID acs\_sdb\_acs109 Submitter Adam Sedgwick  
 Analysis Name acs\_sdb\_acs109\_342666\_81\_01\_46937.d Supervisor Steve Bull  
 Method used Confirm Formula Negative 50to500 loop inj.m Acquisition Date 11/02/2015 17:07:35  
 Ionisation Mode negative electrospray (ESI)

## -MS, 1.0-1.3min #(29-37), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	193.0507	2880	20.2	94	1672.5
2	198.9401	2468	17.3	85	1236.6
3	200.9373	2431	17.1	81	1163.9
4	226.9711	2622	18.4	94	682.0
5	228.9690	2685	18.9	100	670.8
6	255.2332	4190	29.4	107	687.9
7	256.9808	14229	100.0	602	2284.1
8	258.9793	13695	96.2	575	2214.3
9	265.1478	4475	31.4	177	796.3
10	283.2670	2531	17.8	87	638.7

## Generate Molecular Formula Parameters

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

Expected Formula C<sub>10</sub>H<sub>11</sub>BrO<sub>3</sub>

Adduct(s): H, Na

#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	256.9808	256.981332	4.00	0.0134	C <sub>10</sub> H <sub>10</sub> BrO <sub>3</sub>

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