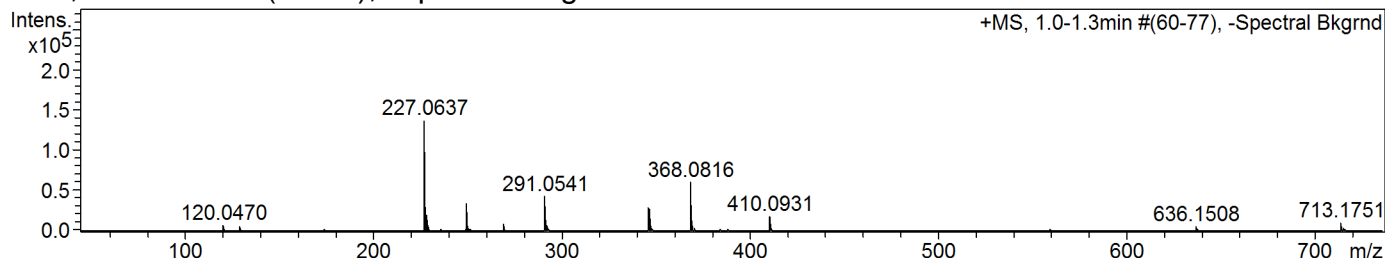


# Confirmation of Expected Formula

Sample-ID acs\_sdb\_acs289 Submitter Adam Sedgwick  
 Analysis Name acs\_sdb\_acs289\_345602\_22\_01\_50183.d Supervisor Steve Bull  
 Method used Confirm Formula Positive 50to500 loop inj.m Acquisition Date 24/11/2015 12:49:50  
 Ionisation Mode positive electrospray (ESI)

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



#	m/z	I	I %	Area	S/N
1	227.0637	137370	100.0	6078	28180.5
2	228.0650	19405	14.1	916	3965.6
3	249.0443	33685	24.5	1794	6376.9
4	269.0743	8277	6.0	480	1817.2
5	291.0541	43074	31.4	2646	12123.6
6	346.0991	28869	21.0	2146	12568.5
7	368.0816	60576	44.1	4517	6906.3
8	369.0832	12867	9.4	994	1419.3
9	410.0931	18629	13.6	1642	2078.8
10	713.1751	10212	7.4	1339	2576.8

## 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 C13 H10 N2 S Adduct(s): H, Na

#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	227.0637	227.064294	0.10	0.0094	C 13 H 11 N 2 S 1
1	249.0443	249.046239	5.70	0.0117	C 13 H 10 N 2 Na 1 S 1

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