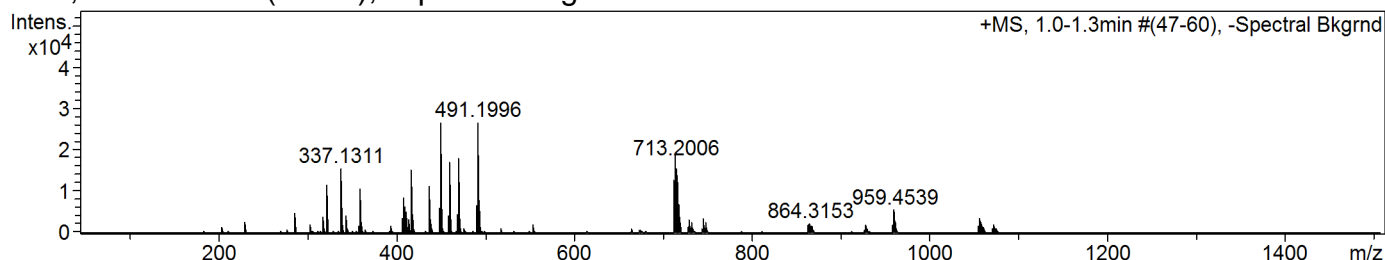


# Confirmation of Expected Formula

Sample-ID acs\_sdb\_acs245 Submitter Adam Sedgwick  
 Analysis Name acs\_sdb\_acs245\_344502\_73\_01\_48993.d Supervisor Steve Bull  
 Method used Confirm Formula Positive 50to1500 loop inj.m Acquisition Date 03/08/2015 11:21:05  
 Ionisation Mode positive electrospray (ESI)

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



#	m/z	I	I %	Area	S/N
1	321.1370	11593	43.3	845	1826.1
2	337.1311	15586	58.3	969	2000.4
3	417.1833	15081	56.4	1456	1003.2
4	449.2082	26647	99.6	2320	1485.3
5	459.1710	16963	63.4	1594	900.1
6	469.2171	18055	67.5	1756	913.8
7	491.1996	26747	100.0	2775	1371.7
8	712.1999	12794	47.8	1854	1560.5
9	713.2006	17384	65.0	2848	2124.6
10	715.1972	15585	58.3	1757	1912.3

## 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>24</sub> H<sub>23</sub> B F<sub>2</sub> N<sub>2</sub> O<sub>3</sub> **Adduct(s):** H, Na

#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	437.1885	437.184805	-8.80	0.0247	C <sub>24</sub> H <sub>24</sub> B F <sub>2</sub> N <sub>2</sub> O <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