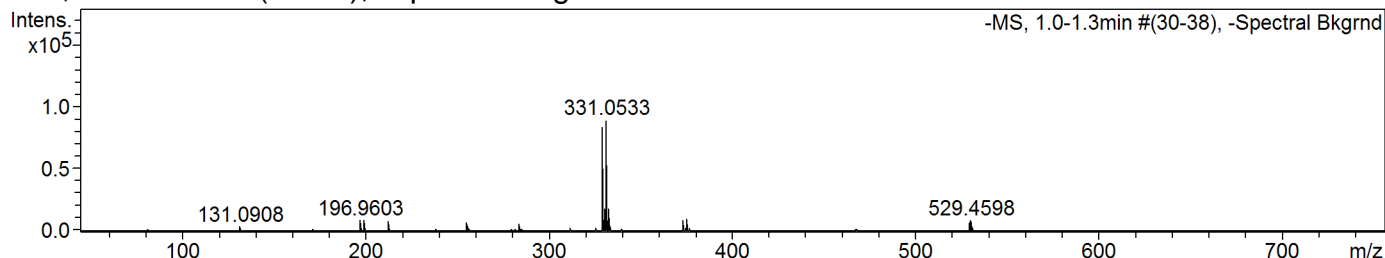


## Confirmation of Expected Formula

Sample-ID acs\_sdb\_acs128 Submitter Adam Sedgwick  
Analysis Name acs\_sdb\_acs128\_343090\_17\_01\_47380.d Supervisor Steve Bull  
Method used Confirm Formula Negative 50to500 loop inj.m Acquisition Date 13/03/2015 11:45:43  
Ionisation Mode negative electrospray (ESI)

### -MS, 1.0-1.3min #(30-38), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	196.9603	8603	9.7	282	694.8
2	198.9590	8562	9.6	278	676.0
3	212.0861	7832	8.8	72	543.2
4	329.0549	83273	93.6	4849	3251.8
5	330.0591	17417	19.6	997	672.3
6	331.0533	89006	100.0	5030	3400.3
7	332.0558	18090	20.3	940	683.4
8	373.0463	8932	10.0	533	460.0
9	375.0434	9669	10.9	572	532.1
10	529.4598	8158	9.2	672	2533.4

### 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** C14 H22 Br O2 Si

**Adduct(s):** H, Na

#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
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Note: Sigma fits < 0.05 indicates high probability of correct MF, and mass accuracy of 5ppm or better is generally acceptable for publication