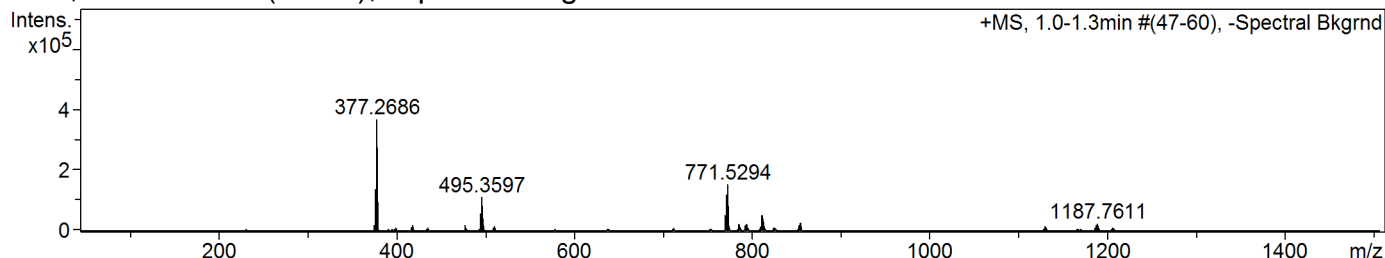


# Confirmation of Expected Formula

Sample-ID acs\_sdb\_acs259 Submitter Adam Sedgwick  
 Analysis Name acs\_sdb\_acs259\_344828\_4\_01\_49353.d Supervisor Steve Bull  
 Method used Confirm Formula Positive 50to1500 loop inj.m Acquisition Date 02/09/2015 14:17:39  
 Ionisation Mode positive electrospray (ESI)

## +MS, 1.0-1.3min #(47-60), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	376.2652	138559	37.8	7386	3785.5
2	377.2686	366614	100.0	12772	9905.9
3	378.2621	77361	21.1	4617	2067.7
4	494.3602	51267	14.0	5792	1936.4
5	495.3597	109445	29.9	10629	4177.9
6	769.5267	50499	13.8	8618	389.6
7	770.5281	121149	33.0	16966	924.9
8	771.5294	152096	41.5	16263	1149.2
9	772.5219	73589	20.1	8715	550.4
10	811.5121	50626	13.8	6015	520.3

## 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 C<sub>34</sub> H<sub>54</sub> B<sub>2</sub> N<sub>2</sub> O<sub>4</sub>

Adduct(s): H, Na

#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	577.4350	577.434794	0.60	0.0387	C <sub>34</sub> H <sub>55</sub> B <sub>2</sub> N <sub>2</sub> O <sub>4</sub>

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